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1. General Methods.

Unless otherwise specified, all reactions were conducted under anhydrous conditions in an argon atmosphere. Commercial reagents (Energy Chemical, etc.) were used without further purification. Solvents were purified according to the methods described in *Purification of Laboratory Chemicals* (Peerrin, D. D.; Armarego, W. L. and Perrins, D. R., Pergamon Press: Oxford, 1980). Yields refer to chromatographically and spectroscopically (1H NMR) homogeneous materials. Reactions were monitored by Thin Layer Chromatography supplied by Yantai Chemicals (China) visualized by UV or stained with ethanolic solution of phosphomolybdic acid and cerium sulfate. If not specially mentioned, flash column chromatography was performed using E. Merck silica gel (60, particle size 0.040–0.063 mm). NMR spectra were acquired on a Bruker 400 MHz NMR spectrometer (AVANCE III) at ambient temperature with $CDCl_3$ as the solvent unless otherwise stated and calibrated by using $CDCl_3$ as internal references. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, b = broad, m = multiple. High-resolution mass spectra (HRMS) were recorded on a Bruker Apex IV FTMS mass spectrometer using ESI (electrospray ionization) as ionization method. Optical rotations were recorded on an AUTOPOL II digital polarimeter.

breviations:

LDA = lithium diisopropylamide

BHT = 2,6-di-*tert*-butyl-4-methylphenol

TBSOTf = *tert*-butyldimethylsilyl trifluoromethanesulfonate

IBX = 2-iodoxybenzoic acid

DMP = Dess-Martin periodinane

Me-CBS = 5,5-diphenyl-2-methyl-3,4-propano-1,3,2-oxazaborolidin

KHMDS = potassium bis(trimethylsilyl)amide

TBD = 1,5,7-triazabicyclo[4.4.0]dec-5-ene

NBS = N-bromosuccinimide

BPO = dibenzoyl peroxide

rt = room temperature

DMSO = dimethyl sulfoxide

DMF = N, N-dimethylformamide

2. Supplementary Figures.

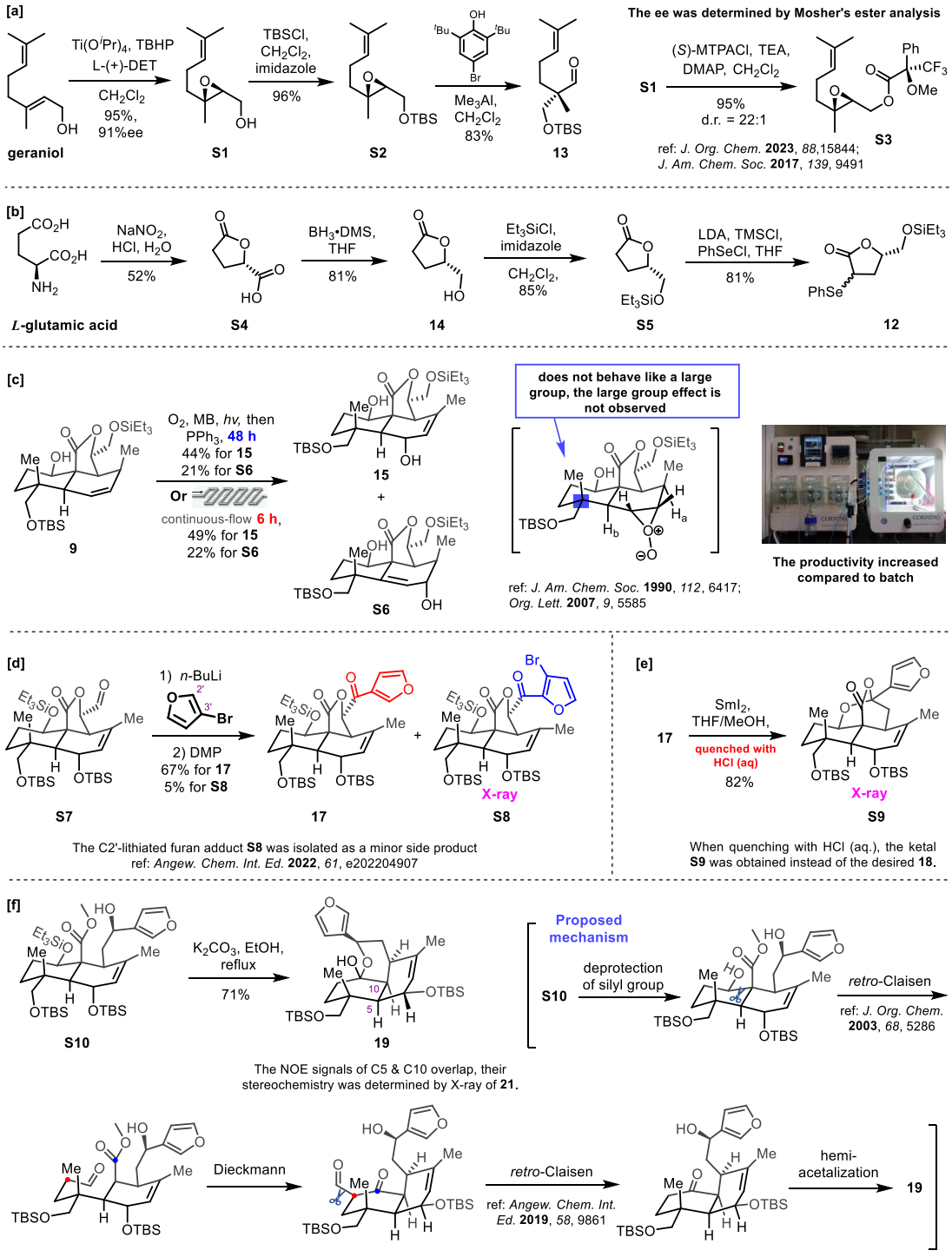


Figure S1. Synthesis of the common intermediate **8**. **a** Synthesis of the aldehyde **13**. **b** Synthesis of the selenolactone **12**. **c** Ene reaction of alkene **9**. **d** Regioselective lithiation of the furan moiety. **e** Formation of the fused cyclic ketal **S9**. **f** Proposed mechanism for the formation of degradation product **19**.

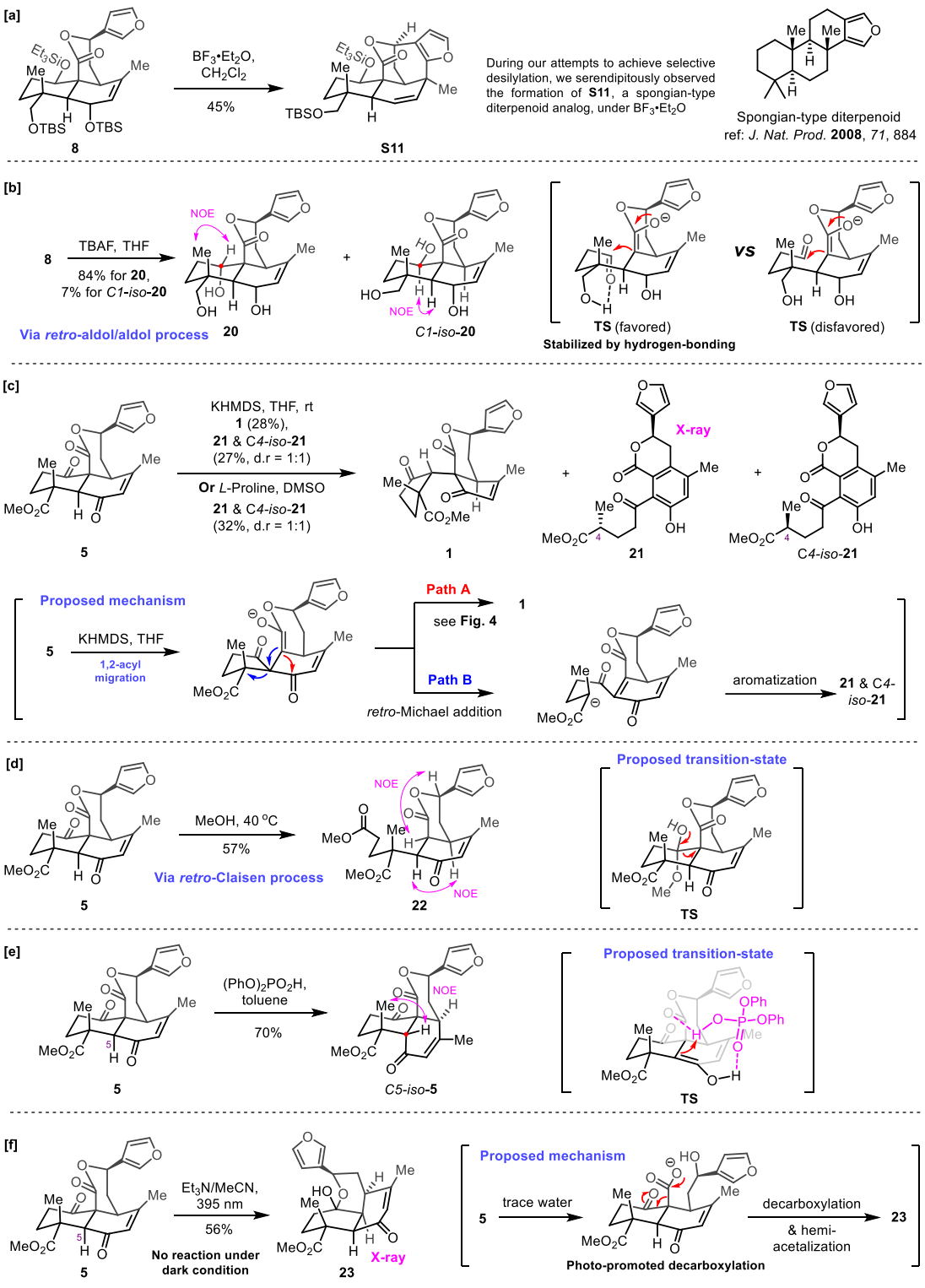


Figure S2. Synthesis of hapmnioide A (**1**) and haploide O (**2**). **a** Serendipitous formation of **S11**. **b** Proposed mechanism for the formation of C-1 isomer **20**. **c** Proposed mechanism for the formation of aromatized product **21**. **d** Proposed mechanism for the formation of **22**. **e** Proposed isomerization pathway for ketone **5**. **f** Proposed mechanism for the formation of degradation product **23**.

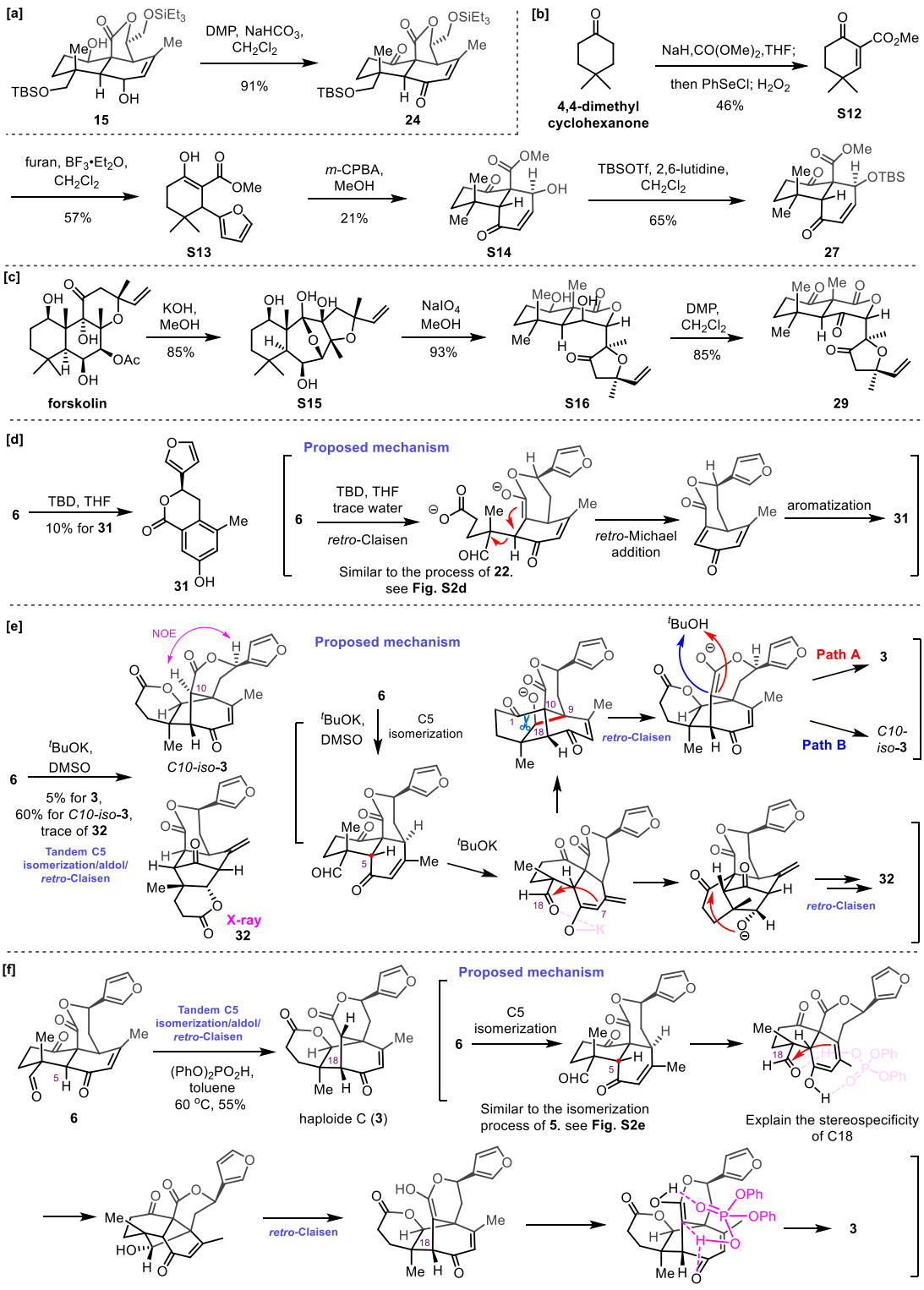


Figure S3. Synthesis of haploide C (**3**). **a** Synthesis of γ-lactone **24**. **b** Synthesis of *cis*-decalin **27**. **c** Synthesis of δ-lactone **29**. **d** Proposed mechanism for the formation of **31**. **e** Proposed isomerization pathway for *C10-iso*-**3** and **32**. **f** Proposed mechanism for the formation of **3**.

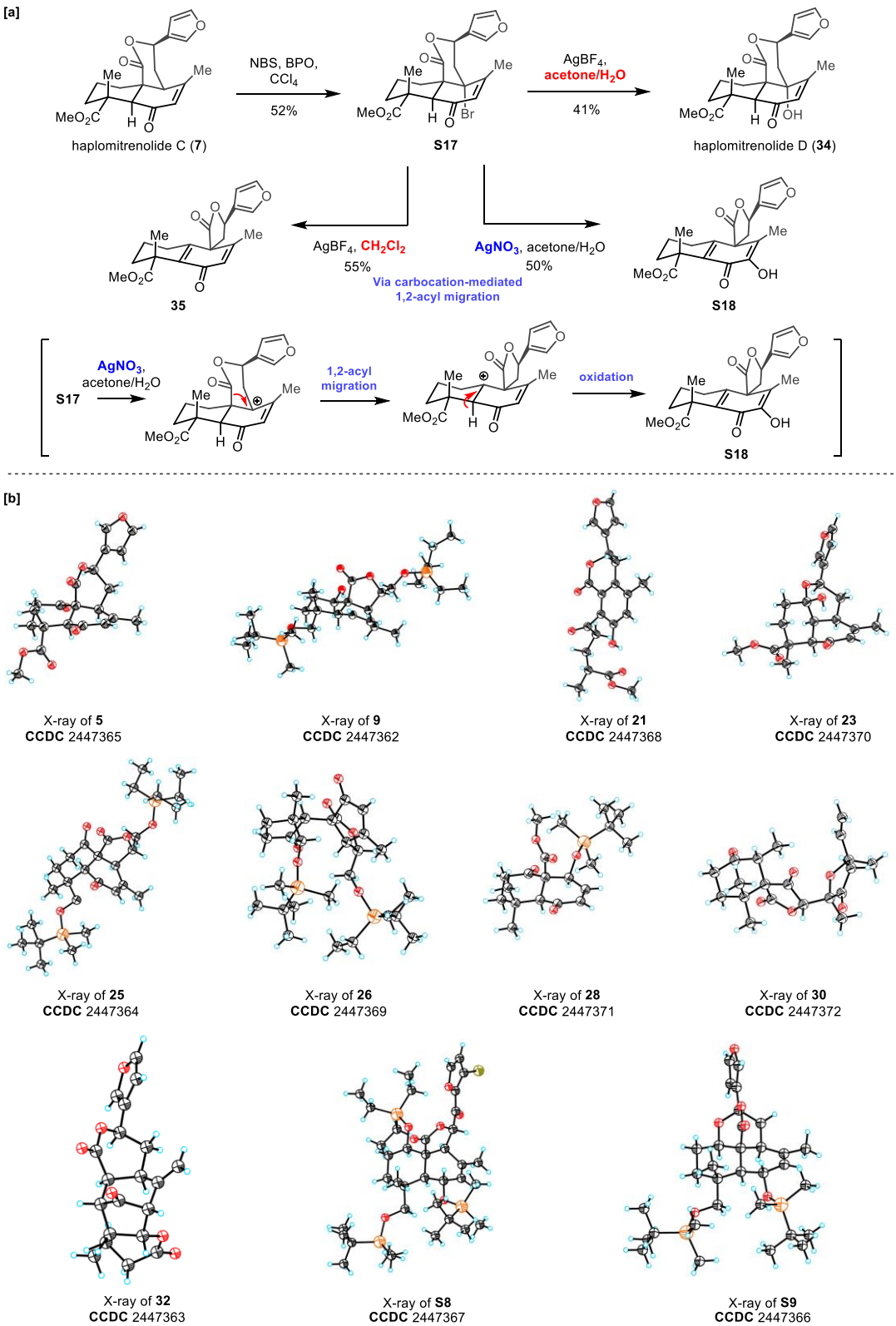
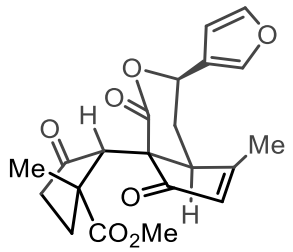


Figure S4. Synthesis of haplomitrenolide D (**34**). **a** Synthesis of the haploide O skeleton **35** via a carbocation-mediated 1,2-acyl migration. **b** Crystallographic data deposited under accession numbers.

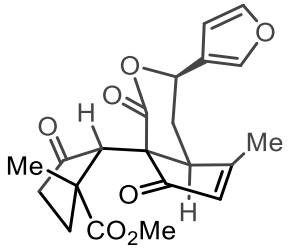
3. Comparison of NMR Spectra of *Haplomitrium* diterpenoids.



hapmnioide A (**1**)

Table 1: Comparison of ^{1}H NMR Spectral Data of hapmnioide A (**1**)

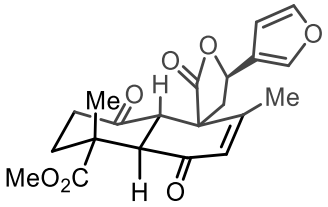
Natural hapmnioide A ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Synthetic hapmnioide A ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Δδ/ppm
7.46, br s	7.46, s	0
7.39, t (1.6)	7.39, t (1.6)	0
6.39, d (0.8)	6.38, s	+0.01
5.92, m	5.94 – 5.90, m	-
5.88, s	5.88, s	0
3.65, s	3.65, s	0
3.62, s	3.62, s	0
3.41, dd (11.2, 6.0)	3.39, dd (11.3, 6.1)	+0.02
2.57, ddd (14.0, 4.0, 2.0)	2.58 – 2.48, m	-
2.41, m	2.42 – 2.32, m	-
2.17, m	2.18 – 2.10, m	-
2.06, s	2.06, s	0
1.94, m	1.98 – 1.88, m	-
1.52, dt (13.6, 11.2)	1.51 – 1.41, m	-
1.34, s	1.33, s	+0.01



hapmnioide A (**1**)

Table 2: Comparison of ^{13}C NMR Spectral Data of hapmnioide A (**1**)

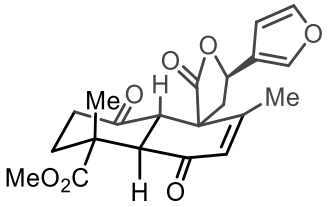
Natural hapmnioide A ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]	Synthetic hapmnioide A ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]	Δδ/ppm
17.4	17.4	0
24.1	24.1	0
32.8	32.9	-0.1
36.3	36.3	0
36.6	36.7	-0.1
45.6	45.6	0
48.7	48.8	-0.1
52.6	52.6	0
58.0	58.0	0
68.1	68.2	-0.1
72.6	72.6	0
108.5	108.5	0
124.4	124.3	+0.1
127.2	127.2	0
140.0	140.0	0
143.8	143.8	0
168.8	168.8	0
175.1	175.1	0
180.9	180.9	0
199.2	199.3	-0.1
213.6	213.6	0



haploide O (**2**)

Table 3: Comparison of ^{1}H NMR Spectral Data of haploide O (**2**)

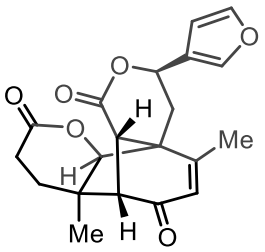
Natural haploide O ^{1}H NMR (600 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Synthetic haploide O ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Δδ/ppm
7.49, br s	7.49, s	0
7.46, t (1.5)	7.46, t (1.8)	0
6.43, br s	6.42, s	+0.01
5.93, dd (9.0, 6.8)	5.95 – 5.89, m	-
5.83, br s	5.83, s	0
3.75, s	3.75, s	0
3.51, d (14.6)	3.49, d (14.6)	+0.02
3.42, d (14.6)	3.40, d (14.6)	+0.02
3.00, dd (13.8, 9.2)	2.97, dd (13.9, 9.1)	+0.03
2.60, m	2.62 – 2.46, m	-
2.12, m	2.14 – 2.05, m	-
2.03, m	2.04 – 1.96, m	-
1.90, s	1.90, s	0
1.41, s	1.41, s	0



haploide O (**2**)

Table 4: Comparison of ^{13}C NMR Spectral Data of haploide O (**2**)

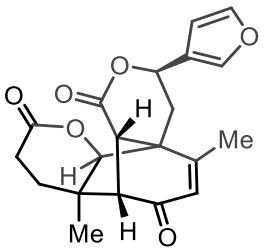
Natural haploide O ^{13}C NMR (150 MHz, $CDCl_3$) δ [ppm]	Synthetic haploide O ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]	Δδ/ppm
14.8	14.8	0
19.7	19.7	0
35.2	35.2	0
36.3	36.2	+0.1
36.6	36.6	0
42.7	42.7	0
51.0	50.9	+0.1
52.0	52.0	0
52.7	52.7	0
53.9	53.9	0
73.2	73.1	+0.1
108.4	108.3	+0.1
125.2	125.1	+0.1
127.1	127.1	0
139.4	139.4	0
144.5	144.5	0
159.5	159.5	0
176.7	176.6	+0.1
177.2	177.2	0
194.5	194.4	+0.1
207.3	207.3	0



haploide C (**3**)

Table 5: Comparison of ^{1}H NMR Spectral Data of haploide C (**3**)

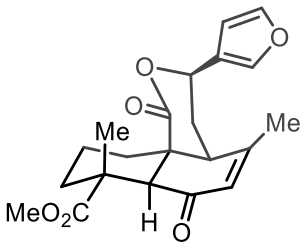
Natural haploide C ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Synthetic haploide C ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Δδ/ppm
7.44, br s	7.44, s	0
7.42, t (1.5)	7.42, t (1.8)	0
6.40, br s	6.39, s	+0.01
6.00, dd (9.3, 5.6)	5.99, dd (9.4, 5.6)	+0.01
5.86, br s	5.86, s	0
4.15, s	4.14, s	+0.01
3.36, s	3.38, s	-0.02
3.00, s	2.99, s	+0.01
2.88, dd (14.6, 5.6)	2.85, dd (14.6, 5.6)	+0.03
2.54, td (17.2, 3.1)	2.53, dt (17.0, 3.1)	+0.01
2.39, td (14.7, 4.2)	2.41 – 2.28, m	-
2.22, m	2.24, 2.14, m	-
2.07, s	2.07, s	0
1.82, dt (13.8, 3.4)	1.79, dt (13.9, 3.6)	+0.03
1.17, s	1.17, s	0



haploide C (**3**)

Table 6: Comparison of ^{13}C NMR Spectral Data of haploide C (**3**)

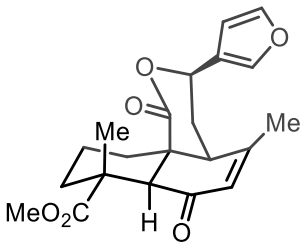
Natural haploide C ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]	Synthetic haploide C ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]	Δδ/ppm
19.2	19.2	0
25.3	25.3	0
27.1	27.1	0
29.9	29.9	0
32.2	32.2	0
43.3	43.3	0
52.1	52.1	0
54.0	54.0	0
59.9	59.9	0
74.0	74.0	0
88.7	88.7	0
108.3	108.3	0
125.8	125.8	0
128.2	128.3	-0.1
139.7	139.7	0
144.2	144.2	0
163.2	163.1	+0.1
169.3	169.2	+0.1
171.1	170.9	+0.2
197.9	197.8	+0.1



haplomitrenolide C (**7**)

Table 7: Comparison of ^{1}H NMR Spectral Data of haplomitrenolide C (**7**)

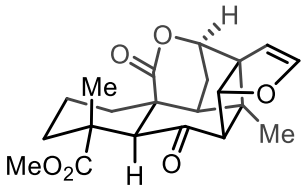
Natural haplomitrenolide C ^{1}H NMR (400 MHz, C_5D_5N) δ [ppm, mult, *J* (Hz)]	Synthetic haplomitrenolide C ^{1}H NMR (400 MHz, C_5D_5N) δ [ppm, mult, *J* (Hz)]	Δδ/ppm
7.76, br s	7.76, s	0
7.67, dd (2.4, 1.4)	7.67, s	0
6.58, br s	6.58, s	0
5.97, dd (8.0, 4.9)	5.99 – 5.93, m	-
5.97, s	5.99 – 5.93, m	-
3.70, s	3.69, s	+0.01
3.62, s	3.61, s	+0.01
2.93, br d (8.0)	2.92, d (8.2)	+0.01
2.71, ddd (14.7, 8.0, 8.0)	2.74 – 2.65, m	-
2.60, br d (13.2)	2.59, d (13.2)	+0.01
2.39, ddd (14.7, 4.9, 2.0)	2.38, dd (14.8, 6.2)	+0.01
2.06, s	2.06, s	0
1.79 – 1.55, m	1.80-1.74, m	-
1.79 – 1.55, m	1.70 – 1.55, m	-
1.67, s	1.67, s	0



haplomitrenolide C (**7**)

Table 8: Comparison of ^{13}C NMR Spectral Data of haplomitrenolide C (**7**)

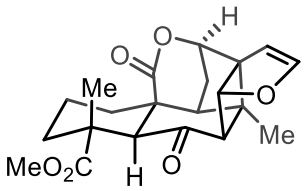
Natural haplomitrenolide C ^{13}C NMR (100 MHz, C_5D_5N) δ [ppm]	Synthetic haplomitrenolide C ^{13}C NMR (100 MHz, C_5D_5N) δ [ppm]	Δδ/ppm
18.6	18.6	0
19.2	19.2	0
22.2	22.2	0
28.2	28.1	+0.1
32.7	32.5	+0.2
38.3	38.2	+0.1
43.9	43.8	+0.1
49.1	48.9	+0.2
50.3	50.3	0
52.3	52.3	0
57.2	57.1	+0.1
72.3	72.2	+0.1
109.0	109.0	0
127.5	127.5	0
128.8	128.7	+0.1
139.9	139.9	0
144.6	144.6	0
158.2	158.3	-0.1
172.3	172.3	0
179.0	179.0	0
194.6	194.7	-0.1



haplomitrin A (**4**)

Table 9: Comparison of ^{1}H NMR Spectral Data of haplomitrin A (**4**)

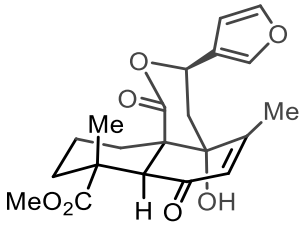
Natural haplomitrin A ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Synthetic haplomitrin A ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Δδ/ppm
6.52, d (2.8)	6.52, d (2.8)	0
4.77, d (2.8)	4.76, d (2.8)	+0.01
4.72, d (3.2)	4.72, d (3.1)	0
4.55, br s	4.55, s	0
3.69, s	3.69, s	0
3.03, s	3.03, s	0
2.91, d (3.2)	2.90, d (3.1)	+0.01
2.39, br d (13.6)	2.37, d (13.6)	+0.02
2.33, d (13.6)	2.32, d (13.6)	+0.01
2.14, dd (4.8, 2.0)	2.16 – 2.12, m	-
2.10, ddd (14.0, 3.2, 3.2)	2.10 – 2.06, m	-
1.86, m	1.87 – 1.83, m	-
1.82, m	1.82 – 1.78, m	-
1.72, s	1.72, s	0
1.62, m	1.63 – 1.59, m	-
1.45, m	1.45 – 1.40, m	-
1.39, m	1.39 – 1.34, m	-
1.24, s	1.25, s	-0.01



haplomitrin A (**4**)

Table 10: Comparison of ^{13}C NMR Spectral Data of haplomitrin A (**4**)

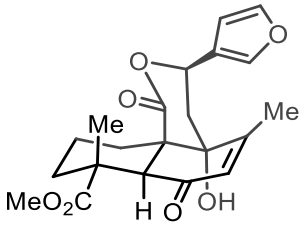
Natural haplomitrin A ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]	Synthetic haplomitrin A ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]	Δδ/ppm
16.5	16.5	0
17.6	17.6	0
23.0	23.0	0
33.7	33.7	0
37.9	37.9	0
38.6	38.6	0
43.5	43.4	+0.1
47.1	47.1	0
50.1	50.0	+0.1
52.6	52.7	-0.1
55.3	55.2	+0.1
56.4	56.3	+0.1
59.4	59.4	0
66.8	66.8	0
80.3	80.2	+0.1
83.1	83.1	0
100.2	100.2	0
150.7	150.6	+0.1
172.3	172.3	0
179.4	179.5	-0.1
204.8	204.8	0



haplomitrenolide D (**34**)

Table 11: Comparison of ^{1}H NMR Spectral Data of haplomitrenolide D (**34**)

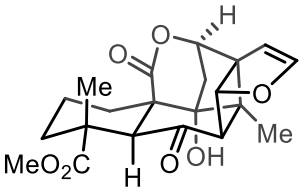
Natural haplomitrenolide D ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Synthetic haplomitrenolide D ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Δδ/ppm
7.43, t (2.0)	7.42, s	0.01
7.39, br s	7.39, s	0
6.35, br s	6.34, s	0.01
	5.75, s	-
5.69, m	5.68, dd (9.3, 5.0)	-
3.73, s	3.76, s	-0.03
3.70, s	3.70, s	0
2.59, m	2.65 – 2.55, m	-
2.17, m	2.21 – 2.09, m	-
1.74, s	1.74, s	0
1.72, m	1.73 – 1.69, m	-
1.58, s	1.59, s	-0.01
1.54, m	1.56 – 1.50, m	-



haplomitrenolide D (**34**)

Table 12: Comparison of ^{13}C NMR Spectral Data of haplomitrenolide D (**34**)

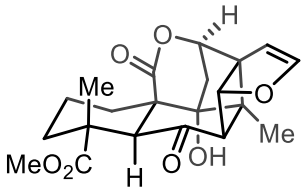
Natural haplomitrenolide D ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]	Synthetic haplomitrenolide D ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]	Δδ/ppm
18.0	18.0	0
18.5	18.5	0
19.7	19.7	0
27.1	27.1	0
35.3	35.2	+0.1
37.5	37.5	0
43.5	43.5	0
49.0	49.0	0
52.8	52.8	0
55.3	55.3	0
69.9	69.9	0
74.1	74.2	-0.1
108.1	108.1	0
126.6	126.6	0
129.8	129.8	0
139.2	139.3	-0.1
144.3	144.3	0
155.6	155.3	+0.3
172.7	172.6	0
179.9	179.8	0
194.9	194.6	+0.3



haplomitrin C (**36**)

Table 13: Comparison of ^{1}H NMR Spectral Data of haplomintrin C (**36**)

Natural haplomintrin C ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Synthetic haplomintrin C ^{1}H NMR (400 MHz, $CDCl_3$) δ [ppm, mult, *J* (Hz)]	Δδ/ppm
6.53, d (2.8)	6.53, d (2.8)	0
4.78, m	4.81 – 4.76, m	-
4.41, d (3.2)	4.42, d (3.4)	-0.01
3.69, s	3.69, s	0
3.65, s	3.64, s	+0.01
2.85, d (3.2)	2.86, d (3.3)	-0.01
2.61, s	2.48, s	0.13
2.42, d (12.8)	2.43, d (13.1)	-0.01
2.36, m	2.40 – 2.32, m	-
1.93, m	2.03 – 1.84, m	-
1.79, m	1.80 – 1.77, m	-
1.76, s	1.76, s	0
1.64, m	1.66 – 1.62, m	-
1.41, td (13.2, 3.2)	1.45 – 1.35, m	-
1.22, s	1.23, s	-0.01



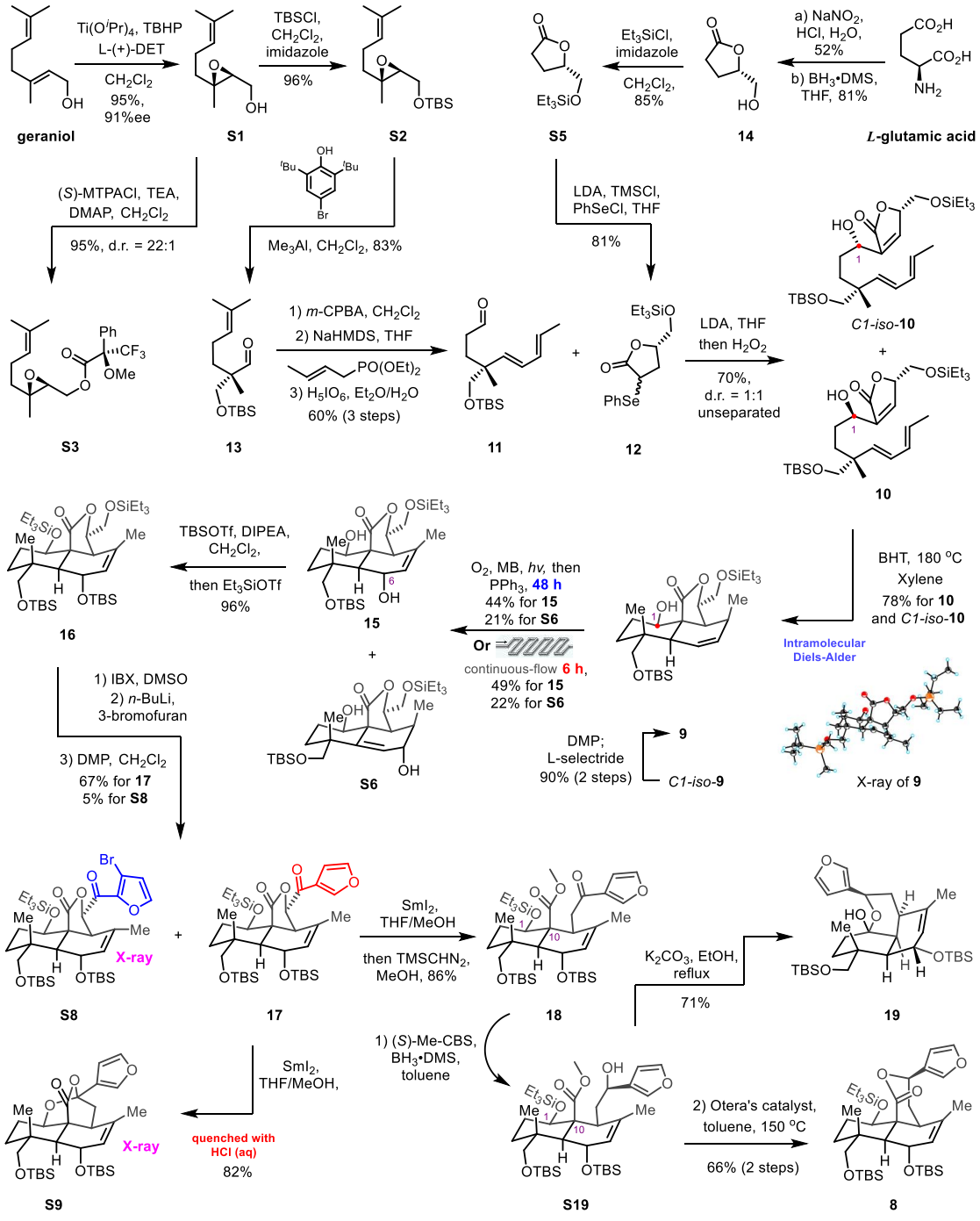
haplomitrin C (**36**)

Table 14: Comparison of ^{13}C NMR Spectral Data of haplomintrin C (**36**)

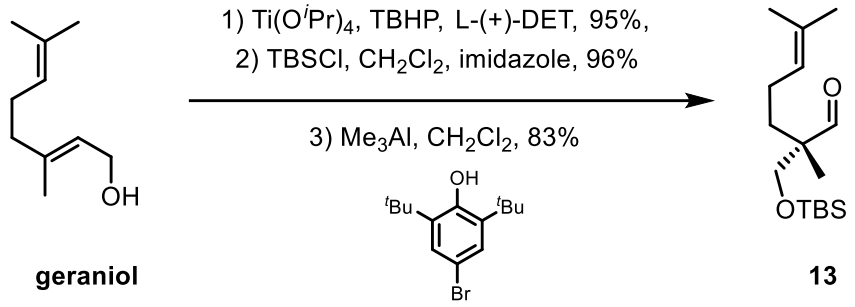
Natural haplomintrin C ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]	Synthetic haplomintrin C ^{13}C NMR (100 MHz, $CDCl_3$) δ [ppm]	Δδ/ppm
17.1	17.1	0
17.2	17.2	0
18.7	18.7	0
29.6	29.6	0
37.3	37.4	-0.1
39.1	39.1	0
43.4	43.4	0
51.7	51.7	0
52.0	51.9	+0.1
52.7	52.77	-0.07
52.8	52.8	0
57.1	57.0	+0.1
67.5	67.5	0
78.4	78.4	0
79.2	79.3	-0.1
80.1	80.1	0
100.4	100.4	0
150.8	150.8	0
173.8	173.8	0
179.7	179.8	-0.1
204.7	204.7	0

4. Experimental Procedures and Characterizations.

4.1 Synthesis of the common intermediate ***8***



Aldehyde 13



geraniol **13**

The aldehyde **13** was synthesized using established literature protocols.[1,2]

To a flamed-dried flask was added activated 4 Å molecular sieves (2.33 g) and DCM (40 mL). After cooled to -25 °C, titanium (IV) isopropoxide (5.92 mL, 20.0 mmol, 1.0 equiv.) and *L*-(+)-Diethyl-tartrate (3.26 mL, 20.0 mmol, 1.0 equiv.) were added. After stirring for 5 minutes at the same temperature, geraniol (3.08 g, 20 mmol, 1.0 equiv.) and TBHP (7.27 mL, 5– 6 M in decane, 40.0 mmol, 2.0 equiv..) were added. The mixture was stirred for 5 h at -25 °C before quenched by adding H_2O (40 mL). Then an aqueous solution of tartaric acid (40 mL, 20%) was added and the suspension was stirred overnight. The aqueous phase was extracted with DCM (80 mL x 5) and the combined organic layers were washed with brine (200 mL), dried over $NaSO_4$, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 2/1) to afford epoxide **S1** (3.23 g, 95%.) as a colorless oil.

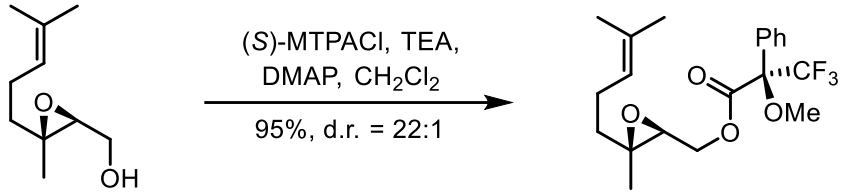
To the solution of **S1** (3.1 g, 18.2 mmol, 1.0 equiv.), imidazole (3.1 g, 45.5 mmol, 2.5 equiv.) and DMAP (1.33 g, 10.9 mmol, 0.6 equiv.) in CH_2Cl_2 (44 mL) was added TBSCl (3.57 g, 23.7 mmol, 1.3 equiv.) at 0 °C, followed by 1 h stirring at the same temperature. The reaction was quenched with H_2O (20 mL) and extracted with CH_2Cl_2 (50 mL × 3). The combined organic layers were washed with brine (100 mL) and dried over Na_2SO_4, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 5/1) to yield **S2** (4.97 g, 96%) as a colorless oil.

To a solution of 4-bromo-2,6-di-*tert*-butylphenol (11.1 g, 38.9 mmol, 2.3 equiv.) in CH_2Cl_2 (110 mL) was added Me_3Al (13.5 mL, 1M in toluene, 13.5 mmol, 0.8 equiv.). After stirring for 1 h at room temperature, the solution was cooled to -78 °C and a solution of epoxide **S2** (4.81 g, 16.9 mmol, 1.0 equiv.) in CH_2Cl_2 (20 mL) was added. Followed by 2.5 h stirring at -78 °C before quenched with NaF (3.85 g) and H_2O (1.9 mL). The mixture was stirred for additional 0.5 h at -78 °C and 0.5 h at 0 °C before Na_2SO_4 was added. The mixture was filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 30/1) afforded aldehyde **13** (4.0 g, 83%) as a reddish-brown oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.54 (s, 1H), 5.10 – 5.00 (m, 1H), 3.67 (d, *J* = 9.9 Hz, 1H), 3.55 (d, *J* = 10.0 Hz, 1H), 2.00 – 1.80 (m, 2H), 1.66 (s, 3H), 1.60 – 1.54 (m, 1H), 1.57 (s, 3H), 1.45 (ddd, *J* = 13.6, 10.9, 5.8 Hz, 1H), 1.03 (s, 3H), 0.86 (s, 9H), 0.02 (s, 6H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 206.46, 132.32, 124.02, 66.91, 51.41, 32.54, 25.88, 25.79, 22.57, 18.30, 17.77, 16.05, -5.52.

Eater S3



S1 **S3**

The eater **S3** was synthesized using established literature protocols.[3,4]

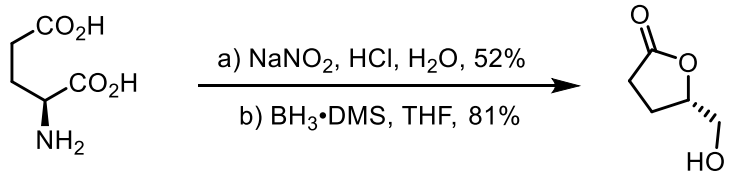
To a solution of **S1** (50 mg, 294 μmol, 1.0 equiv.) in CH_2Cl_2 (5 mL) were added TEA (81.7 μL, 588 μmol, 2.0 equiv.), DMAP (35.9 mg, 294 μmol, 1.0 equiv.) and (S)-MTPACl (66 μL, 353 μmol, 1.2 equiv.) at 0 ℃, followed by 2 h stirring at room temperature before quenched with saturated aqueous $NaHCO_3$ (2 mL). The mixture was extracted with CH_2Cl_2 (5 mL × 3) and the combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 15/1) on silica gel to provide eater **S3** (108 mg, 95%) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.50 (m, 2H), 7.45 – 7.37 (m, 3H), 5.05 (t, *J* = 7.2 Hz, 1H), 4.44 (dd, *J* = 12.0, 4.8 Hz, 1H), 4.38 (dd, *J* = 12.0, 6.6 Hz, 1H), 3.58 (s, 3H), 3.01 (dd, *J* = 6.5, 4.8 Hz, 1H), 2.10 – 1.98 (m, 2H), 1.70 – 1.63 (m, 1H), 1.67 (s, 3H), 1.59 (s, 3H), 1.46 (ddd, *J* = 13.8, 9.5, 6.8 Hz, 1H), 1.32 (s, 3H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.64, 132.51, 132.17, 129.88, 128.65, 127.42, 124.79, 123.23, 121.92, 84.98, 84.70, 65.23, 60.99, 58.98, 55.69, 38.34, 25.78, 23.74, 17.78, 16.94;

^{19}F NMR (376 MHz, $CDCl_3$) δ -71.65, -71.73.

Alcohol 14



***L*-glutamic acid** **14**

The alcohol **14** was synthesized using established literature protocols.[5]

To a solution of (*L*)-glutamic acid (5.0 g, 34 mmol, 1.0 equiv.) in deionised water (34 mL) and HCl (13.25 mL, 3N) was added a solution of sodium nitrite (2.8 g) in deionised water (20 mL) via a dropping funnel over 2 h at 0 °C. After completion of the addition, the reaction was stirred for 16 h at room temperature. After the reaction is complete, add solid NaCl until saturated. The aqueous layer was

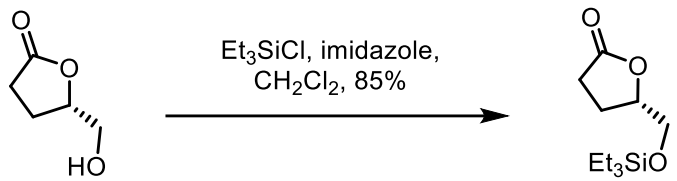
extracted with EtOAc (50 mL × 3). The combined organic layers were washed with brine (100 mL), dried over Na_2SO_4, filtered, concentrated and dried under vacuum to yield carboxylic acid (2.3 g, 52%), which was used in the next step without further purification. To a solution of carboxylic acid (2.3 g, 17.7 mmol, 1.0 equiv.) in anhydrous THF (56 mL) was added BH_3·DMS (10.6 mL, 2 M in THF, 21.2 mmol, 1.2 equiv.) dropwise. The reaction was stirred at room temperature for 6 h and then quenched with MeOH (10 mL) cautiously. The mixture was concentrated and purified by flash column chromatography (CH_2Cl_2/methanol = 15/1) to yield eater **14** (1.66 g, 81%) as a colorless oil.

Opt. Rot. $[\alpha]_D^{20}$ = +18.2° (c 0.32, EtOH) [Lit. [5]: $[\alpha]_D^{20}$ = +15.8° (c 2.0, EtOH)]

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.63 – 4.55 (m, 1H), 3.83 (dd, *J* = 12.5, 2.9 Hz, 1H), 3.59 (dd, *J* = 12.5, 4.6 Hz, 1H), 3.55 – 3.38 (m, 1H), 2.64 – 2.41 (m, 2H), 2.28 – 2.17 (m, 1H), 2.15 – 2.02 (m, 1H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 178.23, 81.09, 63.97, 28.74, 23.15.

Silyl ether S5



14 **S5**

To a solution of **14** (7.4 g, 63.73 mmol, 1.0 equiv.) in CH_2Cl_2 (150 mL) was added imidazole (10.85 g, 159.33 mmol, 2.5 equiv.), DMAP (4.67 g, 38.24 mmol, 0.6 equiv.) and TESCl (13.91 mL, 82.85 mmol, 1.3 equiv.), followed by stirring for 45 minutes at rt. The reaction mixture was quenched with saturated aqueous $NaHCO_3$ (30 mL) and extracted with CH_2Cl_2 (50 mL × 3). The combined organic layers were washed with brine (100 mL) and dried over Na_2SO_4, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 8/1) to yield **S5** (12.48 g, 85%) as a colorless oil.

TLC R*f* = 0.6 (Petroleum ether/Ethyl acetate = 4/1; phosphomolybdic acid).

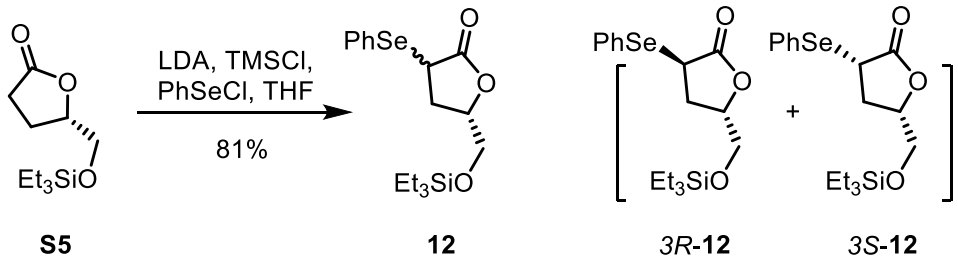
Opt. Rot. $[\alpha]_D^{20}$ = +17.6° (c 0.325, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 4.56 (ddd, *J* = 8.1, 5.6, 2.6 Hz, 1H), 3.83 (dd, *J* = 11.3, 3.2 Hz, 1H), 3.66 (dd, *J* = 11.3, 3.3 Hz, 1H), 2.58 (ddd, *J* = 17.5, 10.1, 7.2 Hz, 1H), 2.43 (ddd, *J* = 17.6, 10.0, 6.3 Hz, 1H), 2.32 – 2.08 (m, 2H), 0.92 (t, *J* = 8.0 Hz, 9H), 0.58 (q, *J* = 8.0 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 177.71, 80.23, 64.65, 28.64, 23.68, 6.70, 4.31.

HRMS (ESI) calcd for $C_{11}H_{22}O_3Si$ $[M+Na]^+$: 253.1230, found 253.1230.

Selenolactone 12



S5 **12** *3R*-**12** *3S*-**12**

Under argon atmosphere, to a solution of **S5** (3 g, 13.02 mmol, 1.0 equiv.) in anhydrous THF (54 mL) was added LDA (9.77 mL, 2 M in THF/Hexane, 19.53 mmol, 1.5 equiv.) dropwise at -78 °C, followed by 1 h stirring at the same temperature. TMSCl (2.48 mL, 19.53 mmol, 1.5 equiv.) was added and the mixture was stirred at -78 °C for 1 h. After that, PhSeCl (2.74 g, 14.32 mmol, 1.1 equiv.) was added, followed by stirring overnight at rt. The reaction mixture was quenched with H_2O (20 mL) and the aqueous layer was extracted with EtOAc (30 mL × 3). The combined organic layers were washed with brine (50 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 10/1) to yield **12** (4.07 g, 81 %) as a red-brown oil.

Data of *3R*-**12**.

TLC R*f* = 0.7 (Petroleum ether/Ethyl acetate = 20/1; UV/phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = +24.0° (c 0.23, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.46 (m, 2H), 7.26 – 7.12 (m, 3H), 4.19 (tt, *J* = 6.3, 3.0 Hz, 1H), 3.88 (dd, *J* = 9.1, 5.5 Hz, 1H), 3.66 (dd, *J* = 11.5, 3.0 Hz, 1H), 3.46 (dd, *J* = 11.4, 3.1 Hz, 1H), 2.50 (ddd, *J* = 13.5, 9.3, 6.0 Hz, 1H), 2.12 (ddd, *J* = 13.4, 7.5, 5.4 Hz, 1H), 0.76 (t, *J* = 8.0 Hz, 9H), 0.42 (q, *J* = 8.0 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 176.19, 135.77, 129.45, 129.04, 126.98, 78.90, 64.04, 37.24, 32.19, 6.74, 4.32.

HRMS (ESI) calcd for $C_{17}H_{26}O_3SeSi$ $[M+Na]^+$: 409.0709, found 409.0702.

Data of *3S*-**12**.

TLC R*f* = 0.7 (Petroleum ether/Ethyl acetate = 20/1; UV/phosphomolybdic acid).

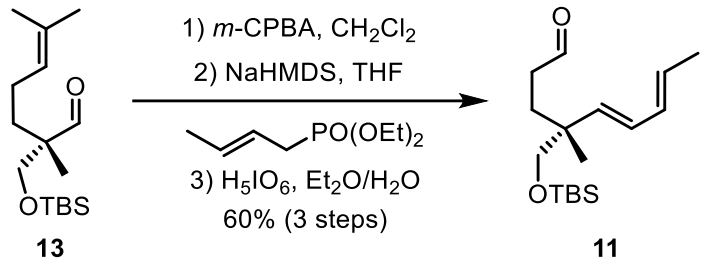
Opt. Rot. $[\alpha]_D^{20}$ = +39.2° (c 0.545, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.3 Hz, 2H), 7.26 – 7.15 (m, 3H), 4.38 (tt, *J* = 7.3, 4.4 Hz, 1H), 3.88 (dd, *J* = 9.9, 8.5 Hz, 1H), 3.56 (dd, *J* = 11.3, 4.2 Hz, 1H), 3.49 (dd, *J* = 11.3, 4.5 Hz, 1H), 2.58 (ddd, *J* = 13.6, 9.9, 7.3 Hz, 1H), 2.17 – 2.06 (m, 1H), 0.83 (t, *J* = 7.9 Hz, 9H), 0.48 (q, *J* = 7.9 Hz, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 176.19, 135.47, 129.42, 128.81, 127.87, 78.91, 63.98, 37.18, 31.85, 6.80, 4.35.

HRMS (ESI) calcd for $C_{17}H_{26}O_3SeSi$ $[M+Na]^+$: 409.0709, found 409.0703.

Aldehyde 11



13 (7 g, 24.6 mmol, 1.0 equiv.) was dissolved in CH_2Cl_2 (250 mL) at 0 °C, and $NaHCO_3$ (10.33 g, 123 mmol, 5.0 equiv.) and *m*-CPBA (5.09 g, 29.52 mmol, 1.2 equiv.) was added. The mixture was stirred at 0 °C for 1 h. Aqueous $Na_2S_2O_3$ solution (50 mL) was added to quench the reaction. The mixture was stirred for 0.5 h and extracted with CH_2Cl_2 (100 mL × 3). The combined organic layers were washed with brine (100 mL), dried over Na_2SO_4, concentrated in vacuo, and purified by flash column chromatography (Petroleum ether/Ethyl acetate =20/1) to yield epoxide (5.77 g, 78%) as a colorless oil.

Under argon atmosphere, to a solution of epoxide (1.28 g, 6.66 mmol, 2.0 equiv.) in anhydrous THF (33 mL) was added NaHMDS (5 mL, 2 M in THF, 10 mmol, 3.0 equiv.) at -78 °C. After 5 mintues, the mixture was warmed up to 0 °C and stirred for 1 h. Sub (1 g, 3.33 mmol, 1.0 equiv.) was added and the reaction was stirred at rt for 2 h. The reaction was quenched with saturated aqueous NH_4Cl (10 mL). The aqueous layer was extracted with EtOAc (20 mL × 3). The combined organic layers were washed with brine (20 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 20/1) to yield diene (1.01 g, 90%) as a light yellow oil.

To a solution of diene (2.7 g, 7.97 mmol, 1.0 equiv.) in Et_2O (44 mL) was added H_5IO_6 (2 g, 8.77 mmol, 1.1 equiv.) in THF (9 mL), followed by stirring for 1.5 h at the same temperature. The reaction mixture was quenched with H_2O (20 mL) and the aqueous layer was extracted with EtOAc (30 mL × 3). The combined organic layers were washed with brine (50 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 20/1) to yield **11** (2 g, 85 %) as a colorless oil.

TLC R*f* = 0.7 (Petroleum ether/Ethyl acetate = 20/1; phosphomolybdic acid).

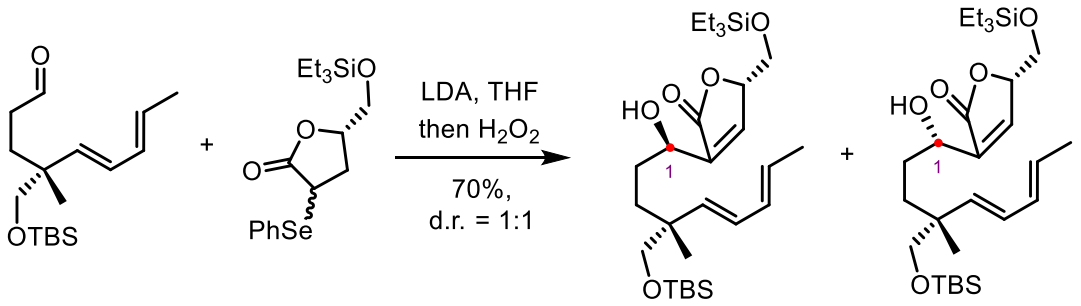
Opt. Rot. $[\alpha]_D^{20}$ = -2.74° (c 0.325, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.73 (t, *J* = 1.9 Hz, 1H), 6.06 – 5.89 (m, 2H), 5.68 – 5.57 (m, 1H), 5.42 (d, *J* = 14.5 Hz, 1H), 3.39 – 3.29 (m, 2H), 2.35 (td, *J* = 8.0, 1.8 Hz, 2H), 1.80 – 1.67 (m, 5H), 0.96 (s, 3H), 0.88 (s, 9H), 0.01 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 203.18, 136.42, 131.88, 129.47, 128.22, 70.63, 40.88, 39.64, 29.40, 26.00, 20.94, 18.40, 18.20, -5.38, -5.39.

HRMS (ESI) calcd for $C_{17}H_{32}O_2Si$ $[M+Na]^+$: 319.2064, found 319.2064.

Trienolide 10



11 **12** **10** *C1-iso*-**10**

Under argon atmosphere, to a solution of **12** (2.6 g, 6.83 mmol, 1.0 equiv.) and HMPA (5.95 mL, 34.2 mmol, 5.0 equiv.) in anhydrous THF (100 mL) was added LDA (4.1 mL, 2M in THF/Hexane, 8.2 mmol, 1.2 equiv.) dropwise at -78 °C, followed by 0.5 h stirring at the same temperature. After 0.5 h stirring at rt, **11** (2.43 g, 8.2 mmol, 1.2 equiv.) was added at -78 °C. The reaction mixture was stirred at -78 °C and quenched with saturated aqueous NH_4Cl (50 mL). The aqueous layer was extracted with EtOAc (100 mL × 3). The combined organic layers were washed with brine (100 mL), dried over Na_2SO_4, filtered, concentrated to give a crude residue. The residue was dissolved in THF (68 mL) and EtOAc (68 mL), and $NaHCO_3$ (5.74 g, 68.3 mmol, 10 equiv.) and H_2O_2 (6 mL, 30wt.% in H_2O) were added. The reaction mixture was stirred at rt for 1 h and quenched with saturated aqueous $Na_2S_2O_3$ (50 mL). The aqueous layer was extracted with EtOAc (100 mL × 3). The combined organic layers were washed with brine (100 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 8/1) to yield **10** and *C1-iso*-**10** (2.5 g, 70 %) as a colorless oil.

Data of **10**.

TLC R*f* = 0.45 (Petroleum ether/Ethyl acetate = 3/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = -10.1° (c 0.44, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (s, 1H), 6.09 – 5.90 (m, 2H), 5.65 – 5.55 (m, 1H), 5.46 (d, *J* = 14.9 Hz, 1H), 4.97 (s, 1H), 4.44 (s, 1H), 3.89 (dd, *J* = 10.7, 4.7 Hz, 1H), 3.77 (dd, *J* = 10.8, 5.3 Hz, 1H), 3.42 – 3.28 (m, 2H), 2.66 (s, 1H), 1.73 (d, *J* = 6.5 Hz, 3H), 1.60 – 1.50 (m, 2H), 1.47 – 1.28 (m, 2H), 0.96 (s, 3H), 0.94 (t, *J* = 7.9 Hz, 9H), 0.88 (s, 9H), 0.59 (q, *J* = 7.9 Hz, 6H), 0.01 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.67, 146.33, 137.52, 137.28, 132.10, 128.91, 127.74, 81.83, 70.52, 67.79, 63.05, 40.98, 32.84, 30.27, 26.04, 21.26, 18.44, 18.21, 6.80, 4.37, -5.34.

HRMS (ESI) calcd for $C_{28}H_{52}O_5Si_2$ $[M+Na]^+$: 547.3245, found 547.3245.

Data of *C1-iso*-**10**.

TLC R*f* = 0.7 (Petroleum ether/Ethyl acetate = 3/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = -6.0° (c 0.295, MeOH).

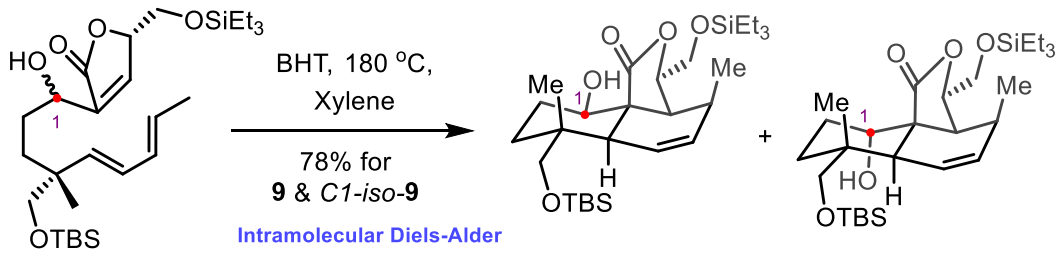
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (t, *J* = 1.5 Hz, 1H), 6.04 – 5.91 (m, 2H), 5.65 – 5.56 (m, 1H), 5.45 (d, *J* = 14.8 Hz, 1H), 4.99 – 4.93 (m, 1H), 4.43 (s, 1H), 3.88 (dd, *J* = 10.7, 4.9 Hz, 1H), 3.76 (dd, *J* = 10.8, 5.4 Hz, 1H), 3.38 – 3.27

(m, 2H), 2.59 (s, 1H), 1.73 (d, *J* = 6.4 Hz, 3H), 1.62 – 1.53 (m, 2H), 1.46 – 1.23 (m, 2H), 0.97 (s, 3H), 0.94 (t, *J* = 7.9 Hz, 9H), 0.88 (s, 9H), 0.60 (q, *J* = 7.9 Hz, 6H), 0.01 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.56, 146.32, 137.60, 137.33, 132.10, 128.90, 127.70, 81.85, 70.58, 67.95, 63.18, 40.99, 32.83, 30.39, 26.03, 21.10, 18.42, 18.19, 6.78, 4.37, -5.35.

HRMS (ESI) calcd for $C_{28}H_{52}O_5Si_2$ $[M+Na]^+$: 547.3245, found 547.3244.

***trans*-Decalin 9**



10 & *C1-iso*-**10** **9** *C1-iso*-**9**

A mixture of **10** and *C1-iso*-**10** (600 mg, 1.14 mmol, 1.0 equiv.), BHT (12.6 mg, 0.057 mmol, 0.05 equiv.) and anhydrous xylene (114 mL) was added to a 350 mL sealed tube and the mixture was bubbled with argon balloon for 1 h. Then the reaction mixture was refluxed at 180 °C for 60 h. After being cooled to ambient temperature, the solution was concentrated in vacuo and the residue was purified by flash column chromatography (Petroleum ether/Ethyl acetate = 20/1) to yield **9** and *C1-iso*-**9** (468 mg, 78%) as a white solid and a colorless oil.

Data of **9**.

TLC R*f* = 0.45 (Petroleum ether/Ethyl acetate = 10/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = +7.4° (c 0.755, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.04 – 5.97 (m, 1H), 5.73 – 5.66 (m, 1H), 4.02 – 3.99 (m, 1H), 3.98 – 3.92 (m, 1H), 3.71 – 3.65 (m, 1H), 3.64 – 3.58 (m, 1H), 3.45 (s, 1H), 3.25 (d, *J* = 9.8 Hz, 1H), 3.06 (d, *J* = 9.7 Hz, 1H), 2.69 (t, *J* = 5.4 Hz, 1H), 2.44 – 2.31 (m, 2H), 2.29 – 2.23 (m, 1H), 1.76 – 1.66 (m, 2H), 1.37 – 1.30 (m, 1H), 1.20 – 1.15 (m, 6H), 0.99 – 0.94 (m, 9H), 0.85 (s, 9H), 0.65 (q, *J* = 8.2 Hz, 6H), -0.01 (s, 3H), -0.05 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 177.04, 133.78, 131.75, 78.59, 76.63, 71.38, 65.08, 59.73, 48.32, 42.06, 36.46, 32.18, 31.72, 26.46, 25.97, 18.32, 17.85, 15.89, 6.74, 4.09, -5.47, -5.49.

HRMS (ESI) calcd for $C_{28}H_{52}O_5Si_2$ $[M+Na]^+$: 547.3245, found 547.3244.

Data of *C1-iso*-**9**.

TLC R*f* = 0.55 (Petroleum ether/Ethyl acetate = 10/1; phosphomolybdic acid).

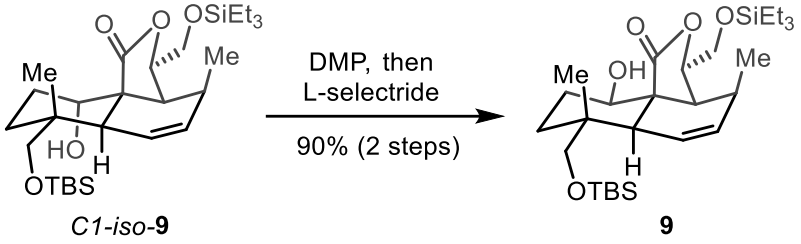
Opt. Rot. $[\alpha]_D^{20}$ = +25.8° (c 0.79, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.99 – 5.93 (m, 1H), 5.74 – 5.67 (m, 1H), 4.06 (q, *J* = 3.6 Hz, 1H), 3.98 (s, 1H), 3.78 (dd, *J* = 11.1, 2.9 Hz, 1H), 3.51 (dd, *J* = 11.1, 3.5 Hz, 1H), 3.27 (d, *J* = 9.7 Hz, 1H), 3.07 (d, *J* = 9.7 Hz, 1H), 2.92 (t, *J* =

5.0 Hz, 1H), 2.71 – 2.60 (m, 2H), 2.39 – 2.29 (m, 1H), 1.96 (td, *J* = 14.3, 3.9 Hz, 1H), 1.66 – 1.58 (m, 2H), 1.18 – 1.11 (m, 7H), 0.95 (t, *J* = 7.9 Hz, 9H), 0.86 (s, 9H), 0.60 (q, *J* = 7.9 Hz, 6H), -0.00 (s, 3H), -0.04 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 178.55, 134.24, 130.83, 78.99, 71.99, 69.40, 65.42, 57.78, 46.81, 37.48, 36.51, 32.29, 26.75, 25.96, 25.08, 18.28, 17.82, 16.07, 6.81, 4.44, 4.42, -5.45, -5.50.

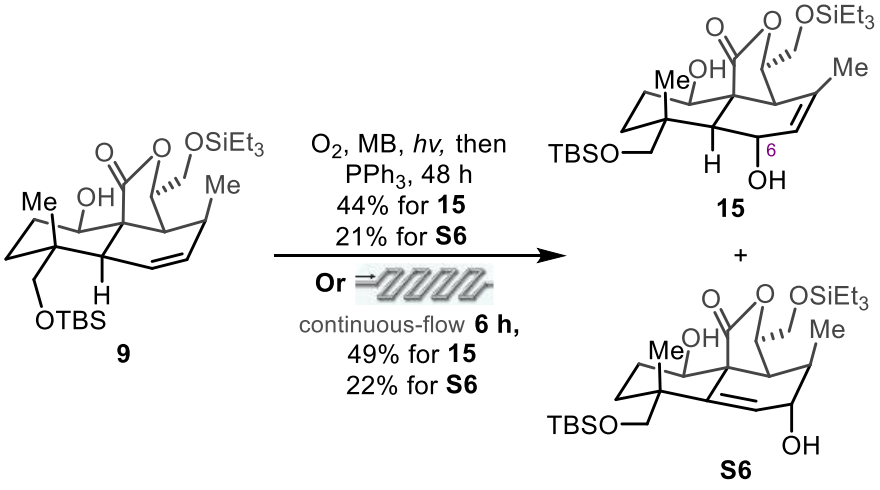
HRMS (ESI) calcd for $C_{28}H_{52}O_5Si_2$ $[M+Na]^+$: 547.3245, found 547.3245.



C1-iso-**9** **9**

Dess-Martin periodinane (40.4 mg, 95.2 μmol, 2.0 equiv.) was added to a solution of *C1-iso*-**9** (25 mg, 47.6 μmol, 1.0 equiv.) and $NaHCO_3$ (20 mg, 0.238 mmol, 5.0 equiv.) in CH_2Cl_2 (1 mL). The mixture was stirred at rt for 2 h and quenched with saturated aqueous $Na_2S_2O_3$ (3 mL). The layers were separated and the aqueous phase was extracted with CH_2Cl_2 (5 mL × 3). The combined organic layers were washed with brine (10 mL) and dried over Na_2SO_4. The solvent was removed under vacuum to give a residue, and the residue was dissolved in anhydrous THF (4 mL). The mixture was cooled to -78 °C and L-selectride (95.2 μL, 95.2 μmol, 2.0 equiv.) was added under argon atmosphere, followed by 0.5 h stirring at the same temperature. The mixture was then quenched with saturated aqueous NH_4Cl (1 mL) and extracted with EtOAc (5 mL × 3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/ethyl acetate = 15/1) to yield **9** (22.5 mg, 90%) as a white solid.

Allyl alcohol 15



To an oxygen bubbled solution of **9** (100 mg, 0.19 mmol, 1.0 equiv.) in anhydrous MeCN (19 mL) was added methylene blue (30.4 mg, 0.095 mmol, 0.5 equiv.) at 0 °C. Under oxygen atmosphere, the mixture was irradiated with a fluorescent lamp (23 W, PHILIPS®, distance 2 cm) for 48 h at the same temperature. The light source and oxygen balloon were removed before PPh_3 (249 mg, 0.95 mmol, 5.0 equiv.) was added. After the reaction mixture was stirred at rt for 2 h, the solvent was concentrated under reduced pressure. The residue was purified by flash column chromatography (Petroleum ether/ethyl acetate = 5/1) to yield **15** (45.2 mg, 44%, brms 52%), **S6** (21.6 mg, 21%), **9** (16 mg, 16%) as white solids.

Or: To a solution of **9** (100 mg, 0.19 mmol, 1.0 equiv.) in anhydrous MeCN (19 mL) was added methylene blue (30.4 mg, 0.095 mmol, 0.5 equiv.). The reaction mixture and oxygen gas were mixed in the advanced-flow reactors equipped with 4 fluorescent lamps (24 W, Leishi®, distance 2 cm) at 0 °C for 6 h before collected into a round-bottom flask. PPh_3 (249 mg, 0.95 mmol, 5.0 equiv.) was added, followed by stirring for 2 h at rt. The mixture was concentrated under reduced pressure. The residue was purified by flash column chromatography (Petroleum ether/ethyl acetate = 5/1) to yield **15** (50 mg, 49%, brms 55%), **S6** (23 mg, 22%), **9** (12 mg, 12%) as white solids.

Data of **15**.

TLC R*f* = 0.5 (Petroleum ether/Ethyl acetate = 5/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = -4.5° (c 0.2, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.59 (t, *J* = 1.5 Hz, 1H), 4.34 (d, *J* = 5.4 Hz, 1H), 4.11 (dd, *J* = 10.9, 4.9 Hz, 1H), 4.08 – 3.99 (m, 2H), 3.84 (dd, *J* = 10.9, 4.5 Hz, 1H), 3.56 – 3.50 (m, 2H), 3.34 – 3.27 (m, 2H), 2.78 (dd, *J* = 3.7, 1.6 Hz, 1H), 2.21 – 2.06 (m, 1H), 1.72 (s, 3H), 1.70 – 1.64 (m, 1H), 1.60 (d, *J* = 10.5 Hz, 1H), 1.43 – 1.38 (m, 2H), 1.32 (s, 3H), 0.97 (t, *J* = 8.0 Hz, 9H), 0.90 (s, 9H), 0.65 (q, *J* = 7.9 Hz, 6H), 0.07 (s, 3H), 0.07 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 175.60, 133.69, 132.14, 84.74, 78.27, 75.02, 66.57, 64.27, 54.10, 51.73, 50.07, 38.11, 35.79, 27.63, 25.95, 20.91, 18.46, 18.34, 6.78, 4.26, -5.35.

HRMS (ESI) calcd for $C_{28}H_{52}O_6Si_2$ $[M+Na]^+$: 563.3195, found 563.3195.

Data of **S6**.

TLC R*f* = 0.2 (Petroleum ether/Ethyl acetate = 5/1; phosphomolybdic acid).

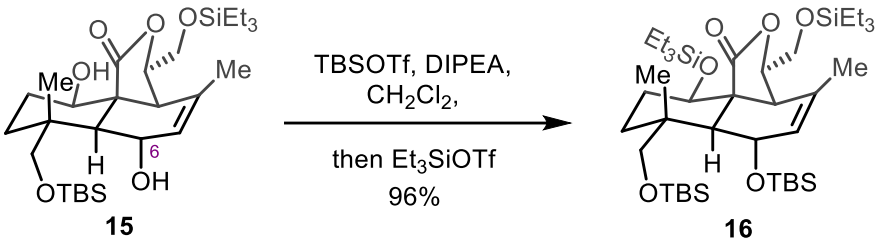
Opt. Rot. $[\alpha]_D^{20}$ = -24° (c 0.23, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.88 (s, 1H), 4.31 (t, *J* = 6.3 Hz, 1H), 4.01 – 3.90 (m, 2H), 3.67 (dd, *J* = 11.7, 4.6 Hz, 1H), 3.52 – 3.41 (m, 3H), 2.89 (dd, *J* = 8.3, 4.6 Hz, 1H), 2.62 – 2.47 (m, 2H), 1.86 – 1.78 (m, 1H), 1.57 (dt, *J* = 14.1, 4.3 Hz, 2H), 1.44 – 1.36 (m, 1H), 1.23 (s, 3H), 1.14 (d, *J* = 6.9 Hz, 3H), 0.96 (t, *J* = 7.9 Hz, 9H), 0.88 (s, 9H), 0.63 (q, *J* = 8.0 Hz, 6H), 0.03 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 175.35, 138.15, 133.07, 77.68, 74.76, 72.32, 69.13, 65.36, 55.88, 42.66, 41.10, 35.70, 32.67, 26.43, 26.01, 22.75, 18.33, 14.90, 6.78, 4.30, -5.34, -5.45.

HRMS (ESI) calcd for $C_{28}H_{52}O_6Si_2$ $[M+Na]^+$: 563.3195, found 563.3195.

Silyl ether 16



To a flamed-dried flask was added **15** (400 mg, 0.74 mmol, 1.0 equiv.), CH_2Cl_2 (15 mL), DIPEA (2.6 mL, 14.8 mmol, 20 equiv.) and TBSOTf (850 μL, 3.7 mmol, 5.0 equiv.) sequentially. The reaction was stirred at rt until completely consumption of starting material. Then TESOTf (837 μL, 3.7 mmol, 5.0 equiv.) was added, followed by 2 h stirring at the same temperature. Saturated aqueous $NaHCO_3$ (10 mL) was added to quenched the reaction. The layers were separated and the aqueous phase was extracted with CH_2Cl_2 (10 mL × 3). The combined organic layers were washed with brine (20 mL) and dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 50/1) to yield **16** (547 mg, 96%) as a white solid.

TLC R*f* = 0.6 (Petroleum ether/Ethyl acetate = 30/1; phosphomolybdic acid).

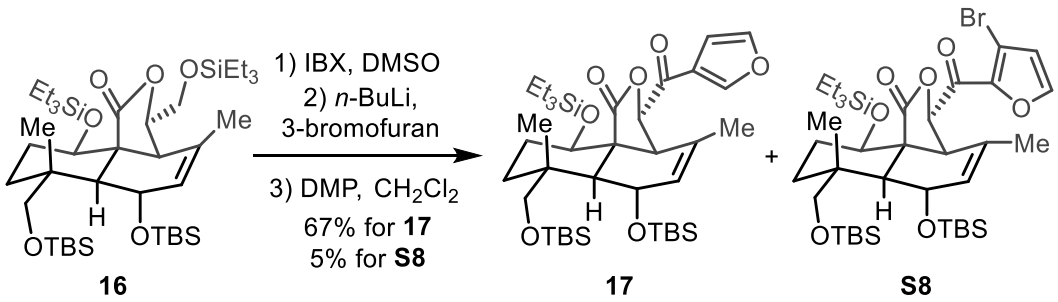
Opt. Rot. $[\alpha]_D^{20}$ = +12.9° (c 0.66, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.52 (s, 1H), 4.10 (d, *J* = 10.4 Hz, 1H), 3.93 – 3.87 (m, 1H), 3.83 – 3.78 (m, 2H), 3.72 (d, *J* = 8.8 Hz, 1H), 3.47 (dd, *J* = 11.5, 3.3 Hz, 1H), 3.33 (d, *J* = 8.8 Hz, 1H), 2.63 (d, *J* = 3.4 Hz, 1H), 2.34 (dt, *J* = 16.0, 11.5 Hz, 1H), 1.81 (d, *J* = 10.4 Hz, 1H), 1.71 (s, 3H), 1.65 – 1.60 (m, 1H), 1.46 – 1.37 (m, 1H), 1.33 – 1.27 (m, 1H), 1.18 (s, 3H), 1.00 – 0.93 (m, 18H), 0.91 (s, 9H), 0.86 (s, 9H), 0.63 (dq, *J* = 16.1, 8.2 Hz, 12H), 0.08 (s, 6H), -0.01 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 176.48, 134.76, 134.03, 86.10, 80.24, 72.67, 69.98, 64.73, 53.74, 50.86, 50.73, 38.30, 34.75, 27.19, 26.30, 26.00, 25.97, 21.36, 18.29, 18.20, 18.17, 7.01, 6.88, 5.46, 4.58, -3.94, -4.91, -5.14.

HRMS (ESI) calcd for $C_{40}H_{80}O_6Si_4$ $[M+Na]^+$: 791.4924, found 791.4923.

Furyl ketone 17



To a solution of **16** (50 mg, 0.065 mmol, 1.0 equiv.) in DMSO (3 mL) and CH_2Cl_2 (3

mL) was added H_2O (47 μL, 2.6 mmol, 40 equiv.) and IBX (109 mg, 0.39 mmol,6.0 equiv.), followed by vigorously stirring at room temperature for 24 h. The reaction was quenched with saturated aqueous $Na_2S_2O_3$ (5 mL). The aqueous phase was extracted with EtOAc (10 mL × 3). The combined organic layers were washed with H_2O (20 mL) and brine (20 mL), dried over Na_2SO_4, concentrated to give a crude unstable aldehyde, which was used directly without further purification.

Under argon atmosphere, to a solution of 3-bromofuran (117 μL, 1.3 mmol, 20 equiv.) and anhydrous THF (1.3 mL) was added *n*-BuLi (609 μL, 0.975 mmol, 15 equiv.) dropwise at -78 °C, followed by 1 h stirring at the same temperature. The crude aldehyde in THF (1 mL) was added dropwise. After 2 h stirring at -78 °C, the reaction was quenched with saturated aqueous NH_4Cl (1 mL) and extracted with EtOAc (5 mL × 3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, concentrated to give a crude furfuryl alcohol.

The alcohol was dissolved in CH_2Cl_2 (1.3 mL), and $NaHCO_3$ (27.3 mg, 0.325 mmol, 5.0 equiv.) and Dess-Martin periodinane (55 mg, 0.13 mmol, 2.0 equiv.) was added at 5 °C. The mixture was stirred at 5 °C for 24 h and quenched with saturated aqueous $Na_2S_2O_3$ (5 mL). The layers were separated and the aqueous phase was extracted with CH_2Cl_2 (5 mL × 3). The combined organic layers were washed with brine (10 mL) and dried over Na_2SO_4, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 15/1) to yield **17** (31.3 mg, 67%) and **S8** (2.6 mg, 5%) as a white solid.

Data of **17**.

TLC R*f* = 0.7 (Petroleum ether/Ethyl acetate = 15/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = +37.4° (c 0.255, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41 (d, *J* = 1.3 Hz, 1H), 7.41 (t, *J* = 1.7 Hz, 1H), 6.84 (d, *J* = 1.9 Hz, 1H), 5.59 – 5.53 (m, 1H), 4.41 (d, *J* = 2.8 Hz, 1H), 4.19 (dq, *J* = 10.5, 1.9 Hz, 1H), 3.74 (d, *J* = 8.9 Hz, 1H), 3.51 (dd, *J* = 11.5, 3.2 Hz, 1H), 3.36 (t, *J* = 2.2 Hz, 1H), 3.31 (d, *J* = 8.8 Hz, 1H), 2.27 – 2.13 (m, 1H), 1.93 (d, *J* = 10.4 Hz, 1H), 1.78 (s, 3H), 1.65 – 1.55 (m, 2H), 1.40 – 1.35 (m, 1H), 1.22 (s, 3H), 0.91 (s, 9H), 0.86 (s, 9H), 0.76 (t, *J* = 7.9 Hz, 9H), 0.45 – 0.23 (m, 6H), 0.11 (s, 6H), -0.01 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 191.50, 176.09, 150.64, 142.99, 133.98, 133.79, 124.89, 110.01, 87.06, 80.82, 72.49, 69.65, 53.02, 50.42, 49.30, 38.18, 34.79, 27.05, 26.77, 26.31, 25.96, 20.75, 18.34, 18.29, 18.24, 6.81, 4.83, -3.78, -3.85, -4.90, -5.15.

HRMS (ESI) calcd for $C_{38}H_{66}O_7Si_3$ $[M+Na]^+$: 741.4009, found 741.4009.

Data of **S8**.

TLC R*f* = 0.4 (Petroleum ether/Ethyl acetate = 15/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = +44.5° (c 0.2, MeOH).

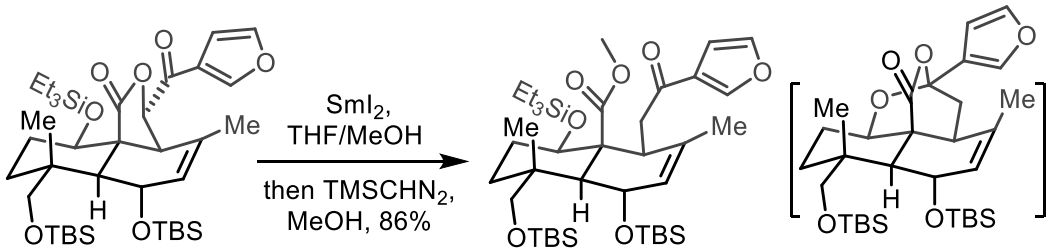
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 1.8 Hz, 1H), 6.66 (d, *J* = 1.8 Hz, 1H), 5.56 (s, 1H), 4.58 (d, *J* = 3.0 Hz, 1H), 4.23 – 4.16 (m, 1H), 3.70 (d, *J* = 8.9 Hz, 1H), 3.56 (dd, *J* = 11.3, 3.3 Hz, 2H), 3.38 (d, *J* = 8.9 Hz, 1H), 2.23 – 2.10 (m, 1H), 1.89 (d, *J* = 10.3 Hz, 1H), 1.71 (s, 3H), 1.63 – 1.55 (m, 2H), 1.44 – 1.40 (m, 1H), 1.22 (s, 3H), 0.91 (s, 9H), 0.87 (s, 9H), 0.80 (t, *J* = 7.9 Hz,

9H), 0.52 – 0.38 (m, 6H), 0.10 (s, 6H), -0.01 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 182.72, 175.98, 146.99, 146.34, 134.42, 133.68, 117.64, 110.72, 85.93, 80.49, 72.58, 69.67, 53.15, 49.50, 48.81, 38.13, 34.50, 26.90, 26.30, 25.97, 20.90, 18.30, 18.22, 18.18, 6.96, 5.05, -3.83, -3.87, -4.93, -5.12.

HRMS (ESI) calcd for $C_{38}H_{65}BrO_7Si_3$ $[M+Na]^+$: 819.3114, found 819.3114.

Methyl ester 18



17 **18** **S9**

To a flamed-dried, round-bottomed flask was added **17** (240 mg, 0.33 mmol, 1.0 equiv.), THF (33.3 mL) and MeOH (3.33 mL). The reaction vessel was degassed and purged with argon balloon for three times. The reaction mixture was cooled to -78 °C and SmI_2 (16.5 mL, 0.1 M in THF, 1.65 mmol, 5.0 equiv.) was added under argon atmosphere, followed by 1 h stirring at the same temperature before EtOAc (10 mL) and saturated aqueous $Na_2S_2O_3$ (20 mL) was added (**Caution: Quenching with Aqueous HCl gives compound S9**). After separating the phases, the aqueous layer was exacted with EtOAc (30 mL × 3). The combined organic layers were washed with brine (30 mL), dried over Na_2SO_4, filtered, concentrated to give a crude residue. The residue was dissolved in MeOH (5 mL) and $TMSCHN_2$ (825 μL, 2 M in hexane, 1.65 mmol, 5.0 equiv.) was added dropwise. The mixture was stirred for 1 h at rt and quenched with silica gel powder (100 mg). The solvent was removed under reduced pressure and the residue was purified by flash column chromatography (Petroleum ether/Ethyl acetate = 50/1) to yield **18** (210 mg, 86 %).

Data of **18**.

TLC R*f* = 0.63 (Petroleum ether/Ethyl acetate = 15/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = +33.5° (c 0.15, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, *J* = 1.1 Hz, 1H), 7.43 (t, *J* = 1.7 Hz, 1H), 6.77 (dd, *J* = 1.9, 0.8 Hz, 1H), 5.31 (s, 1H), 4.43 (d, *J* = 9.7 Hz, 1H), 3.83 – 3.73 (m, 3H), 3.66 (s, 3H), 3.37 (d, *J* = 9.0 Hz, 1H), 3.30 (d, *J* = 9.4 Hz, 1H), 3.14 – 3.03 (m, 1H), 2.22 – 2.10 (m, 1H), 1.78 – 1.65 (m, 3H), 1.47 (s, 3H), 1.37 – 1.31 (m, 1H), 0.99 (s, 3H), 0.91 (s, 9H), 0.89 (s, 9H), 0.86 (t, *J* = 8.0 Hz, 9H), 0.47 (qd, *J* = 8.0, 1.5 Hz, 6H), 0.12 (s, 3H), 0.10 (s, 3H), 0.01 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 194.55, 173.58, 146.62, 144.14, 135.73, 128.56, 127.83, 108.84, 79.84, 73.59, 69.94, 56.34, 52.62, 50.67, 45.19, 42.51,

38.58, 33.63, 28.88, 26.45, 26.08, 21.32, 18.47, 18.37, 16.22, 7.02, 5.68, -3.12, -3.31, -4.95, -5.08.

HRMS (ESI) calcd for $C_{39}H_{70}O_7Si_3$ [M+Na]$^+$: 757.4322, found 757.4322.

Data of **S9**.

TLC R*f* = 0.6 (Petroleum ether/Ethyl acetate = 15/1; phosphomolybdic acid).

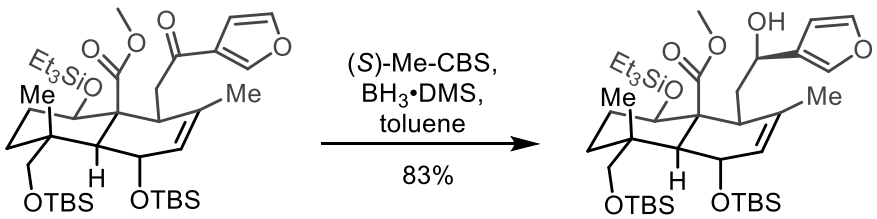
Opt. Rot. $[\alpha]_D^{20}$ = +20.6° (c 0.27, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (s, 1H), 7.40 (t, *J* = 1.7 Hz, 1H), 6.49 (d, *J* = 1.9 Hz, 1H), 5.40 (s, 1H), 5.25 (d, *J* = 9.2 Hz, 1H), 3.89 – 3.82 (m, 1H), 3.58 (d, *J* = 9.6 Hz, 1H), 3.45 (d, *J* = 9.4 Hz, 1H), 2.83 (t, *J* = 8.7 Hz, 1H), 2.54 (dd, *J* = 13.8, 11.0 Hz, 1H), 2.16 (dd, *J* = 13.9, 6.0 Hz, 1H), 1.91 – 1.85 (m, 1H), 1.81 (d, *J* = 9.3 Hz, 1H), 1.74 – 1.66 (m, 1H), 1.64 (s, 3H), 1.47 – 1.37 (m, 2H), 1.11 (s, 3H), 0.91 (s, 9H), 0.89 (s, 9H), 0.15 (s, 3H), 0.14 (s, 3H), 0.01 (s, 3H), 0.00 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.30, 143.57, 140.24, 131.33, 129.90, 124.97, 108.15, 100.33, 80.87, 72.92, 68.46, 49.36, 48.33, 42.77, 38.49, 37.20, 33.82, 29.84, 28.07, 26.32, 26.07, 19.50, 18.31, 17.83, -3.00, -3.39, -5.02, -5.05.

HRMS (ESI) calcd for $C_{32}H_{52}O_6Si_2$ [M+Na]$^+$: 611.3195, found 611.3140.

Alcohol S19



18 **S19**

To a flamed-dried, round-bottomed flask was added (*S*)-2-Methyl-CBS-oxazaborolidine (14 mL, 1 M in toluene, 14 mmol, 50 equiv.), anhydrous toluene (14 mL) and BH_3·DMS (14 mL, 2 M in toluene, 28 mmol, 100 equiv.) under argon atmosphere, followed by 1 h stirring at rt. After the reaction mixture was cooled to -20 °C, **18** (206 mg, 0.28 mmol, 1.0 equiv.) in anhydrous toluene (28 mL) was added slowly. The rection was stirred at the same temperature for 24 h. MeOH (30 mL) was added dropwise at -78 °C to quench the reaction. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography (Petroleum ether/Ethyl acetate = 30/1) to yield **S19** (171 mg, 83%).

TLC R*f* = 0.49 (Petroleum ether/Ethyl acetate = 15/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = +39.5° (c 0.25, MeOH).

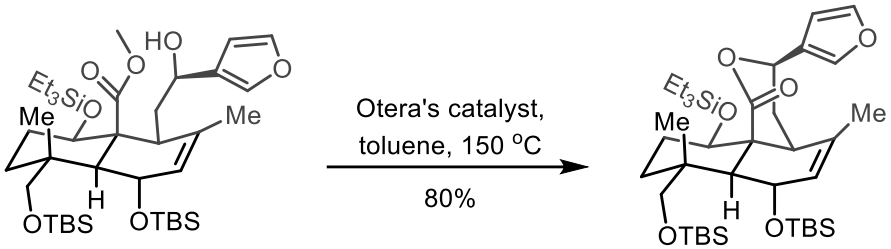
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.34 (m, 2H), 6.38 (d, *J* = 1.9 Hz, 1H), 5.31 (d, *J* = 2.4 Hz, 1H), 4.68 – 4.61 (m, 1H), 4.37 (d, *J* = 9.8 Hz, 1H), 4.03 (dd, *J* = 10.0, 4.2 Hz, 1H), 3.74 (d, *J* = 9.3 Hz, 1H), 3.58 (s, 3H), 3.32 (d, *J* = 9.3 Hz, 1H), 2.65 – 2.53 (m, 2H), 2.43 (d, *J* = 5.8 Hz, 1H), 2.22 – 2.11 (m, 1H),

2.04 (ddd, *J* = 15.6, 7.9, 2.3 Hz, 1H), 1.76 (s, 3H), 1.73 – 1.67 (m, 2H), 1.43 – 1.33 (m, 1H), 1.03 (s, 3H), 0.94 – 0.88 (m, 27H), 0.62 (q, *J* = 7.9 Hz, 6H), 0.12 (s, 3H), 0.10 (s, 3H), 0.00 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.33, 143.22, 138.59, 136.97, 130.28, 128.79, 108.85, 79.39, 73.06, 70.39, 68.04, 58.12, 52.46, 50.63, 49.43, 38.35, 38.30, 32.69, 29.04, 26.43, 26.07, 21.90, 18.46, 18.35, 16.45, 7.10, 6.28, -3.29, -3.31, -4.99, -5.12.

HRMS (ESI) calcd for $C_{39}H_{72}O_7Si_3$ $[M+Na]^+$: 759.4478, found 759.4478.

δ-lactone 8



S19 **8**

A mixture of **S19** (20 mg, 0.027 mmol, 1.0 equiv.), anhydrous toluene (114 mL) and Otera's catalyst (4 mg, 6.75 μmol, 0.25 equiv.) was added to a 15 mL sealed tube and the mixture was purged with argon balloon for three times. Then the reaction mixture was refluxed at 150 °C for 6 h. After being cooled to ambient temperature, the solution was concentrated in vacuo and the residue was purified by flash column chromatography (Petroleum ether/Ethyl acetate = 50/1) to yield **8** (15.3 mg, 80%) as a white solid.

TLC R*f* = 0.7 (Petroleum ether/Ethyl acetate = 15/1; phosphomolybdic acid).

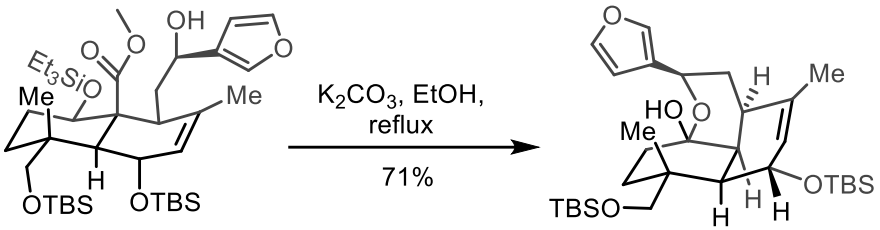
Opt. Rot. $[\alpha]_D^{20}$ = +30.9° (c 0.34, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (s, 1H), 7.25 (s, 1H), 6.28 (d, *J* = 1.8 Hz, 1H), 5.53 (d, *J* = 8.7 Hz, 1H), 5.27 (s, 1H), 4.46 (d, *J* = 9.9 Hz, 1H), 3.78 (dd, *J* = 10.5, 3.9 Hz, 1H), 3.59 (d, *J* = 8.9 Hz, 1H), 3.42 (d, *J* = 8.9 Hz, 1H), 3.04 – 2.94 (m, 1H), 2.47 (s, 1H), 2.10 – 1.94 (m, 2H), 1.76 (d, *J* = 10.0 Hz, 1H), 1.64 – 1.45 (m, 3H), 1.38 (s, 3H), 1.25 (s, 3H), 0.98 (t, *J* = 7.9 Hz, 9H), 0.89 (s, 9H), 0.87 (s, 9H), 0.66 (q, *J* = 7.9 Hz, 6H), 0.11 (s, 3H), 0.10 (s, 3H), -0.01 (s, 3H), -0.02 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.48, 143.20, 139.10, 134.28, 132.39, 127.93, 108.39, 80.50, 73.14, 72.88, 70.22, 53.23, 50.23, 48.03, 37.78, 33.70, 28.45, 28.04, 26.40, 26.04, 21.26, 18.45, 18.39, 18.33, 7.07, 5.64, -3.34, -3.63, -5.00, -5.09.

HRMS (ESI) calcd for $C_{38}H_{68}O_6Si_3$ $[M+Na]^+$: 727.4216, found 727.4213.

Hemiketal 19



S19 **19**

A mixture of **S19** (13.4 mg, 18.2 μmol, 1.0 equiv.), anhydrous ethanol (1.8 mL) and potassium carbonate (12.6 mg, 91 μmol, 5.0 equiv.) was added to a 15 mL sealed tube and the mixture was purged with argon balloon for three times. Then the reaction mixture was refluxed at 150 °C for 15 h. After being cooled to ambient temperature, the reaction mixture was diluted with H_2O (5 mL) and EtOAc (5 mL). After separating the phases, the aqueous layer was exacted with EtOAc (5 mL × 3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 15/1) to yield **19** (7.3 mg, 71%) as a white solid.

TLC R*f* = 0.45 (Petroleum ether/Ethyl acetate = 15/1; phosphomolybdic acid).

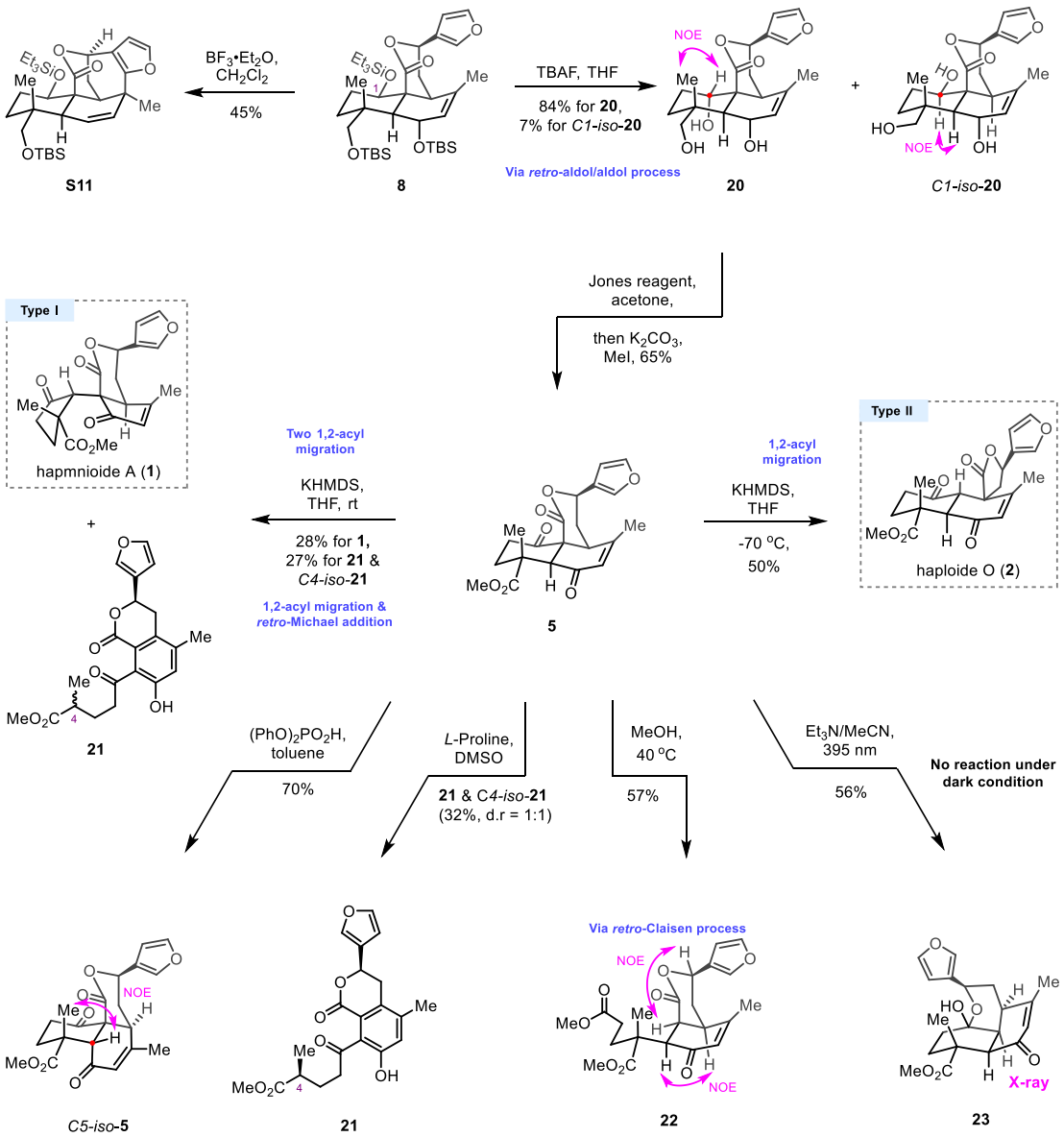
Opt. Rot. $[\alpha]_D^{20}$ = +17.2° (c 0.06, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 (d, *J* = 1.6 Hz, 1H), 7.38 (t, *J* = 1.8 Hz, 1H), 6.42 (d, *J* = 1.8 Hz, 1H), 5.32 (s, 1H), 5.11 (dd, *J* = 11.8, 2.7 Hz, 1H), 4.35 – 4.28 (m, 1H), 3.84 (d, *J* = 9.6 Hz, 1H), 3.34 (d, *J* = 9.7 Hz, 1H), 2.63 (t, *J* = 11.5 Hz, 1H), 2.14 (dt, *J* = 12.9, 3.1 Hz, 1H), 1.82 – 1.73 (m, 2H), 1.64 (s, 3H), 1.55 – 1.51 (m, 2H), 1.37 – 1.29 (m, 3H), 0.98 (s, 3H), 0.90 (s, 9H), 0.89 (s, 9H), 0.09 (s, 3H), 0.09 (s, 3H), 0.02 (s, 3H), 0.01 (s, 3H).

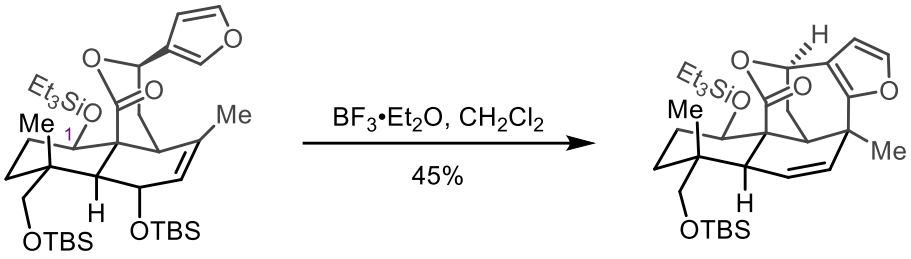
^{13}C NMR (100 MHz, $CDCl_3$) δ 143.25, 139.36, 136.86, 127.42, 126.56, 109.11, 96.95, 73.21, 69.87, 65.46, 45.75, 44.98, 39.21, 37.20, 34.86, 34.47, 32.53, 29.85, 26.35, 26.08, 20.07, 18.36, 15.88, -2.56, -2.85, -5.05, -5.15

HRMS (ESI) calcd for $C_{31}H_{54}O_5Si_2$ $[M+Na]^+$: 585.3402, found 585.3402.

*4.2 Synthesis of hapmnioide A (**1**) and haploide O (**2**)*



Olefin S11



8 **S11**

To a solution of **8** (3 mg, 4.3 μmol, 1.0 equiv.) in CH_2Cl_2 (860 μL) was added BF_3•Et_2O (0.14 μL, 1.1 μmol, 0.25 equiv.) at 0 °C. The mixture was stirred at the same temperature for 0.5 h before quenched with saturated aqueous Na_2CO_3 (2 mL). The layers were separated and the aqueous phase was extracted with CH_2Cl_2 (3 mL × 3). The combined organic layers were washed with brine (5 mL), dried over Na_2SO_4, filtered, concentrated in vacuo, and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 15/1) to yield **S11** (1.1 mg, 45%) as a white solid.

TLC R*f* = 0.5 (Petroleum ether/Ethyl acetate = 15/1; phosphomolybdic acid).

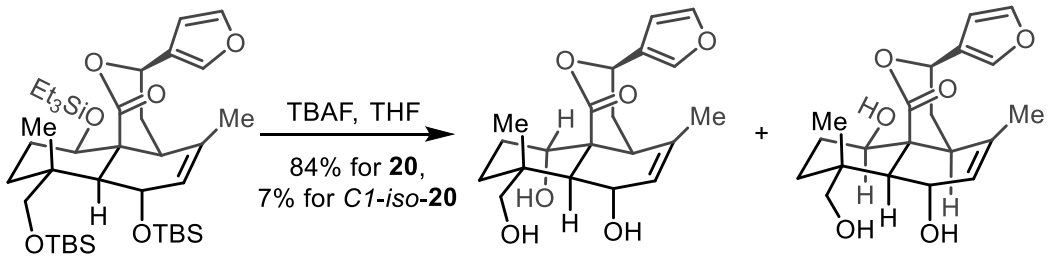
Opt. Rot. $[\alpha]_D^{20}$ = +57.9° (c 0.125, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 (d, *J* = 1.9 Hz, 1H), 6.26 (d, *J* = 1.9 Hz, 1H), 5.79 (dd, *J* = 9.8, 3.0 Hz, 1H), 5.57 (dd, *J* = 9.8, 2.8 Hz, 1H), 5.18 (d, *J* = 4.8 Hz, 1H), 3.71 (dd, *J* = 10.7, 3.6 Hz, 1H), 3.63 – 3.54 (m, 1H), 3.36 (d, *J* = 9.9 Hz, 1H), 3.03 (d, *J* = 10.0 Hz, 1H), 2.45 (s, 1H), 2.30 (s, 1H), 2.02 – 1.89 (m, 2H), 1.72 – 1.65 (m, 2H), 1.40 (s, 3H), 1.30 – 1.20 (m, 1H), 1.07 (s, 3H), 0.99 (t, *J* = 7.9 Hz, 9H), 0.90 (s, 9H), 0.67 (q, *J* = 8.0 Hz, 6H), 0.02 (s, 3H), 0.03 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 171.56, 156.30, 140.95, 132.29, 125.48, 120.28, 108.34, 80.22, 71.64, 69.99, 54.95, 52.66, 42.72, 40.38, 36.84, 32.25, 29.51, 27.10, 26.02, 18.33, 7.11, 5.87, -5.33, -5.37.

HRMS (ESI) calcd for $C_{32}H_{52}O_5Si_2$ $[M+Na]^+$: 595.3245, found 595.3245.

Triol 20



8 **20** *C1-iso*-**20**

To a solution of **8** (52.5 mg, 74.4 μmol, 1.0equiv.) in anhydrous THF (7 mL) was added TBAF (372 μL, 1 M in THF, 0.372 mmol, 5.0 equiv.). The reaction was stirred

at rt overnight and quenched with saturated aqueous NH_4Cl (5 mL). The aqueous layer was extracted with EtOAc (5 mL × 3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (CH_2Cl_2/methanol = 20/1) to yield **20** and *C1-iso*-**20** (24.6 mg, 91%) as a white solid.

Data of **20**

TLC R*f* = 0.4 (CH_2Cl_2/methanol = 15/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = +69.3° (c 0.1, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (t, *J* = 1.8 Hz, 1H), 7.38 (s, 1H), 6.41 (d, *J* = 2.0 Hz, 1H), 5.74 (dd, *J* = 9.6, 3.7 Hz, 1H), 5.29 (s, 1H), 4.47 (d, *J* = 9.7 Hz, 1H), 4.25 (dd, *J* = 4.0, 2.0 Hz, 1H), 3.41 – 3.33 (m, 2H), 3.09 – 3.01 (m, 1H), 2.86 – 2.74 (m, 1H), 2.26 – 2.18 (m, 1H), 1.95 – 1.65 (m, 4H), 1.49 (s, 3H), 1.28 (s, 3H), 1.07 (dt, *J* = 12.9, 3.3 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.76, 144.96, 140.18, 137.26, 129.21, 128.87, 109.28, 76.21, 74.58, 68.50, 66.52, 55.29, 42.61, 38.41, 29.89, 27.25, 27.05, 21.77, 19.36.

HRMS (ESI) calcd for $C_{20}H_{26}O_6$ $[M+Na]^+$: 385.1622, found 385.1622.

Data of *C1-iso*-**20**

TLC R*f* = 0.42 (CH_2Cl_2/methanol = 15/1; phosphomolybdic acid).

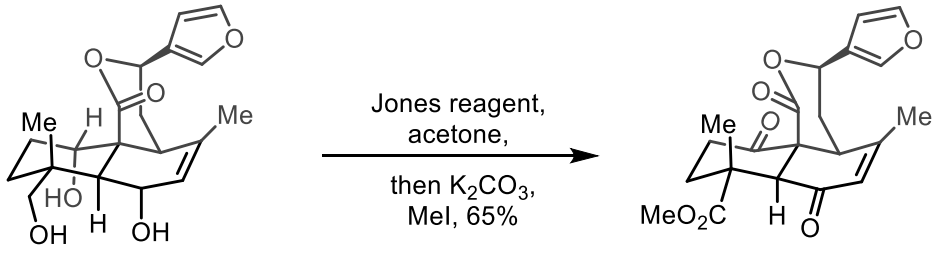
Opt. Rot. $[\alpha]_D^{20}$ = +10° (c 0.175, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (t, *J* = 1.7 Hz, 1H), 7.30 (s, 1H), 6.37 (s, 1H), 5.65 (d, *J* = 9.8 Hz, 1H), 5.31 (s, 1H), 4.34 (d, *J* = 10.2 Hz, 1H), 3.78 (dd, *J* = 10.2, 4.4 Hz, 1H), 3.53 (d, *J* = 10.9 Hz, 1H), 3.41 – 3.33 (m, 1H), 3.17 (ddd, *J* = 14.3, 9.8, 6.5 Hz, 1H), 2.62 (s, 1H), 2.26 (d, *J* = 14.0 Hz, 1H), 1.92 – 1.81 (m, 1H), 1.76 – 1.68 (m, 1H), 1.65 (d, *J* = 10.1 Hz, 1H), 1.58 – 1.49 (m, 1H), 1.43 (s, 3H), 1.42 – 1.36 (m, 1H), 1.29 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 174.70, 144.71, 139.87, 137.40, 131.04, 129.73, 109.26, 77.30, 75.59, 74.78, 68.79, 54.52, 52.13, 48.79, 38.68, 34.82, 29.67, 28.23, 21.50, 18.56.

HRMS (ESI) calcd for $C_{20}H_{26}O_6$ $[M+Na]^+$: 385.1622, found 385.1622.

β-Ketoester 5



20 **5**

To a solution of **20** and *C1-iso*-**20** (12 mg, 33.1 μmol, 1.0 equiv.) in acetone (3.3 mL) was added freshly prepared Jones' reagent (66.2 μL, 2.5 M, 0.166 mmol, 5.0 equiv.). The mixture was stirred for 5 h at the same temperature. K_2CO_3 (69 mg, 0.5 mmol,

15.0 equiv.) and MeI (20.6 μL, 0.331 mmol, 10.0 equiv.) were added, followed by vigorous stirring for 5 h at rt. The reaction mixture was filtered through a short plug of celite and rinsed with EtOAc (10 mL × 3). The combined filtrate was washed with H_2O (20 mL) and brine (20 mL) and dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 2/1) to yield **5** (8.3 mg, 65%).

TLC R*f* = 0.5 (Petroleum ether/Ethyl acetate = 3/2; phosphomolybdic acid).

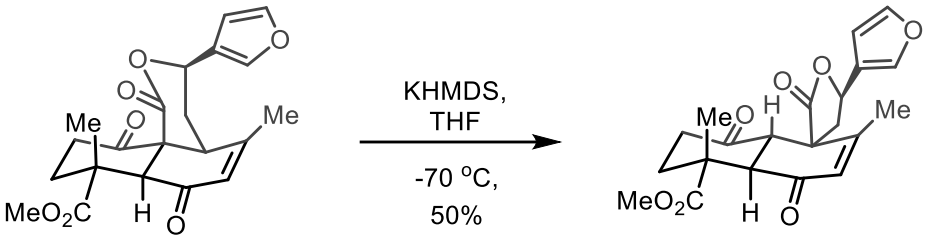
Opt. Rot. $[\alpha]_D^{20}$ = +129.2° (c 0.3, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (s, 1H), 7.41 (s, 1H), 6.39 (s, 1H), 5.87 (s, 1H), 5.26 (dd, *J* = 11.7, 3.4 Hz, 1H), 3.89 – 3.82 (m, 1H), 3.71 (s, 3H), 3.58 (s, 1H), 2.87 – 2.73 (m, 2H), 2.59 – 2.53 (m, 1H), 2.13 – 1.98 (m, 3H), 1.95 (s, 3H), 1.80 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 205.69, 191.60, 177.01, 166.92, 155.66, 144.05, 139.92, 127.15, 123.82, 108.25, 72.85, 64.90, 58.12, 53.03, 43.92, 40.70, 40.08, 37.73, 35.02, 21.82, 18.23.

HRMS (ESI) calcd for $C_{21}H_{22}O_7$ $[M+Na]^+$: 409.1258, found 409.1258

haploide O (2)



Under argon atmosphere, to a solution of **5** (6.0 mg, 15.52 μmol, 1.0 equiv.) in anhydrous THF (15 mL) was added KHMDS (31.0 μL, 1M in THF, 31.0 mmol, 2.0 equiv.) at -70 °C, followed by 24 h stirring at the same temperature. The reaction was quenched with saturated aqueous NH_4Cl (2 mL). The aqueous layer was extracted with EtOAc (5 mL × 3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 2/1) to yield **2** (3.0 mg, 55%) as a white solid.

TLC R*f* = 0.5 (Petroleum ether/Ethyl acetate = 3/2; phosphomolybdic acid).

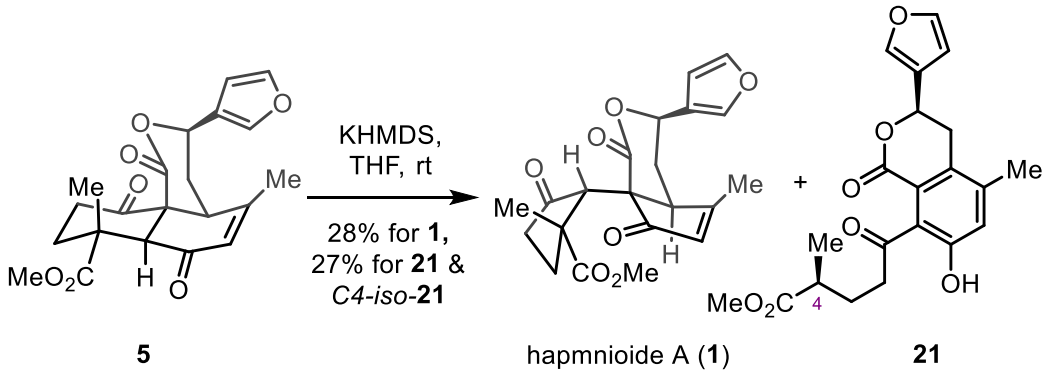
Opt. Rot. $[\alpha]_D^{20}$ = -30° (c 0.1, MeOH). [Lit. [6]: $[\alpha]_D^{20}$ = -45.64 (c 1.5, MeOH)].

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (s, 1H), 7.46 (t, *J* = 1.8 Hz, 1H), 6.42 (s, 1H), 5.95 – 5.89 (m, 1H), 5.83 (s, 1H), 3.75 (s, 3H), 3.49 (d, *J* = 14.6 Hz, 1H), 3.40 (d, *J* = 14.6 Hz, 1H), 2.97 (dd, *J* = 13.9, 9.1 Hz, 1H), 2.62 – 2.46 (m, 2H), 2.11 – 1.96 (m, 3H), 1.90 (s, 3H), 1.41 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 207.25, 194.41, 177.23, 176.63, 159.47 144.46, 139.37, 127.05, 125.13, 108.34, 73.13, 53.86, 52.72, 52.01, 50.91, 42.68, 36.55, 36.22, 35.16, 19.72, 14.80.

HRMS (ESI) calcd for $C_{21}H_{22}O_7$ $[M+Na]^+$: 409.1258, found 409.1258.

hapmnioide A (1)



Under argon atmosphere, to a solution of compound **5** (7.8 mg, 20.2 μmol, 1.0 equiv.) in anhydrous THF (2 mL) was added KHMDS (10.1 μL, 1M in anhydrous THF, 10.1 μmol, 0.5 equiv.) at 0 °C, followed by 5 minutes stirring at the same temperature. The reaction mixture was warmed to room temperature, and stirred for 24 h before quenched with saturated aqueous NH_4Cl (2 mL). The aqueous layer was extracted with ethyl acetate (5 mL × 3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (CH_2Cl_2/methanol = 50/1) to yield **1** (2.2 mg, 28%) and **21** & *C4-iso*-**21** (2.1 mg, 27%) as white solids.

Data of **1**

TLC R*f* = 0.38 (CH_2Cl_2/methanol = 50/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = -153.6° (c 0.08, MeCN). [Lit. [7]: $[\alpha]_D^{20}$ = -213.1° (c 0.1, MeCN)].

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (s, 1H), 7.39 (t, *J* = 1.6 Hz, 1H), 6.38 (s, 1H), 5.94 – 5.90 (m, 1H), 5.88 (s, 1H), 3.65 (s, 3H), 3.62 (s, 1H), 3.39 (dd, *J* = 11.3, 6.1 Hz, 1H), 2.58 – 2.48 (m, 1H), 2.42 – 2.32 (m, 2H), 2.18 – 2.10 (m, 1H), 2.06 (s, 3H), 1.98 – 1.88 (m, 1H), 1.51 – 1.41 (m, 1H), 1.33 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 213.63, 199.25, 180.92, 175.10, 168.79, 143.79, 140.04, 127.21, 124.33, 108.49, 72.55, 68.20, 58.01, 52.58, 48.80, 45.56, 36.65, 36.33, 32.87, 24.05, 17.44.

HRMS (ESI) calcd for $C_{21}H_{22}O_7$ $[M+Na]^+$: 409.1258, found 409.1257.

Data of **21** & *C4-iso*-**21**

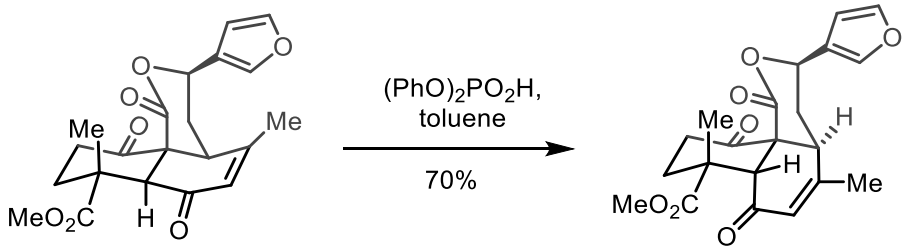
TLC R*f* = 0.34 (CH_2Cl_2/methanol = 50/1; phosphomolybdic acid).

^{1}H NMR (400 MHz, $CDCl_3$) δ 9.26 (s, 1H), 7.60 – 7.54 (m, 1H), 7.49 – 7.43 (m, 1H), 7.06 (s, 1H), 6.54 – 6.49 (m, 1H), 5.63 – 5.55 (m, 1H), 3.67 – 3.61 (m, 3H), 3.14 – 3.00 (m, 2H), 2.92 – 2.80 (m, 1H), 2.72 – 2.62 (m, 1H), 2.56 – 2.45 (m, 1H), 2.31 (s, 3H), 2.06 – 1.96 (m, 1H), 1.92 – 1.82 (m, 1H), 1.18 – 1.12 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 207.31, 207.23, 176.95, 176.83, 164.35, 156.12, 144.03, 141.12, 140.77, 140.72, 140.42, 131.13, 131.01, 125.35, 124.73, 122.72, 122.46, 108.77, 72.69, 72.67, 51.83, 41.65, 41.21, 38.93, 38.76, 31.68, 31.58, 29.33, 29.19, 19.55, 17.44, 17.06.

HRMS (ESI) calcd for $C_{21}H_{22}O_7$ [M+Na]$^+$: 409.1258, found 409.1258.

Isomerized product *C5-iso*-5



5 *C5-iso*-**5**

To a solution of **5** (4.7 mg, 12.2 μmol, 1.0 equiv.) in anhydrous toluene (1.2 mL) was added $(PhO)_2POOH$ (3.7 mg, 14.6 μmol, 1.2 equiv.) under argon atmosphere. The reaction was stirred at 90 °C overnight. The mixture was concentrated in vacuo and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 3/2) to yield *C5-iso*-**5** (3.3 mg, 70%) as a white solid.

TLC R*f* = 0.45 (Petroleum ether/Ethyl acetate = 3/2; phosphomolybdic acid).

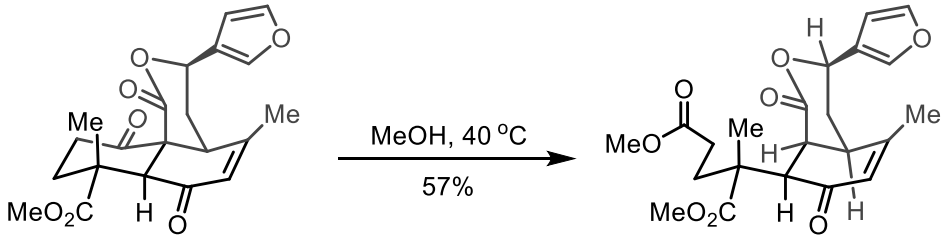
Opt. Rot. $[\alpha]_D^{20}$ = -55.3° (c 0.12, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (s, 1H), 7.45 (s, 1H), 6.43 (s, 1H), 5.83 (s, 1H), 5.46 (dd, *J* = 10.1, 5.1 Hz, 1H), 3.71 (s, 1H), 3.68 (s, 3H), 3.40 (dd, *J* = 9.6, 5.5 Hz, 1H), 2.98 – 2.78 (m, 2H), 2.41 (dt, *J* = 13.3, 5.3 Hz, 1H), 2.28 – 2.15 (m, 2H), 2.05 – 1.95 (m, 1H), 1.98 (s, 3H), 1.49 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 206.30, 192.94, 176.60, 171.30, 160.93, 144.23, 139.84, 126.94, 124.38, 108.22, 74.58, 60.81, 55.26, 52.25, 43.64, 38.94, 36.71, 32.07, 31.74, 24.32, 22.66.

HRMS (ESI) calcd for $C_{21}H_{22}O_7$ [M+Na]$^+$: 409.1258, found 409.1258.

Ring-opening product 22



5 **22**

The reaction flask containing **5** (3 mg, 7.8 μmol, 1.0 equiv.) and anhydrous methanol (8 mL) was attached to a rotary evaporator and concentrated at 40°C to afford the crude product, which was purified by flash column chromatography (Petroleum ether/Ethyl acetate = 1/1) to yield **22** (1.9 mg, 57%) as a white solid.

TLC R*f* = 0.4 (Petroleum ether/Ethyl acetate = 1/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = +35.7° (c 0.1, MeOH).

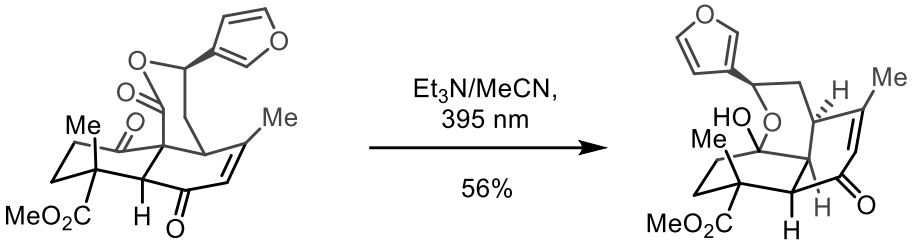
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52 (s, 1H), 7.45 (s, 1H), 6.46 (s, 1H), 5.88 (s, 1H),

5.55 (d, *J* = 11.9 Hz, 1H), 3.71 (s, 3H), 3.68 (s, 3H), 3.55 – 3.50 (m, 1H), 3.46 – 3.38 (m, 1H), 3.25 (d, *J* = 2.6 Hz, 1H), 2.62 (t, *J* = 12.8 Hz, 1H), 2.46 – 2.36 (m, 1H), 2.18 – 2.03 (m, 2H), 1.91 (s, 3H), 1.86 (d, *J* = 8.4 Hz, 2H), 1.33 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 193.80, 176.59, 173.86, 170.36, 155.07, 144.06, 140.01, 128.78, 123.17, 108.50, 71.87, 54.18, 52.46, 52.02, 45.17, 40.32, 39.64, 34.97, 34.02, 29.08, 20.87, 18.21.

HRMS (ESI) calcd for $C_{22}H_{26}O_8$ [M+Na]$^+$: 441.1520, found 441.1520.

Decarboxylation product 23



5 **23**

To a solution of **5** (3 mg, 7.8 μmol, 1.0 equiv.) in anhydrous MeCN (1.5 mL) was added TEA (300 μL) and the reaction vessel was degassed and purged with argon balloon for three times. Then the reaction mixture was stirred for 48 h under LED irradiation (395 nm, 20W, distance ~ 2 cm) under an argon atmosphere at room temperature. The solvent was removed under reduced pressure and the residue was purified by flash column chromatography (Petroleum ether/Ethyl acetate = 3/1) to yield **23** (1.6 mg, 56%) as a white solid.

TLC R*f* = 0.75 (Petroleum ether/Ethyl acetate = 3/2; phosphomolybdic acid).

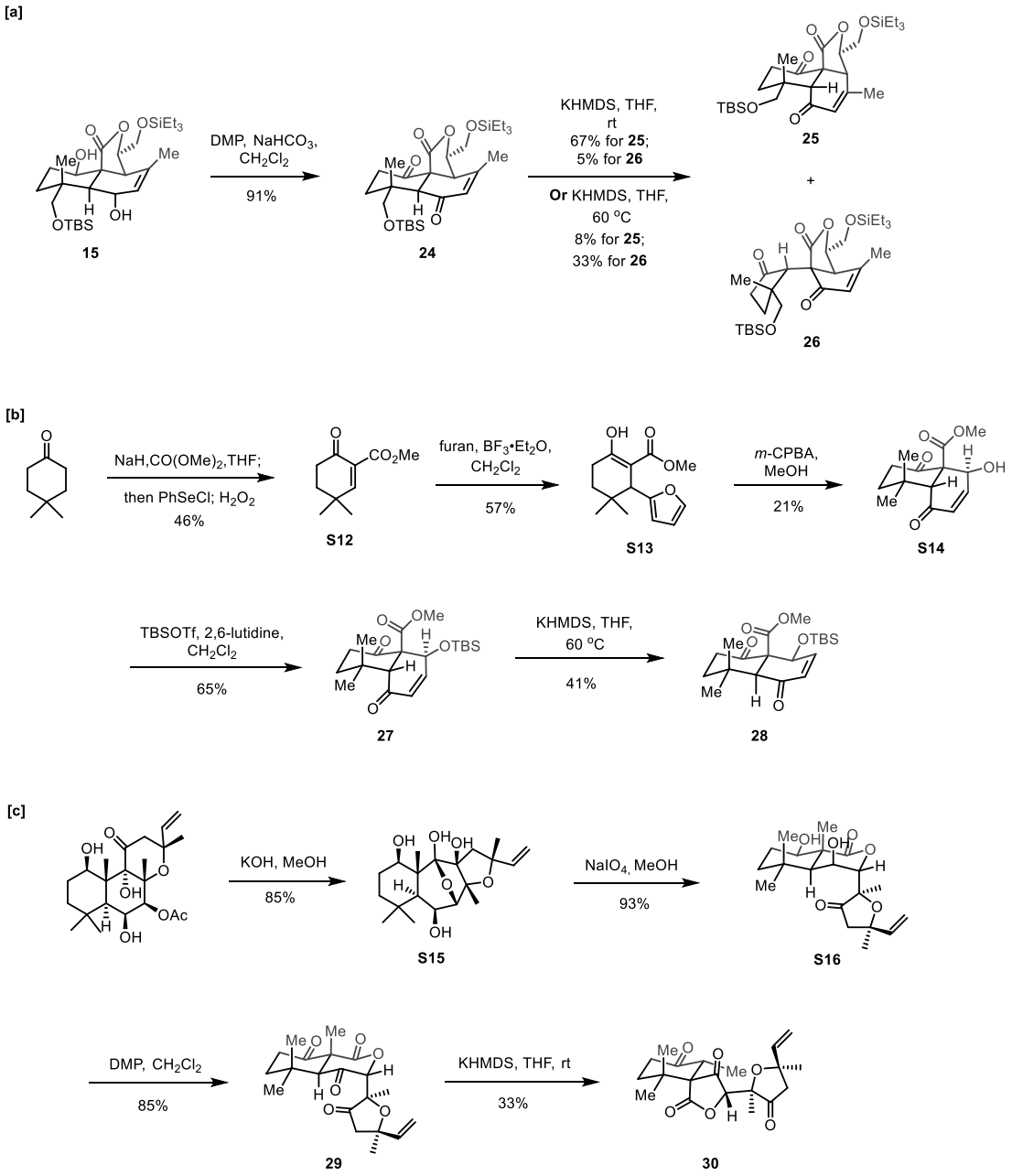
Opt. Rot. $[\alpha]_D^{20}$ = +27.4° (c 0.18, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (s, 1H), 7.38 (s, 1H), 6.38 (s, 1H), 5.79 (s, 1H), 4.89 (dd, *J* = 9.8, 4.9 Hz, 1H), 3.73 (s, 3H), 3.29 (d, *J* = 6.0 Hz, 1H), 2.98 (q, *J* = 9.4 Hz, 1H), 2.62 (t, *J* = 7.2 Hz, 1H), 2.26 – 2.18 (m, 2H), 2.08 – 1.98 (m, 2H), 1.86 (s, 3H), 1.71 – 1.65 (m, 2H), 1.62 (s, 3H).

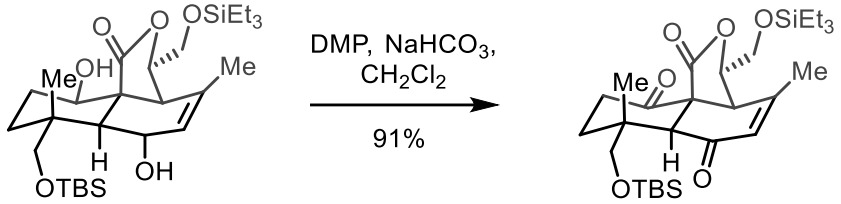
^{13}C NMR (100 MHz, $CDCl_3$) δ 198.60, 177.73, 156.30, 143.61, 139.43, 127.42, 127.40, 108.60, 97.32, 66.59, 52.35, 47.95, 47.03, 40.00, 38.93, 35.43, 34.17, 27.32, 24.81, 20.94.

HRMS (ESI) calcd for $C_{20}H_{24}O_6$ [M+Na]$^+$: 383.1465, found 383.1465.

4.3 Late-stage 1,2-acyl migrations of polycyclic terpenoids



γ-Lactone 24



15 **24**

Dess-Martin periodinane (305 mg, 0.72 mmol, 3.0 equiv.) was added to a solution of **15** (128 mg, 0.24 mmol, 1.0 equiv.) and $NaHCO_3$ (101 mg, 1.2 mmol, 5.0 equiv.) in CH_2Cl_2 (24 mL), followed by stirring for 2 h at rt. The mixture was quenched with saturated aqueous $Na_2S_2O_3$ (10 mL). The layers were separated and the aqueous phase was extracted with CH_2Cl_2 (10 mL × 3). The combined organic layers were washed with brine (20 mL) and dried over Na_2SO_4, concentrated and purified by flash column chromatography (Petroleum ether/ethyl acetate = 15/1) to yield **24** (117 mg, 91%) as a white solid.

TLC R*f* = 0.6 (Petroleum ether/Ethyl acetate = 10/1; phosphomolybdic acid).

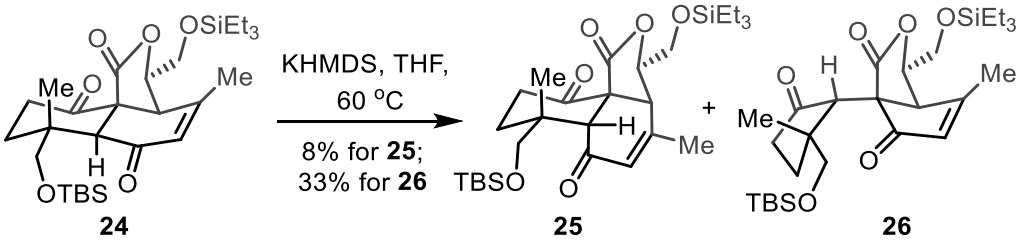
Opt. Rot. $[\alpha]_D^{20}$ = +36.5° (c 0.65, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.89 (s, 1H), 4.32 – 4.24 (m, 1H), 3.92 (d, *J* = 9.5 Hz, 1H), 3.86 (s, 1H), 3.76 (d, *J* = 7.0 Hz, 2H), 3.25 (s, 1H), 3.19 (td, *J* = 13.8, 5.3 Hz, 1H), 3.11 (d, *J* = 9.5 Hz, 1H), 2.40 (dt, *J* = 13.0, 3.9 Hz, 1H), 2.09 (td, *J* = 14.0, 3.7 Hz, 1H), 1.98 (s, 3H), 1.63 (t, *J* = 4.8 Hz, 1H), 1.59 (s, 3H), 0.99 (t, *J* = 8.0 Hz, 9H), 0.79 (s, 9H), 0.66 (q, *J* = 7.9 Hz, 6H), -0.03 (s, 3H), -0.08 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 204.20, 194.11, 171.17, 153.44, 128.60, 81.81, 69.91, 63.19, 61.67, 51.01, 45.71, 37.67, 37.48, 35.56, 25.93, 21.36, 18.48, 18.34, 6.85, 4.44, -5.40, -5.55.

HRMS (ESI) calcd for $C_{28}H_{48}O_6Si_2$ $[M+Na]^+$: 559.2882, found 559.2882.

Hapmnioide A analog 26



24 **25** **26**

Under argon atmosphere, to a solution of **24** (9 mg, 16.8 μmol, 1.0 equiv.) in anhydrous THF (1.7 mL) was added KHMDS (16.8 μL, 1M in THF, 16.8 μmol, 1.0 equiv.) at rt, followed by stirring overnight at 60 °C. The reaction mixture was quenched with saturated aqueous NH_4Cl (2 mL). The aqueous layer was extracted with EtOAc (5 mL × 3). The combined organic layers were washed with brine (10

mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 8/1) to yield **25** (0.7 mg, 8%) and **26** (3 mg, 33%) as white solids.

Data of **25**

TLC R*f* = 0.5 (Petroleum ether/Ethyl acetate = 8/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = -34.6° (c 0.1, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.05 – 6.02 (m, 1H), 4.24 – 4.18 (m, 1H), 3.92 – 3.85 (m, 1H), 3.80 – 3.72 (m, 1H), 3.49 – 3.39 (m, 2H), 3.27 – 3.21 (m, 2H), 2.64 (dd, *J* = 8.6, 6.0 Hz, 2H), 2.13 (dt, *J* = 12.8, 6.1 Hz, 1H), 2.03 (s, 3H), 1.91 (dt, *J* = 14.0, 8.6 Hz, 1H), 1.08 (s, 3H), 0.97 (t, *J* = 7.9 Hz, 9H), 0.87 (s, 9H), 0.64 (q, *J* = 7.7 Hz, 6H), 0.02 (s, 3H), 0.01 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 205.74, 194.09, 173.72, 155.74, 128.77, 82.63, 67.90, 62.84, 59.39, 55.20, 44.11, 37.68, 34.77, 33.61, 26.14, 25.53, 22.31, 18.72, 6.84, 4.41, -5.39, -5.49.

HRMS (ESI) calcd for $C_{28}H_{48}O_6Si_2$ $[M+Na]^+$: 559.2882, found 559.2882.

Data of **26**

TLC R*f* = 0.4 (Petroleum ether/Ethyl acetate = 5/1; phosphomolybdic acid).

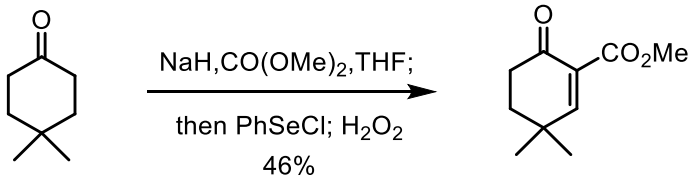
Opt. Rot. $[\alpha]_D^{20}$ = -102.2° (c 0.37, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.00 (s, 1H), 4.17 – 4.07 (m, 2H), 3.90 (dd, *J* = 9.9, 7.4 Hz, 1H), 3.62 (d, *J* = 3.7 Hz, 1H), 3.35 (s, 1H), 3.23 (s, 2H), 2.36 – 2.24 (m, 2H), 2.22 (s, 3H), 1.96 – 1.81 (m, 2H), 1.00 – 0.95 (m, 12H), 0.89 (s, 9H), 0.66 (q, *J* = 7.9 Hz, 6H), 0.05 (s, 3H), 0.04 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 214.62, 200.09, 180.08, 171.98, 128.54, 81.31, 69.08, 64.47, 61.55, 60.01, 51.43, 44.71, 34.42, 34.22, 26.16, 25.17, 18.34, 18.29, 6.92, 4.50, -5.23, -5.49.

HRMS (ESI) calcd for $C_{28}H_{48}O_6Si_2$ $[M+Na]^+$: 559.2882, found 559.2882.

Enone S12



S12

Dimethyl carbonate (58.2 mL, 691.2 mmol, 12.0 equiv.) and a solution of 4,4-dimethylcyclohexanone (7.27g, 57.6mmol, 1.0 equiv.) in anhydrous THF (88 mL) were added to a suspension of NaH (3.2 g, 80.6 mmol, 60% dispersion in mineral oil, 1.4 equiv.) in anhydrous THF (20 mL). The mixture was heated to reflux for 5 h. Until completely consumption of starting material, the mixture was cooled to 0 °C and acetic acid (100 mL of a 10% aqueous solution) was added to quench the reaction. The organic layer was separated and the aqueous phase was extracted with EtOAc (100 mL × 3). The combined organic layers were washed with brine (150 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column

chromatography (Petroleum ether/Ethyl acetate = 15/1) to yield β-keto ester (7.5 g, 71%) as a colorless oil.

To a flamed-dried, round-bottomed flask was added PhSeCl (2.08 g, 10.86 mmol, 1.0 equiv.), pyridine (878 μL, 10.86 mmol, 1.0 equiv.), and CH_2Cl_2 (72 mL) at 0 °C. After 15 min stirring at 0 °C, a solution of β-keto ester (2 g, 10.86 mmol, 1.0 equiv.) in CH_2Cl_2 (8 mL) was added, followed by stirring overnight at rt. Aqueous HCl (40 mL, 10% solution) was added and the organic layer were separated. After the organic layer was cooled to -5 °C, Hydrogen peroxide (3.6 mL, 30 wt% in water) was added dropwise in 4 portions at 15-min intervals and stirred for 1 h at the same temperature. The reaction mixture was diluted with H_2O (20 mL), and the organic layer was separated. The aqueous phase was extracted with CH_2Cl_2 (50 mL × 3). The combined organic layers were washed with brine (10 mL) and dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 5/1) to yield **S12** (1.29 g, 65%) as a white solid.

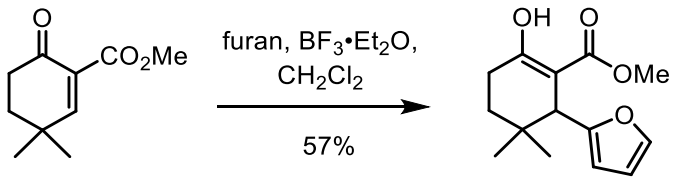
TLC R*f* = 0.15 (Petroleum ether/Ethyl acetate = 10/1; phosphomolybdic acid).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (s, 1H), 3.76 (s, 3H), 2.50 (t, *J* = 6.8 Hz, 2H), 1.86 (t, *J* = 6.8 Hz, 2H), 1.20 (s, 6H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 194.51, 165.34, 164.67, 129.97, 52.27, 35.44, 35.26, 33.57, 27.39.

HRMS (ESI) calcd for $C_{10}H_{14}O_3$ $[M+Na]^+$: 205.0835, found 205.0835.

Furan addition product S13



S12 **S13**

To a solution of **S12** (1.54 g, 8.45 mmol, 1.0 equiv.) in anhydrous CH_2Cl_2 (40 mL) was added furan (12.3 mL, 169 mmol, 20.0 equiv.) and BF_3•Et_2O (209 μL, 1.69 mmol, 0.2 equiv.) at -60 °C. The mixture was stirred at rt for 4 h before quenched with saturated aqueous $NaHCO_3$ (20 mL). The layers were separated and the aqueous phase was extracted with CH_2Cl_2 (30 mL × 3). The combined organic layers were washed with brine (50 mL), dried over Na_2SO_4, filtered, concentrated in vacuo, and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 20/1) to yield **S13** (1.2 g, 57%) as a colorless oil.

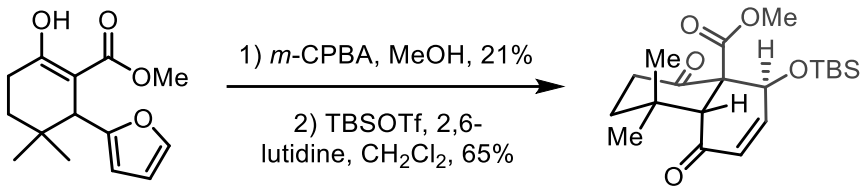
TLC R*f* = 0.75 (Petroleum ether/Ethyl acetate = 10/1; phosphomolybdic acid).

^{1}H NMR (400 MHz, $CDCl_3$) δ 12.37 (s, 1H), 7.29 – 7.26 (m, 1H), 6.25 (dd, *J* = 3.3, 1.9 Hz, 1H), 5.89 (d, *J* = 3.2 Hz, 1H), 3.62 (s, 3H), 3.47 (s, 1H), 2.41 – 2.35 (m, 2H), 1.83 – 1.72 (m, 1H), 1.29 – 1.19 (m, 1H), 1.03 (s, 3H), 0.73 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 173.03, 172.43, 157.91, 140.76, 110.05, 106.63, 98.71, 51.67, 43.67, 33.32, 29.95, 28.73, 26.54, 26.10.

HRMS (ESI) calcd for $C_{14}H_{18}O_4$ [M+Na]$^+$: 273.1097, found 273.1097.

Open-chain methyl ester 27



S13 **27**

To a solution of **S13** (1.2 g, 4.8 mmol, 1.0 equiv.) in dry methanol (30 mL) was added *m*-CPBA (1.5 g, 8.64 mmol, 1.8 equiv.) in 2 portions at 0 °C, followed by stirring for 5 h at 0 °C and 48 h at 5 °C. Methanol was evaporated under reduced pressure to give a residue, which was dissolved in CH_2Cl_2 (15 mL), and KF (307 mg, 5.28 mmol, 1.1 equiv.) was added at 5 °C. The suspension was stirred overnight at the same temperature and filtered through a short plug of Celite and rinsed with CH_2Cl_2 (15 mL × 3). The combined filtrate was concentrated in vacuo and purified by flash column chromatography (CH_2Cl_2/methanol = 40/1) to yield *cis*-decalin product (268 mg, 21%) as a colorless oil.

To a flamed-dried flask was added *cis*-decalin product (100 mg, 0.38 mmol, 1.0 equiv.), CH_2Cl_2 (2.5 mL), 2,6-lutidine (177 μL, 1.52 mmol, 4.0 equiv.) and TBSOTf (175 μL, 0.76 mmol, 2.0 equiv.) sequentially. The reaction was stirred at rt until completely consumption of starting material. The 1N HCl solution (5 mL) was added to quenched the reaction. The layers were separated and the aqueous phase was extracted with CH_2Cl_2 (5mL × 3). The combined organic layers were washed with brine (10 mL) and dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 10/1) to yield **27** (94 mg, 65%) as a white solid.

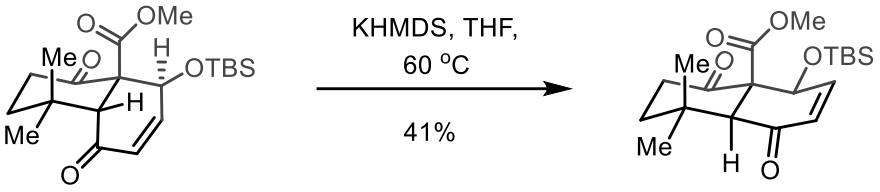
TLC R*f* = 0.6 (Petroleum ether/Ethyl acetate = 5/1; phosphomolybdic acid).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.01 (dd, *J* = 9.9, 5.6 Hz, 1H), 5.97 (d, *J* = 9.9 Hz, 1H), 4.92 (d, *J* = 5.6 Hz, 1H), 3.81 (s, 1H), 3.77 (s, 3H), 2.45 – 2.37 (m, 2H), 2.17 – 2.07 (m, 1H), 1.62 – 1.43 (m, 4H), 1.34 (s, 3H), 0.78 (s, 9H), 0.70 (s, 3H), 0.01 (s, 3H), -0.01 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 207.23, 198.45, 169.10, 147.21, 131.29, 66.45, 65.87, 55.19, 53.31, 35.55, 35.28, 33.99, 31.54, 25.54, 22.44, 17.87, -3.77, -5.11.

HRMS (ESI) calcd for $C_{20}H_{32}O_5Si$ [M+Na]$^+$: 403.1911, found 403.1911.

***trans*-Decalin 28**



27 **28**

Under argon atmosphere, to a solution of **27** (10 mg, 26.3 μmol, 1.0 equiv.) in anhydrous THF (2.6 mL) was added KHMDS (26.3 μL, 1M in THF, 26.3 μmol, 1.0 equiv.) at rt, followed by stirring overnight at 60 °C. The reaction mixture was quenched with saturated aqueous NH_4Cl (3 mL). The aqueous layer was extracted with EtOAc (5 mL × 3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 15/1) to yield **28** (4.1 mg, 41%) as a white solid.

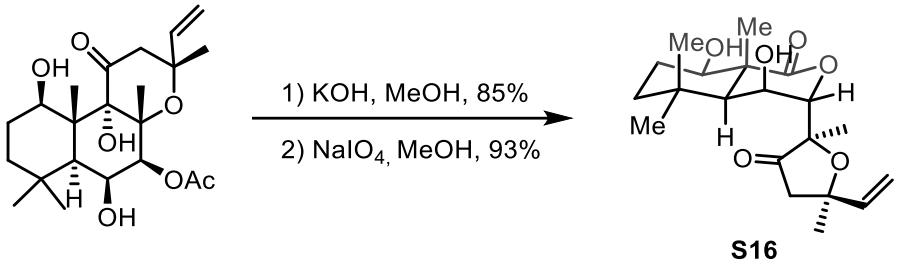
TLC R*f* = 0.55 (Petroleum ether/Ethyl acetate = 10/1; phosphomolybdic acid).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.33 (dd, *J* = 10.4, 2.3 Hz, 1H), 5.96 (dd, *J* = 10.4, 2.2 Hz, 1H), 5.18 (t, *J* = 2.3 Hz, 1H), 3.67 (s, 3H), 2.96 (td, *J* = 14.3, 5.8 Hz, 1H), 2.44 (s, 1H), 2.36 (dt, *J* = 13.5, 3.6 Hz, 1H), 1.72 – 1.65 (m, 1H), 1.62 – 1.56 (m, 1H), 1.24 (s, 3H), 1.19 (s, 3H), 0.83 (s, 9H), 0.20 (s, 3H), 0.16 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 205.11, 195.23, 169.72, 144.82, 129.61, 69.34, 68.11, 59.37, 52.33, 43.34, 37.64, 32.99, 30.40, 25.71, 19.70, 18.11, -4.54, -4.79.

HRMS (ESI) calcd for $C_{20}H_{32}O_5Si$ $[M+Na]^+$: 403.1911, found 403.1911.

δ-Lactone S16



S16

The δ-Lactone **S16** was synthesized using established literature protocols.[8]

To a solution of forskolin (410 mg, 1.0 mmol, 1.0 equiv.) in anhydrous MeOH (10 mL) was added KOH (729 mg, 13.0 mmol, 13.0 equiv.), followed by 8 h stirring at 65 °C. MeOH was removed under vacuum, and EtOAc (10 mL) and H_2O (10 mL) were added. The aqueous layer was extracted with EtOAc (10 mL × 3). The combined organic layers were washed with brine (20 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 1/1) to yield hemiacetal S15 (313 mg, 85%) as a white solid.

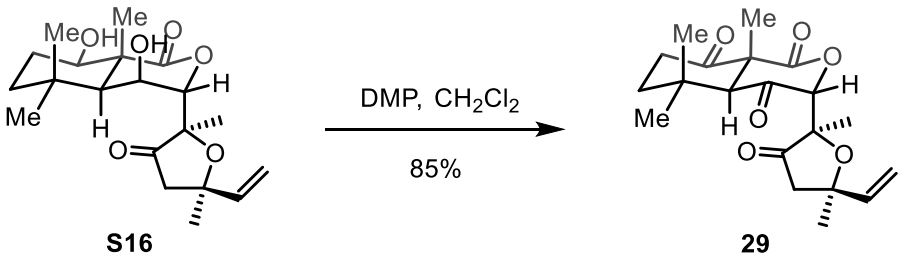
The **S15** (110 mg, 0.3 mmol, 1.0 equiv.), sodium periodate (513 mg, 2.4 mmol, 8.0 equiv.) and silica gel (144 mg, 2.4mmol, 8.0 equiv.) were added to a round-

bottomed flask containing CH_2Cl_2: H_2O: MeOH (5:1:1, 6 mL), the mixture was carried out at 45 °C for 12 h and then filtered through a short plug of celite and rinsed with EtOAc (10 mL × 3). The combined filtrate was concentrated and the residue was purified by flash column chromatography (Petroleum ether/Ethyl acetate = 1/1) to yield **S16** (110 mg, 93%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.95 (dd, *J* = 17.4, 10.7 Hz, 1H), 5.23 – 5.09 (m, 2H), 4.57 – 4.48 (m, 1H), 4.37 (d, *J* = 2.8 Hz, 1H), 4.23 (d, *J* = 1.6 Hz, 1H), 3.77 – 3.68 (m, 1H), 2.82 (d, *J* = 18.0 Hz, 1H), 2.53 (d, *J* = 5.0 Hz, 1H), 2.44 (d, *J* = 18.0 Hz, 1H), 1.73 – 1.64 (m, 3H), 1.53 (s, 3H), 1.44 – 1.36 (s, 4H), 1.35 – 1.27 (s, 4H), 1.23 (s, 3H), 1.05 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 215.25, 179.45, 142.21, 114.00, 88.06, 83.37, 79.39, 74.68, 64.27, 48.02, 46.64, 45.89, 41.22, 34.20, 31.90, 27.95, 25.36, 24.60, 21.32, 14.40.

trans-[6.6]-Bicyclic δ-lactones 29



S16 **29**

Dess-Martin periodinane (577 mg, 1.36 mmol, 4.0 equiv.) was added to a solution of **S16** (125 mg, 0.34 mmol, 1.0 equiv.) and $NaHCO_3$ (143 mg, 1.7 mmol, 5.0 equiv.) in CH_2Cl_2 (17 mL), followed by 2 h stirring at rt. The mixture was quenched with saturated aqueous $Na_2S_2O_3$ (10 mL). The layers were separated and the aqueous phase was extracted with CH_2Cl_2 (10 mL × 3). The combined organic layers were washed with brine (20 mL) and dried over Na_2SO_4, concentrated and purified by flash column chromatography (Petroleum ether/ethyl acetate = 2/1) to yield **29** (105 mg, 85%) as a white solid.

TLC R*f* = 0.55 (Petroleum ether/Ethyl acetate = 3/2; phosphomolybdic acid).

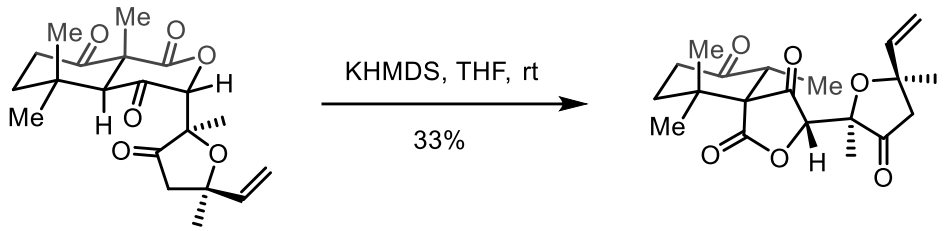
Opt. Rot. $[\alpha]_D^{20}$ = +189.6° (c 0.38, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.04 (dd, *J* = 17.4, 10.8 Hz, 1H), 5.32 – 5.13 (m, 2H), 4.44 (s, 1H), 3.56 (s, 1H), 2.96 – 2.86 (m, 1H), 2.58 (t, *J* = 7.7 Hz, 2H), 2.55 – 2.48 (m, 1H), 1.86 – 1.77 (m, 1H), 1.69 – 1.61 (m, 1H), 1.46 (s, 3H), 1.43 (s, 3H), 1.37 (s, 3H), 1.25 (s, 3H), 1.22 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 212.84, 203.57, 200.99, 166.51, 142.16, 114.28, 85.61, 84.10, 79.71, 57.34, 52.15, 47.43, 39.55, 35.48, 31.60, 30.13, 28.19, 22.84, 20.59, 19.27.

HRMS (ESI) calcd for $C_{20}H_{26}O_6$ $[M+Na]^+$: 385.1622, found 385.1622.

1,2-Ester migration product 30



29 **30**

Under argon atmosphere, to a solution of **29** (10 mg, 27.6 μmol, 1.0 equiv.) in anhydrous THF (2.8 mL) was added KHMDS (13.8 μL, 1M in THF, 13.8 μmol, 0.5 equiv.) at 0 °C, followed by 5 minutes stirring at the same temperature. The reaction mixture was warmed to rt, and stirred for 24 h before quenched with saturated aqueous NH_4Cl (3 mL). The aqueous layer was extracted with EtOAc (5 mL × 3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 3/1) to yield **30** (3.3 mg, 33%) as a white solid.

TLC R*f* = 0.3 (Petroleum ether/Ethyl acetate = 3/2; phosphomolybdic acid).

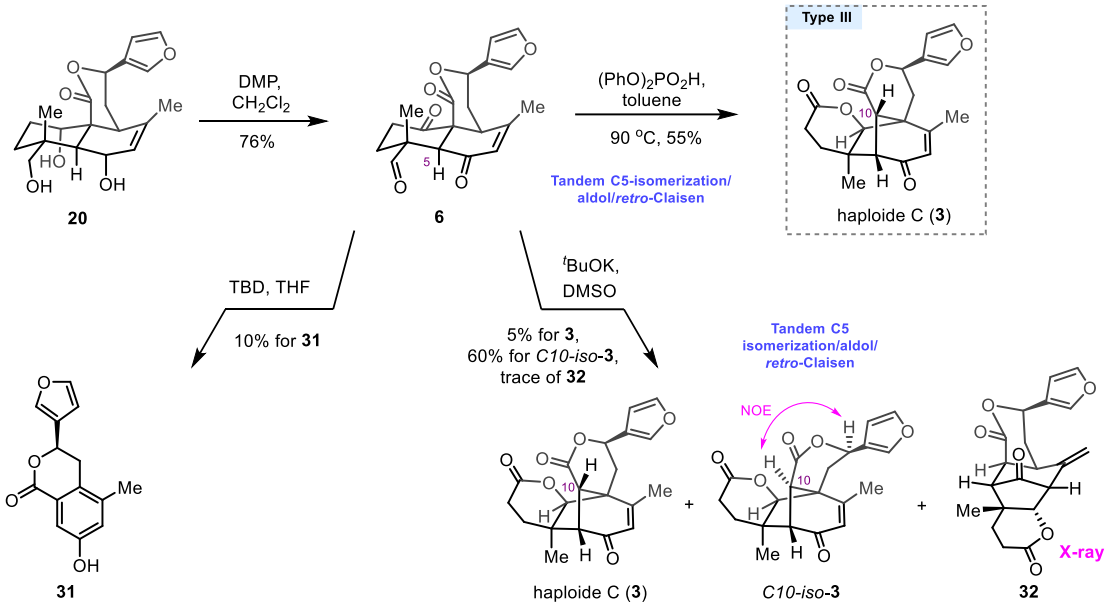
Opt. Rot. $[\alpha]_D^{20}$ = +32.1° (c 0.4, MeCN).

^{1}H NMR (400 MHz, $CDCl_3$) δ 5.91 (dd, *J* = 17.6, 10.8 Hz, 1H), 5.21 – 5.08 (m, 2H), 4.62 (s, 1H), 3.11 – 3.04 (m, 1H), 2.79 (q, *J* = 6.6 Hz, 1H), 2.62 – 2.54 (m, 1H), 2.52 – 2.48 (m, 2H), 2.43 – 2.36 (m, 1H), 1.58 – 1.55 (m, 1H), 1.51 (s, 3H), 1.47 (s, 3H), 1.25 (s, 3H), 1.05 (s, 3H), 0.96 (d, *J* = 6.6 Hz, 3H).

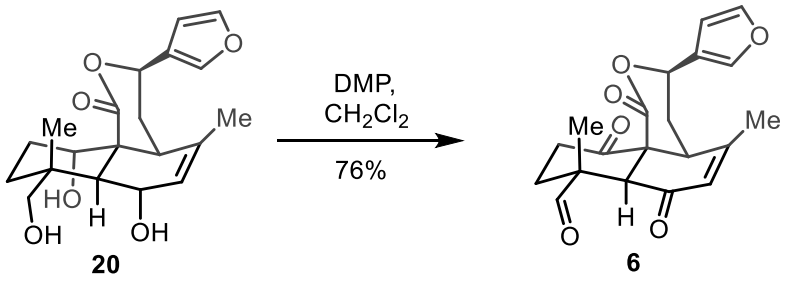
^{13}C NMR (100 MHz, $CDCl_3$) δ 213.93, 207.61, 206.25, 172.98, 141.77, 114.24, 89.25, 82.77, 80.15, 64.29, 46.99, 42.11, 38.09, 36.82, 36.13, 27.85, 26.89, 22.82, 21.38, 11.15.

HRMS (ESI) calcd for $C_{20}H_{26}O_6$ $[M+Na]^+$: 385.1622, found 385.1621.

*4.4 Synthesis of haploide C (**3**)*



Aldehyde 6



Dess-Martin periodinane (28 mg, 66.3 μmol, 3.0 equiv.) was added to a solution of **20** and *C1-iso*-**20** (8 mg, 22.1 μmol, 1.0 equiv.) and $NaHCO_3$ (9.2 mg, 0.11 mmol, 5.0 equiv.) in CH_2Cl_2 (2 mL), followed by 2 h stirring at rt. The mixture was quenched with saturated aqueous $Na_2S_2O_3$ (5 mL). The layers were separated and the aqueous phase was extracted with CH_2Cl_2 (5 mL × 3). The combined organic layers were washed with brine (10 mL) and dried over Na_2SO_4, concentrated and purified by flash column chromatography (Petroleum ether/ethyl acetate = 2/1) to yield **6** (6 mg, 76%) as a white solid.

TLC R*f* = 0.5 (Petroleum ether/Ethyl acetate = 3/2; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = +178.4° (c 0.2, MeOH).

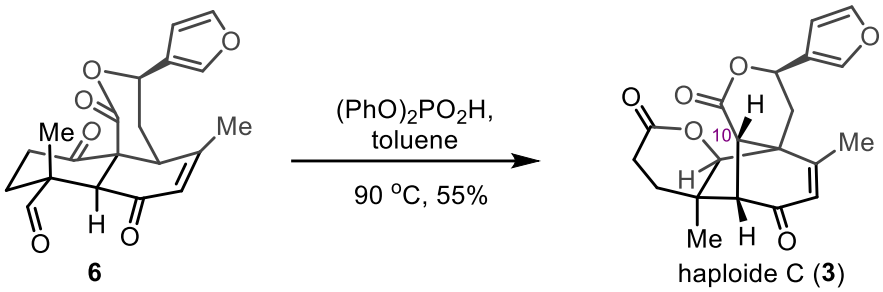
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.71 (s, 1H), 7.44 (s, 1H), 7.42 (t, *J* = 1.8 Hz, 1H), 6.39 (s, 1H), 5.87 (s, 1H), 5.25 (dd, *J* = 11.7, 3.5 Hz, 1H), 3.83 (t, *J* = 9.1 Hz, 1H), 3.26 (s, 1H), 2.85 – 2.75 (m, 2H), 2.58 (dt, *J* = 12.1, 3.5 Hz, 1H), 2.06 – 1.95 (m, 2H), 1.96 (s, 3H), 1.85 (s, 3H), 1.84 – 1.76 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 205.49, 205.28, 191.05, 167.10, 156.72, 144.10, 139.94, 126.81, 123.74, 108.23, 72.78, 64.84, 58.88, 46.53, 40.35,

37.03, 34.83, 21.92, 18.88.

HRMS (ESI) calcd for $C_{20}H_{20}O_6$ [M+Na]$^+$: 379.1152, found 379.1152.

Haploide C (3)



To a solution of **6** (6 mg, 16.8 μmol, 1.0 equiv.) in anhydrous toluene (1.7 mL) was added $(PhO)_2PO_2H$ (5 mg, 0.02 mmol, 1.2 equiv.) under argon atmosphere. The reaction was stirred at 90 °C overnight. The mixture was concentrated in vacuo and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 1/2) to yield **3** (3.3 mg, 55%) as a white solid.

TLC R*f* = 0.46 (Petroleum ether/Ethyl acetate = 1/2; phosphomolybdic acid).

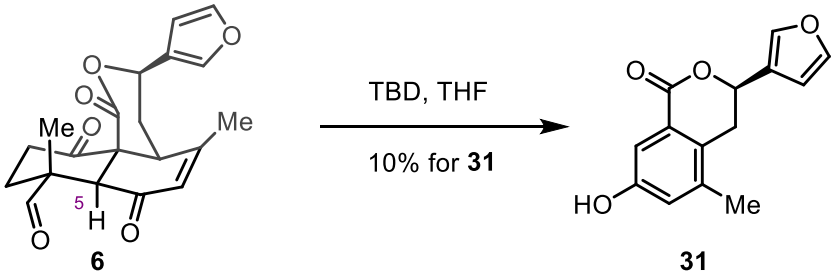
Opt. Rot. $[\alpha]_D^{20}$ = -94.2° (c 0.165, MeOH). [Lit. [6]: $[\alpha]_D^{20}$ = -38.7° (c 0.1, MeOH)].

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (s, 1H), 7.42 (t, *J* = 1.8 Hz, 1H), 6.39 (s, 1H), 5.99 (dd, *J* = 9.4, 5.6 Hz, 1H), 5.86 (s, 1H), 4.14 (s, 1H), 3.38 (s, 1H), 2.99 (s, 1H), 2.85 (dd, *J* = 14.6, 5.6 Hz, 1H), 2.53 (dt, *J* = 17.0, 3.1 Hz, 1H), 2.41 – 2.28 (m, 1H), 2.17 (dd, *J* = 14.6, 9.4 Hz, 2H), 2.07 (s, 3H), 1.79 (dt, *J* = 13.9, 3.6 Hz, 1H), 1.17 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.80, 170.94, 169.23, 163.09, 144.21, 139.70, 128.26, 125.79, 108.26, 88.72, 74.00, 59.86, 53.96, 52.13, 43.26, 32.16, 29.91, 27.13, 25.34, 19.15.

HRMS (ESI) calcd for $C_{20}H_{20}O_6$ [M+Na]$^+$: 379.1152, found 379.1152.

B-ring aromatized product 31



To a solution of **6** (10 mg, 28.1 μmol, 1.0 equiv.) in THF (2.8 mL) was added TBD (4.7 mg, 33.7 μmol, 1.2 equiv.), followed by 24 h stirring at rt before quenched with saturated aqueous NH_4Cl (2 mL). The aqueous layer was extracted with EtOAc (5 mL × 3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography

(Petroleum ether/Ethyl acetate = 3/2) to yield **31** (0.7 mg, 10%) as a white solid.

TLC R*f* = 0.45 (Petroleum ether/Ethyl acetate = 3/2).

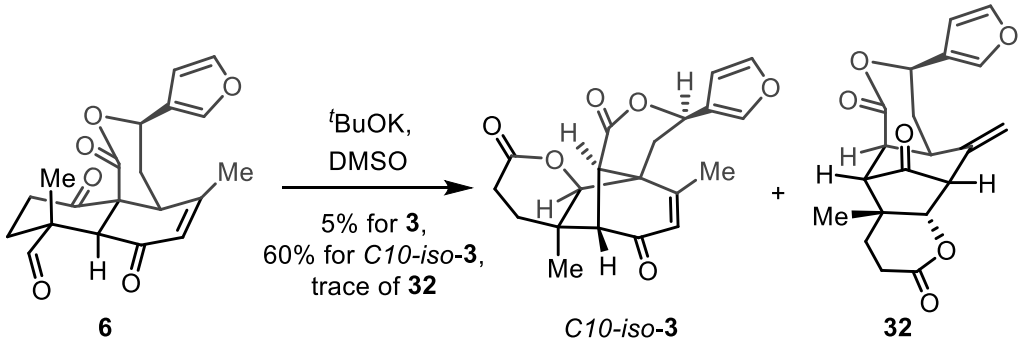
Opt. Rot. $[\alpha]_D^{20}$ = +15.4° (c 0.1, MeCN).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (s, 1H), 7.49 – 7.42 (m, 2H), 6.97 (s, 1H), 6.50 (s, 1H), 5.52 (dd, *J* = 9.8, 4.8 Hz, 1H), 5.08 (s, 1H), 3.14 – 3.02 (m, 2H), 2.30 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 165.67, 154.79, 143.83, 140.27, 137.32, 129.81, 126.10, 124.24, 123.11, 114.12, 108.83, 73.07, 30.65, 19.13.

HRMS (ESI) calcd for $C_{14}H_{12}O_4$ $[M+Na]^+$: 267.0628, found 267.0628.

C10-iso-3 and 32



To a flamed-dried flask was added **6** (7.0 mg, 19.6 μmol, 1.0 equiv.), anhydrous DMSO (2 mL) and *t*-BuOK (2.4 mg, 19.6 μmol, 1.0 equiv.), followed by stirring overnight at rt. The reaction was quenched with saturated aqueous NH_4Cl (5 mL) and extracted with EtOAc (5 mL × 3). The combined organic layers were washed with H_2O (10 mL) and brine (20 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/ethyl acetate = 1/1) to yield *C10-iso*-**3** (4.2 mg, 60%) as a white solid, **3** (0.3 mg, 5%), and trace of **32**.

Data of *C10-iso*-**3**

TLC R*f* = 0.4 (Petroleum ether/Ethyl acetate = 1/2; phosphomolybdic acid).

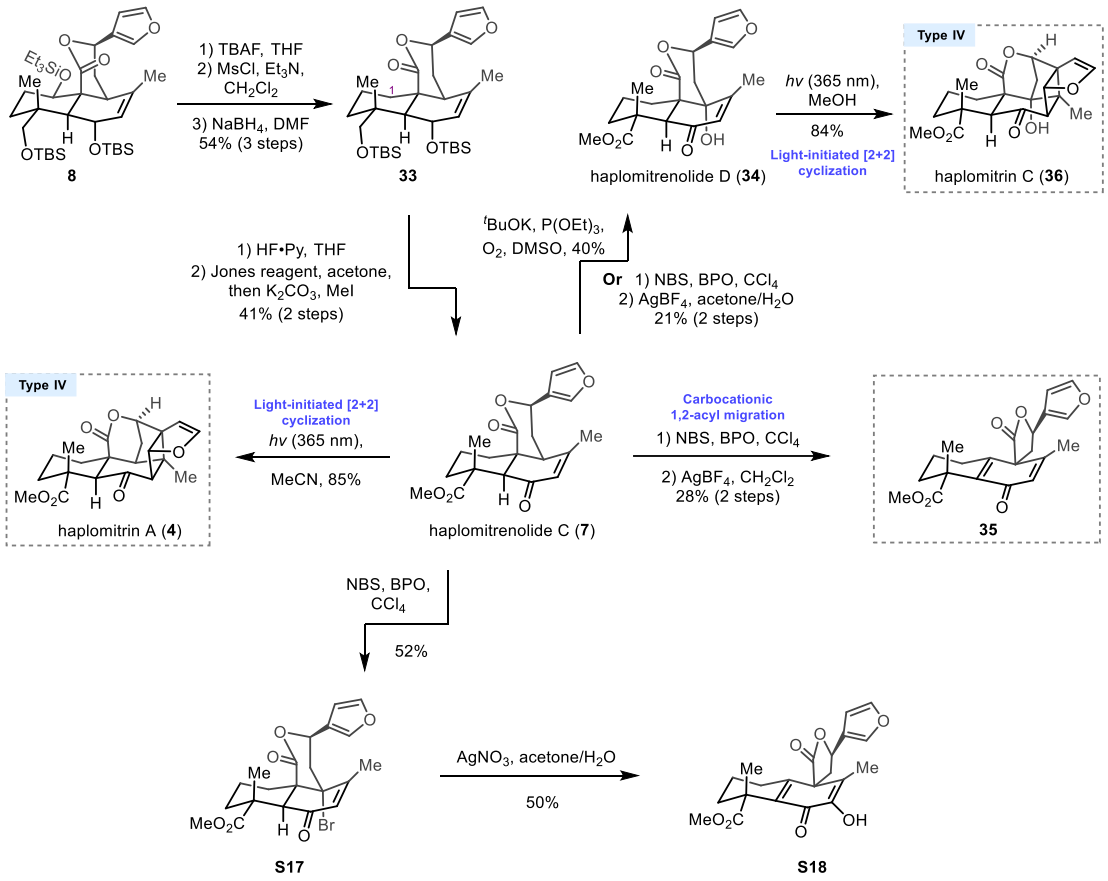
Opt. Rot. $[\alpha]_D^{20}$ = -39.3° (c 0.15, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (s, 1H), 7.47 – 7.43 (m, 1H), 6.44 (s, 1H), 6.00 (s, 1H), 5.36 (dd, *J* = 11.0, 5.9 Hz, 1H), 3.99 (s, 1H), 3.51 (d, *J* = 4.6 Hz, 1H), 3.08 (dd, *J* = 14.8, 5.8 Hz, 1H), 2.90 (d, *J* = 4.7 Hz, 1H), 2.66 (d, *J* = 17.2 Hz, 1H), 2.53 – 2.34 (m, 2H), 2.01 (s, 3H), 1.99 – 1.94 (m, 1H), 1.87 – 1.77 (m, 1H), 1.21 (s, 3H).

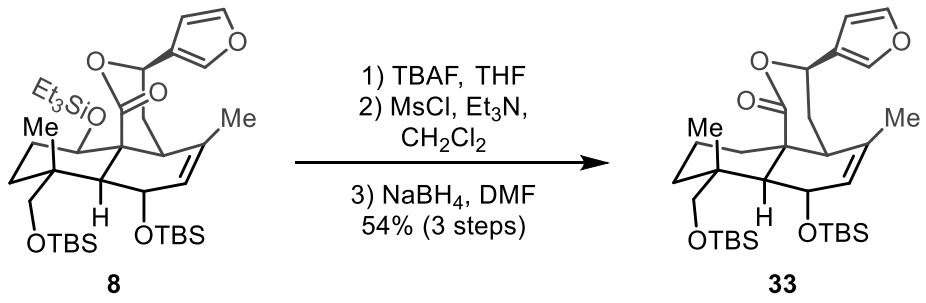
^{13}C NMR (100 MHz, $CDCl_3$) δ 195.72, 171.40, 170.55, 157.68, 144.16, 139.81, 129.60, 108.44, 85.53, 73.15, 57.46, 54.26, 49.65, 43.42, 33.54, 31.04, 27.74, 23.89, 21.26.

HRMS (ESI) calcd for $C_{20}H_{20}O_6$ $[M+Na]^+$: 379.1152, found 379.1151.

*4.5 Synthesis of haplomitrins A/C (**4**/**36**)*



Silyl ether 33



To a solution of **8** (31.3 mg, 44.4 μmol, 1.0 equiv.) in anhydrous THF (17.75 mL) was added TBAF (44.4 μL, 1 M in THF, 44.4 μmol, 1.0 equiv.) at 0 °C. The reaction was stirred at the same temperature for 1 h and quenched with saturated aqueous NH_4Cl (10 mL). The aqueous layer was extracted with EtOAc (20 mL × 3). The combined organic layers were washed with brine (30 mL), dried over Na_2SO_4, filtered, concentrated to give a crude residue.

The residue was directly dissolved in CH_2Cl_2 (4 mL). TEA (123 μL, 888 μmol, 20.0 equiv.), DMAP (10.8 mg, 88.8 μmol, 2.0 equiv.) and MsCl (34.4 μL, 444 μmol, 10.0

equiv.) were added, followed by stirring overnight at rt. The reaction was quenched with saturated aqueous $NaHCO_3$ (5 mL). The aqueous layer was extracted with CH_2Cl_2 (10 mL × 3). The combined organic layers were washed with brine (10 mL), dried over Na_2SO_4, filtered, concentrated to give a crude mesylate.

$NaBH_4$ (33.6 mg, 888 μmol, 20.0 equiv.) was added to a solution of crude mesylate in DMF (4 mL) and the reaction mixture was stirred at 80 °C for 6 h before quenched with saturated aqueous NH_4Cl (10 mL). The mixture was extracted with EtOAc (15 mL × 3). The combined organic layers were washed with H_2O (20 mL) and brine (20 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/ethyl acetate = 15/1) to yield **33** (13.8 mg, 54%) as a white solid.

TLC R*f* = 0.5 (Petroleum ether/Ethyl acetate = 15/1; phosphomolybdic acid).

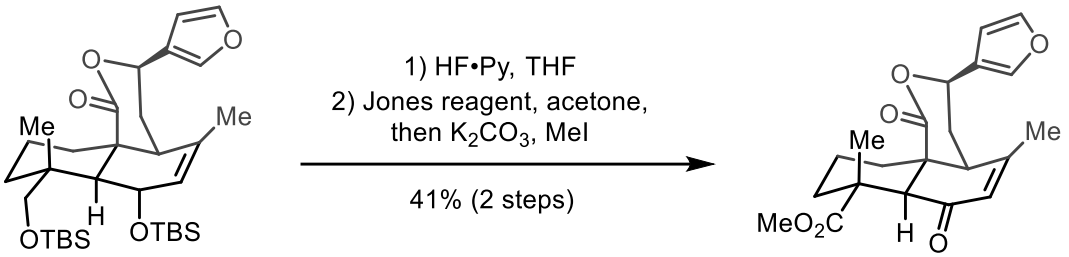
Opt. Rot. $[\alpha]_D^{20}$ = +38.7° (c 0.26, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (s, 1H), 7.34 (s, 1H), 6.33 (s, 1H), 5.58 (dd, *J* = 8.2, 5.1 Hz, 1H), 5.30 (s, 1H), 4.70 (d, *J* = 9.7 Hz, 1H), 3.60 (d, *J* = 8.9 Hz, 1H), 3.44 (d, *J* = 9.0 Hz, 1H), 2.54 (dt, *J* = 14.8, 7.8 Hz, 1H), 2.47 – 2.41 (m, 1H), 2.29 (d, *J* = 13.2 Hz, 1H), 2.08 (dt, *J* = 14.4, 4.3 Hz, 1H), 1.76 (d, *J* = 9.8 Hz, 1H), 1.53 – 1.43 (m, 4H), 1.47 (s, 3H), 1.34 (dt, *J* = 13.2, 6.2 Hz, 1H), 1.22 (s, 3H), 0.89 (s, 9H), 0.88 (s, 9H), 0.12 (s, 3H), 0.11 (s, 3H), 0.00 (s, 3H), 0.00 (s 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.91, 143.60, 139.26, 134.15, 130.99, 127.25, 108.35, 73.28, 71.82, 69.81, 49.67, 48.32, 47.62, 38.09, 36.79, 35.19, 28.24, 26.39, 26.09, 21.42, 18.77, 18.37, 18.30, -3.22, -3.57, -4.99, -5.07.

HRMS (ESI) calcd for $C_{32}H_{54}O_5Si_2$ $[M+Na]^+$: 597.3402, found 597.3402.

Haplomitrenolide C (7)



33 haplomitrenolide C (**7**)

To a solution of **33** (9 mg, 15.7 μmol, 1.0 equiv.) in THF (1.5 mL) was added HF·Py (150 μL, 70wt.% in Pyridine), followed by stirring overnight at rt. Saturated aqueous $NaHCO_3$ (5 mL) was added slowly to quench the reaction. The aqueous layer was extracted with EtOAc (10 mL × 3). The combined organic layers were washed with H_2O (20 mL) and brine (20 mL), dried over Na_2SO_4, filtered, concentrated to give a crude diol.

The diol was dissolved in acetone (1.5 mL) and freshly prepared Jones' reagent (31.3 μL, 2.5 M, 78.5 μmol, 5.0 equiv.) was added at 0 °C. The mixture was stirred for 5 h at the same temperature. K_2CO_3 (32.5 mg, 235.5 μmol, 15.0 equiv.) and MeI

(9.8 μL, 157 μmol, 10.0 equiv.) were added, followed by vigorous stirring for 5 h at rt. The reaction mixture was filtered through a short plug of Celite and rinsed with EtOAc (10 mL × 3). The combined filtrate was washed with H_2O (20 mL) and brine (20 mL) and dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 1/1) to yield **7** (2.4 mg, 41%).

TLC R*f* = 0.47 (Petroleum ether/Ethyl acetate = 1/1; phosphomolybdic acid).

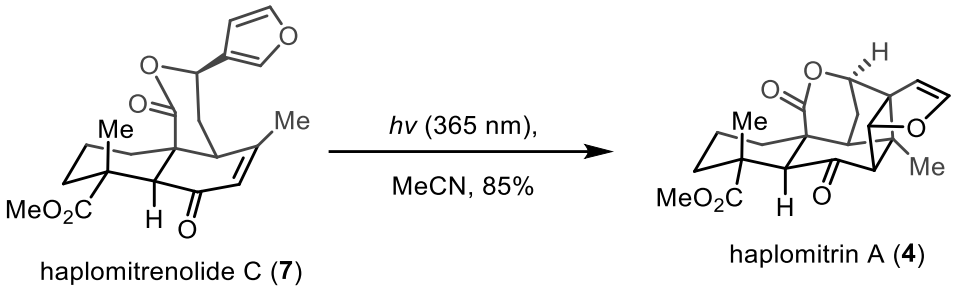
Opt. Rot. $[\alpha]_D^{20}$ = +41.8° (c 0.1, Pyridine). [Lit. [9]: $[\alpha]_D^{20}$ = +121.2 (c 0.25, Pyridine)].

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.67 (s, 1H), 6.58 (s, 1H), 5.99 – 5.93 (m, 2H), 3.69 (s, 3H), 3.61 (s, 1H), 2.92 (d, *J* = 8.2 Hz, 1H), 2.74 – 2.65 (m, 1H), 2.59 (d, *J* = 13.2 Hz, 1H), 2.38 (dd, *J* = 14.8, 6.2 Hz, 1H), 2.06 (s, 3H), 1.80 – 1.74 (m, 1H), 1.70 – 1.55 (m, 4H), 1.67 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 194.74, 179.02, 172.32, 158.33, 144.64, 139.92, 128.68, 127.48, 109.01, 72.16, 57.14, 52.30, 50.29, 48.93, 43.83, 38.21, 32.45, 28.08, 22.23, 19.16, 18.63.

HRMS (ESI) calcd for $C_{21}H_{24}O_6$ $[M+Na]^+$: 395.1465, found 395.1465.

Haplomitrin A (4)



haplomitrenolide C (**7**) haplomitrin A (**4**)

To an oven dried quartz tube was added **20** (2 mg, 5.37 μmol, 1.0 equiv.) and anhydrous MeCN (6 mL). The solution was bubbled with argon balloon for 1 h before irradiated with a UV lamp (365 nm, distance ~ 1 cm) for 6 h at ambient temperature (~ 45 °C). The solvent was concentrated under reduced pressure. The residue was purified by flash column chromatography (Petroleum ether/ethyl acetate = 3/2) to yield **4** (1.7 mg, 85%).

TLC R*f* = 0.72 (Petroleum ether/Ethyl acetate = 1/1; phosphomolybdic acid).

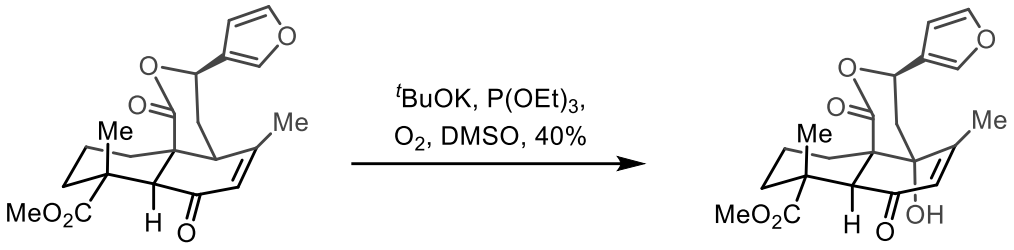
Opt. Rot. $[\alpha]_D^{20}$ = -4.7° (c 0.1, MeCN). [Lit. [10]: $[\alpha]_D^{20}$ = +36.4 (c 0.1, MeCN)].

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.52 (d, *J* = 2.8 Hz, 1H), 4.76 (d, *J* = 2.8 Hz, 1H), 4.72 (d, *J* = 3.1 Hz, 1H), 4.55 (s, 1H), 3.69 (s, 3H), 3.03 (s, 1H), 2.90 (d, *J* = 3.1 Hz, 1H), 2.37 (d, *J* = 13.6 Hz, 1H), 2.32 (d, *J* = 13.6 Hz, 1H), 2.16 – 2.12 (m, 1H), 2.10 – 2.06 (m, 1H), 1.87 – 1.83 (m, 1H), 1.82 – 1.78 (m, 1H), 1.72 (s, 3H), 1.63 – 1.59 (m, 1H), 1.45 – 1.40 (m, 1H), 1.39 – 1.34 (m, 1H), 1.25 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 179.46, 172.34, 150.63, 100.21, 83.08, 80.22, 66.79, 59.35, 56.33, 55.18, 52.70, 50.03, 47.05, 43.42, 38.57, 37.90, 33.71, 23.00, 17.60, 16.46.

HRMS (ESI) calcd for $C_{21}H_{24}O_6$ $[M+Na]^+$: 395.1465, found 395.1465.

Haplomitrenolide D (34)



haplomitrenolide C (**7**) haplomitrenolide D (**34**)

To a flamed-dried flask was added **7** (10 mg, 2.69 μmol, 1.0 equiv.), DMSO (2.7 mL), *t*-BuOK (3 mg, 2.69 μmol, 1.0 equiv.). After stirring for 10 minutes at rt, $P(OEt)_3$ (9.2 μL, 5.38 μmol, 2.0 equiv.) was added. The mixture was purged with oxygen balloon for three times and stirred at rt for 9 h under oxygen atmosphere. The reaction was quenched with saturated aqueous NH_4Cl (10 mL) and extracted with EtOAc (15 mL × 3). The combined organic layers were washed with H_2O (20 mL × 2) and brine (20 mL), dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/ethyl acetate = 1/1) to yield **34** (4.2 mg, 40%) as a white solid.

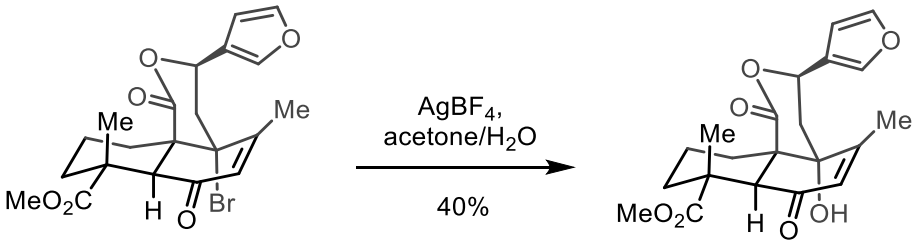
TLC R*f* = 0.3 (Petroleum ether/Ethyl acetate = 1/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = +3.8° (c 0.1, MeCN). [Lit. [9]: $[\alpha]_D^{20}$ = +36.4 (c 0.1, MeCN)].

^{1}H NMR (400 MHz, $CDCl_3$) δ7.42 (s, 1H), 7.39 (s, 1H), 6.34 (s, 1H), 5.75 (s, 1H), 5.68 (dd, *J* = 9.3, 5.0 Hz, 1H), 3.76 (s, 1H), 3.70 (s, 3H), 2.65 – 2.55 (m, 2H), 2.21 – 2.09 (m, 2H), 1.74 (s, 3H), 1.73 – 1.69 (m, 2H), 1.59 (s, 3H), 1.56 – 1.50 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 194.63, 179.82, 172.58, 155.34, 144.32, 139.25, 129.81, 126.59, 108.06, 74.17, 69.88, 55.26, 52.82, 49.00, 43.52, 37.50, 35.23, 27.06, 19.74, 18.45, 18.01.

HRMS (ESI) calcd for $C_{21}H_{24}O_7$ $[M+Na]^+$: 411.1414, found 411.1415.

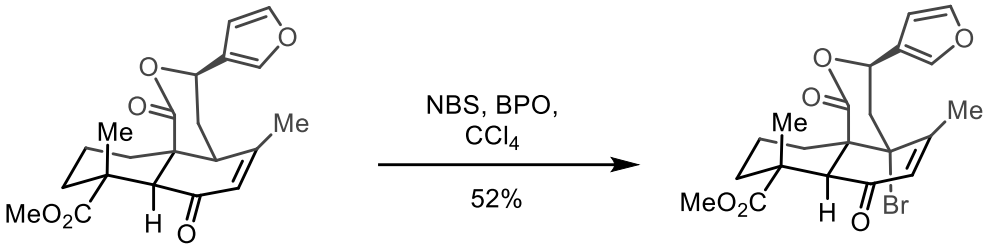


S17 haplomitrenolide D (**34**)

To a solution of **S17** (2 mg, 4.43 μmol, 1.0 equiv.) in acetone (500 μL) and H_2O (50 μL) was added $AgBF_4$ (4.3 mg, 22.2 μmol, 5.0 equiv.), followed by stirring for 24 h at rt. The mixture was filtered through a short plug of Celite and rinsed with EtOAc (5 mL × 3). The combined filtrate was washed with brine (10 mL) and dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography

(Petroleum ether/Ethyl acetate = 1/1) to yield **34** (0.8 mg, 41%).

Brominated product S17



haplomitrenolide C (**7**) **S17**

Under argon atmosphere, to a solution of **7** (12.5 mg, 33.6 μmol) in degassed anhydrous CCl_4 (3.4 mL) was added NBS (6.3 mg, 35.3 μmol, 1.05 equiv.) and BPO (1.63 mg, 6.72 μmol, 0.2 equiv.). The solution was purged with argon balloon for three times and stirred at 85 °C for 24 h. After being cooled to ambient temperature, the solution was concentrated in vacuo and the residue was purified by flash column chromatography (Petroleum ether/Ethyl acetate = 2/1) to yield **S17** (7.9 mg, 52%) as a white solid.

TLC R*f* = 0.48 (Petroleum ether/Ethyl acetate = 2/1; phosphomolybdic acid).

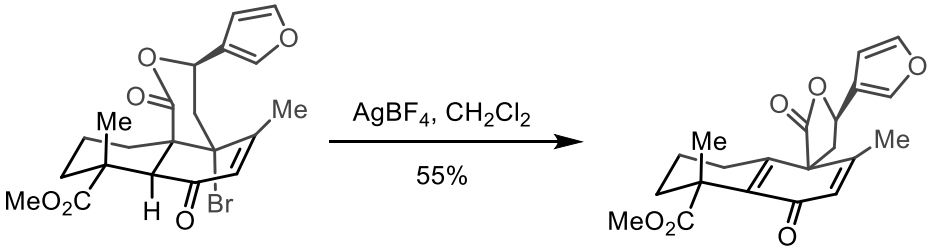
Opt. Rot. $[\alpha]_D^{20}$ = -137.09° (c 0.33, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (t, *J* = 1.7 Hz, 1H), 7.36 (s, 1H), 6.33 (s, 1H), 5.77 (s, 1H), 5.63 (dd, *J* = 9.7, 3.4 Hz, 1H), 4.15 (s, 1H), 3.72 (s, 3H), 3.30 (dd, *J* = 14.7, 9.6 Hz, 1H), 3.05 (dd, *J* = 14.7, 3.5 Hz, 1H), 2.41 – 2.22 (m, 2H), 1.82 (s, 3H), 1.81 – 1.75 (m, 2H), 1.70 – 1.64 (m, 1H), 1.62 (s, 3H), 1.58 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 193.37, 178.77, 168.64, 154.44, 144.53, 139.40, 129.29, 125.96, 107.77, 72.22, 71.50, 55.75, 53.26, 52.79, 43.63, 38.85, 37.13, 30.99, 19.43, 18.17, 17.60.

HRMS (ESI) calcd for $C_{21}H_{23}BrO_6$ $[M+Na]^+$: 473.0570, found 473.0570.

Lactone 35



S17 **35**

To a solution of **S17** (6 mg, 13.3 μmol, 1.0 equiv.) in CH_2Cl_2 (1.3 mL) was added $AgBF_4$ (5.2 mg, 26.6 μmol, 2.0 equiv.), followed by stirring for 1 h at rt. The mixture was concentrated and purified by flash column chromatography (Petroleum

ether/Ethyl acetate = 1/1) to yield **35** (2.7 mg, 55%).

TLC R*f* = 0.4 (Petroleum ether/Ethyl acetate = 1/1; phosphomolybdic acid).

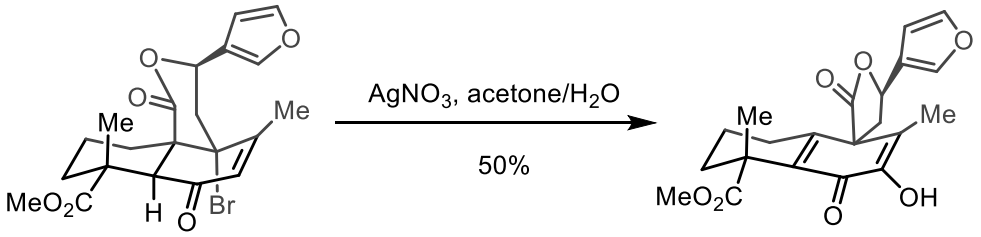
Opt. Rot. $[\alpha]_D^{20}$ = -3.21° (c 0.14, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (s, 1H), 7.51 (s, 1H), 6.45 (s, 1H), 6.23 (s, 1H), 5.71 (t, *J* = 8.5 Hz, 1H), 3.63 (s, 3H), 2.88 (dd, *J* = 14.4, 8.2 Hz, 1H), 2.66 (dd, *J* = 14.5, 8.9 Hz, 1H), 2.62 – 2.51 (m, 1H), 2.35 – 2.25 (m, 1H), 2.01 (s, 3H), 1.95 – 1.88 (m, 1H), 1.87 – 1.78 (m, 3H), 1.43 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 183.59, 177.55, 174.33, 153.09, 150.32, 144.84, 139.93, 137.26, 129.69, 124.23, 107.96, 73.23, 57.64, 52.25, 43.10, 40.45, 34.98, 27.22, 22.77, 19.94, 18.10.

HRMS (ESI) calcd for $C_{21}H_{22}O_6$ $[M+Na]^+$: 393.1309, found 393.1309.

C7-oxidized product S18



To a solution of **S17** (3 mg, 6.7 μmol, 1.0 equiv.) in acetone (665 μL) and H_2O (74 μL) was added $AgNO_3$ (3.4 mg, 20 μmol, 3.0 equiv.), followed by stirring for 24 h at rt. The mixture was filtered through a short plug of Celite and rinsed with EtOAc (5 mL × 3). The combined filtrate was washed with brine (10 mL) and dried over Na_2SO_4, filtered, concentrated and purified by flash column chromatography (Petroleum ether/Ethyl acetate = 1/1) to yield **S18** (1.3 mg, 50%).

TLC Rf = 0.4 (Petroleum ether/Ethyl acetate = 2/1; phosphomolybdic acid).

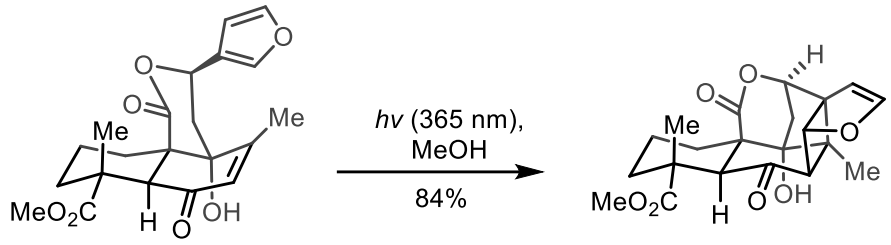
Opt. Rot. $[\alpha]_D^{20}$ = -6.27° (c 0.053, MeOH).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (s, 1H), 7.51 (s, 1H), 6.52 (s, 1H), 6.47 (s, 1H), 5.69 (t, *J* = 8.6 Hz, 1H), 3.64 (s, 3H), 2.87 (dd, *J* = 14.4, 8.2 Hz, 1H), 2.71 (dd, *J* = 14.4, 9.1 Hz, 1H), 2.66 – 2.56 (m, 1H), 2.38 – 2.29 (m, 1H), 1.98 – 1.90 (m, 4H), 1.88 – 1.81 (m, 3H), 1.46 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 178.97, 177.22, 174.51, 152.77, 145.12, 144.82, 140.05, 135.38, 124.20, 122.86, 108.02, 73.06, 57.82, 52.36, 43.60, 40.12, 34.74, 27.45, 22.61, 18.03, 12.97.

HRMS (ESI) calcd for $C_{21}H_{22}O_7$ $[M+Na]^+$: 409.1258, found 409.1258.

Haplomintrin C (36)



haplomitrenolide D (**34**) haplomitrin C (**36**)

To an oven dried quartz tube was added **34** (2.6 mg, 6.7 μmol, 1.0 equiv.) and anhydrous MeOH (7 mL). The solution was bubbled with argon balloon for 1 h before irradiated with a UV lamp (365 nm, distance ~ 1 cm) for 6 h at ambient temperature (~ 45 °C). The solvent was concentrated under reduced pressure. The residue was purified by flash column chromatography (Petroleum ether/ethyl acetate = 1/1) to yield **36** (2.1 mg, 84%).

TLC Rf = 0.37 (Petroleum ether/Ethyl acetate = 1/1; phosphomolybdic acid).

Opt. Rot. $[\alpha]_D^{20}$ = -4.76° (c 0.11, MeCN). [Lit. [10]: $[\alpha]_D^{20}$ = -1.6 (c 0.1, MeCN)].

^{1}H NMR (400 MHz, $CDCl_3$) δ 6.53 (d, *J* = 2.8 Hz, 1H), 4.81 -4.76 (m, 2H), 4.42 (d, *J* = 3.4 Hz, 1H), 3.69 (s, 3H), 3.64 (s, 1H), 2.86 (d, *J* = 3.3 Hz, 1H), 2.48 (s, 1H), 2.43 (d, *J* = 13.1 Hz, 1H), 2.40 – 2.32 (m, 1H), 2.03 – 1.84 (m, 3H), 1.80 – 1.77 (m ,1H), 1.76 (s, 3H), 1.66 – 1.62 (m, 1H), 1.45 – 1.35 (m, 1H), 1.23 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 204.65, 179.8, 173.78, 150.81, 100.37, 80.05, 79.26, 78.35, 67.54, 57.03, 52.79, 52.77, 51.93, 51.68, 43.44, 39.12, 37.35, 29.62, 18.68, 17.15, 17.13.

HRMS (ESI) calcd for $C_{21}H_{24}O_7$ $[M+Na]^+$: 411.1414, found 411.1414.

5. References.

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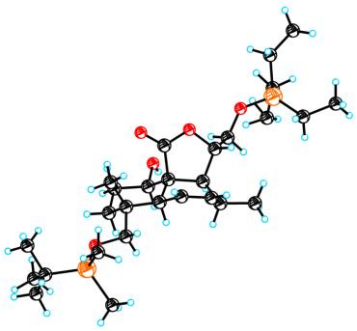
6. Single X-ray Crystal Diffraction data



9

Table 1. Crystal data and structure refinement for 9.

CCDC number	2447362
Empirical formula	$C_{28}H_{52}O_5Si_2$
Formula weight	524.87
Temperature/K	150.00
Crystal system	monoclinic
Space group	$P2_1$
a/Å	11.6306(3)
b/Å	7.2049(2)
c/Å	19.7989(4)
α/°	90
β/°	99.972(2)
γ/°	90
Volume/Å^3	1634.03(7)
Z	2
ρ_{calc}g/cm^3	1.067
μ/mm^{-1}	1.225
F(000)	576.0
Crystal size/mm^3	0.05 × 0.04 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	4.532 to 136.538
Index ranges	-13 ≤ h ≤ 13, -8 ≤ k ≤ 8, -17 ≤ l ≤ 23
Reflections collected	15549
Independent reflections	5604 [R_{int} = 0.0366, R_{sigma} = 0.0462]
Data/restraints/parameters	5604/635/335
Goodness-of-fit on F^2	1.212
Final R indexes [I>=2σ (I)]	R_1 = 0.1129, wR_2 = 0.3169
Final R indexes [all data]	R_1 = 0.1455, wR_2 = 0.3538
Largest diff. peak/hole / e Å^{-3}	0.46/-0.60
Flack parameter	0.05(2)

Table 2. Atomic coordinates and U_{eq} [Å^2] for 9.

Atom	***x***	***y***	***z***	U_{eq}
Si3	0.2565(3)	0.5987(7)	0.72547(16)	0.1344(12)
Si26	0.2016(3)	0.2974(10)	0.09726(16)	0.1290(12)
O34	0.3264(7)	0.8043(12)	0.4139(3)	0.1109(19)
O10	0.2662(6)	0.6875(12)	0.5032(3)	0.1057(18)

O22	0.5162(6)	0.5220(13)	0.4888(3)	0.0996(17)
H22	0.560407	0.442083	0.510547	0.149
O25	0.2751(7)	0.3655(15)	0.1710(3)	0.122(2)
C13	0.2795(8)	0.3600(16)	0.4862(4)	0.0938(12)
H13	0.345232	0.284972	0.511870	0.113
O7	0.2778(8)	0.6308(15)	0.6474(3)	0.134(2)
C12	0.3237(8)	0.4654(16)	0.4272(5)	0.0915(11)
C17	0.2546(7)	0.3987(17)	0.3551(4)	0.0929(11)
H17	0.269843	0.262142	0.355083	0.111
C9	0.2462(8)	0.5108(16)	0.5339(5)	0.0944(13)
H9	0.161622	0.498802	0.536905	0.113
C11	0.3030(7)	0.6688(17)	0.4445(4)	0.0929(13)
C20	0.4933(8)	0.5210(17)	0.3647(4)	0.0942(13)
H20A	0.578020	0.498346	0.367782	0.113
H20B	0.480274	0.656783	0.363383	0.113
C18	0.2929(8)	0.4665(16)	0.2896(5)	0.0952(13)
C21	0.4529(8)	0.4403(16)	0.4271(4)	0.0910(13)
H21	0.469899	0.304169	0.428365	0.109
C14	0.1749(8)	0.2281(16)	0.4600(5)	0.0946(13)
H14	0.207197	0.125301	0.434969	0.113
C16	0.1243(8)	0.4115(17)	0.3570(5)	0.0955(12)
H16	0.072043	0.478374	0.323435	0.115
C8	0.3172(9)	0.5005(18)	0.6040(5)	0.1016(18)
H8A	0.311510	0.374164	0.622870	0.122
H8B	0.400172	0.524937	0.601690	0.122
C15	0.0877(8)	0.3219(17)	0.4093(5)	0.0963(13)
H15	0.007423	0.319728	0.413044	0.116
C19	0.4277(8)	0.4340(16)	0.2999(4)	0.0947(13)
H19A	0.443132	0.298809	0.301093	0.114
H19B	0.457763	0.486014	0.260025	0.114
C23	0.2638(8)	0.6607(18)	0.2673(5)	0.1048(19)
H23A	0.181538	0.685446	0.269129	0.157
H23B	0.277597	0.677847	0.220274	0.157
H23C	0.313146	0.746779	0.297925	0.157
C33	0.1264(9)	0.1360(18)	0.5194(5)	0.109(2)
H33A	0.068292	0.042318	0.500993	0.163
H33B	0.089849	0.230461	0.544298	0.163
H33C	0.190383	0.076590	0.550672	0.163
C24	0.2359(9)	0.3307(18)	0.2343(4)	0.1008(15)
H24A	0.255815	0.201830	0.249358	0.121
H24B	0.149931	0.344148	0.227673	0.121
C29	0.2884(15)	0.365(3)	0.0319(8)	0.156(3)
C35	0.2434(15)	0.8366(9)	0.7561(7)	0.162(2)
H35A	0.312025	0.903748	0.744904	0.194
H35B	0.174497	0.889700	0.725866	0.194
C2	0.1292(11)	0.446(2)	0.7204(7)	0.166(2)
H2A	0.074707	0.479500	0.677994	0.199
H2B	0.156322	0.318152	0.713971	0.199
C30	0.2200(17)	0.320(4)	-0.0370(8)	0.180(4)
H30A	0.203493	0.186743	-0.039821	0.271
H30B	0.265226	0.354884	-0.072450	0.271
H30C	0.146400	0.389413	-0.043927	0.271
C28	0.1661(16)	0.034(3)	0.1035(9)	0.178(4)
H28A	0.224521	-0.024082	0.138747	0.267
H28B	0.167609	-0.025511	0.059141	0.267
H28C	0.088479	0.019600	0.115651	0.267

C32	0.4119(15)	0.329(4)	0.0533(8)	0.180(4)
H32A	0.453021	0.420818	0.085310	0.270
H32B	0.451868	0.316256	0.013883	0.270
H32C	0.411101	0.209298	0.076536	0.270
C31	0.3147(17)	0.568(3)	0.0318(9)	0.184(4)
H31A	0.256677	0.653728	0.007425	0.276
H31B	0.385333	0.571133	0.011059	0.276
H31C	0.334205	0.604316	0.080105	0.276
C4	0.3910(11)	0.591(3)	0.7892(9)	0.161(2)
H4A	0.436910	0.705792	0.786405	0.193
H4B	0.371763	0.582846	0.835900	0.193
C27	0.0575(15)	0.408(3)	0.0802(8)	0.173(4)
H27A	0.060286	0.525470	0.105223	0.259
H27B	-0.000112	0.325430	0.095450	0.259
H27C	0.035216	0.431110	0.030951	0.259
C5	0.4629(14)	0.421(2)	0.7750(9)	0.169(3)
H5AA	0.413318	0.309827	0.771158	0.254
H5AB	0.528771	0.404375	0.812699	0.254
H5AC	0.492371	0.439085	0.731987	0.254
H5BD	0.473694	0.349560	0.734326	0.254
H5BE	0.506153	0.360917	0.816137	0.254
H5BF	0.492058	0.547258	0.771475	0.254
C1	0.0573(15)	0.439(4)	0.7787(8)	0.198(5)
H1A	-0.026128	0.442215	0.759272	0.296
H1B	0.076921	0.546469	0.808991	0.296
H1C	0.075238	0.324601	0.805110	0.296
C36	0.2328(16)	0.899(3)	0.8291(7)	0.185(4)
H36A	0.230971	1.034631	0.831071	0.278
H36B	0.299935	0.852591	0.861600	0.278
H36C	0.160669	0.848639	0.841181	0.278
C6	0.341(2)	0.427(5)	0.7793(17)	0.161(2)
H6A	0.333661	0.451073	0.827566	0.193
H6B	0.306967	0.302880	0.766917	0.193

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic displacement parameters [Å²] for 9. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si3	0.153(2)	0.171(3)	0.0874(17)	−0.0153(17)	0.0453(16)	−0.010(2)
Si26	0.147(2)	0.155(3)	0.0830(17)	−0.0067(17)	0.0141(15)	−0.010(2)
O34	0.153(5)	0.090(4)	0.096(4)	0.006(3)	0.037(4)	0.014(4)
O10	0.133(4)	0.097(4)	0.091(4)	−0.013(3)	0.031(3)	0.020(3)
O22	0.099(4)	0.106(4)	0.089(4)	0.003(3)	0.002(3)	0.003(3)
O25	0.140(5)	0.152(5)	0.074(3)	−0.011(4)	0.021(3)	−0.017(4)
C13	0.102(2)	0.103(2)	0.082(2)	−0.009(2)	0.0286(19)	0.002(2)
O7	0.192(6)	0.135(5)	0.082(4)	−0.020(4)	0.041(4)	0.011(5)
C12	0.099(2)	0.100(2)	0.080(2)	−0.0108(18)	0.0279(18)	0.0016(18)
C17	0.099(2)	0.103(2)	0.081(2)	−0.0100(19)	0.0264(18)	0.0006(19)
C9	0.104(2)	0.102(2)	0.083(2)	−0.011(2)	0.030(2)	0.003(2)
C11	0.101(2)	0.100(2)	0.081(2)	−0.010(2)	0.025(2)	0.003(2)
C20	0.100(2)	0.104(3)	0.082(2)	−0.006(2)	0.025(2)	0.001(2)
C18	0.102(2)	0.106(2)	0.081(2)	−0.009(2)	0.024(2)	−0.002(2)
C21	0.097(2)	0.101(2)	0.080(2)	−0.007(2)	0.028(2)	0.001(2)
C14	0.103(2)	0.102(3)	0.083(2)	−0.011(2)	0.029(2)	−0.001(2)
C16	0.101(2)	0.105(2)	0.083(2)	−0.011(2)	0.024(2)	0.001(2)

C8	0.115(4)	0.110(4)	0.083(3)	−0.011(3)	0.027(3)	0.001(3)
C15	0.102(2)	0.104(3)	0.086(2)	−0.013(2)	0.028(2)	0.000(2)
C19	0.102(2)	0.106(3)	0.081(2)	−0.009(2)	0.028(2)	−0.001(2)
C23	0.111(4)	0.116(4)	0.087(4)	−0.007(3)	0.018(3)	0.002(4)
C33	0.119(4)	0.112(5)	0.102(4)	−0.004(4)	0.040(4)	0.000(4)
C24	0.110(3)	0.113(3)	0.081(3)	−0.008(3)	0.023(2)	−0.003(3)
C29	0.178(5)	0.189(6)	0.103(4)	−0.001(5)	0.031(4)	−0.003(5)
C35	0.183(4)	0.191(5)	0.117(4)	−0.016(4)	0.042(3)	−0.009(4)
C2	0.186(4)	0.194(5)	0.123(4)	−0.014(4)	0.040(4)	−0.011(4)
C30	0.211(8)	0.215(8)	0.116(6)	0.006(7)	0.031(6)	−0.005(7)
C28	0.200(8)	0.193(9)	0.132(7)	−0.008(7)	0.003(7)	−0.011(8)
C32	0.199(7)	0.215(8)	0.128(6)	0.010(7)	0.034(6)	0.003(7)
C31	0.210(8)	0.212(8)	0.134(6)	0.016(7)	0.040(6)	−0.011(7)
C4	0.180(4)	0.192(5)	0.115(4)	−0.014(4)	0.039(4)	−0.007(4)
C27	0.182(7)	0.204(7)	0.130(6)	0.000(7)	0.018(6)	0.002(7)
C5	0.189(5)	0.197(6)	0.124(5)	−0.015(5)	0.034(5)	−0.003(5)
C1	0.210(10)	0.216(11)	0.170(9)	−0.008(9)	0.041(8)	−0.023(9)
C36	0.207(7)	0.211(8)	0.142(7)	−0.012(7)	0.042(6)	−0.006(7)
C6	0.181(4)	0.191(5)	0.115(4)	−0.015(4)	0.039(4)	−0.008(4)

Table 4. Bond lengths and angles for 9.

Atom–Atom	Length [Å]
Si3–O7	1.623(8)
Si3–C35	1.8330(14)
Si3–C2	1.8334(14)
Si3–C4	1.8327(14)
Si3–C6	1.81(2)
Si26–O25	1.634(7)
Si26–C29	1.839(16)
Si26–C28	1.95(2)
Si26–C27	1.833(18)
O34–C11	1.205(12)
O10–C9	1.447(12)
O10–C11	1.314(10)
O22–H22	0.8400
O22–C21	1.438(11)
O25–C24	1.429(11)
C13–H13	1.0000
C13–C12	1.554(13)
C13–C9	1.532(13)
C13–C14	1.561(14)
O7–C8	1.402(12)
C12–C17	1.586(13)
C12–C11	1.534(15)
C12–C21	1.513(12)
C17–H17	1.0000
C17–C18	1.524(12)
C17–C16	1.526(12)
C9–H9	1.0000
C9–C8	1.490(14)
C20–H20A	0.9900
C20–H20B	0.9900
C20–C21	1.511(12)
C20–C19	1.512(13)
C18–C19	1.564(13)

C18–C23	1.488(16)
C18–C24	1.531(13)
C21–H21	1.0000
C14–H14	1.0000
C14–C15	1.462(14)
C14–C33	1.540(14)
C16–H16	0.9500
C16–C15	1.349(13)
C8–H8A	0.9900
C8–H8B	0.9900
C15–H15	0.9500
C19–H19A	0.9900
C19–H19B	0.9900
C23–H23A	0.9800
C23–H23B	0.9800
C23–H23C	0.9800
C33–H33A	0.9800
C33–H33B	0.9800
C33–H33C	0.9800
C24–H24A	0.9900
C24–H24B	0.9900
C29–C30	1.49(2)
C29–C32	1.45(2)
C29–C31	1.49(3)
C35–H35A	0.9900
C35–H35B	0.9900
C35–C36	1.5395(14)
C2–H2A	0.9900
C2–H2B	0.9900
C2–C1	1.5398(14)
C30–H30A	0.9800
C30–H30B	0.9800
C30–H30C	0.9800
C28–H28A	0.9800
C28–H28B	0.9800
C28–H28C	0.9800
C32–H32A	0.9800
C32–H32B	0.9800
C32–H32C	0.9800
C31–H31A	0.9800
C31–H31B	0.9800
C31–H31C	0.9800
C4–H4A	0.9900
C4–H4B	0.9900
C4–C5	1.5394(14)
C27–H27A	0.9800
C27–H27B	0.9800
C27–H27C	0.9800
C5–H5AA	0.9800
C5–H5AB	0.9800
C5–H5AC	0.9800
C5–H5BD	0.9800
C5–H5BE	0.9800
C5–H5BF	0.9800
C5–C6	1.43(2)
C1–H1A	0.9800

C1–H1B	0.9800
C1–H1C	0.9800
C36–H36A	0.9800
C36–H36B	0.9800
C36–H36C	0.9800
C6–H6A	0.9900
C6–H6B	0.9900

Atom–Atom–Atom	**Angle [°]**
O7–Si3–C35	102.5(6)
O7–Si3–C2	106.7(5)
O7–Si3–C4	114.0(9)
O7–Si3–C6	120.1(11)
C35–Si3–C2	117.8(8)
C4–Si3–C35	84.9(8)
C4–Si3–C2	127.2(11)
C6–Si3–C35	120.9(15)
C6–Si3–C2	88.5(13)
O25–Si26–C29	106.4(6)
O25–Si26–C28	108.6(6)
O25–Si26–C27	110.8(7)
C29–Si26–C28	116.7(9)
C27–Si26–C29	110.6(8)
C27–Si26–C28	103.7(9)
C11–O10–C9	112.4(7)
C21–O22–H22	109.5
C24–O25–Si26	122.3(6)
C12–C13–H13	108.8
C12–C13–C14	112.8(7)
C9–C13–H13	108.8
C9–C13–C12	105.6(8)
C9–C13–C14	111.8(7)
C14–C13–H13	108.8
C8–O7–Si3	127.4(8)
C13–C12–C17	110.3(7)
C11–C12–C13	102.3(7)
C11–C12–C17	114.6(8)
C21–C12–C13	113.6(8)
C21–C12–C17	108.1(7)
C21–C12–C11	108.0(8)
C12–C17–H17	103.7
C18–C17–C12	119.5(8)
C18–C17–H17	103.7
C18–C17–C16	116.1(8)
C16–C17–C12	108.1(7)
C16–C17–H17	103.7
O10–C9–C13	106.8(7)
O10–C9–H9	109.4
O10–C9–C8	109.4(8)
C13–C9–H9	109.4
C8–C9–C13	112.4(8)
C8–C9–H9	109.4
O34–C11–O10	119.9(9)
O34–C11–C12	127.1(8)
O10–C11–C12	112.6(8)
H20A–C20–H20B	108.1

C21–C20–H20A	109.5
C21–C20–H20B	109.5
C21–C20–C19	110.6(8)
C19–C20–H20A	109.5
C19–C20–H20B	109.5
C17–C18–C19	106.0(7)
C17–C18–C24	104.4(8)
C23–C18–C17	117.9(8)
C23–C18–C19	110.5(8)
C23–C18–C24	110.0(8)
C24–C18–C19	107.3(7)
O22–C21–C12	108.2(7)
O22–C21–C20	110.5(7)
O22–C21–H21	108.0
C12–C21–H21	108.0
C20–C21–C12	113.9(8)
C20–C21–H21	108.0
C13–C14–H14	106.1
C15–C14–C13	110.8(8)
C15–C14–H14	106.1
C15–C14–C33	115.0(8)
C33–C14–C13	112.1(7)
C33–C14–H14	106.1
C17–C16–H16	122.1
C15–C16–C17	115.8(9)
C15–C16–H16	122.1
O7–C8–C9	110.5(9)
O7–C8–H8A	109.5
O7–C8–H8B	109.5
C9–C8–H8A	109.5
C9–C8–H8B	109.5
H8A–C8–H8B	108.1
C14–C15–H15	120.8
C16–C15–C14	118.4(8)
C16–C15–H15	120.8
C20–C19–C18	113.3(7)
C20–C19–H19A	108.9
C20–C19–H19B	108.9
C18–C19–H19A	108.9
C18–C19–H19B	108.9
H19A–C19–H19B	107.7
C18–C23–H23A	109.5
C18–C23–H23B	109.5
C18–C23–H23C	109.5
H23A–C23–H23B	109.5
H23A–C23–H23C	109.5
H23B–C23–H23C	109.5
C14–C33–H33A	109.5
C14–C33–H33B	109.5
C14–C33–H33C	109.5
H33A–C33–H33B	109.5
H33A–C33–H33C	109.5
H33B–C33–H33C	109.5
O25–C24–C18	110.5(8)
O25–C24–H24A	109.6
O25–C24–H24B	109.6

C18–C24–H24A	109.6
C18–C24–H24B	109.6
H24A–C24–H24B	108.1
C30–C29–Si26	108.4(13)
C30–C29–C31	106.7(16)
C32–C29–Si26	112.6(12)
C32–C29–C30	125.1(16)
C32–C29–C31	88.9(17)
C31–C29–Si26	113.4(13)
Si3–C35–H35A	105.5
Si3–C35–H35B	105.5
H35A–C35–H35B	106.0
C36–C35–Si3	127.4(12)
C36–C35–H35A	105.5
C36–C35–H35B	105.5
Si3–C2–H2A	107.0
Si3–C2–H2B	107.0
H2A–C2–H2B	106.8
C1–C2–Si3	121.1(10)
C1–C2–H2A	107.0
C1–C2–H2B	107.0
C29–C30–H30A	109.5
C29–C30–H30B	109.5
C29–C30–H30C	109.5
H30A–C30–H30B	109.5
H30A–C30–H30C	109.5
H30B–C30–H30C	109.5
Si26–C28–H28A	109.5
Si26–C28–H28B	109.5
Si26–C28–H28C	109.5
H28A–C28–H28B	109.5
H28A–C28–H28C	109.5
H28B–C28–H28C	109.5
C29–C32–H32A	114.7
C29–C32–H32B	111.6
C29–C32–H32C	101.8
H32A–C32–H32B	109.5
H32A–C32–H32C	109.5
H32B–C32–H32C	109.5
C29–C31–H31A	119.7
C29–C31–H31B	102.3
C29–C31–H31C	106.0
H31A–C31–H31B	109.5
H31A–C31–H31C	109.5
H31B–C31–H31C	109.5
Si3–C4–H4A	109.9
Si3–C4–H4B	109.9
H4A–C4–H4B	108.3
C5–C4–Si3	108.9(10)
C5–C4–H4A	109.9
C5–C4–H4B	109.9
Si26–C27–H27A	109.5
Si26–C27–H27B	109.5
Si26–C27–H27C	109.5
H27A–C27–H27B	109.5
H27A–C27–H27C	109.5

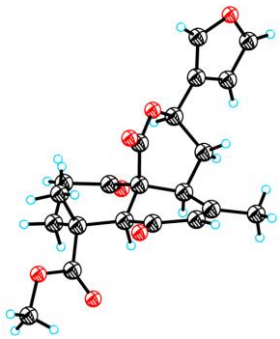
H27B–C27–H27C	109.5
C4–C5–H5AA	109.5
C4–C5–H5AB	109.5
C4–C5–H5AC	109.5
H5AA–C5–H5AB	109.5
H5AA–C5–H5AC	109.5
H5AB–C5–H5AC	109.5
H5BD–C5–H5BE	109.5
H5BD–C5–H5BF	109.5
H5BE–C5–H5BF	109.5
C6–C5–H5BD	109.5
C6–C5–H5BE	109.5
C6–C5–H5BF	109.5
C2–C1–H1A	109.5
C2–C1–H1B	109.5
C2–C1–H1C	109.5
H1A–C1–H1B	109.5
H1A–C1–H1C	109.5
H1B–C1–H1C	109.5
C35–C36–H36A	109.5
C35–C36–H36B	109.5
C35–C36–H36C	109.5
H36A–C36–H36B	109.5
H36A–C36–H36C	109.5
H36B–C36–H36C	109.5
Si3–C6–H6A	108.5
Si3–C6–H6B	108.5
C5–C6–Si3	115.3(19)
C5–C6–H6A	108.5
C5–C6–H6B	108.5
H6A–C6–H6B	107.5

Table 5. Torsion angles for 9.

Atom–Atom–Atom–Atom	Torsion Angle [°]
Si3–O7–C8–C9	135.5(9)
Si26–O25–C24–C18	−158.8(7)
O10–C9–C8–O7	66.3(10)
O25–Si26–C29–C30	−175.2(13)
O25–Si26–C29–C32	42.2(17)
O25–Si26–C29–C31	−56.9(15)
C13–C12–C17–C18	−172.9(8)
C13–C12–C17–C16	51.4(10)
C13–C12–C11–O34	178.1(10)
C13–C12–C11–O10	5.2(10)
C13–C12–C21–O22	−64.4(10)
C13–C12–C21–C20	172.4(8)
C13–C9–C8–O7	−175.2(9)
C13–C14–C15–C16	49.4(11)
O7–Si3–C35–C36	−174.3(15)
O7–Si3–C2–C1	−158.3(15)
O7–Si3–C4–C5	−64.7(17)
O7–Si3–C6–C5	42(3)
C12–C13–C9–O10	1.7(9)
C12–C13–C9–C8	−118.2(9)
C12–C13–C14–C15	−45.9(10)

C12–C13–C14–C33	−175.8(8)
C12–C17–C18–C19	49.1(11)
C12–C17–C18–C23	−75.3(11)
C12–C17–C18–C24	162.3(8)
C12–C17–C16–C15	−54.0(11)
C17–C12–C11–O34	−62.5(12)
C17–C12–C11–O10	124.5(8)
C17–C12–C21–O22	172.9(8)
C17–C12–C21–C20	49.6(11)
C17–C18–C19–C20	−53.8(11)
C17–C18–C24–O25	−173.5(8)
C17–C16–C15–C14	2.2(13)
C9–O10–C11–O34	−178.0(9)
C9–O10–C11–C12	−4.4(10)
C9–C13–C12–C17	−126.1(8)
C9–C13–C12–C11	−3.8(9)
C9–C13–C12–C21	112.3(9)
C9–C13–C14–C15	72.9(10)
C9–C13–C14–C33	−57.0(11)
C11–O10–C9–C13	1.6(10)
C11–O10–C9–C8	123.5(8)
C11–C12–C17–C18	72.4(10)
C11–C12–C17–C16	−63.4(10)
C11–C12–C21–O22	48.4(9)
C11–C12–C21–C20	−74.9(9)
C18–C17–C16–C15	168.6(9)
C21–C12–C17–C18	−48.1(12)
C21–C12–C17–C16	176.2(8)
C21–C12–C11–O34	58.0(12)
C21–C12–C11–O10	−114.9(8)
C21–C20–C19–C18	60.6(11)
C14–C13–C12–C17	−3.8(11)
C14–C13–C12–C11	118.5(8)
C14–C13–C12–C21	−125.4(8)
C14–C13–C9–O10	−121.3(8)
C14–C13–C9–C8	118.8(9)
C16–C17–C18–C19	−178.5(8)
C16–C17–C18–C23	57.1(12)
C16–C17–C18–C24	−65.3(10)
C19–C20–C21–O22	179.5(7)
C19–C20–C21–C12	−58.5(11)
C19–C18–C24–O25	−61.3(10)
C23–C18–C19–C20	75.0(10)
C23–C18–C24–O25	59.0(11)
C33–C14–C15–C16	177.7(9)
C24–C18–C19–C20	−165.0(8)
C29–Si26–O25–C24	−177.9(10)
C35–Si3–O7–C8	165.8(10)
C35–Si3–C2–C1	−43.9(18)
C35–Si3–C4–C5	−166.1(16)
C35–Si3–C6–C5	−88(3)
C2–Si3–O7–C8	−69.7(11)
C2–Si3–C35–C36	68.9(18)
C2–Si3–C4–C5	72.6(18)
C2–Si3–C6–C5	151(3)
C28–Si26–O25–C24	−51.4(12)

C28–Si26–C29–C30	63.4(16)
C28–Si26–C29–C32	−79.2(17)
C28–Si26–C29–C31	−178.3(13)
C4–Si3–O7–C8	75.9(12)
C4–Si3–C35–C36	−60.8(17)
C4–Si3–C2–C1	61.9(19)
C27–Si26–O25–C24	61.9(12)
C27–Si26–C29–C30	−54.8(17)
C27–Si26–C29–C32	162.6(16)
C27–Si26–C29–C31	63.5(16)
C6–Si3–O7–C8	28.4(18)
C6–Si3–C35–C36	−37(2)
C6–Si3–C2–C1	80.6(19)



5

Table 1 Crystal data and structure refinement for compound 5.

CCDC number	2447365
Empirical formula	$C_{21}H_{22}O_7$
Formula weight	386.4
Temperature/K	273.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	10.2359(2)
b/Å	12.2092(3)
c/Å	15.0097(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	1875.79(8)
Z	4
ρ_{calc}g/cm^3	1.361
μ/mm^{-1}	0.859
F(000)	808.0
Crystal size/mm^3	0.2 × 0.15 × 0.1
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	9.338 to 137.002
Index ranges	-11 ≤ h ≤ 12, -14 ≤ k ≤ 14, -18 ≤ l ≤ 18
Reflections collected	17179
Independent reflections	3418 [R_{int} = 0.0482, R_{sigma} = 0.0370]
Data/restraints/parameters	3418/15/236

Goodness-of-fit on F^2	1.083
Final R indexes [I>=2σ (I)]	R_1 = 0.0777, wR_2 = 0.2296
Final R indexes [all data]	R_1 = 0.0861, wR_2 = 0.2431
Largest diff. peak/hole / e $Å^{-3}$	0.45/-0.59
Flack parameter	0.17(9)

Table 2 Atomic coordinates and U_{eq} [$Å^2$] for 5.

Atom	***x***	***y***	***z***	U_{eq}
O6	0.4411(4)	0.2986(3)	0.3901(2)	0.0727(10)
O5	0.5386(3)	0.4403(3)	0.4467(3)	0.0753(11)
O4	0.1065(4)	0.3798(4)	0.4256(4)	0.1022(16)
O1	0.3327(6)	0.8128(3)	0.5654(4)	0.1080(17)
O3	0.5075(6)	0.5738(5)	0.6401(4)	0.123(2)
O2	0.2310(7)	0.6905(4)	0.6494(4)	0.123(2)
C5	0.3145(4)	0.4133(3)	0.4923(3)	0.0476(10)
C4	0.3270(4)	0.5165(3)	0.5517(3)	0.0544(10)
H4	0.248111	0.514799	0.588697	0.065
C6	0.4408(4)	0.3881(4)	0.4414(3)	0.0534(10)
C21	0.2006(5)	0.4363(5)	0.4282(3)	0.0661(13)
C10	0.4372(6)	0.4994(5)	0.6175(4)	0.0762(16)
C7	0.2836(5)	0.3116(4)	0.5489(3)	0.0574(11)
H7	0.190633	0.313925	0.564556	0.069
C8	0.3609(7)	0.3091(5)	0.6339(3)	0.0783(18)
C13	0.3366(5)	0.2198(4)	0.3990(4)	0.0652(13)
H13	0.258028	0.245306	0.367887	0.078
C2	0.2931(6)	0.7120(4)	0.5848(5)	0.0828(18)
C3	0.3245(6)	0.6327(4)	0.5087(4)	0.0702(14)
C12	0.3093(6)	0.2042(4)	0.4970(4)	0.0715(15)
H12A	0.383243	0.167029	0.523878	0.086
H12B	0.233770	0.156797	0.503455	0.086
C9	0.4382(8)	0.3925(6)	0.6586(3)	0.087(2)
H9	0.496178	0.380648	0.705285	0.105
C23	0.2059(7)	0.6365(5)	0.4462(5)	0.0879(18)
H23A	0.204484	0.706174	0.415239	0.105
H23B	0.126447	0.630881	0.481174	0.105
C11	0.3465(11)	0.2086(6)	0.6900(5)	0.122(4)
H11A	0.415040	0.206541	0.733623	0.183
H11B	0.351916	0.144776	0.652806	0.183
H11C	0.263342	0.209939	0.719518	0.183
C22	0.2098(8)	0.5429(6)	0.3777(4)	0.094(2)
H22A	0.137259	0.549483	0.336427	0.113
H22B	0.290592	0.545632	0.343964	0.113
C20	0.5298(15)	0.0228(11)	0.2665(11)	0.0998(14)
H20	0.597941	0.002963	0.228791	0.120
C24	0.4472(8)	0.6655(5)	0.4570(6)	0.108(3)
H24A	0.521713	0.661991	0.495673	0.161
H24B	0.437371	0.738902	0.434958	0.161
H24C	0.459409	0.616303	0.407797	0.161
C1	0.3019(10)	0.8972(5)	0.6303(8)	0.125(3)
H1A	0.212995	0.920409	0.622517	0.187
H1B	0.359238	0.958540	0.621985	0.187
H1C	0.313012	0.868386	0.689343	0.187
C16	0.3806(12)	−0.0689(4)	0.3414(10)	0.0998(14)
H16	0.354470	−0.141682	0.344969	0.120
O7	0.4941(10)	−0.0292(8)	0.2976(8)	0.0998(14)
C18	0.4976(8)	0.0864(8)	0.3080(7)	0.0998(14)

H18	0.561581	0.133091	0.285815	0.120
C14	0.3862(6)	0.1181(4)	0.3582(5)	0.0998(14)
C15	0.3139(9)	0.0222(6)	0.3788(8)	0.0998(14)
H15	0.236507	0.019466	0.411179	0.120
C19	0.4920(10)	0.1279(9)	0.2975(8)	0.0998(14)
H19	0.530868	0.193585	0.280603	0.120
C17	0.3522(14)	0.0054(5)	0.3581(10)	0.0998(14)
H17	0.281212	−0.022468	0.389341	0.120
O8	0.4242(11)	−0.0509(8)	0.3136(8)	0.0998(14)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 3 Anisotropic displacement parameters [Å²] for 5. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O6	0.076(2)	0.066(2)	0.076(2)	−0.0129(17)	0.0230(18)	−0.0054(19)
O5	0.0527(18)	0.065(2)	0.108(3)	0.001(2)	0.0108(18)	−0.0070(16)
O4	0.055(2)	0.115(4)	0.136(4)	−0.031(3)	−0.030(2)	0.006(2)
O1	0.121(4)	0.049(2)	0.153(4)	−0.008(2)	−0.002(4)	0.000(2)
O3	0.109(4)	0.105(4)	0.156(5)	−0.054(4)	−0.060(4)	0.003(3)
O2	0.149(5)	0.075(3)	0.145(5)	−0.039(3)	0.054(4)	−0.015(3)
C5	0.048(2)	0.044(2)	0.050(2)	0.0005(17)	−0.0018(17)	−0.0007(16)
C4	0.055(2)	0.045(2)	0.063(2)	−0.0004(19)	0.000(2)	0.0002(18)
C6	0.052(2)	0.051(2)	0.057(2)	0.0077(18)	0.0024(19)	0.0014(19)
C21	0.058(3)	0.071(3)	0.069(3)	−0.010(2)	−0.011(2)	0.014(2)
C10	0.081(4)	0.068(3)	0.079(3)	−0.029(3)	−0.021(3)	0.016(3)
C7	0.058(2)	0.047(2)	0.067(3)	0.003(2)	0.017(2)	0.0000(19)
C8	0.117(5)	0.069(3)	0.049(2)	0.008(2)	0.014(3)	0.041(3)
C13	0.055(3)	0.069(3)	0.072(3)	−0.016(2)	−0.008(2)	0.003(2)
C2	0.073(3)	0.047(3)	0.128(5)	−0.010(3)	−0.009(4)	0.005(2)
C3	0.067(3)	0.045(2)	0.098(4)	0.003(2)	0.008(3)	0.004(2)
C12	0.078(3)	0.047(2)	0.090(4)	−0.010(2)	0.021(3)	−0.010(2)
C9	0.112(5)	0.101(5)	0.049(3)	−0.008(3)	−0.017(3)	0.045(4)
C23	0.099(4)	0.068(3)	0.097(4)	0.018(3)	−0.005(4)	0.026(3)
C11	0.186(9)	0.094(5)	0.085(4)	0.039(4)	0.056(5)	0.066(6)
C22	0.109(5)	0.097(5)	0.077(3)	0.016(3)	−0.016(3)	0.040(4)
C20	0.098(3)	0.087(2)	0.114(3)	−0.043(2)	0.009(2)	0.019(2)
C24	0.112(5)	0.048(3)	0.162(7)	0.020(4)	0.047(5)	−0.003(3)
C1	0.119(6)	0.055(3)	0.200(10)	−0.036(5)	−0.039(6)	0.020(4)
C16	0.098(3)	0.087(2)	0.114(3)	−0.043(2)	0.009(2)	0.019(2)
O7	0.098(3)	0.087(2)	0.114(3)	−0.043(2)	0.009(2)	0.019(2)
C18	0.098(3)	0.087(2)	0.114(3)	−0.043(2)	0.009(2)	0.019(2)
C14	0.098(3)	0.087(2)	0.114(3)	−0.043(2)	0.009(2)	0.019(2)
C15	0.098(3)	0.087(2)	0.114(3)	−0.043(2)	0.009(2)	0.019(2)
C19	0.098(3)	0.087(2)	0.114(3)	−0.043(2)	0.009(2)	0.019(2)
C17	0.098(3)	0.087(2)	0.114(3)	−0.043(2)	0.009(2)	0.019(2)
O8	0.098(3)	0.087(2)	0.114(3)	−0.043(2)	0.009(2)	0.019(2)

Table 4 Bond lengths and angles for 5.

Atom–Atom	Length [Å]
O6–C6	1.337(6)
O6–C13	1.445(6)
O5–C6	1.190(6)
O4–C21	1.186(7)
O1–C2	1.328(8)
O1–C1	1.453(10)
O3–C10	1.207(8)

O2–C2	1.189(9)
C5–C4	1.548(6)
C5–C6	1.533(6)
C5–C21	1.538(6)
C5–C7	1.537(6)
C4–H4	0.9800
C4–C10	1.515(7)
C4–C3	1.559(6)
C21–C22	1.509(9)
C10–C9	1.444(9)
C7–H7	0.9800
C7–C8	1.502(8)
C7–C12	1.549(7)
C8–C9	1.341(11)
C8–C11	1.495(8)
C13–H13	0.9800
C13–C12	1.511(8)
C13–C14	1.475(6)
C2–C3	1.532(9)
C3–C23	1.535(10)
C3–C24	1.530(9)
C12–H12A	0.9700
C12–H12B	0.9700
C9–H9	0.9300
C23–H23A	0.9700
C23–H23B	0.9700
C23–C22	1.539(10)
C11–H11A	0.9600
C11–H11B	0.9600
C11–H11C	0.9600
C22–H22A	0.9700
C22–H22B	0.9700
C20–H20	0.9300
C20–C19	1.4193(11)
C20–O8	1.57(2)
C24–H24A	0.9600
C24–H24B	0.9600
C24–H24C	0.9600
C1–H1A	0.9600
C1–H1B	0.9600
C1–H1C	0.9600
C16–H16	0.9300
C16–O7	1.4200
C16–C15	1.4200
O7–C18	1.4200
C18–H18	0.9300
C18–C14	1.4200
C14–C15	1.4200
C14–C19	1.4198(12)
C14–C17	1.4195(11)
C15–H15	0.9300
C19–H19	0.9300
C17–H17	0.9300
C17–O8	1.209(15)

Atom–Atom–Atom	**Angle [°]**

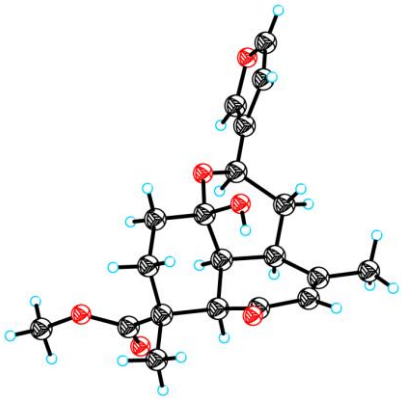
C6–O6–C13	119.3(4)
C2–O1–C1	116.3(7)
C6–C5–C4	112.4(3)
C6–C5–C21	111.3(4)
C6–C5–C7	106.7(3)
C21–C5–C4	105.9(4)
C7–C5–C4	110.9(3)
C7–C5–C21	109.7(4)
C5–C4–H4	103.9
C5–C4–C3	120.1(4)
C10–C4–C5	108.9(4)
C10–C4–H4	103.9
C10–C4–C3	114.0(5)
C3–C4–H4	103.9
O6–C6–C5	117.0(4)
O5–C6–O6	118.3(4)
O5–C6–C5	124.7(4)
O4–C21–C5	122.0(5)
O4–C21–C22	122.4(5)
C22–C21–C5	115.2(5)
O3–C10–C4	121.6(6)
O3–C10–C9	123.8(6)
C9–C10–C4	114.1(5)
C5–C7–H7	108.0
C5–C7–C12	111.8(4)
C8–C7–C5	112.2(4)
C8–C7–H7	108.0
C8–C7–C12	108.7(4)
C12–C7–H7	108.0
C9–C8–C7	122.0(5)
C9–C8–C11	121.7(6)
C11–C8–C7	116.3(7)
O6–C13–H13	110.6
O6–C13–C12	108.1(4)
O6–C13–C14	105.5(4)
C12–C13–H13	110.6
C14–C13–H13	110.6
C14–C13–C12	111.2(5)
O1–C2–C3	110.9(6)
O2–C2–O1	123.2(6)
O2–C2–C3	125.5(5)
C2–C3–C4	105.7(5)
C2–C3–C23	105.7(5)
C23–C3–C4	107.0(5)
C24–C3–C4	115.8(5)
C24–C3–C2	112.7(6)
C24–C3–C23	109.4(6)
C7–C12–H12A	108.6
C7–C12–H12B	108.6
C13–C12–C7	114.5(4)
C13–C12–H12A	108.6
C13–C12–H12B	108.6
H12A–C12–H12B	107.6
C10–C9–H9	117.8
C8–C9–C10	124.4(5)
C8–C9–H9	117.8

C3–C23–H23A	109.3
C3–C23–H23B	109.3
C3–C23–C22	111.5(5)
H23A–C23–H23B	108.0
C22–C23–H23A	109.3
C22–C23–H23B	109.3
C8–C11–H11A	109.5
C8–C11–H11B	109.5
C8–C11–H11C	109.5
H11A–C11–H11B	109.5
H11A–C11–H11C	109.5
H11B–C11–H11C	109.5
C21–C22–C23	107.6(5)
C21–C22–H22A	110.2
C21–C22–H22B	110.2
C23–C22–H22A	110.2
C23–C22–H22B	110.2
H22A–C22–H22B	108.5
C19–C20–H20	129.7
C19–C20–O8	100.5(9)
O8–C20–H20	129.7
C3–C24–H24A	109.5
C3–C24–H24B	109.5
C3–C24–H24C	109.5
H24A–C24–H24B	109.5
H24A–C24–H24C	109.5
H24B–C24–H24C	109.5
O1–C1–H1A	109.5
O1–C1–H1B	109.5
O1–C1–H1C	109.5
H1A–C1–H1B	109.5
H1A–C1–H1C	109.5
H1B–C1–H1C	109.5
O7–C16–H16	126.0
C15–C16–H16	126.0
C15–C16–O7	108.0
C18–O7–C16	108.0
O7–C18–H18	126.0
O7–C18–C14	108.0
C14–C18–H18	126.0
C18–C14–C13	136.6(5)
C15–C14–C13	115.1(5)
C15–C14–C18	108.0
C19–C14–C13	117.3(6)
C17–C14–C13	137.1(7)
C17–C14–C19	105.5(7)
C16–C15–C14	108.0
C16–C15–H15	126.0
C14–C15–H15	126.0
C20–C19–C14	110.0(9)
C20–C19–H19	125.0
C14–C19–H19	125.0
C14–C17–H17	123.1
O8–C17–C14	113.8(10)
O8–C17–H17	123.1
C17–O8–C20	109.9(9)

Table 5 Torsion angles for 5.

Atom–Atom–Atom–Atom	Torsion Angle [°]
O6–C13–C12–C7	53.0(6)
O6–C13–C14–C18	−8.1(11)
O6–C13–C14–C15	164.8(7)
O6–C13–C14–C19	−20.5(11)
O6–C13–C14–C17	164.1(13)
O4–C21–C22–C23	109.7(7)
O1–C2–C3–C4	157.8(5)
O1–C2–C3–C23	−88.9(6)
O1–C2–C3–C24	30.5(7)
O3–C10–C9–C8	−179.8(7)
O2–C2–C3–C4	−28.7(9)
O2–C2–C3–C23	84.5(8)
O2–C2–C3–C24	−156.1(8)
C5–C4–C10–O3	144.1(6)
C5–C4–C10–C9	−43.9(6)
C5–C4–C3–C2	161.7(4)
C5–C4–C3–C23	49.4(6)
C5–C4–C3–C24	−72.9(7)
C5–C21–C22–C23	−63.0(7)
C5–C7–C8–C9	5.5(7)
C5–C7–C8–C11	−174.9(5)
C5–C7–C12–C13	−9.8(7)
C4–C5–C6–O6	178.3(4)
C4–C5–C6–O5	0.7(6)
C4–C5–C21–O4	−120.5(5)
C4–C5–C21–C22	52.2(6)
C4–C5–C7–C8	−41.4(5)
C4–C5–C7–C12	−163.7(4)
C4–C10–C9–C8	8.5(9)
C4–C3–C23–C22	−55.3(7)
C6–O6–C13–C12	−42.5(6)
C6–O6–C13–C14	−161.6(5)
C6–C5–C4–C10	−58.7(5)
C6–C5–C4–C3	75.4(5)
C6–C5–C21–O4	117.0(5)
C6–C5–C21–C22	−70.3(6)
C6–C5–C7–C8	81.3(4)
C6–C5–C7–C12	−41.0(5)
C21–C5–C4–C10	179.6(4)
C21–C5–C4–C3	−46.3(6)
C21–C5–C6–O6	−63.1(5)
C21–C5–C6–O5	119.3(5)
C21–C5–C7–C8	−158.0(4)
C21–C5–C7–C12	79.7(5)
C10–C4–C3–C2	−66.4(6)
C10–C4–C3–C23	−178.7(5)
C10–C4–C3–C24	59.1(7)
C7–C5–C4–C10	60.6(5)
C7–C5–C4–C3	−165.2(4)
C7–C5–C6–O6	56.5(5)
C7–C5–C6–O5	−121.1(5)
C7–C5–C21–O4	−0.8(7)
C7–C5–C21–C22	171.8(4)
C7–C8–C9–C10	12.3(9)

C8–C7–C12–C13	−134.1(5)
C13–O6–C6–O5	165.1(5)
C13–O6–C6–C5	−12.7(6)
C13–C14–C15–C16	−174.9(7)
C13–C14–C19–C20	178.5(10)
C13–C14–C17–O8	−179.6(10)
C2–C3–C23–C22	−167.6(6)
C3–C4–C10–O3	7.0(8)
C3–C4–C10–C9	178.9(5)
C3–C23–C22–C21	63.6(7)
C12–C7–C8–C9	129.6(6)
C12–C7–C8–C11	−50.8(6)
C12–C13–C14–C18	−125.1(9)
C12–C13–C14–C15	47.8(8)
C12–C13–C14–C19	−137.5(9)
C12–C13–C14–C17	47.2(15)
C11–C8–C9–C10	−167.3(6)
C24–C3–C23–C22	70.9(7)
C1–O1–C2–O2	3.0(11)
C1–O1–C2–C3	176.7(6)
C16–O7–C18–C14	0.0
O7–C16–C15–C14	0.0
O7–C18–C14–C13	173.2(10)
O7–C18–C14–C15	0.0
C18–C14–C15–C16	0.0
C14–C13–C12–C7	168.3(5)
C14–C17–O8–C20	−2.6(18)
C15–C16–O7–C18	0.0
C19–C20–O8–C17	−0.5(16)
C19–C14–C17–O8	4.7(17)
C17–C14–C19–C20	−4.8(16)
O8–C20–C19–C14	3.3(15)



23

Table 1 Crystal data and structure refinement for 23.

CCDC number	2447370
Empirical formula	$C_{85}H_{57}Ag_9F_{54}N_{18}O_{12}$
Formula weight	3519.31
Temperature/K	100(1)
Crystal system	trigonal
Space group	$P3_121$
a/Å	12.82180(10)
b/Å	12.82180(10)
c/Å	115.3089(11)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	16416.9(3)
Z	6
ρ_{calc}g/cm^3	2.136
μ/mm^{-1}	14.076
F(000)	10188.0
Crystal size/mm^3	0.13 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54178)
2θ range for data collection/°	4.598 to 141.898
Index ranges	-11 ≤ h ≤ 14, -15 ≤ k ≤ 14, -141 ≤ l ≤ 139
Reflections collected	45033
Independent reflections	19677 [R_{int} = 0.0837, R_{sigma} = 0.1167]
Data/restraints/parameters	19677/1118/1612
Goodness-of-fit on F^2	1.121
Final R indexes [I>=2σ (I)]	R_1 = 0.1291, wR_2 = 0.2932
Final R indexes [all data]	R_1 = 0.1361, wR_2 = 0.2973
Largest diff. peak/hole / e Å^{-3}	1.86/-1.76
Flack parameter	0.12(3)

Table 2 Atomic coordinates and U_{eq} [Å^2] for 23.

Atom	***x***	***y***	***z***	U_{eq}
Ag10	0.5783(3)	1.000000	0.333333	0.0376(8)
Ag4	0.4578(2)	0.1612(2)	0.40498(2)	0.0383(5)
Ag3	0.4628(2)	0.1415(2)	0.43485(2)	0.0390(5)
Ag7	0.4600(2)	0.5435(2)	0.48738(2)	0.0393(6)

Ag1	0.5850(2)	0.4299(2)	0.42422(2)	0.0408(6)
Ag8	0.2782(3)	0.2782(3)	0.500000	0.0424(8)
Ag2	0.7664(2)	0.3290(2)	0.43559(2)	0.0419(6)
Ag6	0.7675(2)	0.3271(2)	0.40585(2)	0.0415(6)
Ag5	0.6135(2)	0.4533(2)	0.39502(2)	0.0402(6)
Ag9	0.3731(3)	1.0426(3)	0.31912(3)	0.0597(8)
O2	0.943(2)	0.528(2)	0.4795(2)	0.040(4)
O3	0.871(2)	0.470(2)	0.4606(2)	0.052(6)
H3	0.806631	0.435767	0.456807	0.078
F53	0.021(2)	0.0278(19)	0.4694(2)	0.068(7)
N4	0.584(3)	0.081(3)	0.4418(3)	0.052(5)
F48	0.639(2)	0.800(2)	0.47532(18)	0.055(5)
F23	0.462(3)	0.529(2)	0.3751(2)	0.067(6)
O5	0.523(3)	0.342(2)	0.49100(19)	0.046(6)
F43	0.8479(19)	1.117(2)	0.3245(2)	0.060(6)
O4	0.599(2)	0.358(2)	0.44894(19)	0.040(5)
O8	0.948(2)	0.403(2)	0.3537(2)	0.051(5)
N10	0.857(3)	0.501(3)	0.3980(3)	0.048(5)
N18	0.245(2)	0.298(3)	0.4826(2)	0.042(5)
C39	0.806(4)	0.806(4)	0.500000	0.035(7)
H39	0.879932	0.879927	0.499999	0.042
N3	0.695(3)	0.153(3)	0.4422(3)	0.054(6)
O11	0.520(2)	0.175(2)	0.34197(19)	0.046(6)
F14	0.040(2)	−0.001(2)	0.4334(3)	0.076(7)
F21	0.180(3)	−0.007(2)	0.3905(2)	0.084(8)
F47	0.594(3)	0.880(3)	0.4894(2)	0.080(7)
F22	0.309(3)	0.528(3)	0.3818(2)	0.079(7)
F46	0.771(3)	0.955(2)	0.4828(3)	0.087(8)
O6	0.534(3)	0.175(2)	0.4909(2)	0.059(6)
N17	0.321(3)	0.405(3)	0.4775(2)	0.036(5)
F15	0.188(2)	−0.035(3)	0.4326(3)	0.077(7)
N15	0.630(3)	1.106(3)	0.3182(3)	0.048(5)
F4	1.160(2)	0.659(3)	0.4287(3)	0.085(8)
O10	0.598(2)	0.248(2)	0.38430(19)	0.044(5)
F30	1.046(2)	0.476(2)	0.4091(3)	0.074(7)
F6	1.035(3)	0.488(3)	0.4355(3)	0.091(8)
F27	0.923(3)	0.840(3)	0.3821(3)	0.101(9)
F44	0.893(3)	1.298(2)	0.3246(2)	0.075(7)
N7	0.366(3)	0.240(3)	0.3978(3)	0.044(5)
F35	0.378(3)	−0.236(3)	0.4140(3)	0.084(8)
F1	0.688(3)	0.671(2)	0.4103(2)	0.070(6)
F33	0.911(2)	0.222(2)	0.4217(3)	0.072(6)
N6	0.401(3)	0.330(3)	0.4261(3)	0.045(5)
N9	0.799(3)	0.552(3)	0.3938(3)	0.051(6)
O9	0.871(3)	0.387(3)	0.3722(2)	0.065(7)
H9	0.806217	0.355287	0.375921	0.098
N1	0.772(3)	0.543(3)	0.4242(3)	0.061(7)
F41	0.427(3)	1.059(3)	0.2893(3)	0.115(12)
C59	0.626(3)	0.410(3)	0.4690(3)	0.042(5)
H59	0.570162	0.437194	0.471989	0.050
N11	0.682(3)	0.153(3)	0.4119(2)	0.042(5)
N5	0.351(3)	0.209(3)	0.4299(3)	0.046(5)
C61	0.692(3)	0.561(3)	0.4522(3)	0.043(6)
H61	0.674405	0.579602	0.444712	0.052
O12	0.551(3)	0.362(2)	0.3416(2)	0.054(5)
C13	0.212(4)	0.257(4)	0.4286(3)	0.051(6)

H13	0.134705	0.249828	0.428849	0.061
F24	0.470(3)	0.601(2)	0.3921(2)	0.072(6)
F52	0.031(2)	0.092(3)	0.4871(2)	0.087(8)
F36	0.343(2)	−0.119(3)	0.4038(3)	0.088(8)
C54	0.750(3)	0.496(3)	0.4747(3)	0.037(5)
H54	0.735410	0.491414	0.483240	0.044
F29	1.180(3)	0.622(3)	0.3995(2)	0.077(7)
C45	0.171(3)	0.224(4)	0.4744(3)	0.050(6)
F34	0.331(3)	−0.114(2)	0.4218(3)	0.091(9)
C14	0.311(4)	0.354(4)	0.4251(4)	0.058(5)
C55	0.842(3)	0.458(3)	0.4727(3)	0.041(5)
F49	0.432(3)	0.602(2)	0.4629(2)	0.079(7)
F12	0.412(3)	−0.210(3)	0.4404(3)	0.093(8)
F50	0.260(3)	0.521(3)	0.4531(2)	0.085(8)
F18	0.442(3)	0.546(3)	0.4197(3)	0.108(9)
N16	0.623(3)	0.663(3)	0.4959(2)	0.049(7)
N8	0.425(3)	0.355(3)	0.3947(2)	0.044(5)
F13	0.165(3)	0.038(3)	0.4478(3)	0.093(9)
N2	0.843(3)	0.507(3)	0.4287(3)	0.051(6)
F11	0.349(3)	−0.093(3)	0.4481(3)	0.091(8)
C7	0.746(4)	0.094(4)	0.4478(4)	0.058(6)
F7	0.939(3)	0.273(4)	0.4483(3)	0.107(9)
F2	0.859(3)	0.819(2)	0.4103(3)	0.091(8)
N12	0.560(3)	0.087(3)	0.4113(3)	0.043(5)
F19	0.167(3)	0.032(2)	0.4073(2)	0.091(9)
C79	0.625(4)	0.208(3)	0.3642(3)	0.045(6)
H79	0.567273	0.125081	0.361312	0.055
C77	0.676(4)	0.425(3)	0.3619(3)	0.047(6)
H77A	0.686552	0.438498	0.370407	0.056
H77B	0.652236	0.481073	0.358662	0.056
F9	0.933(3)	0.107(3)	0.4467(3)	0.094(8)
C60	0.634(3)	0.434(3)	0.4562(3)	0.039(5)
C27	0.723(3)	0.075(3)	0.4145(3)	0.050(5)
F51	0.403(3)	0.480(3)	0.4494(3)	0.090(8)
C23	0.996(4)	0.668(3)	0.3894(4)	0.052(6)
H23	1.070155	0.731776	0.386549	0.062
C82	0.752(4)	0.100(3)	0.3747(3)	0.043(5)
F45	0.939(3)	1.229(3)	0.3105(3)	0.096(9)
F8	0.899(3)	0.163(3)	0.4624(2)	0.089(8)
C78	0.577(4)	0.295(3)	0.3596(3)	0.042(5)
C58	0.569(3)	0.274(3)	0.4731(3)	0.041(5)
F17	0.275(3)	0.464(3)	0.4111(2)	0.085(7)
F28	1.073(3)	0.454(3)	0.3915(3)	0.085(8)
F54	0.157(3)	0.043(2)	0.4812(3)	0.089(8)
C57	0.666(3)	0.243(3)	0.4712(3)	0.041(6)
H57A	0.679688	0.243571	0.462731	0.049
H57B	0.636126	0.159949	0.473987	0.049
C20	0.395(5)	0.504(4)	0.3853(4)	0.063(7)
C74	0.752(4)	0.246(3)	0.3587(3)	0.049(6)
H74	0.737666	0.231174	0.350139	0.058
C24	0.981(3)	0.567(3)	0.3956(3)	0.047(5)
F31	0.908(2)	0.155(3)	0.4051(3)	0.089(8)
C22	0.881(4)	0.657(4)	0.3883(4)	0.059(6)
C17	0.249(4)	0.194(4)	0.3945(4)	0.055(6)
F20	0.049(3)	0.046(2)	0.3949(3)	0.094(9)
C56	0.787(2)	0.326(3)	0.4771(3)	0.041(5)

H56A	0.843507	0.296977	0.475430	0.049
H56B	0.774939	0.324032	0.485569	0.049
C44	0.196(3)	0.283(4)	0.4639(3)	0.050(6)
H44	0.160200	0.251066	0.456566	0.060
C81	0.685(3)	0.129(3)	0.3810(3)	0.044(6)
H81	0.669538	0.100112	0.388767	0.053
F10	0.421(3)	−0.182(3)	0.4586(3)	0.103(10)
C21	0.854(5)	0.729(5)	0.3822(5)	0.083(8)
O1	1.287(3)	0.843(4)	0.4935(3)	0.094(9)
C19	0.341(4)	0.379(4)	0.3897(3)	0.047(5)
C65	0.546(4)	0.275(4)	0.4864(3)	0.051(6)
C37	0.740(4)	1.176(4)	0.3128(3)	0.052(6)
C40	0.703(3)	0.780(3)	0.4942(3)	0.043(6)
C43	0.288(4)	0.400(3)	0.4665(3)	0.045(5)
F40	0.479(3)	1.237(4)	0.2948(3)	0.127(12)
F32	0.883(3)	0.046(3)	0.4201(3)	0.094(8)
F5	1.080(3)	0.648(3)	0.4448(3)	0.101(9)
C36	0.711(4)	1.198(4)	0.3018(4)	0.055(6)
H36	0.766647	1.237532	0.295674	0.066
O7	1.275(3)	0.408(4)	0.3400(3)	0.091(8)
F16	0.279(3)	0.508(3)	0.4283(3)	0.092(8)
C12	0.234(4)	0.168(4)	0.4318(4)	0.055(6)
C51	0.972(3)	0.645(4)	0.4822(3)	0.058(6)
H51	0.929853	0.645701	0.489439	0.070
C52	0.940(3)	0.707(4)	0.4721(3)	0.053(7)
H52A	0.968137	0.792430	0.473988	0.063
H52B	0.978854	0.704226	0.464739	0.063
C80	0.633(3)	0.201(3)	0.3771(3)	0.039(5)
C76	0.800(4)	0.452(4)	0.3563(3)	0.052(6)
H76A	0.791608	0.447167	0.347800	0.062
H76B	0.862627	0.534897	0.358351	0.062
C62	0.767(4)	0.650(3)	0.4592(3)	0.046(6)
C6	0.869(5)	0.158(5)	0.4511(5)	0.074(7)
N14	0.544(3)	1.100(3)	0.3113(3)	0.053(5)
C64	0.445(4)	0.193(4)	0.4673(3)	0.052(8)
H64A	0.453328	0.202456	0.458858	0.079
H64B	0.387193	0.216845	0.470003	0.079
H64C	0.415609	0.108827	0.469360	0.079
C42	0.350(4)	0.503(4)	0.4580(4)	0.055(6)
C28	0.624(4)	−0.045(4)	0.4152(3)	0.060(7)
H28	0.625317	−0.117480	0.416647	0.072
C30	0.389(5)	−0.117(5)	0.4126(4)	0.075(8)
C2	0.836(4)	0.658(3)	0.4212(4)	0.068(7)
C4	0.956(3)	0.600(4)	0.4292(4)	0.069(7)
C9	0.553(4)	−0.023(4)	0.4471(4)	0.063(6)
C63	0.828(4)	0.778(4)	0.4552(3)	0.052(8)
H63A	0.838024	0.830726	0.461767	0.078
H63B	0.778611	0.786774	0.449223	0.078
H63C	0.907243	0.800472	0.451961	0.078
C73	0.792(4)	0.160(4)	0.3629(3)	0.049(6)
H73	0.759670	0.092219	0.357204	0.058
F37	0.010(3)	1.048(4)	0.3095(4)	0.134(11)
C29	0.525(3)	−0.033(4)	0.4133(4)	0.055(6)
C10	0.425(5)	−0.125(5)	0.4478(5)	0.076(7)
C75	0.843(4)	0.371(4)	0.3599(3)	0.053(6)
C3	0.954(4)	0.708(4)	0.4239(4)	0.070(8)

H3A	1.017303	0.788676	0.422821	0.084
C46	0.094(4)	0.098(4)	0.4775(4)	0.065(7)
C16	0.166(5)	0.073(4)	0.3966(4)	0.071(8)
C69	1.207(4)	0.442(5)	0.3562(4)	0.068(8)
H69	1.204967	0.474213	0.363573	0.082
F38	0.088(4)	0.947(4)	0.3046(4)	0.166(15)
C5	1.050(5)	0.597(5)	0.4339(5)	0.086(9)
C83	0.799(4)	0.022(4)	0.3786(3)	0.050(8)
H83A	0.886483	0.069813	0.379350	0.075
H83B	0.777386	−0.042006	0.372893	0.075
H83C	0.763117	−0.013327	0.386117	0.075
C68	1.098(4)	0.360(5)	0.3493(4)	0.069(7)
C25	1.060(4)	0.527(4)	0.3992(4)	0.062(7)
C15	0.328(5)	0.465(5)	0.4211(4)	0.066(7)
C8	0.659(4)	−0.011(4)	0.4517(4)	0.062(6)
H8	0.667222	−0.067033	0.456498	0.074
C35	0.592(4)	1.156(4)	0.3014(4)	0.063(6)
C85	0.548(4)	0.265(3)	0.3465(3)	0.049(6)
C41	0.679(4)	0.849(4)	0.4859(4)	0.060(7)
C71	0.980(4)	0.318(4)	0.3519(4)	0.061(6)
H71	0.935468	0.275670	0.344691	0.074
F25	0.743(3)	0.712(3)	0.3847(3)	0.114(9)
C47	1.157(4)	0.778(5)	0.4942(4)	0.085(9)
H47	1.111278	0.776014	0.500691	0.102
C66	0.496(4)	0.155(4)	0.5030(4)	0.067(10)
H66A	0.426948	0.073593	0.503938	0.100
H66B	0.473660	0.214257	0.505433	0.100
H66C	0.562854	0.163301	0.507873	0.100
F3	0.756(3)	0.779(3)	0.4253(3)	0.100(9)
N13	0.217(6)	1.010(6)	0.3278(4)	0.121(12)
C11	0.147(4)	0.036(4)	0.4369(4)	0.066(7)
C26	0.853(4)	0.119(4)	0.4149(4)	0.058(6)
C53	0.801(3)	0.634(3)	0.4710(3)	0.046(6)
H53	0.767178	0.670109	0.476484	0.055
C84	0.459(4)	0.266(3)	0.3650(3)	0.056(10)
H84A	0.396875	0.185029	0.362722	0.084
H84B	0.435884	0.324638	0.362335	0.084
H84C	0.467082	0.270680	0.373460	0.084
C1	0.775(5)	0.733(4)	0.4169(4)	0.072(8)
C72	0.920(4)	0.218(4)	0.3619(4)	0.060(7)
H72A	0.942838	0.155729	0.360528	0.072
H72B	0.956083	0.256824	0.369446	0.072
C38	0.842(4)	1.195(4)	0.3178(4)	0.062(7)
C34	0.524(3)	1.164(3)	0.2924(3)	0.091(8)
F42	0.584(3)	1.206(4)	0.2823(3)	0.141(14)
C49	1.204(4)	0.744(5)	0.4766(4)	0.081(9)
H49	1.198116	0.714055	0.468889	0.097
C18	0.233(4)	0.284(4)	0.3894(4)	0.056(6)
H18	0.160937	0.277873	0.386427	0.067
C86	0.510(4)	0.348(4)	0.3294(4)	0.066(10)
H86A	0.578806	0.373576	0.324201	0.099
H86B	0.472883	0.397870	0.328046	0.099
H86C	0.450488	0.263382	0.327906	0.099
F26	0.825(4)	0.694(3)	0.3711(3)	0.119(10)
F39	0.195(4)	1.129(4)	0.3079(4)	0.175(16)
C70	1.304(5)	0.463(5)	0.3509(5)	0.082(9)

H70	1.382691	0.509643	0.353894	0.098
C50	1.303(5)	0.818(5)	0.4823(4)	0.090(9)
H50	1.380903	0.851235	0.478911	0.108
C48	1.111(4)	0.718(5)	0.4839(4)	0.073(8)
C32	0.117(8)	1.018(8)	0.32383(18)	0.128(12)
C33	0.102(3)	1.030(4)	0.3126(5)	0.144(12)
C67	1.155(5)	0.354(5)	0.3401(5)	0.085(9)
H67	1.109965	0.310652	0.333423	0.102
C31	0.061(10)	1.000000	0.333333	0.134(14)
H31	−0.012856	1.000000	0.333333	0.161

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 3 Anisotropic displacement parameters [Å²] for 23. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ag10	0.0355(13)	0.043(2)	0.0366(15)	0.0133(14)	0.0067(7)	0.0217(10)
Ag4	0.0342(13)	0.0300(12)	0.0455(12)	0.0058(10)	0.0040(10)	0.0121(10)
Ag3	0.0344(13)	0.0267(11)	0.0520(13)	−0.0005(10)	−0.0036(10)	0.0124(10)
Ag7	0.0321(12)	0.0341(12)	0.0354(11)	0.0029(9)	−0.0053(10)	0.0043(10)
Ag1	0.0483(15)	0.0334(12)	0.0465(13)	0.0062(10)	0.0023(11)	0.0248(12)
Ag8	0.0324(12)	0.0324(12)	0.0401(17)	0.0037(8)	−0.0037(8)	−0.0005(15)
Ag2	0.0324(12)	0.0409(14)	0.0546(14)	0.0076(11)	0.0032(11)	0.0199(11)
Ag6	0.0371(13)	0.0373(13)	0.0521(13)	0.0064(11)	0.0039(11)	0.0203(11)
Ag5	0.0333(13)	0.0282(12)	0.0561(14)	0.0087(10)	0.0039(10)	0.0132(11)
Ag9	0.0462(17)	0.0581(19)	0.078(2)	0.0130(15)	−0.0063(14)	0.0283(15)
O2	0.020(8)	0.052(9)	0.052(9)	−0.005(8)	−0.006(7)	0.021(7)
O3	0.029(12)	0.052(14)	0.052(12)	−0.009(11)	−0.017(10)	0.003(11)
F53	0.048(12)	0.029(10)	0.101(15)	−0.002(10)	−0.040(11)	0.000(10)
N4	0.054(11)	0.063(12)	0.067(11)	0.018(10)	0.008(10)	0.052(10)
F48	0.079(14)	0.050(12)	0.049(10)	0.010(9)	−0.005(10)	0.041(11)
F23	0.094(16)	0.056(13)	0.074(13)	0.018(11)	0.027(12)	0.054(12)
O5	0.069(15)	0.043(12)	0.037(11)	0.005(10)	−0.005(10)	0.037(11)
F43	0.037(11)	0.075(14)	0.080(13)	0.036(12)	0.013(10)	0.035(11)
O4	0.041(12)	0.035(11)	0.043(11)	−0.005(9)	−0.003(9)	0.019(10)
O8	0.054(10)	0.047(10)	0.063(10)	0.008(9)	−0.003(8)	0.032(8)
N10	0.048(11)	0.034(10)	0.067(11)	−0.005(9)	0.004(10)	0.024(9)
N18	0.031(9)	0.043(10)	0.052(10)	−0.002(9)	−0.025(8)	0.019(8)
C39	0.029(9)	0.029(9)	0.050(14)	0.003(7)	−0.003(7)	0.016(11)
N3	0.053(11)	0.069(12)	0.066(11)	0.015(10)	0.002(10)	0.050(10)
O11	0.049(13)	0.047(13)	0.036(10)	−0.003(10)	−0.003(10)	0.020(11)
F14	0.050(13)	0.053(14)	0.113(17)	−0.005(13)	0.004(13)	0.015(11)
F21	0.072(15)	0.047(13)	0.102(16)	−0.016(12)	0.041(13)	0.006(12)
F47	0.079(16)	0.074(16)	0.083(15)	0.005(13)	−0.008(13)	0.036(13)
F22	0.081(16)	0.082(16)	0.101(16)	0.026(14)	0.003(13)	0.060(13)
F46	0.071(16)	0.052(13)	0.114(17)	0.043(13)	−0.016(14)	0.013(12)
O6	0.070(12)	0.043(11)	0.064(11)	0.001(10)	0.011(11)	0.028(10)
N17	0.037(10)	0.038(9)	0.045(10)	−0.004(8)	−0.019(8)	0.028(8)
F15	0.045(13)	0.075(15)	0.109(17)	−0.003(14)	0.006(12)	0.028(12)
N15	0.051(11)	0.057(11)	0.058(11)	0.027(9)	0.018(9)	0.044(9)
F4	0.045(13)	0.075(16)	0.098(16)	0.010(14)	0.023(12)	0.001(12)
O10	0.044(12)	0.047(13)	0.040(11)	−0.008(10)	0.003(9)	0.022(11)
F30	0.027(10)	0.068(15)	0.122(18)	0.008(14)	−0.008(11)	0.019(11)
F6	0.050(14)	0.085(18)	0.13(2)	0.015(16)	−0.007(14)	0.028(13)
F27	0.099(19)	0.053(14)	0.134(19)	0.027(15)	−0.035(16)	0.025(14)
F44	0.069(15)	0.064(14)	0.102(16)	0.005(13)	−0.017(13)	0.040(12)

N7	0.046(9)	0.038(9)	0.055(10)	−0.005(8)	−0.004(8)	0.026(8)
F35	0.078(16)	0.075(16)	0.091(16)	0.009(14)	0.011(14)	0.032(14)
F1	0.081(9)	0.060(9)	0.079(9)	0.005(7)	−0.001(7)	0.041(7)
F33	0.059(14)	0.050(13)	0.108(17)	0.004(12)	−0.004(13)	0.028(11)
N6	0.049(9)	0.050(10)	0.054(9)	−0.004(8)	0.000(8)	0.039(8)
N9	0.045(11)	0.041(10)	0.073(12)	0.006(10)	−0.001(10)	0.026(9)
O9	0.065(16)	0.063(16)	0.051(13)	−0.001(12)	−0.009(12)	0.019(13)
N1	0.053(12)	0.040(11)	0.062(12)	0.001(10)	0.017(10)	0.002(10)
F41	0.089(18)	0.11(2)	0.095(17)	0.059(16)	−0.033(15)	0.013(16)
C59	0.038(9)	0.041(9)	0.048(9)	−0.002(8)	0.002(8)	0.021(8)
N11	0.050(10)	0.044(10)	0.049(10)	0.010(9)	0.009(9)	0.036(9)
N5	0.038(10)	0.060(11)	0.052(10)	−0.006(9)	−0.003(9)	0.033(9)
C61	0.040(11)	0.032(10)	0.049(10)	−0.007(9)	0.001(9)	0.012(9)
O12	0.068(12)	0.038(10)	0.058(11)	0.007(9)	−0.003(10)	0.029(9)
C13	0.042(10)	0.061(10)	0.062(10)	−0.009(9)	0.010(9)	0.035(9)
F24	0.084(16)	0.053(13)	0.106(16)	0.005(12)	−0.011(13)	0.056(12)
F52	0.053(14)	0.065(15)	0.094(16)	−0.016(13)	0.006(13)	−0.006(12)
F36	0.054(14)	0.061(15)	0.106(17)	0.030(14)	−0.003(13)	−0.003(12)
C54	0.033(9)	0.039(9)	0.047(9)	−0.007(8)	0.001(8)	0.025(7)
F29	0.069(9)	0.078(9)	0.087(9)	0.006(7)	−0.004(7)	0.039(7)
C45	0.035(9)	0.041(10)	0.062(10)	0.007(9)	−0.025(9)	0.011(8)
F34	0.087(17)	0.048(14)	0.105(17)	0.010(13)	0.021(15)	0.007(13)
C14	0.058(6)	0.060(6)	0.060(6)	−0.001(4)	0.001(4)	0.032(4)
C55	0.029(8)	0.045(9)	0.053(9)	−0.005(8)	−0.003(8)	0.022(7)
F49	0.102(18)	0.048(13)	0.076(14)	−0.003(11)	−0.019(13)	0.028(13)
F12	0.110(19)	0.053(14)	0.125(19)	−0.006(14)	0.007(16)	0.048(14)
F50	0.088(17)	0.082(16)	0.093(16)	0.025(14)	−0.005(14)	0.048(14)
F18	0.082(18)	0.087(18)	0.15(2)	0.026(17)	−0.002(17)	0.042(15)
N16	0.039(12)	0.035(12)	0.046(12)	−0.018(10)	−0.007(10)	−0.002(10)
N8	0.044(6)	0.043(6)	0.047(6)	0.000(4)	−0.002(4)	0.024(4)
F13	0.078(17)	0.066(15)	0.109(18)	−0.011(15)	−0.006(15)	0.015(14)
N2	0.052(12)	0.023(10)	0.064(12)	0.007(9)	0.012(10)	0.009(9)
F11	0.100(19)	0.067(15)	0.114(18)	0.017(14)	0.018(16)	0.046(14)
C7	0.054(10)	0.076(12)	0.075(11)	0.016(10)	0.000(10)	0.055(9)
F7	0.092(18)	0.12(2)	0.118(19)	0.016(17)	−0.030(16)	0.056(16)
F2	0.108(19)	0.025(10)	0.114(17)	0.032(11)	0.008(15)	0.013(12)
N12	0.051(10)	0.042(10)	0.052(10)	0.012(9)	0.003(9)	0.036(9)
F19	0.086(17)	0.050(13)	0.080(15)	−0.007(12)	0.000(14)	−0.009(13)
C79	0.051(10)	0.029(9)	0.048(9)	0.001(8)	−0.003(8)	0.014(8)
C77	0.057(11)	0.022(10)	0.055(11)	−0.005(9)	0.000(10)	0.016(9)
F9	0.075(16)	0.12(2)	0.099(17)	−0.019(16)	−0.001(14)	0.057(15)
C60	0.035(10)	0.037(10)	0.047(10)	−0.004(9)	0.003(8)	0.019(8)
C27	0.056(10)	0.050(10)	0.063(10)	0.009(9)	0.004(9)	0.042(9)
F51	0.091(18)	0.073(16)	0.094(17)	0.011(14)	0.001(15)	0.033(14)
C23	0.049(11)	0.039(11)	0.076(12)	0.012(10)	0.003(10)	0.028(9)
C82	0.050(10)	0.038(10)	0.051(10)	0.001(9)	0.002(9)	0.029(9)
F45	0.069(16)	0.099(19)	0.102(17)	0.036(15)	0.035(14)	0.029(15)
F8	0.066(15)	0.12(2)	0.080(15)	0.006(15)	−0.010(13)	0.046(15)
C78	0.054(10)	0.026(8)	0.050(9)	0.002(8)	−0.002(8)	0.022(8)
C58	0.042(9)	0.038(9)	0.054(9)	−0.001(8)	0.005(8)	0.028(8)
F17	0.101(18)	0.105(18)	0.076(15)	0.008(14)	−0.004(14)	0.072(15)
F28	0.075(10)	0.093(10)	0.095(10)	−0.003(7)	−0.005(7)	0.048(7)
F54	0.063(15)	0.057(14)	0.121(18)	0.010(14)	−0.037(14)	0.009(12)
C57	0.036(10)	0.035(10)	0.055(11)	0.000(9)	0.009(9)	0.021(9)
C20	0.067(11)	0.057(11)	0.077(12)	0.003(10)	0.005(11)	0.039(10)
C74	0.048(9)	0.043(9)	0.048(9)	0.000(8)	−0.002(8)	0.017(8)

C24	0.044(10)	0.041(9)	0.073(11)	0.008(9)	0.000(9)	0.034(8)
F31	0.052(14)	0.12(2)	0.093(16)	−0.005(16)	0.001(12)	0.038(14)
C22	0.054(11)	0.045(10)	0.081(11)	0.020(9)	−0.003(10)	0.028(9)
C17	0.050(10)	0.049(10)	0.070(10)	−0.010(9)	0.003(9)	0.027(9)
F20	0.059(15)	0.044(13)	0.15(2)	−0.016(14)	0.006(15)	0.002(12)
C56	0.034(10)	0.039(10)	0.059(11)	0.004(9)	0.005(9)	0.024(8)
C44	0.041(10)	0.039(11)	0.059(11)	0.004(10)	−0.018(10)	0.012(9)
C81	0.052(11)	0.035(10)	0.049(11)	0.000(9)	0.004(10)	0.024(9)
F10	0.11(2)	0.083(18)	0.098(17)	0.034(15)	0.011(16)	0.033(16)
C21	0.076(13)	0.058(12)	0.103(13)	0.033(12)	−0.012(12)	0.025(11)
O1	0.053(12)	0.097(15)	0.079(12)	−0.006(13)	−0.010(11)	−0.002(12)
C19	0.051(9)	0.045(9)	0.064(9)	−0.002(8)	0.002(8)	0.040(7)
C65	0.056(11)	0.043(10)	0.059(11)	0.002(9)	0.004(10)	0.029(9)
C37	0.053(10)	0.058(11)	0.063(11)	0.022(9)	0.017(9)	0.041(9)
C40	0.043(10)	0.031(9)	0.048(11)	−0.007(8)	−0.013(8)	0.013(9)
C43	0.047(10)	0.040(9)	0.055(10)	0.000(8)	−0.016(9)	0.026(8)
F40	0.10(2)	0.12(2)	0.14(2)	0.043(19)	−0.046(18)	0.046(17)
F32	0.091(10)	0.095(10)	0.104(10)	0.005(7)	−0.007(7)	0.052(7)
F5	0.083(18)	0.088(19)	0.114(19)	0.000(16)	−0.002(16)	0.028(15)
C36	0.055(11)	0.060(12)	0.064(12)	0.032(10)	0.013(10)	0.039(10)
O7	0.053(12)	0.087(15)	0.102(14)	0.012(13)	0.010(12)	0.012(12)
F16	0.127(19)	0.098(17)	0.088(16)	−0.002(14)	0.017(15)	0.084(15)
C12	0.039(9)	0.066(10)	0.064(10)	−0.008(9)	0.004(9)	0.029(9)
C51	0.031(9)	0.065(10)	0.058(10)	−0.009(9)	−0.003(9)	0.010(9)
C52	0.033(10)	0.056(11)	0.052(10)	−0.009(10)	−0.003(10)	0.008(10)
C80	0.050(10)	0.028(9)	0.047(10)	−0.006(8)	−0.002(9)	0.025(8)
C76	0.053(11)	0.039(10)	0.057(11)	−0.002(10)	0.001(10)	0.018(10)
C62	0.043(10)	0.037(10)	0.048(10)	−0.001(9)	0.001(9)	0.012(9)
C6	0.060(12)	0.095(13)	0.085(12)	0.010(12)	−0.003(11)	0.052(11)
N14	0.050(11)	0.063(11)	0.067(11)	0.037(10)	0.008(9)	0.043(9)
C64	0.060(18)	0.045(17)	0.060(17)	0.012(14)	0.005(15)	0.033(14)
C42	0.063(12)	0.045(11)	0.068(12)	0.001(10)	−0.013(10)	0.035(10)
C28	0.061(12)	0.052(11)	0.061(11)	0.009(10)	0.001(11)	0.025(10)
C30	0.071(12)	0.054(12)	0.073(12)	0.010(11)	0.003(11)	0.011(11)
C2	0.060(11)	0.044(10)	0.071(11)	−0.001(10)	0.018(10)	0.004(10)
C4	0.060(11)	0.038(10)	0.076(12)	0.002(10)	0.012(10)	0.001(10)
C9	0.069(11)	0.062(11)	0.076(11)	0.019(10)	0.008(10)	0.046(10)
C63	0.039(16)	0.053(18)	0.058(17)	−0.002(15)	−0.007(14)	0.018(15)
C73	0.045(10)	0.049(10)	0.052(9)	−0.003(9)	0.004(9)	0.024(9)
F37	0.09(2)	0.17(3)	0.18(2)	0.02(2)	−0.008(19)	0.091(19)
C29	0.059(11)	0.046(10)	0.059(10)	0.009(9)	0.004(10)	0.025(9)
C10	0.083(13)	0.063(12)	0.093(13)	0.014(11)	0.015(12)	0.045(11)
C75	0.053(9)	0.046(9)	0.055(9)	0.002(8)	0.000(8)	0.021(8)
C3	0.059(12)	0.040(11)	0.074(12)	0.002(11)	0.010(11)	−0.004(11)
C46	0.042(11)	0.047(11)	0.080(12)	0.006(11)	−0.031(10)	0.002(10)
C16	0.061(12)	0.048(11)	0.082(12)	−0.018(11)	0.013(11)	0.011(11)
C69	0.043(12)	0.075(14)	0.086(14)	0.007(13)	0.001(12)	0.029(11)
F38	0.14(2)	0.20(3)	0.16(3)	0.03(2)	−0.01(2)	0.09(2)
C5	0.063(12)	0.063(12)	0.097(13)	0.004(12)	0.013(12)	0.004(12)
C83	0.054(10)	0.050(10)	0.054(10)	0.001(7)	−0.004(7)	0.031(7)
C68	0.049(11)	0.071(12)	0.082(12)	0.008(11)	0.003(10)	0.027(10)
C25	0.046(11)	0.059(11)	0.084(12)	0.003(10)	−0.008(10)	0.028(10)
C15	0.073(11)	0.073(11)	0.075(11)	0.008(10)	0.005(10)	0.054(10)
C8	0.062(12)	0.068(12)	0.073(12)	0.018(11)	0.009(11)	0.046(10)
C35	0.054(11)	0.070(11)	0.074(11)	0.038(10)	0.004(10)	0.038(9)
C85	0.063(11)	0.031(9)	0.049(10)	0.006(9)	−0.002(9)	0.020(9)

C41	0.063(12)	0.042(11)	0.062(12)	0.003(10)	−0.009(10)	0.016(10)
C71	0.053(10)	0.061(10)	0.068(10)	0.009(10)	0.000(9)	0.026(9)
F25	0.101(17)	0.090(16)	0.147(18)	0.064(15)	0.004(16)	0.046(14)
C47	0.041(12)	0.088(15)	0.076(13)	−0.009(13)	−0.006(11)	−0.005(12)
C66	0.08(2)	0.06(2)	0.067(19)	0.009(17)	0.020(17)	0.038(17)
F3	0.11(2)	0.081(17)	0.095(17)	0.009(15)	0.022(16)	0.041(16)
N13	0.120(13)	0.122(13)	0.123(13)	0.001(4)	0.000(4)	0.063(7)
C11	0.044(11)	0.069(12)	0.083(12)	−0.007(11)	0.004(11)	0.027(10)
C26	0.056(11)	0.065(11)	0.081(12)	0.013(10)	−0.003(10)	0.051(9)
C53	0.039(9)	0.043(9)	0.048(9)	−0.008(8)	−0.002(8)	0.014(8)
C84	0.048(18)	0.028(15)	0.060(18)	0.002(14)	−0.012(16)	−0.005(14)
C1	0.080(13)	0.042(11)	0.080(12)	0.003(11)	0.018(11)	0.020(11)
C72	0.052(11)	0.059(11)	0.062(11)	0.002(10)	0.002(10)	0.022(10)
C38	0.058(11)	0.067(12)	0.073(12)	0.024(11)	0.015(10)	0.040(10)
C34	0.070(13)	0.094(14)	0.094(13)	0.050(12)	−0.017(12)	0.030(11)
F42	0.10(2)	0.14(2)	0.109(19)	0.074(17)	−0.028(16)	−0.002(18)
C49	0.041(12)	0.091(15)	0.074(13)	−0.006(13)	−0.005(11)	0.005(12)
C18	0.050(11)	0.054(11)	0.071(11)	−0.005(10)	−0.006(10)	0.033(9)
C86	0.070(12)	0.064(11)	0.067(11)	0.002(7)	−0.005(7)	0.036(8)
F26	0.118(19)	0.087(16)	0.121(18)	0.038(15)	−0.027(16)	0.029(15)
F39	0.13(2)	0.20(3)	0.17(2)	0.07(2)	−0.04(2)	0.06(2)
C70	0.048(13)	0.084(15)	0.093(15)	0.009(13)	0.005(13)	0.017(13)
C50	0.048(13)	0.098(16)	0.078(13)	−0.005(14)	−0.004(12)	0.003(13)
C48	0.034(10)	0.083(13)	0.068(11)	−0.009(11)	−0.004(10)	0.004(10)
C32	0.118(15)	0.141(16)	0.138(15)	0.015(12)	−0.003(10)	0.074(11)
C33	0.121(16)	0.163(18)	0.152(17)	0.025(15)	−0.011(14)	0.074(15)
C67	0.053(13)	0.084(15)	0.095(14)	0.006(13)	0.005(12)	0.017(12)
C31	0.12(2)	0.14(2)	0.14(2)	0.014(17)	0.007(8)	0.072(10)

Table 4 Bond lengths and angles for 23.

Atom–Atom	Length [Å]
Ag10–Ag9#1	3.368(4)
Ag10–Ag9	3.367(4)
Ag10–N15#1	2.10(3)
Ag10–N15	2.10(3)
Ag4–N7	2.07(3)
Ag4–N12	2.09(3)
Ag3–N4	2.20(3)
Ag3–N5	2.10(3)
Ag7–Ag8	3.345(4)
Ag7–N17	2.11(3)
Ag7–N16	2.11(3)
Ag1–N6	2.06(3)
Ag1–N1	2.10(3)
Ag8–N18#2	2.09(3)
Ag8–N18	2.09(3)
Ag2–N3	2.11(4)
Ag2–N2	2.13(3)
Ag6–Ag5	3.357(4)
Ag6–N10	2.13(3)
Ag6–N11	2.06(3)
Ag5–N9	2.07(3)
Ag5–N8	2.10(3)
Ag9–N14	2.13(3)
Ag9–N13	2.09(6)

O2–C55	1.39(4)
O2–C51	1.39(5)
O3–H3	0.8402
O3–C55	1.44(4)
F53–C46	1.31(5)
N4–N3	1.25(5)
N4–C9	1.33(5)
F48–C41	1.36(5)
F23–C20	1.40(5)
O5–C65	1.16(5)
F43–C38	1.29(5)
O4–C60	1.19(4)
O8–C75	1.40(5)
O8–C71	1.36(5)
N10–N9	1.30(4)
N10–C24	1.41(5)
N18–N17	1.35(4)
N18–C45	1.35(4)
C39–H39	0.9500
C39–C40#2	1.37(5)
C39–C40	1.37(5)
N3–C7	1.38(4)
O11–C85	1.15(4)
F14–C11	1.27(5)
F21–C16	1.33(5)
F47–C41	1.40(6)
F22–C20	1.35(5)
F46–C41	1.33(5)
O6–C65	1.32(5)
O6–C66	1.46(5)
N17–C43	1.33(4)
F15–C11	1.36(5)
N15–C37	1.39(5)
N15–N14	1.34(4)
F4–C5	1.37(6)
O10–C80	1.24(4)
F30–C25	1.28(5)
F6–C5	1.32(7)
F27–C21	1.24(6)
F44–C38	1.39(6)
N7–N8	1.33(4)
N7–C17	1.36(5)
F35–C30	1.47(6)
F1–C1	1.26(6)
F33–C26	1.39(5)
N6–N5	1.41(5)
N6–C14	1.34(5)
N9–C22	1.37(5)
O9–H9	0.8398
O9–C75	1.45(4)
N1–N2	1.31(5)
N1–C2	1.32(5)
F41–C34	1.349(14)
C59–H59	1.0000
C59–C54	1.56(5)
C59–C60	1.50(5)

C59–C58	1.59(5)
N11–N12	1.37(4)
N11–C27	1.37(4)
N5–C12	1.34(5)
C61–H61	0.9500
C61–C60	1.49(5)
C61–C62	1.34(5)
O12–C85	1.36(4)
O12–C86	1.48(5)
C13–H13	0.9500
C13–C14	1.32(6)
C13–C12	1.34(6)
F24–C20	1.38(5)
F52–C46	1.36(6)
F36–C30	1.17(5)
C54–H54	1.0000
C54–C55	1.50(4)
C54–C53	1.62(5)
F29–C25	1.41(5)
C45–C44	1.37(5)
C45–C46	1.46(6)
F34–C30	1.31(6)
C14–C15	1.41(6)
C55–C56	1.55(5)
F49–C42	1.30(5)
F12–C10	1.33(6)
F50–C42	1.41(5)
F18–C15	1.31(6)
N16–N16#2	1.30(6)
N16–C40	1.35(5)
N8–C19	1.37(4)
F13–C11	1.28(5)
N2–C4	1.34(5)
F11–C10	1.22(6)
C7–C6	1.42(7)
C7–C8	1.33(6)
F7–C6	1.32(7)
F2–C1	1.33(5)
N12–C29	1.39(5)
F19–C16	1.34(6)
C79–H79	1.0000
C79–C78	1.61(5)
C79–C74	1.58(5)
C79–C80	1.51(5)
C77–H77A	0.9900
C77–H77B	0.9900
C77–C78	1.53(5)
C77–C76	1.59(6)
F9–C6	1.38(6)
C27–C28	1.43(6)
C27–C26	1.46(5)
F51–C42	1.32(5)
C23–H23	0.9500
C23–C24	1.40(5)
C23–C22	1.42(6)
C82–C81	1.31(5)

C82–C73	1.52(5)
C82–C83	1.47(5)
F45–C38	1.38(5)
F8–C6	1.35(5)
C78–C85	1.56(5)
C78–C84	1.50(6)
C58–C57	1.50(4)
C58–C65	1.56(5)
C58–C64	1.55(6)
F17–C15	1.33(5)
F28–C25	1.36(5)
F54–C46	1.39(5)
C57–H57A	0.9900
C57–H57B	0.9900
C57–C56	1.534(14)
C20–C19	1.48(6)
C74–H74	1.0000
C74–C73	1.52(6)
C74–C75	1.44(6)
C24–C25	1.41(5)
F31–C26	1.29(5)
C22–C21	1.34(6)
C17–C16	1.39(6)
C17–C18	1.40(6)
F20–C16	1.38(6)
C56–H56A	0.9900
C56–H56B	0.9900
C44–H44	0.9500
C44–C43	1.41(5)
C81–H81	0.9500
C81–C80	1.46(5)
F10–C10	1.44(6)
C21–F25	1.37(7)
C21–F26	1.35(7)
O1–C47	1.44(6)
O1–C50	1.37(6)
C19–C18	1.31(6)
C37–C36	1.39(5)
C37–C38	1.34(6)
C40–C41	1.43(6)
C43–C42	1.50(6)
F40–C34	1.345(14)
F32–C26	1.33(5)
F5–C5	1.38(6)
C36–H36	0.9500
C36–C35	1.35(6)
O7–C70	1.40(6)
O7–C67	1.34(6)
F16–C15	1.31(5)
C12–C11	1.61(7)
C51–H51	1.0000
C51–C52	1.57(6)
C51–C48	1.56(5)
C52–H52A	0.9900
C52–H52B	0.9900
C52–C53	1.55(5)

C76–H76A	0.9900
C76–H76B	0.9900
C76–C75	1.44(6)
C62–C63	1.50(5)
C62–C53	1.46(5)
N14–C35	1.31(5)
C64–H64A	0.9800
C64–H64B	0.9800
C64–H64C	0.9800
C28–H28	0.9500
C28–C29	1.37(6)
C30–C29	1.52(6)
C2–C3	1.34(6)
C2–C1	1.59(6)
C4–C3	1.53(6)
C4–C5	1.34(7)
C9–C10	1.51(7)
C9–C8	1.40(6)
C63–H63A	0.9800
C63–H63B	0.9800
C63–H63C	0.9800
C73–H73	1.0000
C73–C72	1.43(6)
F37–C33	1.350(14)
C3–H3A	0.9500
C69–H69	0.9500
C69–C68	1.49(7)
C69–C70	1.29(7)
F38–C33	1.349(14)
C83–H83A	0.9800
C83–H83B	0.9800
C83–H83C	0.9800
C68–C71	1.36(6)
C68–C67	1.32(7)
C8–H8	0.9500
C35–C34	1.39(5)
C71–H71	1.0000
C71–C72	1.61(6)
C47–H47	0.9500
C47–C48	1.37(6)
C66–H66A	0.9800
C66–H66B	0.9800
C66–H66C	0.9800
F3–C1	1.22(5)
N13–N13#1	1.29(10)
N13–C32	1.40(9)
C53–H53	1.0000
C84–H84A	0.9800
C84–H84B	0.9800
C84–H84C	0.9800
C72–H72A	0.9900
C72–H72B	0.9900
C34–F42	1.348(14)
C49–H49	0.9500
C49–C50	1.33(7)
C49–C48	1.36(7)

C18–H18	0.9500
C86–H86A	0.9800
C86–H86B	0.9800
C86–H86C	0.9800
F39–C33	1.348(14)
C70–H70	0.9500
C50–H50	0.9500
C32–C33	1.33(6)
C32–C31	1.27(7)
C67–H67	0.9500
C31–H31	0.9500

Atom–Atom–Atom	**Angle [°]**
Ag9–Ag10–Ag9#1	60.87(13)
N15#1–Ag10–Ag9	118.3(8)
N15–Ag10–Ag9#1	118.3(8)
N15#1–Ag10–Ag9#1	60.7(8)
N15–Ag10–Ag9	60.7(8)
N15–Ag10–N15#1	179.1(16)
N7–Ag4–N12	176.0(13)
N5–Ag3–N4	173.8(13)
N17–Ag7–Ag8	60.8(7)
N17–Ag7–N16	166.2(12)
N16–Ag7–Ag8	117.9(9)
N6–Ag1–N1	172.8(13)
Ag7#2–Ag8–Ag7	62.09(10)
N18–Ag8–Ag7#2	121.9(8)
N18#2–Ag8–Ag7	121.9(8)
N18–Ag8–Ag7	62.5(8)
N18#2–Ag8–Ag7#2	62.5(8)
N18#2–Ag8–N18	175.5(17)
N3–Ag2–N2	178.5(14)
N10–Ag6–Ag5	58.4(9)
N11–Ag6–Ag5	122.0(9)
N11–Ag6–N10	174.4(12)
N9–Ag5–Ag6	63.1(9)
N9–Ag5–N8	174.9(12)
N8–Ag5–Ag6	119.9(9)
N14–Ag9–Ag10	60.8(7)
N13–Ag9–Ag10	119.0(15)
N13–Ag9–N14	172(2)
C55–O2–C51	119(3)
C55–O3–H3	108.4
N3–N4–Ag3	120(2)
N3–N4–C9	112(3)
C9–N4–Ag3	128(3)
C71–O8–C75	118(3)
N9–N10–Ag6	123(3)
N9–N10–C24	113(3)
C24–N10–Ag6	124(2)
N17–N18–Ag8	117.0(19)
C45–N18–Ag8	135(3)
C45–N18–N17	108(3)
C40–C39–H39	127.2
C40#2–C39–H39	127.2

C40–C39–C40#2	106(5)
N4–N3–Ag2	120(2)
N4–N3–C7	107(4)
C7–N3–Ag2	133(3)
C65–O6–C66	114(3)
N18–N17–Ag7	119.7(19)
C43–N17–Ag7	132(3)
C43–N17–N18	109(3)
C37–N15–Ag10	133(2)
N14–N15–Ag10	119(2)
N14–N15–C37	108(3)
N8–N7–Ag4	120(2)
N8–N7–C17	107(3)
C17–N7–Ag4	132(3)
N5–N6–Ag1	118(2)
C14–N6–Ag1	134(3)
C14–N6–N5	108(3)
N10–N9–Ag5	116(3)
N10–N9–C22	108(3)
C22–N9–Ag5	135(3)
C75–O9–H9	108.2
N2–N1–Ag1	120(3)
N2–N1–C2	110(3)
C2–N1–Ag1	129(3)
C54–C59–H59	105.1
C54–C59–C58	113(3)
C60–C59–H59	105.1
C60–C59–C54	109(3)
C60–C59–C58	118(3)
C58–C59–H59	105.1
N12–N11–Ag6	118(2)
N12–N11–C27	108(3)
C27–N11–Ag6	133(3)
N6–N5–Ag3	120(2)
C12–N5–Ag3	131(3)
C12–N5–N6	107(3)
C60–C61–H61	120.1
C62–C61–H61	120.1
C62–C61–C60	120(3)
C85–O12–C86	116(3)
C14–C13–H13	124.0
C14–C13–C12	112(4)
C12–C13–H13	124.0
C59–C54–H54	106.5
C59–C54–C53	112(3)
C55–C54–C59	114(3)
C55–C54–H54	106.5
C55–C54–C53	111(3)
C53–C54–H54	106.5
N18–C45–C44	110(3)
N18–C45–C46	117(3)
C44–C45–C46	132(4)
N6–C14–C15	123(4)
C13–C14–N6	107(4)
C13–C14–C15	130(5)
O2–C55–O3	112(3)

O2–C55–C54	110(3)
O2–C55–C56	107(3)
O3–C55–C54	108(3)
O3–C55–C56	113(3)
C54–C55–C56	107(3)
N16#2–N16–Ag7	119.7(11)
N16#2–N16–C40	108(2)
C40–N16–Ag7	132(3)
N7–N8–Ag5	120(2)
N7–N8–C19	107(3)
C19–N8–Ag5	132(3)
N1–N2–Ag2	120(2)
N1–N2–C4	109(2)
C4–N2–Ag2	131(2)
N3–C7–C6	120(4)
C8–C7–N3	109(4)
C8–C7–C6	129(4)
N11–N12–Ag4	122(2)
N11–N12–C29	107(3)
C29–N12–Ag4	129(3)
C78–C79–H79	107.2
C74–C79–H79	107.2
C74–C79–C78	110(3)
C80–C79–H79	107.2
C80–C79–C78	115(3)
C80–C79–C74	109(3)
H77A–C77–H77B	108.0
C78–C77–H77A	109.4
C78–C77–H77B	109.4
C78–C77–C76	111(3)
C76–C77–H77A	109.4
C76–C77–H77B	109.4
O4–C60–C59	124(3)
O4–C60–C61	118(3)
C61–C60–C59	118(3)
N11–C27–C28	110(3)
N11–C27–C26	120(3)
C28–C27–C26	130(4)
C24–C23–H23	126.4
C24–C23–C22	107(4)
C22–C23–H23	126.4
C81–C82–C73	117(3)
C81–C82–C83	125(3)
C83–C82–C73	118(3)
C77–C78–C79	107(3)
C77–C78–C85	114(3)
C85–C78–C79	105(3)
C84–C78–C79	112(3)
C84–C78–C77	113(3)
C84–C78–C85	105(3)
C57–C58–C59	105(3)
C57–C58–C65	109(3)
C57–C58–C64	118(3)
C65–C58–C59	106(3)
C64–C58–C59	111(3)
C64–C58–C65	107(3)

C58–C57–H57A	108.3
C58–C57–H57B	108.3
C58–C57–C56	116(3)
H57A–C57–H57B	107.4
C56–C57–H57A	108.3
C56–C57–H57B	108.3
F23–C20–C19	116(4)
F22–C20–F23	100(3)
F22–C20–F24	104(4)
F22–C20–C19	111(4)
F24–C20–F23	102(4)
F24–C20–C19	122(4)
C79–C74–H74	106.1
C73–C74–C79	109(3)
C73–C74–H74	106.1
C75–C74–C79	116(3)
C75–C74–H74	106.1
C75–C74–C73	113(4)
C23–C24–N10	104(3)
C23–C24–C25	134(4)
C25–C24–N10	122(4)
N9–C22–C23	108(3)
C21–C22–N9	126(4)
C21–C22–C23	126(5)
N7–C17–C16	120(4)
N7–C17–C18	110(4)
C16–C17–C18	130(5)
C55–C56–H56A	109.3
C55–C56–H56B	109.3
C57–C56–C55	112(3)
C57–C56–H56A	109.3
C57–C56–H56B	109.3
H56A–C56–H56B	108.0
C45–C44–H44	128.0
C45–C44–C43	104(3)
C43–C44–H44	128.0
C82–C81–H81	117.1
C82–C81–C80	126(3)
C80–C81–H81	117.1
F27–C21–C22	122(5)
F27–C21–F25	106(5)
F27–C21–F26	107(4)
C22–C21–F25	113(5)
C22–C21–F26	113(5)
F26–C21–F25	93(4)
C50–O1–C47	100(4)
N8–C19–C20	113(4)
C18–C19–N8	113(4)
C18–C19–C20	134(4)
O5–C65–O6	126(4)
O5–C65–C58	125(4)
O6–C65–C58	108(3)
N15–C37–C36	105(4)
C38–C37–N15	121(4)
C38–C37–C36	134(4)
C39–C40–C41	131(4)

N16–C40–C39	108(3)
N16–C40–C41	120(3)
N17–C43–C44	109(3)
N17–C43–C42	124(4)
C44–C43–C42	126(3)
C37–C36–H36	125.9
C35–C36–C37	108(4)
C35–C36–H36	125.9
C67–O7–C70	101(4)
N5–C12–C13	107(4)
N5–C12–C11	121(4)
C13–C12–C11	132(4)
O2–C51–H51	110.0
O2–C51–C52	113(3)
O2–C51–C48	107(4)
C52–C51–H51	110.0
C48–C51–H51	110.0
C48–C51–C52	107(4)
C51–C52–H52A	110.6
C51–C52–H52B	110.6
H52A–C52–H52B	108.8
C53–C52–C51	105(3)
C53–C52–H52A	110.6
C53–C52–H52B	110.6
O10–C80–C79	125(3)
O10–C80–C81	120(3)
C81–C80–C79	114(3)
C77–C76–H76A	108.5
C77–C76–H76B	108.5
H76A–C76–H76B	107.5
C75–C76–C77	115(3)
C75–C76–H76A	108.5
C75–C76–H76B	108.5
C61–C62–C63	120(3)
C61–C62–C53	126(4)
C53–C62–C63	114(3)
F7–C6–C7	121(4)
F7–C6–F9	102(4)
F7–C6–F8	99(4)
F9–C6–C7	113(5)
F8–C6–C7	120(5)
F8–C6–F9	98(4)
N15–N14–Ag9	116(2)
C35–N14–Ag9	132(3)
C35–N14–N15	110(3)
C58–C64–H64A	109.5
C58–C64–H64B	109.5
C58–C64–H64C	109.5
H64A–C64–H64B	109.5
H64A–C64–H64C	109.5
H64B–C64–H64C	109.5
F49–C42–F50	109(3)
F49–C42–F51	107(4)
F49–C42–C43	113(3)
F50–C42–C43	106(4)
F51–C42–F50	107(4)

F51–C42–C43	114(3)
C27–C28–H28	128.0
C29–C28–C27	104(4)
C29–C28–H28	128.0
F35–C30–C29	102(4)
F36–C30–F35	106(4)
F36–C30–F34	114(6)
F36–C30–C29	116(4)
F34–C30–F35	101(4)
F34–C30–C29	114(4)
N1–C2–C3	113(3)
N1–C2–C1	123(4)
C3–C2–C1	123(4)
N2–C4–C3	107(3)
C5–C4–N2	125(4)
C5–C4–C3	128(4)
N4–C9–C10	123(4)
N4–C9–C8	107(4)
C8–C9–C10	131(4)
C62–C63–H63A	109.5
C62–C63–H63B	109.5
C62–C63–H63C	109.5
H63A–C63–H63B	109.5
H63A–C63–H63C	109.5
H63B–C63–H63C	109.5
C82–C73–C74	120(3)
C82–C73–H73	105.6
C74–C73–H73	105.6
C72–C73–C82	110(3)
C72–C73–C74	108(4)
C72–C73–H73	105.6
N12–C29–C30	113(4)
C28–C29–N12	111(3)
C28–C29–C30	136(4)
F12–C10–F10	100(4)
F12–C10–C9	108(4)
F11–C10–F12	120(5)
F11–C10–F10	109(4)
F11–C10–C9	115(4)
F10–C10–C9	103(4)
O8–C75–O9	109(3)
O8–C75–C74	114(4)
O8–C75–C76	107(3)
C74–C75–O9	105(3)
C76–C75–O9	110(3)
C76–C75–C74	113(4)
C2–C3–C4	100(3)
C2–C3–H3A	129.8
C4–C3–H3A	129.8
F53–C46–F52	110(4)
F53–C46–C45	116(4)
F53–C46–F54	106(4)
F52–C46–C45	109(4)
F52–C46–F54	102(4)
F54–C46–C45	113(3)
F21–C16–F19	99(4)

F21–C16–C17	116(4)
F21–C16–F20	106(4)
F19–C16–C17	116(4)
F19–C16–F20	105(4)
F20–C16–C17	113(5)
C68–C69–H69	124.5
C70–C69–H69	124.5
C70–C69–C68	111(5)
F4–C5–F5	99(4)
F6–C5–F4	104(5)
F6–C5–F5	103(5)
F6–C5–C4	116(5)
C4–C5–F4	119(5)
C4–C5–F5	114(5)
C82–C83–H83A	109.5
C82–C83–H83B	109.5
C82–C83–H83C	109.5
H83A–C83–H83B	109.5
H83A–C83–H83C	109.5
H83B–C83–H83C	109.5
C71–C68–C69	129(5)
C67–C68–C69	97(4)
C67–C68–C71	134(5)
F30–C25–F29	103(3)
F30–C25–F28	105(4)
F30–C25–C24	121(4)
F28–C25–F29	99(4)
F28–C25–C24	114(4)
C24–C25–F29	111(4)
F18–C15–C14	113(4)
F18–C15–F17	105(4)
F17–C15–C14	117(5)
F16–C15–C14	110(4)
F16–C15–F18	109(5)
F16–C15–F17	103(4)
C7–C8–C9	105(4)
C7–C8–H8	127.7
C9–C8–H8	127.7
C36–C35–C34	128(4)
N14–C35–C36	108(3)
N14–C35–C34	123(4)
O11–C85–O12	126(3)
O11–C85–C78	128(3)
O12–C85–C78	106(3)
F48–C41–F47	103(3)
F48–C41–C40	118(4)
F47–C41–C40	115(4)
F46–C41–F48	100(3)
F46–C41–F47	102(4)
F46–C41–C40	118(4)
O8–C71–C68	116(4)
O8–C71–H71	104.4
O8–C71–C72	108(4)
C68–C71–H71	104.4
C68–C71–C72	118(4)
C72–C71–H71	104.4

O1–C47–H47	125.3
C48–C47–O1	109(4)
C48–C47–H47	125.3
O6–C66–H66A	109.5
O6–C66–H66B	109.5
O6–C66–H66C	109.5
H66A–C66–H66B	109.5
H66A–C66–H66C	109.5
H66B–C66–H66C	109.5
N13#1–N13–Ag9	120.2(15)
N13#1–N13–C32	109(2)
C32–N13–Ag9	130(3)
F14–C11–F15	110(4)
F14–C11–F13	118(4)
F14–C11–C12	109(4)
F15–C11–C12	106(3)
F13–C11–F15	104(4)
F13–C11–C12	109(4)
F33–C26–C27	111(3)
F31–C26–F33	103(4)
F31–C26–C27	115(4)
F31–C26–F32	110(4)
F32–C26–F33	102(3)
F32–C26–C27	115(4)
C54–C53–H53	107.7
C52–C53–C54	111(3)
C52–C53–H53	107.7
C62–C53–C54	114(3)
C62–C53–C52	109(3)
C62–C53–H53	107.7
C78–C84–H84A	109.5
C78–C84–H84B	109.5
C78–C84–H84C	109.5
H84A–C84–H84B	109.5
H84A–C84–H84C	109.5
H84B–C84–H84C	109.5
F1–C1–F2	106(4)
F1–C1–C2	111(4)
F2–C1–C2	104(4)
F3–C1–F1	117(5)
F3–C1–F2	109(4)
F3–C1–C2	109(5)
C73–C72–C71	116(4)
C73–C72–H72A	108.3
C73–C72–H72B	108.3
C71–C72–H72A	108.3
C71–C72–H72B	108.3
H72A–C72–H72B	107.4
F43–C38–F44	103(4)
F43–C38–F45	103(3)
F43–C38–C37	123(4)
F45–C38–F44	97(4)
C37–C38–F44	111(4)
C37–C38–F45	115(4)
F41–C34–C35	115(3)
F40–C34–F41	104(4)

F40–C34–C35	113(3)
F40–C34–F42	105(4)
F42–C34–F41	103(3)
F42–C34–C35	115(3)
C50–C49–H49	127.2
C50–C49–C48	106(5)
C48–C49–H49	127.2
C17–C18–H18	128.4
C19–C18–C17	103(4)
C19–C18–H18	128.4
O12–C86–H86A	109.5
O12–C86–H86B	109.5
O12–C86–H86C	109.5
H86A–C86–H86B	109.5
H86A–C86–H86C	109.5
H86B–C86–H86C	109.5
O7–C70–H70	125.0
C69–C70–O7	110(5)
C69–C70–H70	125.0
O1–C50–H50	122.2
C49–C50–O1	116(5)
C49–C50–H50	122.2
C47–C48–C51	120(4)
C49–C48–C51	131(4)
C49–C48–C47	109(4)
C33–C32–N13	121(5)
C31–C32–N13	99(6)
C31–C32–C33	139(9)
F38–C33–F37	99(3)
F39–C33–F37	100(3)
F39–C33–F38	99(3)
C32–C33–F37	118(6)
C32–C33–F38	123(5)
C32–C33–F39	113(5)
O7–C67–H67	119.9
C68–C67–O7	120(5)
C68–C67–H67	119.9
C32–C31–C32#1	123(10)
C32–C31–H31	118.4
C32#1–C31–H31	118.4

Symmetry transformations used to generate equivalent atoms:

#1: 1+X-Y, 2-Y, 0.66667-Z; #2: +Y, +X, 1-Z;

Table 5 Torsion angles for 23.

Atom–Atom–Atom–Atom	Torsion Angle [°]
Ag10–N15–C37–C36	165(3)
Ag10–N15–C37–C38	−7(7)
Ag10–N15–N14–Ag9	24(4)
Ag10–N15–N14–C35	−169(3)
Ag4–N7–N8–Ag5	8(3)
Ag4–N7–N8–C19	177(2)
Ag4–N7–C17–C16	5(6)
Ag4–N7–C17–C18	−176(3)
Ag4–N12–C29–C28	168(3)
Ag4–N12–C29–C30	−11(5)
Ag3–N4–N3–Ag2	−2(4)
Ag3–N4–N3–C7	175(3)
Ag3–N4–C9–C10	8(7)
Ag3–N4–C9–C8	−170(3)
Ag3–N5–C12–C13	169(3)
Ag3–N5–C12–C11	−11(6)
Ag7–N17–C43–C44	175(3)
Ag7–N17–C43–C42	1(6)
Ag7–N16–C40–C39	−165(2)
Ag7–N16–C40–C41	5(6)
Ag1–N6–N5–Ag3	5(3)
Ag1–N6–N5–C12	173(2)
Ag1–N6–C14–C13	−173(3)
Ag1–N6–C14–C15	7(7)
Ag1–N1–N2–Ag2	2(4)
Ag1–N1–N2–C4	−171(3)
Ag1–N1–C2–C3	170(3)
Ag1–N1–C2–C1	1(6)
Ag8–N18–N17–Ag7	−3(3)
Ag8–N18–N17–C43	179(2)
Ag8–N18–C45–C44	−173(3)
Ag8–N18–C45–C46	−1(6)
Ag2–N3–C7–C6	5(7)
Ag2–N3–C7–C8	171(3)
Ag2–N2–C4–C3	−174(3)
Ag2–N2–C4–C5	4(8)
Ag6–N10–N9–Ag5	−1(4)
Ag6–N10–N9–C22	−174(3)
Ag6–N10–C24–C23	174(3)
Ag6–N10–C24–C25	−6(6)
Ag6–N11–N12–Ag4	−2(3)
Ag6–N11–N12–C29	167(2)
Ag6–N11–C27–C28	−163(3)
Ag6–N11–C27–C26	11(6)
Ag5–N9–C22–C23	−171(3)
Ag5–N9–C22–C21	3(8)
Ag5–N8–C19–C20	−10(5)
Ag5–N8–C19–C18	167(3)
Ag9–N14–C35–C36	165(3)
Ag9–N14–C35–C34	−16(8)
Ag9–N13–C32–C33	11(13)
Ag9–N13–C32–C31	−174(4)
O2–C55–C56–C57	173(3)
O2–C51–C52–C53	65(4)

O2–C51–C48–C47	−123(6)
O2–C51–C48–C49	61(8)
O3–C55–C56–C57	−64(4)
N4–N3–C7–C6	−171(4)
N4–N3–C7–C8	−5(5)
N4–C9–C10–F12	106(5)
N4–C9–C10–F11	−31(8)
N4–C9–C10–F10	−149(4)
N4–C9–C8–C7	−6(5)
F23–C20–C19–N8	74(5)
F23–C20–C19–C18	−101(6)
O8–C71–C72–C73	57(5)
N10–N9–C22–C23	0(5)
N10–N9–C22–C21	175(5)
N10–C24–C25–F30	−38(7)
N10–C24–C25–F29	−160(4)
N10–C24–C25–F28	89(5)
N18–N17–C43–C44	−7(4)
N18–N17–C43–C42	180(3)
N18–C45–C44–C43	−2(5)
N18–C45–C46–F53	179(4)
N18–C45–C46–F52	54(5)
N18–C45–C46–F54	−59(6)
C39–C40–C41–F48	121(4)
C39–C40–C41–F47	−118(4)
C39–C40–C41–F46	2(7)
N3–N4–C9–C10	−180(100)
N3–N4–C9–C8	3(5)
N3–C7–C6–F7	−3(8)
N3–C7–C6–F9	−124(5)
N3–C7–C6–F8	121(5)
N3–C7–C8–C9	7(5)
F22–C20–C19–N8	−173(3)
F22–C20–C19–C18	12(7)
N17–N18–C45–C44	−2(4)
N17–N18–C45–C46	171(4)
N17–C43–C42–F49	−8(6)
N17–C43–C42–F50	−128(4)
N17–C43–C42–F51	115(4)
N15–C37–C36–C35	6(5)
N15–C37–C38–F43	32(7)
N15–C37–C38–F44	−91(5)
N15–C37–C38–F45	160(4)
N15–N14–C35–C36	0(6)
N15–N14–C35–C34	180(4)
N7–N8–C19–C20	−177(3)
N7–N8–C19–C18	−1(5)
N7–C17–C16–F21	−69(6)
N7–C17–C16–F19	47(6)
N7–C17–C16–F20	168(4)
N7–C17–C18–C19	1(5)
F35–C30–C29–N12	175(3)
F35–C30–C29–C28	−3(7)
N6–N5–C12–C13	3(4)
N6–N5–C12–C11	−177(3)
N6–C14–C15–F18	−7(7)

N6–C14–C15–F17	114(5)
N6–C14–C15–F16	−129(5)
N9–N10–C24–C23	1(4)
N9–C22–C21–F27	146(6)
N9–C22–C21–F25	19(9)
N9–C22–C21–F26	−85(7)
N1–N2–C4–C3	−2(5)
N1–N2–C4–C5	176(5)
N1–C2–C3–C4	1(5)
N1–C2–C1–F1	−41(6)
N1–C2–C1–F2	−154(4)
N1–C2–C1–F3	89(6)
C59–C54–C55–O2	−171(3)
C59–C54–C55–O3	67(4)
C59–C54–C55–C56	−55(4)
C59–C54–C53–C52	−155(3)
C59–C54–C53–C62	−32(4)
C59–C58–C57–C56	55(4)
C59–C58–C65–O5	31(5)
C59–C58–C65–O6	−161(3)
N11–N12–C29–C28	0(5)
N11–C27–C28–C29	−2(5)
N11–C27–C26–F33	49(5)
N11–C27–C26–F31	−66(5)
N11–C27–C26–F32	164(4)
N5–N6–C14–C13	3(4)
N5–N6–C14–C15	−177(4)
N5–C12–C11–F14	−153(4)
N5–C12–C11–F15	−34(6)
N5–C12–C11–F13	78(5)
C61–C62–C53–C54	7(6)
C61–C62–C53–C52	131(4)
C13–C14–C15–F18	173(5)
C13–C14–C15–F17	−66(7)
C13–C14–C15–F16	51(7)
C13–C12–C11–F14	27(7)
C13–C12–C11–F15	146(5)
C13–C12–C11–F13	−102(6)
F24–C20–C19–N8	−50(5)
F24–C20–C19–C18	134(5)
F36–C30–C29–N12	59(6)
F36–C30–C29–C28	−119(6)
C54–C59–C60–O4	133(3)
C54–C59–C60–C61	−47(4)
C54–C59–C58–C57	−52(4)
C54–C59–C58–C65	63(4)
C54–C59–C58–C64	179(3)
C54–C55–C56–C57	55(4)
C45–N18–N17–Ag7	−176(2)
C45–N18–N17–C43	5(4)
C45–C44–C43–N17	6(5)
C45–C44–C43–C42	179(4)
F34–C30–C29–N12	−77(5)
F34–C30–C29–C28	105(7)
C14–N6–N5–Ag3	−171(2)
C14–N6–N5–C12	−4(4)

C14–C13–C12–N5	−2(5)
C14–C13–C12–C11	178(4)
C55–O2–C51–C52	−35(4)
C55–O2–C51–C48	−152(3)
C55–C54–C53–C52	−27(4)
C55–C54–C53–C62	96(4)
N16#1–N16–C40–C39	13(5)
N16#1–N16–C40–C41	−177(4)
N16–C40–C41–F48	−46(6)
N16–C40–C41–F47	75(5)
N16–C40–C41–F46	−165(4)
N8–N7–C17–C18	−2(4)
N8–C19–C18–C17	0(5)
N2–N1–C2–C3	−3(5)
N2–N1–C2–C1	−172(4)
N2–C4–C3–C2	0(5)
N2–C4–C5–F4	142(5)
N2–C4–C5–F6	17(8)
N2–C4–C5–F5	−102(6)
N12–N11–C27–C28	2(4)
N12–N11–C27–C26	176(4)
C79–C78–C85–O11	28(6)
C79–C78–C85–O12	−158(3)
C79–C74–C73–C82	−29(5)
C79–C74–C73–C72	−157(3)
C79–C74–C75–O8	−172(3)
C79–C74–C75–O9	69(4)
C79–C74–C75–C76	−51(5)
C77–C78–C85–O11	145(4)
C77–C78–C85–O12	−41(4)
C77–C76–C75–O8	177(3)
C77–C76–C75–O9	−66(4)
C77–C76–C75–C74	51(5)
C60–C59–C54–C55	−77(4)
C60–C59–C54–C53	50(4)
C60–C59–C58–C57	77(4)
C60–C59–C58–C65	−168(3)
C60–C59–C58–C64	−52(4)
C60–C61–C62–C63	178(3)
C60–C61–C62–C53	0(6)
C27–N11–N12–Ag4	−170(2)
C27–N11–N12–C29	−1(4)
C27–C28–C29–N12	1(5)
C27–C28–C29–C30	179(100)
C23–C24–C25–F30	142(5)
C23–C24–C25–F29	21(7)
C23–C24–C25–F28	−91(6)
C23–C22–C21–F27	−40(10)
C23–C22–C21–F25	−167(5)
C23–C22–C21–F26	89(7)
C82–C81–C80–O10	−161(4)
C82–C81–C80–C79	19(6)
C82–C73–C72–C71	−162(4)
C78–C79–C74–C73	−179(3)
C78–C79–C74–C75	52(4)
C78–C79–C80–O10	5(5)

C78–C79–C80–C81	−175(3)
C78–C77–C76–C75	−56(5)
C58–C59–C54–C55	57(4)
C58–C59–C54–C53	−176(3)
C58–C59–C60–O4	2(5)
C58–C59–C60–C61	−178(3)
C58–C57–C56–C55	−60(4)
C57–C58–C65–O5	144(4)
C57–C58–C65–O6	−49(4)
C20–C19–C18–C17	175(4)
C74–C79–C78–C77	−53(4)
C74–C79–C78–C85	69(4)
C74–C79–C78–C84	−177(3)
C74–C79–C80–O10	130(4)
C74–C79–C80–C81	−50(4)
C74–C73–C72–C71	−28(5)
C24–N10–N9–Ag5	173(3)
C24–N10–N9–C22	0(5)
C24–C23–C22–N9	1(5)
C24–C23–C22–C21	−174(5)
C22–C23–C24–N10	−1(5)
C17–N7–N8–Ag5	−168(2)
C17–N7–N8–C19	2(4)
C44–C45–C46–F53	−11(8)
C44–C45–C46–F52	−136(5)
C44–C45–C46–F54	112(5)
C44–C43–C42–F49	180(4)
C44–C43–C42–F50	60(5)
C44–C43–C42–F51	−58(6)
C81–C82–C73–C74	−1(6)
C81–C82–C73–C72	126(4)
O1–C47–C48–C51	−177(5)
O1–C47–C48–C49	−1(8)
C65–C58–C57–C56	−58(4)
C37–N15–N14–Ag9	−163(3)
C37–N15–N14–C35	4(5)
C37–C36–C35–N14	−4(6)
C37–C36–C35–C34	176(5)
C40#1–C39–C40–N16	−4.8(18)
C40#1–C39–C40–C41	−173(5)
C36–C37–C38–F43	−138(5)
C36–C37–C38–F44	99(6)
C36–C37–C38–F45	−10(8)
C36–C35–C34–F41	130(5)
C36–C35–C34–F40	−111(6)
C36–C35–C34–F42	10(7)
C12–C13–C14–N6	0(5)
C12–C13–C14–C15	180(100)
C51–O2–C55–O3	91(4)
C51–O2–C55–C54	−30(4)
C51–O2–C55–C56	−146(3)
C51–C52–C53–C54	−30(4)
C51–C52–C53–C62	−156(3)
C52–C51–C48–C47	116(6)
C52–C51–C48–C49	−60(8)
C80–C79–C78–C77	71(4)

C80–C79–C78–C85	−167(3)
C80–C79–C78–C84	−53(4)
C80–C79–C74–C73	54(4)
C80–C79–C74–C75	−75(4)
C76–C77–C78–C79	55(4)
C76–C77–C78–C85	−62(4)
C76–C77–C78–C84	179(3)
C62–C61–C60–O4	−157(4)
C62–C61–C60–C59	22(5)
C6–C7–C8–C9	171(5)
N14–N15–C37–C36	−6(4)
N14–N15–C37–C38	−179(4)
N14–C35–C34–F41	−50(7)
N14–C35–C34–F40	69(6)
N14–C35–C34–F42	−170(5)
C64–C58–C57–C56	180(100)
C64–C58–C65–O5	−87(5)
C64–C58–C65–O6	80(4)
C28–C27–C26–F33	−138(4)
C28–C27–C26–F31	107(5)
C28–C27–C26–F32	−23(7)
C2–N1–N2–Ag2	176(3)
C2–N1–N2–C4	3(5)
C9–N4–N3–Ag2	−175(3)
C9–N4–N3–C7	1(5)
C63–C62–C53–C54	−172(3)
C63–C62–C53–C52	−48(5)
C73–C82–C81–C80	8(6)
C73–C74–C75–O8	61(4)
C73–C74–C75–O9	−58(4)
C73–C74–C75–C76	−177(3)
C10–C9–C8–C7	177(5)
C75–O8–C71–C68	−159(4)
C75–O8–C71–C72	−25(5)
C75–C74–C73–C82	101(4)
C75–C74–C73–C72	−27(5)
C3–C2–C1–F1	150(5)
C3–C2–C1–F2	37(6)
C3–C2–C1–F3	−79(6)
C3–C4–C5–F4	−40(9)
C3–C4–C5–F6	−166(5)
C3–C4–C5–F5	76(7)
C46–C45–C44–C43	−173(5)
C16–C17–C18–C19	180(100)
C69–C68–C71–O8	58(7)
C69–C68–C71–C72	−72(7)
C69–C68–C67–O7	4(7)
C5–C4–C3–C2	−178(6)
C83–C82–C81–C80	−176(4)
C83–C82–C73–C74	−177(4)
C83–C82–C73–C72	−50(5)
C68–C69–C70–O7	4(7)
C68–C71–C72–C73	−169(5)
C8–C7–C6–F7	−166(5)
C8–C7–C6–F9	73(7)
C8–C7–C6–F8	−42(8)

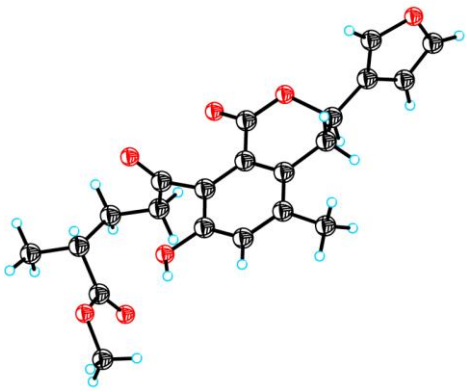
C8–C9–C10–F12	−77(7)
C8–C9–C10–F11	146(5)
C8–C9–C10–F10	28(7)
C71–O8–C75–O9	87(4)
C71–O8–C75–C74	−30(5)
C71–O8–C75–C76	−155(4)
C71–C68–C67–O7	178(6)
C47–O1–C50–C49	−3(7)
C66–O6–C65–O5	−5(7)
C66–O6–C65–C58	−172(3)
N13#2–N13–C32–C33	−175(8)
N13#2–N13–C32–C31	0(11)
N13–C32–C33–F37	−174(6)
N13–C32–C33–F38	62(10)
N13–C32–C33–F39	−58(9)
N13–C32–C31–C32#2	0(4)
C26–C27–C28–C29	−175(4)
C53–C54–C55–O2	62(4)
C53–C54–C55–O3	−61(4)
C53–C54–C55–C56	177(3)
C84–C78–C85–O11	−91(5)
C84–C78–C85–O12	83(4)
C1–C2–C3–C4	171(4)
C38–C37–C36–C35	178(5)
C18–C17–C16–F21	112(6)
C18–C17–C16–F19	−132(5)
C18–C17–C16–F20	−10(7)
C86–O12–C85–O11	2(6)
C86–O12–C85–C78	−172(3)
C70–O7–C67–C68	−2(7)
C70–C69–C68–C71	−179(5)
C70–C69–C68–C67	−4(6)
C50–O1–C47–C48	2(7)
C50–C49–C48–C51	175(6)
C50–C49–C48–C47	−1(8)
C48–C51–C52–C53	−178(3)
C48–C49–C50–O1	2(8)
C33–C32–C31–C32#2	174(13)
C67–O7–C70–C69	−1(6)
C67–C68–C71–O8	−115(7)
C67–C68–C71–C72	115(7)
C31–C32–C33–F37	13(13)
C31–C32–C33–F38	−111(11)
C31–C32–C33–F39	129(10)

Symmetry transformations used to generate equivalent atoms:

#1: +Y, +X, 1-Z; #2: 1+X-Y, 2-Y, 0.66667-Z;

Table 6 Hydrogen bonds for 23.

D–H···A [Å]	d(D–H) [Å]	d(H···A) [Å]	d(D···A) [Å]	<(DHA) [°]
O3–H3···O4	0.84	2.50	3.33(3)	166.2
O9–H9···O10	0.84	2.51	3.34(4)	171.7



21

Table 1 Crystal data and structure refinement for compound 21.

CCDC number	2447368
Empirical formula	$C_{38}H_{33}Ag_3F_{18}N_6O_9$
Formula weight	1383.31
Temperature/K	99.9(5)
Crystal system	orthorhombic
Space group	Pbca
a/Å	15.97820(10)
b/Å	26.0341(2)
c/Å	23.1666(2)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	9636.80(13)
Z	8
ρ_{calc}g/cm^3	1.907
μ/mm^{-1}	10.856
F(000)	5424.0
Crystal size/mm^3	0.25 × 0.15 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	6.79 to 148.142
Index ranges	-18 ≤ h ≤ 19, -31 ≤ k ≤ 32, -28 ≤ l ≤ 22
Reflections collected	33075
Independent reflections	9537 [R_{int} = 0.0630, R_{sigma} = 0.0449]
Data/restraints/parameters	9537/1695/1109
Goodness-of-fit on F^2	1.203
Final R indexes [I>=2σ (I)]	R_1 = 0.1010, wR_2 = 0.2098
Final R indexes [all data]	R_1 = 0.1105, wR_2 = 0.2126
Largest diff. peak/hole / e Å^{-3}	1.94/-2.22

Table 2 Atomic coordinates and U_{eq} [Å^2] for 21.

Atom	*x*	*y*	*z*	U_{eq}
O1	0.3913(4)	0.3543(3)	0.2799(3)	0.0250(15)
O2	0.6543(5)	0.4030(3)	0.1846(3)	0.0328(17)
O3	0.5455(5)	0.4225(3)	0.1273(4)	0.041(2)
O4	0.4652(6)	0.3160(3)	0.1576(3)	0.0351(18)
H4	0.466954	0.309645	0.122112	0.053

O5	0.4417(6)	0.2748(3)	0.3677(3)	0.040(2)
O6	0.4327(5)	0.1916(3)	0.3748(3)	0.0348(17)
C16	0.4539(6)	0.3292(3)	0.2715(4)	0.0199(19)
C17	0.5408(6)	0.3507(4)	0.2808(5)	0.026(2)
H17A	0.563075	0.336806	0.317539	0.031
H17B	0.577456	0.338311	0.249338	0.031
C18	0.5457(7)	0.4083(4)	0.2829(5)	0.029(2)
H18A	0.602855	0.418244	0.295077	0.035
H18B	0.506406	0.420815	0.312884	0.035
C19	0.5258(7)	0.4354(4)	0.2268(5)	0.031(2)
H19	0.466478	0.427889	0.215868	0.037
C20	0.5374(9)	0.4946(4)	0.2322(7)	0.053(4)
H20A	0.504776	0.507320	0.265052	0.079
H20B	0.517943	0.511293	0.196718	0.079
H20C	0.596725	0.502483	0.238209	0.079
C21	0.5822(7)	0.4184(4)	0.1789(5)	0.032(2)
C22	0.5931(9)	0.4063(5)	0.0774(5)	0.045(3)
H22A	0.558878	0.410381	0.042601	0.067
H22B	0.609075	0.370206	0.081780	0.067
H22C	0.643588	0.427499	0.074041	0.067
C23	0.4498(6)	0.2754(3)	0.2470(4)	0.022(2)
C24	0.4564(7)	0.2713(4)	0.1875(4)	0.027(2)
C25	0.4552(7)	0.2232(4)	0.1611(4)	0.028(2)
H25	0.459078	0.221120	0.120297	0.033
C26	0.4485(7)	0.1788(4)	0.1929(5)	0.029(2)
C27	0.4530(9)	0.1270(4)	0.1623(6)	0.044(3)
H27A	0.399205	0.109264	0.166161	0.066
H27B	0.497223	0.106060	0.179901	0.066
H27C	0.465576	0.132306	0.121372	0.066
C28	0.4416(6)	0.1820(4)	0.2524(5)	0.026(2)
C29	0.4423(6)	0.2303(4)	0.2798(4)	0.0208(19)
C30	0.4383(6)	0.2343(4)	0.3433(4)	0.023(2)
C31	0.4344(8)	0.1353(4)	0.2903(5)	0.037(2)
H31A	0.401884	0.108584	0.269792	0.044
H31B	0.491111	0.121360	0.297668	0.044
H31C	0.374595	0.125896	0.293661	0.044
H31D	0.463587	0.106349	0.271224	0.044
Ag1	0.26007(5)	0.35266(3)	0.21462(4)	0.0229(2)
Ag2	0.32135(6)	0.44868(3)	0.30696(4)	0.0261(2)
Ag3	0.26925(6)	0.33322(3)	0.36392(4)	0.0250(2)
F1	0.2229(8)	0.3722(4)	0.0892(4)	0.072(3)
F2	0.2458(9)	0.4354(5)	0.0340(5)	0.081(3)
F3	0.1324(8)	0.4274(6)	0.0785(6)	0.081(3)
F4	0.2605(10)	0.5998(5)	0.1988(7)	0.101(4)
F5	0.3726(7)	0.5703(5)	0.2353(7)	0.087(3)
F6	0.2557(10)	0.5664(5)	0.2688(6)	0.098(3)
F7	0.4866(7)	0.5081(4)	0.3929(5)	0.063(3)
F8	0.3691(8)	0.5461(4)	0.3930(6)	0.073(3)
F9	0.4395(8)	0.5396(4)	0.4715(5)	0.071(3)
F10	0.2066(8)	0.3712(5)	0.5321(6)	0.084(3)
F11	0.2746(8)	0.3133(4)	0.4946(5)	0.072(3)
F12	0.3220(9)	0.3546(6)	0.5657(5)	0.083(4)
F13	0.1301(6)	0.2430(3)	0.4112(4)	0.0426(19)
F14	0.2523(6)	0.2094(4)	0.4091(4)	0.048(2)
F15	0.1456(6)	0.1651(3)	0.3829(4)	0.047(2)
F16	0.2585(7)	0.2332(5)	0.1357(5)	0.094(3)

F17	0.1435(7)	0.2658(4)	0.1385(5)	0.087(3)
F18	0.1557(9)	0.1884(4)	0.1446(6)	0.097(4)
N1	0.2717(7)	0.4291(4)	0.1820(5)	0.029(2)
N2	0.2920(7)	0.4667(4)	0.2206(5)	0.0306(19)
N3	0.3455(7)	0.4352(4)	0.3960(5)	0.031(2)
N4	0.3126(7)	0.3924(4)	0.4200(4)	0.0291(19)
N5	0.2246(7)	0.2745(4)	0.3082(5)	0.0224(18)
N6	0.2266(7)	0.2801(4)	0.2497(5)	0.0257(18)
C1	0.2184(13)	0.4206(8)	0.0841(8)	0.058(3)
C2	0.2481(10)	0.4518(6)	0.1336(6)	0.040(2)
C3	0.2551(11)	0.5046(6)	0.1380(7)	0.047(3)
H3	0.242960	0.529770	0.109517	0.056
C4	0.2829(10)	0.5120(5)	0.1917(8)	0.044(2)
C5	0.3013(12)	0.5613(6)	0.2209(9)	0.052(3)
C6	0.4173(12)	0.5141(7)	0.4251(8)	0.054(3)
C7	0.3760(10)	0.4652(6)	0.4378(7)	0.043(2)
C8	0.3604(10)	0.4428(6)	0.4908(7)	0.045(3)
H8	0.373696	0.455849	0.528015	0.054
C9	0.3214(10)	0.3978(6)	0.4773(6)	0.042(2)
C10	0.2863(12)	0.3592(7)	0.5163(8)	0.053(3)
C11	0.1801(9)	0.2113(5)	0.3800(6)	0.035(2)
C12	0.1900(8)	0.2282(5)	0.3207(5)	0.025(2)
C13	0.1697(9)	0.2028(5)	0.2711(6)	0.029(2)
H13	0.144307	0.170052	0.267175	0.034
C14	0.1961(9)	0.2376(5)	0.2260(6)	0.033(2)
C15	0.1895(8)	0.2304(5)	0.1664(6)	0.042(2)
O7	0.4516(12)	0.0401(8)	0.4459(10)	0.049(3)
C32	0.3950(15)	0.1461(7)	0.3442(9)	0.036(3)
H32	0.334221	0.152977	0.337220	0.043
C33	0.4031(12)	0.1026(8)	0.3863(11)	0.042(3)
C34	0.3392(16)	0.0733(9)	0.4022(12)	0.044(3)
H34	0.283857	0.078950	0.388639	0.053
C35	0.3582(18)	0.0355(11)	0.4388(15)	0.047(3)
H35	0.321522	0.011309	0.456220	0.056
C36	0.4727(14)	0.0845(9)	0.4120(12)	0.047(3)
H36	0.527193	0.098716	0.408295	0.057
O7A	0.3841(12)	0.0388(8)	0.4453(11)	0.049(3)
C32A	0.4696(15)	0.1416(8)	0.3497(9)	0.037(3)
H32A	0.531771	0.145208	0.346931	0.044
C33A	0.4493(12)	0.1008(9)	0.3933(11)	0.043(3)
C34A	0.5070(15)	0.0720(9)	0.4188(11)	0.046(3)
H34A	0.565185	0.076480	0.411926	0.055
C35A	0.4774(18)	0.0363(12)	0.4549(14)	0.048(3)
H35A	0.507723	0.014643	0.480365	0.058
C36A	0.3734(13)	0.0825(10)	0.4085(12)	0.047(3)
H36A	0.321128	0.096318	0.396613	0.056
O8	0.4716(7)	0.3030(4)	0.0458(4)	0.053(2)
H8B	0.481769	0.274209	0.030938	0.079
C37	0.3974(13)	0.3212(8)	0.0249(7)	0.083(5)
H37A	0.399418	0.322102	−0.017318	0.125
H37B	0.387708	0.355905	0.039811	0.125
H37C	0.351798	0.298562	0.037394	0.125
O9	0.4830(9)	0.2841(4)	0.4844(4)	0.078(4)
H9	0.473204	0.273399	0.450852	0.117
C38	0.5328(11)	0.3273(6)	0.4814(6)	0.067(4)
H38A	0.506741	0.352611	0.455820	0.101

H38B	0.587980	0.317875	0.466244	0.101
H38C	0.539120	0.342019	0.520097	0.101
Ag1A	0.2782(3)	0.41459(14)	0.22333(19)	0.0301(10)
Ag2A	0.3137(3)	0.40386(14)	0.36771(18)	0.0319(10)
Ag3A	0.2470(3)	0.29865(16)	0.29066(18)	0.0279(10)
F1A	0.336(2)	0.5170(10)	0.1576(10)	0.059(5)
F2A	0.338(2)	0.5941(7)	0.1858(11)	0.054(5)
F3A	0.2269(17)	0.5507(14)	0.1852(16)	0.071(5)
F4A	0.378(3)	0.5735(9)	0.4277(11)	0.068(5)
F5A	0.460(2)	0.5105(15)	0.4151(16)	0.061(5)
F6A	0.341(2)	0.5081(13)	0.4447(11)	0.066(5)
F7A	0.344(3)	0.3352(13)	0.5587(11)	0.065(6)
F8A	0.375(2)	0.3899(12)	0.4944(13)	0.049(5)
F9A	0.252(2)	0.3898(14)	0.5316(16)	0.067(5)
F10A	0.1206(15)	0.2073(12)	0.3956(14)	0.050(5)
F11A	0.229(2)	0.1936(9)	0.3502(9)	0.046(5)
F12A	0.2163(19)	0.1697(7)	0.4365(11)	0.046(5)
F13A	0.163(2)	0.2118(10)	0.2321(9)	0.054(5)
F14A	0.2416(19)	0.1856(13)	0.1627(15)	0.075(6)
F15A	0.1118(18)	0.2025(11)	0.1475(14)	0.053(6)
F16A	0.299(2)	0.4141(12)	0.0767(14)	0.066(5)
F17A	0.174(2)	0.4214(14)	0.0872(17)	0.070(5)
F18A	0.220(3)	0.3778(12)	0.0217(7)	0.074(6)
N1A	0.313(3)	0.4818(6)	0.2704(7)	0.037(3)
N2A	0.333(3)	0.4754(6)	0.3271(7)	0.037(3)
N3A	0.281(3)	0.3353(8)	0.4124(6)	0.033(3)
N4A	0.253(3)	0.2945(8)	0.3824(6)	0.029(3)
N5A	0.226(3)	0.3052(7)	0.2002(6)	0.032(3)
N6A	0.242(3)	0.3506(7)	0.1729(6)	0.034(4)
C1A	0.312(2)	0.5480(9)	0.1968(10)	0.057(3)
C2A	0.324(3)	0.5306(7)	0.2572(10)	0.050(3)
C3A	0.349(4)	0.5583(8)	0.3051(12)	0.057(4)
H3A	0.359208	0.594116	0.307862	0.068
C4A	0.356(3)	0.5228(8)	0.3466(10)	0.052(4)
C5A	0.392(2)	0.5286(10)	0.4052(10)	0.056(3)
C6A	0.312(2)	0.3594(9)	0.5125(9)	0.055(3)
C7A	0.283(3)	0.3231(10)	0.4685(7)	0.048(4)
C8A	0.247(4)	0.2753(12)	0.4763(8)	0.046(5)
H8A	0.233389	0.258646	0.511595	0.055
C9A	0.235(3)	0.2577(9)	0.4216(8)	0.038(3)
C10A	0.2052(19)	0.2078(8)	0.4020(10)	0.038(3)
C11A	0.1798(19)	0.2183(7)	0.1752(9)	0.052(3)
C12A	0.200(3)	0.2709(8)	0.1603(7)	0.047(3)
C13A	0.202(5)	0.2921(10)	0.1063(8)	0.058(4)
H13A	0.188664	0.276409	0.070473	0.069
C14A	0.231(3)	0.3440(9)	0.1166(7)	0.053(4)
C15A	0.231(2)	0.3849(8)	0.0778(7)	0.064(4)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 3 Anisotropic displacement parameters [Å²] for 21. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.025(3)	0.022(3)	0.028(4)	−0.001(3)	−0.003(3)	0.007(3)
O2	0.035(4)	0.030(4)	0.032(4)	0.000(3)	−0.005(3)	0.003(3)
O3	0.037(4)	0.039(5)	0.048(5)	0.009(4)	−0.005(4)	0.009(4)

O4	0.063(5)	0.022(4)	0.021(4)	0.001(3)	−0.005(4)	−0.001(3)
O5	0.069(6)	0.022(4)	0.029(4)	0.000(3)	−0.016(4)	0.000(4)
O6	0.053(4)	0.023(3)	0.029(4)	0.003(3)	0.008(3)	−0.003(3)
C16	0.024(5)	0.018(4)	0.018(5)	0.003(4)	−0.004(4)	−0.001(4)
C17	0.024(5)	0.027(5)	0.027(6)	0.002(4)	−0.001(4)	−0.002(4)
C18	0.030(5)	0.027(5)	0.031(6)	−0.009(4)	0.001(5)	−0.004(4)
C19	0.031(5)	0.025(5)	0.036(6)	0.005(4)	−0.001(5)	0.002(4)
C20	0.056(8)	0.024(6)	0.078(11)	−0.002(6)	0.019(8)	0.003(6)
C21	0.025(5)	0.023(5)	0.047(7)	0.001(5)	0.002(5)	0.001(4)
C22	0.061(8)	0.044(7)	0.029(7)	0.007(5)	−0.010(6)	0.005(6)
C23	0.018(4)	0.019(4)	0.028(5)	−0.002(4)	−0.002(4)	0.003(3)
C24	0.039(6)	0.022(5)	0.020(5)	−0.001(4)	−0.009(4)	0.004(4)
C25	0.041(6)	0.024(5)	0.017(5)	−0.003(4)	−0.009(4)	0.007(4)
C26	0.036(6)	0.025(5)	0.026(6)	−0.008(4)	−0.010(5)	0.004(4)
C27	0.057(8)	0.024(6)	0.050(8)	−0.006(5)	−0.013(6)	−0.001(5)
C28	0.027(5)	0.023(5)	0.029(6)	−0.001(4)	−0.006(4)	0.003(4)
C29	0.022(5)	0.023(5)	0.017(5)	−0.001(4)	−0.008(4)	0.002(4)
C30	0.021(5)	0.022(5)	0.027(5)	0.007(4)	−0.001(4)	0.001(4)
C31	0.051(6)	0.020(4)	0.039(5)	0.004(4)	−0.011(5)	0.000(4)
Ag1	0.0256(4)	0.0187(4)	0.0242(5)	0.0023(3)	−0.0035(3)	−0.0008(3)
Ag2	0.0325(5)	0.0205(4)	0.0254(5)	−0.0009(3)	0.0024(4)	−0.0013(4)
Ag3	0.0326(5)	0.0217(4)	0.0206(4)	0.0004(3)	−0.0014(4)	−0.0047(3)
F1	0.107(7)	0.065(6)	0.043(5)	−0.008(5)	−0.025(5)	−0.009(6)
F2	0.106(7)	0.093(7)	0.044(5)	0.003(5)	0.000(6)	−0.034(6)
F3	0.061(7)	0.103(8)	0.079(7)	−0.020(6)	−0.009(6)	0.005(6)
F4	0.116(8)	0.056(6)	0.131(8)	−0.008(6)	−0.044(7)	0.007(6)
F5	0.058(6)	0.071(6)	0.131(8)	−0.042(6)	−0.001(6)	−0.010(5)
F6	0.106(7)	0.073(6)	0.114(8)	−0.035(6)	0.022(7)	−0.014(6)
F7	0.067(6)	0.048(5)	0.073(7)	−0.012(5)	0.032(5)	−0.026(5)
F8	0.088(7)	0.039(5)	0.091(7)	0.000(5)	−0.006(6)	−0.014(5)
F9	0.094(7)	0.059(5)	0.059(6)	−0.032(5)	0.010(5)	−0.034(5)
F10	0.069(7)	0.104(8)	0.078(7)	0.030(6)	0.024(6)	−0.004(6)
F11	0.095(6)	0.067(6)	0.054(5)	0.009(5)	0.008(5)	−0.028(5)
F12	0.095(8)	0.111(8)	0.042(6)	0.026(6)	−0.020(6)	−0.040(7)
F13	0.053(5)	0.040(4)	0.034(4)	−0.005(4)	0.012(4)	0.002(4)
F14	0.046(5)	0.053(5)	0.044(5)	0.020(4)	−0.007(4)	−0.008(4)
F15	0.068(5)	0.032(4)	0.041(5)	0.004(3)	0.011(4)	−0.017(4)
F16	0.067(6)	0.163(9)	0.052(6)	−0.009(6)	0.005(5)	0.000(7)
F17	0.118(7)	0.096(7)	0.048(6)	−0.016(5)	−0.015(6)	0.050(6)
F18	0.141(9)	0.072(7)	0.077(7)	−0.018(6)	−0.013(8)	−0.040(7)
N1	0.035(4)	0.024(4)	0.027(5)	0.005(4)	−0.004(4)	−0.001(4)
N2	0.036(4)	0.016(4)	0.040(4)	0.002(3)	−0.001(4)	−0.002(3)
N3	0.042(4)	0.031(4)	0.022(4)	−0.010(4)	0.003(4)	−0.003(4)
N4	0.039(4)	0.030(4)	0.019(4)	−0.005(3)	−0.001(4)	−0.006(4)
N5	0.026(4)	0.018(4)	0.023(4)	−0.003(4)	−0.004(4)	−0.001(3)
N6	0.028(4)	0.018(4)	0.030(4)	−0.004(3)	−0.004(4)	0.001(3)
C1	0.073(6)	0.065(6)	0.037(5)	0.010(5)	−0.011(6)	−0.008(6)
C2	0.052(5)	0.040(5)	0.030(5)	0.015(4)	−0.007(5)	−0.005(5)
C3	0.055(5)	0.033(5)	0.051(6)	0.011(5)	−0.004(5)	−0.001(5)
C4	0.049(5)	0.026(4)	0.058(5)	0.001(4)	−0.001(5)	−0.001(4)
C5	0.057(5)	0.027(5)	0.074(6)	−0.003(5)	−0.002(5)	−0.001(5)
C6	0.067(6)	0.042(5)	0.054(6)	−0.015(5)	0.006(6)	−0.016(5)
C7	0.052(5)	0.038(5)	0.040(5)	−0.012(4)	0.000(5)	−0.012(5)
C8	0.049(6)	0.050(6)	0.036(6)	−0.010(5)	−0.001(5)	−0.016(5)
C9	0.047(5)	0.051(5)	0.030(5)	0.000(4)	−0.001(4)	−0.014(5)
C10	0.055(6)	0.065(6)	0.038(5)	0.001(5)	−0.003(5)	−0.020(5)

C11	0.040(5)	0.030(4)	0.036(5)	0.002(4)	0.003(4)	−0.005(4)
C12	0.029(4)	0.020(4)	0.026(4)	0.000(4)	0.003(4)	−0.001(4)
C13	0.035(5)	0.025(5)	0.026(5)	0.002(4)	0.002(5)	−0.003(4)
C14	0.035(4)	0.031(4)	0.033(4)	−0.002(4)	0.002(4)	−0.002(4)
C15	0.043(5)	0.048(5)	0.034(5)	−0.007(5)	0.000(4)	0.004(5)
O7	0.060(7)	0.040(5)	0.046(5)	0.009(4)	−0.007(6)	−0.002(5)
C32	0.050(6)	0.023(5)	0.035(5)	0.007(5)	−0.006(5)	−0.004(5)
C33	0.055(6)	0.031(5)	0.039(5)	0.008(4)	−0.005(5)	−0.005(5)
C34	0.057(7)	0.033(5)	0.041(6)	0.010(5)	−0.002(6)	−0.005(6)
C35	0.058(8)	0.039(5)	0.044(6)	0.011(5)	−0.006(7)	−0.005(6)
C36	0.059(7)	0.038(5)	0.044(6)	0.009(5)	−0.007(6)	−0.002(6)
O7A	0.060(8)	0.040(5)	0.046(6)	0.013(5)	−0.003(6)	−0.006(6)
C32A	0.050(6)	0.025(5)	0.036(5)	0.008(5)	−0.004(5)	−0.003(5)
C33A	0.055(6)	0.032(5)	0.041(5)	0.010(4)	−0.005(5)	−0.002(5)
C34A	0.057(7)	0.038(6)	0.044(6)	0.007(5)	−0.005(6)	0.000(6)
C35A	0.059(8)	0.040(5)	0.046(6)	0.010(5)	−0.008(7)	−0.001(6)
C36A	0.058(7)	0.038(5)	0.044(5)	0.009(5)	−0.004(6)	−0.003(5)
O8	0.081(7)	0.052(6)	0.024(5)	−0.006(4)	−0.013(4)	0.019(5)
C37	0.110(13)	0.095(12)	0.046(9)	0.009(8)	−0.015(9)	0.033(10)
O9	0.130(10)	0.067(7)	0.036(5)	0.012(5)	−0.023(6)	−0.047(7)
C38	0.094(11)	0.069(9)	0.039(8)	0.011(7)	−0.023(8)	−0.041(8)
Ag1A	0.0317(19)	0.0221(18)	0.036(2)	0.0018(16)	−0.0068(17)	−0.0010(15)
Ag2A	0.041(2)	0.0275(19)	0.027(2)	−0.0073(15)	−0.0004(17)	−0.0011(16)
Ag3A	0.0283(19)	0.0224(19)	0.033(2)	−0.0024(17)	−0.0029(17)	0.0027(15)
F1A	0.072(10)	0.039(10)	0.067(11)	0.002(10)	−0.001(10)	−0.001(10)
F2A	0.065(10)	0.012(9)	0.085(11)	−0.007(9)	0.010(10)	−0.015(9)
F3A	0.073(10)	0.053(9)	0.086(10)	0.006(9)	−0.012(9)	0.005(9)
F4A	0.083(10)	0.054(9)	0.069(10)	−0.019(9)	0.005(10)	−0.016(9)
F5A	0.075(9)	0.047(8)	0.060(9)	−0.014(9)	0.006(9)	−0.019(9)
F6A	0.080(9)	0.053(9)	0.065(9)	−0.017(8)	0.005(9)	−0.015(9)
F7A	0.070(11)	0.076(11)	0.049(10)	0.013(10)	−0.006(10)	−0.016(10)
F8A	0.056(9)	0.057(9)	0.033(9)	−0.005(9)	−0.003(9)	−0.016(9)
F9A	0.065(10)	0.079(10)	0.058(9)	0.004(9)	0.000(9)	−0.020(9)
F10A	0.058(10)	0.043(10)	0.050(10)	0.005(10)	−0.003(10)	−0.004(10)
F11A	0.055(9)	0.041(9)	0.043(9)	0.004(8)	0.004(9)	−0.009(9)
F12A	0.050(10)	0.037(9)	0.050(10)	0.010(9)	−0.002(9)	−0.015(9)
F13A	0.064(10)	0.049(10)	0.050(10)	−0.010(10)	0.015(10)	0.003(10)
F14A	0.079(11)	0.081(11)	0.066(11)	−0.016(10)	0.012(10)	0.004(11)
F15A	0.061(11)	0.056(10)	0.043(10)	−0.014(10)	−0.007(10)	0.018(10)
F16A	0.083(10)	0.071(10)	0.045(9)	0.010(9)	−0.012(9)	−0.014(9)
F17A	0.083(10)	0.078(9)	0.050(9)	0.002(8)	−0.013(9)	−0.007(9)
F18A	0.097(11)	0.079(11)	0.046(10)	0.002(10)	−0.009(10)	−0.019(11)
N1A	0.041(6)	0.026(6)	0.043(6)	0.001(6)	0.002(6)	−0.001(6)
N2A	0.044(6)	0.029(6)	0.038(6)	−0.005(6)	0.003(6)	−0.003(6)
N3A	0.043(6)	0.033(6)	0.023(6)	0.003(5)	−0.002(5)	−0.007(5)
N4A	0.036(6)	0.026(6)	0.025(6)	0.002(6)	−0.002(6)	−0.005(6)
N5A	0.036(5)	0.029(5)	0.030(5)	−0.002(5)	−0.004(5)	0.000(5)
N6A	0.042(7)	0.034(7)	0.027(7)	0.003(7)	−0.006(7)	0.000(7)
C1A	0.061(6)	0.036(5)	0.074(6)	−0.002(5)	−0.003(5)	−0.002(5)
C2A	0.053(5)	0.032(5)	0.065(5)	−0.003(5)	0.001(5)	−0.002(5)
C3A	0.059(8)	0.038(8)	0.074(8)	−0.013(8)	0.006(8)	−0.005(8)
C4A	0.059(7)	0.037(7)	0.059(7)	−0.010(7)	0.004(7)	−0.008(7)
C5A	0.067(6)	0.043(6)	0.058(6)	−0.013(6)	0.005(6)	−0.015(6)
C6A	0.061(6)	0.065(6)	0.040(6)	0.004(6)	−0.001(6)	−0.018(6)
C7A	0.056(6)	0.054(6)	0.035(6)	0.003(6)	0.000(6)	−0.015(6)
C8A	0.055(8)	0.047(8)	0.035(8)	0.004(8)	0.001(8)	−0.013(8)

C9A	0.045(6)	0.036(6)	0.034(6)	0.004(6)	0.002(6)	−0.007(6)
C10A	0.043(6)	0.034(6)	0.036(6)	0.004(6)	0.004(6)	−0.006(6)
C11A	0.057(6)	0.057(6)	0.042(6)	−0.011(6)	−0.002(6)	0.003(6)
C12A	0.050(6)	0.054(6)	0.039(6)	−0.007(5)	−0.002(5)	0.005(5)
C13A	0.063(8)	0.070(8)	0.040(8)	−0.009(8)	−0.006(8)	0.005(8)
C14A	0.065(7)	0.059(7)	0.036(7)	−0.002(7)	−0.008(7)	−0.002(7)
C15A	0.079(7)	0.070(7)	0.042(7)	0.001(7)	−0.010(7)	−0.009(7)

Table 4 Bond lengths and angles for 21.

Atom–Atom	Length [Å]
O1–C16	1.210(11)
O1–Ag1	2.586(7)
O2–C21	1.227(13)
O3–C21	1.336(14)
O3–C22	1.446(15)
O4–H4	0.8400
O4–C24	1.361(12)
O5–C30	1.198(12)
O6–C30	1.334(12)
O6–C32	1.51(2)
O6–C32A	1.54(2)
C16–C17	1.512(13)
C16–C23	1.515(13)
C17–H17A	0.9900
C17–H17B	0.9900
C17–C18	1.504(14)
C18–H18A	0.9900
C18–H18B	0.9900
C18–C19	1.513(15)
C19–H19	1.0000
C19–C20	1.558(15)
C19–C21	1.495(15)
C20–H20A	0.9800
C20–H20B	0.9800
C20–H20C	0.9800
C22–H22A	0.9800
C22–H22B	0.9800
C22–H22C	0.9800
C23–C24	1.386(14)
C23–C29	1.403(13)
C24–C25	1.392(13)
C25–H25	0.9500
C25–C26	1.374(15)
C26–C27	1.525(14)
C26–C28	1.386(15)
C27–H27A	0.9800
C27–H27B	0.9800
C27–H27C	0.9800
C28–C29	1.409(13)
C28–C31	1.505(14)
C29–C30	1.475(14)
C31–H31A	0.9900
C31–H31B	0.9900
C31–H31C	0.9900
C31–H31D	0.9900

C31–C32	1.43(3)
C31–C32A	1.50(3)
Ag1–N1	2.138(10)
Ag1–N6	2.126(10)
Ag2–N2	2.108(12)
Ag2–N3	2.127(11)
Ag3–N4	2.131(10)
Ag3–N5	2.124(10)
F1–C1	1.27(2)
F2–C1	1.30(2)
F3–C1	1.39(2)
F4–C5	1.30(2)
F5–C5	1.21(2)
F6–C5	1.33(2)
F7–C6	1.344(18)
F8–C6	1.36(2)
F9–C6	1.314(19)
F10–C10	1.36(2)
F11–C10	1.31(2)
F12–C10	1.28(2)
F13–C11	1.359(16)
F14–C11	1.337(16)
F15–C11	1.326(16)
F16–C15	1.313(11)
F17–C15	1.344(12)
F18–C15	1.321(11)
N1–N2	1.363(15)
N1–C2	1.323(17)
N2–C4	1.365(18)
N3–N4	1.353(15)
N3–C7	1.335(17)
N4–C9	1.343(18)
N5–N6	1.363(15)
N5–C12	1.359(16)
N6–C14	1.328(16)
C1–C2	1.48(2)
C2–C3	1.38(2)
C3–H3	0.9500
C3–C4	1.33(2)
C4–C5	1.48(2)
C6–C7	1.46(2)
C7–C8	1.38(2)
C8–H8	0.9500
C8–C9	1.36(2)
C9–C10	1.46(2)
C11–C12	1.449(19)
C12–C13	1.363(18)
C13–H13	0.9500
C13–C14	1.447(18)
C14–C15	1.396(19)
O7–C35	1.51(2)
O7–C36	1.44(2)
C32–H32	1.0000
C32–C33	1.50(2)
C33–C34	1.33(2)
C33–C36	1.347(10)

C34–H34	0.9500
C34–C35	1.335(10)
C35–H35	0.9500
C36–H36	0.9500
O7A–C35A	1.51(2)
O7A–C36A	1.43(2)
C32A–H32A	1.0000
C32A–C33A	1.50(2)
C33A–C34A	1.33(2)
C33A–C36A	1.351(13)
C34A–H34A	0.9500
C34A–C35A	1.337(13)
C35A–H35A	0.9500
C36A–H36A	0.9500
O8–H8B	0.8400
O8–C37	1.364(19)
C37–H37A	0.9800
C37–H37B	0.9800
C37–H37C	0.9800
O9–H9	0.8400
O9–C38	1.378(16)
C38–H38A	0.9800
C38–H38B	0.9800
C38–H38C	0.9800
Ag1A–N1A	2.133(12)
Ag1A–N6A	2.116(12)
Ag2A–N2A	2.110(13)
Ag2A–N3A	2.129(13)
Ag3A–N4A	2.130(12)
Ag3A–N5A	2.129(12)
F1A–C1A	1.27(2)
F2A–C1A	1.29(2)
F3A–C1A	1.39(2)
F4A–C5A	1.30(2)
F5A–C5A	1.21(2)
F6A–C5A	1.34(2)
F7A–C6A	1.35(2)
F8A–C6A	1.36(2)
F9A–C6A	1.31(2)
F10A–C10A	1.36(2)
F11A–C10A	1.31(2)
F12A–C10A	1.29(2)
F13A–C11A	1.356(18)
F14A–C11A	1.333(19)
F15A–C11A	1.327(18)
F16A–C15A	1.325(9)
F17A–C15A	1.343(10)
F18A–C15A	1.326(9)
N1A–N2A	1.364(16)
N1A–C2A	1.319(18)
N2A–C4A	1.365(19)
N3A–N4A	1.344(16)
N3A–C7A	1.338(18)
N4A–C9A	1.351(19)
N5A–N6A	1.367(17)
N5A–C12A	1.348(18)

N6A–C14A	1.327(18)
C1A–C2A	1.48(2)
C2A–C3A	1.38(2)
C3A–H3A	0.9500
C3A–C4A	1.34(2)
C4A–C5A	1.48(2)
C6A–C7A	1.46(2)
C7A–C8A	1.39(2)
C8A–H8A	0.9500
C8A–C9A	1.36(2)
C9A–C10A	1.46(2)
C11A–C12A	1.45(2)
C12A–C13A	1.369(19)
C13A–H13A	0.9500
C13A–C14A	1.45(2)
C14A–C15A	1.39(2)

Atom–Atom–Atom	**Angle [°]**
C16–O1–Ag1	124.6(6)
C21–O3–C22	117.5(9)
C24–O4–H4	109.5
C30–O6–C32	115.1(10)
C30–O6–C32A	118.1(10)
O1–C16–C17	122.4(8)
O1–C16–C23	121.6(8)
C17–C16–C23	115.8(8)
C16–C17–H17A	108.5
C16–C17–H17B	108.5
H17A–C17–H17B	107.5
C18–C17–C16	114.9(8)
C18–C17–H17A	108.5
C18–C17–H17B	108.5
C17–C18–H18A	108.5
C17–C18–H18B	108.5
C17–C18–C19	115.2(9)
H18A–C18–H18B	107.5
C19–C18–H18A	108.5
C19–C18–H18B	108.5
C18–C19–H19	109.0
C18–C19–C20	111.5(10)
C20–C19–H19	109.0
C21–C19–C18	111.9(9)
C21–C19–H19	109.0
C21–C19–C20	106.3(9)
C19–C20–H20A	109.5
C19–C20–H20B	109.5
C19–C20–H20C	109.5
H20A–C20–H20B	109.5
H20A–C20–H20C	109.5
H20B–C20–H20C	109.5
O2–C21–O3	122.2(11)
O2–C21–C19	125.7(11)
O3–C21–C19	112.1(9)
O3–C22–H22A	109.5
O3–C22–H22B	109.5
O3–C22–H22C	109.5

H22A–C22–H22B	109.5
H22A–C22–H22C	109.5
H22B–C22–H22C	109.5
C24–C23–C16	116.1(8)
C24–C23–C29	118.8(9)
C29–C23–C16	125.1(9)
O4–C24–C23	116.6(9)
O4–C24–C25	123.1(9)
C23–C24–C25	120.2(9)
C24–C25–H25	119.2
C26–C25–C24	121.5(10)
C26–C25–H25	119.2
C25–C26–C27	119.6(10)
C25–C26–C28	119.2(9)
C28–C26–C27	121.2(10)
C26–C27–H27A	109.5
C26–C27–H27B	109.5
C26–C27–H27C	109.5
H27A–C27–H27B	109.5
H27A–C27–H27C	109.5
H27B–C27–H27C	109.5
C26–C28–C29	120.1(9)
C26–C28–C31	122.6(9)
C29–C28–C31	117.3(10)
C23–C29–C28	120.1(9)
C23–C29–C30	119.0(9)
C28–C29–C30	120.9(9)
O5–C30–O6	118.5(10)
O5–C30–C29	122.2(9)
O6–C30–C29	119.3(9)
C28–C31–H31A	109.1
C28–C31–H31B	109.1
C28–C31–H31C	108.6
C28–C31–H31D	108.6
H31A–C31–H31B	107.8
H31C–C31–H31D	107.5
C32–C31–C28	112.6(11)
C32–C31–H31A	109.1
C32–C31–H31B	109.1
C32A–C31–C28	114.8(11)
C32A–C31–H31C	108.6
C32A–C31–H31D	108.6
N1–Ag1–O1	96.9(3)
N6–Ag1–O1	89.7(3)
N6–Ag1–N1	170.1(4)
N2–Ag2–N3	175.8(4)
N5–Ag3–N4	179.3(4)
N2–N1–Ag1	117.2(8)
C2–N1–Ag1	133.6(10)
C2–N1–N2	107.8(11)
N1–N2–Ag2	121.1(8)
N1–N2–C4	105.9(12)
C4–N2–Ag2	133.0(10)
N4–N3–Ag2	117.7(8)
C7–N3–Ag2	132.3(10)
C7–N3–N4	108.9(11)

N3–N4–Ag3	118.1(8)
C9–N4–Ag3	135.4(10)
C9–N4–N3	106.3(11)
N6–N5–Ag3	121.3(9)
C12–N5–Ag3	130.2(9)
C12–N5–N6	108.4(10)
N5–N6–Ag1	118.7(8)
C14–N6–Ag1	132.4(9)
C14–N6–N5	108.4(11)
F1–C1–F2	111.0(18)
F1–C1–F3	101.0(17)
F1–C1–C2	117.0(15)
F2–C1–F3	102.2(15)
F2–C1–C2	114.9(16)
F3–C1–C2	108.6(16)
N1–C2–C1	120.3(14)
N1–C2–C3	110.9(14)
C3–C2–C1	128.8(14)
C2–C3–H3	128.1
C4–C3–C2	103.9(14)
C4–C3–H3	128.1
N2–C4–C5	120.3(15)
C3–C4–N2	111.6(13)
C3–C4–C5	128.1(15)
F4–C5–F6	88.6(15)
F4–C5–C4	112.9(16)
F5–C5–F4	115.5(16)
F5–C5–F6	105.5(18)
F5–C5–C4	118.8(16)
F6–C5–C4	110.9(15)
F7–C6–F8	103.6(14)
F7–C6–C7	112.4(13)
F8–C6–C7	112.9(16)
F9–C6–F7	106.8(15)
F9–C6–F8	106.9(14)
F9–C6–C7	113.5(15)
N3–C7–C6	121.8(14)
N3–C7–C8	109.5(13)
C8–C7–C6	128.7(14)
C7–C8–H8	128.0
C9–C8–C7	103.9(13)
C9–C8–H8	128.0
N4–C9–C8	111.3(13)
N4–C9–C10	119.9(14)
C8–C9–C10	128.6(15)
F10–C10–C9	111.6(16)
F11–C10–F10	100.3(14)
F11–C10–C9	116.4(15)
F12–C10–F10	101.4(15)
F12–C10–F11	108.6(17)
F12–C10–C9	116.4(15)
F13–C11–C12	112.6(11)
F14–C11–F13	105.1(12)
F14–C11–C12	113.3(11)
F15–C11–F13	106.3(11)
F15–C11–F14	107.5(12)

F15–C11–C12	111.6(12)
N5–C12–C11	121.0(11)
N5–C12–C13	110.2(11)
C13–C12–C11	128.7(12)
C12–C13–H13	128.1
C12–C13–C14	103.8(11)
C14–C13–H13	128.1
N6–C14–C13	109.1(12)
N6–C14–C15	123.3(13)
C15–C14–C13	127.5(12)
F16–C15–F17	99.3(10)
F16–C15–F18	100.4(10)
F16–C15–C14	117.7(12)
F17–C15–C14	115.1(12)
F18–C15–F17	99.2(10)
F18–C15–C14	121.3(13)
C36–O7–C35	103.8(14)
O6–C32–H32	108.9
C31–C32–O6	113.0(15)
C31–C32–H32	108.9
C31–C32–C33	112.4(18)
C33–C32–O6	104.6(16)
C33–C32–H32	108.9
C34–C33–C32	123.2(16)
C34–C33–C36	108.1(16)
C36–C33–C32	128.6(15)
C33–C34–H34	122.4
C33–C34–C35	115(2)
C35–C34–H34	122.4
O7–C35–H35	128.2
C34–C35–O7	103.6(19)
C34–C35–H35	128.2
O7–C36–H36	125.4
C33–C36–O7	109.2(16)
C33–C36–H36	125.4
C36A–O7A–C35A	103.9(14)
O6–C32A–H32A	108.9
C31–C32A–O6	107.2(14)
C31–C32A–H32A	108.9
C31–C32A–C33A	117.4(17)
C33A–C32A–O6	105.1(17)
C33A–C32A–H32A	108.9
C34A–C33A–C32A	123.3(16)
C34A–C33A–C36A	108.0(16)
C36A–C33A–C32A	128.2(15)
C33A–C34A–H34A	122.4
C33A–C34A–C35A	115(2)
C35A–C34A–H34A	122.4
O7A–C35A–H35A	128.4
C34A–C35A–O7A	103.2(19)
C34A–C35A–H35A	128.4
O7A–C36A–H36A	125.4
C33A–C36A–O7A	109.1(16)
C33A–C36A–H36A	125.4
C37–O8–H8B	109.5
O8–C37–H37A	109.5

O8–C37–H37B	109.5
O8–C37–H37C	109.5
H37A–C37–H37B	109.5
H37A–C37–H37C	109.5
H37B–C37–H37C	109.5
C38–O9–H9	109.5
O9–C38–H38A	109.5
O9–C38–H38B	109.5
O9–C38–H38C	109.5
H38A–C38–H38B	109.5
H38A–C38–H38C	109.5
H38B–C38–H38C	109.5
N6A–Ag1A–N1A	176.8(8)
N2A–Ag2A–N3A	173.5(17)
N5A–Ag3A–N4A	173.3(18)
N2A–N1A–Ag1A	117.0(9)
C2A–N1A–Ag1A	134.9(11)
C2A–N1A–N2A	107.9(12)
N1A–N2A–Ag2A	120.1(9)
N1A–N2A–C4A	105.8(12)
C4A–N2A–Ag2A	133.7(12)
N4A–N3A–Ag2A	119.4(9)
C7A–N3A–Ag2A	131.7(11)
C7A–N3A–N4A	108.9(12)
N3A–N4A–Ag3A	119.5(9)
N3A–N4A–C9A	106.4(12)
C9A–N4A–Ag3A	134.1(11)
N6A–N5A–Ag3A	119.7(9)
C12A–N5A–Ag3A	132.1(10)
C12A–N5A–N6A	108.2(11)
N5A–N6A–Ag1A	118.5(9)
C14A–N6A–Ag1A	133.0(11)
C14A–N6A–N5A	108.5(12)
F1A–C1A–F2A	111(2)
F1A–C1A–F3A	100.7(18)
F1A–C1A–C2A	116.4(17)
F2A–C1A–F3A	102.8(17)
F2A–C1A–C2A	115.5(18)
F3A–C1A–C2A	108.4(18)
N1A–C2A–C1A	119.7(15)
N1A–C2A–C3A	110.8(15)
C3A–C2A–C1A	129.4(16)
C2A–C3A–H3A	128.0
C4A–C3A–C2A	104.0(15)
C4A–C3A–H3A	128.0
N2A–C4A–C5A	119.9(17)
C3A–C4A–N2A	111.4(14)
C3A–C4A–C5A	128.4(17)
F4A–C5A–F6A	88.9(17)
F4A–C5A–C4A	113.2(18)
F5A–C5A–F4A	115.4(18)
F5A–C5A–F6A	105(2)
F5A–C5A–C4A	118.7(18)
F6A–C5A–C4A	110.6(17)
F7A–C6A–F8A	103.5(17)
F7A–C6A–C7A	111.8(15)

F8A–C6A–C7A	113.4(18)
F9A–C6A–F7A	106.9(18)
F9A–C6A–F8A	107.0(16)
F9A–C6A–C7A	113.6(17)
N3A–C7A–C6A	122.1(15)
N3A–C7A–C8A	109.2(14)
C8A–C7A–C6A	128.3(16)
C7A–C8A–H8A	128.1
C9A–C8A–C7A	103.7(15)
C9A–C8A–H8A	128.1
N4A–C9A–C8A	111.1(15)
N4A–C9A–C10A	119.5(15)
C8A–C9A–C10A	129.3(16)
F10A–C10A–C9A	111.7(18)
F11A–C10A–F10A	100.4(16)
F11A–C10A–C9A	116.2(17)
F12A–C10A–F10A	101.5(17)
F12A–C10A–F11A	108.2(18)
F12A–C10A–C9A	116.7(17)
F13A–C11A–C12A	113.0(14)
F14A–C11A–F13A	106.1(15)
F14A–C11A–C12A	112.7(14)
F15A–C11A–F13A	105.7(14)
F15A–C11A–F14A	107.7(14)
F15A–C11A–C12A	111.1(15)
N5A–C12A–C11A	122.0(13)
N5A–C12A–C13A	110.6(12)
C13A–C12A–C11A	127.1(13)
C12A–C13A–H13A	128.2
C12A–C13A–C14A	103.5(12)
C14A–C13A–H13A	128.2
N6A–C14A–C13A	109.0(13)
N6A–C14A–C15A	122.3(15)
C15A–C14A–C13A	127.6(15)
F16A–C15A–F17A	99.2(10)
F16A–C15A–F18A	100.2(10)
F16A–C15A–C14A	117.3(14)
F17A–C15A–C14A	115.4(13)
F18A–C15A–F17A	99.2(10)
F18A–C15A–C14A	121.7(15)

Table 5 Torsion angles for 21.

Atom–Atom–Atom–Atom	Torsion Angle [°]
O1–C16–C17–C18	−18.2(14)
O1–C16–C23–C24	92.4(12)
O1–C16–C23–C29	−89.4(12)
O4–C24–C25–C26	178.1(10)
O6–C32–C33–C34	127(3)
O6–C32–C33–C36	−56(3)
O6–C32A–C33A–C34A	−122(3)
O6–C32A–C33A–C36A	66(3)
C16–C17–C18–C19	−66.8(12)
C16–C23–C24–O4	−0.5(14)
C16–C23–C24–C25	178.5(9)
C16–C23–C29–C28	−178.0(9)
C16–C23–C29–C30	−0.3(14)
C17–C16–C23–C24	−83.5(11)
C17–C16–C23–C29	94.7(12)
C17–C18–C19–C20	−176.8(10)
C17–C18–C19–C21	−57.8(12)
C18–C19–C21–O2	−29.1(15)
C18–C19–C21–O3	152.0(9)
C20–C19–C21–O2	92.8(13)
C20–C19–C21–O3	−86.1(12)
C22–O3–C21–O2	2.1(16)
C22–O3–C21–C19	−178.9(9)
C23–C16–C17–C18	157.7(9)
C23–C24–C25–C26	−0.8(17)
C23–C29–C30–O5	−0.3(15)
C23–C29–C30–O6	−178.8(9)
C24–C23–C29–C28	0.1(14)
C24–C23–C29–C30	177.8(9)
C24–C25–C26–C27	−176.2(11)
C24–C25–C26–C28	1.0(17)
C25–C26–C28–C29	−0.7(16)
C25–C26–C28–C31	−179.7(10)
C26–C28–C29–C23	0.1(15)
C26–C28–C29–C30	−177.5(10)
C26–C28–C31–C32	−156.0(14)
C26–C28–C31–C32A	150.6(14)
C27–C26–C28–C29	176.5(10)
C27–C26–C28–C31	−2.6(17)
C28–C29–C30–O5	177.4(10)
C28–C29–C30–O6	−1.1(15)
C28–C31–C32–O6	−50.5(18)
C28–C31–C32–C33	−168.6(13)
C28–C31–C32A–O6	50.0(18)
C28–C31–C32A–C33A	167.9(15)
C29–C23–C24–O4	−178.7(9)
C29–C23–C24–C25	0.2(16)
C29–C28–C31–C32	24.9(17)
C29–C28–C31–C32A	−28.5(17)
C30–O6–C32–C31	52.3(18)
C30–O6–C32–C33	174.9(13)
C30–O6–C32A–C31	−51.3(17)
C30–O6–C32A–C33A	−177.0(12)
C31–C28–C29–C23	179.2(10)

C31–C28–C29–C30	1.6(14)
C31–C32–C33–C34	−110(3)
C31–C32–C33–C36	67(3)
C31–C32A–C33A–C34A	119(3)
C31–C32A–C33A–C36A	−53(4)
Ag1–O1–C16–C17	139.7(8)
Ag1–O1–C16–C23	−36.0(12)
Ag1–N1–N2–Ag2	5.5(13)
Ag1–N1–N2–C4	−170.9(10)
Ag1–N1–C2–C1	−12(2)
Ag1–N1–C2–C3	167.6(11)
Ag1–N6–C14–C13	−169.1(9)
Ag1–N6–C14–C15	9(2)
Ag2–N2–C4–C3	−173.4(12)
Ag2–N2–C4–C5	5(2)
Ag2–N3–N4–Ag3	16.4(12)
Ag2–N3–N4–C9	−167.6(10)
Ag2–N3–C7–C6	−14(2)
Ag2–N3–C7–C8	165.2(11)
Ag3–N4–C9–C8	174.1(11)
Ag3–N4–C9–C10	−9(3)
Ag3–N5–N6–Ag1	−8.2(12)
Ag3–N5–N6–C14	179.2(8)
Ag3–N5–C12–C11	−1.4(18)
Ag3–N5–C12–C13	179.6(9)
F1–C1–C2–N1	−5(3)
F1–C1–C2–C3	175.5(19)
F2–C1–C2–N1	−138.0(17)
F2–C1–C2–C3	43(3)
F3–C1–C2–N1	108.3(18)
F3–C1–C2–C3	−71(2)
F7–C6–C7–N3	−62(2)
F7–C6–C7–C8	119.4(19)
F8–C6–C7–N3	54.9(19)
F8–C6–C7–C8	−124(2)
F9–C6–C7–N3	176.8(16)
F9–C6–C7–C8	−2(3)
F13–C11–C12–N5	60.9(16)
F13–C11–C12–C13	−120.3(15)
F14–C11–C12–N5	−58.2(17)
F14–C11–C12–C13	120.6(15)
F15–C11–C12–N5	−179.7(11)
F15–C11–C12–C13	−1(2)
N1–N2–C4–C3	2.3(18)
N1–N2–C4–C5	−179.0(14)
N1–C2–C3–C4	−1(2)
N2–N1–C2–C1	−177.2(14)
N2–N1–C2–C3	2.3(18)
N2–C4–C5–F4	−154.3(17)
N2–C4–C5–F5	66(3)
N2–C4–C5–F6	−57(2)
N3–N4–C9–C8	−0.8(19)
N3–N4–C9–C10	175.6(15)
N3–C7–C8–C9	2(2)
N4–N3–C7–C6	178.9(14)
N4–N3–C7–C8	−2.2(18)

N4–C9–C10–F10	−91(2)
N4–C9–C10–F11	24(3)
N4–C9–C10–F12	153.7(17)
N5–N6–C14–C13	2.1(15)
N5–N6–C14–C15	−179.8(12)
N5–C12–C13–C14	0.7(14)
N6–N5–C12–C11	179.5(11)
N6–N5–C12–C13	0.5(14)
N6–C14–C15–F16	58.8(18)
N6–C14–C15–F17	−57.8(18)
N6–C14–C15–F18	−177.3(12)
C1–C2–C3–C4	178.6(18)
C2–N1–N2–Ag2	173.6(10)
C2–N1–N2–C4	−2.7(16)
C2–C3–C4–N2	−1(2)
C2–C3–C4–C5	−179.5(17)
C3–C4–C5–F4	24(3)
C3–C4–C5–F5	−116(2)
C3–C4–C5–F6	122(2)
C6–C7–C8–C9	−179.6(17)
C7–N3–N4–Ag3	−174.1(10)
C7–N3–N4–C9	1.9(16)
C7–C8–C9–N4	0(2)
C7–C8–C9–C10	−176.6(18)
C8–C9–C10–F10	85(2)
C8–C9–C10–F11	−160.5(18)
C8–C9–C10–F12	−31(3)
C11–C12–C13–C14	−178.2(13)
C12–N5–N6–Ag1	171.0(8)
C12–N5–N6–C14	−1.6(14)
C12–C13–C14–N6	−1.8(15)
C12–C13–C14–C15	−179.8(14)
C13–C14–C15–F16	−123.4(15)
C13–C14–C15–F17	120.0(15)
C13–C14–C15–F18	0(2)
C32–O6–C30–O5	156.5(14)
C32–O6–C30–C29	−25.0(16)
C32–C33–C34–C35	178(3)
C32–C33–C36–O7	−176(3)
C33–C34–C35–O7	−2(4)
C34–C33–C36–O7	1(3)
C35–O7–C36–C33	−2(3)
C36–O7–C35–C34	3(3)
C36–C33–C34–C35	1(4)
C32A–O6–C30–O5	−151.1(13)
C32A–O6–C30–C29	27.4(16)
C32A–C33A–C34A–C35A	−178(3)
C32A–C33A–C36A–O7A	172(3)
C33A–C34A–C35A–O7A	8(4)
C34A–C33A–C36A–O7A	−1(3)
C35A–O7A–C36A–C33A	5(3)
C36A–O7A–C35A–C34A	−7(3)
C36A–C33A–C34A–C35A	−5(4)
Ag1A–N1A–N2A–Ag2A	−9(5)
Ag1A–N1A–N2A–C4A	178(3)
Ag1A–N1A–C2A–C1A	−1(8)

Ag1A–N1A–C2A–C3A	−178(5)
Ag1A–N6A–C14A–C13A	−178(5)
Ag1A–N6A–C14A–C15A	−9(7)
Ag2A–N2A–C4A–C3A	−171(5)
Ag2A–N2A–C4A–C5A	15(7)
Ag2A–N3A–N4A–Ag3A	2(5)
Ag2A–N3A–N4A–C9A	−178(3)
Ag2A–N3A–C7A–C6A	0(7)
Ag2A–N3A–C7A–C8A	174(4)
Ag3A–N4A–C9A–C8A	−177(4)
Ag3A–N4A–C9A–C10A	1(7)
Ag3A–N5A–N6A–Ag1A	−5(5)
Ag3A–N5A–N6A–C14A	175(4)
Ag3A–N5A–C12A–C11A	1(7)
Ag3A–N5A–C12A–C13A	−175(5)
F1A–C1A–C2A–N1A	−36(5)
F1A–C1A–C2A–C3A	140(6)
F2A–C1A–C2A–N1A	−169(4)
F2A–C1A–C2A–C3A	8(6)
F3A–C1A–C2A–N1A	76(5)
F3A–C1A–C2A–C3A	−107(6)
F7A–C6A–C7A–N3A	−152(5)
F7A–C6A–C7A–C8A	35(6)
F8A–C6A–C7A–N3A	−36(5)
F8A–C6A–C7A–C8A	152(6)
F9A–C6A–C7A–N3A	87(5)
F9A–C6A–C7A–C8A	−86(6)
F13A–C11A–C12A–N5A	20(5)
F13A–C11A–C12A–C13A	−165(6)
F14A–C11A–C12A–N5A	−100(5)
F14A–C11A–C12A–C13A	75(6)
F15A–C11A–C12A–N5A	139(4)
F15A–C11A–C12A–C13A	−46(6)
N1A–N2A–C4A–C3A	1(6)
N1A–N2A–C4A–C5A	−173(4)
N1A–C2A–C3A–C4A	3(7)
N2A–N1A–C2A–C1A	175(4)
N2A–N1A–C2A–C3A	−2(7)
N2A–C4A–C5A–F4A	−152(4)
N2A–C4A–C5A–F5A	67(5)
N2A–C4A–C5A–F6A	−54(4)
N3A–N4A–C9A–C8A	3(6)
N3A–N4A–C9A–C10A	−179(4)
N3A–C7A–C8A–C9A	8(6)
N4A–N3A–C7A–C6A	179(4)
N4A–N3A–C7A–C8A	−7(6)
N4A–C9A–C10A–F10A	−87(4)
N4A–C9A–C10A–F11A	27(5)
N4A–C9A–C10A–F12A	157(4)
N5A–N6A–C14A–C13A	2(6)
N5A–N6A–C14A–C15A	171(4)
N5A–C12A–C13A–C14A	−1(7)
N6A–N5A–C12A–C11A	178(4)
N6A–N5A–C12A–C13A	3(7)
N6A–C14A–C15A–F16A	57(5)
N6A–C14A–C15A–F17A	−59(5)

N6A–C14A–C15A–F18A	−180(4)
C1A–C2A–C3A–C4A	−174(4)
C2A–N1A–N2A–Ag2A	174(4)
C2A–N1A–N2A–C4A	1(6)
C2A–C3A–C4A–N2A	−2(7)
C2A–C3A–C4A–C5A	171(4)
C3A–C4A–C5A–F4A	35(6)
C3A–C4A–C5A–F5A	−105(6)
C3A–C4A–C5A–F6A	133(6)
C6A–C7A–C8A–C9A	−178(4)
C7A–N3A–N4A–Ag3A	−177(4)
C7A–N3A–N4A–C9A	2(6)
C7A–C8A–C9A–N4A	−7(6)
C7A–C8A–C9A–C10A	175(4)
C8A–C9A–C10A–F10A	90(6)
C8A–C9A–C10A–F11A	−155(5)
C8A–C9A–C10A–F12A	−26(6)
C11A–C12A–C13A–C14A	−177(4)
C12A–N5A–N6A–Ag1A	177(4)
C12A–N5A–N6A–C14A	−3(6)
C12A–C13A–C14A–N6A	−1(7)
C12A–C13A–C14A–C15A	−169(4)
C13A–C14A–C15A–F16A	−136(5)
C13A–C14A–C15A–F17A	107(5)
C13A–C14A–C15A–F18A	−13(6)

Table 6 Hydrogen bonds for 21.

D–H···A [Å]	d(D–H) [Å]	d(H···A) [Å]	d(D···A) [Å]	<(DHA) [°]
O4–H4···O8	0.84	1.78	2.616(11)	174.2
C17–H17B···O2	0.99	2.57	3.182(13)	120.0
C27–H27C···F12#1	0.98	2.65	3.103(17)	108.2
C27–H27C···F7A#1	0.98	2.57	3.13(3)	116.0
C32A–H32A···F15A#2	1.00	1.97	2.77(3)	135.5
O8–H8B···O9#1	0.84	1.86	2.683(14)	165.0
C37–H37B···F16A	0.98	2.24	3.12(5)	149.1
O9–H9···O5	0.84	1.99	2.792(12)	159.3
C38–H38A···F8A	0.98	2.48	3.02(4)	113.9

Symmetry transformations used to generate equivalent atoms:

#1: +X, 0.5-Y, -0.5+Z; #2: 0.5+X, +Y, 0.5-Z;

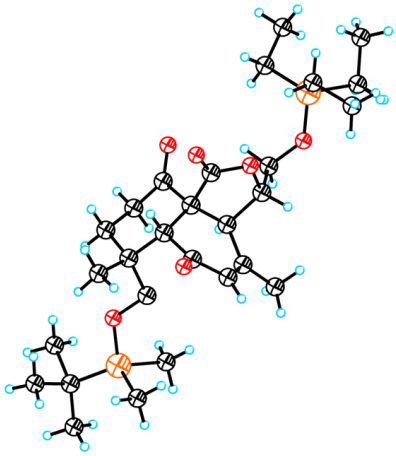


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Table 1 Crystal data and structure refinement for compound 25

CCDC number	2447364
Empirical formula	$C_{28}H_{48}O_6Si_2$
Formula weight	536.84
Temperature/K	273.15
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.885
b/Å	13.433
c/Å	34.799
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3218.4
Z	4
ρ_{calc}g/cm^3	1.108
μ/mm^{-1}	1.282
F(000)	1168.0
Crystal size/mm^3	0.22 × 0.2 × 0.18
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	5.078 to 133.13
Index ranges	-8 ≤ h ≤ 8, -15 ≤ k ≤ 15, 0 ≤ l ≤ 41
Reflections collected	11135
Independent reflections	5644 [R_{int} = 0.1090, R_{sigma} = 0.1010]
Data/restraints/parameters	5644/431/439
Goodness-of-fit on F^2	0.930
Final R indexes [I>=2σ (I)]	R_1 = 0.1164, wR_2 = 0.3028
Final R indexes [all data]	R_1 = 0.1653, wR_2 = 0.3498
Largest diff. peak/hole / e Å^{-3}	0.33/-0.27
Flack parameter	0.45(9)

Table 2 Atomic coordinates and U_{eq} [Å^2] for 25.

Atom	*x*	*y*	*z*	U_{eq}
C1	1.165541	0.602860	0.308710	0.253(12)
H1A	1.139290	0.656240	0.291120	0.380

H1B	1.055870	0.558790	0.309610	0.380
H1C	1.278050	0.566780	0.300250	0.380
C2	1.203121	0.645841	0.349090	0.209(5)
H2A	1.164260	0.715033	0.351215	0.251
H2B	1.337238	0.638194	0.357100	0.251
C3	0.744(4)	0.6915(19)	0.3621(10)	0.218(9)
H3A	0.779589	0.717797	0.386729	0.326
H3B	0.821669	0.722077	0.342489	0.326
H3C	0.609070	0.705367	0.357269	0.326
C4	0.783(2)	0.5783(15)	0.3610(9)	0.207(5)
H4A	0.760978	0.552459	0.335284	0.248
H4B	0.696773	0.543799	0.378616	0.248
C5	1.235(7)	0.418(2)	0.3360(10)	0.239(10)
H5A	1.351380	0.456950	0.336778	0.359
H5B	1.267370	0.348560	0.335148	0.359
H5C	1.160651	0.435290	0.313628	0.359
C6	1.118(3)	0.4313(10)	0.3734(8)	0.208(5)
H6A	1.199350	0.416429	0.395485	0.250
H6B	1.007504	0.386662	0.373700	0.250
C7	1.0280(15)	0.5596(9)	0.4529(3)	0.142(3)
H7A	1.141184	0.579442	0.467597	0.170
H7B	1.032268	0.487966	0.449608	0.170
C8	0.8448(15)	0.5880(7)	0.4748(3)	0.130(3)
H8	0.833147	0.660747	0.474842	0.156
C9	0.8254(12)	0.5505(5)	0.5161(2)	0.111(2)
H9	0.953368	0.530300	0.525686	0.133
C10	0.6941(12)	0.4605(6)	0.5142(2)	0.109(2)
C11	0.5919(17)	0.4746(6)	0.4769(3)	0.131(3)
C12	0.5413(13)	0.4451(7)	0.5465(2)	0.121(3)
H12	0.441510	0.401256	0.535661	0.145
C13	0.4432(15)	0.5429(8)	0.5541(3)	0.127(3)
C14	0.5638(15)	0.6312(7)	0.5549(3)	0.126(3)
H14	0.511741	0.688538	0.565851	0.151
C15	0.7473(14)	0.6361(5)	0.5409(3)	0.121(3)
C16	0.8776(19)	0.7210(7)	0.5468(4)	0.164(4)
H16A	0.896346	0.754138	0.522640	0.246
H16B	0.822596	0.766808	0.564990	0.246
H16C	1.000376	0.697518	0.556230	0.246
C17	0.8212(13)	0.3644(6)	0.5089(3)	0.118(3)
C18	0.9049(16)	0.3253(6)	0.5452(3)	0.129(3)
H18A	0.991156	0.374281	0.556534	0.155
H18B	0.978839	0.265260	0.540137	0.155
C19	0.7347(18)	0.3024(6)	0.5729(3)	0.138(3)
H19A	0.649794	0.253902	0.560910	0.166
H19B	0.786863	0.272367	0.596096	0.166
C20	0.6160(15)	0.3922(7)	0.5840(3)	0.127(3)
C21	0.439(2)	0.3571(10)	0.6073(4)	0.165(4)
H21A	0.478941	0.331348	0.631794	0.247
H21B	0.353541	0.412578	0.611034	0.247
H21C	0.373431	0.306038	0.593085	0.247
C22	0.7352(19)	0.4649(7)	0.6085(3)	0.144(3)
C23	1.078(4)	0.5563(19)	0.6599(7)	0.178(2)
H23A	1.031037	0.596613	0.639034	0.267
H23B	1.123797	0.598573	0.680174	0.267
H23C	1.182197	0.514963	0.650944	0.267
C24	0.670(4)	0.565(2)	0.6961(7)	0.178(2)

H24A	0.722310	0.607095	0.715807	0.267
H24B	0.629560	0.605135	0.674677	0.267
H24C	0.560480	0.529045	0.705977	0.267
C25	1.034(5)	0.435(2)	0.7532(6)	0.178(2)
H25A	1.058854	0.385627	0.772579	0.267
H25B	1.154264	0.463627	0.744899	0.267
H25C	0.952054	0.486097	0.763699	0.267
C26	0.932(4)	0.3856(18)	0.7179(5)	0.1779(18)
C27	1.056(5)	0.2989(18)	0.6952(7)	0.178(2)
H27A	1.176543	0.325309	0.685970	0.268
H27B	1.081143	0.247309	0.713660	0.268
H27C	0.983042	0.271989	0.674140	0.268
C28	0.766(4)	0.321(2)	0.7308(7)	0.178(2)
H28A	0.813021	0.269392	0.747402	0.268
H28B	0.672281	0.360802	0.744402	0.268
H28C	0.705841	0.291992	0.708622	0.268
O1	1.0331(13)	0.6056(5)	0.4169(2)	0.154(3)
O2	0.6706(10)	0.5452(5)	0.45507(19)	0.136(2)
O3	0.4405(11)	0.4336(5)	0.46667(19)	0.145(2)
O4	0.8499(12)	0.3315(4)	0.4774(2)	0.136(2)
O5	0.2700(11)	0.5450(6)	0.5613(2)	0.153(2)
O6	0.7983(16)	0.4133(6)	0.6429(2)	0.1766(18)
Si1	1.0367(7)	0.5608(3)	0.37518(10)	0.1813(18)
Si2	0.871(2)	0.4730(9)	0.6807(3)	0.1772(18)
C5A	0.928(6)	0.4034(19)	0.3313(7)	0.244(11)
H5AA	0.925599	0.332042	0.330045	0.366
H5AB	0.802089	0.428992	0.324385	0.366
H5AC	1.023299	0.428602	0.313725	0.366
C2A	1.2973(18)	0.5533(16)	0.3639(8)	0.212(5)
H2AA	1.322259	0.580241	0.338507	0.254
H2AB	1.372081	0.591113	0.382477	0.254
C1A	1.354(4)	0.4439(19)	0.365420	0.247(8)
H1AA	1.272177	0.398785	0.379460	0.371
H1AB	1.333677	0.434715	0.338360	0.371
H1AC	1.487377	0.430985	0.371570	0.371
C4A	0.909(3)	0.6497(15)	0.3433(7)	0.209(5)
H4AA	0.876427	0.618220	0.319039	0.251
H4AB	0.789365	0.672502	0.355301	0.251
C3A	1.047(5)	0.7364(16)	0.3370(8)	0.231(8)
H3AA	1.167564	0.722724	0.349668	0.346
H3AB	1.069404	0.744834	0.309928	0.346
H3AC	0.991204	0.796284	0.347278	0.346
C6A	0.917(3)	0.4369(11)	0.3736(6)	0.204(5)
H6AA	0.985201	0.390029	0.390058	0.245
H6AB	0.783512	0.441690	0.382090	0.245
C23A	1.054(4)	0.5568(19)	0.6783(7)	0.178(2)
H23D	0.998938	0.610151	0.663434	0.266
H23E	1.089798	0.581191	0.703194	0.266
H23F	1.166598	0.531351	0.665404	0.266
C24A	0.651(4)	0.509(2)	0.7120(7)	0.178(2)
H24D	0.689074	0.533986	0.736813	0.267
H24E	0.598214	0.562946	0.697053	0.267
H24F	0.554224	0.458496	0.715173	0.267
C25A	0.983(5)	0.377(2)	0.7565(6)	0.178(2)
H25D	1.053422	0.324457	0.768870	0.267
H25E	1.059202	0.436727	0.756620	0.267

H25F	0.863122	0.388477	0.769940	0.267
C26A	0.949(4)	0.3479(19)	0.7134(6)	0.1779(19)
C27A	1.155(5)	0.337(2)	0.6923(7)	0.179(2)
H27D	1.230755	0.396564	0.692774	0.268
H27E	1.224975	0.284294	0.705014	0.268
H27F	1.130265	0.317774	0.666144	0.268
C28A	0.825(5)	0.261(2)	0.7130(7)	0.178(2)
H28D	0.888360	0.206838	0.726023	0.268
H28E	0.706710	0.277208	0.726063	0.268
H28F	0.797260	0.241968	0.687033	0.268
Si2A	0.861(3)	0.4521(10)	0.6843(4)	0.1773(18)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 3 Anisotropic displacement parameters [Å²] for 25. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.28(3)	0.29(2)	0.190(15)	0.021(18)	0.01(2)	−0.04(2)
C2	0.229(10)	0.227(10)	0.172(9)	0.019(9)	0.015(9)	−0.007(9)
C3	0.227(18)	0.244(14)	0.181(17)	0.011(17)	−0.005(17)	0.027(16)
C4	0.218(9)	0.234(10)	0.169(10)	0.014(10)	−0.007(9)	0.009(10)
C5	0.28(2)	0.243(17)	0.199(17)	0.003(17)	0.028(16)	0.016(19)
C6	0.233(10)	0.217(8)	0.174(9)	0.002(9)	0.005(10)	0.012(9)
C7	0.116(6)	0.172(8)	0.136(7)	−0.004(7)	−0.005(6)	0.011(6)
C8	0.125(7)	0.124(5)	0.140(7)	0.000(5)	−0.006(6)	−0.002(5)
C9	0.104(5)	0.107(4)	0.122(5)	−0.005(4)	−0.009(4)	0.011(4)
C10	0.112(5)	0.116(5)	0.099(5)	0.005(4)	−0.009(4)	0.000(5)
C11	0.154(9)	0.093(5)	0.145(7)	−0.002(5)	−0.010(7)	−0.009(5)
C12	0.114(5)	0.129(6)	0.119(6)	−0.014(5)	−0.016(5)	−0.002(5)
C13	0.116(7)	0.148(7)	0.116(6)	−0.008(5)	−0.014(5)	0.024(6)
C14	0.118(7)	0.117(6)	0.143(7)	−0.005(5)	−0.011(6)	0.024(5)
C15	0.117(7)	0.086(4)	0.161(8)	0.011(4)	−0.017(6)	0.005(4)
C16	0.180(10)	0.115(6)	0.197(10)	−0.018(6)	−0.019(9)	0.006(7)
C17	0.107(6)	0.106(5)	0.140(7)	0.004(5)	0.003(5)	−0.012(4)
C18	0.133(7)	0.102(5)	0.152(7)	−0.011(5)	−0.011(6)	0.024(5)
C19	0.154(9)	0.115(5)	0.146(7)	−0.007(5)	−0.010(7)	0.006(6)
C20	0.119(6)	0.128(6)	0.134(7)	−0.004(5)	−0.006(6)	−0.006(5)
C21	0.156(10)	0.166(8)	0.173(10)	0.014(7)	−0.001(8)	0.010(8)
C22	0.181(9)	0.133(6)	0.119(6)	−0.004(5)	−0.018(6)	−0.009(7)
C23	0.207(4)	0.189(4)	0.138(3)	0.000(3)	−0.032(3)	−0.006(4)
C24	0.207(4)	0.189(4)	0.139(3)	0.000(3)	−0.031(3)	−0.005(4)
C25	0.207(4)	0.189(4)	0.139(3)	0.001(3)	−0.032(3)	−0.006(3)
C26	0.207(3)	0.189(4)	0.138(3)	0.000(2)	−0.032(2)	−0.006(3)
C27	0.207(4)	0.189(4)	0.139(3)	0.000(3)	−0.032(3)	−0.005(3)
C28	0.207(3)	0.189(4)	0.139(3)	0.000(3)	−0.032(3)	−0.006(3)
O1	0.176(6)	0.152(5)	0.135(5)	0.023(4)	0.023(5)	−0.008(4)
O2	0.132(4)	0.135(4)	0.140(4)	0.006(4)	−0.026(4)	0.012(4)
O3	0.134(5)	0.161(5)	0.141(5)	0.001(4)	−0.022(4)	−0.016(4)
O4	0.154(5)	0.123(4)	0.132(4)	−0.011(3)	0.002(4)	0.015(4)
O5	0.102(4)	0.192(6)	0.165(6)	−0.014(5)	−0.004(4)	0.016(4)
O6	0.206(3)	0.187(4)	0.136(3)	0.000(2)	−0.033(2)	−0.006(3)
Si1	0.205(4)	0.202(3)	0.137(3)	0.012(2)	0.002(2)	−0.001(3)
Si2	0.206(3)	0.188(4)	0.137(2)	0.000(2)	−0.033(2)	−0.006(3)
C5A	0.30(3)	0.219(18)	0.215(16)	−0.048(16)	−0.02(2)	0.02(2)
C2A	0.223(9)	0.237(9)	0.175(9)	0.004(9)	0.008(9)	0.000(9)
C1A	0.270(16)	0.250(13)	0.221(16)	0.017(15)	−0.003(16)	0.018(15)

C4A	0.231(10)	0.232(9)	0.165(9)	0.023(8)	−0.006(9)	0.011(9)
C3A	0.259(18)	0.235(15)	0.199(15)	0.019(14)	0.009(16)	0.001(14)
C6A	0.229(10)	0.210(8)	0.174(9)	−0.004(8)	0.005(10)	0.009(9)
C23A	0.207(4)	0.189(4)	0.137(3)	0.000(3)	−0.032(3)	−0.006(3)
C24A	0.207(4)	0.189(4)	0.138(3)	0.000(3)	−0.031(3)	−0.005(3)
C25A	0.207(4)	0.189(4)	0.139(3)	0.001(3)	−0.032(3)	−0.006(3)
C26A	0.207(3)	0.189(4)	0.138(3)	0.000(2)	−0.032(2)	−0.006(3)
C27A	0.207(4)	0.189(4)	0.140(3)	0.001(3)	−0.032(3)	−0.006(3)
C28A	0.207(4)	0.189(4)	0.139(3)	0.000(3)	−0.032(3)	−0.006(3)
Si2A	0.206(3)	0.188(4)	0.137(2)	0.000(2)	−0.033(2)	−0.006(3)

Table 4 Bond lengths and angles for 25.

Atom–Atom	Length [Å]
C1–H1A	0.9599
C1–H1B	0.9600
C1–H1C	0.9600
C1–C2	1.5410
C2–H2A	0.9700
C2–H2B	0.9700
C2–Si1	1.855(4)
C3–H3A	0.9600
C3–H3B	0.9600
C3–H3C	0.9601
C3–C4	1.545(13)
C4–H4A	0.9700
C4–H4B	0.9700
C4–Si1	1.833(12)
C5–H5A	0.9600
C5–H5B	0.9600
C5–H5C	0.9600
C5–C6	1.538(13)
C6–H6A	0.9700
C6–H6B	0.9700
C6–Si1	1.829(12)
C7–H7A	0.9700
C7–H7B	0.9700
C7–C8	1.522(14)
C7–O1	1.397(12)
C8–H8	0.9800
C8–C9	1.531(13)
C8–O2	1.497(12)
C9–H9	0.9800
C9–C10	1.511(11)
C9–C15	1.535(12)
C10–C11	1.487(14)
C10–C12	1.553(12)
C10–C17	1.570(12)
C11–O2	1.331(11)
C11–O3	1.232(11)
C12–H12	0.9800
C12–C13	1.501(13)
C12–C20	1.573(12)
C13–C14	1.449(15)
C13–O5	1.219(12)
C14–H14	0.9300

C14–C15	1.356(14)
C15–C16	1.466(14)
C16–H16A	0.9604
C16–H16B	0.9598
C16–H16C	0.9599
C17–C18	1.483(13)
C17–O4	1.199(11)
C18–H18A	0.9700
C18–H18B	0.9700
C18–C19	1.549(15)
C19–H19A	0.9700
C19–H19B	0.9700
C19–C20	1.507(14)
C20–C21	1.535(16)
C20–C22	1.534(14)
C21–H21A	0.9594
C21–H21B	0.9597
C21–H21C	0.9606
C22–O6	1.451(12)
C23–H23A	0.9602
C23–H23B	0.9600
C23–H23C	0.9600
C23–Si2	1.95(2)
C24–H24A	0.9598
C24–H24B	0.9599
C24–H24C	0.9600
C24–Si2	1.93(2)
C25–H25A	0.9598
C25–H25B	0.9600
C25–H25C	0.9599
C25–C26	1.56(2)
C26–C27	1.64(3)
C26–C28	1.50(3)
C26–Si2	1.80(2)
C27–H27A	0.9599
C27–H27B	0.9601
C27–H27C	0.9598
C28–H28A	0.9600
C28–H28B	0.9600
C28–H28C	0.9601
O1–Si1	1.570(8)
O6–Si2	1.620(14)
O6–Si2A	1.591(14)
Si1–C2A	1.840(11)
Si1–C4A	1.853(11)
Si1–C6A	1.857(11)
C5A–H5AA	0.9601
C5A–H5AB	0.9599
C5A–H5AC	0.9598
C5A–C6A	1.543(13)
C2A–H2AA	0.9700
C2A–H2AB	0.9700
C2A–C1A	1.521(13)
C1A–H1AA	0.9602
C1A–H1AB	0.9598
C1A–H1AC	0.9600

C4A–H4AA	0.9700
C4A–H4AB	0.9700
C4A–C3A	1.521(13)
C3A–H3AA	0.9598
C3A–H3AB	0.9601
C3A–H3AC	0.9600
C6A–H6AA	0.9700
C6A–H6AB	0.9700
C23A–H23D	0.9600
C23A–H23E	0.9599
C23A–H23F	0.9600
C23A–Si2A	1.94(2)
C24A–H24D	0.9600
C24A–H24E	0.9600
C24A–H24F	0.9600
C24A–Si2A	1.90(2)
C25A–H25D	0.9600
C25A–H25E	0.9600
C25A–H25F	0.9599
C25A–C26A	1.57(2)
C26A–C27A	1.61(3)
C26A–C28A	1.44(3)
C26A–Si2A	1.83(2)
C27A–H27D	0.9599
C27A–H27E	0.9600
C27A–H27F	0.9600
C28A–H28D	0.9598
C28A–H28E	0.9600
C28A–H28F	0.9601

Atom–Atom–Atom	**Angle [°]**
H1A–C1–H1B	109.5
H1A–C1–H1C	109.5
H1B–C1–H1C	109.5
C2–C1–H1A	109.5
C2–C1–H1B	109.5
C2–C1–H1C	109.5
C1–C2–H2A	112.5
C1–C2–H2B	112.5
C1–C2–Si1	96.42(13)
H2A–C2–H2B	110.0
Si1–C2–H2A	112.5
Si1–C2–H2B	112.5
H3A–C3–H3B	109.5
H3A–C3–H3C	109.4
H3B–C3–H3C	109.5
C4–C3–H3A	109.9
C4–C3–H3B	107.8
C4–C3–H3C	110.7
C3–C4–H4A	110.4
C3–C4–H4B	110.4
C3–C4–Si1	106.5(12)
H4A–C4–H4B	108.6
Si1–C4–H4A	110.4
Si1–C4–H4B	110.4
H5A–C5–H5B	109.5

H5A–C5–H5C	109.5
H5B–C5–H5C	109.5
C6–C5–H5A	110.5
C6–C5–H5B	105.2
C6–C5–H5C	112.5
C5–C6–H6A	110.2
C5–C6–H6B	110.2
C5–C6–Si1	107.4(12)
H6A–C6–H6B	108.5
Si1–C6–H6A	110.2
Si1–C6–H6B	110.2
H7A–C7–H7B	108.0
C8–C7–H7A	109.4
C8–C7–H7B	109.4
O1–C7–H7A	109.4
O1–C7–H7B	109.4
O1–C7–C8	111.1(9)
C7–C8–H8	108.6
C7–C8–C9	117.4(8)
C9–C8–H8	108.6
O2–C8–C7	109.8(7)
O2–C8–H8	108.6
O2–C8–C9	103.5(7)
C8–C9–H9	109.4
C8–C9–C15	108.2(6)
C10–C9–C8	105.9(7)
C10–C9–H9	109.4
C10–C9–C15	114.5(7)
C15–C9–H9	109.4
C9–C10–C12	118.6(6)
C9–C10–C17	109.3(6)
C11–C10–C9	102.7(7)
C11–C10–C12	109.1(8)
C11–C10–C17	105.5(7)
C12–C10–C17	110.6(6)
O2–C11–C10	113.4(9)
O3–C11–C10	126.6(9)
O3–C11–O2	119.8(10)
C10–C12–H12	106.1
C10–C12–C20	116.1(7)
C13–C12–C10	108.4(7)
C13–C12–H12	106.1
C13–C12–C20	113.4(7)
C20–C12–H12	106.1
C14–C13–C12	117.6(8)
O5–C13–C12	119.8(10)
O5–C13–C14	122.5(9)
C13–C14–H14	117.8
C15–C14–C13	124.5(8)
C15–C14–H14	117.8
C14–C15–C9	119.5(8)
C14–C15–C16	123.9(9)
C16–C15–C9	116.6(8)
C15–C16–H16A	108.7
C15–C16–H16B	110.4
C15–C16–H16C	109.3

H16A–C16–H16B	109.5
H16A–C16–H16C	109.5
H16B–C16–H16C	109.5
C18–C17–C10	114.1(8)
O4–C17–C10	120.1(8)
O4–C17–C18	125.7(8)
C17–C18–H18A	110.1
C17–C18–H18B	110.1
C17–C18–C19	107.8(9)
H18A–C18–H18B	108.5
C19–C18–H18A	110.1
C19–C18–H18B	110.1
C18–C19–H19A	108.7
C18–C19–H19B	108.7
H19A–C19–H19B	107.6
C20–C19–C18	114.2(7)
C20–C19–H19A	108.7
C20–C19–H19B	108.7
C19–C20–C12	109.0(8)
C19–C20–C21	108.6(8)
C19–C20–C22	111.2(9)
C21–C20–C12	108.5(8)
C22–C20–C12	110.4(7)
C22–C20–C21	109.0(9)
C20–C21–H21A	110.8
C20–C21–H21B	108.8
C20–C21–H21C	108.8
H21A–C21–H21B	109.6
H21A–C21–H21C	109.5
H21B–C21–H21C	109.4
O6–C22–C20	108.3(8)
H23A–C23–H23B	109.5
H23A–C23–H23C	109.5
H23B–C23–H23C	109.5
Si2–C23–H23A	111.1
Si2–C23–H23B	107.8
Si2–C23–H23C	109.6
H24A–C24–H24B	109.5
H24A–C24–H24C	109.5
H24B–C24–H24C	109.5
Si2–C24–H24A	107.8
Si2–C24–H24B	110.7
Si2–C24–H24C	109.9
H25A–C25–H25B	109.5
H25A–C25–H25C	109.5
H25B–C25–H25C	109.5
C26–C25–H25A	109.9
C26–C25–H25B	108.7
C26–C25–H25C	109.8
C25–C26–C27	116.4(19)
C25–C26–Si2	113.2(17)
C27–C26–Si2	103.8(14)
C28–C26–C25	110.5(19)
C28–C26–C27	97(2)
C28–C26–Si2	114.5(16)
C26–C27–H27A	110.4

C26–C27–H27B	106.6
C26–C27–H27C	111.3
H27A–C27–H27B	109.5
H27A–C27–H27C	109.5
H27B–C27–H27C	109.5
C26–C28–H28A	109.9
C26–C28–H28B	109.8
C26–C28–H28C	108.8
H28A–C28–H28B	109.5
H28A–C28–H28C	109.5
H28B–C28–H28C	109.5
C7–O1–Si1	131.3(7)
C11–O2–C8	109.8(8)
C22–O6–Si2	121.7(8)
C22–O6–Si2A	132.2(8)
C4–Si1–C2	112.2(6)
C6–Si1–C2	112.3(6)
C6–Si1–C4	113.9(7)
O1–Si1–C2	103.1(4)
O1–Si1–C4	100.7(11)
O1–Si1–C6	113.6(10)
O1–Si1–C2A	103.5(10)
O1–Si1–C4A	107.4(10)
O1–Si1–C6A	111.3(7)
C2A–Si1–C4A	111.8(7)
C2A–Si1–C6A	112.1(7)
C4A–Si1–C6A	110.5(6)
C24–Si2–C23	105.0(13)
C26–Si2–C23	118.2(13)
C26–Si2–C24	112.8(13)
O6–Si2–C23	102.0(10)
O6–Si2–C24	108.7(11)
O6–Si2–C26	109.4(9)
H5AA–C5A–H5AB	109.5
H5AA–C5A–H5AC	109.5
H5AB–C5A–H5AC	109.5
C6A–C5A–H5AA	109.4
C6A–C5A–H5AB	95.4
C6A–C5A–H5AC	122.4
Si1–C2A–H2AA	110.3
Si1–C2A–H2AB	110.3
H2AA–C2A–H2AB	108.5
C1A–C2A–Si1	107.1(12)
C1A–C2A–H2AA	110.3
C1A–C2A–H2AB	110.3
C2A–C1A–H1AA	118.6
C2A–C1A–H1AB	93.1
C2A–C1A–H1AC	115.3
H1AA–C1A–H1AB	109.5
H1AA–C1A–H1AC	109.5
H1AB–C1A–H1AC	109.5
Si1–C4A–H4AA	110.4
Si1–C4A–H4AB	110.4
H4AA–C4A–H4AB	108.6
C3A–C4A–Si1	106.4(12)
C3A–C4A–H4AA	110.4

C3A–C4A–H4AB	110.4
C4A–C3A–H3AA	109.2
C4A–C3A–H3AB	109.5
C4A–C3A–H3AC	109.7
H3AA–C3A–H3AB	109.5
H3AA–C3A–H3AC	109.5
H3AB–C3A–H3AC	109.4
Si1–C6A–H6AA	110.6
Si1–C6A–H6AB	110.6
C5A–C6A–Si1	105.6(11)
C5A–C6A–H6AA	110.6
C5A–C6A–H6AB	110.6
H6AA–C6A–H6AB	108.8
H23D–C23A–H23E	109.5
H23D–C23A–H23F	109.5
H23E–C23A–H23F	109.5
Si2A–C23A–H23D	109.3
Si2A–C23A–H23E	109.0
Si2A–C23A–H23F	110.1
H24D–C24A–H24E	109.5
H24D–C24A–H24F	109.5
H24E–C24A–H24F	109.5
Si2A–C24A–H24D	112.7
Si2A–C24A–H24E	108.3
Si2A–C24A–H24F	107.3
H25D–C25A–H25E	109.5
H25D–C25A–H25F	109.5
H25E–C25A–H25F	109.5
C26A–C25A–H25D	108.8
C26A–C25A–H25E	107.2
C26A–C25A–H25F	112.3
C25A–C26A–C27A	109.2(19)
C25A–C26A–Si2A	112.8(18)
C27A–C26A–Si2A	96.3(14)
C28A–C26A–C25A	107(2)
C28A–C26A–C27A	116(2)
C28A–C26A–Si2A	114.8(17)
C26A–C27A–H27D	113.2
C26A–C27A–H27E	107.6
C26A–C27A–H27F	107.6
H27D–C27A–H27E	109.5
H27D–C27A–H27F	109.5
H27E–C27A–H27F	109.5
C26A–C28A–H28D	110.1
C26A–C28A–H28E	108.3
C26A–C28A–H28F	110.0
H28D–C28A–H28E	109.5
H28D–C28A–H28F	109.5
H28E–C28A–H28F	109.5
O6–Si2A–C23A	109.0(10)
O6–Si2A–C24A	112.6(12)
O6–Si2A–C26A	109.8(10)
C24A–Si2A–C23A	106.3(13)
C26A–Si2A–C23A	112.9(13)
C26A–Si2A–C24A	106.2(13)

Table 5 Torsion angles for 25.

Atom–Atom–Atom–Atom	Torsion Angle [°]
C1–C2–Si1–C4	−64.2(11)
C1–C2–Si1–C6	65.7(10)
C1–C2–Si1–O1	−171.7(4)
C3–C4–Si1–C2	−48(3)
C3–C4–Si1–C6	−177(2)
C3–C4–Si1–O1	61(2)
C5–C6–Si1–C2	−28(3)
C5–C6–Si1–C4	101(2)
C5–C6–Si1–O1	−145(2)
C7–C8–C9–C10	−99.9(9)
C7–C8–C9–C15	136.9(9)
C7–C8–O2–C11	111.9(9)
C7–O1–Si1–C2	−142.1(9)
C7–O1–Si1–C4	101.9(11)
C7–O1–Si1–C6	−20.3(12)
C7–O1–Si1–C2A	−93.0(12)
C7–O1–Si1–C4A	148.6(11)
C7–O1–Si1–C6A	27.6(13)
C8–C7–O1–Si1	−118.4(10)
C8–C9–C10–C11	−20.2(9)
C8–C9–C10–C12	−140.6(7)
C8–C9–C10–C17	91.4(8)
C8–C9–C15–C14	109.9(9)
C8–C9–C15–C16	−68.0(10)
C9–C8–O2–C11	−14.2(9)
C9–C10–C11–O2	12.3(10)
C9–C10–C11–O3	−162.2(9)
C9–C10–C12–C13	44.9(9)
C9–C10–C12–C20	−84.0(9)
C9–C10–C17–C18	81.8(9)
C9–C10–C17–O4	−95.1(9)
C10–C9–C15–C14	−7.9(11)
C10–C9–C15–C16	174.2(8)
C10–C11–O2–C8	1.3(10)
C10–C12–C13–C14	−41.7(10)
C10–C12–C13–O5	142.3(8)
C10–C12–C20–C19	−46.1(10)
C10–C12–C20–C21	−164.2(8)
C10–C12–C20–C22	76.4(10)
C10–C17–C18–C19	58.4(9)
C11–C10–C12–C13	−72.1(8)
C11–C10–C12–C20	159.0(7)
C11–C10–C17–C18	−168.4(8)
C11–C10–C17–O4	14.7(11)
C12–C10–C11–O2	139.0(8)
C12–C10–C11–O3	−35.5(12)
C12–C10–C17–C18	−50.5(10)
C12–C10–C17–O4	132.6(9)
C12–C13–C14–C15	16.0(14)
C12–C20–C22–O6	179.2(8)
C13–C12–C20–C19	−172.5(9)
C13–C12–C20–C21	69.3(10)
C13–C12–C20–C22	−50.1(11)
C13–C14–C15–C9	11.3(14)

C13–C14–C15–C16	−170.9(9)
C15–C9–C10–C11	98.9(8)
C15–C9–C10–C12	−21.5(10)
C15–C9–C10–C17	−149.4(7)
C17–C10–C11–O2	−102.2(8)
C17–C10–C11–O3	83.4(11)
C17–C10–C12–C13	172.2(7)
C17–C10–C12–C20	43.3(9)
C17–C18–C19–C20	−62.4(10)
C18–C19–C20–C12	55.0(11)
C18–C19–C20–C21	173.2(8)
C18–C19–C20–C22	−66.9(11)
C19–C20–C22–O6	−59.6(12)
C20–C12–C13–C14	88.7(10)
C20–C12–C13–O5	−87.3(10)
C20–C22–O6–Si2	−161.6(11)
C20–C22–O6–Si2A	−156.7(13)
C21–C20–C22–O6	60.1(11)
C22–O6–Si2–C23	−55.4(15)
C22–O6–Si2–C24	55.1(15)
C22–O6–Si2–C26	178.6(13)
C22–O6–Si2A–C23A	−50.1(19)
C22–O6–Si2A–C24A	67.7(18)
C22–O6–Si2A–C26A	−174.2(14)
C25–C26–Si2–C23	55(2)
C25–C26–Si2–C24	−68(2)
C25–C26–Si2–O6	171.1(18)
C27–C26–Si2–C23	−72.1(19)
C27–C26–Si2–C24	165.0(17)
C27–C26–Si2–O6	44(2)
C28–C26–Si2–C23	−177.1(19)
C28–C26–Si2–C24	60(2)
C28–C26–Si2–O6	−61(2)
O1–C7–C8–C9	−175.1(8)
O1–C7–C8–O2	67.1(11)
O1–Si1–C2A–C1A	107.1(14)
O1–Si1–C4A–C3A	75(2)
O1–Si1–C6A–C5A	178.8(19)
O2–C8–C9–C10	21.2(8)
O2–C8–C9–C15	−102.0(7)
O3–C11–O2–C8	176.2(8)
O4–C17–C18–C19	−124.9(10)
O5–C13–C14–C15	−168.2(10)
C2A–Si1–C4A–C3A	−38(2)
C2A–Si1–C6A–C5A	−66(2)
C4A–Si1–C2A–C1A	−137.6(15)
C4A–Si1–C6A–C5A	60(2)
C6A–Si1–C2A–C1A	−12.9(19)
C6A–Si1–C4A–C3A	−163.3(18)
C25A–C26A–Si2A–O6	−171.0(19)
C25A–C26A–Si2A–C23A	67(2)
C25A–C26A–Si2A–C24A	−49(2)
C27A–C26A–Si2A–O6	75.0(17)
C27A–C26A–Si2A–C23A	−46.8(19)
C27A–C26A–Si2A–C24A	−162.9(16)
C28A–C26A–Si2A–O6	−48(3)

C28A–C26A–Si2A–C23A	−169(2)
C28A–C26A–Si2A–C24A	74(2)

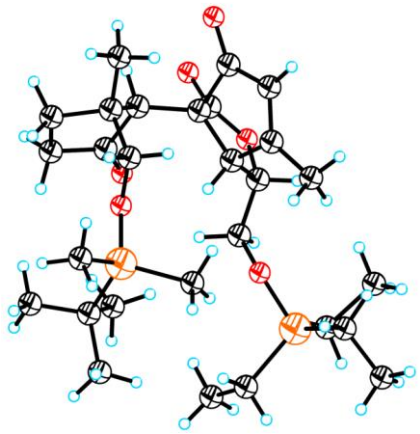

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Table 1. Crystal data and structure refinement for compound 26.

CCDC number	2447369
Empirical formula	$C_{92}H_{108}Ag_6F_{36}N_{12}O_{12}Si_4$
Formula weight	3017.48
Temperature/K	105(8)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	12.8463(5)
b/Å	16.5989(7)
c/Å	54.638(4)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	11650.8(11)
Z	4
ρ_{calc}g/cm^3	1.720
μ/mm^{-1}	9.375
F(000)	6008.0
Crystal size/mm^3	0.1 × 0.09 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	6.47 to 179.224
Index ranges	-10 ≤ h ≤ 16, -20 ≤ k ≤ 18, -65 ≤ l ≤ 67
Reflections collected	36844
Independent reflections	20891 [R_{int} = 0.0708, R_{sigma} = 0.1037]
Data/restraints/parameters	20891/924/1462
Goodness-of-fit on F^2	1.061

Final R indexes [I>=2σ (I)]	R_1 = 0.0966, wR_2 = 0.2598
Final R indexes [all data]	R_1 = 0.1243, wR_2 = 0.2839
Largest diff. peak/hole / e Å^{-3}	2.18/-2.16
Flack parameter	0.016(7)

Table 2. Atomic coordinates and U_{eq} [Å^2] for 26.

Atom	*x*	*y*	*z*	U_{eq}
Ag83	0.77324(12)	0.50834(9)	0.68732(3)	0.0414(3)
Ag89	0.58159(12)	0.37606(10)	0.67343(3)	0.0427(4)
Ag60	0.71530(12)	0.70620(10)	0.58857(3)	0.0445(4)
Ag92	0.83171(12)	0.32597(9)	0.65670(3)	0.0435(4)
Ag43	0.67825(13)	0.50866(10)	0.56826(3)	0.0499(4)
Ag57	0.47292(13)	0.62150(11)	0.58641(3)	0.0485(4)
Si21	0.6521(6)	0.4595(4)	0.43217(14)	0.0598(11)
Si15	0.4897(6)	0.5086(6)	0.80064(16)	0.0690(12)
Si20	0.9643(7)	0.4463(6)	0.81906(16)	0.0680(13)
Si19	0.2595(7)	0.4289(5)	0.48180(17)	0.0681(12)
O144	0.6388(14)	0.3538(12)	0.7336(4)	0.0636(12)
O134	0.9556(15)	0.4123(12)	0.7902(4)	0.0666(13)
F78	1.0642(12)	0.6958(10)	0.6195(3)	0.075(2)
O31	0.6775(13)	0.5041(11)	0.5185(3)	0.0586(18)
O14	0.4800(14)	0.6205(11)	0.5309(3)	0.0619(12)
F116	0.6988(11)	0.6347(9)	0.7444(3)	0.065(2)
F77	0.9145(12)	0.7573(10)	0.6151(3)	0.075(2)
N59	0.5858(19)	0.7791(15)	0.5972(5)	0.0681(16)
F99	1.0494(12)	0.2854(10)	0.6393(3)	0.073(2)
F119	0.9733(12)	0.6308(10)	0.7004(3)	0.072(2)
N44	0.524(2)	0.4564(18)	0.5681(6)	0.090(2)
F68	0.2464(12)	0.8338(10)	0.6110(3)	0.071(2)
F118	0.5845(11)	0.7169(9)	0.7314(3)	0.064(2)
F117	0.7140(11)	0.6810(9)	0.7084(3)	0.063(2)
F105	0.3865(12)	0.2483(10)	0.6574(4)	0.077(2)
F110	0.7775(12)	0.1311(11)	0.5929(4)	0.079(2)
O4	0.6892(14)	0.5199(10)	0.4550(3)	0.0595(12)
F37	1.0277(12)	0.7518(11)	0.5852(3)	0.075(2)
N58	0.4869(19)	0.7434(15)	0.5976(5)	0.0681(16)
O161	0.7512(14)	0.3349(12)	0.7029(3)	0.0622(19)
F114	0.2806(10)	0.4959(9)	0.7116(3)	0.068(2)
F71	0.7364(12)	0.8966(9)	0.5901(3)	0.070(2)
F67	0.2728(12)	0.7214(10)	0.5913(3)	0.071(2)
F79	1.0951(12)	0.6540(9)	0.6754(3)	0.071(2)
O162	0.8343(14)	0.4798(12)	0.7357(3)	0.0632(19)
F109	0.8162(13)	0.0961(11)	0.6286(4)	0.081(2)
O153	0.5840(15)	0.4499(12)	0.7912(4)	0.0674(12)
N45	0.449(2)	0.4996(18)	0.5766(6)	0.090(2)
F112	0.3401(11)	0.4370(10)	0.6799(3)	0.070(2)
N90	0.6037(18)	0.2851(16)	0.6479(5)	0.0756(18)
F104	0.4071(12)	0.3359(10)	0.6288(4)	0.077(2)
F97	1.1876(12)	0.3550(10)	0.6372(3)	0.074(2)
O29	0.6610(15)	0.8002(11)	0.5043(3)	0.0627(19)
F54	0.2349(14)	0.5547(12)	0.5741(4)	0.091(2)
C9	0.735(2)	0.5410(16)	0.5055(5)	0.0596(12)
N93	0.9541(18)	0.4097(15)	0.6663(5)	0.0698(17)
O18	0.3681(15)	0.4821(11)	0.4861(4)	0.0663(12)
O16	0.6331(15)	0.6638(11)	0.5452(3)	0.0617(18)

F70	0.6376(12)	0.9859(10)	0.6076(3)	0.072(2)
F120	0.9396(12)	0.6615(10)	0.6644(3)	0.070(2)
N61	0.8468(18)	0.6291(17)	0.5845(5)	0.0764(18)
F50	0.6489(14)	0.3148(12)	0.5651(4)	0.093(2)
N82	0.9248(17)	0.4859(15)	0.6722(5)	0.0696(17)
F98	1.1477(12)	0.3021(10)	0.6708(4)	0.076(2)
F66	0.2992(12)	0.7275(10)	0.6301(3)	0.070(2)
F106	0.3780(12)	0.2128(11)	0.6185(4)	0.077(2)
C145	0.641(2)	0.3609(18)	0.7595(5)	0.0644(12)
H145	0.585405	0.325627	0.766442	0.077
F51	0.5870(15)	0.3257(12)	0.5315(4)	0.093(2)
F56	0.2636(14)	0.5067(12)	0.6091(4)	0.093(2)
F72	0.7109(13)	0.8964(10)	0.6301(3)	0.071(2)
N88	0.5427(16)	0.4767(13)	0.6958(5)	0.0640(16)
C143	0.734(2)	0.3374(18)	0.7244(5)	0.0634(12)
N42	0.8332(19)	0.5507(16)	0.5790(5)	0.0770(18)
F113	0.3615(11)	0.3880(10)	0.7148(3)	0.070(2)
C142	0.810(2)	0.3126(18)	0.7449(5)	0.0639(11)
N91	0.7074(18)	0.2600(16)	0.6421(5)	0.0758(18)
C26	0.470(2)	0.6905(16)	0.4725(5)	0.0616(13)
O150	0.8479(14)	0.1809(12)	0.7266(4)	0.0664(19)
C5	0.719(2)	0.5981(15)	0.4508(5)	0.0597(12)
H5A	0.656445	0.631426	0.447795	0.072
H5B	0.762983	0.600204	0.435917	0.072
C15	0.576(2)	0.6456(16)	0.5282(5)	0.0614(12)
C124	0.5159(11)	0.5889(13)	0.6441(3)	0.073(9)
H124	0.445283	0.601087	0.647724	0.087
C123	0.5421(15)	0.5142(11)	0.6344(3)	0.073(9)
H123	0.489313	0.475415	0.631312	0.088
C122	0.6454(17)	0.4964(9)	0.6291(3)	0.077(9)
H122	0.663246	0.445392	0.622446	0.092
C121	0.7225(12)	0.5532(12)	0.6336(3)	0.086(10)
H121	0.793151	0.541040	0.629992	0.103
C126	0.6964(12)	0.6279(11)	0.6433(3)	0.060(6)
H126	0.749123	0.666713	0.646405	0.071
C125	0.5931(13)	0.6457(10)	0.6486(3)	0.073(9)
H125	0.575190	0.696738	0.655271	0.087
C46	0.364(3)	0.455(2)	0.5763(8)	0.091(2)
C152	0.616(2)	0.4487(18)	0.7661(5)	0.0658(12)
H15A	0.678805	0.482864	0.763877	0.079
H15B	0.560149	0.469681	0.755468	0.079
N84	0.6192(16)	0.5286(13)	0.7023(5)	0.0638(16)
C11	0.607(2)	0.6599(16)	0.5013(5)	0.0611(11)
C103	0.430(2)	0.258(2)	0.6340(7)	0.0765(18)
C133	0.996(2)	0.3352(19)	0.7830(5)	0.0656(12)
H13A	0.946623	0.292411	0.787737	0.079
H13B	1.062747	0.325229	0.791622	0.079
F74	0.9870(13)	0.3830(12)	0.5959(4)	0.082(2)
C13	0.440(2)	0.5931(16)	0.5075(5)	0.0626(12)
H13	0.370599	0.619019	0.504915	0.075
C128	0.912(2)	0.4438(18)	0.7386(5)	0.0638(13)
C62	0.576(2)	0.8557(18)	0.6040(6)	0.0686(16)
C63	0.469(2)	0.8685(19)	0.6097(6)	0.0685(16)
H63	0.437399	0.916689	0.615511	0.082
C12	0.514(2)	0.6236(17)	0.4874(5)	0.0617(12)
H12	0.537501	0.578234	0.476627	0.074

C38	0.985(2)	0.705(2)	0.6036(7)	0.0754(18)
C102	0.542(2)	0.244(2)	0.6332(7)	0.0760(18)
C7	0.875(2)	0.5798(16)	0.4775(5)	0.0598(13)
H7A	0.932060	0.611228	0.485061	0.072
H7B	0.901035	0.555729	0.462026	0.072
C101	0.596(2)	0.1915(19)	0.6191(7)	0.0762(18)
H101	0.567768	0.155252	0.607410	0.091
C28	0.599(2)	0.7503(17)	0.4954(5)	0.0614(12)
C17	0.424(2)	0.5003(17)	0.5083(5)	0.0644(12)
H17A	0.491231	0.471786	0.508774	0.077
H17B	0.382321	0.484602	0.522853	0.077
C107	0.791(2)	0.163(2)	0.6165(7)	0.0780(18)
C87	0.4582(19)	0.5037(17)	0.7060(6)	0.0650(15)
C130	1.015(2)	0.3319(19)	0.7553(5)	0.0646(12)
C49	0.560(3)	0.321(2)	0.5543(8)	0.092(2)
F52	0.5162(15)	0.2460(12)	0.5556(4)	0.094(2)
C86	0.475(2)	0.5751(17)	0.7190(6)	0.0644(16)
H86	0.427235	0.605742	0.728411	0.077
C6	0.780(2)	0.6335(16)	0.4726(5)	0.0599(11)
C64	0.419(2)	0.7949(19)	0.6048(6)	0.0685(16)
C95	1.092(2)	0.4890(18)	0.6620(6)	0.0701(17)
H95	1.161061	0.507488	0.659201	0.084
F55	0.1851(14)	0.4352(12)	0.5828(4)	0.092(2)
C30	0.378(2)	0.6796(17)	0.4571(5)	0.062(2)
H30A	0.398080	0.650978	0.442130	0.093
H30B	0.349272	0.732371	0.452843	0.093
H30C	0.326016	0.648144	0.466006	0.093
C35	0.606(2)	0.3548(16)	0.4705(5)	0.061(2)
H35A	0.659075	0.367079	0.482946	0.091
H35B	0.576365	0.301580	0.473793	0.091
H35C	0.551130	0.395598	0.471169	0.091
C100	0.701(2)	0.201(2)	0.6250(7)	0.0766(18)
C146	0.750(2)	0.3275(19)	0.7680(5)	0.0641(12)
H146	0.786404	0.366755	0.778907	0.077
C10	0.721(2)	0.6302(16)	0.4975(5)	0.0601(11)
H10	0.764078	0.662525	0.509129	0.072
C94	1.053(2)	0.4126(18)	0.6584(7)	0.0705(16)
C48	0.489(3)	0.381(2)	0.5640(8)	0.091(2)
C155	0.485(2)	0.500(2)	0.8352(5)	0.0694(14)
H15C	0.424831	0.530829	0.841389	0.083
H15D	0.474664	0.442670	0.839693	0.083
C47	0.390(3)	0.380(2)	0.5690(8)	0.091(2)
H47	0.344814	0.334478	0.567736	0.109
C129	0.914(2)	0.3514(18)	0.7396(5)	0.0640(12)
H129	0.932182	0.334128	0.722605	0.077
C80	1.006(2)	0.6149(19)	0.6775(6)	0.0703(17)
C8	0.835(2)	0.5123(16)	0.4954(5)	0.0597(13)
H8A	0.825584	0.460903	0.486516	0.072
H8B	0.886406	0.503560	0.508740	0.072
C41	0.909(2)	0.507(2)	0.5860(7)	0.0778(17)
C27	0.518(2)	0.7621(17)	0.4777(5)	0.0615(13)
H27	0.500874	0.812420	0.470529	0.074
C149	0.819(2)	0.2175(19)	0.7437(5)	0.0643(13)
C69	0.662(2)	0.9082(18)	0.6070(6)	0.0695(16)
C1	0.744(2)	0.4679(16)	0.4050(5)	0.0608(19)
H1A	0.766791	0.524051	0.403144	0.091

H1B	0.708676	0.450375	0.390098	0.091
H1C	0.805475	0.433710	0.407825	0.091
C40	0.984(2)	0.556(2)	0.5961(7)	0.0770(18)
H40	1.049549	0.541483	0.602491	0.092
C148	0.776(2)	0.1855(19)	0.7670(5)	0.0642(13)
H148	0.775002	0.130401	0.771641	0.077
C85	0.580(2)	0.5899(17)	0.7149(6)	0.0639(15)
C65	0.310(2)	0.7716(19)	0.6088(6)	0.0694(16)
C127	1.022(2)	0.4751(18)	0.7425(5)	0.0641(13)
H12A	1.046084	0.503625	0.727691	0.077
H12B	1.023034	0.513167	0.756451	0.077
C115	0.652(2)	0.6555(16)	0.7240(6)	0.0639(16)
C96	1.104(2)	0.3374(18)	0.6506(7)	0.0720(17)
C39	0.940(2)	0.634(2)	0.5949(7)	0.0762(17)
C147	0.737(2)	0.2462(19)	0.7804(5)	0.0641(13)
C131	1.089(2)	0.4052(18)	0.7476(5)	0.0644(13)
H13C	1.137678	0.417891	0.761075	0.077
H13D	1.129558	0.390863	0.732898	0.077
C25	0.137(2)	0.5057(18)	0.5201(6)	0.070(2)
H25A	0.091728	0.528227	0.507450	0.104
H25B	0.192503	0.544386	0.523954	0.104
H25C	0.096285	0.494899	0.534913	0.104
C33	0.658(2)	0.3553(16)	0.4446(5)	0.0605(13)
C111	0.359(2)	0.4584(18)	0.7032(6)	0.0669(16)
C34	0.768(2)	0.3288(16)	0.4472(5)	0.062(2)
H34A	0.799500	0.324340	0.430933	0.093
H34B	0.770051	0.276285	0.455363	0.093
H34C	0.806297	0.368379	0.456940	0.093
C32	0.815(2)	0.7205(15)	0.4659(5)	0.0603(19)
H32A	0.836454	0.749029	0.480801	0.090
H32B	0.757457	0.749273	0.458154	0.090
H32C	0.874313	0.718061	0.454530	0.090
C81	1.006(2)	0.5340(18)	0.6708(6)	0.0699(16)
C3	0.516(2)	0.4877(16)	0.4221(5)	0.0605(19)
H3A	0.465307	0.465372	0.433580	0.091
H3B	0.503072	0.465960	0.405669	0.091
H3C	0.509504	0.546549	0.421675	0.091
C151	0.689(2)	0.2425(19)	0.8048(5)	0.064(2)
H15E	0.739390	0.259754	0.817219	0.097
H15F	0.666837	0.187133	0.808266	0.097
H15G	0.628169	0.278255	0.805283	0.097
C132	1.063(2)	0.2476(18)	0.7508(5)	0.0653(19)
H13E	1.009000	0.206338	0.751698	0.098
H13F	1.116263	0.236867	0.763353	0.098
H13G	1.095949	0.246330	0.734599	0.098
C159	0.512(2)	0.6126(19)	0.7912(6)	0.0694(14)
H15H	0.579322	0.630887	0.797849	0.083
H15I	0.516676	0.614374	0.773085	0.083
C139	0.893(2)	0.5806(19)	0.8451(5)	0.070(2)
H13H	0.824804	0.563765	0.851155	0.104
H13I	0.897993	0.639520	0.845488	0.104
H13J	0.947702	0.557568	0.855559	0.104
C20	0.188(2)	0.4849(18)	0.4577(6)	0.0685(14)
H20A	0.174011	0.540228	0.463663	0.082
H20B	0.232952	0.489358	0.443068	0.082
C24	0.188(2)	0.4227(18)	0.5104(6)	0.0686(14)

H24A	0.132042	0.382490	0.508376	0.082
H24B	0.236194	0.402136	0.523123	0.082
C23	0.344(2)	0.2721(18)	0.4876(6)	0.070(2)
H23A	0.372201	0.223836	0.479713	0.104
H23B	0.287552	0.256548	0.498766	0.104
H23C	0.399063	0.299087	0.496899	0.104
C21	0.084(2)	0.4464(18)	0.4501(6)	0.069(2)
H21A	0.046573	0.483130	0.439152	0.104
H21B	0.041906	0.435937	0.464669	0.104
H21C	0.097714	0.395567	0.441532	0.104
C22	0.303(2)	0.3272(18)	0.4689(6)	0.0686(14)
H22A	0.243204	0.301280	0.460627	0.082
H22B	0.357693	0.336453	0.456404	0.082
C138	0.907(2)	0.5522(19)	0.8200(6)	0.0690(14)
C137	0.859(2)	0.3863(19)	0.8362(5)	0.069(2)
H13K	0.791262	0.396954	0.828782	0.103
H13L	0.858409	0.402664	0.853392	0.103
H13M	0.874989	0.328608	0.835047	0.103
C136	1.088(2)	0.4313(19)	0.8321(5)	0.069(2)
H13N	1.128825	0.394900	0.821726	0.103
H13O	1.080406	0.407540	0.848438	0.103
H13P	1.124215	0.483154	0.833468	0.103
C141	0.830(2)	0.566(2)	0.8021(5)	0.070(2)
H14A	0.861598	0.562870	0.785790	0.105
H14B	0.799904	0.619625	0.804504	0.105
H14C	0.775490	0.525131	0.803583	0.105
C157	0.368(2)	0.4770(19)	0.7857(6)	0.0695(14)
H15J	0.310052	0.512566	0.790826	0.083
H15K	0.375210	0.480215	0.767732	0.083
C140	1.007(2)	0.6061(19)	0.8102(6)	0.070(2)
H14D	1.071996	0.584259	0.817056	0.106
H14E	0.999059	0.662220	0.815361	0.106
H14F	1.010612	0.603637	0.792258	0.106
C36	0.597(2)	0.2948(16)	0.4282(5)	0.062(2)
H36A	0.522476	0.300516	0.431033	0.092
H36B	0.619085	0.239749	0.432099	0.092
H36C	0.612750	0.306174	0.410923	0.092
C158	0.345(2)	0.3859(19)	0.7939(6)	0.070(2)
H15L	0.390090	0.349217	0.784739	0.105
H15M	0.271790	0.372850	0.790458	0.105
H15N	0.358136	0.380006	0.811458	0.105
C156	0.589(2)	0.5322(19)	0.8480(6)	0.070(2)
H15O	0.607597	0.584602	0.841023	0.105
H15P	0.645449	0.493821	0.845276	0.105
H15Q	0.576616	0.538163	0.865636	0.105
C160	0.433(2)	0.6675(19)	0.7988(6)	0.071(2)
H16A	0.364898	0.649234	0.792727	0.106
H16B	0.447661	0.721280	0.792306	0.106
H16C	0.430964	0.669807	0.816759	0.106
C73	0.913(2)	0.416(2)	0.5833(7)	0.0799(18)
C53	0.259(3)	0.488(2)	0.5856(8)	0.091(2)
F76	0.8313(13)	0.3796(11)	0.5910(4)	0.081(2)
F108	0.8802(12)	0.2068(11)	0.6148(4)	0.080(2)
F75	0.9151(14)	0.3974(11)	0.5594(4)	0.084(2)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic displacement parameters [Å²] for 26. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ag83	0.0340(7)	0.0384(7)	0.0518(8)	0.0019(6)	0.0041(6)	−0.0021(6)
Ag89	0.0335(8)	0.0437(8)	0.0510(8)	−0.0062(7)	0.0034(6)	0.0003(6)
Ag60	0.0342(8)	0.0496(8)	0.0496(8)	−0.0076(7)	0.0050(7)	−0.0053(7)
Ag92	0.0321(7)	0.0401(7)	0.0584(9)	−0.0039(7)	0.0029(7)	−0.0023(6)
Ag43	0.0388(8)	0.0501(9)	0.0608(9)	−0.0052(8)	−0.0013(7)	−0.0031(7)
Ag57	0.0399(8)	0.0509(9)	0.0547(9)	−0.0070(8)	0.0023(7)	−0.0058(7)
Si21	0.058(3)	0.055(2)	0.067(3)	−0.015(2)	−0.003(2)	0.000(2)
Si15	0.055(2)	0.079(3)	0.073(3)	−0.003(2)	0.003(2)	−0.003(2)
Si20	0.055(3)	0.080(3)	0.070(3)	0.003(2)	−0.003(2)	0.000(2)
Si19	0.057(3)	0.065(2)	0.081(3)	−0.005(2)	−0.003(2)	−0.002(2)
O144	0.049(2)	0.075(3)	0.067(3)	0.003(2)	0.001(2)	−0.001(2)
O134	0.053(2)	0.078(3)	0.068(3)	0.003(2)	−0.002(2)	0.000(2)
F78	0.043(4)	0.080(4)	0.100(5)	−0.014(4)	−0.002(4)	−0.002(4)
O31	0.052(4)	0.055(3)	0.068(4)	−0.011(3)	−0.004(3)	0.002(3)
O14	0.056(2)	0.058(2)	0.071(3)	−0.010(2)	−0.003(2)	0.001(2)
F116	0.037(4)	0.060(4)	0.097(5)	−0.012(4)	−0.003(4)	−0.005(3)
F77	0.044(4)	0.078(4)	0.102(5)	−0.016(4)	0.000(4)	−0.001(4)
N59	0.054(3)	0.069(4)	0.082(4)	−0.008(3)	0.006(3)	−0.002(3)
F99	0.048(4)	0.068(4)	0.103(5)	−0.004(4)	0.009(4)	0.000(4)
F119	0.053(4)	0.066(4)	0.097(5)	−0.004(4)	0.008(4)	−0.007(4)
N44	0.064(4)	0.080(4)	0.126(5)	−0.021(4)	0.017(4)	−0.008(3)
F68	0.054(4)	0.073(4)	0.085(4)	−0.006(4)	0.008(4)	0.000(4)
F118	0.036(4)	0.057(4)	0.098(5)	−0.013(4)	−0.001(4)	−0.003(3)
F117	0.036(4)	0.059(4)	0.096(5)	−0.012(4)	−0.002(4)	−0.006(3)
F105	0.043(4)	0.077(4)	0.112(5)	−0.020(4)	0.000(4)	−0.003(4)
F110	0.046(4)	0.080(4)	0.111(5)	−0.024(4)	0.001(4)	0.001(4)
O4	0.057(2)	0.055(2)	0.067(3)	−0.014(2)	−0.003(2)	0.000(2)
F37	0.045(4)	0.079(4)	0.101(5)	−0.012(4)	0.001(4)	−0.002(4)
N58	0.054(3)	0.069(4)	0.081(4)	−0.008(3)	0.006(3)	−0.002(3)
O161	0.048(3)	0.074(4)	0.064(4)	0.005(3)	0.000(3)	−0.001(3)
F114	0.037(3)	0.066(4)	0.103(5)	−0.015(4)	0.000(4)	−0.003(3)
F71	0.056(4)	0.068(4)	0.085(4)	−0.008(4)	0.007(4)	−0.005(4)
F67	0.055(4)	0.075(4)	0.084(4)	−0.007(4)	0.005(4)	−0.002(4)
F79	0.048(4)	0.065(4)	0.100(5)	−0.003(4)	0.007(4)	−0.009(3)
O162	0.048(3)	0.076(4)	0.065(4)	0.003(3)	0.000(3)	0.000(3)
F109	0.048(4)	0.080(4)	0.114(5)	−0.021(4)	−0.001(4)	0.002(4)
O153	0.053(2)	0.078(3)	0.071(3)	−0.001(2)	0.003(2)	−0.002(2)
N45	0.064(4)	0.081(4)	0.126(5)	−0.021(4)	0.017(4)	−0.009(3)
F112	0.037(3)	0.070(4)	0.103(5)	−0.014(4)	−0.002(4)	−0.006(3)
N90	0.041(3)	0.075(4)	0.110(5)	−0.021(4)	−0.001(3)	−0.002(3)
F104	0.044(4)	0.075(4)	0.112(5)	−0.019(4)	−0.002(4)	0.000(4)
F97	0.047(4)	0.070(4)	0.104(5)	−0.003(4)	0.012(4)	−0.001(4)
O29	0.059(4)	0.058(3)	0.070(4)	−0.011(3)	−0.003(3)	0.001(3)
F54	0.063(5)	0.083(5)	0.127(6)	−0.021(5)	0.019(5)	−0.007(4)
C9	0.055(3)	0.056(2)	0.068(3)	−0.012(2)	−0.004(2)	0.001(2)
N93	0.046(3)	0.065(3)	0.098(4)	−0.003(3)	0.008(3)	−0.004(3)
O18	0.057(3)	0.063(2)	0.078(3)	−0.007(2)	−0.003(2)	−0.001(2)
O16	0.057(4)	0.059(3)	0.070(4)	−0.012(3)	−0.004(3)	0.003(3)
F70	0.060(4)	0.069(4)	0.087(4)	−0.009(4)	0.005(4)	−0.004(4)
F120	0.048(4)	0.066(4)	0.098(5)	−0.003(4)	0.004(4)	−0.003(3)
N61	0.047(3)	0.079(4)	0.103(4)	−0.014(4)	0.001(3)	−0.001(3)
F50	0.068(5)	0.082(5)	0.128(6)	−0.022(5)	0.013(5)	−0.004(4)

N82	0.046(3)	0.065(3)	0.098(4)	−0.003(3)	0.008(3)	−0.005(3)
F98	0.052(4)	0.072(4)	0.103(5)	−0.002(4)	0.007(4)	0.002(4)
F66	0.055(4)	0.073(4)	0.082(4)	−0.004(4)	0.006(4)	−0.003(4)
F106	0.044(4)	0.077(4)	0.112(5)	−0.022(4)	−0.003(4)	−0.003(4)
C145	0.050(2)	0.076(3)	0.068(2)	0.002(2)	0.001(2)	−0.002(2)
F51	0.070(5)	0.083(5)	0.128(6)	−0.021(5)	0.016(5)	−0.005(4)
F56	0.067(5)	0.084(5)	0.127(6)	−0.021(5)	0.022(5)	−0.009(4)
F72	0.056(4)	0.072(4)	0.085(4)	−0.009(4)	0.006(4)	−0.005(4)
N88	0.034(3)	0.060(3)	0.098(4)	−0.013(3)	−0.002(3)	−0.004(3)
C143	0.049(2)	0.075(3)	0.066(2)	0.003(2)	0.001(2)	−0.001(2)
N42	0.048(3)	0.079(4)	0.104(4)	−0.014(4)	0.001(3)	−0.001(3)
F113	0.038(4)	0.066(4)	0.106(5)	−0.010(4)	−0.002(4)	−0.005(3)
C142	0.049(2)	0.076(2)	0.067(2)	0.003(2)	0.000(2)	−0.001(2)
N91	0.042(3)	0.076(4)	0.110(5)	−0.021(4)	−0.001(3)	−0.001(3)
C26	0.057(3)	0.058(2)	0.071(3)	−0.010(2)	−0.003(2)	0.001(2)
O150	0.053(3)	0.077(4)	0.070(4)	0.004(3)	0.000(3)	0.000(3)
C5	0.056(2)	0.055(2)	0.068(2)	−0.013(2)	−0.004(2)	0.000(2)
C15	0.056(2)	0.058(2)	0.070(3)	−0.011(2)	−0.004(2)	0.002(2)
C124	0.08(2)	0.11(3)	0.031(11)	0.022(14)	0.004(12)	−0.003(18)
C123	0.07(2)	0.10(2)	0.047(14)	0.035(16)	−0.009(13)	−0.013(18)
C122	0.09(2)	0.08(2)	0.062(16)	0.043(16)	−0.001(15)	−0.001(18)
C121	0.07(2)	0.12(3)	0.073(19)	0.045(19)	0.003(17)	0.02(2)
C125	0.059(16)	0.10(2)	0.062(15)	0.053(15)	−0.022(13)	−0.036(16)
C46	0.064(4)	0.081(4)	0.126(5)	−0.021(4)	0.017(4)	−0.009(3)
C152	0.051(2)	0.077(3)	0.069(3)	0.000(2)	0.002(2)	−0.002(2)
N84	0.034(3)	0.060(3)	0.098(4)	−0.013(3)	−0.001(3)	−0.004(3)
C11	0.056(2)	0.057(2)	0.070(2)	−0.011(2)	−0.004(2)	0.001(2)
C103	0.043(3)	0.076(4)	0.111(5)	−0.021(4)	−0.001(3)	−0.002(3)
C133	0.052(2)	0.078(3)	0.067(3)	0.003(2)	−0.001(2)	−0.001(2)
F74	0.053(4)	0.082(4)	0.111(5)	−0.013(4)	0.002(4)	0.001(4)
C13	0.056(2)	0.059(2)	0.072(2)	−0.010(2)	−0.003(2)	0.001(2)
C128	0.049(2)	0.076(3)	0.066(3)	0.003(2)	0.000(2)	−0.001(2)
C62	0.055(3)	0.069(3)	0.082(4)	−0.008(3)	0.006(3)	−0.003(3)
C63	0.054(3)	0.069(3)	0.082(4)	−0.008(3)	0.006(3)	−0.003(3)
C12	0.056(2)	0.058(2)	0.071(2)	−0.010(2)	−0.003(2)	0.001(2)
C38	0.045(3)	0.079(4)	0.102(4)	−0.014(4)	0.001(3)	−0.001(3)
C102	0.042(3)	0.076(4)	0.110(5)	−0.021(4)	−0.001(3)	−0.002(3)
C7	0.055(3)	0.056(2)	0.068(3)	−0.012(2)	−0.004(2)	0.001(2)
C101	0.042(3)	0.076(4)	0.110(5)	−0.021(4)	−0.001(3)	−0.001(3)
C28	0.057(3)	0.057(2)	0.070(3)	−0.011(2)	−0.003(2)	0.001(2)
C17	0.057(2)	0.061(2)	0.075(3)	−0.008(2)	−0.003(2)	0.000(2)
C107	0.044(3)	0.078(4)	0.112(5)	−0.022(4)	0.000(3)	0.000(3)
C87	0.034(3)	0.061(3)	0.099(4)	−0.013(3)	−0.001(3)	−0.004(3)
C130	0.050(2)	0.077(3)	0.067(2)	0.003(2)	0.000(2)	−0.001(2)
C49	0.067(4)	0.081(4)	0.127(5)	−0.021(4)	0.016(4)	−0.007(3)
F52	0.070(5)	0.081(5)	0.130(6)	−0.021(5)	0.015(5)	−0.006(4)
C86	0.034(3)	0.060(3)	0.098(4)	−0.013(3)	−0.001(3)	−0.004(3)
C6	0.056(2)	0.056(2)	0.068(2)	−0.012(2)	−0.004(2)	0.000(2)
C64	0.054(3)	0.070(3)	0.082(4)	−0.007(3)	0.006(3)	−0.002(3)
C95	0.046(3)	0.066(3)	0.098(4)	−0.003(3)	0.008(3)	−0.004(3)
F55	0.064(5)	0.084(5)	0.129(6)	−0.022(5)	0.020(5)	−0.010(4)
C30	0.057(4)	0.058(4)	0.071(4)	−0.010(3)	−0.003(3)	0.001(3)
C35	0.058(4)	0.056(4)	0.068(4)	−0.014(4)	−0.002(4)	−0.001(4)
C100	0.043(3)	0.076(4)	0.111(5)	−0.022(4)	−0.001(3)	−0.001(3)
C146	0.049(2)	0.076(3)	0.067(2)	0.003(2)	0.001(2)	−0.001(2)
C10	0.055(2)	0.056(2)	0.069(2)	−0.012(2)	−0.004(2)	0.001(2)

C94	0.046(3)	0.066(3)	0.099(4)	−0.003(3)	0.008(3)	−0.004(3)
C48	0.065(4)	0.081(4)	0.126(5)	−0.021(4)	0.016(4)	−0.008(3)
C155	0.056(3)	0.079(3)	0.074(3)	−0.003(3)	0.003(3)	−0.003(3)
C47	0.065(4)	0.081(4)	0.126(5)	−0.021(4)	0.017(4)	−0.008(3)
C129	0.049(2)	0.076(3)	0.066(2)	0.003(2)	0.000(2)	−0.001(2)
C80	0.048(3)	0.065(3)	0.098(4)	−0.003(3)	0.007(3)	−0.005(3)
C8	0.055(3)	0.056(2)	0.068(3)	−0.012(2)	−0.004(2)	0.001(2)
C41	0.049(3)	0.079(4)	0.105(4)	−0.014(4)	0.001(3)	0.000(3)
C27	0.057(3)	0.058(2)	0.070(3)	−0.010(2)	−0.003(2)	0.001(2)
C149	0.050(2)	0.076(3)	0.067(3)	0.003(2)	0.000(2)	−0.001(2)
C69	0.056(3)	0.069(3)	0.084(4)	−0.008(3)	0.006(3)	−0.004(3)
C1	0.059(4)	0.056(3)	0.067(4)	−0.015(3)	−0.003(3)	−0.001(3)
C40	0.048(3)	0.079(4)	0.104(4)	−0.014(4)	0.001(3)	0.000(3)
C148	0.049(3)	0.076(3)	0.067(3)	0.003(2)	0.001(2)	−0.001(2)
C85	0.035(3)	0.060(3)	0.098(4)	−0.013(3)	−0.002(3)	−0.004(3)
C65	0.054(3)	0.071(4)	0.083(4)	−0.007(3)	0.006(3)	−0.002(3)
C127	0.049(3)	0.077(3)	0.066(3)	0.004(3)	0.000(2)	−0.001(2)
C115	0.035(3)	0.059(3)	0.097(4)	−0.013(3)	−0.002(3)	−0.004(3)
C96	0.047(3)	0.068(3)	0.101(4)	−0.003(3)	0.009(3)	−0.002(3)
C39	0.047(3)	0.079(4)	0.103(4)	−0.014(4)	0.001(3)	−0.001(3)
C147	0.049(2)	0.076(3)	0.067(3)	0.003(2)	0.001(2)	−0.001(2)
C131	0.050(3)	0.077(3)	0.067(3)	0.003(2)	0.000(2)	−0.001(2)
C25	0.059(4)	0.068(4)	0.082(4)	−0.005(4)	−0.002(4)	−0.002(4)
C33	0.058(3)	0.056(3)	0.067(3)	−0.015(2)	−0.003(2)	0.000(2)
C111	0.036(3)	0.064(3)	0.101(4)	−0.013(3)	−0.002(3)	−0.004(3)
C34	0.060(4)	0.057(4)	0.069(4)	−0.014(4)	−0.002(4)	0.000(4)
C32	0.056(4)	0.056(3)	0.069(4)	−0.012(3)	−0.004(3)	0.000(3)
C81	0.046(3)	0.065(3)	0.098(4)	−0.003(3)	0.008(3)	−0.005(3)
C3	0.058(4)	0.056(3)	0.068(4)	−0.015(3)	−0.004(3)	0.000(3)
C151	0.049(4)	0.076(4)	0.068(4)	0.005(4)	0.000(3)	−0.001(4)
C132	0.051(4)	0.078(4)	0.068(4)	0.003(3)	0.001(3)	0.000(3)
C159	0.055(3)	0.079(3)	0.074(3)	−0.003(3)	0.003(3)	−0.003(3)
C139	0.058(4)	0.080(4)	0.071(4)	0.002(4)	−0.004(4)	0.000(4)
C20	0.058(3)	0.066(3)	0.082(3)	−0.005(3)	−0.003(3)	−0.003(3)
C24	0.058(3)	0.066(3)	0.082(3)	−0.005(3)	−0.003(3)	−0.002(3)
C23	0.058(4)	0.067(4)	0.083(4)	−0.005(4)	−0.001(4)	−0.003(4)
C21	0.058(4)	0.068(4)	0.083(4)	−0.006(4)	−0.003(4)	−0.003(4)
C22	0.058(3)	0.066(3)	0.082(3)	−0.005(3)	−0.002(3)	−0.003(3)
C138	0.056(3)	0.080(3)	0.070(3)	0.003(3)	−0.003(3)	0.000(3)
C137	0.056(4)	0.080(4)	0.070(4)	0.002(4)	−0.003(3)	0.000(4)
C136	0.055(4)	0.081(4)	0.070(4)	0.003(4)	−0.003(3)	0.000(4)
C141	0.058(4)	0.081(4)	0.071(4)	0.002(4)	−0.003(4)	0.000(4)
C157	0.055(3)	0.079(3)	0.074(3)	−0.003(3)	0.003(3)	−0.003(3)
C140	0.058(4)	0.081(4)	0.072(4)	0.003(4)	−0.003(4)	0.000(4)
C36	0.060(4)	0.057(4)	0.068(4)	−0.014(4)	−0.003(4)	−0.001(4)
C158	0.055(4)	0.080(4)	0.075(4)	−0.003(4)	0.003(4)	−0.003(4)
C156	0.057(4)	0.079(4)	0.074(4)	−0.003(4)	0.002(4)	−0.004(4)
C160	0.057(4)	0.080(4)	0.075(4)	−0.004(4)	0.003(4)	−0.003(4)
C73	0.052(3)	0.081(4)	0.107(4)	−0.013(4)	0.001(3)	0.001(3)
C53	0.065(4)	0.082(4)	0.127(5)	−0.021(4)	0.019(4)	−0.009(3)
F76	0.054(4)	0.080(4)	0.110(5)	−0.012(4)	0.000(4)	0.002(4)
F108	0.045(4)	0.079(4)	0.115(5)	−0.023(4)	0.002(4)	−0.001(4)
F75	0.059(4)	0.083(4)	0.110(5)	−0.014(4)	0.003(4)	0.001(4)

Table 4. Bond lengths and angles for 26.

Atom–Atom	Length [Å]
Ag83–N82	2.15(2)
Ag83–N84	2.17(2)
Ag89–N90	2.07(3)
Ag89–N88	2.13(2)
Ag60–N59	2.11(2)
Ag60–N61	2.13(3)
Ag92–N93	2.16(2)
Ag92–N91	2.09(2)
Ag43–N44	2.16(3)
Ag43–N42	2.19(3)
Ag57–N58	2.12(3)
Ag57–N45	2.11(3)
Si21–O4	1.668(18)
Si21–C1	1.91(3)
Si21–C33	1.86(3)
Si21–C3	1.89(3)
Si15–O153	1.64(2)
Si15–C155	1.89(3)
Si15–C159	1.83(3)
Si15–C157	1.84(3)
Si20–O134	1.68(2)
Si20–C138	1.91(3)
Si20–C137	1.92(3)
Si20–C136	1.76(3)
Si19–O18	1.67(2)
Si19–C20	1.86(3)
Si19–C24	1.81(3)
Si19–C22	1.91(3)
O144–C145	1.42(3)
O144–C143	1.34(3)
O134–C133	1.44(4)
F78–C38	1.35(4)
O31–C9	1.20(3)
O14–C15	1.31(3)
O14–C13	1.45(3)
F116–C115	1.32(3)
F77–C38	1.40(3)
N59–N58	1.40(3)
N59–C62	1.33(4)
F99–C96	1.27(3)
F119–C80	1.35(4)
N44–N45	1.29(4)
N44–C48	1.35(4)
F68–C65	1.32(3)
F118–C115	1.40(3)
F117–C115	1.24(3)
F105–C103	1.41(4)
F110–C107	1.40(4)
O4–C5	1.37(3)
F37–C38	1.38(4)
N58–C64	1.28(4)
O161–C143	1.20(3)
F114–C111	1.27(3)
F71–C69	1.34(3)
F67–C65	1.35(3)

F79–C80	1.32(3)
O162–C128	1.18(3)
F109–C107	1.33(4)
O153–C152	1.43(3)
N45–C46	1.31(4)
F112–C111	1.34(4)
N90–N91	1.43(3)
N90–C102	1.33(4)
F104–C103	1.35(4)
F97–C96	1.34(3)
O29–C28	1.25(3)
F54–C53	1.32(4)
C9–C10	1.55(4)
C9–C8	1.48(4)
N93–N82	1.36(3)
N93–C94	1.34(4)
O18–C17	1.44(3)
O16–C15	1.22(3)
F70–C69	1.33(3)
F120–C80	1.36(3)
N61–N42	1.35(4)
N61–C39	1.33(4)
F50–C49	1.29(4)
N82–C81	1.31(4)
F98–C96	1.37(4)
F66–C65	1.38(4)
F106–C103	1.32(3)
C145–H145	1.0000
C145–C152	1.54(4)
C145–C146	1.57(4)
F51–C49	1.29(4)
F56–C53	1.32(4)
F72–C69	1.42(4)
N88–N84	1.35(3)
N88–C87	1.30(3)
C143–C142	1.55(4)
N42–C41	1.27(4)
F113–C111	1.33(4)
C142–C146	1.50(4)
C142–C129	1.51(4)
C142–C149	1.58(4)
N91–C100	1.36(4)
C26–C12	1.49(4)
C26–C30	1.46(4)
C26–C27	1.37(4)
O150–C149	1.17(3)
C5–H5A	0.9900
C5–H5B	0.9900
C5–C6	1.54(4)
C15–C11	1.54(4)
C124–H124	0.9500
C124–C123	1.3900
C124–C125	1.3900
C123–H123	0.9500
C123–C122	1.3900
C122–H122	0.9500

C122–C121	1.3900
C121–H121	0.9500
C121–C126	1.3900
C126–H126	0.9500
C126–C125	1.3900
C125–H125	0.9500
C46–C47	1.36(5)
C46–C53	1.54(5)
C152–H15A	0.9900
C152–H15B	0.9900
N84–C85	1.33(3)
C11–C12	1.53(4)
C11–C28	1.54(4)
C11–C10	1.56(4)
C103–C102	1.45(4)
C133–H13A	0.9900
C133–H13B	0.9900
C133–C130	1.53(4)
F74–C73	1.30(4)
C13–H13	1.0000
C13–C12	1.54(4)
C13–C17	1.56(4)
C128–C129	1.54(4)
C128–C127	1.51(4)
C62–C63	1.43(4)
C62–C69	1.42(4)
C63–H63	0.9500
C63–C64	1.40(4)
C12–H12	1.0000
C38–C39	1.41(4)
C102–C101	1.35(4)
C7–H7A	0.9900
C7–H7B	0.9900
C7–C6	1.53(4)
C7–C8	1.57(4)
C101–H101	0.9500
C101–C100	1.40(4)
C28–C27	1.43(4)
C17–H17A	0.9900
C17–H17B	0.9900
C107–C100	1.39(4)
C107–F108	1.37(3)
C87–C86	1.40(4)
C87–C111	1.49(4)
C130–C129	1.58(4)
C130–C131	1.60(4)
C130–C132	1.55(4)
C49–F52	1.38(4)
C49–C48	1.45(5)
C86–H86	0.9500
C86–C85	1.39(4)
C6–C10	1.56(4)
C6–C32	1.56(4)
C64–C65	1.47(4)
C95–H95	0.9500
C95–C94	1.38(4)

C95–C81	1.42(4)
F55–C53	1.29(4)
C30–H30A	0.9800
C30–H30B	0.9800
C30–H30C	0.9800
C35–H35A	0.9800
C35–H35B	0.9800
C35–H35C	0.9800
C35–C33	1.56(4)
C146–H146	1.0000
C146–C147	1.52(4)
C10–H10	1.0000
C94–C96	1.47(4)
C48–C47	1.30(5)
C155–H15C	0.9900
C155–H15D	0.9900
C155–C156	1.60(4)
C47–H47	0.9500
C129–H129	1.0000
C80–C81	1.39(4)
C8–H8A	0.9900
C8–H8B	0.9900
C41–C40	1.37(4)
C41–C73	1.52(5)
C27–H27	0.9500
C149–C148	1.49(4)
C1–H1A	0.9800
C1–H1B	0.9800
C1–H1C	0.9800
C40–H40	0.9500
C40–C39	1.40(5)
C148–H148	0.9500
C148–C147	1.34(4)
C85–C115	1.51(4)
C127–H12A	0.9900
C127–H12B	0.9900
C127–C131	1.47(4)
C147–C151	1.47(4)
C131–H13C	0.9900
C131–H13D	0.9900
C25–H25A	0.9800
C25–H25B	0.9800
C25–H25C	0.9800
C25–C24	1.62(4)
C33–C34	1.49(4)
C33–C36	1.55(3)
C34–H34A	0.9800
C34–H34B	0.9800
C34–H34C	0.9800
C32–H32A	0.9800
C32–H32B	0.9800
C32–H32C	0.9800
C3–H3A	0.9800
C3–H3B	0.9800
C3–H3C	0.9800
C151–H15E	0.9800

C151–H15F	0.9800
C151–H15G	0.9800
C132–H13E	0.9800
C132–H13F	0.9800
C132–H13G	0.9800
C159–H15H	0.9900
C159–H15I	0.9900
C159–C160	1.43(4)
C139–H13H	0.9800
C139–H13I	0.9800
C139–H13J	0.9800
C139–C138	1.46(4)
C20–H20A	0.9900
C20–H20B	0.9900
C20–C21	1.54(4)
C24–H24A	0.9900
C24–H24B	0.9900
C23–H23A	0.9800
C23–H23B	0.9800
C23–H23C	0.9800
C23–C22	1.47(4)
C21–H21A	0.9800
C21–H21B	0.9800
C21–H21C	0.9800
C22–H22A	0.9900
C22–H22B	0.9900
C138–C141	1.41(4)
C138–C140	1.66(4)
C137–H13K	0.9800
C137–H13L	0.9800
C137–H13M	0.9800
C136–H13N	0.9800
C136–H13O	0.9800
C136–H13P	0.9800
C141–H14A	0.9800
C141–H14B	0.9800
C141–H14C	0.9800
C157–H15J	0.9900
C157–H15K	0.9900
C157–C158	1.60(4)
C140–H14D	0.9800
C140–H14E	0.9800
C140–H14F	0.9800
C36–H36A	0.9800
C36–H36B	0.9800
C36–H36C	0.9800
C158–H15L	0.9800
C158–H15M	0.9800
C158–H15N	0.9800
C156–H15O	0.9800
C156–H15P	0.9800
C156–H15Q	0.9800
C160–H16A	0.9800
C160–H16B	0.9800
C160–H16C	0.9800
C73–F76	1.28(4)

C73–F75	1.34(4)

Atom–Atom–Atom	**Angle [°]**
N82–Ag83–N84	178.8(9)
N90–Ag89–N88	171.5(10)
N59–Ag60–N61	173.0(11)
N91–Ag92–N93	169.3(11)
N44–Ag43–N42	164.1(12)
N45–Ag57–N58	175.9(10)
O4–Si21–C1	111.0(11)
O4–Si21–C33	105.9(11)
O4–Si21–C3	109.5(11)
C33–Si21–C1	109.3(13)
C33–Si21–C3	111.9(13)
C3–Si21–C1	109.2(12)
O153–Si15–C155	107.0(13)
O153–Si15–C159	111.0(13)
O153–Si15–C157	108.6(13)
C159–Si15–C155	111.1(15)
C159–Si15–C157	106.0(14)
C157–Si15–C155	113.1(14)
O134–Si20–C138	108.0(12)
O134–Si20–C137	103.7(12)
O134–Si20–C136	113.2(13)
C138–Si20–C137	101.2(14)
C136–Si20–C138	117.8(15)
C136–Si20–C137	111.3(14)
O18–Si19–C20	104.5(12)
O18–Si19–C24	109.3(13)
O18–Si19–C22	105.9(12)
C20–Si19–C22	109.0(14)
C24–Si19–C20	112.9(14)
C24–Si19–C22	114.5(14)
C143–O144–C145	112(2)
C133–O134–Si20	122.1(18)
C15–O14–C13	110(2)
N58–N59–Ag60	118.4(18)
C62–N59–Ag60	133(2)
C62–N59–N58	108(2)
N45–N44–Ag43	117(2)
N45–N44–C48	109(3)
C48–N44–Ag43	133(2)
C5–O4–Si21	121.6(17)
N59–N58–Ag57	118.4(17)
C64–N58–Ag57	132(2)
C64–N58–N59	110(2)
C152–O153–Si15	121.7(18)
N44–N45–Ag57	121(2)
N44–N45–C46	108(3)
C46–N45–Ag57	131(2)
N91–N90–Ag89	119.2(17)
C102–N90–Ag89	135(2)
C102–N90–N91	106(2)
O31–C9–C10	125(3)
O31–C9–C8	127(3)
C8–C9–C10	108(2)

N82–N93–Ag92	117.1(17)
C94–N93–Ag92	129(2)
C94–N93–N82	108(2)
C17–O18–Si19	130.2(19)
N42–N61–Ag60	120.0(19)
C39–N61–Ag60	129(2)
C39–N61–N42	106(3)
N93–N82–Ag83	120.3(17)
C81–N82–Ag83	129(2)
C81–N82–N93	109(2)
O144–C145–H145	108.4
O144–C145–C152	108(2)
O144–C145–C146	107(2)
C152–C145–H145	108.4
C152–C145–C146	117(3)
C146–C145–H145	108.4
N84–N88–Ag89	118.7(16)
C87–N88–Ag89	135.4(18)
C87–N88–N84	106(2)
O144–C143–C142	111(2)
O161–C143–O144	123(3)
O161–C143–C142	125(3)
N61–N42–Ag43	119.1(19)
C41–N42–Ag43	127(2)
C41–N42–N61	112(3)
C143–C142–C149	106(2)
C146–C142–C143	104(2)
C146–C142–C129	123(3)
C146–C142–C149	104(2)
C129–C142–C143	108(2)
C129–C142–C149	111(2)
N90–N91–Ag92	118.3(18)
C100–N91–Ag92	133(2)
C100–N91–N90	108(2)
C30–C26–C12	122(2)
C27–C26–C12	111(2)
C27–C26–C30	126(3)
O4–C5–H5A	109.2
O4–C5–H5B	109.2
O4–C5–C6	112(2)
H5A–C5–H5B	107.9
C6–C5–H5A	109.2
C6–C5–H5B	109.2
O14–C15–C11	113(2)
O16–C15–O14	124(3)
O16–C15–C11	122(3)
C123–C124–H124	120.0
C123–C124–C125	120.0
C125–C124–H124	120.0
C124–C123–H123	120.0
C124–C123–C122	120.0
C122–C123–H123	120.0
C123–C122–H122	120.0
C121–C122–C123	120.0
C121–C122–H122	120.0
C122–C121–H121	120.0

C122–C121–C126	120.0
C126–C121–H121	120.0
C121–C126–H126	120.0
C125–C126–C121	120.0
C125–C126–H126	120.0
C124–C125–H125	120.0
C126–C125–C124	120.0
C126–C125–H125	120.0
N45–C46–C47	108(3)
N45–C46–C53	122(3)
C47–C46–C53	129(3)
O153–C152–C145	107(2)
O153–C152–H15A	110.2
O153–C152–H15B	110.2
C145–C152–H15A	110.2
C145–C152–H15B	110.2
H15A–C152–H15B	108.5
N88–N84–Ag83	117.7(17)
C85–N84–Ag83	131.2(17)
C85–N84–N88	111(2)
C15–C11–C10	109(2)
C12–C11–C15	102(2)
C12–C11–C28	103(2)
C12–C11–C10	122(2)
C28–C11–C15	109(2)
C28–C11–C10	110(2)
F105–C103–C102	114(3)
F104–C103–F105	102(2)
F104–C103–C102	112(3)
F106–C103–F105	108(2)
F106–C103–F104	107(3)
F106–C103–C102	113(3)
O134–C133–H13A	109.4
O134–C133–H13B	109.4
O134–C133–C130	111(2)
H13A–C133–H13B	108.0
C130–C133–H13A	109.4
C130–C133–H13B	109.4
O14–C13–H13	108.0
O14–C13–C12	108(2)
O14–C13–C17	110(2)
C12–C13–H13	108.0
C12–C13–C17	115(2)
C17–C13–H13	108.0
O162–C128–C129	122(3)
O162–C128–C127	129(3)
C127–C128–C129	109(2)
N59–C62–C63	107(3)
N59–C62–C69	123(3)
C69–C62–C63	130(3)
C62–C63–H63	127.4
C64–C63–C62	105(3)
C64–C63–H63	127.4
C26–C12–C11	106(2)
C26–C12–C13	113(2)
C26–C12–H12	110.9

C11–C12–C13	105(2)
C11–C12–H12	110.9
C13–C12–H12	110.9
F78–C38–F77	106(3)
F78–C38–F37	104(2)
F78–C38–C39	115(3)
F77–C38–C39	114(2)
F37–C38–F77	104(3)
F37–C38–C39	113(3)
N90–C102–C103	119(3)
N90–C102–C101	112(3)
C101–C102–C103	129(3)
H7A–C7–H7B	108.8
C6–C7–H7A	110.7
C6–C7–H7B	110.7
C6–C7–C8	105(2)
C8–C7–H7A	110.7
C8–C7–H7B	110.7
C102–C101–H101	126.4
C102–C101–C100	107(3)
C100–C101–H101	126.4
O29–C28–C11	122(3)
O29–C28–C27	129(3)
C27–C28–C11	109(2)
O18–C17–C13	105(2)
O18–C17–H17A	110.8
O18–C17–H17B	110.8
C13–C17–H17A	110.8
C13–C17–H17B	110.8
H17A–C17–H17B	108.9
F109–C107–F110	100(2)
F109–C107–C100	115(3)
F109–C107–F108	106(2)
C100–C107–F110	112(3)
F108–C107–F110	104(3)
F108–C107–C100	118(3)
N88–C87–C86	112(2)
N88–C87–C111	120(2)
C86–C87–C111	128(2)
C133–C130–C129	114(2)
C133–C130–C131	109(2)
C133–C130–C132	104(2)
C129–C130–C131	101(2)
C132–C130–C129	115(2)
C132–C130–C131	114(2)
F50–C49–F51	102(3)
F50–C49–F52	105(3)
F50–C49–C48	117(3)
F51–C49–F52	102(3)
F51–C49–C48	119(4)
F52–C49–C48	110(3)
C87–C86–H86	128.7
C85–C86–C87	103(2)
C85–C86–H86	128.7
C5–C6–C10	114(2)
C5–C6–C32	109(2)

C7–C6–C5	109(2)
C7–C6–C10	102(2)
C7–C6–C32	111(2)
C32–C6–C10	112(2)
N58–C64–C63	110(3)
N58–C64–C65	121(3)
C63–C64–C65	129(3)
C94–C95–H95	127.8
C94–C95–C81	104(2)
C81–C95–H95	127.8
C26–C30–H30A	109.5
C26–C30–H30B	109.5
C26–C30–H30C	109.5
H30A–C30–H30B	109.5
H30A–C30–H30C	109.5
H30B–C30–H30C	109.5
H35A–C35–H35B	109.5
H35A–C35–H35C	109.5
H35B–C35–H35C	109.5
C33–C35–H35A	109.5
C33–C35–H35B	109.5
C33–C35–H35C	109.5
N91–C100–C101	107(3)
N91–C100–C107	120(3)
C101–C100–C107	132(3)
C145–C146–H146	111.4
C142–C146–C145	105(2)
C142–C146–H146	111.4
C142–C146–C147	106(2)
C147–C146–C145	111(2)
C147–C146–H146	111.4
C9–C10–C11	112(2)
C9–C10–C6	103(2)
C9–C10–H10	105.4
C11–C10–H10	105.4
C6–C10–C11	124(2)
C6–C10–H10	105.4
N93–C94–C95	109(3)
N93–C94–C96	119(3)
C95–C94–C96	132(3)
N44–C48–C49	119(3)
C47–C48–N44	108(3)
C47–C48–C49	133(4)
Si15–C155–H15C	109.0
Si15–C155–H15D	109.0
H15C–C155–H15D	107.8
C156–C155–Si15	113(2)
C156–C155–H15C	109.0
C156–C155–H15D	109.0
C46–C47–H47	126.7
C48–C47–C46	107(3)
C48–C47–H47	126.7
C142–C129–C128	115(2)
C142–C129–C130	122(2)
C142–C129–H129	104.9
C128–C129–C130	104(2)

C128–C129–H129	104.9
C130–C129–H129	104.9
F119–C80–F120	100(2)
F119–C80–C81	115(3)
F79–C80–F119	105(2)
F79–C80–F120	103(2)
F79–C80–C81	117(3)
F120–C80–C81	114(3)
C9–C8–C7	107(2)
C9–C8–H8A	110.4
C9–C8–H8B	110.4
C7–C8–H8A	110.4
C7–C8–H8B	110.4
H8A–C8–H8B	108.6
N42–C41–C40	109(3)
N42–C41–C73	124(3)
C40–C41–C73	128(3)
C26–C27–C28	110(3)
C26–C27–H27	124.8
C28–C27–H27	124.8
O150–C149–C142	125(3)
O150–C149–C148	128(3)
C148–C149–C142	107(2)
F71–C69–F72	106(2)
F71–C69–C62	113(3)
F70–C69–F71	109(2)
F70–C69–F72	102(2)
F70–C69–C62	114(3)
C62–C69–F72	111(3)
Si21–C1–H1A	109.5
Si21–C1–H1B	109.5
Si21–C1–H1C	109.5
H1A–C1–H1B	109.5
H1A–C1–H1C	109.5
H1B–C1–H1C	109.5
C41–C40–H40	127.8
C41–C40–C39	104(3)
C39–C40–H40	127.8
C149–C148–H148	125.1
C147–C148–C149	110(3)
C147–C148–H148	125.1
N84–C85–C86	108(2)
N84–C85–C115	120(2)
C86–C85–C115	132(3)
F68–C65–F67	109(2)
F68–C65–F66	106(2)
F68–C65–C64	113(3)
F67–C65–F66	103(2)
F67–C65–C64	113(3)
F66–C65–C64	111(3)
C128–C127–H12A	110.2
C128–C127–H12B	110.2
H12A–C127–H12B	108.5
C131–C127–C128	108(2)
C131–C127–H12A	110.2
C131–C127–H12B	110.2

F116–C115–F118	103(2)
F116–C115–C85	112(2)
F118–C115–C85	104.4(19)
F117–C115–F116	112(2)
F117–C115–F118	110(2)
F117–C115–C85	114(3)
F99–C96–F97	109(3)
F99–C96–F98	109(2)
F99–C96–C94	118(3)
F97–C96–F98	102(2)
F97–C96–C94	109(2)
F98–C96–C94	108(3)
N61–C39–C38	124(3)
N61–C39–C40	109(3)
C40–C39–C38	126(3)
C148–C147–C146	113(3)
C148–C147–C151	128(3)
C151–C147–C146	119(3)
C130–C131–H13C	110.2
C130–C131–H13D	110.2
C127–C131–C130	107(2)
C127–C131–H13C	110.2
C127–C131–H13D	110.2
H13C–C131–H13D	108.5
H25A–C25–H25B	109.5
H25A–C25–H25C	109.5
H25B–C25–H25C	109.5
C24–C25–H25A	109.5
C24–C25–H25B	109.5
C24–C25–H25C	109.5
C35–C33–Si21	108.7(17)
C34–C33–Si21	110(2)
C34–C33–C35	108(2)
C34–C33–C36	110(2)
C36–C33–Si21	112(2)
C36–C33–C35	108(2)
F114–C111–F112	109(2)
F114–C111–F113	106(2)
F114–C111–C87	113(2)
F112–C111–C87	113(3)
F113–C111–F112	103(2)
F113–C111–C87	112(2)
C33–C34–H34A	109.5
C33–C34–H34B	109.5
C33–C34–H34C	109.5
H34A–C34–H34B	109.5
H34A–C34–H34C	109.5
H34B–C34–H34C	109.5
C6–C32–H32A	109.5
C6–C32–H32B	109.5
C6–C32–H32C	109.5
H32A–C32–H32B	109.5
H32A–C32–H32C	109.5
H32B–C32–H32C	109.5
N82–C81–C95	109(3)
N82–C81–C80	125(3)

C80–C81–C95	126(3)
Si21–C3–H3A	109.5
Si21–C3–H3B	109.5
Si21–C3–H3C	109.5
H3A–C3–H3B	109.5
H3A–C3–H3C	109.5
H3B–C3–H3C	109.5
C147–C151–H15E	109.5
C147–C151–H15F	109.5
C147–C151–H15G	109.5
H15E–C151–H15F	109.5
H15E–C151–H15G	109.5
H15F–C151–H15G	109.5
C130–C132–H13E	109.5
C130–C132–H13F	109.5
C130–C132–H13G	109.5
H13E–C132–H13F	109.5
H13E–C132–H13G	109.5
H13F–C132–H13G	109.5
Si15–C159–H15H	108.7
Si15–C159–H15I	108.7
H15H–C159–H15I	107.6
C160–C159–Si15	114(2)
C160–C159–H15H	108.7
C160–C159–H15I	108.7
H13H–C139–H13I	109.5
H13H–C139–H13J	109.5
H13I–C139–H13J	109.5
C138–C139–H13H	109.5
C138–C139–H13I	109.5
C138–C139–H13J	109.5
Si19–C20–H20A	108.6
Si19–C20–H20B	108.6
H20A–C20–H20B	107.6
C21–C20–Si19	114(2)
C21–C20–H20A	108.6
C21–C20–H20B	108.6
Si19–C24–H24A	108.3
Si19–C24–H24B	108.3
C25–C24–Si19	116(2)
C25–C24–H24A	108.3
C25–C24–H24B	108.3
H24A–C24–H24B	107.4
H23A–C23–H23B	109.5
H23A–C23–H23C	109.5
H23B–C23–H23C	109.5
C22–C23–H23A	109.5
C22–C23–H23B	109.5
C22–C23–H23C	109.5
C20–C21–H21A	109.5
C20–C21–H21B	109.5
C20–C21–H21C	109.5
H21A–C21–H21B	109.5
H21A–C21–H21C	109.5
H21B–C21–H21C	109.5
Si19–C22–H22A	108.9

Si19–C22–H22B	108.9
C23–C22–Si19	113(2)
C23–C22–H22A	108.9
C23–C22–H22B	108.9
H22A–C22–H22B	107.7
C139–C138–Si20	112(2)
C139–C138–C140	103(2)
C141–C138–Si20	114(2)
C141–C138–C139	121(3)
C141–C138–C140	103(2)
C140–C138–Si20	100.9(19)
Si20–C137–H13K	109.5
Si20–C137–H13L	109.5
Si20–C137–H13M	109.5
H13K–C137–H13L	109.5
H13K–C137–H13M	109.5
H13L–C137–H13M	109.5
Si20–C136–H13N	109.5
Si20–C136–H13O	109.5
Si20–C136–H13P	109.5
H13N–C136–H13O	109.5
H13N–C136–H13P	109.5
H13O–C136–H13P	109.5
C138–C141–H14A	109.5
C138–C141–H14B	109.5
C138–C141–H14C	109.5
H14A–C141–H14B	109.5
H14A–C141–H14C	109.5
H14B–C141–H14C	109.5
Si15–C157–H15J	110.2
Si15–C157–H15K	110.2
H15J–C157–H15K	108.5
C158–C157–Si15	108(2)
C158–C157–H15J	110.2
C158–C157–H15K	110.2
C138–C140–H14D	109.5
C138–C140–H14E	109.5
C138–C140–H14F	109.5
H14D–C140–H14E	109.5
H14D–C140–H14F	109.5
H14E–C140–H14F	109.5
C33–C36–H36A	109.5
C33–C36–H36B	109.5
C33–C36–H36C	109.5
H36A–C36–H36B	109.5
H36A–C36–H36C	109.5
H36B–C36–H36C	109.5
C157–C158–H15L	109.5
C157–C158–H15M	109.5
C157–C158–H15N	109.5
H15L–C158–H15M	109.5
H15L–C158–H15N	109.5
H15M–C158–H15N	109.5
C155–C156–H15O	109.5
C155–C156–H15P	109.5
C155–C156–H15Q	109.5

H15O–C156–H15P	109.5
H15O–C156–H15Q	109.5
H15P–C156–H15Q	109.5
C159–C160–H16A	109.5
C159–C160–H16B	109.5
C159–C160–H16C	109.5
H16A–C160–H16B	109.5
H16A–C160–H16C	109.5
H16B–C160–H16C	109.5
F74–C73–C41	113(3)
F74–C73–F75	114(3)
F76–C73–F74	103(3)
F76–C73–C41	115(3)
F76–C73–F75	103(3)
F75–C73–C41	109(3)
F54–C53–F56	106(3)
F54–C53–C46	110(3)
F56–C53–C46	111(3)
F55–C53–F54	110(3)
F55–C53–F56	108(3)
F55–C53–C46	112(3)

Table 5. Torsion angles for 26.

Atom–Atom–Atom–Atom	Torsion Angle [°]
Ag83–N82–C81–C95	173(2)
Ag83–N82–C81–C80	−5(5)
Ag83–N84–C85–C86	177(2)
Ag83–N84–C85–C115	−9(5)
Ag89–N90–N91–Ag92	−7(3)
Ag89–N90–N91–C100	−179(2)
Ag89–N90–C102–C103	−2(6)
Ag89–N90–C102–C101	178(3)
Ag89–N88–N84–Ag83	4(3)
Ag89–N88–N84–C85	176(2)
Ag89–N88–C87–C86	−179(2)
Ag89–N88–C87–C111	2(5)
Ag60–N59–N58–Ag57	−6(3)
Ag60–N59–N58–C64	175(2)
Ag60–N59–C62–C63	−174(2)
Ag60–N59–C62–C69	0(5)
Ag60–N61–N42–Ag43	10(3)
Ag60–N61–N42–C41	−155(3)
Ag60–N61–C39–C38	−25(5)
Ag60–N61–C39–C40	154(3)
Ag92–N93–N82–Ag83	27(3)
Ag92–N93–N82–C81	−162(2)
Ag92–N93–C94–C95	159(2)
Ag92–N93–C94–C96	−28(5)
Ag92–N91–C100–C101	−168(3)
Ag92–N91–C100–C107	12(6)
Ag43–N44–N45–Ag57	7(4)
Ag43–N44–N45–C46	−176(3)
Ag43–N44–C48–C49	−11(7)
Ag43–N44–C48–C47	173(3)
Ag43–N42–C41–C40	−167(2)
Ag43–N42–C41–C73	13(5)
Ag57–N58–C64–C63	−179(2)
Ag57–N58–C64–C65	6(5)
Ag57–N45–C46–C47	−179(3)
Ag57–N45–C46–C53	−5(7)
Si21–O4–C5–C6	−162.7(17)
Si15–O153–C152–C145	−141(2)
Si20–O134–C133–C130	−159.2(19)
Si19–O18–C17–C13	−130(2)
O144–C145–C152–O153	161(2)
O144–C145–C146–C142	7(3)
O144–C145–C146–C147	−107(3)
O144–C143–C142–C146	−7(3)
O144–C143–C142–C129	−139(3)
O144–C143–C142–C149	102(3)
O134–C133–C130–C129	−56(3)
O134–C133–C130–C131	55(3)
O134–C133–C130–C132	177(2)
F78–C38–C39–N61	162(3)
F78–C38–C39–C40	−17(5)
O31–C9–C10–C11	−18(4)
O31–C9–C10–C6	−154(3)
O31–C9–C8–C7	174(3)

O14–C15–C11–C12	−10(3)
O14–C15–C11–C28	99(3)
O14–C15–C11–C10	−141(2)
O14–C13–C12–C26	−107(3)
O14–C13–C12–C11	8(3)
O14–C13–C17–O18	171(2)
F77–C38–C39–N61	39(5)
F77–C38–C39–C40	−140(4)
N59–N58–C64–C63	0(4)
N59–N58–C64–C65	−175(3)
N59–C62–C63–C64	−2(4)
N59–C62–C69–F71	38(5)
N59–C62–C69–F70	164(3)
N59–C62–C69–F72	−81(4)
F119–C80–C81–N82	54(5)
F119–C80–C81–C95	−124(3)
N44–N45–C46–C47	5(5)
N44–N45–C46–C53	179(4)
N44–C48–C47–C46	0(5)
F105–C103–C102–N90	−56(4)
F105–C103–C102–C101	124(4)
F110–C107–C100–N91	−155(3)
F110–C107–C100–C101	25(6)
O4–Si21–C33–C35	45(2)
O4–Si21–C33–C34	−73(2)
O4–Si21–C33–C36	164.6(18)
O4–C5–C6–C7	57(3)
O4–C5–C6–C10	−56(3)
O4–C5–C6–C32	177(2)
F37–C38–C39–N61	−79(4)
F37–C38–C39–C40	102(4)
N58–N59–C62–C63	2(3)
N58–N59–C62–C69	176(3)
N58–C64–C65–F68	−166(3)
N58–C64–C65–F67	−41(4)
N58–C64–C65–F66	75(4)
O161–C143–C142–C146	180(3)
O161–C143–C142–C129	48(4)
O161–C143–C142–C149	−71(4)
F79–C80–C81–N82	178(3)
F79–C80–C81–C95	0(6)
O162–C128–C129–C142	−19(4)
O162–C128–C129–C130	−155(3)
O162–C128–C127–C131	175(3)
F109–C107–C100–N91	92(4)
F109–C107–C100–C101	−88(5)
O153–Si15–C155–C156	64(2)
O153–Si15–C159–C160	−180(2)
O153–Si15–C157–C158	61(2)
N45–N44–C48–C49	180(4)
N45–N44–C48–C47	3(5)
N45–C46–C47–C48	−3(5)
N45–C46–C53–F54	56(5)
N45–C46–C53–F56	−61(5)
N45–C46–C53–F55	178(4)
N90–N91–C100–C101	3(4)

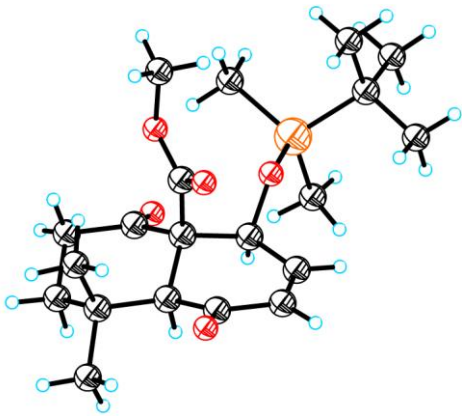
N90–N91–C100–C107	−177(3)
N90–C102–C101–C100	−1(5)
F104–C103–C102–N90	59(5)
F104–C103–C102–C101	−121(4)
O29–C28–C27–C26	178(3)
N93–N82–C81–C95	4(4)
N93–N82–C81–C80	−175(3)
N93–C94–C96–F99	37(5)
N93–C94–C96–F97	162(3)
N93–C94–C96–F98	−88(4)
O18–Si19–C20–C21	179(2)
O18–Si19–C24–C25	69(2)
O16–C15–C11–C12	177(2)
O16–C15–C11–C28	−74(3)
O16–C15–C11–C10	46(3)
F120–C80–C81–N82	−61(5)
F120–C80–C81–C95	120(3)
N61–N42–C41–C40	−3(4)
N61–N42–C41–C73	177(3)
F50–C49–C48–N44	50(6)
F50–C49–C48–C47	−135(5)
N82–N93–C94–C95	7(4)
N82–N93–C94–C96	−180(3)
F106–C103–C102–N90	−180(3)
F106–C103–C102–C101	0(6)
C145–O144–C143–O161	−174(3)
C145–O144–C143–C142	13(3)
C145–C146–C147–C148	110(3)
C145–C146–C147–C151	−71(3)
F51–C49–C48–N44	−74(5)
F51–C49–C48–C47	102(6)
N88–N84–C85–C86	6(4)
N88–N84–C85–C115	−180(3)
N88–C87–C86–C85	2(4)
N88–C87–C111–F114	−173(3)
N88–C87–C111–F112	−48(4)
N88–C87–C111–F113	68(4)
C143–O144–C145–C152	114(3)
C143–O144–C145–C146	−12(3)
C143–C142–C146–C145	0(3)
C143–C142–C146–C147	117(2)
C143–C142–C129–C128	60(3)
C143–C142–C129–C130	−174(3)
C143–C142–C149–O150	60(4)
C143–C142–C149–C148	−115(2)
N42–N61–C39–C38	−180(3)
N42–N61–C39–C40	−1(4)
N42–C41–C40–C39	2(4)
N42–C41–C73–F74	−167(3)
N42–C41–C73–F76	−50(5)
N42–C41–C73–F75	65(4)
C142–C146–C147–C148	−4(3)
C142–C146–C147–C151	175(2)
C142–C149–C148–C147	4(3)
N91–N90–C102–C103	−177(3)
N91–N90–C102–C101	3(4)

O150–C149–C148–C147	−170(3)
C5–C6–C10–C9	79(3)
C5–C6–C10–C11	−50(3)
C15–O14–C13–C12	−14(3)
C15–O14–C13–C17	112(3)
C15–C11–C12–C26	121(2)
C15–C11–C12–C13	1(3)
C15–C11–C28–O29	70(3)
C15–C11–C28–C27	−115(3)
C15–C11–C10–C9	55(3)
C15–C11–C10–C6	179(2)
C124–C123–C122–C121	0.0
C123–C124–C125–C126	0.0
C123–C122–C121–C126	0.0
C122–C121–C126–C125	0.0
C121–C126–C125–C124	0.0
C125–C124–C123–C122	0.0
C152–C145–C146–C142	−113(3)
C152–C145–C146–C147	132(3)
N84–N88–C87–C86	1(4)
N84–N88–C87–C111	−178(3)
N84–C85–C115–F116	−82(4)
N84–C85–C115–F118	168(3)
N84–C85–C115–F117	47(4)
C11–C28–C27–C26	3(3)
C103–C102–C101–C100	179(4)
C133–C130–C129–C142	−48(4)
C133–C130–C129–C128	84(3)
C133–C130–C131–C127	−88(3)
C13–O14–C15–O16	−172(3)
C13–O14–C15–C11	15(3)
C128–C127–C131–C130	−18(3)
C62–N59–N58–Ag57	178(2)
C62–N59–N58–C64	−1(4)
C62–C63–C64–N58	1(4)
C62–C63–C64–C65	176(3)
C63–C62–C69–F71	−149(3)
C63–C62–C69–F70	−24(5)
C63–C62–C69–F72	92(4)
C63–C64–C65–F68	19(5)
C63–C64–C65–F67	145(3)
C63–C64–C65–F66	−100(4)
C12–C26–C27–C28	1(4)
C12–C11–C28–O29	178(3)
C12–C11–C28–C27	−6(3)
C12–C11–C10–C9	−64(4)
C12–C11–C10–C6	60(4)
C12–C13–C17–O18	−68(3)
C102–N90–N91–Ag92	169(2)
C102–N90–N91–C100	−3(4)
C102–C101–C100–N91	−1(4)
C102–C101–C100–C107	179(4)
C7–C6–C10–C9	−39(3)
C7–C6–C10–C11	−167(2)
C28–C11–C12–C26	7(3)
C28–C11–C12–C13	−113(2)

C28–C11–C10–C9	175(2)
C28–C11–C10–C6	−61(3)
C17–C13–C12–C26	130(3)
C17–C13–C12–C11	−115(3)
C87–N88–N84–Ag83	−177(2)
C87–N88–N84–C85	−4(3)
C87–C86–C85–N84	−5(4)
C87–C86–C85–C115	−178(3)
C49–C48–C47–C46	−176(5)
F52–C49–C48–N44	169(4)
F52–C49–C48–C47	−15(8)
C86–C87–C111–F114	9(5)
C86–C87–C111–F112	133(3)
C86–C87–C111–F113	−111(3)
C86–C85–C115–F116	91(4)
C86–C85–C115–F118	−19(5)
C86–C85–C115–F117	−140(3)
C6–C7–C8–C9	−16(3)
C95–C94–C96–F99	−152(4)
C95–C94–C96–F97	−26(5)
C95–C94–C96–F98	84(5)
C30–C26–C12–C11	−178(3)
C30–C26–C12–C13	−64(3)
C30–C26–C27–C28	174(3)
C146–C145–C152–O153	−79(3)
C146–C142–C129–C128	−61(4)
C146–C142–C129–C130	66(4)
C146–C142–C149–O150	168(3)
C146–C142–C149–C148	−6(3)
C10–C9–C8–C7	−9(3)
C10–C11–C12–C26	−118(3)
C10–C11–C12–C13	122(3)
C10–C11–C28–O29	−50(4)
C10–C11–C28–C27	126(3)
C94–N93–N82–Ag83	−177(2)
C94–N93–N82–C81	−7(4)
C94–C95–C81–N82	1(4)
C94–C95–C81–C80	179(4)
C48–N44–N45–Ag57	178(3)
C48–N44–N45–C46	−5(5)
C155–Si15–O153–C152	−173(2)
C155–Si15–C159–C160	−61(3)
C155–Si15–C157–C158	−57(2)
C47–C46–C53–F54	−132(5)
C47–C46–C53–F56	112(5)
C47–C46–C53–F55	−9(7)
C129–C142–C146–C145	122(3)
C129–C142–C146–C147	−120(3)
C129–C142–C149–O150	−58(4)
C129–C142–C149–C148	128(2)
C129–C128–C127–C131	−4(3)
C129–C130–C131–C127	32(3)
C8–C9–C10–C11	165(2)
C8–C9–C10–C6	30(3)
C8–C7–C6–C5	−88(3)
C8–C7–C6–C10	34(2)

C8–C7–C6–C32	153(2)
C41–C40–C39–N61	−1(4)
C41–C40–C39–C38	178(4)
C27–C26–C12–C11	−6(3)
C27–C26–C12–C13	109(3)
C149–C142–C146–C145	−111(3)
C149–C142–C146–C147	6(3)
C149–C142–C129–C128	176(2)
C149–C142–C129–C130	−57(4)
C149–C148–C147–C146	0(3)
C149–C148–C147–C151	−179(3)
C69–C62–C63–C64	−175(3)
C1–Si21–O4–C5	45(2)
C1–Si21–C33–C35	165.0(18)
C1–Si21–C33–C34	46(2)
C1–Si21–C33–C36	−76(2)
C40–C41–C73–F74	13(6)
C40–C41–C73–F76	130(4)
C40–C41–C73–F75	−115(4)
C127–C128–C129–C142	160(2)
C127–C128–C129–C130	24(3)
C39–N61–N42–Ag43	168(2)
C39–N61–N42–C41	2(4)
C131–C130–C129–C142	−164(3)
C131–C130–C129–C128	−33(3)
C33–Si21–O4–C5	164(2)
C111–C87–C86–C85	−179(3)
C32–C6–C10–C9	−157(2)
C32–C6–C10–C11	75(3)
C81–C95–C94–N93	−5(4)
C81–C95–C94–C96	−177(4)
C3–Si21–O4–C5	−76(2)
C3–Si21–C33–C35	−74(2)
C3–Si21–C33–C34	167.5(18)
C3–Si21–C33–C36	45(2)
C132–C130–C129–C142	73(4)
C132–C130–C129–C128	−156(2)
C132–C130–C131–C127	156(2)
C159–Si15–O153–C152	−52(2)
C159–Si15–C155–C156	−58(3)
C159–Si15–C157–C158	−179(2)
C20–Si19–O18–C17	141(2)
C20–Si19–C24–C25	−47(3)
C24–Si19–O18–C17	20(3)
C24–Si19–C20–C21	−62(3)
C22–Si19–O18–C17	−104(2)
C22–Si19–C20–C21	66(2)
C22–Si19–C24–C25	−172(2)
C138–Si20–O134–C133	177(2)
C137–Si20–O134–C133	−76(2)
C136–Si20–O134–C133	45(2)
C157–Si15–O153–C152	64(2)
C157–Si15–C155–C156	−177(2)
C157–Si15–C159–C160	62(3)
C73–C41–C40–C39	−178(4)
C53–C46–C47–C48	−176(4)

F108–C107–C100–N91	−34(5)
F108–C107–C100–C101	146(4)



28

Crystallographic data of compound **28**

CCDC number	2447371
Empirical formula	$C_{35}H_{35}Ag_3F_{18}N_6O_5Si$
Formula weight	1313.39
Temperature/K	99.9(6)
Crystal system	triclinic
Space group	P-1
a/Å	12.4331(3)
b/Å	12.9634(2)
c/Å	16.4196(2)
α/°	112.543(2)
β/°	97.301(2)
γ/°	105.808(2)
Volume/Å^3	2270.57(8)
Z	2
ρ_{calc}g/cm^3	1.921
μ/mm^{-1}	11.650
F(000)	1288.0
Crystal size/mm^3	0.15 × 0.1 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	6.036 to 148.446
Index ranges	-15 ≤ h ≤ 15, -16 ≤ k ≤ 15, -20 ≤ l ≤ 20
Reflections collected	52816
Independent reflections	8929 [R_{int} = 0.0544, R_{sigma} = 0.0353]
Data/restraints/parameters	8929/1/621
Goodness-of-fit on F^2	1.071

Final R indexes [I>=2σ (I)]	R_1 = 0.0421, wR_2 = 0.1060
Final R indexes [all data]	R_1 = 0.0515, wR_2 = 0.1085
Largest diff. peak/hole / e Å^{-3}	2.22/-1.48

Table 2. Atomic coordinates and U_{eq} [Å^2] for 28.

Atom	*x*	*y*	*z*	U_{eq}
Ag3	0.62358(3)	0.63558(3)	0.16666(2)	0.02827(9)
Ag1	0.44618(2)	0.34051(3)	0.02772(2)	0.02703(9)
Ag2	0.33624(3)	0.53283(3)	0.16821(2)	0.03173(9)
F00D	0.3091(3)	0.8600(3)	0.4228(2)	0.0558(8)
F00F	0.7804(3)	0.8806(3)	0.2867(2)	0.0573(9)
F00H	0.6519(3)	0.1541(3)	-0.0303(2)	0.0630(10)
F00I	0.6870(3)	0.1811(3)	-0.1462(2)	0.0655(10)
F00L	0.1476(3)	-0.0392(3)	-0.0665(3)	0.0666(10)
F00M	0.2449(4)	0.0585(3)	-0.1278(2)	0.0689(11)
F00O	0.2239(3)	0.7315(3)	0.2844(3)	0.0675(10)
F00P	0.7911(3)	0.9520(4)	0.4282(2)	0.0741(11)
F00R	0.7403(3)	1.0372(3)	0.3517(4)	0.0807(13)
F00S	0.3282(3)	0.0624(3)	-0.0064(3)	0.0715(11)
F00T	-0.0653(3)	0.2876(3)	0.0869(4)	0.0780(13)
F00V	0.0681(4)	0.3882(5)	0.2138(3)	0.0926(17)
F00W	0.2920(4)	0.6766(4)	0.3804(4)	0.0849(14)
F005	0.9795(2)	0.6512(2)	0.08042(18)	0.0368(6)
F006	0.8630(2)	0.7367(2)	0.13858(19)	0.0385(6)
F007	0.0563(2)	0.4559(3)	0.11650(19)	0.0410(6)
F009	0.5226(2)	0.1707(3)	-0.1179(2)	0.0458(7)
F10	0.9378(2)	0.6455(3)	0.20155(18)	0.0426(7)
N3	0.2789(3)	0.2764(3)	0.0407(2)	0.0272(7)
N2	0.6165(3)	0.4024(3)	0.0195(2)	0.0263(7)
N1	0.6859(3)	0.5169(3)	0.0735(2)	0.0258(7)
N4	0.2298(3)	0.3548(3)	0.0858(2)	0.0290(8)
N5	0.4440(3)	0.7068(3)	0.2606(3)	0.0315(8)
N6	0.5558(3)	0.7491(3)	0.2594(2)	0.0296(8)
C7	0.6825(4)	0.3440(4)	-0.0222(3)	0.0270(9)
C2	0.1205(4)	0.2925(4)	0.0783(3)	0.0335(10)
C4	0.1994(4)	0.1669(4)	0.0056(3)	0.0301(9)
C10	0.8926(4)	0.6406(4)	0.1211(3)	0.0296(9)
C14	0.4273(4)	0.7900(4)	0.3324(3)	0.0367(10)
C5	0.2291(4)	0.0616(4)	-0.0485(3)	0.0389(11)
C11	0.7289(4)	0.9309(4)	0.3474(3)	0.0391(11)
C6	0.6359(4)	0.2126(4)	-0.0786(3)	0.0353(10)
C12	0.6046(4)	0.8575(4)	0.3287(3)	0.0322(9)
C13	0.5261(4)	0.8872(4)	0.3770(3)	0.0391(11)
H13	0.538078	0.958891	0.429209	0.047
C15	0.3129(5)	0.7640(5)	0.3546(4)	0.0475(13)
C1	0.0454(4)	0.3566(5)	0.1243(4)	0.0419(12)
C9	0.7937(3)	0.5268(4)	0.0643(3)	0.0249(8)
C8	0.7963(4)	0.4198(4)	0.0038(3)	0.0301(9)
H8	0.860686	0.401986	-0.015420	0.036
C3	0.0969(4)	0.1726(4)	0.0282(3)	0.0344(10)
H3	0.026706	0.108574	0.012603	0.041
Si1	0.82224(11)	0.79176(12)	0.66726(9)	0.0362(3)
O1	0.7627(3)	0.7215(3)	0.5549(2)	0.0328(6)
O5	0.5251(3)	0.4447(3)	0.2226(2)	0.0334(7)
O4	0.7659(3)	0.6539(3)	0.3451(2)	0.0324(7)

O3	0.9199(3)	0.6654(3)	0.4412(2)	0.0330(7)
O2	0.8337(3)	0.5140(3)	0.5546(2)	0.0424(8)
C22	0.5734(4)	0.6153(4)	0.4591(3)	0.0325(9)
H22	0.542294	0.667343	0.499058	0.039
C25	0.6402(3)	0.4269(4)	0.3448(3)	0.0257(8)
H25	0.591859	0.381180	0.372358	0.031
C33	0.5177(4)	0.5576(4)	0.3711(3)	0.0326(9)
H33	0.449006	0.569448	0.350893	0.039
C28	0.8587(4)	0.3979(4)	0.4104(3)	0.0387(11)
H28A	0.900521	0.366229	0.444854	0.046
H28B	0.913480	0.438234	0.383936	0.046
C27	0.7569(4)	0.2952(4)	0.3335(3)	0.0376(10)
H27A	0.706224	0.251686	0.360541	0.045
H27B	0.787388	0.238814	0.291828	0.045
C30	0.5783(4)	0.2248(4)	0.2109(3)	0.0388(11)
H30A	0.531767	0.246548	0.171839	0.058
H30B	0.531071	0.194324	0.245759	0.058
H30C	0.605401	0.163044	0.172947	0.058
C21	0.7300(5)	0.7135(5)	0.7218(3)	0.0422(12)
H21A	0.741005	0.637388	0.709587	0.063
H21B	0.648465	0.698539	0.696664	0.063
H21C	0.751900	0.763260	0.787911	0.063
C35	0.9936(4)	0.7625(5)	0.4276(4)	0.0445(12)
H35A	1.072081	0.791668	0.466639	0.067
H35B	0.962586	0.827532	0.443621	0.067
H35C	0.995764	0.733874	0.363499	0.067
C20	0.9751(4)	0.7984(5)	0.6911(4)	0.0471(13)
H20A	1.016145	0.832276	0.654948	0.071
H20B	0.976473	0.717756	0.674629	0.071
H20C	1.013027	0.848610	0.756197	0.071
C18	0.6907(5)	0.9393(5)	0.6740(4)	0.0492(13)
H18A	0.642268	0.896553	0.701795	0.074
H18B	0.661921	0.896597	0.607357	0.074
H18C	0.687872	1.019980	0.694681	0.074
C16	0.8669(6)	1.0184(5)	0.8073(4)	0.0576(15)
H16A	0.818278	0.980213	0.837615	0.086
H16B	0.867384	1.100065	0.826070	0.086
H16C	0.946050	1.020401	0.824620	0.086
C17	0.8179(4)	0.9471(5)	0.7029(3)	0.0433(12)
C19	0.8948(5)	1.0108(5)	0.6571(4)	0.0504(13)
H19A	0.863687	0.967948	0.590629	0.076
H19B	0.973904	1.012067	0.673570	0.076
H19C	0.895606	1.092758	0.678079	0.076
C24	0.7369(4)	0.5343(4)	0.4283(3)	0.0268(8)
C26	0.6838(4)	0.3361(4)	0.2777(3)	0.0299(9)
C32	0.5598(3)	0.4753(4)	0.3041(3)	0.0275(9)
C34	0.8078(4)	0.6237(4)	0.3981(3)	0.0282(9)
C23	0.6820(4)	0.6041(4)	0.4995(3)	0.0289(9)
H23	0.664118	0.563113	0.539389	0.035
C31	0.7548(4)	0.3849(5)	0.2226(3)	0.0368(10)
H31A	0.825099	0.451473	0.264190	0.055
H31B	0.708707	0.412709	0.188429	0.055
H31C	0.776282	0.321675	0.179832	0.055
C29	0.8147(4)	0.4853(4)	0.4732(3)	0.0322(9)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic displacement parameters [Å²] for 28. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ag3	0.02807(16)	0.02537(16)	0.02990(16)	0.00731(12)	0.01398(12)	0.01134(12)
Ag1	0.02177(15)	0.02599(16)	0.02820(15)	0.00673(12)	0.00913(11)	0.00717(12)
Ag2	0.03310(17)	0.02783(17)	0.03391(17)	0.00978(13)	0.01418(13)	0.01317(13)
F00D	0.0586(19)	0.0519(19)	0.0549(19)	0.0082(15)	0.0360(16)	0.0289(16)
F00F	0.0446(17)	0.0451(18)	0.0541(19)	−0.0011(15)	0.0241(15)	0.0025(14)
F00H	0.086(3)	0.0335(17)	0.058(2)	0.0180(15)	−0.0068(18)	0.0174(17)
F00I	0.071(2)	0.0449(19)	0.064(2)	−0.0014(16)	0.0434(19)	0.0217(17)
F00L	0.063(2)	0.0278(16)	0.088(3)	0.0089(16)	0.0399(19)	−0.0015(15)
F00M	0.105(3)	0.056(2)	0.058(2)	0.0238(18)	0.050(2)	0.036(2)
F00O	0.0409(18)	0.070(2)	0.065(2)	0.0048(18)	0.0227(16)	0.0130(17)
F00P	0.052(2)	0.094(3)	0.048(2)	0.023(2)	0.0000(16)	0.001(2)
F00R	0.060(2)	0.0376(19)	0.148(4)	0.043(2)	0.036(2)	0.0150(17)
F00S	0.061(2)	0.045(2)	0.082(3)	0.0018(18)	−0.0047(19)	0.0300(17)
F00T	0.0369(17)	0.056(2)	0.161(4)	0.056(3)	0.050(2)	0.0233(16)
F00V	0.133(4)	0.170(5)	0.063(2)	0.077(3)	0.069(3)	0.126(4)
F00W	0.092(3)	0.074(3)	0.149(4)	0.074(3)	0.094(3)	0.053(2)
F005	0.0258(12)	0.0421(16)	0.0395(14)	0.0148(12)	0.0175(11)	0.0079(11)
F006	0.0335(14)	0.0282(14)	0.0477(16)	0.0093(12)	0.0146(12)	0.0108(11)
F007	0.0370(14)	0.0430(16)	0.0447(15)	0.0151(13)	0.0168(12)	0.0200(13)
F009	0.0382(15)	0.0331(15)	0.0473(16)	0.0032(13)	0.0017(12)	0.0101(12)
F10	0.0375(14)	0.0491(17)	0.0290(13)	0.0158(12)	0.0023(11)	0.0021(13)
N3	0.0254(17)	0.0248(18)	0.0286(17)	0.0081(14)	0.0075(14)	0.0097(14)
N2	0.0245(16)	0.0224(18)	0.0269(17)	0.0042(14)	0.0087(13)	0.0096(14)
N1	0.0239(16)	0.0241(18)	0.0260(17)	0.0060(14)	0.0109(13)	0.0086(14)
N4	0.0255(17)	0.033(2)	0.0330(18)	0.0154(16)	0.0139(14)	0.0126(15)
N5	0.0326(19)	0.0279(19)	0.0354(19)	0.0093(16)	0.0170(16)	0.0159(16)
N6	0.0314(18)	0.0234(18)	0.0297(18)	0.0056(15)	0.0127(15)	0.0099(15)
C7	0.027(2)	0.028(2)	0.0238(19)	0.0079(17)	0.0108(16)	0.0096(17)
C2	0.028(2)	0.044(3)	0.038(2)	0.025(2)	0.0148(18)	0.013(2)
C4	0.026(2)	0.028(2)	0.029(2)	0.0114(18)	0.0061(16)	0.0014(17)
C10	0.024(2)	0.036(2)	0.027(2)	0.0122(18)	0.0108(16)	0.0085(18)
C14	0.042(3)	0.029(2)	0.042(3)	0.012(2)	0.022(2)	0.017(2)
C5	0.039(3)	0.031(2)	0.042(3)	0.011(2)	0.013(2)	0.010(2)
C11	0.041(3)	0.031(3)	0.036(2)	0.007(2)	0.013(2)	0.009(2)
C6	0.037(2)	0.032(2)	0.034(2)	0.007(2)	0.0136(19)	0.016(2)
C12	0.041(2)	0.025(2)	0.029(2)	0.0066(18)	0.0152(19)	0.0151(19)
C13	0.049(3)	0.032(3)	0.037(2)	0.011(2)	0.021(2)	0.016(2)
C15	0.052(3)	0.038(3)	0.061(3)	0.019(3)	0.035(3)	0.024(3)
C1	0.041(3)	0.057(3)	0.051(3)	0.035(3)	0.025(2)	0.030(3)
C9	0.0236(19)	0.029(2)	0.0252(19)	0.0123(17)	0.0108(15)	0.0103(17)
C8	0.028(2)	0.035(2)	0.029(2)	0.0113(18)	0.0130(17)	0.0146(19)
C3	0.027(2)	0.040(3)	0.039(2)	0.021(2)	0.0111(18)	0.0077(19)
Si1	0.0327(6)	0.0356(7)	0.0331(6)	0.0102(5)	0.0078(5)	0.0087(5)
O1	0.0338(16)	0.0267(16)	0.0302(10)	0.0067(12)	0.0090(11)	0.0075(13)
O5	0.0305(15)	0.0350(17)	0.0311(16)	0.0116(14)	0.0067(12)	0.0108(13)
O4	0.0339(16)	0.0331(17)	0.0307(15)	0.0163(14)	0.0097(13)	0.0084(14)
O3	0.0268(15)	0.0327(17)	0.0312(15)	0.0110(13)	0.0087(12)	0.0023(13)
O2	0.046(2)	0.049(2)	0.0352(18)	0.0190(16)	0.0066(15)	0.0206(17)
C22	0.029(2)	0.029(2)	0.036(2)	0.0097(19)	0.0151(18)	0.0092(18)
C25	0.0243(19)	0.023(2)	0.0259(19)	0.0083(17)	0.0082(16)	0.0061(16)
C33	0.028(2)	0.030(2)	0.035(2)	0.0103(19)	0.0081(18)	0.0092(18)
C28	0.038(2)	0.034(3)	0.044(3)	0.013(2)	0.007(2)	0.019(2)

C27	0.039(2)	0.032(3)	0.041(3)	0.013(2)	0.012(2)	0.014(2)
C30	0.036(2)	0.026(2)	0.040(3)	0.002(2)	0.009(2)	0.008(2)
C21	0.043(3)	0.044(3)	0.030(2)	0.015(2)	0.006(2)	0.005(2)
C35	0.034(2)	0.047(3)	0.041(3)	0.019(2)	0.011(2)	−0.004(2)
C20	0.028(2)	0.043(3)	0.053(3)	0.006(2)	0.004(2)	0.013(2)
C18	0.053(3)	0.042(3)	0.056(3)	0.017(3)	0.020(3)	0.025(3)
C16	0.071(4)	0.040(3)	0.040(3)	0.002(2)	0.005(3)	0.014(3)
C17	0.039(3)	0.041(3)	0.038(3)	0.011(2)	0.009(2)	0.007(2)
C19	0.056(3)	0.035(3)	0.058(3)	0.022(3)	0.016(3)	0.010(2)
C24	0.027(2)	0.024(2)	0.027(2)	0.0088(17)	0.0077(16)	0.0068(17)
C26	0.030(2)	0.024(2)	0.029(2)	0.0047(17)	0.0084(17)	0.0093(18)
C32	0.0239(19)	0.025(2)	0.028(2)	0.0094(17)	0.0074(16)	0.0039(17)
C34	0.027(2)	0.023(2)	0.027(2)	0.0046(17)	0.0111(16)	0.0065(17)
C23	0.034(2)	0.025(2)	0.027(2)	0.0099(17)	0.0117(17)	0.0093(18)
C31	0.035(2)	0.041(3)	0.034(2)	0.011(2)	0.0159(19)	0.016(2)
C29	0.030(2)	0.031(2)	0.031(2)	0.0148(19)	0.0054(17)	0.0054(18)

Table 4. Bond lengths and angles for 28.

Atom–Atom	Length [Å]
Ag3–Ag1$^{\#1}$	3.3521(4)
Ag3–N1	2.110(3)
Ag3–N6	2.117(3)
Ag1–N3	2.090(3)
Ag1–N2	2.091(3)
Ag2–N4	2.097(4)
Ag2–N5	2.097(4)
F00D–C15	1.334(6)
F00F–C11	1.313(5)
F00H–C6	1.321(6)
F00I–C6	1.332(5)
F00L–C5	1.315(6)
F00M–C5	1.328(6)
F00O–C15	1.334(7)
F00P–C11	1.334(6)
F00R–C11	1.318(6)
F00S–C5	1.329(6)
F00T–C1	1.328(6)
F00V–C1	1.333(6)
F00W–C15	1.328(7)
F005–C10	1.343(5)
F006–C10	1.331(5)
F007–C1	1.314(6)
F009–C6	1.333(6)
F10–C10	1.340(5)
N3–N4	1.352(5)
N3–C4	1.337(5)
N2–N1	1.354(5)
N2–C7	1.341(5)
N1–C9	1.346(5)
N4–C2	1.340(6)
N5–N6	1.353(5)
N5–C14	1.344(6)
N6–C12	1.331(6)
C7–C6	1.488(6)
C7–C8	1.385(6)
C2–C1	1.502(7)
C2–C3	1.374(7)

C4–C5	1.489(7)
C4–C3	1.384(6)
C10–C9	1.491(6)
C14–C13	1.361(7)
C14–C15	1.495(7)
C11–C12	1.497(7)
C12–C13	1.377(6)
C13–H13	0.9500
C9–C8	1.374(6)
C8–H8	0.9500
C3–H3	0.9500
Si1–O1	1.667(3)
Si1–C21	1.864(5)
Si1–C20	1.862(5)
Si1–C17	1.888(6)
O1–C23	1.422(5)
O5–C32	1.220(5)
O4–C34	1.199(5)
O3–C35	1.453(6)
O3–C34	1.335(5)
O2–C29	1.212(5)
C22–H22	0.9500
C22–C33	1.327(6)
C22–C23	1.496(6)
C25–H25	1.0000
C25–C24	1.572(6)
C25–C26	1.549(6)
C25–C32	1.527(6)
C33–H33	0.9500
C33–C32	1.474(6)
C28–H28A	0.9900
C28–H28B	0.9900
C28–C27	1.535(7)
C28–C29	1.494(7)
C27–H27A	0.9900
C27–H27B	0.9900
C27–C26	1.540(7)
C30–H30A	0.9800
C30–H30B	0.9800
C30–H30C	0.9800
C30–C26	1.547(6)
C21–H21A	0.9800
C21–H21B	0.9800
C21–H21C	0.9800
C35–H35A	0.9800
C35–H35B	0.9800
C35–H35C	0.9800
C20–H20A	0.9800
C20–H20B	0.9800
C20–H20C	0.9800
C18–H18A	0.9800
C18–H18B	0.9800
C18–H18C	0.9800
C18–C17	1.556(8)
C16–H16A	0.9800
C16–H16B	0.9800

C16–H16C	0.9800
C16–C17	1.541(7)
C17–C19	1.546(7)
C19–H19A	0.9800
C19–H19B	0.9800
C19–H19C	0.9800
C24–C34	1.537(6)
C24–C23	1.543(6)
C24–C29	1.548(6)
C26–C31	1.529(6)
C23–H23	1.0000
C31–H31A	0.9800
C31–H31B	0.9800
C31–H31C	0.9800

Atom–Atom–Atom	**Angle [°]**
N1–Ag3–Ag1$^{\#1}$	75.68(10)
N1–Ag3–N6	177.87(13)
N6–Ag3–Ag1$^{\#1}$	104.76(10)
N3–Ag1–Ag3$^{\#1}$	98.35(10)
N3–Ag1–N2	177.26(14)
N2–Ag1–Ag3$^{\#1}$	84.32(10)
N4–Ag2–N5	174.80(15)
N4–N3–Ag1	119.4(3)
C4–N3–Ag1	132.6(3)
C4–N3–N4	107.8(3)
N1–N2–Ag1	120.4(2)
C7–N2–Ag1	131.3(3)
C7–N2–N1	107.5(3)
N2–N1–Ag3	120.5(2)
C9–N1–Ag3	131.2(3)
C9–N1–N2	107.5(3)
N3–N4–Ag2	118.5(3)
C2–N4–Ag2	132.5(3)
C2–N4–N3	107.9(4)
N6–N5–Ag2	120.7(3)
C14–N5–Ag2	131.6(3)
C14–N5–N6	107.5(4)
N5–N6–Ag3	119.4(3)
C12–N6–Ag3	132.7(3)
C12–N6–N5	107.5(3)
N2–C7–C6	121.4(4)
N2–C7–C8	110.8(4)
C8–C7–C6	127.4(4)
N4–C2–C1	119.7(4)
N4–C2–C3	110.3(4)
C3–C2–C1	130.0(4)
N3–C4–C5	119.8(4)
N3–C4–C3	110.2(4)
C3–C4–C5	130.0(4)
F005–C10–C9	111.5(3)
F006–C10–F005	107.5(4)
F006–C10–F10	107.3(4)
F006–C10–C9	113.0(4)
F10–C10–F005	105.9(3)
F10–C10–C9	111.3(4)

N5–C14–C13	110.5(4)
N5–C14–C15	119.4(4)
C13–C14–C15	130.1(4)
F00L–C5–F00M	107.3(4)
F00L–C5–F00S	108.1(5)
F00L–C5–C4	111.7(4)
F00M–C5–F00S	104.6(4)
F00M–C5–C4	112.2(4)
F00S–C5–C4	112.4(4)
F00F–C11–F00P	106.2(4)
F00F–C11–F00R	108.1(4)
F00F–C11–C12	113.5(4)
F00P–C11–C12	111.8(4)
F00R–C11–F00P	105.1(5)
F00R–C11–C12	111.7(4)
F00H–C6–F00I	107.4(4)
F00H–C6–F009	106.7(4)
F00H–C6–C7	112.3(4)
F00I–C6–F009	106.3(4)
F00I–C6–C7	110.9(4)
F009–C6–C7	112.9(4)
N6–C12–C11	121.7(4)
N6–C12–C13	110.6(4)
C13–C12–C11	127.7(4)
C14–C13–C12	103.9(4)
C14–C13–H13	128.0
C12–C13–H13	128.0
F00D–C15–C14	110.8(5)
F00O–C15–F00D	106.7(4)
F00O–C15–C14	113.1(5)
F00W–C15–F00D	107.3(5)
F00W–C15–F00O	106.5(5)
F00W–C15–C14	112.1(5)
F00T–C1–F00V	108.3(5)
F00T–C1–C2	109.8(5)
F00V–C1–C2	113.1(4)
F007–C1–F00T	106.6(4)
F007–C1–F00V	105.3(5)
F007–C1–C2	113.4(4)
N1–C9–C10	120.5(4)
N1–C9–C8	110.9(4)
C8–C9–C10	128.4(4)
C7–C8–H8	128.4
C9–C8–C7	103.3(4)
C9–C8–H8	128.4
C2–C3–C4	103.8(4)
C2–C3–H3	128.1
C4–C3–H3	128.1
O1–Si1–C21	108.0(2)
O1–Si1–C20	109.6(2)
O1–Si1–C17	104.9(2)
C21–Si1–C17	110.2(2)
C20–Si1–C21	113.8(3)
C20–Si1–C17	110.0(2)
C23–O1–Si1	130.4(3)
C34–O3–C35	116.0(4)

C33–C22–H22	117.8
C33–C22–C23	124.4(4)
C23–C22–H22	117.8
C24–C25–H25	104.7
C26–C25–H25	104.7
C26–C25–C24	115.2(3)
C32–C25–H25	104.7
C32–C25–C24	108.7(3)
C32–C25–C26	117.4(3)
C22–C33–H33	119.2
C22–C33–C32	121.6(4)
C32–C33–H33	119.2
H28A–C28–H28B	108.2
C27–C28–H28A	109.7
C27–C28–H28B	109.7
C29–C28–H28A	109.7
C29–C28–H28B	109.7
C29–C28–C27	109.7(4)
C28–C27–H27A	108.8
C28–C27–H27B	108.8
C28–C27–C26	113.7(4)
H27A–C27–H27B	107.7
C26–C27–H27A	108.8
C26–C27–H27B	108.8
H30A–C30–H30B	109.5
H30A–C30–H30C	109.5
H30B–C30–H30C	109.5
C26–C30–H30A	109.5
C26–C30–H30B	109.5
C26–C30–H30C	109.5
Si1–C21–H21A	109.5
Si1–C21–H21B	109.5
Si1–C21–H21C	109.5
H21A–C21–H21B	109.5
H21A–C21–H21C	109.5
H21B–C21–H21C	109.5
O3–C35–H35A	109.5
O3–C35–H35B	109.5
O3–C35–H35C	109.5
H35A–C35–H35B	109.5
H35A–C35–H35C	109.5
H35B–C35–H35C	109.5
Si1–C20–H20A	109.5
Si1–C20–H20B	109.5
Si1–C20–H20C	109.5
H20A–C20–H20B	109.5
H20A–C20–H20C	109.5
H20B–C20–H20C	109.5
H18A–C18–H18B	109.5
H18A–C18–H18C	109.5
H18B–C18–H18C	109.5
C17–C18–H18A	109.5
C17–C18–H18B	109.5
C17–C18–H18C	109.5
H16A–C16–H16B	109.5
H16A–C16–H16C	109.5

H16B–C16–H16C	109.5
C17–C16–H16A	109.5
C17–C16–H16B	109.5
C17–C16–H16C	109.5
C18–C17–Si1	109.4(4)
C16–C17–Si1	109.0(4)
C16–C17–C18	110.5(5)
C16–C17–C19	108.3(5)
C19–C17–Si1	109.6(4)
C19–C17–C18	110.1(5)
C17–C19–H19A	109.5
C17–C19–H19B	109.5
C17–C19–H19C	109.5
H19A–C19–H19B	109.5
H19A–C19–H19C	109.5
H19B–C19–H19C	109.5
C34–C24–C25	110.7(3)
C34–C24–C23	106.1(3)
C34–C24–C29	111.5(3)
C23–C24–C25	110.4(3)
C23–C24–C29	109.1(3)
C29–C24–C25	109.0(3)
C27–C26–C25	107.9(4)
C27–C26–C30	107.1(4)
C30–C26–C25	108.9(3)
C31–C26–C25	114.0(4)
C31–C26–C27	109.8(4)
C31–C26–C30	109.0(4)
O5–C32–C25	124.5(4)
O5–C32–C33	120.6(4)
C33–C32–C25	114.7(4)
O4–C34–O3	125.4(4)
O4–C34–C24	123.7(4)
O3–C34–C24	110.9(4)
O1–C23–C22	107.5(4)
O1–C23–C24	109.2(3)
O1–C23–H23	108.6
C22–C23–C24	114.2(4)
C22–C23–H23	108.6
C24–C23–H23	108.6
C26–C31–H31A	109.5
C26–C31–H31B	109.5
C26–C31–H31C	109.5
H31A–C31–H31B	109.5
H31A–C31–H31C	109.5
H31B–C31–H31C	109.5
O2–C29–C28	123.1(4)
O2–C29–C24	120.5(4)
C28–C29–C24	116.3(4)

Symmetry transformations used to generate equivalent atoms:

#1: 1-X, 1-Y, -Z;

Table 5. Torsion angles for 28.

Atom–Atom–Atom–Atom	Torsion Angle [°]
Ag3–N1–C9–C10	−5.5(6)
Ag3–N1–C9–C8	170.1(3)
Ag3–N6–C12–C11	8.2(7)
Ag3–N6–C12–C13	−171.4(3)
Ag1–N3–N4–Ag2	−15.3(4)
Ag1–N3–N4–C2	175.1(3)
Ag1–N3–C4–C5	6.0(6)
Ag1–N3–C4–C3	−174.3(3)
Ag1–N2–N1–Ag3	−0.2(4)
Ag1–N2–N1–C9	170.7(3)
Ag1–N2–C7–C6	3.3(6)
Ag1–N2–C7–C8	−169.6(3)
Ag2–N4–C2–C1	10.8(6)
Ag2–N4–C2–C3	−167.6(3)
Ag2–N5–N6–Ag3	−2.5(4)
Ag2–N5–N6–C12	−175.8(3)
Ag2–N5–C14–C13	175.1(3)
Ag2–N5–C14–C15	−2.0(7)
F00F–C11–C12–N6	3.5(7)
F00F–C11–C12–C13	−177.1(5)
F00P–C11–C12–N6	−116.6(5)
F00P–C11–C12–C13	62.9(7)
F00R–C11–C12–N6	126.0(5)
F00R–C11–C12–C13	−54.6(7)
F005–C10–C9–N1	−155.6(4)
F005–C10–C9–C8	29.7(6)
F006–C10–C9–N1	−34.4(5)
F006–C10–C9–C8	150.9(4)
F10–C10–C9–N1	86.4(5)
F10–C10–C9–C8	−88.3(5)
N3–N4–C2–C1	178.4(4)
N3–N4–C2–C3	−0.1(5)
N3–C4–C5–F00L	170.8(4)
N3–C4–C5–F00M	−68.5(6)
N3–C4–C5–F00S	49.1(6)
N3–C4–C3–C2	0.4(5)
N2–N1–C9–C10	−175.0(4)
N2–N1–C9–C8	0.5(5)
N2–C7–C6–F00H	−90.8(5)
N2–C7–C6–F00I	149.1(4)
N2–C7–C6–F009	30.0(6)
N2–C7–C8–C9	0.3(5)
N1–N2–C7–C6	172.9(4)
N1–N2–C7–C8	0.0(5)
N1–C9–C8–C7	−0.5(5)
N4–N3–C4–C5	179.7(4)
N4–N3–C4–C3	−0.5(5)
N4–C2–C1–F00T	160.8(4)
N4–C2–C1–F00V	−78.1(6)
N4–C2–C1–F007	41.8(6)
N4–C2–C3–C4	−0.2(5)
N5–N6–C12–C11	−179.7(4)
N5–N6–C12–C13	0.7(5)
N5–C14–C13–C12	−0.8(6)

N5–C14–C15–F00D	−174.7(5)
N5–C14–C15–F00O	−55.0(7)
N5–C14–C15–F00W	65.4(7)
N6–N5–C14–C13	1.3(6)
N6–N5–C14–C15	−175.8(4)
N6–C12–C13–C14	0.0(6)
C7–N2–N1–Ag3	−171.2(3)
C7–N2–N1–C9	−0.3(4)
C4–N3–N4–Ag2	169.9(3)
C4–N3–N4–C2	0.4(5)
C10–C9–C8–C7	174.6(4)
C14–N5–N6–Ag3	172.1(3)
C14–N5–N6–C12	−1.2(5)
C5–C4–C3–C2	−179.9(5)
C11–C12–C13–C14	−179.5(5)
C6–C7–C8–C9	−172.1(4)
C13–C14–C15–F00D	8.8(9)
C13–C14–C15–F00O	128.5(6)
C13–C14–C15–F00W	−111.0(7)
C15–C14–C13–C12	175.9(5)
C1–C2–C3–C4	−178.5(5)
C8–C7–C6–F00H	81.0(6)
C8–C7–C6–F00I	−39.2(7)
C8–C7–C6–F009	−158.3(4)
C3–C2–C1–F00T	−21.0(7)
C3–C2–C1–F00V	100.1(7)
C3–C2–C1–F007	−140.1(5)
C3–C4–C5–F00L	−8.9(7)
C3–C4–C5–F00M	111.8(6)
C3–C4–C5–F00S	−130.6(5)
Si1–O1–C23–C22	116.0(4)
Si1–O1–C23–C24	−119.6(3)
O1–Si1–C17–C18	56.8(4)
O1–Si1–C17–C16	177.7(4)
O1–Si1–C17–C19	−64.0(4)
C22–C33–C32–O5	−162.8(4)
C22–C33–C32–C25	21.6(6)
C25–C24–C34–O4	41.8(5)
C25–C24–C34–O3	−140.6(3)
C25–C24–C23–O1	−158.1(3)
C25–C24–C23–C22	−37.8(5)
C25–C24–C29–O2	−128.0(4)
C25–C24–C29–C28	49.2(5)
C33–C22–C23–O1	130.7(5)
C33–C22–C23–C24	9.3(6)
C28–C27–C26–C25	−56.8(5)
C28–C27–C26–C30	−173.9(4)
C28–C27–C26–C31	67.9(5)
C27–C28–C29–O2	123.4(5)
C27–C28–C29–C24	−53.7(5)
C21–Si1–O1–C23	−19.8(4)
C21–Si1–C17–C18	−59.2(4)
C21–Si1–C17–C16	61.7(4)
C21–Si1–C17–C19	−180.0(4)
C35–O3–C34–O4	5.6(6)
C35–O3–C34–C24	−172.0(4)

C20–Si1–O1–C23	104.6(4)
C20–Si1–C17–C18	174.5(4)
C20–Si1–C17–C16	−64.6(4)
C20–Si1–C17–C19	53.7(4)
C17–Si1–O1–C23	−137.4(4)
C24–C25–C26–C27	53.1(5)
C24–C25–C26–C30	169.0(4)
C24–C25–C26–C31	−69.0(5)
C24–C25–C32–O5	135.3(4)
C24–C25–C32–C33	−49.3(4)
C26–C25–C24–C34	74.1(5)
C26–C25–C24–C23	−168.8(3)
C26–C25–C24–C29	−48.9(5)
C26–C25–C32–O5	2.3(6)
C26–C25–C32–C33	177.6(4)
C32–C25–C24–C34	−60.1(4)
C32–C25–C24–C23	57.0(4)
C32–C25–C24–C29	176.9(3)
C32–C25–C26–C27	−176.8(4)
C32–C25–C26–C30	−60.9(5)
C32–C25–C26–C31	61.0(5)
C34–C24–C23–O1	−38.2(4)
C34–C24–C23–C22	82.2(4)
C34–C24–C29–O2	109.5(5)
C34–C24–C29–C28	−73.3(5)
C23–C22–C33–C32	−0.2(7)
C23–C24–C34–O4	−78.0(5)
C23–C24–C34–O3	99.6(4)
C23–C24–C29–O2	−7.3(6)
C23–C24–C29–C28	169.8(4)
C29–C28–C27–C26	57.5(5)
C29–C24–C34–O4	163.3(4)
C29–C24–C34–O3	−19.1(5)
C29–C24–C23–O1	82.1(4)
C29–C24–C23–C22	−157.5(4)

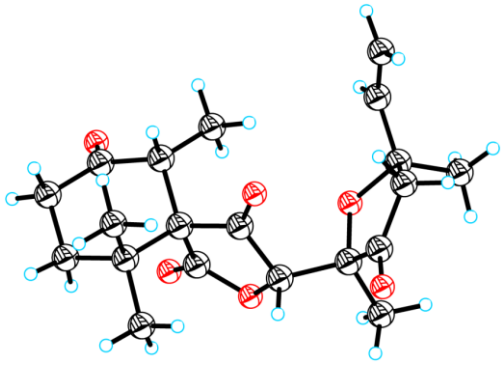


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Table 1. Crystal data and structure refinement for compound 30

CCDC number	2447372
Empirical formula	$C_{50}H_{32}Ag_6F_{36}N_{12}O_6$
Formula weight	2228.09
Temperature/K	99.9(4)
Crystal system	trigonal
Space group	$P3_1$
a/Å	21.49560(10)
b/Å	21.49560(10)
c/Å	38.2395(3)
α/°	90
β/°	90
γ/°	120
Volume/Å^3	15301.77(19)
Z	9
ρ_{calc}g/cm^3	2.176
μ/mm^{-1}	15.030
F(000)	9630.0
Crystal size/mm^3	0.15 × 0.13 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	4.746 to 148
Index ranges	-25 ≤ h ≤ 20, -26 ≤ k ≤ 26, -46 ≤ l ≤ 47
Reflections collected	116881
Independent reflections	40139 [R_{int} = 0.0621, R_{sigma} = 0.0599]
Data/restraints/parameters	40139/55/2986
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0522, wR_2 = 0.1298
Final R indexes [all data]	R_1 = 0.0573, wR_2 = 0.1322
Largest diff. peak/hole / e Å^{-3}	2.02/-1.49
Flack parameter	-0.004(3)

Table 2. Atomic coordinates and U_{eq} [Å^2] for 30.

Atom	***x***	***y***	***z***	U_{eq}
Ag23	0.46667(5)	0.68117(5)	0.67200(3)	0.02720(19)
Ag22	0.25013(5)	0.64674(5)	0.60397(3)	0.02825(19)
Ag1	0.41981(5)	0.66368(5)	0.59238(3)	0.02795(19)
Ag2	0.30789(5)	0.67507(5)	0.68663(3)	0.02707(19)
Ag11	0.95580(5)	0.85348(5)	0.52936(3)	0.02896(19)

Ag13	0.94859(5)	0.99265(5)	0.57760(3)	0.0285(2)
Ag3	0.30690(5)	0.51910(5)	0.65215(3)	0.0302(2)
Ag4	1.05794(5)	0.99189(5)	0.47615(3)	0.0311(2)
Ag5	1.10908(5)	1.00717(5)	0.56010(3)	0.0302(2)
Ag41	0.75677(5)	0.34588(5)	0.48052(3)	0.0340(2)
Ag6	0.26171(5)	0.50486(5)	0.57076(3)	0.0323(2)
Ag16	0.88271(5)	0.96374(5)	0.48953(3)	0.0333(2)
Ag42	0.58911(5)	0.31972(5)	0.48934(3)	0.0335(2)
Ag7	0.90622(5)	0.84468(5)	0.44106(3)	0.0361(2)
Ag56	0.71374(5)	0.36500(5)	0.40036(3)	0.0348(2)
Ag38	0.61828(6)	0.19781(6)	0.43752(3)	0.0375(2)
Ag59	0.58798(6)	0.22224(6)	0.35296(4)	0.0444(3)
Ag73	0.53203(7)	0.32092(8)	0.40131(4)	0.0524(3)
F258	0.5499(4)	0.7089(5)	0.5497(3)	0.048(2)
F300	0.3701(5)	0.8825(5)	0.7526(3)	0.051(2)
F144	0.7190(4)	0.7007(5)	0.5016(3)	0.045(2)
F257	0.5949(4)	0.6390(5)	0.5537(3)	0.044(2)
F280	0.6103(4)	0.7092(4)	0.6226(3)	0.043(2)
O321	0.3208(5)	0.6483(6)	0.5409(3)	0.037(2)
O198	0.8885(5)	0.9055(5)	0.6891(2)	0.0307(19)
F146	0.7501(5)	0.6637(4)	0.5470(3)	0.048(2)
F55	0.8753(5)	0.4535(6)	0.5467(4)	0.065(3)
O317	0.3695(5)	0.7511(6)	0.4648(3)	0.038(2)
F159	1.0085(6)	1.1936(6)	0.6514(3)	0.058(3)
F103	0.7403(6)	0.1106(6)	0.3739(3)	0.058(3)
F282	0.6481(5)	0.6345(5)	0.6286(3)	0.051(2)
F145	0.8287(5)	0.7240(5)	0.5069(3)	0.046(2)
F125	0.9609(5)	0.7393(5)	0.4908(3)	0.059(3)
F292	0.2544(6)	0.8038(6)	0.5885(3)	0.056(3)
F188	1.1878(4)	1.1250(5)	0.5047(3)	0.047(2)
F244	0.1210(6)	0.3522(5)	0.5632(3)	0.053(2)
F270	0.1723(5)	0.3844(5)	0.6386(3)	0.047(2)
F281	0.6145(5)	0.6718(6)	0.6734(3)	0.051(2)
N134	0.8550(5)	0.8949(6)	0.5641(3)	0.028(2)
F296	0.5557(5)	0.8011(5)	0.6194(3)	0.057(3)
F49	0.5565(5)	0.4090(6)	0.5419(4)	0.069(3)
O311	0.2728(5)	0.6225(5)	0.4300(2)	0.032(2)
F158	0.9333(5)	1.1029(5)	0.6223(3)	0.054(3)
O212	0.9057(6)	0.7308(6)	0.5759(3)	0.044(2)
F51	0.6086(6)	0.5159(6)	0.5212(3)	0.055(3)
F274	0.1595(6)	0.6740(6)	0.6878(3)	0.061(3)
O22	0.5189(5)	0.2168(6)	0.6041(3)	0.039(2)
F127	1.0280(8)	0.6968(5)	0.5100(3)	0.067(3)
F126	1.0471(5)	0.7459(5)	0.4598(2)	0.048(2)
F285	0.3092(5)	0.3963(5)	0.6168(3)	0.056(3)
O202	1.0078(5)	0.9672(5)	0.7595(3)	0.037(2)
F298	0.5770(5)	0.9076(5)	0.6284(3)	0.055(3)
O19	0.6543(6)	0.2625(6)	0.5642(3)	0.043(2)
F86	0.8300(6)	0.4965(5)	0.4360(3)	0.065(3)
O216	1.0197(5)	0.9471(5)	0.6481(3)	0.033(2)
O218	0.9588(5)	0.8136(5)	0.7121(3)	0.034(2)
F92	0.8702(5)	0.4073(6)	0.4001(3)	0.068(3)
F284	0.3935(5)	0.3890(5)	0.5895(3)	0.053(3)
F157	0.9928(7)	1.2053(6)	0.5974(3)	0.069(3)
N119	1.0592(6)	0.8672(6)	0.5203(3)	0.031(2)
F256	0.5693(5)	0.6633(6)	0.5031(3)	0.056(3)

N135	0.8568(5)	0.8435(5)	0.5445(3)	0.027(2)
F35	0.4974(5)	0.0773(5)	0.3979(3)	0.057(3)
F269	0.0626(4)	0.3601(4)	0.6355(3)	0.044(2)
N166	0.7915(6)	0.8753(6)	0.4670(4)	0.035(3)
O324	0.2095(6)	0.6820(6)	0.4989(3)	0.042(2)
F271	0.1042(5)	0.3459(4)	0.6838(3)	0.051(2)
N263	0.2106(6)	0.5179(5)	0.6654(3)	0.027(2)
F174	0.6502(7)	0.9093(7)	0.4617(4)	0.077(4)
O330	0.1386(6)	0.7256(7)	0.3695(3)	0.050(3)
O217	1.0086(5)	0.8943(5)	0.5974(3)	0.034(2)
F184	0.8692(5)	1.0823(7)	0.5419(3)	0.065(3)
O20	0.6473(5)	0.2223(6)	0.5102(3)	0.040(2)
N237	0.1599(6)	0.4961(5)	0.5764(3)	0.028(2)
F104	0.6431(6)	0.0935(6)	0.3980(3)	0.070(3)
F243	0.0159(5)	0.3289(5)	0.5488(4)	0.075(4)
F178	0.7718(7)	0.6949(5)	0.4206(4)	0.069(3)
F84	0.8242(8)	0.5703(7)	0.3999(3)	0.095(5)
F286	0.3792(6)	0.3677(5)	0.6444(3)	0.062(3)
N233	0.4694(6)	0.5961(5)	0.6466(3)	0.026(2)
F245	0.1043(8)	0.3884(6)	0.5148(3)	0.076(4)
F37	0.4089(6)	0.0017(6)	0.4298(3)	0.070(3)
F54	0.8958(6)	0.5112(10)	0.4989(4)	0.094(5)
N264	0.2107(6)	0.5767(5)	0.6782(3)	0.026(2)
F183	0.8756(6)	1.1118(7)	0.4880(3)	0.069(3)
F187	1.2046(5)	1.2246(5)	0.5242(4)	0.065(3)
F155	1.2552(5)	1.1527(7)	0.5751(3)	0.069(3)
F294	0.2431(5)	0.7825(6)	0.6434(3)	0.059(3)
N254	0.4225(6)	0.5846(6)	0.5593(3)	0.029(2)
C203	1.0096(7)	0.9291(7)	0.6849(3)	0.027(3)
H203	1.057303	0.955036	0.696850	0.032
F302	0.2968(5)	0.7949(6)	0.7215(4)	0.073(4)
F293	0.3088(6)	0.8901(5)	0.6250(3)	0.062(3)
N58	0.6971(7)	0.2511(6)	0.3502(3)	0.037(3)
N226	0.4043(6)	0.7690(6)	0.7001(3)	0.029(2)
N167	0.8017(6)	0.8288(6)	0.4473(4)	0.037(3)
O21	0.5787(7)	0.1124(6)	0.6190(3)	0.048(3)
N40	0.7757(6)	0.2710(7)	0.4543(3)	0.036(3)
O24	0.6329(6)	0.2611(6)	0.6763(3)	0.046(3)
N234	0.4092(6)	0.5324(6)	0.6405(3)	0.031(3)
O325	0.2210(5)	0.6337(5)	0.3822(2)	0.0292(19)
N147	1.0417(6)	1.0870(6)	0.5935(3)	0.030(2)
F50	0.6236(6)	0.4991(8)	0.5741(3)	0.069(3)
N44	0.7423(6)	0.4200(6)	0.5093(3)	0.032(2)
N164	0.9746(6)	1.0608(6)	0.5052(3)	0.030(2)
F261	0.2696(6)	0.3756(6)	0.5399(4)	0.087(5)
F297	0.5592(5)	0.8675(8)	0.5770(3)	0.074(4)
F301	0.3677(8)	0.8972(7)	0.6979(3)	0.075(4)
F108	0.8903(6)	0.3128(7)	0.5080(3)	0.069(3)
F36	0.3902(6)	0.0548(6)	0.3891(3)	0.067(3)
F67	0.4553(7)	0.0653(6)	0.3138(4)	0.081(4)
F154	1.2391(7)	1.1185(10)	0.6264(4)	0.093(5)
N57	0.7463(6)	0.3087(6)	0.3677(3)	0.032(2)
F191	1.2058(6)	1.0266(9)	0.4542(4)	0.110(6)
N287	0.4659(6)	0.7662(6)	0.6984(3)	0.028(2)
N169	1.0097(6)	0.8652(6)	0.4274(3)	0.034(3)
N43	0.6753(6)	0.4119(6)	0.5129(3)	0.032(2)

F194	1.0036(6)	0.7488(7)	0.3601(4)	0.086(5)
N75	0.6836(8)	0.4346(6)	0.4240(3)	0.041(3)
F107	0.9552(5)	0.3067(7)	0.4673(4)	0.077(4)
N39	0.7239(7)	0.2144(8)	0.4367(4)	0.042(3)
C323	0.2159(7)	0.6558(7)	0.4722(4)	0.030(3)
F248	-0.0003(6)	0.5605(8)	0.6035(5)	0.104(6)
F193	0.9288(7)	0.7834(7)	0.3660(4)	0.083(4)
F85	0.8334(8)	0.5936(6)	0.4550(3)	0.081(4)
N74	0.6134(8)	0.4174(8)	0.4250(4)	0.048(3)
N120	1.1180(6)	0.9262(6)	0.5333(3)	0.030(2)
C199	0.9597(7)	0.9531(7)	0.7013(4)	0.028(3)
F53	0.9013(5)	0.5633(5)	0.5474(4)	0.072(3)
C204	0.9825(7)	0.8492(7)	0.6864(4)	0.029(3)
N116	1.0694(5)	0.9237(6)	0.4399(3)	0.029(2)
F66	0.3872(7)	0.0831(6)	0.2782(4)	0.083(4)
N230	0.4114(5)	0.7532(5)	0.6113(3)	0.025(2)
C313	0.3458(7)	0.6828(8)	0.4805(4)	0.034(3)
N229	0.3446(5)	0.7464(6)	0.6139(3)	0.027(2)
C148	1.0540(7)	1.1444(6)	0.6117(4)	0.032(3)
N238	0.1559(6)	0.5524(6)	0.5881(3)	0.029(2)
F97	0.6547(7)	0.1809(6)	0.2808(3)	0.070(3)
N31	0.5156(6)	0.1830(6)	0.4453(3)	0.033(2)
C114	1.1025(8)	0.8725(8)	0.3977(4)	0.039(3)
H114	1.130550	0.862438	0.382031	0.047
N151	1.1059(6)	1.0881(6)	0.5884(3)	0.030(2)
F96	0.7334(8)	0.1489(7)	0.2881(4)	0.084(4)
C266	0.0960(8)	0.4858(7)	0.6799(4)	0.033(3)
H266	0.045451	0.458596	0.683196	0.040
F102	0.7062(8)	0.0502(6)	0.4212(3)	0.081(4)
C206	1.0640(8)	0.8186(8)	0.6505(4)	0.037(3)
F190	1.2443(7)	0.9637(9)	0.4351(6)	0.125(7)
N30	0.5034(6)	0.2249(6)	0.4674(4)	0.036(3)
C265	0.1439(7)	0.5581(7)	0.6871(4)	0.034(3)
C113	1.0282(7)	0.8350(8)	0.4023(4)	0.036(3)
F182	0.9272(6)	1.1926(6)	0.5268(4)	0.077(4)
N250	0.3612(6)	0.5214(6)	0.5540(3)	0.033(3)
N160	1.0428(6)	1.0718(6)	0.5009(3)	0.030(2)
F176	0.6516(8)	0.8584(10)	0.5093(4)	0.094(5)
F68	0.5022(6)	0.1572(6)	0.2805(4)	0.071(3)
C137	0.7442(8)	0.8005(8)	0.5629(4)	0.038(3)
H137	0.694191	0.769633	0.566650	0.045
C7	0.6096(8)	0.1544(8)	0.5961(4)	0.038(3)
F131	1.2870(7)	0.9452(8)	0.5491(7)	0.134(8)
C162	1.0511(8)	1.1779(8)	0.5151(4)	0.041(3)
H162	1.069703	1.227098	0.520757	0.049
C277	0.5034(7)	0.5225(7)	0.6232(4)	0.034(3)
H277	0.532156	0.504270	0.613932	0.041
C5	0.5894(8)	0.2576(9)	0.6175(4)	0.039(3)
F186	1.1866(6)	1.1999(9)	0.4699(3)	0.090(5)
C242	0.0850(9)	0.3799(8)	0.5481(4)	0.041(3)
C205	0.9948(7)	0.8264(7)	0.6509(4)	0.029(3)
C136	0.7903(7)	0.7869(6)	0.5436(4)	0.029(3)
F175	0.7417(7)	0.9584(9)	0.4941(6)	0.137(9)
F273	0.0576(6)	0.5891(7)	0.7009(5)	0.107(6)
F303	0.6196(8)	0.8314(12)	0.6910(4)	0.109(6)
F275	0.1460(12)	0.6232(9)	0.7359(3)	0.113(7)

N60	0.4812(7)	0.2009(7)	0.3485(5)	0.055(4)
C215	1.0071(6)	0.8896(7)	0.6283(4)	0.025(3)
F80	0.4961(8)	0.4233(8)	0.4602(5)	0.098(5)
C267	0.1425(7)	0.4646(7)	0.6667(4)	0.030(3)
F249	0.1064(8)	0.6375(8)	0.6161(5)	0.103(6)
C211	0.8594(8)	0.7638(8)	0.6363(4)	0.039(3)
H21A	0.848983	0.772708	0.660125	0.058
H21B	0.818681	0.719218	0.627424	0.058
H21C	0.867472	0.803888	0.621158	0.058
C6	0.6398(8)	0.2364(8)	0.5997(4)	0.036(3)
H6	0.686108	0.257931	0.612936	0.044
F82	0.5507(10)	0.5348(9)	0.4517(4)	0.108(6)
C210	0.9261(7)	0.7567(6)	0.6366(4)	0.032(3)
H210	0.916564	0.716196	0.652698	0.039
F262	0.3434(6)	0.3755(8)	0.5034(6)	0.143(10)
C276	0.4285(7)	0.4863(7)	0.6267(4)	0.036(3)
C224	0.4892(9)	0.8663(8)	0.7272(5)	0.045(4)
H224	0.512583	0.909768	0.740128	0.054
F179	0.7695(10)	0.7544(8)	0.3775(4)	0.091(5)
C289	0.4260(8)	0.8634(8)	0.6186(4)	0.036(3)
H289	0.446929	0.913931	0.621295	0.044
C255	0.5471(8)	0.6490(8)	0.5364(4)	0.038(3)
C241	0.0954(7)	0.4472(7)	0.5644(4)	0.031(3)
F106	0.9211(6)	0.3861(6)	0.4655(4)	0.074(3)
C138	0.7878(7)	0.8702(7)	0.5758(4)	0.032(3)
C139	0.7659(7)	0.9114(8)	0.5984(5)	0.043(4)
C115	1.1255(7)	0.9281(8)	0.4217(4)	0.033(3)
C315	0.3696(8)	0.7731(8)	0.5257(4)	0.039(3)
H31A	0.404692	0.792079	0.545103	0.047
H31B	0.329249	0.781392	0.531062	0.047
F27	0.3364(6)	0.1903(9)	0.5010(5)	0.114(6)
C25	0.4030(8)	0.1237(9)	0.6202(5)	0.051(4)
H25	0.386175	0.123698	0.597280	0.061
C123	1.0804(8)	0.8213(8)	0.5086(4)	0.037(3)
C46	0.7520(8)	0.5114(8)	0.5431(4)	0.040(3)
H46	0.771242	0.553637	0.556963	0.048
C214	1.1307(8)	0.8889(9)	0.6603(5)	0.044(4)
H21D	1.135506	0.927039	0.644559	0.066
H21E	1.173202	0.883538	0.658208	0.066
H21F	1.126263	0.901417	0.684457	0.066
C225	0.4190(7)	0.8292(7)	0.7166(4)	0.032(3)
C295	0.5383(8)	0.8491(7)	0.6104(4)	0.033(3)
C156	0.9977(8)	1.1628(7)	0.6210(4)	0.035(3)
N61	0.4585(7)	0.2358(10)	0.3705(5)	0.072(6)
F153	1.2762(6)	1.2269(8)	0.6166(6)	0.118(7)
O16	0.5403(8)	0.0632(8)	0.4798(4)	0.070(4)
C278	0.5260(7)	0.5894(7)	0.6358(4)	0.027(3)
C290	0.3541(7)	0.8113(7)	0.6177(4)	0.032(3)
C314	0.3432(8)	0.6952(9)	0.5199(4)	0.037(3)
C209	0.9431(8)	0.7385(7)	0.6010(4)	0.036(3)
C149	1.1271(8)	1.1864(8)	0.6187(5)	0.042(4)
H149	1.151000	1.230731	0.631008	0.050
F95	0.6408(9)	0.1084(6)	0.3212(4)	0.094(5)
C307	0.1195(8)	0.6868(9)	0.3944(5)	0.040(3)
C253	0.4742(7)	0.5866(7)	0.5384(4)	0.032(3)
C2	0.4649(8)	0.1927(9)	0.6325(5)	0.045(4)

C45	0.7874(8)	0.4789(8)	0.5272(4)	0.039(3)
C100	0.7522(9)	0.1743(9)	0.4250(4)	0.045(4)
C163	0.9799(9)	1.1232(8)	0.5132(4)	0.039(3)
C200	0.9556(7)	0.9402(7)	0.7401(4)	0.031(3)
F140	0.8170(7)	0.9534(10)	0.6208(4)	0.106(6)
C279	0.5993(8)	0.6513(7)	0.6402(4)	0.035(3)
F260	0.2789(8)	0.4234(9)	0.4922(5)	0.119(7)
C99	0.8229(9)	0.2044(9)	0.4357(5)	0.046(4)
H99	0.855572	0.187570	0.431480	0.055
C223	0.5188(7)	0.8258(7)	0.7147(4)	0.034(3)
C268	0.1206(8)	0.3891(8)	0.6564(4)	0.038(3)
C308	0.1624(9)	0.7046(8)	0.4276(4)	0.040(3)
H308	0.133600	0.710969	0.446380	0.048
F129	1.2770(11)	1.0247(10)	0.5241(6)	0.172(12)
C310	0.2220(7)	0.6317(7)	0.4137(4)	0.030(3)
F91	0.9318(7)	0.3739(10)	0.3710(6)	0.120(6)
F304	0.5906(8)	0.7879(11)	0.7401(6)	0.131(8)
C23	0.6208(10)	0.3393(9)	0.6130(5)	0.048(4)
H23A	0.617074	0.350040	0.588452	0.072
H23B	0.671318	0.364702	0.620154	0.072
H23C	0.593732	0.355091	0.627618	0.072
C327	0.1129(10)	0.5027(8)	0.4464(6)	0.054(5)
H32A	0.143754	0.502490	0.427598	0.081
H32B	0.066837	0.457658	0.445942	0.081
H32C	0.136410	0.507599	0.469002	0.081
C143	0.7727(7)	0.7197(7)	0.5251(4)	0.036(3)
C252	0.4460(8)	0.5232(10)	0.5196(5)	0.054(5)
H252	0.470130	0.509987	0.502959	0.065
C89	0.8110(9)	0.3210(8)	0.3567(4)	0.043(4)
C4	0.5827(7)	0.2373(7)	0.6557(4)	0.036(3)
C88	0.8033(10)	0.2703(10)	0.3325(5)	0.053(4)
H88	0.840026	0.266147	0.320753	0.063
C161	1.0878(8)	1.1429(7)	0.5066(4)	0.034(3)
C48	0.6163(8)	0.4721(8)	0.5422(4)	0.040(3)
C101	0.7105(10)	0.1074(9)	0.4049(5)	0.051(4)
C309	0.1735(7)	0.6404(7)	0.4390(4)	0.030(3)
C77	0.6780(16)	0.5288(12)	0.4427(5)	0.072(7)
H77	0.690465	0.575293	0.450948	0.087
F221	0.6332(7)	0.8956(9)	0.7353(6)	0.138(9)
C76	0.7250(11)	0.5040(9)	0.4343(4)	0.051(4)
C14	0.7573(10)	0.1921(10)	0.5716(5)	0.053(4)
H14A	0.762710	0.235690	0.560628	0.080
H14B	0.798883	0.186884	0.565866	0.080
H14C	0.754152	0.195538	0.597062	0.080
C197	0.8365(8)	0.8845(8)	0.7179(4)	0.036(3)
C47	0.6809(7)	0.4650(7)	0.5331(4)	0.031(3)
F247	0.0671(11)	0.6274(9)	0.5657(4)	0.108(6)
C124	1.0288(10)	0.7515(8)	0.4926(4)	0.046(4)
C189	1.1998(8)	0.9875(9)	0.4282(4)	0.044(4)
C312	0.2708(8)	0.6312(8)	0.4675(4)	0.035(3)
H312	0.252737	0.583520	0.479138	0.042
F111	0.9357(9)	0.7170(7)	0.4043(4)	0.122(7)
C316	0.4049(8)	0.8079(8)	0.4911(4)	0.042(3)
F180	0.6719(6)	0.6754(8)	0.4028(6)	0.118(7)
C240	0.0475(8)	0.4708(8)	0.5688(4)	0.038(3)
H240	-0.002114	0.446871	0.562892	0.046

C196	0.7756(8)	0.8115(8)	0.7096(4)	0.037(3)
H196	0.759092	0.803183	0.686085	0.044
C291	0.2892(8)	0.8222(8)	0.6188(5)	0.041(3)
F142	0.7589(14)	0.9579(11)	0.5817(5)	0.138(7)
C283	0.3773(9)	0.4097(8)	0.6192(5)	0.046(4)
C8	0.6229(8)	0.1402(8)	0.5588(4)	0.040(3)
C98	0.8348(8)	0.2654(9)	0.4541(4)	0.038(3)
C306	0.0482(9)	0.6164(10)	0.3962(5)	0.051(4)
H30A	0.016220	0.620828	0.413462	0.061
H30B	0.024273	0.605810	0.373119	0.061
C272	0.1275(8)	0.6120(8)	0.7033(4)	0.040(3)
C172	0.7231(7)	0.8573(9)	0.4636(5)	0.044(4)
F141	0.7103(8)	0.8732(7)	0.6160(6)	0.135(8)
C87	0.7319(9)	0.2281(9)	0.3293(4)	0.042(3)
F192	1.2290(8)	1.0258(10)	0.4008(4)	0.144(9)
F110	0.4290(9)	0.2924(9)	0.4932(6)	0.113(6)
C29	0.4336(7)	0.1934(8)	0.4746(5)	0.043(4)
C246	0.0660(7)	0.5900(8)	0.5935(4)	0.038(3)
C9	0.5539(8)	0.0774(8)	0.5416(5)	0.041(3)
H9	0.539222	0.033850	0.556392	0.049
C219	0.9866(9)	1.0321(8)	0.6928(4)	0.040(3)
H21G	0.957086	1.047999	0.705194	0.060
H21H	0.983318	1.037647	0.667587	0.060
H21I	1.036759	1.061249	0.700321	0.060
C201	0.8794(7)	0.8891(8)	0.7508(4)	0.033(3)
H20A	0.864932	0.908067	0.770917	0.039
H20B	0.872864	0.841468	0.757087	0.039
C208	1.0096(9)	0.7318(8)	0.5992(4)	0.042(3)
H20C	1.001285	0.688855	0.612530	0.050
H20D	1.018752	0.724846	0.574524	0.050
C207	1.0744(7)	0.7965(7)	0.6136(4)	0.034(3)
H20E	1.087950	0.837337	0.597449	0.040
H20F	1.114797	0.786732	0.614174	0.040
C185	1.1669(8)	1.1729(8)	0.5009(4)	0.042(4)
C305	0.0605(9)	0.5555(9)	0.4068(5)	0.047(4)
H30C	0.088088	0.548445	0.388056	0.056
H30D	0.013243	0.510890	0.408431	0.056
C34	0.4409(11)	0.0652(9)	0.4157(5)	0.059(5)
C32	0.4499(8)	0.1248(8)	0.4387(4)	0.044(4)
C1	0.4411(9)	0.2469(9)	0.6385(6)	0.053(4)
H1A	0.423171	0.255563	0.616516	0.079
H1B	0.481943	0.292060	0.646796	0.079
H1C	0.402811	0.228515	0.656055	0.079
C18	0.6422(7)	0.2108(7)	0.5410(4)	0.033(3)
F93	0.8961(9)	0.4422(9)	0.3495(4)	0.116(6)
C299	0.3633(8)	0.8521(9)	0.7220(4)	0.040(3)
C239	0.0886(7)	0.5382(7)	0.5838(4)	0.032(3)
C288	0.4605(7)	0.8227(7)	0.6145(4)	0.029(3)
C150	1.1572(7)	1.1489(8)	0.6036(4)	0.039(3)
C329	0.2330(9)	0.7748(8)	0.4247(5)	0.043(4)
H32D	0.262971	0.770233	0.406664	0.065
H32E	0.258148	0.786099	0.447165	0.065
H32F	0.223597	0.813463	0.418203	0.065
C322	0.3960(10)	0.6530(11)	0.4729(4)	0.051(4)
H32G	0.442353	0.683226	0.484349	0.077
H32H	0.403188	0.653007	0.447577	0.077

H32I	0.374475	0.603823	0.481823	0.077
C222	0.5922(9)	0.8380(10)	0.7195(5)	0.050(4)
C13	0.6899(9)	0.1277(10)	0.5584(5)	0.049(4)
C220	0.8079(9)	0.9374(9)	0.7198(5)	0.046(4)
H22A	0.848416	0.986629	0.721653	0.069
H22B	0.776789	0.926346	0.740264	0.069
H22C	0.780435	0.932994	0.698539	0.069
C64	0.4297(9)	0.1570(9)	0.3267(6)	0.061(6)
C152	1.2341(9)	1.1645(10)	0.6055(5)	0.051(4)
C195	0.7425(9)	0.7576(9)	0.7314(5)	0.048(4)
H19A	0.756958	0.763126	0.755237	0.057
H19B	0.704039	0.713025	0.723436	0.057
C128	1.2452(9)	0.9701(10)	0.5429(7)	0.066(6)
C171	0.6879(9)	0.7992(10)	0.4409(5)	0.054(4)
H171	0.639097	0.775784	0.433610	0.065
C112	0.9742(9)	0.7705(10)	0.3835(5)	0.051(4)
C251	0.3762(8)	0.4838(9)	0.5300(5)	0.050(5)
C328	0.0564(10)	0.5683(11)	0.4720(5)	0.058(5)
H32J	0.008419	0.525489	0.471672	0.086
H32K	0.051929	0.611410	0.470336	0.086
H32L	0.080655	0.569527	0.493921	0.086
C122	1.1531(9)	0.8506(8)	0.5139(5)	0.051(4)
H122	1.182245	0.830371	0.508105	0.061
C17	0.4917(8)	0.0912(9)	0.5415(5)	0.047(4)
H17A	0.483933	0.103236	0.565193	0.071
H17B	0.448270	0.047958	0.533461	0.071
H17C	0.502348	0.131198	0.525697	0.071
C28	0.4040(9)	0.2254(10)	0.4997(6)	0.055(5)
C10	0.5739(10)	0.0620(10)	0.5064(6)	0.058(5)
C319	0.3951(9)	0.8682(9)	0.4794(4)	0.049(4)
H319	0.405725	0.882564	0.455643	0.059
F130	1.2424(7)	0.9953(14)	0.5742(6)	0.155(10)
C33	0.3969(8)	0.1282(8)	0.4577(5)	0.046(4)
H33	0.347115	0.093824	0.458795	0.055
C105	0.9000(8)	0.3178(11)	0.4733(5)	0.053(4)
C3	0.5059(9)	0.1854(10)	0.6643(5)	0.048(4)
H3A	0.491383	0.198650	0.686337	0.058
H3B	0.497370	0.135817	0.666290	0.058
C318	0.4853(8)	0.8331(11)	0.4917(5)	0.060(5)
H31C	0.510779	0.878178	0.504876	0.090
H31D	0.503714	0.840818	0.467754	0.090
H31E	0.492784	0.796454	0.503039	0.090
F81	0.5108(13)	0.4624(16)	0.4082(5)	0.156(10)
C90	0.8780(8)	0.3865(10)	0.3697(5)	0.050(4)
C121	1.1742(8)	0.9160(8)	0.5296(5)	0.043(4)
C52	0.8641(8)	0.5019(9)	0.5299(5)	0.050(4)
C94	0.6892(12)	0.1674(11)	0.3048(6)	0.064(5)
C213	1.0559(9)	0.7610(9)	0.6770(5)	0.045(4)
H21J	1.050564	0.775606	0.700555	0.067
H21K	1.098585	0.755776	0.676109	0.067
H21L	1.013264	0.715059	0.671109	0.067
F109	0.4295(10)	0.2285(13)	0.5315(5)	0.129(7)
C326	0.1000(8)	0.5659(8)	0.4412(4)	0.041(3)
C15	0.6741(14)	0.0619(13)	0.5819(7)	0.080(7)
H15A	0.711097	0.048682	0.577951	0.121
H15B	0.626894	0.021156	0.575954	0.121

H15C	0.674552	0.074608	0.606546	0.121
C63	0.3694(10)	0.1634(14)	0.3333(7)	0.074(7)
H63	0.324963	0.140984	0.321150	0.089
C62	0.3879(10)	0.2074(14)	0.3603(7)	0.073(7)
C170	0.7401(7)	0.7837(8)	0.4316(5)	0.041(4)
C26	0.3690(10)	0.0627(11)	0.6375(6)	0.065(5)
H26A	0.383453	0.059443	0.660542	0.078
H26B	0.329979	0.021951	0.626818	0.078
C12	0.7024(10)	0.1128(12)	0.5211(6)	0.066(6)
H12A	0.742391	0.102468	0.520739	0.079
H12B	0.716720	0.156174	0.506725	0.079
C259	0.3179(10)	0.4141(12)	0.5169(7)	0.070(7)
C11	0.6340(12)	0.0479(10)	0.5047(6)	0.066(5)
H11A	0.643603	0.041363	0.480004	0.080
H11B	0.621680	0.003274	0.517615	0.080
C181	0.9138(10)	1.1281(9)	0.5179(5)	0.048(4)
C78	0.6122(14)	0.4741(11)	0.4368(5)	0.062(6)
C320	0.3728(13)	0.9040(10)	0.4991(6)	0.069(6)
H32M	0.361521	0.891548	0.523036	0.083
H32N	0.368099	0.942035	0.489310	0.083
C65	0.4428(10)	0.1163(9)	0.3005(6)	0.062(5)
C83	0.8022(12)	0.5402(10)	0.4314(5)	0.062(5)
C69	0.3460(13)	0.236(2)	0.3767(9)	0.104(11)
F70	0.2885(14)	0.220(2)	0.3631(9)	0.26(2)
F72	0.3779(14)	0.3038(17)	0.3826(12)	0.25(2)
C177	0.7363(9)	0.7270(9)	0.4078(6)	0.055(5)
C173	0.6916(9)	0.8967(11)	0.4817(6)	0.062(5)
C79	0.5424(15)	0.4730(15)	0.4403(7)	0.079(7)
F71	0.3300(19)	0.215(2)	0.4096(8)	0.211(16)

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic displacement parameters [Å²] for 30. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ag23	0.0252(4)	0.0183(4)	0.0397(5)	−0.0017(3)	0.0038(4)	0.0121(4)
Ag22	0.0193(4)	0.0217(4)	0.0418(5)	−0.0018(4)	−0.0003(4)	0.0088(3)
Ag1	0.0224(4)	0.0212(4)	0.0419(5)	−0.0055(4)	−0.0023(4)	0.0121(4)
Ag2	0.0220(4)	0.0179(4)	0.0405(5)	−0.0007(3)	0.0001(4)	0.0094(3)
Ag11	0.0209(4)	0.0239(4)	0.0422(5)	−0.0007(4)	0.0027(4)	0.0113(4)
Ag13	0.0180(4)	0.0166(4)	0.0487(6)	0.0003(4)	0.0019(4)	0.0070(3)
Ag3	0.0243(4)	0.0221(4)	0.0442(5)	−0.0035(4)	0.0025(4)	0.0116(4)
Ag4	0.0220(4)	0.0273(5)	0.0424(5)	−0.0001(4)	0.0000(4)	0.0111(4)
Ag5	0.0221(4)	0.0227(4)	0.0448(5)	0.0010(4)	0.0036(4)	0.0104(4)
Ag41	0.0238(5)	0.0309(5)	0.0495(6)	−0.0054(4)	0.0015(4)	0.0153(4)
Ag6	0.0179(4)	0.0230(4)	0.0547(6)	−0.0060(4)	0.0001(4)	0.0093(4)
Ag16	0.0210(4)	0.0277(5)	0.0472(6)	0.0010(4)	0.0029(4)	0.0092(4)
Ag42	0.0183(4)	0.0275(5)	0.0510(6)	0.0005(4)	0.0012(4)	0.0087(4)
Ag7	0.0169(4)	0.0234(5)	0.0645(7)	0.0022(4)	0.0031(4)	0.0075(4)
Ag56	0.0271(5)	0.0298(5)	0.0461(6)	−0.0029(4)	0.0017(4)	0.0131(4)
Ag38	0.0281(5)	0.0385(6)	0.0447(6)	−0.0014(4)	−0.0001(4)	0.0157(4)
Ag59	0.0270(5)	0.0259(5)	0.0723(8)	0.0040(5)	−0.0102(5)	0.0073(4)
Ag73	0.0362(6)	0.0624(8)	0.0648(8)	0.0178(6)	0.0107(5)	0.0293(6)
F258	0.025(4)	0.028(4)	0.089(7)	−0.006(4)	0.007(4)	0.011(4)
F300	0.054(6)	0.049(5)	0.064(6)	−0.017(5)	0.000(5)	0.036(5)
F144	0.024(4)	0.034(5)	0.068(6)	−0.009(4)	−0.012(4)	0.008(4)

F257	0.020(4)	0.043(5)	0.067(6)	−0.004(4)	−0.003(4)	0.016(4)
F280	0.028(4)	0.026(4)	0.070(6)	0.005(4)	0.004(4)	0.010(3)
O321	0.034(5)	0.039(6)	0.034(5)	0.006(4)	0.000(4)	0.015(4)
O198	0.025(5)	0.030(5)	0.038(5)	−0.005(4)	−0.006(4)	0.015(4)
F146	0.045(5)	0.020(4)	0.079(7)	0.003(4)	0.001(5)	0.016(4)
F55	0.031(5)	0.051(6)	0.119(10)	−0.015(6)	−0.018(5)	0.025(5)
O317	0.028(5)	0.047(6)	0.031(5)	0.002(4)	0.000(4)	0.014(5)
F159	0.053(6)	0.066(7)	0.067(7)	−0.027(5)	−0.004(5)	0.038(5)
F103	0.062(7)	0.052(6)	0.062(6)	−0.010(5)	0.011(5)	0.030(5)
F282	0.031(5)	0.051(5)	0.080(7)	−0.001(5)	0.007(4)	0.028(4)
F145	0.029(4)	0.037(5)	0.071(6)	−0.017(4)	−0.002(4)	0.017(4)
F125	0.038(5)	0.032(5)	0.093(8)	−0.025(5)	0.018(5)	0.006(4)
F292	0.055(6)	0.062(6)	0.074(7)	−0.017(5)	−0.022(5)	0.046(5)
F188	0.024(4)	0.034(5)	0.080(7)	−0.010(4)	−0.004(4)	0.011(4)
F244	0.053(6)	0.034(5)	0.075(7)	−0.011(4)	−0.011(5)	0.024(4)
F270	0.033(4)	0.030(4)	0.075(7)	−0.010(4)	−0.001(4)	0.013(4)
F281	0.040(5)	0.056(6)	0.055(6)	−0.011(5)	−0.008(4)	0.021(5)
N134	0.009(4)	0.021(5)	0.050(7)	−0.004(4)	0.003(4)	0.006(4)
F296	0.024(4)	0.031(5)	0.117(9)	0.006(5)	−0.005(5)	0.013(4)
F49	0.027(5)	0.049(6)	0.132(11)	0.001(6)	0.018(5)	0.020(4)
O311	0.034(5)	0.039(5)	0.028(5)	−0.001(4)	−0.001(4)	0.023(4)
F158	0.027(4)	0.033(5)	0.101(8)	−0.009(5)	0.005(5)	0.014(4)
O212	0.049(6)	0.044(6)	0.047(6)	−0.003(5)	−0.003(5)	0.029(5)
F51	0.055(6)	0.056(6)	0.078(7)	0.004(5)	0.001(5)	0.045(5)
F274	0.066(7)	0.047(6)	0.086(8)	0.007(5)	0.017(6)	0.040(5)
O22	0.031(5)	0.035(5)	0.050(6)	−0.010(4)	−0.008(4)	0.015(4)
F127	0.113(10)	0.033(5)	0.056(6)	−0.003(4)	−0.007(6)	0.037(6)
F126	0.054(6)	0.055(6)	0.048(5)	−0.003(4)	0.006(4)	0.036(5)
F285	0.035(5)	0.025(4)	0.098(8)	−0.016(5)	0.010(5)	0.008(4)
O202	0.036(5)	0.032(5)	0.041(6)	−0.004(4)	−0.001(4)	0.016(4)
F298	0.032(5)	0.032(5)	0.090(8)	−0.022(5)	−0.008(5)	0.008(4)
O19	0.044(6)	0.030(5)	0.053(7)	0.001(5)	0.002(5)	0.016(5)
F86	0.043(6)	0.036(5)	0.089(8)	−0.016(5)	0.004(5)	0.000(5)
O216	0.032(5)	0.025(5)	0.038(5)	0.000(4)	0.004(4)	0.012(4)
O218	0.037(5)	0.036(5)	0.037(5)	0.005(4)	0.004(4)	0.024(4)
F92	0.024(5)	0.064(7)	0.078(7)	−0.016(6)	0.002(4)	−0.006(4)
F284	0.049(5)	0.029(4)	0.079(7)	−0.018(4)	0.012(5)	0.018(4)
F157	0.088(8)	0.067(7)	0.081(8)	0.029(6)	0.020(6)	0.060(7)
N119	0.035(6)	0.029(6)	0.041(6)	0.003(5)	0.006(5)	0.024(5)
F256	0.033(5)	0.075(7)	0.052(6)	0.001(5)	0.002(4)	0.020(5)
N135	0.019(5)	0.018(5)	0.037(6)	0.001(4)	0.002(4)	0.004(4)
F35	0.043(5)	0.043(5)	0.073(7)	−0.009(5)	0.000(5)	0.013(4)
F269	0.028(4)	0.022(4)	0.070(6)	−0.006(4)	−0.015(4)	0.003(3)
N166	0.019(5)	0.026(6)	0.058(8)	0.004(5)	0.007(5)	0.011(5)
O324	0.036(5)	0.046(6)	0.040(6)	−0.009(5)	0.005(4)	0.018(5)
F271	0.056(6)	0.022(4)	0.068(6)	0.010(4)	−0.006(5)	0.013(4)
N263	0.020(5)	0.013(5)	0.047(7)	−0.001(4)	0.001(4)	0.006(4)
F174	0.063(7)	0.081(8)	0.108(10)	0.009(7)	0.009(7)	0.052(7)
O330	0.043(6)	0.057(7)	0.061(7)	0.002(6)	−0.007(5)	0.034(6)
O217	0.032(5)	0.032(5)	0.040(6)	0.001(4)	0.004(4)	0.017(4)
F184	0.037(5)	0.072(7)	0.097(9)	−0.001(6)	0.011(5)	0.035(5)
O20	0.028(5)	0.037(6)	0.046(6)	0.004(4)	0.003(4)	0.010(4)
N237	0.024(5)	0.015(5)	0.046(7)	−0.001(4)	0.000(5)	0.010(4)
F104	0.052(6)	0.058(7)	0.095(9)	−0.036(6)	−0.001(6)	0.024(5)
F243	0.029(5)	0.031(5)	0.148(12)	−0.021(6)	−0.025(6)	0.002(4)
F178	0.078(8)	0.033(5)	0.104(9)	−0.005(5)	−0.004(7)	0.034(6)

F84	0.099(10)	0.063(8)	0.053(7)	0.012(6)	0.017(7)	−0.012(7)
F286	0.075(7)	0.030(5)	0.078(7)	0.003(5)	0.010(6)	0.024(5)
N233	0.024(5)	0.019(5)	0.039(6)	0.000(4)	0.003(4)	0.014(4)
F245	0.120(11)	0.051(6)	0.061(7)	−0.010(5)	0.007(7)	0.046(7)
F37	0.065(7)	0.035(5)	0.093(9)	0.003(5)	0.011(6)	0.013(5)
F54	0.032(6)	0.152(14)	0.085(9)	−0.020(9)	0.009(6)	0.036(7)
N264	0.025(5)	0.016(5)	0.037(6)	−0.003(4)	−0.002(4)	0.010(4)
F183	0.056(6)	0.085(8)	0.090(8)	−0.023(7)	−0.029(6)	0.054(6)
F187	0.028(5)	0.033(5)	0.116(10)	−0.019(5)	−0.015(5)	0.001(4)
F155	0.028(5)	0.092(9)	0.077(8)	−0.012(6)	0.002(5)	0.021(5)
F294	0.039(5)	0.068(7)	0.085(8)	0.015(6)	0.021(5)	0.037(5)
N254	0.018(5)	0.027(5)	0.042(6)	−0.004(5)	0.003(4)	0.011(4)
C203	0.027(6)	0.025(6)	0.029(6)	0.000(5)	−0.003(5)	0.013(5)
F302	0.031(5)	0.052(6)	0.148(12)	−0.043(7)	−0.019(6)	0.028(5)
F293	0.053(6)	0.039(5)	0.112(9)	−0.011(5)	−0.008(6)	0.036(5)
N58	0.037(7)	0.026(6)	0.049(7)	−0.004(5)	−0.004(5)	0.016(5)
N226	0.028(6)	0.028(6)	0.036(6)	−0.001(4)	0.002(4)	0.018(5)
N167	0.020(5)	0.019(5)	0.065(8)	−0.001(5)	0.006(5)	0.004(4)
O21	0.052(7)	0.042(6)	0.049(7)	0.008(5)	0.007(5)	0.024(6)
N40	0.028(6)	0.037(6)	0.048(7)	−0.015(5)	−0.005(5)	0.020(5)
O24	0.042(6)	0.045(6)	0.046(6)	−0.004(5)	−0.005(5)	0.020(5)
N234	0.018(5)	0.019(5)	0.060(8)	−0.003(5)	0.007(5)	0.013(4)
O325	0.025(4)	0.029(5)	0.036(5)	−0.006(4)	−0.002(4)	0.015(4)
N147	0.023(5)	0.025(5)	0.046(7)	0.005(5)	0.003(5)	0.015(5)
F50	0.064(7)	0.111(10)	0.061(7)	−0.015(6)	0.004(5)	0.065(7)
N44	0.016(5)	0.018(5)	0.050(7)	−0.002(5)	0.000(4)	0.001(4)
N164	0.028(6)	0.024(5)	0.040(6)	−0.003(4)	−0.002(5)	0.014(5)
F261	0.040(6)	0.038(6)	0.159(14)	−0.037(7)	0.006(7)	0.002(5)
F297	0.031(5)	0.124(11)	0.050(6)	0.008(6)	0.005(4)	0.026(6)
F301	0.102(10)	0.092(9)	0.074(8)	0.019(7)	0.013(7)	0.080(8)
F108	0.049(6)	0.095(9)	0.069(7)	−0.027(6)	−0.013(5)	0.040(6)
F36	0.056(7)	0.054(6)	0.069(7)	−0.005(5)	−0.019(5)	0.011(5)
F67	0.081(9)	0.046(6)	0.110(10)	0.015(6)	−0.025(7)	0.028(6)
F154	0.053(7)	0.155(14)	0.095(10)	0.022(9)	−0.004(6)	0.071(9)
N57	0.019(5)	0.029(6)	0.045(7)	−0.007(5)	−0.007(5)	0.010(5)
F191	0.024(5)	0.114(12)	0.138(13)	−0.071(10)	0.013(6)	−0.006(6)
N287	0.019(5)	0.018(5)	0.039(6)	−0.001(4)	0.002(4)	0.005(4)
N169	0.025(6)	0.023(5)	0.054(7)	−0.002(5)	0.008(5)	0.010(5)
N43	0.023(5)	0.029(6)	0.049(7)	0.001(5)	0.003(5)	0.016(5)
F194	0.048(6)	0.068(8)	0.143(12)	−0.068(8)	−0.006(7)	0.029(6)
N75	0.065(9)	0.027(6)	0.043(7)	−0.001(5)	0.006(6)	0.032(6)
F107	0.034(5)	0.107(10)	0.108(10)	−0.046(8)	−0.020(6)	0.049(6)
N39	0.039(7)	0.049(8)	0.049(8)	−0.008(6)	0.000(6)	0.030(6)
C323	0.021(6)	0.032(7)	0.036(7)	0.001(5)	0.007(5)	0.012(5)
F248	0.037(6)	0.076(9)	0.198(17)	−0.028(10)	0.028(8)	0.027(6)
F193	0.066(8)	0.089(9)	0.116(10)	−0.057(8)	−0.052(7)	0.057(7)
F85	0.119(11)	0.031(5)	0.071(8)	−0.018(5)	−0.005(7)	0.022(6)
N74	0.059(9)	0.058(9)	0.052(8)	0.012(7)	0.017(7)	0.049(8)
N120	0.018(5)	0.023(5)	0.046(7)	0.002(5)	0.005(4)	0.007(4)
C199	0.022(6)	0.023(6)	0.038(7)	−0.007(5)	−0.005(5)	0.011(5)
F53	0.028(5)	0.035(5)	0.134(11)	−0.025(6)	−0.011(6)	0.003(4)
C204	0.019(6)	0.030(7)	0.036(7)	0.005(5)	0.000(5)	0.012(5)
N116	0.015(5)	0.029(6)	0.042(6)	0.003(5)	0.003(4)	0.010(4)
F66	0.059(7)	0.052(7)	0.110(10)	0.007(6)	−0.034(7)	0.008(6)
N230	0.021(5)	0.013(5)	0.034(6)	−0.003(4)	−0.002(4)	0.002(4)
C313	0.029(7)	0.044(8)	0.027(7)	0.004(6)	0.001(5)	0.016(6)

N229	0.014(5)	0.025(5)	0.041(6)	0.003(4)	0.002(4)	0.008(4)
C148	0.027(7)	0.010(5)	0.049(8)	−0.007(5)	0.001(6)	0.003(5)
N238	0.030(6)	0.020(5)	0.043(6)	0.003(4)	0.004(5)	0.016(5)
F97	0.083(8)	0.063(7)	0.076(8)	−0.028(6)	−0.036(6)	0.046(7)
N31	0.026(6)	0.018(5)	0.045(7)	0.000(4)	0.003(5)	0.004(4)
C114	0.027(7)	0.041(8)	0.046(9)	−0.009(6)	−0.006(6)	0.015(6)
N151	0.018(5)	0.022(5)	0.042(6)	−0.002(4)	0.000(4)	0.003(4)
F96	0.094(9)	0.086(9)	0.113(10)	−0.050(8)	−0.038(8)	0.076(8)
C266	0.030(7)	0.028(7)	0.048(8)	0.004(6)	0.007(6)	0.020(6)
F102	0.123(12)	0.039(6)	0.077(8)	0.005(5)	0.012(8)	0.038(7)
C206	0.033(7)	0.036(8)	0.042(8)	0.005(6)	0.008(6)	0.018(6)
F190	0.027(6)	0.088(11)	0.25(2)	−0.020(12)	−0.025(9)	0.020(7)
N30	0.021(6)	0.025(6)	0.056(8)	0.003(5)	0.004(5)	0.006(5)
C265	0.027(7)	0.023(6)	0.041(8)	−0.001(5)	0.002(6)	0.005(5)
C113	0.022(6)	0.036(8)	0.049(8)	−0.001(6)	−0.002(6)	0.014(6)
F182	0.064(7)	0.049(6)	0.140(12)	−0.032(7)	−0.024(7)	0.044(6)
N250	0.019(5)	0.017(5)	0.064(8)	−0.011(5)	0.002(5)	0.009(4)
N160	0.028(6)	0.025(5)	0.036(6)	−0.002(4)	0.000(4)	0.012(5)
F176	0.090(10)	0.150(14)	0.086(9)	0.017(9)	0.026(8)	0.092(11)
F68	0.053(7)	0.046(6)	0.102(9)	0.002(6)	−0.008(6)	0.017(5)
C137	0.023(7)	0.030(7)	0.058(9)	0.001(6)	0.003(6)	0.012(6)
C7	0.029(7)	0.031(7)	0.054(9)	0.002(6)	−0.004(6)	0.015(6)
F131	0.035(7)	0.070(9)	0.30(3)	−0.021(12)	−0.033(10)	0.031(7)
C162	0.038(8)	0.034(8)	0.053(9)	−0.004(6)	−0.007(7)	0.019(7)
C277	0.026(7)	0.030(7)	0.047(8)	0.003(6)	0.008(6)	0.016(6)
C5	0.031(7)	0.042(8)	0.041(8)	−0.003(6)	−0.002(6)	0.016(6)
F186	0.042(6)	0.137(13)	0.073(8)	0.049(8)	0.013(6)	0.032(7)
C242	0.043(8)	0.024(7)	0.056(10)	−0.012(6)	−0.012(7)	0.017(6)
C205	0.030(7)	0.023(6)	0.037(7)	0.001(5)	0.003(5)	0.016(5)
C136	0.017(6)	0.013(5)	0.053(8)	0.006(5)	0.002(5)	0.004(5)
F175	0.034(6)	0.089(11)	0.28(2)	−0.102(13)	−0.012(10)	0.026(7)
F273	0.026(5)	0.053(7)	0.234(19)	−0.037(9)	0.030(8)	0.013(5)
F303	0.063(8)	0.204(19)	0.077(9)	−0.029(10)	−0.003(7)	0.079(11)
F275	0.24(2)	0.139(13)	0.051(7)	−0.017(8)	−0.011(9)	0.163(16)
N60	0.029(7)	0.028(7)	0.101(13)	0.012(7)	−0.008(7)	0.009(6)
C215	0.014(5)	0.023(6)	0.039(7)	0.003(5)	0.002(5)	0.009(5)
F80	0.065(9)	0.085(10)	0.157(15)	0.001(10)	0.019(9)	0.048(8)
C267	0.020(6)	0.025(6)	0.045(8)	0.004(5)	0.001(5)	0.011(5)
F249	0.090(10)	0.097(10)	0.162(15)	−0.083(10)	−0.066(10)	0.078(9)
C211	0.027(7)	0.037(8)	0.051(9)	0.004(6)	0.004(6)	0.016(6)
C6	0.036(8)	0.039(8)	0.041(8)	0.002(6)	0.002(6)	0.024(7)
F82	0.163(15)	0.118(12)	0.115(12)	0.046(10)	0.061(11)	0.125(13)
C210	0.022(6)	0.013(5)	0.055(9)	0.006(5)	0.005(6)	0.004(5)
F262	0.038(6)	0.084(10)	0.28(2)	−0.122(13)	0.016(10)	0.010(6)
C276	0.028(7)	0.014(6)	0.070(10)	−0.008(6)	0.004(6)	0.014(5)
C224	0.045(9)	0.031(8)	0.060(10)	−0.013(7)	−0.005(7)	0.020(7)
F179	0.152(14)	0.071(8)	0.075(9)	−0.001(7)	0.002(9)	0.074(10)
C289	0.042(8)	0.027(7)	0.046(8)	0.002(6)	0.003(6)	0.022(6)
C255	0.028(7)	0.032(7)	0.047(9)	−0.007(6)	−0.002(6)	0.010(6)
C241	0.017(6)	0.024(6)	0.045(8)	−0.003(5)	−0.003(5)	0.006(5)
F106	0.042(6)	0.042(6)	0.116(10)	−0.009(6)	−0.019(6)	0.005(5)
C138	0.012(5)	0.025(6)	0.058(9)	0.005(6)	0.006(5)	0.009(5)
C139	0.019(6)	0.031(7)	0.076(11)	−0.007(7)	0.002(7)	0.011(6)
C115	0.023(6)	0.031(7)	0.045(8)	−0.001(6)	0.002(5)	0.014(6)
C315	0.027(7)	0.036(8)	0.045(8)	0.005(6)	0.003(6)	0.008(6)
F27	0.024(5)	0.108(11)	0.184(15)	−0.056(10)	0.020(7)	0.013(6)

C25	0.027(8)	0.045(9)	0.073(12)	−0.005(8)	0.006(7)	0.013(7)
C123	0.037(8)	0.036(7)	0.051(9)	0.007(6)	0.012(6)	0.029(7)
C46	0.035(8)	0.023(7)	0.063(10)	−0.004(6)	0.006(7)	0.016(6)
C214	0.023(7)	0.046(9)	0.070(11)	0.001(7)	0.002(7)	0.023(7)
C225	0.030(7)	0.015(6)	0.051(8)	−0.010(5)	0.000(6)	0.010(5)
C295	0.031(7)	0.022(6)	0.044(8)	0.005(5)	0.003(6)	0.012(6)
C156	0.033(7)	0.025(7)	0.047(8)	0.002(6)	0.000(6)	0.014(6)
N61	0.015(6)	0.080(12)	0.113(15)	0.046(11)	0.006(7)	0.017(7)
F153	0.027(6)	0.073(9)	0.23(2)	−0.082(11)	−0.025(8)	0.007(6)
O16	0.059(9)	0.069(9)	0.080(10)	−0.005(7)	−0.009(7)	0.032(8)
C278	0.017(6)	0.026(6)	0.040(7)	0.004(5)	0.004(5)	0.012(5)
C290	0.024(6)	0.028(7)	0.046(8)	−0.008(6)	0.000(5)	0.015(6)
C314	0.027(7)	0.052(9)	0.035(7)	0.008(7)	0.000(5)	0.022(7)
C209	0.031(7)	0.022(6)	0.051(9)	−0.002(6)	0.002(6)	0.011(6)
C149	0.034(8)	0.022(7)	0.061(10)	−0.008(6)	−0.003(7)	0.007(6)
F95	0.110(11)	0.028(6)	0.101(10)	−0.014(6)	−0.027(8)	0.002(6)
C307	0.029(7)	0.042(8)	0.059(10)	−0.009(7)	−0.003(6)	0.025(7)
C253	0.022(6)	0.027(7)	0.048(8)	−0.008(6)	0.000(5)	0.013(5)
C2	0.028(7)	0.047(9)	0.059(10)	−0.013(7)	−0.009(7)	0.018(7)
C45	0.028(7)	0.035(8)	0.055(9)	−0.001(7)	0.003(6)	0.016(6)
C100	0.049(9)	0.049(9)	0.050(9)	−0.001(7)	0.005(7)	0.035(8)
C163	0.047(9)	0.029(7)	0.050(9)	−0.006(6)	−0.005(7)	0.025(7)
C200	0.020(6)	0.019(6)	0.048(8)	−0.008(5)	−0.001(5)	0.006(5)
F140	0.064(8)	0.136(12)	0.129(12)	−0.083(10)	−0.010(7)	0.057(8)
C279	0.031(7)	0.023(6)	0.052(9)	0.000(6)	0.003(6)	0.016(6)
F260	0.074(10)	0.106(13)	0.124(14)	−0.056(11)	−0.036(9)	0.004(9)
C99	0.043(9)	0.042(9)	0.060(10)	−0.002(7)	0.009(7)	0.027(7)
C223	0.027(7)	0.020(6)	0.047(8)	−0.014(5)	−0.006(6)	0.007(5)
C268	0.033(7)	0.032(7)	0.049(9)	−0.004(6)	−0.009(6)	0.016(6)
C308	0.042(8)	0.037(8)	0.046(8)	−0.007(6)	−0.001(6)	0.023(7)
F129	0.118(14)	0.091(12)	0.159(18)	0.061(12)	−0.070(13)	−0.058(11)
C310	0.029(7)	0.028(7)	0.036(7)	0.001(5)	−0.002(5)	0.017(6)
F91	0.039(6)	0.130(13)	0.201(16)	−0.072(12)	−0.027(8)	0.050(8)
F304	0.044(8)	0.143(16)	0.20(2)	0.056(14)	−0.009(10)	0.045(9)
C23	0.056(10)	0.038(8)	0.059(10)	−0.006(7)	−0.005(8)	0.029(8)
C327	0.044(9)	0.025(8)	0.079(13)	0.002(8)	0.012(8)	0.007(7)
C143	0.019(6)	0.019(6)	0.065(10)	0.000(6)	0.005(6)	0.006(5)
C252	0.025(7)	0.048(10)	0.080(13)	−0.031(9)	−0.005(7)	0.012(7)
C89	0.044(9)	0.032(8)	0.053(9)	−0.003(7)	0.010(7)	0.020(7)
C4	0.023(6)	0.021(6)	0.058(9)	−0.007(6)	−0.007(6)	0.007(5)
C88	0.042(9)	0.053(10)	0.073(12)	−0.001(9)	0.002(8)	0.031(8)
C161	0.031(7)	0.024(6)	0.037(7)	0.001(5)	−0.002(6)	0.006(6)
C48	0.024(7)	0.031(7)	0.062(10)	0.002(7)	0.012(6)	0.012(6)
C101	0.061(11)	0.033(8)	0.061(11)	0.000(7)	0.007(8)	0.025(8)
C309	0.017(6)	0.029(7)	0.037(7)	−0.007(5)	−0.001(5)	0.006(5)
C77	0.14(2)	0.059(13)	0.042(10)	0.008(9)	0.021(12)	0.069(16)
F221	0.036(7)	0.105(12)	0.27(2)	−0.117(14)	−0.053(10)	0.033(7)
C76	0.084(13)	0.035(8)	0.043(9)	0.005(7)	0.014(9)	0.037(9)
C14	0.046(10)	0.056(11)	0.068(12)	−0.003(9)	−0.001(8)	0.033(9)
C197	0.028(7)	0.034(7)	0.047(8)	−0.002(6)	0.000(6)	0.017(6)
C47	0.022(6)	0.032(7)	0.042(8)	0.002(6)	0.007(5)	0.015(6)
F247	0.197(18)	0.128(13)	0.079(9)	0.037(9)	0.040(10)	0.141(14)
C124	0.065(11)	0.027(7)	0.051(9)	0.009(6)	0.021(8)	0.027(8)
C189	0.024(7)	0.050(9)	0.049(9)	−0.008(7)	0.000(6)	0.012(7)
C312	0.033(7)	0.040(8)	0.032(7)	0.003(6)	0.001(6)	0.018(6)
F111	0.117(13)	0.049(7)	0.089(10)	0.007(7)	−0.020(9)	−0.041(8)

C316	0.032(8)	0.035(8)	0.044(8)	0.000(6)	0.002(6)	0.005(6)
F180	0.027(6)	0.081(10)	0.221(19)	−0.081(11)	−0.034(8)	0.008(6)
C240	0.028(7)	0.028(7)	0.057(9)	−0.001(6)	−0.006(6)	0.013(6)
C196	0.032(7)	0.037(8)	0.047(8)	−0.009(6)	−0.010(6)	0.021(6)
C291	0.039(8)	0.033(8)	0.060(10)	−0.002(7)	0.004(7)	0.024(7)
F142	0.26(2)	0.133(13)	0.114(12)	−0.011(10)	0.002(13)	0.169(15)
C283	0.045(9)	0.024(7)	0.055(10)	−0.006(6)	0.017(7)	0.006(7)
C8	0.027(7)	0.023(7)	0.063(10)	0.003(6)	−0.001(6)	0.006(6)
C98	0.026(7)	0.048(9)	0.051(9)	−0.001(7)	0.006(6)	0.026(7)
C306	0.042(9)	0.056(10)	0.056(10)	−0.005(8)	−0.015(8)	0.026(8)
C272	0.042(8)	0.038(8)	0.051(9)	−0.001(7)	0.006(7)	0.029(7)
C172	0.016(6)	0.044(9)	0.067(11)	0.001(7)	−0.001(6)	0.012(6)
F141	0.080(9)	0.058(8)	0.234(18)	−0.032(9)	0.096(11)	0.009(7)
C87	0.049(9)	0.039(8)	0.047(9)	−0.005(7)	−0.002(7)	0.029(7)
F192	0.070(9)	0.138(15)	0.084(10)	0.042(10)	−0.012(8)	−0.053(10)
F110	0.084(10)	0.082(10)	0.181(15)	0.003(10)	0.049(10)	0.048(8)
C29	0.014(6)	0.037(8)	0.067(10)	0.004(7)	−0.005(6)	0.005(6)
C246	0.020(6)	0.039(8)	0.056(9)	−0.002(7)	−0.003(6)	0.016(6)
C9	0.035(8)	0.024(7)	0.061(10)	−0.007(6)	0.003(7)	0.012(6)
C219	0.045(9)	0.035(8)	0.046(9)	−0.003(6)	0.000(7)	0.024(7)
C201	0.018(6)	0.039(8)	0.040(8)	−0.002(6)	−0.002(5)	0.013(6)
C208	0.048(9)	0.036(8)	0.049(9)	0.004(6)	0.011(7)	0.027(7)
C207	0.032(7)	0.027(7)	0.049(8)	0.004(6)	0.013(6)	0.021(6)
C185	0.023(7)	0.029(7)	0.051(9)	0.013(6)	−0.002(6)	−0.006(6)
C305	0.032(8)	0.035(8)	0.068(11)	−0.011(7)	−0.002(7)	0.013(7)
C34	0.064(12)	0.025(8)	0.057(11)	0.003(7)	0.021(9)	−0.001(8)
C32	0.023(7)	0.030(7)	0.057(10)	0.016(7)	0.005(6)	−0.003(6)
C1	0.030(8)	0.041(9)	0.089(14)	−0.008(8)	−0.003(8)	0.018(7)
C18	0.025(6)	0.027(7)	0.044(8)	−0.003(6)	−0.007(6)	0.010(5)
F93	0.093(10)	0.077(9)	0.098(10)	0.023(8)	−0.002(8)	−0.017(8)
C299	0.035(8)	0.044(8)	0.054(9)	−0.013(7)	−0.004(6)	0.031(7)
C239	0.015(6)	0.031(7)	0.044(8)	0.002(6)	−0.004(5)	0.008(5)
C288	0.027(6)	0.021(6)	0.036(7)	−0.003(5)	0.000(5)	0.011(5)
C150	0.022(7)	0.036(8)	0.050(9)	−0.009(6)	−0.003(6)	0.008(6)
C329	0.047(9)	0.031(7)	0.056(10)	−0.007(7)	0.001(7)	0.024(7)
C322	0.055(10)	0.074(12)	0.038(9)	−0.005(8)	−0.004(7)	0.042(10)
C222	0.037(9)	0.052(10)	0.070(12)	−0.011(8)	−0.002(8)	0.029(8)
C13	0.042(9)	0.053(10)	0.064(11)	−0.005(8)	−0.009(8)	0.033(8)
C220	0.046(9)	0.046(9)	0.056(10)	−0.011(7)	−0.004(7)	0.031(8)
C64	0.026(8)	0.030(8)	0.102(16)	0.018(9)	−0.020(9)	−0.006(7)
C152	0.027(8)	0.058(11)	0.057(10)	−0.015(8)	−0.005(7)	0.012(7)
C195	0.039(8)	0.034(8)	0.058(10)	0.002(7)	−0.008(7)	0.009(7)
C128	0.021(8)	0.036(9)	0.13(2)	−0.006(10)	0.020(9)	0.007(7)
C171	0.028(8)	0.045(9)	0.084(13)	−0.005(9)	−0.006(8)	0.015(7)
C112	0.041(9)	0.045(10)	0.061(11)	−0.013(8)	−0.009(8)	0.017(8)
C251	0.024(7)	0.041(9)	0.087(13)	−0.030(8)	0.002(7)	0.017(7)
C328	0.041(9)	0.054(11)	0.058(11)	−0.005(8)	0.015(8)	0.009(8)
C122	0.044(9)	0.029(7)	0.094(14)	0.007(8)	0.018(9)	0.029(7)
C17	0.031(8)	0.039(9)	0.066(11)	−0.011(7)	−0.003(7)	0.012(7)
C28	0.034(9)	0.045(10)	0.081(14)	−0.008(9)	0.004(8)	0.016(8)
C10	0.041(9)	0.045(10)	0.072(13)	0.006(9)	−0.002(9)	0.010(8)
C319	0.047(9)	0.035(8)	0.040(9)	0.004(7)	−0.003(7)	0.001(7)
F130	0.033(7)	0.24(2)	0.170(18)	−0.106(18)	−0.030(9)	0.049(11)
C33	0.022(7)	0.031(8)	0.069(11)	0.002(7)	0.000(7)	0.001(6)
C105	0.026(8)	0.073(12)	0.065(11)	−0.016(9)	0.000(7)	0.029(8)
C3	0.042(9)	0.057(10)	0.048(9)	0.000(8)	0.000(7)	0.026(8)

C318	0.020(7)	0.074(13)	0.057(11)	0.004(9)	−0.003(7)	0.000(8)
F81	0.19(2)	0.31(3)	0.098(12)	−0.021(15)	−0.020(13)	0.22(2)
C90	0.015(6)	0.049(10)	0.072(12)	−0.004(8)	0.004(7)	0.007(6)
C121	0.025(7)	0.037(8)	0.077(11)	0.000(7)	0.009(7)	0.022(6)
C52	0.024(7)	0.044(9)	0.077(12)	−0.002(8)	0.004(7)	0.013(7)
C94	0.076(14)	0.051(11)	0.069(13)	−0.022(9)	−0.023(11)	0.036(11)
C213	0.040(8)	0.052(9)	0.061(10)	0.001(8)	0.002(7)	0.037(8)
F109	0.112(12)	0.201(18)	0.107(12)	−0.050(12)	−0.012(10)	0.103(13)
C326	0.025(7)	0.030(7)	0.058(10)	−0.009(6)	0.003(6)	0.005(6)
C15	0.088(17)	0.063(13)	0.12(2)	0.010(13)	−0.007(14)	0.058(14)
C63	0.032(9)	0.087(16)	0.085(16)	0.032(13)	−0.001(10)	0.016(10)
C62	0.027(9)	0.097(18)	0.088(16)	0.023(14)	0.005(9)	0.028(10)
C170	0.010(6)	0.031(7)	0.073(11)	−0.001(7)	−0.007(6)	0.003(5)
C26	0.039(10)	0.061(12)	0.083(14)	−0.005(10)	−0.002(9)	0.016(9)
C12	0.036(9)	0.074(14)	0.090(15)	−0.021(11)	−0.007(9)	0.031(10)
C259	0.031(9)	0.059(12)	0.110(18)	−0.047(12)	−0.007(10)	0.015(9)
C11	0.071(13)	0.041(10)	0.087(15)	−0.001(9)	0.013(11)	0.028(10)
C181	0.050(10)	0.031(8)	0.065(11)	−0.009(7)	−0.007(8)	0.022(7)
C78	0.108(18)	0.056(12)	0.050(10)	0.018(9)	0.025(11)	0.061(13)
C320	0.087(15)	0.032(9)	0.063(12)	0.007(8)	0.005(11)	0.011(10)
C65	0.038(9)	0.027(8)	0.104(16)	0.006(9)	−0.017(10)	0.005(7)
C83	0.074(14)	0.042(10)	0.055(11)	−0.004(8)	0.011(10)	0.017(10)
C69	0.039(12)	0.15(3)	0.13(3)	0.03(2)	0.033(14)	0.057(17)
F70	0.13(2)	0.48(6)	0.26(3)	−0.12(4)	−0.06(2)	0.22(3)
F72	0.12(2)	0.16(2)	0.51(7)	0.01(3)	0.11(3)	0.10(2)
C177	0.034(8)	0.031(8)	0.101(16)	−0.007(9)	−0.003(9)	0.016(7)
C173	0.031(8)	0.051(11)	0.110(17)	−0.008(10)	0.003(9)	0.026(8)
C79	0.086(17)	0.096(18)	0.098(18)	0.008(14)	0.016(14)	0.078(16)
F71	0.25(3)	0.36(5)	0.16(2)	0.04(3)	0.05(2)	0.26(4)

Table 4. Bond lengths and angles for 30.

Atom–Atom	Length [Å]
Ag23–Ag1	3.1698(14)
Ag23–N233	2.096(10)
Ag23–N287	2.097(11)
Ag22–Ag2	3.3388(14)
Ag22–N229	2.123(11)
Ag22–N238	2.115(12)
Ag1–N254	2.142(11)
Ag1–N230	2.146(10)
Ag2–N264	2.127(10)
Ag2–N226	2.110(12)
Ag11–Ag4	3.3586(14)
Ag11–N119	2.121(11)
Ag11–N135	2.111(11)
Ag13–Ag5	3.3719(13)
Ag13–N134	2.122(10)
Ag13–N147	2.105(12)
Ag3–Ag6	3.2292(15)
Ag3–N263	2.119(11)
Ag3–N234	2.119(10)
Ag4–Ag5	3.3556(15)
Ag4–N116	2.121(11)
Ag4–N160	2.123(11)
Ag5–N120	2.110(11)

Ag5–N151	2.079(11)
Ag41–Ag42	3.3751(13)
Ag41–Ag56	3.2861(15)
Ag41–N40	2.102(11)
Ag41–N44	2.083(12)
Ag6–N237	2.111(11)
Ag6–N250	2.086(11)
Ag16–N166	2.115(12)
Ag16–N164	2.120(11)
Ag42–N43	2.120(12)
Ag42–N30	2.121(12)
Ag7–N167	2.110(12)
Ag7–N169	2.107(11)
Ag56–N57	2.088(12)
Ag56–N75	2.107(12)
Ag38–N39	2.116(13)
Ag38–N31	2.087(12)
Ag59–N58	2.107(13)
Ag59–N60	2.111(14)
Ag73–N74	2.135(17)
Ag73–N61	2.08(2)
F258–C255	1.356(17)
F300–C299	1.312(18)
F144–C143	1.354(18)
F257–C255	1.327(17)
F280–C279	1.329(16)
O321–C314	1.187(18)
O198–C199	1.428(15)
O198–C197	1.468(18)
F146–C143	1.344(17)
F55–C52	1.34(2)
O317–C313	1.424(18)
O317–C316	1.465(19)
F159–C156	1.299(18)
F103–C101	1.33(2)
F282–C279	1.344(16)
F145–C143	1.351(16)
F125–C124	1.35(2)
F292–C291	1.33(2)
F188–C185	1.321(19)
F244–C242	1.322(18)
F270–C268	1.350(18)
F281–C279	1.331(18)
N134–N135	1.351(15)
N134–C138	1.340(16)
F296–C295	1.309(16)
F49–C48	1.321(17)
O311–C310	1.357(16)
O311–C312	1.447(17)
F158–C156	1.339(17)
O212–C209	1.209(19)
F51–C48	1.312(19)
F274–C272	1.298(19)
O22–C5	1.416(18)
O22–C2	1.48(2)
F127–C124	1.342(18)

F126–C124	1.339(18)
F285–C283	1.35(2)
O202–C200	1.223(17)
F298–C295	1.303(17)
O19–C6	1.443(18)
O19–C18	1.340(18)
F86–C83	1.35(3)
O216–C203	1.448(16)
O216–C215	1.356(16)
O218–C204	1.194(16)
F92–C90	1.29(2)
F284–C283	1.329(18)
F157–C156	1.326(17)
N119–N120	1.360(16)
N119–C123	1.351(17)
F256–C255	1.343(18)
N135–C136	1.337(16)
F35–C34	1.30(2)
F269–C268	1.343(16)
N166–N167	1.356(17)
N166–C172	1.326(18)
O324–C323	1.208(17)
F271–C268	1.324(18)
N263–N264	1.354(14)
N263–C267	1.334(17)
F174–C173	1.30(2)
O330–C307	1.19(2)
O217–C215	1.184(16)
F184–C181	1.34(2)
O20–C18	1.198(18)
N237–N238	1.335(15)
N237–C241	1.335(16)
F104–C101	1.35(2)
F243–C242	1.335(18)
F178–C177	1.35(2)
F84–C83	1.34(2)
F286–C283	1.33(2)
N233–N234	1.353(15)
N233–C278	1.360(16)
F245–C242	1.32(2)
F37–C34	1.30(2)
F54–C52	1.33(2)
N264–C265	1.328(18)
F183–C181	1.35(2)
F187–C185	1.336(19)
F155–C152	1.32(2)
F294–C291	1.322(19)
N254–N250	1.353(15)
N254–C253	1.354(17)
C203–H203	1.0000
C203–C199	1.538(18)
C203–C204	1.514(18)
F302–C299	1.340(19)
F293–C291	1.322(17)
N58–N57	1.339(16)
N58–C87	1.35(2)

N226–N287	1.355(15)
N226–C225	1.328(16)
N167–C170	1.330(18)
O21–C7	1.195(19)
N40–N39	1.348(18)
N40–C98	1.333(17)
O24–C4	1.222(18)
N234–C276	1.358(15)
O325–C310	1.204(16)
N147–C148	1.322(17)
N147–N151	1.381(15)
F50–C48	1.324(19)
N44–N43	1.369(15)
N44–C45	1.336(19)
N164–N160	1.374(16)
N164–C163	1.323(18)
F261–C259	1.30(3)
F297–C295	1.347(18)
F301–C299	1.31(2)
F108–C105	1.34(2)
F36–C34	1.43(2)
F67–C65	1.35(2)
F154–C152	1.32(2)
N57–C89	1.347(19)
F191–C189	1.27(2)
N287–C223	1.365(16)
N169–N116	1.358(16)
N169–C113	1.324(19)
N43–C47	1.333(18)
F194–C112	1.31(2)
N75–N74	1.36(2)
N75–C76	1.36(2)
F107–C105	1.340(18)
N39–C100	1.354(19)
C323–C309	1.498(19)
C323–C312	1.527(19)
F248–C246	1.296(18)
F193–C112	1.32(2)
F85–C83	1.34(2)
N74–C78	1.31(2)
N120–C121	1.339(17)
C199–C200	1.50(2)
C199–C219	1.529(19)
F53–C52	1.33(2)
C204–C205	1.510(19)
N116–C115	1.352(17)
F66–C65	1.34(2)
N230–N229	1.373(14)
N230–C288	1.335(16)
C313–C314	1.53(2)
C313–C312	1.51(2)
C313–C322	1.53(2)
N229–C290	1.314(17)
C148–C156	1.49(2)
C148–C149	1.39(2)
N238–C239	1.330(17)

F97–C94	1.30(2)
N31–N30	1.353(17)
N31–C32	1.363(18)
C114–H114	0.9500
C114–C113	1.39(2)
C114–C115	1.39(2)
N151–C150	1.350(18)
F96–C94	1.36(2)
C266–H266	0.9500
C266–C265	1.397(19)
C266–C267	1.385(18)
F102–C101	1.34(2)
C206–C205	1.580(19)
C206–C214	1.52(2)
C206–C207	1.54(2)
C206–C213	1.54(2)
F190–C189	1.32(2)
N30–C29	1.329(18)
C265–C272	1.50(2)
C113–C112	1.48(2)
F182–C181	1.312(18)
N250–C251	1.365(18)
N160–C161	1.357(17)
F176–C173	1.35(3)
F68–C65	1.37(2)
C137–H137	0.9500
C137–C136	1.38(2)
C137–C138	1.40(2)
C7–C6	1.55(2)
C7–C8	1.52(2)
F131–C128	1.28(2)
C162–H162	0.9500
C162–C163	1.39(2)
C162–C161	1.37(2)
C277–H277	0.9500
C277–C276	1.402(19)
C277–C278	1.355(19)
C5–C6	1.53(2)
C5–C23	1.54(2)
C5–C4	1.51(2)
F186–C185	1.293(19)
C242–C241	1.484(19)
C205–C215	1.518(17)
C205–C210	1.584(18)
C136–C143	1.478(19)
F175–C173	1.31(2)
F273–C272	1.331(19)
F303–C222	1.28(2)
F275–C272	1.29(2)
N60–N61	1.37(3)
N60–C64	1.33(2)
F80–C79	1.28(3)
C267–C268	1.50(2)
F249–C246	1.285(19)
C211–H21A	0.9800
C211–H21B	0.9800

C211–H21C	0.9800
C211–C210	1.515(19)
C6–H6	1.0000
F82–C79	1.32(3)
C210–H210	1.0000
C210–C209	1.51(2)
F262–C259	1.31(2)
C276–C283	1.480(19)
C224–H224	0.9500
C224–C225	1.37(2)
C224–C223	1.39(2)
F179–C177	1.33(3)
C289–H289	0.9500
C289–C290	1.38(2)
C289–C288	1.410(19)
C255–C253	1.469(19)
C241–C240	1.37(2)
F106–C105	1.34(2)
C138–C139	1.48(2)
C139–F140	1.33(2)
C139–F142	1.26(2)
C139–F141	1.25(2)
C115–C189	1.48(2)
C315–H31A	0.9900
C315–H31B	0.9900
C315–C314	1.49(2)
C315–C316	1.52(2)
F27–C28	1.26(2)
C25–H25	0.9500
C25–C2	1.49(2)
C25–C26	1.31(3)
C123–C124	1.48(2)
C123–C122	1.38(2)
C46–H46	0.9500
C46–C45	1.40(2)
C46–C47	1.40(2)
C214–H21D	0.9800
C214–H21E	0.9800
C214–H21F	0.9800
C225–C299	1.518(18)
C295–C288	1.481(19)
N61–C62	1.38(2)
F153–C152	1.26(2)
O16–C10	1.26(2)
C278–C279	1.479(19)
C290–C291	1.525(19)
C209–C208	1.51(2)
C149–H149	0.9500
C149–C150	1.39(2)
F95–C94	1.33(3)
C307–C308	1.50(2)
C307–C306	1.53(2)
C253–C252	1.38(2)
C2–C1	1.51(2)
C2–C3	1.56(2)
C45–C52	1.47(2)

C100–C99	1.38(2)
C100–C101	1.47(2)
C163–C181	1.49(2)
C200–C201	1.503(18)
F260–C259	1.34(3)
C99–H99	0.9500
C99–C98	1.39(2)
C223–C222	1.48(2)
C308–H308	1.0000
C308–C309	1.57(2)
C308–C329	1.52(2)
F129–C128	1.25(3)
C310–C309	1.501(18)
F91–C90	1.31(2)
F304–C222	1.32(3)
C23–H23A	0.9800
C23–H23B	0.9800
C23–H23C	0.9800
C327–H32A	0.9800
C327–H32B	0.9800
C327–H32C	0.9800
C327–C326	1.53(2)
C252–H252	0.9500
C252–C251	1.36(2)
C89–C88	1.37(2)
C89–C90	1.51(2)
C4–C3	1.50(2)
C88–H88	0.9500
C88–C87	1.34(2)
C161–C185	1.50(2)
C48–C47	1.511(18)
C309–C326	1.594(18)
C77–H77	0.9500
C77–C76	1.40(3)
C77–C78	1.33(4)
F221–C222	1.26(2)
C76–C83	1.44(3)
C14–H14A	0.9800
C14–H14B	0.9800
C14–H14C	0.9800
C14–C13	1.51(3)
C197–C196	1.49(2)
C197–C201	1.53(2)
C197–C220	1.54(2)
F247–C246	1.33(2)
C189–F192	1.29(2)
C312–H312	1.0000
F111–C112	1.30(2)
C316–C319	1.48(2)
C316–C318	1.53(2)
F180–C177	1.28(2)
C240–H240	0.9500
C240–C239	1.39(2)
C196–H196	0.9500
C196–C195	1.31(2)
C8–C9	1.57(2)

C8–C18	1.52(2)
C8–C13	1.59(2)
C98–C105	1.48(2)
C306–H30A	0.9900
C306–H30B	0.9900
C306–C305	1.51(2)
C172–C171	1.39(2)
C172–C173	1.49(2)
C87–C94	1.49(2)
F110–C28	1.28(2)
C29–C28	1.50(3)
C29–C33	1.38(2)
C246–C239	1.47(2)
C9–H9	1.0000
C9–C17	1.51(2)
C9–C10	1.50(3)
C219–H21G	0.9800
C219–H21H	0.9800
C219–H21I	0.9800
C201–H20A	0.9900
C201–H20B	0.9900
C208–H20C	0.9900
C208–H20D	0.9900
C208–C207	1.50(2)
C207–H20E	0.9900
C207–H20F	0.9900
C305–H30C	0.9900
C305–H30D	0.9900
C305–C326	1.52(2)
C34–C32	1.49(3)
C32–C33	1.38(2)
C1–H1A	0.9800
C1–H1B	0.9800
C1–H1C	0.9800
F93–C90	1.31(2)
C150–C152	1.52(2)
C329–H32D	0.9800
C329–H32E	0.9800
C329–H32F	0.9800
C322–H32G	0.9800
C322–H32H	0.9800
C322–H32I	0.9800
C13–C15	1.57(3)
C13–C12	1.51(3)
C220–H22A	0.9800
C220–H22B	0.9800
C220–H22C	0.9800
C64–C63	1.39(3)
C64–C65	1.45(3)
C195–H19A	0.9500
C195–H19B	0.9500
C128–F130	1.33(3)
C128–C121	1.47(2)
C171–H171	0.9500
C171–C170	1.37(2)
C251–C259	1.48(2)

C328–H32J	0.9800
C328–H32K	0.9800
C328–H32L	0.9800
C328–C326	1.52(2)
C122–H122	0.9500
C122–C121	1.38(2)
C17–H17A	0.9800
C17–H17B	0.9800
C17–H17C	0.9800
C28–F109	1.32(3)
C10–C11	1.47(3)
C319–H319	0.9500
C319–C320	1.32(3)
C33–H33	0.9500
C3–H3A	0.9900
C3–H3B	0.9900
C318–H31C	0.9800
C318–H31D	0.9800
C318–H31E	0.9800
F81–C79	1.37(3)
C213–H21J	0.9800
C213–H21K	0.9800
C213–H21L	0.9800
C15–H15A	0.9800
C15–H15B	0.9800
C15–H15C	0.9800
C63–H63	0.9500
C63–C62	1.32(4)
C62–C69	1.46(4)
C170–C177	1.49(2)
C26–H26A	0.9500
C26–H26B	0.9500
C12–H12A	0.9900
C12–H12B	0.9900
C12–C11	1.57(3)
C11–H11A	0.9900
C11–H11B	0.9900
C78–C79	1.49(3)
C320–H32M	0.9500
C320–H32N	0.9500
C69–F70	1.23(3)
C69–F72	1.29(4)
C69–F71	1.32(4)

Atom–Atom–Atom	**Angle [°]**
N233–Ag23–Ag1	66.3(3)
N233–Ag23–N287	178.5(5)
N287–Ag23–Ag1	115.2(3)
N229–Ag22–Ag2	64.2(3)
N238–Ag22–Ag2	122.4(3)
N238–Ag22–N229	173.2(4)
N254–Ag1–Ag23	121.9(3)
N254–Ag1–N230	163.3(4)
N230–Ag1–Ag23	74.6(3)
N264–Ag2–Ag22	65.5(3)
N226–Ag2–Ag22	120.2(3)

N226–Ag2–N264	174.2(4)
N119–Ag11–Ag4	66.6(3)
N135–Ag11–Ag4	115.8(3)
N135–Ag11–N119	173.3(5)
N134–Ag13–Ag5	117.6(3)
N147–Ag13–Ag5	62.1(3)
N147–Ag13–N134	176.9(5)
N263–Ag3–Ag6	89.0(3)
N263–Ag3–N234	173.7(4)
N234–Ag3–Ag6	93.0(4)
Ag5–Ag4–Ag11	62.89(3)
N116–Ag4–Ag11	92.0(3)
N116–Ag4–Ag5	123.2(3)
N116–Ag4–N160	165.6(4)
N160–Ag4–Ag11	98.6(3)
N160–Ag4–Ag5	70.7(3)
Ag4–Ag5–Ag13	84.88(3)
N120–Ag5–Ag13	122.1(3)
N120–Ag5–Ag4	67.3(3)
N151–Ag5–Ag13	60.9(3)
N151–Ag5–Ag4	115.7(3)
N151–Ag5–N120	176.4(5)
Ag56–Ag41–Ag42	76.72(3)
N40–Ag41–Ag42	121.3(3)
N40–Ag41–Ag56	80.0(4)
N44–Ag41–Ag42	61.3(3)
N44–Ag41–Ag56	103.7(3)
N44–Ag41–N40	176.1(5)
N237–Ag6–Ag3	99.2(3)
N250–Ag6–Ag3	92.6(4)
N250–Ag6–N237	167.2(5)
N166–Ag16–N164	171.4(5)
N43–Ag42–Ag41	61.7(3)
N43–Ag42–N30	177.6(5)
N30–Ag42–Ag41	117.6(3)
N169–Ag7–N167	171.6(5)
N57–Ag56–Ag41	106.7(3)
N57–Ag56–N75	168.2(5)
N75–Ag56–Ag41	84.0(4)
N31–Ag38–N39	172.5(5)
N58–Ag59–N60	171.5(6)
N61–Ag73–N74	170.6(6)
C199–O198–C197	110.8(10)
C313–O317–C316	109.8(11)
N135–N134–Ag13	122.9(7)
C138–N134–Ag13	127.7(9)
C138–N134–N135	109.0(10)
C310–O311–C312	111.1(10)
C5–O22–C2	111.1(11)
C18–O19–C6	112.6(11)
C215–O216–C203	111.4(10)
N120–N119–Ag11	119.3(8)
C123–N119–Ag11	131.6(10)
C123–N119–N120	107.9(11)
N134–N135–Ag11	120.6(7)
C136–N135–Ag11	130.6(9)

C136–N135–N134	107.7(10)
N167–N166–Ag16	118.0(8)
C172–N166–Ag16	134.2(11)
C172–N166–N167	107.1(13)
N264–N263–Ag3	121.9(8)
C267–N263–Ag3	131.6(9)
C267–N263–N264	106.1(10)
N238–N237–Ag6	119.2(8)
C241–N237–Ag6	131.1(9)
C241–N237–N238	108.5(11)
N234–N233–Ag23	122.3(8)
N234–N233–C278	107.0(10)
C278–N233–Ag23	130.6(9)
N263–N264–Ag2	121.7(8)
C265–N264–Ag2	129.6(9)
C265–N264–N263	108.3(10)
N250–N254–Ag1	119.1(8)
N250–N254–C253	108.4(11)
C253–N254–Ag1	132.1(9)
O216–C203–H203	108.7
O216–C203–C199	110.2(10)
O216–C203–C204	105.1(10)
C199–C203–H203	108.7
C204–C203–H203	108.7
C204–C203–C199	115.4(11)
N57–N58–Ag59	119.7(9)
N57–N58–C87	108.0(12)
C87–N58–Ag59	131.6(11)
N287–N226–Ag2	117.4(8)
C225–N226–Ag2	133.6(9)
C225–N226–N287	107.7(11)
N166–N167–Ag7	119.8(9)
C170–N167–Ag7	131.2(11)
C170–N167–N166	108.6(12)
N39–N40–Ag41	122.7(9)
C98–N40–Ag41	129.0(10)
C98–N40–N39	108.0(12)
N233–N234–Ag3	120.1(7)
N233–N234–C276	108.7(10)
C276–N234–Ag3	131.2(9)
C148–N147–Ag13	134.5(9)
C148–N147–N151	109.0(11)
N151–N147–Ag13	115.8(8)
N43–N44–Ag41	120.4(8)
C45–N44–Ag41	132.9(10)
C45–N44–N43	106.8(11)
N160–N164–Ag16	121.6(8)
C163–N164–Ag16	129.0(10)
C163–N164–N160	108.1(11)
N58–N57–Ag56	119.7(9)
N58–N57–C89	106.6(12)
C89–N57–Ag56	133.4(10)
N226–N287–Ag23	119.7(8)
N226–N287–C223	108.1(11)
C223–N287–Ag23	132.2(9)
N116–N169–Ag7	121.1(8)

C113–N169–Ag7	128.4(10)
C113–N169–N116	109.4(11)
N44–N43–Ag42	116.6(8)
C47–N43–Ag42	135.2(9)
C47–N43–N44	108.1(11)
N74–N75–Ag56	120.8(10)
C76–N75–Ag56	129.7(12)
C76–N75–N74	108.5(13)
N40–N39–Ag38	118.5(9)
N40–N39–C100	108.0(13)
C100–N39–Ag38	133.0(12)
O324–C323–C309	128.4(13)
O324–C323–C312	123.3(13)
C309–C323–C312	108.3(11)
N75–N74–Ag73	120.6(10)
C78–N74–Ag73	131.4(15)
C78–N74–N75	107.0(17)
N119–N120–Ag5	121.5(8)
C121–N120–Ag5	130.4(10)
C121–N120–N119	107.6(12)
O198–C199–C203	107.7(10)
O198–C199–C200	104.2(10)
O198–C199–C219	113.8(11)
C200–C199–C203	109.1(10)
C200–C199–C219	111.6(11)
C219–C199–C203	110.2(11)
O218–C204–C203	123.8(13)
O218–C204–C205	128.3(13)
C205–C204–C203	107.8(11)
N169–N116–Ag4	119.2(8)
C115–N116–Ag4	134.1(9)
C115–N116–N169	106.3(11)
N229–N230–Ag1	118.8(7)
C288–N230–Ag1	131.3(9)
C288–N230–N229	108.2(10)
O317–C313–C314	105.1(12)
O317–C313–C312	108.6(11)
O317–C313–C322	112.7(13)
C314–C313–C322	110.7(12)
C312–C313–C314	109.5(11)
C312–C313–C322	110.1(14)
N230–N229–Ag22	121.1(8)
C290–N229–Ag22	130.9(9)
C290–N229–N230	107.2(10)
N147–C148–C156	124.3(12)
N147–C148–C149	109.9(13)
C149–C148–C156	125.7(12)
N237–N238–Ag22	120.0(8)
C239–N238–Ag22	131.8(9)
C239–N238–N237	107.8(11)
N30–N31–Ag38	122.1(9)
N30–N31–C32	105.6(12)
C32–N31–Ag38	130.2(11)
C113–C114–H114	128.4
C115–C114–H114	128.4
C115–C114–C113	103.2(13)

N147–N151–Ag5	120.6(8)
C150–N151–Ag5	133.0(10)
C150–N151–N147	106.3(11)
C265–C266–H266	129.6
C267–C266–H266	129.6
C267–C266–C265	100.7(12)
C214–C206–C205	111.2(12)
C214–C206–C207	108.9(12)
C214–C206–C213	108.0(13)
C207–C206–C205	109.3(12)
C213–C206–C205	110.1(11)
C213–C206–C207	109.4(12)
N31–N30–Ag42	121.4(9)
C29–N30–Ag42	128.7(11)
C29–N30–N31	109.6(12)
N264–C265–C266	111.7(12)
N264–C265–C272	120.5(12)
C266–C265–C272	127.8(13)
N169–C113–C114	110.2(13)
N169–C113–C112	121.6(13)
C114–C113–C112	128.2(15)
N254–N250–Ag6	121.7(8)
N254–N250–C251	107.2(11)
C251–N250–Ag6	129.2(9)
N164–N160–Ag4	119.8(8)
C161–N160–Ag4	132.1(10)
C161–N160–N164	105.8(11)
C136–C137–H137	127.9
C136–C137–C138	104.3(12)
C138–C137–H137	127.9
O21–C7–C6	123.6(15)
O21–C7–C8	129.0(14)
C8–C7–C6	107.3(12)
C163–C162–H162	128.8
C161–C162–H162	128.8
C161–C162–C163	102.5(13)
C276–C277–H277	127.5
C278–C277–H277	127.5
C278–C277–C276	104.9(11)
O22–C5–C6	110.7(12)
O22–C5–C23	112.7(13)
O22–C5–C4	104.7(12)
C6–C5–C23	108.6(13)
C4–C5–C6	108.9(12)
C4–C5–C23	111.1(13)
F244–C242–F243	106.5(13)
F244–C242–F245	105.6(14)
F244–C242–C241	114.8(13)
F243–C242–C241	110.8(13)
F245–C242–F243	105.9(14)
F245–C242–C241	112.6(13)
C204–C205–C206	111.8(11)
C204–C205–C215	101.6(10)
C204–C205–C210	112.7(11)
C206–C205–C210	112.2(11)
C215–C205–C206	109.7(11)

C215–C205–C210	108.2(11)
N135–C136–C137	110.3(12)
N135–C136–C143	122.4(12)
C137–C136–C143	127.2(12)
N61–N60–Ag59	118.5(11)
C64–N60–Ag59	129.5(15)
C64–N60–N61	112.0(16)
O216–C215–C205	111.4(11)
O217–C215–O216	119.5(11)
O217–C215–C205	129.1(12)
N263–C267–C266	113.1(12)
N263–C267–C268	122.5(12)
C266–C267–C268	124.3(13)
H21A–C211–H21B	109.5
H21A–C211–H21C	109.5
H21B–C211–H21C	109.5
C210–C211–H21A	109.5
C210–C211–H21B	109.5
C210–C211–H21C	109.5
O19–C6–C7	104.1(12)
O19–C6–C5	110.6(12)
O19–C6–H6	109.0
C7–C6–H6	109.0
C5–C6–C7	114.9(13)
C5–C6–H6	109.0
C205–C210–H210	107.4
C211–C210–C205	112.9(11)
C211–C210–H210	107.4
C209–C210–C205	108.9(11)
C209–C210–C211	112.5(13)
C209–C210–H210	107.4
N234–C276–C277	108.4(11)
N234–C276–C283	124.0(13)
C277–C276–C283	127.5(12)
C225–C224–H224	127.8
C225–C224–C223	104.5(13)
C223–C224–H224	127.8
C290–C289–H289	128.8
C290–C289–C288	102.4(12)
C288–C289–H289	128.8
F258–C255–C253	111.7(12)
F257–C255–F258	107.2(12)
F257–C255–F256	107.0(12)
F257–C255–C253	112.7(13)
F256–C255–F258	107.3(13)
F256–C255–C253	110.6(12)
N237–C241–C242	120.2(12)
N237–C241–C240	110.1(12)
C240–C241–C242	129.7(13)
N134–C138–C137	108.7(12)
N134–C138–C139	124.1(12)
C137–C138–C139	127.2(12)
F140–C139–C138	112.5(12)
F142–C139–C138	112.3(16)
F142–C139–F140	100.1(17)
F141–C139–C138	114.0(13)

F141–C139–F140	107.2(19)
F141–C139–F142	109.8(19)
N116–C115–C114	111.0(12)
N116–C115–C189	120.8(13)
C114–C115–C189	128.2(13)
H31A–C315–H31B	109.0
C314–C315–H31A	111.0
C314–C315–H31B	111.0
C314–C315–C316	103.8(13)
C316–C315–H31A	111.0
C316–C315–H31B	111.0
C2–C25–H25	116.2
C26–C25–H25	116.2
C26–C25–C2	128(2)
N119–C123–C124	121.5(13)
N119–C123–C122	109.6(14)
C122–C123–C124	128.9(13)
C45–C46–H46	129.3
C47–C46–H46	129.3
C47–C46–C45	101.4(13)
C206–C214–H21D	109.5
C206–C214–H21E	109.5
C206–C214–H21F	109.5
H21D–C214–H21E	109.5
H21D–C214–H21F	109.5
H21E–C214–H21F	109.5
N226–C225–C224	111.2(12)
N226–C225–C299	122.6(12)
C224–C225–C299	126.2(12)
F296–C295–F297	107.1(13)
F296–C295–C288	112.6(11)
F298–C295–F296	109.1(13)
F298–C295–F297	104.9(12)
F298–C295–C288	111.7(12)
F297–C295–C288	111.1(12)
F159–C156–F158	107.1(13)
F159–C156–F157	108.2(13)
F159–C156–C148	112.8(12)
F158–C156–C148	109.7(11)
F157–C156–F158	106.7(13)
F157–C156–C148	112.0(13)
N60–N61–Ag73	120.5(10)
N60–N61–C62	101(2)
C62–N61–Ag73	137.0(19)
N233–C278–C279	118.5(11)
C277–C278–N233	110.9(11)
C277–C278–C279	130.5(12)
N229–C290–C289	112.4(12)
N229–C290–C291	119.8(12)
C289–C290–C291	127.8(12)
O321–C314–C313	123.4(15)
O321–C314–C315	128.2(15)
C315–C314–C313	108.4(12)
O212–C209–C210	121.3(14)
O212–C209–C208	123.2(14)
C208–C209–C210	115.5(13)

C148–C149–H149	127.9
C150–C149–C148	104.2(12)
C150–C149–H149	127.9
O330–C307–C308	122.9(15)
O330–C307–C306	123.6(15)
C308–C307–C306	113.5(15)
N254–C253–C255	122.9(12)
N254–C253–C252	109.1(12)
C252–C253–C255	128.0(13)
O22–C2–C25	105.8(13)
O22–C2–C1	110.5(15)
O22–C2–C3	102.9(12)
C25–C2–C1	109.9(13)
C25–C2–C3	114.4(16)
C1–C2–C3	112.8(15)
N44–C45–C46	112.1(13)
N44–C45–C52	121.1(14)
C46–C45–C52	126.8(15)
N39–C100–C99	110.0(15)
N39–C100–C101	123.1(16)
C99–C100–C101	126.8(15)
N164–C163–C162	111.7(14)
N164–C163–C181	119.8(14)
C162–C163–C181	128.4(13)
O202–C200–C199	123.8(12)
O202–C200–C201	125.9(14)
C201–C200–C199	110.2(11)
F280–C279–F282	106.7(12)
F280–C279–F281	105.9(11)
F280–C279–C278	113.3(12)
F282–C279–C278	110.2(11)
F281–C279–F282	107.9(12)
F281–C279–C278	112.4(12)
C100–C99–H99	128.4
C100–C99–C98	103.2(13)
C98–C99–H99	128.4
N287–C223–C224	108.4(13)
N287–C223–C222	122.5(13)
C224–C223–C222	128.8(13)
F270–C268–C267	112.8(12)
F269–C268–F270	105.9(12)
F269–C268–C267	112.0(12)
F271–C268–F270	106.6(12)
F271–C268–F269	106.6(12)
F271–C268–C267	112.5(13)
C307–C308–H308	107.3
C307–C308–C309	110.7(12)
C307–C308–C329	111.8(14)
C309–C308–H308	107.3
C329–C308–H308	107.3
C329–C308–C309	112.1(12)
O311–C310–C309	112.3(11)
O325–C310–O311	119.8(12)
O325–C310–C309	127.9(12)
C5–C23–H23A	109.5
C5–C23–H23B	109.5

C5–C23–H23C	109.5
H23A–C23–H23B	109.5
H23A–C23–H23C	109.5
H23B–C23–H23C	109.5
H32A–C327–H32B	109.5
H32A–C327–H32C	109.5
H32B–C327–H32C	109.5
C326–C327–H32A	109.5
C326–C327–H32B	109.5
C326–C327–H32C	109.5
F144–C143–C136	112.0(11)
F146–C143–F144	105.7(10)
F146–C143–F145	107.1(11)
F146–C143–C136	112.1(13)
F145–C143–F144	106.0(13)
F145–C143–C136	113.3(11)
C253–C252–H252	127.3
C251–C252–C253	105.4(14)
C251–C252–H252	127.3
N57–C89–C88	110.7(15)
N57–C89–C90	119.2(13)
C88–C89–C90	130.0(15)
O24–C4–C5	124.4(13)
O24–C4–C3	125.8(15)
C3–C4–C5	109.8(12)
C89–C88–H88	128.1
C87–C88–C89	103.8(15)
C87–C88–H88	128.1
N160–C161–C162	111.9(13)
N160–C161–C185	118.5(13)
C162–C161–C185	129.5(14)
F49–C48–F50	107.4(14)
F49–C48–C47	111.5(12)
F51–C48–F49	108.9(14)
F51–C48–F50	106.2(13)
F51–C48–C47	112.5(12)
F50–C48–C47	110.1(13)
F103–C101–F104	105.8(16)
F103–C101–F102	105.8(14)
F103–C101–C100	111.8(15)
F104–C101–C100	112.2(14)
F102–C101–F104	108.3(16)
F102–C101–C100	112.5(16)
C323–C309–C308	112.5(11)
C323–C309–C310	101.0(10)
C323–C309–C326	111.4(12)
C308–C309–C326	112.7(12)
C310–C309–C308	110.5(12)
C310–C309–C326	108.0(11)
C76–C77–H77	127.0
C78–C77–H77	127.0
C78–C77–C76	106.1(18)
N75–C76–C77	106.5(19)
N75–C76–C83	121.1(16)
C77–C76–C83	131.9(19)
H14A–C14–H14B	109.5

H14A–C14–H14C	109.5
H14B–C14–H14C	109.5
C13–C14–H14A	109.5
C13–C14–H14B	109.5
C13–C14–H14C	109.5
O198–C197–C196	107.3(12)
O198–C197–C201	104.8(11)
O198–C197–C220	109.3(12)
C196–C197–C201	115.2(13)
C196–C197–C220	108.8(12)
C201–C197–C220	111.2(13)
N43–C47–C46	111.6(12)
N43–C47–C48	121.7(13)
C46–C47–C48	126.6(13)
F125–C124–C123	114.0(12)
F127–C124–F125	108.4(14)
F127–C124–C123	111.1(15)
F126–C124–F125	105.7(15)
F126–C124–F127	105.2(12)
F126–C124–C123	111.9(13)
F191–C189–F190	104.4(17)
F191–C189–C115	114.2(13)
F191–C189–F192	111.1(19)
F190–C189–C115	112.2(15)
F192–C189–F190	101.2(18)
F192–C189–C115	112.7(14)
O311–C312–C323	103.8(11)
O311–C312–C313	109.4(11)
O311–C312–H312	109.3
C323–C312–H312	109.3
C313–C312–C323	115.5(12)
C313–C312–H312	109.3
O317–C316–C315	105.2(12)
O317–C316–C319	106.3(13)
O317–C316–C318	109.3(14)
C315–C316–C318	110.9(14)
C319–C316–C315	115.9(14)
C319–C316–C318	109.0(14)
C241–C240–H240	128.3
C241–C240–C239	103.4(12)
C239–C240–H240	128.3
C197–C196–H196	116.7
C195–C196–C197	126.7(15)
C195–C196–H196	116.7
F292–C291–C290	110.6(13)
F294–C291–F292	107.5(14)
F294–C291–F293	108.0(13)
F294–C291–C290	111.7(13)
F293–C291–F292	107.7(13)
F293–C291–C290	111.2(13)
F285–C283–C276	112.0(13)
F284–C283–F285	108.0(14)
F284–C283–F286	106.8(13)
F284–C283–C276	111.3(13)
F286–C283–F285	107.6(13)
F286–C283–C276	110.8(15)

C7–C8–C9	112.0(12)
C7–C8–C18	101.8(12)
C7–C8–C13	108.7(13)
C9–C8–C13	113.4(13)
C18–C8–C9	110.0(13)
C18–C8–C13	110.2(13)
N40–C98–C99	110.7(14)
N40–C98–C105	120.7(14)
C99–C98–C105	128.5(14)
C307–C306–H30A	109.6
C307–C306–H30B	109.6
H30A–C306–H30B	108.1
C305–C306–C307	110.3(13)
C305–C306–H30A	109.6
C305–C306–H30B	109.6
F274–C272–C265	113.3(13)
F274–C272–F273	105.6(14)
F273–C272–C265	110.0(13)
F275–C272–F274	107.0(15)
F275–C272–C265	111.9(13)
F275–C272–F273	108.7(17)
N166–C172–C171	110.5(15)
N166–C172–C173	122.5(15)
C171–C172–C173	126.9(14)
N58–C87–C94	118.8(16)
C88–C87–N58	110.9(15)
C88–C87–C94	130.0(17)
N30–C29–C28	121.9(15)
N30–C29–C33	110.4(15)
C33–C29–C28	127.6(14)
F248–C246–F247	102.4(15)
F248–C246–C239	113.8(13)
F249–C246–F248	109.3(16)
F249–C246–F247	104.8(17)
F249–C246–C239	115.1(12)
F247–C246–C239	110.3(14)
C8–C9–H9	106.9
C17–C9–C8	112.6(12)
C17–C9–H9	106.9
C10–C9–C8	108.3(13)
C10–C9–H9	106.9
C10–C9–C17	114.9(15)
C199–C219–H21G	109.5
C199–C219–H21H	109.5
C199–C219–H21I	109.5
H21G–C219–H21H	109.5
H21G–C219–H21I	109.5
H21H–C219–H21I	109.5
C200–C201–C197	102.9(12)
C200–C201–H20A	111.2
C200–C201–H20B	111.2
C197–C201–H20A	111.2
C197–C201–H20B	111.2
H20A–C201–H20B	109.1
C209–C208–H20C	109.1
C209–C208–H20D	109.1

H20C–C208–H20D	107.9
C207–C208–C209	112.4(12)
C207–C208–H20C	109.1
C207–C208–H20D	109.1
C206–C207–H20E	108.7
C206–C207–H20F	108.7
C208–C207–C206	114.3(12)
C208–C207–H20E	108.7
C208–C207–H20F	108.7
H20E–C207–H20F	107.6
F188–C185–F187	105.9(12)
F188–C185–C161	113.7(11)
F187–C185–C161	110.1(14)
F186–C185–F188	106.7(16)
F186–C185–F187	108.2(14)
F186–C185–C161	111.9(13)
C306–C305–H30C	108.4
C306–C305–H30D	108.4
C306–C305–C326	115.5(14)
H30C–C305–H30D	107.5
C326–C305–H30C	108.4
C326–C305–H30D	108.4
F35–C34–F36	102.7(15)
F35–C34–C32	115.6(14)
F37–C34–F35	112.3(17)
F37–C34–F36	99.8(14)
F37–C34–C32	115.7(15)
F36–C34–C32	108.5(17)
N31–C32–C34	121.9(15)
N31–C32–C33	111.0(15)
C33–C32–C34	126.9(14)
C2–C1–H1A	109.5
C2–C1–H1B	109.5
C2–C1–H1C	109.5
H1A–C1–H1B	109.5
H1A–C1–H1C	109.5
H1B–C1–H1C	109.5
O19–C18–C8	112.1(13)
O20–C18–O19	121.2(13)
O20–C18–C8	126.7(14)
F300–C299–F302	105.8(13)
F300–C299–C225	111.9(12)
F302–C299–C225	110.6(12)
F301–C299–F300	108.0(13)
F301–C299–F302	108.6(14)
F301–C299–C225	111.6(13)
N238–C239–C240	110.1(13)
N238–C239–C246	121.8(12)
C240–C239–C246	128.0(12)
N230–C288–C289	109.8(12)
N230–C288–C295	121.9(12)
C289–C288–C295	128.0(12)
N151–C150–C149	110.5(13)
N151–C150–C152	120.5(14)
C149–C150–C152	128.7(14)
C308–C329–H32D	109.5

C308–C329–H32E	109.5
C308–C329–H32F	109.5
H32D–C329–H32E	109.5
H32D–C329–H32F	109.5
H32E–C329–H32F	109.5
C313–C322–H32G	109.5
C313–C322–H32H	109.5
C313–C322–H32I	109.5
H32G–C322–H32H	109.5
H32G–C322–H32I	109.5
H32H–C322–H32I	109.5
F303–C222–C223	112.6(16)
F303–C222–F304	104.2(18)
F304–C222–C223	109.9(15)
F221–C222–F303	112.4(19)
F221–C222–C223	113.2(14)
F221–C222–F304	104(2)
C14–C13–C8	112.2(14)
C14–C13–C15	108.1(16)
C14–C13–C12	108.7(16)
C15–C13–C8	110.0(16)
C12–C13–C8	108.5(14)
C12–C13–C15	109.3(17)
C197–C220–H22A	109.5
C197–C220–H22B	109.5
C197–C220–H22C	109.5
H22A–C220–H22B	109.5
H22A–C220–H22C	109.5
H22B–C220–H22C	109.5
N60–C64–C63	108(2)
N60–C64–C65	121.1(18)
C63–C64–C65	131.1(19)
F155–C152–F154	103.0(17)
F155–C152–C150	111.0(14)
F154–C152–C150	110.6(15)
F153–C152–F155	111.8(17)
F153–C152–F154	108.0(18)
F153–C152–C150	112.1(16)
C196–C195–H19A	120.0
C196–C195–H19B	120.0
H19A–C195–H19B	120.0
F131–C128–F130	101(2)
F131–C128–C121	113.7(16)
F129–C128–F131	109(2)
F129–C128–F130	104(2)
F129–C128–C121	114(2)
F130–C128–C121	113.1(15)
C172–C171–H171	128.2
C170–C171–C172	103.6(14)
C170–C171–H171	128.2
F194–C112–F193	105.5(16)
F194–C112–C113	112.0(14)
F193–C112–C113	111.4(15)
F111–C112–F194	108.1(18)
F111–C112–F193	106.7(17)
F111–C112–C113	112.7(16)

N250–C251–C259	119.8(14)
C252–C251–N250	110.0(14)
C252–C251–C259	129.9(15)
H32J–C328–H32K	109.5
H32J–C328–H32L	109.5
H32K–C328–H32L	109.5
C326–C328–H32J	109.5
C326–C328–H32K	109.5
C326–C328–H32L	109.5
C123–C122–H122	127.8
C123–C122–C121	104.5(12)
C121–C122–H122	127.8
C9–C17–H17A	109.5
C9–C17–H17B	109.5
C9–C17–H17C	109.5
H17A–C17–H17B	109.5
H17A–C17–H17C	109.5
H17B–C17–H17C	109.5
F27–C28–F110	113.0(19)
F27–C28–C29	112.2(16)
F27–C28–F109	109(2)
F110–C28–C29	110.8(17)
F110–C28–F109	101.0(19)
F109–C28–C29	110.6(17)
O16–C10–C9	119.4(19)
O16–C10–C11	123(2)
C11–C10–C9	117.8(18)
C316–C319–H319	117.0
C320–C319–C316	126.0(17)
C320–C319–H319	117.0
C29–C33–C32	103.4(13)
C29–C33–H33	128.3
C32–C33–H33	128.3
F108–C105–C98	112.3(15)
F107–C105–F108	105.7(15)
F107–C105–C98	111.5(14)
F106–C105–F108	105.1(15)
F106–C105–F107	108.3(15)
F106–C105–C98	113.4(15)
C2–C3–H3A	111.2
C2–C3–H3B	111.2
C4–C3–C2	102.9(14)
C4–C3–H3A	111.2
C4–C3–H3B	111.2
H3A–C3–H3B	109.1
C316–C318–H31C	109.5
C316–C318–H31D	109.5
C316–C318–H31E	109.5
H31C–C318–H31D	109.5
H31C–C318–H31E	109.5
H31D–C318–H31E	109.5
F92–C90–F91	108.6(17)
F92–C90–C89	113.2(13)
F92–C90–F93	104.3(17)
F91–C90–C89	110.3(16)
F93–C90–F91	108.7(17)

F93–C90–C89	111.5(16)
N120–C121–C128	119.9(14)
N120–C121–C122	110.4(14)
C122–C121–C128	129.6(14)
F55–C52–C45	112.2(14)
F54–C52–F55	105.4(15)
F54–C52–C45	113.1(16)
F53–C52–F55	106.0(15)
F53–C52–F54	106.9(15)
F53–C52–C45	112.6(14)
F97–C94–F96	107.0(17)
F97–C94–F95	106.5(18)
F97–C94–C87	114.7(16)
F96–C94–C87	109.8(17)
F95–C94–F96	105.8(17)
F95–C94–C87	112.5(17)
C206–C213–H21J	109.5
C206–C213–H21K	109.5
C206–C213–H21L	109.5
H21J–C213–H21K	109.5
H21J–C213–H21L	109.5
H21K–C213–H21L	109.5
C327–C326–C309	111.7(13)
C305–C326–C327	108.6(14)
C305–C326–C309	107.6(13)
C305–C326–C328	111.5(14)
C328–C326–C327	108.5(16)
C328–C326–C309	108.9(12)
C13–C15–H15A	109.5
C13–C15–H15B	109.5
C13–C15–H15C	109.5
H15A–C15–H15B	109.5
H15A–C15–H15C	109.5
H15B–C15–H15C	109.5
C64–C63–H63	127.7
C62–C63–C64	104.6(19)
C62–C63–H63	127.7
N61–C62–C69	118(3)
C63–C62–N61	114(2)
C63–C62–C69	128(2)
N167–C170–C171	110.1(15)
N167–C170–C177	120.0(13)
C171–C170–C177	129.9(14)
C25–C26–H26A	120.0
C25–C26–H26B	120.0
H26A–C26–H26B	120.0
C13–C12–H12A	109.1
C13–C12–H12B	109.1
C13–C12–C11	112.3(17)
H12A–C12–H12B	107.9
C11–C12–H12A	109.1
C11–C12–H12B	109.1
F261–C259–F262	109(2)
F261–C259–F260	102.2(16)
F261–C259–C251	114.7(18)
F262–C259–F260	108(2)

F262–C259–C251	111.3(15)
F260–C259–C251	111(2)
C10–C11–C12	109.1(16)
C10–C11–H11A	109.9
C10–C11–H11B	109.9
C12–C11–H11A	109.9
C12–C11–H11B	109.9
H11A–C11–H11B	108.3
F184–C181–F183	105.8(15)
F184–C181–C163	112.9(14)
F183–C181–C163	111.2(15)
F182–C181–F184	107.3(15)
F182–C181–F183	106.1(14)
F182–C181–C163	113.1(14)
N74–C78–C77	112(2)
N74–C78–C79	120(2)
C77–C78–C79	128(2)
C319–C320–H32M	120.0
C319–C320–H32N	120.0
H32M–C320–H32N	120.0
F67–C65–F68	103.5(16)
F67–C65–C64	114.0(19)
F66–C65–F67	106.9(14)
F66–C65–F68	106.5(19)
F66–C65–C64	111.7(17)
F68–C65–C64	113.5(14)
F86–C83–C76	113.7(15)
F84–C83–F86	106.4(18)
F84–C83–F85	106.6(16)
F84–C83–C76	111.3(19)
F85–C83–F86	107.4(19)
F85–C83–C76	111.0(18)
F70–C69–C62	117(3)
F70–C69–F72	106(4)
F70–C69–F71	105(3)
F72–C69–C62	118(2)
F72–C69–F71	96(4)
F71–C69–C62	113(3)
F178–C177–C170	112.3(17)
F179–C177–F178	103.1(15)
F179–C177–C170	111.7(15)
F180–C177–F178	104.7(16)
F180–C177–F179	111(2)
F180–C177–C170	113.1(15)
F174–C173–F176	106.9(14)
F174–C173–F175	107.5(18)
F174–C173–C172	113.4(19)
F176–C173–C172	110.5(16)
F175–C173–F176	107(2)
F175–C173–C172	111.6(14)
F80–C79–F82	107.4(19)
F80–C79–F81	106(3)
F80–C79–C78	115.0(19)
F82–C79–F81	106(2)
F82–C79–C78	113(2)
F81–C79–C78	109.5(19)

Table 5. Torsion angles for 30.

Atom–Atom–Atom–Atom	Torsion Angle [°]
Ag23–N233–N234–Ag3	6.0(14)
Ag23–N233–N234–C276	−174.5(10)
Ag23–N233–C278–C277	174.7(10)
Ag23–N233–C278–C279	−3.4(19)
Ag23–N287–C223–C224	178.2(11)
Ag23–N287–C223–C222	−6(2)
Ag22–N229–C290–C289	−170.7(10)
Ag22–N229–C290–C291	7(2)
Ag22–N238–C239–C240	172.4(10)
Ag22–N238–C239–C246	−6(2)
Ag1–N254–N250–Ag6	9.4(15)
Ag1–N254–N250–C251	175.1(12)
Ag1–N254–C253–C255	5(2)
Ag1–N254–C253–C252	−173.5(12)
Ag1–N230–N229–Ag22	5.3(13)
Ag1–N230–N229–C290	−165.1(9)
Ag1–N230–C288–C289	163.3(10)
Ag1–N230–C288–C295	−11(2)
Ag2–N264–C265–C266	−174.0(10)
Ag2–N264–C265–C272	5(2)
Ag2–N226–N287–Ag23	14.4(12)
Ag2–N226–N287–C223	−167.8(9)
Ag2–N226–C225–C224	163.9(12)
Ag2–N226–C225–C299	−17(2)
Ag11–N119–N120–Ag5	−3.1(13)
Ag11–N119–N120–C121	169.0(10)
Ag11–N119–C123–C124	13(2)
Ag11–N119–C123–C122	−167.6(12)
Ag11–N135–C136–C137	167.1(10)
Ag11–N135–C136–C143	−11(2)
Ag13–N134–N135–Ag11	5.4(14)
Ag13–N134–N135–C136	174.5(9)
Ag13–N134–C138–C137	−174.1(10)
Ag13–N134–C138–C139	6(2)
Ag13–N147–C148–C156	−12(2)
Ag13–N147–C148–C149	171.4(11)
Ag13–N147–N151–Ag5	8.8(13)
Ag13–N147–N151–C150	−173.4(10)
Ag3–N263–N264–Ag2	−0.4(14)
Ag3–N263–N264–C265	−174.2(9)
Ag3–N263–C267–C266	174.2(10)
Ag3–N263–C267–C268	−3(2)
Ag3–N234–C276–C277	177.9(11)
Ag3–N234–C276–C283	−6(2)
Ag4–N116–C115–C114	−172.3(10)
Ag4–N116–C115–C189	7(2)
Ag4–N160–C161–C162	163.6(11)
Ag4–N160–C161–C185	−13(2)
Ag5–N120–C121–C128	−6(3)
Ag5–N120–C121–C122	171.8(12)
Ag5–N151–C150–C149	178.2(11)
Ag5–N151–C150–C152	−7(2)
Ag41–N40–N39–Ag38	−2.9(16)
Ag41–N40–N39–C100	−175.9(11)

Ag41–N40–C98–C99	175.0(11)
Ag41–N40–C98–C105	−2(2)
Ag41–N44–N43–Ag42	1.8(13)
Ag41–N44–N43–C47	178.3(9)
Ag41–N44–C45–C46	−178.9(11)
Ag41–N44–C45–C52	−1(2)
Ag6–N237–N238–Ag22	−4.0(13)
Ag6–N237–N238–C239	169.6(9)
Ag6–N237–C241–C242	10(2)
Ag6–N237–C241–C240	−168.2(11)
Ag6–N250–C251–C252	162.9(14)
Ag6–N250–C251–C259	−11(3)
Ag16–N166–N167–Ag7	1.8(14)
Ag16–N166–N167–C170	−171.1(10)
Ag16–N166–C172–C171	169.1(13)
Ag16–N166–C172–C173	−10(3)
Ag16–N164–N160–Ag4	2.5(13)
Ag16–N164–N160–C161	167.5(9)
Ag16–N164–C163–C162	−167.3(11)
Ag16–N164–C163–C181	11(2)
Ag42–N43–C47–C46	176.8(11)
Ag42–N43–C47–C48	−5(2)
Ag42–N30–C29–C28	4(2)
Ag42–N30–C29–C33	−172.7(11)
Ag7–N167–C170–C171	−172.2(12)
Ag7–N167–C170–C177	8(2)
Ag7–N169–N116–Ag4	3.8(14)
Ag7–N169–N116–C115	−169.5(9)
Ag7–N169–C113–C114	169.2(11)
Ag7–N169–C113–C112	−11(2)
Ag56–N57–C89–C88	−174.3(12)
Ag56–N57–C89–C90	2(2)
Ag56–N75–N74–Ag73	−1.9(15)
Ag56–N75–N74–C78	−171.8(11)
Ag56–N75–C76–C77	170.0(12)
Ag56–N75–C76–C83	−3(2)
Ag38–N39–C100–C99	−170.4(12)
Ag38–N39–C100–C101	8(3)
Ag38–N31–N30–Ag42	10.4(15)
Ag38–N31–N30–C29	−163.6(11)
Ag38–N31–C32–C34	−16(2)
Ag38–N31–C32–C33	160.4(12)
Ag59–N58–N57–Ag56	4.2(15)
Ag59–N58–N57–C89	−170.0(10)
Ag59–N58–C87–C88	169.0(12)
Ag59–N58–C87–C94	−6(2)
Ag59–N60–N61–Ag73	10.9(17)
Ag59–N60–N61–C62	−178.8(13)
Ag59–N60–C64–C63	−178.3(13)
Ag59–N60–C64–C65	−2(3)
Ag73–N74–C78–C77	−166.5(13)
Ag73–N74–C78–C79	10(3)
Ag73–N61–C62–C63	163.8(17)
Ag73–N61–C62–C69	−8(4)
F258–C255–C253–N254	−17(2)
F258–C255–C253–C252	160.8(17)

F257–C255–C253–N254	103.5(16)
F257–C255–C253–C252	−78(2)
O198–C199–C200–O202	173.9(12)
O198–C199–C200–C201	−5.0(14)
O198–C197–C196–C195	137.5(16)
O198–C197–C201–C200	22.7(14)
O317–C313–C314–O321	174.7(13)
O317–C313–C314–C315	−2.6(15)
O317–C313–C312–O311	62.8(14)
O317–C313–C312–C323	−53.9(15)
O317–C316–C319–C320	132.0(19)
F244–C242–C241–N237	38(2)
F244–C242–C241–C240	−144.1(16)
N134–N135–C136–C137	−0.5(16)
N134–N135–C136–C143	−178.4(13)
N134–C138–C139–F140	−34(2)
N134–C138–C139–F142	78(2)
N134–C138–C139–F141	−156.7(19)
F296–C295–C288–N230	−29(2)
F296–C295–C288–C289	157.4(15)
F49–C48–C47–N43	28(2)
F49–C48–C47–C46	−154.1(16)
O311–C310–C309–C323	15.3(14)
O311–C310–C309–C308	134.6(12)
O311–C310–C309–C326	−101.7(13)
O212–C209–C208–C207	126.2(16)
F51–C48–C47–N43	−95.0(17)
F51–C48–C47–C46	83(2)
O22–C5–C6–O19	72.1(16)
O22–C5–C6–C7	−45.4(17)
O22–C5–C4–O24	179.3(14)
O22–C5–C4–C3	−1.8(16)
O22–C2–C3–C4	26.3(16)
O202–C200–C201–C197	170.0(13)
F298–C295–C288–N230	−152.4(13)
F298–C295–C288–C289	34(2)
O216–C203–C199–O198	72.7(13)
O216–C203–C199–C200	−174.7(10)
O216–C203–C199–C219	−51.9(14)
O216–C203–C204–O218	−169.2(12)
O216–C203–C204–C205	13.6(13)
O218–C204–C205–C206	−76.7(17)
O218–C204–C205–C215	166.3(13)
O218–C204–C205–C210	50.8(18)
N119–N120–C121–C128	−177.3(17)
N119–N120–C121–C122	0.6(19)
N119–C123–C124–F125	1(2)
N119–C123–C124–F127	−122.2(16)
N119–C123–C124–F126	120.6(16)
N119–C123–C122–C121	0(2)
F256–C255–C253–N254	−136.8(14)
F256–C255–C253–C252	41(2)
N135–N134–C138–C137	−0.8(16)
N135–N134–C138–C139	179.2(14)
N135–C136–C143–F144	−125.5(14)
N135–C136–C143–F146	115.8(14)

N135–C136–C143–F145	−6(2)
F35–C34–C32–N31	−11(3)
F35–C34–C32–C33	173.5(17)
N166–N167–C170–C171	−0.4(19)
N166–N167–C170–C177	179.4(15)
N166–C172–C171–C170	1(2)
N166–C172–C173–F174	136.3(18)
N166–C172–C173–F176	−104(2)
N166–C172–C173–F175	15(3)
O324–C323–C309–C308	45(2)
O324–C323–C309–C310	162.6(15)
O324–C323–C309–C326	−83.0(18)
O324–C323–C312–O311	−165.0(13)
O324–C323–C312–C313	−45.3(19)
N263–N264–C265–C266	−0.8(17)
N263–N264–C265–C272	178.1(13)
N263–C267–C268–F270	−14(2)
N263–C267–C268–F269	−133.6(14)
N263–C267–C268–F271	106.4(16)
O330–C307–C308–C309	−128.4(15)
O330–C307–C308–C329	−3(2)
O330–C307–C306–C305	127.5(17)
N237–N238–C239–C240	−0.1(16)
N237–N238–C239–C246	−178.8(13)
N237–C241–C240–C239	0.9(17)
F243–C242–C241–N237	158.8(14)
F243–C242–C241–C240	−23(2)
N233–N234–C276–C277	−1.4(18)
N233–N234–C276–C283	175.0(15)
N233–C278–C279–F280	−61.6(17)
N233–C278–C279–F282	178.9(12)
N233–C278–C279–F281	58.5(16)
F245–C242–C241–N237	−82.7(18)
F245–C242–C241–C240	95(2)
F37–C34–C32–N31	123.2(19)
F37–C34–C32–C33	−52(3)
N264–N263–C267–C266	0.5(16)
N264–N263–C267–C268	−176.6(13)
N264–C265–C272–F274	45(2)
N264–C265–C272–F273	162.5(16)
N264–C265–C272–F275	−77(2)
N254–N250–C251–C252	−1(2)
N254–N250–C251–C259	−175.5(19)
N254–C253–C252–C251	0(2)
C203–O216–C215–O217	175.2(11)
C203–O216–C215–C205	−6.8(13)
C203–C199–C200–O202	59.1(16)
C203–C199–C200–C201	−119.8(12)
C203–C204–C205–C206	100.3(12)
C203–C204–C205–C215	−16.6(13)
C203–C204–C205–C210	−132.2(11)
N58–N57–C89–C88	−1.3(19)
N58–N57–C89–C90	175.3(15)
N58–C87–C94–F97	64(3)
N58–C87–C94–F96	−175.5(16)
N58–C87–C94–F95	−58(2)

N226–N287–C223–C224	0.7(17)
N226–N287–C223–C222	176.2(15)
N226–C225–C299–F300	142.5(15)
N226–C225–C299–F302	25(2)
N226–C225–C299–F301	−96.3(18)
N167–N166–C172–C171	−0.9(19)
N167–N166–C172–C173	179.9(17)
N167–C170–C177–F178	42(2)
N167–C170–C177–F179	−73(2)
N167–C170–C177–F180	160.5(19)
O21–C7–C6–O19	−165.0(14)
O21–C7–C6–C5	−44(2)
O21–C7–C8–C9	45(2)
O21–C7–C8–C18	162.6(16)
O21–C7–C8–C13	−81.1(19)
N40–N39–C100–C99	1.2(19)
N40–N39–C100–C101	179.3(15)
N40–C98–C105–F108	67(2)
N40–C98–C105–F107	−174.6(16)
N40–C98–C105–F106	−52(2)
O24–C4–C3–C2	163.3(15)
N234–N233–C278–C277	−0.6(16)
N234–N233–C278–C279	−178.6(12)
N234–C276–C283–F285	20(2)
N234–C276–C283–F284	141.0(16)
N234–C276–C283–F286	−100.3(19)
O325–C310–C309–C323	−162.8(14)
O325–C310–C309–C308	−43.5(19)
O325–C310–C309–C326	80.3(18)
N147–C148–C156–F159	145.7(14)
N147–C148–C156–F158	26(2)
N147–C148–C156–F157	−91.8(17)
N147–C148–C149–C150	−0.9(18)
N147–N151–C150–C149	0.7(17)
N147–N151–C150–C152	175.2(14)
F50–C48–C47–N43	146.7(14)
F50–C48–C47–C46	−35(2)
N44–N43–C47–C46	1.2(17)
N44–N43–C47–C48	179.7(13)
N44–C45–C52–F55	−63(2)
N44–C45–C52–F54	56(2)
N44–C45–C52–F53	177.1(15)
N164–N160–C161–C162	1.2(16)
N164–N160–C161–C185	−175.1(12)
N164–C163–C181–F184	56(2)
N164–C163–C181–F183	−63(2)
N164–C163–C181–F182	178.1(15)
F297–C295–C288–N230	90.9(16)
F297–C295–C288–C289	−82.5(19)
F36–C34–C32–N31	−125.7(16)
F36–C34–C32–C33	59(2)
N57–N58–C87–C88	−0.9(19)
N57–N58–C87–C94	−175.5(15)
N57–C89–C88–C87	1(2)
N57–C89–C90–F92	28(2)
N57–C89–C90–F91	149.7(18)

N57–C89–C90–F93	−89(2)
N287–N226–C225–C224	−2.1(17)
N287–N226–C225–C299	177.3(13)
N287–C223–C222–F303	51(2)
N287–C223–C222–F304	−64(2)
N287–C223–C222–F221	−179.6(19)
N169–N116–C115–C114	−0.4(16)
N169–N116–C115–C189	178.7(14)
N169–C113–C112–F194	−179.2(16)
N169–C113–C112–F193	63(2)
N169–C113–C112–F111	−57(2)
N43–N44–C45–C46	−0.1(18)
N43–N44–C45–C52	177.7(15)
N75–N74–C78–C77	2(2)
N75–N74–C78–C79	178.7(17)
N75–C76–C83–F86	−33(3)
N75–C76–C83–F84	87(2)
N75–C76–C83–F85	−154.2(17)
N39–N40–C98–C99	0.6(19)
N39–N40–C98–C105	−176.3(15)
N39–C100–C99–C98	−1(2)
N39–C100–C101–F103	122.3(18)
N39–C100–C101–F104	4(2)
N39–C100–C101–F102	−118.8(19)
C323–C309–C326–C327	−61.7(17)
C323–C309–C326–C305	179.2(12)
C323–C309–C326–C328	58.2(17)
F248–C246–C239–N238	−149.0(16)
F248–C246–C239–C240	33(2)
N74–N75–C76–C77	1.6(18)
N74–N75–C76–C83	−171.6(16)
N74–C78–C79–F80	58(3)
N74–C78–C79–F82	−178.3(18)
N74–C78–C79–F81	−61(3)
N120–N119–C123–C124	−179.7(13)
N120–N119–C123–C122	0.0(17)
C199–O198–C197–C196	−151.1(11)
C199–O198–C197–C201	−28.1(14)
C199–O198–C197–C220	91.2(13)
C199–C203–C204–O218	−47.7(17)
C199–C203–C204–C205	135.1(11)
C199–C200–C201–C197	−11.2(14)
C204–C203–C199–O198	−46.0(14)
C204–C203–C199–C200	66.5(14)
C204–C203–C199–C219	−170.6(12)
C204–C205–C215–O216	14.6(13)
C204–C205–C215–O217	−167.6(13)
C204–C205–C210–C211	53.6(16)
C204–C205–C210–C209	179.3(11)
N116–N169–C113–C114	1.2(18)
N116–N169–C113–C112	−179.3(14)
N116–C115–C189–F191	8(2)
N116–C115–C189–F190	126.3(18)
N116–C115–C189–F192	−120(2)
N230–N229–C290–C289	−1.5(17)
N230–N229–C290–C291	175.7(13)

C313–O317–C316–C315	−28.8(15)
C313–O317–C316–C319	−152.2(12)
C313–O317–C316–C318	90.3(15)
N229–N230–C288–C289	−1.4(15)
N229–N230–C288–C295	−175.8(12)
N229–C290–C291–F292	−64.4(19)
N229–C290–C291–F294	55(2)
N229–C290–C291–F293	176.0(14)
C148–N147–N151–Ag5	−179.1(9)
C148–N147–N151–C150	−1.3(16)
C148–C149–C150–N151	0.1(19)
C148–C149–C150–C152	−173.9(17)
N238–N237–C241–C242	177.1(13)
N238–N237–C241–C240	−1.0(17)
N31–N30–C29–C28	177.1(16)
N31–N30–C29–C33	0.7(19)
N31–C32–C33–C29	3.2(19)
C114–C113–C112–F194	0(3)
C114–C113–C112–F193	−117.7(19)
C114–C113–C112–F111	122(2)
C114–C115–C189–F191	−173.2(18)
C114–C115–C189–F190	−55(2)
C114–C115–C189–F192	59(3)
N151–N147–C148–C156	177.6(13)
N151–N147–C148–C149	1.3(17)
N151–C150–C152–F155	46(2)
N151–C150–C152–F154	−67(2)
N151–C150–C152–F153	172.0(18)
C266–C265–C272–F274	−136.7(16)
C266–C265–C272–F273	−19(2)
C266–C265–C272–F275	102(2)
C266–C267–C268–F270	169.0(13)
C266–C267–C268–F269	50(2)
C266–C267–C268–F271	−70.4(18)
C206–C205–C215–O216	−103.8(12)
C206–C205–C215–O217	74.0(17)
C206–C205–C210–C211	−179.1(12)
C206–C205–C210–C209	−53.4(15)
N30–N31–C32–C34	−179.0(15)
N30–N31–C32–C33	−2.8(18)
N30–C29–C28–F27	175.1(19)
N30–C29–C28–F110	48(3)
N30–C29–C28–F109	−63(2)
N30–C29–C33–C32	−2(2)
C265–C266–C267–N263	−0.9(17)
C265–C266–C267–C268	176.1(14)
C113–N169–N116–Ag4	172.8(10)
C113–N169–N116–C115	−0.5(16)
C113–C114–C115–N116	1.1(17)
C113–C114–C115–C189	−178.0(16)
N250–N254–C253–C255	177.6(14)
N250–N254–C253–C252	−0.9(18)
N250–C251–C259–F261	−36(3)
N250–C251–C259–F262	−160(2)
N250–C251–C259–F260	80(3)
N160–N164–C163–C162	−0.7(18)

N160–N164–C163–C181	177.3(14)
N160–C161–C185–F188	−26(2)
N160–C161–C185–F187	−144.7(14)
N160–C161–C185–F186	94.9(18)
C137–C136–C143–F144	57(2)
C137–C136–C143–F146	−61.7(19)
C137–C136–C143–F145	177.0(14)
C137–C138–C139–F140	145.6(18)
C137–C138–C139–F142	−102(2)
C137–C138–C139–F141	23(3)
C7–C8–C9–C17	57.9(18)
C7–C8–C9–C10	−174.0(14)
C7–C8–C18–O19	12.0(15)
C7–C8–C18–O20	−168.5(14)
C7–C8–C13–C14	−60.5(18)
C7–C8–C13–C15	59.8(19)
C7–C8–C13–C12	179.4(15)
F131–C128–C121–N120	157(2)
F131–C128–C121–C122	−20(4)
C162–C163–C181–F184	−126.4(18)
C162–C163–C181–F183	115.0(19)
C162–C163–C181–F182	−4(3)
C162–C161–C185–F188	158.4(15)
C162–C161–C185–F187	40(2)
C162–C161–C185–F186	−81(2)
C277–C276–C283–F285	−164.3(16)
C277–C276–C283–F284	−43(3)
C277–C276–C283–F286	75(2)
C277–C278–C279–F280	120.8(16)
C277–C278–C279–F282	1(2)
C277–C278–C279–F281	−119.1(17)
C5–O22–C2–C25	−150.3(13)
C5–O22–C2–C1	90.8(15)
C5–O22–C2–C3	−29.9(16)
C5–C4–C3–C2	−15.6(17)
C242–C241–C240–C239	−177.0(15)
C205–C206–C207–C208	−52.5(16)
C205–C210–C209–O212	−126.2(14)
C205–C210–C209–C208	53.1(15)
C136–C137–C138–N134	0.5(17)
C136–C137–C138–C139	−179.5(15)
N60–N61–C62–C63	−4(2)
N60–N61–C62–C69	−176(2)
N60–C64–C63–C62	−4(2)
N60–C64–C65–F67	67(2)
N60–C64–C65–F66	−171.5(16)
N60–C64–C65–F68	−51(2)
C215–O216–C203–C199	−129.2(11)
C215–O216–C203–C204	−4.3(13)
C215–C205–C210–C211	−57.9(15)
C215–C205–C210–C209	67.8(13)
C267–N263–N264–Ag2	174.0(9)
C267–N263–N264–C265	0.2(15)
C267–C266–C265–N264	1.0(17)
C267–C266–C265–C272	−177.7(15)
F249–C246–C239–N238	−22(2)

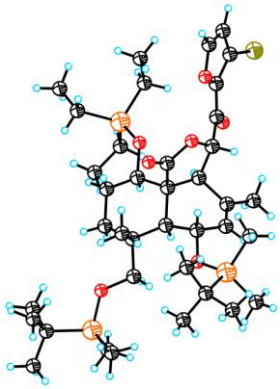
F249–C246–C239–C240	159.8(18)
C211–C210–C209–O212	−0.2(19)
C211–C210–C209–C208	179.1(12)
C6–O19–C18–O20	175.3(13)
C6–O19–C18–C8	−5.1(16)
C6–C7–C8–C9	−131.3(13)
C6–C7–C8–C18	−13.8(14)
C6–C7–C8–C13	102.6(14)
C6–C5–C4–O24	60.8(19)
C6–C5–C4–C3	−120.2(14)
C210–C205–C215–O216	133.4(11)
C210–C205–C215–O217	−48.8(17)
C210–C209–C208–C207	−53.1(17)
C276–C277–C278–N233	−0.3(17)
C276–C277–C278–C279	177.5(15)
C224–C225–C299–F300	−38(2)
C224–C225–C299–F302	−155.8(17)
C224–C225–C299–F301	83(2)
C224–C223–C222–F303	−134(2)
C224–C223–C222–F304	110(2)
C224–C223–C222–F221	−5(3)
C289–C290–C291–F292	112.4(17)
C289–C290–C291–F294	−128.0(17)
C289–C290–C291–F293	−7(2)
C255–C253–C252–C251	−178.3(17)
C241–N237–N238–Ag22	−172.9(9)
C241–N237–N238–C239	0.7(15)
C241–C240–C239–N238	−0.5(17)
C241–C240–C239–C246	178.1(15)
C138–N134–N135–Ag11	−168.3(9)
C138–N134–N135–C136	0.8(15)
C138–C137–C136–N135	0.0(17)
C138–C137–C136–C143	177.8(14)
C115–C114–C113–N169	−1.4(18)
C115–C114–C113–C112	179.1(16)
C315–C316–C319–C320	16(3)
C25–C2–C3–C4	140.5(14)
C123–N119–N120–Ag5	−172.5(9)
C123–N119–N120–C121	−0.4(16)
C123–C122–C121–N120	−1(2)
C123–C122–C121–C128	177(2)
C46–C45–C52–F55	114.1(19)
C46–C45–C52–F54	−126.8(19)
C46–C45–C52–F53	−5(3)
C214–C206–C205–C204	−58.8(16)
C214–C206–C205–C215	53.1(16)
C214–C206–C205–C210	173.4(12)
C214–C206–C207–C208	−174.1(12)
C225–N226–N287–Ag23	−177.0(9)
C225–N226–N287–C223	0.9(15)
C225–C224–C223–N287	−1.9(19)
C225–C224–C223–C222	−177.1(17)
C156–C148–C149–C150	−177.0(15)
N61–N60–C64–C63	2(2)
N61–N60–C64–C65	178.2(16)
N61–C62–C69–F70	167(3)

N61–C62–C69–F72	39(5)
N61–C62–C69–F71	−72(4)
O16–C10–C11–C12	122(2)
C278–N233–N234–Ag3	−178.2(9)
C278–N233–N234–C276	1.2(16)
C278–C277–C276–N234	1.0(18)
C278–C277–C276–C283	−175.2(17)
C290–C289–C288–N230	0.5(16)
C290–C289–C288–C295	174.5(14)
C314–C313–C312–O311	177.0(11)
C314–C313–C312–C323	60.4(16)
C314–C315–C316–O317	25.4(15)
C314–C315–C316–C319	142.4(13)
C314–C315–C316–C318	−92.7(16)
C209–C208–C207–C206	52.0(18)
C149–C148–C156–F159	−39(2)
C149–C148–C156–F158	−157.9(15)
C149–C148–C156–F157	84(2)
C149–C150–C152–F155	−140.4(19)
C149–C150–C152–F154	106(2)
C149–C150–C152–F153	−15(3)
C307–C308–C309–C323	−179.7(12)
C307–C308–C309–C310	68.2(15)
C307–C308–C309–C326	−52.8(16)
C307–C306–C305–C326	57(2)
C253–N254–N250–Ag6	−164.3(10)
C253–N254–N250–C251	1.3(17)
C253–C252–C251–N250	1(2)
C253–C252–C251–C259	174(2)
C2–O22–C5–C6	137.5(13)
C2–O22–C5–C23	−100.7(15)
C2–O22–C5–C4	20.2(16)
C45–N44–N43–Ag42	−177.2(10)
C45–N44–N43–C47	−0.7(16)
C45–C46–C47–N43	−1.2(17)
C45–C46–C47–C48	−179.6(15)
C100–C99–C98–N40	0.1(19)
C100–C99–C98–C105	176.7(18)
C163–N164–N160–Ag4	−165.3(10)
C163–N164–N160–C161	−0.3(15)
C163–C162–C161–N160	−1.6(18)
C163–C162–C161–C185	174.2(15)
C99–C100–C101–F103	−60(2)
C99–C100–C101–F104	−178.8(17)
C99–C100–C101–F102	59(2)
C99–C98–C105–F108	−109.4(19)
C99–C98–C105–F107	9(3)
C99–C98–C105–F106	131.6(18)
C223–C224–C225–N226	2.5(19)
C223–C224–C225–C299	−177.0(15)
C308–C307–C306–C305	−54.9(19)
C308–C309–C326–C327	170.7(14)
C308–C309–C326–C305	51.6(16)
C308–C309–C326–C328	−69.4(17)
F129–C128–C121–N120	−77(3)
F129–C128–C121–C122	106(3)

C310–O311–C312–C323	−6.1(14)
C310–O311–C312–C313	−130.0(12)
C310–C309–C326–C327	48.3(17)
C310–C309–C326–C305	−70.7(15)
C310–C309–C326–C328	168.2(14)
C23–C5–C6–O19	−52.1(16)
C23–C5–C6–C7	−169.7(13)
C23–C5–C4–O24	−59(2)
C23–C5–C4–C3	120.2(15)
C252–C251–C259–F261	151(2)
C252–C251–C259–F262	27(4)
C252–C251–C259–F260	−93(3)
C89–C88–C87–N58	0(2)
C89–C88–C87–C94	174.0(18)
C4–C5–C6–O19	−173.3(11)
C4–C5–C6–C7	69.2(16)
C88–C89–C90–F92	−156.4(19)
C88–C89–C90–F91	−34(3)
C88–C89–C90–F93	86(2)
C88–C87–C94–F97	−109(2)
C88–C87–C94–F96	11(3)
C88–C87–C94–F95	129(2)
C161–C162–C163–N164	1.4(18)
C161–C162–C163–C181	−176.4(16)
C101–C100–C99–C98	−178.8(17)
C309–C323–C312–O311	15.9(14)
C309–C323–C312–C313	135.6(12)
C77–C76–C83–F86	155.8(19)
C77–C76–C83–F84	−84(3)
C77–C76–C83–F85	35(3)
C77–C78–C79–F80	−126(3)
C77–C78–C79–F82	−2(3)
C77–C78–C79–F81	115(3)
C76–N75–N74–Ag73	167.8(10)
C76–N75–N74–C78	−2.2(18)
C76–C77–C78–N74	−1(2)
C76–C77–C78–C79	−177(2)
C14–C13–C12–C11	−178.2(16)
C197–O198–C199–C203	136.4(11)
C197–O198–C199–C200	20.6(13)
C197–O198–C199–C219	−101.1(13)
C47–C46–C45–N44	0.8(18)
C47–C46–C45–C52	−176.8(17)
F247–C246–C239–N238	96.5(18)
F247–C246–C239–C240	−82(2)
C124–C123–C122–C121	−179.9(16)
C312–O311–C310–O325	172.3(12)
C312–O311–C310–C309	−5.9(15)
C312–C323–C309–C308	−136.3(12)
C312–C323–C309–C310	−18.4(14)
C312–C323–C309–C326	96.1(13)
C312–C313–C314–O321	58.2(18)
C312–C313–C314–C315	−119.1(13)
C316–O317–C313–C314	19.5(14)
C316–O317–C313–C312	136.6(12)
C316–O317–C313–C322	−101.1(14)

C316–C315–C314–O321	168.8(15)
C316–C315–C314–C313	−14.1(15)
C196–C197–C201–C200	140.4(12)
C8–C7–C6–O19	11.5(15)
C8–C7–C6–C5	132.7(13)
C8–C9–C10–O16	−125.0(17)
C8–C9–C10–C11	53(2)
C8–C13–C12–C11	−56(2)
C98–N40–N39–Ag38	171.9(11)
C98–N40–N39–C100	−1.1(18)
C306–C307–C308–C309	53.9(17)
C306–C307–C308–C329	179.7(13)
C306–C305–C326–C327	−175.6(14)
C306–C305–C326–C309	−54.5(18)
C306–C305–C326–C328	64.9(19)
C172–N166–N167–Ag7	173.7(11)
C172–N166–N167–C170	0.8(17)
C172–C171–C170–N167	0(2)
C172–C171–C170–C177	−179.9(19)
C87–N58–N57–Ag56	175.5(10)
C87–N58–N57–C89	1.3(17)
C9–C8–C18–O19	131.0(13)
C9–C8–C18–O20	−50(2)
C9–C8–C13–C14	174.2(15)
C9–C8–C13–C15	−66(2)
C9–C8–C13–C12	54(2)
C9–C10–C11–C12	−56(2)
C219–C199–C200–O202	−62.9(17)
C219–C199–C200–C201	118.2(13)
C201–C197–C196–C195	21(2)
C207–C206–C205–C204	−179.0(11)
C207–C206–C205–C215	−67.1(14)
C207–C206–C205–C210	53.2(15)
C34–C32–C33–C29	179.1(17)
C32–N31–N30–Ag42	175.3(10)
C32–N31–N30–C29	1.3(17)
C1–C2–C3–C4	−92.8(16)
C18–O19–C6–C7	−4.1(15)
C18–O19–C6–C5	−128.1(13)
C18–C8–C9–C17	−54.6(18)
C18–C8–C9–C10	73.5(17)
C18–C8–C13–C14	50.4(19)
C18–C8–C13–C15	170.7(16)
C18–C8–C13–C12	−69.8(18)
C288–N230–N229–Ag22	172.2(9)
C288–N230–N229–C290	1.7(15)
C288–C289–C290–N229	0.7(17)
C288–C289–C290–C291	−176.3(15)
C329–C308–C309–C323	54.7(16)
C329–C308–C309–C310	−57.4(16)
C329–C308–C309–C326	−178.4(13)
C322–C313–C314–O321	−63.5(19)
C322–C313–C314–C315	119.3(14)
C322–C313–C312–O311	−61.0(15)
C322–C313–C312–C323	−177.6(12)
C13–C8–C9–C17	−178.5(15)

C13–C8–C9–C10	−50.4(19)
C13–C8–C18–O19	−103.3(15)
C13–C8–C18–O20	76.2(18)
C13–C12–C11–C10	57(2)
C220–C197–C196–C195	−104.5(19)
C220–C197–C201–C200	−95.2(14)
C64–N60–N61–Ag73	−169.2(12)
C64–N60–N61–C62	1(2)
C64–C63–C62–N61	5(3)
C64–C63–C62–C69	176(3)
C171–C172–C173–F174	−43(3)
C171–C172–C173–F176	77(3)
C171–C172–C173–F175	−164(2)
C171–C170–C177–F178	−138.0(19)
C171–C170–C177–F179	107(2)
C171–C170–C177–F180	−20(3)
C122–C123–C124–F125	−179.1(17)
C122–C123–C124–F127	58(2)
C122–C123–C124–F126	−59(2)
C17–C9–C10–O16	2(2)
C17–C9–C10–C11	−179.8(15)
C28–C29–C33–C32	−178.5(18)
F130–C128–C121–N120	43(3)
F130–C128–C121–C122	−135(2)
C33–C29–C28–F27	−9(3)
C33–C29–C28–F110	−137(2)
C33–C29–C28–F109	112(2)
C318–C316–C319–C320	−110(2)
C90–C89–C88–C87	−175.4(18)
C213–C206–C205–C204	60.8(16)
C213–C206–C205–C215	172.7(12)
C213–C206–C205–C210	−66.9(16)
C213–C206–C207–C208	68.1(16)
C15–C13–C12–C11	64(2)
C63–C64–C65–F67	−117(2)
C63–C64–C65–F66	4(3)
C63–C64–C65–F68	125(2)
C63–C62–C69–F70	−4(5)
C63–C62–C69–F72	−132(4)
C63–C62–C69–F71	117(4)
C26–C25–C2–O22	130.9(19)
C26–C25–C2–C1	−110(2)
C26–C25–C2–C3	18(3)
C78–C77–C76–N75	0(2)
C78–C77–C76–C83	172(2)
C65–C64–C63–C62	180(2)
C173–C172–C171–C170	179.8(19)



S8

Table 1. Crystal data and structure refinement for compound S8

CCDC number	2447367
Empirical formula	$C_{38}H_{65}BrO_7Si_3$
Formula weight	798.08
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	6.6015(3)
b/Å	29.7627(10)
c/Å	21.7016(12)
α/°	90
β/°	97.068(5)
γ/°	90
Volume/Å^3	4231.5(3)
Z	4
ρ_{calc}g/cm^3	1.253
μ/mm^{-1}	2.486
F(000)	1704.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	5.064 to 133.19
Index ranges	-7 ≤ h ≤ 5, -35 ≤ k ≤ 31, -25 ≤ l ≤ 24
Reflections collected	21000
Independent reflections	10747 [R_{int} = 0.1411, R_{sigma} = 0.1528]
Data/restraints/parameters	10747/625/913
Goodness-of-fit on F^2	1.166
Final R indexes [I>=2σ (I)]	R_1 = 0.1202, wR_2 = 0.3142
Final R indexes [all data]	R_1 = 0.1654, wR_2 = 0.3342
Largest diff. peak/hole / e Å^{-3}	2.01/-1.25
Flack parameter	0.07(3)

Table 2. Atomic coordinates and U_{eq} [Å^2] for S8

Atom	*x*	*y*	*z*	U_{eq}
Si70	0.2598(7)	0.39242(15)	-0.1400(2)	0.0324(9)
Si43	0.6452(8)	0.57831(16)	0.6605(2)	0.0401(11)

Si52	0.3458(8)	0.68320(16)	-0.0185(2)	0.0436(11)
Si78	0.0102(7)	0.40623(15)	0.1169(2)	0.0359(10)
Si5	0.1745(8)	0.57116(16)	0.3854(2)	0.0401(11)
Si33	0.5618(7)	0.29028(15)	0.5285(2)	0.0366(10)
O8	0.3059(16)	0.5367(4)	0.4362(5)	0.030(2)
O53	0.2335(16)	0.6384(3)	0.0083(5)	0.027(2)
O77	0.1661(15)	0.4392(3)	0.0827(5)	0.028(2)
O94	-0.1634(16)	0.5732(4)	0.0296(5)	0.035(2)
O93	0.4458(18)	0.6623(4)	0.1614(6)	0.048(3)
O17	0.1297(17)	0.3756(4)	0.3991(5)	0.037(2)
O57	0.0020(16)	0.6021(4)	0.1146(5)	0.032(2)
O32	0.4393(18)	0.3367(4)	0.4997(5)	0.036(2)
O42	0.5345(19)	0.5332(4)	0.6276(5)	0.038(2)
O69	0.1807(18)	0.4386(4)	-0.1100(5)	0.037(2)
O31	0.0364(18)	0.4039(4)	0.4856(5)	0.041(3)
O88	-0.0566(19)	0.6636(4)	0.2034(6)	0.047(3)
O30	0.538(2)	0.3194(4)	0.3393(6)	0.048(3)
C86	0.271(3)	0.6504(6)	0.1657(8)	0.038(3)
C87	0.128(3)	0.6800(6)	0.1926(8)	0.043(3)
C60	0.432(2)	0.5376(5)	0.1487(7)	0.028(3)
C62	0.179(2)	0.4867(5)	0.0906(6)	0.027(3)
H62	0.048107	0.497667	0.101714	0.032
C63	0.230(2)	0.5124(5)	0.0333(6)	0.024(3)
H63	0.376824	0.507746	0.032827	0.029
C20	0.523(2)	0.4403(5)	0.3627(7)	0.030(3)
C18	0.301(3)	0.3728(6)	0.3652(8)	0.035(3)
H18	0.264594	0.389578	0.326627	0.042
C61	0.346(2)	0.4976(5)	0.1436(7)	0.030(3)
H61	0.388382	0.475613	0.172848	0.036
C10	0.433(2)	0.4640(5)	0.4822(7)	0.030(3)
H10	0.577971	0.468840	0.479333	0.036
C55	0.209(2)	0.5643(5)	0.0487(6)	0.025(2)
C64	0.130(2)	0.4961(5)	-0.0324(6)	0.026(3)
C65	0.201(3)	0.5292(6)	-0.0804(7)	0.035(3)
H65A	0.346534	0.525244	-0.081193	0.042
H65B	0.133379	0.521407	-0.121269	0.042
C66	0.161(3)	0.5775(5)	-0.0686(7)	0.033(3)
H66A	0.015256	0.582189	-0.069622	0.039
H66B	0.207963	0.595617	-0.101208	0.039
C40	0.189(3)	0.4868(6)	0.5633(8)	0.038(4)
H40A	0.107131	0.460346	0.554811	0.057
H40B	0.131069	0.511112	0.537856	0.057
H40C	0.191806	0.494772	0.606310	0.057
C54	0.270(2)	0.5928(5)	-0.0053(6)	0.026(3)
H54	0.417129	0.589064	-0.006092	0.031
C22	0.654(3)	0.4302(6)	0.3141(8)	0.039(4)
H22A	0.788385	0.422452	0.333196	0.059
H22B	0.661790	0.456189	0.288246	0.059
H22C	0.597291	0.405528	0.289278	0.059
C11	0.406(2)	0.4777(5)	0.5490(7)	0.031(3)
C68	0.235(2)	0.4513(5)	-0.0455(6)	0.030(3)
H68A	0.381963	0.454648	-0.036787	0.036
H68B	0.192631	0.427967	-0.018619	0.036
C56	-0.005(2)	0.5785(5)	0.0590(6)	0.026(3)
C46	0.647(3)	0.5683(6)	0.7452(8)	0.043(3)
C13	0.448(2)	0.3947(5)	0.5778(6)	0.029(3)

H13A	0.514409	0.374393	0.608962	0.034
H13B	0.302010	0.391680	0.577920	0.034
C59	0.345(2)	0.5755(5)	0.1103(6)	0.027(3)
H59	0.455317	0.595496	0.101311	0.033
C83	0.013(3)	0.3191(6)	0.1643(9)	0.049(4)
H83A	-0.007885	0.329996	0.204592	0.074
H83B	0.078008	0.290163	0.168289	0.074
H83C	-0.115667	0.316496	0.138777	0.074
C14	0.500(2)	0.3813(5)	0.5176(7)	0.030(3)
H14	0.648118	0.383520	0.518271	0.036
C73	0.181(3)	0.3984(6)	-0.2254(7)	0.038(3)
C85	0.609(2)	0.5485(6)	0.1957(8)	0.035(4)
H85A	0.570636	0.571732	0.222704	0.053
H85B	0.720764	0.558637	0.175015	0.053
H85C	0.648710	0.522134	0.219636	0.053
C16	0.170(2)	0.3980(5)	0.4534(7)	0.032(3)
C19	0.470(2)	0.3998(6)	0.4038(7)	0.032(3)
H19	0.591137	0.380716	0.412537	0.038
C12	0.510(3)	0.4427(6)	0.5959(7)	0.033(3)
H12A	0.657083	0.445610	0.597955	0.040
H12B	0.472707	0.449071	0.636913	0.040
C47	0.424(3)	0.5675(8)	0.7623(9)	0.057(5)
H47A	0.379745	0.597673	0.768956	0.086
H47B	0.419359	0.550230	0.799451	0.086
H47C	0.334869	0.554147	0.728917	0.086
C23	0.361(3)	0.3258(6)	0.3465(8)	0.040(3)
C41	0.528(3)	0.5217(6)	0.5622(7)	0.035(3)
H41A	0.665176	0.517946	0.551669	0.041
H41B	0.462613	0.545755	0.536852	0.041
C51	0.257(3)	0.7316(7)	0.0267(10)	0.056(4)
H51A	0.109021	0.732634	0.020101	0.067
H51B	0.297580	0.726246	0.070604	0.067
C74	0.286(3)	0.3613(6)	-0.2620(9)	0.050(5)
H74A	0.430713	0.366699	-0.258056	0.075
H74B	0.231453	0.362379	-0.305071	0.075
H74C	0.260906	0.332289	-0.245349	0.075
C67	-0.098(3)	0.4908(6)	-0.0419(8)	0.037(4)
H67A	-0.142271	0.476631	-0.006112	0.055
H67B	-0.137018	0.472541	-0.077918	0.055
H67C	-0.161206	0.519809	-0.047797	0.055
C90	-0.044(3)	0.7342(8)	0.2344(9)	0.054(4)
H90	-0.081683	0.761168	0.251433	0.065
C7	0.008(3)	0.5395(7)	0.3269(10)	0.058(5)
H7A	0.065639	0.539477	0.288451	0.086
H7B	-0.124479	0.553369	0.320849	0.086
H7C	-0.004973	0.509174	0.340914	0.086
C34	0.467(3)	0.2717(7)	0.6020(8)	0.049(4)
H34A	0.499313	0.294788	0.633303	0.059
H34B	0.319688	0.268951	0.594786	0.059
C38	0.494(3)	0.2459(6)	0.4684(10)	0.050(4)
H38A	0.516920	0.257739	0.428240	0.060
H38B	0.585815	0.220581	0.477419	0.060
C9	0.323(3)	0.4891(5)	0.4258(7)	0.030(3)
H9	0.184978	0.476600	0.416196	0.036
C76	-0.048(3)	0.3950(7)	-0.2393(7)	0.043(4)
H76A	-0.093392	0.367824	-0.221505	0.064

H76B	-0.085598	0.394486	-0.283469	0.064
H76C	-0.109690	0.420373	-0.221881	0.064
C6	0.361(3)	0.6052(7)	0.3444(9)	0.046(4)
H6A	0.445951	0.622808	0.374385	0.069
H6B	0.286870	0.624729	0.314532	0.069
H6C	0.444805	0.585231	0.323723	0.069
C81	0.150(3)	0.3520(6)	0.1341(8)	0.038(3)
C49	0.749(3)	0.5227(7)	0.7631(9)	0.046(4)
H49A	0.691368	0.499937	0.735018	0.070
H49B	0.726725	0.515051	0.804714	0.070
H49C	0.893197	0.524902	0.760843	0.070
C58	0.197(3)	0.6020(6)	0.1479(7)	0.035(3)
H58	0.189162	0.585473	0.186623	0.043
C36	0.846(3)	0.2999(6)	0.5409(9)	0.042(3)
H36A	0.914275	0.271023	0.541792	0.050
H36B	0.884794	0.316563	0.505744	0.050
C4	0.157(3)	0.6309(7)	0.4826(9)	0.046(4)
H4A	0.196772	0.608666	0.513704	0.069
H4B	0.082407	0.654435	0.500139	0.069
H4C	0.276284	0.643338	0.467885	0.069
C21	0.439(2)	0.4801(5)	0.3722(7)	0.031(3)
H21	0.453640	0.503203	0.344335	0.037
C75	0.245(4)	0.4448(7)	-0.2472(9)	0.055(5)
H75A	0.188435	0.467743	-0.223271	0.082
H75B	0.195170	0.448661	-0.290319	0.082
H75C	0.391168	0.447105	-0.241596	0.082
C2	0.025(3)	0.6098(6)	0.4298(9)	0.045(4)
C39	0.277(3)	0.2291(8)	0.4644(9)	0.053(5)
H39A	0.251864	0.208349	0.430401	0.080
H39B	0.185009	0.254009	0.457725	0.080
H39C	0.257219	0.214182	0.502377	0.080
C72	0.538(3)	0.3883(8)	-0.1195(10)	0.052(5)
H72A	0.594111	0.417684	-0.110645	0.078
H72B	0.598138	0.375443	-0.153630	0.078
H72C	0.568165	0.369487	-0.083551	0.078
C45	0.497(3)	0.6298(6)	0.6316(10)	0.054(5)
H45A	0.472642	0.629047	0.587062	0.081
H45B	0.574408	0.656183	0.644624	0.081
H45C	0.369286	0.630357	0.648320	0.081
C15	0.396(2)	0.4126(5)	0.4643(7)	0.029(3)
C89	-0.152(3)	0.6992(7)	0.2294(9)	0.052(4)
H89	-0.281382	0.697471	0.241693	0.062
C71	0.145(3)	0.3415(6)	-0.1093(8)	0.041(4)
H71A	0.186477	0.339268	-0.065460	0.061
H71B	0.189922	0.315393	-0.129714	0.061
H71C	-0.001152	0.343571	-0.116926	0.061
C50	0.337(4)	0.7757(7)	0.0102(11)	0.063(5)
H50A	0.302463	0.780897	-0.033459	0.094
H50B	0.482859	0.776061	0.020289	0.094
H50C	0.278195	0.798897	0.033125	0.094
C35	0.557(3)	0.2271(7)	0.6273(10)	0.057(5)
H35A	0.496543	0.202836	0.602296	0.086
H35B	0.529309	0.223223	0.669392	0.086
H35C	0.702029	0.227120	0.626147	0.086
C82	0.347(3)	0.3592(8)	0.1768(11)	0.062(5)
H82A	0.443839	0.374312	0.154613	0.093

H82B	0.400818	0.330713	0.191399	0.093
H82C	0.319567	0.377278	0.211559	0.093
C84	0.204(3)	0.3320(7)	0.0719(9)	0.051(5)
H84A	0.089970	0.314760	0.052797	0.076
H84B	0.321134	0.312964	0.079952	0.076
H84C	0.232249	0.355957	0.044661	0.076
C37	0.921(3)	0.3249(7)	0.5991(10)	0.052(5)
H37A	0.880235	0.355773	0.594837	0.078
H37B	1.067592	0.323168	0.606282	0.078
H37C	0.864569	0.311706	0.633537	0.078
C97	0.236(4)	0.6937(8)	-0.1046(11)	0.061(4)
H97A	0.296724	0.720737	-0.119115	0.074
H97B	0.273672	0.668812	-0.129656	0.074
C80	-0.231(3)	0.3971(8)	0.0618(11)	0.062(5)
H80A	-0.301320	0.425177	0.054482	0.094
H80B	-0.317326	0.376135	0.079789	0.094
H80C	-0.196513	0.385362	0.023254	0.094
C1	-0.065(3)	0.6490(7)	0.3860(9)	0.051(5)
H1A	0.044419	0.667820	0.375742	0.076
H1B	-0.157702	0.666600	0.406809	0.076
H1C	-0.136064	0.636588	0.348614	0.076
C48	0.764(4)	0.6048(7)	0.7838(9)	0.058(5)
H48A	0.907478	0.600913	0.782574	0.087
H48B	0.734514	0.602857	0.825947	0.087
H48C	0.722552	0.633755	0.767108	0.087
C79	-0.053(4)	0.4319(8)	0.1889(11)	0.067(6)
H79A	0.066567	0.445723	0.210411	0.101
H79B	-0.101851	0.409123	0.214778	0.101
H79C	-0.157185	0.454169	0.179199	0.101
C98	0.015(5)	0.6985(10)	-0.1136(13)	0.086(7)
H98A	-0.031396	0.700957	-0.157155	0.129
H98B	-0.022902	0.725066	-0.092662	0.129
H98C	-0.046383	0.672706	-0.096916	0.129
C3	-0.156(3)	0.5841(7)	0.4531(9)	0.048(4)
H3A	-0.274480	0.586639	0.422939	0.072
H3B	-0.184659	0.596718	0.491814	0.072
H3C	-0.120288	0.552962	0.459015	0.072
C95	0.625(4)	0.6800(8)	-0.0128(11)	0.067(4)
H95A	0.666771	0.652241	-0.031035	0.080
H95B	0.678464	0.705048	-0.034519	0.080
C96	0.697(5)	0.6816(11)	0.0496(17)	0.104(8)
H96A	0.836582	0.672004	0.055802	0.157
H96B	0.616058	0.662094	0.072077	0.157
H96C	0.687250	0.711823	0.064490	0.157
Br92	0.3524(4)	0.76516(7)	0.20539(11)	0.0615(7)
C91	0.149(3)	0.7263(7)	0.2097(9)	0.052(4)
Br29	0.4262(4)	0.23287(8)	0.25291(11)	0.0675(7)
C24	0.211(3)	0.2909(7)	0.3331(9)	0.050(3)
C25	0.220(3)	0.2508(7)	0.2966(10)	0.053(4)
O28	0.029(2)	0.2947(5)	0.3487(7)	0.059(3)
C26	0.022(3)	0.2331(8)	0.2983(10)	0.059(4)
H26	-0.026043	0.206247	0.279890	0.071
C27	-0.079(3)	0.2586(8)	0.3280(11)	0.062(4)
H27	-0.213560	0.253265	0.334968	0.075
C44	0.912(4)	0.5871(8)	0.6419(12)	0.068(6)
H44A	0.975685	0.558440	0.637160	0.102

H44B	0.989201	0.603373	0.675139	0.102
H44C	0.909171	0.603850	0.604069	0.102

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic displacement parameters [Å²] for S8. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si70	0.036(2)	0.030(2)	0.034(2)	−0.0072(18)	0.0136(17)	−0.0041(19)
Si43	0.048(3)	0.033(2)	0.039(2)	−0.0046(19)	0.0053(19)	−0.006(2)
Si52	0.059(3)	0.028(2)	0.047(3)	0.004(2)	0.017(2)	−0.007(2)
Si78	0.037(2)	0.027(2)	0.046(2)	0.0022(19)	0.0154(19)	−0.005(2)
Si5	0.042(3)	0.029(2)	0.046(2)	0.0043(19)	−0.0060(19)	−0.001(2)
Si33	0.044(3)	0.025(2)	0.042(2)	0.0018(18)	0.0062(18)	0.000(2)
O8	0.034(5)	0.024(5)	0.032(5)	0.010(4)	0.004(4)	−0.002(4)
O53	0.033(5)	0.020(4)	0.030(4)	0.002(4)	0.008(4)	−0.003(4)
O77	0.030(5)	0.025(5)	0.031(4)	0.002(4)	0.010(4)	−0.001(4)
O94	0.025(6)	0.031(6)	0.051(6)	−0.010(5)	0.005(5)	0.007(5)
O93	0.032(7)	0.043(7)	0.069(8)	−0.025(6)	0.006(5)	−0.006(6)
O17	0.041(6)	0.029(5)	0.040(5)	−0.008(4)	0.001(4)	0.000(5)
O57	0.024(5)	0.033(5)	0.041(5)	−0.011(4)	0.011(4)	0.001(4)
O32	0.046(6)	0.028(5)	0.033(5)	−0.002(4)	0.002(4)	−0.003(5)
O42	0.053(6)	0.029(5)	0.032(5)	−0.003(4)	0.010(4)	−0.007(5)
O69	0.051(6)	0.033(5)	0.028(5)	−0.002(4)	0.004(4)	0.006(5)
O31	0.042(6)	0.033(6)	0.046(6)	0.002(5)	−0.003(5)	−0.007(5)
O88	0.047(6)	0.040(6)	0.053(6)	−0.016(5)	0.007(5)	0.006(5)
O30	0.056(8)	0.041(7)	0.048(7)	−0.004(6)	0.016(6)	0.003(6)
C86	0.041(7)	0.033(7)	0.039(6)	−0.009(6)	0.000(6)	0.004(6)
C87	0.044(7)	0.036(6)	0.049(6)	−0.005(6)	−0.002(6)	0.007(6)
C60	0.025(6)	0.033(6)	0.028(6)	−0.003(5)	0.011(5)	−0.001(5)
C62	0.034(6)	0.023(5)	0.024(5)	0.005(5)	0.008(5)	0.001(5)
C63	0.033(6)	0.020(5)	0.020(5)	0.004(5)	0.006(5)	0.000(5)
C20	0.038(7)	0.025(6)	0.027(6)	−0.001(5)	0.010(5)	−0.005(6)
C18	0.040(6)	0.032(6)	0.036(6)	−0.002(5)	0.012(5)	−0.004(6)
C61	0.032(7)	0.032(6)	0.026(6)	0.002(5)	0.005(5)	0.003(6)
C10	0.035(6)	0.024(6)	0.030(5)	0.004(5)	0.002(5)	−0.002(5)
C55	0.032(5)	0.024(5)	0.020(5)	0.007(4)	0.006(4)	−0.002(5)
C64	0.034(6)	0.024(5)	0.021(5)	0.001(5)	0.005(5)	0.002(5)
C65	0.040(7)	0.034(7)	0.032(6)	0.008(6)	0.005(5)	0.006(6)
C66	0.037(7)	0.029(6)	0.033(6)	0.008(6)	0.006(5)	0.005(6)
C40	0.042(9)	0.028(8)	0.045(9)	0.005(7)	0.007(7)	0.000(7)
C54	0.031(6)	0.026(6)	0.023(5)	0.008(5)	0.008(5)	0.000(5)
C22	0.052(10)	0.035(9)	0.033(8)	−0.004(7)	0.015(7)	0.006(8)
C11	0.038(6)	0.029(6)	0.027(5)	0.006(5)	0.007(5)	−0.004(5)
C68	0.039(7)	0.031(6)	0.019(6)	−0.004(5)	0.002(5)	0.004(6)
C56	0.028(6)	0.023(6)	0.029(6)	0.003(5)	0.010(5)	0.005(5)
C46	0.054(8)	0.033(7)	0.041(7)	−0.004(6)	−0.002(6)	0.003(7)
C13	0.033(6)	0.031(6)	0.023(5)	0.004(5)	0.007(5)	−0.002(6)
C59	0.036(6)	0.022(5)	0.024(5)	−0.002(5)	0.009(5)	−0.003(5)
C83	0.066(12)	0.033(9)	0.049(10)	0.006(8)	0.010(8)	−0.015(9)
C14	0.033(6)	0.025(6)	0.032(5)	0.004(5)	0.001(5)	0.003(5)
C73	0.053(7)	0.032(7)	0.031(6)	−0.007(6)	0.023(6)	−0.013(6)
C85	0.032(8)	0.035(8)	0.042(8)	0.006(7)	0.013(6)	−0.013(7)
C16	0.040(6)	0.024(6)	0.034(6)	−0.006(5)	0.011(5)	0.001(6)
C19	0.034(6)	0.032(6)	0.029(6)	−0.002(5)	0.007(5)	−0.001(5)
C12	0.035(7)	0.033(7)	0.034(6)	0.003(6)	0.009(5)	−0.002(6)

C47	0.076(13)	0.053(11)	0.042(9)	−0.013(8)	0.007(9)	0.013(10)
C23	0.042(7)	0.034(7)	0.045(7)	−0.001(6)	0.008(6)	−0.002(6)
C41	0.048(7)	0.030(6)	0.027(6)	0.002(5)	0.009(5)	−0.002(6)
C51	0.067(9)	0.039(8)	0.062(8)	0.002(7)	0.014(7)	−0.004(8)
C74	0.067(12)	0.038(9)	0.051(10)	−0.012(8)	0.031(9)	−0.007(9)
C67	0.047(10)	0.025(8)	0.038(8)	−0.011(6)	0.000(7)	0.005(7)
C90	0.050(8)	0.049(8)	0.060(8)	−0.014(7)	−0.006(7)	0.018(7)
C7	0.062(12)	0.046(10)	0.060(11)	−0.007(9)	−0.014(9)	0.015(10)
C34	0.059(8)	0.041(8)	0.045(7)	−0.007(7)	−0.001(7)	−0.006(7)
C38	0.058(8)	0.030(7)	0.061(8)	0.006(7)	0.006(7)	0.005(7)
C9	0.038(6)	0.024(6)	0.029(5)	0.001(5)	0.006(5)	−0.003(5)
C76	0.051(10)	0.048(10)	0.030(8)	0.003(7)	0.009(7)	−0.008(8)
C6	0.048(10)	0.044(10)	0.048(9)	0.011(8)	0.014(8)	0.001(8)
C81	0.043(7)	0.031(7)	0.042(7)	0.000(6)	0.012(6)	−0.009(6)
C49	0.054(11)	0.040(9)	0.044(9)	−0.001(8)	0.000(8)	0.004(8)
C58	0.042(6)	0.030(6)	0.034(6)	−0.007(5)	0.002(5)	0.003(6)
C36	0.039(8)	0.030(7)	0.057(8)	0.000(6)	0.008(6)	0.002(6)
C4	0.039(10)	0.046(10)	0.053(10)	−0.014(8)	0.004(8)	0.004(8)
C21	0.042(7)	0.024(6)	0.027(6)	0.005(5)	0.008(5)	−0.005(6)
C75	0.080(13)	0.040(10)	0.049(10)	−0.002(8)	0.029(9)	0.001(9)
C2	0.045(7)	0.034(7)	0.055(7)	0.001(6)	0.000(6)	−0.001(6)
C39	0.057(11)	0.049(10)	0.056(10)	−0.003(9)	0.016(8)	−0.006(10)
C72	0.038(9)	0.054(11)	0.065(11)	−0.017(9)	0.013(8)	0.010(9)
C45	0.072(12)	0.029(9)	0.059(11)	0.004(8)	0.001(9)	−0.010(9)
C15	0.035(6)	0.025(5)	0.028(5)	0.001(5)	0.006(5)	−0.001(5)
C89	0.049(8)	0.047(7)	0.059(8)	−0.014(7)	0.003(7)	0.010(7)
C71	0.052(10)	0.029(8)	0.043(9)	−0.010(7)	0.010(7)	−0.014(8)
C50	0.079(13)	0.037(11)	0.073(12)	0.009(9)	0.015(10)	−0.003(10)
C35	0.071(13)	0.044(11)	0.058(11)	0.018(9)	0.010(9)	−0.009(10)
C82	0.067(13)	0.057(12)	0.060(11)	0.005(10)	0.001(10)	−0.008(10)
C84	0.059(11)	0.051(11)	0.046(9)	0.010(8)	0.025(8)	−0.004(9)
C37	0.048(11)	0.045(10)	0.065(11)	0.014(9)	0.011(9)	0.001(9)
C97	0.081(9)	0.041(8)	0.064(9)	0.003(7)	0.017(8)	−0.006(8)
C80	0.058(11)	0.045(11)	0.087(13)	0.024(10)	0.019(10)	−0.014(10)
C1	0.068(12)	0.036(9)	0.053(10)	0.007(8)	0.026(9)	0.011(9)
C48	0.087(14)	0.039(10)	0.043(10)	0.001(8)	−0.016(9)	−0.008(10)
C79	0.083(14)	0.049(11)	0.080(13)	−0.003(10)	0.055(11)	0.003(11)
C98	0.119(17)	0.060(13)	0.074(14)	−0.002(12)	−0.008(13)	−0.002(14)
C3	0.056(11)	0.042(10)	0.051(10)	0.003(8)	0.024(8)	−0.002(9)
C95	0.085(10)	0.044(8)	0.076(9)	0.007(8)	0.024(8)	−0.002(8)
C96	0.125(19)	0.063(14)	0.126(19)	0.026(15)	0.017(16)	−0.001(15)
Br92	0.0705(15)	0.0357(10)	0.0754(14)	−0.0099(10)	−0.0023(11)	0.0007(10)
C91	0.057(7)	0.040(7)	0.055(7)	−0.010(7)	−0.009(6)	0.017(7)
Br29	0.0858(17)	0.0460(12)	0.0717(15)	−0.0094(11)	0.0131(12)	0.0035(12)
C24	0.044(7)	0.041(7)	0.064(7)	−0.006(6)	0.010(6)	−0.001(6)
C25	0.047(7)	0.056(8)	0.057(8)	−0.005(7)	0.005(7)	−0.011(7)
O28	0.050(7)	0.048(7)	0.080(7)	−0.016(6)	0.012(6)	0.000(6)
C26	0.049(8)	0.054(8)	0.074(9)	−0.009(8)	0.010(7)	−0.011(8)
C27	0.049(8)	0.053(8)	0.086(9)	−0.014(8)	0.014(7)	−0.008(8)
C44	0.072(13)	0.055(12)	0.076(13)	−0.008(11)	0.004(11)	−0.010(11)

Table 4. Bond lengths and angles for S8.

Atom–Atom	Length [Å]
Si70–O69	1.633(12)
Si70–C73	1.871(17)

Si70–C72	1.842(19)
Si70–C71	1.854(18)
Si43–O42	1.649(12)
Si43–C46	1.862(19)
Si43–C45	1.88(2)
Si43–C44	1.87(2)
Si52–O53	1.666(11)
Si52–C51	1.88(2)
Si52–C97	1.95(2)
Si52–C95	1.84(2)
Si78–O77	1.662(11)
Si78–C81	1.874(19)
Si78–C80	1.89(2)
Si78–C79	1.83(2)
Si5–O8	1.669(11)
Si5–C7	1.83(2)
Si5–C6	1.897(19)
Si5–C2	1.86(2)
Si33–O32	1.681(12)
Si33–C34	1.87(2)
Si33–C38	1.87(2)
Si33–C36	1.885(19)
O8–C9	1.441(18)
O53–C54	1.415(17)
O77–C62	1.424(18)
O94–C56	1.165(18)
O93–C86	1.22(2)
O17–C18	1.43(2)
O17–C16	1.351(18)
O57–C56	1.393(18)
O57–C58	1.40(2)
O32–C14	1.427(18)
O42–C41	1.455(19)
O69–C68	1.452(17)
O31–C16	1.203(19)
O88–C87	1.36(2)
O88–C89	1.39(2)
O30–C23	1.21(2)
C86–C87	1.46(3)
C86–C58	1.55(2)
C87–C91	1.43(3)
C60–C61	1.32(2)
C60–C59	1.48(2)
C60–C85	1.49(2)
C62–H62	0.9800
C62–C63	1.535(19)
C62–C61	1.53(2)
C63–H63	0.9800
C63–C55	1.59(2)
C63–C64	1.574(19)
C20–C22	1.48(2)
C20–C19	1.56(2)
C20–C21	1.33(2)
C18–H18	0.9800
C18–C19	1.54(2)
C18–C23	1.52(2)

C61–H61	0.9300
C10–H10	0.9800
C10–C11	1.54(2)
C10–C9	1.54(2)
C10–C15	1.59(2)
C55–C54	1.540(19)
C55–C56	1.52(2)
C55–C59	1.55(2)
C64–C65	1.55(2)
C64–C68	1.55(2)
C64–C67	1.50(2)
C65–H65A	0.9700
C65–H65B	0.9700
C65–C66	1.49(2)
C66–H66A	0.9700
C66–H66B	0.9700
C66–C54	1.54(2)
C40–H40A	0.9600
C40–H40B	0.9600
C40–H40C	0.9600
C40–C11	1.53(2)
C54–H54	0.9800
C22–H22A	0.9600
C22–H22B	0.9600
C22–H22C	0.9600
C11–C12	1.55(2)
C11–C41	1.54(2)
C68–H68A	0.9700
C68–H68B	0.9700
C46–C47	1.56(3)
C46–C49	1.54(3)
C46–C48	1.52(3)
C13–H13A	0.9700
C13–H13B	0.9700
C13–C14	1.45(2)
C13–C12	1.52(2)
C59–H59	0.9800
C59–C58	1.56(2)
C83–H83A	0.9600
C83–H83B	0.9600
C83–H83C	0.9600
C83–C81	1.53(2)
C14–H14	0.9800
C14–C15	1.58(2)
C73–C74	1.57(2)
C73–C76	1.51(3)
C73–C75	1.54(3)
C85–H85A	0.9600
C85–H85B	0.9600
C85–H85C	0.9600
C16–C15	1.54(2)
C19–H19	0.9800
C19–C15	1.50(2)
C12–H12A	0.9700
C12–H12B	0.9700
C47–H47A	0.9600

C47–H47B	0.9600
C47–H47C	0.9600
C23–C24	1.44(3)
C41–H41A	0.9700
C41–H41B	0.9700
C51–H51A	0.9700
C51–H51B	0.9700
C51–C50	1.48(3)
C74–H74A	0.9600
C74–H74B	0.9600
C74–H74C	0.9600
C67–H67A	0.9600
C67–H67B	0.9600
C67–H67C	0.9600
C90–H90	0.9300
C90–C89	1.26(3)
C90–C91	1.46(3)
C7–H7A	0.9600
C7–H7B	0.9600
C7–H7C	0.9600
C34–H34A	0.9700
C34–H34B	0.9700
C34–C35	1.53(3)
C38–H38A	0.9700
C38–H38B	0.9700
C38–C39	1.51(3)
C9–H9	0.9800
C9–C21	1.49(2)
C76–H76A	0.9600
C76–H76B	0.9600
C76–H76C	0.9600
C6–H6A	0.9600
C6–H6B	0.9600
C6–H6C	0.9600
C81–C82	1.51(3)
C81–C84	1.55(3)
C49–H49A	0.9600
C49–H49B	0.9600
C49–H49C	0.9600
C58–H58	0.9800
C36–H36A	0.9700
C36–H36B	0.9700
C36–C37	1.50(3)
C4–H4A	0.9600
C4–H4B	0.9600
C4–H4C	0.9600
C4–C2	1.49(3)
C21–H21	0.9300
C75–H75A	0.9600
C75–H75B	0.9600
C75–H75C	0.9600
C2–C1	1.58(3)
C2–C3	1.55(3)
C39–H39A	0.9600
C39–H39B	0.9600
C39–H39C	0.9600

C72–H72A	0.9600
C72–H72B	0.9600
C72–H72C	0.9600
C45–H45A	0.9600
C45–H45B	0.9600
C45–H45C	0.9600
C89–H89	0.9300
C71–H71A	0.9600
C71–H71B	0.9600
C71–H71C	0.9600
C50–H50A	0.9600
C50–H50B	0.9600
C50–H50C	0.9600
C35–H35A	0.9600
C35–H35B	0.9600
C35–H35C	0.9600
C82–H82A	0.9600
C82–H82B	0.9600
C82–H82C	0.9600
C84–H84A	0.9600
C84–H84B	0.9600
C84–H84C	0.9600
C37–H37A	0.9600
C37–H37B	0.9600
C37–H37C	0.9600
C97–H97A	0.9700
C97–H97B	0.9700
C97–C98	1.45(4)
C80–H80A	0.9600
C80–H80B	0.9600
C80–H80C	0.9600
C1–H1A	0.9600
C1–H1B	0.9600
C1–H1C	0.9600
C48–H48A	0.9600
C48–H48B	0.9600
C48–H48C	0.9600
C79–H79A	0.9600
C79–H79B	0.9600
C79–H79C	0.9600
C98–H98A	0.9600
C98–H98B	0.9600
C98–H98C	0.9600
C3–H3A	0.9600
C3–H3B	0.9600
C3–H3C	0.9600
C95–H95A	0.9700
C95–H95B	0.9700
C95–C96	1.38(4)
C96–H96A	0.9600
C96–H96B	0.9600
C96–H96C	0.9600
Br92–C91	1.78(2)
Br29–C25	1.83(2)
C24–C25	1.44(3)
C24–O28	1.29(2)

C25–C26	1.42(3)
O28–C27	1.34(2)
C26–H26	0.9300
C26–C27	1.24(3)
C27–H27	0.9300
C44–H44A	0.9600
C44–H44B	0.9600
C44–H44C	0.9600

Atom–Atom–Atom	**Angle [°]**
O69–Si70–C73	104.6(7)
O69–Si70–C72	108.6(8)
O69–Si70–C71	112.3(7)
C72–Si70–C73	113.1(9)
C72–Si70–C71	107.4(10)
C71–Si70–C73	110.9(8)
O42–Si43–C46	104.2(7)
O42–Si43–C45	109.6(8)
O42–Si43–C44	113.5(9)
C46–Si43–C45	113.6(9)
C46–Si43–C44	110.0(10)
C44–Si43–C45	106.2(11)
O53–Si52–C51	104.6(8)
O53–Si52–C97	109.5(8)
O53–Si52–C95	115.0(9)
C51–Si52–C97	106.0(10)
C95–Si52–C51	112.4(11)
C95–Si52–C97	109.0(11)
O77–Si78–C81	106.2(7)
O77–Si78–C80	108.8(7)
O77–Si78–C79	110.7(8)
C81–Si78–C80	111.0(9)
C79–Si78–C81	110.4(10)
C79–Si78–C80	109.7(12)
O8–Si5–C7	111.1(8)
O8–Si5–C6	108.8(7)
O8–Si5–C2	107.6(7)
C7–Si5–C6	108.6(10)
C7–Si5–C2	111.4(9)
C2–Si5–C6	109.2(9)
O32–Si33–C34	111.4(8)
O32–Si33–C38	105.0(7)
O32–Si33–C36	110.7(7)
C34–Si33–C38	108.1(9)
C34–Si33–C36	110.8(9)
C38–Si33–C36	110.8(9)
C9–O8–Si5	123.0(9)
C54–O53–Si52	126.9(9)
C62–O77–Si78	124.2(10)
C16–O17–C18	113.2(12)
C56–O57–C58	112.2(11)
C14–O32–Si33	123.8(9)
C41–O42–Si43	124.9(10)
C68–O69–Si70	123.4(10)
C87–O88–C89	104.8(15)
O93–C86–C87	121.2(16)

O93–C86–C58	121.1(15)
C87–C86–C58	117.5(16)
O88–C87–C86	119.2(16)
O88–C87–C91	111.4(17)
C91–C87–C86	129.4(19)
C61–C60–C59	120.6(13)
C61–C60–C85	123.2(14)
C59–C60–C85	116.0(14)
O77–C62–H62	108.7
O77–C62–C63	114.4(12)
O77–C62–C61	109.2(12)
C63–C62–H62	108.7
C61–C62–H62	108.7
C61–C62–C63	107.0(12)
C62–C63–H63	104.7
C62–C63–C55	106.3(11)
C62–C63–C64	118.1(12)
C55–C63–H63	104.7
C64–C63–H63	104.7
C64–C63–C55	116.9(11)
C22–C20–C19	116.3(14)
C21–C20–C22	125.6(14)
C21–C20–C19	118.0(13)
O17–C18–H18	106.5
O17–C18–C19	104.9(12)
O17–C18–C23	116.1(14)
C19–C18–H18	106.5
C23–C18–H18	106.5
C23–C18–C19	115.5(15)
C60–C61–C62	121.3(14)
C60–C61–H61	119.4
C62–C61–H61	119.4
C11–C10–H10	104.3
C11–C10–C9	121.7(13)
C11–C10–C15	117.1(12)
C9–C10–H10	104.3
C9–C10–C15	103.2(12)
C15–C10–H10	104.3
C54–C55–C63	109.6(11)
C54–C55–C59	111.0(12)
C56–C55–C63	114.2(12)
C56–C55–C54	107.3(11)
C56–C55–C59	105.3(12)
C59–C55–C63	109.4(11)
C65–C64–C63	106.5(12)
C68–C64–C63	106.4(11)
C68–C64–C65	104.1(12)
C67–C64–C63	117.4(12)
C67–C64–C65	111.0(13)
C67–C64–C68	110.5(12)
C64–C65–H65A	108.5
C64–C65–H65B	108.5
H65A–C65–H65B	107.5
C66–C65–C64	115.0(13)
C66–C65–H65A	108.5
C66–C65–H65B	108.5

C65–C66–H66A	109.3
C65–C66–H66B	109.3
C65–C66–C54	111.5(13)
H66A–C66–H66B	108.0
C54–C66–H66A	109.3
C54–C66–H66B	109.3
H40A–C40–H40B	109.5
H40A–C40–H40C	109.5
H40B–C40–H40C	109.5
C11–C40–H40A	109.5
C11–C40–H40B	109.5
C11–C40–H40C	109.5
O53–C54–C55	107.5(11)
O53–C54–C66	113.4(12)
O53–C54–H54	107.8
C55–C54–H54	107.8
C66–C54–C55	112.3(12)
C66–C54–H54	107.8
C20–C22–H22A	109.5
C20–C22–H22B	109.5
C20–C22–H22C	109.5
H22A–C22–H22B	109.5
H22A–C22–H22C	109.5
H22B–C22–H22C	109.5
C10–C11–C12	110.4(13)
C10–C11–C41	106.4(12)
C40–C11–C10	117.2(13)
C40–C11–C12	109.6(12)
C40–C11–C41	106.8(13)
C41–C11–C12	105.6(12)
O69–C68–C64	109.7(11)
O69–C68–H68A	109.7
O69–C68–H68B	109.7
C64–C68–H68A	109.7
C64–C68–H68B	109.7
H68A–C68–H68B	108.2
O94–C56–O57	118.5(13)
O94–C56–C55	132.0(14)
O57–C56–C55	109.5(12)
C47–C46–Si43	110.2(12)
C49–C46–Si43	109.9(13)
C49–C46–C47	108.9(16)
C48–C46–Si43	111.7(13)
C48–C46–C47	107.9(16)
C48–C46–C49	108.2(15)
H13A–C13–H13B	107.6
C14–C13–H13A	108.7
C14–C13–H13B	108.7
C14–C13–C12	114.1(13)
C12–C13–H13A	108.7
C12–C13–H13B	108.7
C60–C59–C55	117.8(13)
C60–C59–H59	109.1
C60–C59–C58	108.3(12)
C55–C59–H59	109.1
C55–C59–C58	103.2(12)

C58–C59–H59	109.1
H83A–C83–H83B	109.5
H83A–C83–H83C	109.5
H83B–C83–H83C	109.5
C81–C83–H83A	109.5
C81–C83–H83B	109.5
C81–C83–H83C	109.5
O32–C14–C13	114.5(13)
O32–C14–H14	108.3
O32–C14–C15	105.6(11)
C13–C14–H14	108.3
C13–C14–C15	111.7(13)
C15–C14–H14	108.3
C74–C73–Si70	110.5(13)
C76–C73–Si70	109.9(10)
C76–C73–C74	110.2(15)
C76–C73–C75	107.7(16)
C75–C73–Si70	109.7(12)
C75–C73–C74	108.8(13)
C60–C85–H85A	109.5
C60–C85–H85B	109.5
C60–C85–H85C	109.5
H85A–C85–H85B	109.5
H85A–C85–H85C	109.5
H85B–C85–H85C	109.5
O17–C16–C15	110.8(12)
O31–C16–O17	119.9(15)
O31–C16–C15	129.3(14)
C20–C19–H19	108.8
C18–C19–C20	106.9(12)
C18–C19–H19	108.8
C15–C19–C20	114.9(13)
C15–C19–C18	108.4(13)
C15–C19–H19	108.8
C11–C12–H12A	109.2
C11–C12–H12B	109.2
C13–C12–C11	112.1(13)
C13–C12–H12A	109.2
C13–C12–H12B	109.2
H12A–C12–H12B	107.9
C46–C47–H47A	109.5
C46–C47–H47B	109.5
C46–C47–H47C	109.5
H47A–C47–H47B	109.5
H47A–C47–H47C	109.5
H47B–C47–H47C	109.5
O30–C23–C18	117.8(16)
O30–C23–C24	120.7(17)
C24–C23–C18	121.4(16)
O42–C41–C11	109.4(12)
O42–C41–H41A	109.8
O42–C41–H41B	109.8
C11–C41–H41A	109.8
C11–C41–H41B	109.8
H41A–C41–H41B	108.2
Si52–C51–H51A	108.7

Si52–C51–H51B	108.7
H51A–C51–H51B	107.6
C50–C51–Si52	114.3(15)
C50–C51–H51A	108.7
C50–C51–H51B	108.7
C73–C74–H74A	109.5
C73–C74–H74B	109.5
C73–C74–H74C	109.5
H74A–C74–H74B	109.5
H74A–C74–H74C	109.5
H74B–C74–H74C	109.5
C64–C67–H67A	109.5
C64–C67–H67B	109.5
C64–C67–H67C	109.5
H67A–C67–H67B	109.5
H67A–C67–H67C	109.5
H67B–C67–H67C	109.5
C89–C90–H90	124.9
C89–C90–C91	110.1(19)
C91–C90–H90	124.9
Si5–C7–H7A	109.5
Si5–C7–H7B	109.5
Si5–C7–H7C	109.5
H7A–C7–H7B	109.5
H7A–C7–H7C	109.5
H7B–C7–H7C	109.5
Si33–C34–H34A	108.7
Si33–C34–H34B	108.7
H34A–C34–H34B	107.6
C35–C34–Si33	114.0(14)
C35–C34–H34A	108.7
C35–C34–H34B	108.7
Si33–C38–H38A	108.6
Si33–C38–H38B	108.6
H38A–C38–H38B	107.6
C39–C38–Si33	114.7(14)
C39–C38–H38A	108.6
C39–C38–H38B	108.6
O8–C9–C10	113.0(12)
O8–C9–H9	108.6
O8–C9–C21	110.8(12)
C10–C9–H9	108.6
C21–C9–C10	107.1(13)
C21–C9–H9	108.6
C73–C76–H76A	109.5
C73–C76–H76B	109.5
C73–C76–H76C	109.5
H76A–C76–H76B	109.5
H76A–C76–H76C	109.5
H76B–C76–H76C	109.5
Si5–C6–H6A	109.5
Si5–C6–H6B	109.5
Si5–C6–H6C	109.5
H6A–C6–H6B	109.5
H6A–C6–H6C	109.5
H6B–C6–H6C	109.5

C83–C81–Si78	109.4(13)
C83–C81–C84	109.5(15)
C82–C81–Si78	111.4(14)
C82–C81–C83	109.5(16)
C82–C81–C84	108.6(17)
C84–C81–Si78	108.5(13)
C46–C49–H49A	109.5
C46–C49–H49B	109.5
C46–C49–H49C	109.5
H49A–C49–H49B	109.5
H49A–C49–H49C	109.5
H49B–C49–H49C	109.5
O57–C58–C86	111.3(13)
O57–C58–C59	109.0(12)
O57–C58–H58	107.5
C86–C58–C59	113.8(14)
C86–C58–H58	107.5
C59–C58–H58	107.5
Si33–C36–H36A	108.6
Si33–C36–H36B	108.6
H36A–C36–H36B	107.6
C37–C36–Si33	114.7(13)
C37–C36–H36A	108.6
C37–C36–H36B	108.6
H4A–C4–H4B	109.5
H4A–C4–H4C	109.5
H4B–C4–H4C	109.5
C2–C4–H4A	109.5
C2–C4–H4B	109.5
C2–C4–H4C	109.5
C20–C21–C9	122.9(14)
C20–C21–H21	118.6
C9–C21–H21	118.6
C73–C75–H75A	109.5
C73–C75–H75B	109.5
C73–C75–H75C	109.5
H75A–C75–H75B	109.5
H75A–C75–H75C	109.5
H75B–C75–H75C	109.5
C4–C2–Si5	111.2(13)
C4–C2–C1	107.0(16)
C4–C2–C3	111.0(16)
C1–C2–Si5	109.2(13)
C3–C2–Si5	110.0(13)
C3–C2–C1	108.3(16)
C38–C39–H39A	109.5
C38–C39–H39B	109.5
C38–C39–H39C	109.5
H39A–C39–H39B	109.5
H39A–C39–H39C	109.5
H39B–C39–H39C	109.5
Si70–C72–H72A	109.5
Si70–C72–H72B	109.5
Si70–C72–H72C	109.5
H72A–C72–H72B	109.5
H72A–C72–H72C	109.5

H72B–C72–H72C	109.5
Si43–C45–H45A	109.5
Si43–C45–H45B	109.5
Si43–C45–H45C	109.5
H45A–C45–H45B	109.5
H45A–C45–H45C	109.5
H45B–C45–H45C	109.5
C14–C15–C10	110.5(12)
C16–C15–C10	115.1(13)
C16–C15–C14	105.7(12)
C19–C15–C10	113.7(13)
C19–C15–C14	109.4(13)
C19–C15–C16	101.9(12)
O88–C89–H89	123.5
C90–C89–O88	112.9(18)
C90–C89–H89	123.5
Si70–C71–H71A	109.5
Si70–C71–H71B	109.5
Si70–C71–H71C	109.5
H71A–C71–H71B	109.5
H71A–C71–H71C	109.5
H71B–C71–H71C	109.5
C51–C50–H50A	109.5
C51–C50–H50B	109.5
C51–C50–H50C	109.5
H50A–C50–H50B	109.5
H50A–C50–H50C	109.5
H50B–C50–H50C	109.5
C34–C35–H35A	109.5
C34–C35–H35B	109.5
C34–C35–H35C	109.5
H35A–C35–H35B	109.5
H35A–C35–H35C	109.5
H35B–C35–H35C	109.5
C81–C82–H82A	109.5
C81–C82–H82B	109.5
C81–C82–H82C	109.5
H82A–C82–H82B	109.5
H82A–C82–H82C	109.5
H82B–C82–H82C	109.5
C81–C84–H84A	109.5
C81–C84–H84B	109.5
C81–C84–H84C	109.5
H84A–C84–H84B	109.5
H84A–C84–H84C	109.5
H84B–C84–H84C	109.5
C36–C37–H37A	109.5
C36–C37–H37B	109.5
C36–C37–H37C	109.5
H37A–C37–H37B	109.5
H37A–C37–H37C	109.5
H37B–C37–H37C	109.5
Si52–C97–H97A	108.9
Si52–C97–H97B	108.9
H97A–C97–H97B	107.7
C98–C97–Si52	113.3(17)

C98–C97–H97A	108.9
C98–C97–H97B	108.9
Si78–C80–H80A	109.5
Si78–C80–H80B	109.5
Si78–C80–H80C	109.5
H80A–C80–H80B	109.5
H80A–C80–H80C	109.5
H80B–C80–H80C	109.5
C2–C1–H1A	109.5
C2–C1–H1B	109.5
C2–C1–H1C	109.5
H1A–C1–H1B	109.5
H1A–C1–H1C	109.5
H1B–C1–H1C	109.5
C46–C48–H48A	109.5
C46–C48–H48B	109.5
C46–C48–H48C	109.5
H48A–C48–H48B	109.5
H48A–C48–H48C	109.5
H48B–C48–H48C	109.5
Si78–C79–H79A	109.5
Si78–C79–H79B	109.5
Si78–C79–H79C	109.5
H79A–C79–H79B	109.5
H79A–C79–H79C	109.5
H79B–C79–H79C	109.5
C97–C98–H98A	109.5
C97–C98–H98B	109.5
C97–C98–H98C	109.5
H98A–C98–H98B	109.5
H98A–C98–H98C	109.5
H98B–C98–H98C	109.5
C2–C3–H3A	109.5
C2–C3–H3B	109.5
C2–C3–H3C	109.5
H3A–C3–H3B	109.5
H3A–C3–H3C	109.5
H3B–C3–H3C	109.5
Si52–C95–H95A	110.4
Si52–C95–H95B	110.4
H95A–C95–H95B	108.6
C96–C95–Si52	106(2)
C96–C95–H95A	110.4
C96–C95–H95B	110.4
C95–C96–H96A	109.5
C95–C96–H96B	109.5
C95–C96–H96C	109.5
H96A–C96–H96B	109.5
H96A–C96–H96C	109.5
H96B–C96–H96C	109.5
C87–C91–C90	100.7(18)
C87–C91–Br92	131.6(16)
C90–C91–Br92	127.6(15)
C25–C24–C23	129.3(18)
O28–C24–C23	121.6(17)
O28–C24–C25	108.8(17)

C24–C25–Br29	127.8(15)
C26–C25–Br29	130.8(16)
C26–C25–C24	101.1(18)
C24–O28–C27	108.6(16)
C25–C26–H26	125.0
C27–C26–C25	110(2)
C27–C26–H26	125.0
O28–C27–H27	124.3
C26–C27–O28	111(2)
C26–C27–H27	124.3
Si43–C44–H44A	109.5
Si43–C44–H44B	109.5
Si43–C44–H44C	109.5
H44A–C44–H44B	109.5
H44A–C44–H44C	109.5
H44B–C44–H44C	109.5

Table 5. Torsion angles for S8.

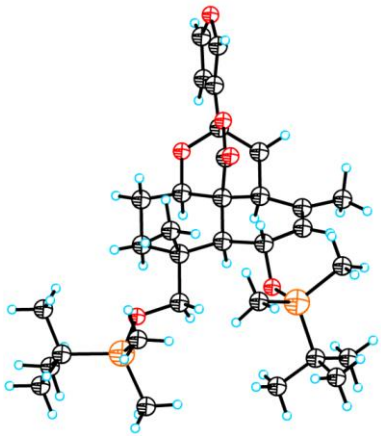
Atom–Atom–Atom–Atom	Torsion Angle [°]
Si70–O69–C68–C64	−178.5(10)
Si43–O42–C41–C11	−178.6(11)
Si52–O53–C54–C55	155.8(10)
Si52–O53–C54–C66	−79.5(15)
Si78–O77–C62–C63	−147.5(10)
Si78–O77–C62–C61	92.6(14)
Si5–O8–C9–C10	−174.0(10)
Si5–O8–C9–C21	65.8(16)
Si33–O32–C14–C13	−75.9(16)
Si33–O32–C14–C15	160.8(10)
O8–Si5–C2–C4	50.5(15)
O8–Si5–C2–C1	168.4(12)
O8–Si5–C2–C3	−72.9(13)
O8–C9–C21–C20	161.8(15)
O53–Si52–C51–C50	−179.5(16)
O53–Si52–C95–C96	−68(2)
O77–Si78–C81–C83	−178.5(11)
O77–Si78–C81–C82	60.4(14)
O77–Si78–C81–C84	−59.1(13)
O77–C62–C63–C55	172.9(12)
O77–C62–C63–C64	39.3(18)
O77–C62–C61–C60	159.2(14)
O93–C86–C87–O88	−172.1(16)
O93–C86–C87–C91	9(3)
O93–C86–C58–O57	−137.8(16)
O93–C86–C58–C59	−14(2)
O17–C18–C19–C20	−117.1(13)
O17–C18–C19–C15	7.3(17)
O17–C18–C23–O30	−153.1(15)
O17–C18–C23–C24	31(2)
O17–C16–C15–C10	130.2(13)
O17–C16–C15–C14	−107.7(14)
O17–C16–C15–C19	6.7(17)
O32–Si33–C34–C35	174.2(13)
O32–Si33–C38–C39	−72.3(15)
O32–Si33–C36–C37	80.1(15)

O32–C14–C15–C10	174.0(12)
O32–C14–C15–C16	49.0(15)
O32–C14–C15–C19	−60.1(16)
O42–Si43–C46–C47	−65.7(14)
O42–Si43–C46–C49	54.2(14)
O42–Si43–C46–C48	174.3(14)
O69–Si70–C73–C74	168.2(11)
O69–Si70–C73–C76	−70.0(13)
O69–Si70–C73–C75	48.3(14)
O31–C16–C15–C10	−50(2)
O31–C16–C15–C14	72(2)
O31–C16–C15–C19	−173.5(17)
O88–C87–C91–C90	2.3(19)
O88–C87–C91–Br92	−179.1(14)
O30–C23–C24–C25	−18(3)
O30–C23–C24–O28	169.9(18)
C86–C87–C91–C90	−178.7(17)
C86–C87–C91–Br92	0(3)
C87–O88–C89–C90	0(2)
C87–C86–C58–O57	47(2)
C87–C86–C58–C59	170.8(14)
C60–C59–C58–O57	−121.0(14)
C60–C59–C58–C86	114.0(15)
C62–C63–C55–C54	176.7(12)
C62–C63–C55–C56	−63.0(15)
C62–C63–C55–C59	54.8(15)
C62–C63–C64–C65	177.7(13)
C62–C63–C64–C68	−71.7(16)
C62–C63–C64–C67	52.6(18)
C63–C62–C61–C60	34.8(19)
C63–C55–C54–O53	175.6(12)
C63–C55–C54–C66	50.2(16)
C63–C55–C56–O94	−51(2)
C63–C55–C56–O57	129.1(12)
C63–C55–C59–C60	−11.8(18)
C63–C55–C59–C58	−131.0(13)
C63–C64–C65–C66	−54.0(17)
C63–C64–C68–O69	−168.7(12)
C20–C19–C15–C10	−13.2(19)
C20–C19–C15–C14	−137.2(14)
C20–C19–C15–C16	111.2(14)
C18–O17–C16–O31	177.8(15)
C18–O17–C16–C15	−2.4(18)
C18–C19–C15–C10	−132.6(14)
C18–C19–C15–C14	103.3(15)
C18–C19–C15–C16	−8.2(17)
C18–C23–C24–C25	157.5(19)
C18–C23–C24–O28	−15(3)
C61–C60–C59–C55	−23(2)
C61–C60–C59–C58	93.6(17)
C61–C62–C63–C55	−66.1(15)
C61–C62–C63–C64	160.4(13)
C10–C11–C12–C13	−49.4(17)
C10–C11–C41–O42	−171.7(13)
C10–C9–C21–C20	38(2)
C55–C63–C64–C65	48.9(16)

C55–C63–C64–C68	159.6(13)
C55–C63–C64–C67	−76.1(17)
C55–C59–C58–O57	4.5(16)
C55–C59–C58–C86	−120.4(14)
C64–C63–C55–C54	−49.1(17)
C64–C63–C55–C56	71.2(15)
C64–C63–C55–C59	−171.0(12)
C64–C65–C66–C54	60.1(18)
C65–C64–C68–O69	−56.4(16)
C65–C66–C54–O53	−179.1(13)
C65–C66–C54–C55	−57.0(17)
C40–C11–C12–C13	81.1(16)
C40–C11–C41–O42	62.4(16)
C54–C55–C56–O94	70(2)
C54–C55–C56–O57	−109.3(13)
C54–C55–C59–C60	−132.8(14)
C54–C55–C59–C58	107.9(14)
C22–C20–C19–C18	−78.4(18)
C22–C20–C19–C15	161.3(14)
C22–C20–C21–C9	−174.4(15)
C11–C10–C9–O8	36(2)
C11–C10–C9–C21	158.4(14)
C11–C10–C15–C14	−43.4(18)
C11–C10–C15–C16	76.1(17)
C11–C10–C15–C19	−166.9(14)
C68–C64–C65–C66	−166.3(14)
C56–O57–C58–C86	127.4(14)
C56–O57–C58–C59	1.0(17)
C56–C55–C54–O53	51.1(15)
C56–C55–C54–C66	−74.2(15)
C56–C55–C59–C60	111.4(14)
C56–C55–C59–C58	−7.9(15)
C46–Si43–O42–C41	−169.3(13)
C13–C14–C15–C10	48.9(17)
C13–C14–C15–C16	−76.1(15)
C13–C14–C15–C19	174.8(13)
C59–C60–C61–C62	11(2)
C59–C55–C54–O53	−63.4(15)
C59–C55–C54–C66	171.2(12)
C59–C55–C56–O94	−171.4(16)
C59–C55–C56–O57	9.0(15)
C14–C13–C12–C11	59.8(18)
C73–Si70–O69–C68	−170.7(12)
C85–C60–C61–C62	−173.8(14)
C85–C60–C59–C55	161.6(13)
C85–C60–C59–C58	−81.9(16)
C16–O17–C18–C19	−3.0(17)
C16–O17–C18–C23	125.9(16)
C19–C20–C21–C9	9(2)
C19–C18–C23–O30	−30(2)
C19–C18–C23–C24	154.9(16)
C12–C11–C41–O42	−54.3(16)
C12–C13–C14–O32	−178.9(13)
C12–C13–C14–C15	−58.9(17)
C23–C18–C19–C20	113.7(15)
C23–C18–C19–C15	−122.0(15)

C23–C24–C25–Br29	−3(3)
C23–C24–C25–C26	−176(2)
C23–C24–O28–C27	177.0(19)
C41–C11–C12–C13	−164.1(13)
C51–Si52–O53–C54	−171.8(13)
C51–Si52–C95–C96	51(2)
C67–C64–C65–C66	74.8(17)
C67–C64–C68–O69	62.8(16)
C7–Si5–O8–C9	14.3(15)
C7–Si5–C2–C4	172.5(14)
C7–Si5–C2–C1	−69.6(16)
C7–Si5–C2–C3	49.2(16)
C34–Si33–O32–C14	86.3(13)
C34–Si33–C38–C39	46.7(17)
C34–Si33–C36–C37	−44.0(16)
C38–Si33–O32–C14	−157.0(13)
C38–Si33–C34–C35	59.4(16)
C38–Si33–C36–C37	−163.9(13)
C9–C10–C11–C40	46(2)
C9–C10–C11–C12	172.2(13)
C9–C10–C11–C41	−73.6(18)
C9–C10–C15–C14	180.0(12)
C9–C10–C15–C16	−60.5(16)
C9–C10–C15–C19	56.6(16)
C6–Si5–O8–C9	−105.3(13)
C6–Si5–C2–C4	−67.5(16)
C6–Si5–C2–C1	50.4(15)
C6–Si5–C2–C3	169.1(13)
C81–Si78–O77–C62	−145.3(11)
C58–O57–C56–O94	173.9(14)
C58–O57–C56–C55	−6.4(16)
C58–C86–C87–O88	3(2)
C58–C86–C87–C91	−176.0(17)
C36–Si33–O32–C14	−37.4(14)
C36–Si33–C34–C35	−62.1(16)
C36–Si33–C38–C39	168.2(14)
C21–C20–C19–C18	98.6(16)
C21–C20–C19–C15	−22(2)
C2–Si5–O8–C9	136.5(12)
C72–Si70–O69–C68	−49.7(15)
C72–Si70–C73–C74	50.2(15)
C72–Si70–C73–C76	172.0(13)
C72–Si70–C73–C75	−69.7(15)
C45–Si43–O42–C41	68.9(15)
C45–Si43–C46–C47	53.4(15)
C45–Si43–C46–C49	173.4(13)
C45–Si43–C46–C48	−66.5(17)
C15–C10–C11–C40	−82.4(18)
C15–C10–C11–C12	44.0(18)
C15–C10–C11–C41	158.2(13)
C15–C10–C9–O8	170.1(13)
C15–C10–C9–C21	−67.6(15)
C89–O88–C87–C86	179.2(16)
C89–O88–C87–C91	−1.8(19)
C89–C90–C91–C87	−2(2)
C89–C90–C91–Br92	179.3(16)

C71–Si70–O69–C68	68.9(14)
C71–Si70–C73–C74	−70.5(13)
C71–Si70–C73–C76	51.3(15)
C71–Si70–C73–C75	169.6(13)
C97–Si52–O53–C54	75.1(14)
C97–Si52–C51–C50	−63.8(19)
C97–Si52–C95–C96	168.3(19)
C80–Si78–O77–C62	95.1(13)
C80–Si78–C81–C83	−60.3(15)
C80–Si78–C81–C82	178.5(14)
C80–Si78–C81–C84	59.0(15)
C79–Si78–O77–C62	−25.5(15)
C79–Si78–C81–C83	61.5(15)
C79–Si78–C81–C82	−59.7(17)
C79–Si78–C81–C84	−179.1(13)
C95–Si52–O53–C54	−48.0(15)
C95–Si52–C51–C50	55(2)
C91–C90–C89–O88	1(2)
Br29–C25–C26–C27	−171.5(19)
C24–C25–C26–C27	2(3)
C24–O28–C27–C26	−2(3)
C25–C24–O28–C27	3(2)
C25–C26–C27–O28	0(3)
O28–C24–C25–Br29	170.3(15)
O28–C24–C25–C26	−3(2)
C44–Si43–O42–C41	−49.6(16)
C44–Si43–C46–C47	172.3(14)
C44–Si43–C46–C49	−67.8(15)
C44–Si43–C46–C48	52.3(17)



S9

Table 1. Crystal data and structure refinement for compound S9

CCDC number	2447366
Empirical formula	$C_{32}H_{52}O_6Si_2$
Formula weight	588.93
Temperature/K	99.9(8)
Crystal system	monoclinic
Space group	C2
a/Å	26.0796(5)
b/Å	6.41310(10)
c/Å	21.5662(4)
α/°	90
β/°	110.592(2)
γ/°	90
Volume/Å^3	3376.52(11)
Z	4
ρ_{calc}g/cm^3	1.194
μ/mm^{-1}	1.301
F(000)	1320.0
Crystal size/mm^3	0.3 × 0.03 × 0.02
Radiation	Cu Kα (λ = 1.54178)
2θ range for data collection/°	4.376 to 147.408
Index ranges	-30 ≤ h ≤ 32, -7 ≤ k ≤ 7, -25 ≤ l ≤ 26
Reflections collected	20670
Independent reflections	6551 [R_{int} = 0.0482, R_{sigma} = 0.0487]
Data/restraints/parameters	6551/1/373
Goodness-of-fit on F^2	1.067
Final R indexes [I>=2σ (I)]	R_1 = 0.0469, wR_2 = 0.1213
Final R indexes [all data]	R_1 = 0.0511, wR_2 = 0.1240
Largest diff. peak/hole / e Å^{-3}	0.42/-0.29
Flack parameter	-0.02(2)

Table 2. Atomic coordinates and U_{eq} [Å^2] for S9.

Atom	*x*	*y*	*z*	U_{eq}
Si01	0.37204(4)	0.73200(15)	0.11957(5)	0.0344(2)
Si02	0.19348(4)	0.86151(15)	0.20875(5)	0.0349(2)

O003	0.42120(9)	0.3048(4)	0.48564(11)	0.0331(5)
O004	0.34981(9)	0.8425(4)	0.43658(11)	0.0331(5)
O005	0.37694(10)	0.6205(4)	0.18972(12)	0.0384(6)
O006	0.38283(9)	0.6004(4)	0.51316(11)	0.0305(5)
O007	0.23464(9)	0.6683(4)	0.24688(11)	0.0332(5)
O008	0.46004(12)	0.3621(7)	0.70131(14)	0.0619(9)
C009	0.31991(13)	0.5365(5)	0.32657(16)	0.0280(6)
H009	0.306109	0.401796	0.303320	0.034
C00A	0.35872(12)	0.6599(5)	0.44924(16)	0.0282(6)
C00B	0.38855(13)	0.3745(6)	0.52087(16)	0.0314(7)
C00C	0.26778(13)	0.6670(5)	0.31613(15)	0.0297(7)
H00C	0.278281	0.813035	0.331640	0.036
C00D	0.36155(13)	0.6184(5)	0.29463(16)	0.0300(7)
C00E	0.34518(12)	0.4768(5)	0.40088(16)	0.0260(6)
C00F	0.41835(13)	0.3303(6)	0.59230(17)	0.0358(8)
C00G	0.39766(12)	0.3464(5)	0.41555(16)	0.0298(6)
H00G	0.387366	0.210013	0.391966	0.036
C00H	0.41325(14)	0.4786(6)	0.31701(18)	0.0348(7)
H00A	0.403398	0.339751	0.296131	0.042
H00B	0.440886	0.540349	0.300622	0.042
C00I	0.44228(15)	0.6936(6)	0.11530(17)	0.0364(8)
C00J	0.33102(13)	0.2845(5)	0.49455(16)	0.0300(7)
H00D	0.308593	0.346317	0.518550	0.036
H00E	0.332423	0.131750	0.501494	0.036
C00K	0.33551(14)	0.5973(6)	0.21855(17)	0.0345(7)
H00F	0.317883	0.458951	0.206960	0.041
H00H	0.307031	0.705594	0.200847	0.041
C00L	0.23312(13)	0.5745(6)	0.35280(17)	0.0323(7)
H00L	0.197296	0.629790	0.342562	0.039
C00M	0.24787(13)	0.4241(5)	0.39773(16)	0.0303(7)
C00N	0.43899(14)	0.4501(6)	0.39178(17)	0.0349(7)
H00I	0.472298	0.362752	0.402721	0.042
H00J	0.449528	0.587221	0.413655	0.042
C00O	0.37907(14)	0.8455(5)	0.31099(17)	0.0331(7)
H00K	0.346473	0.933953	0.300590	0.050
H00M	0.400983	0.890371	0.284649	0.050
H00N	0.400977	0.857759	0.358215	0.050
C00P	0.44742(17)	0.7983(7)	0.05396(18)	0.0449(9)
H00O	0.419505	0.741983	0.014060	0.067
H00P	0.483898	0.770950	0.052347	0.067
H00Q	0.442147	0.949052	0.056216	0.067
C00Q	0.30505(12)	0.3340(5)	0.41980(15)	0.0271(6)
H00R	0.302725	0.199552	0.395483	0.033
C00R	0.14434(14)	0.7391(7)	0.13211(18)	0.0403(8)
C00S	0.20816(14)	0.3225(6)	0.42492(17)	0.0361(7)
H00S	0.220005	0.347534	0.472733	0.054
H00T	0.207069	0.172064	0.416542	0.054
H00U	0.171565	0.381753	0.403181	0.054
C00T	0.43230(16)	0.4610(8)	0.64403(19)	0.0473(10)
H00V	0.423722	0.605491	0.640821	0.057
C00U	0.45422(16)	0.4594(7)	0.1145(2)	0.0473(9)
H00W	0.449987	0.392577	0.153243	0.071
H00X	0.491786	0.439305	0.115573	0.071
H00Y	0.428504	0.396750	0.074009	0.071
C00V	0.17606(18)	0.6380(8)	0.0917(2)	0.0511(10)
H00Z	0.197658	0.744610	0.079430	0.077

H	0.150120	0.574739	0.051539	0.077
HA	0.200585	0.530149	0.118469	0.077
C00W	0.31803(15)	0.6056(8)	0.0487(2)	0.0488(10)
H00	0.325846	0.456283	0.048285	0.073
HB	0.317519	0.669066	0.007141	0.073
HC	0.282280	0.625032	0.053339	0.073
C00X	0.48584(18)	0.7897(8)	0.1769(2)	0.0534(11)
H1	0.479032	0.939553	0.178414	0.080
HD	0.522316	0.767623	0.174649	0.080
HE	0.483861	0.722937	0.216901	0.080
C00Y	0.10598(17)	0.9078(8)	0.0891(2)	0.0565(12)
H2	0.086487	0.976961	0.114841	0.085
HF	0.079428	0.842826	0.049777	0.085
HG	0.127650	1.010952	0.075489	0.085
C00Z	0.43890(16)	0.1296(7)	0.6185(2)	0.0501(10)
H3	0.435659	0.003326	0.594447	0.060
C010	0.23312(18)	1.0748(7)	0.1874(3)	0.0633(13)
H01A	0.262261	1.122263	0.227726	0.095
H01B	0.208567	1.191490	0.167630	0.095
H01C	0.249354	1.022571	0.155797	0.095
C011	0.11005(19)	0.5705(9)	0.1504(3)	0.0629(13)
H01D	0.134435	0.462560	0.177352	0.094
H01E	0.084525	0.507616	0.109920	0.094
H01F	0.089395	0.634003	0.175738	0.094
C012	0.1577(2)	0.9791(9)	0.2611(2)	0.0647(14)
H01G	0.133538	0.875092	0.269781	0.097
H01H	0.135966	1.098791	0.238043	0.097
H01I	0.184831	1.025474	0.303226	0.097
C013	0.46345(18)	0.1559(10)	0.6835(2)	0.0616(13)
H013	0.480988	0.048008	0.713668	0.074
C014	0.3549(3)	1.0125(8)	0.1193(3)	0.0678(14)
H01J	0.317322	1.027442	0.118537	0.102
H01K	0.358197	1.079358	0.080001	0.102
H01L	0.380259	1.079086	0.159261	0.102

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 3. Anisotropic displacement parameters [Å²] for S9. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si01	0.0441(5)	0.0325(5)	0.0344(5)	0.0016(4)	0.0235(4)	−0.0003(4)
Si02	0.0344(5)	0.0346(5)	0.0363(5)	0.0048(4)	0.0132(4)	0.0052(4)
O003	0.0276(11)	0.0410(14)	0.0353(12)	0.0092(9)	0.0167(9)	0.0071(9)
O004	0.0391(12)	0.0276(12)	0.0348(12)	−0.0021(10)	0.0159(10)	0.0010(10)
O005	0.0434(13)	0.0417(14)	0.0384(13)	0.0027(11)	0.0245(11)	−0.0011(11)
O006	0.0317(11)	0.0316(12)	0.0299(11)	0.0009(9)	0.0131(9)	−0.0021(9)
O007	0.0312(11)	0.0380(13)	0.0311(12)	0.0015(10)	0.0118(9)	0.0057(10)
O008	0.0478(16)	0.098(3)	0.0349(14)	0.0132(17)	0.0088(12)	0.0043(18)
C009	0.0306(15)	0.0263(15)	0.0308(16)	0.0004(12)	0.0154(13)	0.0019(12)
C00A	0.0241(14)	0.0326(17)	0.0321(16)	−0.0016(13)	0.0152(12)	−0.0028(12)
C00B	0.0323(16)	0.0323(17)	0.0338(16)	0.0037(14)	0.0169(13)	0.0010(13)
C00C	0.0314(15)	0.0309(16)	0.0279(16)	0.0019(12)	0.0119(13)	0.0014(12)
C00D	0.0330(16)	0.0305(17)	0.0321(17)	0.0005(13)	0.0184(13)	−0.0008(13)
C00E	0.0282(14)	0.0250(15)	0.0291(16)	0.0005(12)	0.0153(12)	0.0017(12)
C00F	0.0279(15)	0.049(2)	0.0333(17)	0.0075(15)	0.0143(13)	0.0010(15)
C00G	0.0296(15)	0.0314(16)	0.0338(16)	0.0047(13)	0.0178(13)	0.0036(13)

C00H	0.0363(17)	0.0357(19)	0.0412(19)	0.0049(14)	0.0246(15)	0.0048(14)
C00I	0.0400(18)	0.039(2)	0.0335(17)	−0.0011(14)	0.0175(14)	−0.0106(14)
C00J	0.0312(15)	0.0307(16)	0.0329(17)	0.0016(12)	0.0175(13)	−0.0003(12)
C00K	0.0406(18)	0.0354(18)	0.0352(18)	0.0011(14)	0.0228(15)	−0.0022(14)
C00L	0.0288(15)	0.0366(17)	0.0339(17)	0.0008(13)	0.0140(13)	0.0023(13)
C00M	0.0293(16)	0.0328(17)	0.0326(17)	−0.0024(12)	0.0158(13)	−0.0022(12)
C00N	0.0311(16)	0.0389(18)	0.043(2)	0.0091(15)	0.0226(15)	0.0067(14)
C00O	0.0381(17)	0.0297(17)	0.0359(17)	0.0015(14)	0.0186(14)	−0.0006(14)
C00P	0.048(2)	0.056(2)	0.0363(19)	−0.0032(16)	0.0220(16)	−0.0145(17)
C00Q	0.0275(14)	0.0261(15)	0.0308(15)	0.0002(12)	0.0140(12)	0.0006(12)
C00R	0.0295(16)	0.051(2)	0.0389(18)	0.0094(17)	0.0104(14)	0.0011(16)
C00S	0.0306(16)	0.0421(19)	0.0392(18)	−0.0005(14)	0.0169(14)	−0.0019(14)
C00T	0.0365(19)	0.070(3)	0.035(2)	0.0069(19)	0.0122(16)	0.0037(19)
C00U	0.042(2)	0.049(2)	0.061(3)	0.0007(19)	0.0302(19)	0.0017(17)
C00V	0.052(2)	0.064(3)	0.035(2)	−0.0039(19)	0.0124(17)	0.005(2)
C00W	0.0341(18)	0.069(3)	0.045(2)	0.007(2)	0.0162(16)	0.0004(18)
C00X	0.056(2)	0.065(3)	0.038(2)	−0.0003(18)	0.0151(18)	−0.028(2)
C00Y	0.039(2)	0.075(3)	0.050(2)	0.016(2)	0.0090(18)	0.012(2)
C00Z	0.045(2)	0.051(2)	0.050(2)	0.0220(19)	0.0118(18)	0.0005(18)
C010	0.044(2)	0.038(2)	0.100(4)	0.017(2)	0.015(2)	0.0025(18)
C011	0.045(2)	0.064(3)	0.076(3)	0.008(3)	0.017(2)	−0.014(2)
C012	0.080(3)	0.064(3)	0.055(3)	0.011(2)	0.030(2)	0.038(3)
C013	0.043(2)	0.085(4)	0.051(3)	0.032(3)	0.0096(19)	0.003(2)
C014	0.100(4)	0.044(3)	0.085(4)	0.016(2)	0.065(3)	0.014(3)

Table 4. Bond lengths and angles for S9.

Atom–Atom	Length [Å]
Si01–O005	1.637(3)
Si01–C00I	1.882(4)
Si01–C00W	1.861(4)
Si01–C014	1.853(5)
Si02–O007	1.656(2)
Si02–C00R	1.871(4)
Si02–C010	1.867(5)
Si02–C012	1.859(5)
O003–C00B	1.399(4)
O003–C00G	1.442(4)
O004–C00A	1.206(4)
O005–C00K	1.431(4)
O006–C00A	1.353(4)
O006–C00B	1.460(4)
O007–C00C	1.438(4)
O008–C00T	1.350(5)
O008–C013	1.388(7)
C009–H009	1.0000
C009–C00C	1.544(4)
C009–C00D	1.567(4)
C009–C00E	1.551(4)
C00A–C00E	1.527(4)
C00B–C00F	1.488(5)
C00B–C00J	1.519(4)
C00C–H00C	1.0000
C00C–C00L	1.516(4)
C00D–C00H	1.548(5)
C00D–C00K	1.545(5)

C00D–C00O	1.530(5)
C00E–C00G	1.539(4)
C00E–C00Q	1.549(4)
C00F–C00T	1.340(6)
C00F–C00Z	1.432(6)
C00G–H00G	1.0000
C00G–C00N	1.502(4)
C00H–H00A	0.9900
C00H–H00B	0.9900
C00H–C00N	1.524(5)
C00I–C00P	1.531(5)
C00I–C00U	1.536(6)
C00I–C00X	1.541(5)
C00J–H00D	0.9900
C00J–H00E	0.9900
C00J–C00Q	1.546(4)
C00K–H00F	0.9900
C00K–H00H	0.9900
C00L–H00L	0.9500
C00L–C00M	1.325(5)
C00M–C00Q	1.511(4)
C00M–C00S	1.506(4)
C00N–H00I	0.9900
C00N–H00J	0.9900
C00O–H00K	0.9800
C00O–H00M	0.9800
C00O–H00N	0.9800
C00P–H00O	0.9800
C00P–H00P	0.9800
C00P–H00Q	0.9800
C00Q–H00R	1.0000
C00R–C00V	1.540(6)
C00R–C00Y	1.542(6)
C00R–C011	1.541(6)
C00S–H00S	0.9800
C00S–H00T	0.9800
C00S–H00U	0.9800
C00T–H00V	0.9500
C00U–H00W	0.9800
C00U–H00X	0.9800
C00U–H00Y	0.9800
C00V–H00Z	0.9800
C00V–H	0.9800
C00V–HA	0.9800
C00W–H00	0.9800
C00W–HB	0.9800
C00W–HC	0.9800
C00X–H1	0.9800
C00X–HD	0.9800
C00X–HE	0.9800
C00Y–H2	0.9800
C00Y–HF	0.9800
C00Y–HG	0.9800
C00Z–H3	0.9500
C00Z–C013	1.330(7)
C010–H01A	0.9800

C010–H01B	0.9800
C010–H01C	0.9800
C011–H01D	0.9800
C011–H01E	0.9800
C011–H01F	0.9800
C012–H01G	0.9800
C012–H01H	0.9800
C012–H01I	0.9800
C013–H013	0.9500
C014–H01J	0.9800
C014–H01K	0.9800
C014–H01L	0.9800

Atom–Atom–Atom	**Angle [°]**
O005–Si01–C00I	103.12(15)
O005–Si01–C00W	111.07(17)
O005–Si01–C014	111.5(2)
C00W–Si01–C00I	111.80(17)
C014–Si01–C00I	111.3(2)
C014–Si01–C00W	108.0(3)
O007–Si02–C00R	104.34(16)
O007–Si02–C010	110.61(17)
O007–Si02–C012	112.20(18)
C010–Si02–C00R	110.9(2)
C012–Si02–C00R	111.9(2)
C012–Si02–C010	107.0(3)
C00B–O003–C00G	113.2(2)
C00K–O005–Si01	128.4(2)
C00A–O006–C00B	112.8(3)
C00C–O007–Si02	124.6(2)
C00T–O008–C013	105.1(4)
C00C–C009–H009	104.6
C00C–C009–C00D	117.7(3)
C00C–C009–C00E	108.5(2)
C00D–C009–H009	104.6
C00E–C009–H009	104.6
C00E–C009–C00D	115.4(3)
O004–C00A–O006	119.2(3)
O004–C00A–C00E	127.7(3)
O006–C00A–C00E	113.1(3)
O003–C00B–O006	108.2(3)
O003–C00B–C00F	107.8(3)
O003–C00B–C00J	112.7(3)
O006–C00B–C00F	107.6(3)
O006–C00B–C00J	106.6(3)
C00F–C00B–C00J	113.7(3)
O007–C00C–C009	109.4(2)
O007–C00C–H00C	109.6
O007–C00C–C00L	107.1(3)
C009–C00C–H00C	109.6
C00L–C00C–C009	111.6(3)
C00L–C00C–H00C	109.6
C00H–C00D–C009	109.3(3)
C00K–C00D–C009	108.9(3)
C00K–C00D–C00H	106.8(3)
C00O–C00D–C009	114.5(3)

C00O–C00D–C00H	108.8(3)
C00O–C00D–C00K	108.2(3)
C00A–C00E–C009	115.3(3)
C00A–C00E–C00G	107.6(3)
C00A–C00E–C00Q	106.8(2)
C00G–C00E–C009	111.8(2)
C00G–C00E–C00Q	105.0(2)
C00Q–C00E–C009	109.7(2)
C00T–C00F–C00B	129.3(4)
C00T–C00F–C00Z	106.2(4)
C00Z–C00F–C00B	124.5(4)
O003–C00G–C00E	109.6(2)
O003–C00G–H00G	108.1
O003–C00G–C00N	110.4(3)
C00E–C00G–H00G	108.1
C00N–C00G–C00E	112.5(3)
C00N–C00G–H00G	108.1
C00D–C00H–H00A	108.7
C00D–C00H–H00B	108.7
H00A–C00H–H00B	107.6
C00N–C00H–C00D	114.2(3)
C00N–C00H–H00A	108.7
C00N–C00H–H00B	108.7
C00P–C00I–Si01	111.6(3)
C00P–C00I–C00U	109.8(3)
C00P–C00I–C00X	107.9(3)
C00U–C00I–Si01	109.5(2)
C00U–C00I–C00X	108.1(4)
C00X–C00I–Si01	109.9(3)
C00B–C00J–H00D	109.9
C00B–C00J–H00E	109.9
C00B–C00J–C00Q	109.0(2)
H00D–C00J–H00E	108.3
C00Q–C00J–H00D	109.9
C00Q–C00J–H00E	109.9
O005–C00K–C00D	109.6(3)
O005–C00K–H00F	109.8
O005–C00K–H00H	109.8
C00D–C00K–H00F	109.8
C00D–C00K–H00H	109.8
H00F–C00K–H00H	108.2
C00C–C00L–H00L	116.8
C00M–C00L–C00C	126.4(3)
C00M–C00L–H00L	116.8
C00L–C00M–C00Q	120.6(3)
C00L–C00M–C00S	122.5(3)
C00S–C00M–C00Q	116.7(3)
C00G–C00N–C00H	108.2(3)
C00G–C00N–H00I	110.1
C00G–C00N–H00J	110.1
C00H–C00N–H00I	110.1
C00H–C00N–H00J	110.1
H00I–C00N–H00J	108.4
C00D–C00O–H00K	109.5
C00D–C00O–H00M	109.5
C00D–C00O–H00N	109.5

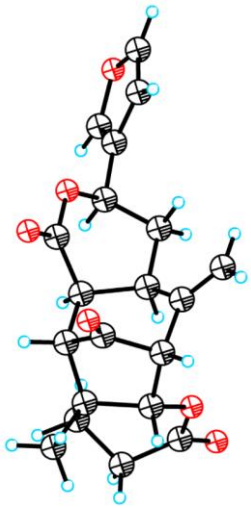
H00K–C00O–H00M	109.5
H00K–C00O–H00N	109.5
H00M–C00O–H00N	109.5
C00I–C00P–H00O	109.5
C00I–C00P–H00P	109.5
C00I–C00P–H00Q	109.5
H00O–C00P–H00P	109.5
H00O–C00P–H00Q	109.5
H00P–C00P–H00Q	109.5
C00E–C00Q–H00R	107.1
C00J–C00Q–C00E	107.9(2)
C00J–C00Q–H00R	107.1
C00M–C00Q–C00E	112.0(3)
C00M–C00Q–C00J	115.4(3)
C00M–C00Q–H00R	107.1
C00V–C00R–Si02	109.8(3)
C00V–C00R–C00Y	108.6(3)
C00V–C00R–C011	109.0(4)
C00Y–C00R–Si02	109.5(3)
C011–C00R–Si02	110.3(3)
C011–C00R–C00Y	109.5(3)
C00M–C00S–H00S	109.5
C00M–C00S–H00T	109.5
C00M–C00S–H00U	109.5
H00S–C00S–H00T	109.5
H00S–C00S–H00U	109.5
H00T–C00S–H00U	109.5
O008–C00T–H00V	124.2
C00F–C00T–O008	111.7(5)
C00F–C00T–H00V	124.2
C00I–C00U–H00W	109.5
C00I–C00U–H00X	109.5
C00I–C00U–H00Y	109.5
H00W–C00U–H00X	109.5
H00W–C00U–H00Y	109.5
H00X–C00U–H00Y	109.5
C00R–C00V–H00Z	109.5
C00R–C00V–H	109.5
C00R–C00V–HA	109.5
H00Z–C00V–H	109.5
H00Z–C00V–HA	109.5
H–C00V–HA	109.5
Si01–C00W–H00	109.5
Si01–C00W–HB	109.5
Si01–C00W–HC	109.5
H00–C00W–HB	109.5
H00–C00W–HC	109.5
HB–C00W–HC	109.5
C00I–C00X–H1	109.5
C00I–C00X–HD	109.5
C00I–C00X–HE	109.5
H1–C00X–HD	109.5
H1–C00X–HE	109.5
HD–C00X–HE	109.5
C00R–C00Y–H2	109.5
C00R–C00Y–HF	109.5

C00R–C00Y–HG	109.5
H2–C00Y–HF	109.5
H2–C00Y–HG	109.5
HF–C00Y–HG	109.5
C00F–C00Z–H3	127.0
C013–C00Z–C00F	106.1(5)
C013–C00Z–H3	127.0
Si02–C010–H01A	109.5
Si02–C010–H01B	109.5
Si02–C010–H01C	109.5
H01A–C010–H01B	109.5
H01A–C010–H01C	109.5
H01B–C010–H01C	109.5
C00R–C011–H01D	109.5
C00R–C011–H01E	109.5
C00R–C011–H01F	109.5
H01D–C011–H01E	109.5
H01D–C011–H01F	109.5
H01E–C011–H01F	109.5
Si02–C012–H01G	109.5
Si02–C012–H01H	109.5
Si02–C012–H01I	109.5
H01G–C012–H01H	109.5
H01G–C012–H01I	109.5
H01H–C012–H01I	109.5
O008–C013–H013	124.5
C00Z–C013–O008	111.0(4)
C00Z–C013–H013	124.5
Si01–C014–H01J	109.5
Si01–C014–H01K	109.5
Si01–C014–H01L	109.5
H01J–C014–H01K	109.5
H01J–C014–H01L	109.5
H01K–C014–H01L	109.5

Table 5. Torsion angles for S9.

Atom–Atom–Atom–Atom	Torsion Angle [°]
Si01–O005–C00K–C00D	−144.0(3)
Si02–O007–C00C–C009	−150.1(2)
Si02–O007–C00C–C00L	88.8(3)
O003–C00B–C00F–C00T	124.7(4)
O003–C00B–C00F–C00Z	−54.1(4)
O003–C00B–C00J–C00Q	−55.1(3)
O003–C00G–C00N–C00H	176.6(3)
O004–C00A–C00E–C009	3.7(5)
O004–C00A–C00E–C00G	129.1(3)
O004–C00A–C00E–C00Q	−118.5(3)
O005–Si01–C00I–C00P	−177.0(2)
O005–Si01–C00I–C00U	61.2(3)
O005–Si01–C00I–C00X	−57.3(3)
O006–C00A–C00E–C009	−177.3(2)
O006–C00A–C00E–C00G	−51.8(3)
O006–C00A–C00E–C00Q	60.5(3)
O006–C00B–C00F–C00T	8.3(5)
O006–C00B–C00F–C00Z	−170.6(3)
O006–C00B–C00J–C00Q	63.4(3)
O007–Si02–C00R–C00V	−56.6(3)
O007–Si02–C00R–C00Y	−175.8(3)
O007–Si02–C00R–C011	63.5(3)
O007–C00C–C00L–C00M	130.9(4)
C009–C00C–C00L–C00M	11.3(5)
C009–C00D–C00H–C00N	−52.3(4)
C009–C00D–C00K–O005	−165.5(3)
C009–C00E–C00G–O003	176.8(2)
C009–C00E–C00G–C00N	53.7(4)
C009–C00E–C00Q–C00J	−178.2(2)
C009–C00E–C00Q–C00M	−50.1(3)
C00A–O006–C00B–O003	60.5(3)
C00A–O006–C00B–C00F	176.7(2)
C00A–O006–C00B–C00J	−60.9(3)
C00A–C00E–C00G–O003	49.3(3)
C00A–C00E–C00G–C00N	−73.9(3)
C00A–C00E–C00Q–C00J	−52.5(3)
C00A–C00E–C00Q–C00M	75.5(3)
C00B–O003–C00G–C00E	5.6(4)
C00B–O003–C00G–C00N	130.0(3)
C00B–O006–C00A–O004	177.3(3)
C00B–O006–C00A–C00E	−1.9(3)
C00B–C00F–C00T–O008	−179.0(3)
C00B–C00F–C00Z–C013	179.0(3)
C00B–C00J–C00Q–C00E	−5.7(3)
C00B–C00J–C00Q–C00M	−131.7(3)
C00C–C009–C00D–C00H	174.1(3)
C00C–C009–C00D–C00K	−69.5(4)
C00C–C009–C00D–C00O	51.7(4)
C00C–C009–C00E–C00A	−56.6(3)
C00C–C009–C00E–C00G	−179.8(3)
C00C–C009–C00E–C00Q	64.1(3)
C00C–C00L–C00M–C00Q	3.1(5)
C00C–C00L–C00M–C00S	−171.6(3)
C00D–C009–C00C–O007	64.8(4)

C00D–C009–C00C–C00L	−177.0(3)
C00D–C009–C00E–C00A	78.0(3)
C00D–C009–C00E–C00G	−45.3(4)
C00D–C009–C00E–C00Q	−161.4(3)
C00D–C00H–C00N–C00G	61.3(4)
C00E–C009–C00C–O007	−162.0(2)
C00E–C009–C00C–C00L	−43.7(4)
C00E–C009–C00D–C00H	43.9(4)
C00E–C009–C00D–C00K	160.3(3)
C00E–C009–C00D–C00O	−78.4(3)
C00E–C00G–C00N–C00H	−60.6(4)
C00F–C00B–C00J–C00Q	−178.2(3)
C00F–C00Z–C013–O008	0.1(5)
C00G–O003–C00B–O006	−61.6(3)
C00G–O003–C00B–C00F	−177.7(3)
C00G–O003–C00B–C00J	56.0(4)
C00G–C00E–C00Q–C00J	61.6(3)
C00G–C00E–C00Q–C00M	−170.4(3)
C00H–C00D–C00K–O005	−47.5(4)
C00I–Si01–O005–C00K	−178.5(3)
C00J–C00B–C00F–C00T	−109.6(4)
C00J–C00B–C00F–C00Z	71.6(4)
C00K–C00D–C00H–C00N	−170.0(3)
C00L–C00M–C00Q–C00E	16.8(4)
C00L–C00M–C00Q–C00J	140.7(3)
C00O–C00D–C00H–C00N	73.4(4)
C00O–C00D–C00K–O005	69.5(3)
C00Q–C00E–C00G–O003	−64.3(3)
C00Q–C00E–C00G–C00N	172.5(3)
C00R–Si02–O007–C00C	−159.8(2)
C00S–C00M–C00Q–C00E	−168.1(3)
C00S–C00M–C00Q–C00J	−44.2(4)
C00T–O008–C013–C00Z	−0.1(5)
C00T–C00F–C00Z–C013	−0.1(5)
C00W–Si01–O005–C00K	−58.6(3)
C00W–Si01–C00I–C00P	63.6(3)
C00W–Si01–C00I–C00U	−58.2(3)
C00W–Si01–C00I–C00X	−176.7(3)
C00Z–C00F–C00T–O008	0.0(4)
C010–Si02–O007–C00C	80.9(3)
C010–Si02–C00R–C00V	62.5(4)
C010–Si02–C00R–C00Y	−56.7(3)
C010–Si02–C00R–C011	−177.4(3)
C012–Si02–O007–C00C	−38.5(3)
C012–Si02–C00R–C00V	−178.2(3)
C012–Si02–C00R–C00Y	62.6(3)
C012–Si02–C00R–C011	−58.0(4)
C013–O008–C00T–C00F	0.1(5)
C014–Si01–O005–C00K	61.9(4)
C014–Si01–C00I–C00P	−57.3(3)
C014–Si01–C00I–C00U	−179.1(3)
C014–Si01–C00I–C00X	62.4(4)



32

Table 1 Crystal data and structure refinement for compound 32.

CCDC number	2447363
Empirical formula	$C_{22}H_{24}O_7$
Formula weight	400.41
Temperature/K	105(8)
Crystal system	monoclinic
Space group	C2
a/Å	22.056(5)
b/Å	6.5546(7)
c/Å	14.279(3)
α/°	90
β/°	110.54(2)
γ/°	90
Volume/Å^3	1933.0(7)
Z	4
ρ_{calc}g/cm^3	1.376
μ/mm^{-1}	0.853
F(000)	848.0
Crystal size/mm^3	0.4 × 0.04 × 0.03
Radiation	Cu Kα (λ = 1.54178)
2θ range for data collection/°	6.61 to 147.286
Index ranges	-22 ≤ h ≤ 26, -5 ≤ k ≤ 7, -17 ≤ l ≤ 15
Reflections collected	4527
Independent reflections	2678 [R_{int} = 0.0653, R_{sigma} = 0.1199]
Data/restraints/parameters	2678/271/345
Goodness-of-fit on F^2	0.962
Final R indexes [I>=2σ (I)]	R_1 = 0.0740, wR_2 = 0.1846
Final R indexes [all data]	R_1 = 0.1350, wR_2 = 0.2309
Largest diff. peak/hole / e Å^{-3}	0.42/-0.30
Flack parameter	0.3(8)

Table 2 Atomic coordinates and U_{eq} [Å^2] for 32.

Atom	***x***	***y***	***z***	U_{eq}
O1	0.5293(3)	1.1919(13)	0.2475(5)	0.0616(18)

O2	0.6478(2)	0.6906(10)	0.4267(4)	0.0424(14)
O3	0.7068(3)	0.4121(10)	0.4746(5)	0.0482(15)
O4	0.7123(3)	0.1419(9)	0.6559(5)	0.0510(17)
O5	0.6877(3)	0.6926(10)	0.8504(5)	0.0494(15)
O6	0.6936(4)	0.9974(11)	0.9192(5)	0.0654(19)
C1	0.5808(4)	1.1560(16)	0.3342(7)	0.048(2)
H1	0.614771	1.250107	0.364597	0.058
C2	0.5762(4)	0.9680(14)	0.3703(7)	0.045(2)
C3	0.5185(4)	0.884(2)	0.3000(8)	0.064(3)
H3	0.502115	0.751118	0.303678	0.077
C4	0.4914(5)	1.019(2)	0.2287(9)	0.070(3)
H4	0.452254	1.000264	0.173649	0.084
C5	0.6232(4)	0.8739(13)	0.4601(7)	0.042(2)
H5	0.659660	0.970767	0.491708	0.050
C6	0.5940(4)	0.8065(14)	0.5369(7)	0.043(2)
H6A	0.557678	0.711758	0.504754	0.052
H6B	0.576306	0.927168	0.560171	0.052
C7	0.6438(4)	0.6996(13)	0.6281(6)	0.0399(19)
H7	0.656688	0.801705	0.683661	0.048
C8	0.7065(4)	0.6484(13)	0.6050(6)	0.0371(19)
H8	0.730849	0.778835	0.609668	0.045
C9	0.6877(4)	0.5726(13)	0.4983(7)	0.040(2)
C10	0.7519(4)	0.4982(12)	0.6790(7)	0.0384(19)
H10	0.788023	0.455958	0.656187	0.046
C11	0.7122(4)	0.3157(13)	0.6875(7)	0.043(2)
C12	0.6723(4)	0.3944(14)	0.7470(7)	0.043(2)
H12	0.654219	0.279864	0.775316	0.051
C13	0.6195(4)	0.5101(14)	0.6680(7)	0.043(2)
C14	0.5600(4)	0.4449(17)	0.6365(8)	0.061(3)
H14A	0.549304	0.322988	0.663127	0.073
H14B	0.527275	0.519254	0.586788	0.073
C15	0.7210(4)	0.5187(13)	0.8291(7)	0.041(2)
H15	0.738323	0.432783	0.890674	0.050
C16	0.7780(4)	0.5661(13)	0.7881(7)	0.041(2)
C17	0.7995(4)	0.7890(13)	0.8107(7)	0.043(2)
H17A	0.845276	0.802912	0.816214	0.052
H17B	0.772861	0.877349	0.755296	0.052
C18	0.7919(5)	0.8569(15)	0.9086(8)	0.054(2)
H18A	0.815560	0.761821	0.963032	0.065
H18B	0.810576	0.994877	0.926851	0.065
C19	0.7224(5)	0.8596(14)	0.8965(7)	0.050(2)
C20	0.8347(4)	0.4260(14)	0.8456(7)	0.045(2)
H20A	0.820565	0.283378	0.835378	0.067
H20B	0.849208	0.458496	0.917107	0.067
H20C	0.870524	0.446747	0.821041	0.067
O7A	1.0414(18)	0.059(7)	1.126(3)	0.063(5)
O8A	0.9305(19)	0.080(7)	0.960(3)	0.062(5)
C21A	1.016(3)	0.253(5)	1.087(3)	0.061(5)
H21A	1.051004	0.354069	1.100532	0.073
H21B	0.985020	0.300542	1.119061	0.073
C22A	0.980(3)	0.228(8)	0.973(3)	0.062(5)
H22A	0.961308	0.359391	0.942260	0.074
H22B	1.010857	0.180782	0.940412	0.074
C23A	0.954(3)	−0.113(6)	1.002(4)	0.063(5)
H23A	0.982751	−0.170234	0.968877	0.075
H23B	0.917442	−0.207535	0.991677	0.075
C24A	0.992(3)	−0.091(7)	1.115(3)	0.065(5)
H24A	0.963038	−0.046376	1.150618	0.078
H24B	1.012017	−0.222567	1.143772	0.078
O7	0.9651(9)	0.082(3)	1.0645(14)	0.065(4)
O8	1.0336(10)	−0.040(3)	0.9444(15)	0.077(5)
C21	0.9911(12)	0.230(3)	1.017(2)	0.062(4)
H21C	1.002180	0.355382	1.057744	0.074
H21D	0.958623	0.265553	0.950698	0.074
C22	1.0524(9)	0.142(3)	1.003(2)	0.051(4)

H22C	1.070704	0.242137	0.968081	0.061
H22D	1.085624	0.110565	1.068659	0.061
C23	1.0061(13)	−0.188(2)	0.991(3)	0.064(5)
H23C	1.038367	−0.226877	1.056327	0.076
H23D	0.994360	−0.311251	0.948490	0.076
C24	0.9454(10)	−0.100(3)	1.006(2)	0.061(4)
H24C	0.911658	−0.068485	0.940666	0.073
H24D	0.927494	−0.200241	1.041421	0.073

U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Table 3 Anisotropic displacement parameters [Å²] for 32. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\, h^2(a^*)^2U_{11} + k^2(b^*)^2U_{22} + \ldots + 2hka^*b^*U_{12}\,]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O1	0.057(4)	0.065(5)	0.059(4)	0.012(4)	0.016(3)	0.021(4)
O2	0.039(3)	0.036(3)	0.050(4)	−0.002(3)	0.013(3)	0.006(3)
O3	0.051(3)	0.032(3)	0.068(4)	−0.002(3)	0.029(3)	0.007(3)
O4	0.056(4)	0.016(3)	0.077(5)	−0.002(3)	0.019(3)	0.005(2)
O5	0.062(4)	0.023(3)	0.065(4)	0.000(3)	0.025(3)	0.012(3)
O6	0.105(5)	0.035(4)	0.064(5)	−0.003(3)	0.038(4)	0.019(4)
C1	0.039(5)	0.050(5)	0.053(6)	0.008(5)	0.014(4)	0.013(4)
C2	0.035(4)	0.044(5)	0.056(6)	0.003(4)	0.017(4)	0.007(4)
C3	0.045(5)	0.073(7)	0.067(7)	0.007(6)	0.011(5)	−0.008(5)
C4	0.051(6)	0.078(8)	0.069(8)	0.006(6)	0.008(5)	0.010(6)
C5	0.040(4)	0.029(4)	0.058(6)	0.003(4)	0.019(4)	0.008(4)
C6	0.041(5)	0.031(4)	0.061(6)	0.003(4)	0.021(4)	0.006(3)
C7	0.042(4)	0.023(4)	0.057(5)	0.005(4)	0.021(4)	0.001(3)
C8	0.035(4)	0.021(4)	0.058(5)	0.003(4)	0.019(4)	0.005(3)
C9	0.031(4)	0.030(4)	0.058(6)	0.001(4)	0.016(4)	−0.002(3)
C10	0.039(4)	0.023(4)	0.057(6)	0.004(4)	0.020(4)	0.003(3)
C11	0.043(5)	0.023(4)	0.058(6)	0.006(4)	0.010(4)	0.006(3)
C12	0.042(4)	0.026(4)	0.062(6)	0.002(4)	0.020(4)	0.000(4)
C13	0.038(4)	0.031(4)	0.062(6)	0.001(4)	0.021(4)	−0.003(4)
C14	0.050(5)	0.046(6)	0.084(8)	0.013(5)	0.020(5)	0.003(4)
C15	0.045(4)	0.025(4)	0.057(6)	0.003(4)	0.023(4)	0.009(4)
C16	0.050(5)	0.021(4)	0.047(5)	0.006(3)	0.011(4)	0.003(3)
C17	0.050(5)	0.027(4)	0.045(5)	0.002(4)	0.006(4)	−0.004(4)
C18	0.074(6)	0.028(4)	0.057(6)	0.002(4)	0.018(5)	−0.006(4)
C19	0.070(6)	0.030(5)	0.053(6)	−0.004(4)	0.025(5)	0.005(4)
C20	0.040(4)	0.031(4)	0.060(6)	0.011(4)	0.013(4)	0.006(4)
O7A	0.061(7)	0.059(7)	0.068(8)	−0.010(7)	0.020(7)	0.000(7)
O8A	0.059(7)	0.056(7)	0.067(8)	−0.005(7)	0.019(7)	0.001(7)
C21A	0.060(8)	0.058(8)	0.065(8)	−0.012(7)	0.022(7)	0.002(7)
C22A	0.061(8)	0.057(7)	0.066(8)	−0.013(7)	0.020(7)	0.004(7)
C23A	0.062(7)	0.055(7)	0.069(8)	−0.011(7)	0.020(7)	−0.001(7)
C24A	0.063(8)	0.058(8)	0.069(9)	−0.010(7)	0.019(7)	0.000(7)
O7	0.062(6)	0.057(6)	0.073(7)	−0.014(6)	0.021(6)	0.001(5)
O8	0.077(8)	0.075(9)	0.075(9)	−0.010(8)	0.023(7)	−0.008(8)
C21	0.060(7)	0.058(7)	0.066(8)	−0.009(6)	0.020(7)	0.005(6)
C22	0.051(7)	0.054(7)	0.056(8)	−0.013(6)	0.027(6)	0.002(6)
C23	0.066(8)	0.056(8)	0.070(9)	−0.010(8)	0.024(7)	−0.005(8)
C24	0.059(7)	0.054(7)	0.067(8)	−0.013(6)	0.019(6)	−0.003(6)

Table 4 Bond lengths and angles for 32.

Atom–Atom	Length [Å]
O1–C1	1.376(11)
O1–C4	1.376(14)
O2–C5	1.466(10)
O2–C9	1.337(9)
O3–C9	1.224(10)
O4–C11	1.226(10)
O5–C15	1.445(9)
O5–C19	1.365(11)
O6–C19	1.212(10)

C1–H1	0.9500
C1–C2	1.353(13)
C2–C3	1.427(13)
C2–C5	1.472(12)
C3–H3	0.9500
C3–C4	1.325(15)
C4–H4	0.9500
C5–H5	1.0000
C5–C6	1.519(12)
C6–H6A	0.9900
C6–H6B	0.9900
C6–C7	1.546(11)
C7–H7	1.0000
C7–C8	1.565(11)
C7–C13	1.540(11)
C8–H8	1.0000
C8–C9	1.516(12)
C8–C10	1.532(11)
C10–H10	1.0000
C10–C11	1.512(11)
C10–C16	1.525(12)
C11–C12	1.512(12)
C12–H12	1.0000
C12–C13	1.512(12)
C12–C15	1.519(12)
C13–C14	1.300(12)
C14–H14A	0.9500
C14–H14B	0.9500
C15–H15	1.0000
C15–C16	1.592(12)
C16–C17	1.535(11)
C16–C20	1.537(11)
C17–H17A	0.9900
C17–H17B	0.9900
C17–C18	1.530(13)
C18–H18A	0.9900
C18–H18B	0.9900
C18–C19	1.481(14)
C20–H20A	0.9800
C20–H20B	0.9800
C20–H20C	0.9800
O7A–C21A	1.420(17)
O7A–C24A	1.430(17)
O8A–C22A	1.428(17)
O8A–C23A	1.417(17)
C21A–H21A	0.9900
C21A–H21B	0.9900
C21A–C22A	1.554(17)
C22A–H22A	0.9900
C22A–H22B	0.9900
C23A–H23A	0.9900
C23A–H23B	0.9900
C23A–C24A	1.542(17)
C24A–H24A	0.9900
C24A–H24B	0.9900
O7–C21	1.418(12)
O7–C24	1.434(12)
O8–C22	1.432(12)
O8–C23	1.422(12)
C21–H21C	0.9900
C21–H21D	0.9900
C21–C22	1.545(12)
C22–H22C	0.9900
C22–H22D	0.9900
C23–H23C	0.9900

C23–H23D	0.9900
C23–C24	1.541(12)
C24–H24C	0.9900
C24–H24D	0.9900

Atom–Atom–Atom	**Angle [°]**
C1–O1–C4	106.7(8)
C9–O2–C5	116.4(6)
C19–O5–C15	119.6(7)
O1–C1–H1	124.8
C2–C1–O1	110.5(9)
C2–C1–H1	124.8
C1–C2–C3	104.6(9)
C1–C2–C5	126.1(8)
C3–C2–C5	129.2(9)
C2–C3–H3	125.3
C4–C3–C2	109.4(11)
C4–C3–H3	125.3
O1–C4–H4	125.6
C3–C4–O1	108.8(9)
C3–C4–H4	125.6
O2–C5–C2	106.7(7)
O2–C5–H5	109.7
O2–C5–C6	107.2(6)
C2–C5–H5	109.7
C2–C5–C6	113.8(7)
C6–C5–H5	109.7
C5–C6–H6A	109.1
C5–C6–H6B	109.1
C5–C6–C7	112.6(6)
H6A–C6–H6B	107.8
C7–C6–H6A	109.1
C7–C6–H6B	109.1
C6–C7–H7	106.6
C6–C7–C8	109.8(7)
C8–C7–H7	106.6
C13–C7–C6	116.1(6)
C13–C7–H7	106.6
C13–C7–C8	110.7(6)
C7–C8–H8	107.3
C9–C8–C7	109.4(6)
C9–C8–H8	107.3
C9–C8–C10	111.4(6)
C10–C8–C7	113.9(7)
C10–C8–H8	107.3
O2–C9–C8	117.0(7)
O3–C9–O2	118.9(8)
O3–C9–C8	124.1(8)
C8–C10–H10	110.9
C11–C10–C8	107.9(6)
C11–C10–H10	110.9
C11–C10–C16	99.8(7)
C16–C10–C8	116.0(7)
C16–C10–H10	110.9
O4–C11–C10	129.1(9)
O4–C11–C12	126.9(8)
C12–C11–C10	104.0(7)
C11–C12–H12	111.4
C11–C12–C15	102.9(6)
C13–C12–C11	101.6(7)
C13–C12–H12	111.4
C13–C12–C15	117.2(7)
C15–C12–H12	111.4
C12–C13–C7	113.8(6)
C14–C13–C7	125.3(8)

C14–C13–C12	120.9(8)
C13–C14–H14A	120.0
C13–C14–H14B	120.0
H14A–C14–H14B	120.0
O5–C15–C12	108.2(6)
O5–C15–H15	109.0
O5–C15–C16	116.6(7)
C12–C15–H15	109.0
C12–C15–C16	104.8(7)
C16–C15–H15	109.0
C10–C16–C15	104.8(7)
C10–C16–C17	118.1(7)
C10–C16–C20	108.4(7)
C17–C16–C15	109.5(7)
C17–C16–C20	108.8(7)
C20–C16–C15	106.7(7)
C16–C17–H17A	109.6
C16–C17–H17B	109.6
H17A–C17–H17B	108.1
C18–C17–C16	110.1(7)
C18–C17–H17A	109.6
C18–C17–H17B	109.6
C17–C18–H18A	109.7
C17–C18–H18B	109.7
H18A–C18–H18B	108.2
C19–C18–C17	109.7(8)
C19–C18–H18A	109.7
C19–C18–H18B	109.7
O5–C19–C18	115.4(7)
O6–C19–O5	117.9(9)
O6–C19–C18	126.6(9)
C16–C20–H20A	109.5
C16–C20–H20B	109.5
C16–C20–H20C	109.5
H20A–C20–H20B	109.5
H20A–C20–H20C	109.5
H20B–C20–H20C	109.5
C21A–O7A–C24A	112.8(19)
C23A–O8A–C22A	113(2)
O7A–C21A–H21A	110.2
O7A–C21A–H21B	110.2
O7A–C21A–C22A	107.7(18)
H21A–C21A–H21B	108.5
C22A–C21A–H21A	110.2
C22A–C21A–H21B	110.2
O8A–C22A–C21A	106.6(18)
O8A–C22A–H22A	110.4
O8A–C22A–H22B	110.4
C21A–C22A–H22A	110.4
C21A–C22A–H22B	110.4
H22A–C22A–H22B	108.6
O8A–C23A–H23A	109.6
O8A–C23A–H23B	109.6
O8A–C23A–C24A	110.3(18)
H23A–C23A–H23B	108.1
C24A–C23A–H23A	109.6
C24A–C23A–H23B	109.6
O7A–C24A–C23A	107.0(18)
O7A–C24A–H24A	110.3
O7A–C24A–H24B	110.3
C23A–C24A–H24A	110.3
C23A–C24A–H24B	110.3
H24A–C24A–H24B	108.6
C21–O7–C24	112.3(14)
C23–O8–C22	112.2(15)

O7–C21–H21C	109.9
O7–C21–H21D	109.9
O7–C21–C22	109.1(14)
H21C–C21–H21D	108.3
C22–C21–H21C	109.9
C22–C21–H21D	109.9
O8–C22–C21	107.3(14)
O8–C22–H22C	110.2
O8–C22–H22D	110.2
C21–C22–H22C	110.2
C21–C22–H22D	110.2
H22C–C22–H22D	108.5
O8–C23–H23C	109.6
O8–C23–H23D	109.6
O8–C23–C24	110.3(14)
H23C–C23–H23D	108.1
C24–C23–H23C	109.6
C24–C23–H23D	109.6
O7–C24–C23	106.9(14)
O7–C24–H24C	110.4
O7–C24–H24D	110.4
C23–C24–H24C	110.4
C23–C24–H24D	110.4
H24C–C24–H24D	108.6

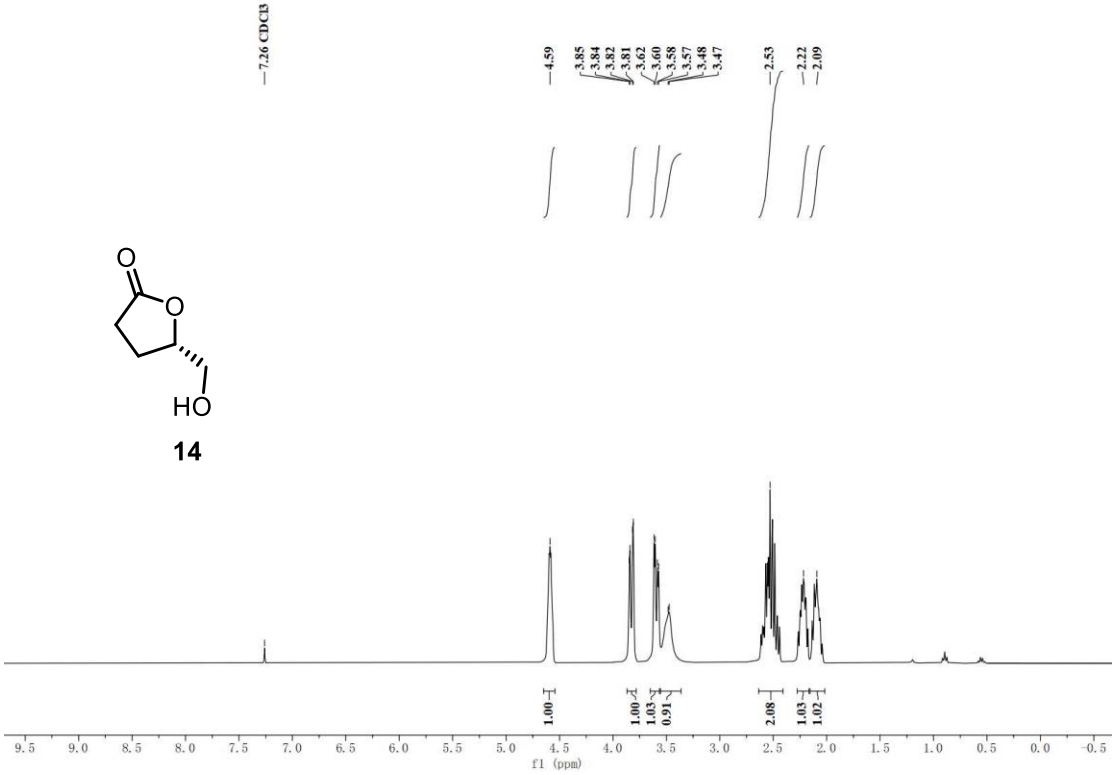
Table 5 Torsion angles for 32.

Atom–Atom–Atom–Atom	Torsion Angle [°]
O1–C1–C2–C3	0.7(10)
O1–C1–C2–C5	178.2(8)
O2–C5–C6–C7	59.6(9)
O4–C11–C12–C13	−102.7(9)
O4–C11–C12–C15	135.6(9)
O5–C15–C16–C10	−109.9(7)
O5–C15–C16–C17	17.7(10)
O5–C15–C16–C20	135.3(7)
C1–O1–C4–C3	−0.4(12)
C1–C2–C3–C4	−1.0(12)
C1–C2–C5–O2	−118.4(9)
C1–C2–C5–C6	123.6(9)
C2–C3–C4–O1	0.8(13)
C2–C5–C6–C7	177.4(7)
C3–C2–C5–O2	58.5(12)
C3–C2–C5–C6	−59.6(13)
C4–O1–C1–C2	−0.3(10)
C5–O2–C9–O3	176.1(7)
C5–O2–C9–C8	−3.8(10)
C5–C2–C3–C4	−178.4(10)
C5–C6–C7–C8	−12.3(10)
C5–C6–C7–C13	−138.8(8)
C6–C7–C8–C9	−40.6(8)
C6–C7–C8–C10	−166.0(7)
C6–C7–C13–C12	171.6(7)
C6–C7–C13–C14	−5.8(13)
C7–C8–C9–O2	52.9(9)
C7–C8–C9–O3	−127.0(8)
C7–C8–C10–C11	50.8(9)
C7–C8–C10–C16	−60.0(9)
C8–C7–C13–C12	45.5(10)
C8–C7–C13–C14	−131.9(10)
C8–C10–C11–O4	108.6(10)
C8–C10–C11–C12	−72.7(8)
C8–C10–C16–C15	80.6(8)
C8–C10–C16–C17	−41.6(10)
C8–C10–C16–C20	−165.9(7)

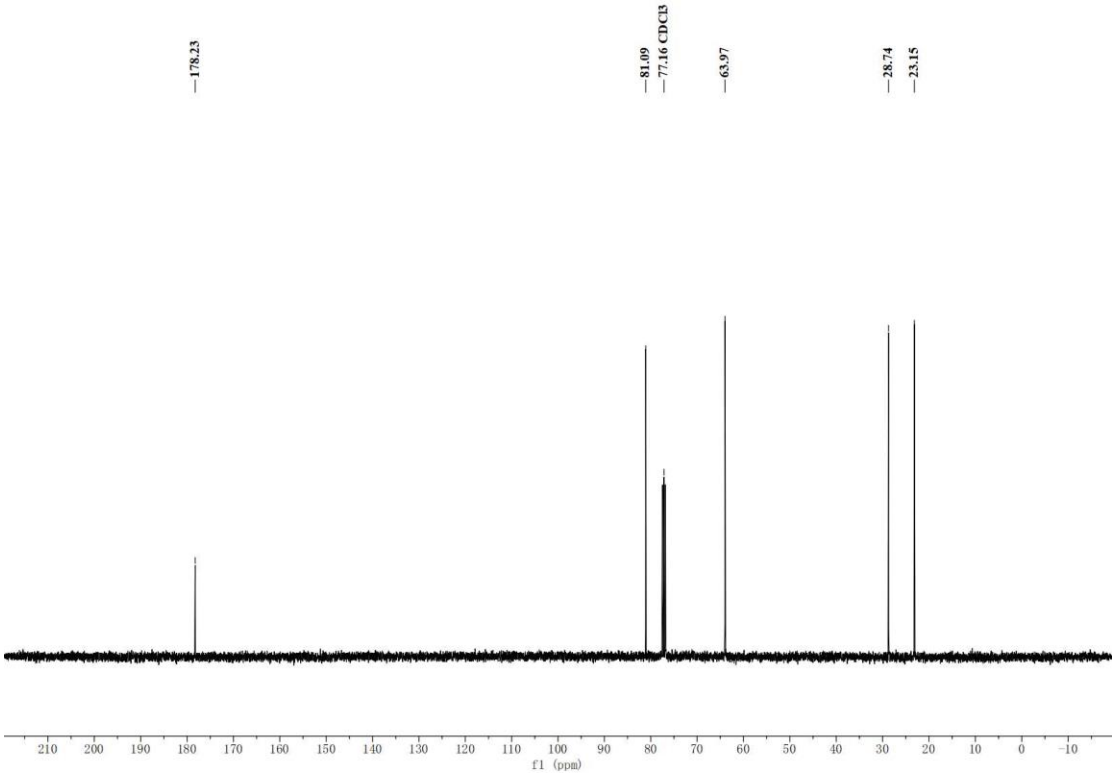
C9–O2–C5–C2	−174.9(7)
C9–O2–C5–C6	−52.6(9)
C9–C8–C10–C11	−73.5(8)
C9–C8–C10–C16	175.7(7)
C10–C8–C9–O2	179.7(6)
C10–C8–C9–O3	−0.2(10)
C10–C11–C12–C13	78.5(7)
C10–C11–C12–C15	−43.2(8)
C10–C16–C17–C18	152.2(8)
C11–C10–C16–C15	−34.9(7)
C11–C10–C16–C17	−157.1(8)
C11–C10–C16–C20	78.7(7)
C11–C12–C13–C7	−66.2(9)
C11–C12–C13–C14	111.3(10)
C11–C12–C15–O5	144.8(6)
C11–C12–C15–C16	19.7(8)
C12–C15–C16–C10	9.7(8)
C12–C15–C16–C17	137.3(7)
C12–C15–C16–C20	−105.1(8)
C13–C7–C8–C9	88.9(8)
C13–C7–C8–C10	−36.5(9)
C13–C12–C15–O5	34.3(10)
C13–C12–C15–C16	−90.8(8)
C15–O5–C19–O6	−175.3(8)
C15–O5–C19–C18	8.0(12)
C15–C12–C13–C7	45.0(11)
C15–C12–C13–C14	−137.4(9)
C15–C16–C17–C18	32.4(9)
C16–C10–C11–O4	−130.0(9)
C16–C10–C11–C12	48.8(7)
C16–C17–C18–C19	−66.0(9)
C17–C18–C19–O5	45.5(11)
C17–C18–C19–O6	−130.9(10)
C19–O5–C15–C12	−159.3(7)
C19–O5–C15–C16	−41.5(11)
C20–C16–C17–C18	−83.8(9)
O7A–C21A–C22A–O8A	60(4)
O8A–C23A–C24A–O7A	−55(4)
C21A–O7A–C24A–C23A	60(3)
C22A–O8A–C23A–C24A	59(4)
C23A–O8A–C22A–C21A	−60(4)
C24A–O7A–C21A–C22A	−64(3)
O7–C21–C22–O8	59(3)
O8–C23–C24–O7	−57(3)
C21–O7–C24–C23	60(2)
C22–O8–C23–C24	60(3)
C23–O8–C22–C21	−59(3)
C24–O7–C21–C22	−62(2)

7. NMR Spectra.

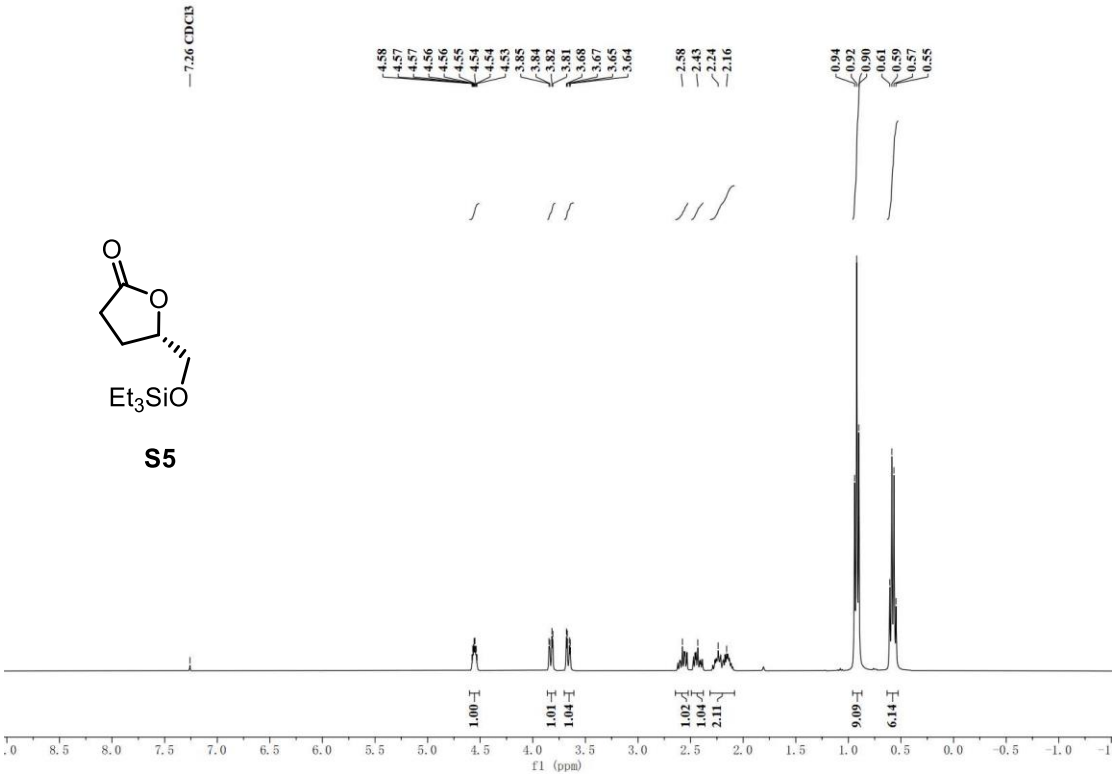
^{1}H NMR spectrum of **14** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **14** (100 MHz, $CDCl_3$)

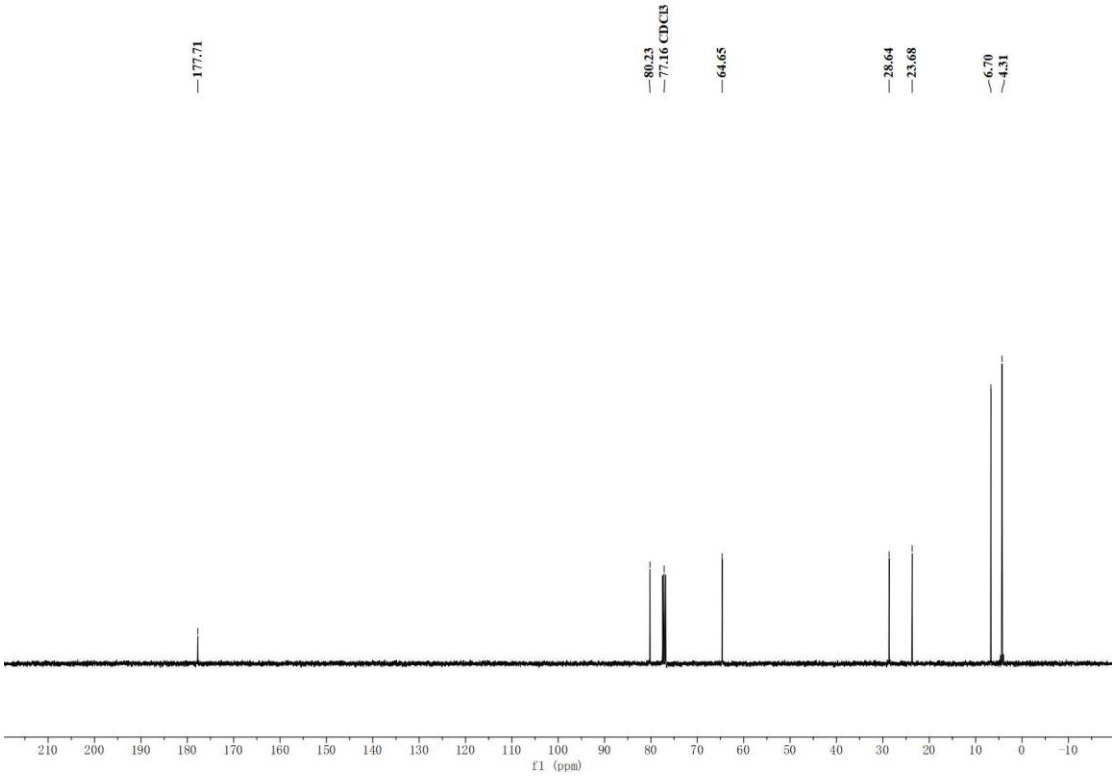


^{1}H NMR spectrum of **S5** (400 MHz, $CDCl_3$)

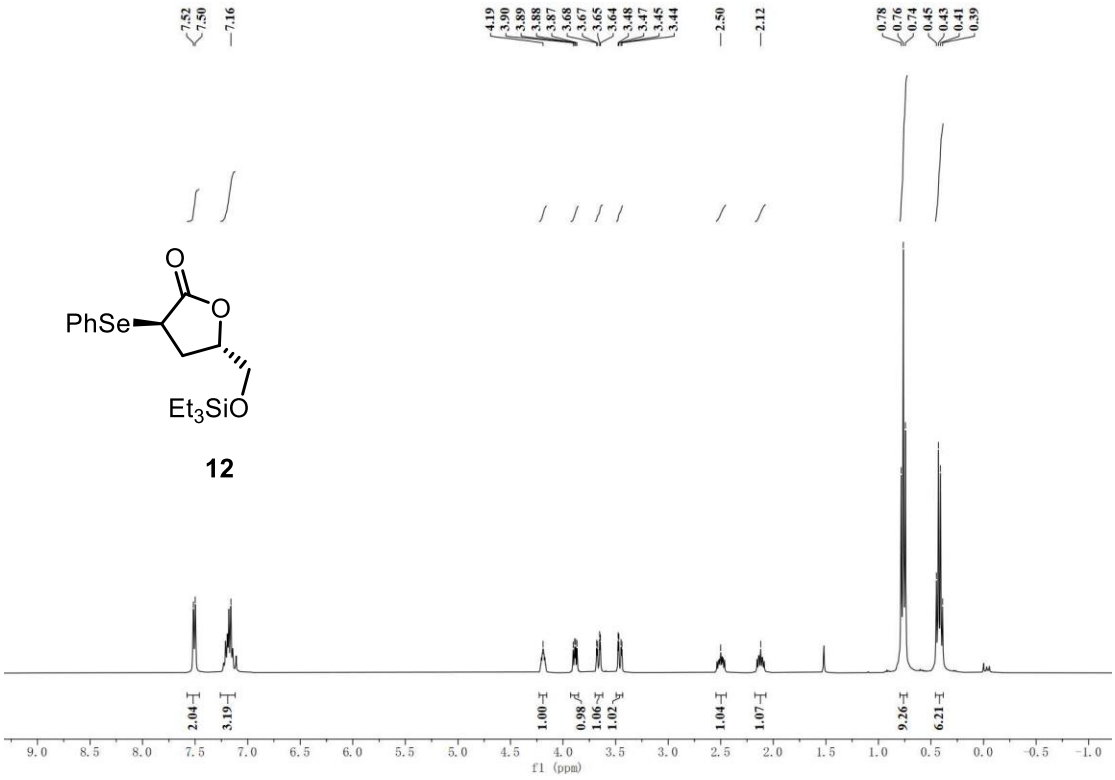


S5

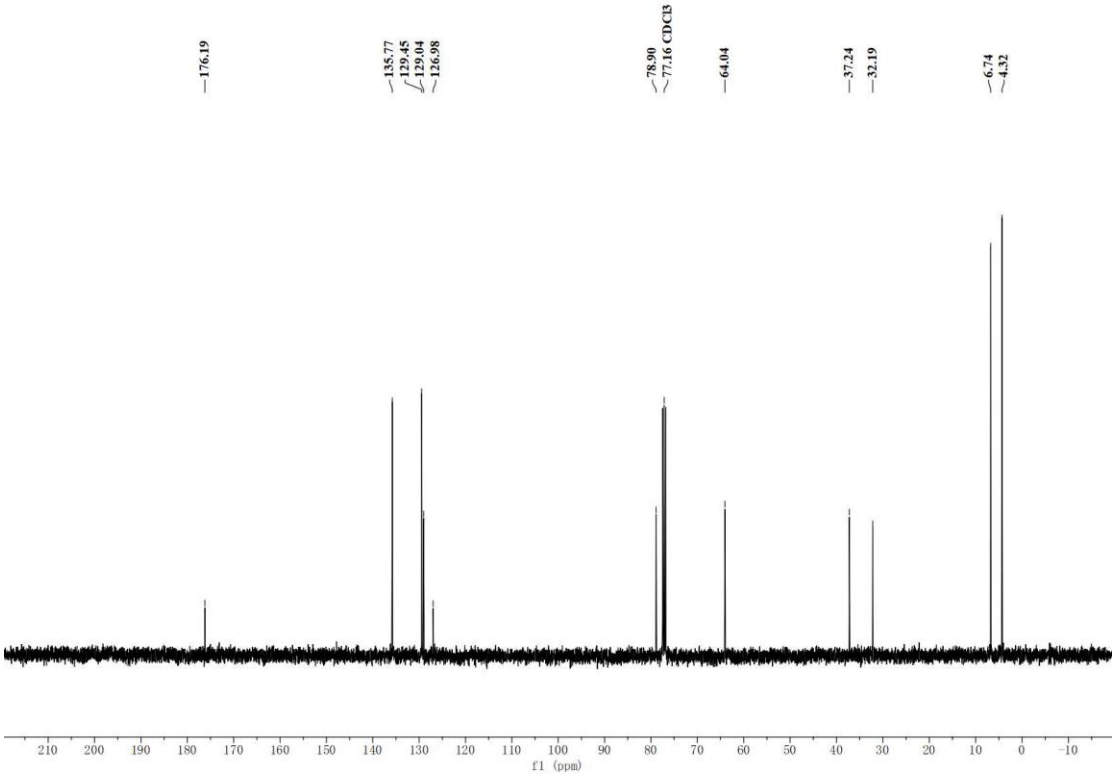
^{13}C NMR spectrum of **S5** (100 MHz, $CDCl_3$)



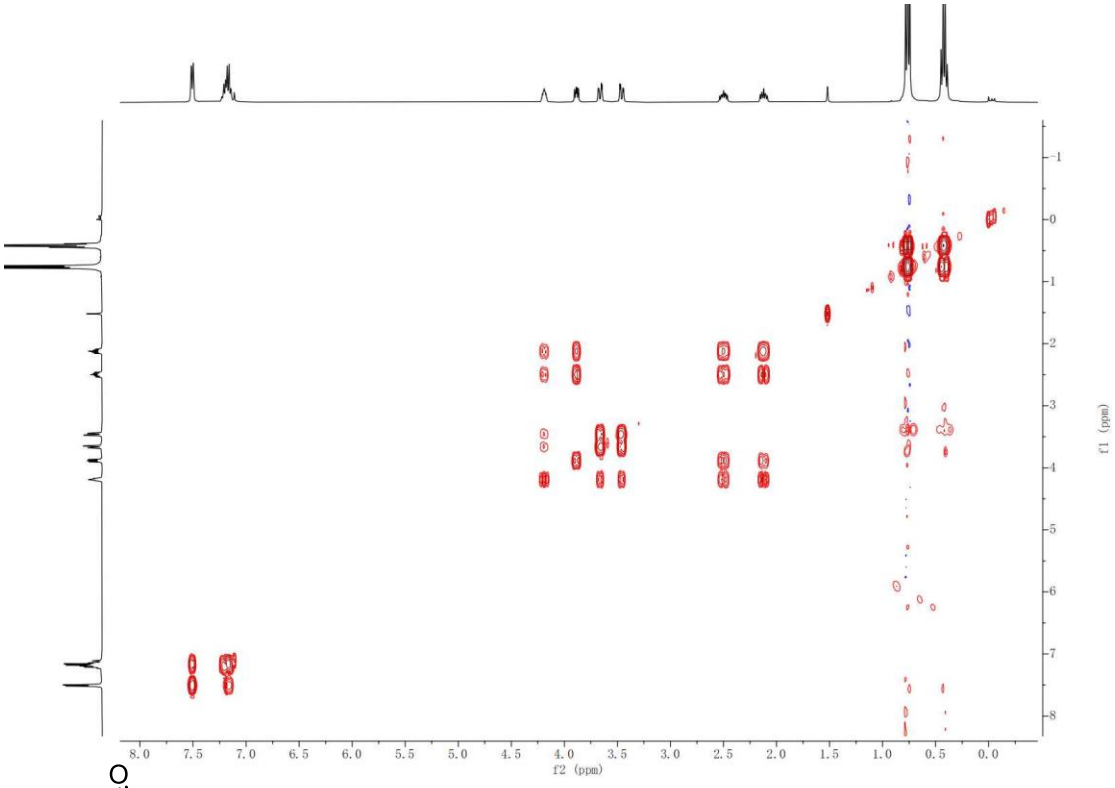
^{1}H NMR spectrum of **12** (400 MHz, $CDCl_3$)

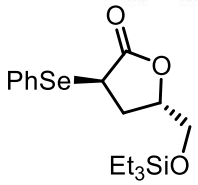


^{13}C NMR spectrum of **12** (100 MHz, $CDCl_3$)



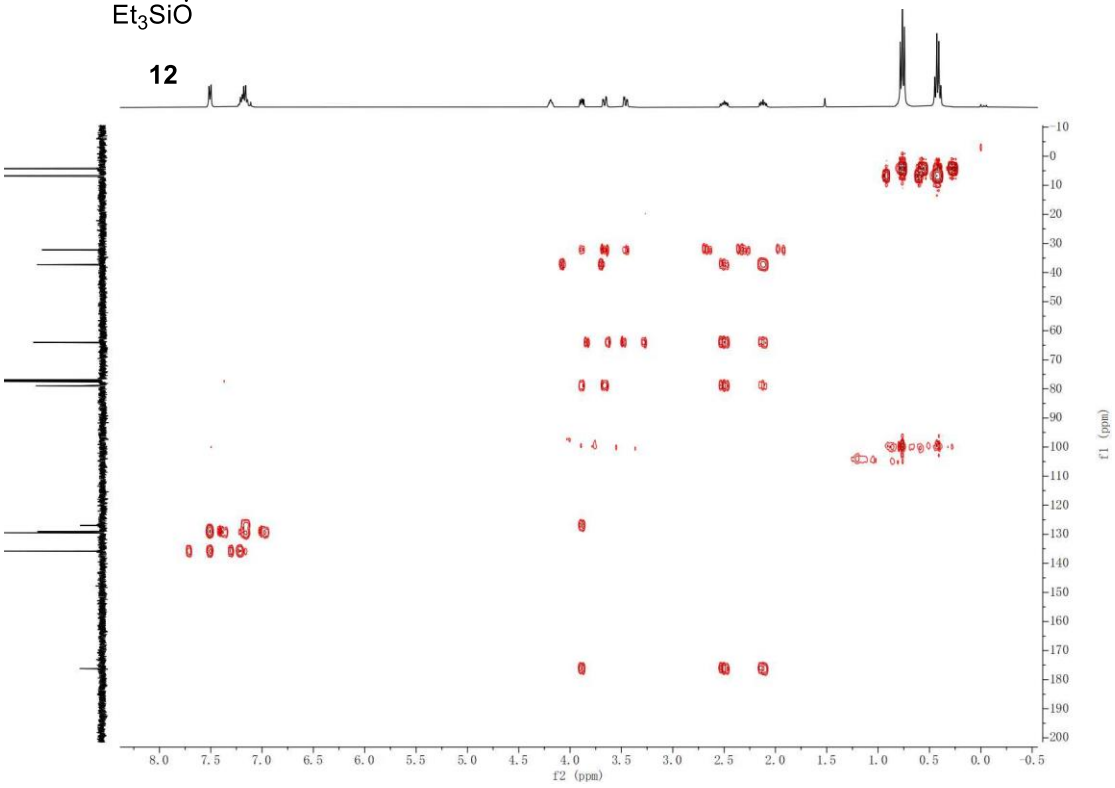
^{1}H-^{1}H COSY spectrum of **12**



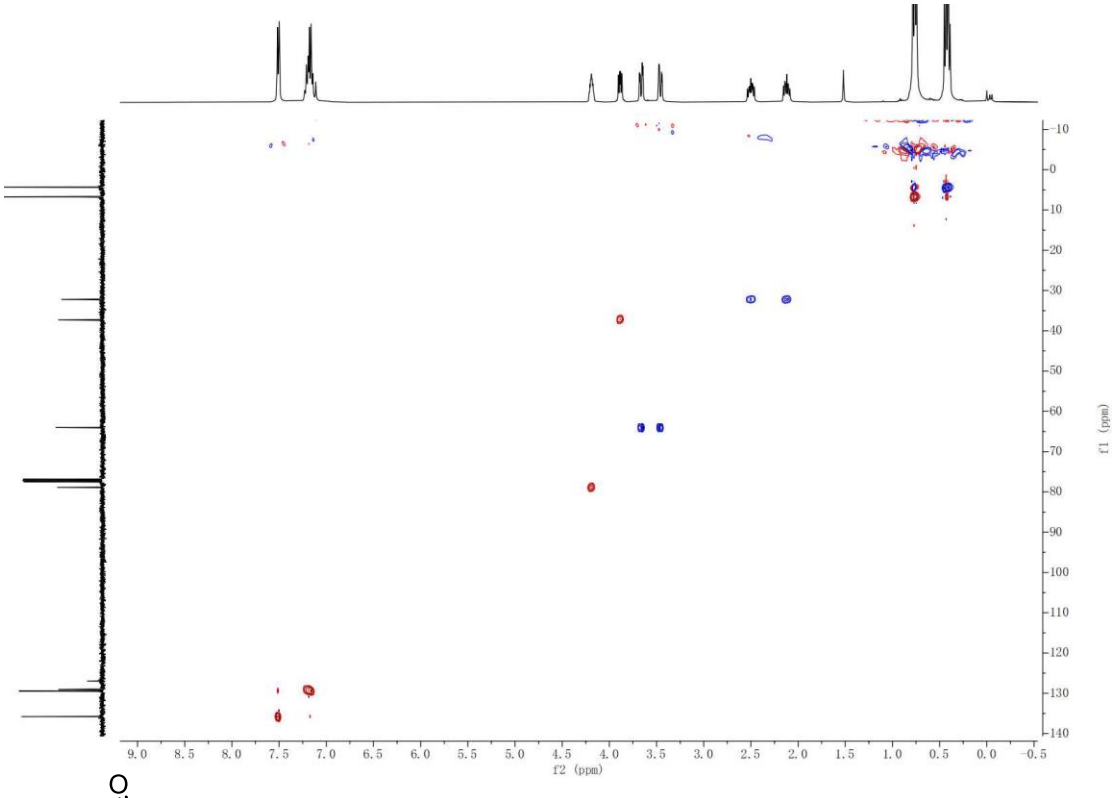


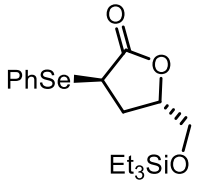
12

HMBC spectrum of **12**



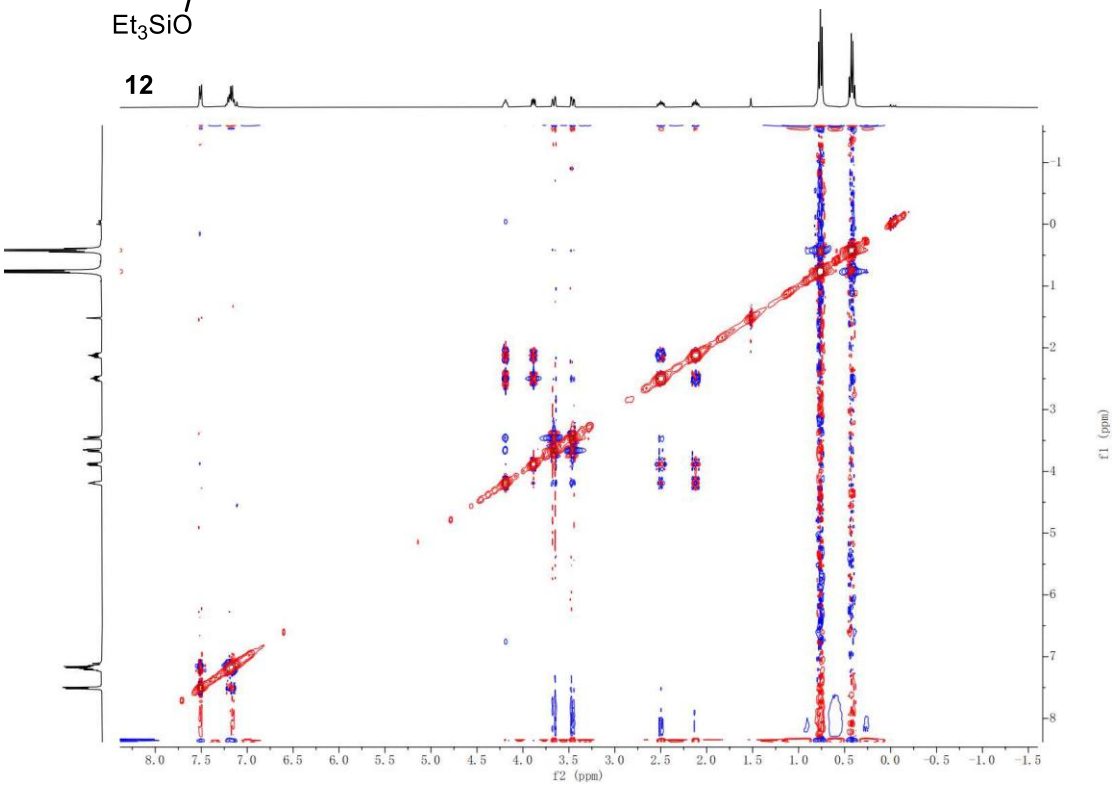
HSQC spectrum of **12**



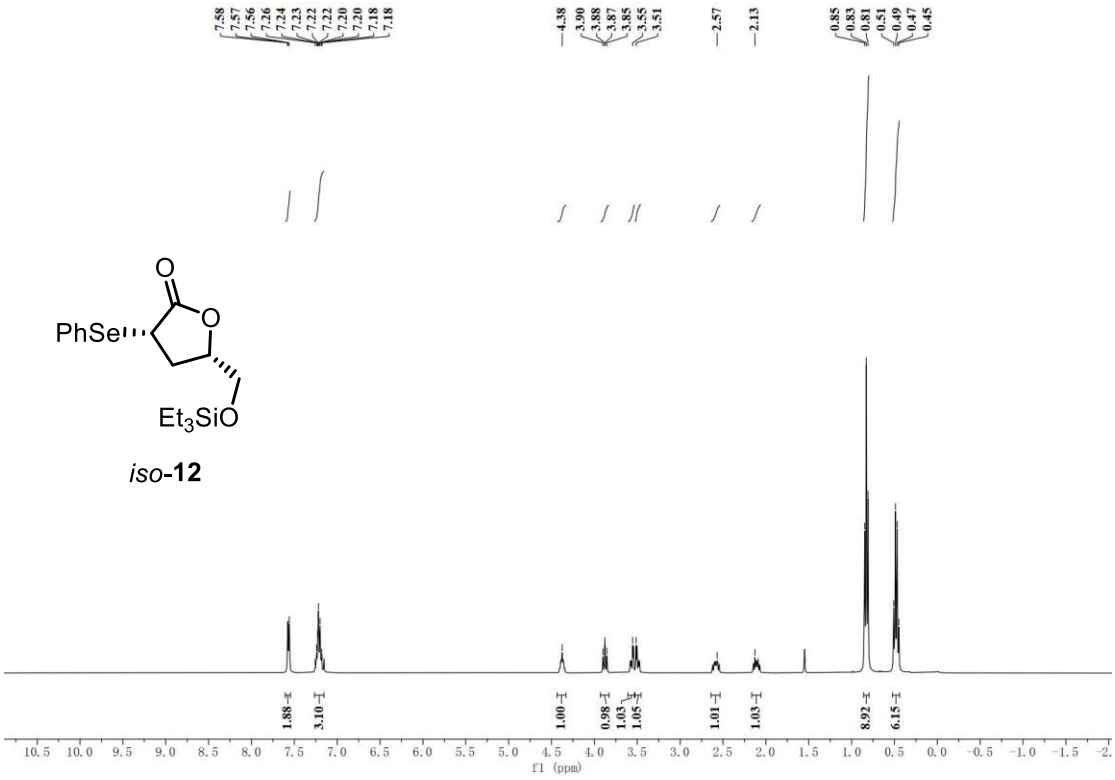


NOESY spectrum of **12**

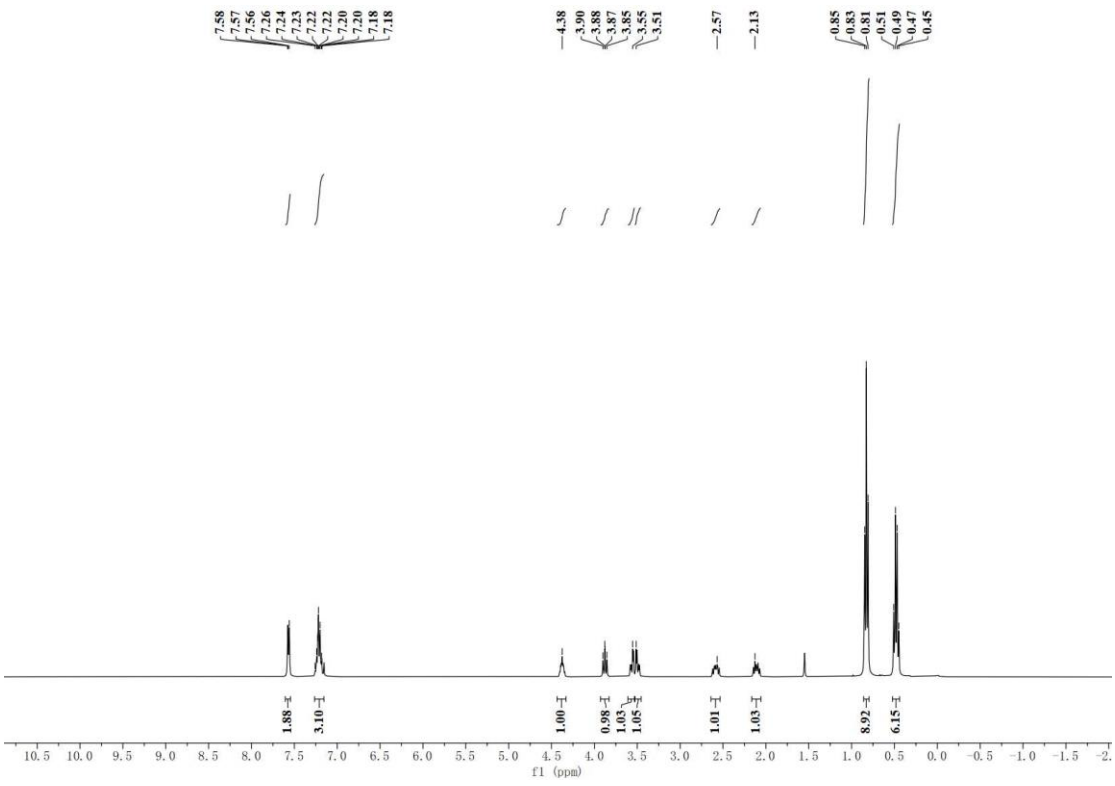
12



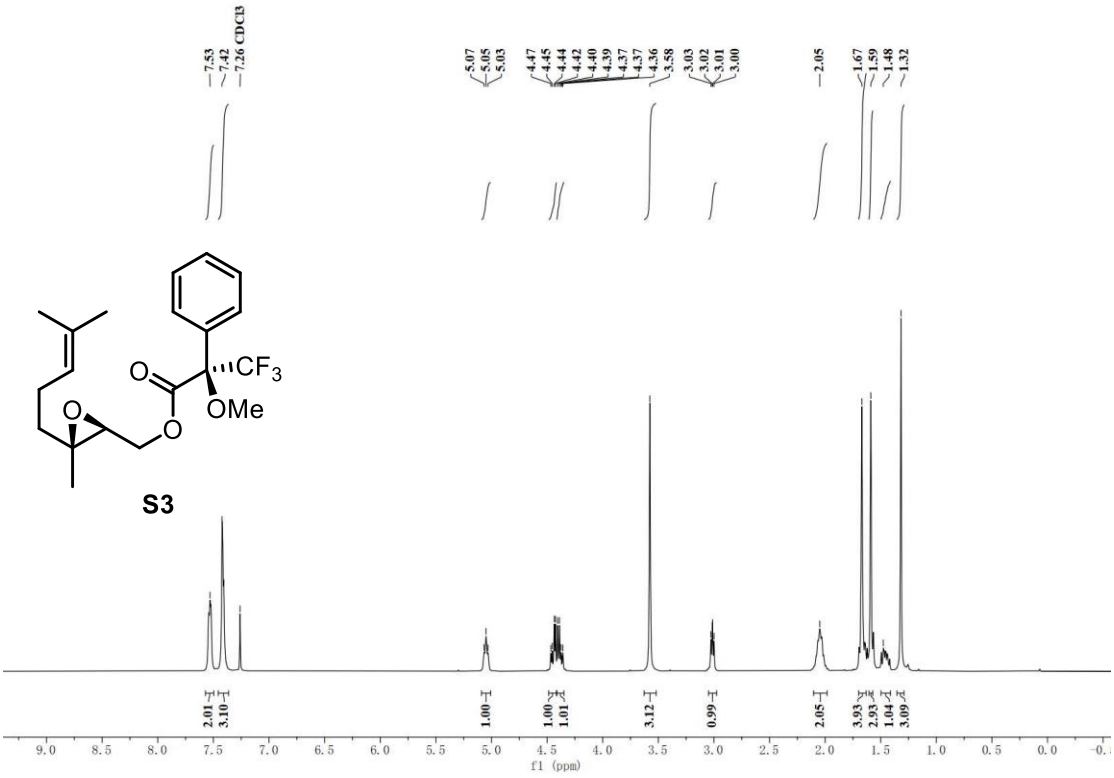
^{1}H NMR spectrum of *iso*-**12**(400 MHz, $CDCl_3$)



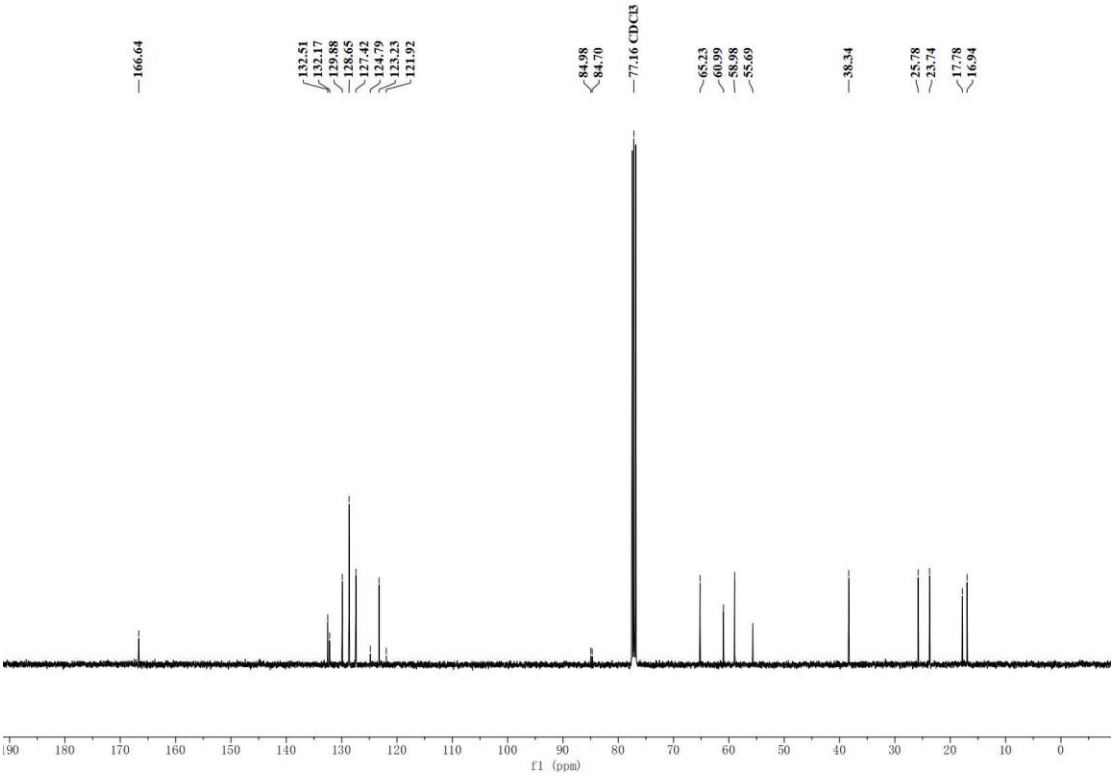
^{13}C NMR spectrum of *iso*-**12** (100 MHz, $CDCl_3$)



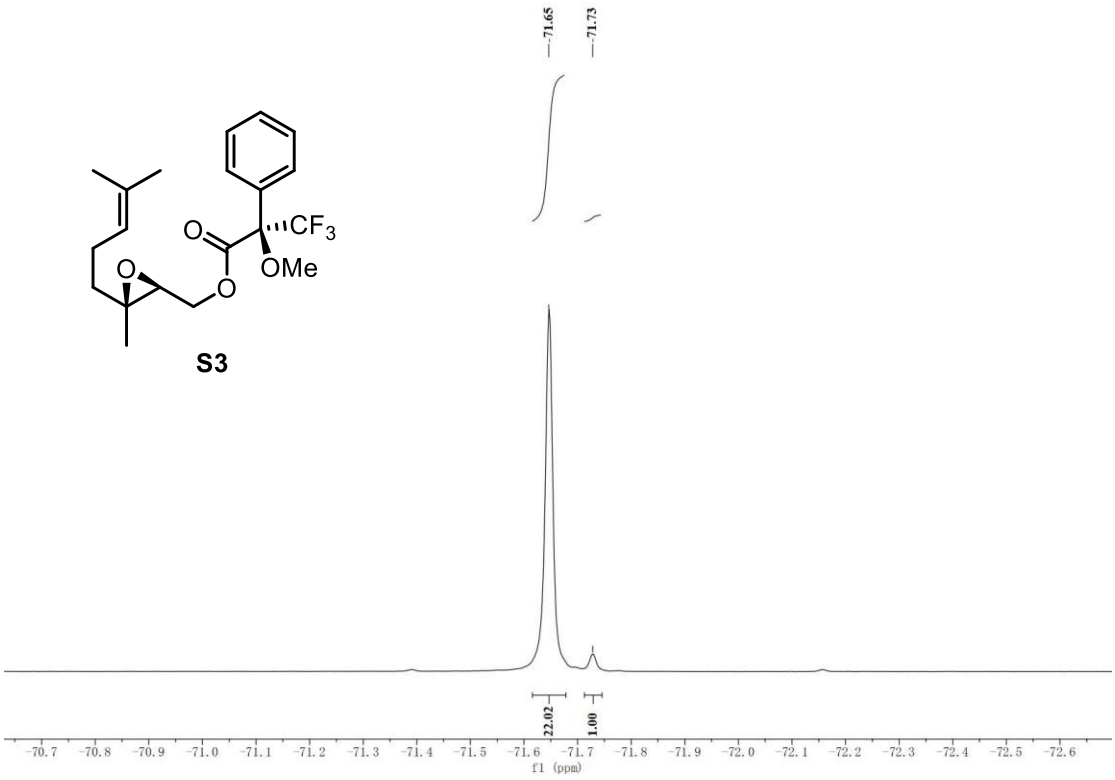
^{1}H NMR spectrum of **MTPA-ester S3** (400 MHz, $CDCl_3$)



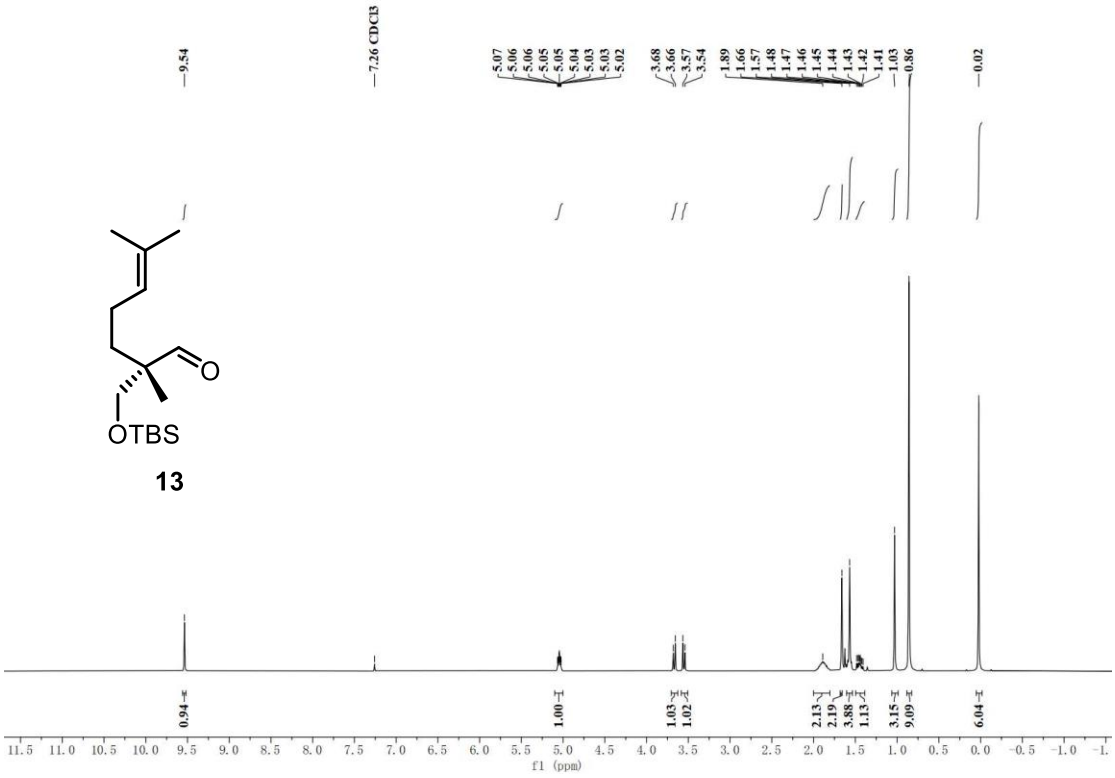
^{13}C NMR spectrum of **MTPA-ester S3** (100 MHz, $CDCl_3$)



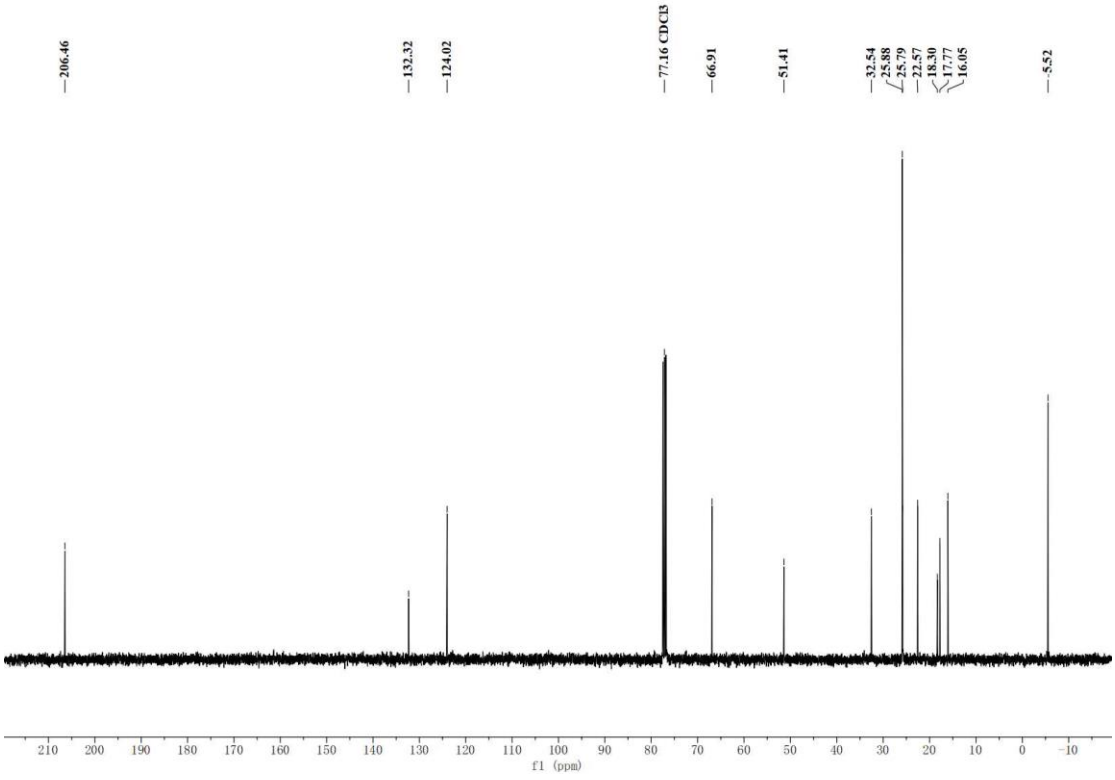
^{19}F NMR spectrum of **S3** (376 MHz, $CDCl_3$)



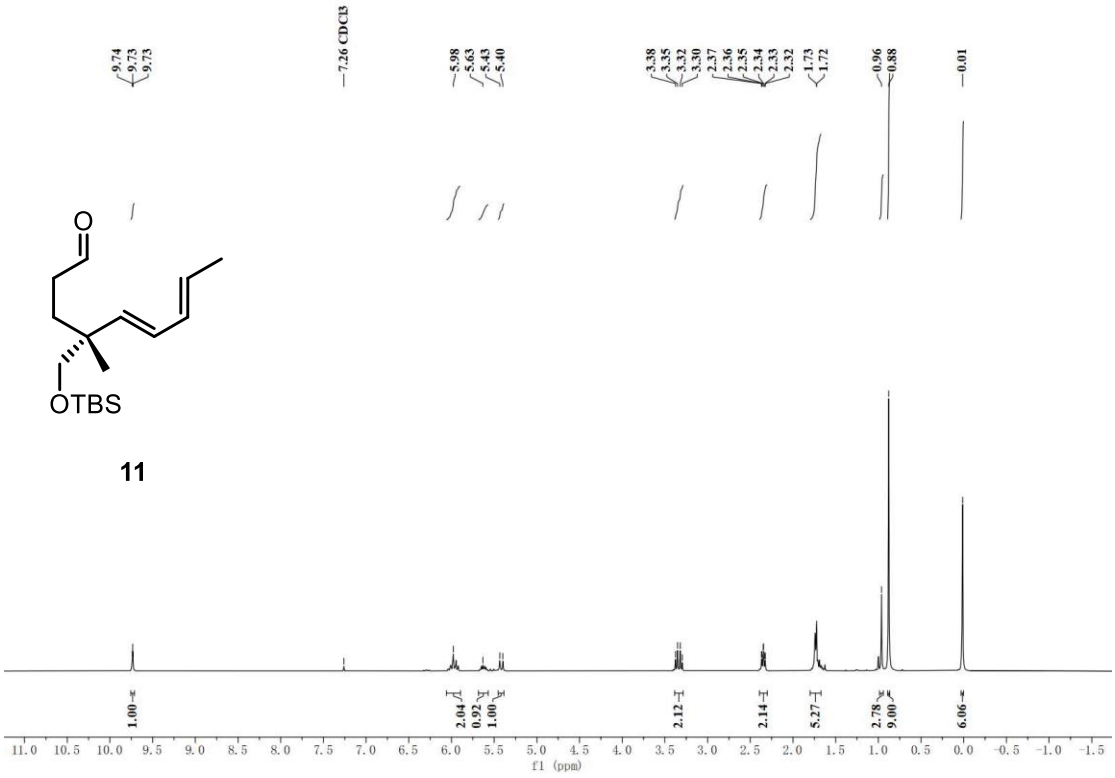
^{1}H NMR spectrum of **13** (400 MHz, $CDCl_3$)



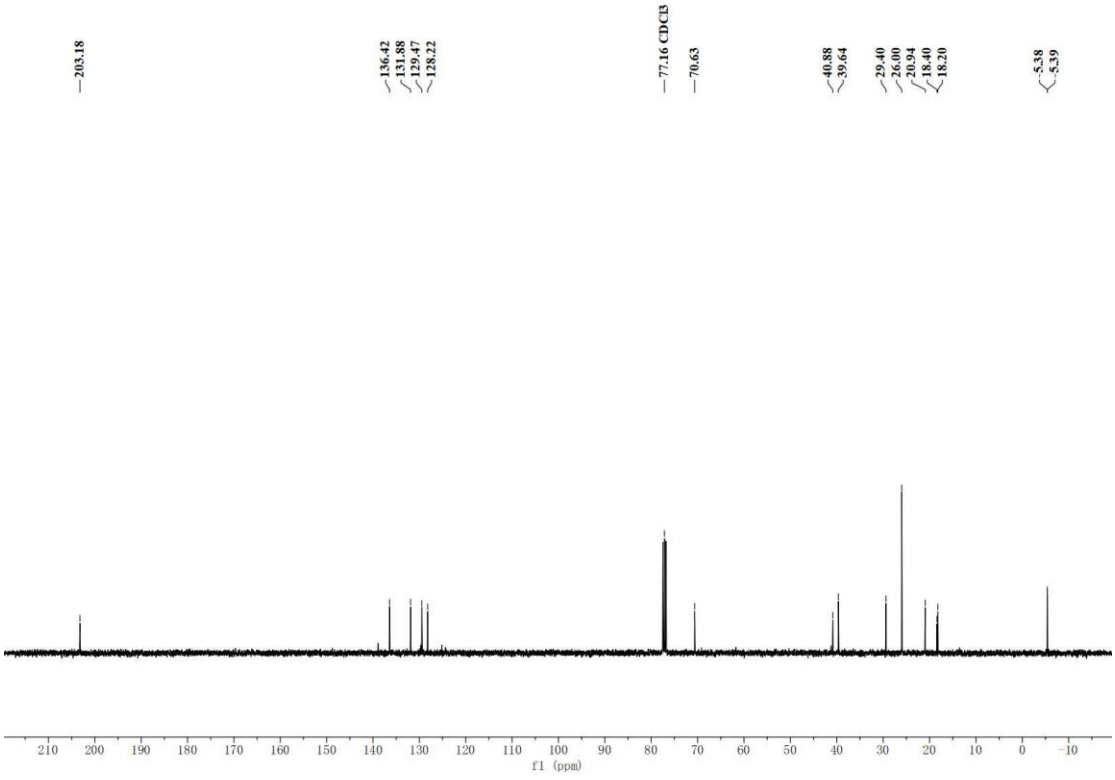
^{13}C NMR spectrum of **13** (100 MHz, $CDCl_3$)



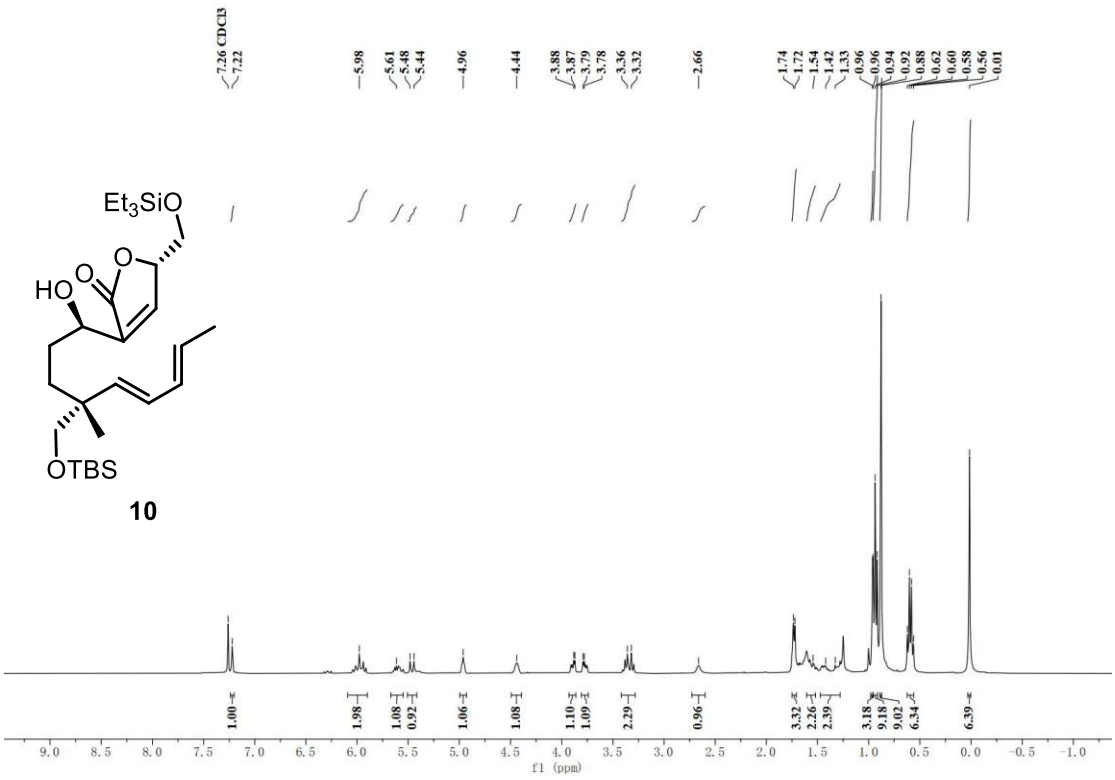
^{1}H NMR spectrum of **11** (400 MHz, $CDCl_3$)



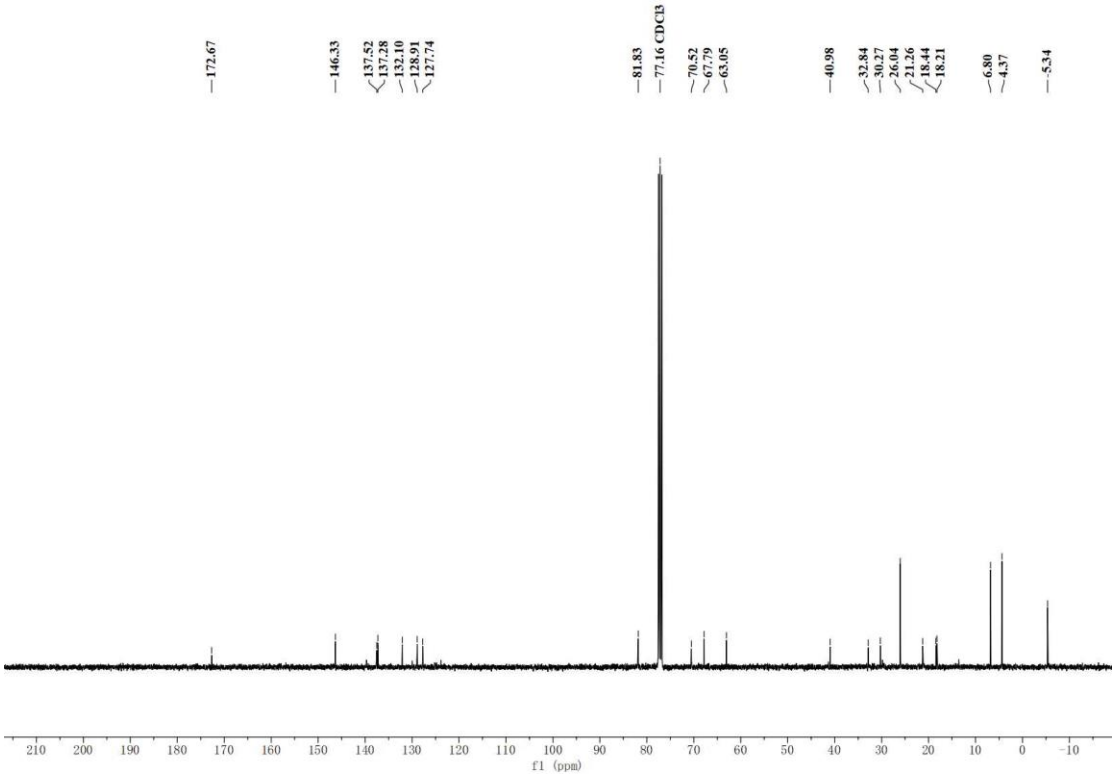
^{13}C NMR spectrum of **11** (100 MHz, $CDCl_3$)



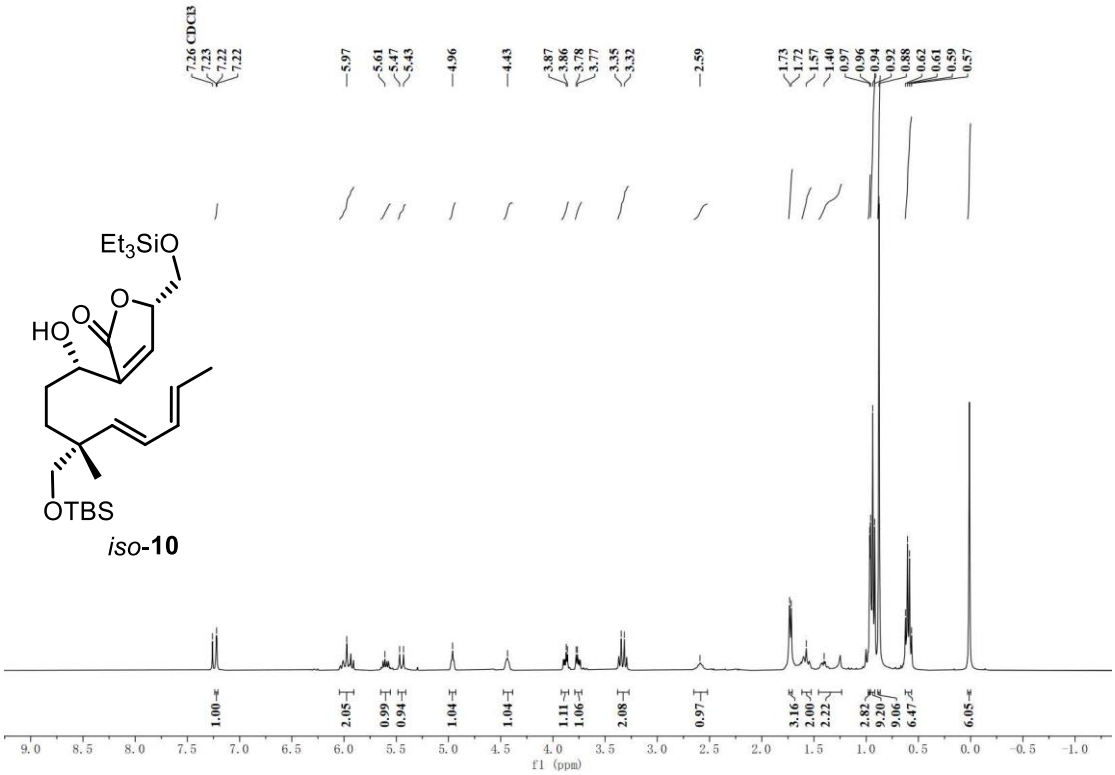
^{1}H NMR spectrum of **10** (400 MHz, $CDCl_3$)



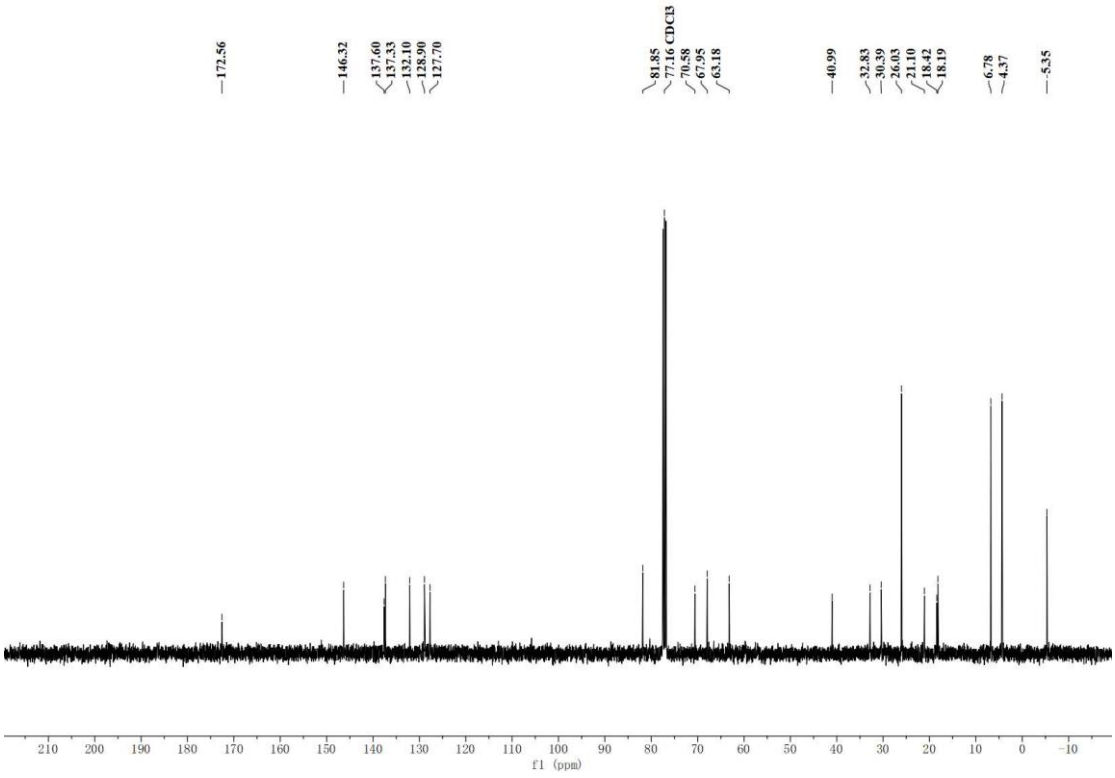
^{13}C NMR spectrum of **10** (100 MHz, $CDCl_3$)



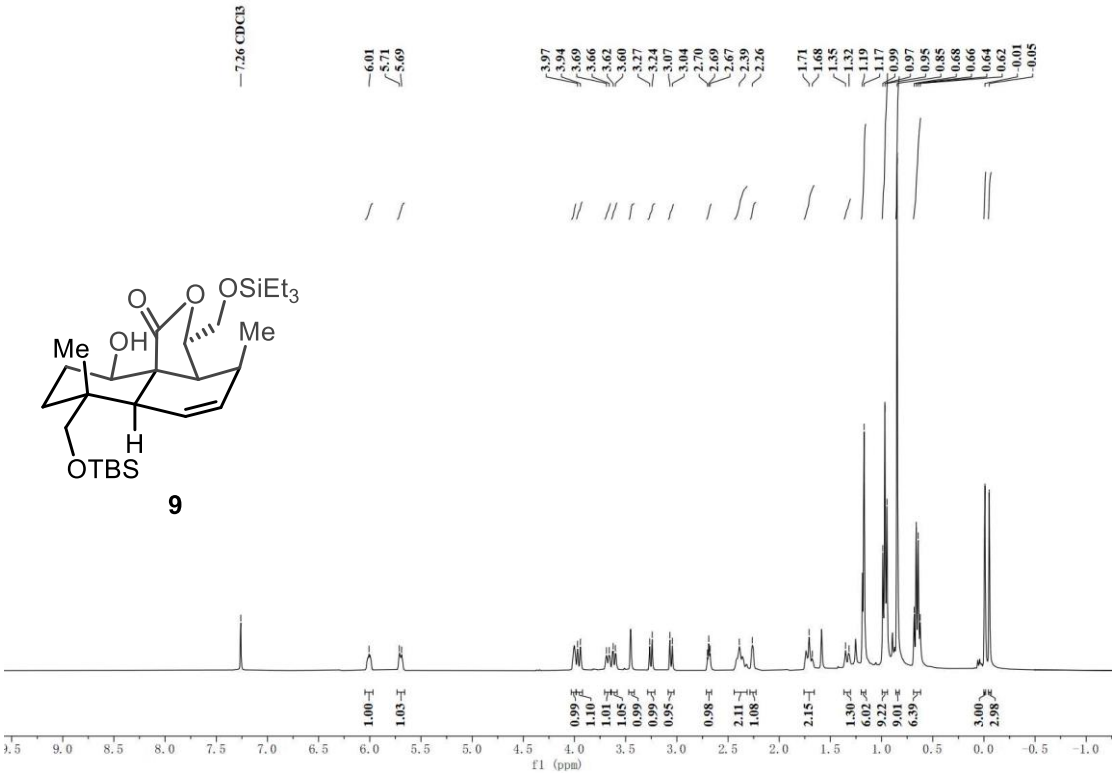
^{1}H NMR spectrum of *iso*-**10** (400 MHz, $CDCl_3$)



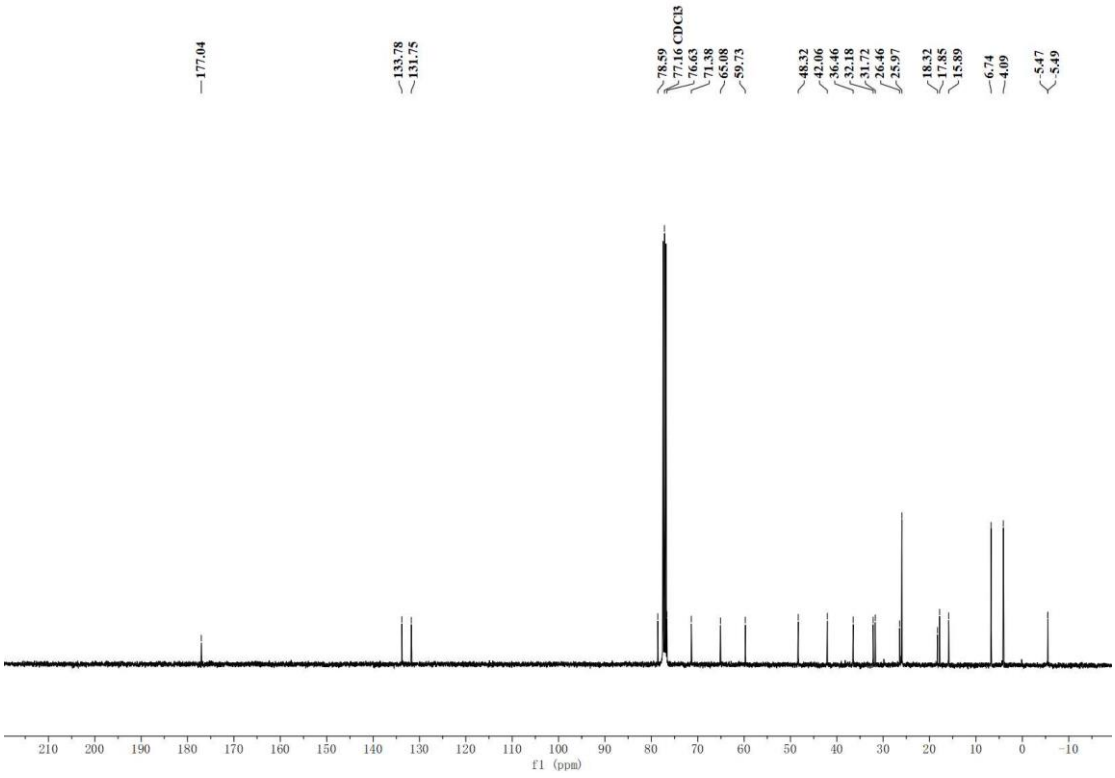
^{13}C NMR spectrum of *iso*-**10** (100 MHz, $CDCl_3$)



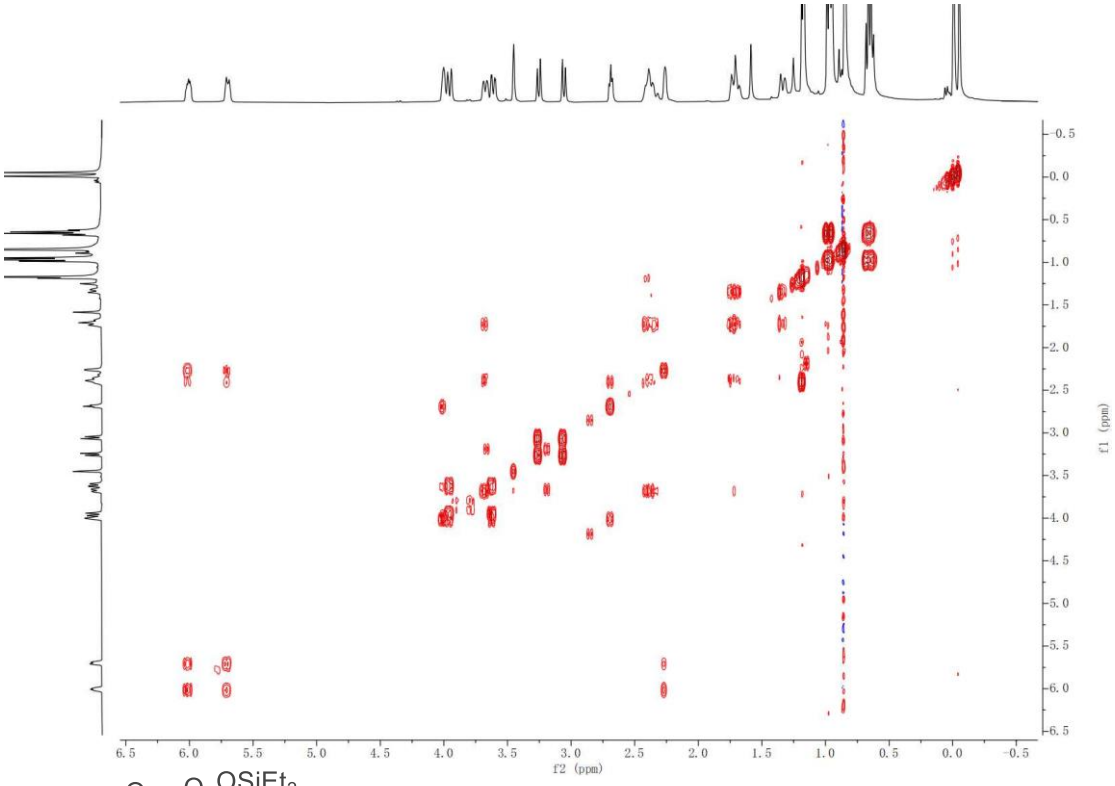
^{1}H NMR spectrum of **9**(400 MHz, $CDCl_3$)

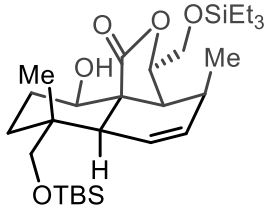


^{13}C NMR spectrum of **9** (100 MHz, $CDCl_3$)

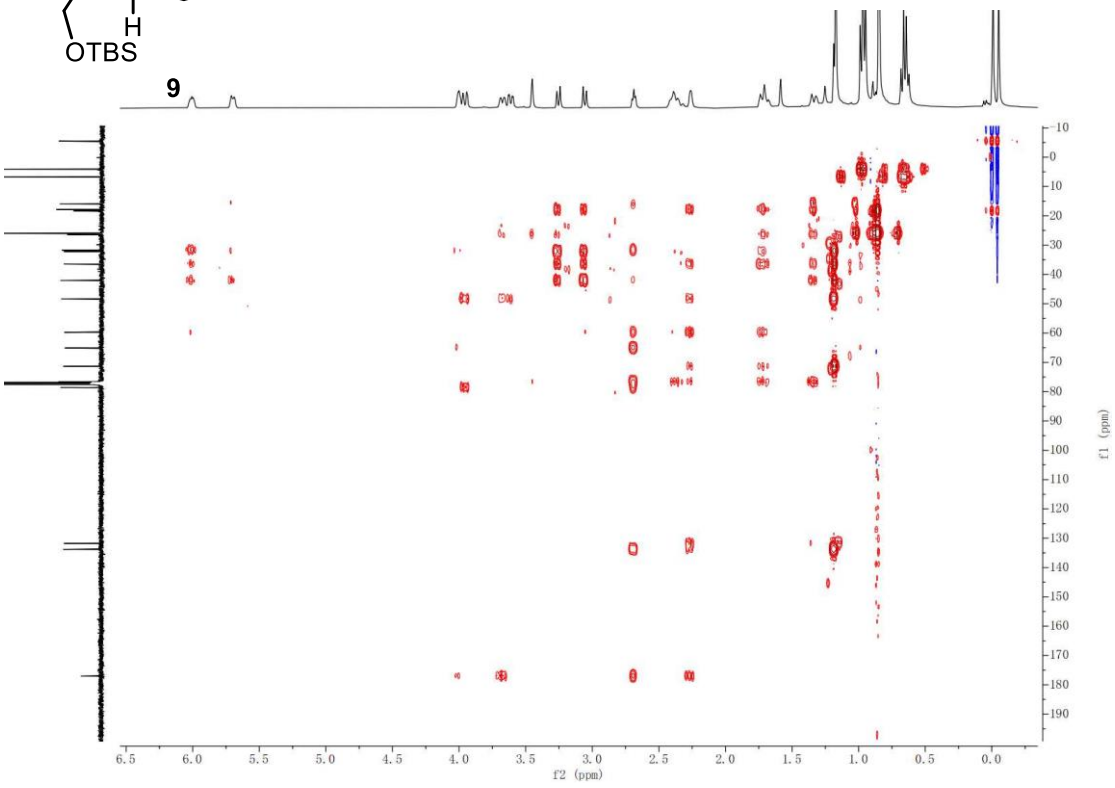


^{1}H-^{1}H COSY spectrum of **9**

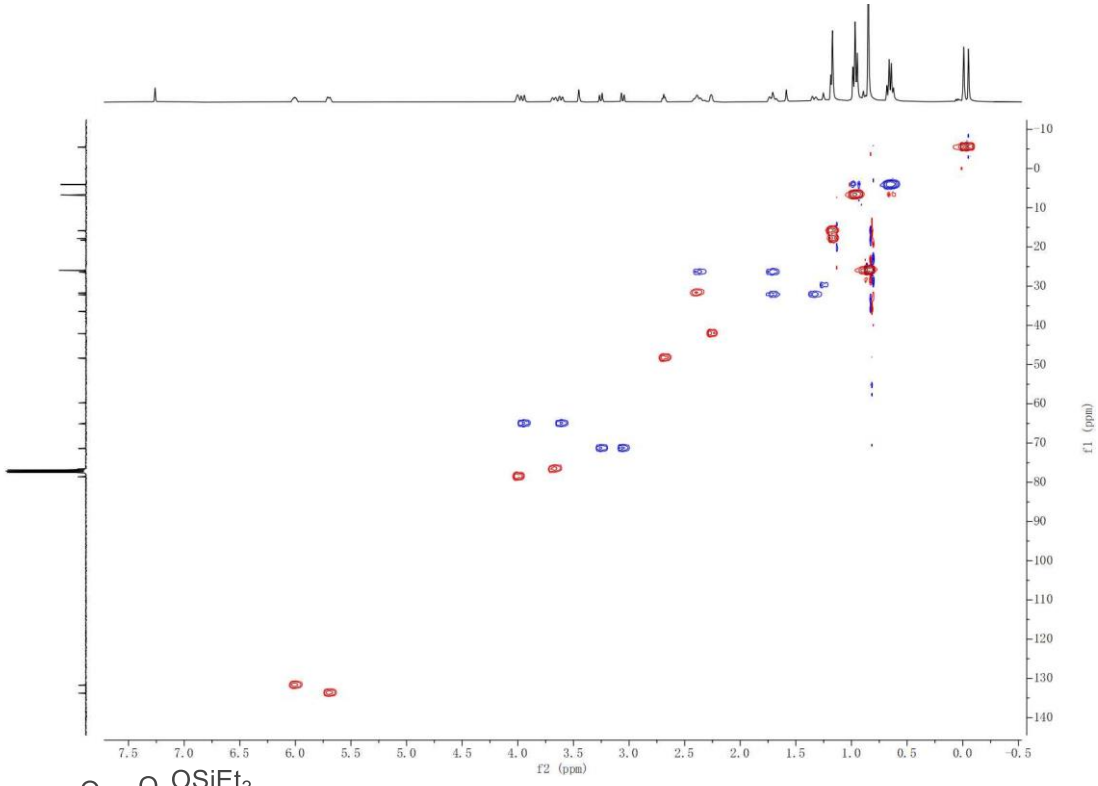


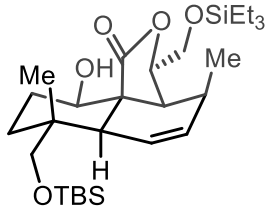


HMBC spectrum of **9**



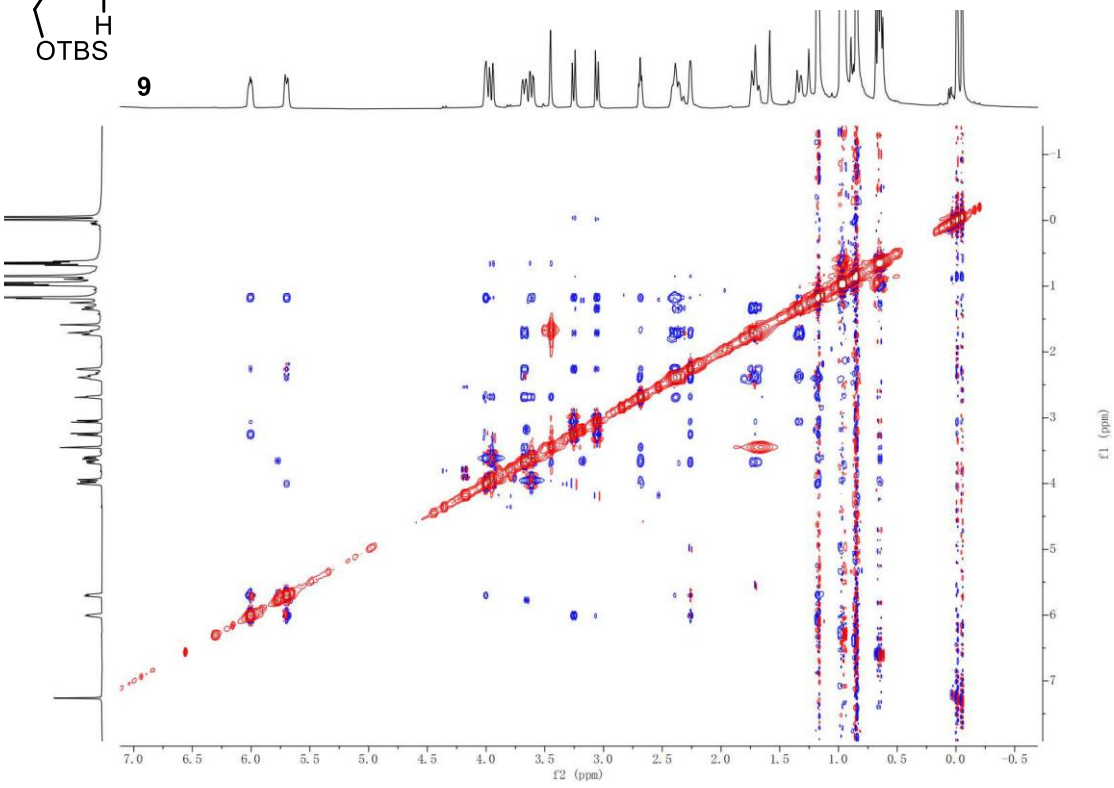
HSQC spectrum of **9**



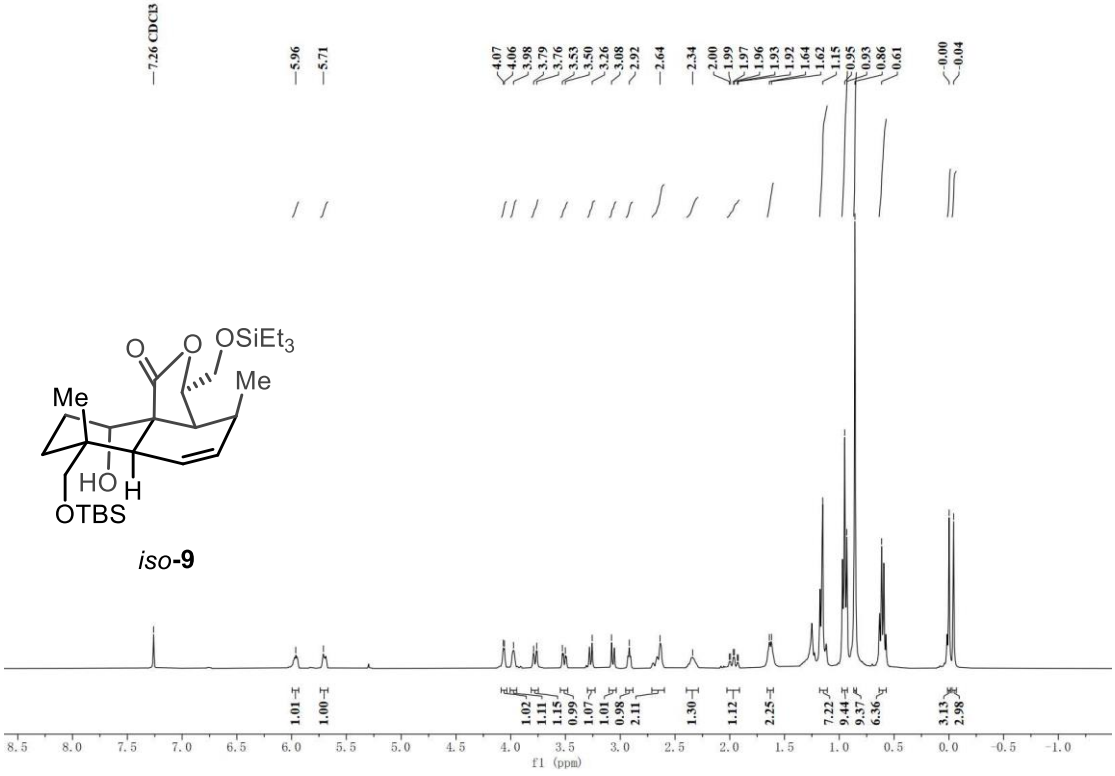


NOESY spectrum of **9**

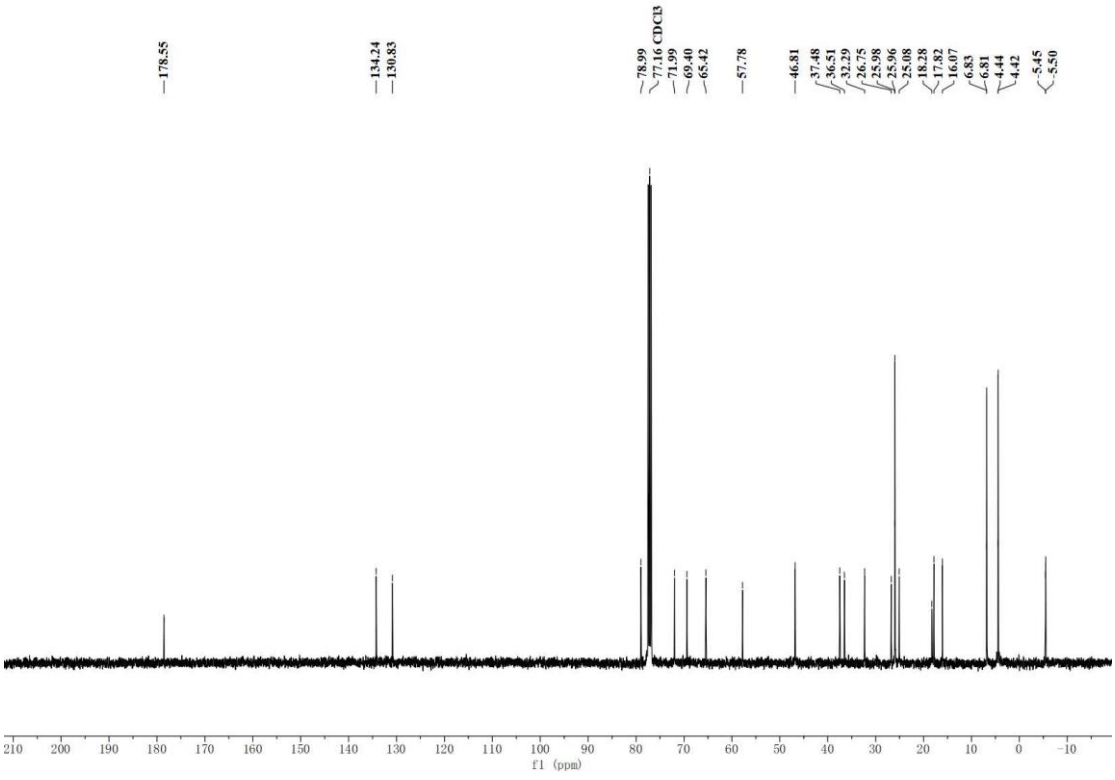
9



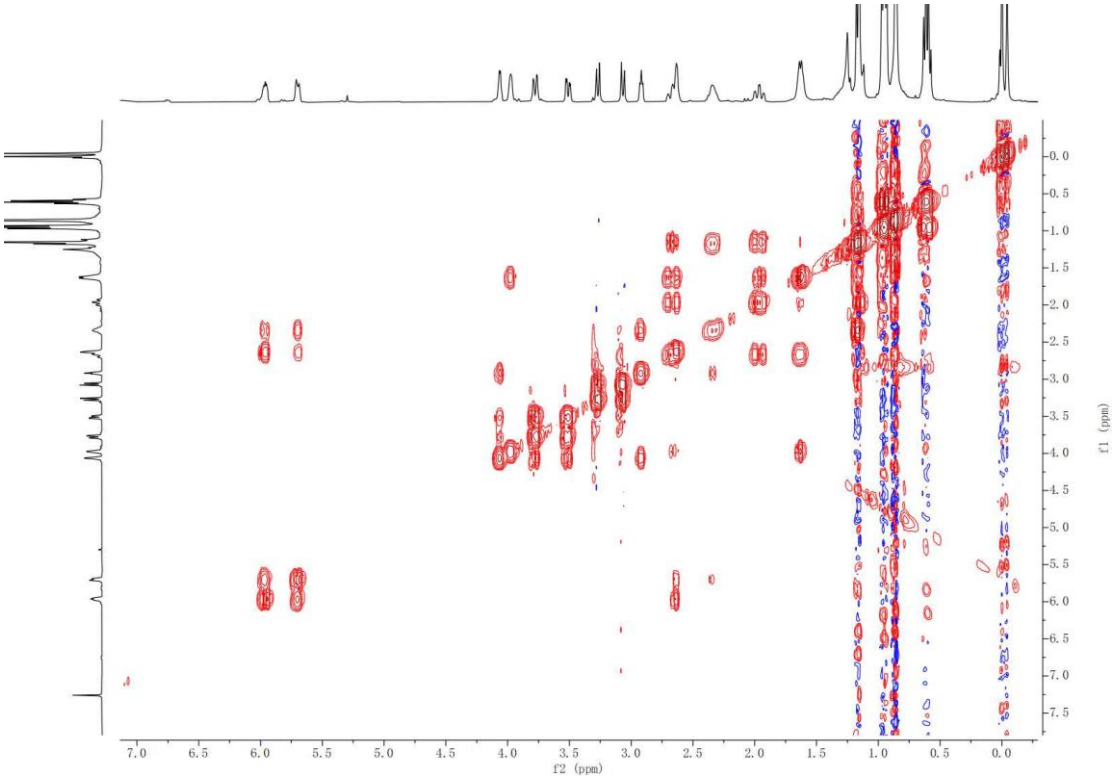
^{1}H NMR spectrum of *iso*-**9** (400 MHz, $CDCl_3$)

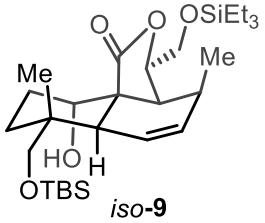


^{13}C NMR spectrum of *iso*-**9** (100 MHz, $CDCl_3$)



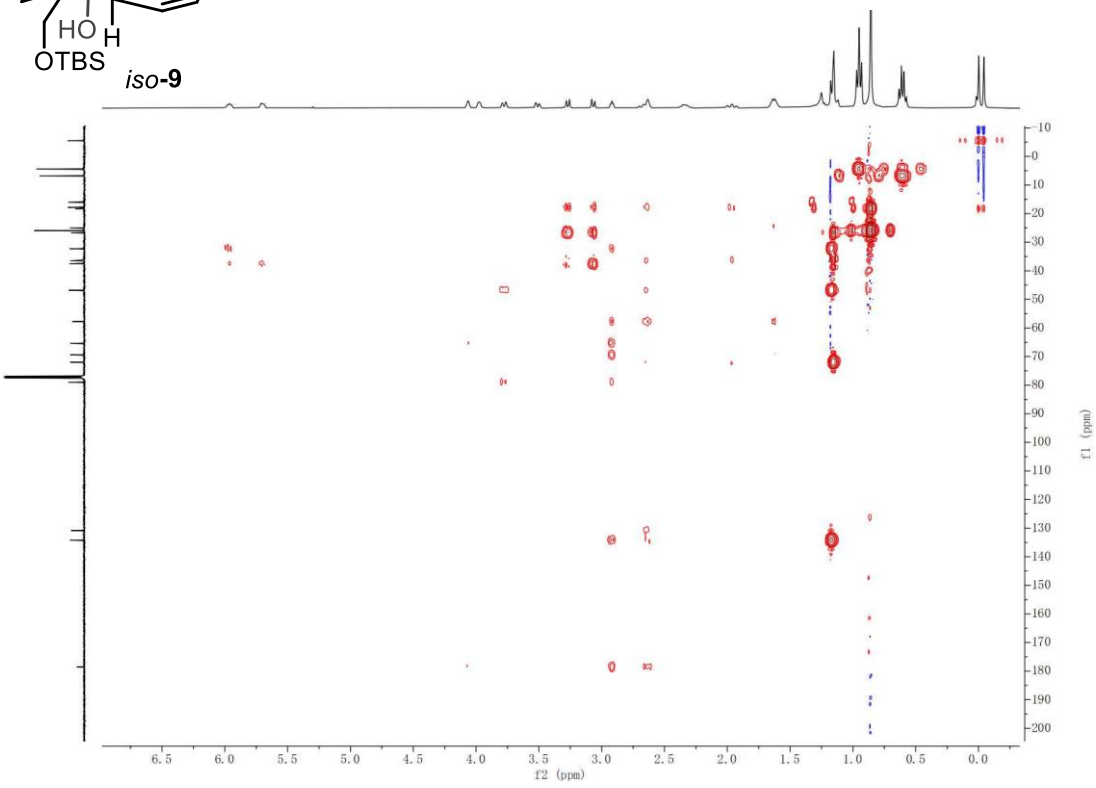
^{1}H-^{1}H COSY spectrum of *iso*-**9**



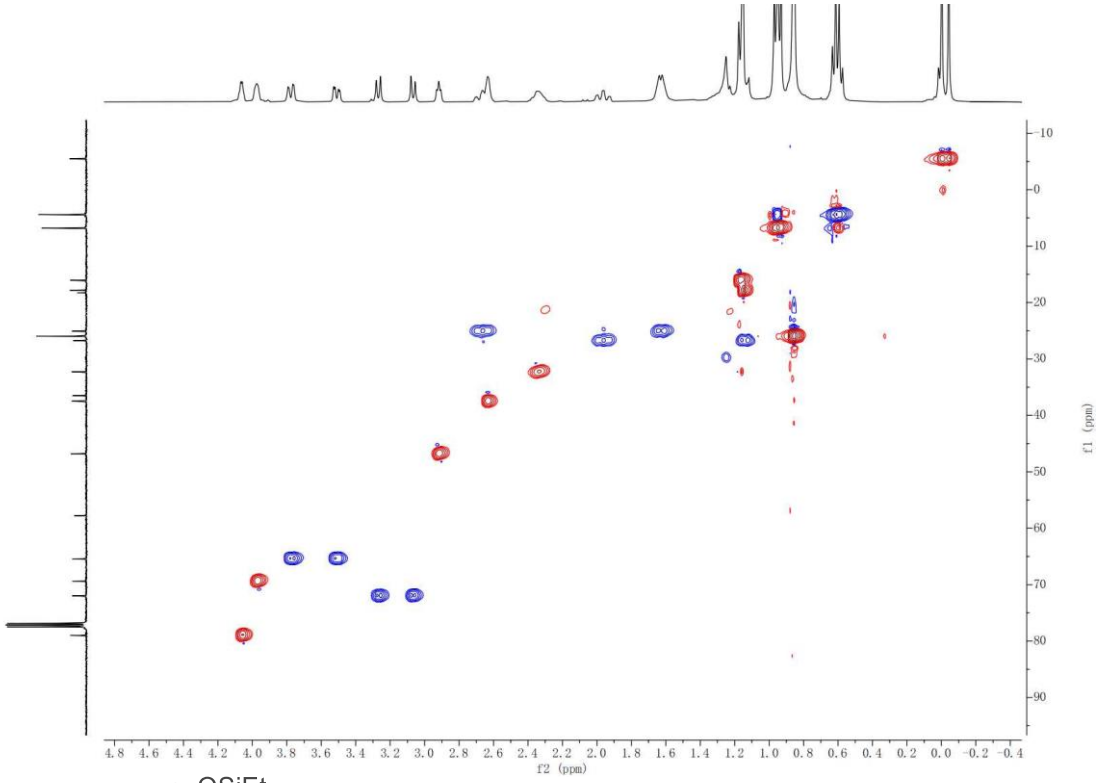


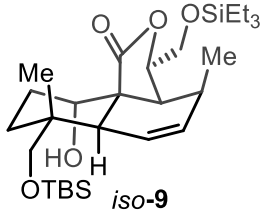
iso-**9**

HMBC spectrum of *iso*-**9**



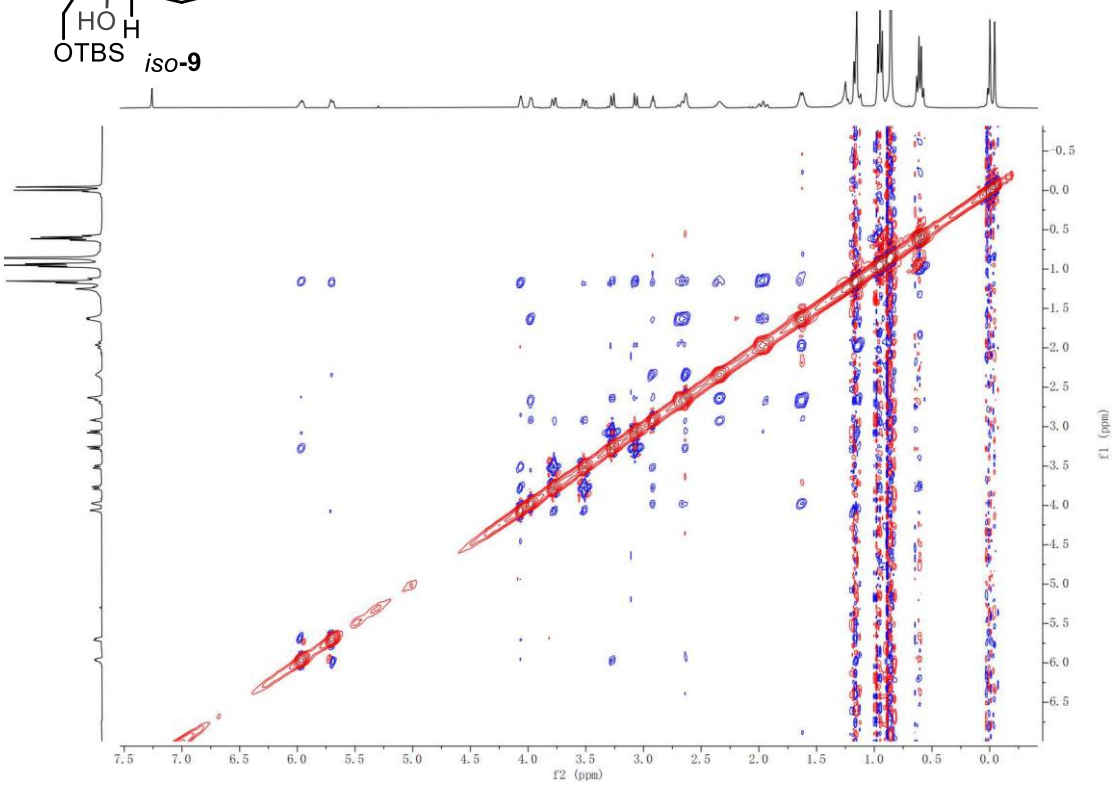
HSQC spectrum of *iso*-**9**



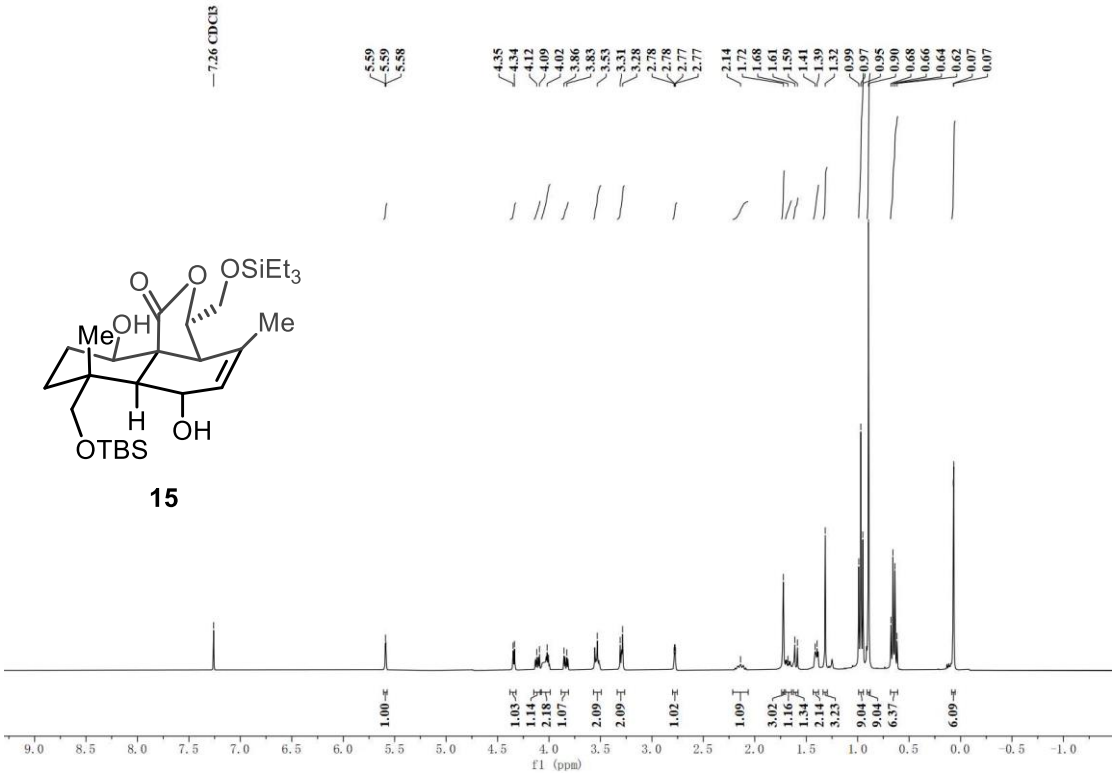


iso-**9**

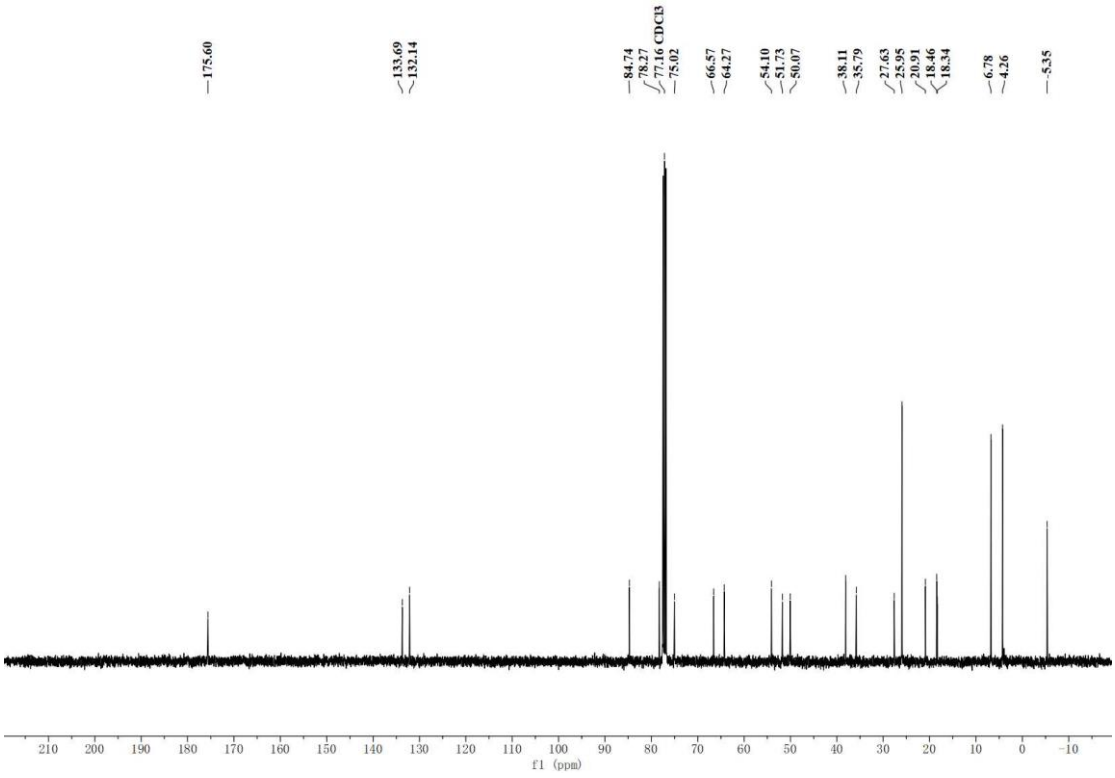
NOESY spectrum of *iso*-**9**



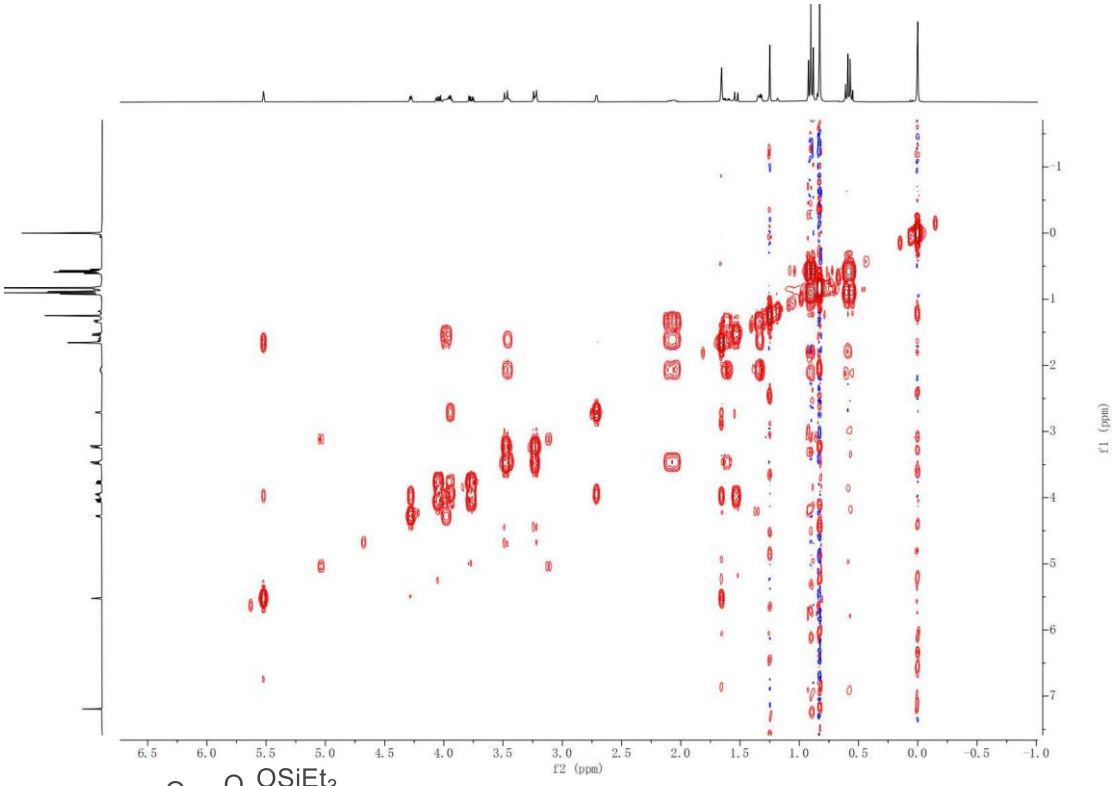
^{1}H NMR spectrum of **15** (400 MHz, $CDCl_3$)

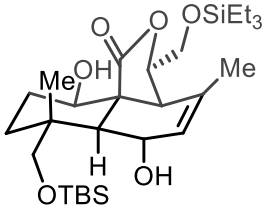


^{13}C NMR spectrum of **15** (100 MHz, $CDCl_3$)



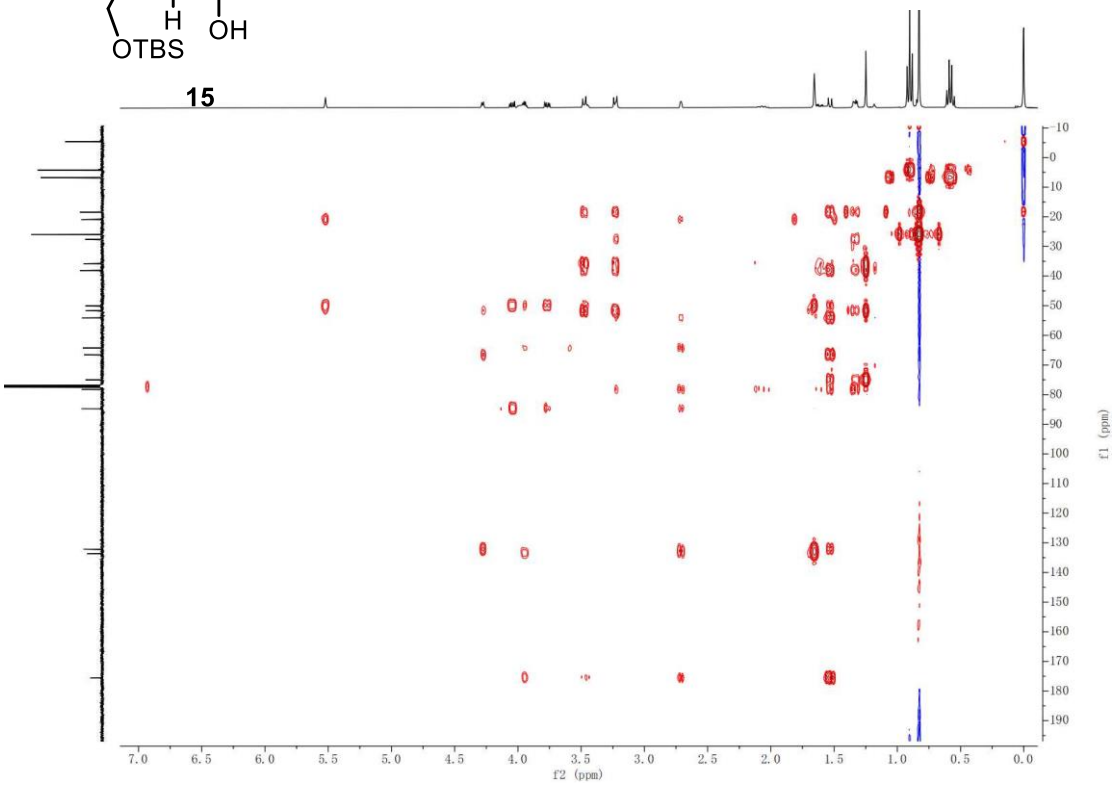
^{1}H-^{1}H COSY spectrum of **15**



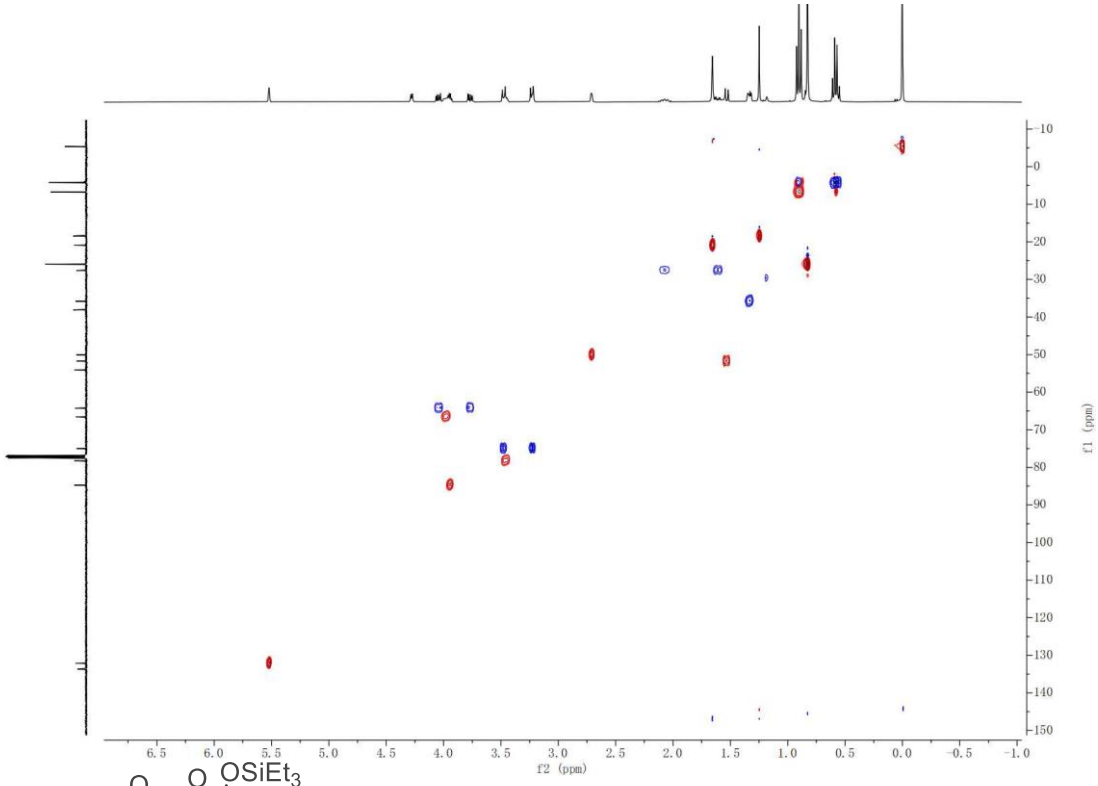


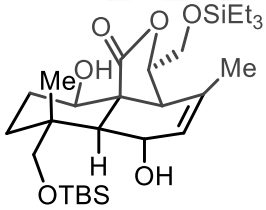
15

HMBC spectrum of **15**



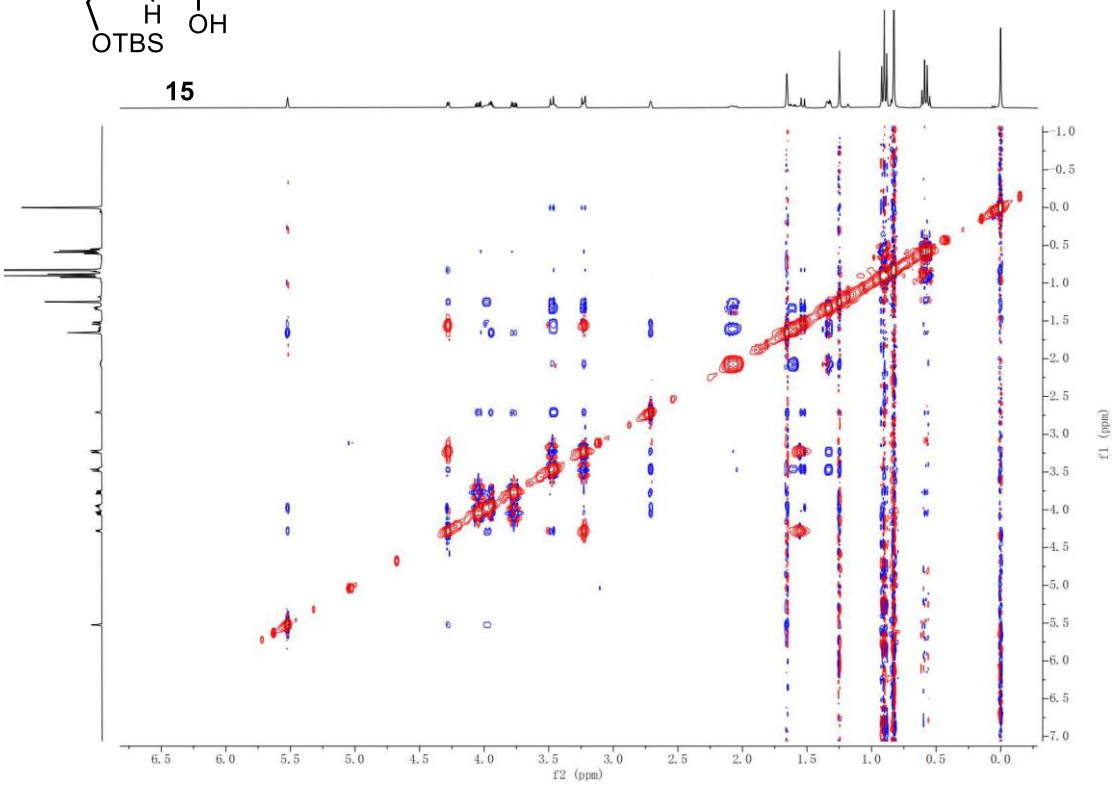
HSQC spectrum of **15**



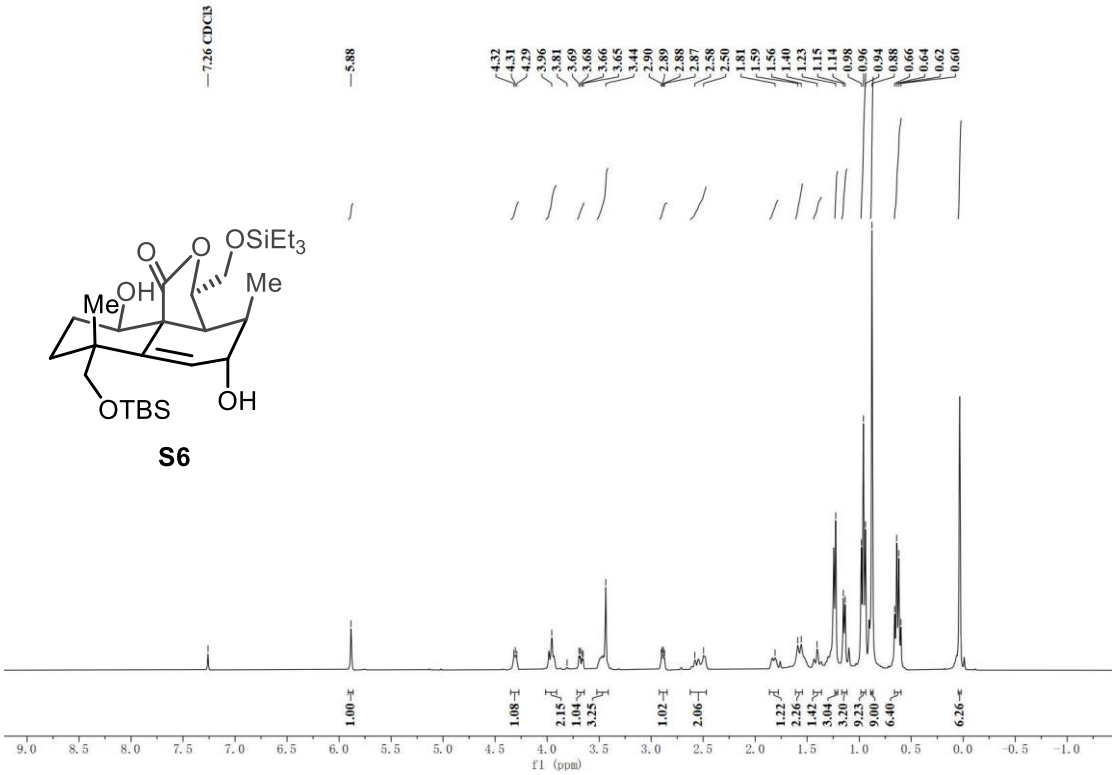


NOESY spectrum of **15**

15

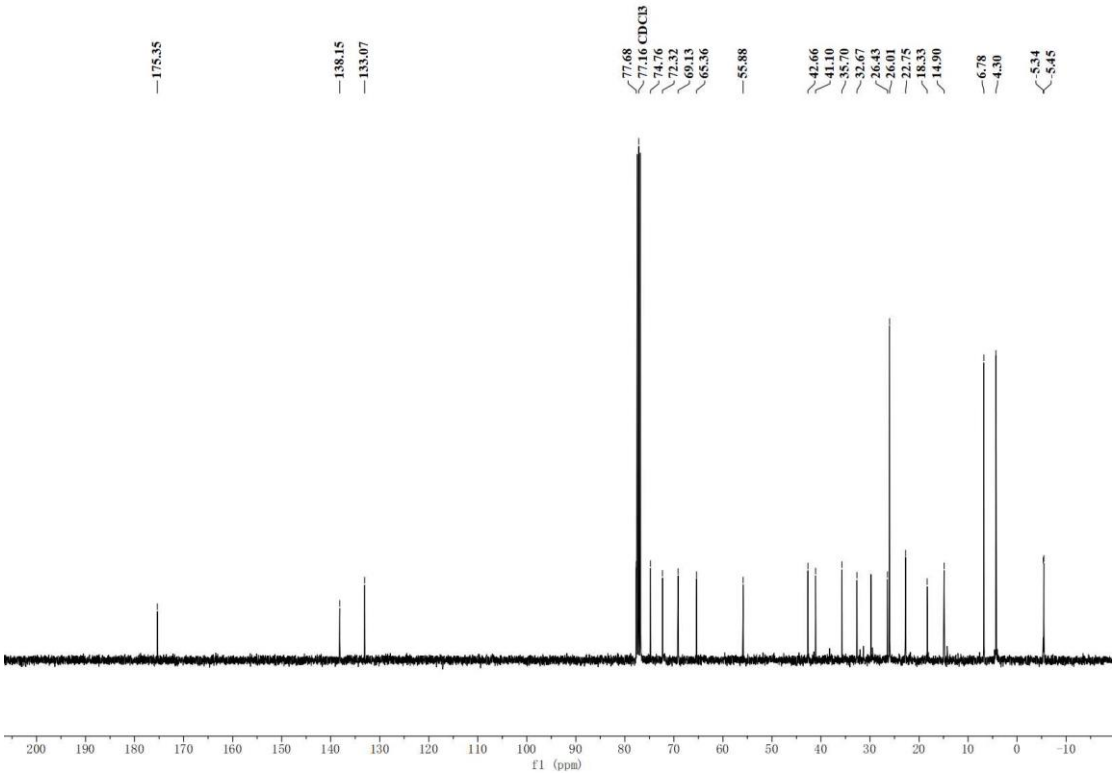


^{1}H NMR spectrum of **S6** (400 MHz, $CDCl_3$)

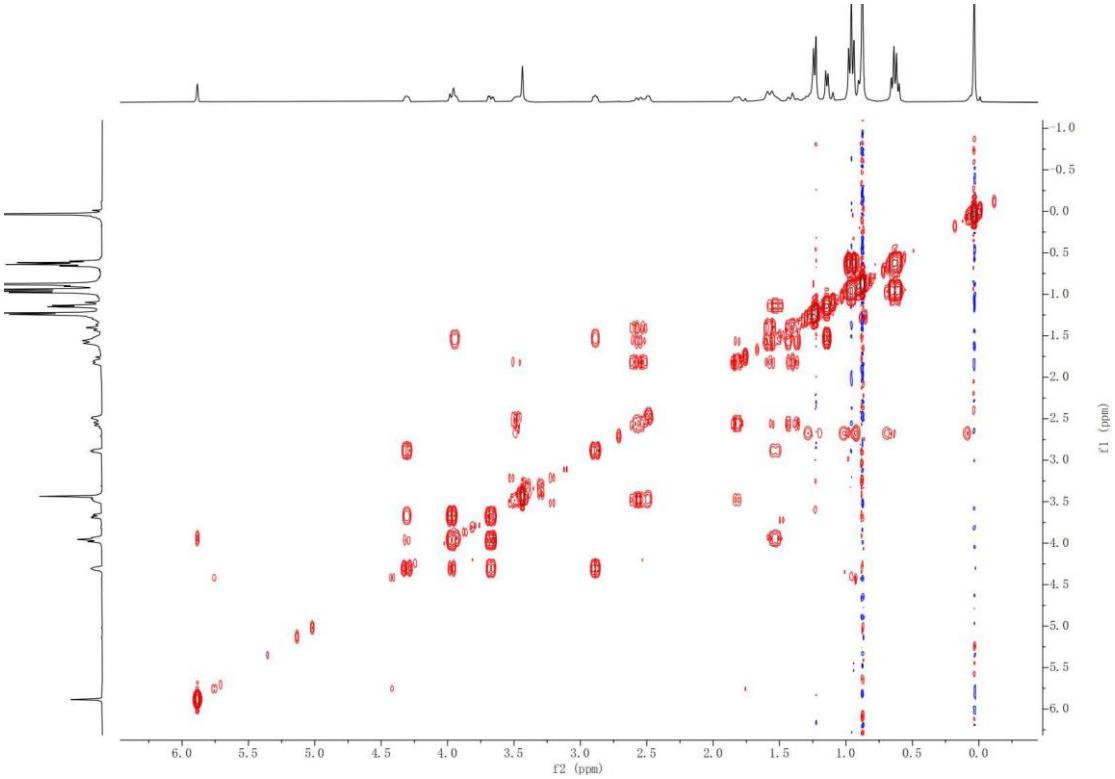


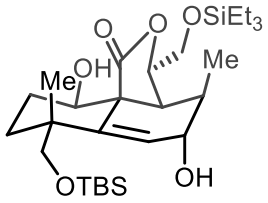
S6

^{13}C NMR spectrum of **S6** (100 MHz, $CDCl_3$)

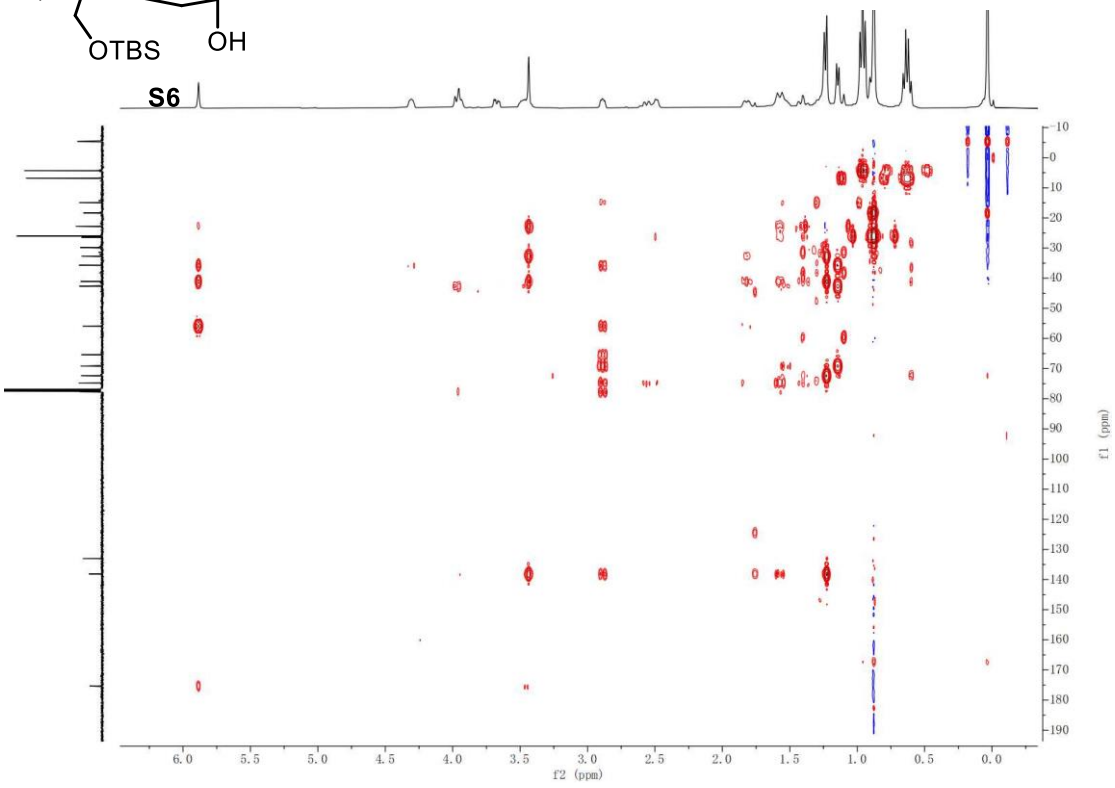


^{1}H-^{1}H COSY spectrum of **S6**

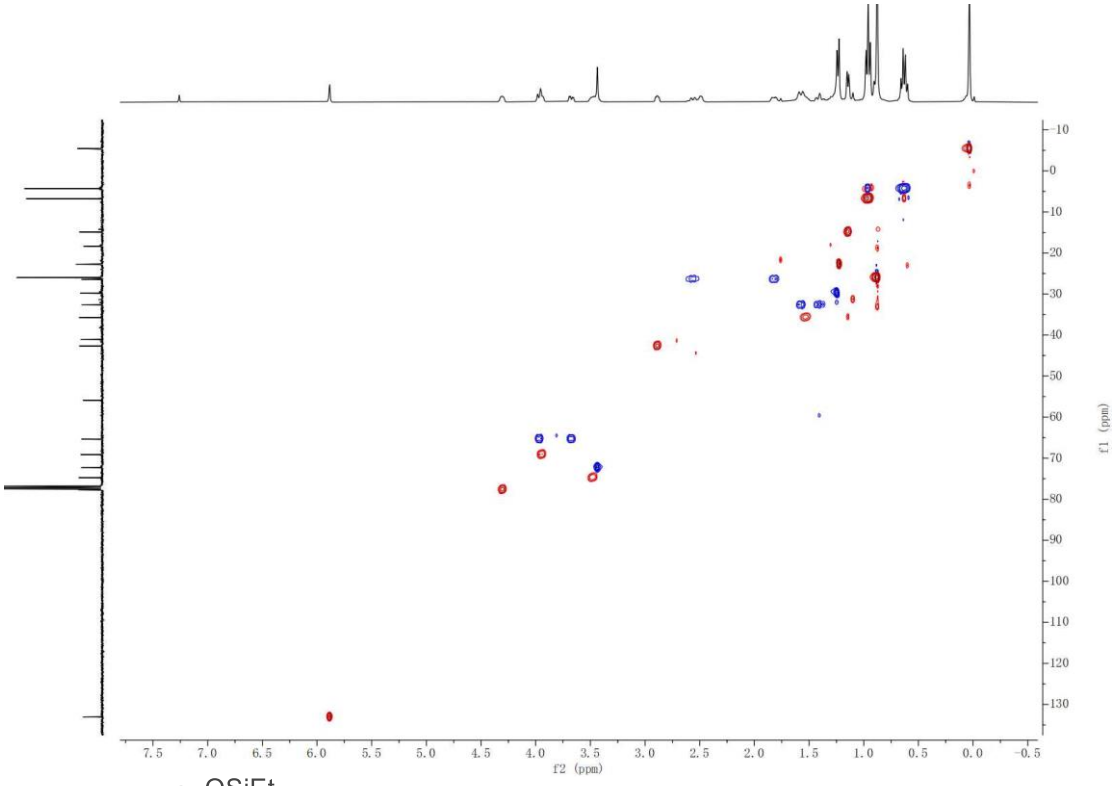


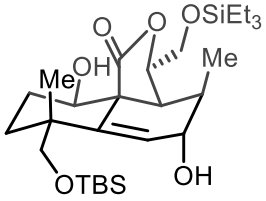


HMBC spectrum of **S6**

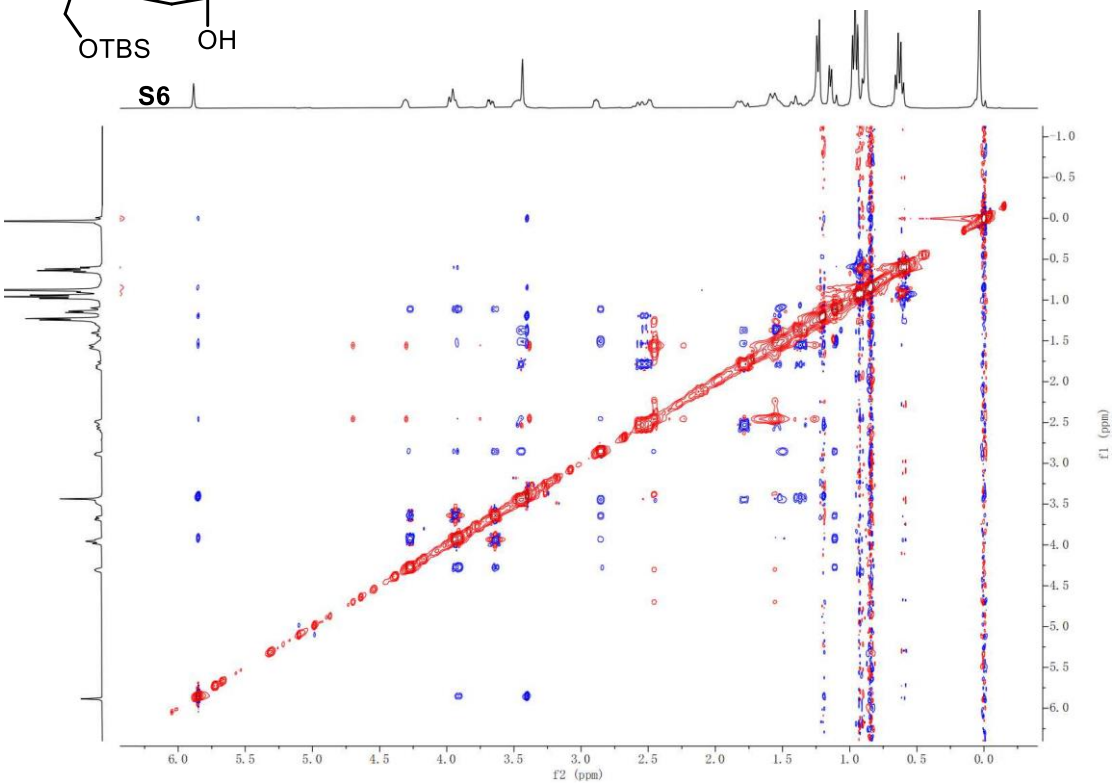


HSQC spectrum of **S6**

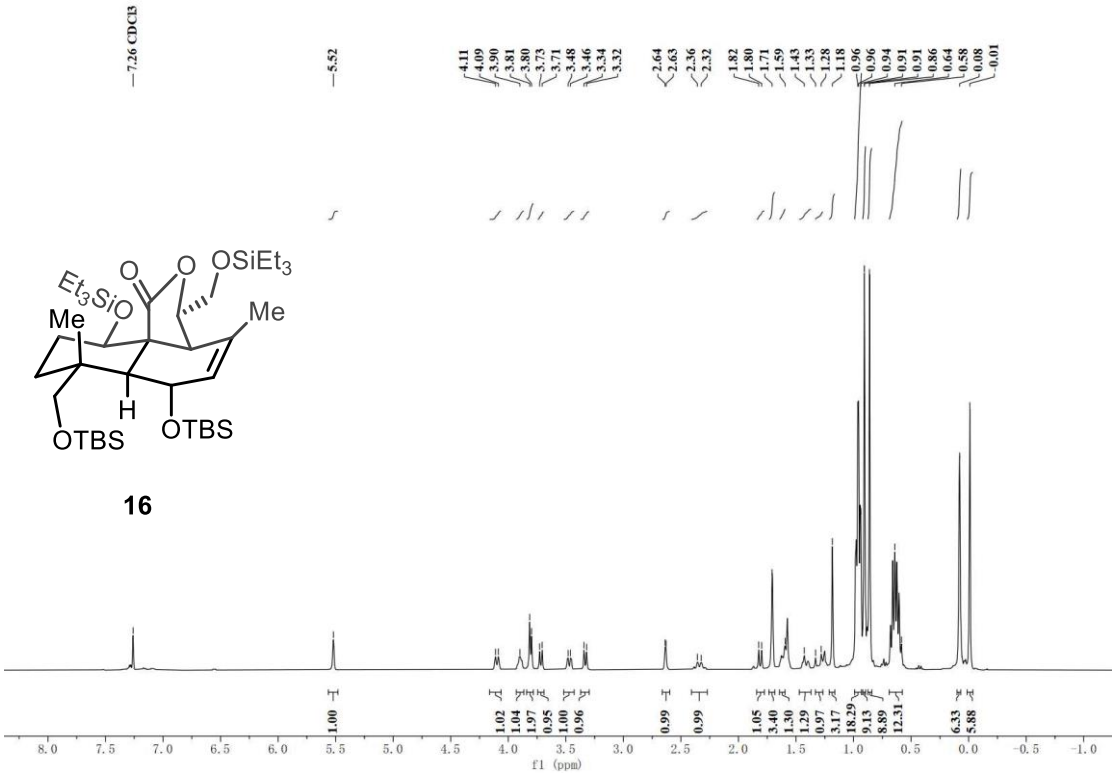




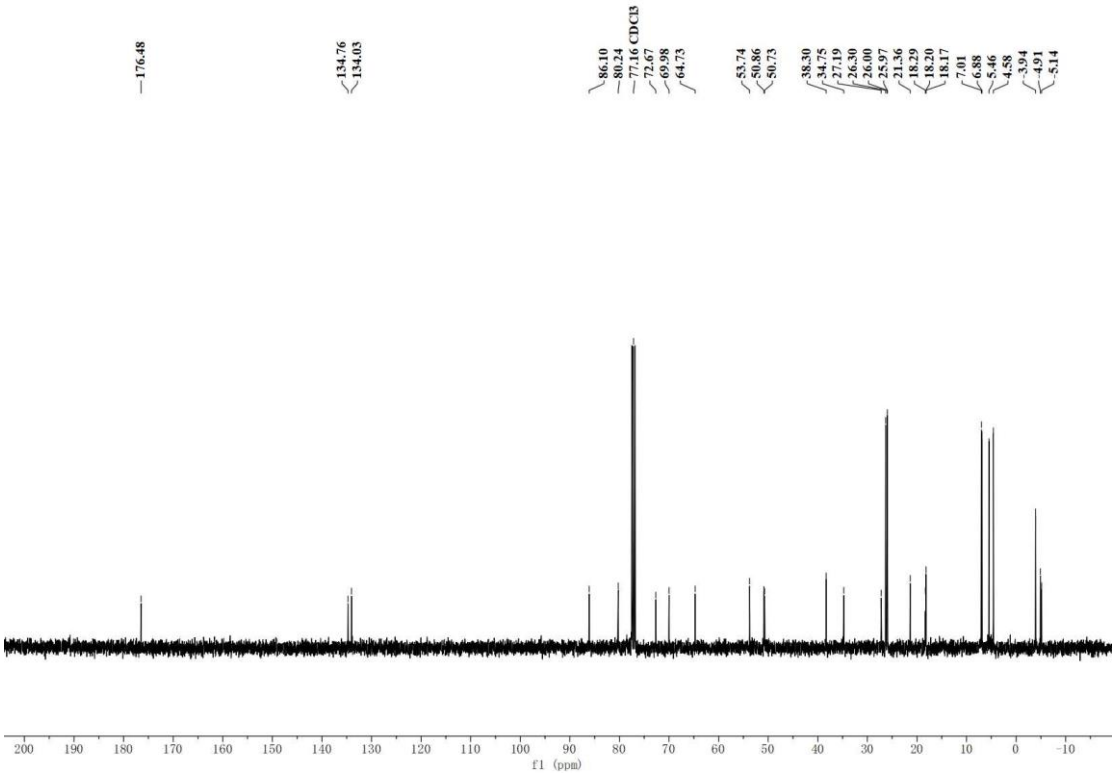
NOESY spectrum of **S6**



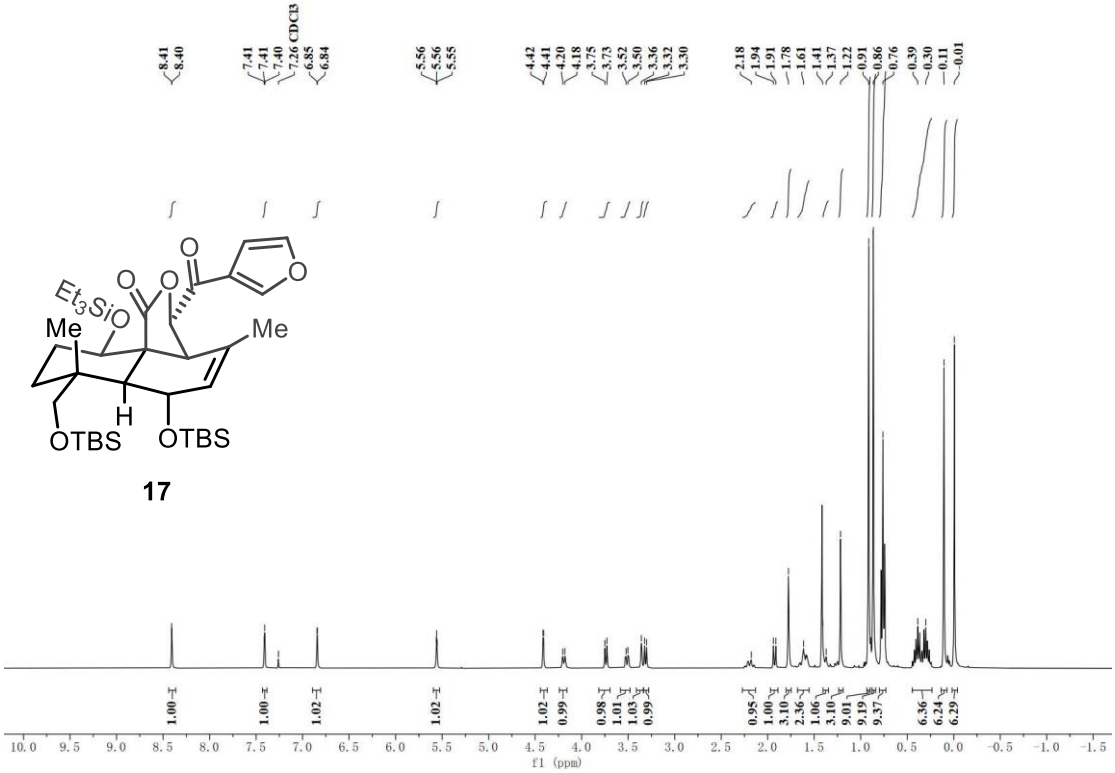
^{1}H NMR spectrum of **16** (400 MHz, $CDCl_3$)



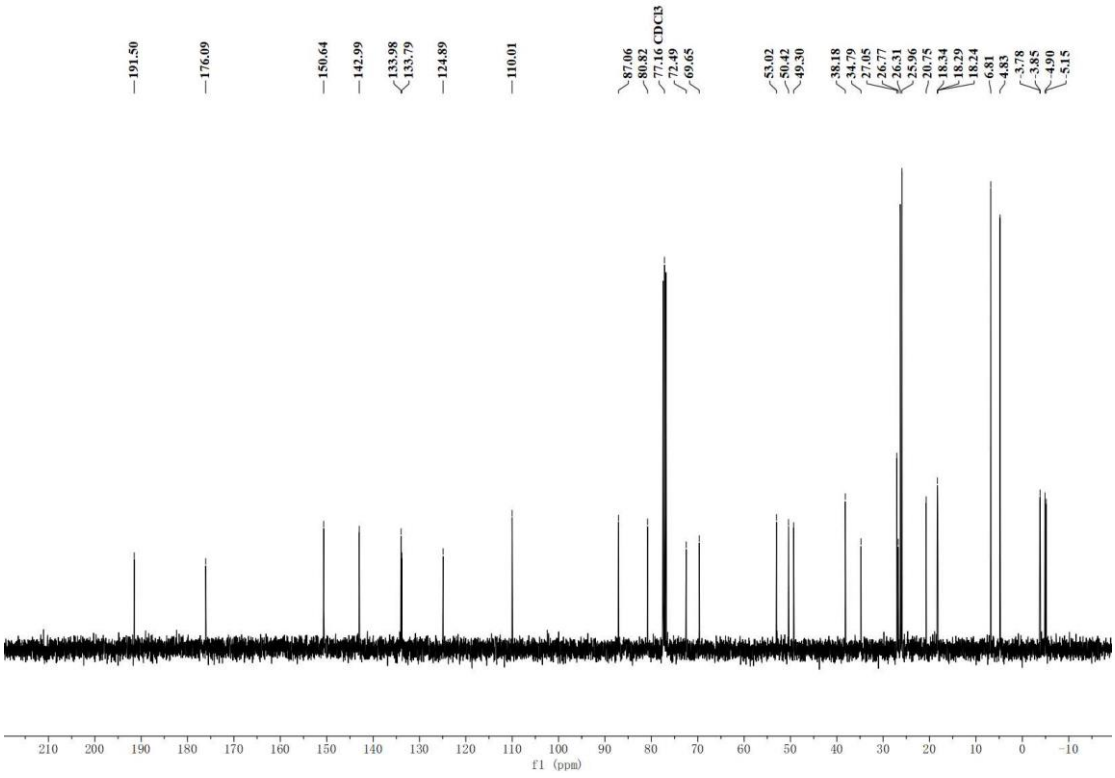
^{13}C NMR spectrum of **16** (100 MHz, $CDCl_3$)



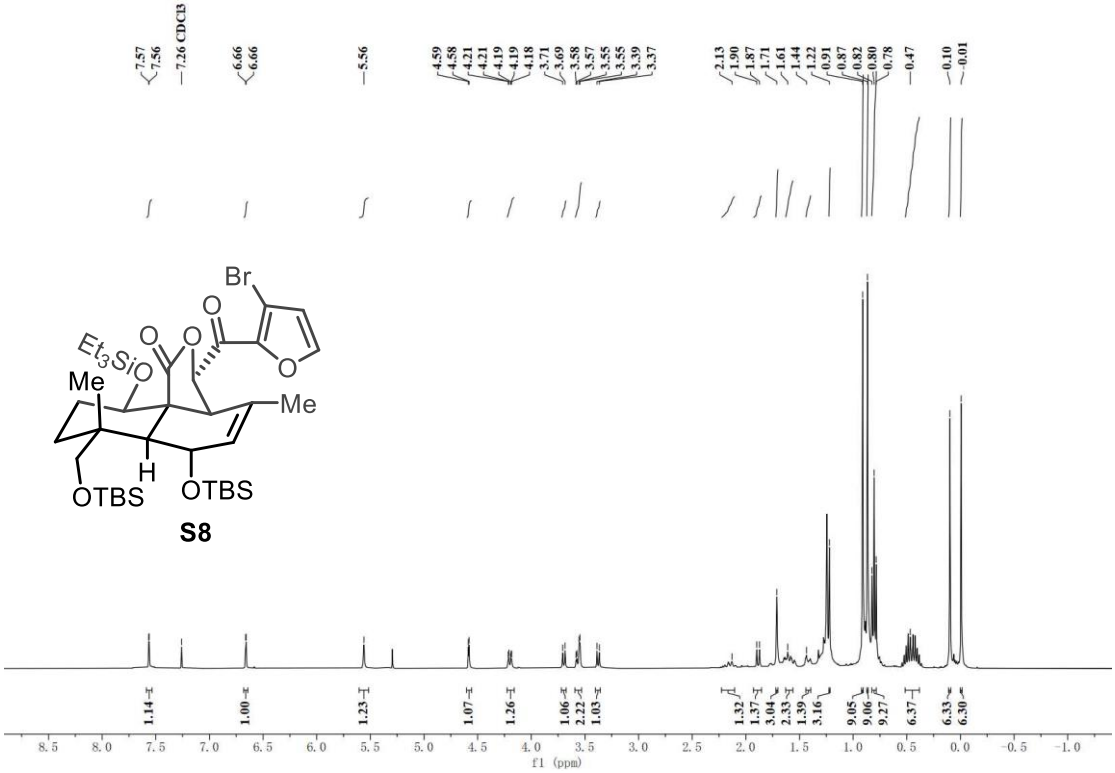
^{1}H NMR spectrum of **17** (400 MHz, $CDCl_3$)



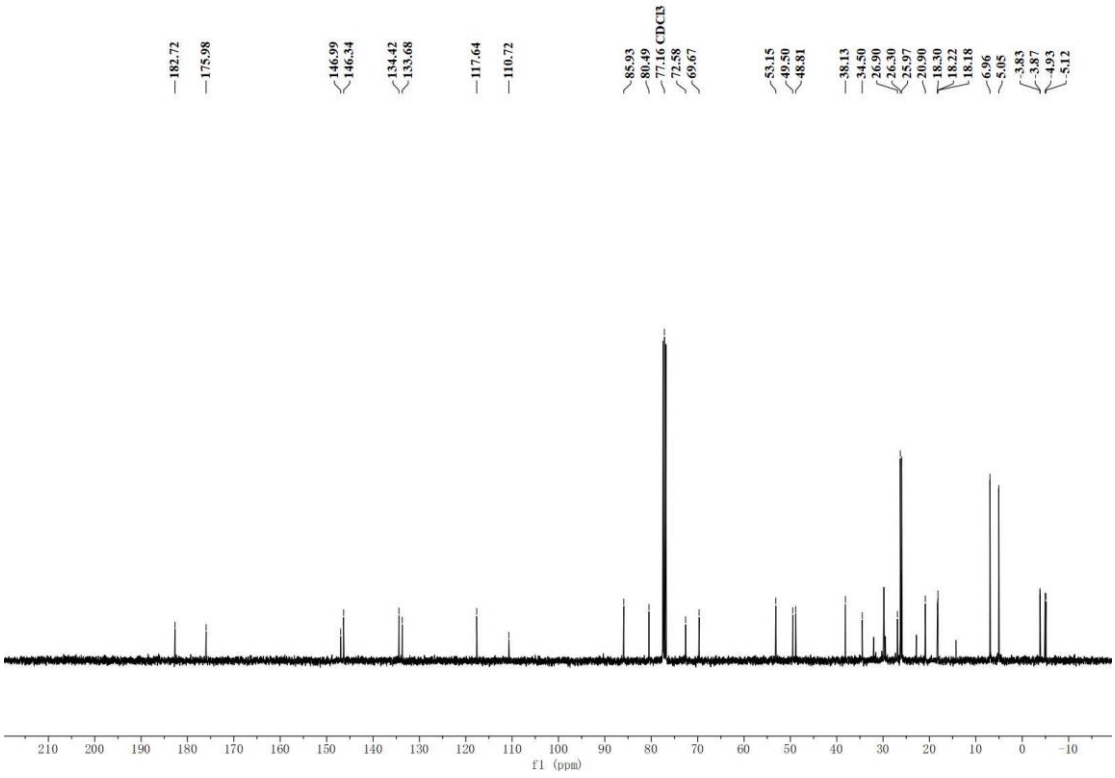
^{13}C NMR spectrum of **17** (100 MHz, $CDCl_3$)



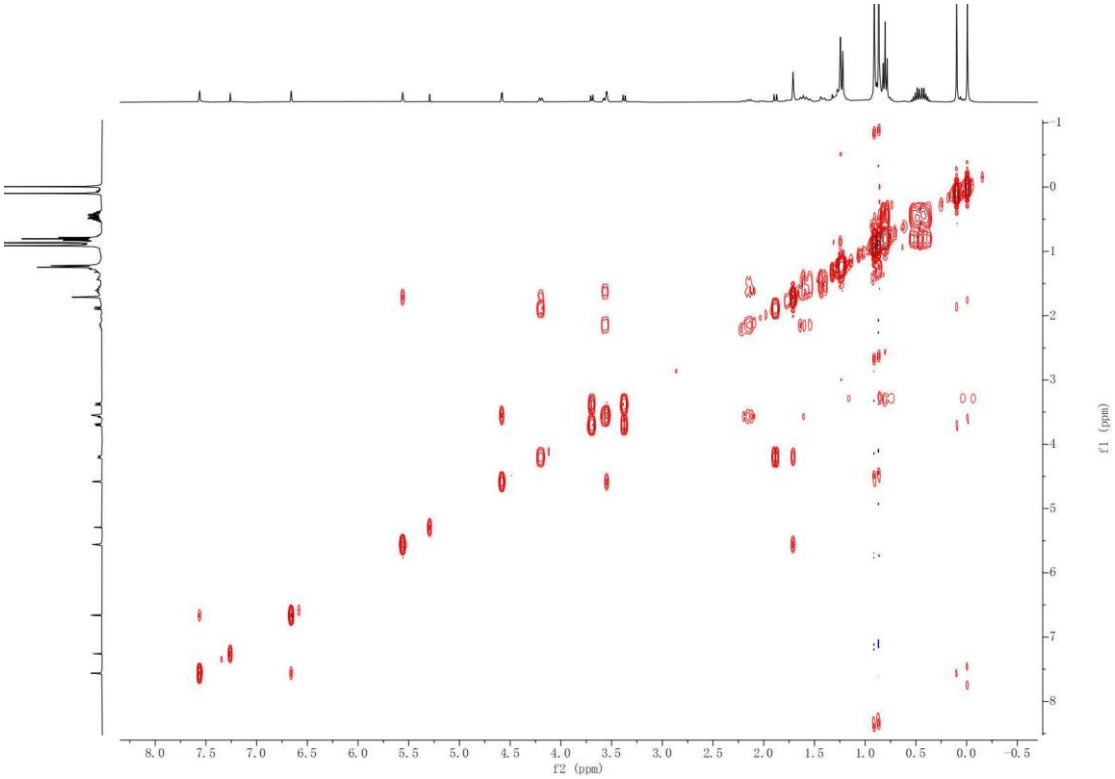
^{1}H NMR spectrum of **S8** (400 MHz, $CDCl_3$)

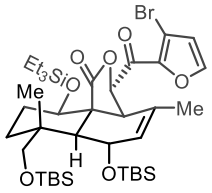


^{13}C NMR spectrum of **S8** (100 MHz, $CDCl_3$)



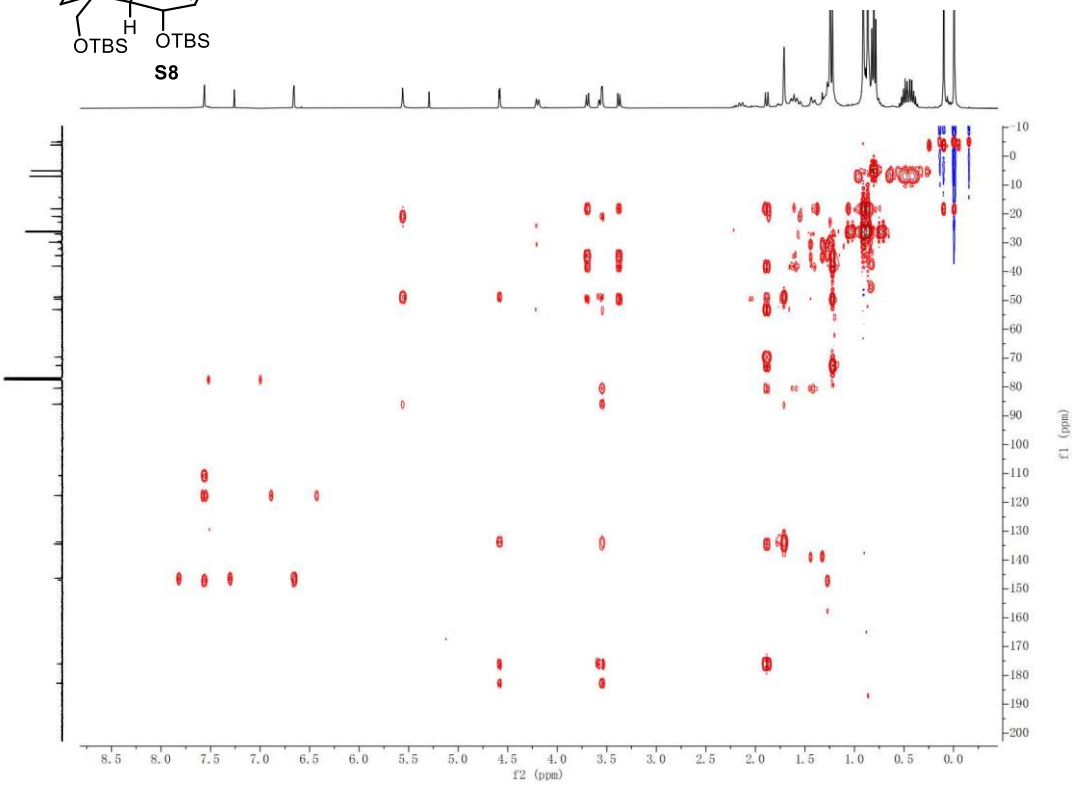
^{1}H-^{1}H COSY spectrum of **S8**



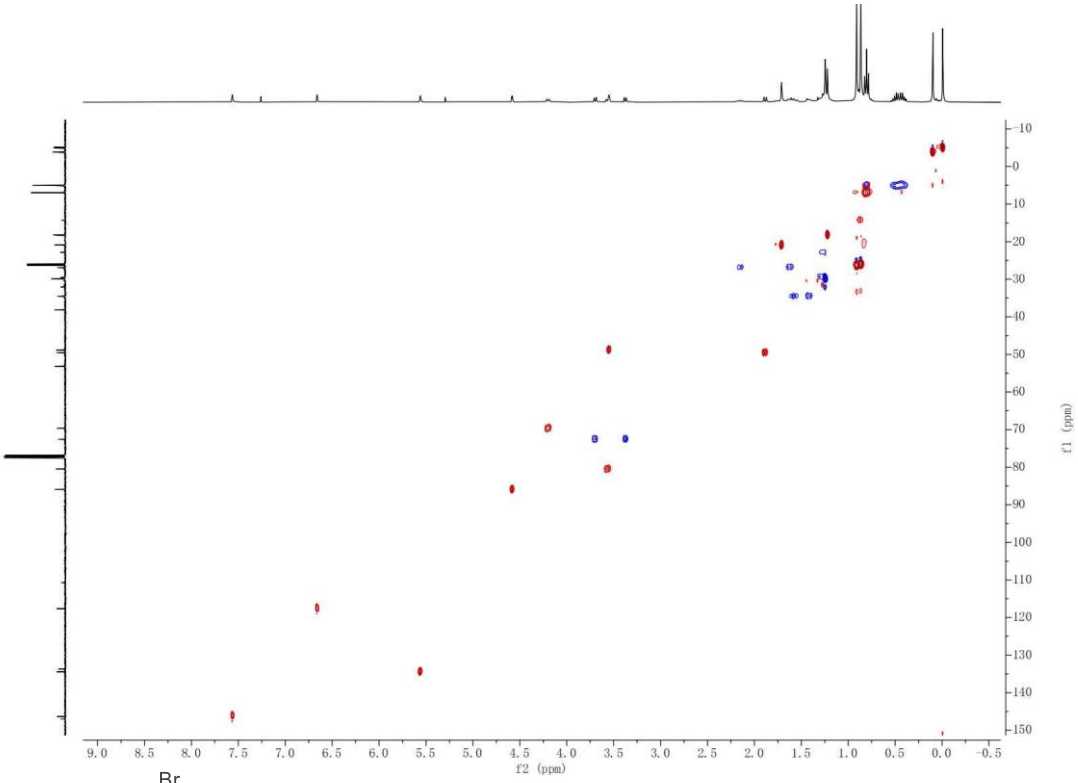


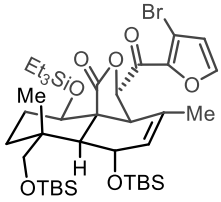
S8

HMBC spectrum of **S8**



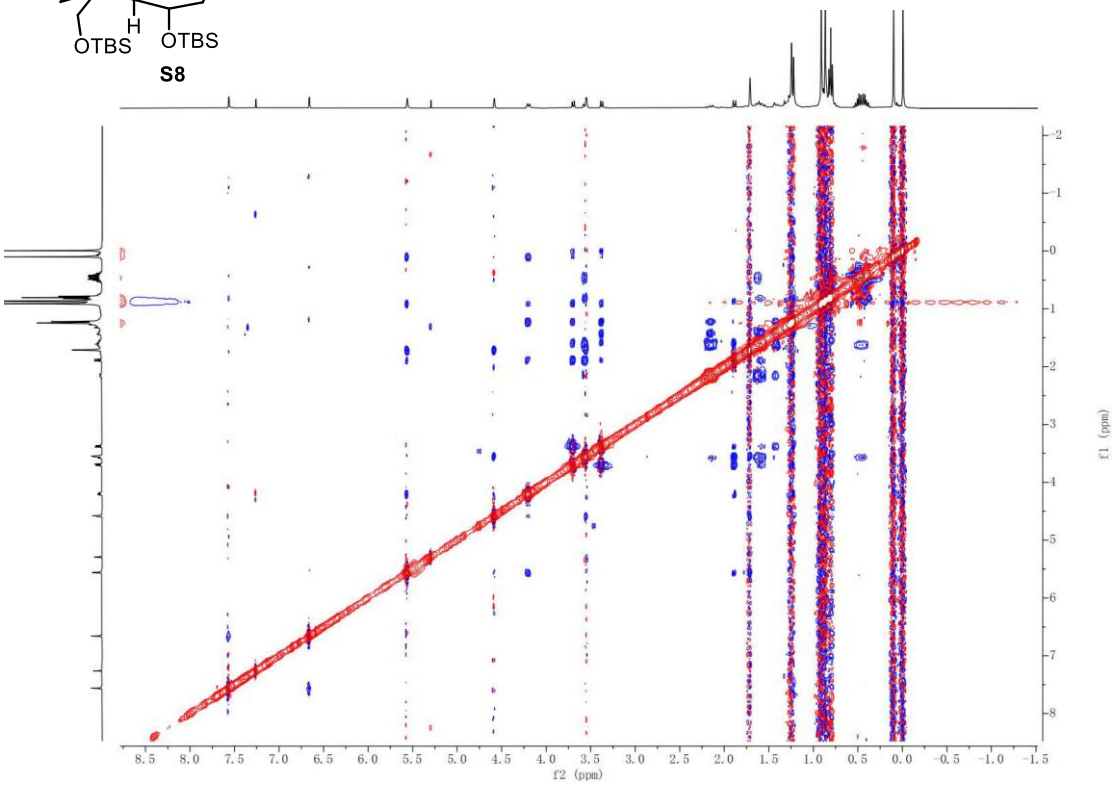
HSQC spectrum of **S8**



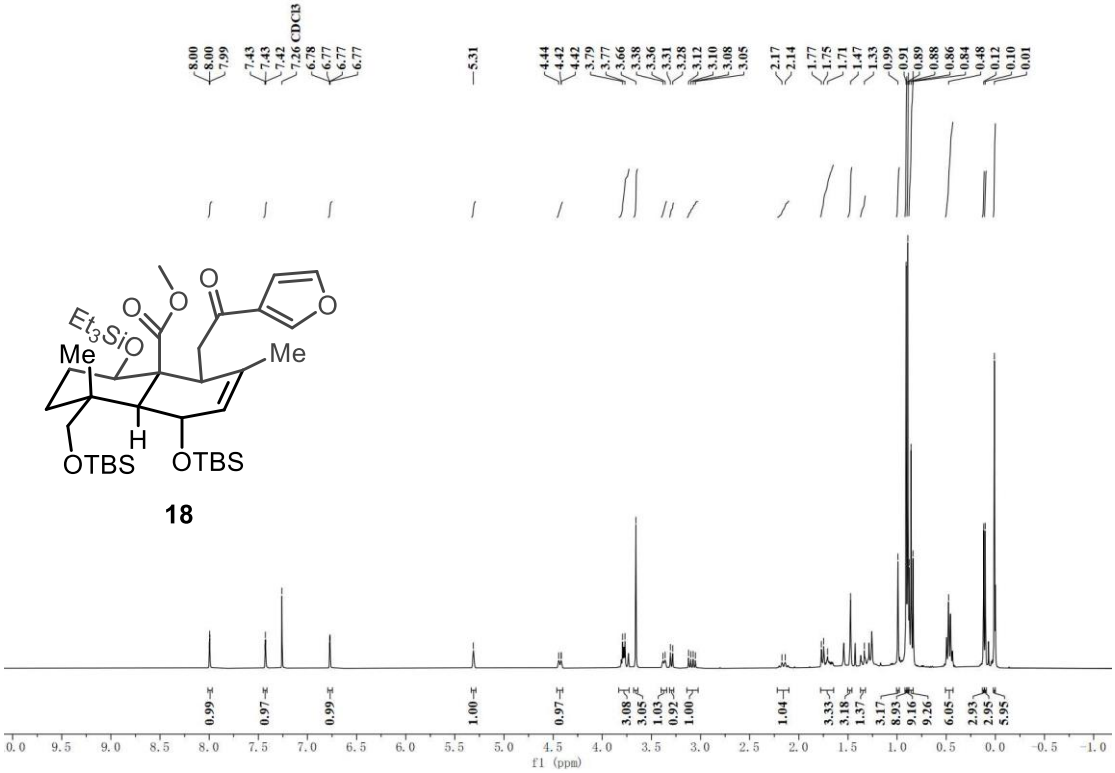


S8

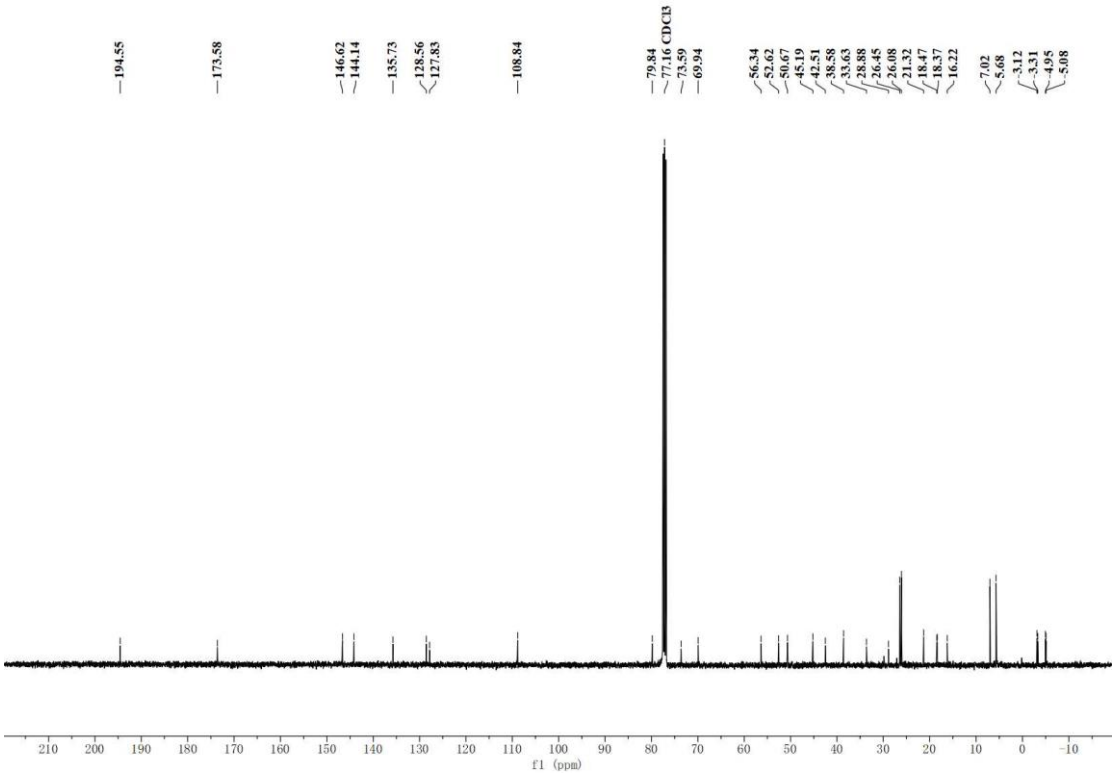
NOESY spectrum of **S8**



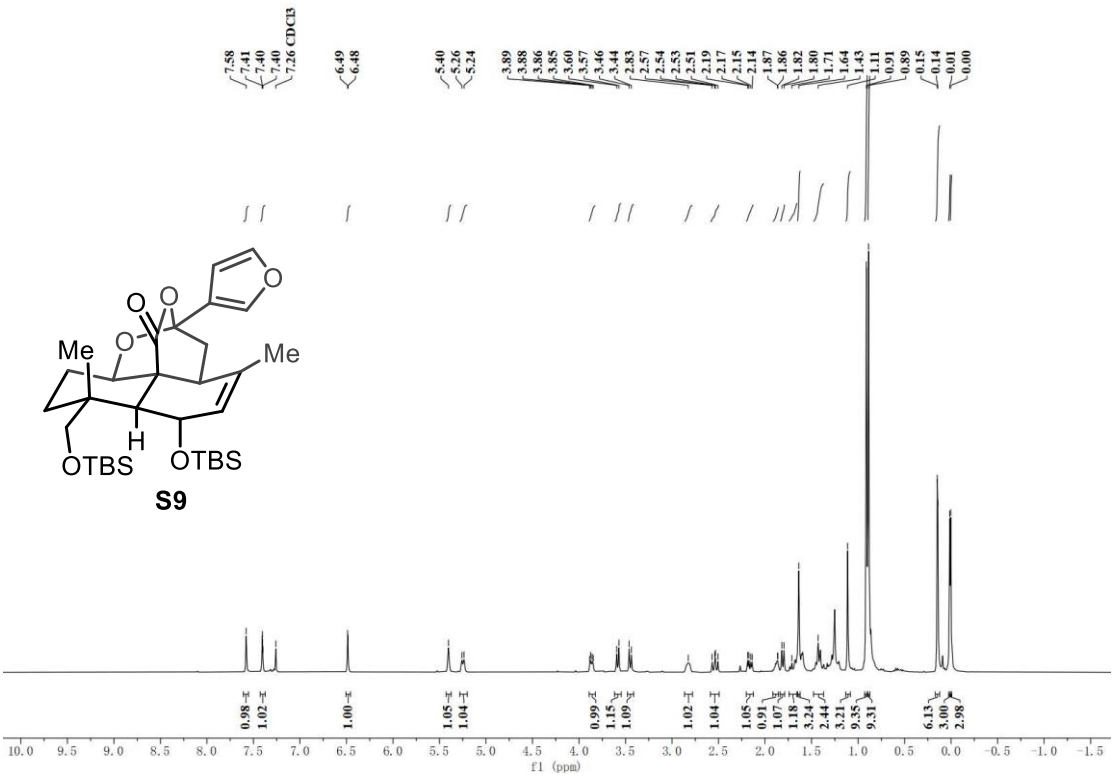
^{1}H NMR spectrum of **18** (400 MHz, $CDCl_3$)



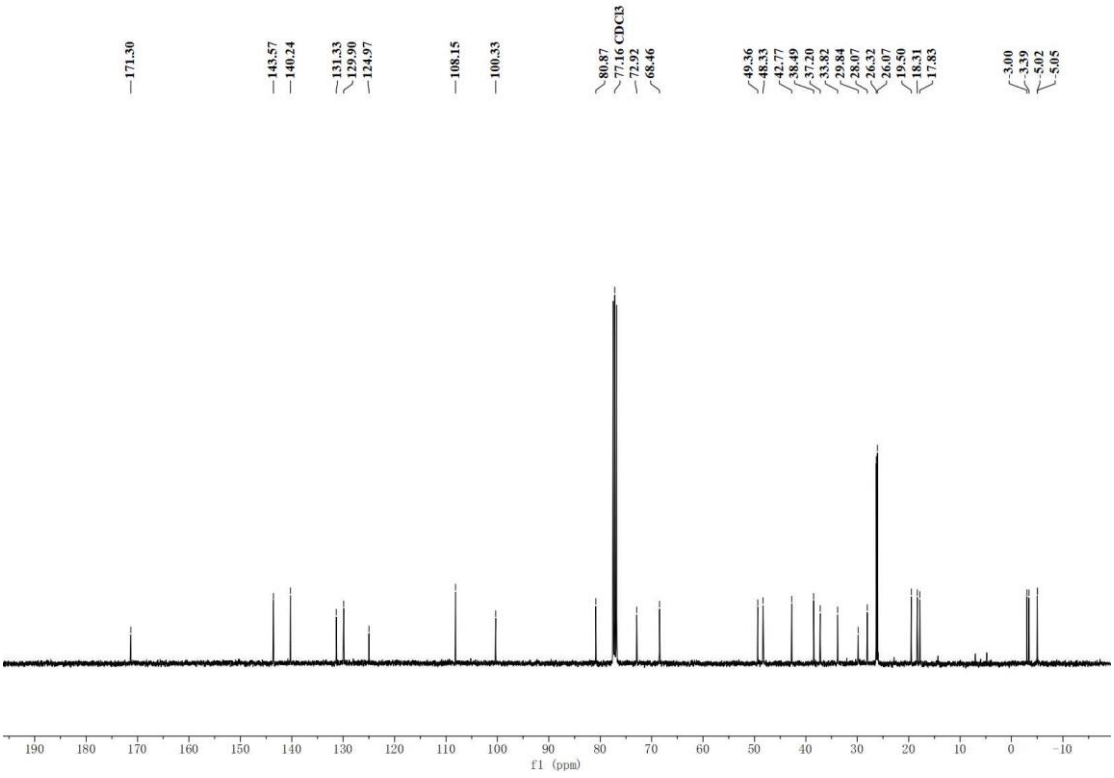
^{13}C NMR spectrum of **18** (100 MHz, $CDCl_3$)



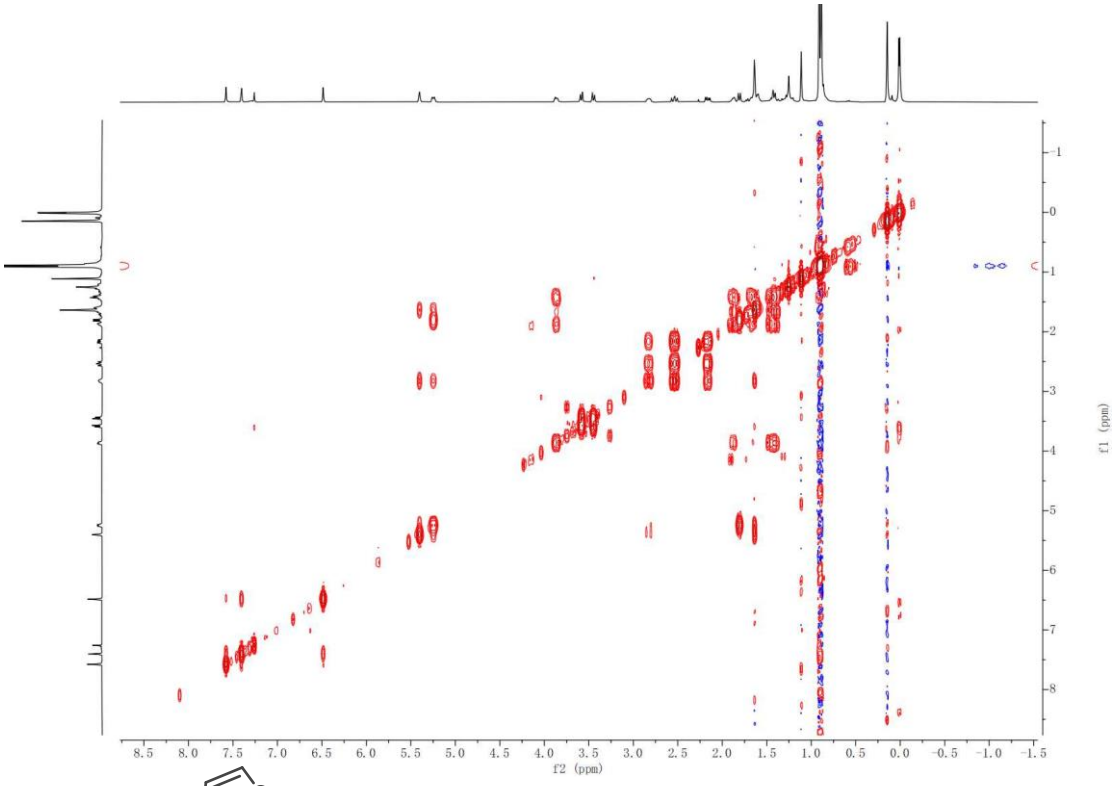
^{1}H NMR spectrum of **S9** (400 MHz, $CDCl_3$)

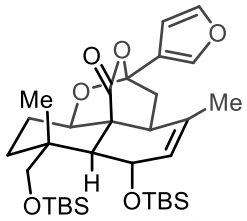


^{13}C NMR spectrum of **S9** (100 MHz, $CDCl_3$)



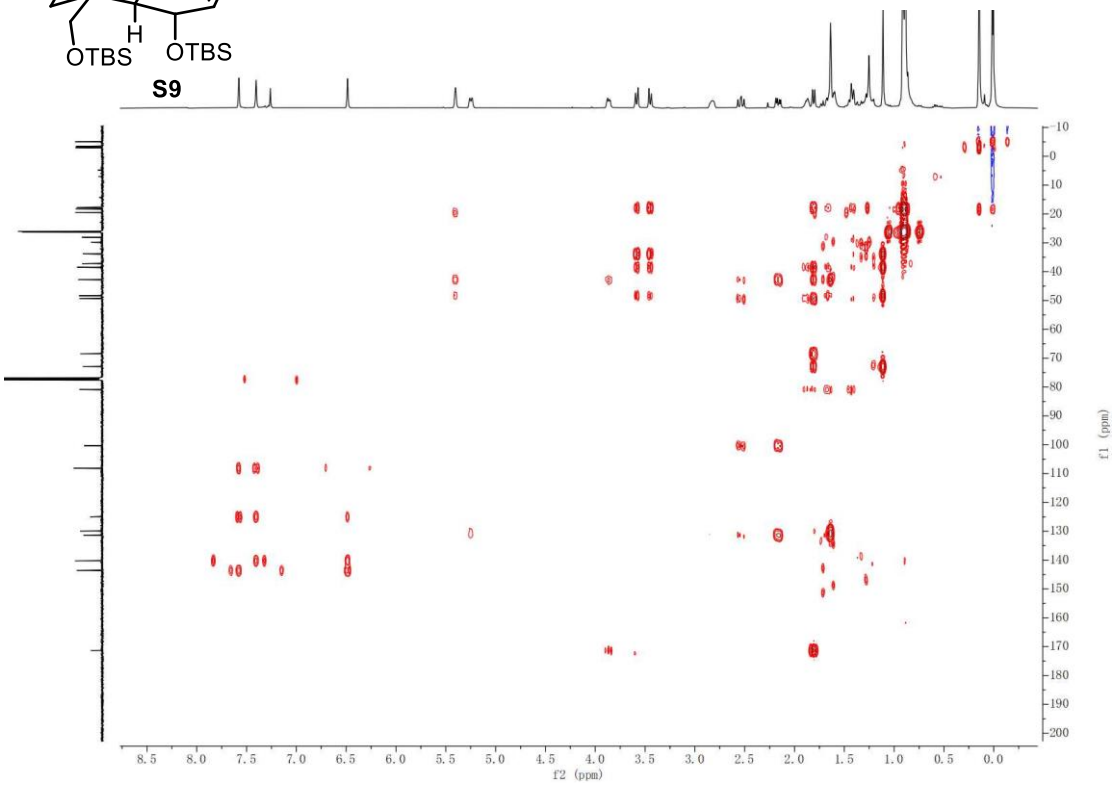
^{1}H-^{1}H COSY spectrum of **S9**



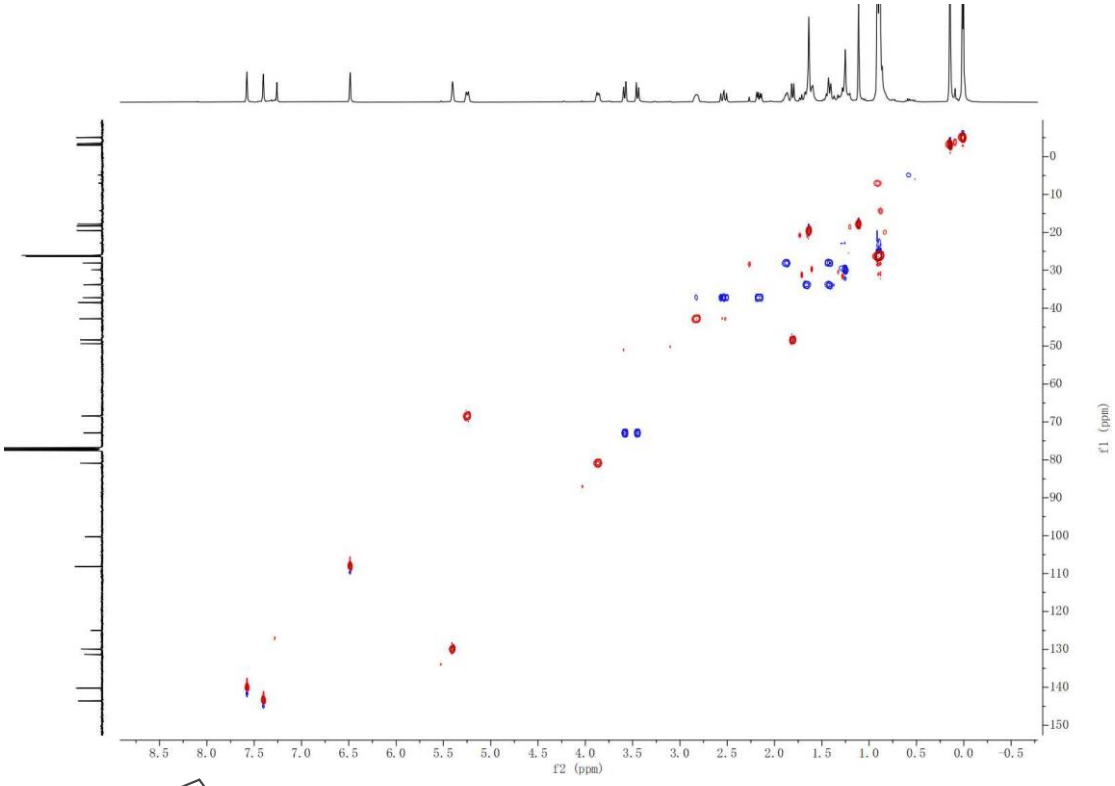


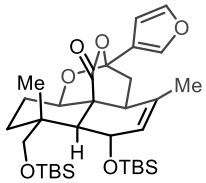
S9

HMBC spectrum of **S9**



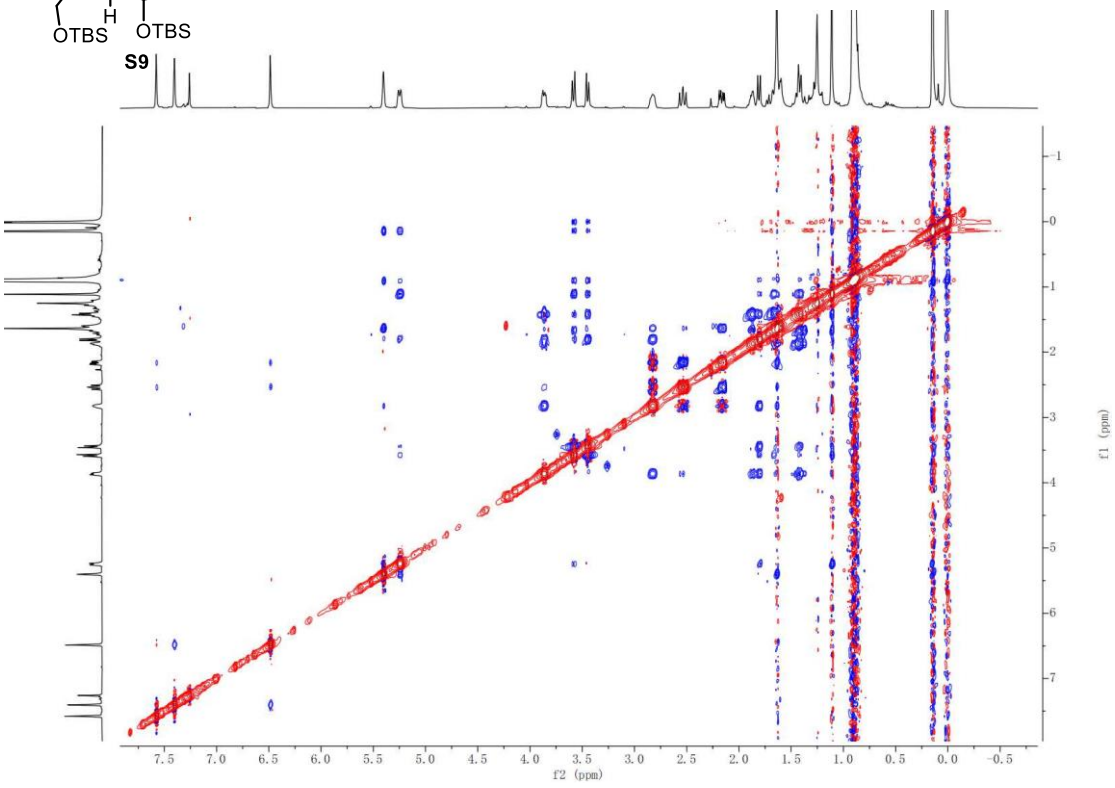
HSQC spectrum of **S9**



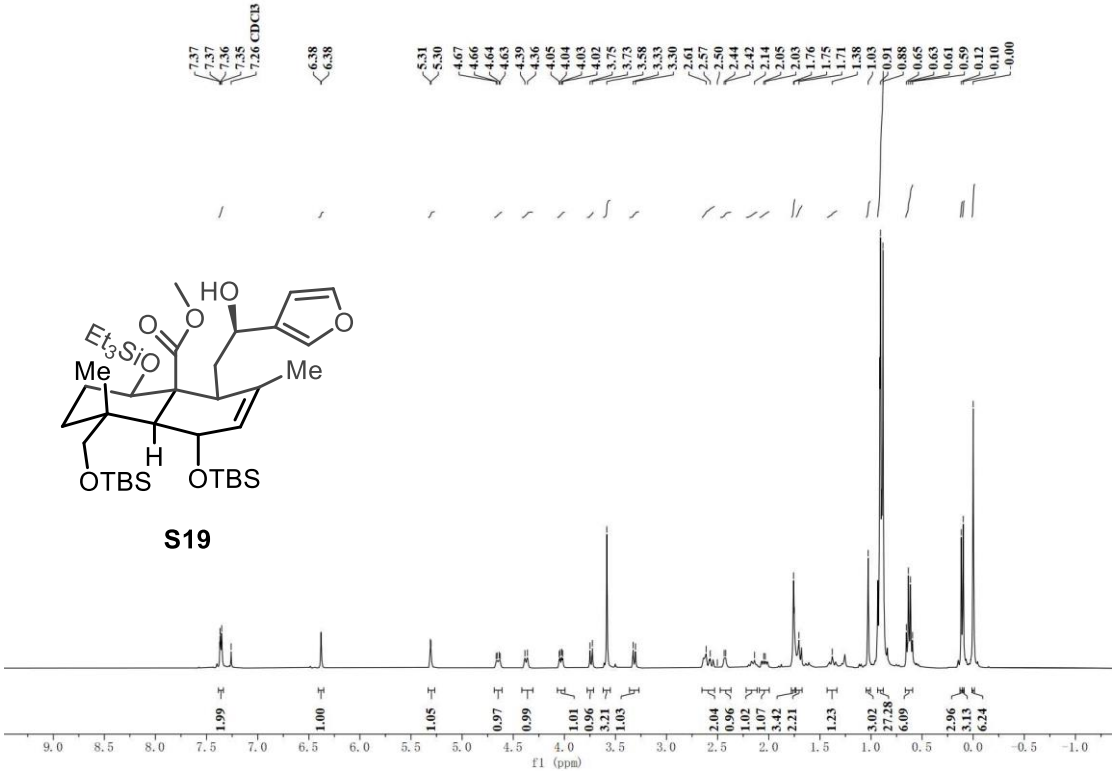


S9

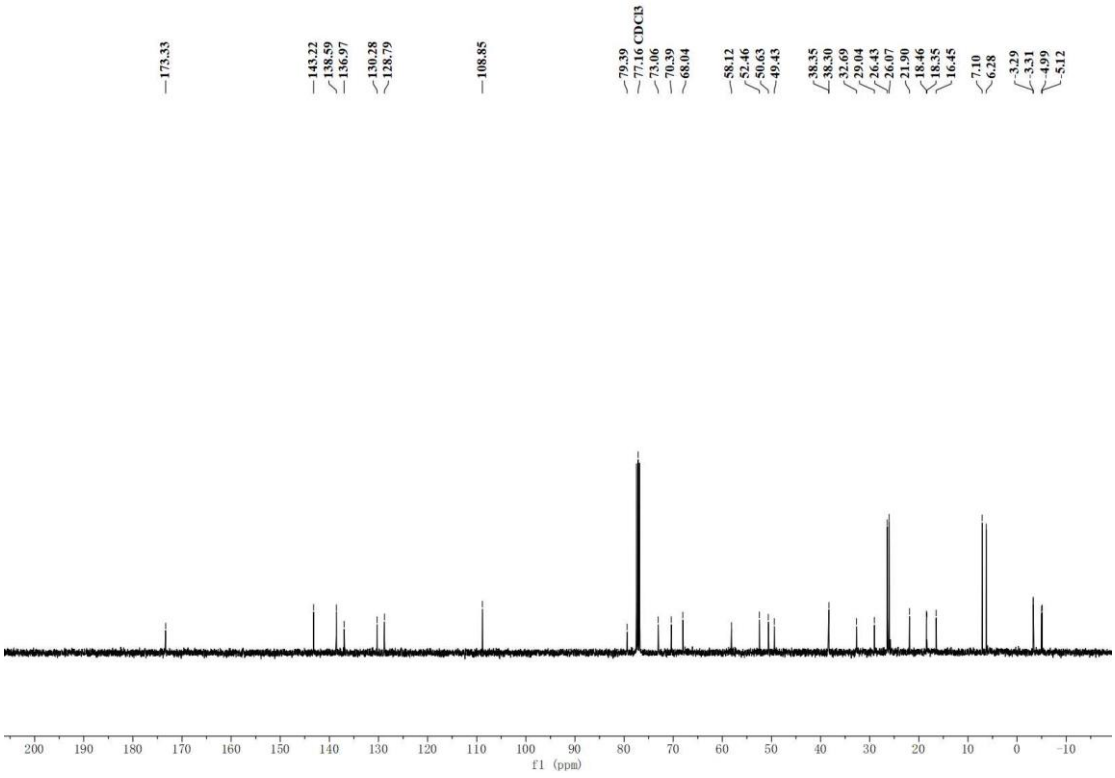
NOESY spectrum of **S9**



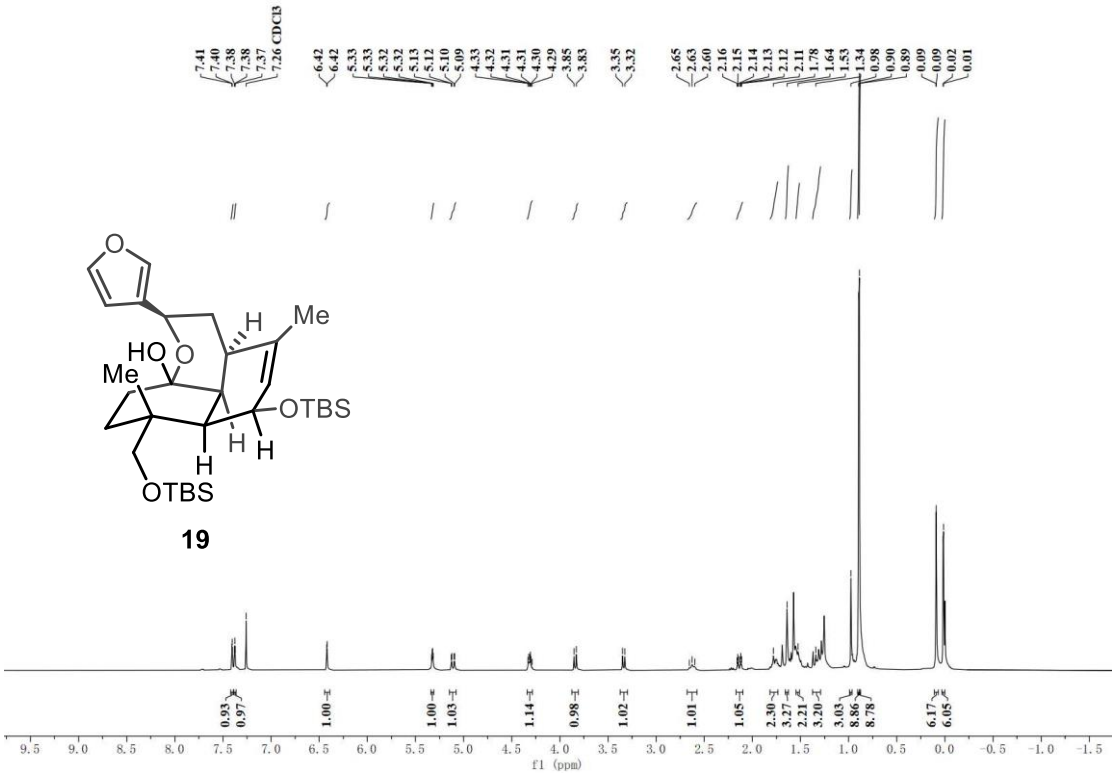
^{1}H NMR spectrum of **S19** (400 MHz, $CDCl_3$)



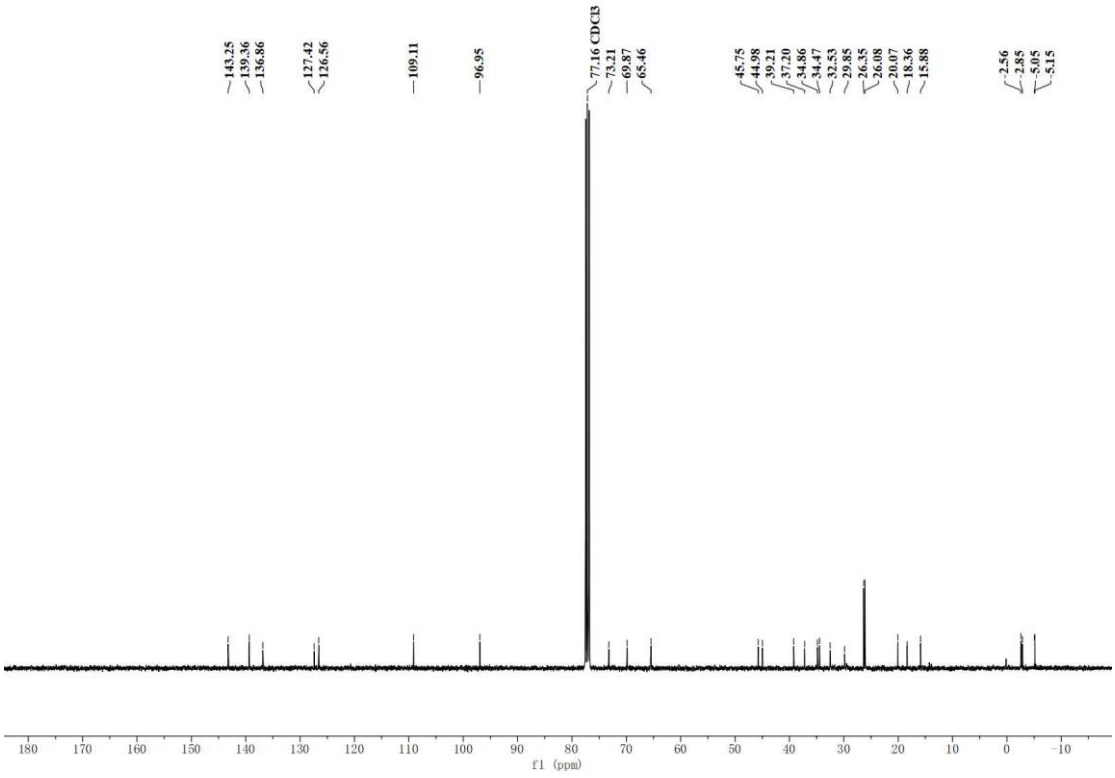
^{13}C NMR spectrum of **S19** (100 MHz, $CDCl_3$)



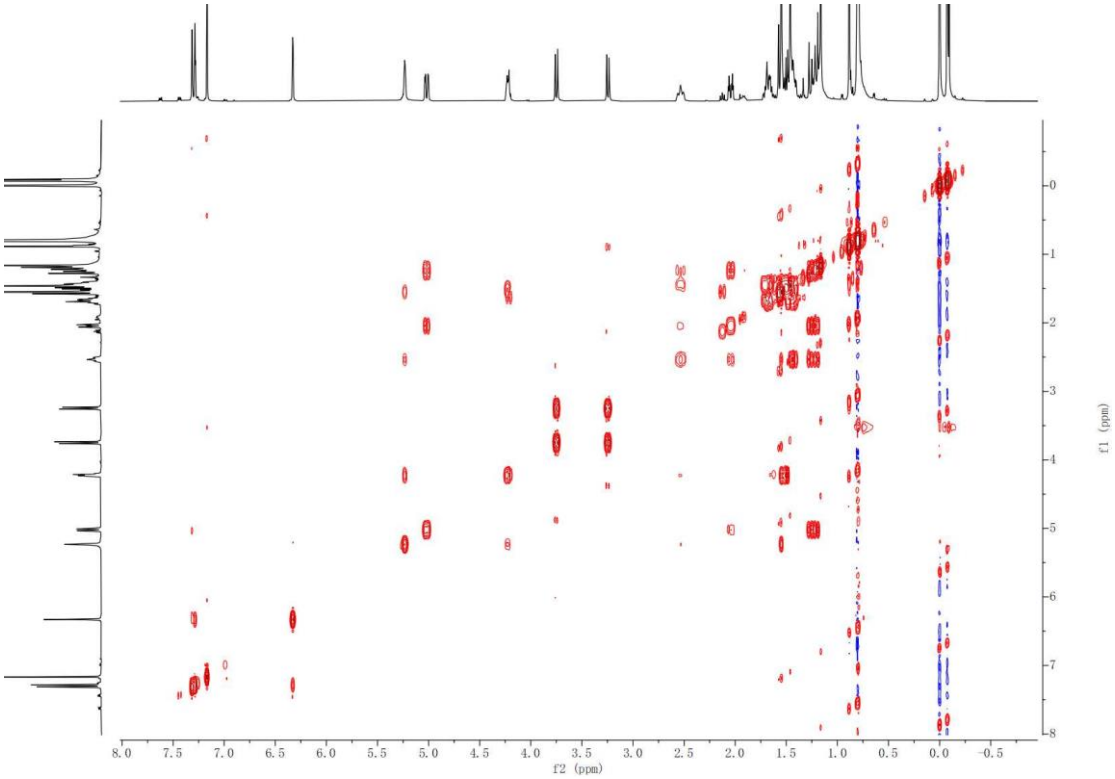
^{1}H NMR spectrum of **19** (400 MHz, $CDCl_3$)

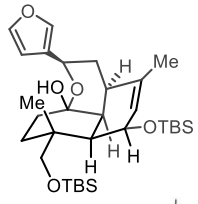


^{13}C NMR spectrum of **19** (100 MHz, $CDCl_3$)



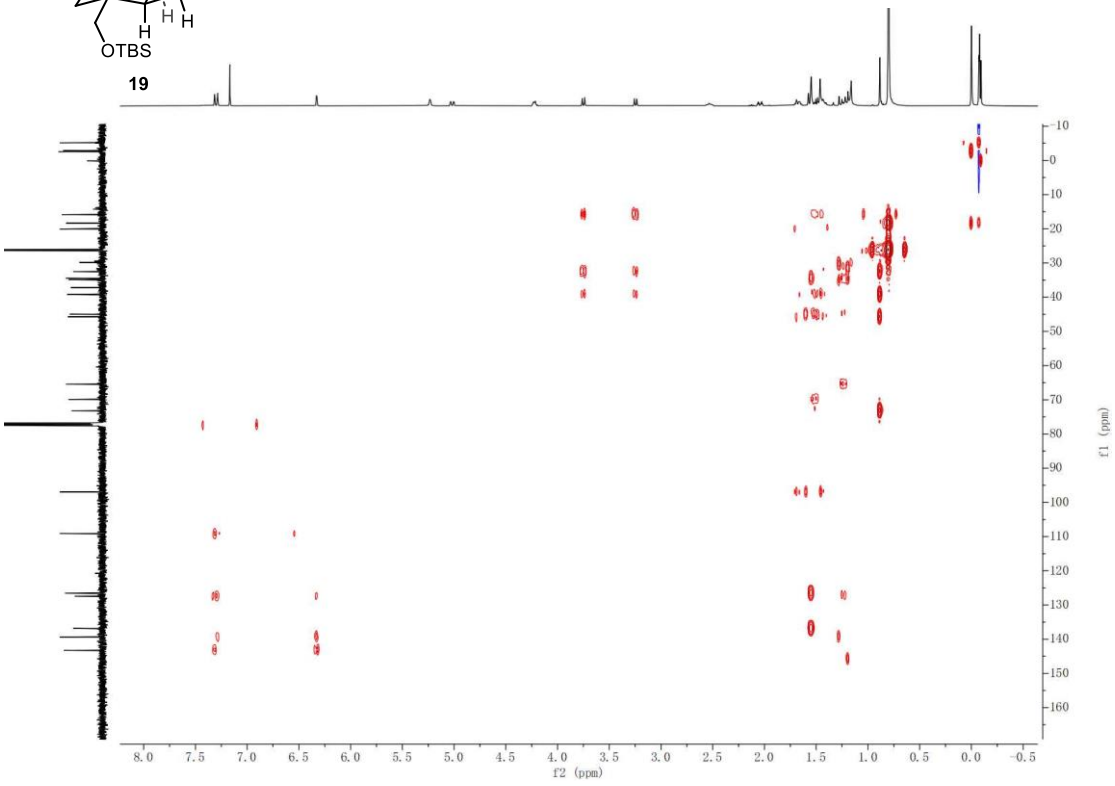
^{1}H-^{1}H COSY spectrum of **19**



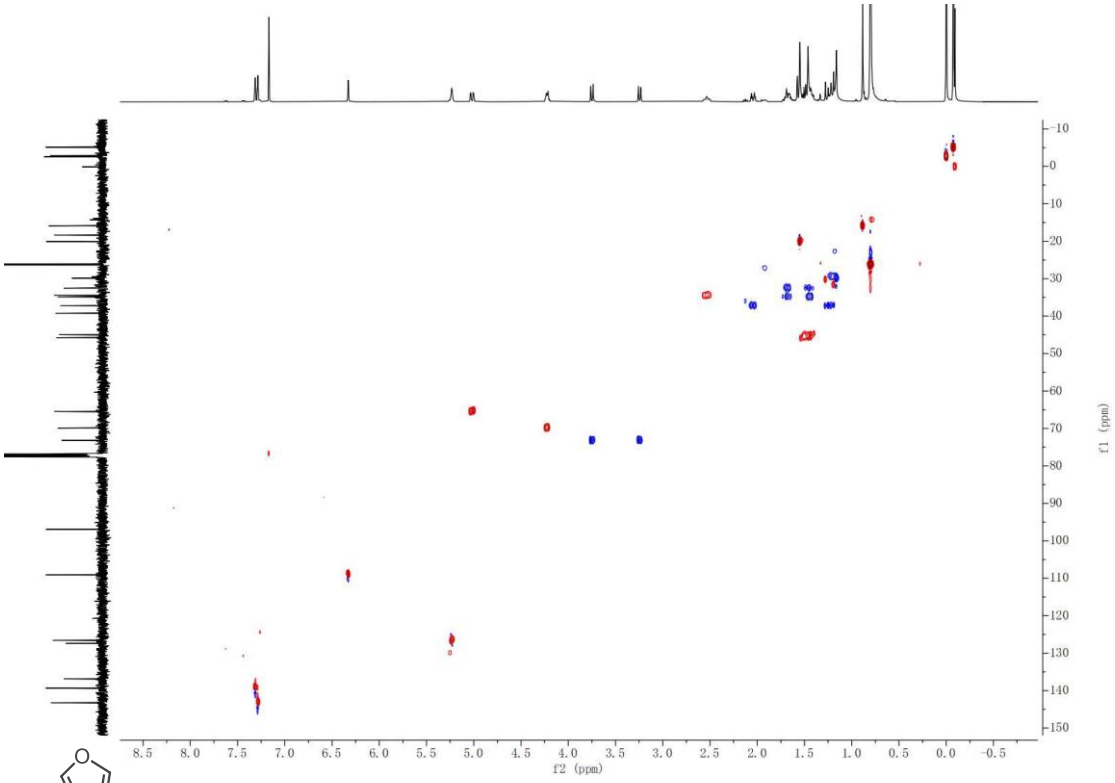


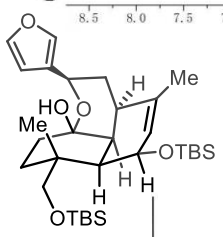
19

HMBC spectrum of **19**



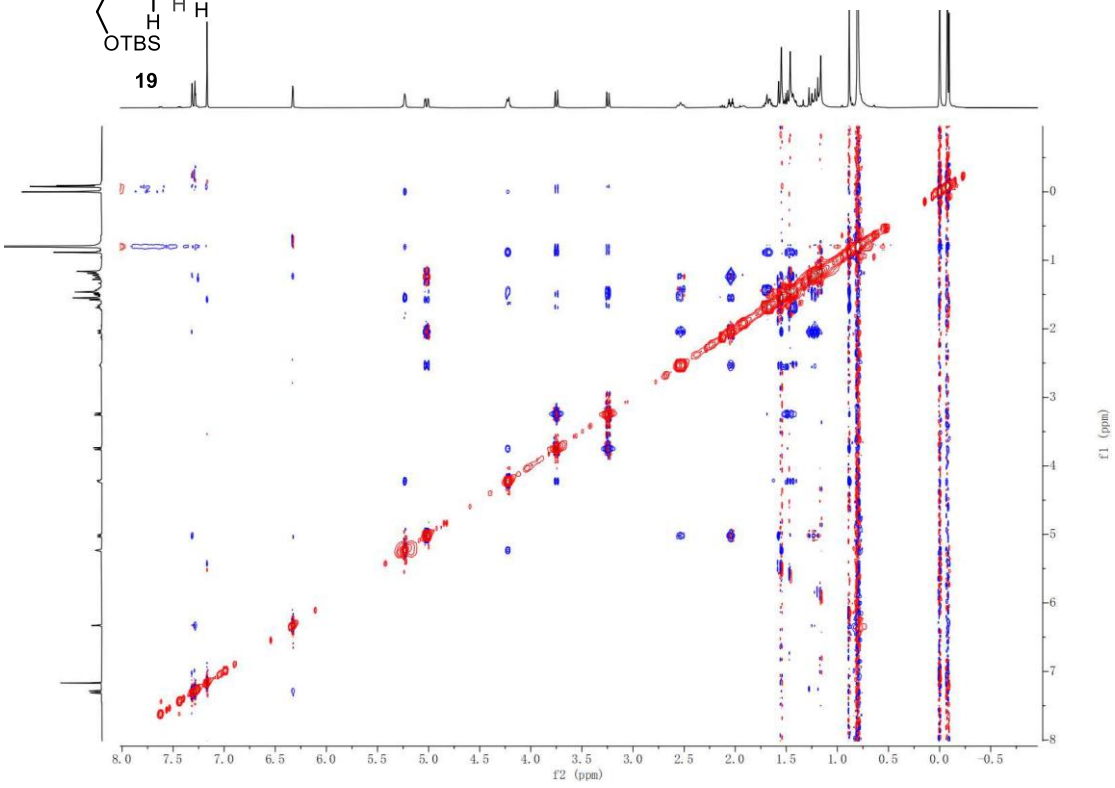
HSQC spectrum of **19**



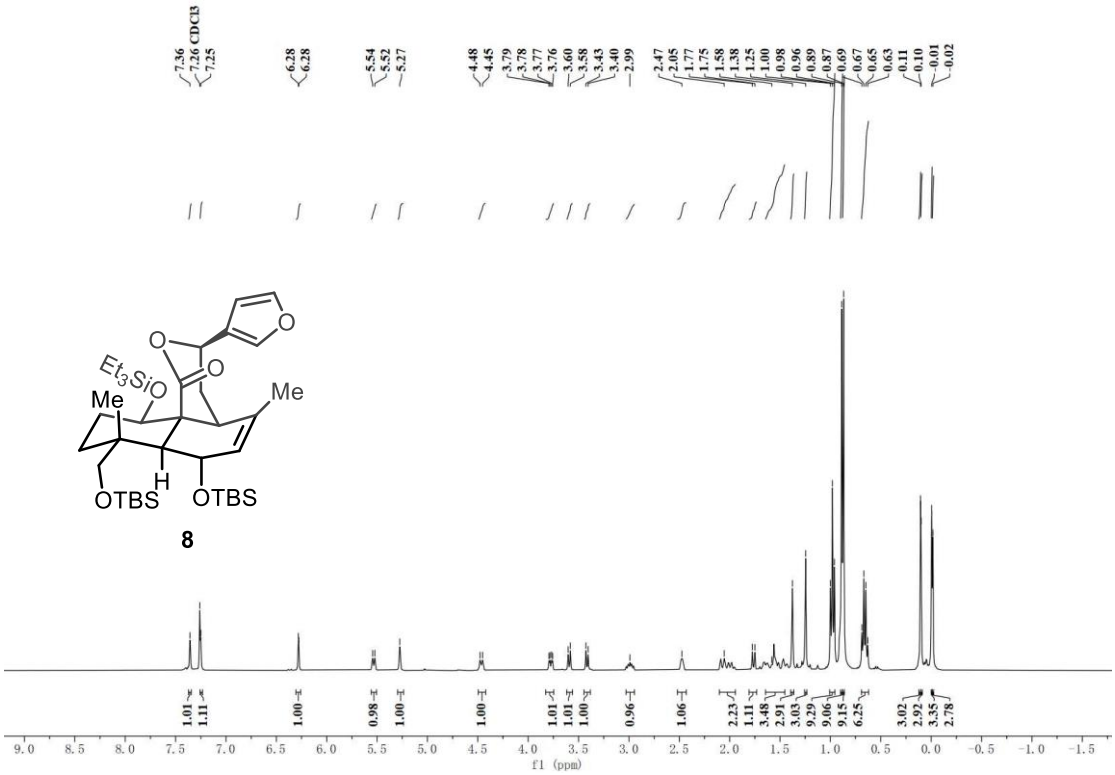


19

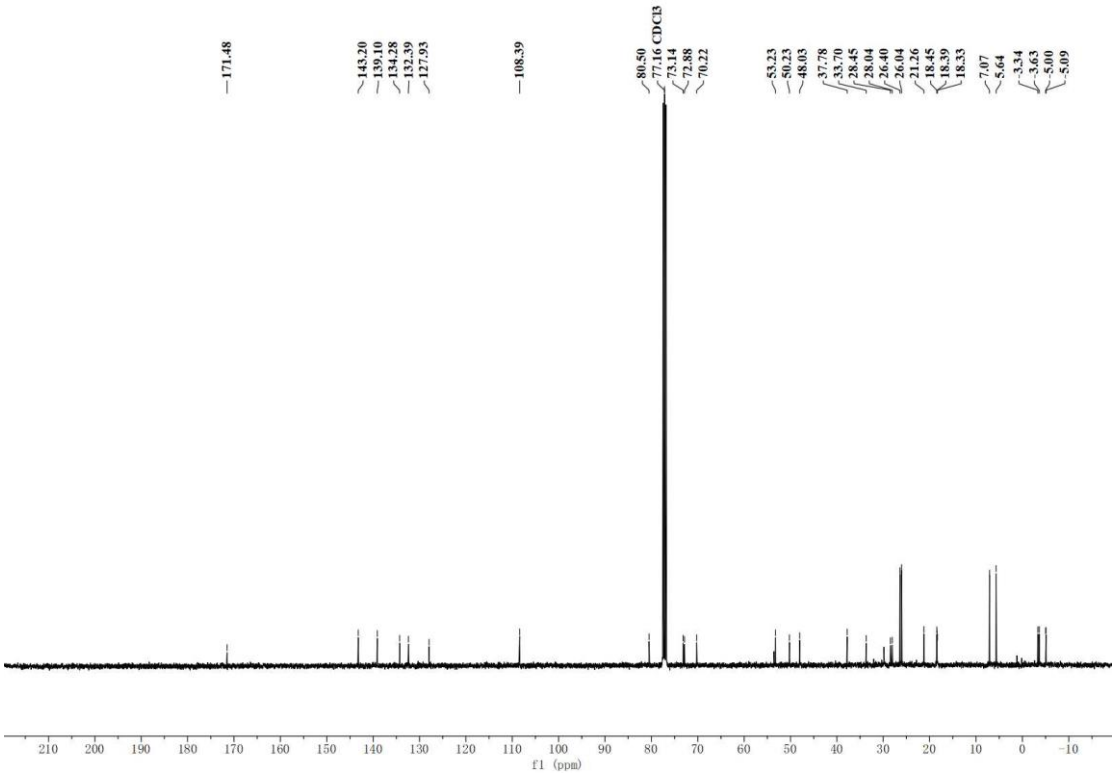
NOESY spectrum of **19**



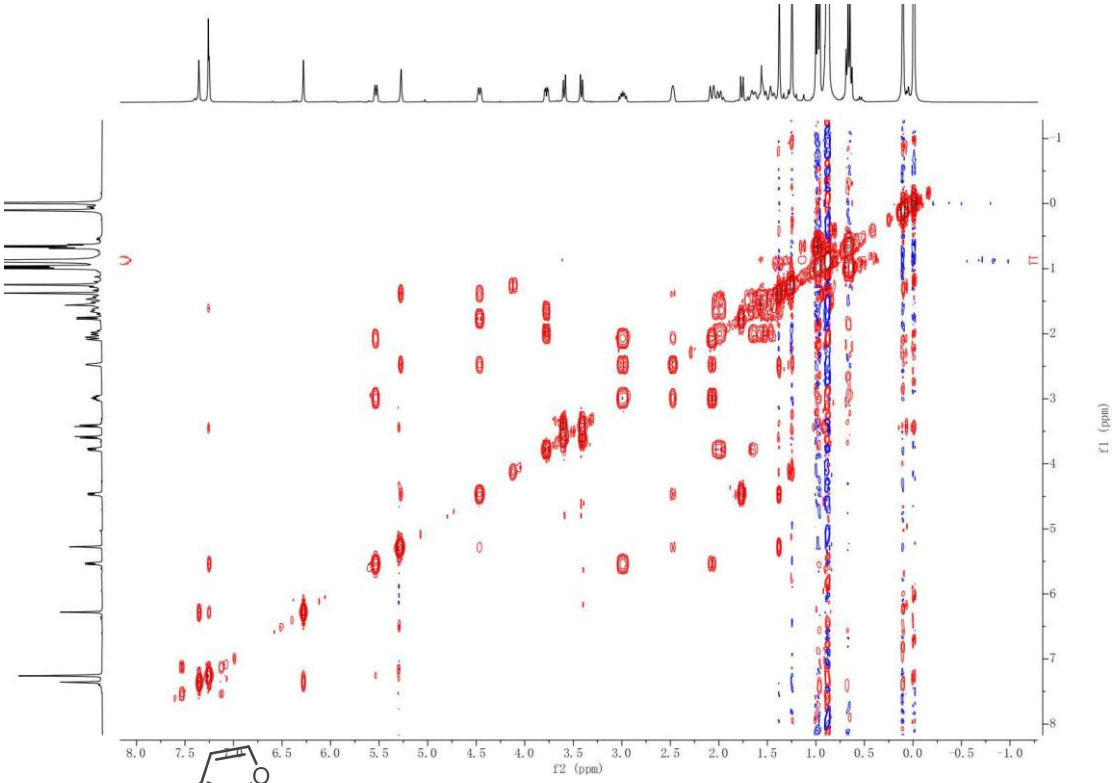
^{1}H NMR spectrum of **8** (400 MHz, $CDCl_3$)

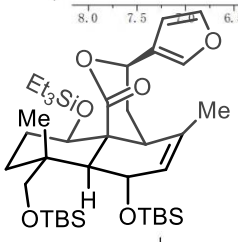


^{13}C NMR spectrum of **8** (100 MHz, $CDCl_3$)



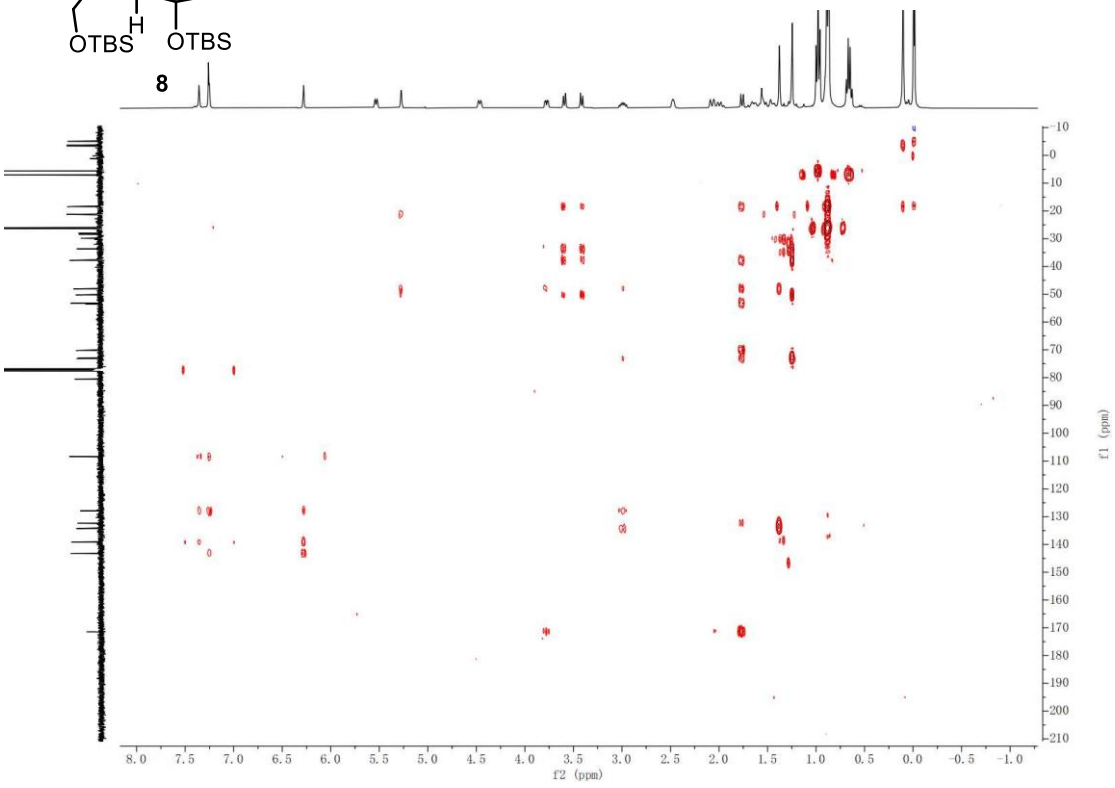
^{1}H-^{1}H COSY spectrum of **8**



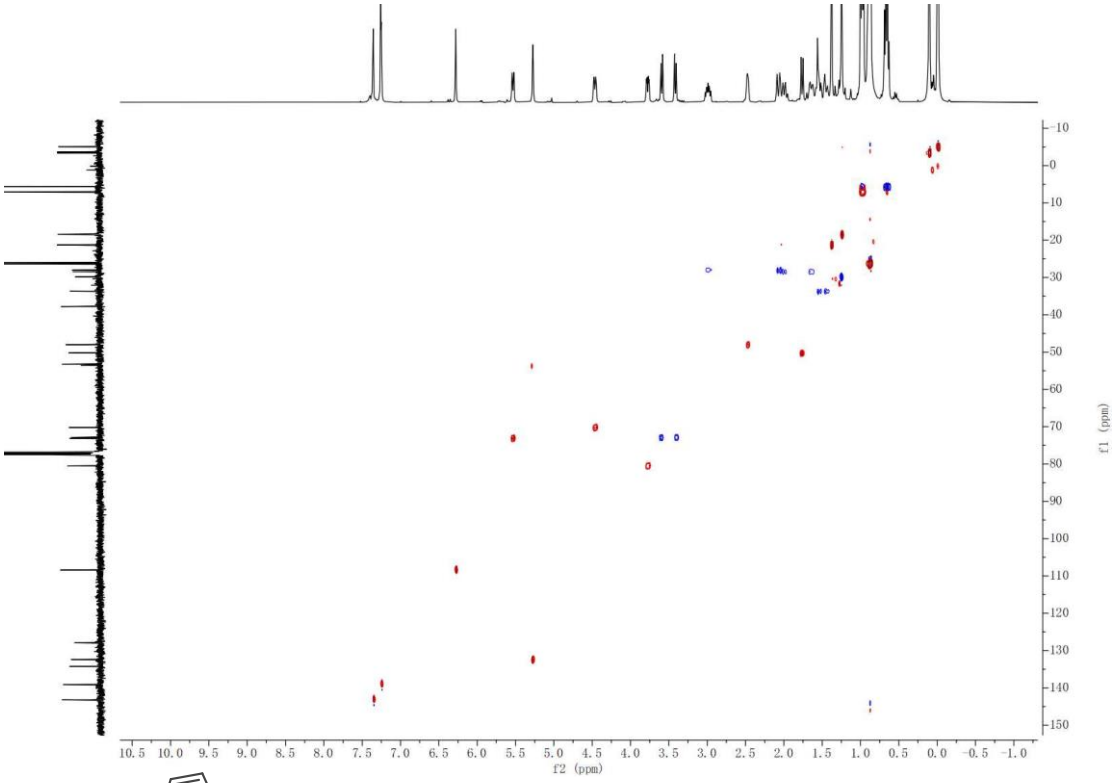


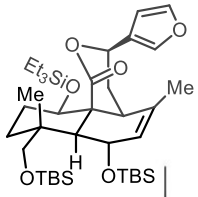
8

HMBC spectrum of **8**



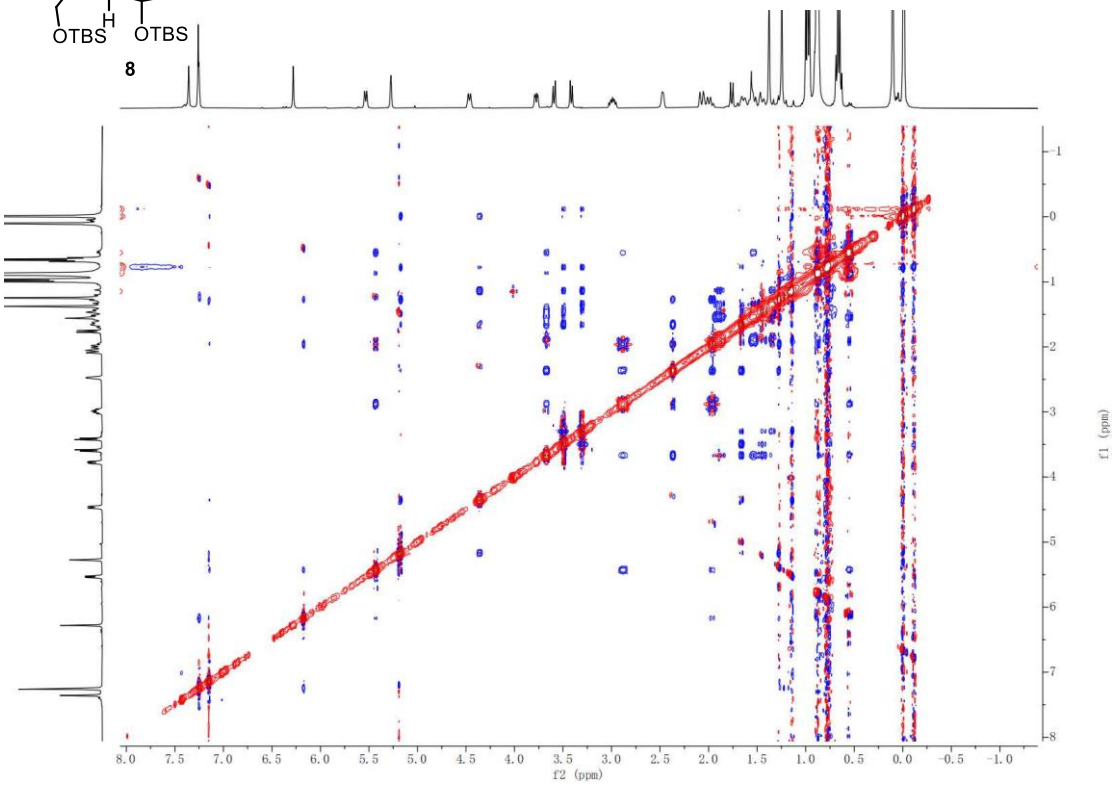
HSQC spectrum of **8**



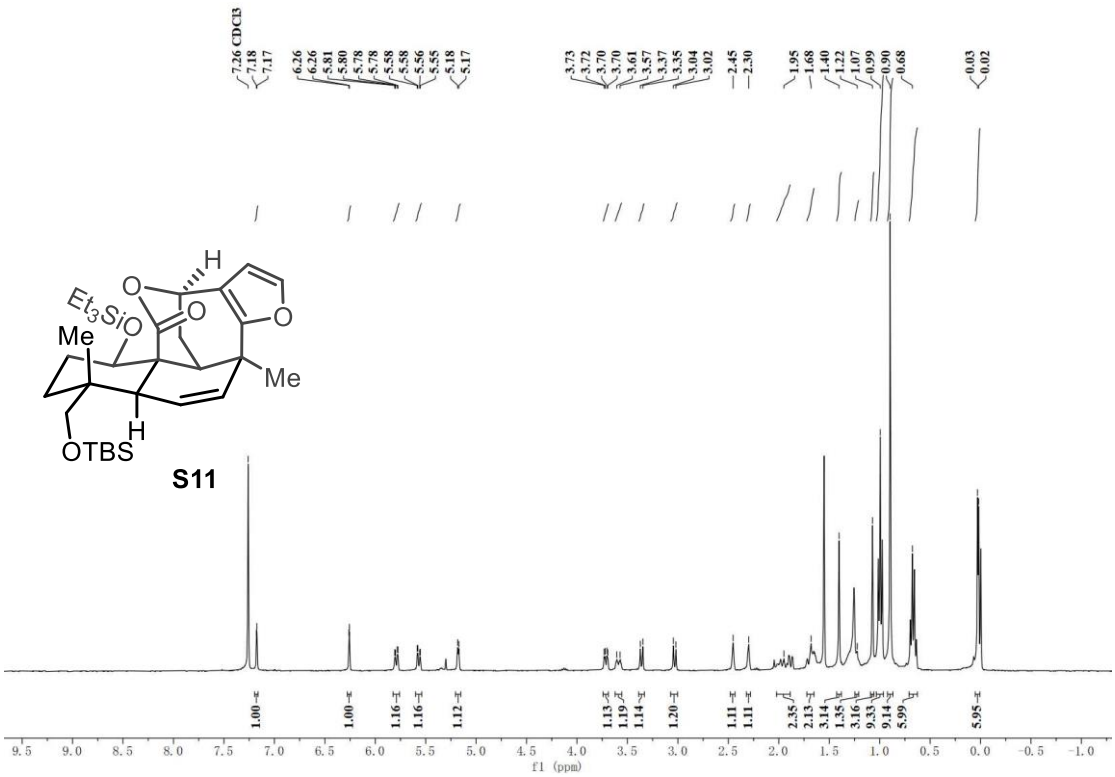


8

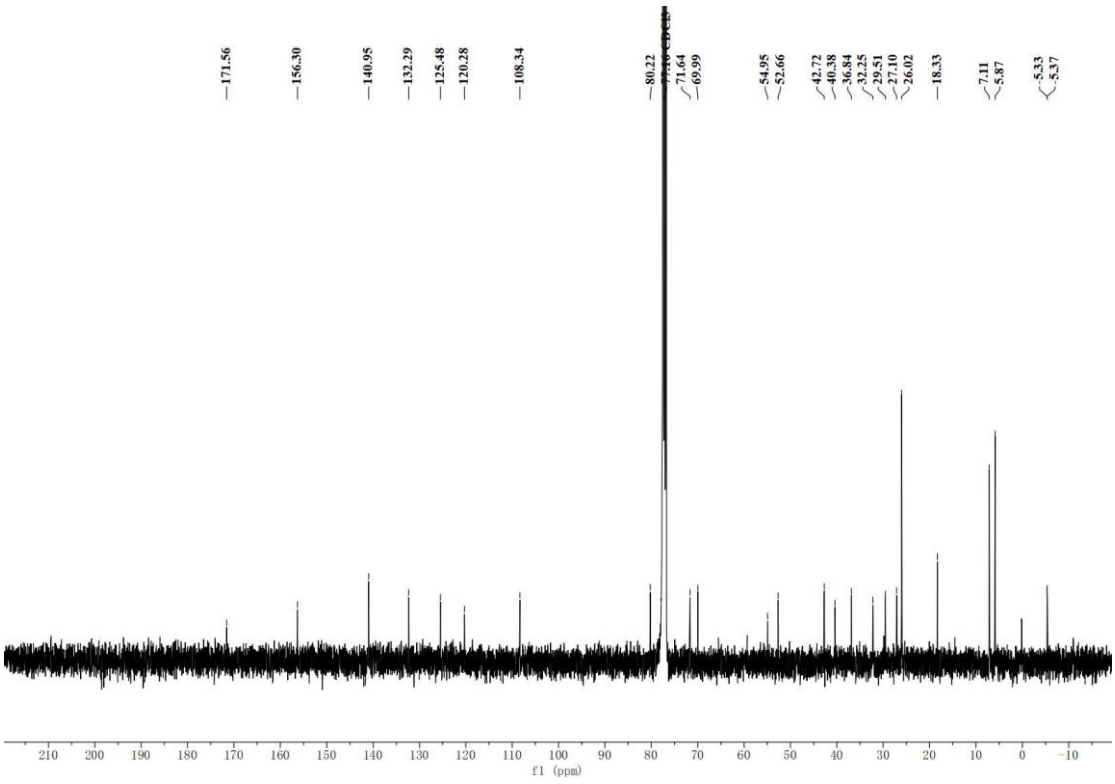
NOESY spectrum of **8**



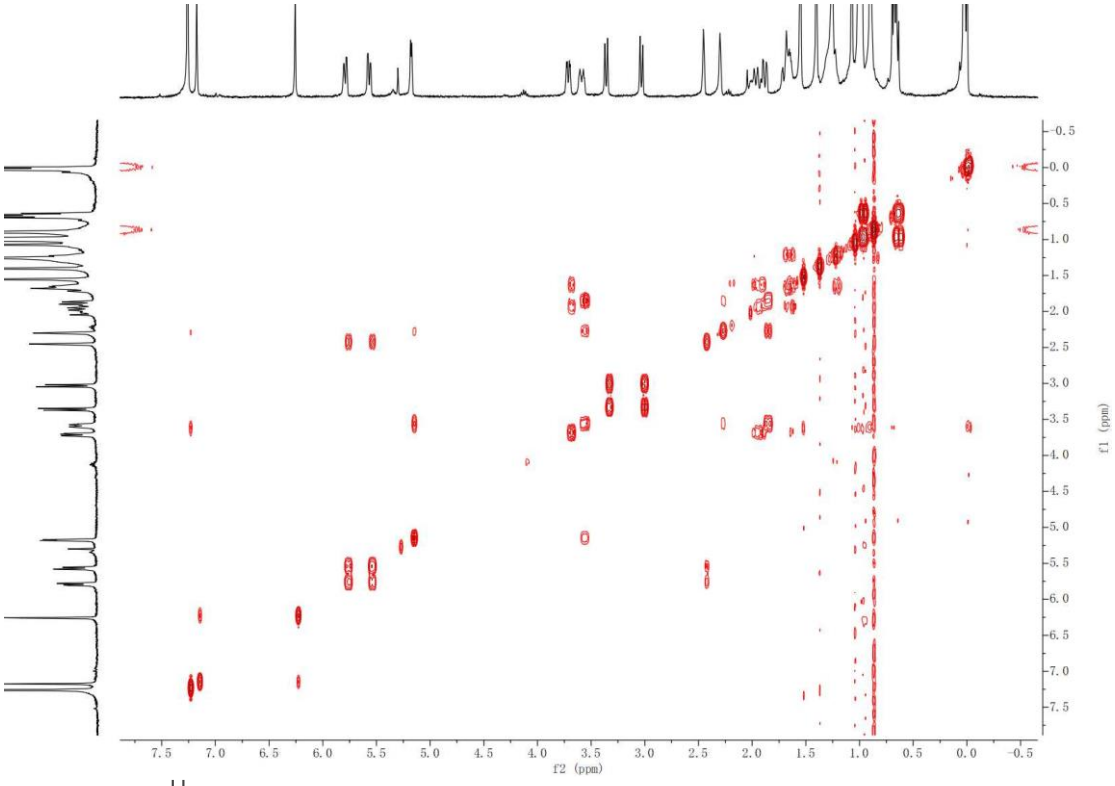
^{1}H NMR spectrum of **S11** (400 MHz, $CDCl_3$)

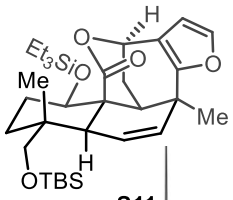


^{13}C NMR spectrum of **S11** (100 MHz, $CDCl_3$)



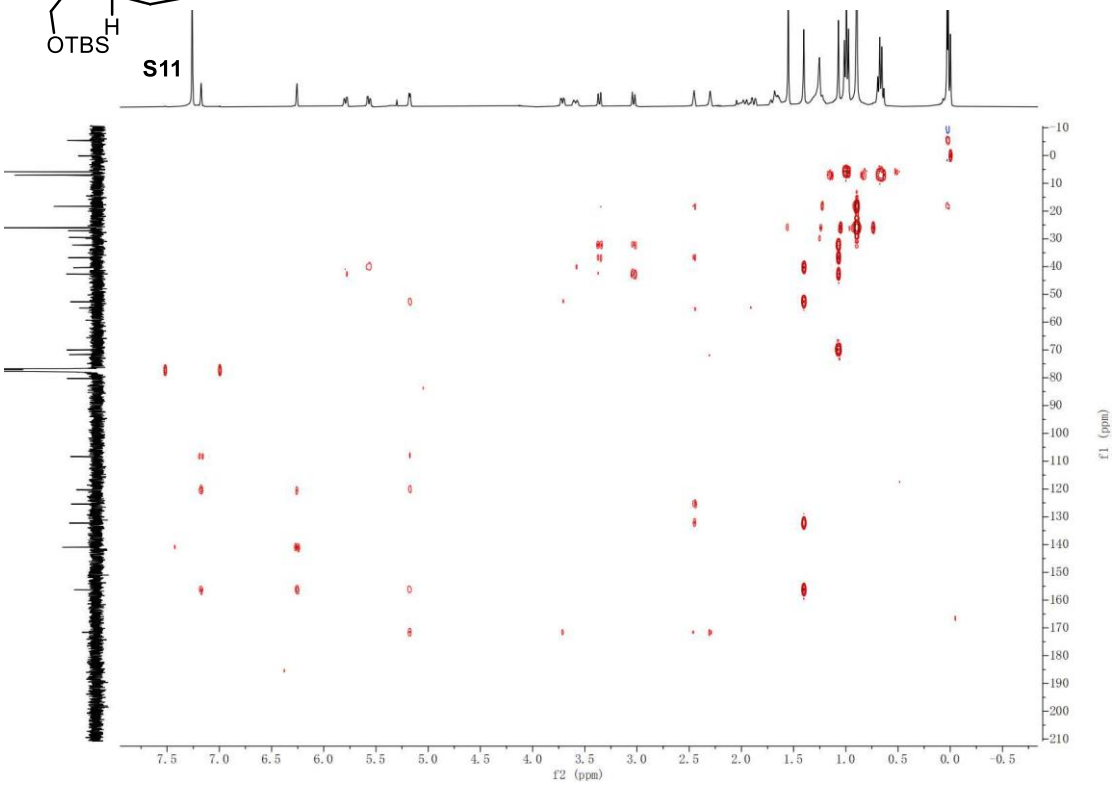
^{1}H-^{1}H COSY spectrum of **S11**



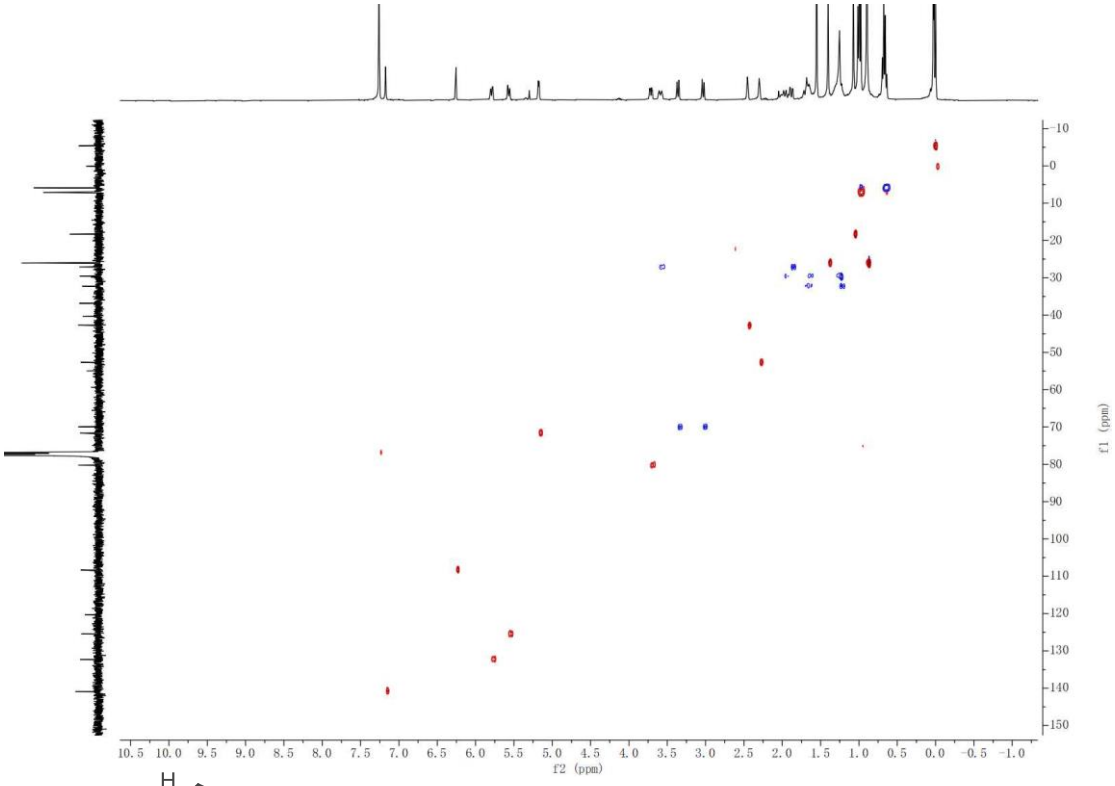


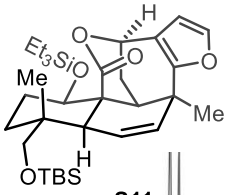
S11

HMBC spectrum of **S11**

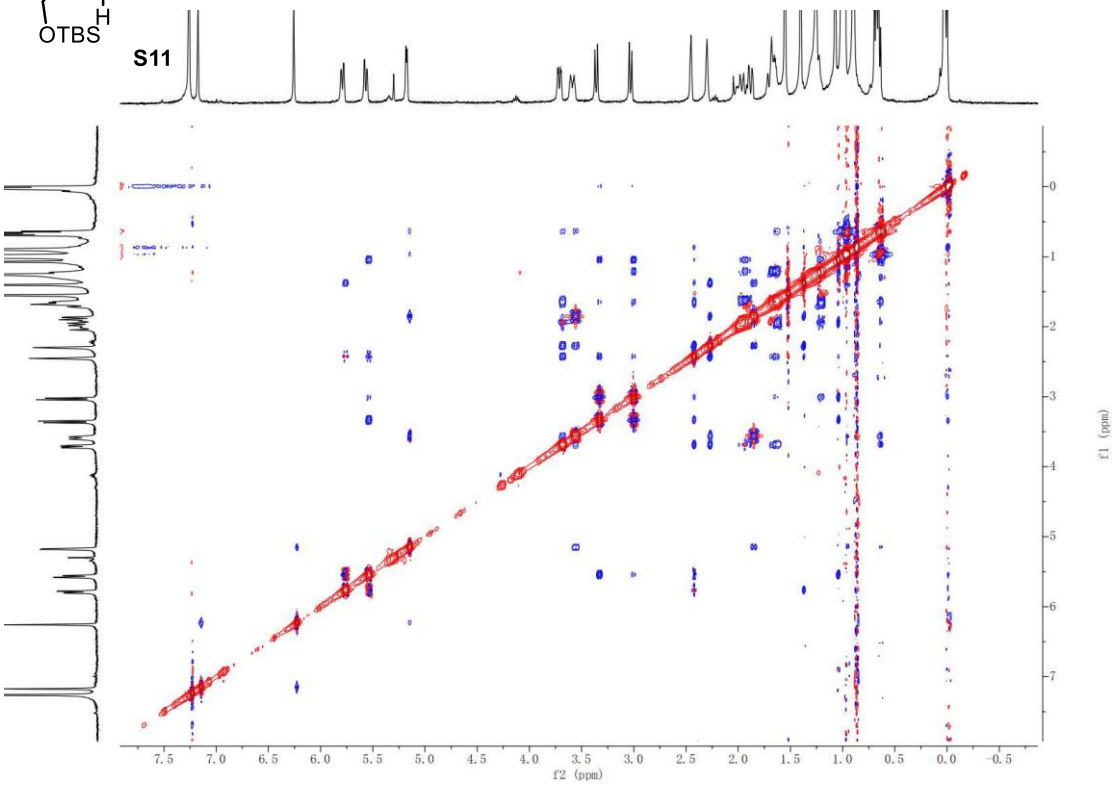


HSQC spectrum of **S11**

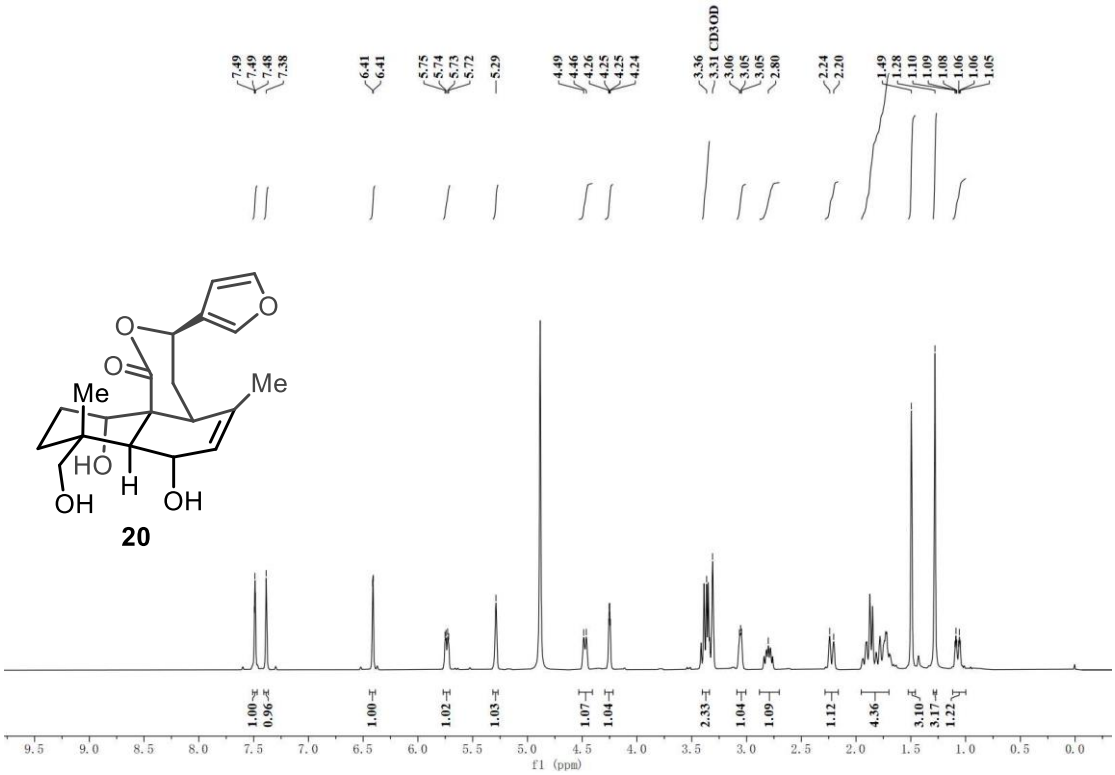




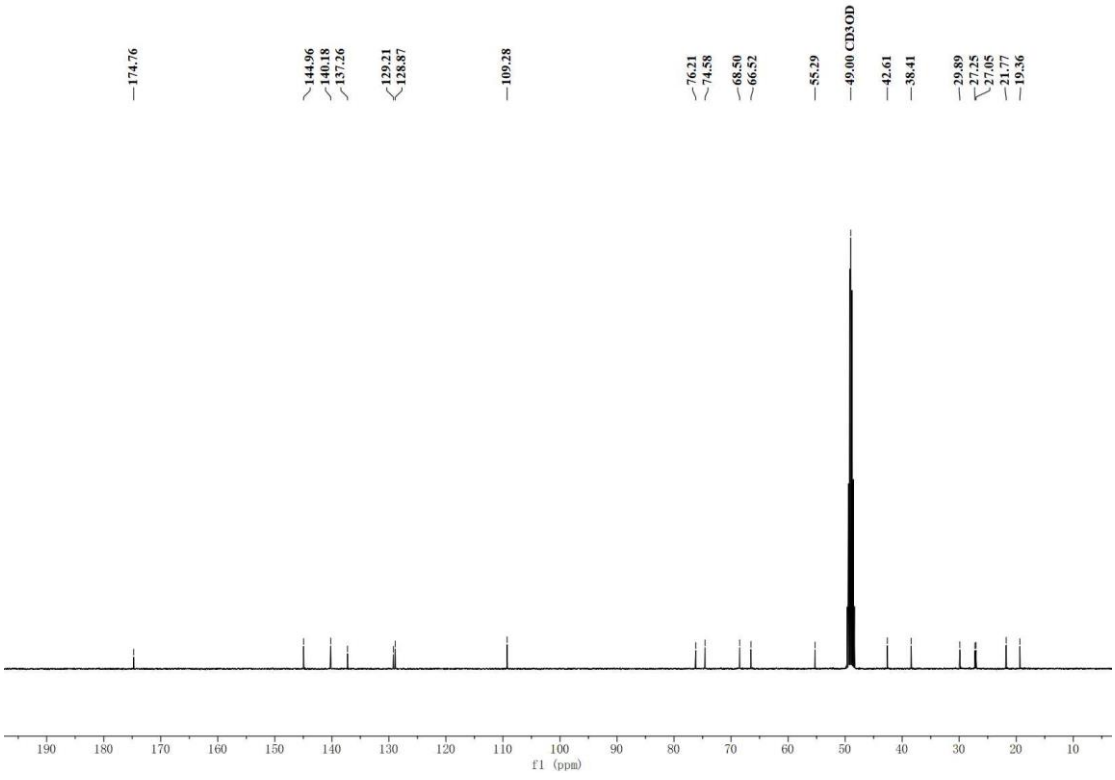
NOESY spectrum of **S11**



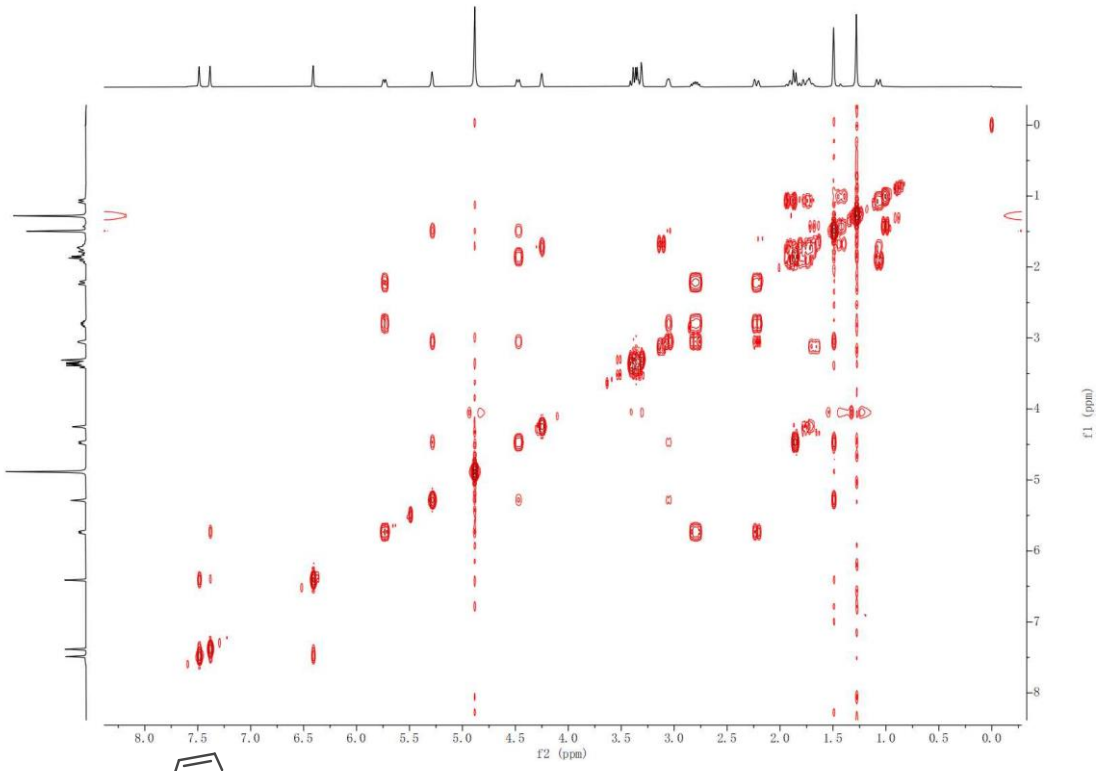
^{1}H NMR spectrum of **20** (400 MHz, CD_3OD)

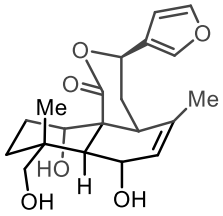


^{13}C NMR spectrum of **20** (100 MHz, CD_3OD)



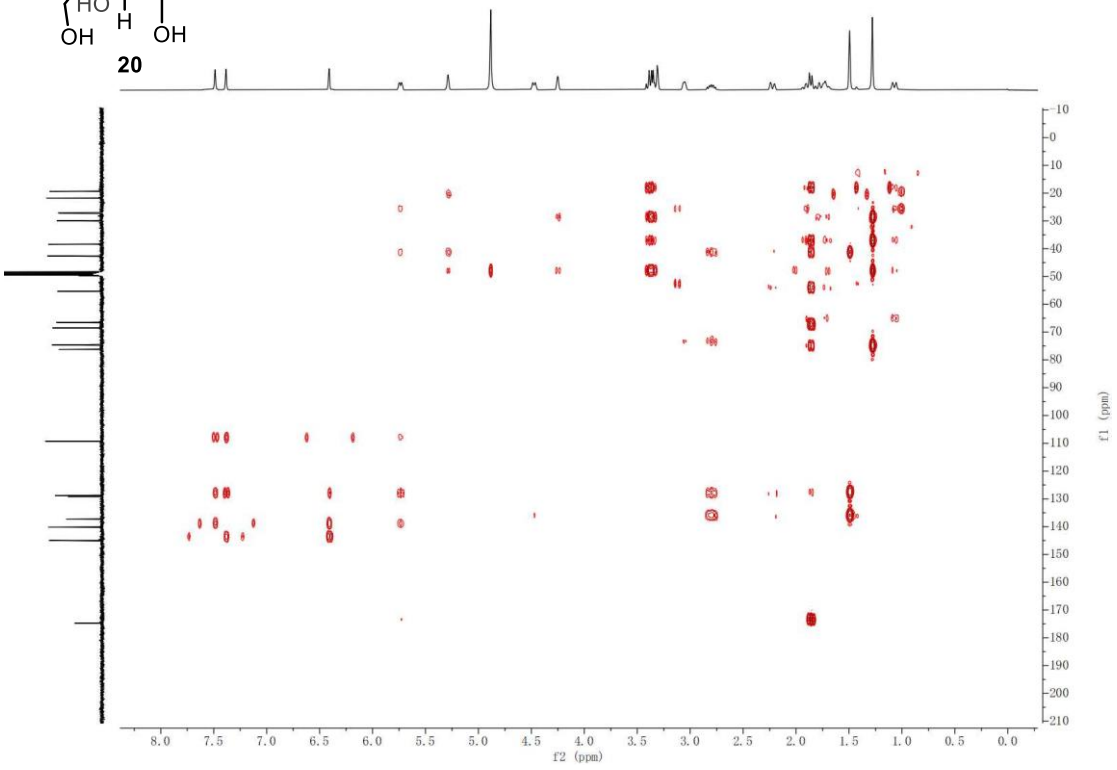
^{1}H-^{1}H COSY spectrum of **20**



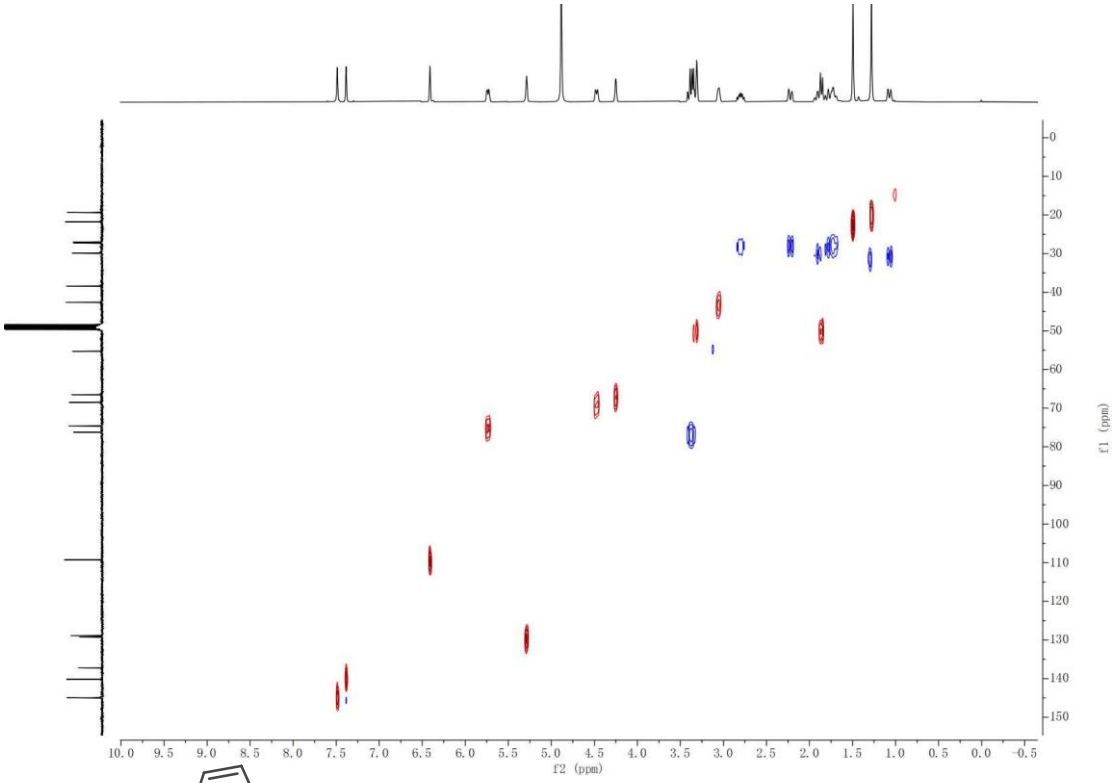


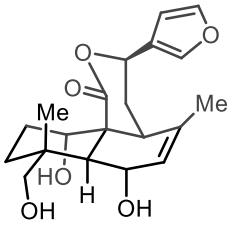
20

HMBC spectrum of **20**



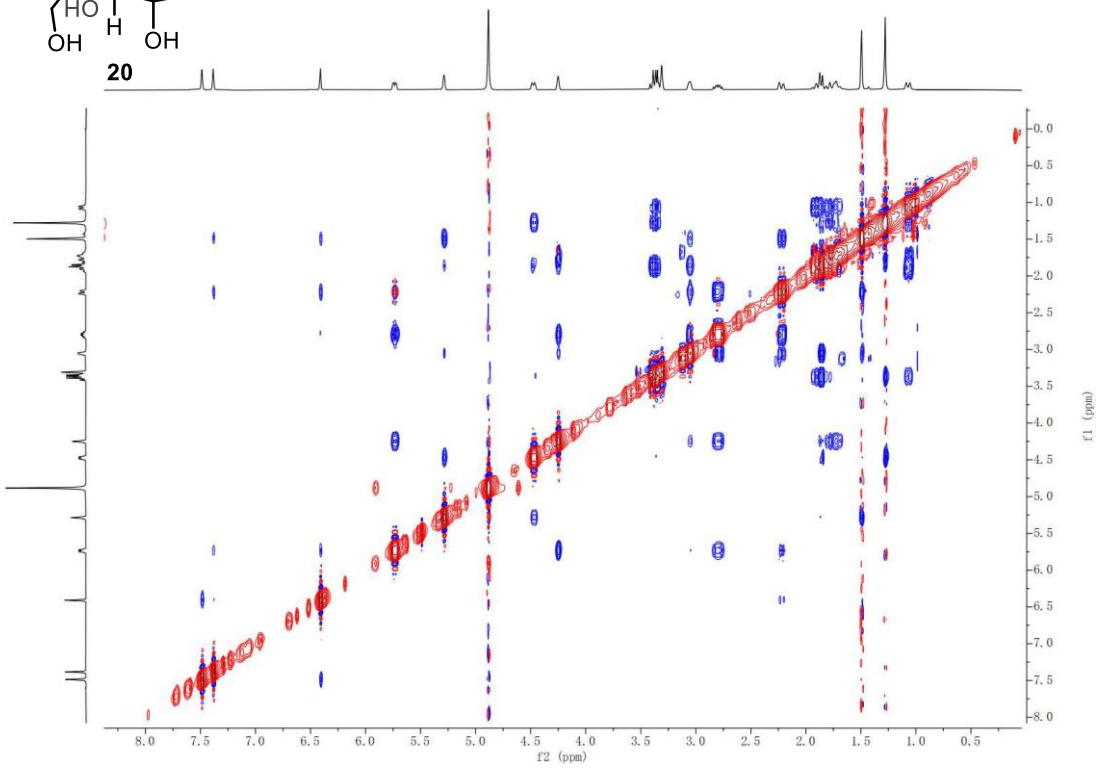
HSQC spectrum of **20**



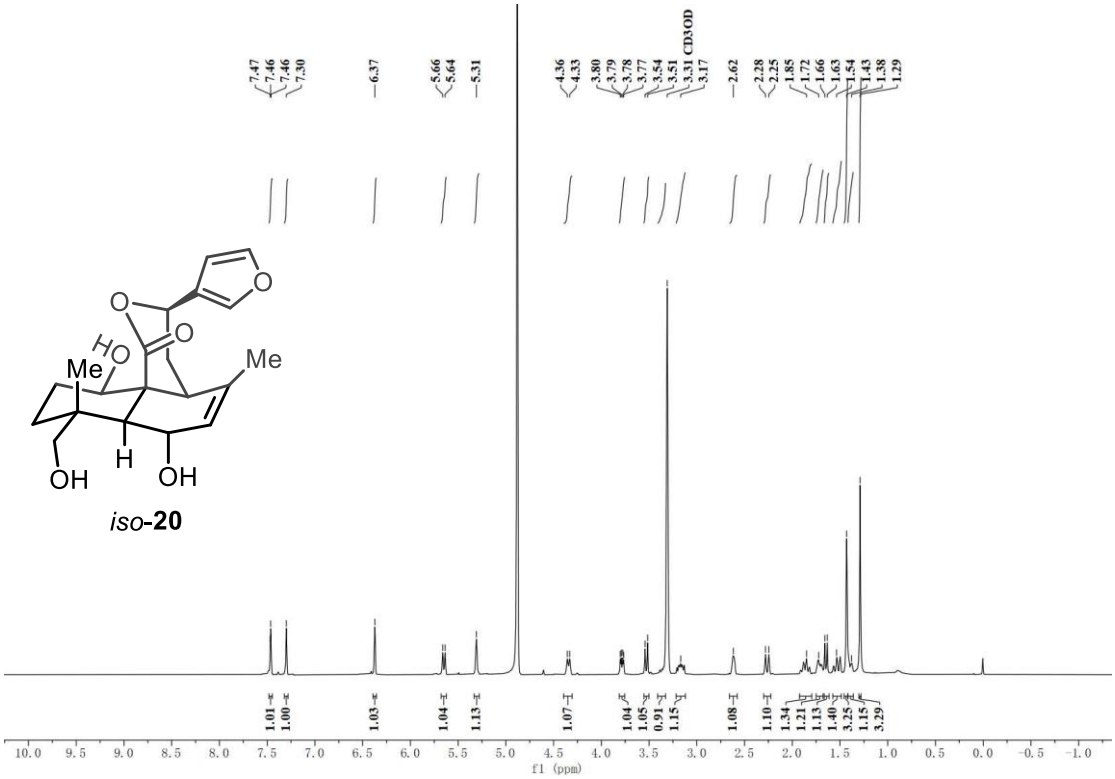


20

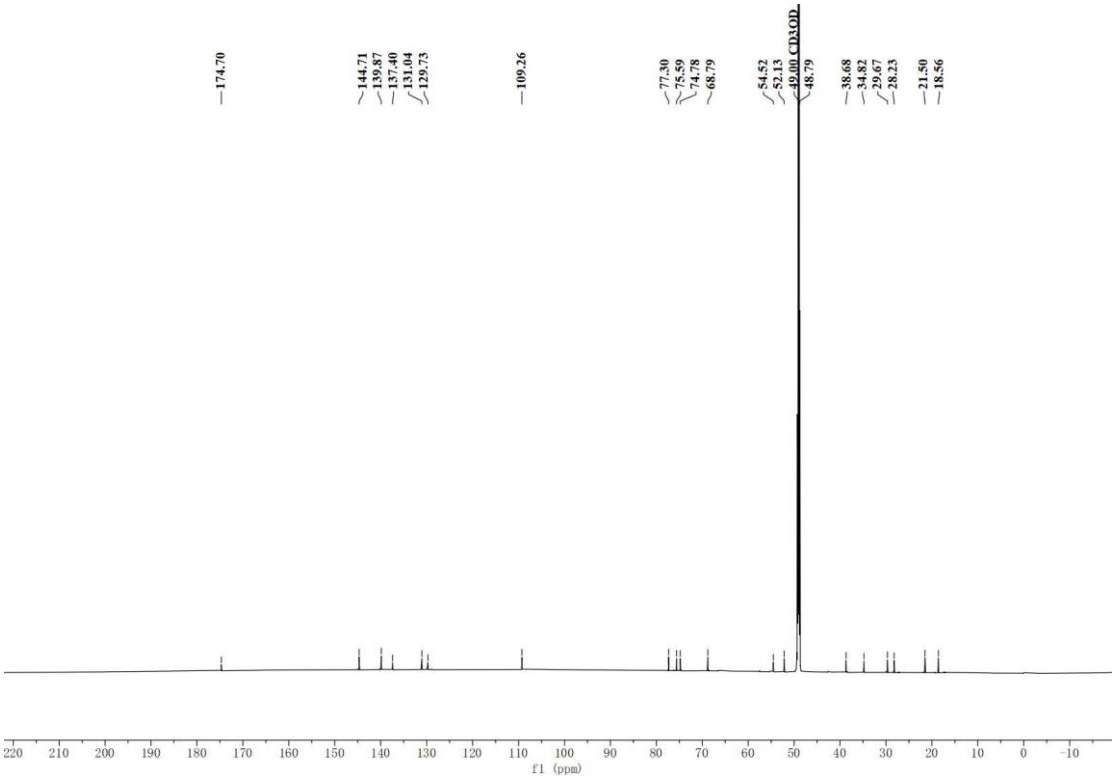
NOESY spectrum of **20**



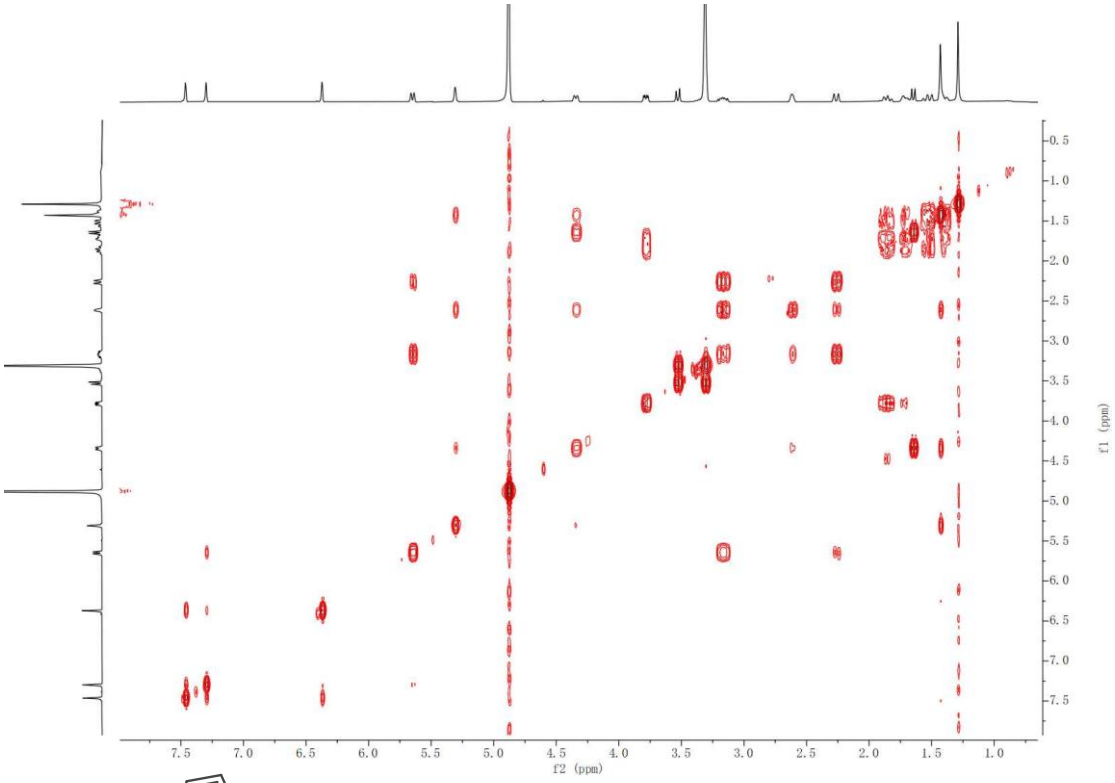
^{1}H NMR spectrum of *iso*-**20** (400 MHz, CD_3OD)

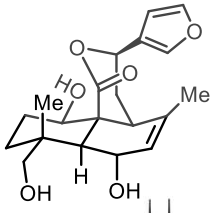


^{13}C NMR spectrum of *iso*-**20** (200 MHz, CD_3OD)



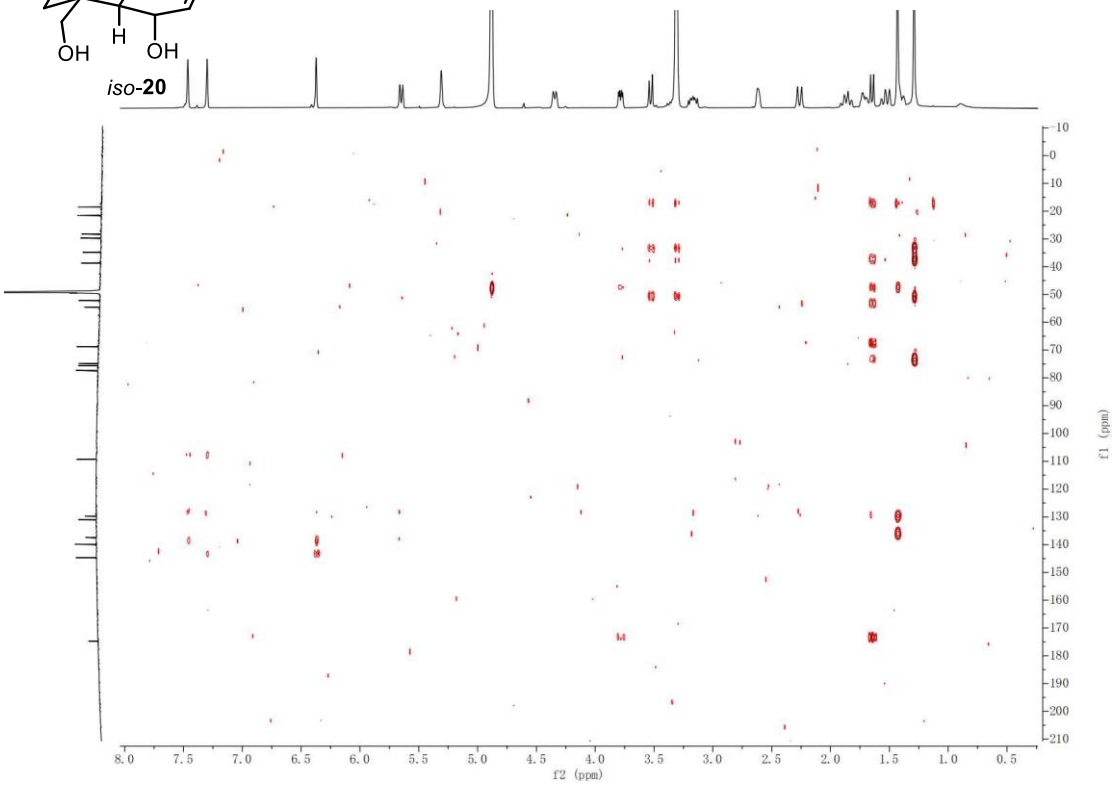
^{1}H-^{1}H COSY spectrum of *iso*-**20**



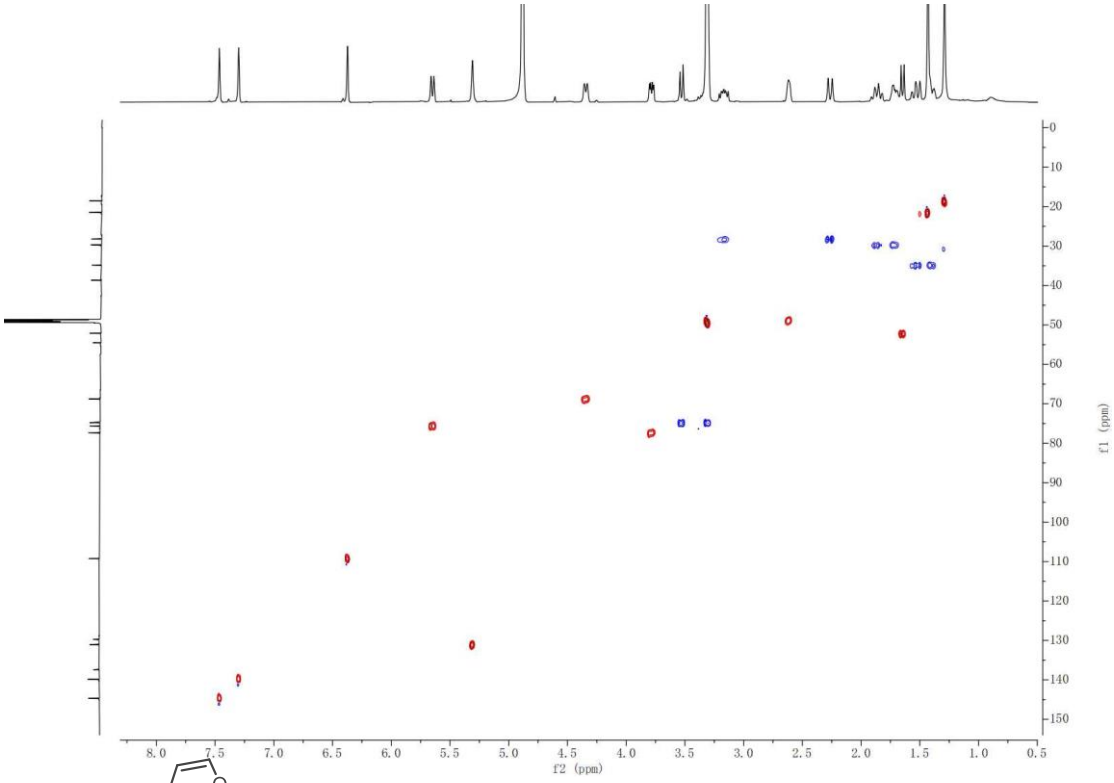


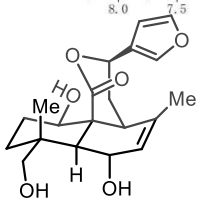
iso-**20**

HMBC spectrum of *iso*-**20**



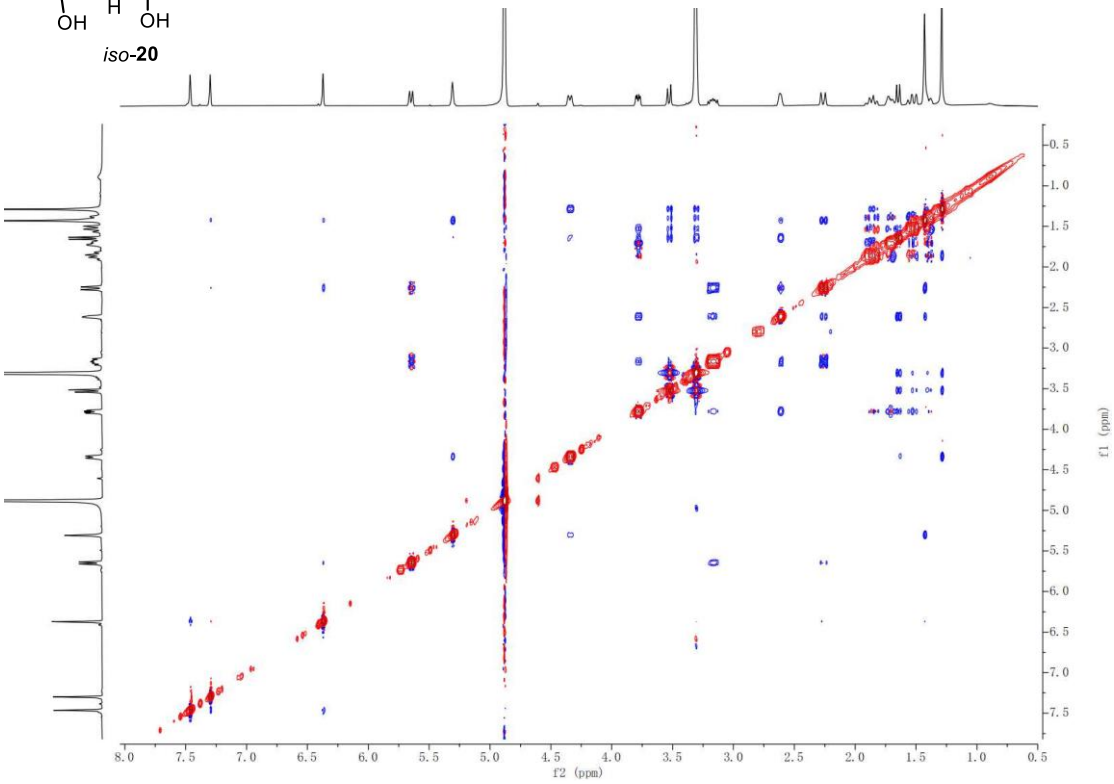
HSQC spectrum of *iso*-**20**



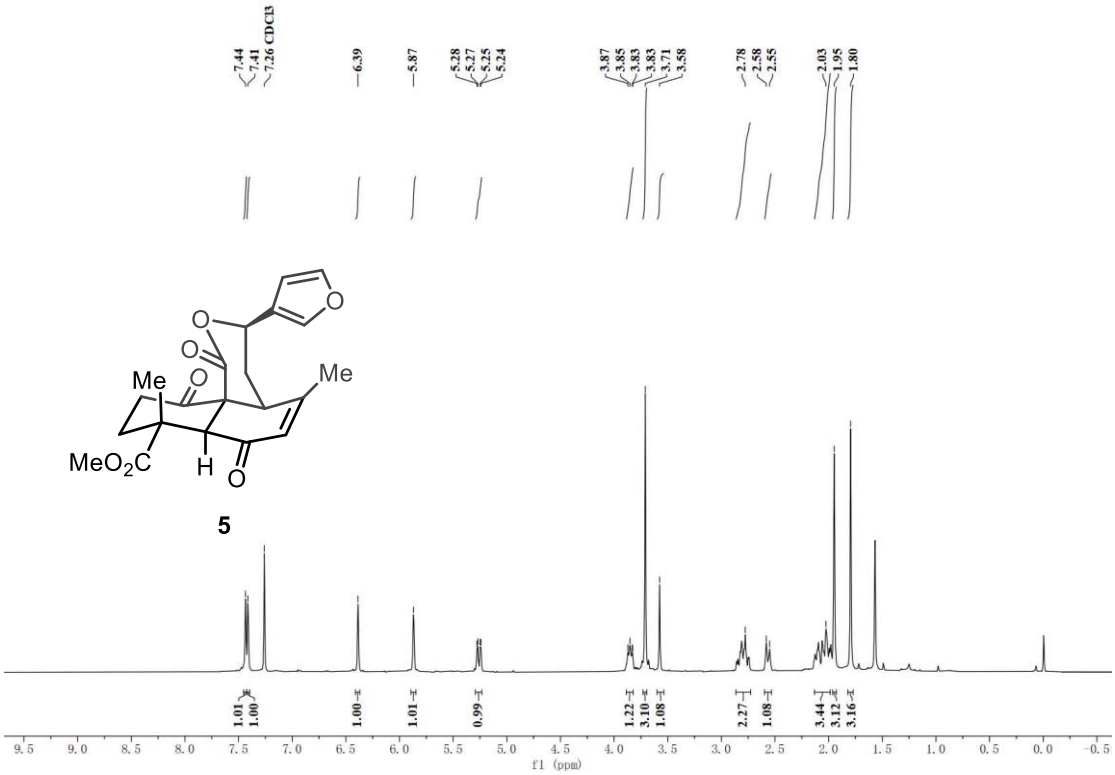


iso-**20**

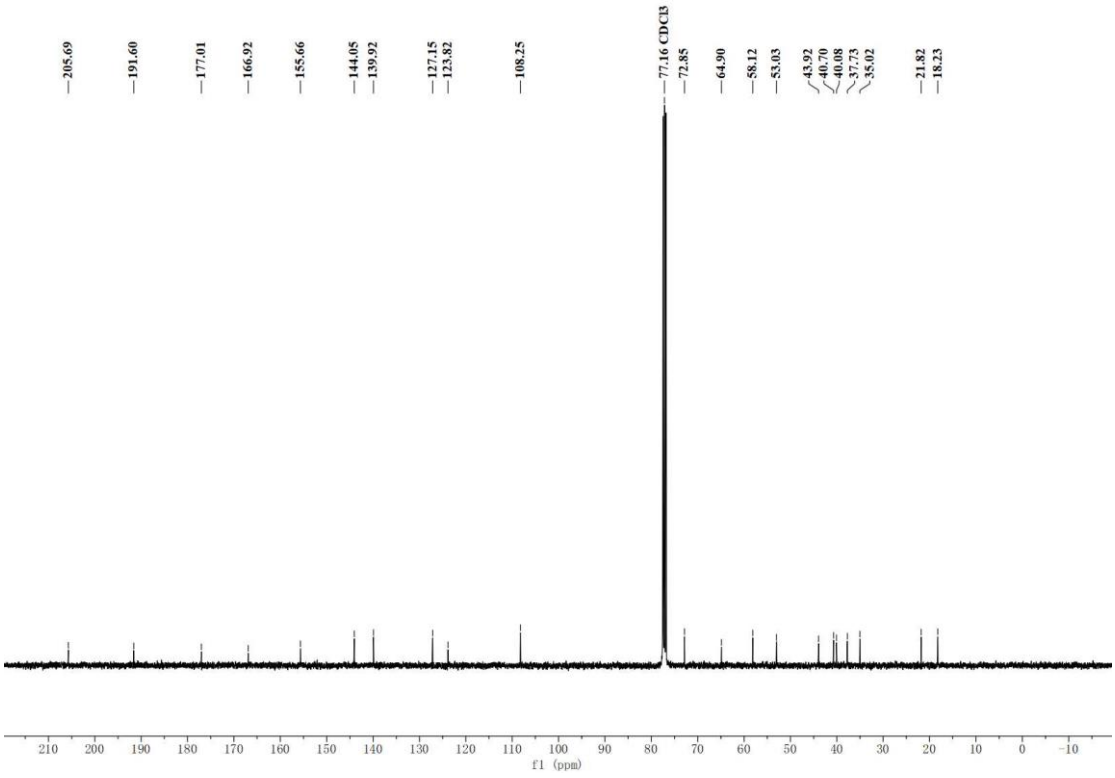
NOESY spectrum of *iso*-**20**



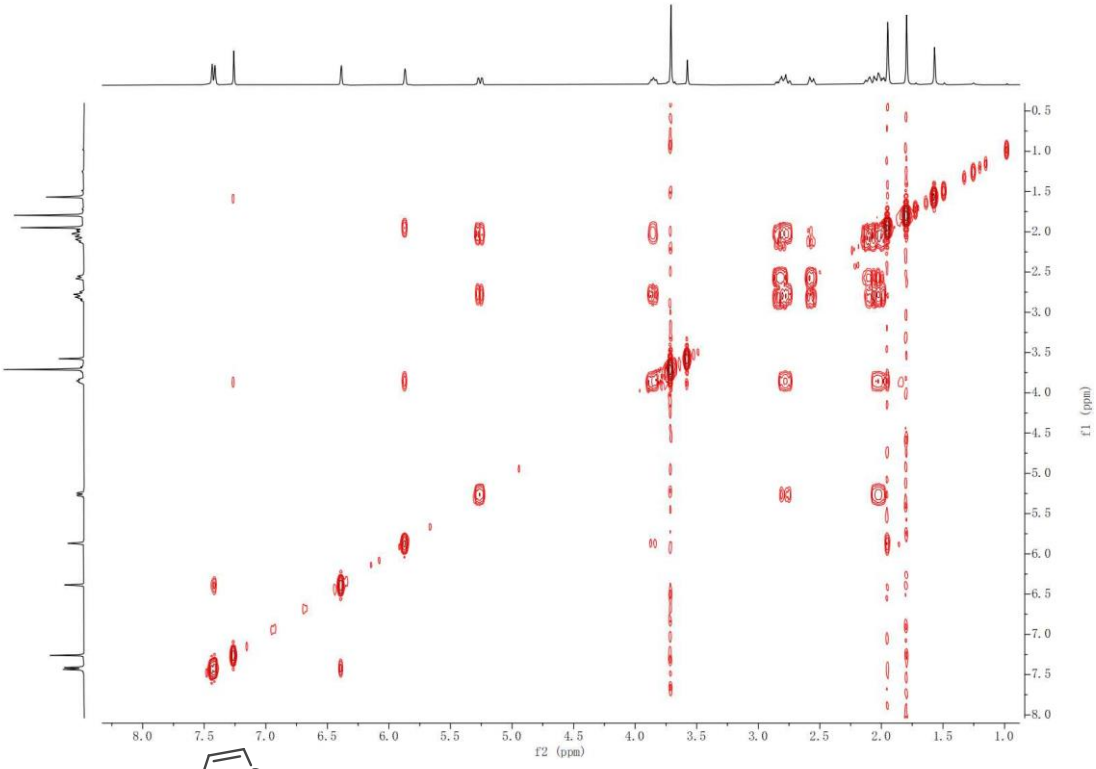
^{1}H NMR spectrum of **5** (400 MHz, $CDCl_3$)

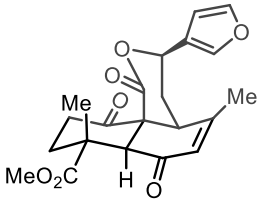


^{13}C NMR spectrum of **5** (100 MHz, $CDCl_3$)



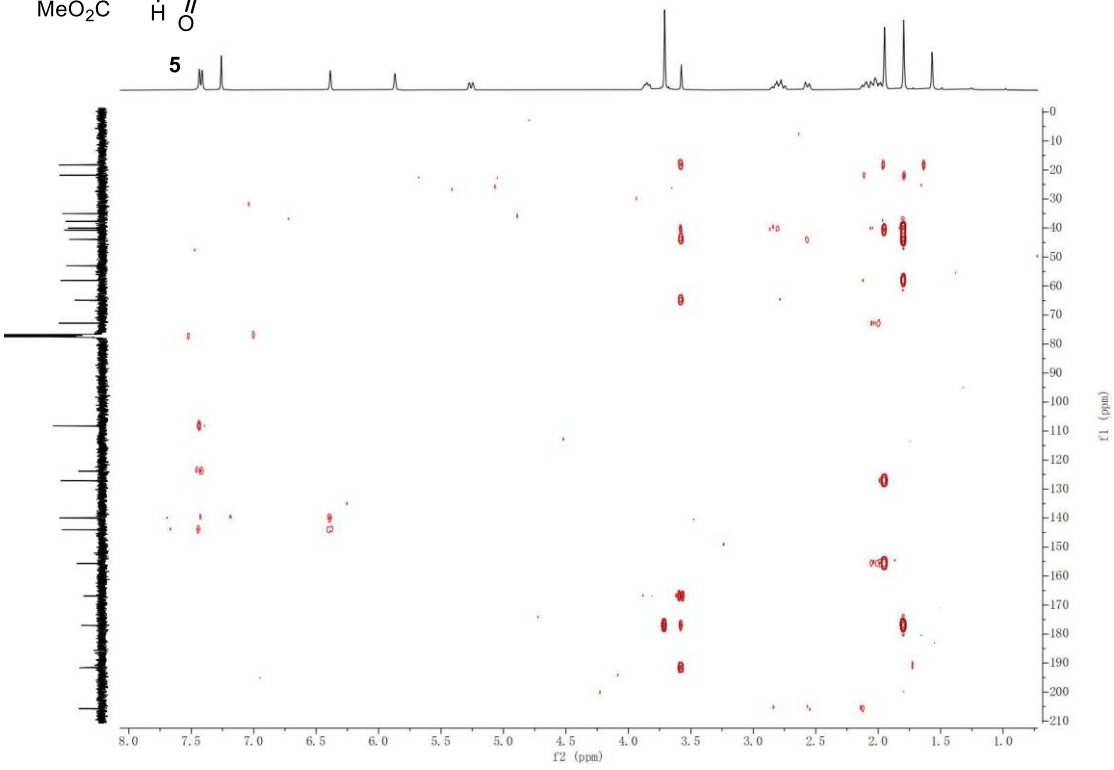
^{1}H-^{1}H COSY spectrum of **5**



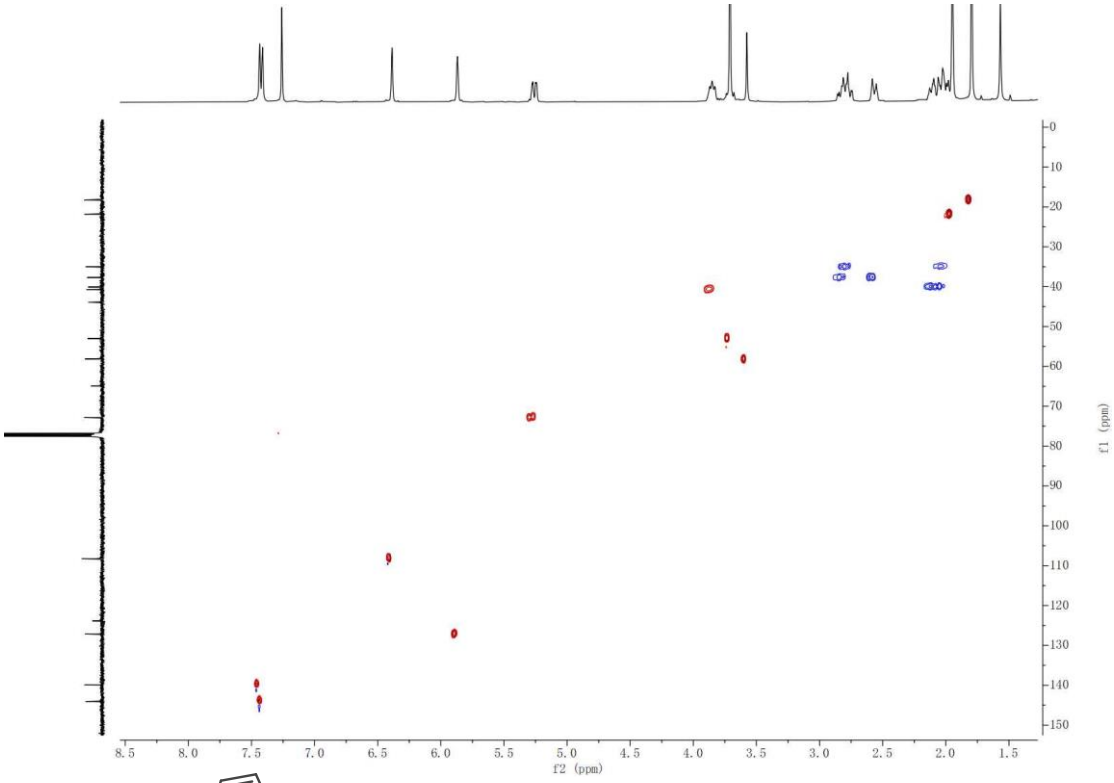


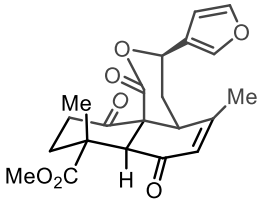
5

HMBC spectrum of **5**



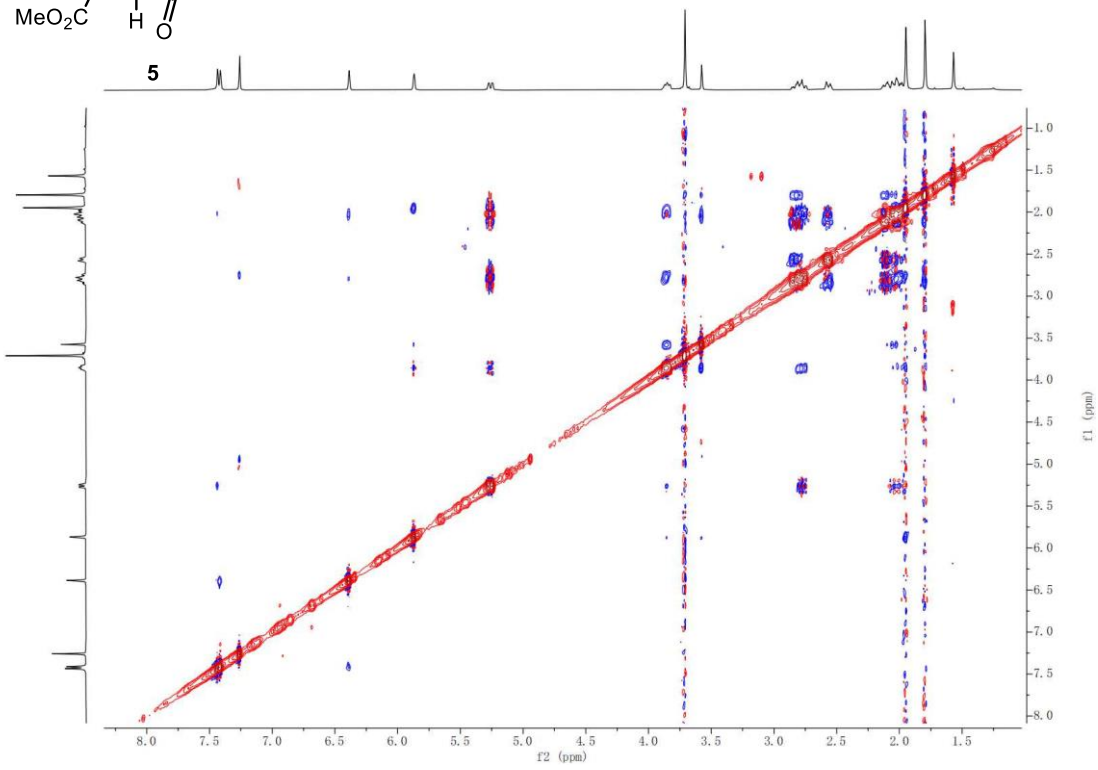
HSQC spectrum of **5**



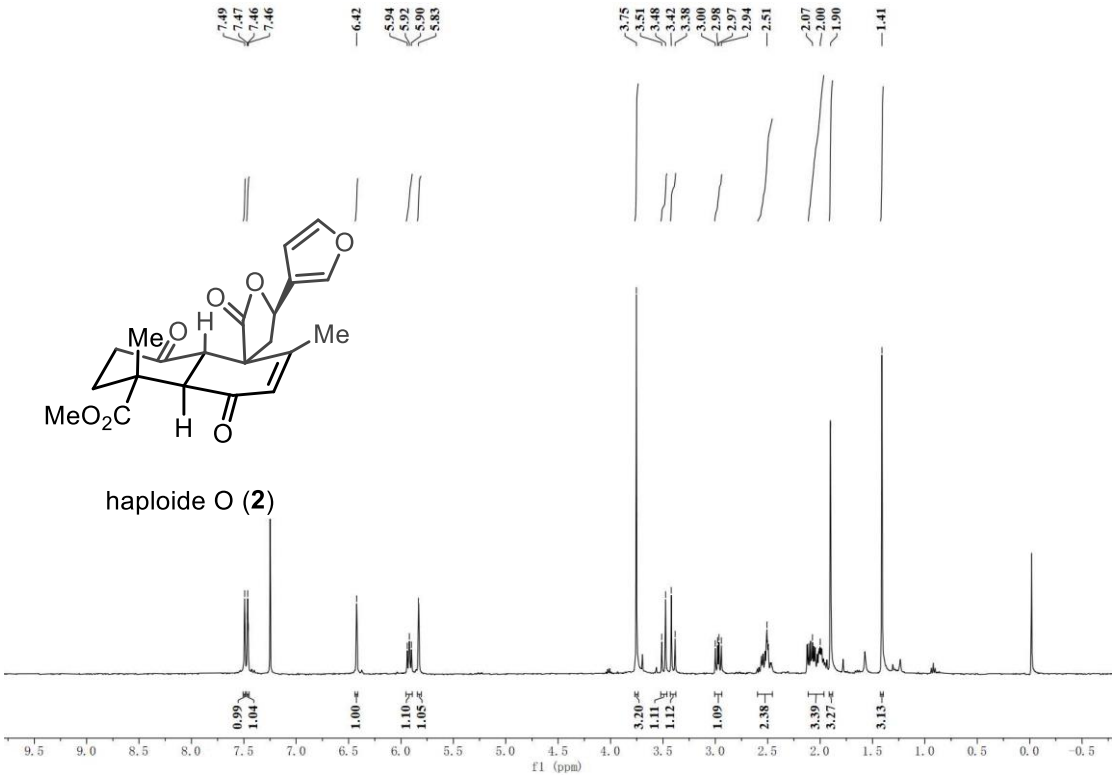


5

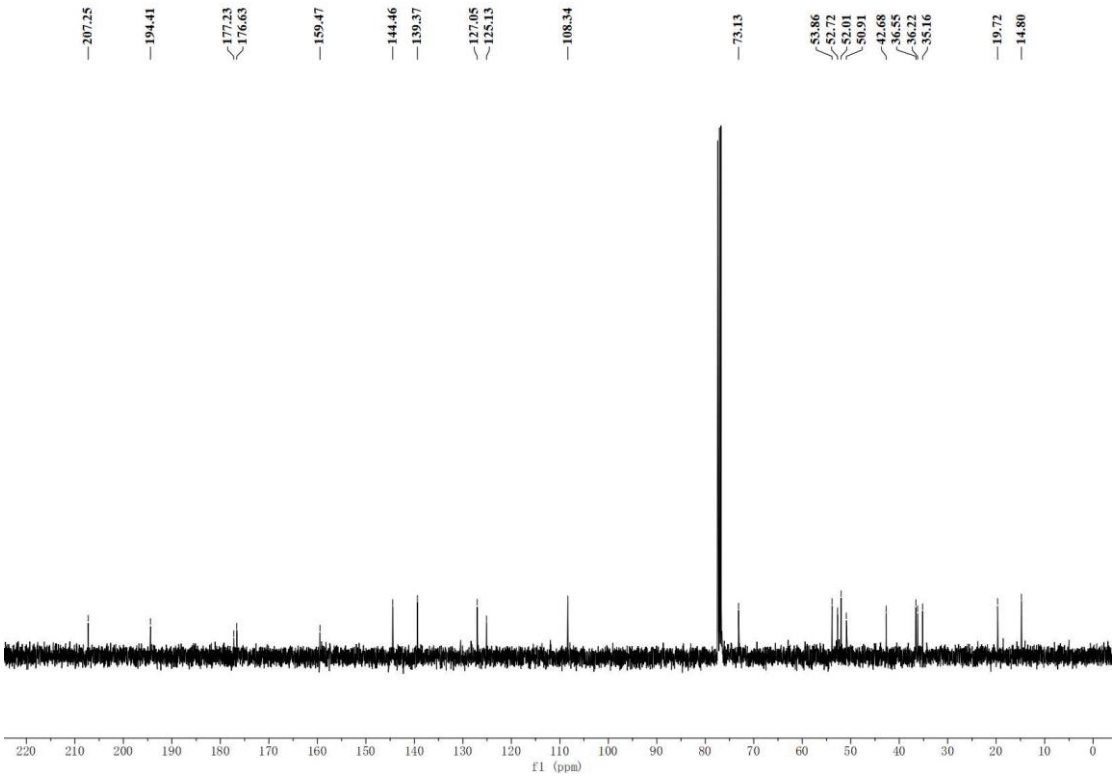
NOESY spectrum of **5**



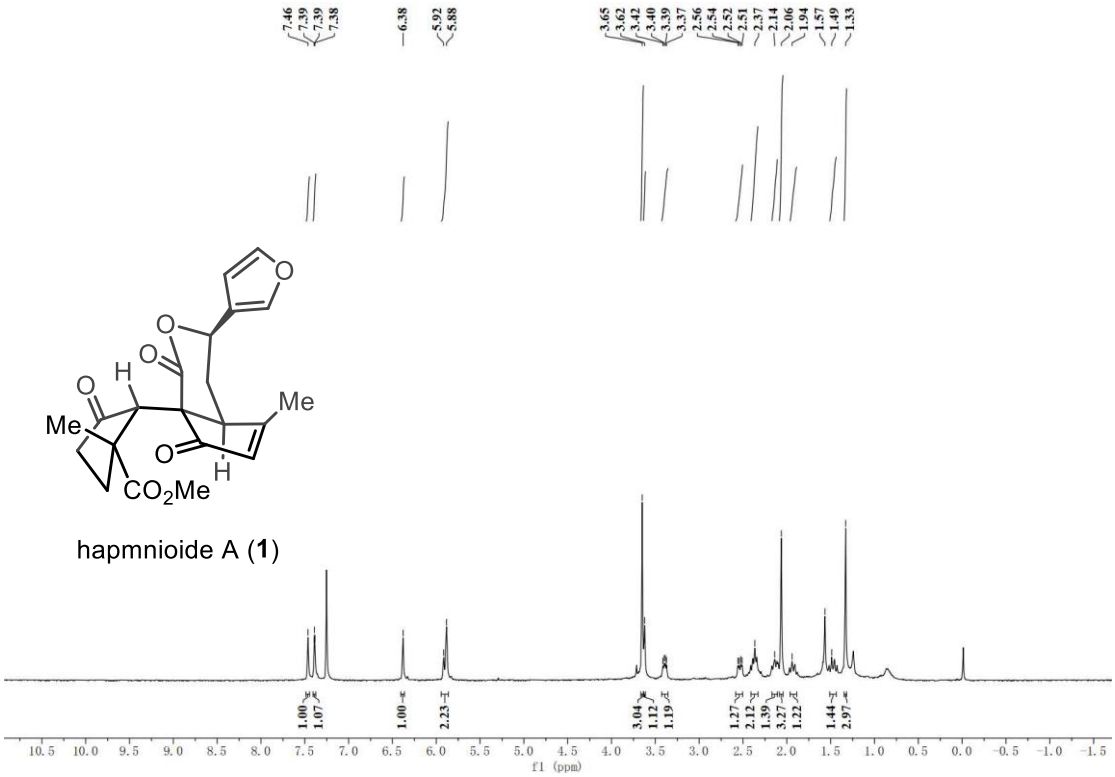
^{1}H NMR spectrum of **2** (400 MHz, $CDCl_3$)



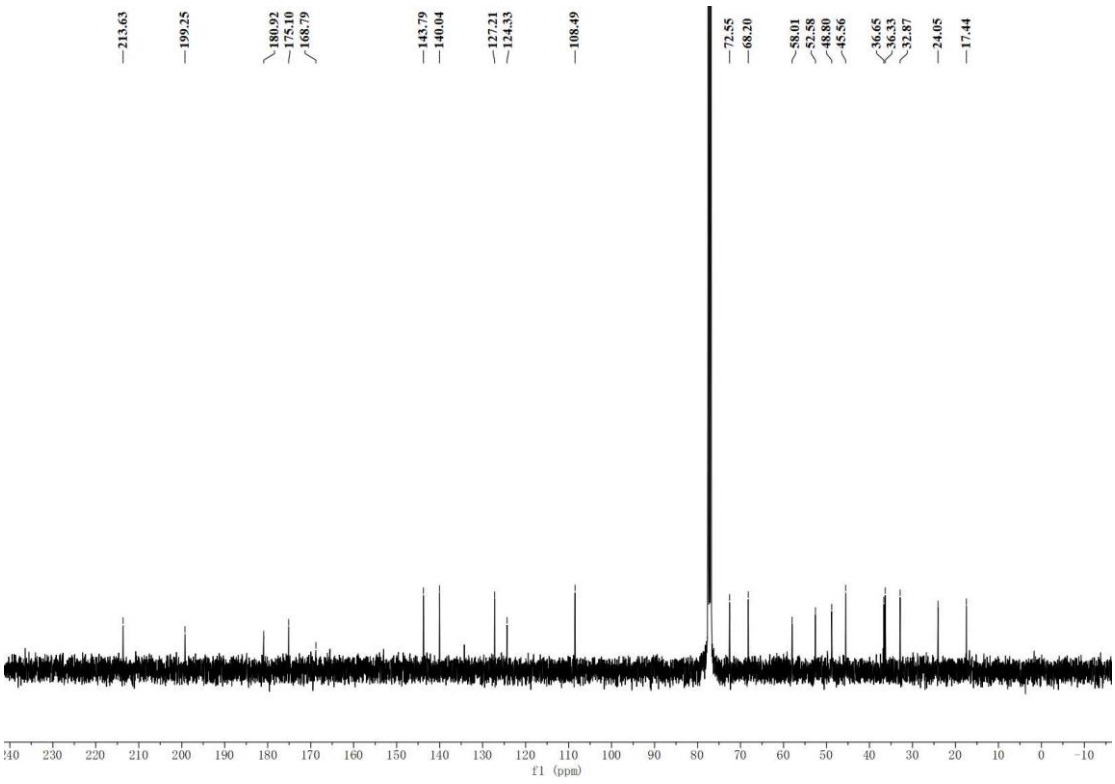
^{13}C NMR spectrum of **2** (100 MHz, $CDCl_3$)



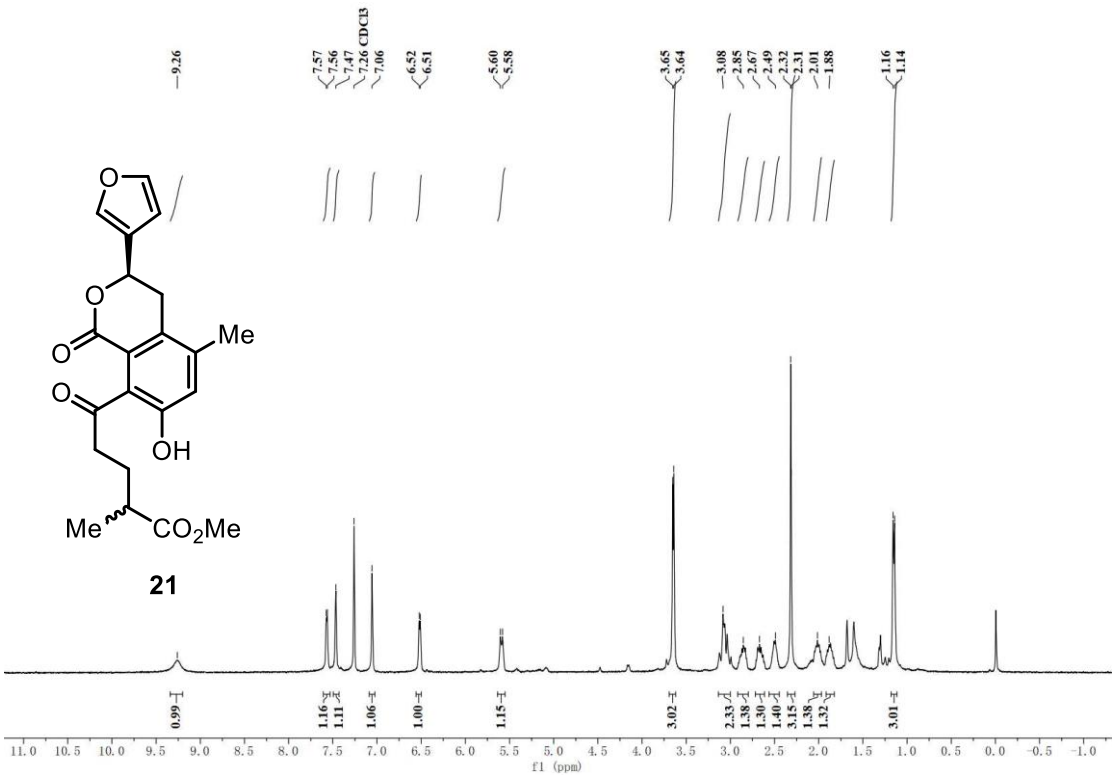
^{1}H NMR spectrum of **1** (400 MHz, $CDCl_3$)



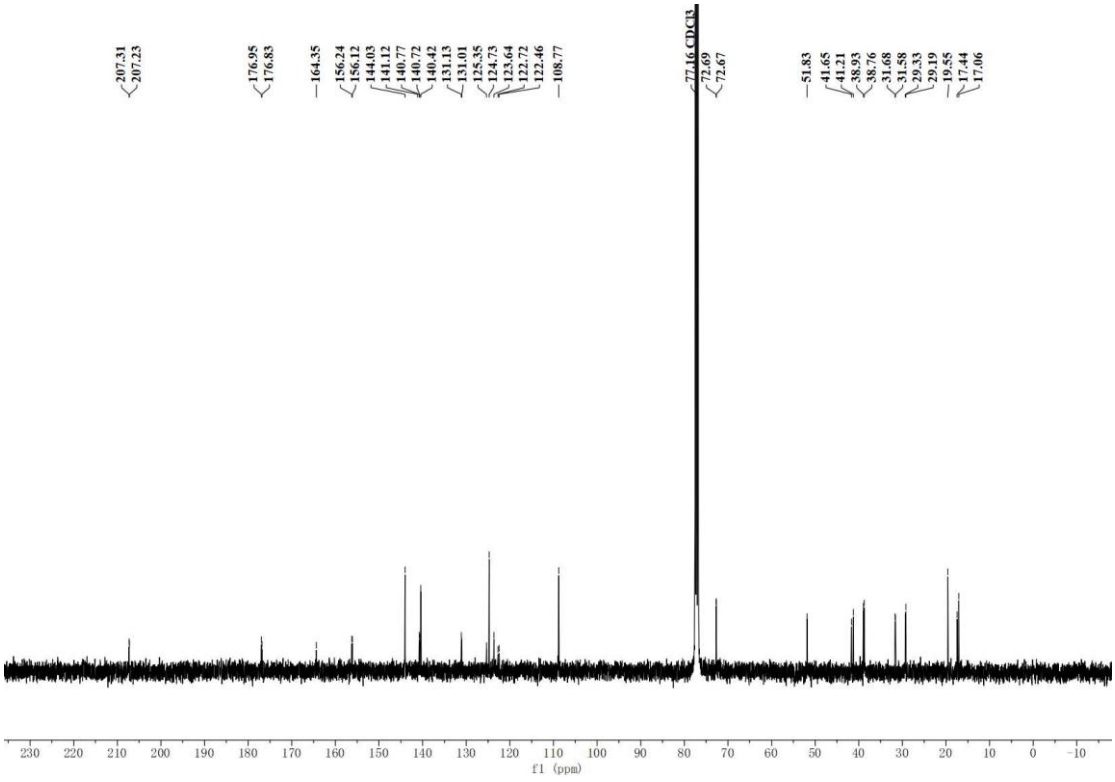
^{13}C NMR spectrum of **1** (100 MHz, $CDCl_3$)



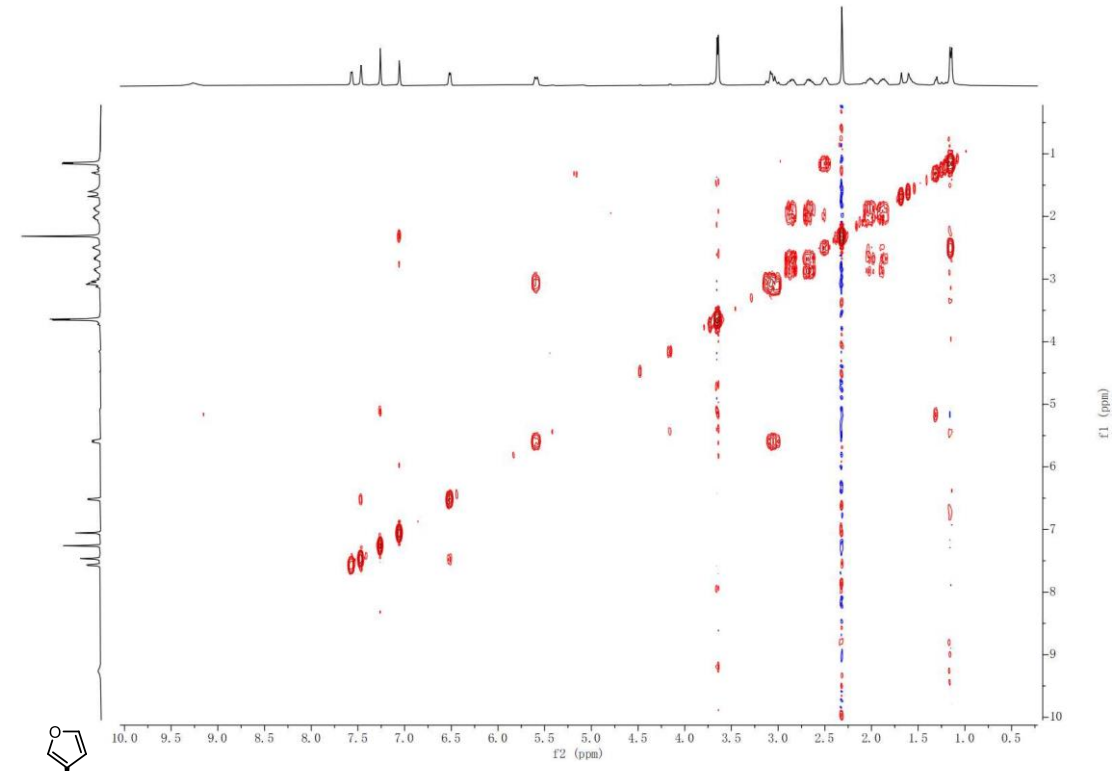
^{1}H NMR spectrum of **21** (400 MHz, $CDCl_3$)

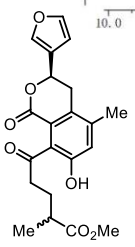


^{13}C NMR spectrum of **21** (100 MHz, $CDCl_3$)



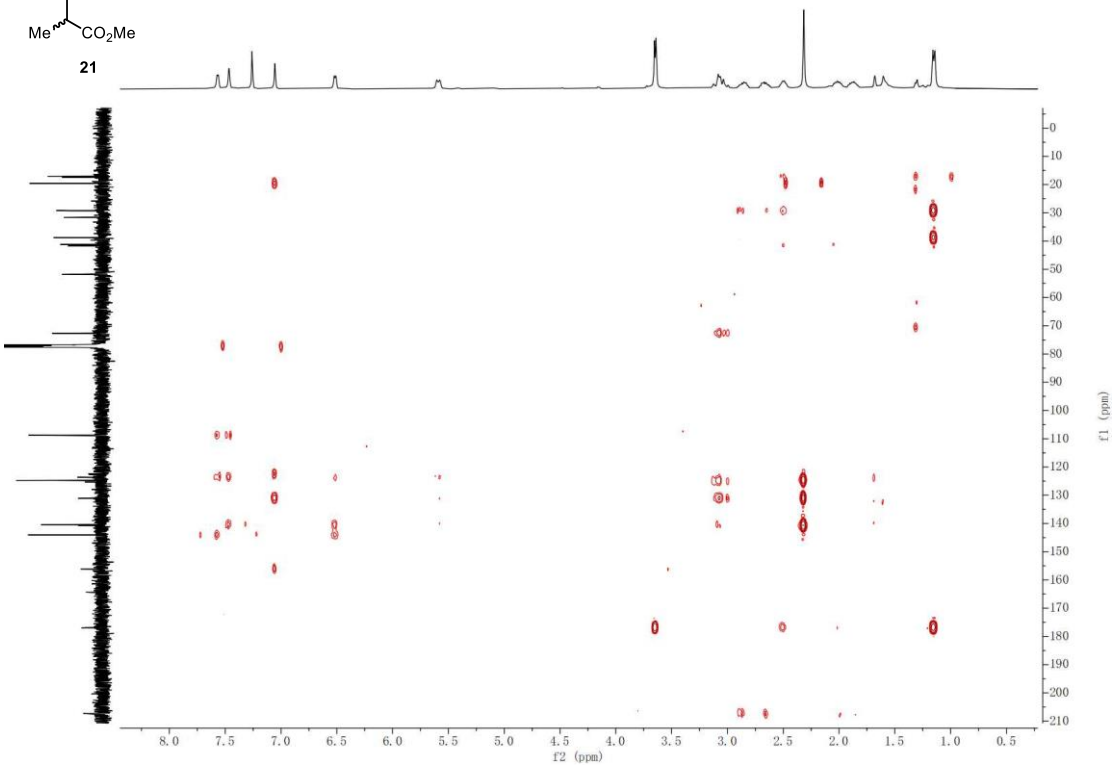
^{1}H-^{1}H COSY spectrum of **21**



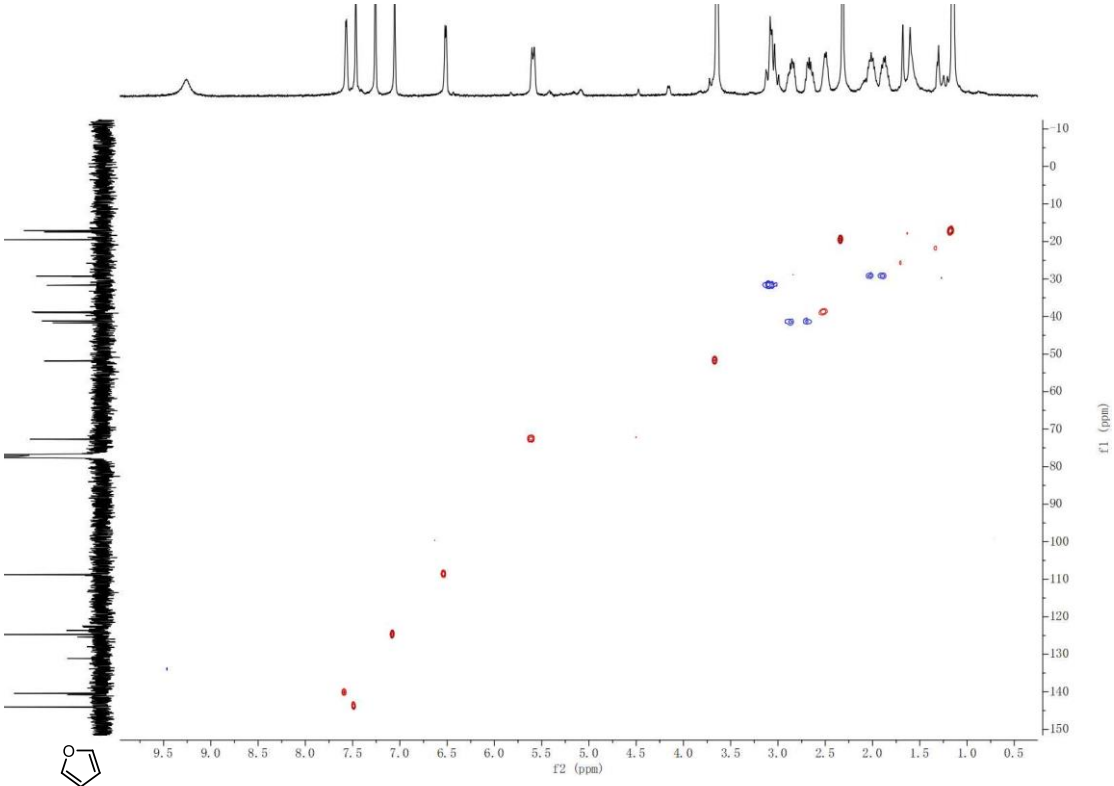


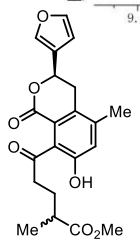
21

HMBC spectrum of **21**



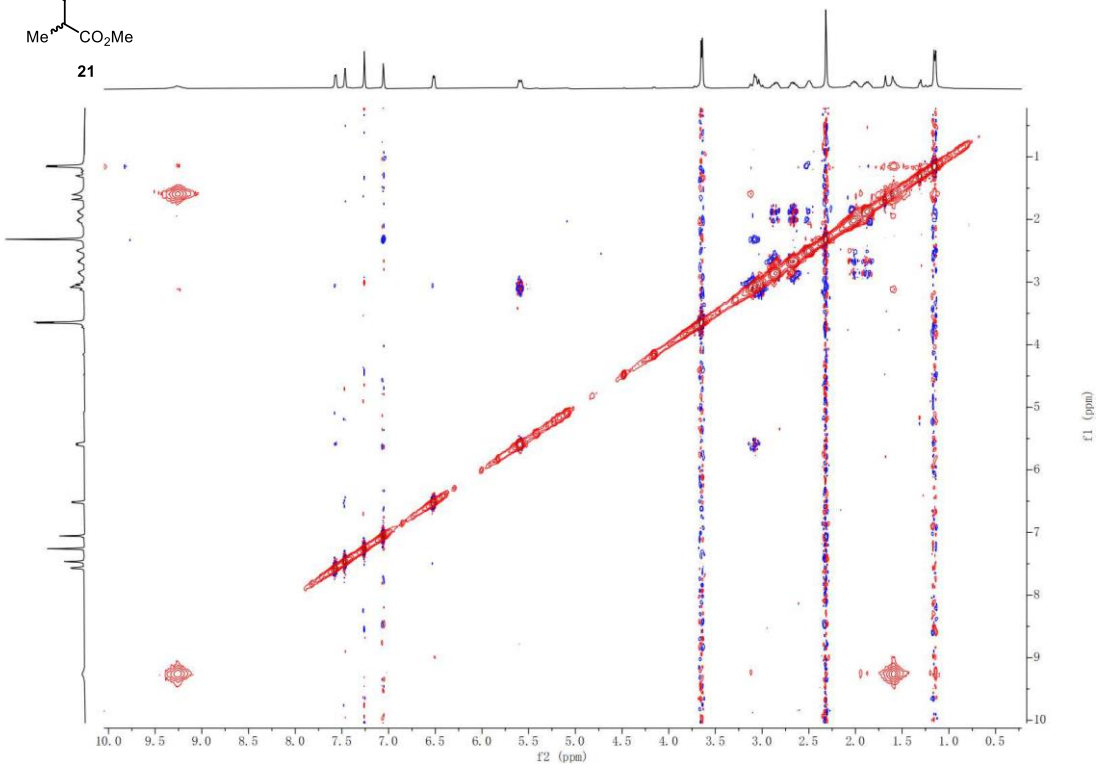
HSQC spectrum of **21**



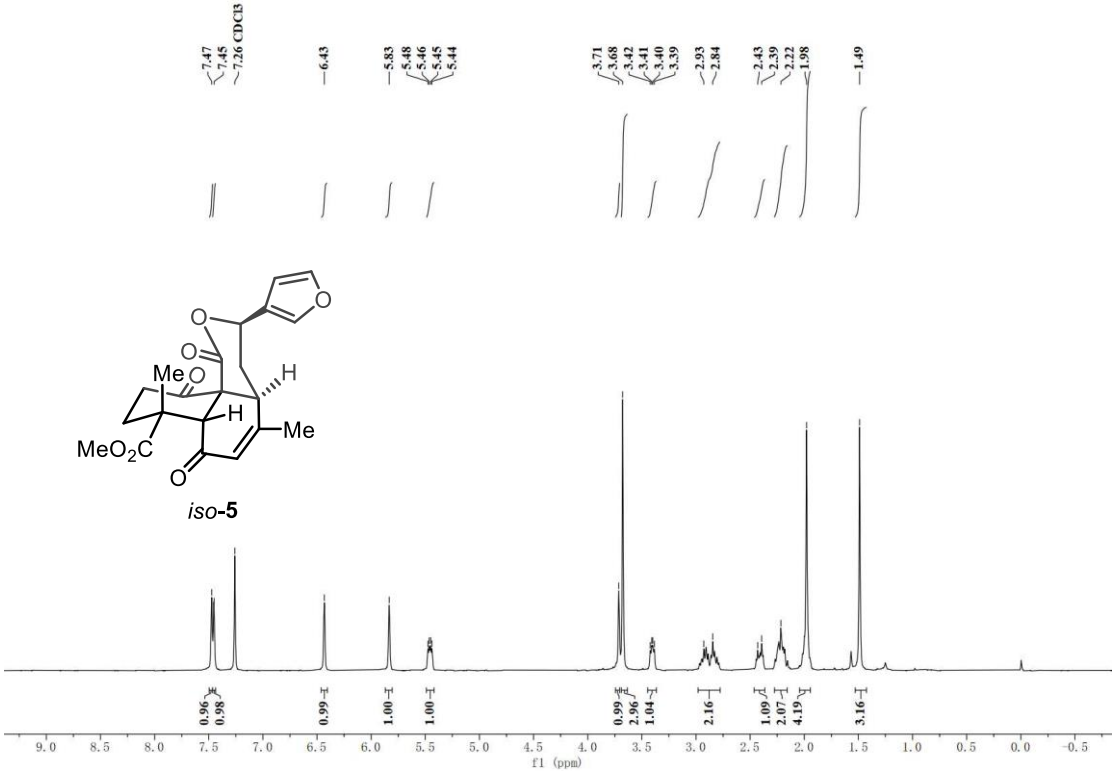


21

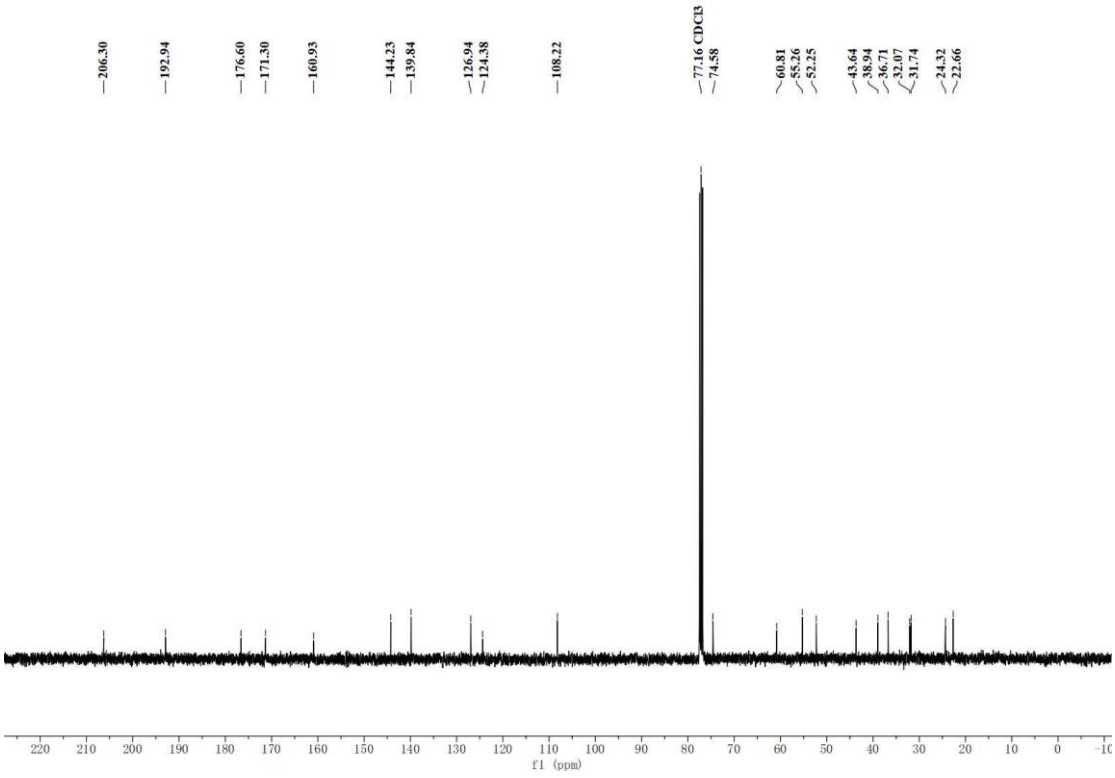
NOESY spectrum of **21**



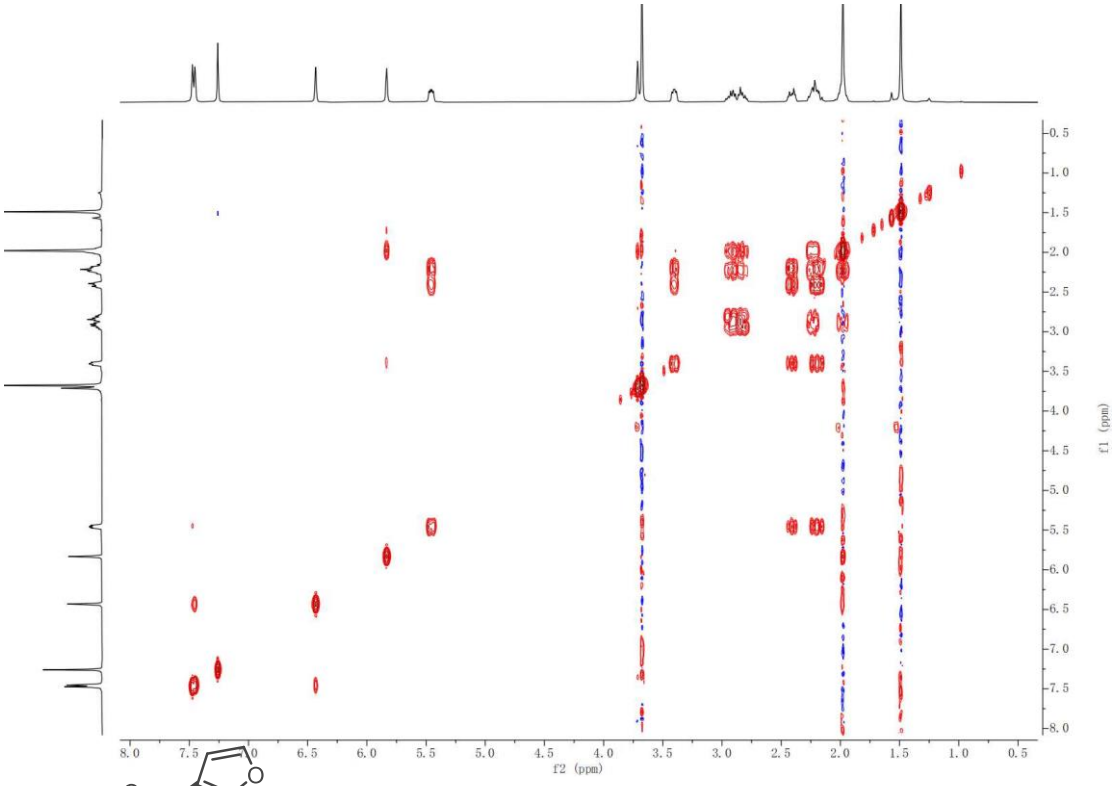
^{1}H NMR spectrum of *iso*-**5** (400 MHz, $CDCl_3$)

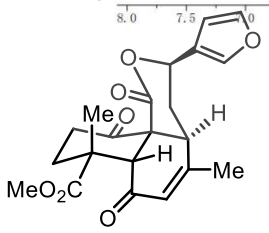


^{13}C NMR spectrum of *iso*-**5** (100 MHz, $CDCl_3$)



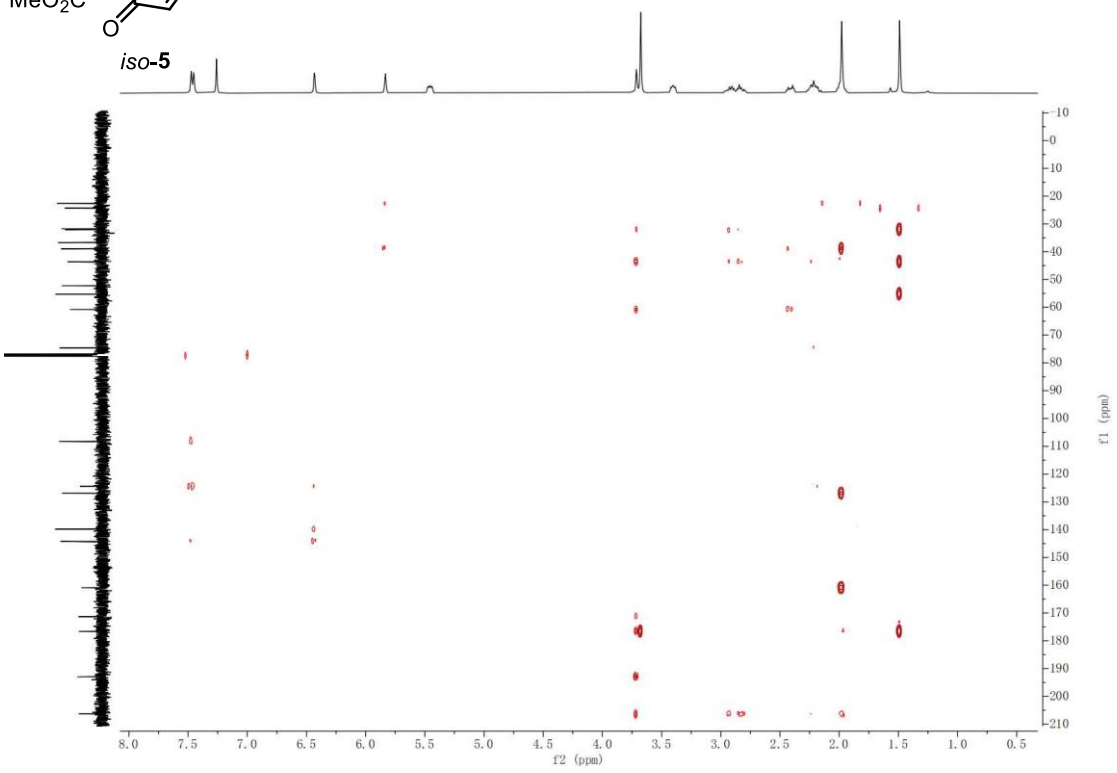
^{1}H-^{1}H COSY spectrum of *iso*-**5**



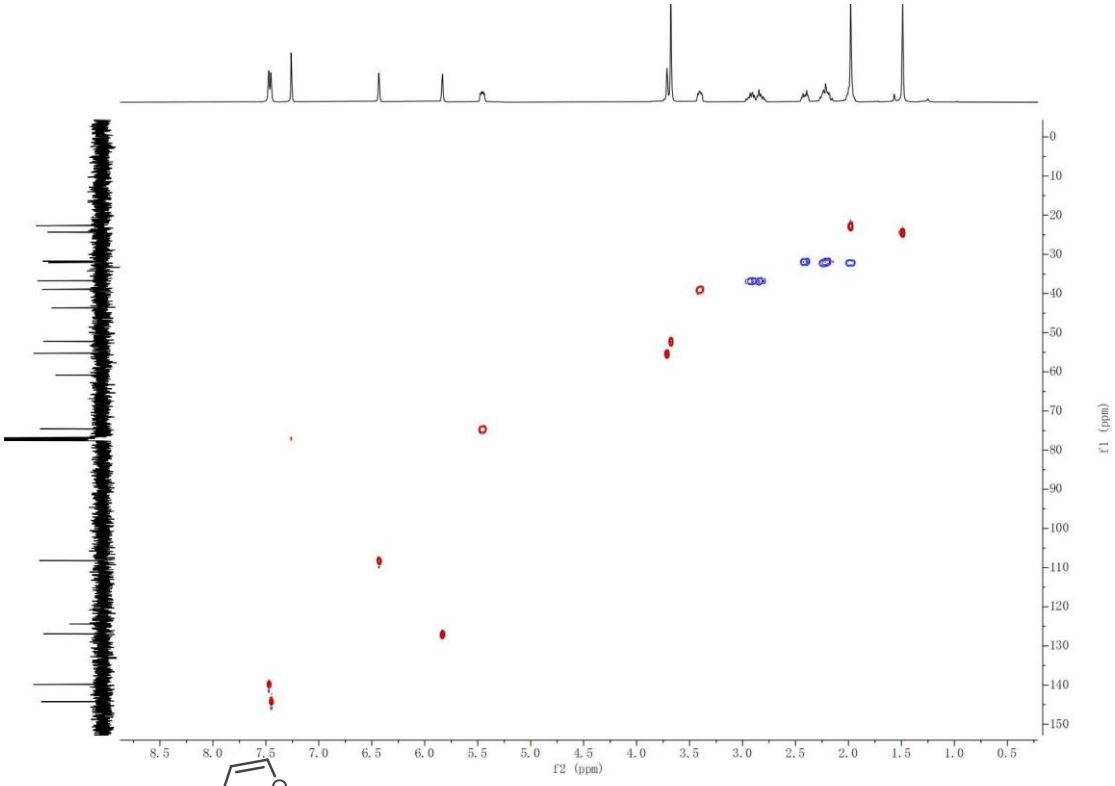


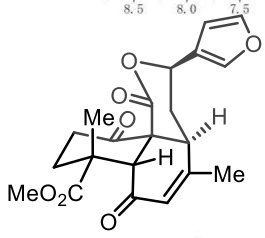
iso-**5**

HMBC spectrum of *iso*-**5**



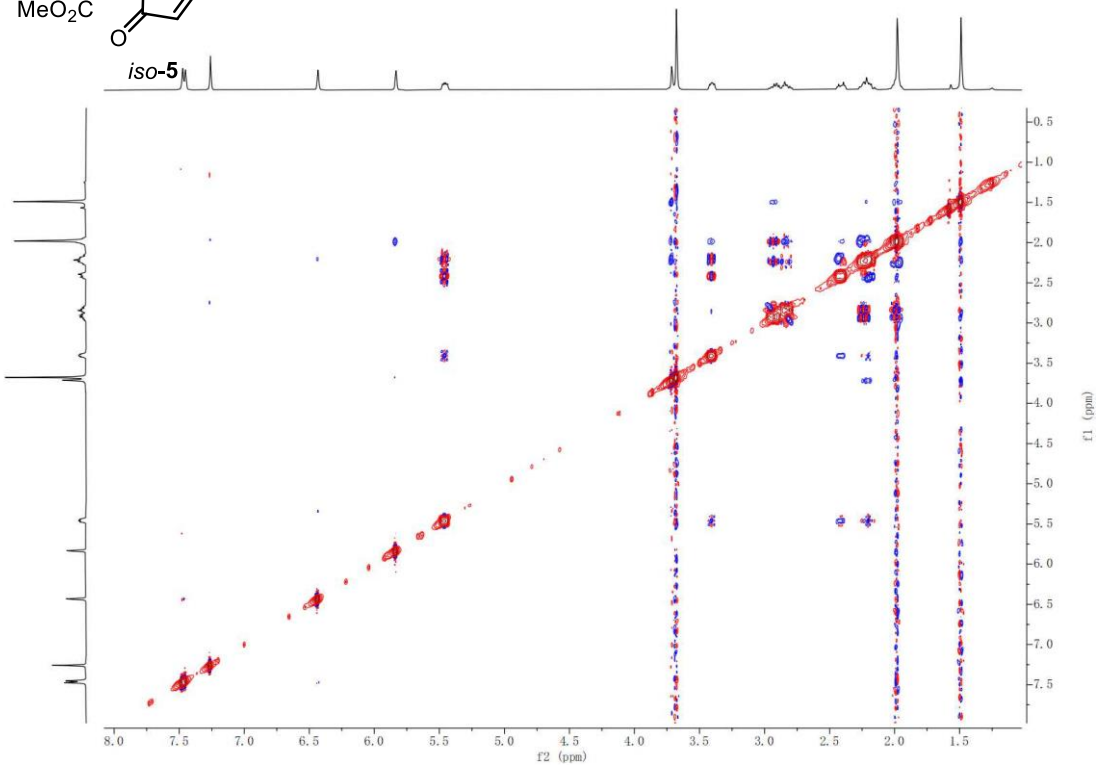
HSQC spectrum of *iso*-**5**



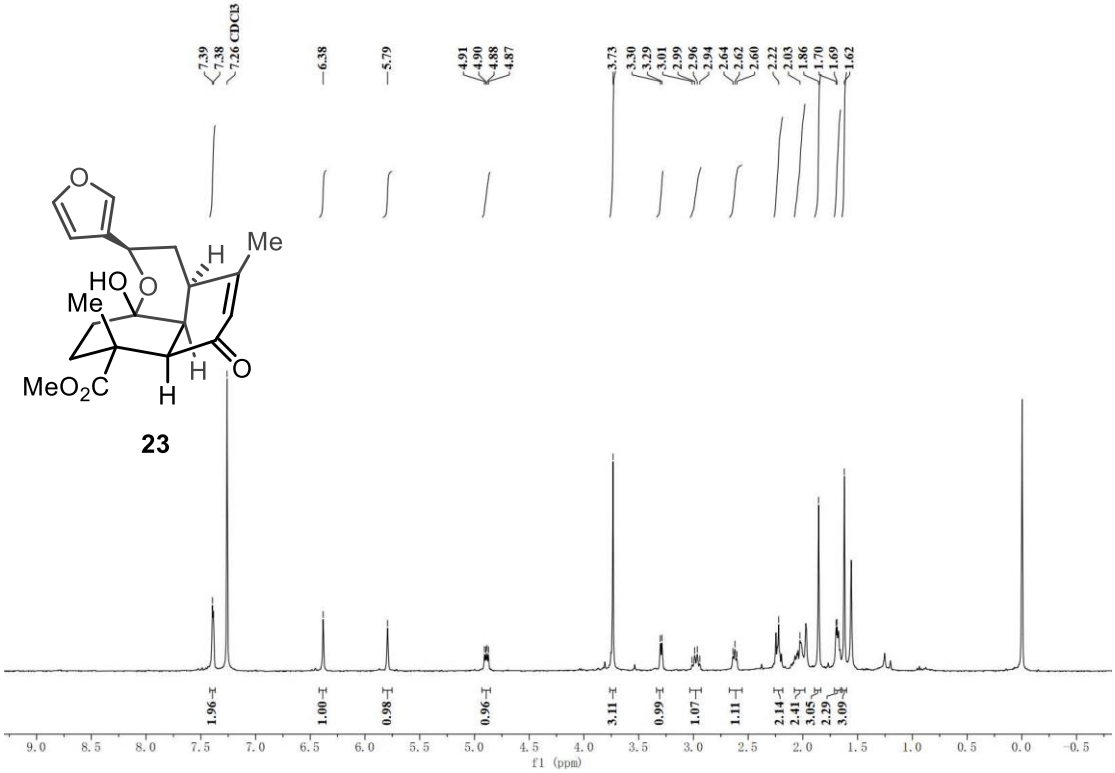


iso-**5**

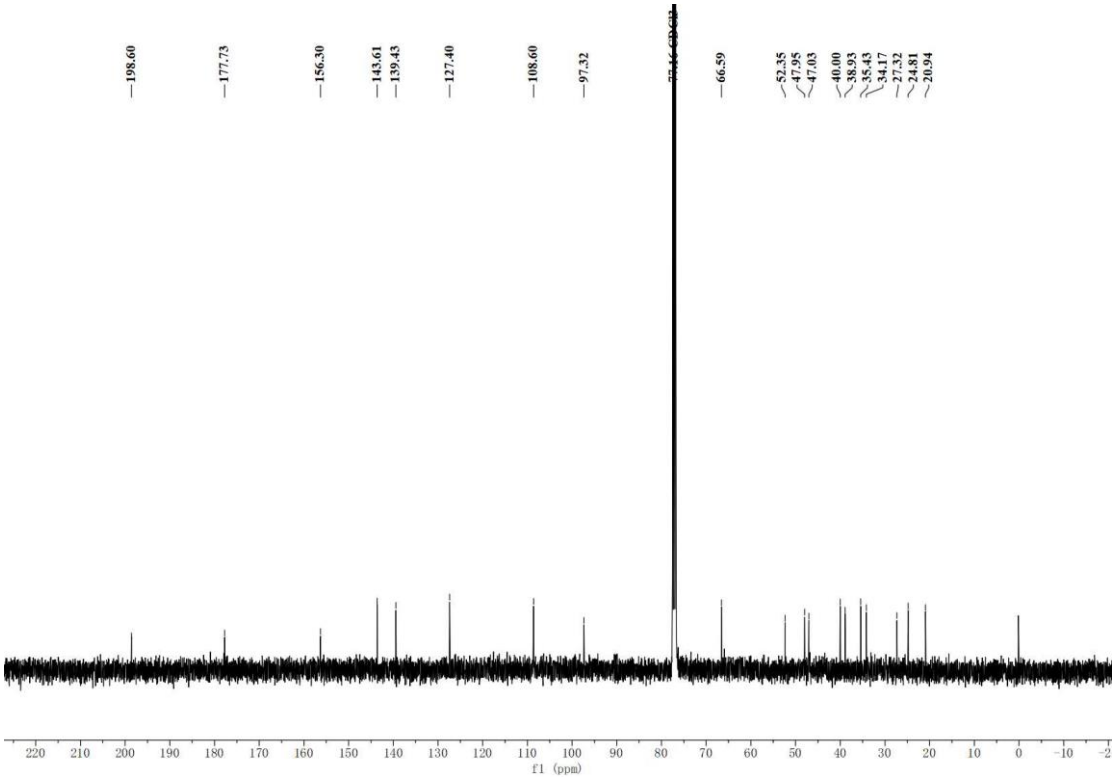
NOESY spectrum of *iso*-**5**



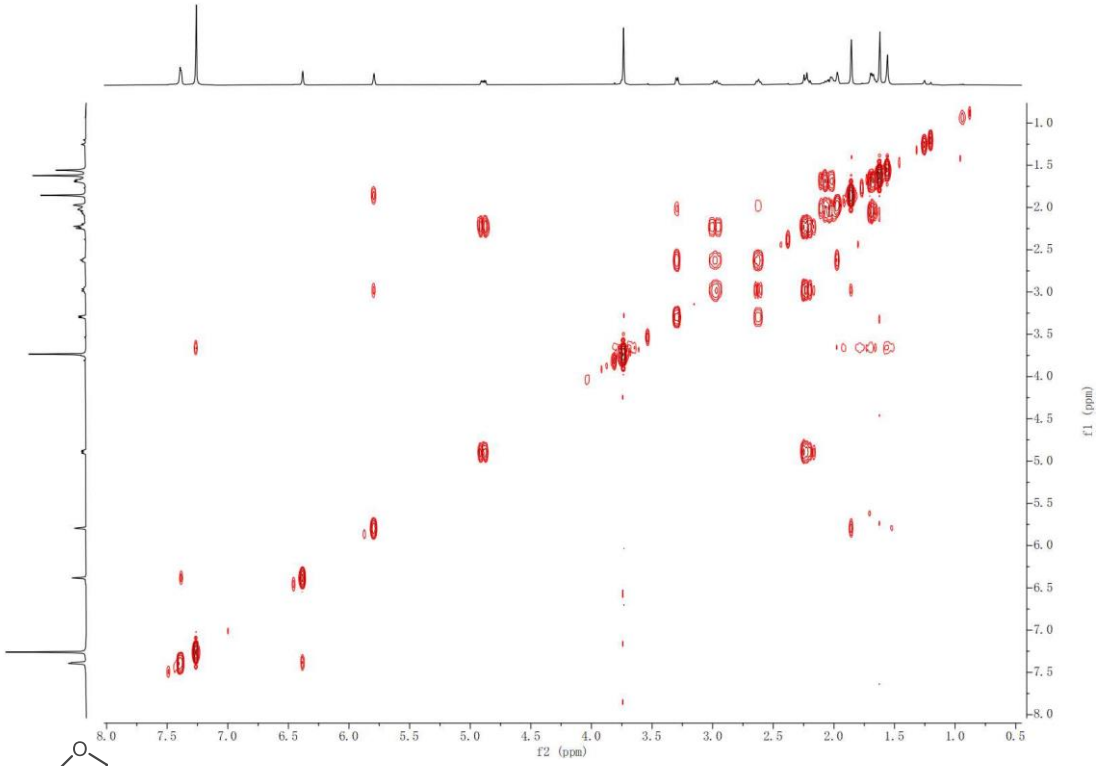
^{1}H NMR spectrum of **23** (400 MHz, $CDCl_3$)

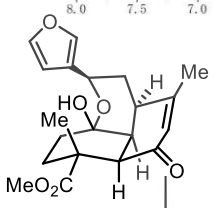


^{13}C NMR spectrum of **23** (100 MHz, $CDCl_3$)



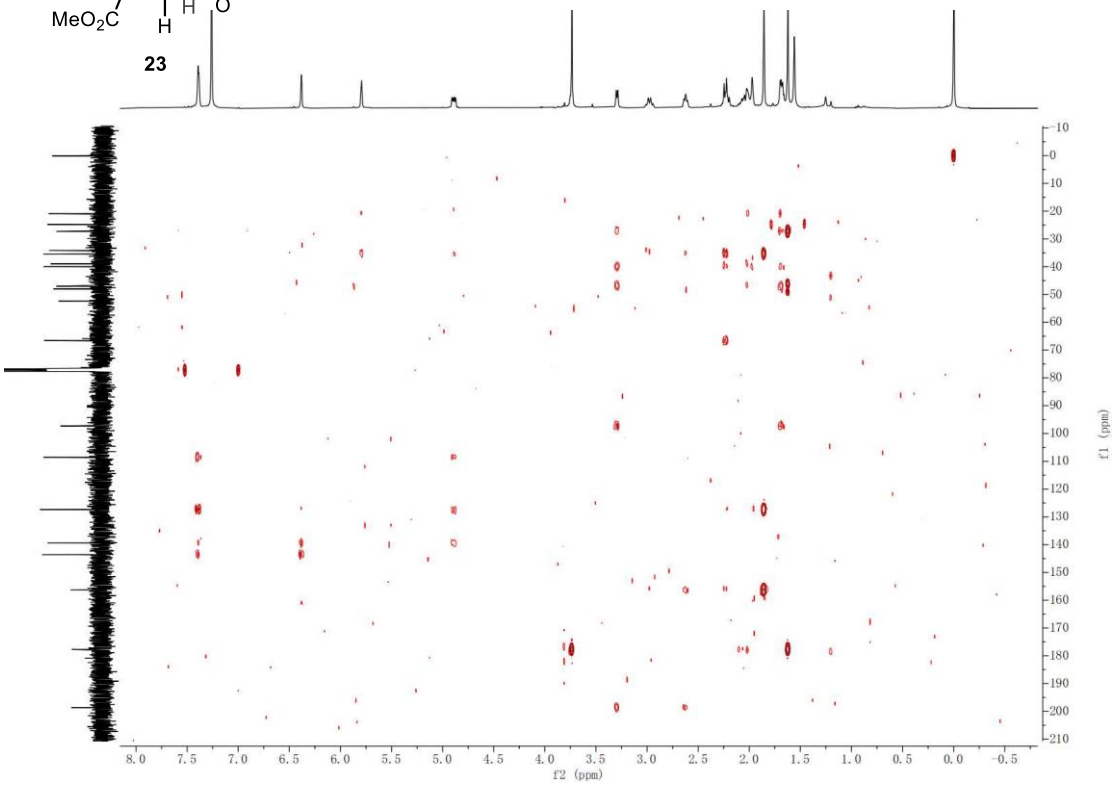
^{1}H-^{1}H COSY spectrum of **23**



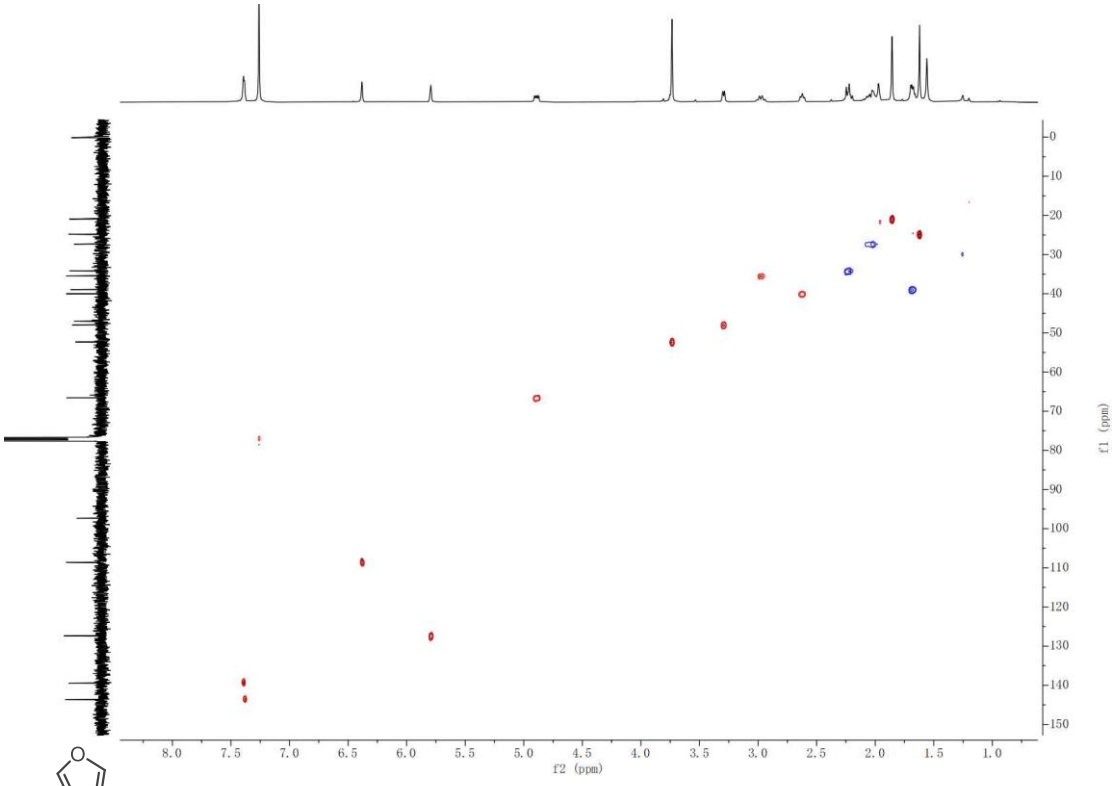


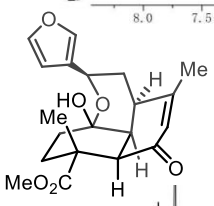
23

HMBC spectrum of **23**



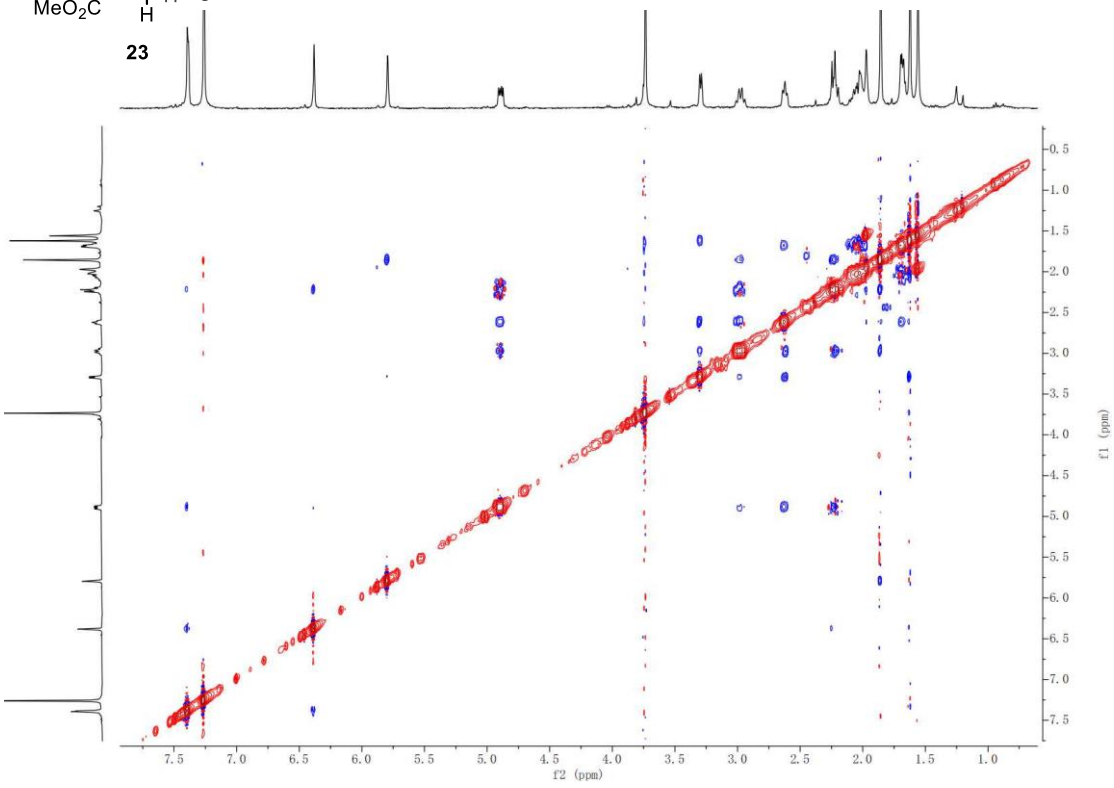
HSQC spectrum of **23**



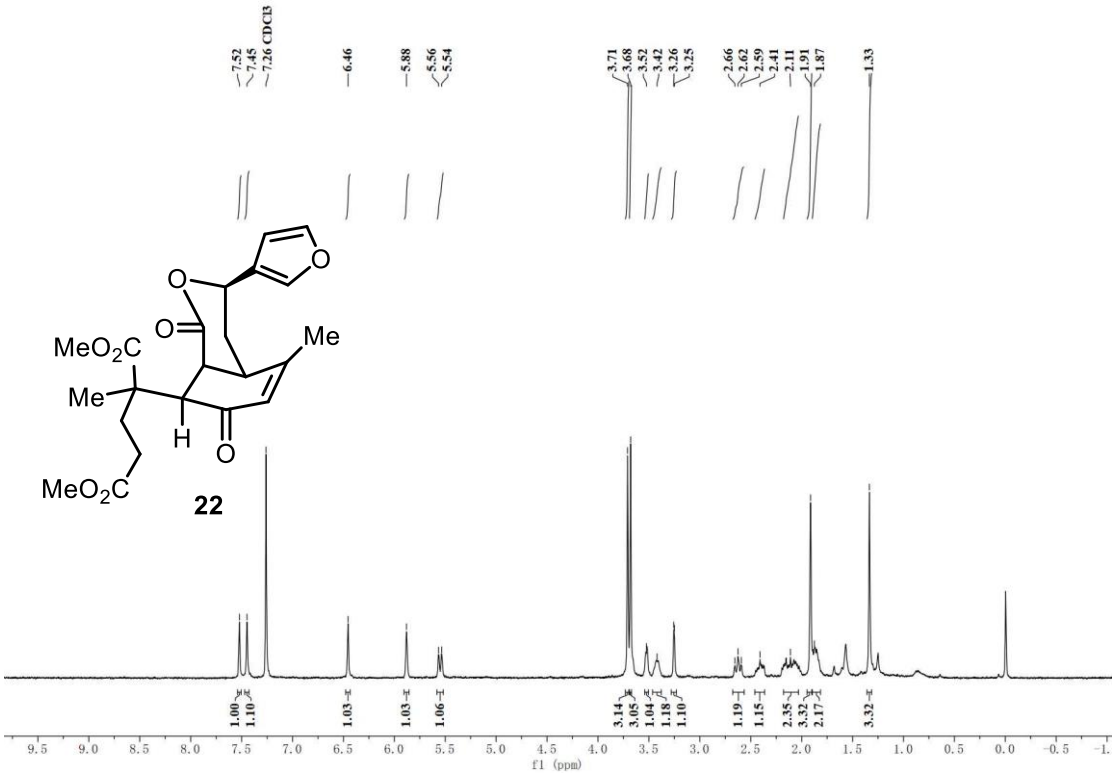


23

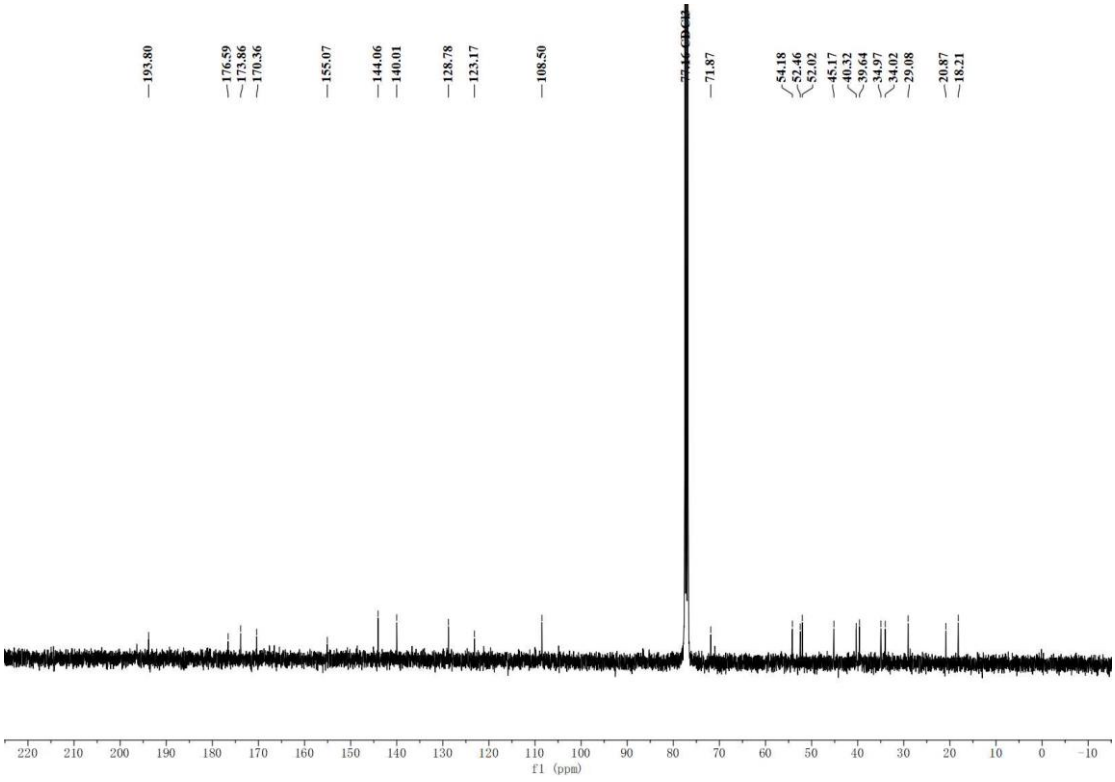
NOESY spectrum of **23**



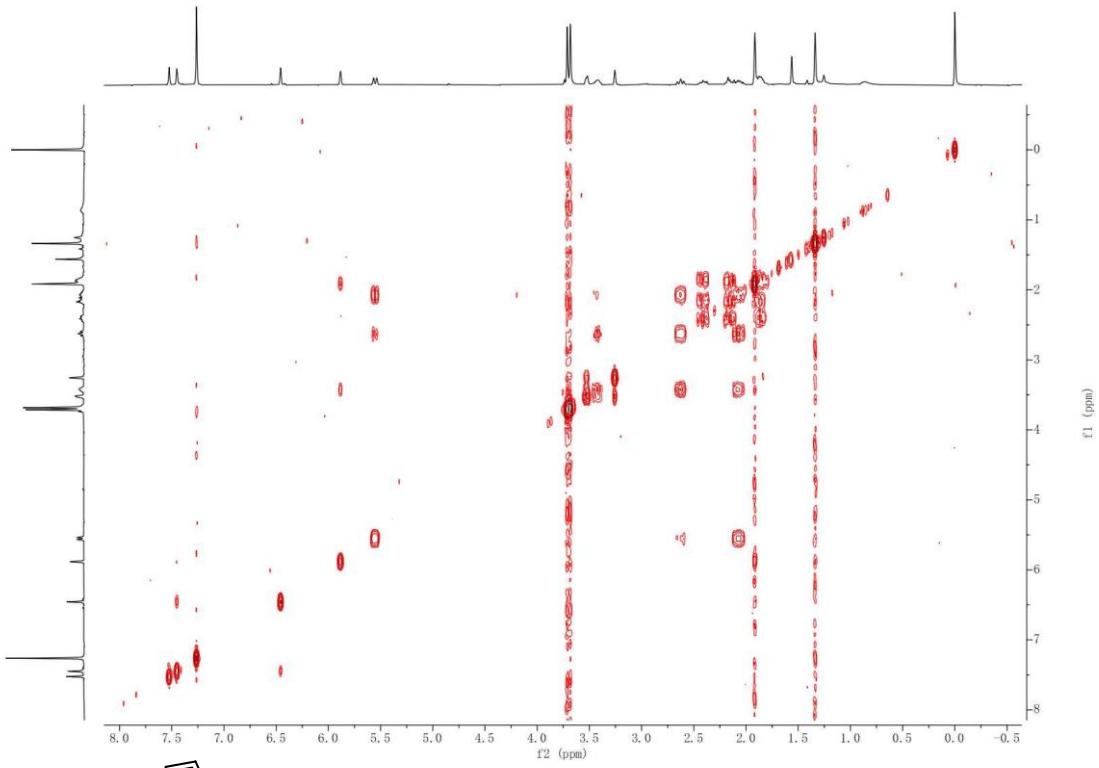
^{1}H NMR spectrum of **22** (400 MHz, $CDCl_3$)

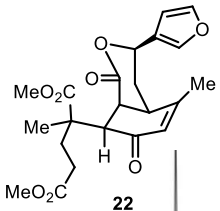


^{13}C NMR spectrum of **22** (100 MHz, $CDCl_3$)



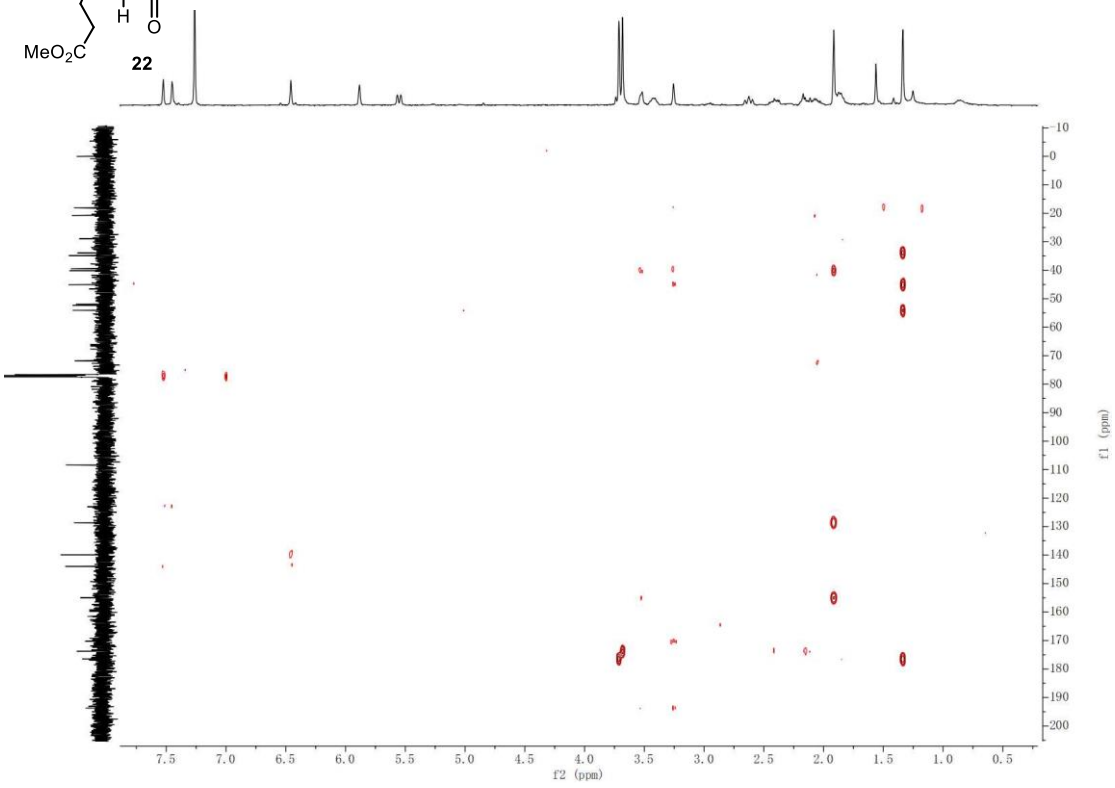
^{1}H-^{1}H COSY spectrum of **22**



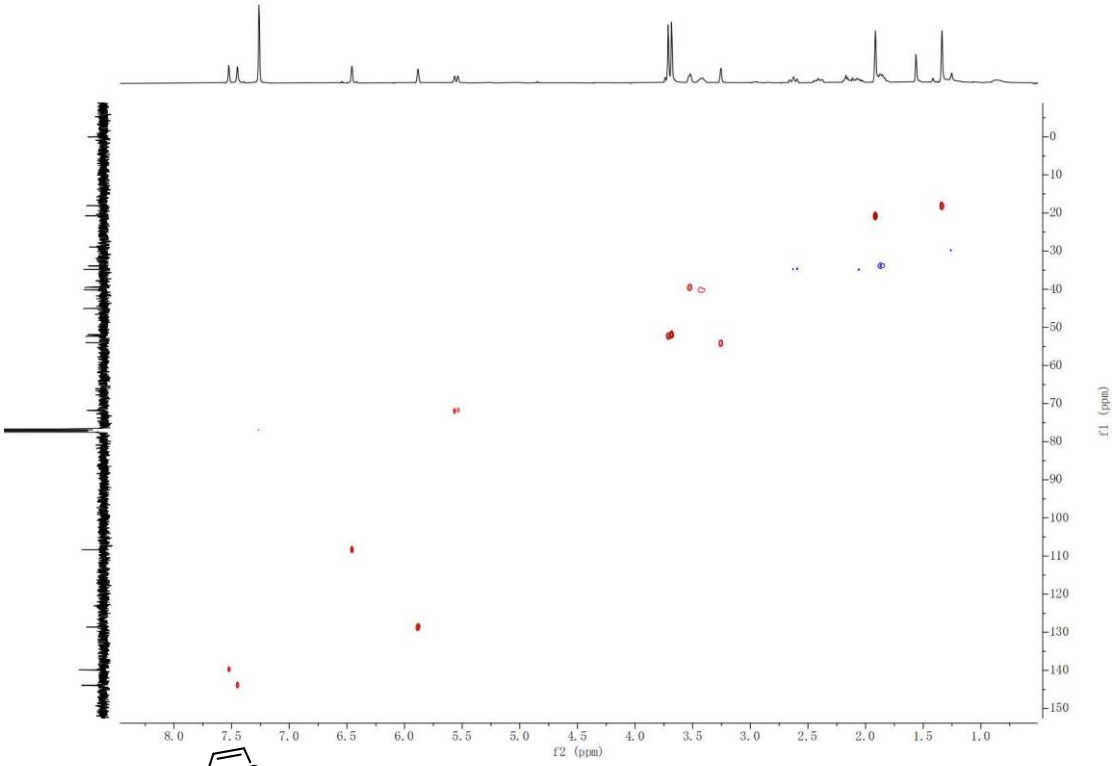


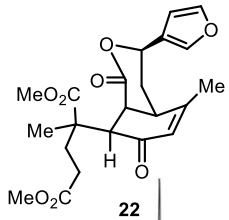
22

HMBC spectrum of **22**



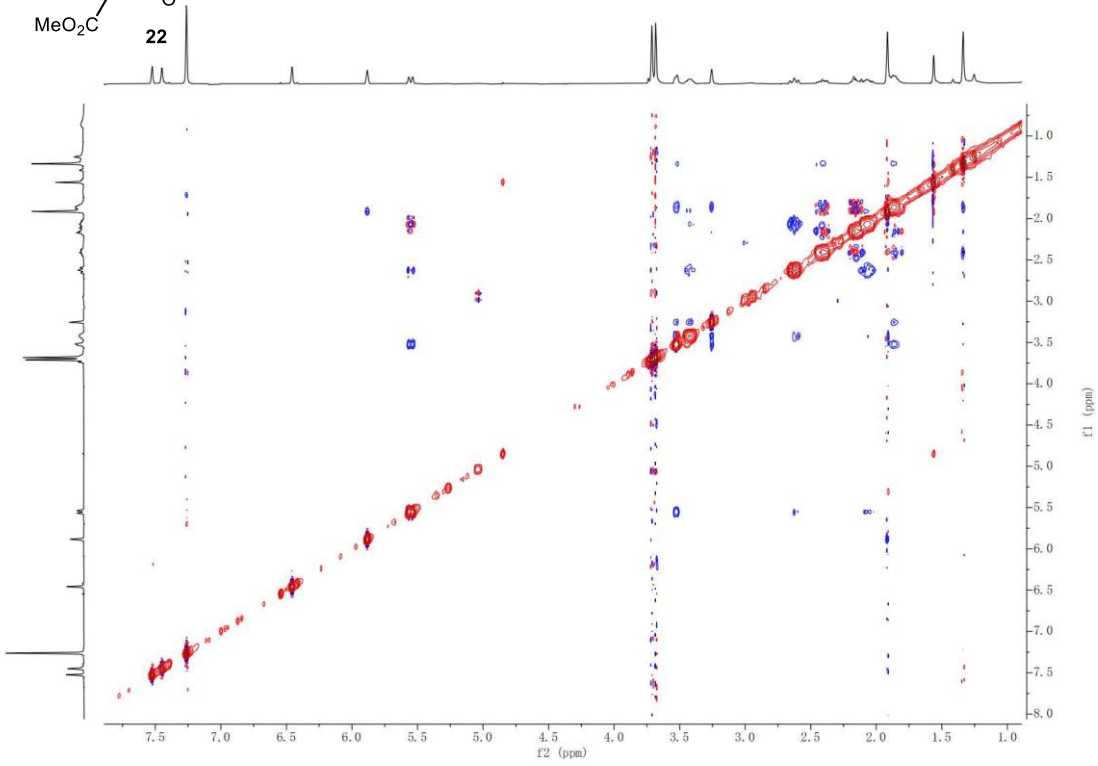
HSQC spectrum of **22**



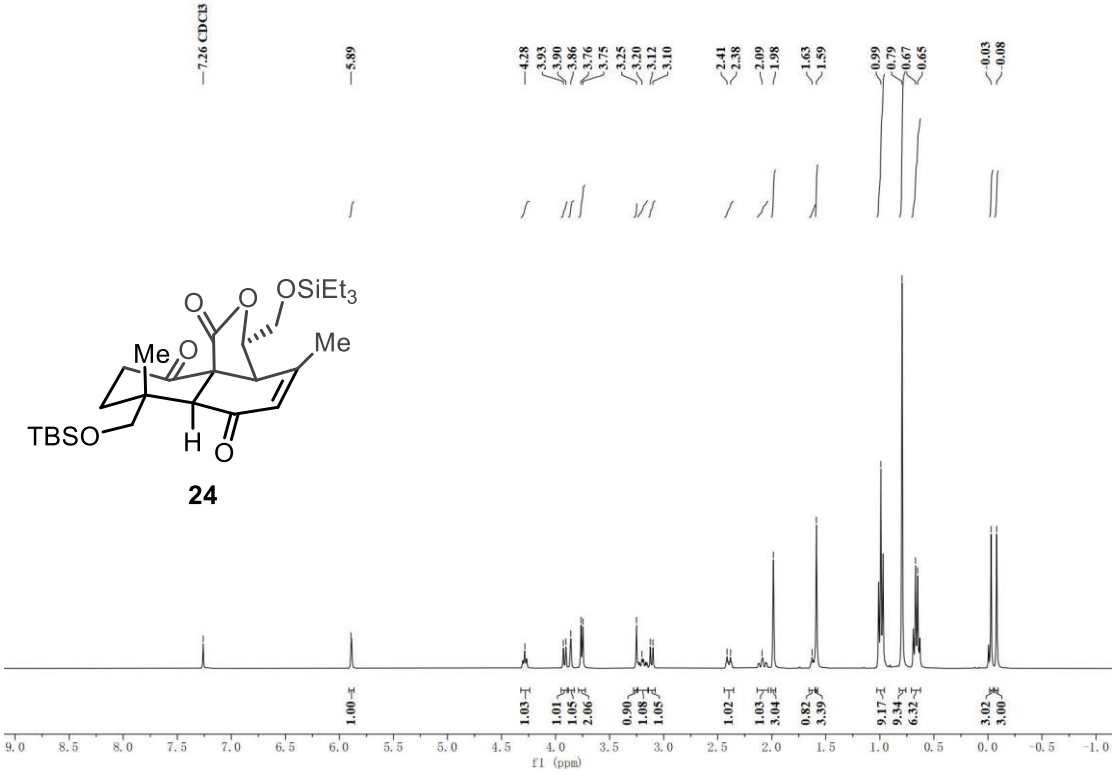


22

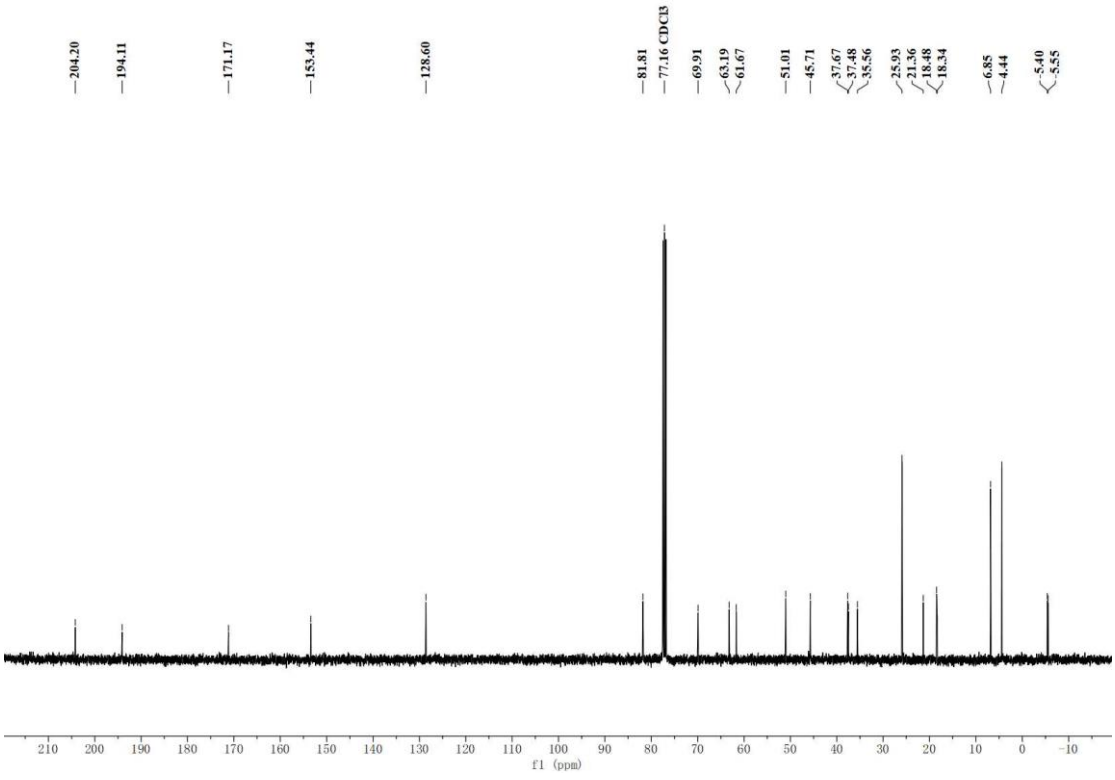
NOESY spectrum of **22**



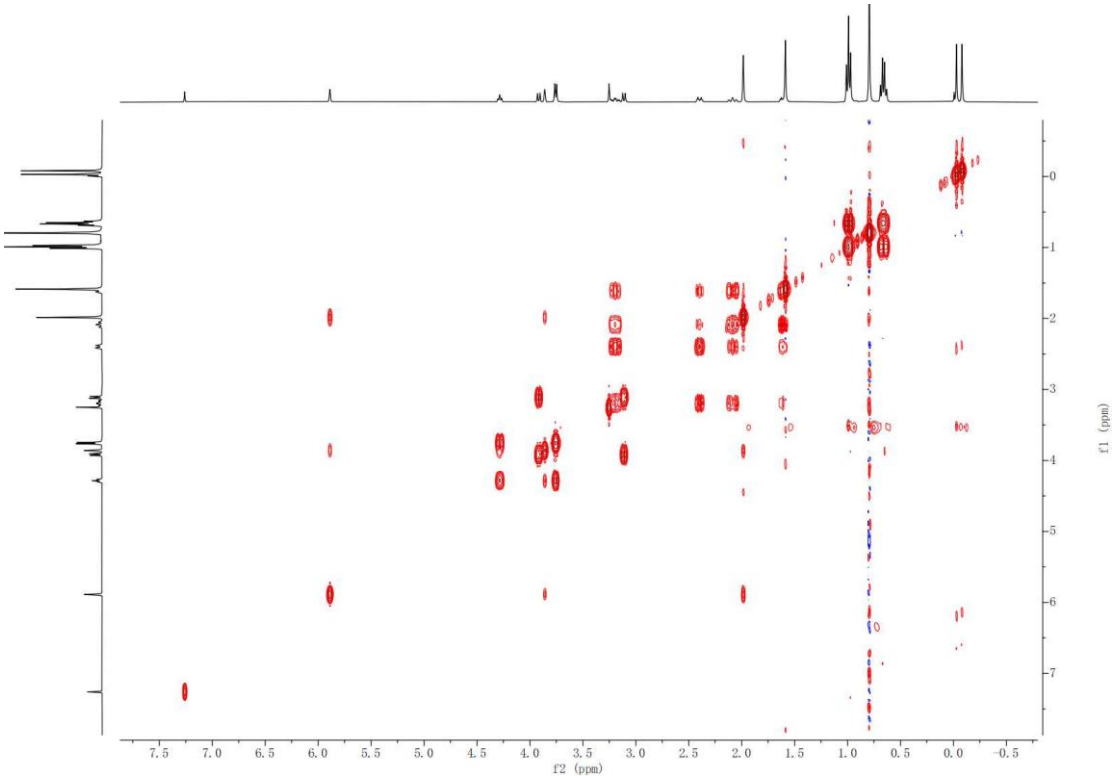
^{1}H NMR spectrum of **24** (400 MHz, $CDCl_3$)

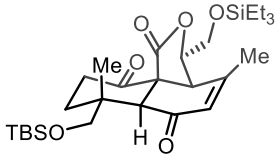


^{13}C NMR spectrum of **24** (100 MHz, $CDCl_3$)



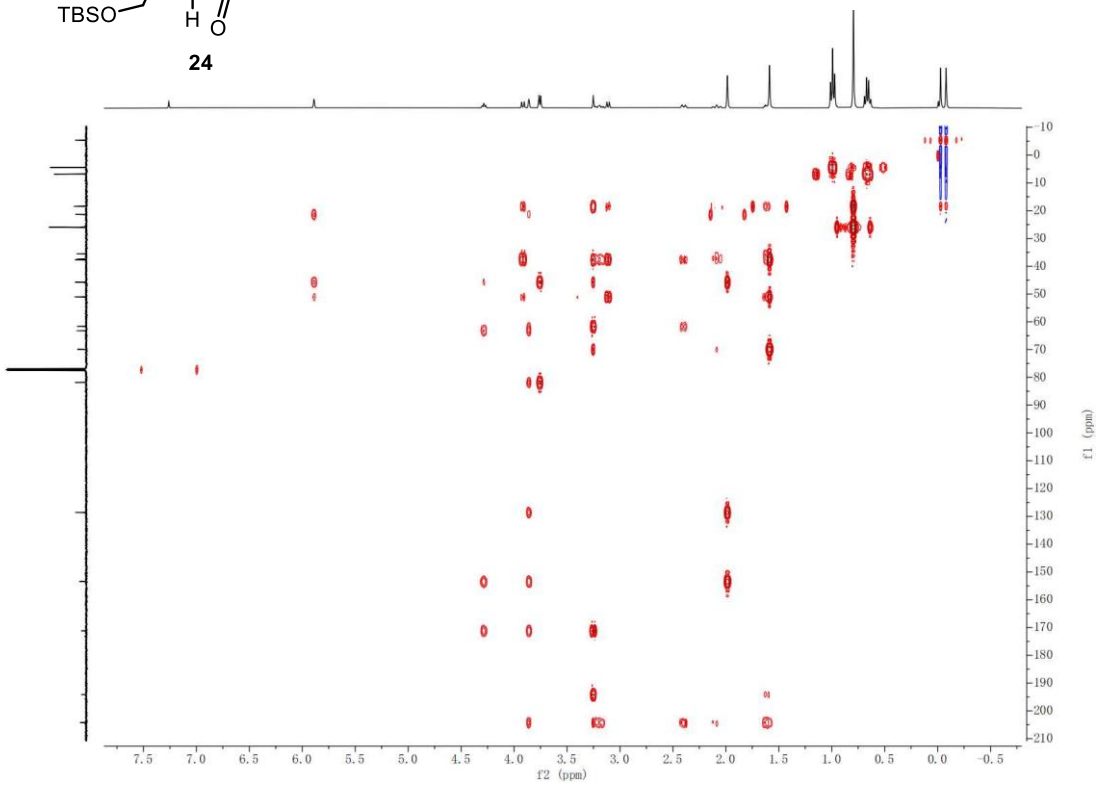
^{1}H-^{1}H COSY spectrum of **24**



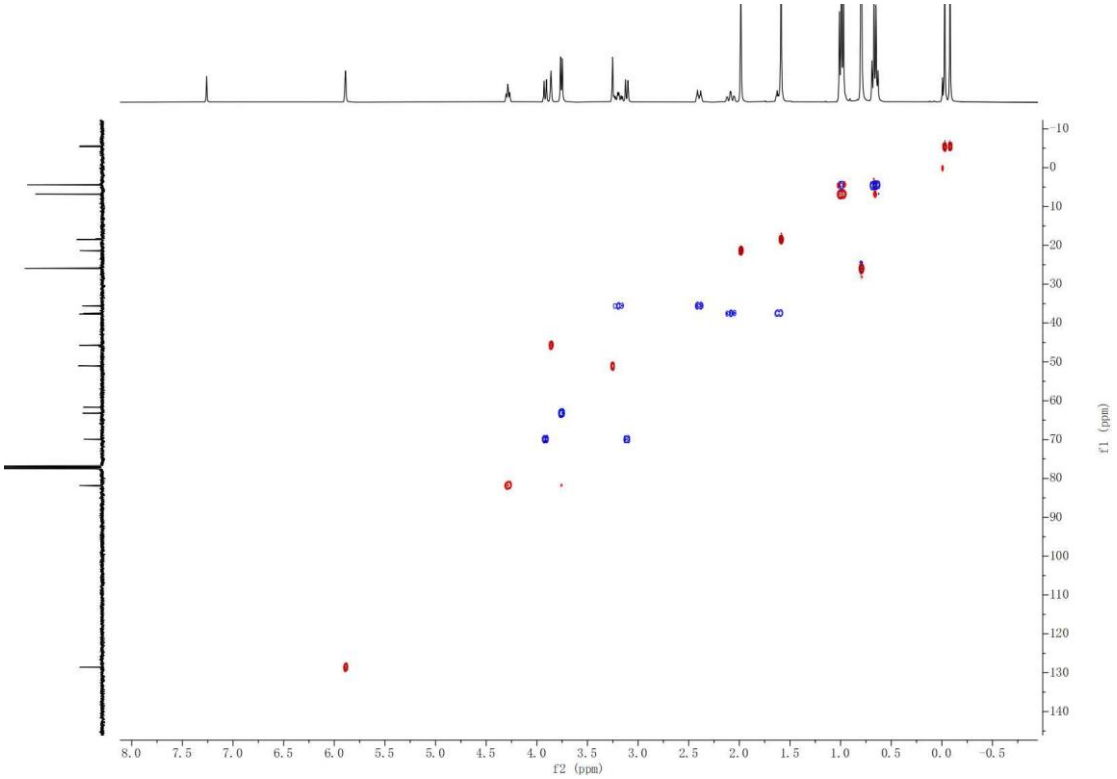


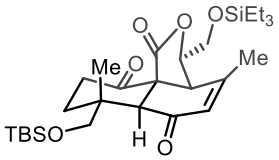
24

HMBC spectrum of **24**



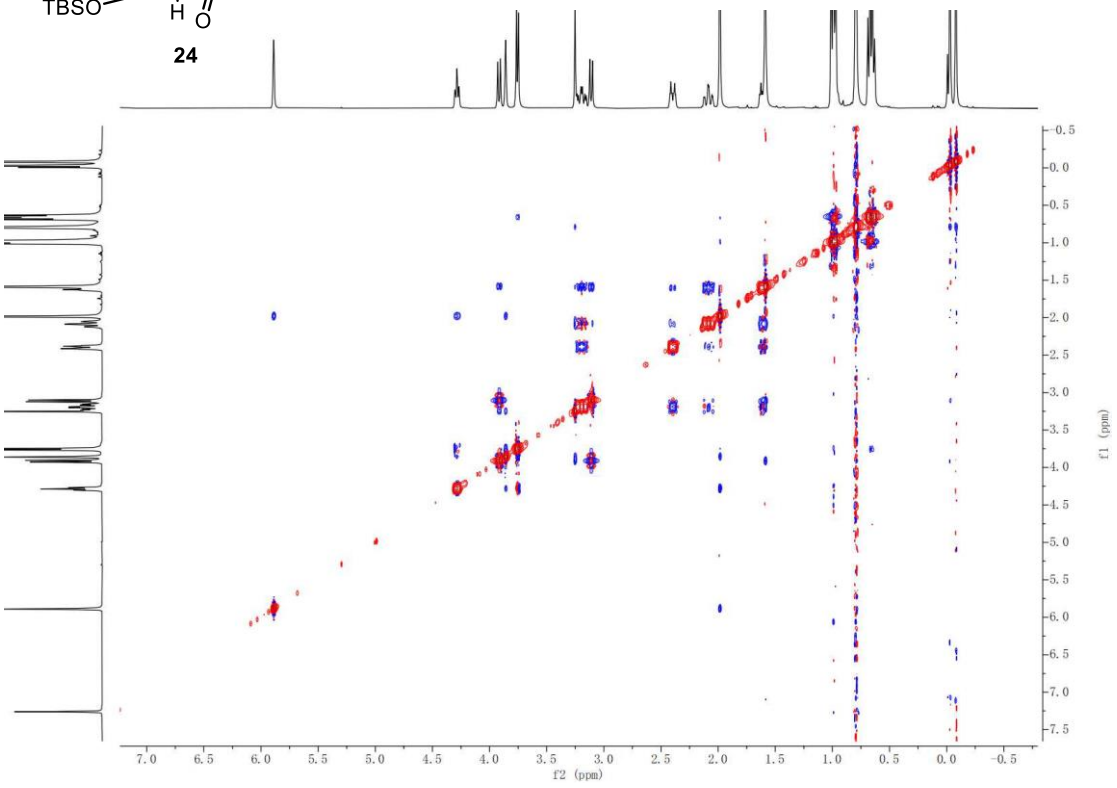
HSQC spectrum of **24**



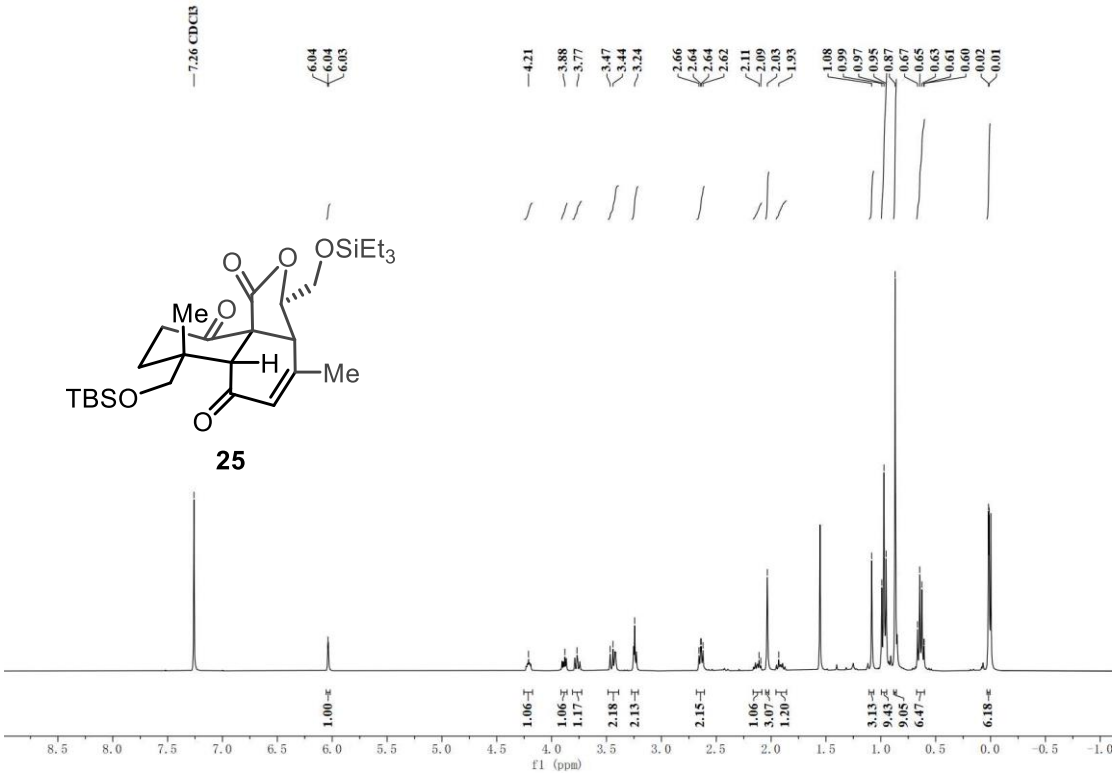


24

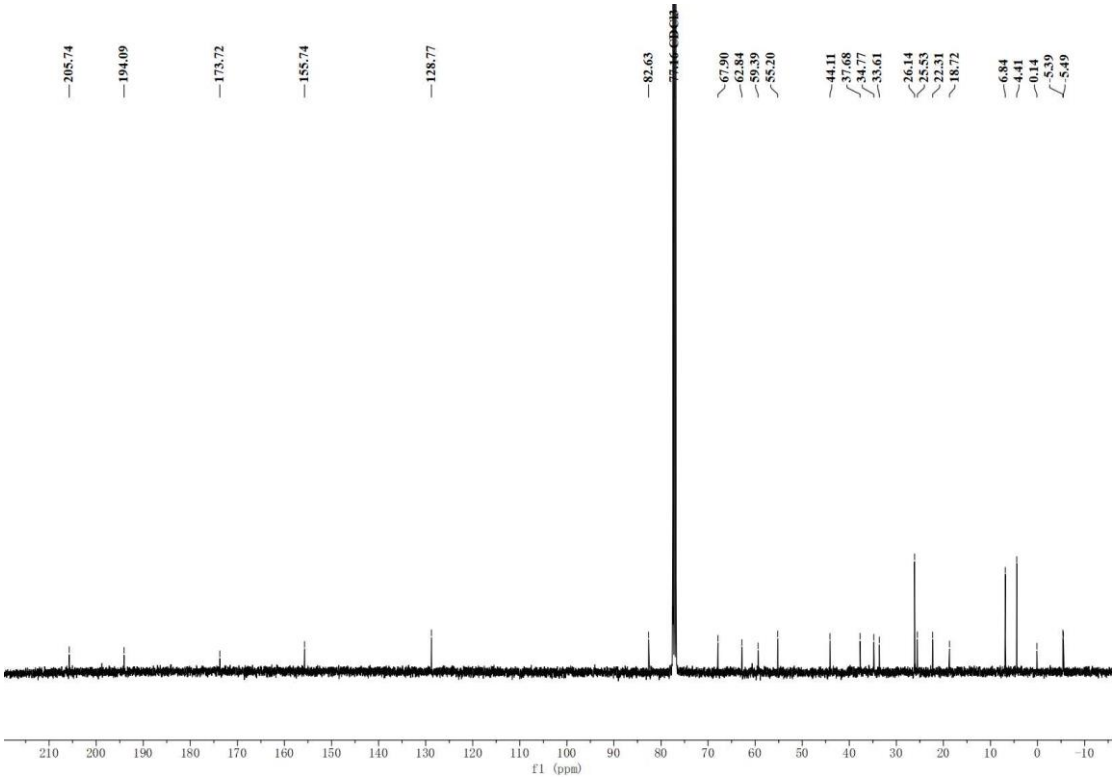
NOESY spectrum of **24**



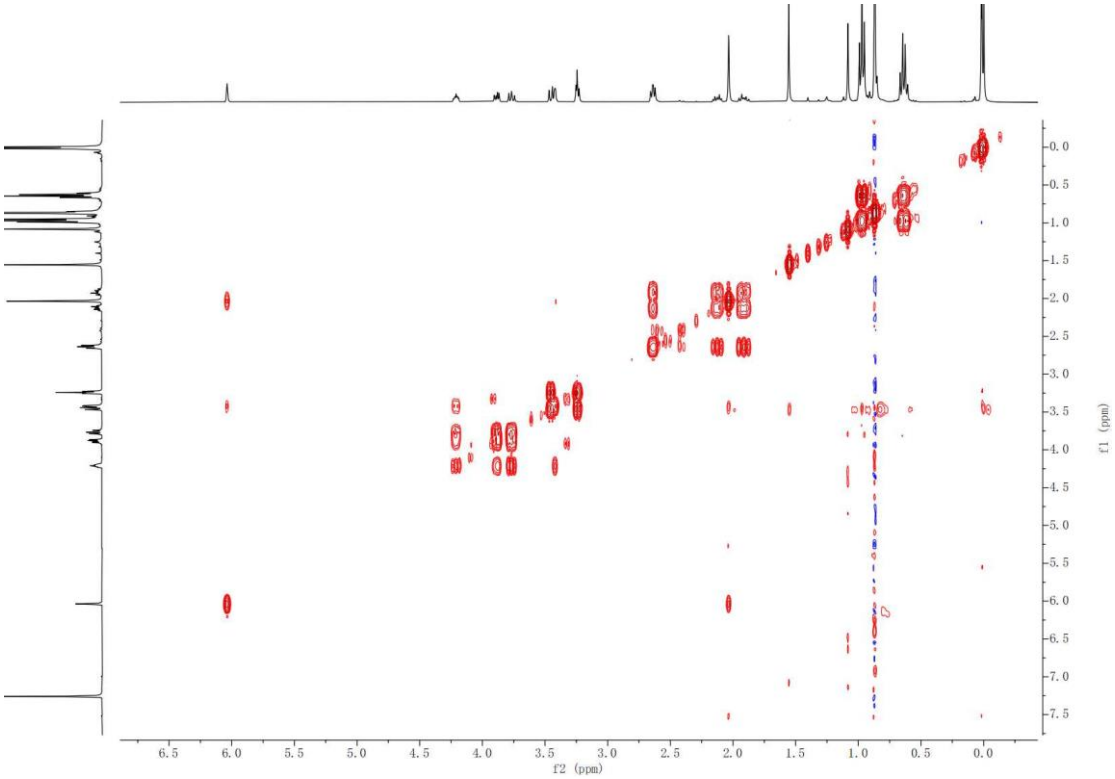
^{1}H NMR spectrum of **25** (400 MHz, $CDCl_3$)

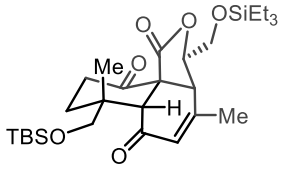


^{13}C NMR spectrum of **25** (100 MHz, $CDCl_3$)



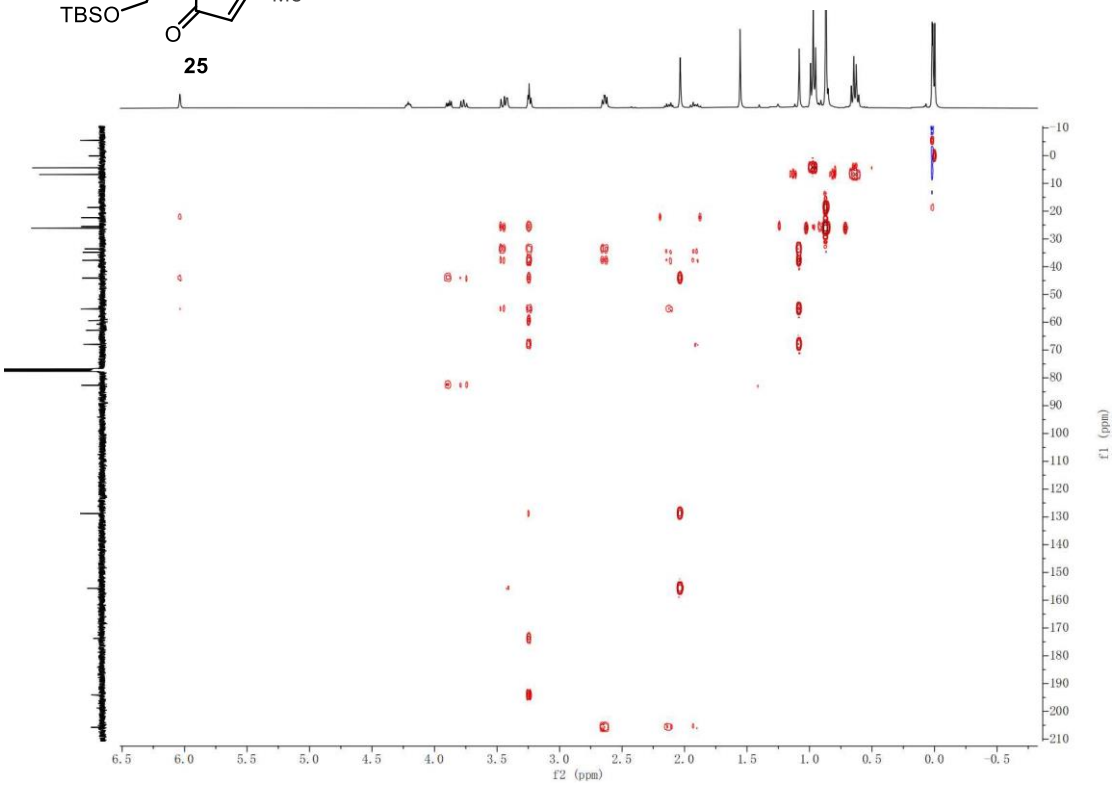
^{1}H-^{1}H COSY spectrum of **25**



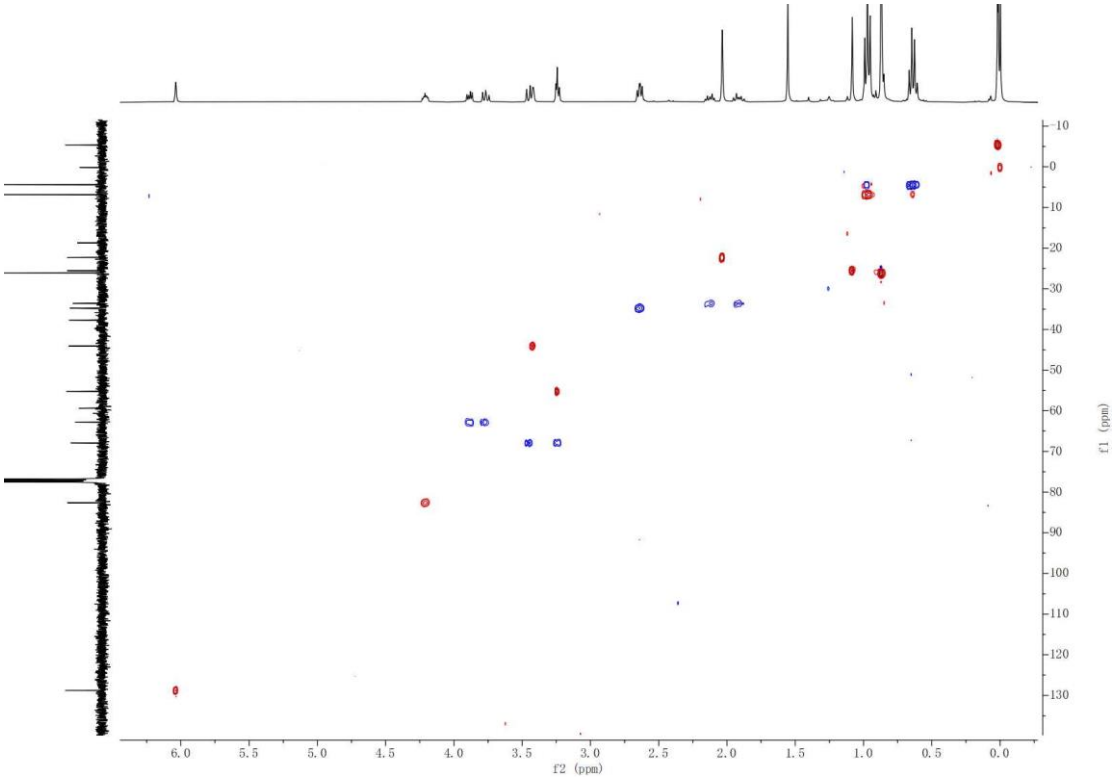


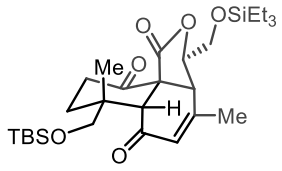
25

HMBC spectrum of **25**



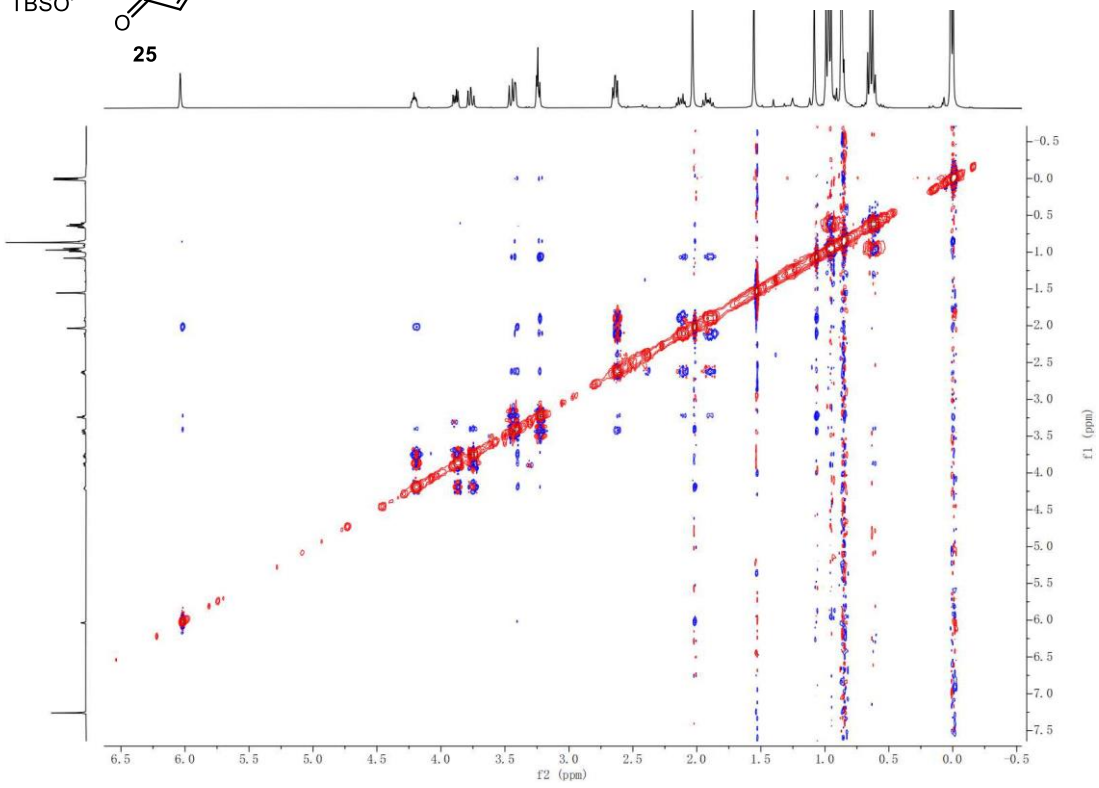
HSQC spectrum of **25**



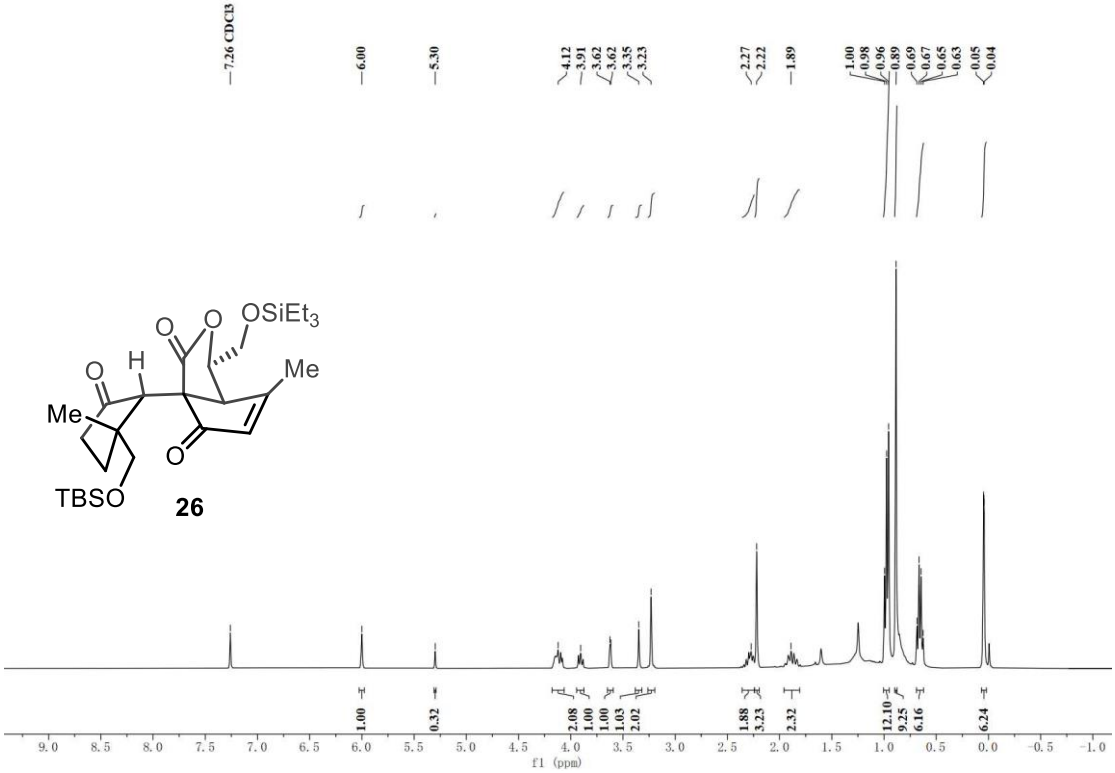


25

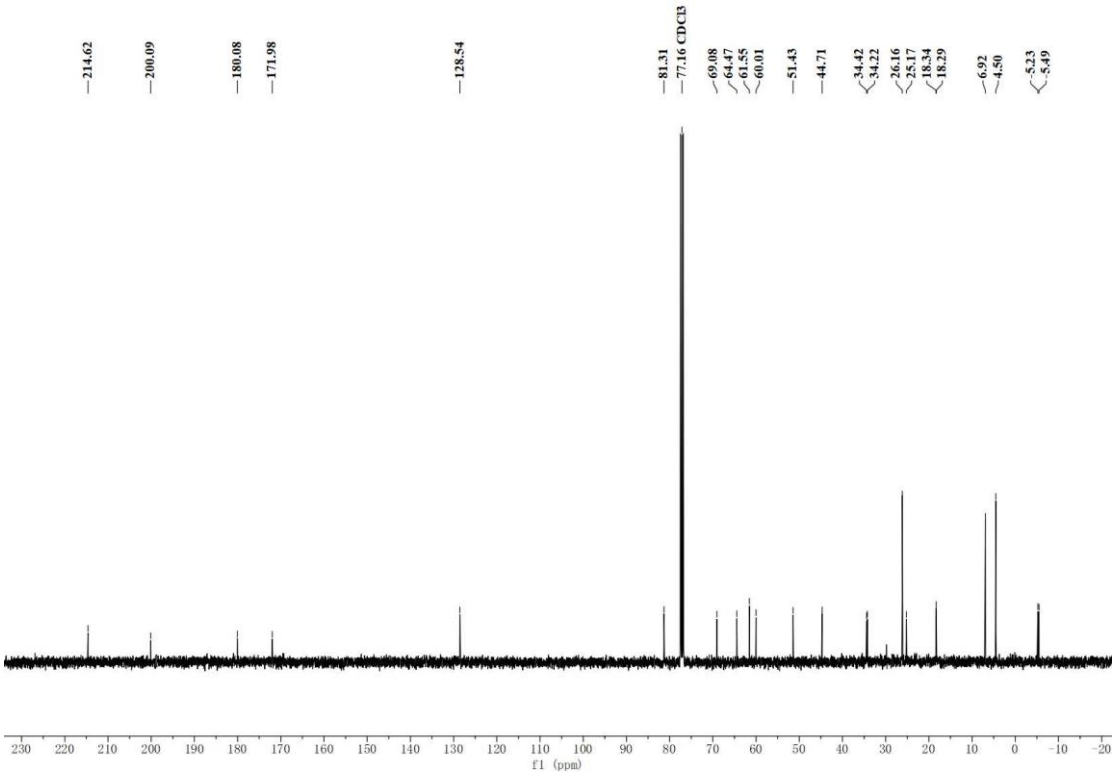
NOESY spectrum of **25**



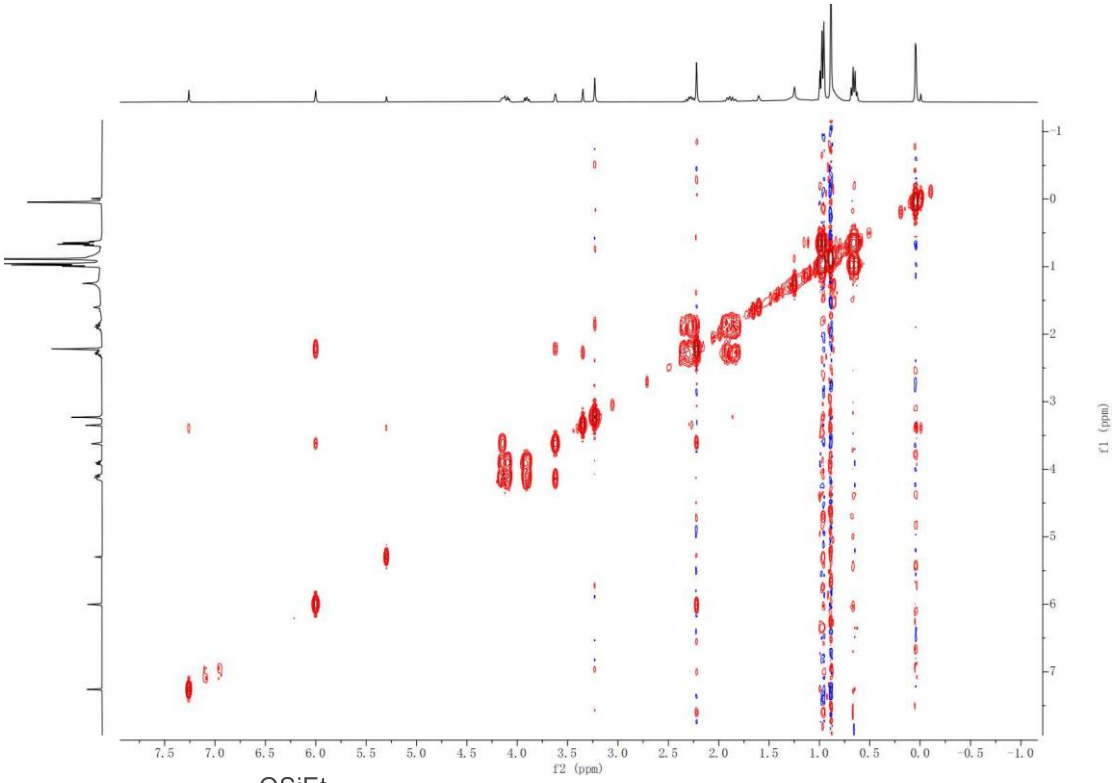
^{1}H NMR spectrum of **26** (400 MHz, $CDCl_3$)

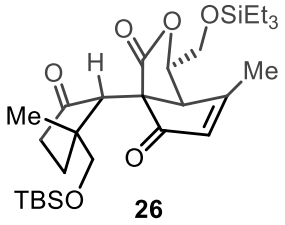


^{13}C NMR spectrum of **26** (100 MHz, $CDCl_3$)



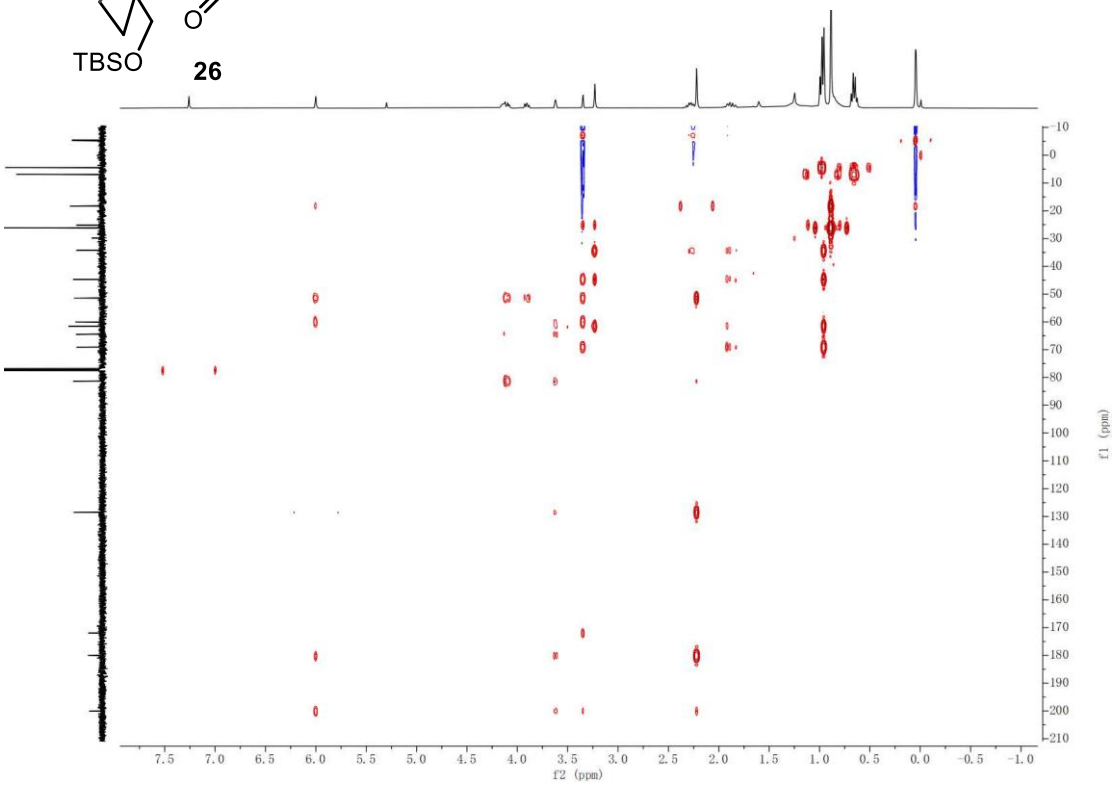
^{1}H-^{1}H COSY spectrum of **26**



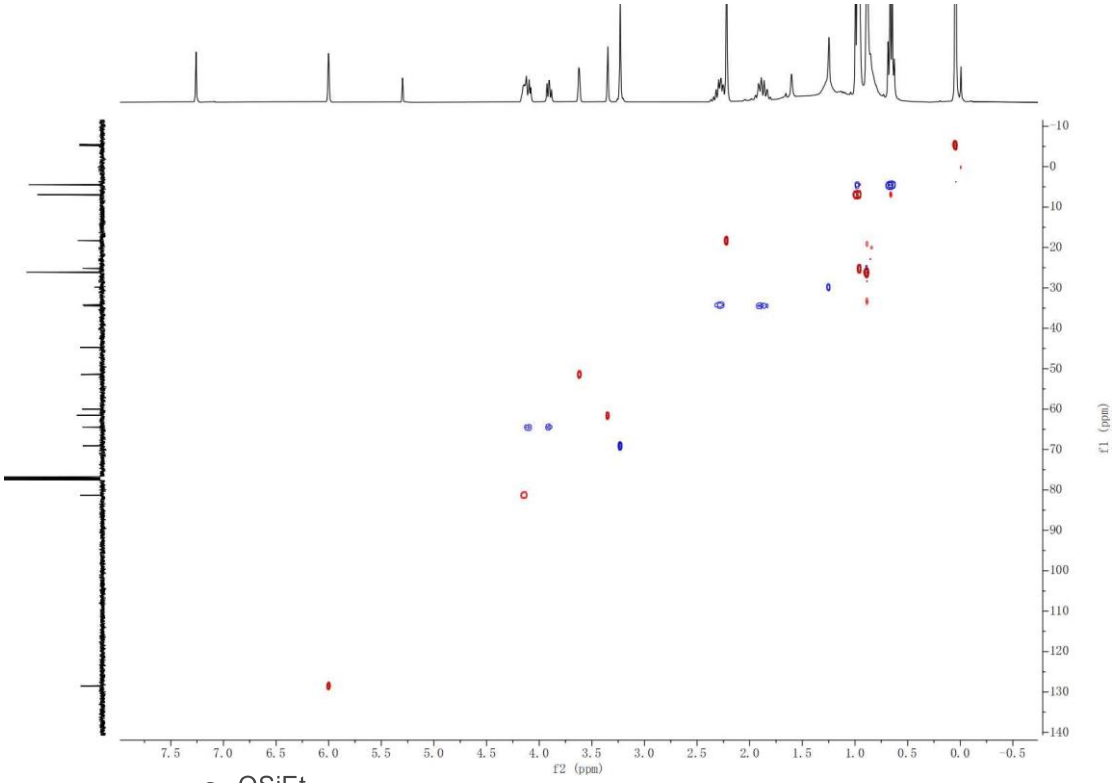


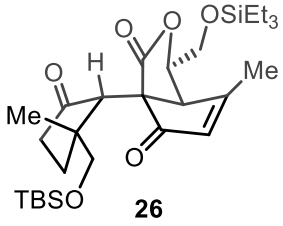
26

HMBC spectrum of **26**



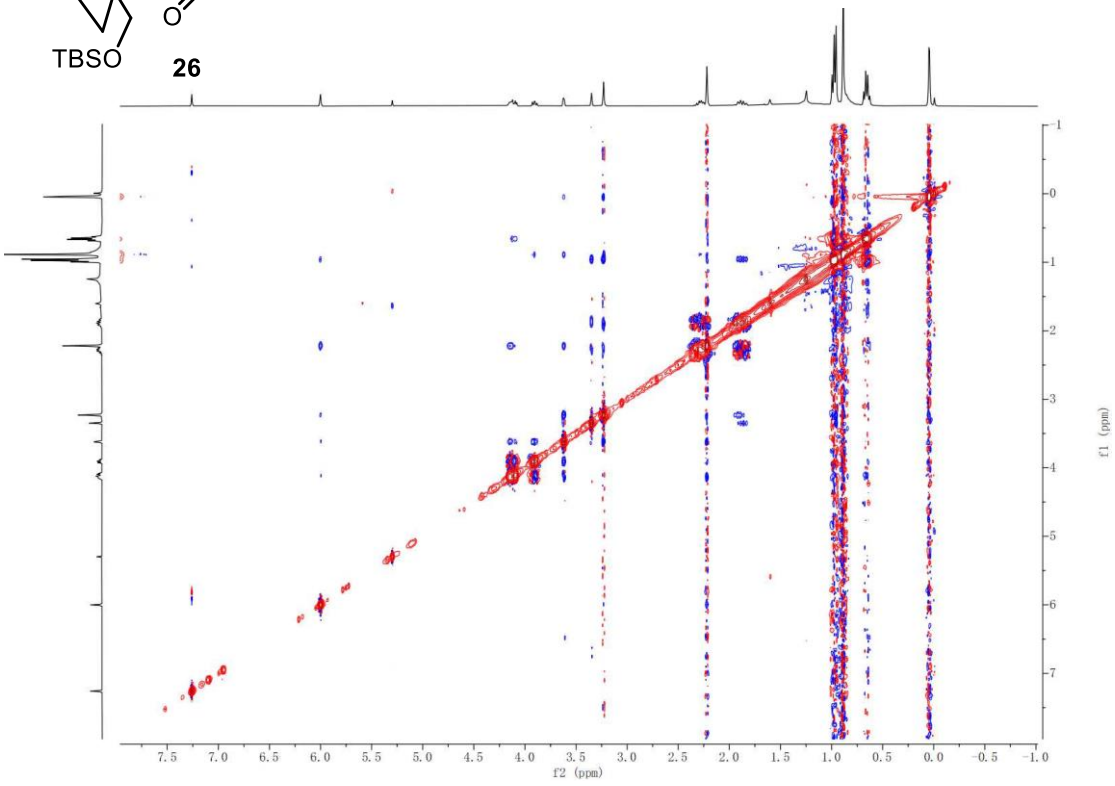
HSQC spectrum of **26**



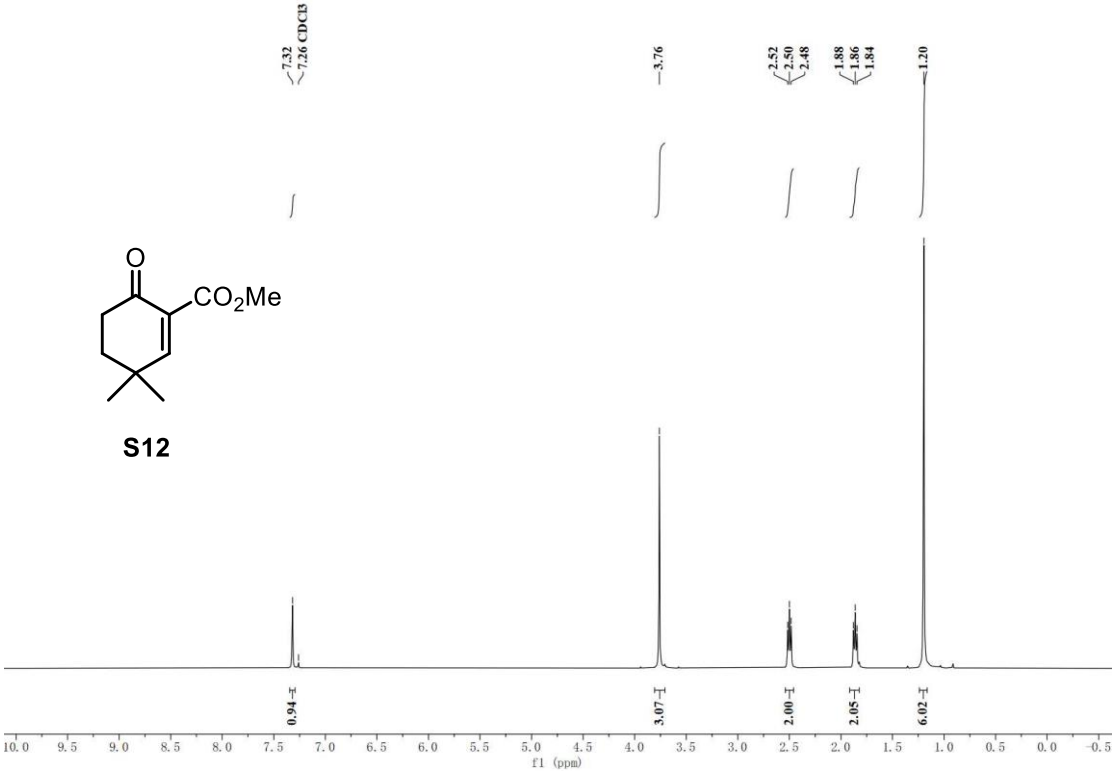


26

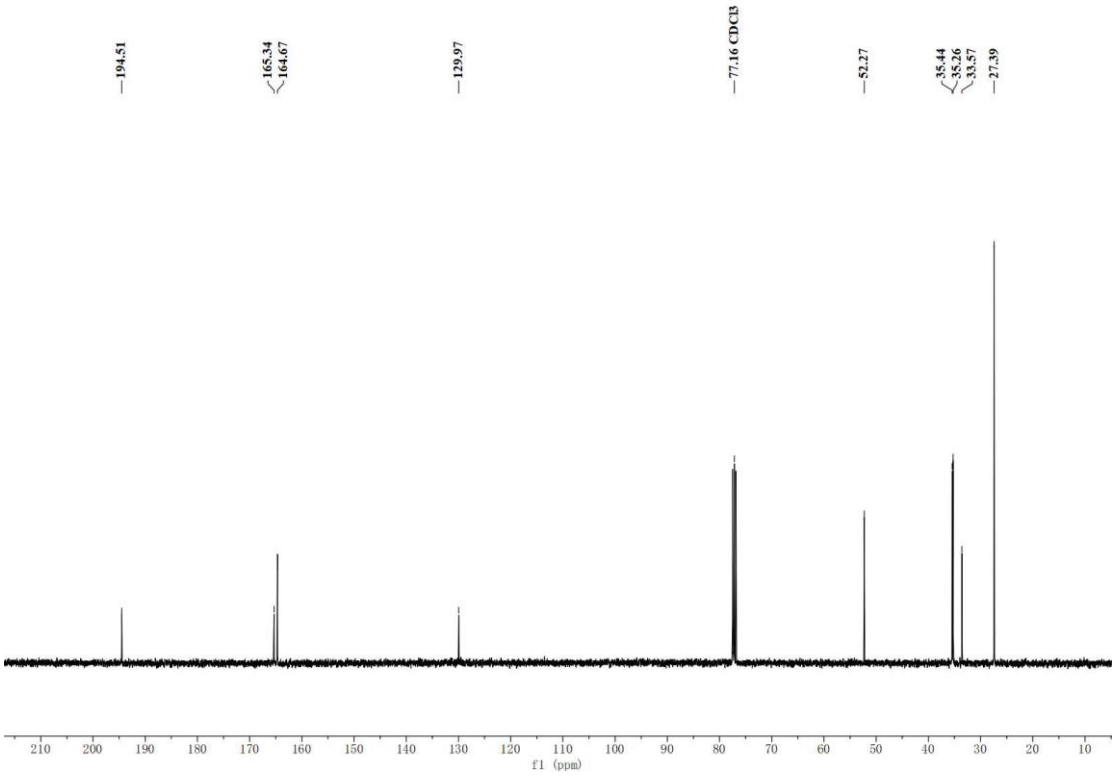
NOESY spectrum of **26**



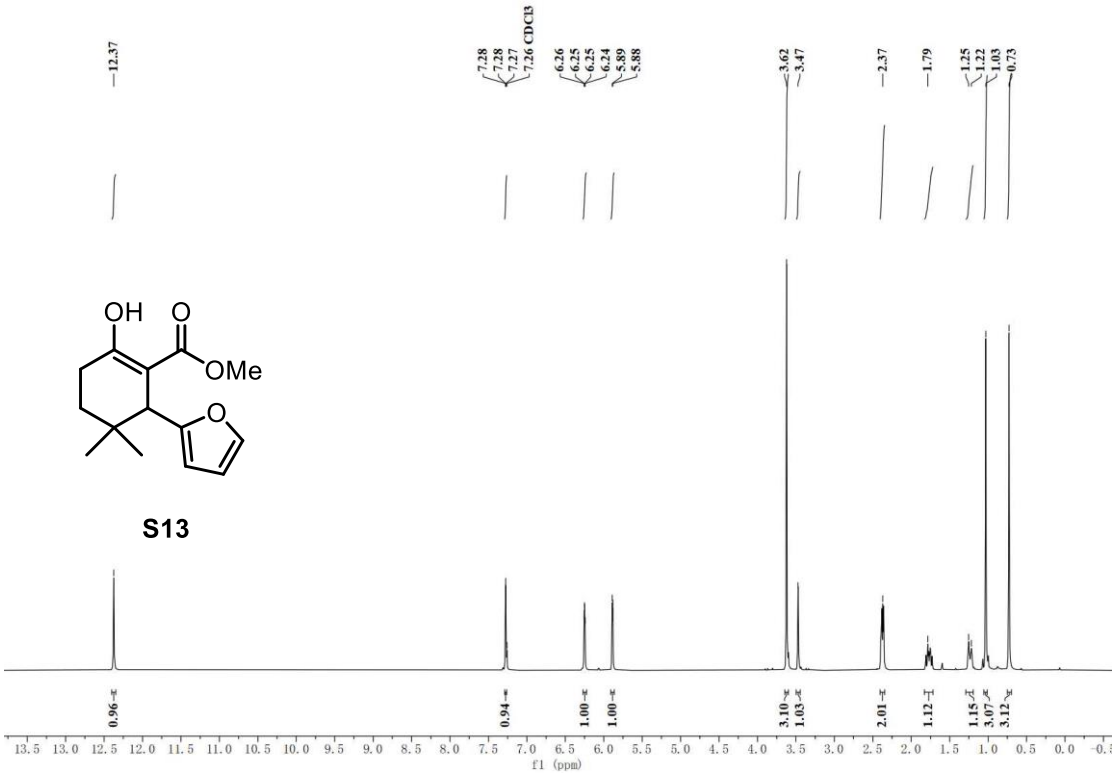
^{1}H NMR spectrum of **S12** (400 MHz, $CDCl_3$)



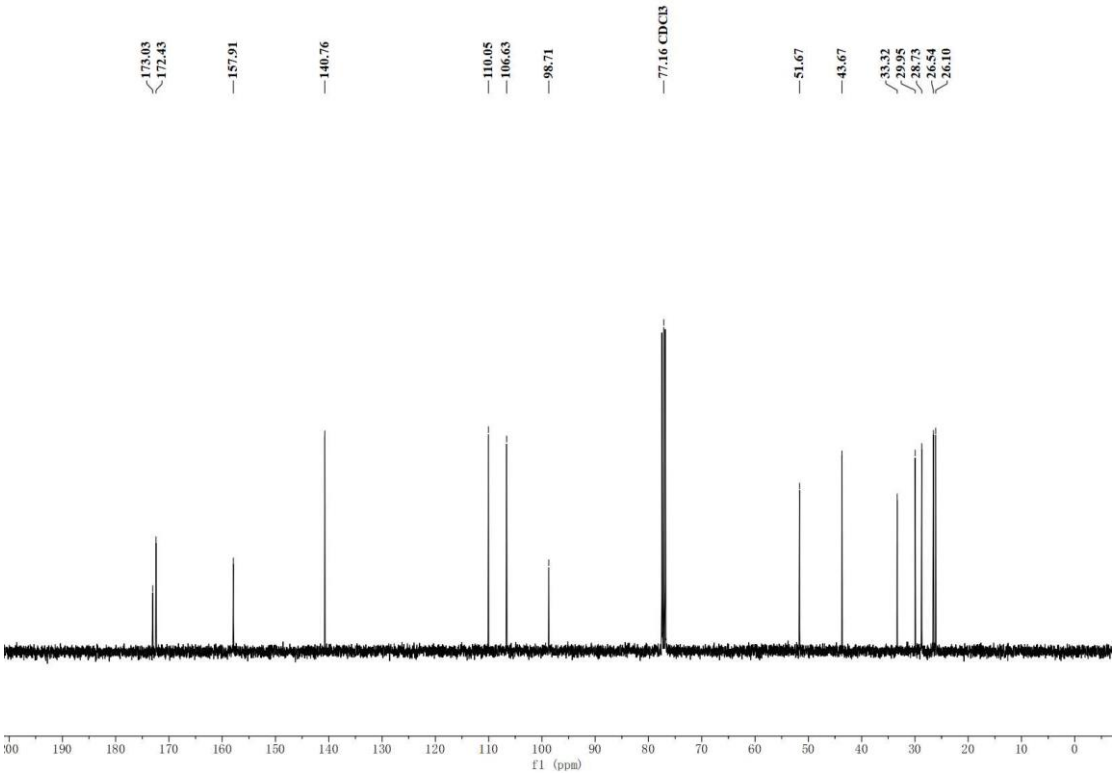
^{13}C NMR spectrum of **S12** (100 MHz, $CDCl_3$)



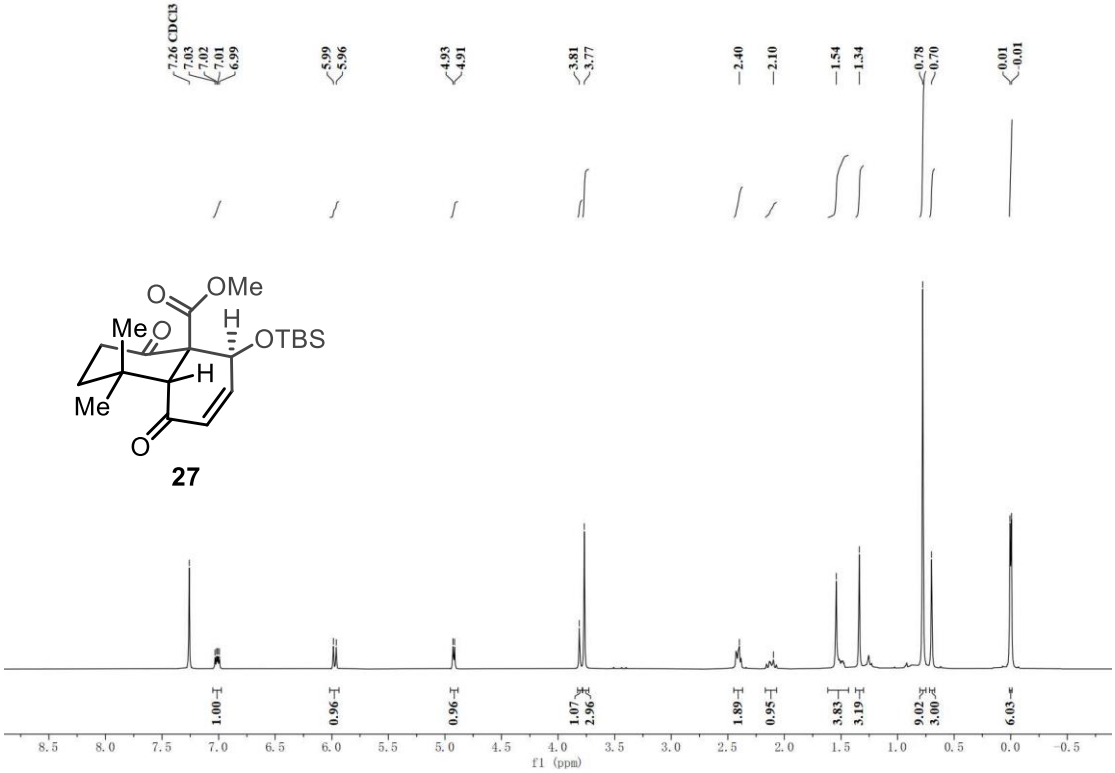
^{1}H NMR spectrum of **S13** (400 MHz, $CDCl_3$)



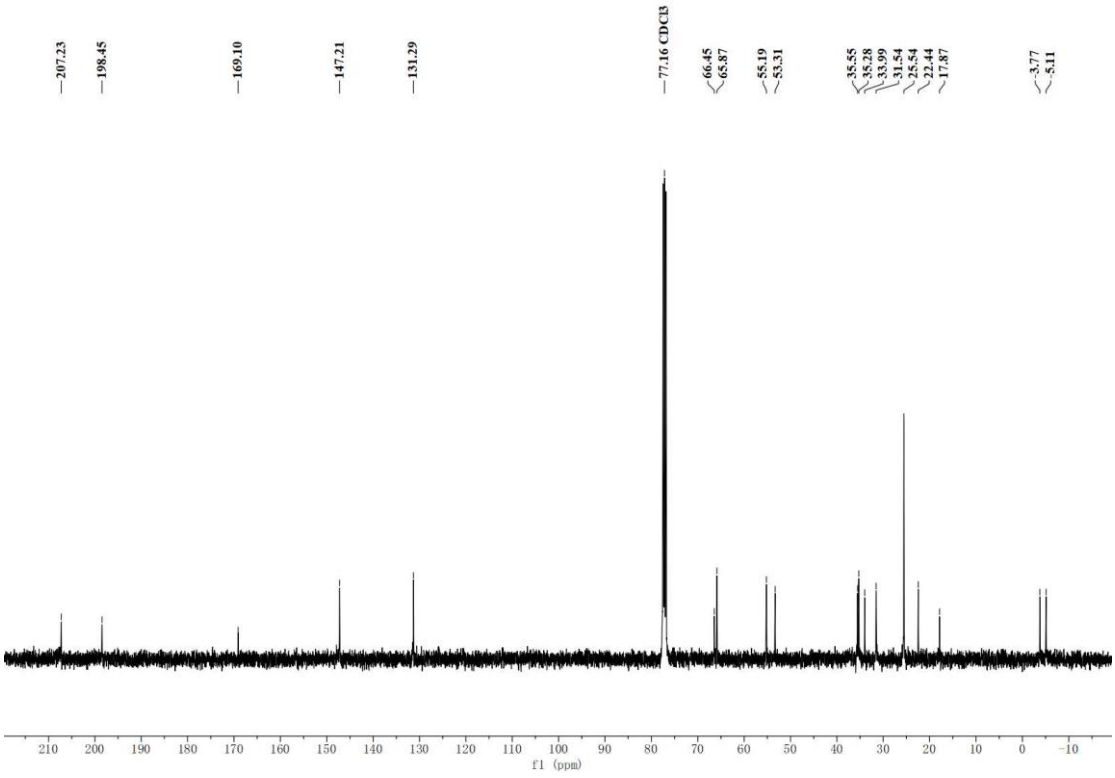
^{13}C NMR spectrum of **S13** (100 MHz, $CDCl_3$)



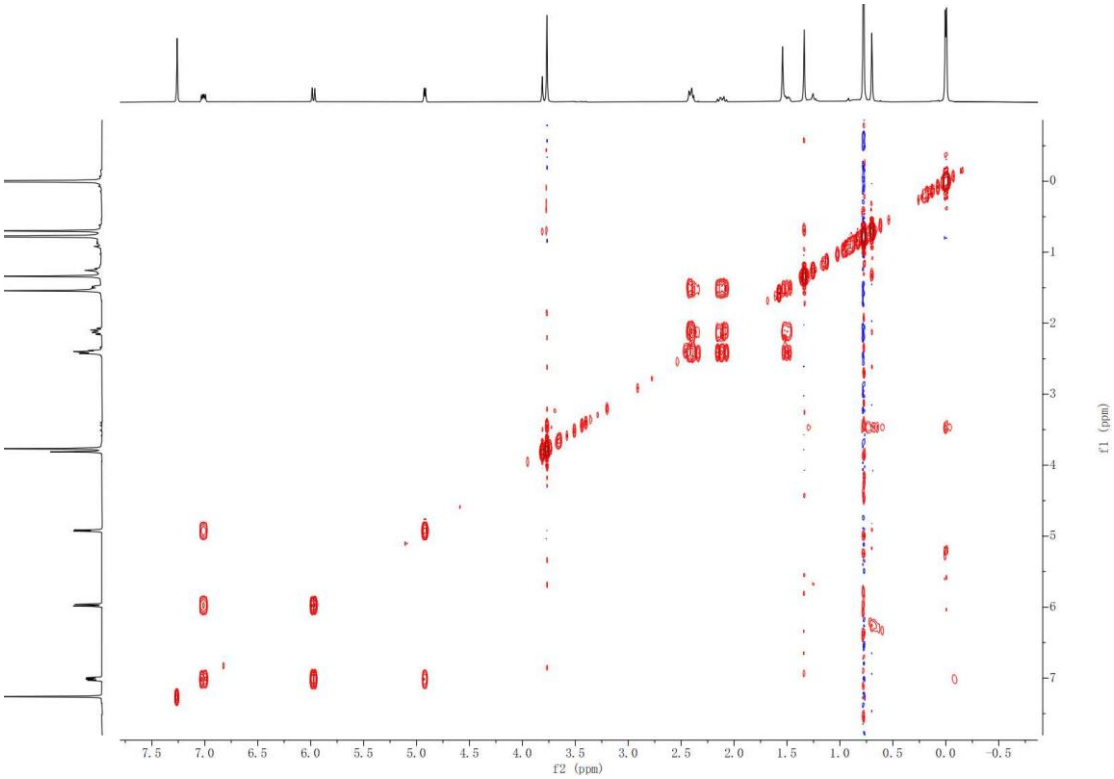
^{1}H NMR spectrum of **27** (400 MHz, $CDCl_3$)

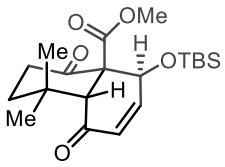


^{13}C NMR spectrum of **27** (100 MHz, $CDCl_3$)



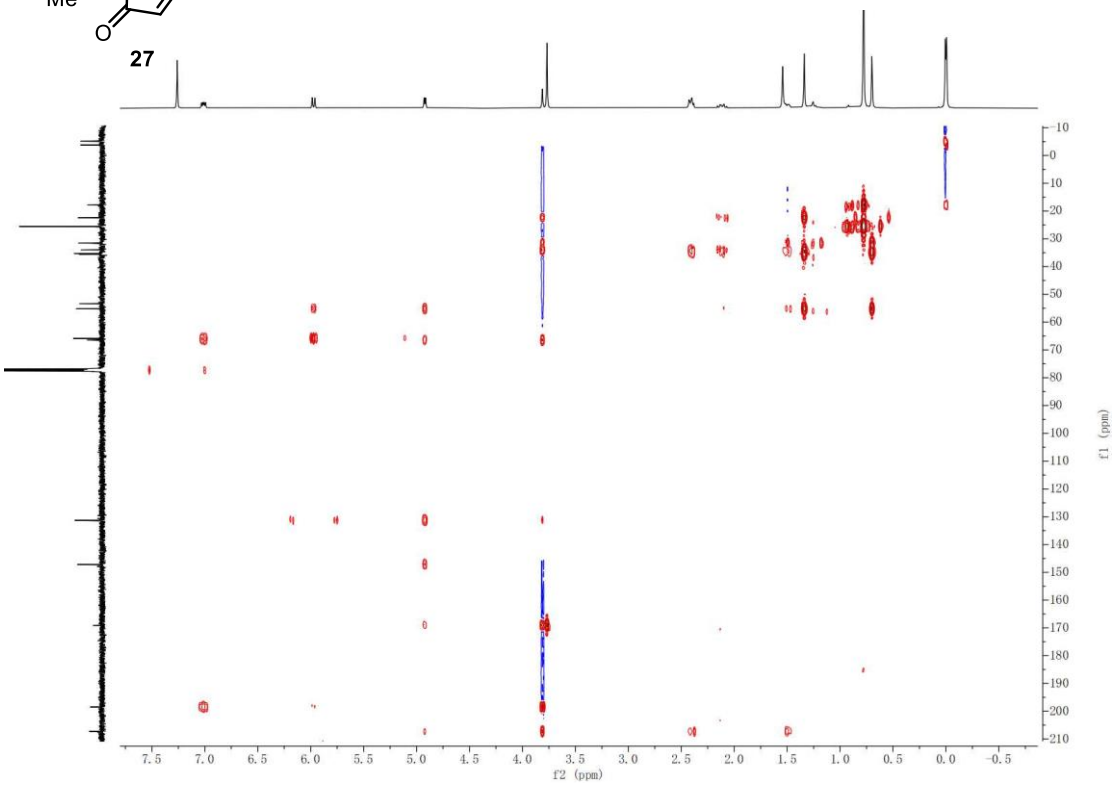
^{1}H-^{1}H COSY spectrum of **27**



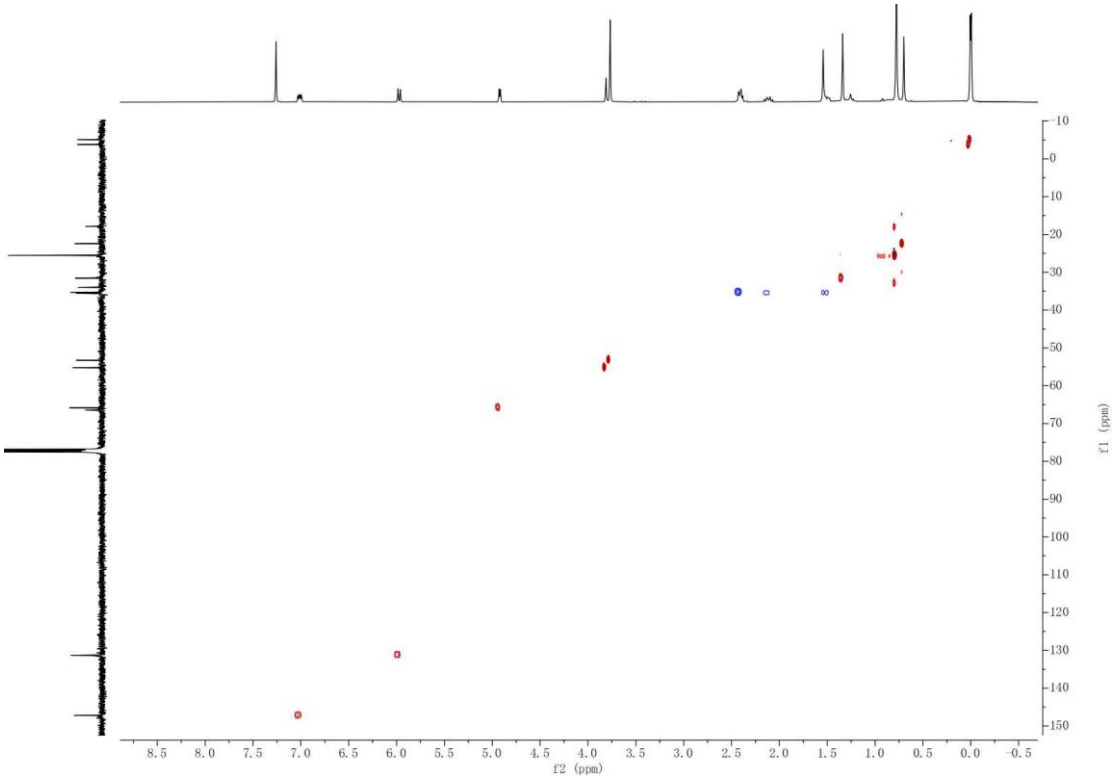


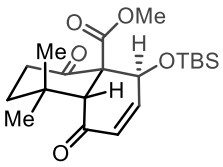
27

HMBC spectrum of **27**



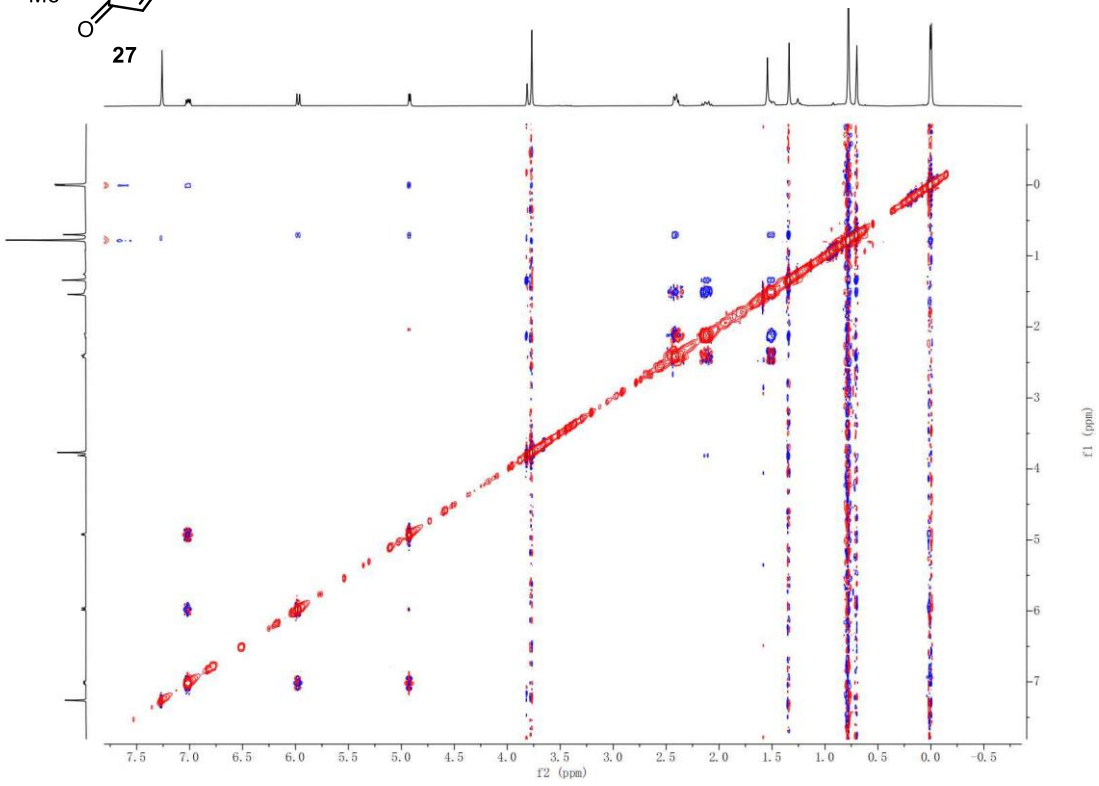
HSQC spectrum of **27**



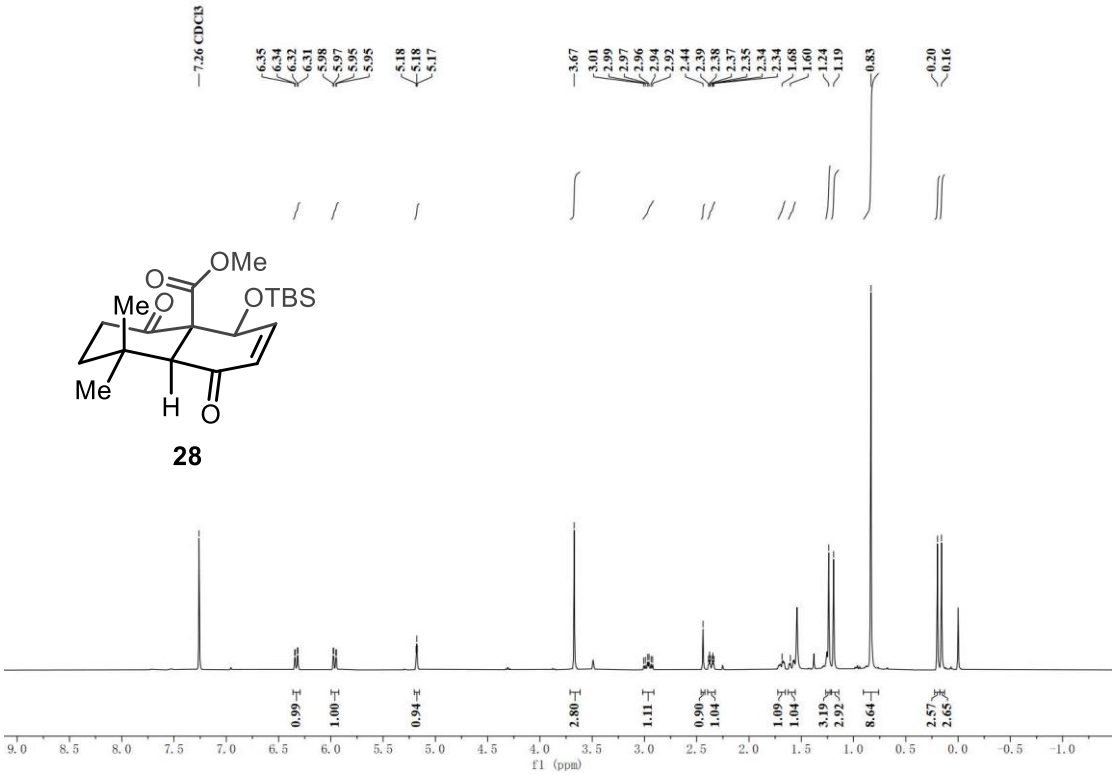


27

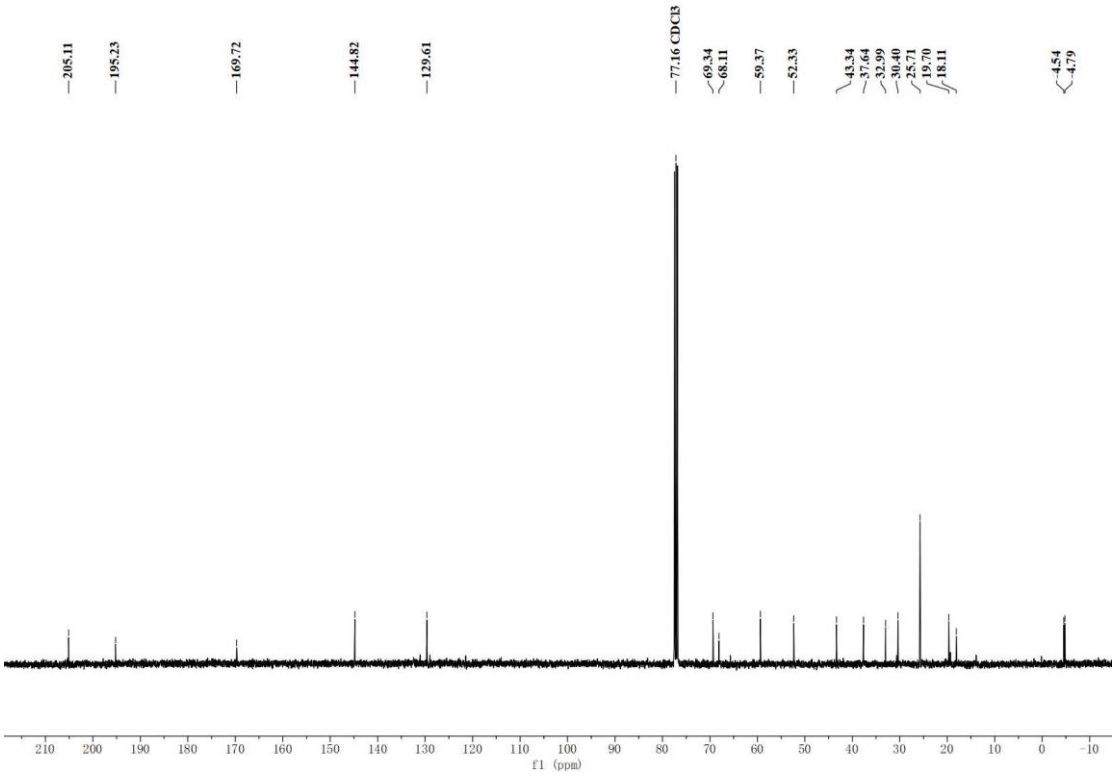
NOESY spectrum of **27**



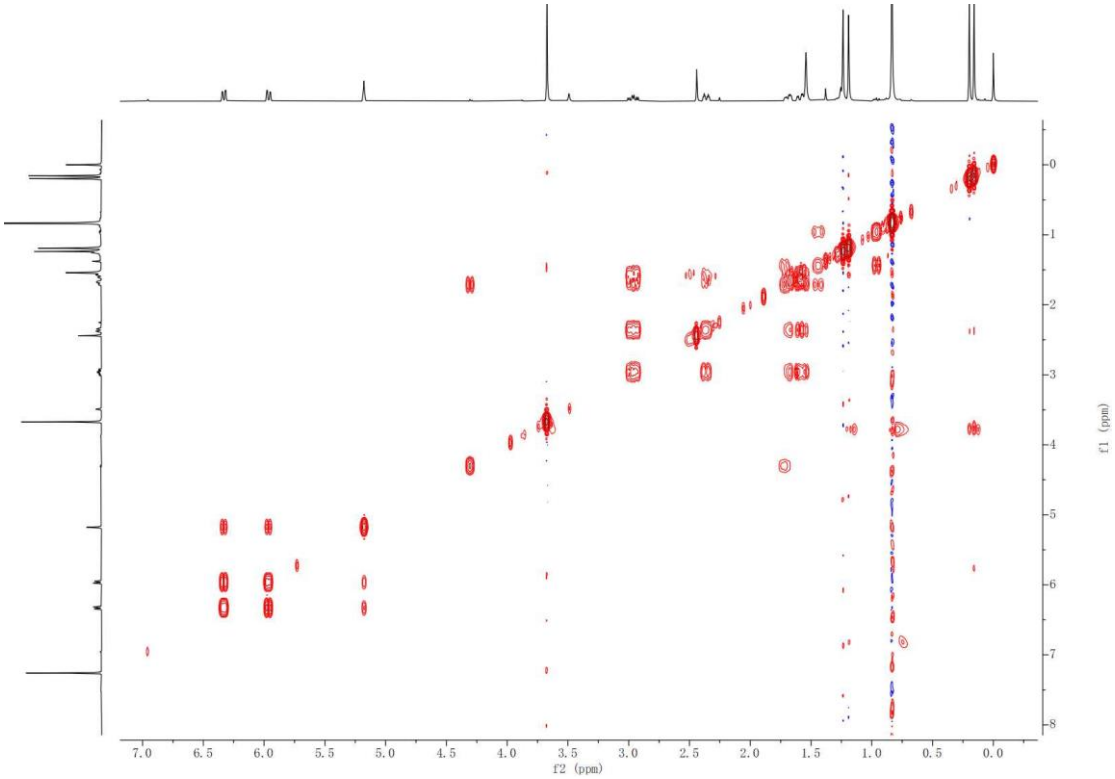
^{1}H NMR spectrum of **28** (400 MHz, $CDCl_3$)

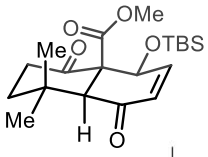


^{13}C NMR spectrum of **28** (100 MHz, $CDCl_3$)



^{1}H-^{1}H COSY spectrum of **28**





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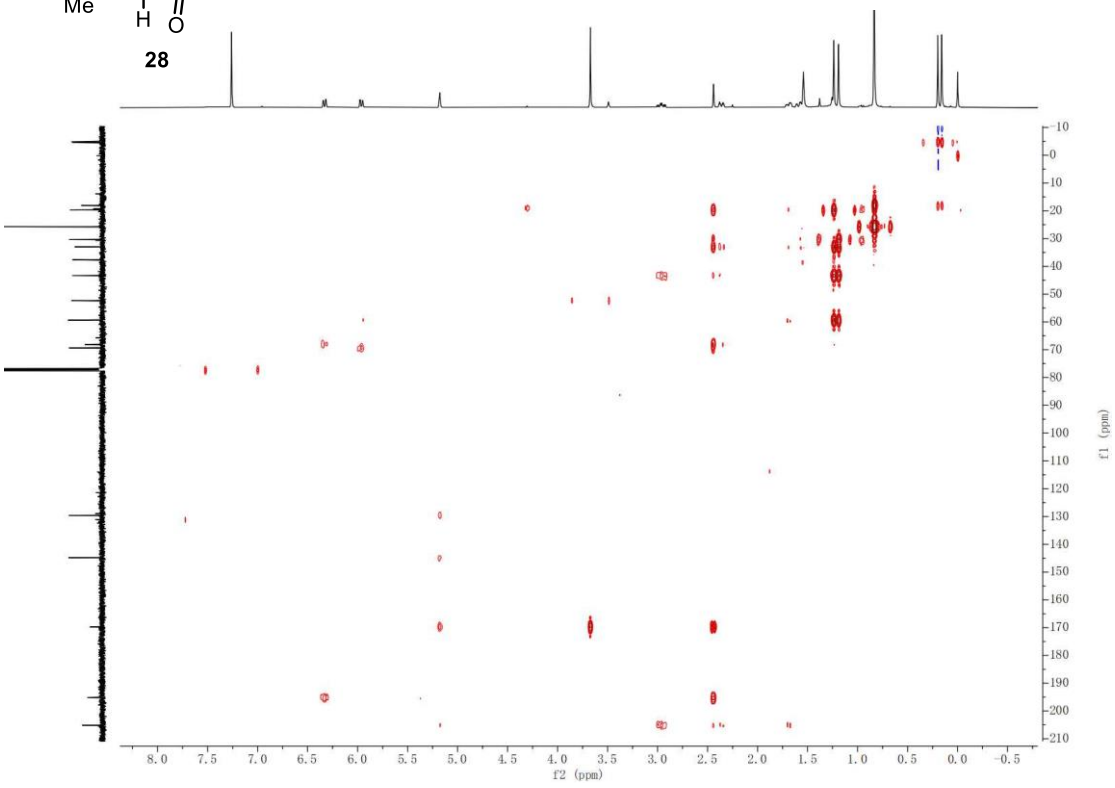
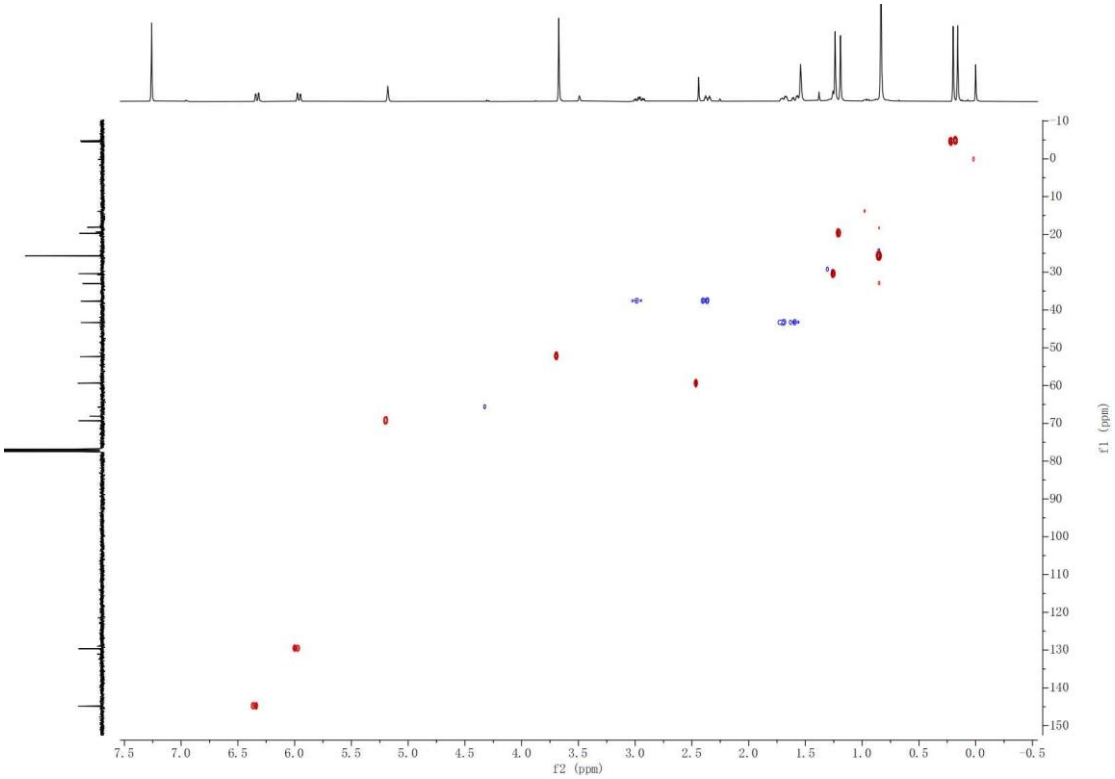
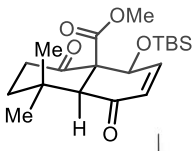
HMBC spectrum of **28**



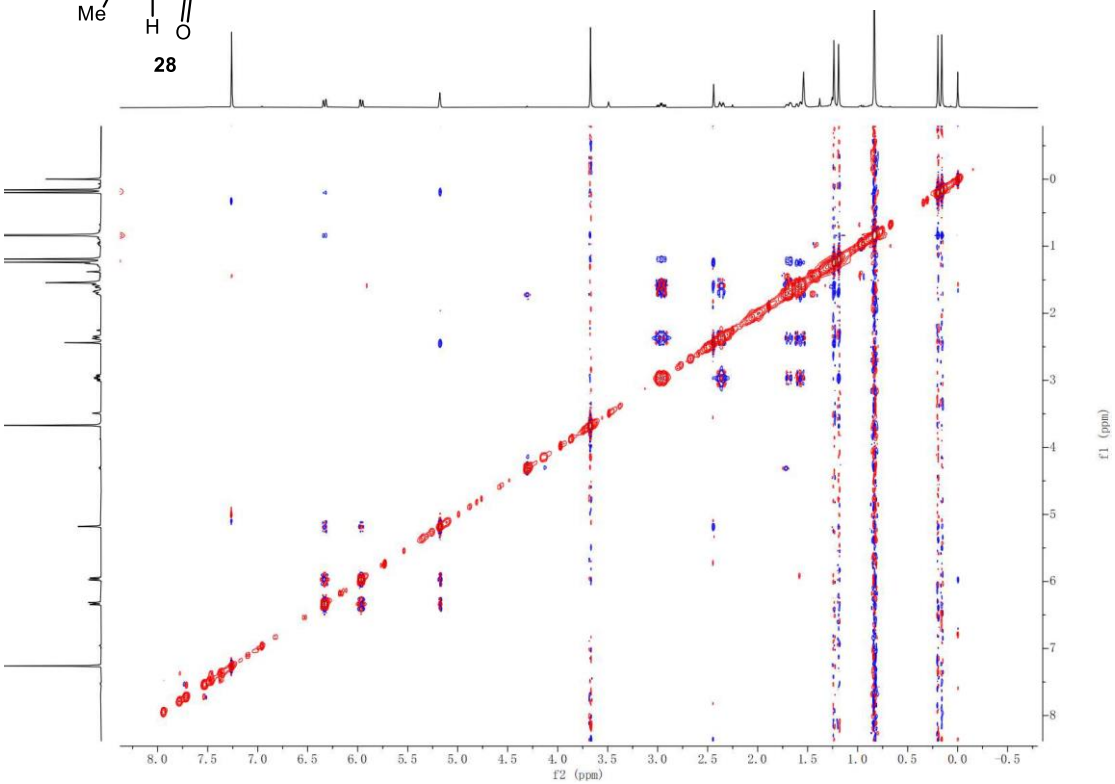
HSQC spectrum of **28**



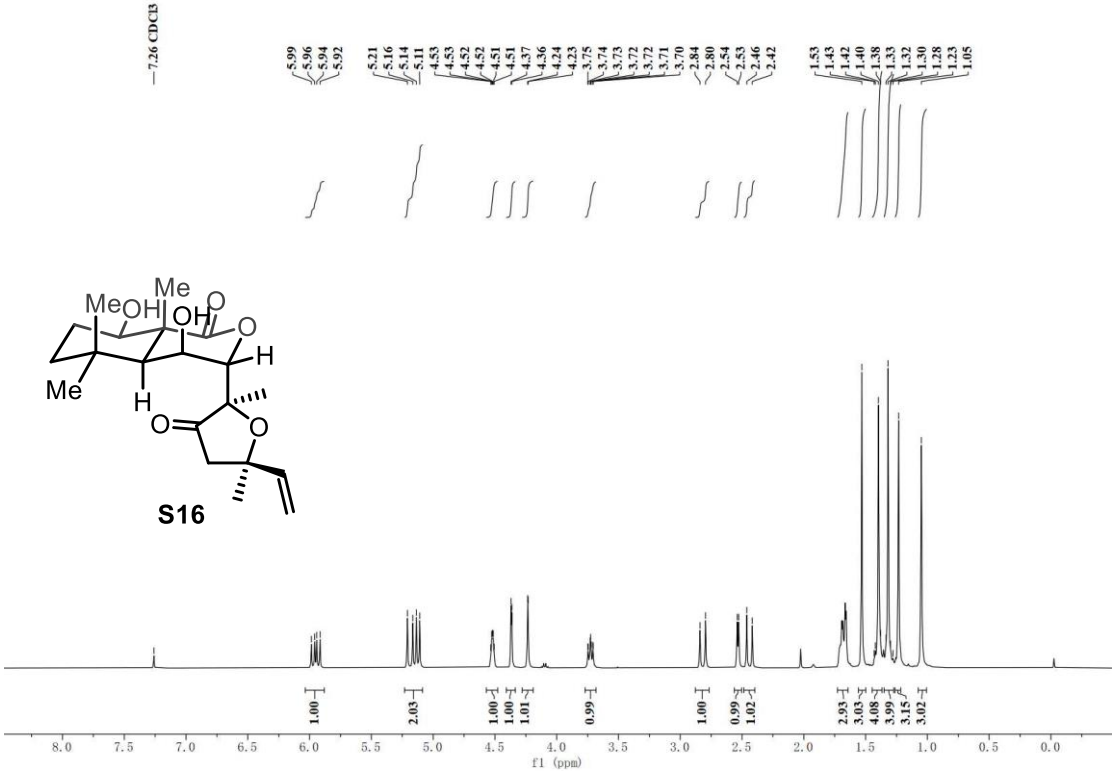


28

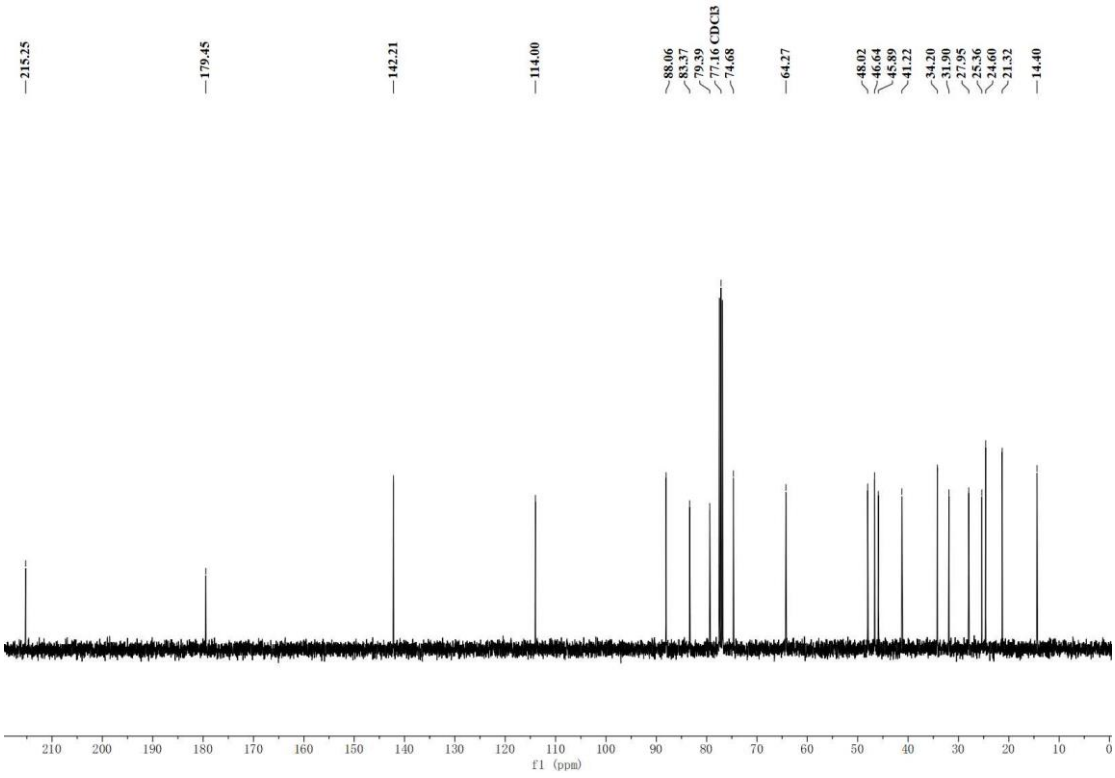
NOESY spectrum of **28**



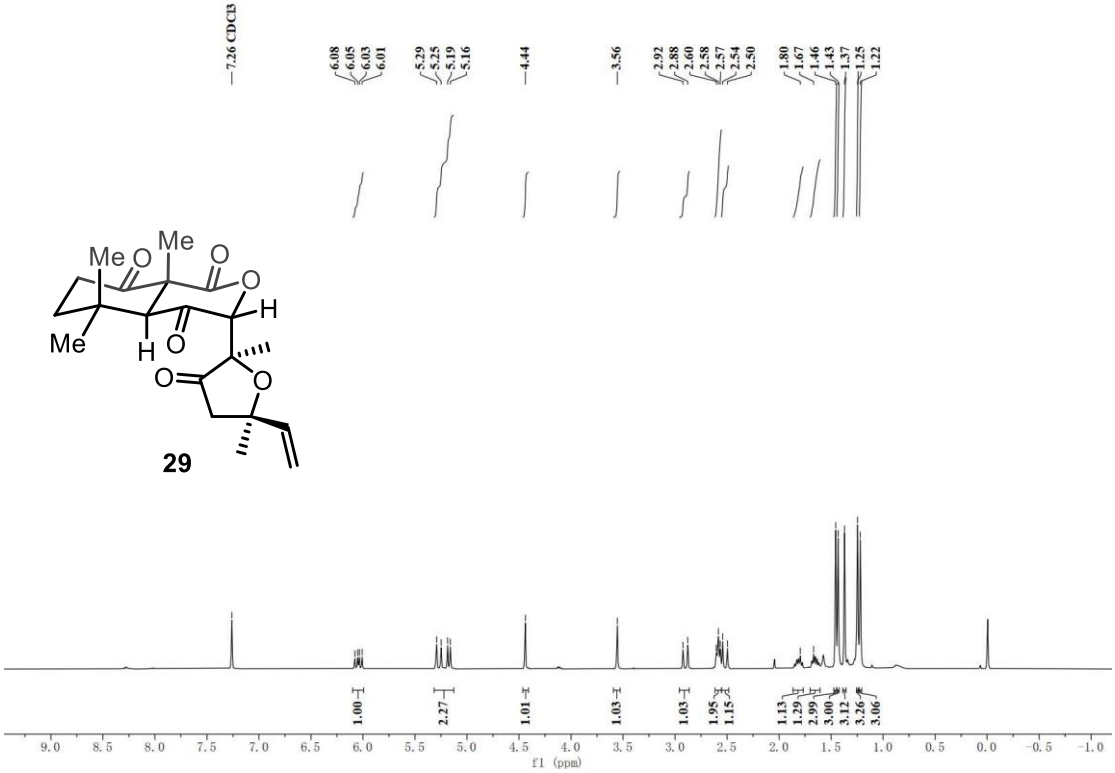
^{1}H NMR spectrum of **S16** (400 MHz, $CDCl_3$)



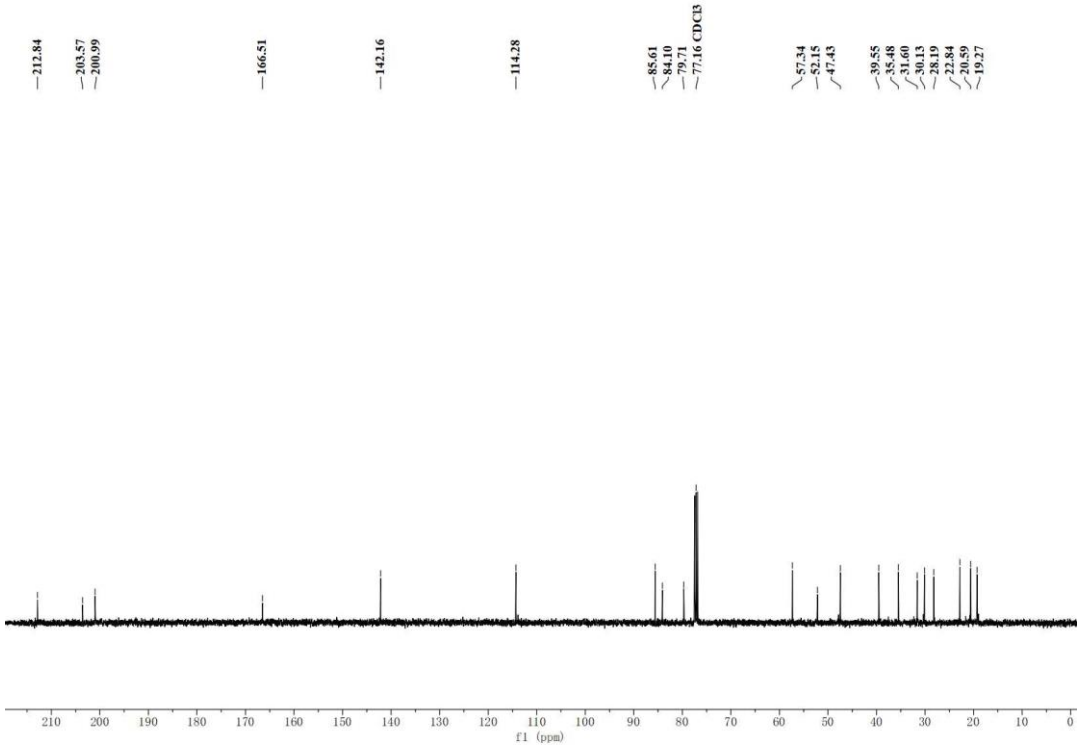
^{13}C NMR spectrum of **S16** (100 MHz, $CDCl_3$)



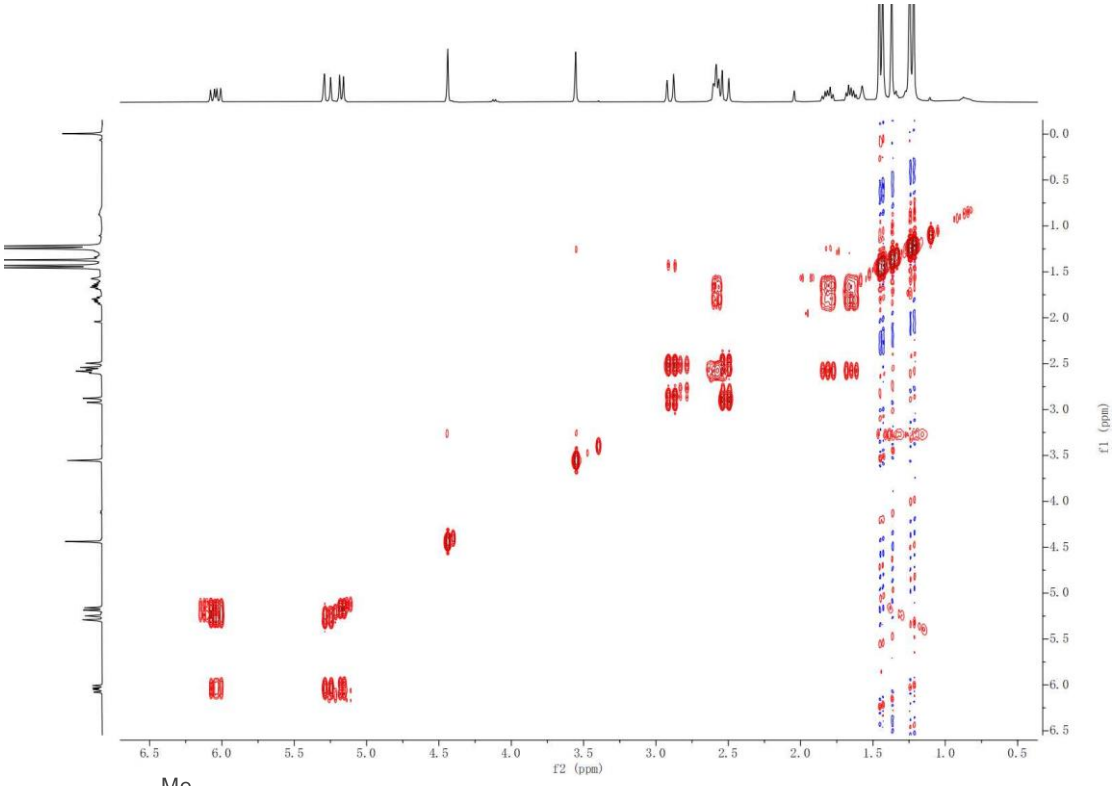
^{1}H NMR spectrum of **29** (400 MHz, $CDCl_3$)

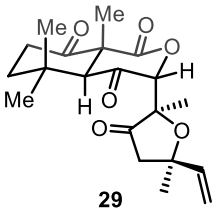


^{13}C NMR spectrum of **29**(100 MHz, $CDCl_3$)



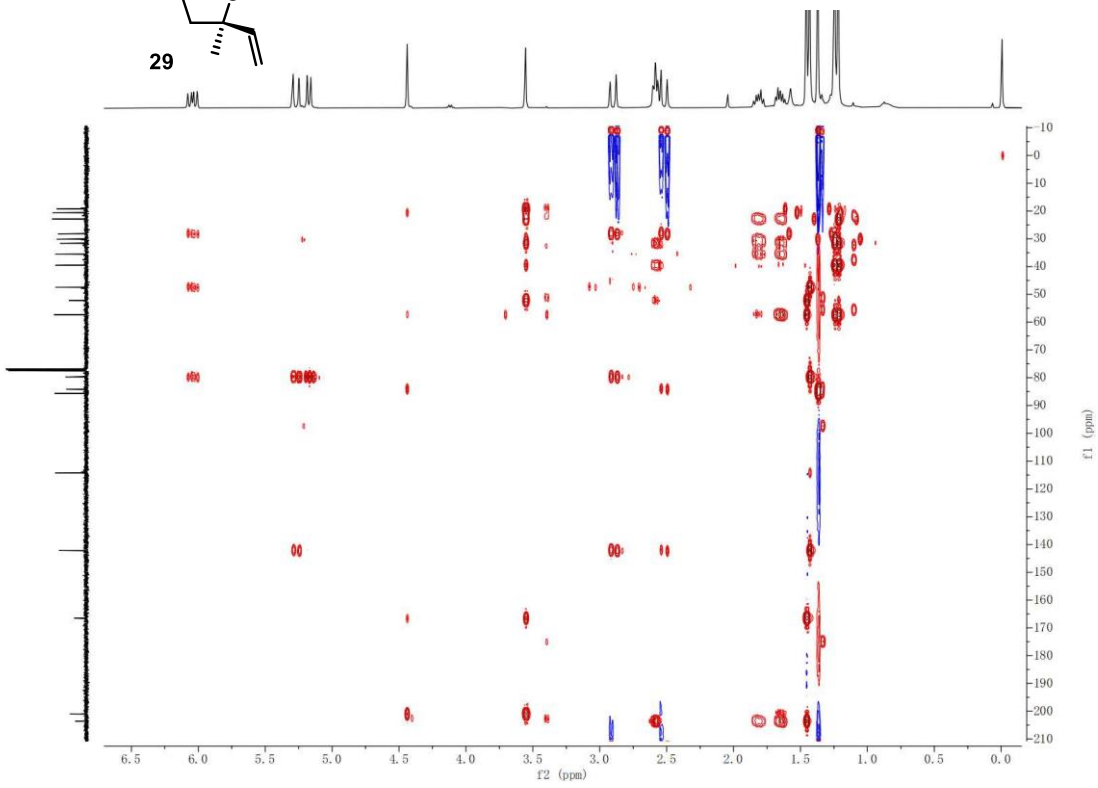
^{1}H-^{1}H COSY spectrum of **29**



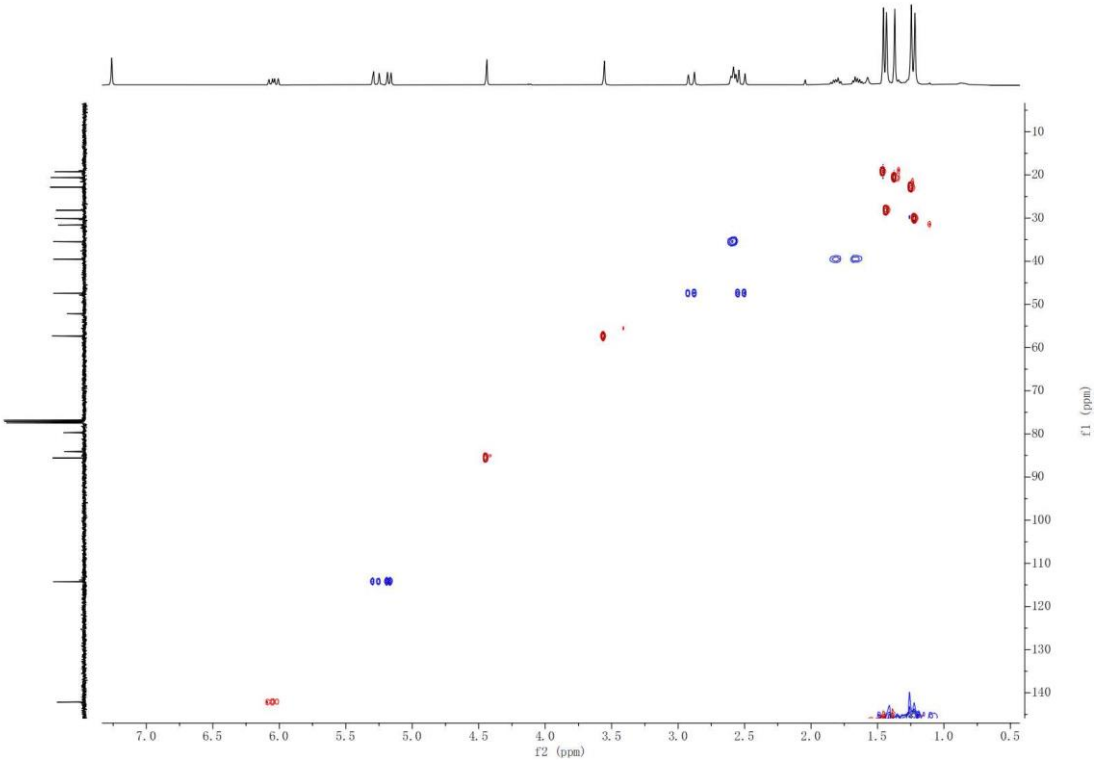


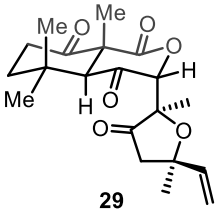
29

HMBC spectrum of **29**



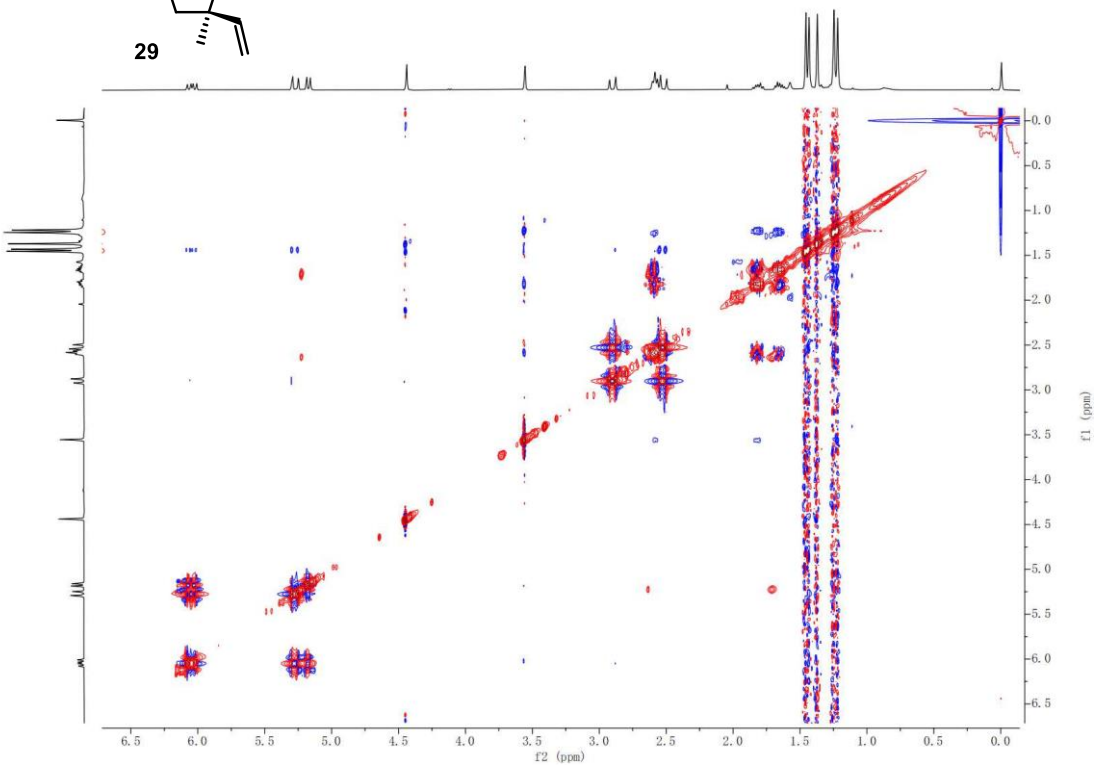
HSQC spectrum of **29**



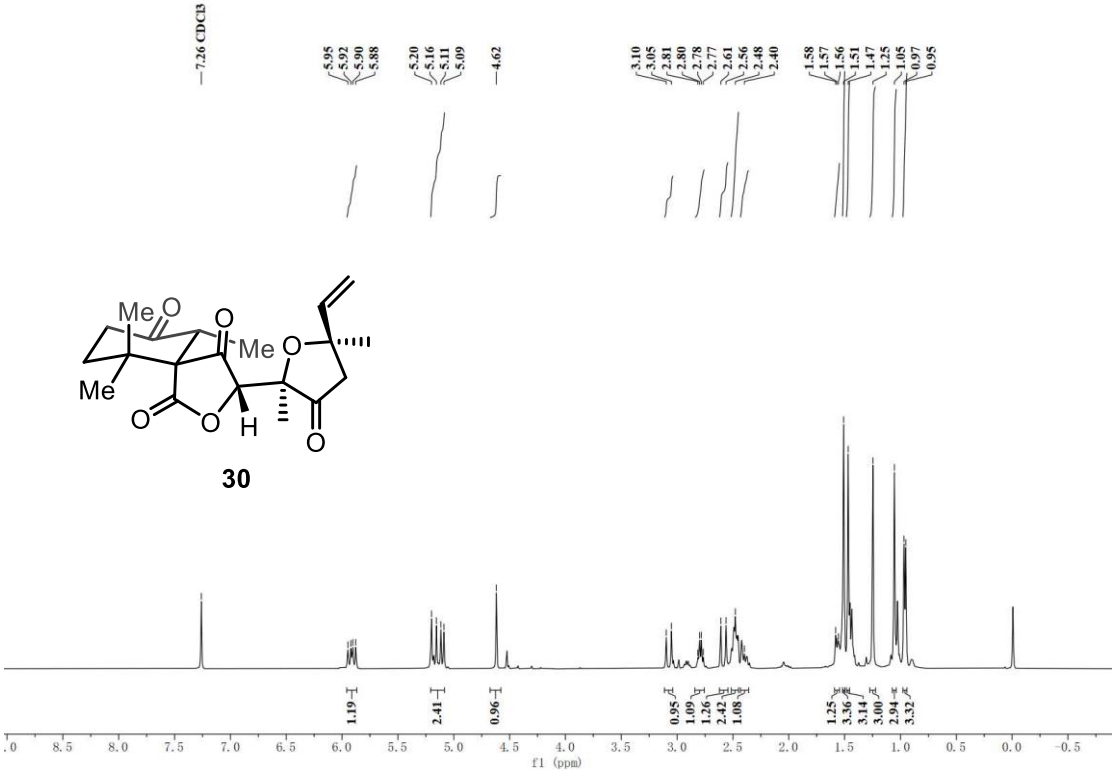


29

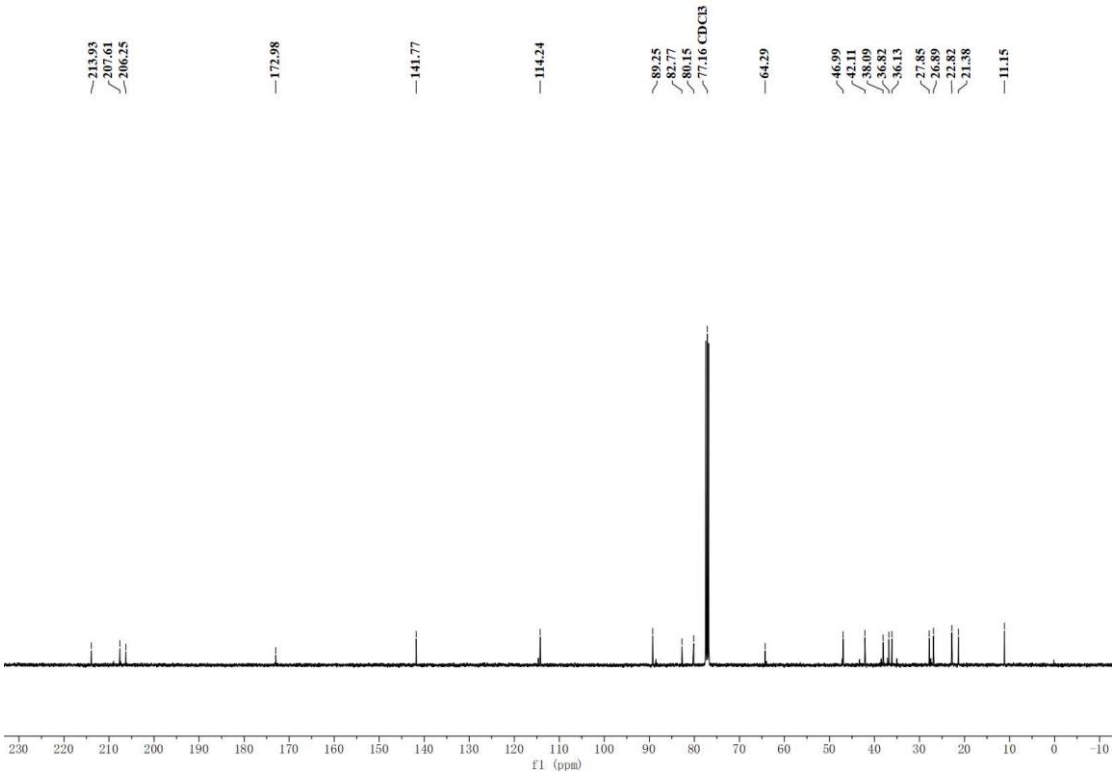
NOESY spectrum of **29**



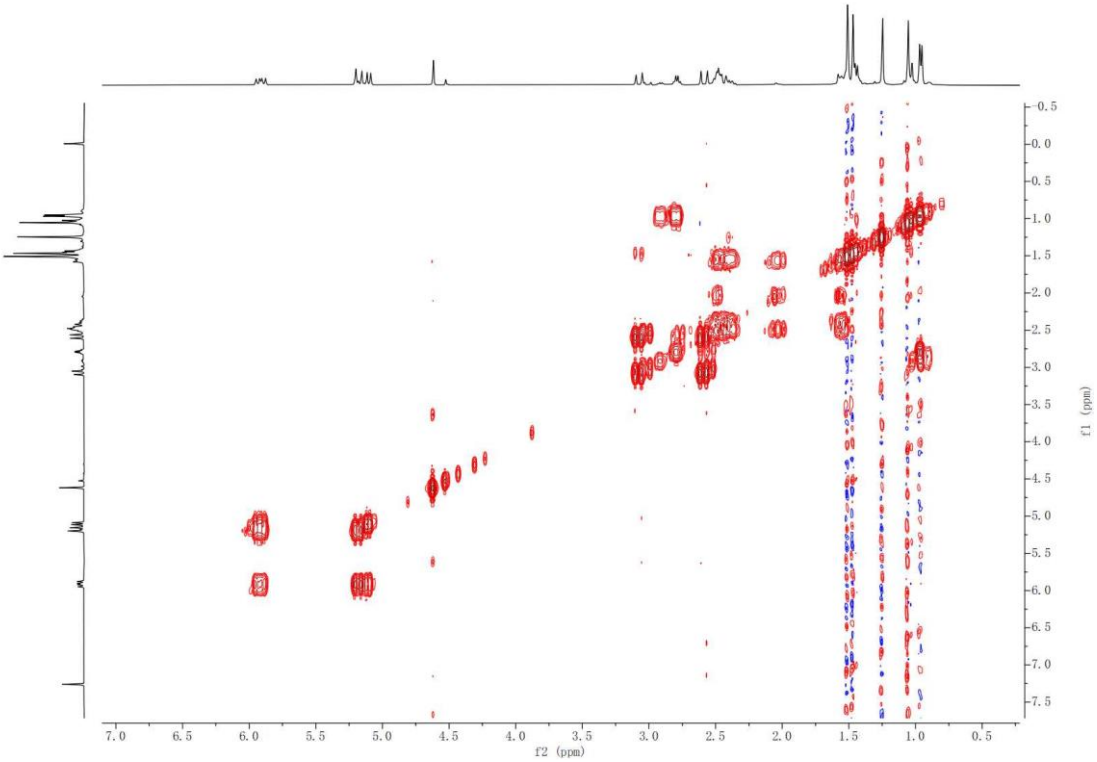
^{1}H NMR spectrum of **30** (400 MHz, $CDCl_3$)

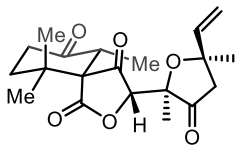


^{13}C NMR spectrum of **30** (100 MHz, $CDCl_3$)



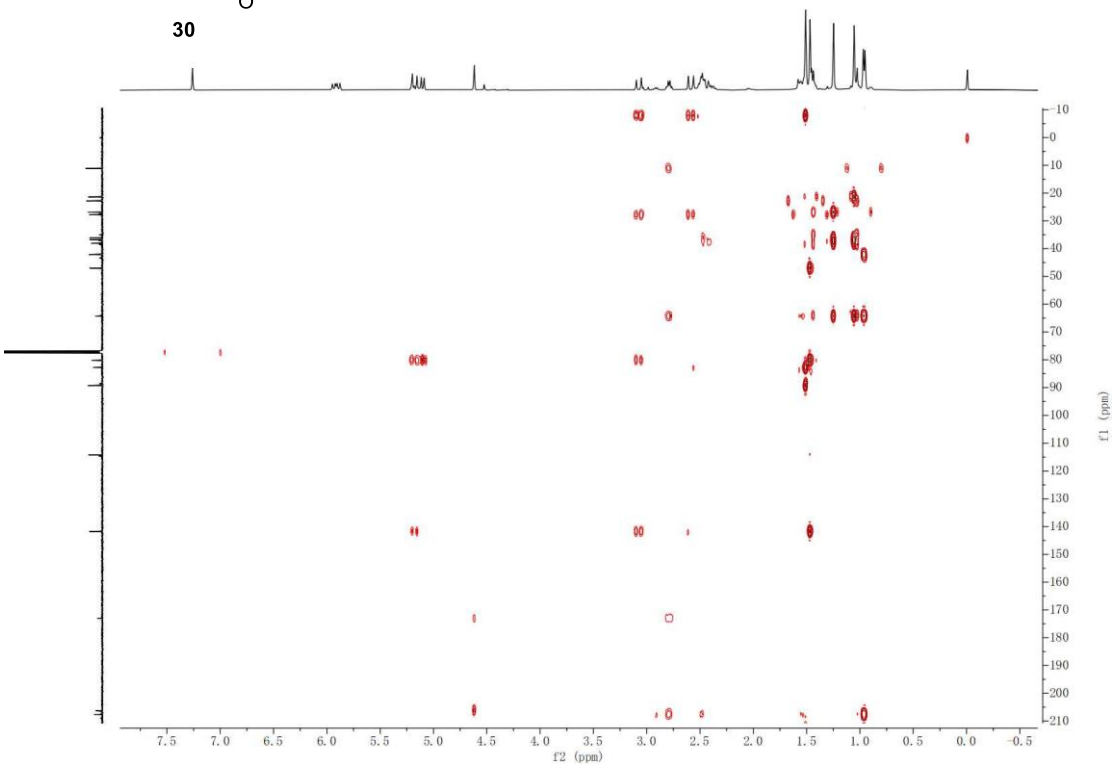
^{1}H-^{1}H COSY spectrum of **30**



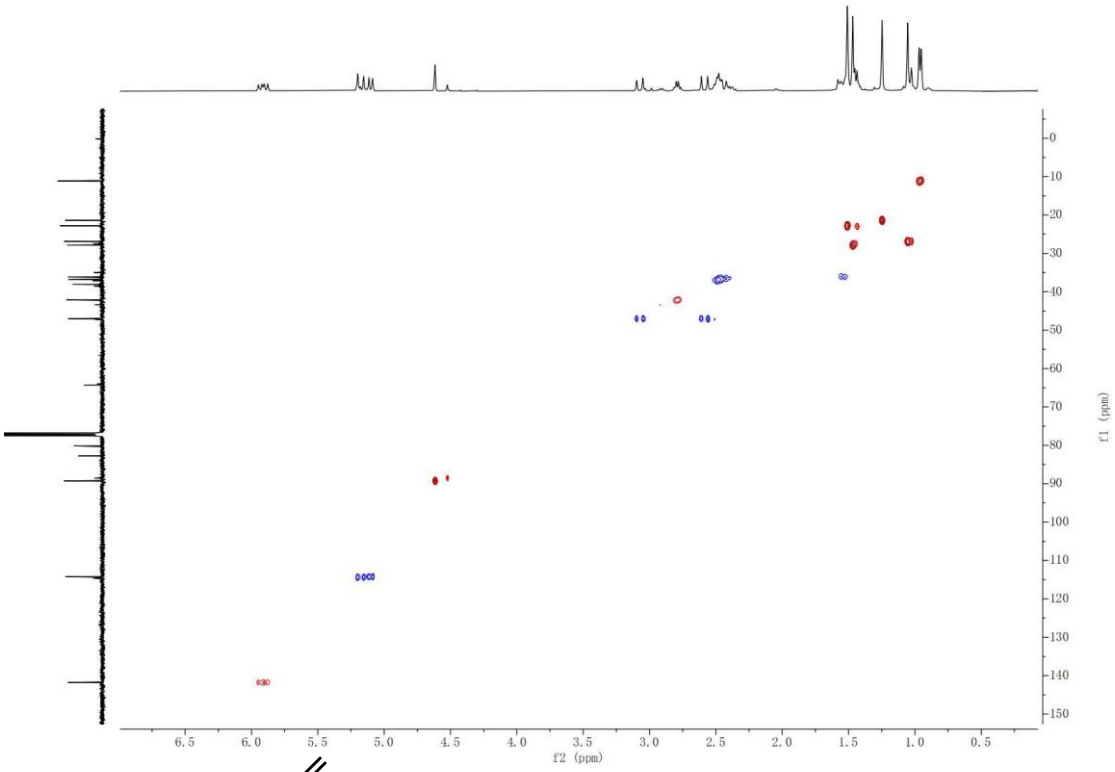


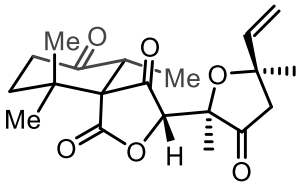
30

HMBC spectrum of **30**



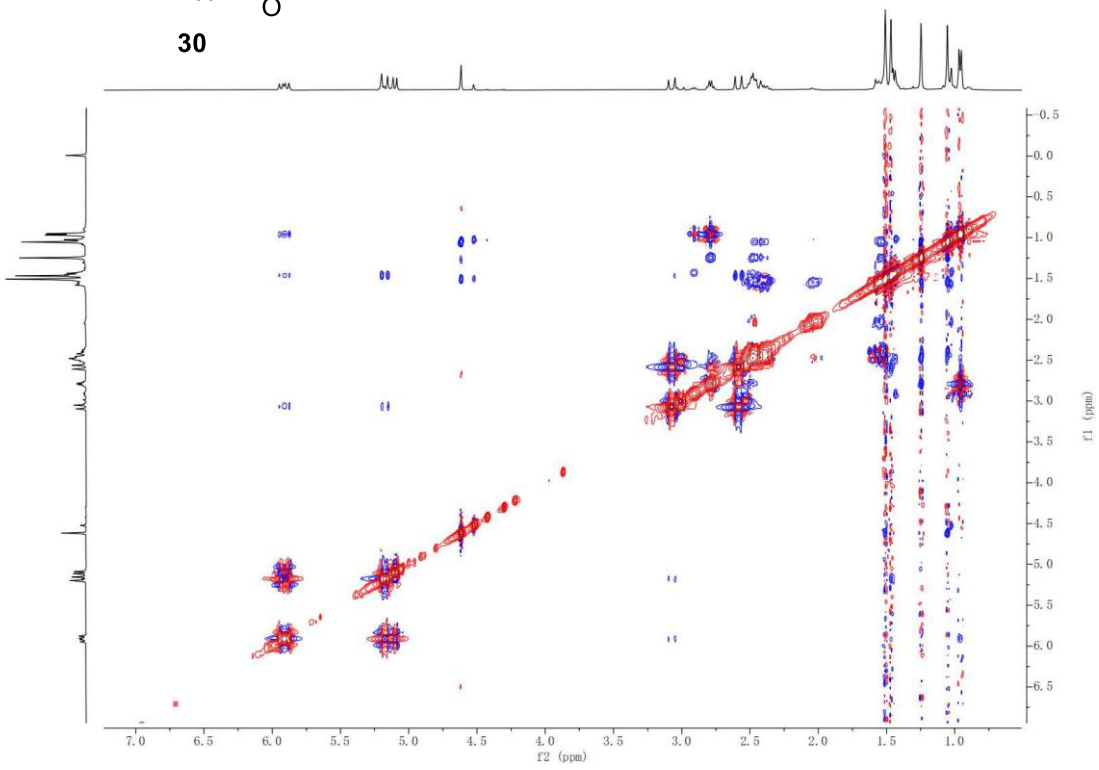
HSQC spectrum of **30**



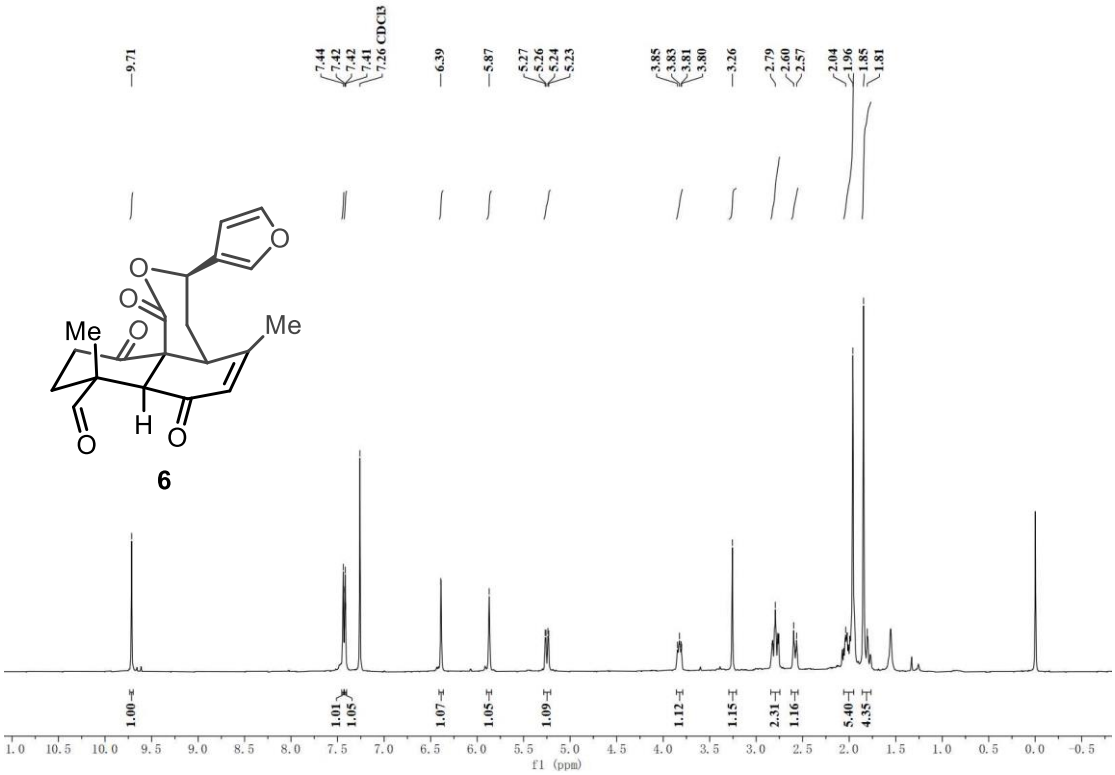


30

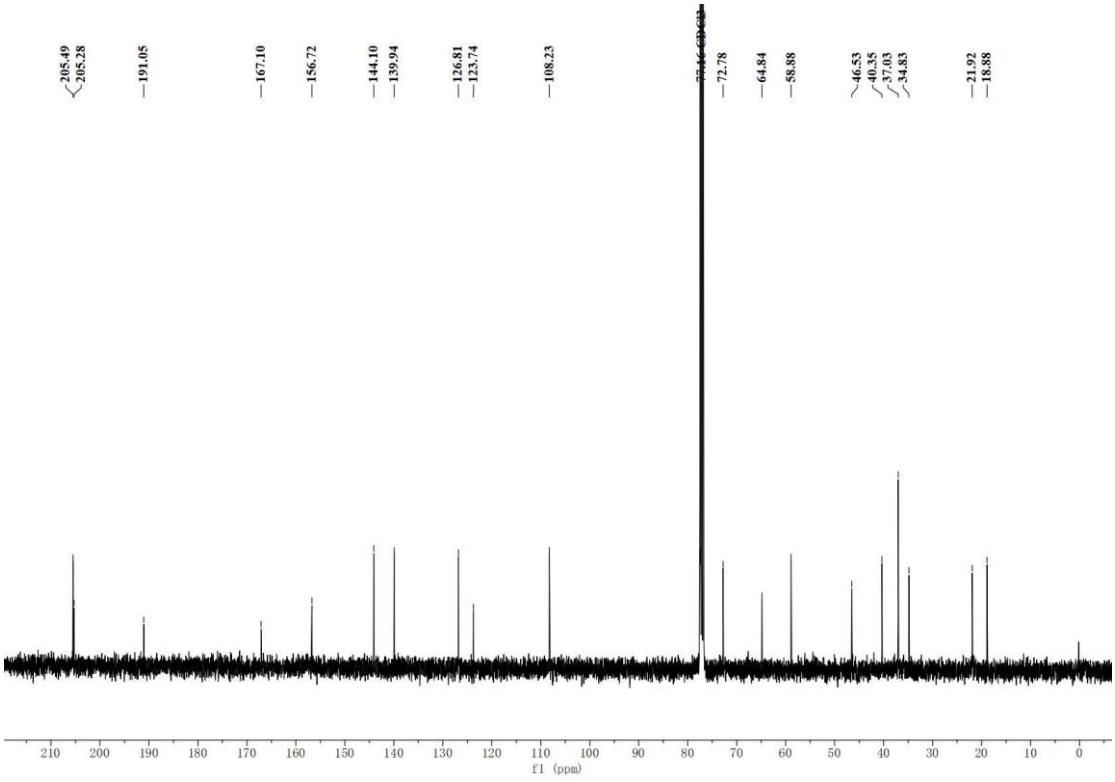
NOESY spectrum of **30**



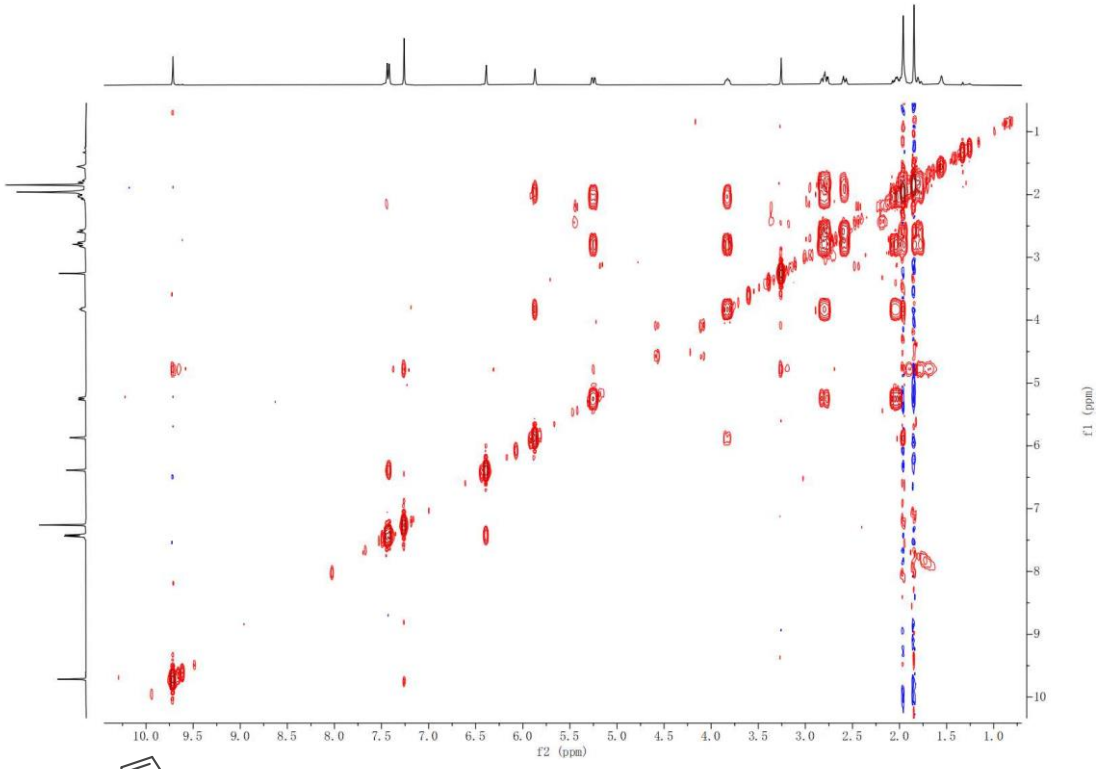
^{1}H NMR spectrum of **6** (400 MHz, $CDCl_3$)

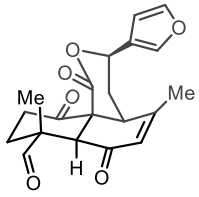


^{13}C NMR spectrum of **6** (100 MHz, $CDCl_3$)



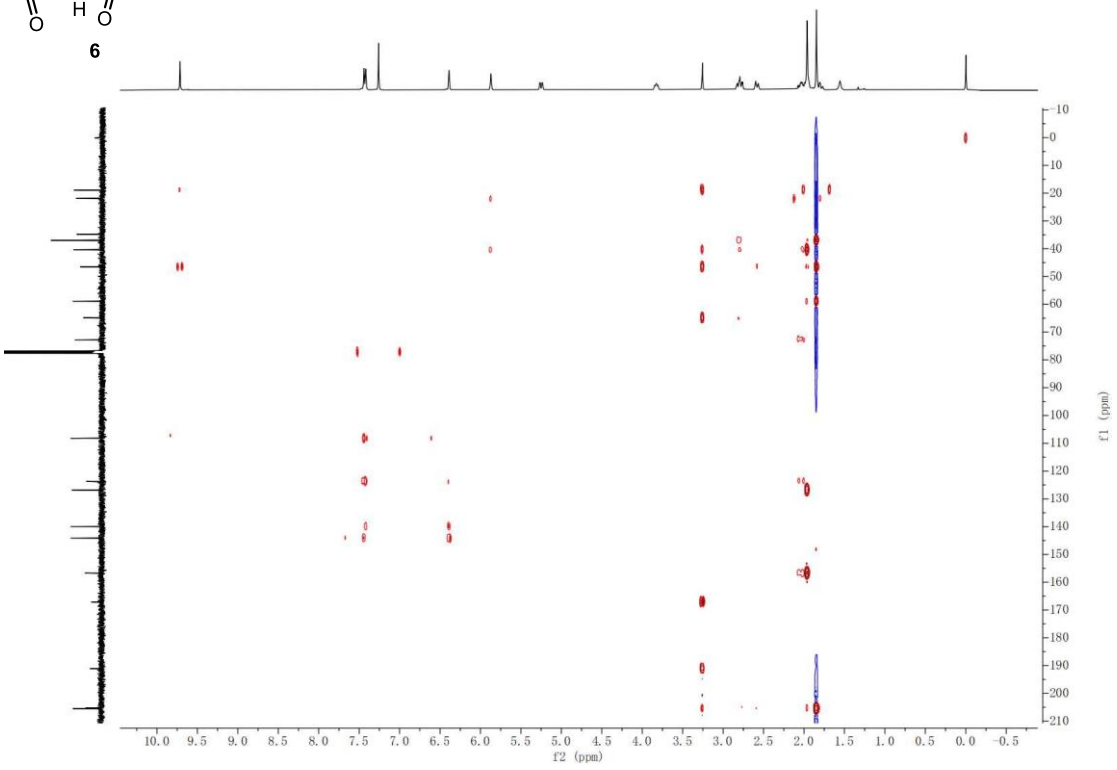
^{1}H-^{1}H COSY spectrum of **6**



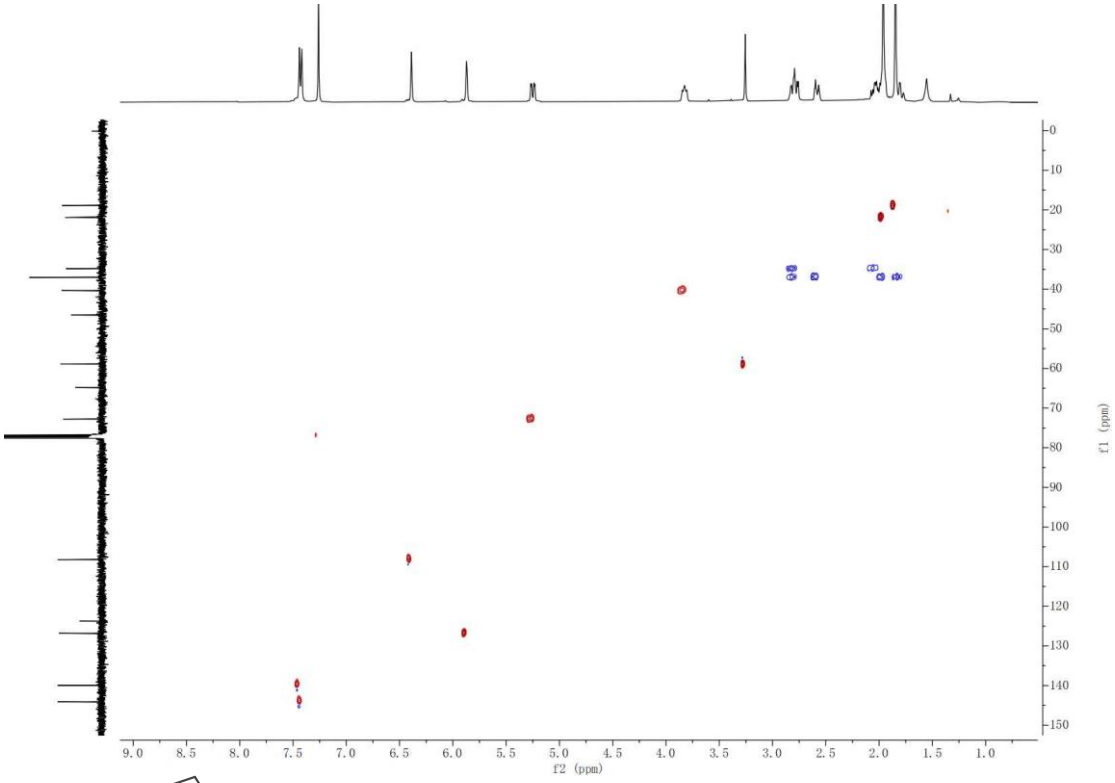


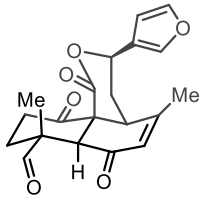
6

HMBC spectrum of **6**



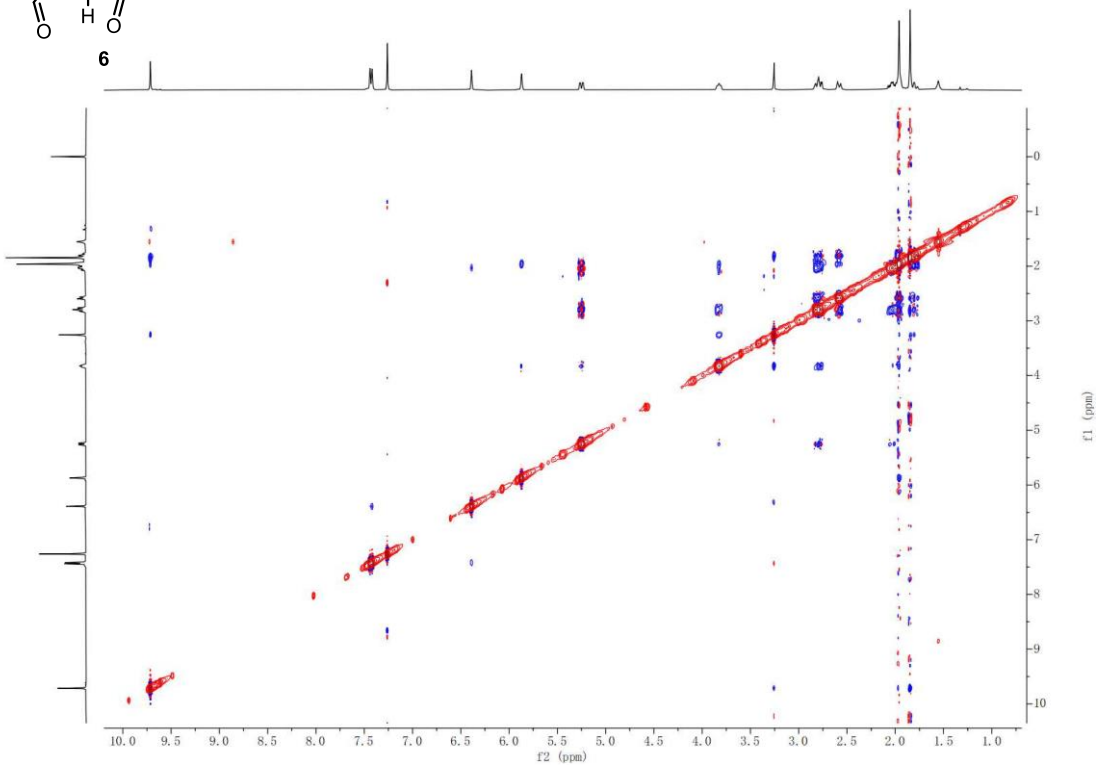
HSQC spectrum of **6**



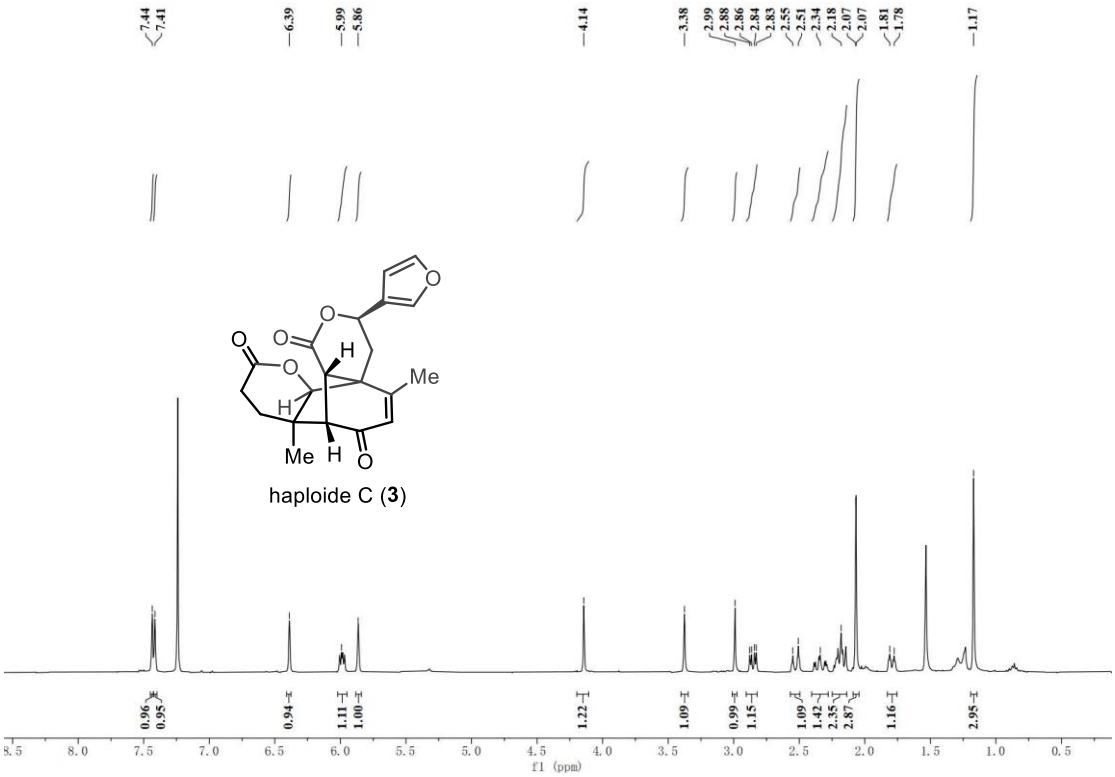


6

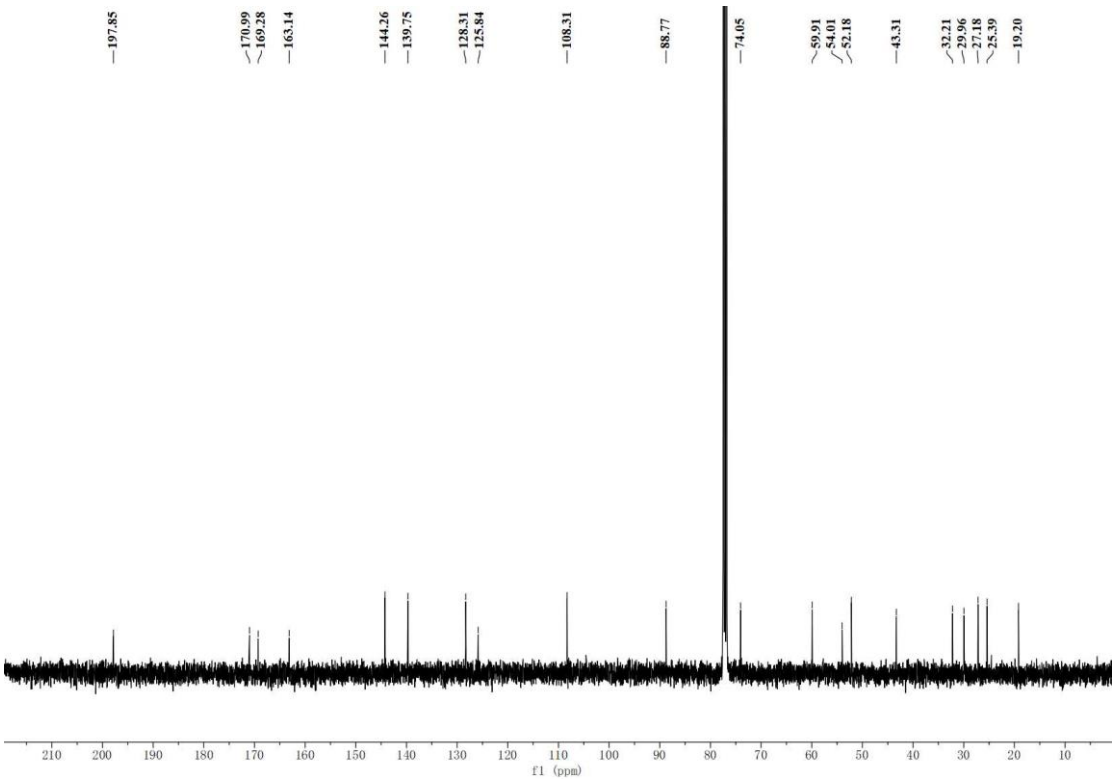
NOESY spectrum of **6**



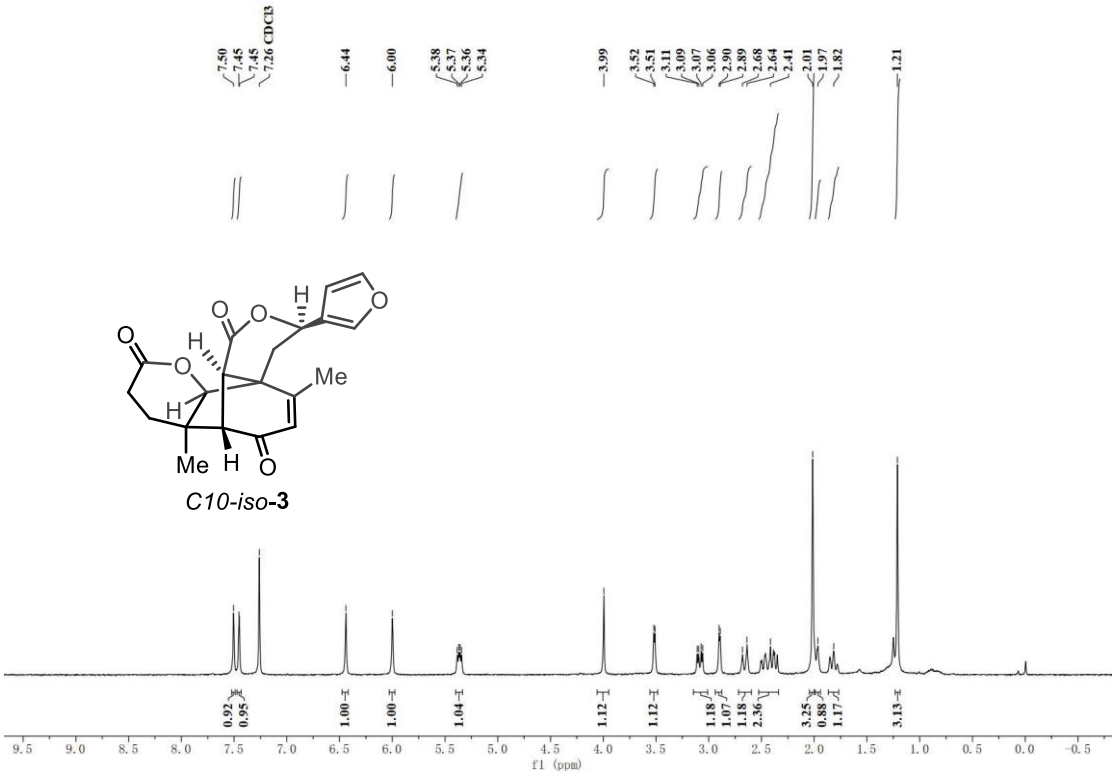
^{1}H NMR spectrum of **3** (400 MHz, $CDCl_3$)



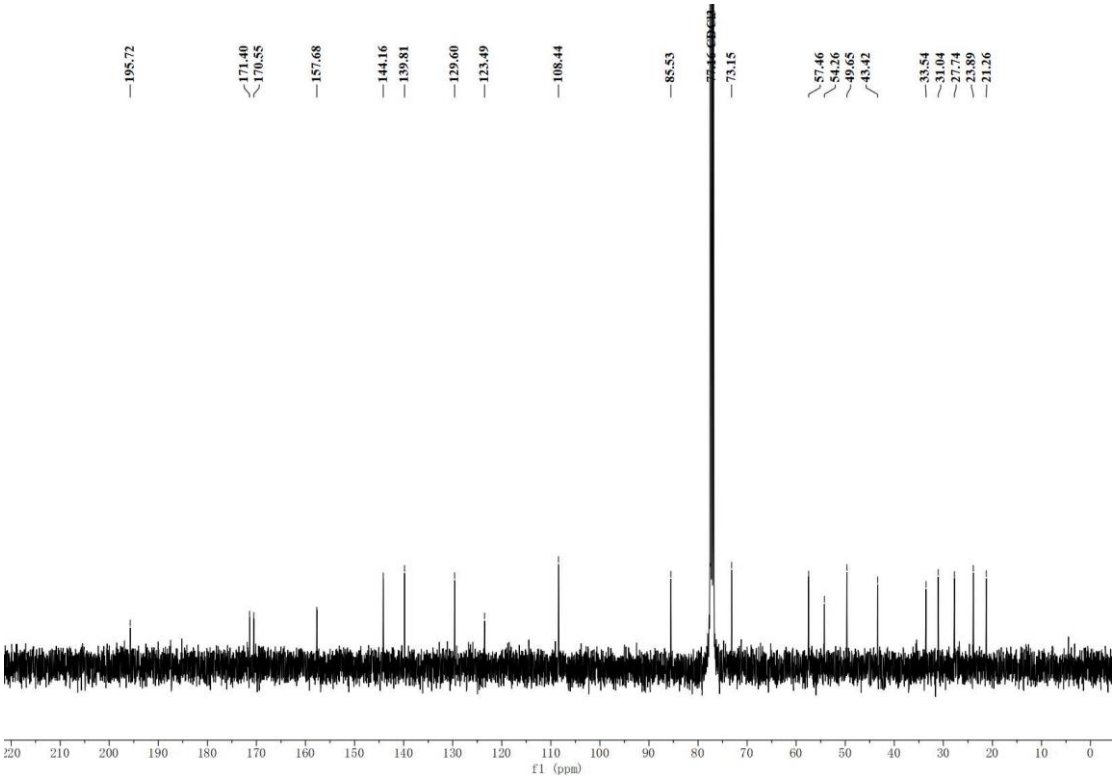
^{13}C NMR spectrum of **3** (100 MHz, $CDCl_3$)



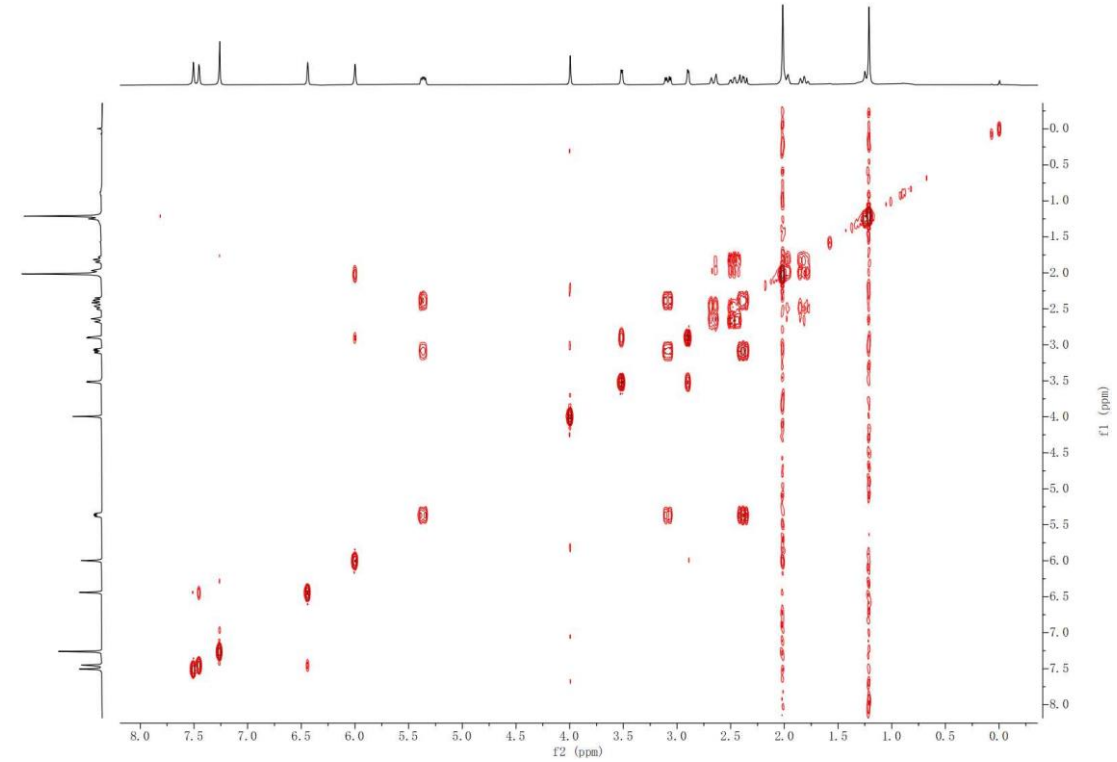
^{1}H NMR spectrum of *iso*-**3** (400 MHz, $CDCl_3$)

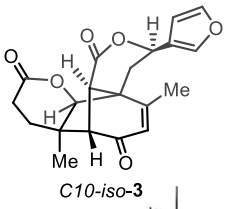


^{13}C NMR spectrum of *iso*-**3** (100 MHz, $CDCl_3$)



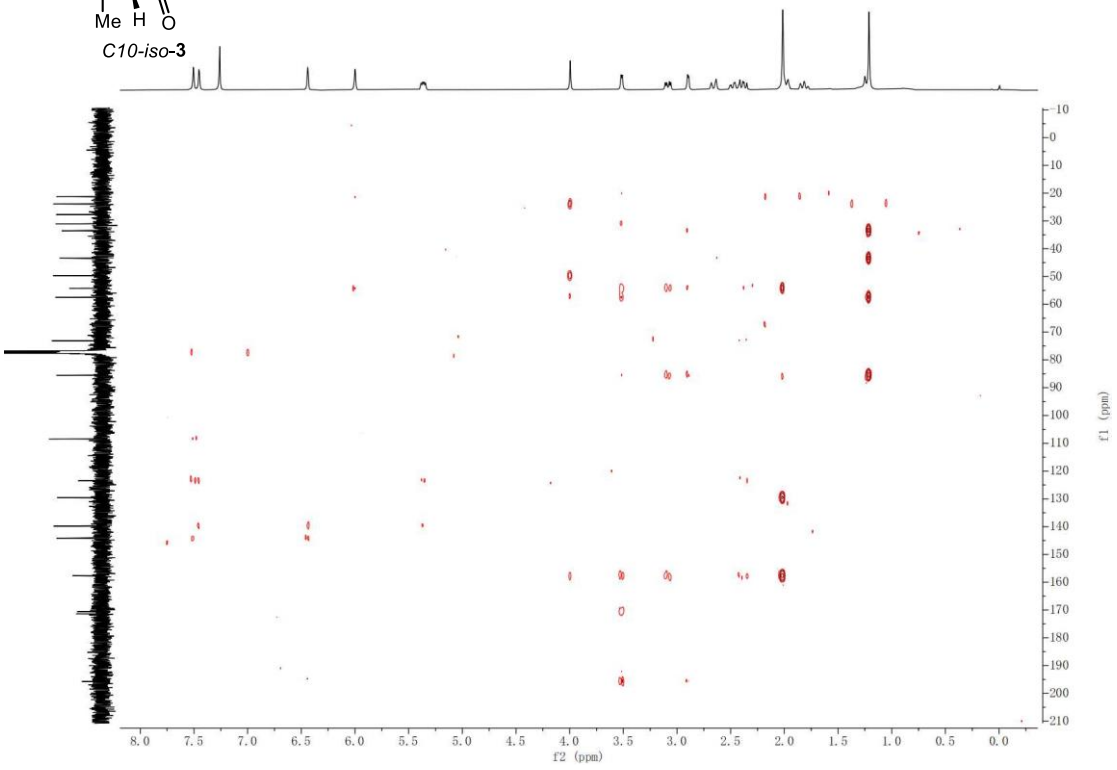
^{1}H-^{1}H COSY spectrum of *iso*-**3**



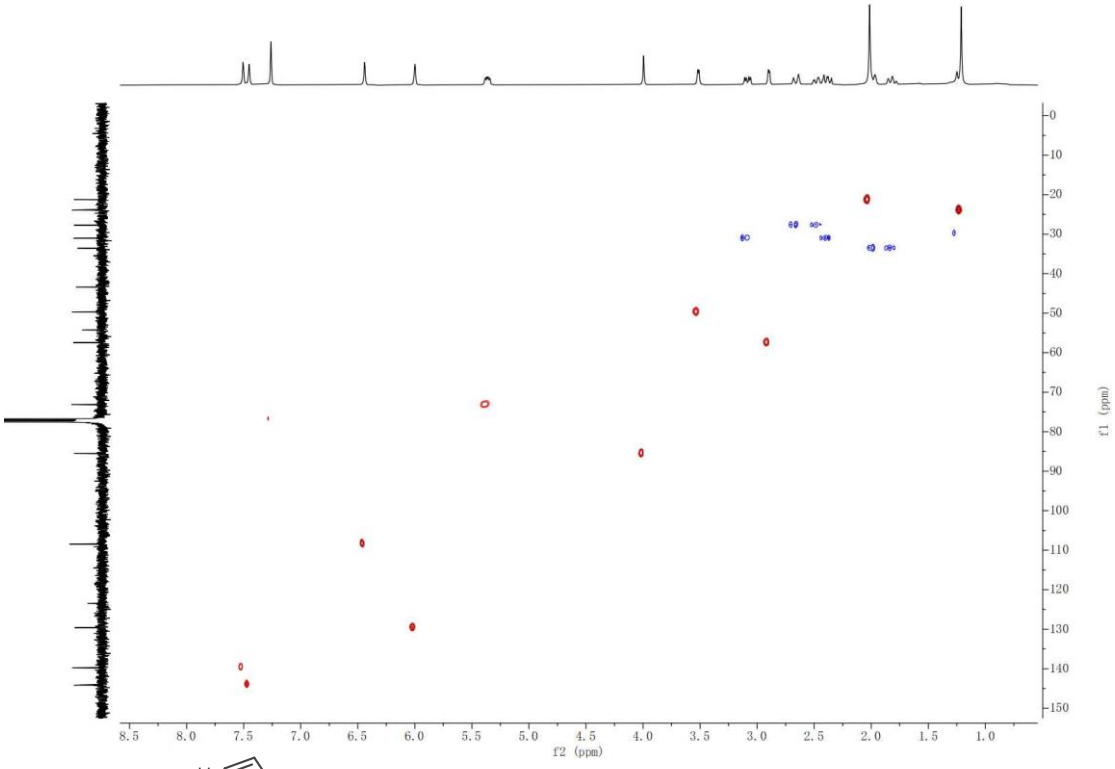


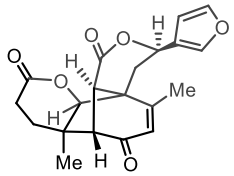
C10-iso-**3**

HMBC spectrum of *iso*-**3**



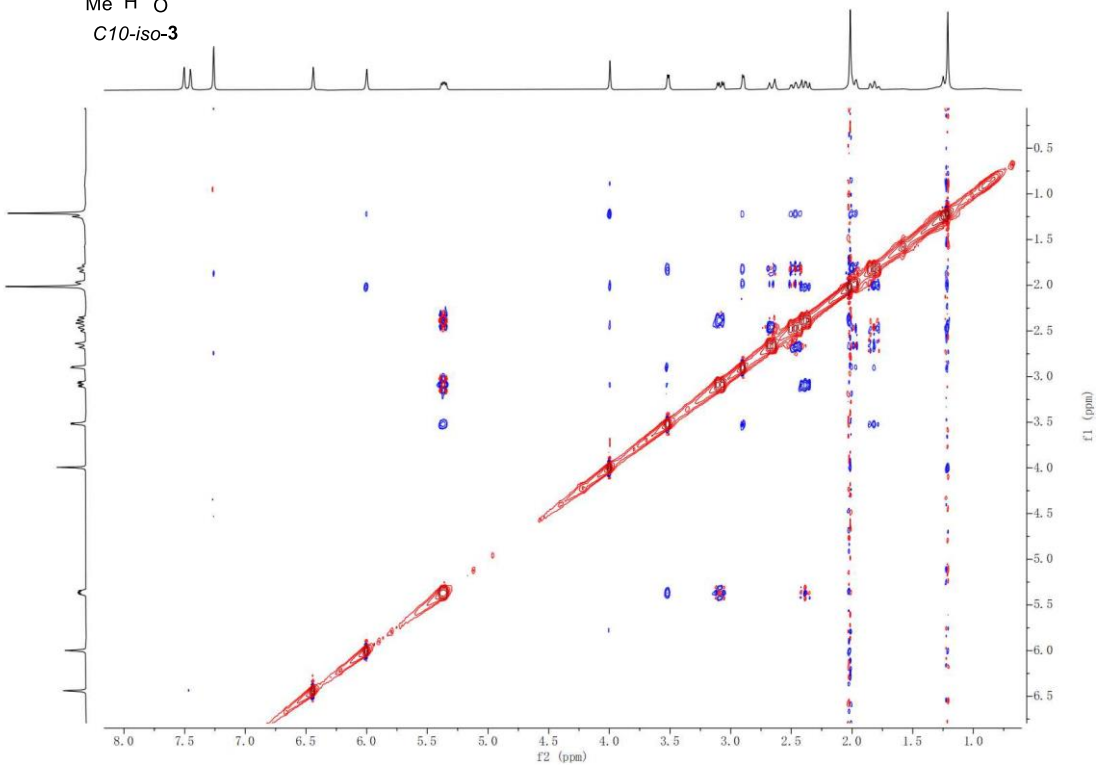
HSQC spectrum of *iso*-**3**



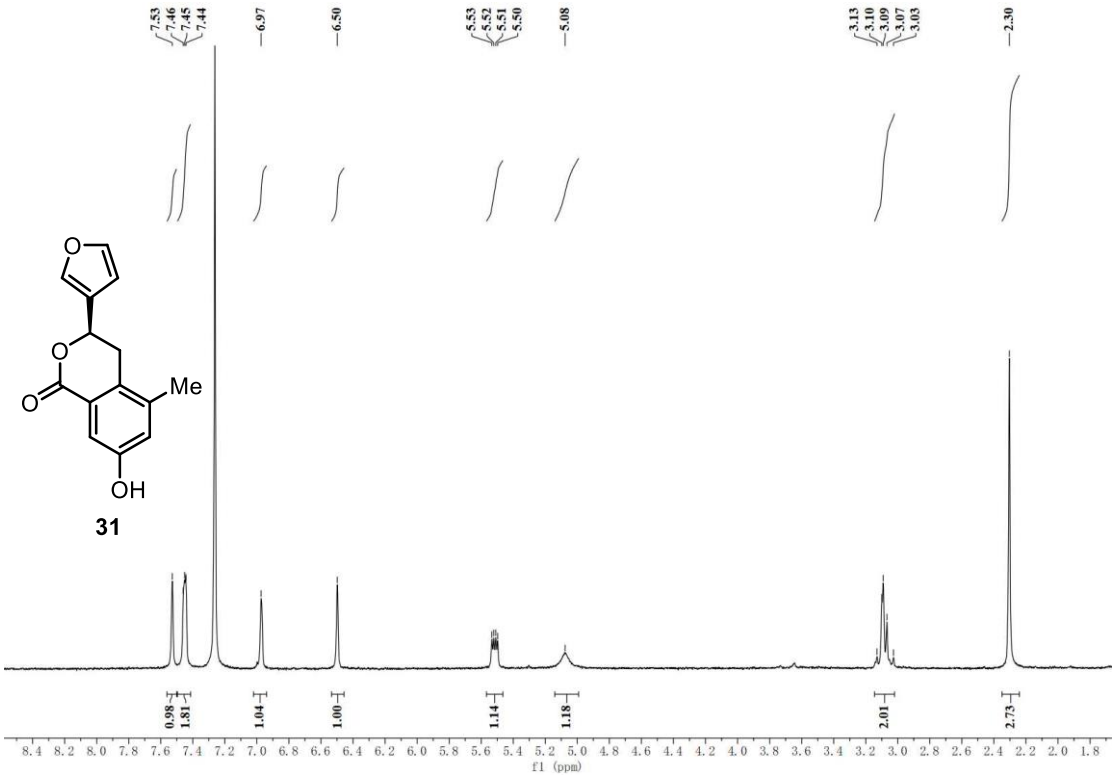


C10-iso-**3**

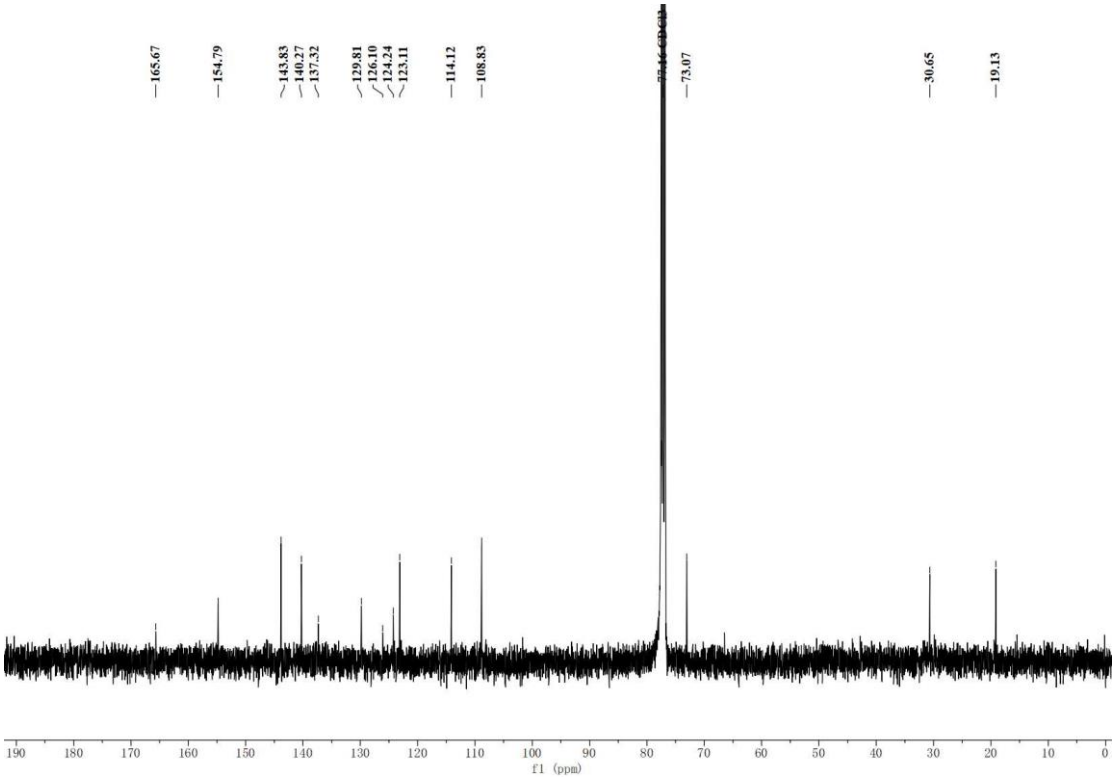
NOESY spectrum of *iso*-**3**



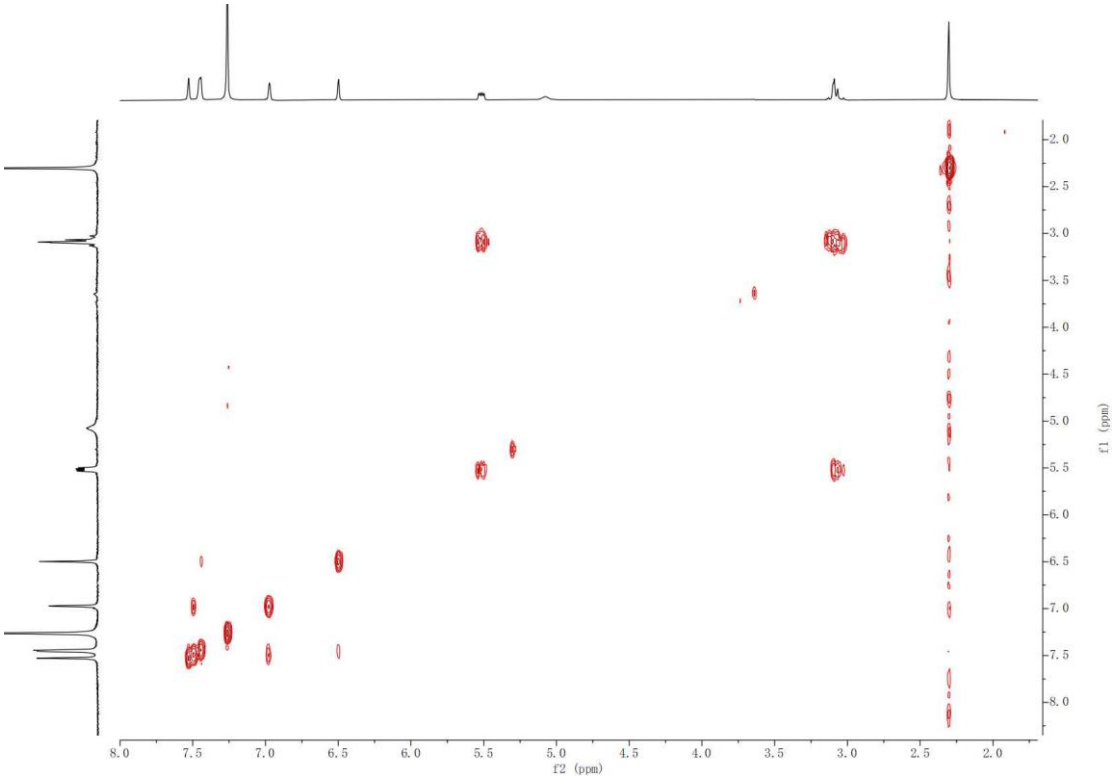
^{1}H NMR spectrum of **31** (400 MHz, $CDCl_3$)

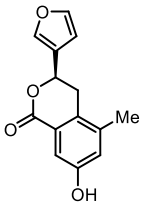


^{13}C NMR spectrum of **31** (100 MHz, $CDCl_3$)



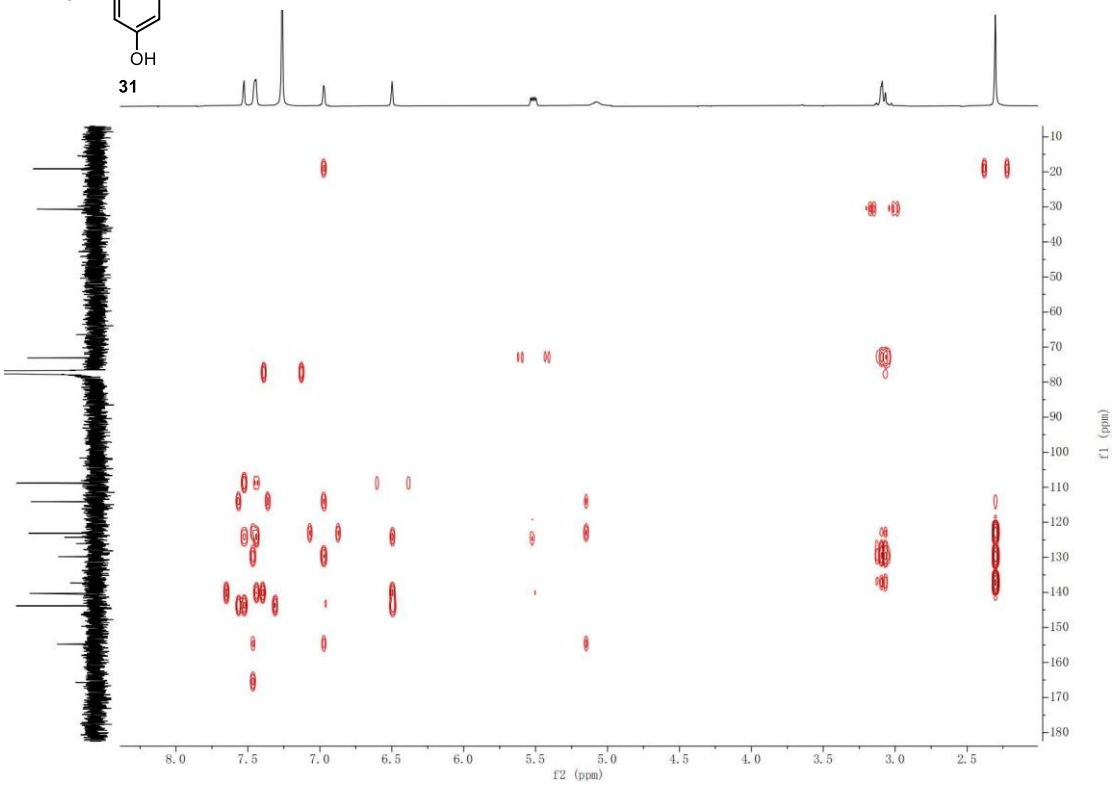
^{1}H-^{1}H COSY spectrum of **31**



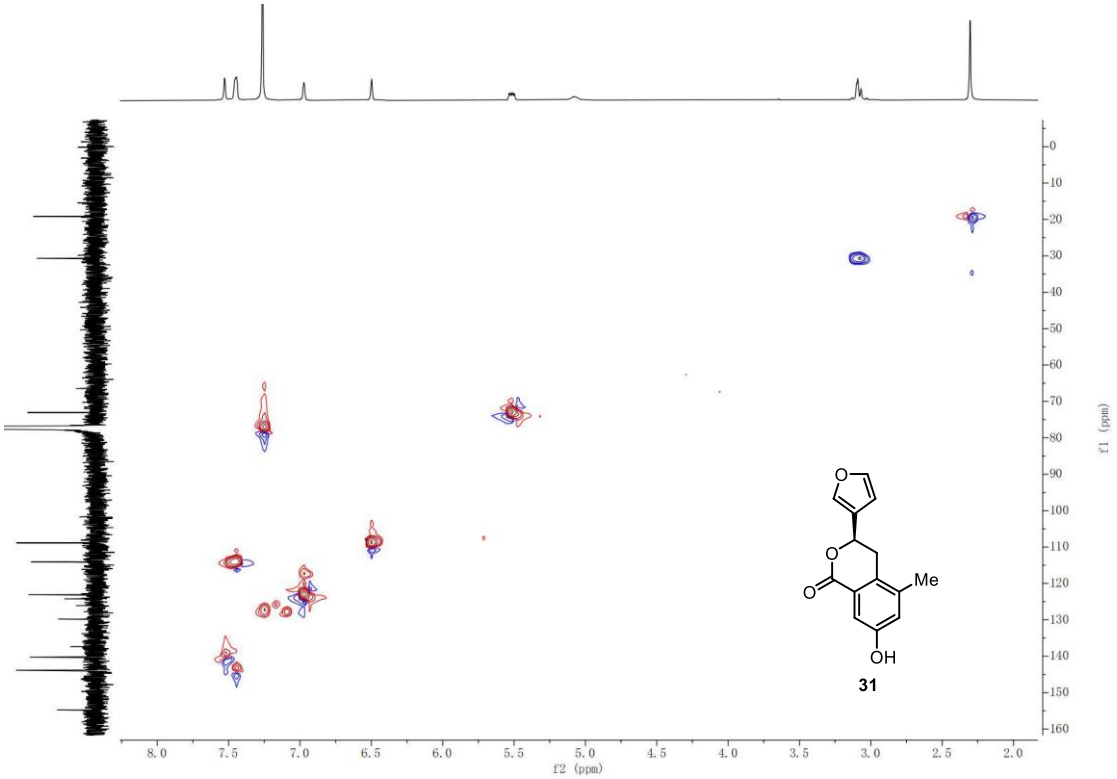


31

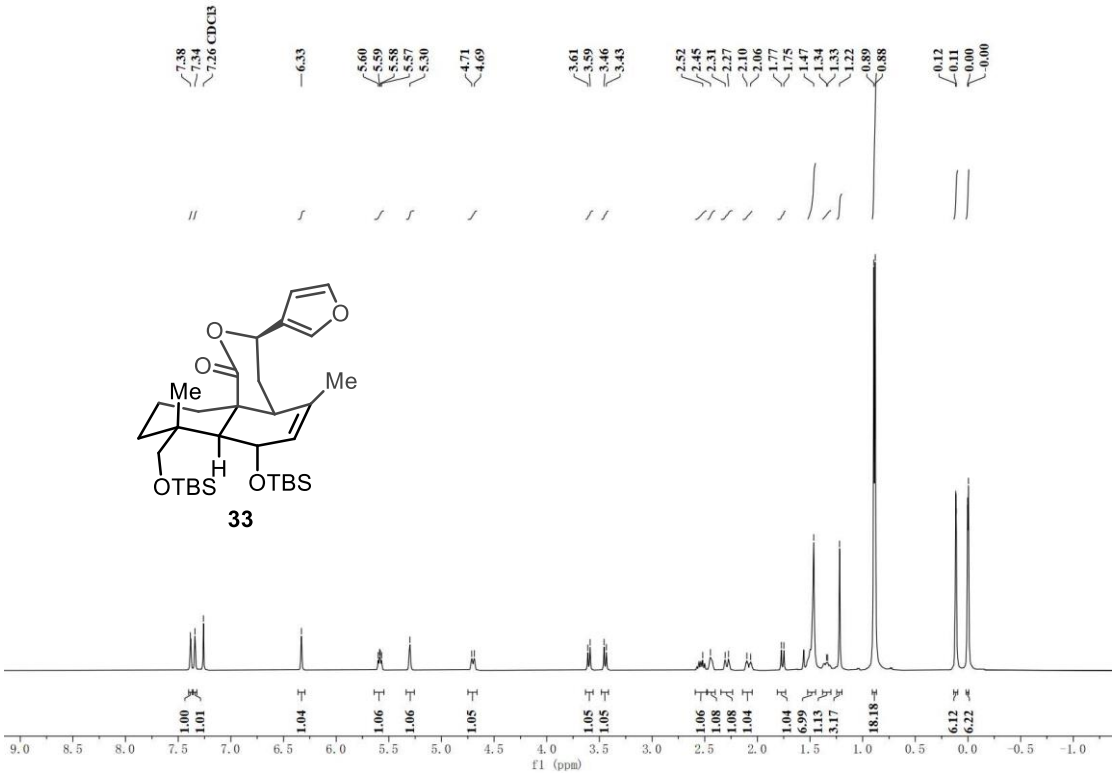
HMBC spectrum of **31**



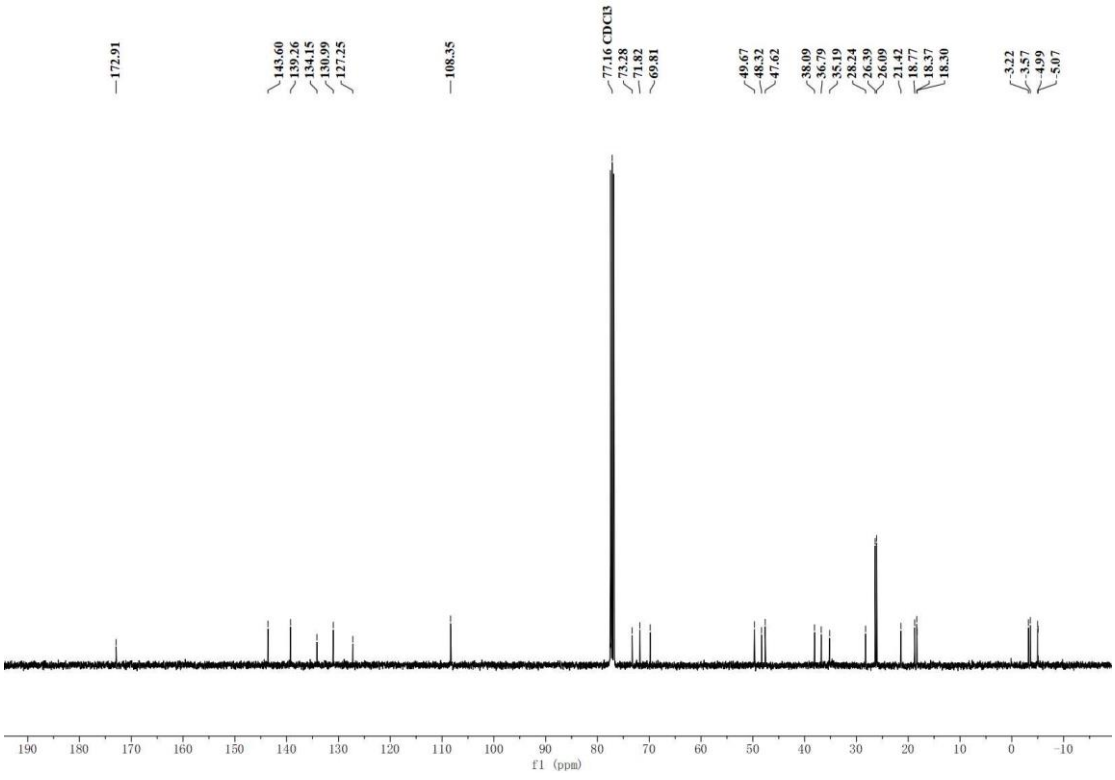
HSQC spectrum of **31**



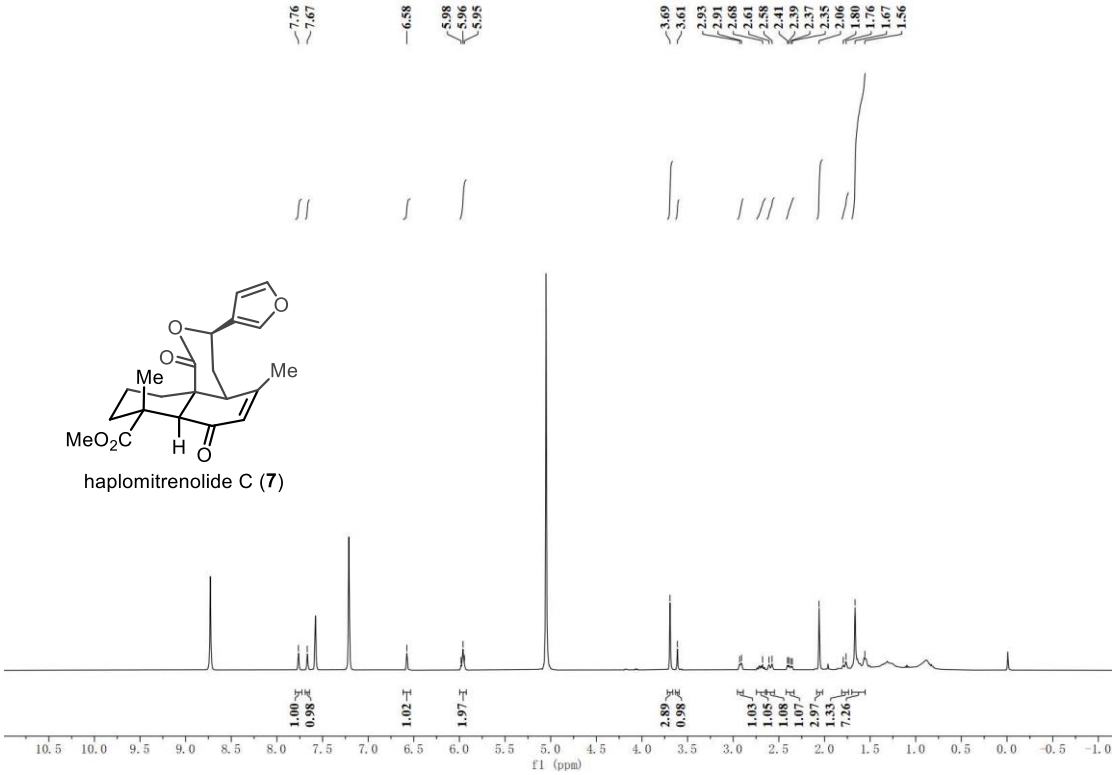
^{1}H NMR spectrum of **33** (400 MHz, $CDCl_3$)



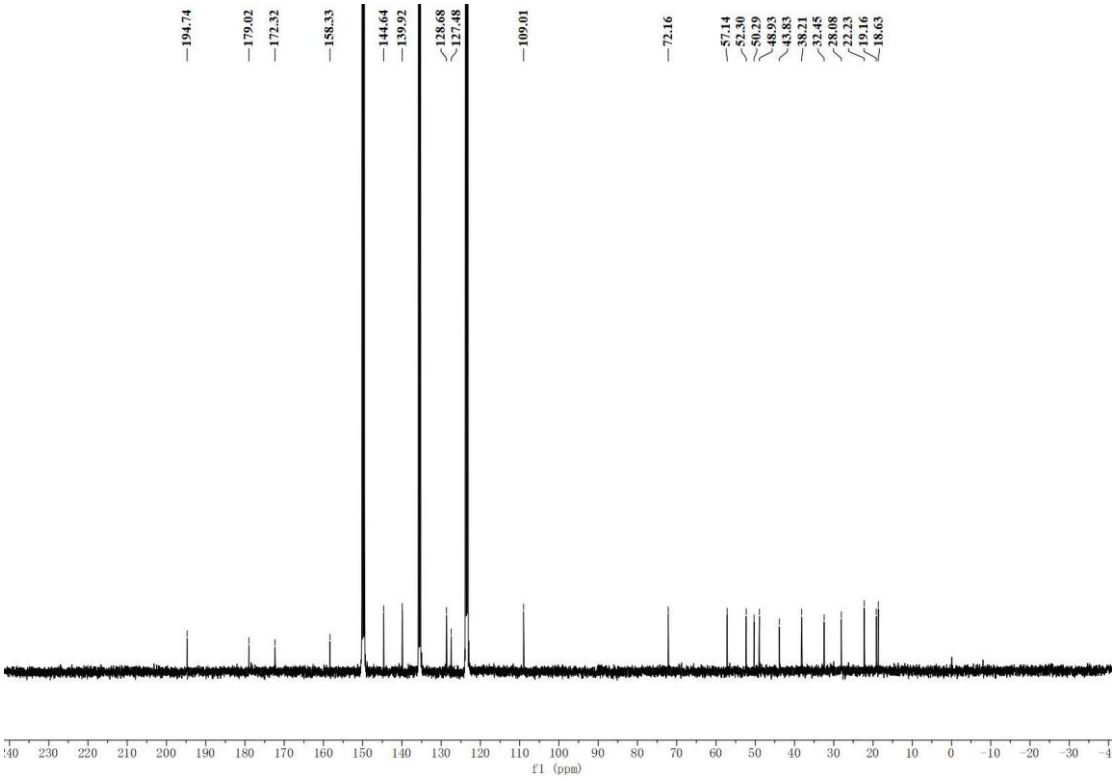
^{13}C NMR spectrum of **33** (100 MHz, $CDCl_3$)



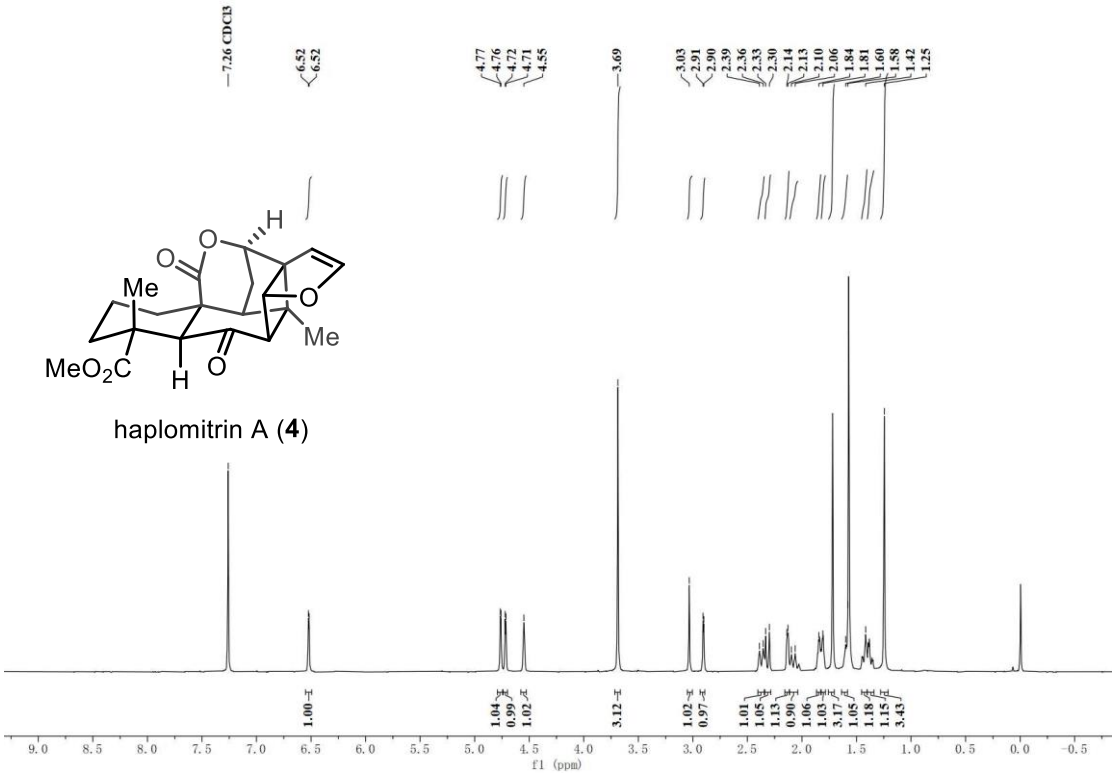
^{1}H NMR spectrum of **7** (400 MHz, C_5D_5N)



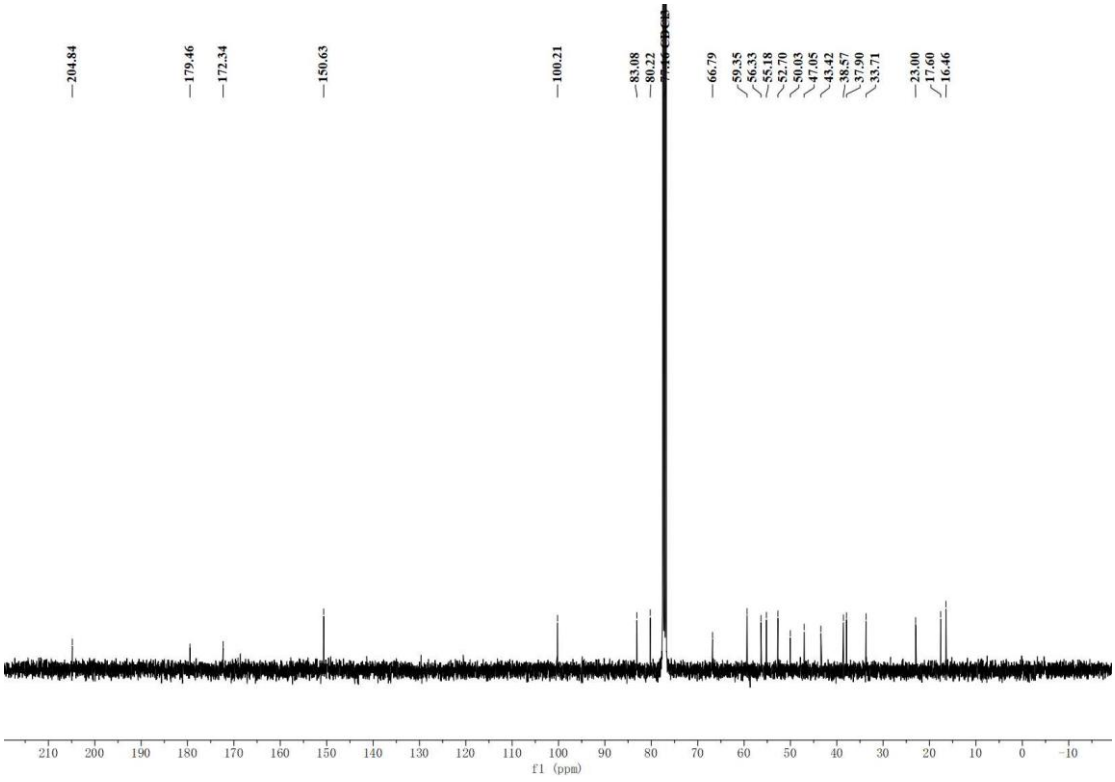
^{13}C NMR spectrum of 20 (100 MHz, C_5D_5N)



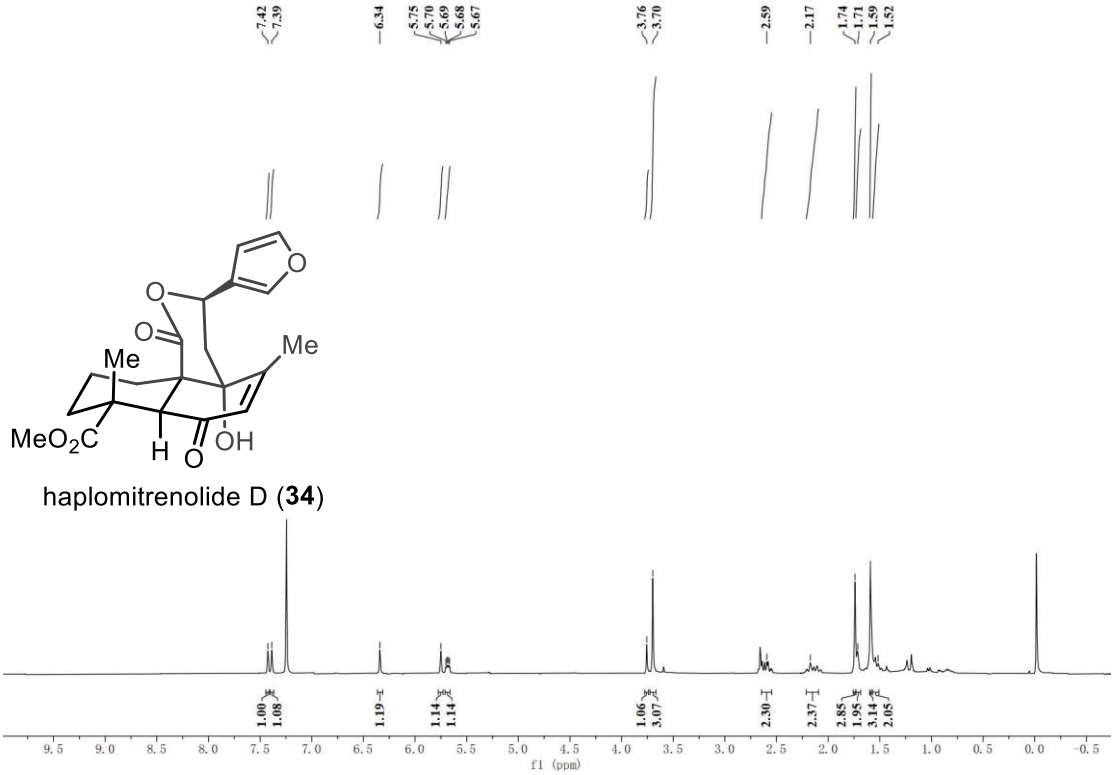
^{1}H NMR spectrum of **4** (400 MHz, $CDCl_3$)



^{13}C NMR spectrum of **4** (100 MHz, $CDCl_3$)

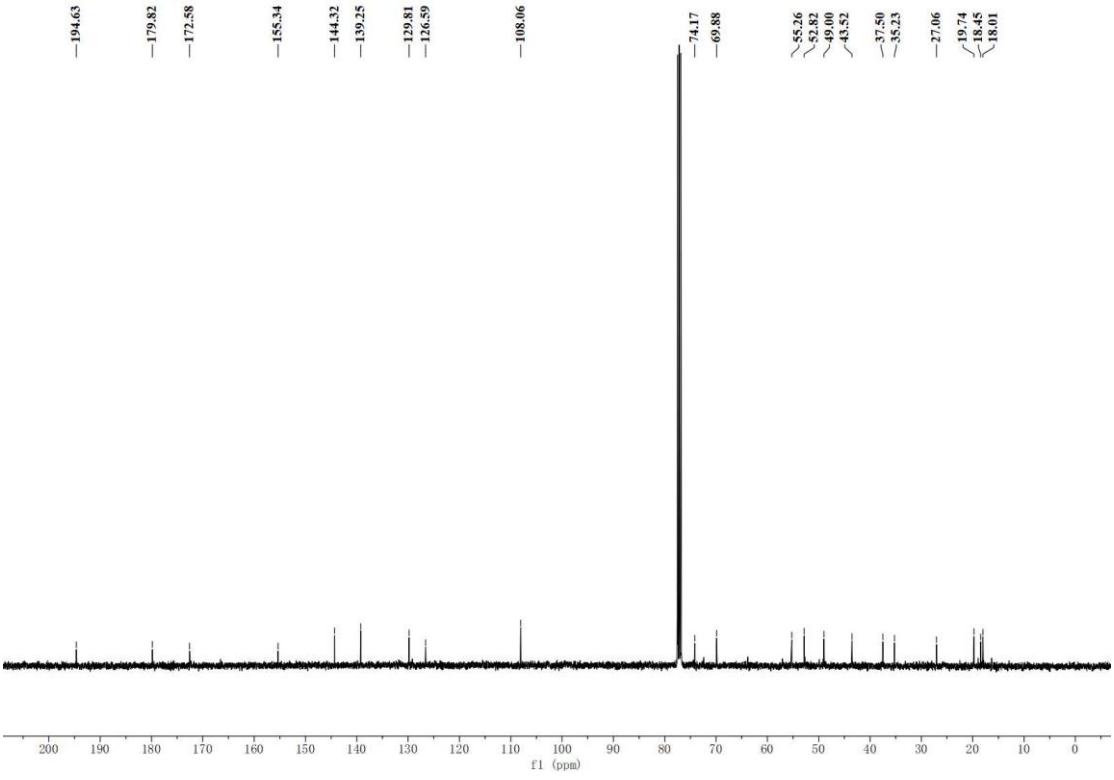


^{1}H NMR spectrum of **34** (400 MHz, $CDCl_3$)

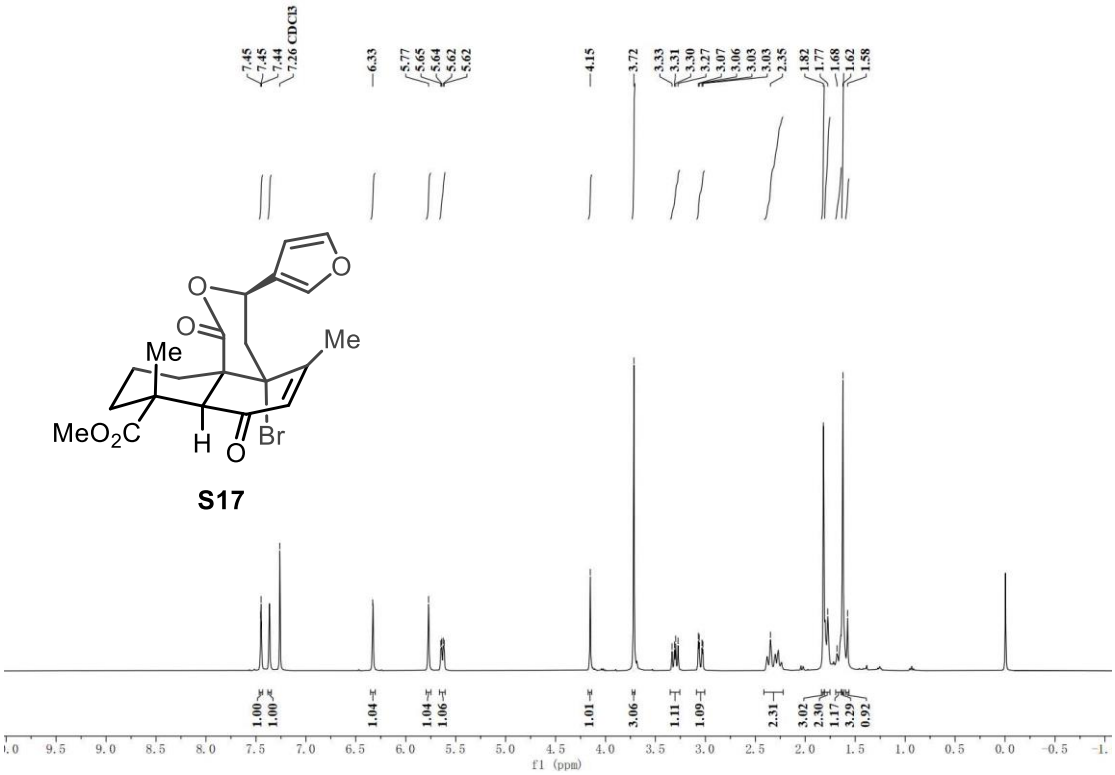


haplomitrenolide D (**34**)

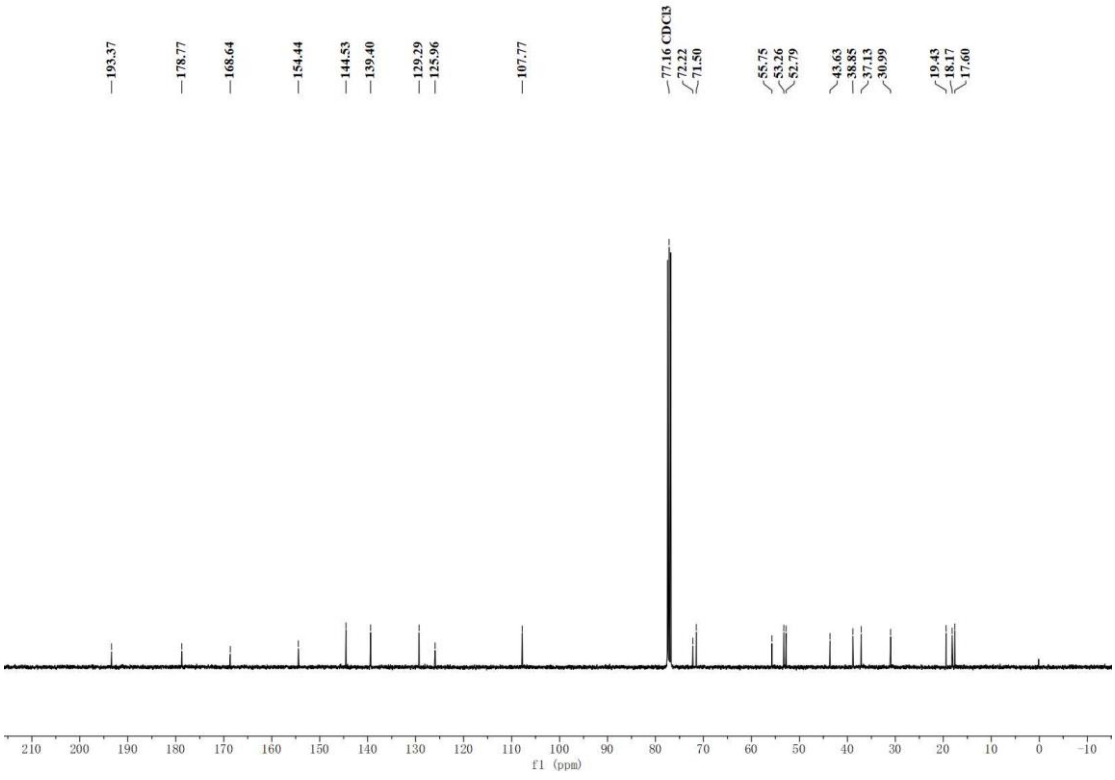
^{13}C NMR spectrum of **34** (100 MHz, $CDCl_3$)



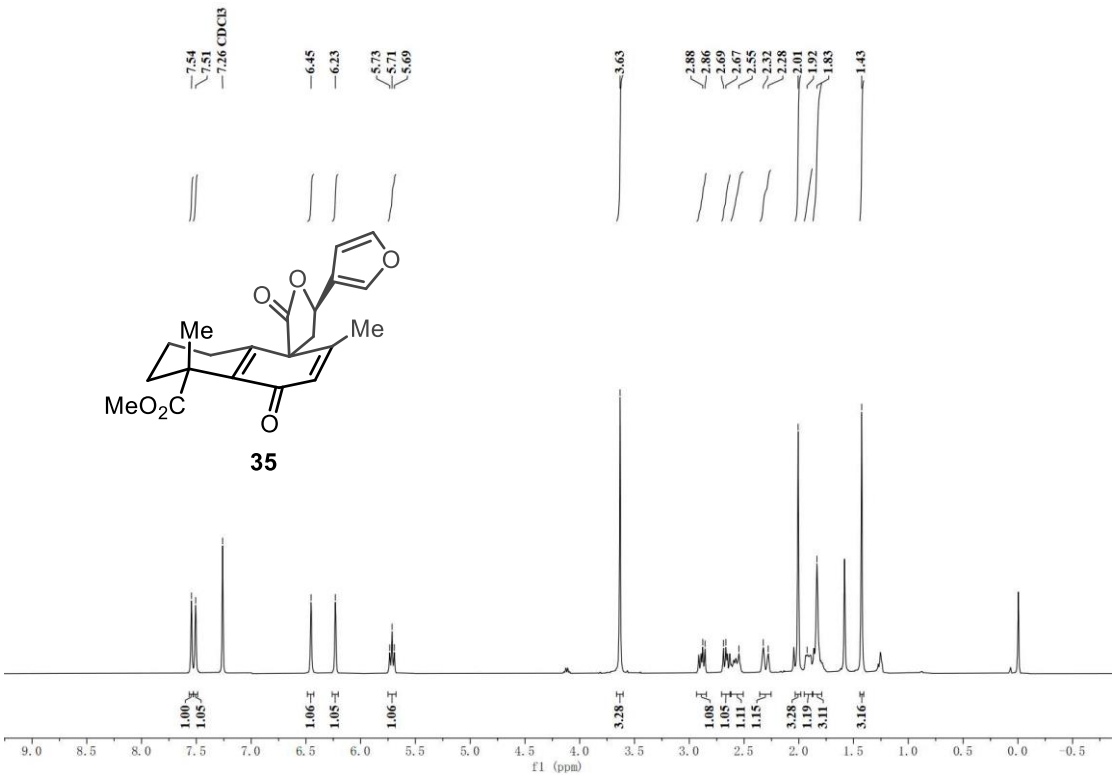
^{1}H NMR spectrum of **S17** (400 MHz, $CDCl_3$)



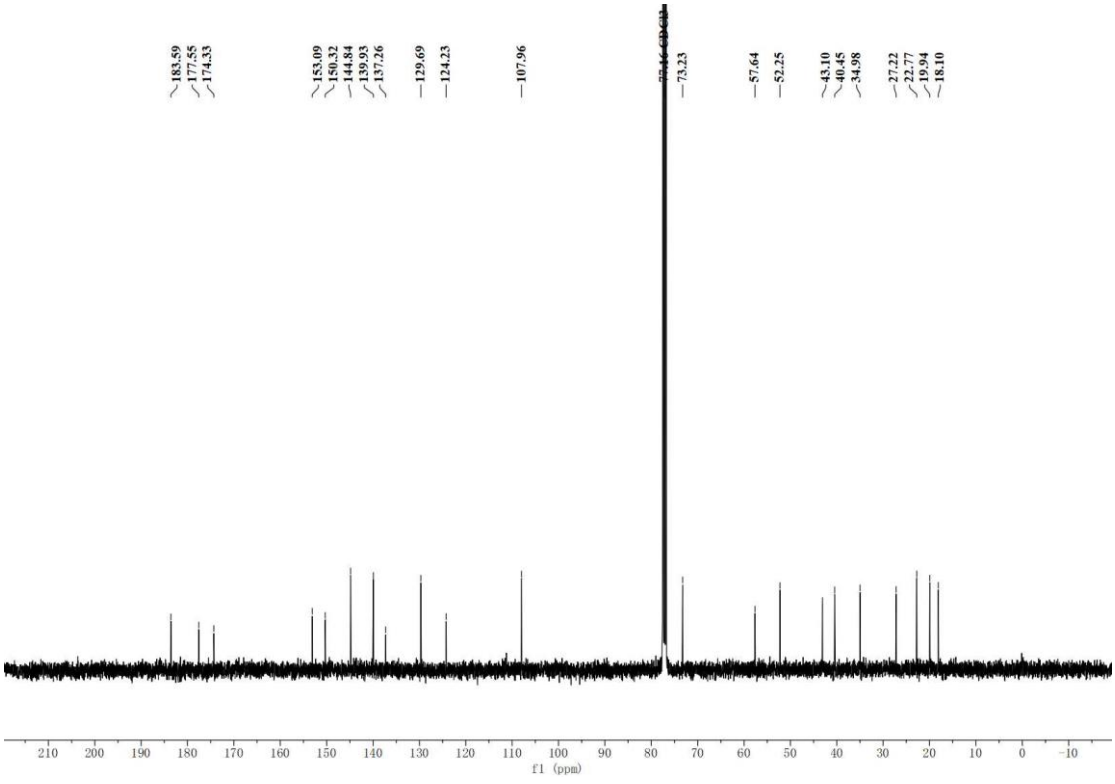
^{13}C NMR spectrum of **S17** (100 MHz, $CDCl_3$)



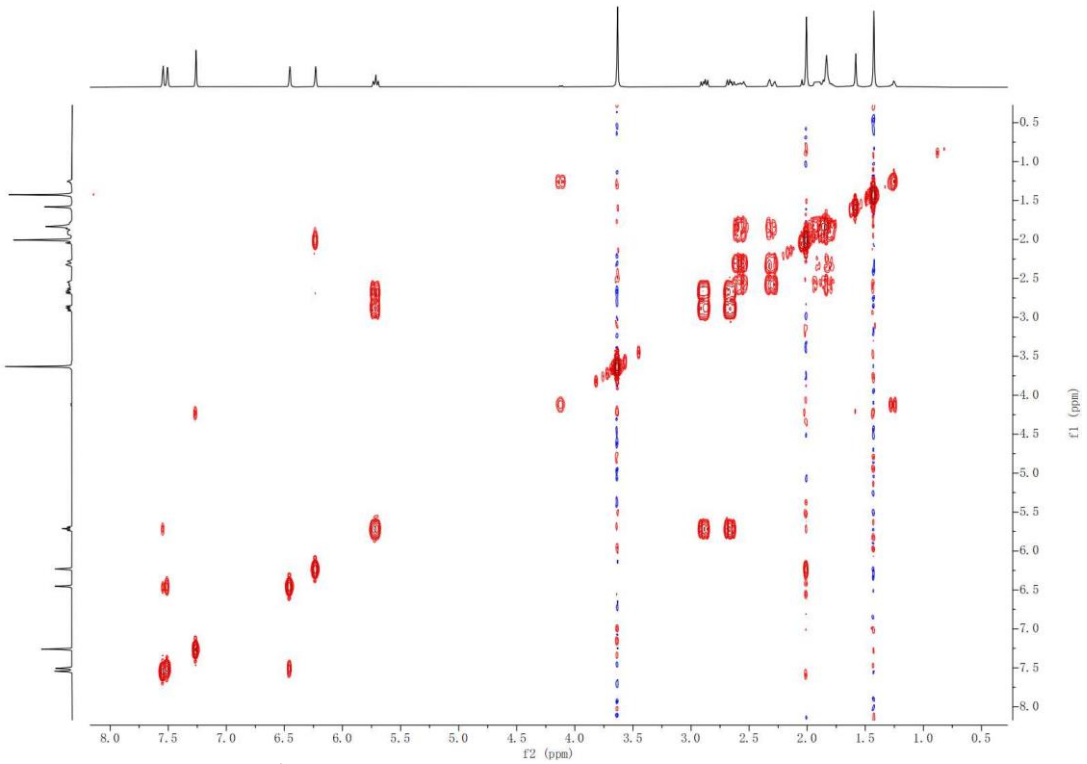
^{1}H NMR spectrum of **35** (400 MHz, $CDCl_3$)

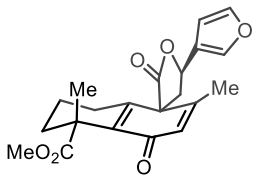


^{13}C NMR spectrum of **35** (100 MHz, $CDCl_3$)



^{1}H-^{1}H COSY spectrum of **35**





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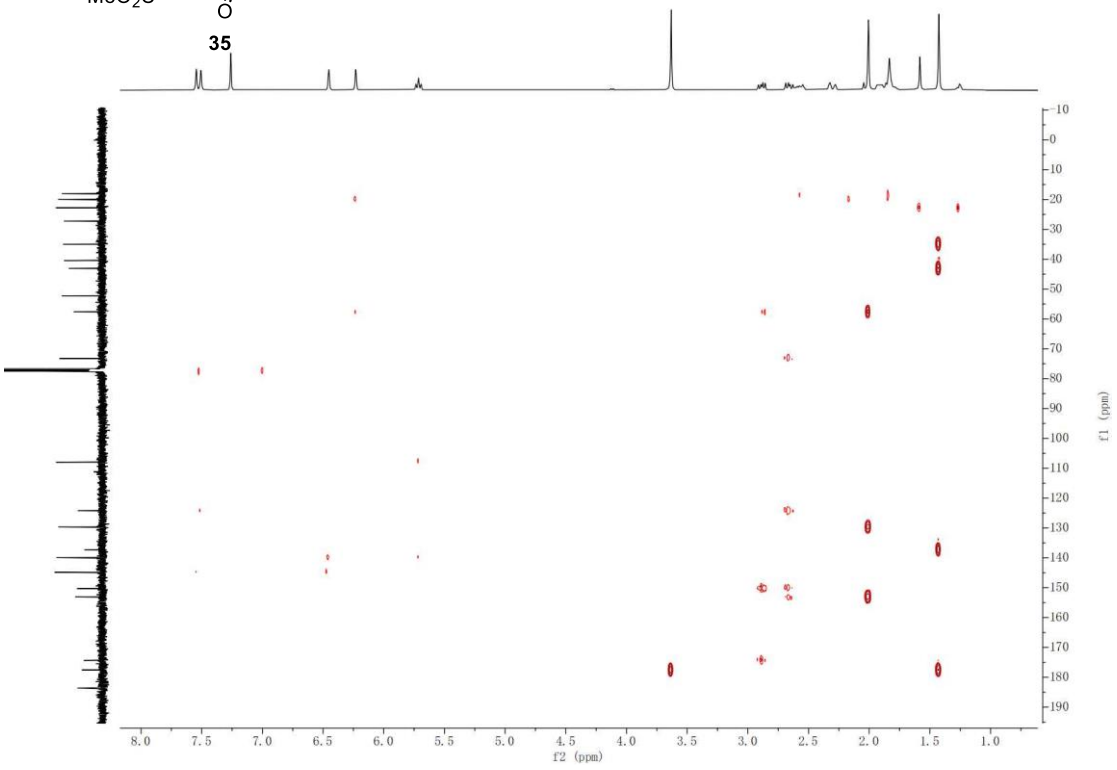
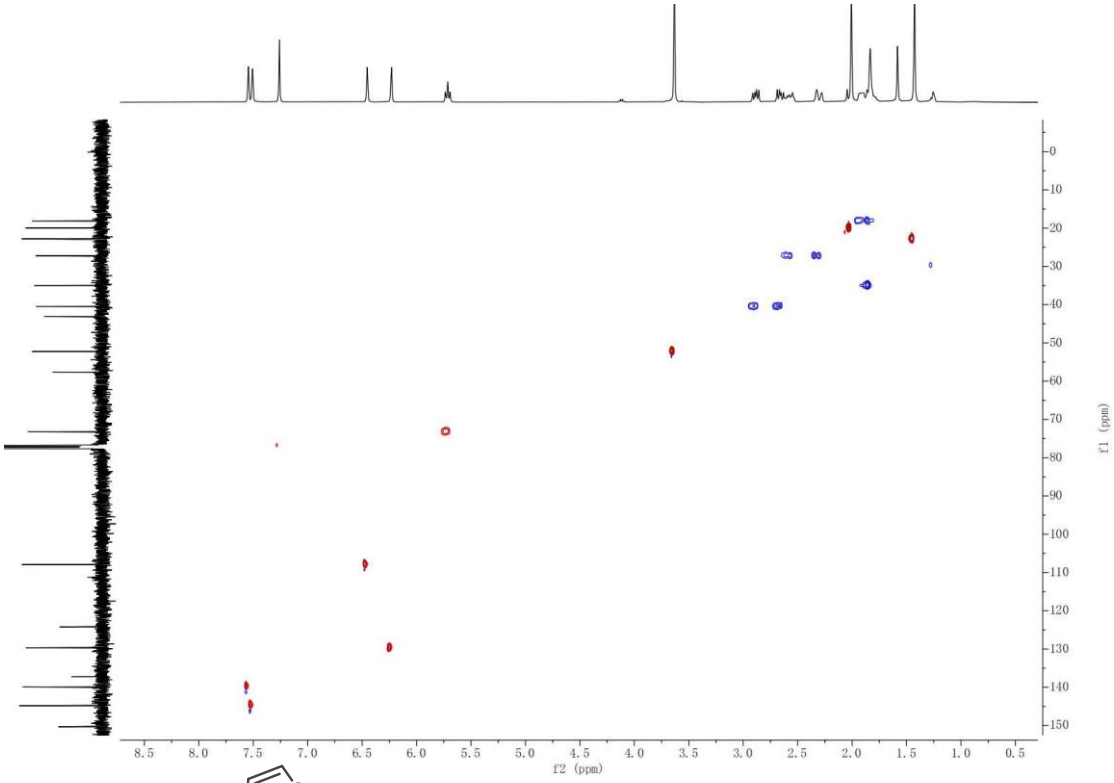
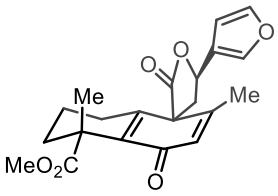
HMBC spectrum of **35**



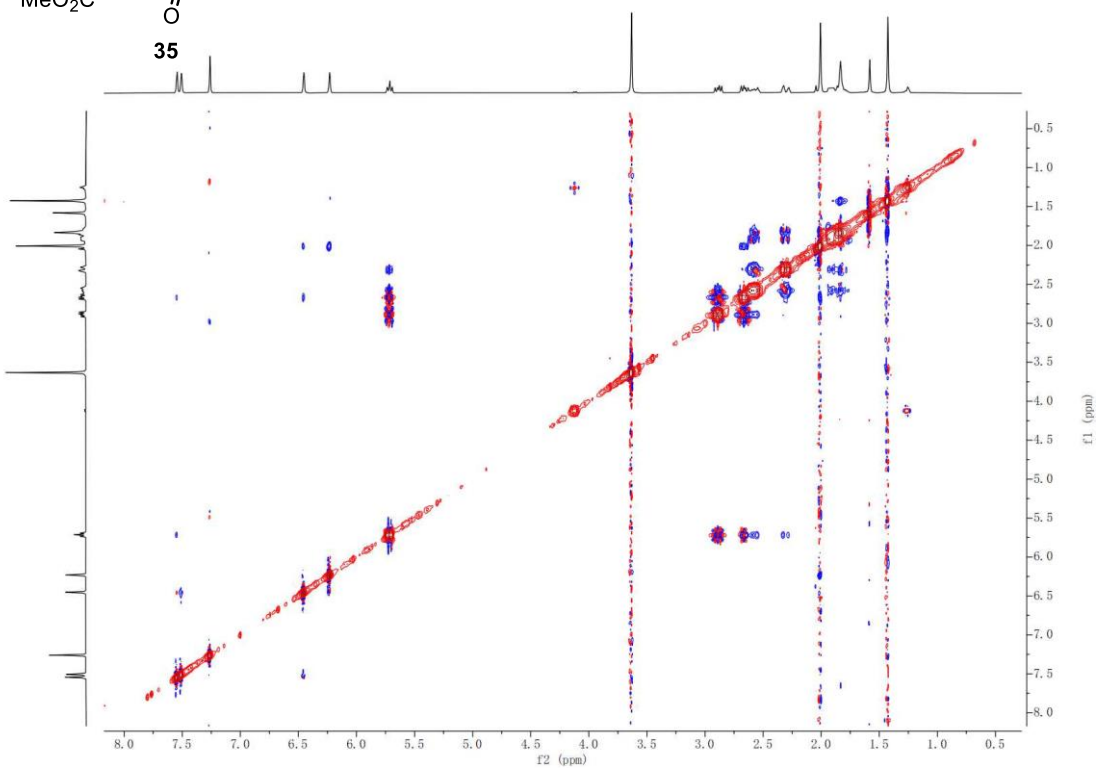
HSQC spectrum of **35**



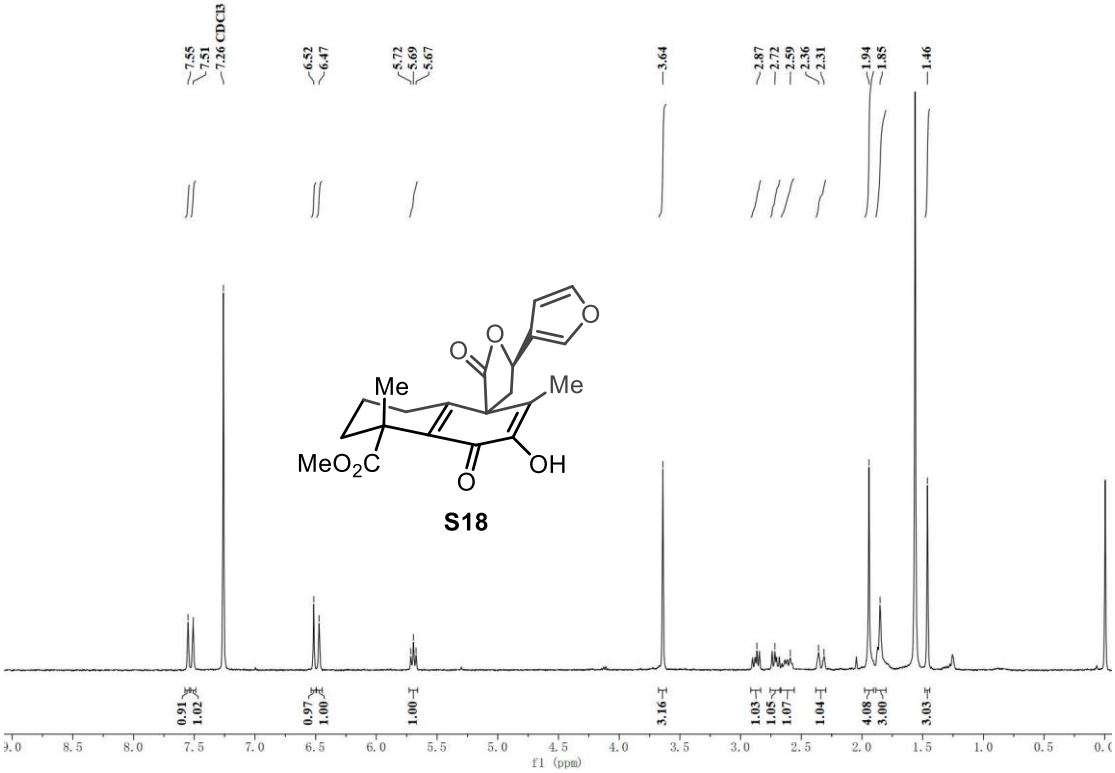


35

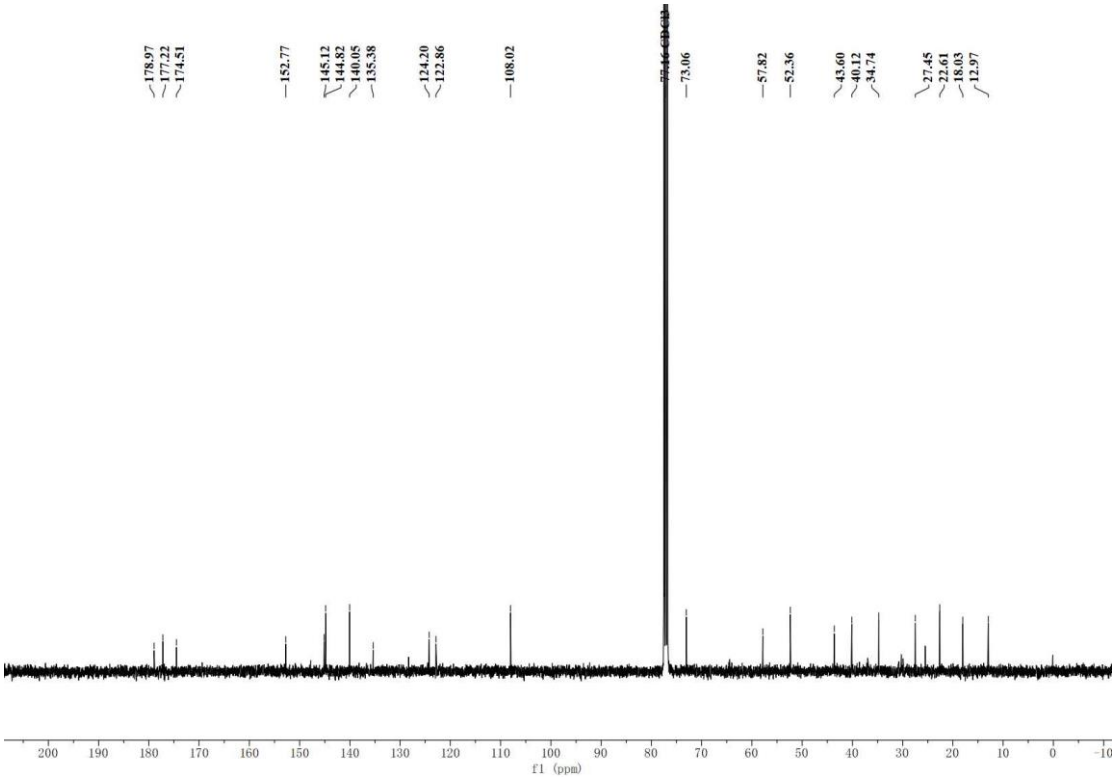
NOESY spectrum of **35**



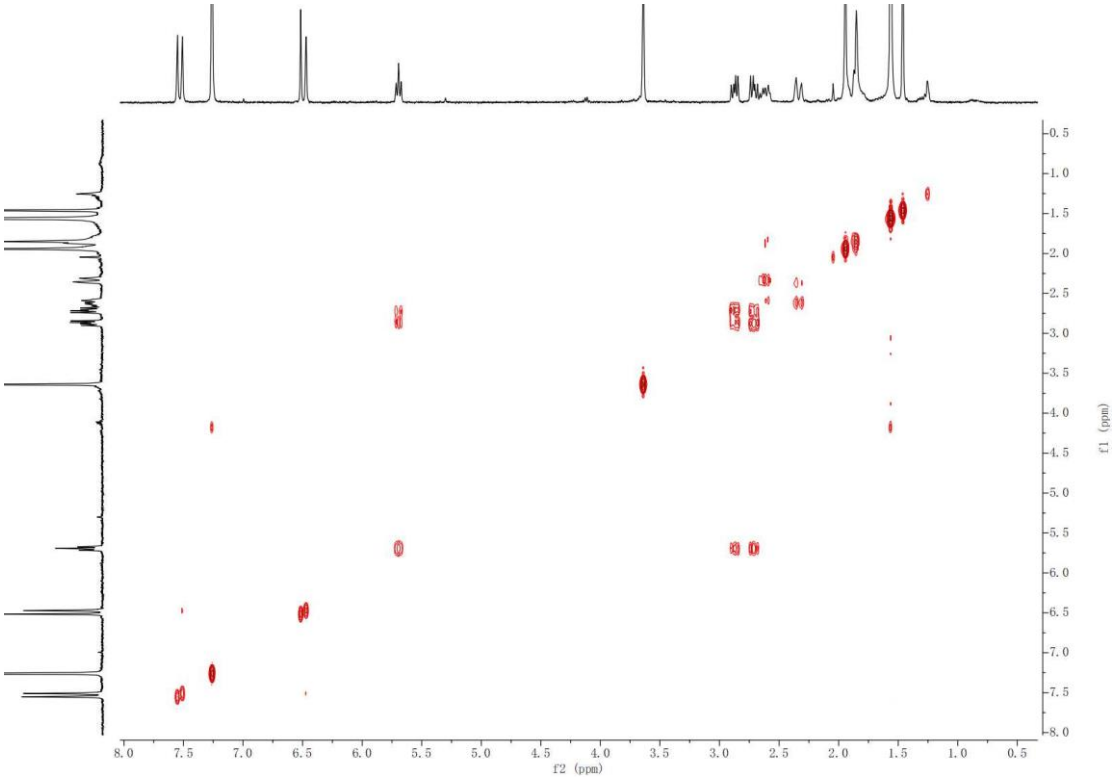
^{1}H NMR spectrum of **S18** (400 MHz, $CDCl_3$)

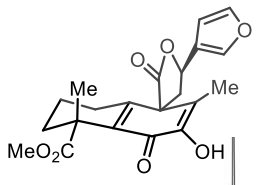


^{13}C NMR spectrum of **S18** (100 MHz, $CDCl_3$)



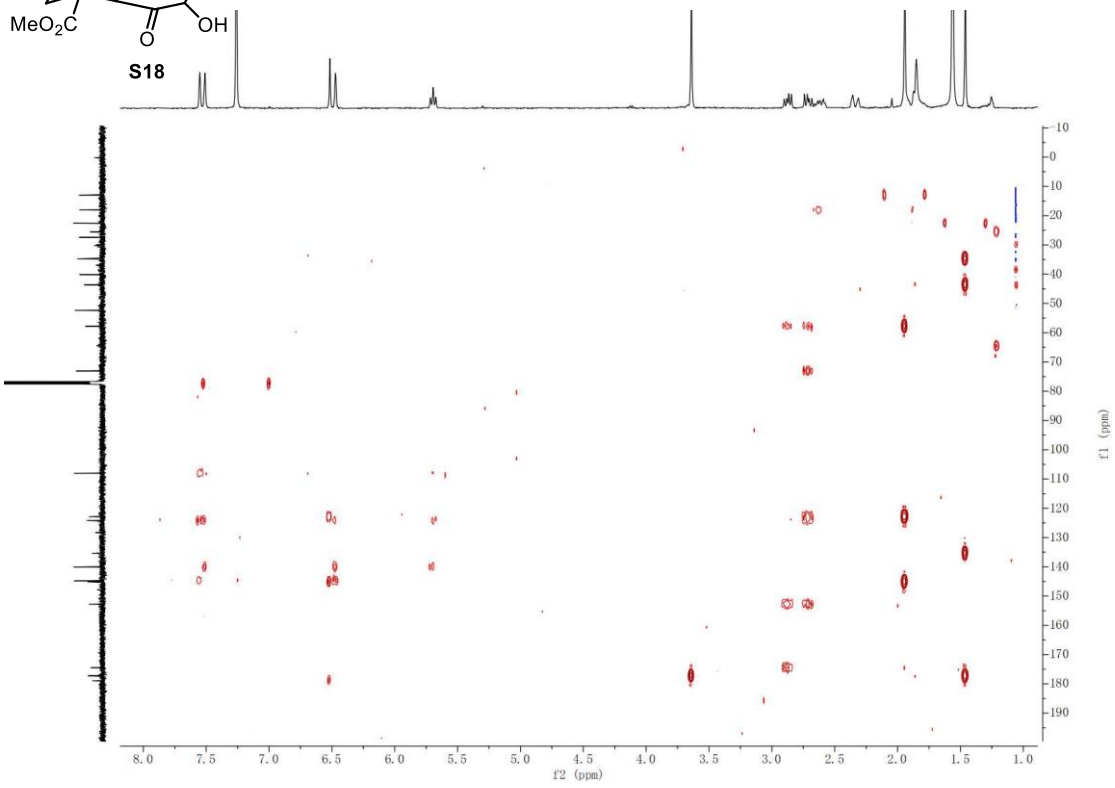
^{1}H-^{1}H COSY spectrum of **S18**



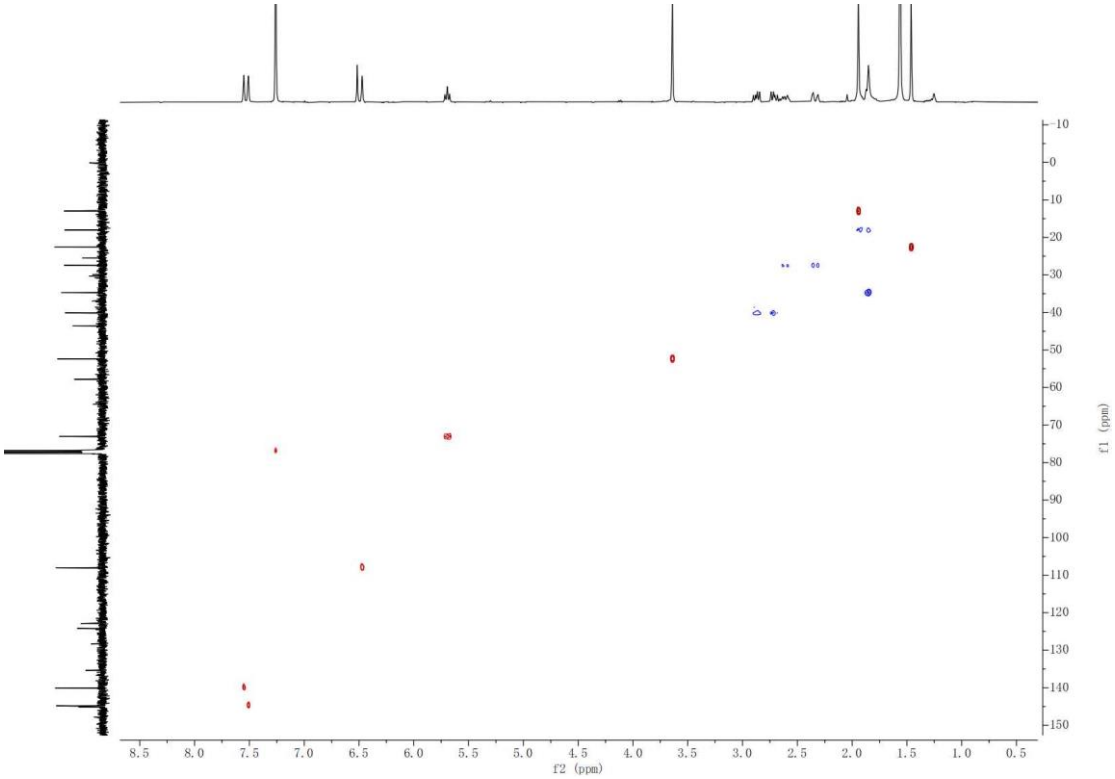


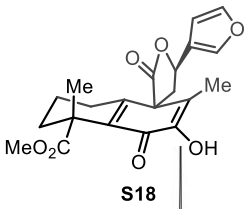
S18

HMBC spectrum of **S18**



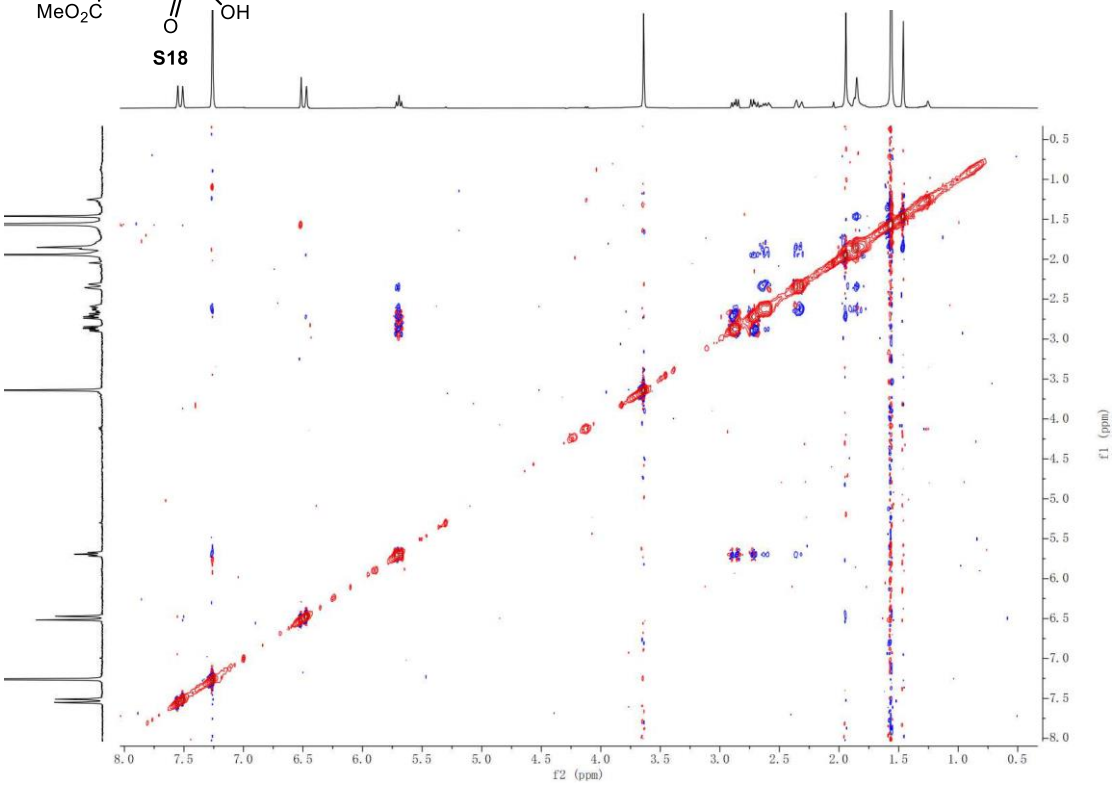
HSQC spectrum of **S18**



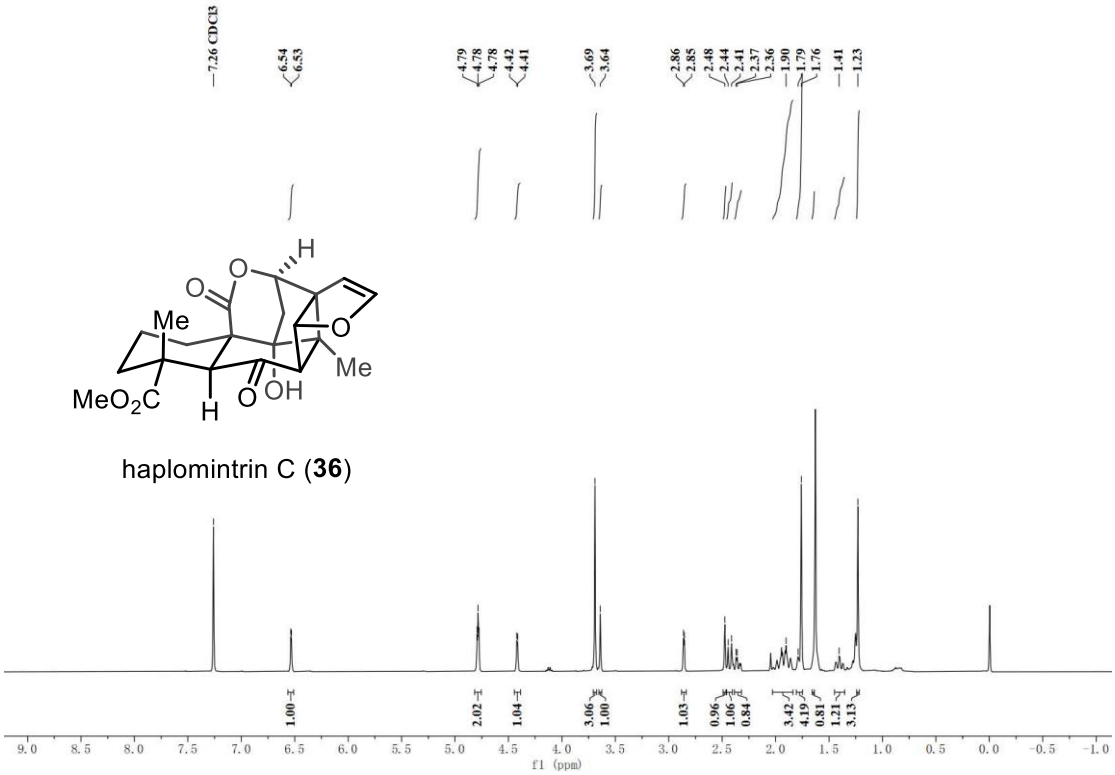


S18

NOESY spectrum of **S18**



^{1}H NMR spectrum of **36** (400 MHz, $CDCl_3$)



haplomintrin C (**36**)

^{13}C NMR spectrum of **36** (100 MHz, $CDCl_3$)