

Electronic Supporting Information

Bioinspired Synthesis of Glycinoeclepin A Enables Chemical Interrogation of Its Plausible Biogenesis

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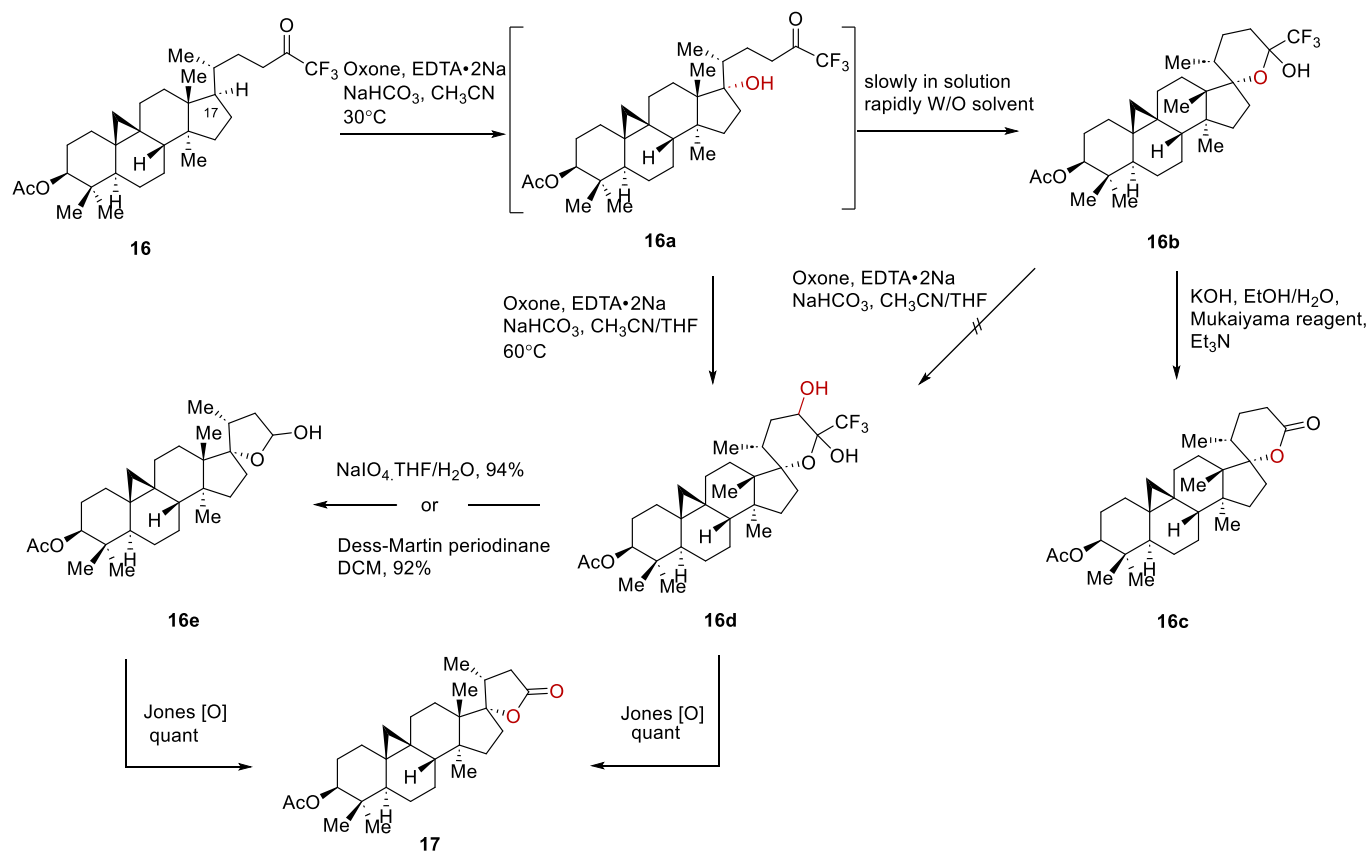
- I Methods**
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I. Methods

All reactions were carried out under a nitrogen atmosphere with dry solvents under anhydrous conditions, unless otherwise noted. Tetrahydrofuran (THF) and 1,4-dioxane were distilled immediately before use from sodium-benzophenoneketyl. Methanol (MeOH) was distilled from magnesium stored under an argon atmosphere. Methylene chloride (CH_2Cl_2), triethylamine (Et_3N) and Pyridine were distilled from calcium hydride and stored under an argon atmosphere. Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. Solvents for chromatography were used as supplied by Titan chemical. Reactions were monitored by thin layer chromatography (TLC) carried out on 0.2 mm Qingdao gel plates (60F-254) using UV light as visualizing agent and aqueous ammonium cerium nitrate/ammonium molybdate or basic aqueous potassium permanganate as developing agent. Huang hai silica gel (60, particle size 0.040–0.063 mm) was used for flash column chromatography.

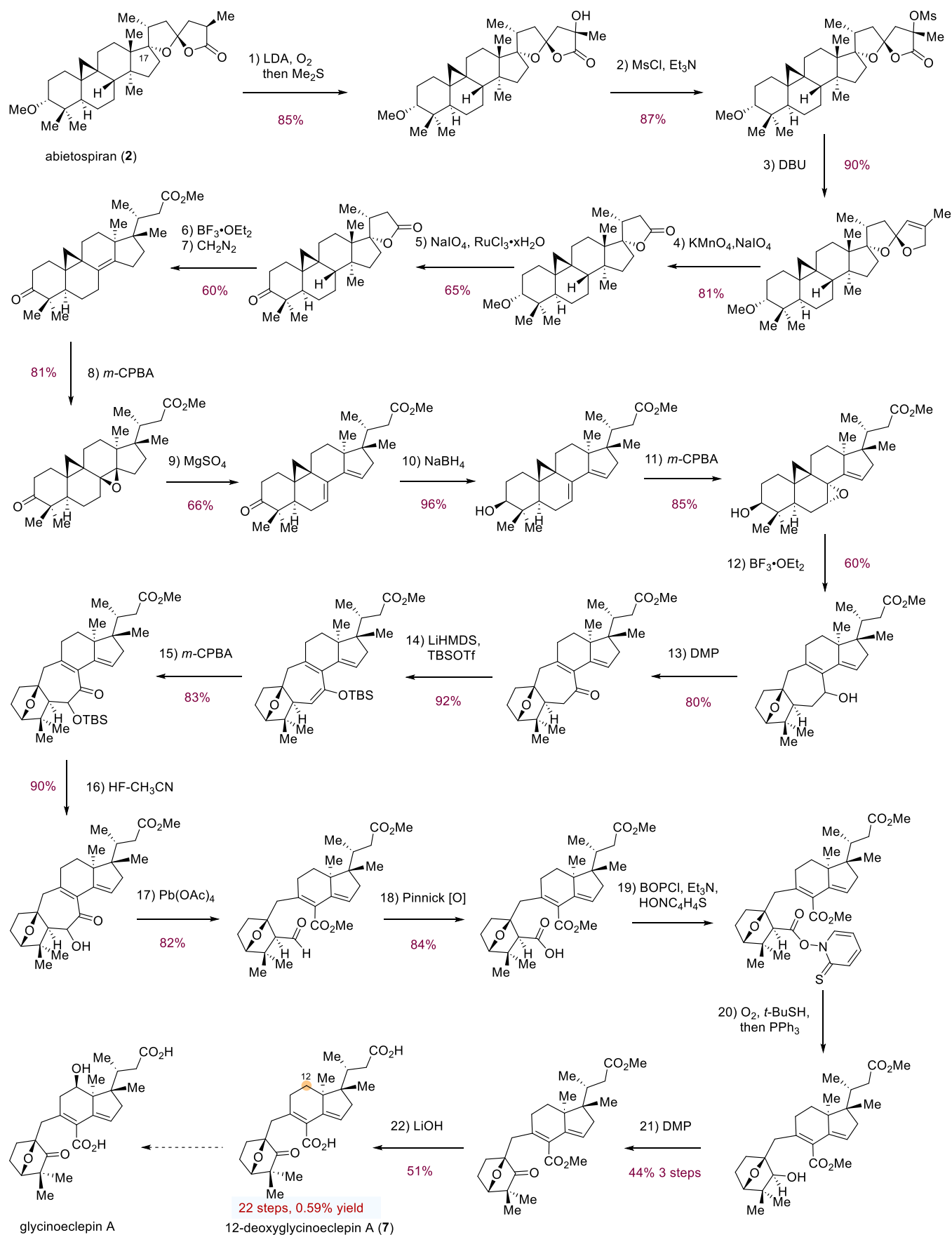
NMR spectra were recorded on Bruker AV III 400 and 800. The spectra were calibrated by using residual undeuterated solvents (for ^1H NMR) and deuterated solvents (for ^{13}C NMR) as internal references: undeuterated chloroform ($\delta_{\text{H}} = 7.26$ ppm) and CDCl_3 ($\delta_{\text{C}} = 77.16$ ppm); undeuterated methanol ($\delta_{\text{H}} = 3.31$ ppm) and methanol- d_4 ($\delta_{\text{C}} = 49.00$ ppm); The following abbreviations are used to designate multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, quint = quintet, br = broad. IR spectra were recorded on a BRUKER Tensor-27 FT-IR spectrometer. Specific Rotation were recorded on Rudolph Autopol V. High-resolution mass spectra (HRMS) were recorded on Agilent G6230 ESI-FT

II. Scheme S1. Control Experiments for decarbonylative C-H oxidation of lactone 17

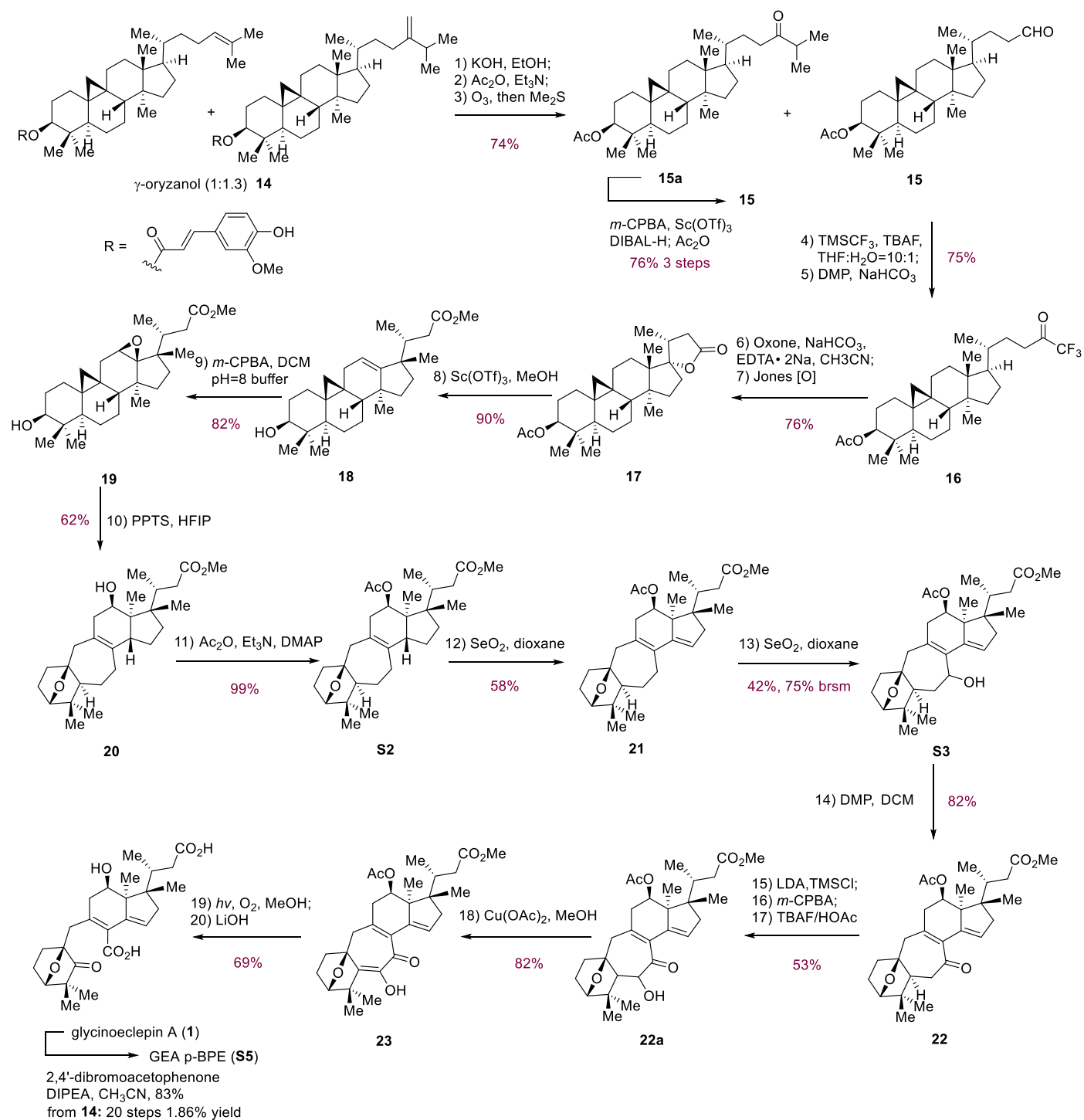


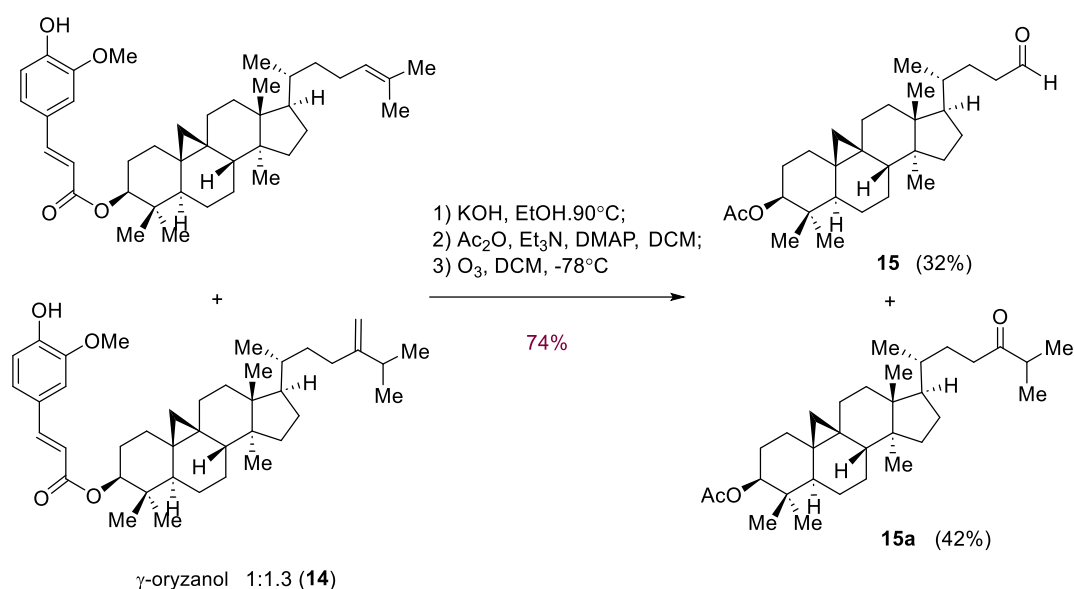
III. Experimental Procedures and Spectroscopic Data of Compound

Scheme S2. Corey's biomimetic Synthesis of 12-deoxyglycinoeclepin A (7)



Scheme S3. Our bioinspired synthesis of glycinoclepin A (1).





To a stirred solution of γ -oryzanol (720 g, 1.19 mol) in EtOH (2.4 L) was added aq KOH (299 mL, 5.97 mol, 20.0 M in H₂O) at 0 °C. The reaction mixture was allowed to stir at 90 °C for 6 h before it was quenched with H₂O (1.0 L), and the mixture was extracted with EtOAc (1.5 L \times 3). The combined extracts were washed with H₂O (1.0 L), brine (1.0 L), and dried over anhydrous Na₂SO₄. The solvent was removed under vacuum to give crude. The residue was purified by flash column chromatography (silica gel, PE : EtOAc = 5 : 1) to give white solid (453 g, 89%).

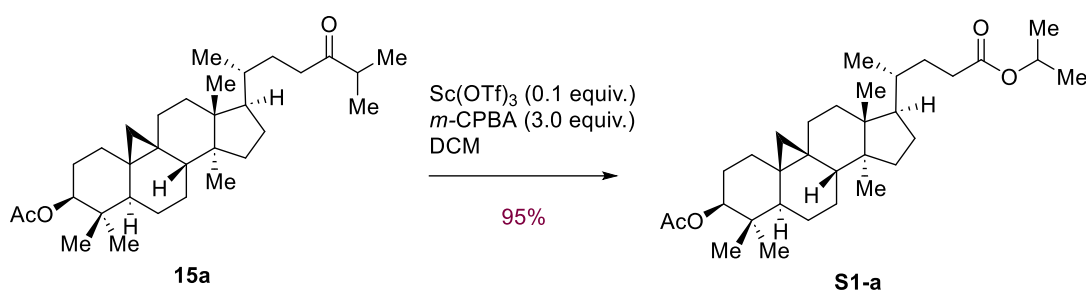
To a stirred solution of the above white solid (450 g, 1.05 mol) in DCM (1.05 L) were sequentially added DMAP (6.4 g, 52.7 mmol) Et₃N (293 mL, 2.1 mol), and Ac₂O (149.5 mL, 1.58 mol) at 0 °C. The reaction mixture was allowed to stir at 25 °C for 1 h before it was quenched with MeOH (22 mL). The solvent was evaporated under vacuum to give crude and was used for the next step without further purification.

To a stirred solution of the above crude (200 g) in DCM (2.9 L) and MeOH (1.4 L) was cooled to -78 °C. Ozone was then bubbled through the solution at -78 °C until material consumption. After the excess ozone was removed by passing a stream of Ar through the mixture for 10 min, excess dimethyl sulfide (157 mL, 2.13 mol) was added, and the cooling bath was removed. After the mixture was stirred for overnight at 25 °C, the solvent was evaporated under vacuum. The residue was purified by flash column chromatography (silica gel, PE : EtOAc = 50 : 1 \rightarrow 20 : 1) to give **15** (61 g, 32%) and **15a** (87 g, 42 %).

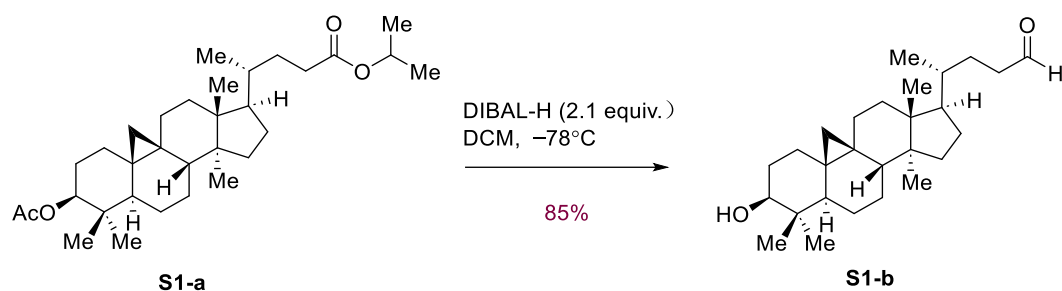
15: white solid, R_f = 0.4 (silica, PE : EtOAc = 10 : 1); $[\alpha]_D^{22}$ = +8.0 (c = 0.1 in CHCl₃); IR (film): ν_{\max} = 2962, 2868, 1731, 1469, 1372, 1247, 1049, 1027, 979 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ = 9.77 (s, 1H), 4.56 (dd, J = 10.7, 5.0 Hz, 1H), 2.54 – 2.43 (m, 1H), 2.41 – 2.32 (m, 1H), 2.05 (s, 3H), 2.01 – 1.90 (m, 2H), 1.86 – 1.76 (m, 2H), 1.61 (t, J = 7.6 Hz, 5H), 1.50 (s, 1H), 1.39 (dd, J = 12.3, 4.4 Hz, 3H), 1.31 (q, J = 4.4, 2.9 Hz, 4H), 1.15 – 1.06 (m, 3H), 0.96 (s, 3H), 0.90 (s, 3H), 0.89 (s, 5H), 0.87 (s, 2H), 0.85 (s, 3H), 0.80 (dd, J = 12.5, 2.6 Hz, 1H), 0.58 (d, J = 4.2 Hz, 1H), 0.34 (d, J = 4.2 Hz, 1H) ppm; ¹³C NMR (101 MHz, CDCl₃): δ = 203.22, 171.02, 80.72, 52.23, 48.93, 47.90, 47.25, 45.44, 41.25, 39.54, 35.77, 35.57, 32.94, 31.71, 29.85, 28.35, 28.19, 26.90, 26.54, 26.07, 25.90, 25.52, 21.44, 21.01, 20.18, 19.39, 18.12, 15.25 ppm. HRMS (m/z): [M+Na]⁺ calcd

for $C_{29}H_{46}O_3Na^+$ 465.3339 found 465.3340.

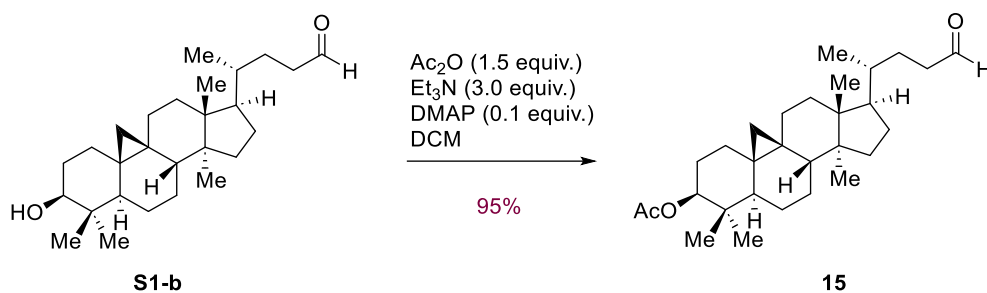
15a: white solid, $R_f = 0.5$ (silica, PE : EtOAc = 10 : 1); $[\alpha]_D^{22} = +12.0$ ($c = 0.1$ in $CHCl_3$); IR (film): $\nu_{max} = 2966, 2869, 1733, 1713, 1468, 1373, 1245, 1026\text{ cm}^{-1}$; 1H NMR (400 MHz, $CDCl_3$): $\delta = 4.62 - 4.43$ (m, 1H), 2.61 (p, $J = 6.9$ Hz, 1H), 2.46 (dd, $J = 10.3, 5.4$ Hz, 1H), 2.37 (td, $J = 10.0, 4.9$ Hz, 1H), 2.04 (s, 3H), 2.01 – 1.89 (m, 2H), 1.81 – 1.71 (m, 2H), 1.64 – 1.47 (m, 8H), 1.43 – 1.22 (m, 8H), 1.09 (s, 3H), 1.08 (s, 3H), 0.95 (s, 3H), 0.89 (d, $J = 3.8$ Hz, 6H), 0.86 (s, 3H), 0.84 (s, 4H), 0.79 (dd, $J = 12.5, 2.5$ Hz, 1H), 0.57 (d, $J = 4.2$ Hz, 1H), 0.33 (d, $J = 4.2$ Hz, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): $\delta = 215.49, 171.05, 80.77, 52.35, 48.94, 47.93, 47.29, 45.43, 40.94, 39.57, 37.64, 35.86, 35.62, 32.98, 31.73, 30.25, 29.88, 28.17, 26.93, 26.60, 26.09, 25.93, 25.55, 21.46, 21.04, 20.23, 19.42, 18.52, 18.44, 18.24, 18.13, 15.27$ ppm; HRMS (m/z): $[M+Na]^+$ calcd for $C_{32}H_{52}O_3Na^+$ 507.3809 found 507.3812.



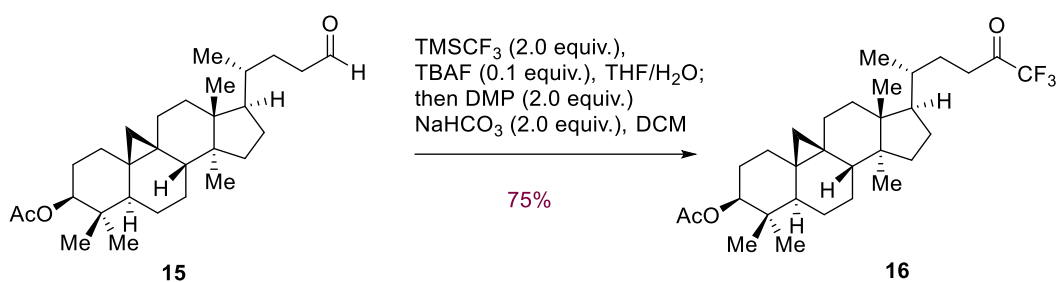
To a stirred solution of **15a** (110 g, 227 mmol) in DCM (227 mL) were sequentially added $Sc(OTf)_3$ (11.2 g, 22.7 mol) and *m*-CPBA (117.5 g, 680.7 mmol) at 0 °C. The reaction mixture was stirred at 25 °C for 24 h. The resultant mixture was quenched with saturated aq. $Na_2S_2O_3$ (500 mL) and extracted with EtOAc (500 mL \times 3). The combined organic phases were washed with saturated aq. $NaHCO_3$ (300 mL) and brine (300 mL), dried over anhydrous Na_2SO_4 . The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 20 : 1) to give **S1-a** (107.9 g, 95%) as a white solid; **S1-a**: $R_f = 0.5$ (silica, PE : EtOAc = 10 : 1); $[\alpha]_D^{21} = +30.0$ ($c = 0.2$ in $CHCl_3$); IR (film): $\nu_{max} = 2967, 2869, 1796, 1772, 1470, 1373, 1246, 1174, 1110\text{ cm}^{-1}$; 1H NMR (400 MHz, $CDCl_3$): $\delta = 5.05 - 4.95$ (m, 1H), 4.56 (dd, $J = 10.5, 5.0$ Hz, 1H), 2.37 – 2.29 (m, 1H), 2.23 – 2.16 (m, 1H), 2.05 (s, 3H), 2.03 – 1.90 (m, 3H), 1.86 – 1.73 (m, 2H), 1.63 – 1.54 (m, 7H), 1.51 (dd, $J = 12.1, 4.8$ Hz, 1H), 1.39 (dd, $J = 12.2, 4.3$ Hz, 1H), 1.35 – 1.25 (m, 8H), 1.23 (s, 3H), 1.22 (s, 3H), 1.16 (d, $J = 7.1$, 1H), 1.15 – 1.06 (m, 2H), 0.95 (s, 3H), 0.89 (s, 3H), 0.87 (d, $J = 6.2$, 1H), 0.86 (s, 1H), 0.85 (s, 3H), 0.79 (dd, $J = 12.6, 2.6$ Hz, 1H), 0.57 (d, $J = 4.2$ Hz, 1H), 0.34 (d, $J = 4.2$ Hz, 1H) ppm; ^{13}C NMR (101 MHz, $CDCl_3$): $\delta = 173.93, 171.06, 80.77, 67.43, 52.22, 48.94, 47.94, 47.28, 45.45, 39.57, 35.76, 35.62, 32.97, 32.00, 31.73, 31.42, 29.88, 28.14, 26.93, 26.59, 26.09, 25.93, 25.55, 22.01, 22.00, 21.47, 21.04, 20.23, 19.42, 18.12, 18.04, 15.27$ ppm; HRMS (m/z): $[M+Na]^+$ calcd for $C_{32}H_{52}O_4Na^+$ 523.3758 found 523.3760.



To a stirred solution of **S1-a** (100 g, 199.7 mmol) in DCM (998 mL) were sequentially added DIBAL-H (419 mL, 419 mmol, 1.0 M in hexane) at -78°C . The reaction mixture was stirred at -78°C for 30 min. The resultant mixture was quenched with saturated aq. potassium sodium tartrate (500 mL) and extracted with EtOAc (500 mL \times 3). The combined organic phases were washed with saturated aq. NaHCO_3 (300 mL) and brine (300 mL), dried over anhydrous Na_2SO_4 . The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 8 : 1) to give **S1-b** (68 g, 85%) as a white solid; **S1-b**: $R_f = 0.4$ (silica, PE : EtOAc = 5 : 1); $[\alpha]_D^{21} = +35$ ($c = 0.2$ in CHCl_3); IR (film): $\nu_{\text{max}} = 3420, 2933, 2867, 1722, 1455, 1376, 1337, 1097, 936 \text{ cm}^{-1}$; $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 9.77$ (t, $J = 1.9$ Hz, 1H), 3.28 (s, 1H), 2.52 – 2.44 (m, 1H), 2.41 – 2.32 (m, 1H), 2.05 – 1.69 (m, 5H), 1.64 – 1.56 (m, 6H), 1.50 (dd, $J = 12.3, 4.7$ Hz, 1H), 1.47 – 1.40 (m, 1H), 1.36 – 1.21 (m, 8H), 1.15 – 1.02 (m, 2H), 0.97 (s, 6H), 0.90 (s, 3H), 0.88 (d, $J = 6.4$ Hz, 3H), 0.81 (s, 3H), 0.55 (d, $J = 4.2$ Hz, 1H), 0.33 (d, $J = 4.2$ Hz, 1H) ppm; $^{13}\text{C NMR}$ (101 MHz, CDCl_3): $\delta = 203.35, 78.93, 52.29, 48.95, 48.10, 47.22, 45.48, 41.29, 40.61, 35.80, 35.65, 33.01, 32.10, 30.51, 30.01, 28.38, 28.23, 26.54, 26.21, 26.14, 25.57, 21.24, 20.06, 19.45, 18.20, 18.14, 14.14$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{27}\text{H}_{44}\text{O}_2\text{Na}^+$ 423.3234 found 423.3235.

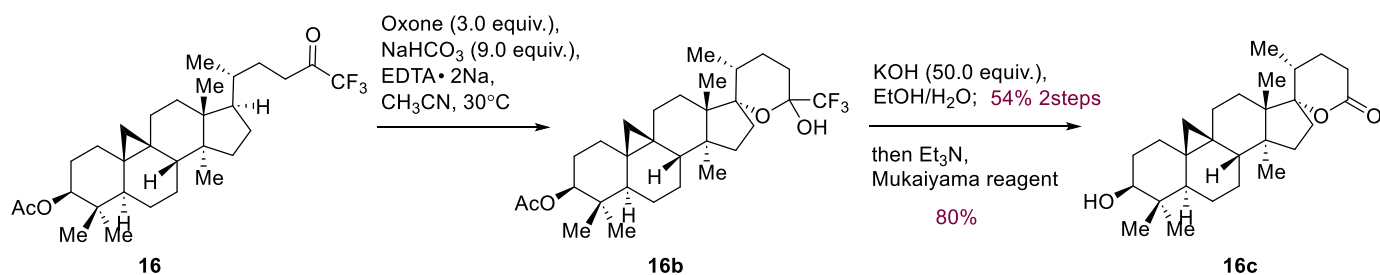


To a stirred solution of **S1-b** (68 g, 169.7 mmol) in DCM (170 mL) were sequentially added DMAP (2.07 g, 16.9 mmol), Et_3N (70.8 mL, 509 mmol) and Ac_2O (24.1 mL, 254.6 mmol) at 0°C . The reaction mixture was allowed to stir at 25°C for 1 h. The resultant mixture was quenched with MeOH (10 mL). The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 20 : 1) to give **15** (71.4 g, 95 %) as a white solid.



To a stirred solution of **15** (120 g, 271.1 mmol) in THF (1.36 L) was sequentially added TMSCF_3 (80.1 mL, 542.2 mmol) and TBAF (27.1 mL, 27.1 mmol, 1.0 M in THF) at 0 °C. The resultant mixture was stirred at 0 °C for 30 min. Then water (136 mL) was added into the reaction mixture. The reaction mixture was allowed to stir at room temperature for 2 h before it was quenched with saturated aq. NH_4Cl (300 mL), and the mixture was extracted with EtOAc (400 mL \times 3). The combined extracts were washed with brine (300 mL) and dried over anhydrous Na_2SO_4 . The solvent was removed under vacuum to give crude as a white solid. The crude was used for the next step reaction without further purification.

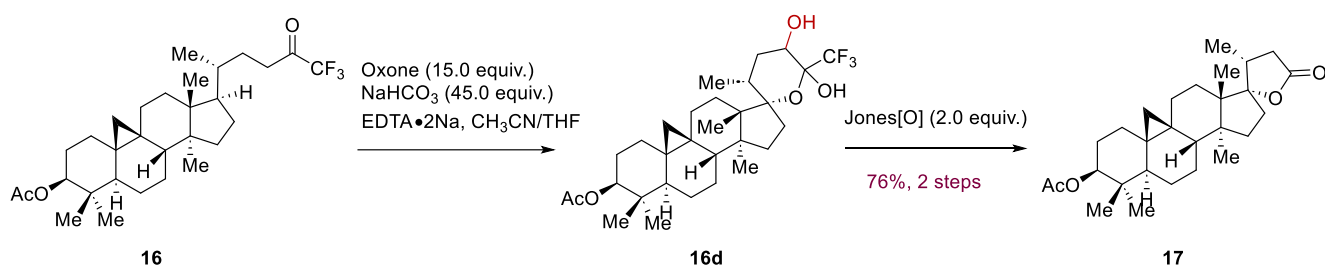
To a stirred solution of the above crude in DCM (542 mL) was sequentially added NaHCO_3 (45.5 g, 542.2 mmol) and Dess-Martin periodinane (230 g, 542.2 mmol) at 0 °C. The reaction mixture was stirred at 25 °C for 2h. The resultant mixture was quenched with saturated aq. $\text{Na}_2\text{S}_2\text{O}_3$ (400 mL) and extracted with DCM (400 mL \times 3). The combined organic phases were washed with brine (300 mL), dried over anhydrous Na_2SO_4 . The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 15 : 1) to give **16** (104 g, 75%) as a white solid; **16**: R_f = 0.5 (silica, PE : EtOAc = 5 : 1); $[\alpha]_D^{21} = +40.4$ ($c = 0.29$ in CHCl_3); IR (film): $\nu_{\text{max}} = 3411, 3041, 2870, 1763, 1732, 1470, 1375, 1248, 1205, 1149, 1040, 895, 739 \text{ cm}^{-1}$; $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 4.56$ (dd, $J = 9.9, 4.6$ Hz, 1H), 2.80 – 2.72 (m, 1H), 2.69 – 2.61 (m, 1H), 2.05 (s, 3H), 2.01 – 1.85 (m, 3H), 1.79 – 1.73 (m, 1H), 1.63 – 1.56 (m, 6H), 1.52 (dd, $J = 12.2, 4.8$ Hz, 1H), 1.49 – 1.23 (m, 7H), 1.16 – 1.07 (m, 3H), 0.96 (s, 3H), 0.90 (s, 3H), 0.89 (s, 3H), 0.88 (d, $J = 6.3$ Hz, 3H), 0.85 (s, 3H), 0.79 (dd, $J = 12.6, 2.7$ Hz, 1H), 0.58 (d, $J = 4.1$ Hz, 1H), 0.34 (d, $J = 4.1$ Hz, 1H) ppm; $^{13}\text{C NMR}$ (400 MHz, CDCl_3): $\delta = 191.12$ (q, $^2J_{\text{F-C}} = 34.5$ Hz), 171.09, 115.76 (q, $^1J_{\text{F-C}} = 292.4$ Hz), 77.16, 52.20, 48.96, 47.93, 47.27, 45.50, 39.56, 35.57, 35.55, 33.79, 32.97, 31.74, 29.87, 28.82, 28.11, 26.91, 26.54, 26.10, 25.92, 25.54, 21.45, 21.03, 20.18, 19.41, 18.13, 18.04, 15.26 ppm; $^{19}\text{F NMR}$ (376 MHz, CDCl_3): $\delta = -79.14$ (s, 3F), HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{30}\text{H}_{45}\text{O}_3\text{F}_3\text{Na}^+$ 533.3213 found 533.3213.



To a stirred solution of **16** (30.0 g, 58.7 mmol) in the mixture solution of CH₃CN (2.7 L) and EDTA•2Na (1×10⁻⁴ M, 1.6 L) was sequentially added NaHCO₃ (44.4 g, 528.7 mmol), Oxone (108.3 g, 176.2 mmol) at room temperature. After 12 h of stirring at room temperature, the mixture was extracted with EtOAc (400 mL × 3). The combined extracts were washed with brine (200 mL) and dried over anhydrous Na₂SO₄. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 10 : 1) to give **16b** (17.0 g, 55 %) as a white solid; **16b** : *R*_f = 0.5 (silica, PE : EtOAc = 3 : 1); [α]_D²⁰ = -11.3 (*c* = 0.12 in CHCl₃); IR (film): ν_{max} = 2961, 2920, 1714, 1649, 1590, 1454, 1385, 1262, 1164, 1027; ¹H NMR (400 MHz, CDCl₃): δ = 4.57 (dt, *J* = 8.3, 4.5 Hz, 1H), 2.70 (s, 1H), 2.23 (d, *J* = 5.1 Hz, 2H), 2.14 – 2.07 (m, 2H), 2.03 – 1.96 (m, 3H), 1.92 – 1.83 (m, 2H), 1.77 (t, *J* = 3.5 Hz, 2H), 1.62 (d, *J* = 8.7 Hz, 1H), 1.57 – 1.48 (m, 3H), 1.46 – 1.36 (m, 3H), 1.34 – 1.25 (m, 4H), 1.22 (d, *J* = 6.8 Hz, 3H), 1.15 (s, 3H), 1.13 (s, 3H), 0.89 (s, 3H), 0.85 (s, 3H), 0.78 (dd, *J* = 12.6, 2.4 Hz, 1H), 0.56 (d, *J* = 4.3 Hz, 1H), 0.39 (d, *J* = 4.2 Hz, 1H). ppm; ¹³C NMR (151 MHz, CDCl₃): δ = 171.20, 123.27 (q, ¹*J*_{F-C} = 287.7 Hz), 94.17 (q, ²*J*_{F-C} = 31.8 Hz), 91.50, 80.79, 52.05, 49.64, 48.61, 47.49, 39.59, 37.81, 36.71, 33.31, 31.78, 30.13, 26.93, 26.56, 26.27, 26.21, 26.11, 25.56, 22.48, 21.49, 21.40, 21.08, 20.67, 20.42, 20.25, 18.65, 15.34 ppm; ¹⁹F NMR (376 MHz, CDCl₃): δ = -86.89 (s, 3F) ppm; HRMS (*m/z*): [M+Na]⁺ calcd for C₃₀H₄₅F₃O₄Na⁺ 549.3162 found 549.3172.

To a stirred solution of **16b** (17 g, 32.3 mmol) in anhydrous EtOH (161 mL) was added KOH (90.5 g, 1.6 mol, 1.1g/mL) at 0 °C. The reaction mixture was allowed to stir at 25°C for 2 h. The reaction was quenched with HCl (1 M) until the pH = 6 and extracted with EtOAc (300 mL × 3). The combined organic phases were washed with brine (200 mL), dried over anhydrous Na₂SO₄, and filtered. The solvent was evaporated under vacuum to give crude and was used for the next step without further purification.

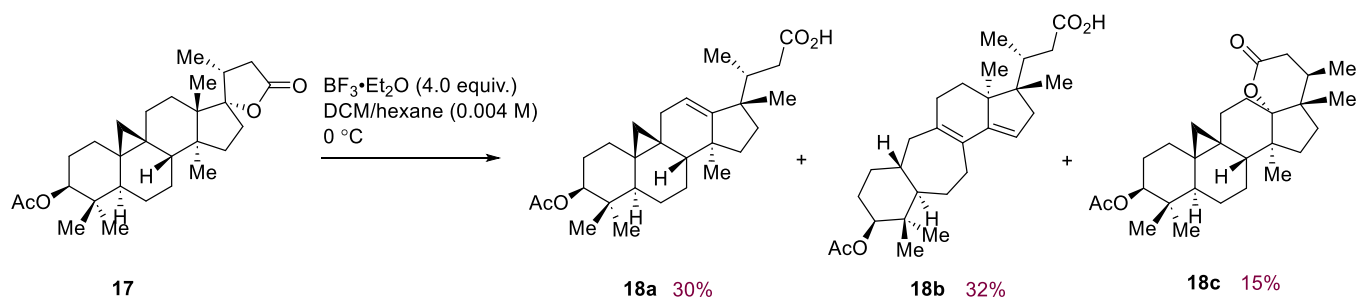
To a stirred solution of the above crude (15.3 g) in DCM (0.64 L) was added Et₃N (17.9 mL, 128.9 mmol) and Mukaiyama reagent (16.5 g, 64.5 mmol) at room temperature. After the mixture was stirred for 30 min at 25 °C, the reaction was quenched with saturated aq. NaHCO₃ (200 mL) and extracted with EtOAc (200 mL × 3). The combined organic phases were washed with brine (400 mL), dried over anhydrous Na₂SO₄, and filtered. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE: EtOAc = 8 : 1) to give **16c** (10.7 g, 80%) as a white solid. **16c** : *R*_f = 0.5 (silica, PE : EtOAc = 2 : 1); [α]_D²⁰ = -10.9 (*c* = 0.11 in CHCl₃); IR (film): ν_{max} = 2958, 2923, 1693, 1585, 1455, 1384, 1348, 1261, 1092, 1019; ¹H NMR (600 MHz, CDCl₃): δ = 3.36 – 3.22 (m, 1H), 2.65 – 2.40 (m, 2H), 2.27 (t, *J* = 12.3 Hz, 1H), 2.18 – 1.97 (m, 5H), 1.81 – 1.69 (m, 1H), 1.57 (tdd, *J* = 25.0, 10.9, 3.9 Hz, 6H), 1.44 (td, *J* = 12.1, 8.4 Hz, 1H), 1.38 (dt, *J* = 10.6, 3.5 Hz, 1H), 1.33 (dd, *J* = 12.4, 4.1 Hz, 2H), 1.29 (dd, *J* = 12.4, 2.0 Hz, 1H), 1.23 (s, 3H), 1.19 (s, 3H), 1.18 – 1.08 (m, 2H), 1.02 (d, *J* = 6.8 Hz, 3H), 0.97 (s, 3H), 0.81 (s, 3H), 0.54 (d, *J* = 4.1 Hz, 1H), 0.54 (d, *J* = 4.1 Hz, 1H), 0.39 (d, *J* = 4.2 Hz, 1H) ppm; ¹³C NMR (151 MHz, CDCl₃): δ = 172.05, 96.88, 78.84, 51.53, 49.84, 49.30, 47.29, 40.61, 39.56, 36.21, 33.06, 32.06, 30.49, 30.27, 26.43, 26.34, 26.21, 25.58, 25.26, 24.85, 21.30, 21.24, 20.93, 20.10, 14.79, 14.17 ppm; HRMS (*m/z*): [M+Na]⁺ calcd for C₂₇H₄₂O₃Na⁺ 437.3026 found 437.3027.



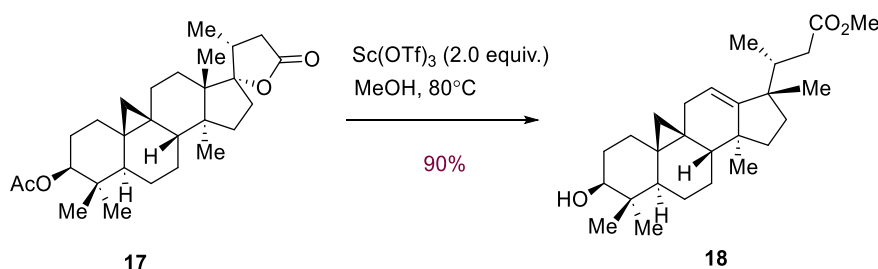
To a stirred solution of **16** (30.0 g, 58.7 mmol) in the mixture solution of CH₃CN/THF = 6:1 (2.7 L) and EDTA•2Na (1×10⁻⁴ M, 1.6 L) was sequentially added NaHCO₃ (44.4 g, 528.7 mmol), Oxone (108.3 g, 176.2 mmol) at 60 °C, After 30 min of stirring at 60 °C, another portion of NaHCO₃ (44.4 g, 528.7 mmol) was added, followed by addition of Oxone (108.3 g, 176.2 mmol). This was repeated for a total of 5 times with 30 min in between additions, and the resulting mixture was stirred for another hour after the last addition. Then the reaction was quenched with water, and the mixture was extracted with EtOAc (400 mL × 3). The combined extracts were washed with brine (200 mL) and dried over anhydrous Na₂SO₄. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 10 : 1) to give **16d** as a white solid. **16d**: *R*_f = 0.47 (silica, PE : EtOAc = 3 : 1); [α]_D²⁰ = +52.0 (*c* = 0.10 in CHCl₃); IR (film): ν_{max} = 2917, 2832, 1732, 1584, 1462, 1364, 1245, 1095, 1070, 1027; ¹H NMR (600 MHz, CDCl₃) δ = 5.63 (td, *J* = 6.1, 2.7 Hz, 1H), 4.56 (q, *J* = 4.6 Hz, 1H), 2.80 (d, *J* = 3.5 Hz, 1H), 2.50 – 2.39 (m, 1H), 2.20 – 2.13 (m, 1H), 2.12 – 2.07 (m, 1H), 2.05 (s, 3H), 1.96 (dt, *J* = 12.6, 6.3 Hz, 1H), 1.88 – 1.80 (m, 2H), 1.77 (dd, *J* = 6.5, 3.7 Hz, 1H), 1.65 – 1.56 (m, 4H), 1.55 (dd, *J* = 12.3, 4.7 Hz, 1H), 1.48 (ddd, *J* = 15.1, 8.7, 3.7 Hz, 1H), 1.43 – 1.38 (m, 2H), 1.35 – 1.22 (m, 4H), 1.19 (s, 3H), 1.16 (s, 3H), 1.14 – 1.08 (m, 3H), 0.95 (d, *J* = 6.7 Hz, 3H), 0.89 (s, 3H), 0.85 (s, 3H), 0.56 (d, *J* = 4.1 Hz, 1H), 0.36 (d, *J* = 4.2 Hz, 1H) ppm; ¹³C NMR (101 MHz, CDCl₃) δ = 171.14, 98.51, 97.21, 80.80, 49.61, 49.26, 48.98, 47.36, 44.17, 42.15, 39.59, 39.36, 36.40, 31.74, 29.96, 26.95, 26.30, 26.21, 26.02, 25.58, 21.49, 21.12, 20.85, 20.72, 20.55, 17.92, 15.31 ppm; ¹⁹F NMR (376 MHz, CDCl₃) δ = -75.14 (s, 3F) ppm; HRMS (*m/z*): [M+Na]⁺ calcd for C₃₀H₄₅F₃O₅Na⁺ 565.3111 found 565.3107.

The above white solid was dissolved in acetone (587 mL) was added Jones reagent (47 mL, 117.5 mmol, 2.5 M) at 0 °C, and the resultant mixture was stirred at 0 °C for 30 min. Then the reaction was quenched with NaOAc (300 mL, 4.0 M in H₂O), extracted with EtOAc (300 mL × 3). The combined extracts were washed with brine (300 mL) and dried over anhydrous Na₂SO₄. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 10 : 1) to give **17** (19.7 g, 76 %) as a white solid. **17**: *R*_f = 0.47 (silica, PE : EtOAc = 3 : 1); [α]_D²⁰ = +34.4 (*c* = 0.25 in CHCl₃); IR (film): ν_{max} = 2959, 1765, 1731, 1469, 1377, 1308, 1241, 1164, 1095, 1032; ¹H NMR (400 MHz, CDCl₃): δ = 4.57 (dd, *J* = 11.3, 4.3 Hz, 1H), 2.74 (dd, *J* = 16.6, 6.4 Hz, 1H), 2.44 (p, *J* = 6.6 Hz, 1H), 2.15 – 2.10 (m, 6H), 2.04 (s, 3H), 1.78 (d, *J* = 8.8 Hz, 1H), 1.64 – 1.54 (m, 6H), 1.48 – 1.39 (m, 3H), 1.24 (s, 3H), 1.14 (s, 4H), 1.10 (d, *J* = 6.5 Hz, 4H), 0.89 (s, 3H), 0.85 (s, 3H), 0.82 – 0.77 (m, 1H), 0.57 (d, *J* = 4.2 Hz, 1H), 0.41 (d, *J* = 4.2 Hz,

1H) ppm; ^{13}C NMR (101 MHz, CDCl_3): $\delta = 177.21, 170.91, 99.41, 80.48, 49.98, 49.21, 49.15, 47.20, 41.12, 39.45, 39.25, 38.76, 35.79, 31.62, 29.96, 26.78, 26.16, 25.96, 25.80, 25.43, 25.13, 21.34, 20.98, 20.46, 20.13, 19.91, 17.34, 15.18$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{28}\text{H}_{42}\text{O}_4\text{Na}^+$ 465.2975 found 465.2979.

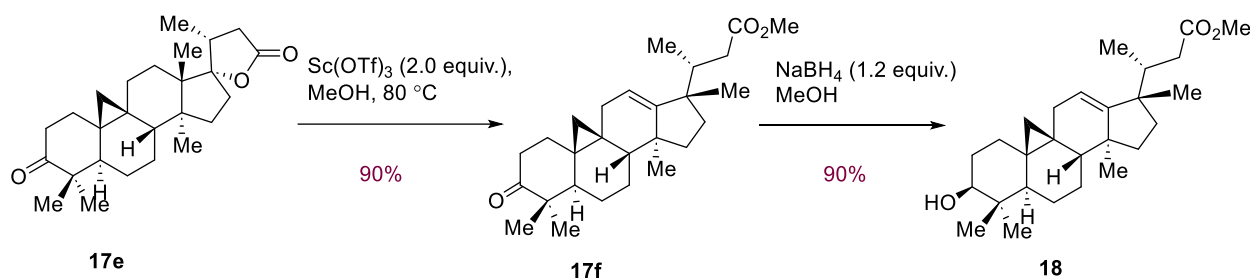


To a stirred solution of **17** (50 mg, 0.113 mmol) in anhydrous DCM/hexane (30 mL/3 mL) was sequentially added $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (56 μL , 0.45 mmol) at 0°C . The reaction mixture was allowed to be stirred at 0°C for 1 h. To this solution H_2O (68 μL) was added over 30 min at 0°C . The reaction was quenched with pH = 7 buffer (15 mL) and extracted with EtOAc (5 mL \times 3). The combined organic phases were washed with brine (15 mL), dried over anhydrous Na_2SO_4 and filtered. The solvent was evaporated under vacuum to give **18c** (7.5 mg, 15%) as a white solid. **18c**: $R_f = 0.40$ (silica, PE : EtOAc = 3 : 1); $[\alpha]_D^{22} = -5.8$ ($c = 0.10$ in CHCl_3); IR (film): $\nu_{\text{max}} = 2957, 2923, 1736, 1648, 1576, 1461, 1259, 1117, 1063, 1024, 799$ cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) $\delta = 4.58$ (dd, $J = 11.4, 4.1$ Hz, 1H), 2.35 (dd, $J = 17.0, 3.2$ Hz, 1H), 2.14 (dt, $J = 12.6, 9.0$ Hz, 3H), 1.94 – 1.83 (m, 0H), 1.80 – 1.65 (m, 1H), 1.67 – 1.58 (m, 1H), 1.54 – 1.37 (m, 3H), 1.34 (dd, $J = 12.9, 4.3$ Hz, 1H), 1.32 – 1.25 (m, 0H), 1.18 – 1.12 (m, 0H), 1.09 (s, 3H), 1.05 (s, 3H), 0.97 (d, $J = 6.8$ Hz, 3H), 0.88 (s, 3H), 0.86 (s, 3H), 0.64 (d, $J = 4.3$ Hz, 1H), 0.09 (d, $J = 4.3$ Hz, 1H) ppm; ^{13}C NMR (101 MHz, CDCl_3) $\delta = 173.74, 171.00, 96.34, 80.38, 52.63, 47.70, 46.21, 39.10, 38.03, 36.35, 35.11, 35.07, 34.60, 33.76, 30.29, 27.56, 26.61, 26.37, 25.52, 24.68, 24.18, 22.22, 21.47, 20.40, 20.29, 19.05, 16.31, 15.21$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{28}\text{H}_{42}\text{O}_4\text{Na}^+$ 465.2975 found 465.2974.



To a stirred solution of **17** (22 g, 49.7 mmol) in anhydrous MeOH (497 mL) was sequentially added $\text{Sc}(\text{OTf})_3$ (48.9 g, 99.4 mmol) at 25°C . The reaction mixture was allowed to stir at 80°C for 5 h. The reaction was quenched with saturated aq. NaHCO_3 (300 mL) and extracted with EtOAc (300 mL \times 3). The combined organic phases were washed with brine (200 mL), dried over anhydrous Na_2SO_4 , and filtered. The solvent was

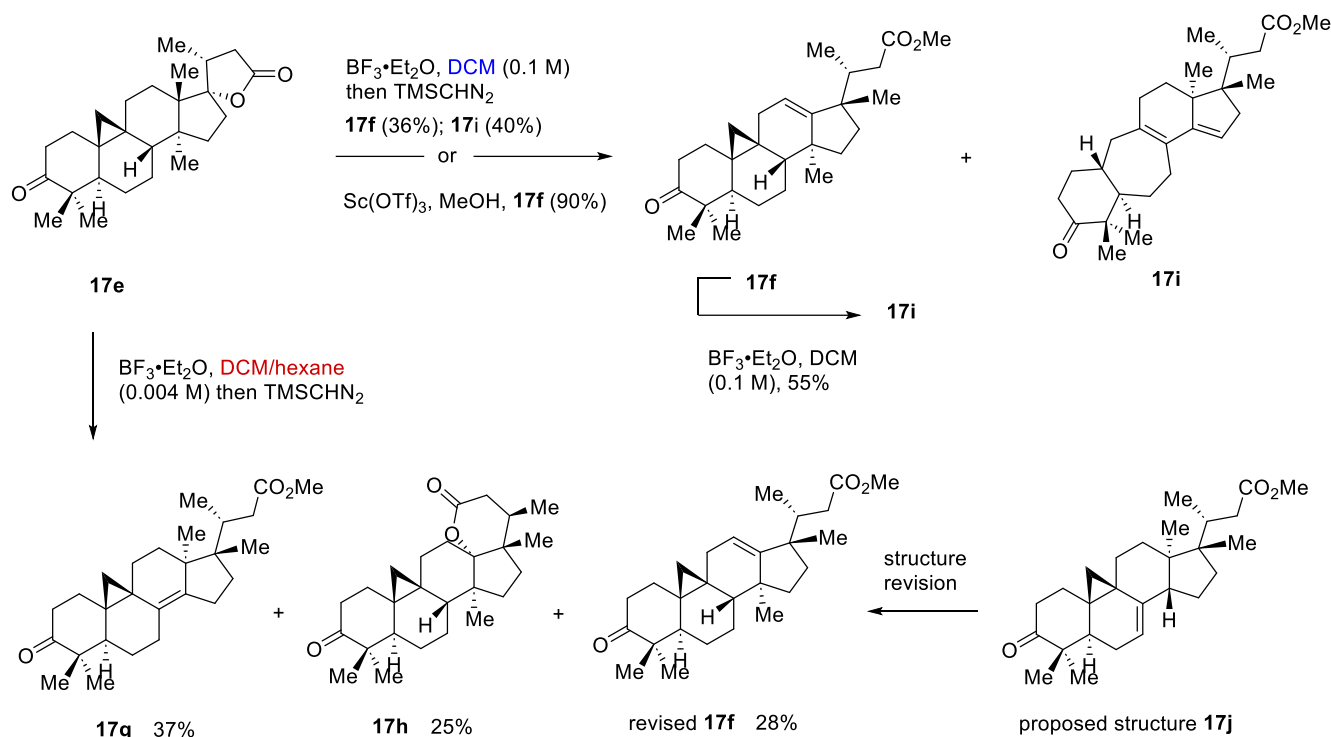
evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE: EtOAc = 6 : 1) to give epoxide **18** (20.4 g, 90%) as a white solid. **18**: $R_f = 0.47$ (silica, PE: EtOAc = 3 : 1); $[\alpha]_D^{22} = +28.2$ ($c = 0.27$ in CHCl_3); IR (film): $\nu_{\text{max}} = 2958, 2930, 2360, 2341, 1731, 1717, 1456, 1374, 1260, 1020 \text{ cm}^{-1}$; $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 5.45$ (dd, $J = 7.7, 2.6 \text{ Hz}$, 1H), 3.67 (s, 3H), 3.31 (dd, $J = 11.0, 4.3 \text{ Hz}$, 1H), 2.60 (dd, $J = 14.6, 3.1 \text{ Hz}$, 1H), 2.40 (dd, $J = 15.6, 2.6 \text{ Hz}$, 1H), 2.14 (ddd, $J = 10.1, 6.7, 3.2 \text{ Hz}$, 1H), 1.98 (dd, $J = 14.6, 11.0 \text{ Hz}$, 1H), 1.81 – 1.72 (m, 2H), 1.66 – 1.48 (m, 8H), 1.40 – 1.24 (m, 4H), 1.21 – 1.06 (m, 2H), 1.00 (s, 3H), 0.99 (s, 3H), 0.90 (d, $J = 6.6 \text{ Hz}$, 3H), 0.87 (s, 3H), 0.81 (s, 3H), 0.51 (d, $J = 4.4 \text{ Hz}$, 1H), 0.17 (d, $J = 4.4 \text{ Hz}$, 1H) ppm; $^{13}\text{C NMR}$ (101 MHz, CDCl_3): $\delta = 174.64, 159.01, 115.83, 78.60, 51.44, 49.99, 48.84, 47.09, 46.38, 40.24, 37.57, 37.51, 35.97, 32.89, 31.51, 31.40, 30.05, 27.82, 26.03, 25.75, 25.59, 25.56, 21.77, 19.81, 17.69, 15.34, 14.06$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{27}\text{H}_{42}\text{O}_3\text{Na}^+$ 437.3026 found 437.3029.



To a stirred solution of **17e** (20 mg, 0.05 mmol) in anhydrous MeOH (0.5 mL) was sequentially added $\text{Sc}(\text{OTf})_3$ (49.4 mg, 0.1 mmol) at 25 °C. The reaction mixture was allowed to stir at 80 °C for 5 h. The reaction was quenched with saturated aq. NaHCO_3 (5 mL) and extracted with EtOAc (5 mL \times 3). The combined organic phases were washed with brine (15 mL), dried over anhydrous Na_2SO_4 , and filtered. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE: EtOAc = 6 : 1) to give epoxide **17f** (18.6 mg, 90%) as a white solid. **17f**: $R_f = 0.8$ (silica, PE: EtOAc = 3 : 1); $[\alpha]_D^{22} = +8.7$ ($c = 0.11$ in CHCl_3); IR (film): $\nu_{\text{max}} = 2957, 2918, 2850, 1740, 1708, 1652, 1593, 1262, 1096, 1025, 804$; $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 5.46$ (dt, $J = 7.6, 2.0 \text{ Hz}$, 1H), 3.65 (d, $J = 1.5 \text{ Hz}$, 3H), 2.79 – 2.65 (m, 1H), 2.58 (dt, $J = 14.8, 2.0 \text{ Hz}$, 1H), 2.44 (d, $J = 15.5 \text{ Hz}$, 1H), 2.34 – 2.24 (m, 1H), 2.18 – 2.08 (m, 1H), 2.01 – 1.88 (m, 2H), 1.81 – 1.72 (m, 1H), 1.66 (dd, $J = 12.0, 3.7 \text{ Hz}$, 1H), 1.60 – 1.50 (m, 7H), 1.42 (dd, $J = 12.3, 5.6 \text{ Hz}$, 1H), 1.20 – 1.14 (m, 2H), 1.08 (s, 3H), 1.05 (s, 3H), 1.00 (s, 3H), 0.88 (d, $J = 6.7 \text{ Hz}$, 3H), 0.86 (s, 3H), 0.72 (d, $J = 4.5 \text{ Hz}$, 1H), 0.40 (d, $J = 4.5 \text{ Hz}$, 1H) ppm; $^{13}\text{C NMR}$ (101 MHz, CDCl_3): $\delta = 216.67, 174.77, 159.46, 115.71, 51.63, 50.13, 50.12, 49.08, 48.67, 46.52, 37.80, 37.67, 37.42, 36.14, 33.09, 32.99, 31.81, 27.69, 26.14, 25.81, 25.72, 23.05, 22.47, 21.14, 20.41, 17.79, 15.51$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{27}\text{H}_{40}\text{O}_3\text{Na}^+$ 435.2870 found 435.2870.

To a stirred solution of **17f** (15 mg, 0.034 mmol) in anhydrous MeOH (0.34 mL) was sequentially added NaBH_4 (1.6 mg, 0.04 mmol) at 0 °C. The reaction mixture was allowed to stirred at 0 °C for 0.5 h. The reaction was quenched with saturated aq. NH_4Cl (5 mL) and extracted with EtOAc (5 mL \times 3). The combined organic

phases were washed with brine (15 mL), dried over anhydrous Na₂SO₄, and filtered. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE: EtOAc = 6 : 1) to give epoxide **18** (12.8 mg, 90%) as a white solid.



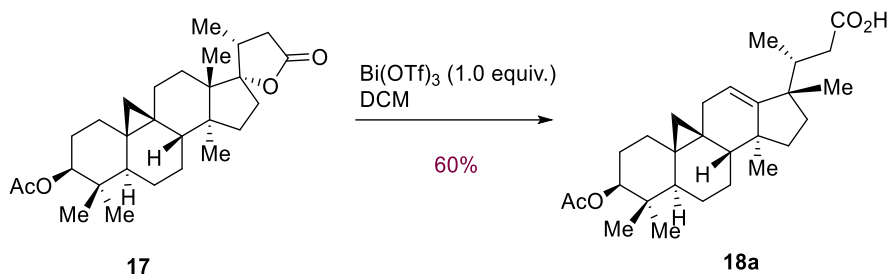
To a stirred solution of **17e** (55 mg, 0.138 mmol) in DCM (1.38 mL) was sequentially added $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (68 μL , 0.55 mmol) at 0 °C. The reaction mixture was allowed to stirred at 0 °C for 2 h. The reaction was quenched with saturated aq. NaHCO₃ (5 mL) and extracted with EtOAc (5 mL \times 3). The combined organic phases were washed with brine (15 mL), dried over anhydrous Na₂SO₄, and filtered. The solvent was evaporated under vacuum to give crude and was used for the next step without further purification as a white solid.

To a stirred solution of the above crude in MeOH (1.38 mL) was added TMSCHN₂ (0.2 mL, 1.38 mmol) at 0 °C and stirred at 15 °C for 30 min. The solvent was evaporated under vacuum. The residue was purified by flash column chromatography (silica gel, PE : EtOAc = 10 : 1) to give **17f** (20 mg, 36 %) and **17i** (22.8 mg, 40 %) as white solid.

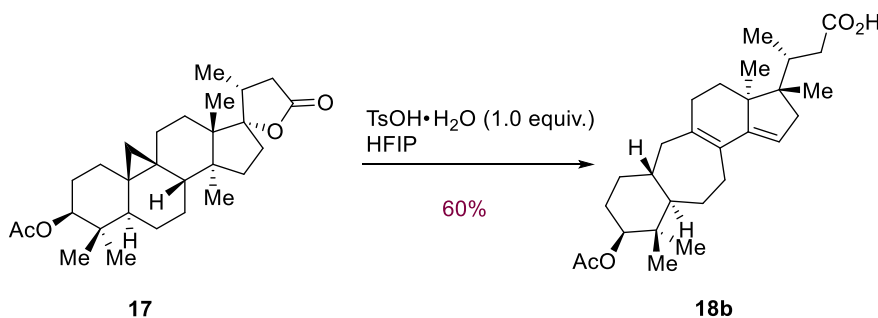
To a stirred solution of **17e** (55 mg, 0.138 mmol) in DCM/hexane (30 mL/3 mL) was sequentially added $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (68 μL , 0.55 mmol) at 0 °C. The reaction mixture was allowed to stirred at 0 °C for 1 h. To this solution H₂O (68 μL) was added over 30 min at 0 °C. The reaction was quenched with pH = 7 buffer (15 mL) and extracted with EtOAc (5 mL \times 3). The combined organic phases were washed with brine (15 mL), dried over anhydrous Na₂SO₄ and filtered. The solvent was evaporated under vacuum to give crude as a yellow oil and was used for the next step without further purification.

To a stirred solution of the above crude in MeOH (1.38 mL) was added TMSCHN₂ (0.2 mL, 1.38 mmol) at 0 °C and stirred at 15 °C for 30 min. The solvent was evaporated under vacuum. The residue was purified by

flash column chromatography (silica gel, PE : EtOAc = 20 : 1) to give **17f** (15.9 mg, 28 %), **17g** (21.1 mg, 37 %) and **17h** (14.2 mg, 25%) as oil. In contrast to the structure **17j** tentatively proposed by Corey and co-workers, our verification experiments indicate that the data are not consistent with that assignment. Herein, we provide a revised structure for **17f**.

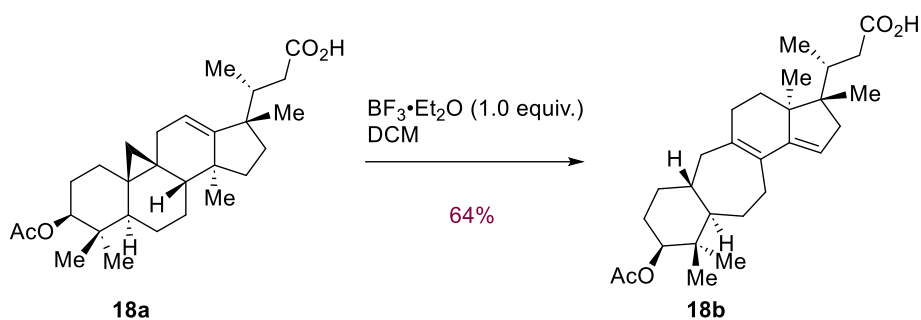


To a stirred solution of **17** (15 mg, 0.03 mmol) in DCM (0.34 mL) was sequentially added Bi(OTf)_3 (22 mg, 0.03 mmol) at 0 °C. The reaction mixture was allowed to stirred at 15 °C for 2.5 h. The reaction was quenched with saturated aq. NaHCO_3 (5 mL) and extracted with EtOAc (5 mL \times 3). The combined organic phases were washed with brine (15 mL), dried over anhydrous Na_2SO_4 , and filtered. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 6 : 1) to give epoxide **18a** (9.0 mg, 60%) as a white solid. **18a**: R_f = 0.2 (silica, PE: EtOAc = 1 : 1); $[\alpha]_D^{22}$ = +29.7 (c = 0.11 in CHCl_3); IR (film): ν_{max} = 2960, 2927, 2853, 1736, 1702, 1590, 1364, 1261, 1100, 1027, 804; $^1\text{H NMR}$ (400 MHz, CDCl_3): δ = 5.46 (dd, J = 7.7, 2.6 Hz, 1H), 4.59 (dd, J = 11.2, 4.2 Hz, 1H), 2.66 (dd, J = 14.8, 2.8 Hz, 1H), 2.41 (dd, J = 15.6, 2.5 Hz, 1H), 2.23 – 2.08 (m, 1H), 2.06 (s, 3H), 2.01 (dd, J = 14.9, 11.2 Hz, 1H), 1.85 – 1.71 (m, 2H), 1.69 (d, J = 13.5 Hz, 1H), 1.64 (d, J = 3.8 Hz, 1H), 1.59 – 1.45 (m, 5H), 1.42 – 1.32 (m, 2H), 1.35 – 1.27 (m, 1H), 1.18 (dt, J = 12.4, 6.0 Hz, 1H), 1.15 – 1.03 (m, 1H), 1.01 (s, 3H), 0.95 (d, J = 6.8 Hz, 3H), 0.89 (s, 3H), 0.88 (s, 3H), 0.87 (s, 3H), 0.85 – 0.76 (m, 1H), 0.53 (d, J = 4.4 Hz, 1H), 0.18 (d, J = 4.4 Hz, 1H) ppm; $^{13}\text{C NMR}$ (151 MHz, CDCl_3): δ = 171.17, 159.14, 116.08, 80.70, 50.03, 49.01, 47.34, 46.51, 39.35, 37.64, 35.93, 33.09, 31.65, 31.20, 29.85, 27.96, 26.66, 26.02, 25.74, 25.69, 25.57, 21.99, 21.50, 19.80, 17.90, 15.45, 15.35 ppm; HRMS (m/z): $[\text{M-H}]^-$ calcd for $\text{C}_{28}\text{H}_{41}\text{O}_4^-$ 441.3010 found 441.2997.

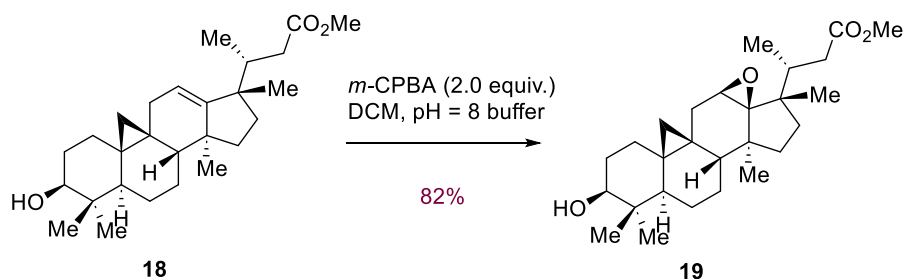


To a stirred solution of **17** (15 mg, 0.03 mmol) in HFIP (0.34 mL) was sequentially added $\text{TsOH}\cdot\text{H}_2\text{O}$ (22 mg, 0.03 mmol) at 0 °C. The reaction mixture was allowed to stirred at 0 °C for 2.5 h. The reaction was quenched

with saturated aq. NaHCO₃ (5 mL) and extracted with EtOAc (5 mL × 3). The combined organic phases were washed with brine (15 mL), dried over anhydrous Na₂SO₄, and filtered. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 6 : 1) to give epoxide **18b** (9 mg, 60%) as a white solid. **18b**: *R*_f = 0.2 (silica, PE : EtOAc = 1 : 1); [α]_D²² = +16.0 (*c* = 0.11 in CHCl₃); IR (film): ν_{max} = 2962, 2927, 1736, 1594, 1265, 1082, 1461, 1381, 1017, 808, 739; ¹H NMR (400 MHz, CDCl₃): δ = 5.32 (s, 1H), 4.50 (dd, *J* = 11.8, 4.4 Hz, 1H), 2.55 (d, *J* = 14.9 Hz, 1H), 2.44 (dd, *J* = 15.3, 7.8 Hz, 2H), 2.35 (d, *J* = 16.5 Hz, 1H), 2.31 – 2.16 (m, 2H), 2.13 – 2.06 (m, 2H), 2.04 (s, 3H), 2.01 (d, *J* = 1.2 Hz, 2H), 2.00 – 1.86 (m, 2H), 1.79 – 1.60 (m, 4H), 1.58 – 1.46 (m, 1H), 1.43 (dd, *J* = 12.5, 5.3 Hz, 1H), 1.29 – 1.12 (m, 2H), 1.07 (t, *J* = 9.9 Hz, 1H), 0.96 (d, *J* = 6.6 Hz, 3H), 0.89 (s, 6H), 0.80 (s, 6H)ppm; ¹³C NMR (101 MHz, CDCl₃): δ = 179.60, 171.10, 147.87, 135.73, 132.46, 115.73, 80.12, 56.24, 50.11, 48.26, 45.23, 42.32, 38.67, 38.04, 35.44, 35.06, 33.96, 30.78, 29.77, 27.32, 27.00, 25.39, 21.48, 17.63, 16.41, 16.08, 14.84ppm; HRMS (*m/z*): [*M*-H]⁻ calcd for C₂₈H₄₁O₄⁻ 441.3010 found 441.3009.

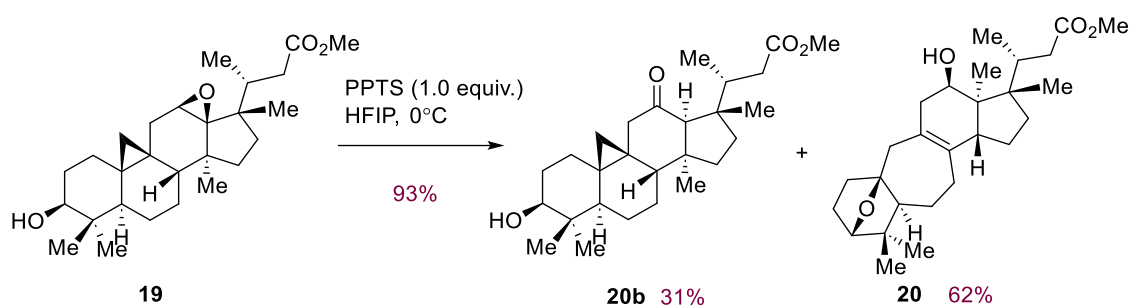


To a stirred solution of **18a** (10 mg, 0.02 mmol) in DCM (0.34 mL) was sequentially added BF₃·Et₂O (3 μL, 0.02 mmol) at 0 °C. The reaction mixture was allowed to be stirred at 15 °C for 2.5 h. The reaction was quenched with saturated aq. NaHCO₃ (5 mL) and extracted with EtOAc (5 mL × 3). The combined organic phases were washed with brine (15 mL), dried over anhydrous Na₂SO₄, and filtered. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 6 : 1) to give epoxide **18b** (6.4 mg, 64%) as a white solid.



To a stirred solution of **18** (18 g, 43.4 mmol) in DCM (217 mL) was sequentially added pH = 8 buffer (109 mL) and *m*-CPBA (17.6 g, 86.8 mmol, 85%) at 0 °C. The reaction mixture was allowed to be stirred at 25 °C for 2h. The reaction was quenched with saturated aq. NaHCO₃ (200 mL) and extracted with DCM (200 mL ×

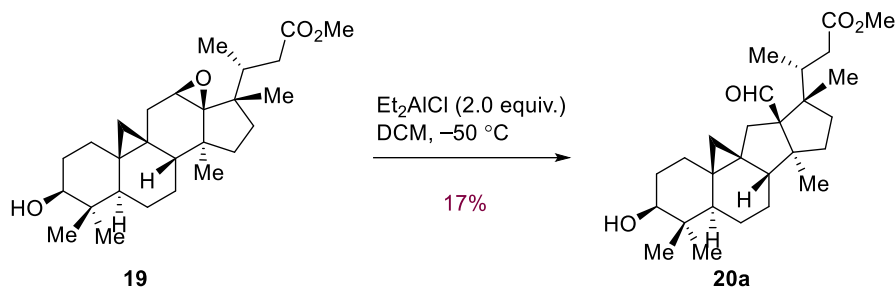
3). The combined organic phases were washed with brine (200 mL), dried over anhydrous Na₂SO₄, and filtered. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 3 : 1) to give epoxide **19** (15.3 g, 82%) as a white solid. **19**: *R*_f = 0.29 (silica, PE : EtOAc = 3 : 1); [α]_D²⁶ = +34.4 (*c* = 0.19 in CHCl₃); IR (film): ν_{\max} = 2959, 2926, 2360, 2341, 1736, 1447, 1364, 1290, 1169, 1030 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ = 3.66 (s, 3H), 3.52 (d, *J* = 4.4 Hz, 1H), 3.26 (dd, *J* = 11.0, 4.3 Hz, 1H), 2.42 (dd, *J* = 14.9, 2.6 Hz, 1H), 2.21 (d, *J* = 15.0 Hz, 1H), 2.09 (ddd, *J* = 9.6, 6.6, 2.8 Hz, 1H), 1.98 (dd, *J* = 14.8, 10.5 Hz, 1H), 1.74 (dq, *J* = 12.8, 6.1 Hz, 3H), 1.63 – 1.33 (m, 10H), 1.21 (dt, *J* = 11.8, 3.7 Hz, 2H), 1.00 (s, 3H), 0.96 (d, *J* = 6.8 Hz, 3H), 0.96 (s, 3H), 0.89 (s, 3H), 0.85 – 0.83 (m, 1H), 0.78 (s, 3H), 0.65 (d, *J* = 4.8 Hz, 1H), 0.21 (d, *J* = 4.8 Hz, 1H) ppm; ¹³C NMR (101 MHz, CDCl₃): δ = 174.04, 78.51, 76.72, 73.93, 57.29, 51.56, 47.05, 45.93, 45.23, 40.29, 38.19, 37.40, 36.35, 35.56, 34.28, 31.71, 29.99, 27.95, 25.41, 25.40, 24.94, 20.38, 19.49, 19.46, 18.99, 16.92, 13.96 ppm; HRMS (*m/z*): [M+Na]⁺ calcd for C₂₇H₄₂O₄Na⁺ 453.2975 found 453.2976.



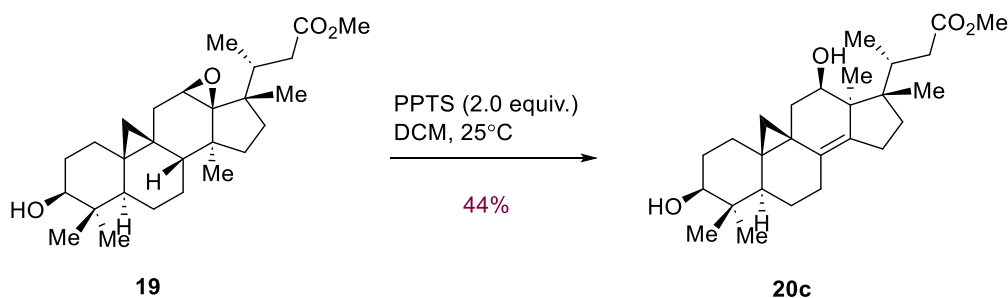
To a stirred solution of **19** (14 g, 32.5 mmol) in HFIP (325 mL) was added PPTS (8.14 g, 32.5 mmol) at 0 °C, and the resultant mixture was stirred at 25 °C for 30 min. The reaction was quenched with saturated aq. NaHCO₃ (100 mL) and the mixture was extracted with EtOAc (200 mL × 3). The combined extracts were washed with brine (100 mL) and dried over with anhydrous Na₂SO₄. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 1 : 1) to give **20b** (4.3 g, 31%) as a white solid. **20b**: *R*_f = 0.17 (silica, PE : EtOAc = 3 : 1); [α]_D²⁰ = -33.6 (*c* = 0.25 in CHCl₃); IR (film): ν_{\max} = 2952, 2828, 1733, 1698, 1558, 1507, 1456, 1362, 1172 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ = 3.68 (s, 3H), 3.33 (dd, *J* = 11.1, 4.3 Hz, 1H), 2.84 – 2.76 (m, 2H), 2.24 (s, 3H), 2.13 – 2.07 (m, 2H), 1.82 – 1.57 (m, 8H), 1.45 – 1.40 (m, 2H), 1.35 (dd, *J* = 12.4, 3.8 Hz, 1H), 1.22 (s, 3H), 1.20 – 1.18 (m, 1H), 1.15 – 1.09 (m, 1H), 1.01 (s, 3H), 0.98 (s, 3H), 0.94 (d, *J* = 5.8 Hz, 3H), 0.93 – 0.86 (m, 1H), 0.82 (s, 3H), 0.62 (d, *J* = 4.8 Hz, 1H), 0.34 (d, *J* = 4.8 Hz, 1H). ppm; ¹³C NMR (101 MHz, CDCl₃): δ = 213.86, 174.93, 78.51, 67.46, 51.56, 49.42, 48.05, 46.89, 46.53, 43.44, 40.99, 40.41, 38.66, 38.44, 36.19, 31.65, 30.05, 26.53, 26.40, 25.66, 25.56, 25.51, 21.52, 21.24, 20.16, 16.05, 14.06 ppm; HRMS (*m/z*): [M+Na]⁺ calcd for C₂₇H₄₂O₄Na⁺ 453.2975 found 453.2978.

20 (8.7 g, 62%), white solid; **20**: *R*_f = 0.17 (silica, PE : EtOAc = 3 : 1); [α]_D²⁰ = -36.9 (*c* = 0.27 in CHCl₃); IR (film): ν_{\max} = 2958, 2926, 2871, 1736, 1457, 1436, 1374, 1299, 1260, 1069 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ = 4.01 (d, *J* = 3.0 Hz, 1H), 3.75 (d, *J* = 5.5 Hz, 1H), 3.69 (s, 3H), 3.21 (d, *J* = 14.0 Hz, 1H), 2.91 (t, *J* = 10.1

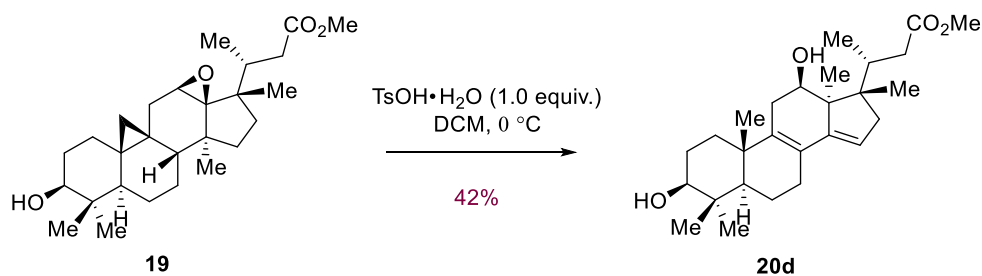
Hz, 1H), 2.65 – 2.58 (m, 2H), 2.41 – 2.36 (m, 1H), 2.30 (ddd, $J = 11.3, 6.6, 2.3$ Hz, 1H), 2.15 (dd, $J = 14.3, 11.3$ Hz, 1H), 2.00 – 1.89 (m, 2H), 1.82 – 1.71 (m, 5H), 1.64 (ddd, $J = 12.9, 10.1, 5.3$ Hz, 1H), 1.48 – 1.34 (m, 5H), 1.32 – 1.26 (m, 2H), 1.08 (s, 3H), 1.04 (s, 3H), 0.96 (s, 3H), 0.90 (d, $J = 6.6$ Hz, 3H), 0.81 (s, 3H) ppm; ^{13}C NMR (400 MHz, CDCl_3): $\delta = 174.27, 132.81, 120.69, 90.30, 84.95, 73.03, 55.30, 51.61, 49.47, 48.76, 45.59, 44.46, 41.74, 38.71, 38.25, 36.76, 36.59, 36.01, 33.35, 25.68, 25.13, 23.33, 22.77, 22.75, 19.95, 16.68, 15.74$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{27}\text{H}_{42}\text{O}_4\text{Na}^+$ 453.2975 found 453.2978.



To a stirred solution of **19** (30.0 mg, 0.07 mmol) in DCM (0.7 mL) was added Et_2AlCl (0.14 mL, 0.14 mmol, 1.0 M in hexane) at $-50\text{ }^\circ\text{C}$, and the resultant mixture was stirred at $-78\text{ }^\circ\text{C}$ for 1 h. The reaction was quenched with saturated aq. NaHCO_3 (10 mL), and the mixture was extracted with DCM (20 mL \times 3). The combined extracts were washed with brine (10 mL) and dried over with anhydrous Na_2SO_4 . The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 6 : 1) to give **20a** (5.1 mg, 17%) as a white solid. **20a**: $R_f = 0.38$ (silica, PE : EtOAc = 2 : 1); $[\alpha]_D^{20} = -7.9$ ($c = 0.11$ in CHCl_3); IR (film): $\nu_{\text{max}} = 2960, 2925, 2868, 1737, 1717, 1460, 1377, 1363, 1260, 1047\text{ cm}^{-1}$; ^1H NMR (400 MHz, CDCl_3): $\delta = 9.82$ (s, 1H), 3.67 – 3.64 (m, 1H), 3.61 (s, 3H), 3.29 (dd, $J = 11.2, 4.2$ Hz, 1H), 2.61 (d, $J = 14.6$ Hz, 1H), 2.24 – 2.12 (m, 2H), 2.02 – 1.91 (m, 5H), 1.81 – 1.76 (m, 2H), 1.68 – 1.53 (m, 7H), 1.49 – 1.42 (m, 2H), 1.11 (s, 3H), 0.97 (s, 3H), 0.93 (d, $J = 6.3$ Hz, 3H), 0.82 (s, 3H), 0.79 (s, 3H), 0.59 (d, $J = 4.4$ Hz, 1H), 0.28 (d, $J = 4.4$ Hz, 1H) ppm; ^{13}C NMR (400 MHz, CDCl_3): $\delta = 204.30, 173.11, 78.73, 73.25, 58.60, 56.57, 51.53, 51.26, 46.68, 40.54, 40.18, 39.79, 36.43, 36.22, 32.65, 32.56, 30.16, 27.68, 27.40, 27.24, 25.59, 25.39, 20.69, 19.59, 18.60, 15.89, 14.07$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{27}\text{H}_{42}\text{O}_4\text{Na}^+$ 453.2975 found 453.2977.

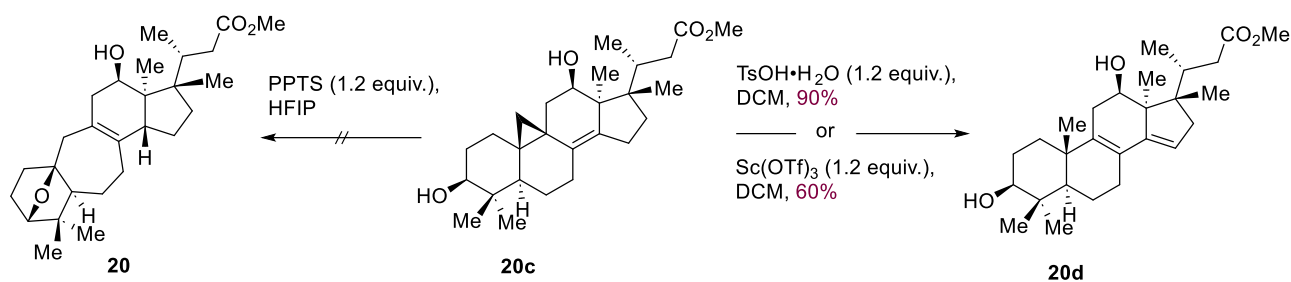


To a stirred solution of **19** (20.0 mg, 0.046 mmol) in DCM (0.46 mL) was added PPTS (23.3 mg, 0.093 mmol) at 0 °C, and the resultant mixture was stirred at 25 °C for 30 min. The reaction was quenched with saturated aq. NaHCO₃ (10 mL), and the mixture was extracted with DCM (10 mL × 3). The combined extracts were washed with brine (10 mL) and dried over with anhydrous Na₂SO₄. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 6 : 1) to give **20c** (8.8 mg, 44%) as a white solid; **20c**: *R*_f = 0.25 (silica, PE : EtOAc = 2 : 1); [α]_D²⁰ = -41.7 (*c* = 0.12 in CHCl₃); IR (film): ν_{max} = 2951, 2928, 1733, 1717, 1456, 1436, 1383, 1300, 1273, 1258 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ = 4.00 (ddd, *J* = 11.8, 4.1, 2.1 Hz, 1H), 3.67 (s, 3H), 3.31 (dd, *J* = 11.5, 3.9 Hz, 1H), 2.69 (d, *J* = 15.0 Hz, 1H), 2.34 – 2.29 (m, 2H), 2.25 – 2.17 (m, 1H), 2.14 – 1.97 (m, 2H), 1.82 (d, *J* = 11.8 Hz, 2H), 1.84 – 1.68 (m, 3H), 1.64 – 1.57 (m, 3H), 1.42 – 1.33 (m, 4H), 1.24 (dd, *J* = 13.7, 3.8 Hz, 1H), 1.15 (tt, *J* = 13.1, 6.6 Hz, 1H), 1.05 (d, *J* = 4.4 Hz, 1H), 1.01 (s, 3H), 1.00 (s, 3H), 0.94 (s, 3H), 0.91 (d, *J* = 6.6 Hz, 3H), 0.82 (s, 3H), 0.53 (d, *J* = 4.4 Hz, 1H) ppm; ¹³C NMR (400 MHz, CDCl₃): δ = 174.66, 138.83, 125.23, 78.24, 75.07, 51.42, 51.40, 50.58, 44.03, 39.94, 37.93, 37.77, 35.99, 34.82, 29.89, 29.43, 25.82, 25.37, 24.39, 23.82, 22.79, 22.13, 19.70, 18.58, 18.14, 16.52, 13.56 ppm; HRMS (*m/z*): [M+Na]⁺ calcd for C₂₇H₄₂O₄Na⁺ 453.2975 found 453.2972.



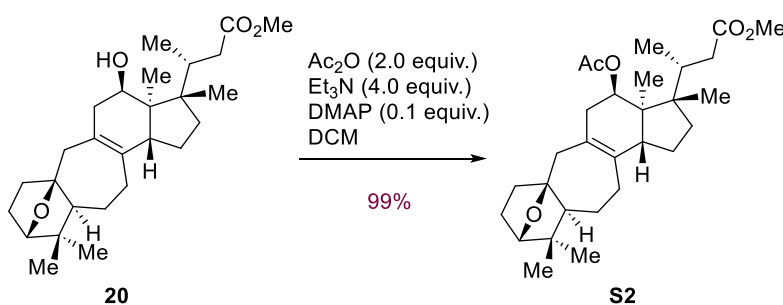
To a stirred solution of **19** (20.0 mg, 0.046 mmol) in DCM (0.46 mL) was added TsOH·H₂O (8.0 mg, 0.046 mmol) at 0 °C, and the resultant mixture was stirred at 0 °C for 30 min. The reaction was quenched with saturated aq. NaHCO₃ (10 mL), and the mixture was extracted with DCM (10 mL × 3). The combined extracts were washed with brine (10 mL) and dried over with anhydrous Na₂SO₄. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 6 : 1) to give **20d** (8.4 mg, 42%) as a white solid; **20d**: *R*_f = 0.21 (silica, PE : EtOAc = 2 : 1); [α]_D²⁰ = -10.5 (*c* = 0.11 in CHCl₃); IR (film): ν_{max} = 2961, 2926, 2852, 1732, 1539, 1435, 1377, 1298, 1261, 1059 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ = 5.53 (s, 1H), 3.99 (d, *J* = 10.2 Hz, 1H), 3.68 (s, 3H), 3.24 (dd, *J* = 11.6, 3.7 Hz, 1H), 2.53 – 2.46 (m, 3H), 2.42 (dd, *J* = 16.7, 5.7 Hz, 1H), 2.34 (d, *J* = 16.3 Hz, 1H), 2.22 – 2.15 (m, 2H), 1.94 (dd, *J* = 16.3, 3.5 Hz, 1H), 1.82 – 1.61 (m, 3H), 1.67 – 1.58 (m, 2H), 1.58 – 1.47 (m, 2H), 1.43 (d, *J* = 10.5 Hz, 1H), 1.21 (dd, *J* = 13.0, 4.0 Hz, 1H), 1.16 (dd, *J* = 12.4, 1.9 Hz, 1H), 1.05 (s, 3H), 1.03 (s, 6H), 0.92 (d, *J* = 6.4 Hz, 3H), 0.91 (s, 3H), 0.84 (s, 3H) ppm; ¹³C NMR (400 MHz, CDCl₃): δ = 174.14, 144.43, 137.46, 123.28, 120.68, 78.72, 72.22, 53.41, 51.50, 51.42, 50.58, 45.84, 38.86, 38.30, 37.65, 35.18, 34.34, 33.61, 27.98, 27.50, 27.00,

19.42, 19.10, 18.46, 18.16, 16.32, 15.51 ppm; HRMS (m/z): $[M+Na]^+$ calcd for $C_{27}H_{42}O_4Na^+$ 453.2975 found 453.2977.



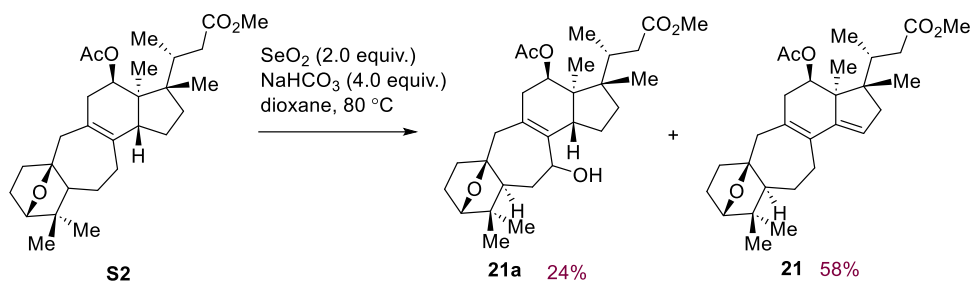
To a stirred solution of **20c** (10.0 mg, 0.023 mmol) in DCM (0.23 mL) was added $TsOH \cdot H_2O$ (5.3 mg, 0.028 mmol) at 0 °C, and the resultant mixture was stirred at 15 °C for 30 min. The reaction was quenched with saturated aq. $NaHCO_3$ (5 mL), and the mixture was extracted with DCM (5 mL \times 3). The combined extracts were washed with brine (10 mL) and dried over with anhydrous Na_2SO_4 . The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 6 : 1) to give **20d** (9 mg, 90%) as a white solid.

To a stirred solution of **20c** (10.0 mg, 0.023 mmol) in DCM (0.23 mL) was added $Sc(OTf)_3$ (13.7 mg, 0.028 mmol) at 0 °C, and the resultant mixture was stirred at 15 °C for 30 min. The reaction was quenched with saturated aq. $NaHCO_3$ (5 mL), and the mixture was extracted with DCM (5 mL \times 3). The combined extracts were washed with brine (10 mL) and dried over with anhydrous Na_2SO_4 . The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 6 : 1) to give **20d** (6 mg, 60%) as a white solid.



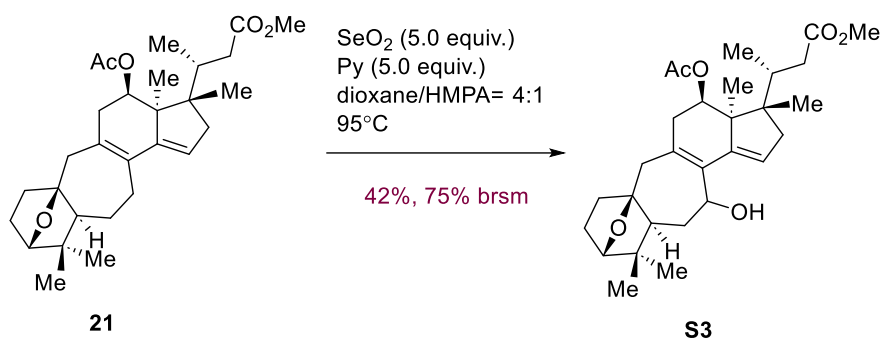
To a stirred solution of **20** (7.5 g, 17.4 mmol) in DCM (34.8 mL) were sequentially added DMAP (213 mg, 1.7 mmol), Et_3N (9.7 mL, 69.7 mmol) and Ac_2O (3.3 mL, 34.8 mmol) at 0 °C. The reaction mixture was allowed to stirred at 25 °C for 30 min, The reaction was quenched with MeOH (5 mL), The solvent was evaporated under vacuum. and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 6 : 1) to give **S2** (8.14 g, 99%) as a white solid. **S2**: R_f = 0.44 (silica, PE : EtOAc = 3 : 1); $[\alpha]_D^{20} = -7.3$ ($c = 0.24$ in $CHCl_3$); IR (film): $\nu_{max} = 2956, 2870, 1733, 1683, 1568, 1507, 1456, 1363, 1173$ cm^{-1} ; 1H NMR (400 MHz, $CDCl_3$): $\delta = 5.18$ (d, $J = 2.9$ Hz, 1H), 3.72 (d, $J = 5.5$ Hz, 1H), 3.65 (s, 3H), 3.14 (d, $J = 14.0$

Hz, 1H), 2.96 (t, $J = 10.1$ Hz, 1H), 2.54 – 2.46 (m, 2H), 2.41 – 2.27 (m, 1H), 2.30 – 2.22 (m, 1H), 2.01 (s, 3H), 1.98 – 1.85 (m, 2H), 1.79 – 1.67 (m, 4H), 1.79 – 1.67 (m, 4H), 1.47 – 1.38 (m, 4H), 1.25 (d, $J = 12.2$ Hz, 1H), 1.01 (s, 3H), 0.94 (s, 3H), 0.87 (s, 3H), 0.86 (s, 3H), 0.84 (d, $J = 6.6$ Hz, 3H) ppm; ^{13}C NMR (101 MHz, CDCl_3): $\delta = 174.11, 170.55, 132.60, 120.81, 90.25, 84.96, 74.00, 55.31, 51.58, 48.47, 47.72, 45.61, 42.76, 40.99, 38.91, 38.03, 36.86, 36.58, 35.69, 33.31, 25.70, 25.15, 23.34, 22.80, 22.77, 22.06, 19.27, 16.63, 15.28$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{29}\text{H}_{44}\text{O}_5\text{Na}^+$ 495.3081 found 495.3084.

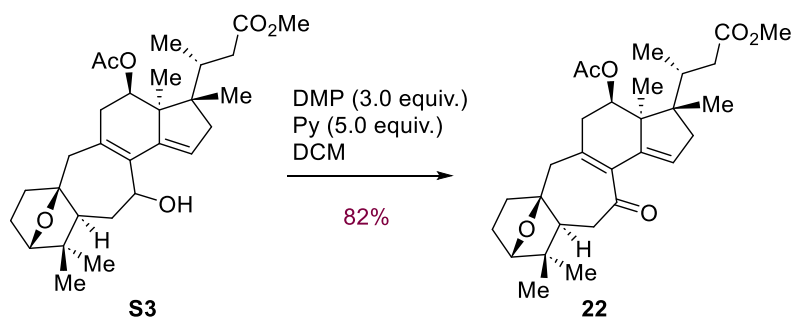


To a stirred solution of **S2** (6.4 g, 13.5 mmol) in dioxane (135 mL) were sequentially added NaHCO_3 (4.55 g, 54.2 mmol) and SeO_2 (3.0 g, 27.1 mmol) at 25 °C. The resultant mixture was allowed to stir at 80 °C for 30 min before it was filtered. The solvent was evaporated under vacuum. The residue was purified by a flash column chromatography (silica gel, PE : EtOAc = 6 : 1 \rightarrow 1 : 1) to give **21a** (1.5 g, 24%) and **21** (3.69 g, 58%) as a white solid. **21a**: $R_f = 0.11$ (silica, PE : EtOAc = 3 : 1); $[\alpha]_D^{20} = -28.7$ ($c = 0.3$ in CHCl_3); IR (film): $\nu_{\text{max}} = 2962, 1733, 1717, 1457, 1436, 1373, 1259, 1099, 1024, 1026 \text{ cm}^{-1}$; ^1H NMR (400 MHz, CDCl_3) $\delta = 5.19$ (d, $J = 4.0$ Hz, 1H), 4.11 (t, $J = 9.0$ Hz, 1H), 3.80 (d, $J = 5.5$ Hz, 1H), 3.66 (s, 3H), 3.29 (t, $J = 10.3$ Hz, 1H), 3.20 (d, $J = 13.8$ Hz, 1H), 2.59 – 2.48 (m, 2H), 2.35 – 2.24 (m, 1H), 2.06 (d, $J = 3.2$ Hz, 1H), 2.03 (s, 3H), 1.99 – 1.88 (m, 4H), 1.81 (d, $J = 13.8$ Hz, 2H), 1.74 (d, $J = 12.4$ Hz, 2H), 1.54 – 1.36 (m, 5H), 1.11 (d, $J = 12.2$ Hz, 1H), 1.03 (s, 3H), 0.99 (s, 3H), 0.91 (s, 3H), 0.87 (d, $J = 6.5$ Hz, 3H), 0.84 (s, 3H) ppm; ^{13}C NMR (400 MHz, CDCl_3): $\delta = 173.96, 170.44, 134.17, 125.59, 88.65, 85.37, 73.48, 73.37, 51.47, 50.45, 48.32, 47.48, 45.19, 41.36, 40.43, 38.61, 37.88, 36.81, 36.17, 35.59, 32.77, 25.57, 24.94, 23.35, 21.88, 19.13, 16.51, 14.95$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{29}\text{H}_{44}\text{O}_6\text{Na}^+$ 511.3030 found 511.3035.

21: $R_f = 0.42$ (silica, PE : EtOAc = 3 : 1); $[\alpha]_D^{20} = -14.3$ ($c = 0.21$ in CHCl_3); IR (film): $\nu_{\text{max}} = 2956, 1733, 1698, 1461, 1437, 1373, 1258, 1200, 1174, 1019, 794 \text{ cm}^{-1}$; ^1H NMR (400 MHz, CDCl_3): $\delta = 5.47$ (s, 1H), 5.20 (s, 1H), 3.75 (d, $J = 5.4$ Hz, 1H), 3.67 (s, 3H), 3.27 (d, $J = 14.0$ Hz, 1H), 2.72 (t, $J = 18.3$ Hz, 2H), 2.44 (d, $J = 14.5$ Hz, 2H), 2.35 (d, $J = 16.1$ Hz, 2H), 2.10 – 2.01 (m, 4H), 1.98 (s, 3H), 1.97 – 1.88 (m, 1H), 1.85 (d, $J = 14.0$ Hz, 1H), 1.77 – 1.66 (m, 2H), 1.58 – 1.52 (m, 2H), 1.22 (d, $J = 13.8$ Hz, 1H), 1.01 (s, 3H), 0.97 (s, 3H), 0.96 (s, 3H), 0.89 (d, $J = 6.6$ Hz, 3H), 0.88 (s, 3H) ppm; ^{13}C NMR (400 MHz, CDCl_3): $\delta = 174.01, 170.89, 146.01, 126.81, 125.68, 119.02, 89.61, 85.09, 73.47, 54.78, 51.60, 51.52, 51.27, 46.00, 45.48, 40.27, 38.20, 36.99, 36.51, 35.30, 30.98, 25.65, 25.19, 23.37, 22.89, 22.10, 19.53, 18.09, 16.46$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{29}\text{H}_{42}\text{O}_5\text{Na}^+$ 493.2924 found 493.2929.

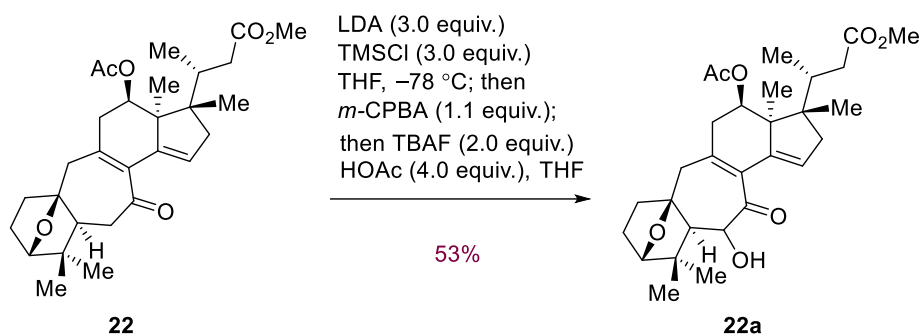


To a stirred solution of **21** (3.0 g, 6.37 mmol) in dioxane/HMPA = 4:1 (64 mL) was sequentially added pyridine (2.6 mL, 31.9 mmol) and SeO_2 (3.5 g, 31.9 mmol) at 95 °C. The resultant mixture was allowed to stir at 95 °C for 1.5 h before it was filtered. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 4:1 → 1:1) to **S3** (1.3 g, 42%, 75% brsm) and **21** (1.32 g) as a white solid. **S3**: R_f = 0.11 (silica, petroleum ether : EtOAc = 3 : 1); $[\alpha]_D^{25} = -17.0$ ($c = 0.33$ in CHCl_3); IR (film): $\nu_{\text{max}} = 3420, 2961, 2926, 1732, 1468, 1435, 1371, 1259, 1019 \text{ cm}^{-1}$; $^1\text{H NMR}$ (400 MHz, CDCl_3): $\delta = 5.72$ (s, 1H), 5.20 (s, 1H), 4.55 (t, $J = 9.2$ Hz, 1H), 3.79 (d, $J = 5.3$ Hz, 1H), 3.34 (d, $J = 14.1$ Hz, 1H), 2.75 (d, $J = 19.5$ Hz, 1H), 2.50 – 2.35 (m, 3H), 2.17 – 1.90 (m, 8H), 1.97 (s, 3H), 1.81 – 1.72 (m, 3H), 1.47 – 1.36 (m, 3H), 1.10 – 1.05 (m, 1H), 1.01 (s, 3H), 0.99 (s, 3H), 0.95 (s, 3H), 0.90 (s, 6H) ppm; $^{13}\text{C NMR}$ (101 MHz, CDCl_3): $\delta = 173.94, 170.84, 144.70, 129.63, 129.48, 120.23, 88.33, 85.61, 72.68, 72.25, 51.66, 51.63, 51.39, 50.14, 46.01, 45.27, 40.48, 38.18, 36.83, 36.21, 35.31, 32.23, 25.63, 25.09, 23.50, 22.02, 19.30, 18.01, 16.47$ ppm; HRMS (m/z): $[\text{M}+\text{H}]^+$ calcd for $\text{C}_{29}\text{H}_{42}\text{O}_6\text{Na}^+$ 509.2874 found 509.2881.



A solution of DMP (2.9 g, 6.78 mmol) in DCM (24 mL) was treated with pyridine (0.91 mL, 11.3 mmol) at 0 °C and stirred for 5 min. To this reaction mixture a solution of **S3** (1.1 g, 2.26 mmol) in DCM (113 mL) was added at 0 °C. The resultant mixture was allowed to stir at 25 °C for 1 h. The reaction was quenched with saturated aq. NaHCO_3 (50 mL), and the mixture was extracted with EtOAc (100 mL × 3). The combined extracts were washed with brine (50 mL) and dried over with anhydrous Na_2SO_4 . The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 3 : 1) to **22** (902 mg, 82%) as a white solid; **22**: R_f = 0.19 (silica, PE : EtOAc = 3 : 1); $[\alpha]_D^{25} = -54.2$ ($c = 0.16$ in CHCl_3); IR (film): $\nu_{\text{max}} = 2962, 2926, 1732, 1671, 1465, 1436, 1371, 1260, 1099, 1029, 803 \text{ cm}^{-1}$; $^1\text{H NMR}$

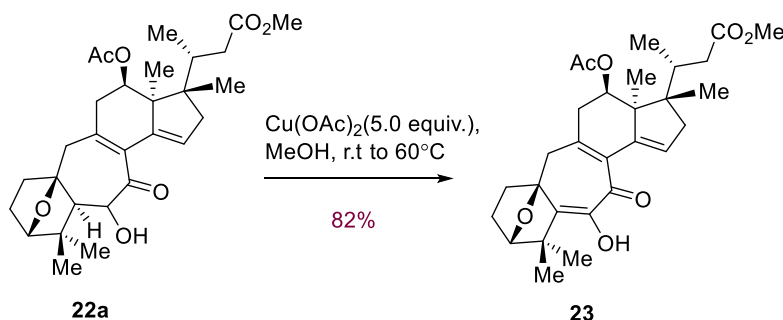
(400 MHz, CDCl₃): δ = 6.08 (s, 1H), 5.22 (s, 1H), 3.85 (d, J = 5.3 Hz, 1H), 3.66 (s, 3H), 3.13 (d, J = 13.4 Hz, 1H), 2.90 (d, J = 20.0 Hz, 1H), 2.55 – 2.38 (m, 4H), 2.31 (dd, J = 18.8, 8.2 Hz, 2H), 2.18 (d, J = 13.5 Hz, 1H), 2.12 – 1.97 (m, 4H), 1.94 (s, 3H), 1.82 – 1.71 (m, 1H), 1.52 (td, J = 6.4, 6.0, 3.0 Hz, 4H), 1.02 (s, 3H), 0.97 (s, 3H), 0.96 (s, 3H), 0.89 (s, 3H), 0.88 (d, J = 6.7 Hz, 1H) ppm; ¹³C NMR (101 MHz, CDCl₃): δ = 203.45, 173.87, 170.84, 138.55, 137.98, 131.91, 125.36, 87.10, 86.54, 71.90, 51.80, 51.66, 50.80, 50.29, 46.36, 44.53, 43.13, 40.11, 38.26, 38.22, 36.03, 35.30, 25.96, 25.57, 23.83, 21.94, 19.25, 17.86, 16.50 ppm; HRMS (m/z): [M+Na]⁺ calcd for C₂₉H₄₀O₆Na⁺ 507.2717 found 507.2719.



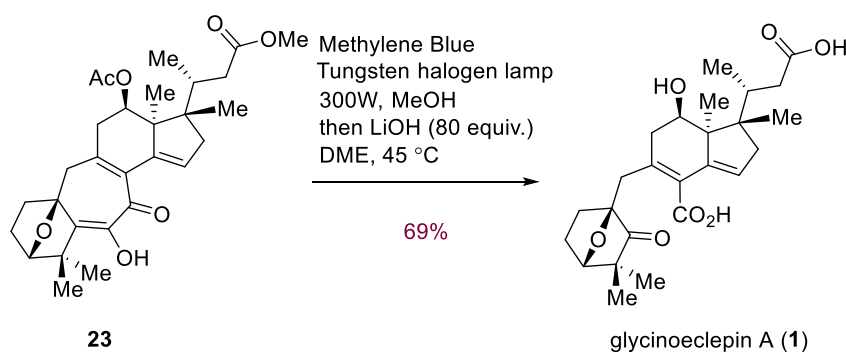
To a stirred solution mixture of **22** (830 mg, 1.71 mmol) in THF (34 mL) was sequentially added LDA (10.3 mL, 5.1 mmol, 0.5 M in THF) at -78 °C, and the resultant mixture was stirred at -78 °C for 30 min. To this solution TMSCl (0.65 mL, 5.1 mmol) was added and the resulting mixture was stirred for 30 min. The reaction was quenched with saturated aq. NaHCO₃ (50 mL) and the mixture was extracted with EtOAc (100 mL \times 3). The combined extracts were washed with brine (50 mL) and dried over with anhydrous Na₂SO₄. The solvent was evaporated under vacuum to give crude product and was used for the next step without further purification. To a stirred solution of above crude product in DCM (91 mL) was sequentially added *m*-CPBA (405 mg, 2.0 mmol, 85%) at 0 °C. The reaction mixture was allowed to stirred at 0 °C for 30 min. The reaction was quenched with ethyl vinyl ether (0.19 mL, 2.0 mmol). The solvent was evaporated under vacuum to give crude product and was used for the next step without further purification.

To a stirred solution mixture of above crude product in THF (36 mL) was sequentially added HOAc (0.4 mL, 7.3 mmol) and TBAF (3.6 mL, 3.6 mmol, 1 M in THF) at 0 °C, and the resultant mixture was stirred at 0 °C for 10 h. The reaction was quenched with saturated aq. NaHCO₃ (50 mL), and the mixture was extracted with EtOAc (50 mL \times 3). The combined extracts were washed with brine (50 mL), and dried over with anhydrous Na₂SO₄. The solvent was evaporated under vacuum to give crude product and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 3 : 1) to give **22a** (474 mg, 53%) as a white solid. **22a**: R_f = 0.29 (silica, PE : EtOAc = 3 : 1). $[\alpha]_D^{25}$ = -78.1 (c = 0.1 in CHCl₃); IR (film): ν_{max} = 3439, 2961, 2924, 1733, 1664, 1457, 1373, 1260, 1094, 1022 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ = 6.55 (s, 1H), 5.25 (s, 1H), 4.14 (d, J = 11.8 Hz, 2H), 3.87 (d, J = 5.6 Hz, 1H), 3.68 (s, 3H), 3.19 (d, J = 14.4 Hz, 1H), 2.98 (d, J = 20.0 Hz, 1H), 2.44 – 2.34 (m, 5H), 2.11 – 2.08 (m, 2H), 2.04 – 1.99 (m, 1H), 1.97 (s, 3H), 1.84 – 1.76 (m, 2H),

1.50 (td, $J = 10.7, 9.5, 3.5$ Hz, 1H), 1.38 (s, 3H), 1.21 (dd, $J = 17.8, 9.9$ Hz, 1H), 1.10 (s, 3H), 0.96 (s, 3H), 0.91 (d, $J = 5.2$ Hz, 3H), 0.91(s, 3H) ppm; ^{13}C NMR (101 MHz, CDCl_3): $\delta = 202.85, 173.72, 170.65, 144.69, 137.86, 129.19, 127.49, 86.63, 86.16, 76.71, 71.58, 54.70, 52.22, 51.57, 50.24, 47.69, 46.42, 41.53, 39.08, 38.12, 36.83, 35.18, 25.03, 24.84, 23.53, 21.80, 19.07, 17.75, 16.40$. ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{29}\text{H}_{40}\text{O}_7\text{Na}^+$ 523.2666 found 523.2663.



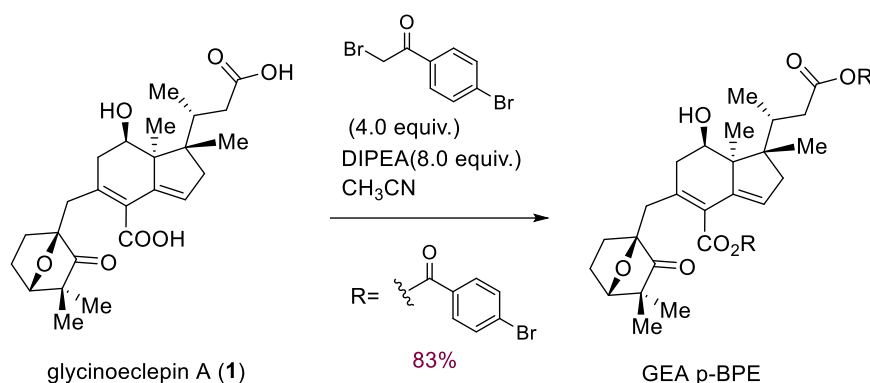
To a stirred solution of **22a** (120 mg, 0.24 mmol) in MeOH (24 mL) was sequentially added $\text{Cu}(\text{OAc})_2$ (217 mg, 1.2 mmol) at 25 °C, and the resultant mixture was stirred at 25 °C for 5 h, then the resultant mixture was stirred at 60 °C for 1 h. The reaction was quenched with saturated aq. NaHCO_3 and extracted with DCM (20 mL \times 3). The combined extracts were washed with brine (20 mL) and dried over anhydrous Na_2SO_4 . The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, PE : EtOAc = 5 : 1) to give **23** (98 mg, 82%) as a white solid. **23**: $R_f = 0.47$ (silica, PE : EtOAc = 3 : 1); $[\alpha]_D^{25} = +51.7$ ($c = 0.12$ in CHCl_3); IR (film): $\nu_{\text{max}} = 3383, 2961, 2965, 1734, 1604, 1457, 1373, 1260, 1092, 1020$ cm^{-1} ; ^1H NMR (400 MHz, CDCl_3): $\delta = 6.59$ (s, 1H), 6.07 (s, 1H), 5.27 (s, 1H), 4.03 (d, $J = 5.0$ Hz, 1H), 3.68 (s, 3H), 3.26 (d, $J = 14.1$ Hz, 1H), 2.89 (d, $J = 20.4$ Hz, 1H), 2.44 – 2.31 (m, 2H), 2.27 (d, $J = 14.2$ Hz, 1H), 2.15 – 2.04 (m, 3H), 1.98 (s, 3H), 1.96 – 1.92 (m, 1H), 1.83 – 1.70 (m, 2H), 1.60 – 1.54 (m, 2H), 1.40 (s, 3H), 1.27 (s, 3H), 0.99 (s, 3H), 0.94 (s, 3H), 0.91 (d, $J = 6.7$ Hz, 3H) ppm; ^{13}C NMR (101 MHz, CDCl_3): $\delta = 187.17, 173.75, 170.74, 143.55, 140.68, 138.63, 136.70, 130.63, 126.01, 86.29, 85.40, 71.68, 51.90, 51.57, 50.79, 48.97, 46.10, 41.00, 39.47, 38.09, 35.19, 31.81, 25.03, 24.23, 21.82, 20.81, 18.90, 17.74, 16.37$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{29}\text{H}_{38}\text{O}_7\text{Na}^+$ 521.2510 found 521.2513.



To a stirred solution of **23** (30 mg, 0.06 mmol) in MeOH (6.0 mL) was sequentially added methylene blue (4.0

mg, 0.012 mmol) at 25 °C, and the resultant mixture was irradiated with a 300 W tungsten halogen lamp for 8 h under oxygen atmosphere. The solvent was evaporated under vacuum to give crude product.

To a stirred solution of above crude product in DME (6.0 mL) was sequentially added LiOH (4.8 mL, 4.78 mmol, 1.0 M in H₂O) at 25 °C, and the resultant mixture was stirred at 45 °C for 8 h. The reaction was quenched by addition of 2.0 M H₂SO₄ at 0 °C and extracted with EtOAc (50 mL × 3). The combined extracts were washed with brine (50 mL) and dried over with anhydrous MgSO₄. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, DCM → PE : EtOAc = 10 : 1) to give glycinoclepin A (**1**) (18 mg, 69%) as a solid. glycinoclepin A (**1**): *R*_f = 0.41 (silica, EtOAc : MeOH = 1 : 1); [α]_D²⁵ = -12.3 (*c* = 0.45 in MeOH); IR (film): ν_{max} = 3419, 2918, 2849, 1705, 1538, 1463, 1385, 1339, 1177, 1017 cm⁻¹; ¹H NMR (400 MHz, CDCl₃): δ = 5.66 (s, 1H), 4.31 (d, *J* = 4.8 Hz, 1H), 4.08 (t, *J* = 2.4 Hz, 1H), 3.04 (d, *J* = 14.6 Hz, 1H), 2.90 (d, *J* = 19.0 Hz, 1H), 2.48 – 2.58 (m, 4H), 2.20 (d, *J* = 17.8 Hz, 1H), 2.16 (dd, *J* = 14.9, 12.0 Hz, 1H), 1.98 – 2.07 (m, 2H), 1.84 (tt, *J* = 11.9, 5.2 Hz, 1H), 1.77 (dd, *J* = 12.0, 3.4 Hz, 1H), 1.45 (ddd, *J* = 13.5, 9.1, 4.5 Hz, 1H), 1.20 (s, 3H), 1.17 (s, 3H), 1.06 (s, 3H), 1.00 (d, *J* = 6.8 Hz, 3H), 0.99 (s, 3H) ppm; ¹³C NMR (201 MHz, CDCl₃): δ = 218.10, 178.01, 176.42, 141.33, 134.01, 125.04, 123.39, 88.45, 83.51, 71.75, 52.62, 51.38, 48.49, 45.87, 39.66, 38.96, 35.21, 33.84, 27.65, 24.84, 22.01, 18.98, 18.42, 17.86, 15.38 ppm; HRMS (*m/z*): [M+Na]⁺ calcd for C₂₅H₃₄O₇Na⁺ 469.2197 found 469.2201.



To a stirred solution of glycinoclepin A (**1**) (3.0 mg, 0.0067 mmol) in DCM (0.13 mL) were sequentially added DIPEA (10 μL, 0.054 mmol) and 2,4'-dibromoacetophenone (7.5 mg, 0.0269 mmol) at 25 °C, and the resultant mixture was stirred at 25 °C for 1 h. The reaction was quenched by addition of saturated aq. NaHCO₃ (10 mL) and extracted with DCM (10 mL × 3). The combined extracts were washed with brine (10 mL), and dried over with anhydrous Na₂SO₄. The solvent was evaporated under vacuum, and the residue was purified by flash column chromatography (silica gel, DCM → DCM : EtOAc = 6 : 1) to give GEA p-BPE (**S4**) (4.7 mg, 83%) as a white solid. GEA p-BPE (**S4**): *R*_f = 0.30 (silica, DCM : EtOAc = 5 : 1); [α]_D²⁵ = -13.8 (*c* = 0.13 in CHCl₃); IR (film): ν_{max} = 2956, 2924, 1760, 1696, 1463, 1367, 1258, 1202, 1060 cm⁻¹; ¹H NMR (400 MHz, CDCl₃ and D₂O): δ = 7.82 (d, *J* = 7.4 Hz, 2H), 7.79 (d, *J* = 7.5 Hz, 2H), 7.65 (d, *J* = 6.1 Hz, 2H), 7.64 (d, *J* = 6.9 Hz, 2H), 6.10 (s, 1H), 5.51 (d, *J* = 16.2 Hz, 1H), 5.37 (d, *J* = 16.3 Hz, 1H), 5.32 (d, *J* = 16.3 Hz, 1H), 5.28 (d, *J* = 16.2 Hz, 1H), 4.25 (d, *J* = 5.0 Hz, 1H), 4.07 (d, *J* = 8.9 Hz, 1H), 3.01 (d, *J* = 14.5 Hz, 1H), 2.88 (d, *J* =

20.2 Hz, 1H), 2.85 (d, $J = 14.6$ Hz, 1H), 2.64 (d, $J = 14.7$ Hz, 1H), 2.61 – 2.55 (m, 1H), 2.47 (d, $J = 16.8$ Hz, 1H), 2.39 (d, $J = 10.6$ Hz, 1H), 2.36 (d, $J = 15.5$ Hz, 1H), 2.08 (dd, $J = 17.0, 3.4$ Hz, 1H), 1.93 – 1.87 (m, 1H), 1.86 – 1.79 (m, 1H), 1.79 – 1.72 (m, 1H), 1.55 (m, 1H), 1.16 (s, 3H), 1.15 (s, 3H), 1.04 (d, $J = 6.6$ Hz, 3H), 1.02 (s, 3H), 0.99 (s, 3H) ppm; ^{13}C NMR (101 MHz, CDCl_3 and D_2O): $\delta = 217.24, 191.58, 191.34, 173.08, 167.11, 139.19, 133.89, 133.11, 132.39, 129.47, 129.40, 129.29, 127.58, 126.92, 88.78, 83.82, 71.67, 66.23, 65.89, 53.66, 51.49, 49.08, 46.34, 41.18, 38.31, 35.44, 33.77, 29.83, 25.37, 23.03, 20.18, 19.42, 18.74, 16.50$ ppm; HRMS (m/z): $[\text{M}+\text{Na}]^+$ calcd for $\text{C}_{41}\text{H}_{44}\text{O}_9\text{Br}_2\text{Na}^+$ 861.1244 found 861.1254.

IV Comparison of the Spectra and Data of previous and our Synthetic GEA p-BPE (S4)

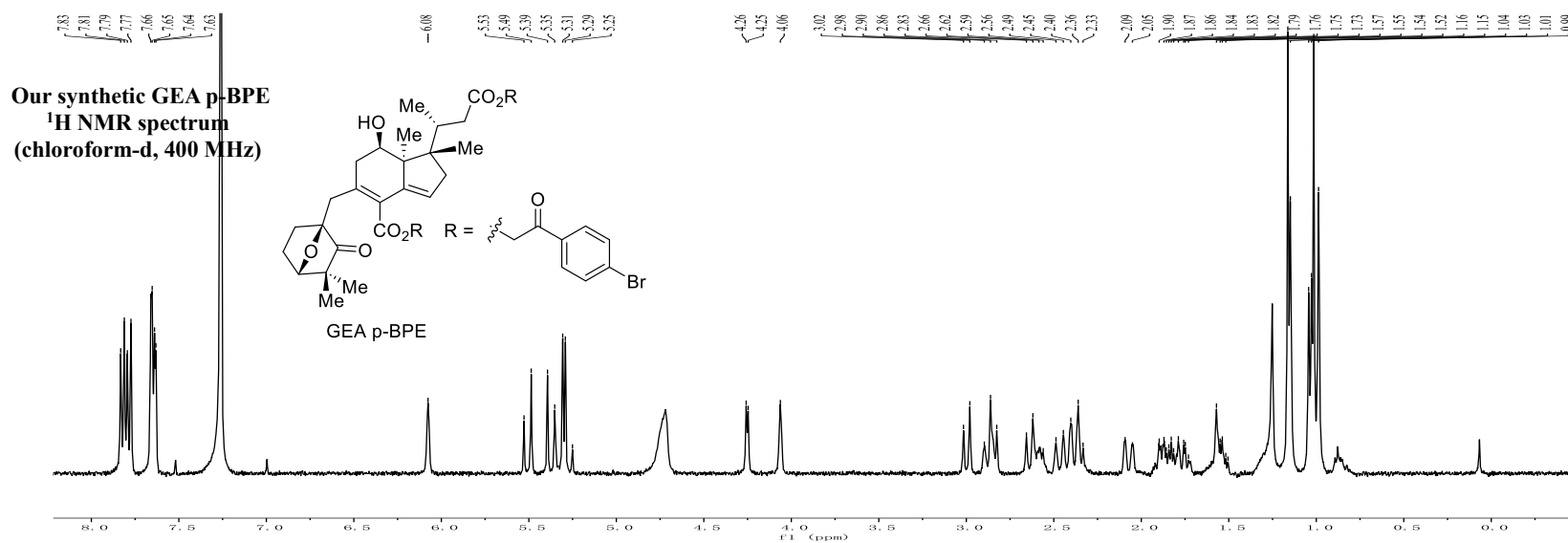
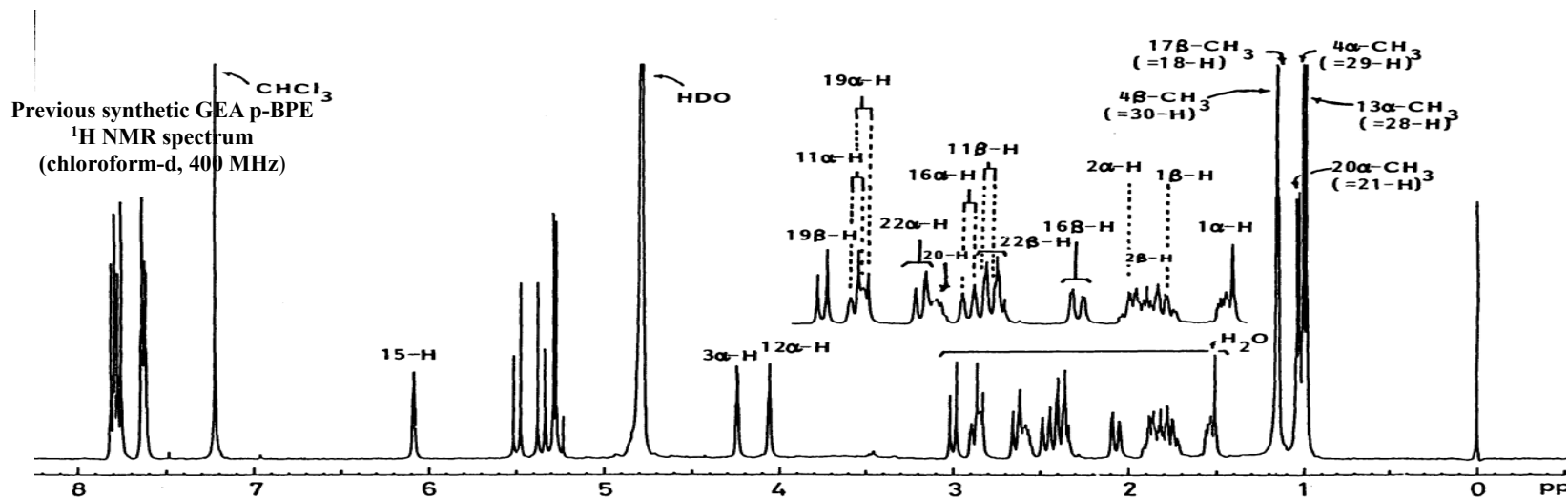
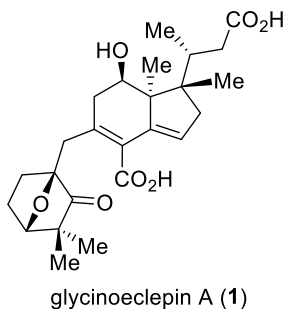
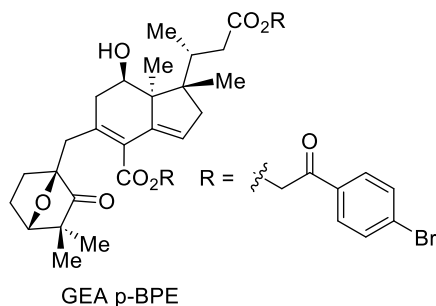


Table S1. Comparison of the ^1H NMR spectroscopic data (Methanol- d_4) of our and previous synthesis glyclnoeclepin A (**1**) (Kenii-Mori et al, *J. Chem. Soc. Perkin. Trans.* **1991**, *1*,2919)

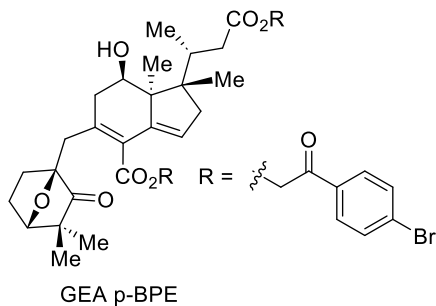


Natural		Synthetic		Err
δ_{H} [ppm, mult, J (Hz)]		δ_{H} [ppm, mult, J (Hz)]		(Natural–Synthetic)
300 MHz		400 MHz		$\Delta\delta_{\text{H}}$ (ppm)
5.66	1 H, s	5.66	1 H, s	0
4.31	1 H, d, 4.8	4.31	1 H, d, 4.8	0
4.08	1 H, br t, 2.0	4.08	1 H, br t, 2.4	0
3.04	1 H, d, 14.5	3.04	2 H, d, 14.6	0
2.90	1 H, br d, 19.0	2.90	1 H, br d, 19.0	0
2.41-2.55	4 H, m	2.48-2.58	4 H, m	–
2.20	1 H, br d, 17.0	2.20	1 H, br d, 17.8	0
2.16	1 H, dd, 15.0, 12.0	2.16	1 H, dd, 14.9, 12.0	0
1.94-2.09	1 H, m	1.98-2.07	1 H, m	–
1.84	1 H, tt, 12.0, 5.0	1.84	1 H, tt, 11.9, 5.2	0
1.77	1 H, dt, 12.0, 3.0	1.76	1 H, dd, 12.0, 3.4	+0.01
1.47	1 H, m	1.45	1 H, ddd, 13.5, 9.1, 4.5	+0.02
1.20	3 H, s	1.20	3 H, s	0
1.16	3 H, s	1.17	3 H, s	–0.01
1.05	3 H, s	1.06	3 H, s	–0.01
1.00	3 H, d, 6.0	1.00	3 H, d, 6.8	0
0.99	3 H, s	0.99	3 H, s	0

Table S2. Comparison of the ^1H NMR spectroscopic data (CDCl_3) of natural and synthetic GEA p-BPE (**S4**)

Natural		Synthetic		Err
δ_{H} [ppm, mult, J (Hz)]		δ_{H} [ppm, mult, J (Hz)]		(Natural–Synthetic)
500 MHz		400 MHz		$\Delta\delta_{\text{H}}$ (ppm)
7.83	2 H, d, 8.5	7.82	2 H, d, 8.4	–0.01
7.79	2 H, d, 8.5	7.79	2 H, d, 8.4	0
7.65	2 H, d, 8.5	7.65	2 H, d, 8.6	0
7.65	2 H, d, 8.5	7.64	2 H, d, 8.4	–0.01
6.08	1 H, dd, 3.5, 1.5	6.08	1 H, s	0
5.51	1 H, d, 16.5	5.51	1 H, d, 16.5	0
5.36	1 H, d, 16.5	5.37	1 H, d, 16.6	–0.01
5.32	1 H, d, 16.5	5.32	1 H, d, 16.3	0
5.28	1 H, d, 16.5	5.28	1 H, d, 16.4	0
4.26	1 H, d, 5.0	4.25	1 H, d, 5.0	–0.01
4.07	1 H, dd, 3, 1.5	4.06	1 H, s	–0.01
3.00	1 H, d, 14.5	3.01	1 H, d, 14.5	–0.01
2.86	1 H, dd, 18, 3	2.88	1 H, d, 19.3	0
2.85	1 H, d, 14.5	2.85	1 H, d, 14.5	0
2.64	1 H, br d, 14.5	2.64	1 H, d, 14.6	0
2.58	1 H, dq, 11.5, 6.5	2.58	1 H, m	0
2.47	1 H, dd, 17, 1.5	2.47	1 H, d, 16.8	0
2.39	1 H, dd, 18, 1.5	2.39	1 H, d, 18.2	0
2.37	1 H, dd, 14.5, 11.5	2.36	1 H, d, 14.8	–0.01
2.08	1 H, dd, 17.0, 3.5	2.08	1 H, dd, 17.0, 3.4	0
1.90	1 H, ddd, 12, 9, 5	1.90	1 H, m	0

1.84	1 H, dddd, 12, 10, 5, 4	1.83	1 H, m	-0.01
1.76	1 H, ddd, 12, 10, 5	1.76	1 H, m	0
1.54	1 H, ddd, 12, 9, 4	1.55	1 H, m	-0.01
1.17	3 H, s	1.16	3 H, s	-0.01
1.15	3 H, s	1.15	3 H, s	0
1.04	3 H, d, 6.5	1.04	3 H, d, 6.6	0
1.02	3 H, s	1.02	3 H, s	0
0.99	br s	0.99	3 H, s	0

Table S3. Comparison of the ^{13}C NMR spectroscopic data (CDCl_3) of natural and synthetic GEA p-BPE (**S4**)

Natural δ_{C} (ppm) 126 MHz	Synthetic δ_{C} (ppm) 201 MHz	Err (Natural–Synthetic) $\Delta\delta_{\text{C}}$ (ppm)
217.1	217.1	0
191.4	191.4	0
191.2	191.2	0
172.9	172.9	0
167.1	167.0	+0.1
139.1	139.0	+0.1
133.8	133.7	+0.1
133.0	133.0	0
132.2	132.2	0
129.3	129.3	0
129.2	129.2	0
129.1	129.1	0
127.4	127.4	0
126.7	126.8	-0.1
88.6	88.6	0
83.7	83.7	0
71.5	71.5	0
66.1	66.1	0
65.7	65.7	0
53.5	53.5	0
51.4	51.4	0

48.9	48.9	0
46.2	46.2	0
41.1	41.0	0
38.2	38.2	0
35.3	35.3	0
33.6	33.6	0
29.7	29.7	0
25.2	25.2	0
22.9	22.9	0
20.0	20.0	0
19.3	19.3	0
18.6	18.6	0
16.4	16.4	0

V DFT calculation

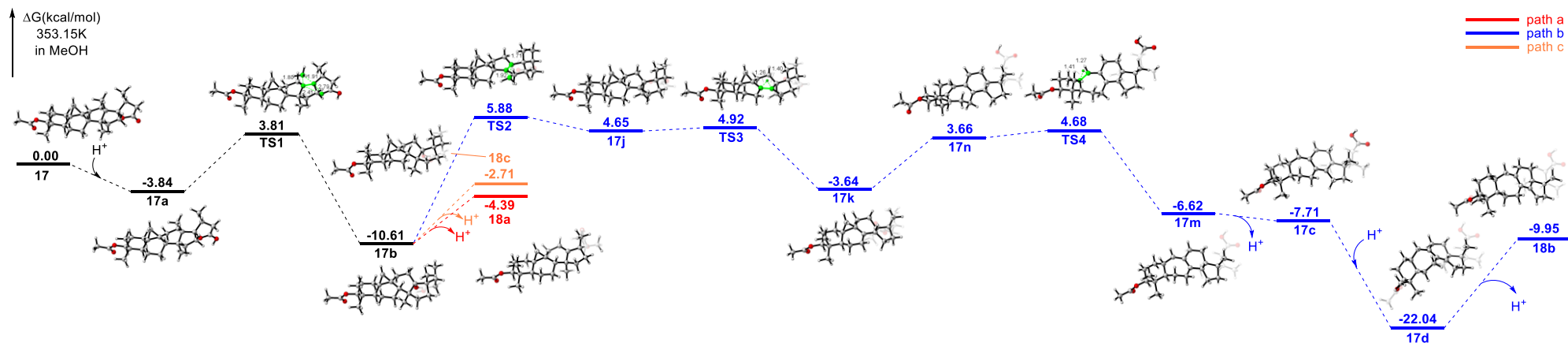
Computational Methods

Geometry optimizations and frequency calculations of stationary points were carried out by using Gaussian 16 Rev. A.03.[1] Geometry optimizations and frequency calculations of stationary points were performed at B3LYP[2] level of theory in gas phase with def2-SVP[3] basis set for all atoms. Empirical dispersion correction has been considered by using Grimme's DFT empirical dispersion correction with the Becke-Jonson (D3BJ) damping function.[4][4] Frequency calculations were conducted at the same level of theory to confirm the presence of local minima (no imaginary frequencies) and transition states (one imaginary frequency) on the PES. Subsequent higher level of single point energies for those structures were calculated at M06-2X-D3[5]/def2-TZVPP[3] level. Solvent effect was modelled by employing the SMD model at the level of M05-2X/6-31G(d),[6] with MeOH as the solvent for the Wagner–Meerwein rearrangement and HFIP as the solvent for the Meinwald rearrangement. Intrinsic reaction coordinate (IRC) calculations were performed to verify that the saddle points found were true TSs connecting the reactants and the products.[7] The thermal correction to the Gibbs free energy was calculated at 353.15 K or 273.15 K and 1 atm using unscaled harmonic frequencies. The calculation of ΔG_{gas} uses a reference state of 1 atm and the calculations of ΔG_{s} use a reference state of 1M. Based on the ΔG_{gas} reference state (28.98 L at 353.15 K or 22.41 L at 273.15 K) from 1 atm to 1M, the Gibbs free energy can be computed by using the equation $\Delta G_{\text{gas}}(1\text{M}) = \Delta G_{\text{gas}}(1\text{ atm}) + RT\ln(28.98/22.41) = \Delta G_{\text{gas}}(1\text{ atm}) + 2.36/1.69\text{ kcal/mol}$. [8] The 3D diagrams of optimized structures were generated with CYLview 2.0.[9]

Note: as HFIP is not by default parametrized within the SMD model implemented in Gaussian, the following parameters were used following a report by Paton and coworkers[10]: $\epsilon_{\text{ps}} = 16.7$; $\epsilon_{\text{psinf}} = 1.625626$; H Bond Acidity = 1.96; h bond basicity = 0.00; Surface Tension At Interface = 23.23; Electronegative Halogenicity = 0.6; Carbon Aromaticity = 0.00

Supplementary Calculation Data

Figure S1. DFT-computed free-energy profiles of the Wagner–Meerwein rearrangement. (SMD(MeOH)-M06-2X-D3/def2-TZVPP//B3LYP-D3(BJ)/def2-SVP, $t = 353.15\text{K}$, MeOH_2^+ was used as the proton source, set 17 and MeOH_2^+ as zero point, $\Delta G/\Delta G^\ddagger$ values are given in $\text{kcal}\cdot\text{mol}^{-1}$).



Scheme S3. The reaction pathway of the Wagner–Meerwein rearrangement

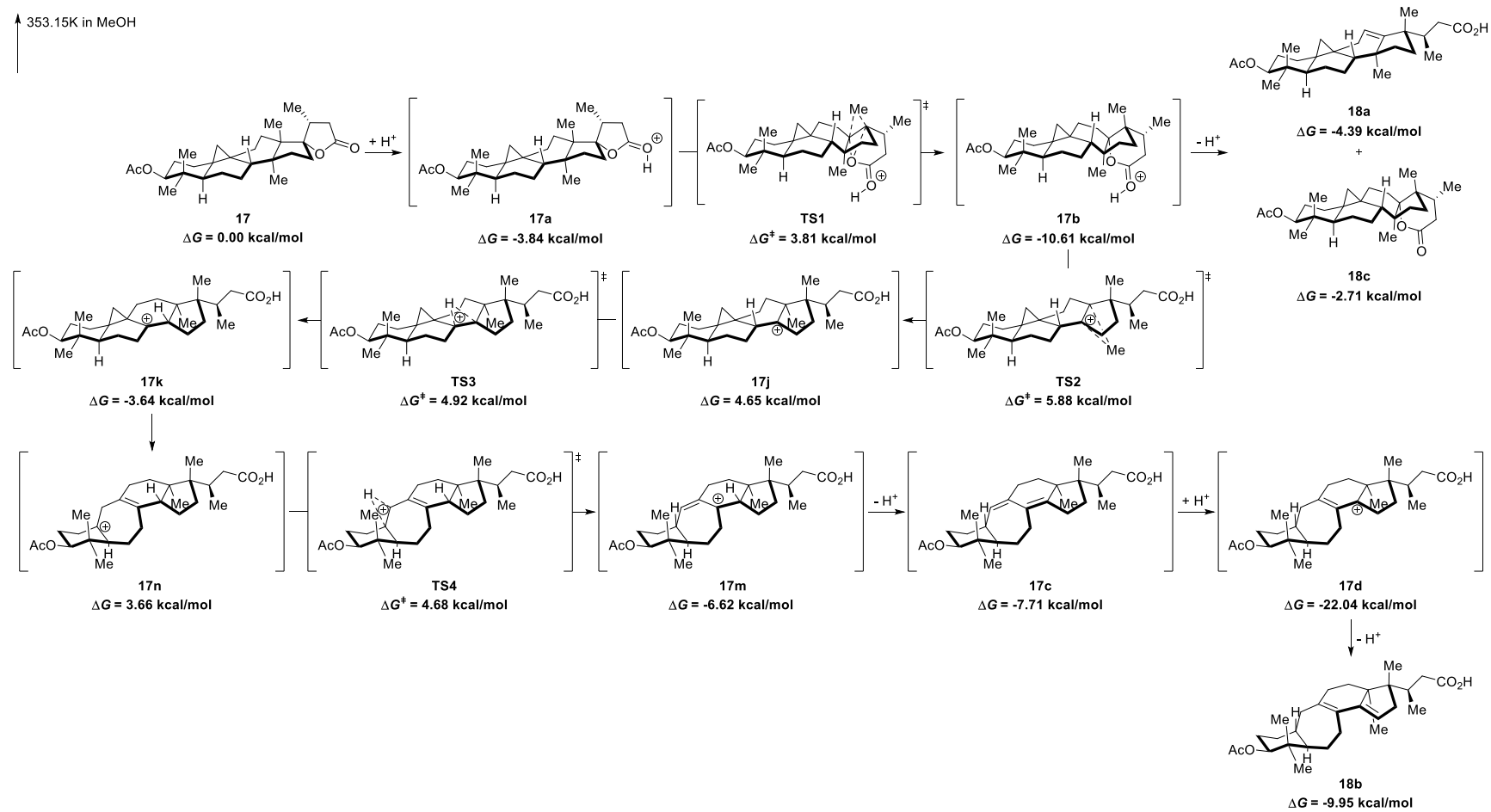
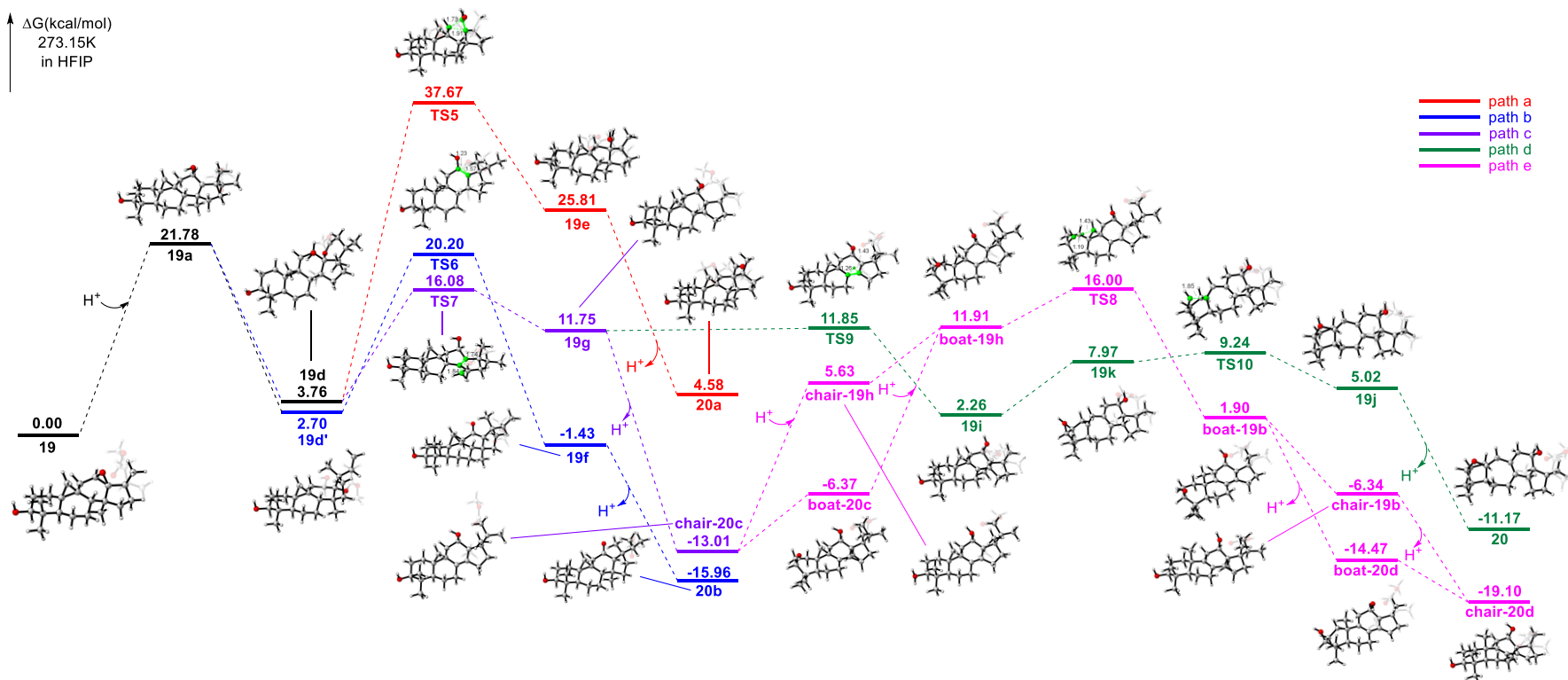
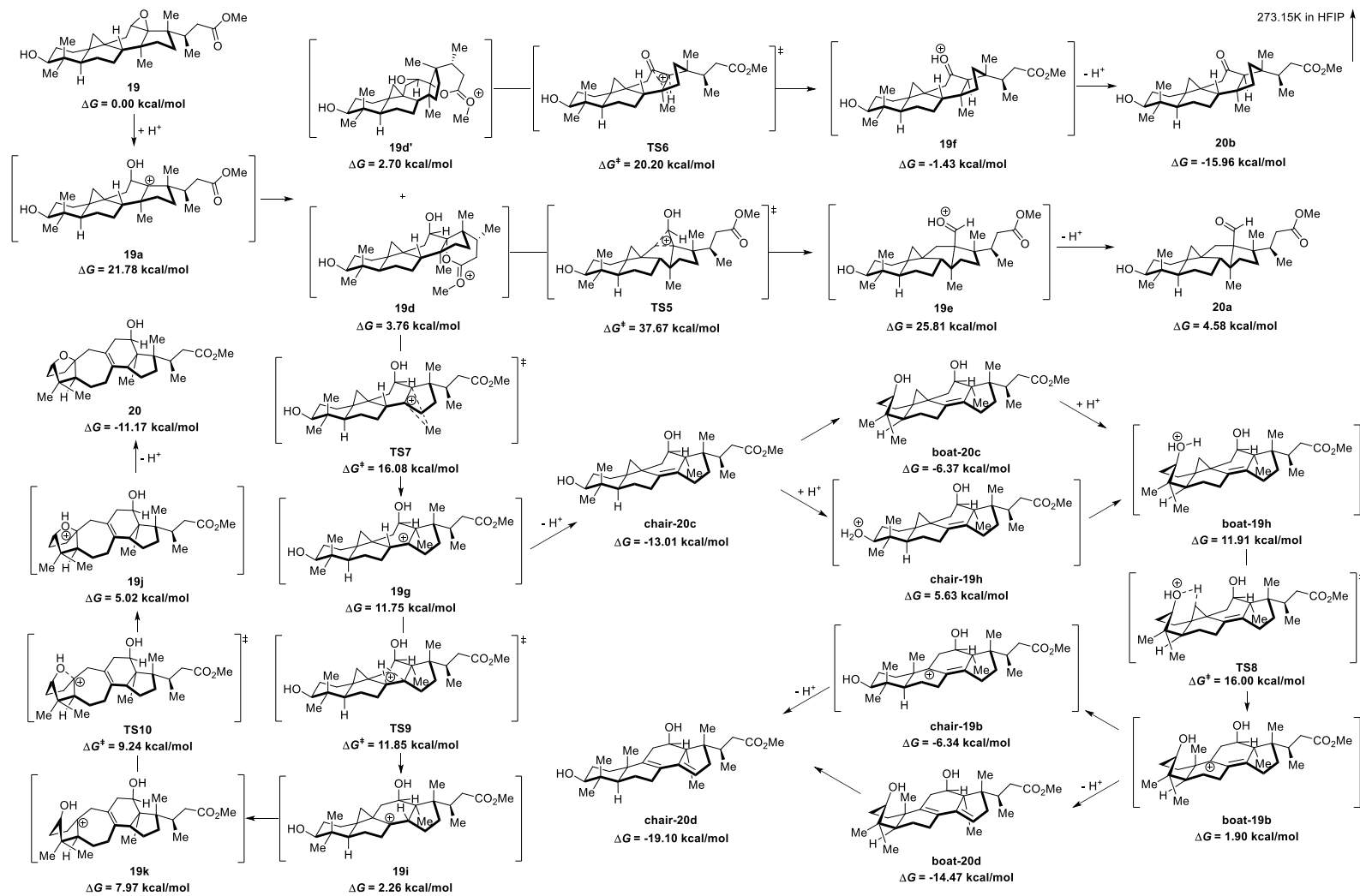


Figure S2. DFT-computed free-energy profiles of the Meinwald rearrangement. (SMD(HFIP)-M06-2X-D3/def2-TZVPP//B3LYP-D3(BJ)/def2-SVP, $t = 273.15\text{K}$, PyH^+ was used as the proton source, set 19 and PyH^+ as zero point, $\Delta G/\Delta G^\ddagger$ values are given in $\text{kcal}\cdot\text{mol}^{-1}$).



Scheme S4. The reaction pathway of the Meinwald rearrangement.



Cartesian Coordinates and Energies

17

Thermal correction to Gibbs free energy (Hartree): 0.583396

Single point energy (Hartree): -1393.147293

Solvation Gibbs free energy (Hartree): -0.028864

G_{sol} (Hartree): -1392.592761

C	2.30298800	-1.54496300	-0.36151700
C	3.76037400	-1.61102900	0.09987600
C	4.51879000	-0.34798800	-0.28593600
C	3.87850000	0.96057200	0.22961600
C	2.40318300	0.95672900	-0.28446400
C	1.63798900	2.26276900	-0.06009400
C	0.23448500	2.14909800	-0.64885500
C	-0.60393700	1.14258000	0.14044300
C	0.10103600	-0.23652800	0.29618700
C	1.62541900	-0.28613700	0.16446700
C	0.97858700	-0.36974900	1.52457700
C	-0.67748900	-1.46789600	-0.18236000
C	-2.19936500	-1.50140700	0.12206000
C	-2.77047600	-0.12514700	0.49069600
C	-2.06178600	0.99730700	-0.35375800
C	-2.95326600	2.22518500	-0.05706700
C	-4.38600100	1.66540900	0.11218400
C	-4.28059800	0.11178600	0.20618300
H	2.48403500	0.85659900	-1.38466400
H	-0.67362000	1.57163800	1.15180300
O	-4.64659600	-0.45991400	-1.08592700
C	-5.98343300	-0.69160800	-1.15486000
C	-6.58565100	-0.40359800	0.21246000
C	-5.36394400	-0.50779800	1.13513200
O	-6.52480500	-1.06341200	-2.15621800
C	-2.55337200	0.11701300	2.00506600
C	-2.10219100	0.74481400	-1.87743200
C	4.65221900	2.13850000	-0.38615800
C	3.97507100	1.05143900	1.76128800
O	5.86997900	-0.41937200	0.21679900
O	6.54755300	-1.57529700	-1.59637200
C	6.78890600	-1.05829400	-0.53336900
C	8.14048600	-1.02727800	0.13617300
C	-5.14754500	-1.97730200	1.51351000
H	2.26502200	-1.54329300	-1.46567100
H	1.78304200	-2.45391400	-0.03347200
H	4.26689300	-2.47669800	-0.35255700
H	3.80207900	-1.73872000	1.19346400
H	4.57725200	-0.29966600	-1.38456400
H	1.57513300	2.50874000	1.01393200
H	2.17807400	3.09280800	-0.53738900
H	-0.26874100	3.12994800	-0.63917000
H	0.32056200	1.84606000	-1.70475500
H	1.01701600	-1.33517400	2.03970400
H	1.03800300	0.49205700	2.19439200
H	-0.52685900	-1.56765100	-1.26782800
H	-0.22200500	-2.36615800	0.25309800
H	-2.73084600	-1.89516800	-0.75474900
H	-2.39130100	-2.20678100	0.94295000
H	-2.90015200	2.97382100	-0.86001300
H	-2.62375000	2.72816100	0.86429700
H	-4.86909700	2.07174700	1.01307900

H	-5.02632800	1.93261200	-0.73946800
H	-7.39920700	-1.10758600	0.43210000
H	-7.01344300	0.61182200	0.19367700
H	-5.47570200	0.09942000	2.04442000
H	-1.50470500	-0.03717100	2.28182300
H	-2.84221100	1.12727000	2.32649200
H	-3.14099700	-0.59465100	2.59677200
H	-3.11976200	0.56555500	-2.23698700
H	-1.71276800	1.62935000	-2.40098300
H	-1.48920500	-0.11053600	-2.18670900
H	4.31984800	3.10259400	0.02494800
H	5.72605800	2.03912100	-0.17155600
H	4.52478800	2.17075500	-1.48067000
H	3.49191300	0.20358800	2.26321000
H	5.02983900	1.06899800	2.07019300
H	3.49993400	1.97355600	2.12812600
H	8.86271400	-1.59358400	-0.46329100
H	8.47784600	0.01510700	0.24477400
H	8.06758000	-1.45227000	1.14853800
H	-4.28323900	-2.12867300	2.17134100
H	-6.03639900	-2.35632500	2.04131500
H	-5.00021600	-2.60223200	0.61950600

17a

Thermal correction to Gibbs free energy (Hartree): 0.595283

Single point energy (Hartree): -1393.493528

Solvation Gibbs free energy (Hartree): -0.103018

G_{sol} (Hartree): -1393.001263

C	2.32379900	-1.55278400	-0.31767800
C	3.78164000	-1.60718400	0.14312800
C	4.54297000	-0.35635800	-0.27878000
C	3.90562100	0.96655500	0.20507900
C	2.43141500	0.95193200	-0.30965400
C	1.66997000	2.26618500	-0.12422200
C	0.26794000	2.14350800	-0.71572400
C	-0.57076000	1.16299700	0.10565600
C	0.12594700	-0.21493300	0.29684500
C	1.65052400	-0.27682300	0.17340300
C	1.00116300	-0.32378200	1.53206000
C	-0.65828400	-1.44671600	-0.16137200
C	-2.16935400	-1.48293600	0.19226900
C	-2.72986200	-0.08932500	0.51978200
C	-2.03827200	1.01495800	-0.36408300
C	-2.92145300	2.25126900	-0.07899900
C	-4.35266500	1.69336200	0.11275800
C	-4.22845700	0.16252600	0.29917800
H	2.51223100	0.81860100	-1.40598700
H	-0.63106300	1.62330900	1.10342300
O	-4.66460100	-0.47730000	-1.09023200
C	-5.90370600	-0.70736100	-1.05572900
C	-6.55450800	-0.42327400	0.24775100
C	-5.32628100	-0.47901100	1.18454600
O	-6.53586800	-1.15601900	-2.08158400
C	-2.49912300	0.19714500	2.03028800
C	-2.11691700	0.73516600	-1.88104900
C	4.67943400	2.12760700	-0.44155100
C	4.00253900	1.09579100	1.73385100
O	5.89149700	-0.41573500	0.21670800
O	6.52213000	-1.66578900	-1.54818600

C	6.79681200	-1.10176300	-0.51862000
C	8.15921400	-1.04945100	0.12125800
C	-5.09419600	-1.93124000	1.61431600
H	2.28377800	-1.58222500	-1.42118400
H	1.80480100	-2.45200700	0.03941200
H	4.28329200	-2.48533600	-0.28850700
H	3.82618200	-1.70745400	1.23927200
H	4.59250200	-0.33755000	-1.37919800
H	1.60544400	2.54552700	0.94123400
H	2.21320600	3.07923700	-0.62443200
H	-0.23014700	3.12709200	-0.73765700
H	0.35952600	1.80654200	-1.76093600
H	1.03589800	-1.27600000	2.07094300
H	1.06448700	0.55432900	2.18000700
H	-0.54099800	-1.54693900	-1.25086400
H	-0.19480000	-2.34665300	0.25845100
H	-2.71731500	-1.92864500	-0.65093700
H	-2.32976400	-2.15046800	1.04987200
H	-2.88189700	2.98601400	-0.89385800
H	-2.59072300	2.77023500	0.83092300
H	-4.84520700	2.12443600	0.99648100
H	-5.00079400	1.92703100	-0.74425200
H	-7.36052300	-1.13590900	0.47040100
H	-7.00598100	0.58286700	0.18233700
H	-5.47960600	0.15494900	2.06737200
H	-1.44476700	0.04075900	2.27939100
H	-2.76923500	1.21856000	2.32882200
H	-3.07478100	-0.49665500	2.65394600
H	-3.14790800	0.72356400	-2.25341500
H	-1.60291600	1.54140300	-2.41969400
H	-1.64373600	-0.20781500	-2.17805600
H	4.35404500	3.10303600	-0.05204300
H	5.75271500	2.02851100	-0.22712000
H	4.55108500	2.13368700	-1.53636800
H	3.52265700	0.26046100	2.25995700
H	5.05774600	1.11905800	2.03912800
H	3.53221600	2.02843600	2.08025300
H	8.86078200	-1.66488600	-0.45349000
H	8.51471200	-0.00784800	0.15289900
H	8.10119700	-1.40480100	1.16091300
H	-4.23631100	-2.03730000	2.28631000
H	-5.98175300	-2.29918600	2.14990700
H	-4.92338200	-2.59508700	0.75243600
H	-5.95105700	-1.27250900	-2.85798600

TS1

Thermal correction to Gibbs free energy (Hartree): 0.589193

Single point energy (Hartree): -1393.480608

Solvation Gibbs free energy (Hartree): -0.097661

G_{sol} (Hartree): -1392.989076

C	2.35514700	-1.57492700	-0.29187300
C	3.80588500	-1.61289100	0.19306200
C	4.58163500	-0.38584200	-0.27253500
C	3.94124100	0.96180600	0.13460400
C	2.47622900	0.92401400	-0.40278400
C	1.72199800	2.25318900	-0.31881000
C	0.31598700	2.10358900	-0.89625500
C	-0.51263800	1.18331700	-0.00145900
C	0.16102800	-0.19776500	0.23153000

C	1.68308100	-0.27443600	0.13499100
C	1.01404800	-0.27782700	1.48728000
C	-0.63889000	-1.41620300	-0.21689600
C	-2.11412100	-1.43269100	0.23198400
C	-2.68924800	-0.04708000	0.38082100
C	-2.00050200	1.07480300	-0.41187000
C	-2.83557400	2.32376500	-0.02851500
C	-4.22728300	1.76674600	0.29949500
C	-3.99652700	0.33717400	0.74569200
H	2.57343800	0.72098300	-1.48671100
H	-0.52492300	1.69273000	0.97729100
O	-4.98246700	-0.95503700	-1.52650500
C	-6.09989000	-0.84072100	-1.06910800
C	-6.38662400	-0.33635300	0.32770300
C	-5.17282800	-0.47158800	1.27370100
O	-7.20828100	-1.11168500	-1.74965700
C	-2.68085600	0.39370700	2.13081600
C	-2.20225800	0.77649700	-1.91555400
C	4.72920600	2.08733400	-0.55584600
C	4.01162500	1.16629400	1.65650600
O	5.91829100	-0.42600200	0.25216500
O	6.57029300	-1.77227700	-1.43192900
C	6.83327800	-1.15606700	-0.43005900
C	8.18450600	-1.07655500	0.22905900
C	-4.93105700	-1.94869400	1.60207000
H	2.32920200	-1.65331600	-1.39299100
H	1.82792500	-2.45544600	0.09920900
H	4.30907900	-2.51174900	-0.19104000
H	3.83360600	-1.66439600	1.29318600
H	4.65223600	-0.41986200	-1.37151600
H	1.65975300	2.61417800	0.72234600
H	2.27231100	3.02101100	-0.87862600
H	-0.17527700	3.08731000	-0.97589100
H	0.38462600	1.69362600	-1.91733800
H	1.04318300	-1.21520500	2.05178500
H	1.07193400	0.61852800	2.11100100
H	-0.59023200	-1.49106700	-1.31318700
H	-0.16692500	-2.33144900	0.15650800
H	-2.73758000	-1.94323800	-0.51767200
H	-2.22691400	-1.99984100	1.16347300
H	-2.86826600	3.06803000	-0.83398900
H	-2.40243500	2.82517500	0.84993800
H	-4.80818600	2.35750400	1.02371700
H	-4.83416600	1.69442300	-0.61650400
H	-7.24023400	-0.88903400	0.74588800
H	-6.72986400	0.70684200	0.23750200
H	-5.47522700	0.04517900	2.20167100
H	-1.58366200	0.43095400	2.10046600
H	-3.03825100	1.35802800	2.50213000
H	-3.00278000	-0.44757800	2.74505000
H	-3.25249200	0.55566400	-2.14585700
H	-1.89476600	1.65470400	-2.49849600
H	-1.60519200	-0.07506200	-2.26075900
H	4.40270900	3.08192300	-0.21916500
H	5.79843200	1.99438800	-0.32003700
H	4.61825600	2.04043300	-1.65150900
H	3.52767900	0.35463600	2.21522200
H	5.06130200	1.20952400	1.97771900
H	3.53214500	2.11266100	1.94947000
H	8.89102300	-1.72756100	-0.29842800

H	8.54705200	-0.03710200	0.20810700
H	8.10674800	-1.37267700	1.28582300
H	-4.12869000	-2.10141500	2.33560900
H	-5.84615700	-2.36937300	2.04262600
H	-4.69058100	-2.53041200	0.70309000
H	-6.96211700	-1.39821900	-2.64818500

17b

Thermal correction to Gibbs free energy (Hartree): 0.594287

Single point energy (Hartree): -1393.507052

Solvation Gibbs free energy (Hartree): -0.099287

G_{sol} (Hartree): -1393.012052

C	-2.05120700	1.27435800	0.82995300
C	-3.56367700	1.25134500	1.03942200
C	-4.23499900	0.43396900	-0.05580400
C	-3.74123900	-1.02826200	-0.13929000
C	-2.19344300	-0.97262100	-0.35713800
C	-1.54392400	-2.35054100	-0.50088800
C	-0.06927600	-2.23761000	-0.88179900
C	0.79989100	-1.33562000	0.03169100
C	0.02094200	-0.31371700	0.88394800
C	-1.47636700	-0.12690900	0.70318300
C	-0.94699200	-0.82979700	1.92905800
C	0.87700700	0.87200200	1.33067000
C	2.32555000	0.42163300	1.51299100
C	2.94941000	0.05659200	0.17594500
C	1.94254400	-0.66412400	-0.80483400
C	2.81345400	-1.74578200	-1.50910700
C	4.26258300	-1.31375800	-1.30465300
C	4.29481700	-0.71709700	0.12517900
H	-2.04653600	-0.44504600	-1.32038900
H	1.30604500	-2.00566000	0.74657200
O	3.19176600	1.48414500	-0.43640100
C	4.29423500	2.00692700	-0.73527600
C	5.60264200	1.32275100	-0.64004400
C	5.55939700	0.15928200	0.35991600
O	4.28271100	3.22176800	-1.18788000
C	4.28193800	-1.87485300	1.14101200
C	1.36494100	0.30340100	-1.85670100
C	-4.41865400	-1.68396200	-1.35447300
C	-4.12655800	-1.80555400	1.13068400
O	-5.65774700	0.42047800	0.14466000
O	-5.85535300	2.39971100	-0.91237900
C	-6.36438500	1.46863700	-0.33964500
C	-7.83531400	1.29693600	-0.06836500
C	5.76069800	0.69760700	1.78218300
H	-1.82537200	1.83102600	-0.09850100
H	-1.57421600	1.82779800	1.65095900
H	-3.96571100	2.27440200	1.01471900
H	-3.80866600	0.82220000	2.02343000
H	-4.03927000	0.92607000	-1.02221800
H	-1.66797200	-2.93600000	0.42176500
H	-2.05272000	-2.92441200	-1.28733900
H	0.37638800	-3.24228700	-0.92571500
H	-0.03931000	-1.85775500	-1.91244500
H	-0.98272900	-0.29433100	2.88212900
H	-1.09282600	-1.90609400	2.02719800
H	0.83648500	1.70661900	0.61255000
H	0.50763700	1.27520000	2.28183800

H	2.93198000	1.18574600	2.01786600
H	2.34800000	-0.46653200	2.15801100
H	2.55353100	-1.85018000	-2.57083900
H	2.64610300	-2.72942800	-1.05056400
H	4.98441300	-2.13571900	-1.41760700
H	4.52888500	-0.55656500	-2.05857900
H	6.36711500	2.07513300	-0.39615900
H	5.83473900	0.98743100	-1.66663800
H	6.41640700	-0.49118000	0.12590500
H	3.44320300	-2.56128200	0.97155900
H	5.21096800	-2.45430900	1.03420300
H	4.22019300	-1.52733400	2.17895900
H	2.15357900	0.70994200	-2.50664100
H	0.66789300	-0.23333000	-2.51031600
H	0.81692200	1.14176600	-1.40918900
H	-4.17739400	-2.75371200	-1.43126400
H	-5.51056200	-1.59875700	-1.26801000
H	-4.11366800	-1.19376600	-2.29354600
H	-3.63441900	-1.41330800	2.03083600
H	-5.21242800	-1.74666500	1.28772100
H	-3.86044000	-2.86871700	1.03828100
H	-8.38036800	2.18277900	-0.41394700
H	-8.20726400	0.40146900	-0.58994900
H	-8.00397400	1.13968700	1.00745900
H	5.74896900	-0.10247500	2.53259400
H	6.73665900	1.19984200	1.85766200
H	4.99282400	1.43429900	2.06543000
H	3.37181300	3.57324300	-1.24870200

18a

Thermal correction to Gibbs free energy (Hartree): 0.573997

Single point energy (Hartree): -1393.143589

Solvation Gibbs free energy (Hartree): -0.030168

G_{sol} (Hartree): -1392.599759

C	-2.28522900	1.52562500	0.10929200
C	-3.75950700	1.65680500	0.49445000
C	-4.59791100	0.59332500	-0.20191300
C	-4.13636300	-0.85663800	0.06850200
C	-2.63153800	-0.92716500	-0.34856200
C	-2.01458700	-2.32642200	-0.28647900
C	-0.58161400	-2.28362800	-0.80778100
C	0.35561100	-1.45482500	0.07818900
C	-0.27343800	-0.11740800	0.54143600
C	-1.77237400	0.11789700	0.37085100
C	-1.20258200	-0.19751500	1.73253300
C	0.66227400	1.09397000	0.49981700
C	2.09005700	0.72622800	0.81286500
C	2.64108000	-0.37338300	0.28544900
C	1.77861600	-1.31939200	-0.54419600
C	2.55736000	-2.65157400	-0.43098400
C	4.02844800	-2.24365900	-0.36087600
C	4.07353700	-0.90614500	0.44125400
C	5.16109900	0.02343100	-0.19683900
C	5.26624400	1.41136400	0.43916300
H	-2.61357600	-0.63975700	-1.41834700
O	-5.97639100	0.71354800	0.20941400
H	0.51822800	-2.03686200	1.00078500
C	1.75732900	-0.82777100	-2.00768100
C	6.54935600	-0.63370200	-0.22660200

C	6.07467100	2.38723000	-0.38283300
O	6.31074200	2.29944800	-1.56330700
O	6.48878200	3.43821100	0.35650100
C	-4.97479800	-1.79142600	-0.81970700
C	-4.36380600	-1.23560700	1.54115500
C	4.35137700	-1.18252300	1.93082200
H	-2.16597500	1.75620500	-0.96499600
H	-1.69920200	2.27631700	0.65575400
H	-4.14354300	2.64849100	0.21203800
H	-3.87582600	1.55533900	1.58526500
H	-4.56011700	0.77671400	-1.28719500
H	-2.03724800	-2.72577100	0.74105700
H	-2.60568700	-3.02133600	-0.89998100
H	-0.17750300	-3.30375100	-0.90752800
H	-0.60931800	-1.85714300	-1.82328500
H	-1.16500400	0.61024800	2.47027800
H	-1.38993500	-1.18228600	2.16670600
H	0.61824700	1.56629500	-0.49942000
H	0.31554500	1.86195100	1.20389500
H	2.65153600	1.39226100	1.47184300
H	2.34864700	-3.34410300	-1.26072100
H	2.26228600	-3.16238400	0.50048200
H	4.66200700	-3.02075000	0.09175500
H	4.41255100	-2.07631700	-1.37899500
H	4.85050800	0.18758700	-1.24171600
H	4.27217200	1.87394900	0.52866200
H	5.68470000	1.37887400	1.45695500
H	2.77765300	-0.62471900	-2.36437300
H	1.31446200	-1.57555300	-2.68201800
H	1.18364300	0.10498700	-2.11064900
H	6.95688900	-0.76149100	0.78903400
H	7.25102800	-0.00735300	-0.79541600
H	6.53074000	-1.62134000	-0.70749900
H	-6.04669600	-1.62188900	-0.64309800
H	-4.77275000	-1.61220900	-1.88848100
H	-4.76710800	-2.84970300	-0.60584700
H	-3.81144200	-0.58543100	2.23147400
H	-5.43252200	-1.15955200	1.78692000
H	-4.04660300	-2.27173200	1.73102400
H	5.35356600	-1.61125100	2.08378100
H	4.27322800	-0.26453200	2.53252600
H	3.61478400	-1.89546800	2.33163000
H	6.95546000	4.03684800	-0.25197400
C	-6.75723800	1.59049600	-0.45097100
C	-8.16068800	1.57830900	0.10245800
H	-8.13942900	1.78654400	1.18278100
H	-8.76921500	2.32746200	-0.41729900
H	-8.60324600	0.57859000	-0.02713000
O	-6.37166500	2.28112300	-1.36205200

18c

Thermal correction to Gibbs free energy (Hartree): 0.580926

Single point energy (Hartree): -1393.146940

Solvation Gibbs free energy (Hartree): -0.031068

G_{sol} (Hartree): -1392.597082

C	-2.04620500	1.36853400	0.65952000
C	-3.55185200	1.34802600	0.91744200
C	-4.24676700	0.43416900	-0.08137700
C	-3.73105900	-1.02228600	-0.06957700

C	-2.19059200	-0.96259000	-0.33684100
C	-1.52171600	-2.33775300	-0.40365200
C	-0.05948300	-2.21723300	-0.82532200
C	0.81888700	-1.27670200	0.03454100
C	0.04091300	-0.19557400	0.81495800
C	-1.45774300	-0.03188500	0.63653900
C	-0.90862900	-0.63584900	1.90938900
C	0.90003300	1.01813900	1.16709200
C	2.33419300	0.56054100	1.42338100
C	2.99458000	0.15034100	0.10173400
C	1.98517700	-0.67751900	-0.81987700
C	2.85572500	-1.82455800	-1.41327800
C	4.30552500	-1.40041700	-1.19496900
C	4.30271900	-0.70047100	0.18476500
H	-2.07925100	-0.50610000	-1.34012900
H	1.29905900	-1.90690400	0.80127300
O	3.22706700	1.42243700	-0.57176700
C	4.39310100	2.05432700	-0.81366100
C	5.66626800	1.25251100	-0.66200600
C	5.58209000	0.15245700	0.39693500
O	4.37132000	3.19462000	-1.19760400
C	4.22152100	-1.78339800	1.27429400
C	1.44555400	0.19800300	-1.96633700
C	-4.43520200	-1.77829500	-1.20916900
C	-4.06809700	-1.70523200	1.26677100
O	-5.66594600	0.41250600	0.18151900
O	-5.98690700	2.26137300	-1.06834200
C	-6.42426500	1.38007400	-0.37031000
C	-7.87506600	1.19892400	0.00177900
C	5.74701500	0.77004000	1.79237900
H	-1.85204400	1.84588400	-0.31825100
H	-1.55069400	1.99520900	1.41307600
H	-3.97106100	2.36075500	0.82139300
H	-3.76087800	0.99854800	1.94101700
H	-4.10389900	0.85021200	-1.09106700
H	-1.61243300	-2.86042600	0.56067100
H	-2.04002300	-2.97146600	-1.13757500
H	0.39897200	-3.21731500	-0.85139700
H	-0.06156600	-1.86543200	-1.86602500
H	-0.93626200	-0.02740400	2.81826800
H	-1.05007200	-1.70220300	2.09219900
H	0.90347500	1.77326300	0.36702200
H	0.50564000	1.51591500	2.06323400
H	2.92526400	1.36509100	1.88034100
H	2.32278800	-0.27640500	2.13425500
H	2.62689600	-2.00379400	-2.47361600
H	2.65893300	-2.77088500	-0.88909400
H	5.01731200	-2.24018100	-1.22869200
H	4.60231200	-0.69596800	-1.98473100
H	6.47288000	1.96736800	-0.44900800
H	5.88642300	0.83484800	-1.65744100
H	6.43235200	-0.53465500	0.24201500
H	3.36814000	-2.45808300	1.12787300
H	5.13675800	-2.39564800	1.24462300
H	4.13600000	-1.36415900	2.28400900
H	2.26577700	0.58214900	-2.58578200
H	0.78833500	-0.38897400	-2.62112600
H	0.87977700	1.06557600	-1.60500800
H	-4.17637400	-2.84674500	-1.21082400
H	-5.52625300	-1.70237500	-1.09790300

H	-4.16291700	-1.35862400	-2.19142500
H	-3.56348100	-1.22922400	2.11781100
H	-5.15164300	-1.66336400	1.44676000
H	-3.77049900	-2.76398400	1.25098300
H	-8.46915300	2.01872000	-0.41853900
H	-8.24035600	0.23424200	-0.38304300
H	-7.98100000	1.17313200	1.09676400
H	5.69126100	0.02309200	2.59572000
H	6.72989700	1.26031500	1.86635500
H	4.98758300	1.54055200	1.99370600

TS2

Thermal correction to Gibbs free energy (Hartree): 0.590101

Single point energy (Hartree): -1393.480597

Solvation Gibbs free energy (Hartree): -0.095276

G_{sol} (Hartree): -1392.985771

C	-2.17244600	1.36127300	0.57858900
C	-3.67419200	1.38888500	0.86596200
C	-4.44166900	0.53661300	-0.13759400
C	-3.97094500	-0.93499600	-0.20628200
C	-2.43975500	-0.88987400	-0.51206900
C	-1.80760400	-2.25396100	-0.78994000
C	-0.33605100	-2.09756000	-1.15574800
C	0.48268300	-1.53999200	0.01960500
C	-0.16275400	-0.32916200	0.73895900
C	-1.65861000	-0.07152100	0.52212000
C	-1.18007700	-0.69617000	1.80299600
C	0.73014900	0.88838100	0.98990200
C	2.19520300	0.54769800	1.26683400
C	2.77091700	-0.39134300	0.23032800
C	1.93442800	-1.40381400	-0.29412000
C	2.75262900	-2.51368300	-0.90317100
C	4.21002500	-2.02505300	-0.81679600
C	4.21866400	-0.95127500	0.30847600
H	-2.34939000	-0.32158900	-1.45822800
H	0.54343300	-2.36060600	0.76650000
O	3.82658200	2.59091700	-0.70289000
C	5.00216000	2.30704500	-0.84823800
C	5.54646500	0.91003700	-1.05768600
C	5.45238200	-0.00053700	0.20137700
O	5.95853400	3.22899000	-0.81168700
C	4.29257300	-1.70562400	1.65845600
C	2.35444100	0.14968300	-1.33740100
C	-4.71842100	-1.61725600	-1.36417400
C	-4.29435400	-1.67538700	1.10164400
O	-5.84103500	0.54670800	0.18138000
O	-6.10512500	2.48972900	-0.92668800
C	-6.57636500	1.58789300	-0.28096000
C	-8.02060000	1.44549700	0.11778200
C	5.76287200	0.81935300	1.46394800
H	-1.97464200	1.85279100	-0.39078700
H	-1.64937100	1.95106000	1.34264100
H	-4.04928900	2.42071800	0.81010400
H	-3.87150300	1.02074500	1.88505800
H	-4.32221100	0.98842400	-1.13556500
H	-1.90708500	-2.92655500	0.07796900
H	-2.33192700	-2.74494300	-1.62032200
H	0.08359800	-3.06381400	-1.47451500
H	-0.24887500	-1.41023300	-2.01622500

H	-1.21281700	-0.08769400	2.71161700
H	-1.37115800	-1.75778100	1.97758800
H	0.67597000	1.58984600	0.14251000
H	0.34832500	1.44972600	1.85122600
H	2.79179700	1.46679800	1.31392900
H	2.28488600	0.04257900	2.24075400
H	2.42233900	-2.78856400	-1.91499700
H	2.57673900	-3.40363300	-0.27550100
H	4.90810800	-2.84177400	-0.58939900
H	4.53434700	-1.60171600	-1.77794900
H	6.60355800	1.00977000	-1.33399400
H	5.03303200	0.46908500	-1.92282100
H	6.28852400	-0.70976200	0.08352100
H	3.52143800	-2.48793400	1.72426500
H	5.27159000	-2.19764100	1.75381300
H	4.16428900	-1.04426600	2.52302000
H	2.90535700	-0.31009100	-2.15663600
H	1.29497200	0.27257000	-1.57912000
H	2.75779900	1.16829800	-1.13407300
H	-4.51909900	-2.69806500	-1.40177200
H	-5.80197800	-1.48827700	-1.23659900
H	-4.43752100	-1.17958500	-2.33610700
H	-3.82333000	-1.21265200	1.97871400
H	-5.38006200	-1.67372300	1.26877900
H	-3.96581100	-2.72455300	1.05438700
H	-8.58398000	2.32385600	-0.21722900
H	-8.44328700	0.53477300	-0.33400900
H	-8.10036400	1.33394300	1.20948900
H	5.98322300	0.18241300	2.32925700
H	6.64941800	1.44687000	1.29159100
H	4.93582600	1.48993500	1.73976200
H	5.54300300	4.09958900	-0.66837600

17j

Thermal correction to Gibbs free energy (Hartree): 0.587961

Single point energy (Hartree): -1393.478680

Solvation Gibbs free energy (Hartree): -0.097021

G_{sol} (Hartree): -1392.987740

C	-2.21283400	1.39360100	0.52576900
C	-3.71254500	1.43484500	0.82086400
C	-4.48719400	0.55511000	-0.15285700
C	-4.02328900	-0.92016900	-0.17574900
C	-2.49312900	-0.89368100	-0.49070200
C	-1.87204500	-2.27288200	-0.71173300
C	-0.40589200	-2.14731200	-1.10619100
C	0.43698500	-1.50515400	0.01726800
C	-0.20307000	-0.28546900	0.71574500
C	-1.70313900	-0.04135500	0.50849400
C	-1.21027400	-0.63213300	1.79845200
C	0.69620500	0.93238400	0.93451900
C	2.16187300	0.57858200	1.19372700
C	2.72646800	-0.32808000	0.10333200
C	1.86569800	-1.41919900	-0.29437000
C	2.65332900	-2.48486000	-0.98156300
C	4.12813900	-2.04956200	-0.85966800
C	4.14381600	-0.98975900	0.27867400
H	-2.40359100	-0.36496400	-1.45942400
H	0.54448100	-2.29820800	0.80243100
O	4.20792600	2.66975100	-0.51328900

C	5.32029000	2.24798000	-0.76033800
C	5.68320700	0.79323200	-0.98368400
C	5.44094500	-0.12203300	0.25164800
O	6.38023200	3.05129900	-0.84435500
C	4.11505700	-1.76821500	1.61439800
C	2.50114500	0.37383700	-1.33991400
C	-4.77997000	-1.63653100	-1.30681900
C	-4.34256700	-1.61546100	1.15778800
O	-5.88508300	0.58103300	0.16950800
O	-6.14286800	2.48818300	-1.00050500
C	-6.61716300	1.61093500	-0.32420100
C	-8.06033800	1.48966300	0.08448900
C	5.73064300	0.65715500	1.54572400
H	-2.01898800	1.85426600	-0.45922100
H	-1.68177900	2.00330700	1.26814700
H	-4.08394200	2.46590900	0.73503300
H	-3.90611900	1.09916200	1.85177700
H	-4.36843900	0.97451300	-1.16500400
H	-1.96618100	-2.90490300	0.18640500
H	-2.40653600	-2.79839100	-1.51412800
H	0.00826000	-3.13251700	-1.36679900
H	-0.32232800	-1.51103700	-2.00429500
H	-1.22862100	-0.00195200	2.69228200
H	-1.40065500	-1.68871100	2.00255300
H	0.62798200	1.61752500	0.07532800
H	0.32805700	1.50680600	1.79343200
H	2.76376100	1.49463400	1.24341800
H	2.25143500	0.06411100	2.16135400
H	2.30014600	-2.63670100	-2.01502000
H	2.43813300	-3.43987300	-0.47144500
H	4.78758500	-2.89592200	-0.62537600
H	4.48549000	-1.62940400	-1.80969100
H	6.75015100	0.76144100	-1.23721300
H	5.14157600	0.44265600	-1.87271400
H	6.23129900	-0.88765600	0.17536100
H	3.29624100	-2.50508400	1.63947200
H	5.05531800	-2.32349700	1.74597900
H	3.98943600	-1.11606800	2.48590100
H	3.05180200	-0.11356900	-2.14713900
H	1.44578600	0.45707800	-1.62903300
H	2.89284100	1.39081700	-1.16378400
H	-4.58589500	-2.71900300	-1.31080900
H	-5.86212900	-1.49899800	-1.17699900
H	-4.50347900	-1.23131200	-2.29393700
H	-3.85795400	-1.13113900	2.01565700
H	-5.42651100	-1.59524600	1.33452500
H	-4.02762300	-2.66975300	1.14085700
H	-8.62113200	2.35744600	-0.28098000
H	-8.48868400	0.56448800	-0.33108300
H	-8.13636100	1.41972300	1.17993900
H	5.87900900	-0.00599300	2.40672900
H	6.65686100	1.23930500	1.42816900
H	4.92737700	1.36524900	1.79266400
H	6.08016700	3.96651500	-0.69282200

TS3

Thermal correction to Gibbs free energy (Hartree): 0.585923

Single point energy (Hartree): -1393.475139

Solvation Gibbs free energy (Hartree): -0.098093

G_{sol} (Hartree): -1392.987309

C	-2.30341500	1.48907700	0.32332700
C	-3.78694900	1.52480800	0.68787000
C	-4.57512600	0.53587600	-0.16138100
C	-4.08023600	-0.92464700	-0.04270400
C	-2.56610800	-0.91841000	-0.43433800
C	-1.93250200	-2.31080400	-0.45044600
C	-0.49424500	-2.25477600	-0.94955500
C	0.39084700	-1.24750100	-0.24077600
C	-0.21976700	-0.08016900	0.47606300
C	-1.75093000	0.07362400	0.40579400
C	-1.12145900	-0.40172100	1.67286200
C	0.68013700	1.14674400	0.59215000
C	2.12089100	0.76316000	0.94911500
C	2.72510000	-0.17605100	-0.10044200
C	1.78196300	-1.27407200	-0.49302600
C	2.55421900	-2.36178700	-1.19700500
C	4.03653100	-2.06870000	-0.85668800
C	4.00639300	-1.01884500	0.29272600
H	-2.52691300	-0.53792100	-1.47294500
H	1.12520800	-1.82160600	0.61291100
O	4.75795700	2.59534400	-0.08338800
C	5.73419200	2.04887800	-0.55007900
C	5.94741800	0.55373900	-0.67369800
C	5.39360700	-0.32041700	0.47859700
O	6.76796000	2.73465300	-1.04851600
C	3.71822300	-1.80725300	1.59221500
C	2.85365600	0.59229000	-1.45802100
C	-4.87462800	-1.77642400	-1.04694900
C	-4.31899700	-1.46696100	1.37640900
O	-5.96067600	0.56943400	0.20444500
O	-6.29101300	2.34408600	-1.14192200
C	-6.72894800	1.53334300	-0.36607800
C	-8.15537700	1.43098900	0.10040400
C	5.58182700	0.39331200	1.82927900
H	-2.17057400	1.85722700	-0.70891600
H	-1.74892700	2.17483200	0.97669800
H	-4.18721900	2.53419500	0.51778100
H	-3.92644900	1.28916600	1.75440700
H	-4.49721300	0.84836400	-1.21543400
H	-1.97589000	-2.77761000	0.54482700
H	-2.49699400	-2.97305200	-1.11925900
H	-0.03016700	-3.25175900	-0.94394300
H	-0.49276200	-1.92955600	-2.00619000
H	-1.04206800	0.29497800	2.51135600
H	-1.24520400	-1.44275500	1.97503700
H	0.65499100	1.72453900	-0.34469600
H	0.29138100	1.81644600	1.36812500
H	2.75023200	1.65933300	1.02018600
H	2.12242900	0.27801900	1.93661800
H	2.33723000	-2.30838800	-2.27683300
H	2.22424000	-3.36126800	-0.87971700
H	4.56884400	-2.97769700	-0.54529100
H	4.56485200	-1.68449700	-1.73899800
H	7.03289400	0.39789100	-0.74411200
H	5.55357800	0.25436700	-1.65712200
H	6.08052000	-1.18383000	0.49840100
H	2.86891700	-2.50300600	1.48730600
H	4.58752900	-2.42973400	1.84934900
H	3.50904400	-1.16129700	2.45248400

H	3.42018100	0.03980300	-2.21500700
H	1.86324800	0.80390700	-1.88391400
H	3.34443500	1.55063200	-1.26357200
H	-4.64851400	-2.84811900	-0.94938900
H	-5.95145200	-1.65275200	-0.86954700
H	-4.66578600	-1.47072000	-2.08507100
H	-3.76506200	-0.90955800	2.14389600
H	-5.38717600	-1.39634500	1.62219500
H	-4.03110100	-2.52614200	1.45192200
H	-8.74356700	2.24898500	-0.33083500
H	-8.57918900	0.46237400	-0.20671900
H	-8.19554700	1.46995900	1.19928900
H	5.54609600	-0.30613300	2.67384300
H	6.57268400	0.87252600	1.85954500
H	4.83545400	1.18061900	1.99245900
H	6.56204700	3.68363600	-0.96981400

17k

Thermal correction to Gibbs free energy (Hartree): 0.588541

Single point energy (Hartree): -1393.494326

Solvation Gibbs free energy (Hartree): -0.095169

G_{sol} (Hartree): -1393.000954

C	-2.08887600	1.02200000	1.05102400
C	-3.61118600	1.17446000	1.13387300
C	-4.28309400	0.59755200	-0.10603200
C	-3.96498000	-0.89695800	-0.34724800
C	-2.40507900	-1.01500200	-0.44817200
C	-1.91571200	-2.43633200	-0.72513600
C	-0.40103400	-2.47226100	-0.87621500
C	0.42186700	-1.62161600	0.01845500
C	-0.11642800	-0.75056900	0.99099300
C	-1.72742900	-0.42628300	0.78707200
C	-1.31737500	-1.29825200	1.86641700
C	0.75351200	0.34375700	1.62350200
C	2.26475400	0.08901400	1.54984700
C	2.66114800	-0.39908800	0.15660400
C	1.88935300	-1.70694800	-0.13960400
C	2.55363400	-2.29091600	-1.40219700
C	3.99199900	-1.70129700	-1.38275400
C	4.14118900	-0.90683800	-0.04903400
H	-2.10510000	-0.37895000	-1.30117800
H	2.10414500	-2.40210900	0.70140400
O	4.01979700	2.79761200	0.37623200
C	4.80059800	2.63088700	-0.53522300
C	5.26187600	1.30247500	-1.09869300
C	5.33415700	0.11060500	-0.11467300
O	5.35676900	3.65693200	-1.19359300
C	4.52403800	-1.94401600	1.03552600
C	2.20099600	0.62848200	-0.90517300
C	-4.59902600	-1.31072200	-1.68487100
C	-4.54183700	-1.76776000	0.78084700
O	-5.70285900	0.73979200	-0.00583700
O	-5.54805700	2.86098200	-0.74347200
C	-6.22953000	1.94159500	-0.36930900
C	-7.72685200	1.93559000	-0.23900700
C	5.85350200	0.58933900	1.25426600
H	-1.70578200	1.64109200	0.22302700
H	-1.62973900	1.39135900	1.97600500
H	-3.86102100	2.24175900	1.21054200

H	-4.00062700	0.67632500	2.03486800
H	-3.94475500	1.17561700	-0.98157800
H	-2.24281100	-3.12076600	0.06956600
H	-2.36404900	-2.81860100	-1.65063600
H	0.00097500	-3.50089800	-0.85835400
H	-0.11253300	-2.11432600	-1.88622700
H	-1.25423900	-0.89706000	2.88034000
H	-1.50286200	-2.37046100	1.81921200
H	0.53335300	1.29251200	1.11338700
H	0.45948300	0.49066300	2.67163900
H	2.78927000	1.02489400	1.78540400
H	2.55230300	-0.65576100	2.30639200
H	2.01632900	-1.98118500	-2.31072300
H	2.55126800	-3.38986400	-1.39466700
H	4.75797600	-2.48627800	-1.45085800
H	4.14425100	-1.04653700	-2.25195000
H	6.26591500	1.47845000	-1.51098600
H	4.63357400	1.08998400	-1.97692100
H	6.14032400	-0.51486100	-0.53501600
H	3.91273800	-2.85723900	0.98914400
H	5.56192300	-2.27139800	0.87681200
H	4.45801900	-1.54806600	2.05634600
H	2.58704100	0.40668200	-1.90642100
H	1.10320300	0.63555500	-0.99453600
H	2.50746900	1.63868200	-0.62407600
H	-4.48315700	-2.38605700	-1.88150800
H	-5.67571400	-1.09510400	-1.66518700
H	-4.15760000	-0.75331800	-2.52666600
H	-4.08318300	-1.56323600	1.75910800
H	-5.61905100	-1.57638900	0.87694200
H	-4.41482700	-2.83841600	0.56406000
H	-8.12125900	2.92907800	-0.48056700
H	-8.15673400	1.18609100	-0.92141000
H	-8.01494600	1.64836200	0.78330100
H	6.27119100	-0.23303100	1.84782300
H	6.66687800	1.31737900	1.10868100
H	5.07543200	1.08850400	1.84477000
H	5.00661100	4.47898400	-0.80646700

17n

Thermal correction to Gibbs free energy (Hartree): 0.583398

Single point energy (Hartree): -1393.467252

Solvation Gibbs free energy (Hartree): -0.105457

G_{sol} (Hartree): -1392.989312

C	3.48737100	-0.96353200	-1.78981200
C	4.80911300	-1.25287700	-1.04887800
C	5.23993400	-0.07353000	-0.18490500
C	4.13896700	0.42111300	0.78162500
C	2.88115800	0.82119500	-0.12505200
C	1.78713500	1.59926500	0.60464100
C	0.54573800	1.87117800	-0.25985900
C	-0.48656800	0.77212800	-0.21967100
C	-0.17000600	-0.53101000	-0.38901800
C	2.45423800	-0.35017500	-0.91775700
C	1.18074600	-1.03921400	-0.80169200
C	-1.18785600	-1.65396100	-0.29859500
C	-2.57810700	-1.22240400	0.19189100
C	-2.96454600	0.13735100	-0.40799600
C	-1.90954100	1.14784100	0.10494600

C	-2.46280700	2.51689400	-0.30866100
C	-3.99997500	2.33688300	-0.20578300
C	-4.30535000	0.82170000	0.07957600
H	3.32452500	1.49453700	-0.88482100
O	-7.29297400	-1.37171800	1.26383500
C	-6.33752000	-1.70926000	0.61240300
C	-5.91367500	-1.11341200	-0.71073300
C	-5.58518800	0.39994000	-0.71070100
O	-5.51738900	-2.71213800	1.01111000
C	-4.51165700	0.62399100	1.59292100
C	-2.92360800	0.06573700	-1.94913600
C	4.64688400	1.67452400	1.50561300
C	3.76601100	-0.65392500	1.81010600
O	6.37412000	-0.43995700	0.59731300
O	7.69990800	-0.06791900	-1.18226300
C	7.59157300	-0.37884300	-0.02568700
C	8.70081800	-0.73597300	0.91991000
C	-6.82602200	1.22448500	-0.33376800
H	3.68077200	-0.20851900	-2.57839600
H	3.10809900	-1.86017000	-2.29783000
H	5.59122800	-1.47015000	-1.78785700
H	4.68853400	-2.14725100	-0.41959800
H	5.53091900	0.75975500	-0.84588500
H	1.48273200	1.07508300	1.52286200
H	2.22348100	2.55450000	0.92357700
H	0.08074100	2.80773400	0.07162300
H	0.85107900	2.05813500	-1.30807000
H	1.07665800	-1.78979000	-1.60347000
H	-1.26677200	-2.12857100	-1.29465800
H	-0.79761800	-2.44723300	0.36390800
H	-3.30373000	-2.01276600	-0.03750300
H	-2.55735900	-1.13995100	1.28831500
H	-2.16236700	2.76646000	-1.33808400
H	-4.42401700	2.96761500	0.58774300
H	-4.47950400	2.65908100	-1.14079600
H	-6.77286900	-1.25868800	-1.38593200
H	-5.08375600	-1.70007200	-1.11994300
H	-5.37611700	0.63029900	-1.76622400
H	-3.67853900	1.03865000	2.17964100
H	-5.42046300	1.14017400	1.92820500
H	-4.60850300	-0.43303700	1.86974800
H	-3.29466600	0.98617600	-2.41833000
H	-1.90204000	-0.09177300	-2.32226000
H	-3.53949800	-0.76344300	-2.32423200
H	5.59508800	1.43185400	2.00457000
H	4.83308500	2.50090600	0.80204400
H	3.94451100	2.02022100	2.27542000
H	2.98921300	-0.29604500	2.50038700
H	3.40952800	-1.59027100	1.35294900
H	4.65273500	-0.90915800	2.40602800
H	9.65129400	-0.76717700	0.37545200
H	8.75715700	0.01420100	1.72411000
H	8.49735300	-1.70784600	1.39341700
H	-7.19554700	0.98576700	0.67119100
H	-6.62705100	2.30391700	-0.39082500
H	-7.64703300	1.00340600	-1.03300600
H	-5.88232700	-3.05284100	1.84734100
H	-2.10062100	3.33051100	0.33619100
H	-1.95556800	1.11701100	1.20887900
H	1.59434200	-1.67403800	0.04859000

TS4

Thermal correction to Gibbs free energy (Hartree): 0.583052

Single point energy (Hartree): -1393.466536

Solvation Gibbs free energy (Hartree): -0.104203

G_{sol} (Hartree): -1392.987687

C	3.49409200	-1.27986100	-1.58081000
C	4.79979000	-1.45136200	-0.80228800
C	5.24130600	-0.13287200	-0.17746700
C	4.16501900	0.52508400	0.72053800
C	2.88465000	0.75403000	-0.17313200
C	1.78996000	1.57476400	0.51055300
C	0.54187800	1.81708700	-0.35169700
C	-0.49658200	0.73087700	-0.25863900
C	-0.19204700	-0.59293100	-0.37769300
C	2.43446000	-0.53067000	-0.81713800
C	1.12103000	-1.08074000	-0.79306100
C	-1.23055600	-1.69873700	-0.25436100
C	-2.61300000	-1.22916600	0.22030500
C	-2.98099600	0.11425200	-0.42499200
C	-1.91004300	1.12862700	0.04846700
C	-2.44830400	2.49624100	-0.39165100
C	-3.98724500	2.33363600	-0.29259300
C	-4.30892900	0.83381200	0.04620300
H	3.23850200	1.34063400	-1.04299900
O	-7.30919400	-1.27674900	1.32746400
C	-6.36560800	-1.65088600	0.67911000
C	-5.94653700	-1.10658000	-0.66775400
C	-5.59848200	0.40121900	-0.72203600
O	-5.55516100	-2.65085900	1.10392900
C	-4.50575000	0.69285600	1.56703200
C	-2.94448900	-0.00718500	-1.96284300
C	4.71074600	1.87921400	1.20003100
C	3.84610300	-0.35740600	1.93722700
O	6.40994100	-0.34249200	0.61432100
O	7.67782700	-0.23350500	-1.24186800
C	7.60508800	-0.36006600	-0.04772300
C	8.74865100	-0.54671900	0.90721900
C	-6.82579000	1.25491100	-0.36635500
H	3.67840200	-0.66034600	-2.47874600
H	3.11209800	-2.24379200	-1.94645400
H	5.58527200	-1.80708000	-1.48235800
H	4.67720000	-2.21153300	-0.01517800
H	5.49803300	0.56808000	-0.98898700
H	1.48939400	1.10451600	1.45955300
H	2.22648600	2.54514200	0.77670000
H	0.08295300	2.76739500	-0.05328100
H	0.82946500	1.95587600	-1.41068700
H	1.06725100	-2.04425200	-1.31937500
H	-1.31553300	-2.20190000	-1.23497100
H	-0.85323300	-2.47325100	0.43587900
H	-3.35009700	-2.01592400	0.01755800
H	-2.59207500	-1.11111500	1.31339100
H	-2.14059800	2.72390200	-1.42368200
H	-4.41070400	2.99768900	0.47328800
H	-4.45662100	2.62444000	-1.24280000
H	-6.81382000	-1.26290100	-1.32991300
H	-5.12891800	-1.71851600	-1.06475700
H	-5.39258200	0.59275400	-1.78600200

H	-3.66245600	1.11663700	2.13317700
H	-5.40378500	1.23495800	1.88993400
H	-4.61653900	-0.35152500	1.88349700
H	-3.29774700	0.90535200	-2.46033100
H	-1.92780500	-0.19843400	-2.33420800
H	-3.57798100	-0.83513200	-2.30987400
H	5.68346700	1.72648800	1.68558200
H	4.85750500	2.57314000	0.35699200
H	4.04727700	2.35702200	1.93331800
H	3.16438700	0.14963600	2.63432100
H	3.39213300	-1.32645500	1.66830900
H	4.77328000	-0.58488400	2.48039200
H	9.68488300	-0.63971300	0.34536400
H	8.80725900	0.31648500	1.58840900
H	8.58286100	-1.44061500	1.52668200
H	-7.19097800	1.05679300	0.64896600
H	-6.61405200	2.32900200	-0.46365400
H	-7.65433300	1.01942400	-1.05171000
H	-5.91711100	-2.96027700	1.95360500
H	-2.07964100	3.31629600	0.24072600
H	-1.94139600	1.12331600	1.15501100
H	1.90210600	-1.39707600	0.16183400

17m

Thermal correction to Gibbs free energy (Hartree): 0.586713

Single point energy (Hartree): -1393.492090

Solvation Gibbs free energy (Hartree): -0.100314

G_{sol} (Hartree): -1393.005692

C	-3.12996600	-2.01267200	0.02533200
C	-4.63206400	-1.74768000	0.04250600
C	-4.92415400	-0.28049000	0.33584700
C	-4.27087700	0.71099400	-0.65643800
C	-2.73782200	0.41834700	-0.65236400
C	-1.92046100	1.33298900	-1.57123400
C	-0.53999900	1.63270600	-1.01457200
C	0.44939000	0.55201000	-0.76918700
C	0.23110400	-0.84519100	-0.89744600
C	-2.42288200	-1.04450400	-0.96969200
C	-1.00621900	-1.44914200	-1.07173500
C	1.40779700	-1.83006000	-0.80316400
C	2.80682300	-1.21694600	-0.69165400
C	2.78182500	0.03084700	0.20030400
C	1.82616100	1.02484900	-0.49595000
C	2.06932800	2.39219100	0.16743000
C	3.53229200	2.30918000	0.66434800
C	4.10236200	0.89760100	0.29334100
H	-2.40148600	0.59559900	0.38645300
O	7.55101600	-0.79404600	-0.13548900
C	6.50167200	-1.32921400	0.11399800
C	5.61062000	-1.01668200	1.29557800
C	5.10243900	0.44125200	1.40260800
O	5.99226100	-2.31348600	-0.66516400
C	4.79591800	0.99366500	-1.07781400
C	2.23424400	-0.30723600	1.60175000
C	-4.52969600	2.13208600	-0.12791600
C	-4.87568900	0.57680800	-2.06340000
O	-6.33697000	-0.05362900	0.32691000
O	-6.47314800	-0.76414900	2.45892000
C	-7.01491700	-0.33348000	1.47349700

C	-8.47921300	-0.02986300	1.32163800
C	6.27538800	1.41589400	1.59064500
H	-2.70581300	-1.85382100	1.03097000
H	-2.92822100	-3.05962700	-0.24848600
H	-5.10214500	-2.36289800	0.82294700
H	-5.08356400	-2.03234300	-0.92077100
H	-4.55118400	-0.05576900	1.34853600
H	-1.83437500	0.88918100	-2.57700300
H	-2.42415500	2.29792900	-1.70939600
H	-0.02216400	2.37348400	-1.65162000
H	-0.62665800	2.17086900	-0.04892100
H	-0.92481600	-2.53194800	-1.24118800
H	1.21936500	-2.47941100	0.06655700
H	1.36429100	-2.49325600	-1.68176500
H	3.50507400	-1.98194800	-0.33157600
H	3.16237500	-0.93723600	-1.69353500
H	1.37351100	2.53692300	1.00806200
H	4.15035200	3.10332000	0.22557200
H	3.56264600	2.45956700	1.75257500
H	6.22668000	-1.21134300	2.18854500
H	4.78130000	-1.73260600	1.32170800
H	4.53415600	0.46283000	2.34510600
H	4.14019100	1.43982100	-1.84332600
H	5.68076600	1.63954700	-1.01395300
H	5.12251700	0.01923300	-1.45950800
H	2.26560200	0.55734300	2.27809100
H	1.18728300	-0.64334300	1.56206000
H	2.81251700	-1.11412000	2.07157800
H	-5.60929100	2.29219000	-0.00591100
H	-4.05290500	2.28558400	0.85381500
H	-4.16245500	2.90725300	-0.81581100
H	-4.45504900	1.32813300	-2.74822200
H	-4.71176700	-0.41440400	-2.51238200
H	-5.96155500	0.73538100	-2.01859800
H	-9.01027700	-0.30997100	2.23839800
H	-8.61849800	1.04361900	1.12074200
H	-8.88956500	-0.57796200	0.46029500
H	6.96941000	1.40076700	0.74112800
H	5.92667500	2.44641200	1.74706700
H	6.85742400	1.12845300	2.47928400
H	6.64241200	-2.47785900	-1.37186900
H	1.90742700	3.22817400	-0.52624100
H	2.20025400	1.12029000	-1.54206700
H	-2.84198500	-1.29911300	-1.96628800

17c

Thermal correction to Gibbs free energy (Hartree): 0.574973

Single point energy (Hartree): -1393.148194

Solvation Gibbs free energy (Hartree): -0.031823

G_{sol} (Hartree): -1392.605044

C	-3.25212500	-2.02870000	0.37843200
C	-4.74202700	-1.72046100	0.26143200
C	-4.96991400	-0.21591600	0.29459600
C	-4.21317900	0.56951000	-0.79972900
C	-2.69753600	0.21393900	-0.66670000
C	-1.80171300	0.91837200	-1.69522100
C	-0.49239000	1.40310900	-1.08771700
C	0.46777400	0.37653600	-0.50735300
C	0.19505100	-1.07526700	-0.47590400

C	-2.43181000	-1.29678300	-0.70053100
C	-0.99091300	-1.71799800	-0.59862400
C	1.39928300	-1.99368200	-0.21847100
C	2.76369500	-1.32146200	-0.32059000
C	2.79057600	-0.00907600	0.48267500
C	1.65104300	0.85262700	-0.04344900
C	2.05052000	2.30717500	-0.03136200
C	3.47052100	2.32546100	0.55015900
C	4.06354600	0.92018300	0.25788400
H	-2.39664100	0.56792200	0.33746800
O	7.59482300	-0.53106500	-0.53890200
C	6.62561000	-1.11778900	-0.12347100
C	5.86103600	-0.78422900	1.13618300
C	5.25770400	0.63966200	1.21827800
O	6.11929500	-2.19814900	-0.76285500
C	4.50142600	0.88991000	-1.21756500
C	2.54546500	-0.28957700	1.98361700
C	-4.42310900	2.06788300	-0.52010700
C	-4.76227500	0.23860800	-2.19763800
O	-6.37851800	0.07007500	0.16083000
O	-6.70092100	-0.17578200	2.37875800
C	-7.13277800	0.06017400	1.27727300
C	-8.56957000	0.38751800	0.95396400
C	6.36080700	1.70701900	1.15044400
H	-2.88402500	-1.71747500	1.37189800
H	-3.08219900	-3.11538500	0.31044500
H	-5.29804300	-2.18012300	1.09231300
H	-5.14968800	-2.13352900	-0.67555100
H	-4.64860000	0.15864100	1.27895700
H	-1.60493500	0.24285300	-2.54413900
H	-2.30795300	1.79639200	-2.12107100
H	0.05860000	1.97978300	-1.85221700
H	-0.73665800	2.14173400	-0.30231100
H	-0.91062200	-2.81311700	-0.56423100
H	1.28619300	-2.43993200	0.78325600
H	1.35642300	-2.83800900	-0.92433700
H	3.54520200	-2.02258900	0.00522700
H	2.96715400	-1.09558400	-1.37605200
H	1.34766400	2.92898600	0.54913400
H	4.08578700	3.13027600	0.12412300
H	3.43497900	2.49527700	1.63829300
H	6.59317800	-0.87781600	1.95567500
H	5.09222800	-1.54647300	1.30084200
H	4.84353100	0.69712800	2.23641300
H	3.66205200	1.14621100	-1.88127500
H	5.30405800	1.61782100	-1.39985000
H	4.86290200	-0.09571100	-1.53285700
H	2.58650100	0.63250100	2.58087000
H	1.54547000	-0.71816900	2.13341500
H	3.27899700	-0.99755200	2.39902900
H	-5.49574300	2.30945600	-0.51929600
H	-4.01030800	2.34624700	0.46316000
H	-3.94186500	2.69918900	-1.28066100
H	-4.25846000	0.84248900	-2.96673300
H	-4.62608300	-0.81875000	-2.46579500
H	-5.83818300	0.45831300	-2.24470400
H	-9.17557900	0.33026000	1.86564100
H	-8.63289200	1.39883700	0.52342900
H	-8.95250600	-0.31268200	0.19636800
H	6.86341600	1.72764700	0.17504400

H	5.96044400	2.70805100	1.36359200
H	7.13761300	1.49441200	1.90161400
H	6.67831400	-2.34119200	-1.54664100
H	2.02798800	2.72351900	-1.05475000
H	-2.79345000	-1.67097800	-1.67942700

17d

Thermal correction to Gibbs free energy (Hartree): 0.586541

Single point energy (Hartree): -1393.517658

Solvation Gibbs free energy (Hartree): -0.099145

G_{sol} (Hartree): -1393.030262

C	-2.72403500	-0.24373500	2.15599100
C	-4.04399500	0.36678000	1.69584200
C	-4.01452300	0.61662500	0.19415600
C	-3.73370100	-0.64663000	-0.65502100
C	-2.37237000	-1.23597000	-0.15082500
C	-1.90183500	-2.43762200	-0.98672600
C	-0.43799300	-2.90836500	-0.73946300
C	0.42464600	-1.88311600	-0.04036500
C	0.15247200	-1.57528600	1.30163300
C	-2.38704700	-1.51472700	1.36977900
C	-1.05952300	-2.15195500	1.92636200
C	0.99951600	-0.63818500	2.08139600
C	2.33502600	-0.28793600	1.42965000
C	2.16915900	-0.00461000	-0.07141000
C	1.39351000	-1.12841800	-0.70100800
C	1.77074900	-1.28170300	-2.13072600
C	2.91877900	-0.29149500	-2.37031500
C	3.48923100	0.04513100	-0.96075500
H	-1.64258000	-0.42163500	-0.31543700
O	6.84192300	1.03035500	0.64372400
C	5.74123700	1.24635800	1.08023400
C	4.64436600	2.00450800	0.36506500
C	4.20057500	1.43094500	-1.00151800
O	5.35304600	0.82179200	2.30617300
C	4.43958400	-1.09102200	-0.54313300
C	1.28826600	1.26399800	-0.29028100
C	-3.60521300	-0.19161700	-2.11987700
C	-4.88911700	-1.65558000	-0.54594800
O	-5.26128100	1.18096100	-0.22967900
O	-4.51785700	3.24376300	0.28417700
C	-5.39474700	2.52927400	-0.13165000
C	-6.75114200	2.97220500	-0.60611100
C	5.35469100	1.47450000	-2.01523800
H	-1.91717800	0.49913900	2.01518400
H	-2.76195000	-0.46473500	3.23425400
H	-4.21919100	1.32177000	2.21171300
H	-4.88433300	-0.29991600	1.94505200
H	-3.22444100	1.35649600	-0.01408500
H	-2.57677500	-3.29117300	-0.82524400
H	-1.99730800	-2.17185400	-2.04669000
H	-0.43725000	-3.82471500	-0.13040800
H	0.01751000	-3.19578200	-1.69513800
H	-1.04041000	-2.02915500	3.01726300
H	0.37020100	0.25688800	2.26541300
H	1.14204800	-1.06123700	3.09080400
H	2.80069800	0.55576600	1.95127800
H	3.01293600	-1.14158000	1.56447400
H	0.89648700	-1.13448300	-2.78920200

H	3.68591500	-0.71291700	-3.03157300
H	2.54370700	0.61850400	-2.86113000
H	5.05358300	3.01020100	0.17682700
H	3.79299700	2.13463700	1.04325000
H	3.44631800	2.14515900	-1.36749000
H	3.93915200	-2.07230500	-0.58754200
H	5.30567900	-1.13434600	-1.21541700
H	4.82032100	-0.97479000	0.47789700
H	1.13847600	1.48843400	-1.35399100
H	0.29390000	1.14566500	0.16139600
H	1.76822300	2.13380800	0.17684300
H	-4.49228900	0.38888100	-2.40655500
H	-2.72123500	0.45221400	-2.26250700
H	-3.53391300	-1.03895800	-2.81605800
H	-4.73191300	-2.51157000	-1.21844800
H	-5.02237900	-2.04951400	0.47183600
H	-5.83183500	-1.17211800	-0.83611400
H	-6.84526700	4.05814500	-0.49274400
H	-6.88927200	2.69012600	-1.66119300
H	-7.53513700	2.46015400	-0.02805400
H	6.20028200	0.84567300	-1.71001400
H	5.02602000	1.17025600	-3.01885700
H	5.73779200	2.50275600	-2.09490600
H	6.12522100	0.38931900	2.71390300
H	-3.16590900	-2.26537100	1.57494900
H	-1.08006500	-3.23129900	1.70994700
H	2.06711000	-2.33360800	-2.29707200

18b

Thermal correction to Gibbs free energy (Hartree): 0.576050

Single point energy (Hartree): -1393.153677

Solvation Gibbs free energy (Hartree): -0.030996

G_{sol} (Hartree): -1392.608623

C	-2.66088400	0.25508100	2.04197700
C	-4.04426200	0.75337100	1.62147900
C	-4.23579200	0.63038000	0.11311000
C	-4.00066500	-0.78588200	-0.46455300
C	-2.58064900	-1.21847100	0.00626100
C	-2.08047600	-2.57031700	-0.52706900
C	-0.57129000	-2.55154200	-0.86137400
C	0.34985700	-1.65774100	-0.04020500
C	0.13124900	-1.31567500	1.25756800
C	-2.42881400	-1.17083100	1.54038400
C	-1.09135300	-1.78135600	2.01406700
C	1.07961100	-0.42826800	2.02852400
C	2.46437600	-0.28136900	1.39947000
C	2.36433300	-0.01586400	-0.11120300
C	1.52670800	-1.13157900	-0.73852400
C	1.99313400	-1.44042000	-1.96385600
C	3.22053100	-0.64692800	-2.31003200
C	3.72393300	-0.10746500	-0.93467100
H	-1.90210900	-0.44612400	-0.39743300
O	7.14831200	1.05113200	0.53742400
C	6.03877900	1.27415600	0.95596900
C	4.91803300	1.93785700	0.19083600
C	4.47162400	1.24471500	-1.12066000
O	5.68005600	0.95925500	2.22335900
C	4.64607800	-1.18421500	-0.33616600
C	1.60869700	1.30681400	-0.37071700

C	-4.03519300	-0.66985100	-1.99820000
C	-5.09391600	-1.76807500	-0.01545100
O	-5.57301900	1.04333700	-0.23981600
O	-4.94507500	3.20661800	-0.33570000
C	-5.79579300	2.35730500	-0.43835300
C	-7.23745400	2.60500200	-0.80725200
C	5.63095300	1.16572300	-2.12515300
H	-1.88246300	0.92017700	1.62680000
H	-2.56085300	0.30088800	3.13886600
H	-4.18358800	1.80733800	1.90525800
H	-4.82712600	0.17035200	2.13404100
H	-3.53533000	1.32338200	-0.37838700
H	-2.31669700	-3.36236600	0.20015700
H	-2.61354600	-2.85420200	-1.44544400
H	-0.17551500	-3.58361500	-0.85892100
H	-0.48037200	-2.21226700	-1.90451700
H	-0.97049700	-1.55682700	3.08534000
H	0.60034000	0.56019000	2.16832800
H	1.18561800	-0.83100400	3.05076200
H	3.03758600	0.50081900	1.91834900
H	3.00532100	-1.22396000	1.56237800
H	1.55032400	-2.16704400	-2.64722200
H	3.98907700	-1.24711800	-2.82423700
H	2.97056500	0.18207000	-3.00061400
H	5.29899000	2.93739600	-0.07797100
H	4.06720500	2.08591800	0.86431800
H	3.73830000	1.93969100	-1.55738000
H	4.12877900	-2.15469400	-0.30687800
H	5.54965400	-1.30512200	-0.94921600
H	4.96296900	-0.95238700	0.68735800
H	1.55448800	1.52992300	-1.44581600
H	0.57294700	1.23261400	-0.01028100
H	2.07543300	2.16419500	0.13726400
H	-4.98558000	-0.22410800	-2.32589900
H	-3.21416200	-0.03233200	-2.36447900
H	-3.94558000	-1.65178800	-2.48471600
H	-4.90317700	-2.77082200	-0.42749500
H	-5.15539700	-1.86411900	1.07779100
H	-6.07788900	-1.43409400	-0.37390600
H	-7.41026000	3.68165100	-0.91963700
H	-7.47500300	2.08589400	-1.74864500
H	-7.89943500	2.19083700	-0.03194000
H	6.44911900	0.52639500	-1.77010300
H	5.28712700	0.79062400	-3.09953900
H	6.05949100	2.16728800	-2.28757900
H	6.46081700	0.55052800	2.63638200
H	-3.21935100	-1.80602300	1.97737500
H	-1.16054700	-2.87823400	1.94811400

MeOH

Thermal correction to Gibbs free energy (Hartree): 0.023254

Single point energy (Hartree): -115.717231

Solvation Gibbs free energy (Hartree): -0.008733

G_{sol} (Hartree): -115.702710

O	-0.74535300	0.12246900	0.00000200
H	-1.13750200	-0.75948400	0.00001500
C	0.65445000	-0.01958700	0.00000100
H	1.09166200	0.99097400	-0.00069200
H	1.04103900	-0.54627700	0.89631400

H 1.04092400 -0.54744900 -0.89566400

MeOH₂⁺

Thermal correction to Gibbs free energy (Hartree): 0.033128

Single point energy (Hartree): -116.012180

Solvation Gibbs free energy (Hartree): -0.126044

G_{sol} (Hartree): -116.105095

O	-0.70319600	-0.00094100	-0.00032600
H	-1.21808100	-0.83128900	0.00094700
C	0.79412800	-0.00212900	0.00008400
H	1.08306400	1.05420000	-0.00217600
H	1.11110000	-0.51098200	0.91719100
H	1.11127400	-0.51479600	-0.91483000
H	-1.22656200	0.82316300	0.00096900

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Thermal correction to Gibbs free energy (Hartree): 0.598661

Single point energy (Hartree): -1354.987751

Solvation Gibbs free energy (Hartree): 0.007301

G_{sol} (Hartree): -1354.381788

C	-2.86041600	2.04282200	-0.37256800
C	-4.28683100	2.51980700	-0.09899500
C	-5.33360000	1.54674900	-0.63536000
C	-5.14490200	0.09523000	-0.10405900
C	-3.67827300	-0.33713900	-0.41966300
C	-3.35945800	-1.79605400	-0.08564200
C	-1.93946600	-2.13722600	-0.52307800
C	-0.86763700	-1.35619300	0.24676200
C	-1.21681900	0.14963600	0.44067000
C	-2.64107600	0.63306400	0.15555500
C	-2.16591800	0.46015100	1.57560300
C	-0.07660200	1.15842800	0.24130300
C	1.26403200	0.62452200	0.69872600
C	1.58373900	-0.78016200	0.43430900
C	0.52985700	-1.56111900	-0.36914100
C	1.08586100	-2.99225300	-0.26305200
C	2.58899600	-2.78749000	-0.48185600
C	2.95929200	-1.50463000	0.32554900
C	4.03845700	-0.64228400	-0.39195800
C	4.63342100	0.44588300	0.51710700
H	-3.58372200	-0.25368000	-1.52064600
O	-6.64717200	2.03974400	-0.42735000
O	1.20068200	-0.34228900	1.74781700
H	-0.81037400	-1.78563900	1.25914700
C	0.57691400	-1.09757700	-1.84693500
C	5.19026400	-1.46131000	-0.99003800
C	5.15403200	1.63479900	-0.25886500
O	4.74466000	2.00479900	-1.33357200
O	6.12311500	2.27877600	0.41754400
C	6.63961400	3.45920300	-0.19584000
C	-6.14017400	-0.80347100	-0.85639000
C	-5.46615300	0.03205800	1.39854800
C	3.42160200	-1.93455300	1.72854800
H	-2.67666900	2.04768600	-1.46283500
H	-2.14777500	2.75372200	0.06592600
H	-4.46463100	3.50863000	-0.55088800
H	-4.42762700	2.63986300	0.99031500
H	-5.22405500	1.49880100	-1.73329500

H	-3.48102500	-1.99164900	0.99278300
H	-4.07094500	-2.45768200	-0.60028200
H	-1.75122200	-3.21572500	-0.40061900
H	-1.85858800	-1.92715000	-1.60237600
H	-1.97725900	1.35979300	2.16930000
H	-2.54296000	-0.38090300	2.16127800
H	0.01605300	1.47529400	-0.81104900
H	-0.29262000	2.07339600	0.81152300
H	2.05880700	1.37240900	0.79351100
H	0.64159200	-3.69041300	-0.98837900
H	0.88950100	-3.39081400	0.74657800
H	3.19429600	-3.65077000	-0.16879600
H	2.77841500	-2.64138400	-1.55470800
H	3.53830800	-0.11924300	-1.22218000
H	3.88847800	0.84796500	1.22067500
H	5.44399000	0.05401100	1.14857500
H	-6.74464800	2.23451000	0.51396700
H	1.58821100	-0.79757800	-2.15453900
H	0.25531700	-1.90468200	-2.52199900
H	-0.08275100	-0.23877500	-2.02670700
H	5.71336500	-2.04586700	-0.21590500
H	5.92933400	-0.79186000	-1.45762400
H	4.84954100	-2.15880200	-1.76724700
H	7.40538400	3.84916500	0.48566700
H	7.08187900	3.22822600	-1.17669500
H	5.84331700	4.20450000	-0.34356800
H	-7.14476900	-0.36016100	-0.80862200
H	-5.86304900	-0.89765200	-1.91943700
H	-6.18974800	-1.81482700	-0.42665000
H	-4.82471900	0.69108300	1.99889200
H	-6.51613500	0.31444500	1.57625300
H	-5.34367400	-0.99012700	1.78551100
H	4.39684600	-2.44198300	1.67132100
H	3.50196300	-1.08454700	2.41663100
H	2.70153400	-2.63516300	2.17625700

19a

Thermal correction to Gibbs free energy (Hartree): 0.608486

Single point energy (Hartree): -1355.330487

Solvation Gibbs free energy (Hartree): -0.059219

G_{sol} (Hartree): -1354.781220

C	-2.82296600	2.05722300	0.20039100
C	-4.27995100	2.45819700	0.43280000
C	-5.24207800	1.70449400	-0.48422600
C	-5.09522300	0.15574700	-0.37971800
C	-3.59719100	-0.19117400	-0.64257000
C	-3.29381900	-1.68832200	-0.72906700
C	-1.83033300	-1.91357700	-1.09470400
C	-0.87736400	-1.41734600	-0.00090600
C	-1.26210100	-0.02506800	0.57800900
C	-2.64906400	0.54827200	0.30905100
C	-2.34296700	-0.03911400	1.65995900
C	-0.10245300	0.94957500	0.80667800
C	1.11016300	0.21125700	1.35215400
C	1.58205500	-0.85989900	0.41474900
C	0.59544600	-1.50592700	-0.45694100
C	1.16269700	-2.93346600	-0.62301600
C	2.68363800	-2.73819500	-0.57608500
C	2.92555900	-1.49891900	0.34546900

C	4.05239500	-0.57406800	-0.26771700
C	4.15573400	0.84386400	0.30584500
H	-3.37652700	0.21928800	-1.64701800
O	-6.57239400	2.13879600	-0.30276300
O	0.77305400	-0.66318300	2.43255300
H	-0.95034700	-2.14453100	0.82623100
C	0.84257900	-0.65172500	-1.77772400
C	5.41335100	-1.27691800	-0.23036600
C	5.09277700	1.69090400	-0.54248600
O	5.12058600	1.64453500	-1.74877600
O	5.84401700	2.49866800	0.20382200
C	6.73294600	3.38057300	-0.50021400
C	-5.97951400	-0.46674200	-1.47248600
C	-5.58579200	-0.33720400	0.99153900
C	3.29680900	-1.94525800	1.79394100
H	-2.51089300	2.37627500	-0.81022300
H	-2.18064000	2.59353500	0.91254200
H	-4.41273900	3.53848800	0.26983700
H	-4.54885900	2.26229200	1.48584400
H	-4.99822400	1.97385200	-1.52738900
H	-3.53378200	-2.20229300	0.21627600
H	-3.93053600	-2.14899100	-1.49570000
H	-1.63928200	-2.98157000	-1.28134100
H	-1.63040200	-1.38439200	-2.04036200
H	-2.24601000	0.65322000	2.50233800
H	-2.78495400	-1.00300900	1.92310300
H	0.18694200	1.49186200	-0.10732700
H	-0.38537600	1.71716600	1.53786400
H	1.90194300	0.88393900	1.69638700
H	0.81568200	-3.41761300	-1.54559200
H	0.81670000	-3.54642800	0.22423000
H	3.20872000	-3.62859600	-0.20735900
H	3.07369200	-2.53010300	-1.58301500
H	3.78382600	-0.44830100	-1.32753600
H	3.18892800	1.36800400	0.24913000
H	4.48378200	0.85989400	1.35486300
H	-6.79116900	2.09054200	0.63729500
H	1.85490300	-0.23462300	-1.87914500
H	0.68899400	-1.32893000	-2.62884400
H	0.12750900	0.17574600	-1.82969600
H	5.84538700	-1.28615500	0.78118600
H	6.11297600	-0.74415600	-0.88980400
H	5.35550900	-2.31335200	-0.59180800
H	7.25566500	3.95937200	0.26917100
H	7.44798600	2.80158600	-1.10191800
H	6.16518600	4.04516600	-1.16701700
H	-6.98746500	-0.03395300	-1.41534200
H	-5.58042700	-0.25415700	-2.47788900
H	-6.07068600	-1.55732600	-1.36212200
H	-5.04485600	0.11767500	1.83307000
H	-6.65510200	-0.10690900	1.11233600
H	-5.48904000	-1.42927600	1.08229100
H	4.23543900	-2.50978800	1.73671800
H	3.43369600	-1.08888600	2.46670400
H	2.52256200	-2.59245600	2.22272200
H	-0.19281600	-0.78571100	2.42345500

19d

Thermal correction to Gibbs free energy (Hartree): 0.617066

Single point energy (Hartree): -1355.361054

Solvation Gibbs free energy (Hartree): -0.065942

G_{sol} (Hartree): -1354.809931

C	2.80868100	1.81732400	-0.57329500
C	4.29211900	1.89754900	-0.93148600
C	5.16319000	1.12702100	0.05907700
C	4.74037800	-0.36610500	0.20673500
C	3.22696400	-0.39459200	0.58609200
C	2.66961900	-1.79122500	0.87105400
C	1.23397400	-1.69653300	1.37647400
C	0.25190800	-1.07828800	0.36343000
C	0.87406900	0.04473500	-0.50098100
C	2.35516100	0.37459700	-0.41291500
C	1.83510200	-0.37076200	-1.61481800
C	-0.12382000	1.12597700	-0.89546500
C	-1.44033000	0.46238600	-1.29852400
C	-2.12400000	-0.13406200	-0.01742300
C	-1.09002300	-0.66589800	1.05844600
C	-1.78616600	-1.91993800	1.66593100
C	-3.26105500	-1.75189500	1.33578700
C	-3.28401300	-1.19730400	-0.10823000
C	-4.70488900	-0.59327600	-0.41742800
C	-4.62095200	0.87696500	-0.87921400
H	3.15390200	0.16605200	1.53835300
O	6.53599700	1.27903100	-0.23642300
O	-1.25558900	-0.46853200	-2.32387700
H	-0.02123100	-1.88804000	-0.33358900
C	-0.86198900	0.35814400	2.18985900
C	-5.58244200	-1.37938800	-1.39267500
C	-3.80376000	1.61578200	0.10494300
O	-2.73332200	1.12906500	0.58611700
O	-4.21938800	2.74450900	0.55105400
C	-3.45182200	3.46611000	1.55634300
C	5.57907700	-0.97294500	1.34355800
C	5.03952200	-1.13581800	-1.09054900
C	-2.92402000	-2.33143600	-1.08719700
H	2.63495400	2.34520100	0.38206500
H	2.21690700	2.34355200	-1.33544800
H	4.62957700	2.94509400	-0.95486700
H	4.44679200	1.49291100	-1.94729800
H	5.03759200	1.59028300	1.05403500
H	2.72954500	-2.43616100	-0.02008400
H	3.28071000	-2.28295100	1.63991600
H	0.86904300	-2.69050000	1.67504800
H	1.26030400	-1.08970200	2.29264800
H	1.78618400	0.17179400	-2.56438000
H	2.08368800	-1.42866500	-1.71982000
H	-0.30389400	1.84594700	-0.08404600
H	0.24369400	1.70585600	-1.75145200
H	-2.11526100	1.23429700	-1.70199200
H	-1.60114100	-2.00433500	2.74514600
H	-1.39743500	-2.83931200	1.20723600
H	-3.84489700	-2.68023200	1.42298100
H	-3.72104300	-1.01919700	2.02070100
H	-5.24460900	-0.57108100	0.54305700
H	-4.13868800	0.93778500	-1.86895400
H	-5.60624400	1.35421400	-0.95716100
H	6.68199400	1.03636500	-1.16034200
H	-1.80179000	0.58964500	2.70841300
H	-0.18554800	-0.06578300	2.93973700

H	-0.42201000	1.30159200	1.84198800
H	-5.15570300	-1.40509400	-2.40532500
H	-6.57818400	-0.91520000	-1.45722900
H	-5.72500600	-2.41446700	-1.05544600
H	-4.00588100	4.39410900	1.72470300
H	-3.39694100	2.86378200	2.47204700
H	-2.44435500	3.66728400	1.17041900
H	6.64132000	-0.75140700	1.17269200
H	5.29932000	-0.54114000	2.31854200
H	5.46436500	-2.06500900	1.40648400
H	4.51067400	-0.73033200	-1.96427600
H	6.11910900	-1.10968500	-1.30402000
H	4.76553700	-2.19688100	-0.99687700
H	-3.59520500	-3.18226500	-0.90816500
H	-3.00351100	-2.02374400	-2.13263900
H	-1.89852200	-2.68744100	-0.94026300
H	-0.33260500	-0.76246300	-2.31268700

19d'

Thermal correction to Gibbs free energy (Hartree): 0.618456

Single point energy (Hartree): -1355.366635

Solvation Gibbs free energy (Hartree): -0.063443

G_{sol} (Hartree): -1354.811621

C	-2.89624400	-1.45873600	-1.31223900
C	-4.35459900	-1.23978700	-1.71782500
C	-5.26053100	-0.97780600	-0.51627800
C	-4.77138800	0.21202400	0.36269200
C	-3.28997500	-0.07715300	0.75555100
C	-2.68498600	0.91619500	1.74718200
C	-1.26919800	0.48840500	2.11303300
C	-0.30053500	0.60974200	0.92706800
C	-0.87192300	-0.05233700	-0.36277300
C	-2.38842600	-0.30435400	-0.46048900
C	-1.77482900	0.86199700	-1.17701600
C	0.03711200	-0.96830100	-1.19314600
C	1.43860700	-1.21672600	-0.64957200
C	2.05983600	-0.06786600	0.14308600
C	1.18059000	0.26424300	1.37659300
C	1.83983800	1.57094400	1.86427500
C	2.10612400	2.36177000	0.58297300
C	2.50891400	1.31056200	-0.49973600
C	4.06326400	1.39866400	-0.67710500
C	4.66449700	0.05295700	-1.10033200
H	-3.31599400	-1.04951200	1.28491000
O	-6.61136400	-0.84922200	-0.90920900
O	2.34508000	-1.61282200	-1.66932400
H	-0.27678300	1.68164600	0.69515000
C	1.22314700	-0.83469400	2.44902000
C	4.53092000	2.51350000	-1.61168300
C	4.34631600	-0.90499600	-0.02229700
O	3.29994100	-0.78530500	0.69219600
O	5.20743900	-1.79931300	0.30036000
C	4.93376300	-2.72861000	1.38416600
C	-5.65346000	0.25150200	1.62112900
C	-4.93558300	1.53998500	-0.39491100
C	1.78292600	1.57700100	-1.82427100
H	-2.81370400	-2.39717600	-0.73364300
H	-2.28870700	-1.59006400	-2.21913400
H	-4.73966700	-2.11476900	-2.26370700

H	-4.41375300	-0.38337100	-2.41251900
H	-5.24019000	-1.87493500	0.12781300
H	-2.68215900	1.94068500	1.33924200
H	-3.29957000	0.95008900	2.65688900
H	-0.89466100	1.09679400	2.95132900
H	-1.31202200	-0.55273800	2.46802100
H	-1.71126500	0.81119000	-2.26878700
H	-1.94602900	1.86988000	-0.79159700
H	-0.42171900	-1.96200900	-1.30796700
H	0.14887600	-0.56799500	-2.20980000
H	1.37128000	-2.03016000	0.09418300
H	2.78513800	1.33271300	2.37983300
H	1.21073900	2.11342300	2.58416100
H	1.20381000	2.90148900	0.26529500
H	2.88675700	3.12357500	0.71504600
H	4.47679300	1.62088100	0.32154300
H	4.21493700	-0.31311600	-2.03544800
H	5.75512800	0.08633600	-1.23066700
H	-6.66955000	-0.17361100	-1.59767600
H	2.25531300	-1.10719800	2.69907000
H	0.75419500	-0.47623100	3.37277500
H	0.68784900	-1.74642100	2.14407400
H	4.27770400	2.30270000	-2.66061800
H	5.62383000	2.62401600	-1.54735500
H	4.08468200	3.48067500	-1.33899100
H	5.78161400	-3.41994500	1.38820900
H	4.87127700	-2.17598200	2.33045700
H	3.99151500	-3.25453800	1.18537100
H	-6.71162100	0.22685100	1.32673300
H	-5.46473500	-0.62164400	2.26716600
H	-5.48591200	1.16110000	2.21654300
H	-4.38226000	1.56567300	-1.34378600
H	-5.99906400	1.71932400	-0.61546800
H	-4.59418900	2.39048300	0.21348300
H	2.00650900	2.59365100	-2.17212500
H	2.07672000	0.86819700	-2.61070200
H	0.69666400	1.52070300	-1.69450500
H	1.98839500	-2.38612500	-2.12754800

TS5

Thermal correction to Gibbs free energy (Hartree): 0.610349

Single point energy (Hartree): -1355.303369

Solvation Gibbs free energy (Hartree): -0.062881

G_{sol} (Hartree): -1354.755902

C	-1.93289900	1.51999600	0.58625100
C	-3.33031700	2.11152600	0.76353000
C	-4.29865300	1.62305500	-0.31378900
C	-4.39857500	0.06831500	-0.38722300
C	-2.95527700	-0.48939600	-0.58898900
C	-2.87714700	-2.00892400	-0.77287900
C	-1.46093800	-2.43743600	-1.15780800
C	-0.39330800	-2.06723400	-0.11213000
C	-0.71824400	-0.79676400	0.72687900
C	-1.98780300	0.00425600	0.49209400
C	-1.83036500	-0.81429900	1.74796800
C	0.54965400	-0.06146000	1.13013500
C	1.56769100	-1.29267200	1.80659100
C	1.88874700	-1.23087600	0.42837800
C	1.01932700	-1.79017300	-0.68235300

C	1.99196800	-2.92307700	-1.07163600
C	3.36302000	-2.19584400	-1.12533600
C	3.36269800	-1.06415000	-0.01368300
C	3.76758800	0.33784200	-0.56438500
C	3.62596600	1.47639400	0.48521000
H	-2.59818400	-0.04156800	-1.53673300
O	-5.55952900	2.24585000	-0.18879300
O	0.85191300	-2.29075400	2.37273900
H	-0.31677600	-2.90504700	0.59060400
C	0.89724400	-0.80557700	-1.87338900
C	5.17626700	0.35140800	-1.16837800
C	2.70952500	2.57592900	-0.01017200
O	1.58331200	2.36517000	-0.42254200
O	3.25513000	3.77980900	0.05865600
C	2.45115100	4.89043900	-0.37568500
C	-5.27304000	-0.28037300	-1.60262800
C	-5.06869300	-0.48660100	0.88059600
C	4.31076300	-1.48927200	1.12221100
H	-1.47429000	1.91724800	-0.33656700
H	-1.28318900	1.84567500	1.41352300
H	-3.29430500	3.21109100	0.72938100
H	-3.72277000	1.83785300	1.75875400
H	-3.91511800	1.96061700	-1.29315900
H	-3.21426200	-2.53521100	0.13392200
H	-3.56355600	-2.31893300	-1.57203500
H	-1.42406600	-3.52409100	-1.32999600
H	-1.24326700	-1.96776800	-2.12508100
H	-1.67196000	-0.26808400	2.68403400
H	-2.40222700	-1.73564100	1.86634000
H	0.94179100	0.65250200	0.37456100
H	0.50301200	0.55249400	2.04078600
H	2.30449300	-0.83242600	2.47311100
H	1.72800900	-3.39235400	-2.02976600
H	1.99001900	-3.70839200	-0.29959900
H	4.19836900	-2.88799700	-0.95954800
H	3.51345500	-1.74866800	-2.11578600
H	3.06771300	0.57154400	-1.37284100
H	3.17840300	1.11389900	1.42463400
H	4.59975300	1.90243800	0.75790700
H	-5.88750400	2.10459300	0.70920700
H	1.85390200	-0.41276200	-2.21935400
H	0.45988700	-1.34294000	-2.72262800
H	0.24838500	0.04757200	-1.63692000
H	5.95455400	0.20359200	-0.40519200
H	5.36429400	1.32677900	-1.64189100
H	5.30384200	-0.41938200	-1.94198800
H	3.07543900	5.78096900	-0.24653000
H	2.16658200	4.76421900	-1.42969200
H	1.54017700	4.96281600	0.23512500
H	-6.20960900	0.29155800	-1.55595300
H	-4.76643400	-0.01672400	-2.54550000
H	-5.52772900	-1.34968300	-1.63742100
H	-4.51446300	-0.24949000	1.79960100
H	-6.08602700	-0.07815700	0.98126100
H	-5.17568900	-1.57992100	0.82785500
H	5.32273400	-1.62980100	0.72092800
H	4.38179400	-0.74313100	1.92755200
H	4.00155100	-2.44739600	1.56655200
H	0.60855600	-2.06268900	3.28179300

19e

Thermal correction to Gibbs free energy (Hartree): 0.611965

Single point energy (Hartree): -1355.315449

Solvation Gibbs free energy (Hartree): -0.071315

G_{sol} (Hartree): -1354.774799

C	-1.87083900	1.58898900	0.49775500
C	-3.23816700	2.20639100	0.79083600
C	-4.30237200	1.75084600	-0.20886700
C	-4.43649200	0.19900500	-0.30358500
C	-3.02118700	-0.37387700	-0.62163600
C	-2.96950600	-1.88466600	-0.87752200
C	-1.57249800	-2.29484500	-1.34828800
C	-0.50552000	-2.06323700	-0.26890600
C	-0.71953300	-0.76222900	0.56070600
C	-1.97649500	0.07624700	0.40371700
C	-1.76900300	-0.73706500	1.65192000
C	0.62380200	-0.07447200	0.82284600
C	1.56984900	-1.81777900	1.80512100
C	1.68217100	-1.24269400	0.48418000
C	0.96691200	-1.90893500	-0.73362600
C	1.94804000	-3.06017200	-0.97570500
C	3.31968300	-2.33498200	-0.92315100
C	3.22096200	-1.12750700	0.10240300
C	3.56347900	0.26891200	-0.49291600
C	3.53198000	1.39513400	0.57237800
H	-2.72199300	0.10499100	-1.57392000
O	-5.53839200	2.38947000	0.03387100
O	0.71579300	-2.69273400	2.19375600
H	-0.57461800	-2.91995900	0.41331500
C	0.97377600	-1.00345700	-1.98633100
C	4.89267300	0.32148600	-1.25476300
C	2.86538700	2.63948300	0.02047300
O	1.75731500	2.63184700	-0.47782200
O	3.61388600	3.72890700	0.14470000
C	3.05289600	4.96118700	-0.33628600
C	-5.40342600	-0.11127300	-1.45759800
C	-5.02384400	-0.36909200	0.99872900
C	4.18470000	-1.43696500	1.26500800
H	-1.48224800	1.98053400	-0.45873900
H	-1.14720800	1.89313200	1.26960500
H	-3.18302400	3.30537900	0.76537000
H	-3.55483500	1.92868300	1.81194000
H	-3.99741500	2.10125700	-1.21089600
H	-3.26274600	-2.45273100	0.02078500
H	-3.69845600	-2.15061500	-1.65468200
H	-1.55795200	-3.35471500	-1.64765400
H	-1.35855600	-1.71164700	-2.25292400
H	-1.53976000	-0.19039400	2.57320700
H	-2.36387600	-1.63998400	1.80359500
H	0.88593700	0.74472300	0.13099100
H	0.68862300	0.36411800	1.83204500
H	2.21653800	-1.39330100	2.58203200
H	1.79413800	-3.57925700	-1.93233700
H	1.86506200	-3.81463300	-0.17560300
H	4.12910800	-3.01950600	-0.63542400
H	3.58051100	-1.96414000	-1.92095100
H	2.77309800	0.51530900	-1.20753400
H	2.93103300	1.10558300	1.44815700
H	4.53595400	1.63911100	0.94368500

H	-5.78539700	2.24488800	0.95685500
H	1.97309400	-0.72484500	-2.32480300
H	0.52183700	-1.56992000	-2.80980900
H	0.38715100	-0.08403000	-1.85703800
H	5.75230400	0.09087700	-0.60690400
H	5.05099200	1.33545400	-1.65255300
H	4.91507900	-0.36939800	-2.10907800
H	3.81193800	5.72932000	-0.15264300
H	2.82907200	4.88497400	-1.40974600
H	2.12515600	5.19537300	0.20495200
H	-6.32152400	0.47923500	-1.33468800
H	-4.96026900	0.15634500	-2.43077800
H	-5.68302900	-1.17455800	-1.48889900
H	-4.41521800	-0.13504900	1.88340700
H	-6.03455200	0.03416400	1.16488800
H	-5.12794900	-1.46285300	0.94391100
H	5.21647600	-1.42774500	0.88877000
H	4.13989700	-0.70871400	2.08953800
H	4.02276200	-2.44518800	1.68305300
H	0.71147400	-2.82678800	3.16010300

20a

Thermal correction to Gibbs free energy (Hartree): 0.599020

Single point energy (Hartree): -1354.987126

Solvation Gibbs free energy (Hartree): 0.013622

G_{sol} (Hartree): -1354.374484

C	-1.92846200	1.70512200	0.33557200
C	-3.27774600	2.33568100	0.68108000
C	-4.40143200	1.82085000	-0.21858100
C	-4.52793300	0.26668600	-0.22462200
C	-3.12857600	-0.31584900	-0.59210900
C	-3.08078300	-1.83737800	-0.77932600
C	-1.69695600	-2.26613200	-1.27372000
C	-0.60961800	-1.99888700	-0.23020300
C	-0.76478500	-0.62635300	0.49659800
C	-2.02756400	0.19052400	0.34355600
C	-1.74867600	-0.53057400	1.64038400
C	0.62504400	0.03489000	0.63946700
C	1.34162800	-1.93240400	1.84060700
C	1.53064100	-1.19931700	0.49833400
C	0.86592400	-1.93534800	-0.70474300
C	1.79212900	-3.14687400	-0.85436700
C	3.19649900	-2.49618600	-0.73198700
C	3.08997800	-1.22514200	0.20544000
C	3.55042600	0.10101600	-0.47518000
C	3.57456400	1.28682300	0.50711400
H	-2.88980600	0.11370400	-1.58520100
O	-5.62882300	2.46642100	0.07866500
O	1.09102600	-3.09183200	2.04922900
H	-0.68996800	-2.79205700	0.52543400
C	0.92038600	-1.14156400	-2.03051500
C	4.90596700	0.01728500	-1.18855800
C	3.24021000	2.59736900	-0.16983100
O	2.46965900	2.72759300	-1.09282000
O	3.87117700	3.63395900	0.40760900
C	3.56480500	4.92734800	-0.11438600
C	-5.56242600	-0.10725200	-1.29860200
C	-5.03297000	-0.23317900	1.13904900
C	3.95993000	-1.47244700	1.45738800

H	-1.61106900	2.03893700	-0.66907200
H	-1.15618600	2.05486100	1.03668300
H	-3.23763500	3.43301400	0.59323100
H	-3.52598300	2.11079600	1.73405000
H	-4.17146900	2.12248600	-1.25575600
H	-3.33098700	-2.35978200	0.15933800
H	-3.84114500	-2.14251600	-1.51251100
H	-1.69461000	-3.33644100	-1.53771500
H	-1.49808200	-1.71395200	-2.20380200
H	-1.47311500	0.07839500	2.50722600
H	-2.32132400	-1.42661500	1.88966200
H	0.81744900	0.78096900	-0.14209100
H	0.72804900	0.54539800	1.60939200
H	1.48721300	-1.23415800	2.70747900
H	1.67172800	-3.67140600	-1.81502700
H	1.61914600	-3.86575200	-0.04552900
H	3.93911000	-3.20628000	-0.33955200
H	3.55571000	-2.20513200	-1.72735400
H	2.80572300	0.36330600	-1.23352200
H	2.81877800	1.16742600	1.29865500
H	4.54020300	1.38587100	1.02278900
H	-5.80725300	2.34355600	1.02025700
H	1.94094100	-0.91967600	-2.35712100
H	0.46982200	-1.75728300	-2.82183100
H	0.36575700	-0.19396100	-1.99550000
H	5.72108400	-0.24843200	-0.49678300
H	5.15741800	0.99395800	-1.63201600
H	4.90503300	-0.71672000	-2.00631500
H	4.15576600	5.64184700	0.47120800
H	3.83215500	4.99094000	-1.17982000
H	2.49062300	5.14447700	-0.01409900
H	-6.47751300	0.48344300	-1.15117000
H	-5.17949200	0.10997100	-2.30945600
H	-5.83066000	-1.17332000	-1.25814600
H	-4.36864500	0.04734000	1.96753900
H	-6.03607300	0.17231600	1.34698600
H	-5.12632400	-1.32912500	1.14677000
H	5.02328000	-1.47864900	1.17491800
H	3.82917100	-0.70477600	2.23364100
H	3.74765800	-2.44835700	1.91551100

TS6

Thermal correction to Gibbs free energy (Hartree): 0.609453

Single point energy (Hartree): -1355.330076

Solvation Gibbs free energy (Hartree): -0.063115

G_{sol} (Hartree): -1354.783738

C	-2.95221700	1.79392800	0.59454500
C	-4.42379600	1.76793700	1.01205600
C	-5.30290000	1.02090700	0.00860100
C	-4.80359300	-0.42733000	-0.28200900
C	-3.30939400	-0.32169500	-0.71394600
C	-2.68663200	-1.62237500	-1.22348000
C	-1.25065600	-1.37558300	-1.68195000
C	-0.35113700	-1.03656000	-0.48946000
C	-0.94722400	0.08601600	0.39539500
C	-2.44442900	0.38099200	0.33713300
C	-1.86650200	-0.37302200	1.50832100
C	-0.00291400	1.24924200	0.70319200
C	1.36868000	0.71063300	1.08807200

C	1.86299900	-0.39136300	0.36369300
C	1.14604400	-0.77597400	-0.92075400
C	1.85362700	-2.10224500	-1.30817400
C	2.47348400	-2.61870400	-0.01243900
C	2.96349900	-1.35354300	0.75699000
C	4.36549300	-0.90241400	0.17547500
C	4.71155100	0.57791800	0.47422100
H	-3.30983700	0.36285400	-1.58427800
O	-6.66195800	1.06421000	0.38625800
O	1.84466500	0.95225800	2.33843500
H	-0.31273100	-1.94271100	0.13752100
C	1.26759600	0.24985300	-2.06433500
C	5.49073100	-1.81774300	0.66958400
C	4.33404900	1.50086500	-0.66265700
O	4.72198200	1.39664700	-1.79486500
O	3.45166300	2.46609700	-0.27720000
C	3.12298500	3.46258400	-1.26454800
C	-5.65000000	-0.98598600	-1.43719800
C	-5.00274900	-1.32194600	0.95236200
C	3.02829400	-1.62001200	2.26949800
H	-2.84114100	2.39000100	-0.32898400
H	-2.36660700	2.30401500	1.37308500
H	-4.81239300	2.79159300	1.12375200
H	-4.51109000	1.28685900	2.00228100
H	-5.26072900	1.56619000	-0.95099800
H	-2.70687000	-2.40963900	-0.45118000
H	-3.27596100	-2.00516400	-2.06727300
H	-0.85890600	-2.25838300	-2.20898900
H	-1.25301100	-0.54397700	-2.40466500
H	-1.82734200	0.14428600	2.47201000
H	-2.04690900	-1.44709200	1.59124700
H	0.07128100	1.93686900	-0.15090400
H	-0.37452000	1.84389900	1.54624500
H	2.17448400	1.14888000	0.27011100
H	2.63201700	-1.89876500	-2.05827200
H	1.15802900	-2.81917000	-1.76250100
H	1.71946000	-3.13764200	0.60016500
H	3.29484600	-3.32867400	-0.17471200
H	4.31601900	-1.00279000	-0.91882500
H	4.28396600	0.92643900	1.42392500
H	5.80493800	0.67039300	0.56285100
H	-6.74424200	0.73613700	1.29155600
H	0.87629400	-0.19887900	-2.98674500
H	0.70296000	1.17468300	-1.88896600
H	2.32064300	0.50160600	-2.25183400
H	6.40587300	-1.60422800	0.09765300
H	5.25753600	-2.88263600	0.53031300
H	5.71484000	-1.65306700	1.73352300
H	2.64778300	3.00055500	-2.14069800
H	2.43969000	4.16285900	-0.77078100
H	4.03546400	3.98139000	-1.58778100
H	-5.47880800	-2.06122700	-1.59384000
H	-6.71534900	-0.83990700	-1.21249400
H	-5.43184600	-0.46137400	-2.38190800
H	-4.49302700	-0.94110300	1.84824100
H	-6.07511900	-1.41059800	1.18370000
H	-4.63661700	-2.34296100	0.76849100
H	3.56428500	-2.56272000	2.44433800
H	3.53717600	-0.82266200	2.82360300
H	2.01923400	-1.72919800	2.69163600

H 1.53608300 1.81507800 2.65022400

19f

Thermal correction to Gibbs free energy (Hartree): 0.611249

Single point energy (Hartree): -1355.367463

Solvation Gibbs free energy (Hartree): -0.061998

G_{sol} (Hartree): -1354.818211

C	-3.06727100	-2.02221200	-0.25985500
C	-4.51007800	-2.09026500	-0.76424100
C	-5.45662000	-1.21006800	0.05233700
C	-4.98819300	0.27426400	0.13722900
C	-3.52410200	0.26808200	0.67462200
C	-2.94579500	1.64533700	1.00395300
C	-1.54528100	1.50229900	1.59424800
C	-0.54878400	0.98492400	0.55283500
C	-1.09325300	-0.25928600	-0.19406100
C	-2.58848500	-0.57813900	-0.19609400
C	-1.93474700	-0.00533300	-1.42692000
C	-0.11469300	-1.44646400	-0.24934800
C	1.19031900	-0.92394200	-0.68769700
C	1.80859400	0.16067800	0.02346900
C	0.89231500	0.78856500	1.12245800
C	1.58722400	2.15057800	1.32453300
C	2.04762200	2.57944100	-0.06120400
C	2.58726800	1.30402800	-0.77145200
C	4.13502900	1.20133700	-0.54924900
C	4.75893400	-0.18091300	-0.88251500
H	-3.57396900	-0.26898700	1.64129000
O	-6.78851300	-1.33942100	-0.39581100
O	1.80095400	-1.44863100	-1.70439400
H	-0.46266700	1.77420000	-0.21022300
C	0.91249700	-0.00471600	2.44068200
C	4.90750100	2.27594500	-1.32870100
C	4.88733100	-1.11736200	0.29517100
O	4.02702600	-1.28028000	1.14979200
O	6.03700500	-1.76818400	0.30958800
C	6.25827900	-2.70347000	1.37929600
C	-5.91190400	0.99480900	1.13258700
C	-5.11369700	0.95737200	-1.23449800
C	2.23301300	1.35234700	-2.26414800
H	-3.00678700	-2.46534300	0.75019800
H	-2.43235800	-2.63724700	-0.91487800
H	-4.88100500	-3.12600300	-0.73439300
H	-4.53990700	-1.77395300	-1.82191700
H	-5.47022600	-1.59540100	1.08721800
H	-2.91705300	2.29312600	0.11135500
H	-3.59864300	2.15054600	1.72798900
H	-1.19615900	2.46821800	1.98869200
H	-1.59661200	0.80953100	2.44944000
H	-1.82841700	-0.67057800	-2.29044600
H	-2.11370000	1.03831500	-1.69446400
H	0.00805100	-1.88159200	0.75618400
H	-0.46188300	-2.24562400	-0.91731600
H	2.60739200	-0.43326500	0.57331500
H	2.45501500	2.00906800	1.98899000
H	0.93393200	2.88846500	1.81014500
H	1.20243700	2.98729100	-0.63552300
H	2.80572900	3.37221200	-0.02362300
H	4.30062200	1.38680200	0.52519800

H	4.16911200	-0.70620700	-1.65163000
H	5.76188100	-0.05596500	-1.31009900
H	-6.81893900	-1.14590800	-1.34216800
H	0.53965000	0.62104800	3.26348600
H	0.28585200	-0.90882100	2.42881000
H	1.93897300	-0.30766000	2.69384400
H	5.95490900	2.30246000	-0.99327800
H	4.49225900	3.28296600	-1.18456400
H	4.91396300	2.06552200	-2.40888200
H	5.48756900	-3.48703300	1.36697700
H	7.24987800	-3.13258300	1.20033800
H	6.22842900	-2.18559800	2.34812900
H	-5.75944900	2.08397500	1.12481500
H	-6.95923500	0.79493800	0.86805100
H	-5.75069400	0.63210000	2.16093700
H	-4.54332000	0.44897300	-2.02442100
H	-6.16924500	0.98862000	-1.54490900
H	-4.76874500	2.00111100	-1.19266800
H	2.55799900	2.31016300	-2.69300300
H	2.70337400	0.55144100	-2.85068200
H	1.14342500	1.28498300	-2.41089300
H	1.31865900	-2.21320000	-2.06943600

20b

Thermal correction to Gibbs free energy (Hartree): 0.599977

Single point energy (Hartree): -1355.020008

Solvation Gibbs free energy (Hartree): 0.012808

G_{sol} (Hartree): -1354.407223

C	3.06654500	2.07371100	-0.02821600
C	4.48077000	2.18656300	-0.60003700
C	5.46007900	1.22159700	0.06563100
C	4.98040500	-0.26009000	0.02796700
C	3.54375600	-0.29815600	0.63319800
C	2.96757100	-1.69787800	0.85609400
C	1.59014900	-1.59789000	1.50611300
C	0.56154800	-0.98443600	0.55139700
C	1.07377800	0.34019600	-0.07465200
C	2.57262700	0.63551600	-0.09510400
C	1.86681500	0.20057400	-1.35668000
C	0.10845300	1.51488200	0.01643500
C	-1.28839200	1.12307300	-0.40520700
C	-1.84366900	-0.14723200	0.20383800
C	-0.86820400	-0.88500900	1.16735100
C	-1.52350200	-2.28088100	1.21230700
C	-1.95146900	-2.56660200	-0.22383900
C	-2.43924100	-1.20799700	-0.81364100
C	-4.00455100	-1.17309200	-0.78681700
C	-4.60911600	0.23670100	-0.97233700
H	3.65020900	0.13604100	1.64696500
O	6.77089200	1.38535700	-0.44917600
O	-1.92453300	1.81955700	-1.17520900
H	0.47442800	-1.69310200	-0.28597900
C	-0.86645200	-0.26400400	2.57352200
C	-4.63992800	-2.13379600	-1.80121200
C	-5.11284300	0.87492900	0.29708300
O	-4.75573100	0.60516500	1.42394300
O	-6.00925300	1.84214000	0.03803400
C	-6.49176600	2.57417400	1.16299400
C	5.94809900	-1.08135600	0.89534100

C	5.03157600	-0.80180500	-1.41020500
C	-1.90075000	-1.02484000	-2.24034800
H	3.06715200	2.40594800	1.02593300
H	2.39966900	2.75628600	-0.57119800
H	4.86931700	3.21107800	-0.48736400
H	4.44936700	1.97856300	-1.68478700
H	5.54165200	1.49981900	1.13126000
H	2.89509500	-2.25588600	-0.09330800
H	3.64388500	-2.27510800	1.50261300
H	1.24809800	-2.59318100	1.82955500
H	1.67922000	-0.98290400	2.41678600
H	1.72533600	0.95034400	-2.14143300
H	2.02861800	-0.81183200	-1.73464100
H	0.05504500	1.88734000	1.05388500
H	0.40995000	2.35752700	-0.61494600
H	-2.68258300	0.19527400	0.82809600
H	-2.41018100	-2.22624100	1.86544000
H	-0.86403300	-3.05554700	1.63220500
H	-1.09992600	-2.94640600	-0.80898600
H	-2.72822800	-3.34231500	-0.27667900
H	-4.28825500	-1.51528200	0.22181500
H	-3.85964700	0.94158200	-1.37208400
H	-5.43912300	0.23521700	-1.69364600
H	6.72538200	1.29961100	-1.41048800
H	-1.89951300	-0.06658400	2.89887600
H	-0.41359700	-0.94876900	3.30592000
H	-0.30970300	0.68279900	2.62968800
H	-4.50273400	-1.77994500	-2.83491300
H	-5.72400200	-2.21180400	-1.62266100
H	-4.22134800	-3.14925300	-1.73725600
H	-7.19323700	3.31825200	0.76636700
H	-7.00258500	1.90783000	1.87448000
H	-5.66345100	3.07236900	1.68929800
H	6.98343100	-0.86455900	0.59668200
H	5.84279900	-0.82148900	1.96168900
H	5.77903800	-2.16328900	0.79023100
H	4.41879200	-0.21585400	-2.10835300
H	6.06952200	-0.80303400	-1.77904800
H	4.67812100	-1.84265800	-1.45320200
H	-2.14640800	-1.89770600	-2.86312600
H	-2.30597800	-0.12747600	-2.72726800
H	-0.80430700	-0.92452000	-2.23300100

TS7

Thermal correction to Gibbs free energy (Hartree): 0.611126

Single point energy (Hartree): -1355.341990

Solvation Gibbs free energy (Hartree): -0.059435

G_{sol} (Hartree): -1354.790300

C	-2.71243700	1.89905500	0.07413200
C	-4.18137300	2.24985700	0.31484200
C	-5.13095800	1.38155800	-0.50921200
C	-4.90482000	-0.14566000	-0.29003400
C	-3.39800300	-0.43582200	-0.56761700
C	-3.02338600	-1.91815700	-0.56898300
C	-1.55365900	-2.10145200	-0.92915400
C	-0.62866400	-1.48921300	0.13346500
C	-1.04174700	-0.06423600	0.59079200
C	-2.46665700	0.41329800	0.30426900
C	-2.09508400	-0.02985200	1.69183000

C	0.06451700	0.99535600	0.63701200
C	1.39818200	0.41071600	1.08252700
C	1.82923700	-0.74118200	0.16269500
C	0.82528700	-1.65371800	-0.20948300
C	1.42766900	-2.99478700	-0.54369500
C	2.93938500	-2.73542500	-0.63239100
C	3.21588900	-1.43579300	0.19211900
C	4.39201600	-0.62498100	-0.43925100
C	4.71141900	0.72928900	0.23257300
H	-3.22176800	-0.08328400	-1.60260400
O	-6.47586200	1.76477600	-0.31908600
O	1.31356100	-0.10953100	2.39511700
H	-0.70157200	-2.14807500	1.02151100
C	1.38764400	-0.45405500	-1.49338500
C	5.67893100	-1.46364700	-0.50362400
C	4.08969000	1.94190000	-0.42177100
O	3.09355300	1.93186700	-1.12676700
O	4.74478000	3.05215600	-0.12283000
C	4.23733500	4.28717000	-0.65421800
C	-5.78367200	-0.89361700	-1.30560300
C	-5.33451500	-0.55286100	1.12874800
C	3.51056800	-1.83119100	1.65355600
H	-2.44031200	2.14810600	-0.96725700
H	-2.07981300	2.52060500	0.72191000
H	-4.37029500	3.30621000	0.07032000
H	-4.41327500	2.12804000	1.38776400
H	-4.93064900	1.57837900	-1.57757700
H	-3.22887500	-2.38493200	0.40870000
H	-3.64263100	-2.45475300	-1.29976800
H	-1.31940700	-3.17006100	-1.04787000
H	-1.35958700	-1.62175500	-1.90505600
H	-2.01317200	0.74106500	2.46454800
H	-2.47410100	-0.98679500	2.05861500
H	0.18455100	1.51296100	-0.32518400
H	-0.19846300	1.77772200	1.36041200
H	2.15940200	1.19670800	1.08990400
H	0.99751600	-3.46292400	-1.43974300
H	1.17495300	-3.65199100	0.30616700
H	3.51971700	-3.58420700	-0.25011800
H	3.24267700	-2.60073900	-1.68111800
H	4.10187600	-0.41058100	-1.47980200
H	4.41333000	0.74612900	1.29432400
H	5.79660700	0.90412700	0.25292200
H	-6.66224300	1.78884600	0.62884600
H	2.00527100	0.47664600	-1.43694900
H	1.83604900	-1.12047700	-2.22963500
H	0.37454500	-0.13962100	-1.75272200
H	6.10384500	-1.63753400	0.49623300
H	6.43977500	-0.93261100	-1.09450300
H	5.52029400	-2.44120200	-0.97949500
H	4.91695700	5.06816400	-0.29689100
H	4.22792600	4.25370700	-1.75261500
H	3.21539200	4.46805700	-0.29152600
H	-6.81024000	-0.50626300	-1.25312300
H	-5.42095100	-0.74196700	-2.33560600
H	-5.81790900	-1.97536000	-1.10857300
H	-4.79831400	-0.00470300	1.91574700
H	-6.41148100	-0.36972100	1.26128700
H	-5.17626100	-1.62773100	1.30238100
H	4.41743600	-2.44943700	1.68695300

H	3.64780900	-0.96451100	2.31082400
H	2.68441000	-2.41562400	2.08110300
H	0.38596400	-0.29806800	2.59496100

19g

Thermal correction to Gibbs free energy (Hartree): 0.609631

Single point energy (Hartree): -1355.344176

Solvation Gibbs free energy (Hartree): -0.062650

G_{sol} (Hartree): -1354.797195

C	-2.80301100	1.97343200	-0.16708600
C	-4.25828500	2.39372900	0.04013900
C	-5.23646100	1.44854400	-0.65459300
C	-5.05179400	-0.03939700	-0.22592100
C	-3.55781700	-0.41628000	-0.47276200
C	-3.23366800	-1.88910100	-0.22211500
C	-1.79098800	-2.20045300	-0.59727400
C	-0.76860200	-1.39136800	0.23264100
C	-1.15760800	0.06520300	0.55760400
C	-2.58887000	0.52514100	0.24913900
C	-2.18230300	0.23416000	1.66420600
C	-0.03085200	1.09587800	0.48603200
C	1.32880500	0.50172700	0.85799900
C	1.68528100	-0.66646900	-0.07627300
C	0.61528300	-1.64669700	-0.15154300
C	1.14076800	-2.95394700	-0.61539100
C	2.66299100	-2.77325900	-0.75352900
C	3.01110400	-1.52393900	0.11205700
C	4.29631500	-0.80655600	-0.38940800
C	4.71750700	0.41211200	0.47583000
H	-3.38776000	-0.24488300	-1.55358700
O	-6.56938500	1.89096900	-0.51621300
O	1.28907500	-0.02384700	2.17481800
H	-0.67104000	-1.90173400	1.22990100
C	1.56523600	-0.16160500	-1.58892600
C	5.48610000	-1.76846600	-0.53102800
C	4.61405300	1.73956800	-0.24136100
O	3.70050200	2.05382400	-0.98032100
O	5.62071900	2.55332500	0.05865700
C	5.59604600	3.86514700	-0.52355500
C	-5.96689100	-0.89402000	-1.11791300
C	-5.47257500	-0.22944800	1.24054400
C	3.17154300	-2.00946000	1.56491100
H	-2.54019100	2.07780200	-1.23509600
H	-2.14303800	2.65452800	0.38692000
H	-4.42238400	3.41278500	-0.34191900
H	-4.48083700	2.42148600	1.12145000
H	-5.03693500	1.49027600	-1.74035300
H	-3.41970000	-2.16834300	0.82724200
H	-3.89376700	-2.52371700	-0.82826700
H	-1.58977500	-3.27609500	-0.48727700
H	-1.63637600	-1.95013400	-1.66095500
H	-2.04716400	1.07856400	2.34621200
H	-2.56756800	-0.66383400	2.15209500
H	0.02628800	1.57367700	-0.50206900
H	-0.23502200	1.91671200	1.18869700
H	2.09757700	1.28107600	0.74962500
H	0.62275300	-3.28707100	-1.53091600
H	0.86229700	-3.70638700	0.14545200
H	3.20596300	-3.66363900	-0.41426600

H	2.93455500	-2.62221600	-1.80743800
H	4.07726400	-0.43110700	-1.39909800
H	4.08790800	0.50772300	1.37469300
H	5.74276200	0.29970300	0.85177800
H	-6.74586900	2.06282200	0.41823800
H	2.13838900	0.77985000	-1.60809400
H	2.00828900	-0.87028200	-2.29305200
H	0.53201900	0.03993500	-1.89842300
H	5.80205800	-2.17934400	0.43983300
H	6.34812300	-1.23187400	-0.95473200
H	5.26619600	-2.61028900	-1.20296800
H	6.49710600	4.37214900	-0.16143500
H	5.60454600	3.79682900	-1.62062900
H	4.69336400	4.40801600	-0.20817500
H	-6.98118400	-0.47262800	-1.10783800
H	-5.61633600	-0.89654900	-2.16314600
H	-6.02940900	-1.93673400	-0.77276300
H	-4.89102300	0.38742500	1.93961400
H	-6.53525500	0.02938700	1.36181800
H	-5.36946300	-1.27875000	1.55449000
H	3.99799600	-2.73182200	1.61701800
H	3.36918000	-1.19626800	2.26916300
H	2.26480300	-2.51363200	1.93020700
H	0.98553200	0.66735400	2.77798500

chair-20c

Thermal correction to Gibbs free energy (Hartree): 0.598534

Single point energy (Hartree): -1355.001948

Solvation Gibbs free energy (Hartree): 0.000885

G_{sol} (Hartree): -1354.402528

C	3.05190800	-1.96758300	-0.63916300
C	4.45197800	-2.39957300	-0.20834700
C	5.49345400	-1.32778900	-0.51468400
C	5.15286900	0.04844500	0.12971100
C	3.71784400	0.45899300	-0.33391200
C	3.27654300	1.83065000	0.18303600
C	1.92728300	2.24907400	-0.39648300
C	0.82839000	1.21351700	-0.28645500
C	1.19691700	-0.21893100	-0.02283600
C	2.66913300	-0.62240500	-0.04310300
C	1.92505700	-0.57728000	1.26603300
C	0.13031500	-1.19396600	-0.49447100
C	-1.26256900	-0.79058700	0.01360700
C	-1.63894900	0.60987600	-0.51538300
C	-0.45437500	1.56024900	-0.49090800
C	-0.98000900	2.96848900	-0.67376300
C	-2.50634400	2.86055400	-0.44927600
C	-2.73818400	1.48436700	0.24067800
C	-4.18826100	0.97136500	0.04515900
C	-4.46013500	-0.36354400	0.77734900
H	3.77388000	0.53770600	-1.43780500
O	6.80095100	-1.77429900	-0.19484000
O	-1.28726000	-0.83488700	1.43534500
C	-2.05264600	0.39090100	-1.99888600
C	-5.26072900	1.99817100	0.43479600
C	-5.10333600	-1.41150600	-0.09539300
O	-4.91742200	-1.55355800	-1.28322300
O	-5.89564600	-2.23674300	0.61522300
C	-6.49035000	-3.31339700	-0.10687100

C	6.18987600	1.06247200	-0.38099900
C	5.26371000	-0.04260700	1.66133400
C	-2.42328800	1.68226700	1.73856100
H	3.02101900	-1.88551100	-1.74109400
H	2.32600200	-2.74542500	-0.36582500
H	4.74836300	-3.33191000	-0.71472300
H	4.45533100	-2.61223900	0.87580200
H	5.51145500	-1.17122900	-1.60781700
H	3.22869200	1.82531500	1.28294400
H	4.02607300	2.58921500	-0.08303900
H	1.60176100	3.19664000	0.06318600
H	2.07038100	2.48080500	-1.46930700
H	1.66393700	-1.53176900	1.73286300
H	2.13424600	0.21634900	1.98383200
H	0.12184600	-1.25217500	-1.59337300
H	0.34118900	-2.21421400	-0.13720800
H	-1.99847500	-1.51334400	-0.38608100
H	-0.74032500	3.37487100	-1.67159600
H	-0.51209000	3.65572700	0.04981700
H	-2.88799800	3.68463500	0.16943400
H	-3.04906200	2.91094500	-1.40453600
H	-4.31560100	0.77841100	-1.02806500
H	-3.52505900	-0.81411900	1.14655000
H	-5.08277200	-0.22280900	1.67262100
H	6.79773400	-2.06675300	0.72594000
H	-2.90679700	-0.29588300	-2.07944100
H	-2.32037700	1.33050600	-2.49762100
H	-1.21454700	-0.03689000	-2.56549700
H	-5.20806100	2.25971200	1.50358600
H	-6.26553000	1.58651800	0.24625800
H	-5.17323200	2.92755200	-0.14650900
H	-7.08898500	-3.87666200	0.61950300
H	-7.13032400	-2.93455500	-0.91804800
H	-5.71921900	-3.96099800	-0.55149900
H	7.20190700	0.66092200	-0.23189900
H	6.05839400	1.25254900	-1.45900500
H	6.12143200	2.02555700	0.14557400
H	4.54221800	-0.74663100	2.09813000
H	6.27783100	-0.35924500	1.95316000
H	5.09430700	0.93776900	2.12938900
H	-3.00997300	2.52774600	2.13004700
H	-2.64318200	0.79586700	2.34036900
H	-1.35950500	1.91089300	1.89234700
H	-0.86847900	-1.65929300	1.71260500

boat-20c

Thermal correction to Gibbs free energy (Hartree): 0.598774

Single point energy (Hartree): -1354.988349

Solvation Gibbs free energy (Hartree): -0.002370

G_{sol} (Hartree): -1354.391945

C	3.16908300	-2.06418600	-0.44971900
C	4.53844700	-2.43875000	0.15253400
C	5.40587300	-1.22810100	0.51576200
C	5.23983400	-0.04359100	-0.47181100
C	3.72142300	0.39531700	-0.57693800
C	3.38084800	1.77422400	-0.00944500
C	1.94994100	2.18600900	-0.37158900
C	0.88478900	1.11321100	-0.24315900
C	1.28389600	-0.29270500	0.09175100

C	2.75965800	-0.66821900	-0.02406900
C	2.13697700	-0.50563500	1.33219400
C	0.20695200	-1.31722700	-0.22112100
C	-1.17171800	-0.87046200	0.28378100
C	-1.57553100	0.46214100	-0.38570400
C	-0.40544100	1.42955600	-0.45039800
C	-0.94242900	2.82183500	-0.70278800
C	-2.46991100	2.70469800	-0.50805400
C	-2.69011100	1.38601600	0.28819200
C	-4.13325700	0.84632500	0.12288900
C	-4.37342600	-0.46146100	0.94395600
H	3.50079400	0.45211900	-1.65947200
O	5.08161800	-0.86233900	1.85131500
O	-1.14200500	-0.74325700	1.70101600
C	-1.98990500	0.09118300	-1.83729900
C	-5.22684600	1.87047200	0.44901100
C	-4.97510900	-1.52311400	0.06762100
O	-4.35847000	-2.38575900	-0.51751300
O	-6.30973700	-1.37320300	-0.06331300
C	-6.96066300	-2.27741100	-0.95359500
C	5.73494900	-0.49686800	-1.85871200
C	6.16632900	1.09811200	-0.01743400
C	-2.39644600	1.70696100	1.76847400
H	3.21011200	-2.09978100	-1.55216000
H	2.42184700	-2.81089500	-0.15127300
H	5.09024800	-3.09108900	-0.54124300
H	4.40672100	-3.01049900	1.08322300
H	6.46925900	-1.54101900	0.47395100
H	3.52882700	1.77544800	1.08115700
H	4.06246900	2.53709900	-0.40993300
H	1.66087600	3.07240000	0.21933300
H	1.95204700	2.53262800	-1.42168300
H	1.96578500	-1.41947700	1.90762100
H	2.38879900	0.35271200	1.95350400
H	0.16139300	-1.50883300	-1.30421400
H	0.44283600	-2.28651200	0.24640100
H	-1.91388100	-1.63731600	-0.00061400
H	-0.68133600	3.19356200	-1.70917200
H	-0.50122200	3.54366600	0.00480200
H	-2.88409700	3.56946200	0.02884700
H	-2.98782200	2.66318000	-1.47792700
H	-4.25380800	0.60247000	-0.94330900
H	-3.43831500	-0.85245500	1.35663500
H	-5.05206200	-0.25546800	1.78409900
H	-2.78874800	-0.66409000	-1.84714000
H	-2.33016000	0.96381800	-2.40894900
H	-1.13143500	-0.32528900	-2.38050600
H	-5.17687600	2.19385800	1.50057300
H	-6.21688600	1.41767600	0.28615700
H	-5.15645400	2.76537700	-0.18660600
H	-8.02489500	-2.01220700	-0.93696900
H	-6.55815300	-2.18022100	-1.97349300
H	-6.82078200	-3.31857200	-0.62600900
H	6.77535000	-0.85840700	-1.81221600
H	5.11673600	-1.30178000	-2.28028600
H	5.70552600	0.34541000	-2.56791900
H	5.88455900	1.51428300	0.96127400
H	7.20518800	0.73511000	0.05171500
H	6.15990900	1.93318000	-0.73302400
H	-2.98093600	2.58717400	2.07840700

H	-2.63301500	0.87498000	2.43805400
H	-1.33275600	1.93502600	1.91931700
H	-0.69051800	-1.51947500	2.05492500
H	5.66440600	-0.14078000	2.11611300

chair-19h

Thermal correction to Gibbs free energy (Hartree): 0.610506

Single point energy (Hartree): -1355.328368

Solvation Gibbs free energy (Hartree): -0.089091

G_{sol} (Hartree): -1354.806954

C	3.05071000	-1.98070700	-0.45082900
C	4.48014200	-2.33372800	0.00157100
C	5.38470700	-1.24158200	-0.48908100
C	5.11619200	0.17237200	0.01729600
C	3.64602000	0.48302900	-0.46782700
C	3.18757200	1.89798300	-0.10336800
C	1.80638200	2.19419000	-0.68670800
C	0.74649100	1.15480800	-0.39250400
C	1.16590000	-0.22759300	0.02586900
C	2.64963100	-0.58593300	-0.00562600
C	1.94066000	-0.40388700	1.31763400
C	0.11711800	-1.28443900	-0.28370800
C	-1.25968700	-0.85764400	0.25864200
C	-1.70435900	0.46159600	-0.41165500
C	-0.55556900	1.44407100	-0.55721400
C	-1.13241100	2.80669000	-0.87220400
C	-2.64240800	2.68459000	-0.56702000
C	-2.80456900	1.38721200	0.27948800
C	-4.24820400	0.82717300	0.19069200
C	-4.43849500	-0.47529100	1.03371200
H	3.67798300	0.43224500	-1.57389200
O	6.86321600	-1.67390800	-0.07738700
O	-1.17871100	-0.73339600	1.67600400
C	-2.16195600	0.06138400	-1.84484800
C	-5.33178800	1.84696600	0.56163900
C	-4.90918900	-1.60874300	0.16427100
O	-4.19315600	-2.45088200	-0.33671500
O	-6.23080400	-1.55220700	-0.05969500
C	-6.77356600	-2.53437200	-0.94529200
C	6.11533400	1.13554400	-0.64893000
C	5.25056200	0.25871400	1.54751500
C	-2.44639000	1.75514000	1.73397600
H	2.99496200	-2.04858000	-1.55161200
H	2.37054800	-2.74502300	-0.05770200
H	4.79233800	-3.30496300	-0.41071100
H	4.50885800	-2.39500900	1.10198100
H	5.49427100	-1.26427700	-1.58142300
H	3.17122000	2.02266300	0.98972800
H	3.89854400	2.64201300	-0.48974200
H	1.47415400	3.18569500	-0.34168300
H	1.91135000	2.28841600	-1.78437800
H	1.71641400	-1.29740400	1.90533700
H	2.14214700	0.47960900	1.92387600
H	0.05859700	-1.46291400	-1.36787400
H	0.37536300	-2.24833500	0.18057200
H	-1.99661200	-1.63435400	0.00167500
H	-0.94618600	3.10077900	-1.91919800
H	-0.65520800	3.58291300	-0.25214500
H	-3.02048900	3.56181300	-0.02547700

H	-3.22608800	2.61863400	-1.49654000
H	-4.42092100	0.57544700	-0.86661600
H	-3.50175100	-0.78003200	1.50932600
H	-5.17892600	-0.30211200	1.82715800
H	6.90785100	-1.90963500	0.87123100
H	-2.94945500	-0.70314300	-1.81059000
H	-2.53600600	0.91838900	-2.41756800
H	-1.32032300	-0.35488300	-2.41455900
H	-5.24928400	2.16269100	1.61320900
H	-6.32479500	1.39176100	0.42793600
H	-5.28858400	2.74616900	-0.06987400
H	-7.85039500	-2.33576100	-0.99807100
H	-6.31873200	-2.45063300	-1.94372400
H	-6.58858000	-3.54832400	-0.56141400
H	7.16889300	0.90549200	-0.39202800
H	6.02221800	1.12715700	-1.74588600
H	5.96242400	2.16546900	-0.30316500
H	4.53049800	-0.38027400	2.07264000
H	6.26834600	-0.00205800	1.88883000
H	5.07993100	1.28970900	1.88328100
H	-3.03465400	2.62951300	2.04980000
H	-2.63012200	0.93783800	2.43707600
H	-1.38257900	2.01574200	1.82714800
H	-1.16816400	-1.62480200	2.04618000
H	7.48360200	-0.92975300	-0.23170900

boat-19h

Thermal correction to Gibbs free energy (Hartree): 0.610627

Single point energy (Hartree): -1355.332476

Solvation Gibbs free energy (Hartree): -0.075091

G_{sol} (Hartree): -1354.796940

C	3.10182400	-2.05111100	-0.54057000
C	4.47680400	-2.45112700	0.04093300
C	5.25580500	-1.25449800	0.54763200
C	5.21545500	-0.00966400	-0.34148200
C	3.70668000	0.41209700	-0.61224000
C	3.31808100	1.81423700	-0.13904700
C	1.92012300	2.18920200	-0.63331800
C	0.84719300	1.14467300	-0.40926400
C	1.24694800	-0.26645600	-0.07502500
C	2.69320000	-0.64280900	-0.13041800
C	1.99516700	-0.46765800	1.26096300
C	0.16723300	-1.29166900	-0.38532200
C	-1.18558200	-0.85915500	0.20478400
C	-1.61813600	0.49235500	-0.40869800
C	-0.45405100	1.45933100	-0.53133900
C	-1.00611700	2.84686900	-0.76590900
C	-2.51533600	2.73734300	-0.45859700
C	-2.69287800	1.40851600	0.33384400
C	-4.14984300	0.88260000	0.23911700
C	-4.36265100	-0.44804400	1.03066800
H	3.58689300	0.41405100	-1.70865200
O	4.61772300	-0.82351300	1.87745500
O	-1.05327400	-0.80665200	1.62626300
C	-2.10051200	0.15673400	-1.85046700
C	-5.20502000	1.91125500	0.66442800
C	-4.80872600	-1.55760800	0.11717600
O	-4.07997700	-2.39932000	-0.36734800
O	-6.11625200	-1.47906200	-0.16084800

C	-6.63698800	-2.43733800	-1.08694100
C	5.88551400	-0.39409300	-1.67753000
C	6.06416700	1.09584900	0.31219700
C	-2.30930800	1.70868700	1.79749900
H	3.13787100	-2.06992400	-1.64121000
H	2.34867800	-2.79110000	-0.24901800
H	5.09631800	-2.95532900	-0.71479600
H	4.37336400	-3.18485000	0.85861200
H	6.28358900	-1.50638400	0.83910700
H	3.37913600	1.88570500	0.95893900
H	4.03352200	2.55178000	-0.52474800
H	1.61735200	3.14602600	-0.17982300
H	1.98784100	2.39252000	-1.71833100
H	1.67613200	-1.35317200	1.81567200
H	2.09096900	0.44207400	1.85783400
H	0.08908400	-1.42265200	-1.47433900
H	0.41811600	-2.27533100	0.03608900
H	-1.94285400	-1.61065800	-0.06094900
H	-0.81522200	3.19374800	-1.79550300
H	-0.50896200	3.57697800	-0.10682900
H	-2.87590800	3.59727600	0.12084800
H	-3.10441400	2.71930400	-1.38668200
H	-4.34094700	0.67812900	-0.82511300
H	-3.43990000	-0.76787600	1.52251000
H	-5.12429200	-0.30210000	1.80930400
H	4.68286000	-1.52018400	2.55668800
H	-2.89398700	-0.60202200	-1.83559000
H	-2.47673100	1.04032600	-2.37937700
H	-1.27299900	-0.24123800	-2.45294400
H	-5.10729400	2.17830800	1.72807900
H	-6.20980900	1.48673700	0.51903300
H	-5.14522300	2.83583100	0.07253400
H	-7.70836000	-2.22365100	-1.17568700
H	-6.14349000	-2.33821900	-2.06524800
H	-6.47826300	-3.46038700	-0.71623100
H	6.91138500	-0.76504000	-1.52602200
H	5.31889700	-1.15604100	-2.23126600
H	5.94761200	0.49847100	-2.31679000
H	5.66220600	1.42745300	1.27793300
H	7.09014900	0.73259100	0.47925200
H	6.13404400	1.97287600	-0.34386200
H	-2.87980000	2.57700300	2.15862000
H	-2.49488300	0.86638400	2.46995500
H	-1.24075400	1.95111100	1.88724800
H	-1.30296100	-1.67142500	1.97353700
H	3.60098900	-0.64982600	1.66459900

TS8

Thermal correction to Gibbs free energy (Hartree): 0.606924

Single point energy (Hartree): -1355.329266

Solvation Gibbs free energy (Hartree): -0.068091

G_{sol} (Hartree): -1354.790433

C	3.09745500	-2.05522200	-0.55119500
C	4.45098300	-2.44982000	0.08049000
C	5.20102800	-1.24435700	0.62139800
C	5.20836500	-0.02185800	-0.30682900
C	3.71478400	0.41157100	-0.62864200
C	3.31457400	1.81511600	-0.16883400
C	1.92575700	2.18721700	-0.68926200

C	0.85091900	1.14737000	-0.45668300
C	1.25498800	-0.26515700	-0.14648100
C	2.67774800	-0.63736700	-0.19230700
C	1.99428500	-0.46128400	1.24843600
C	0.16733500	-1.28872600	-0.43160600
C	-1.17404900	-0.85900900	0.18387500
C	-1.61600800	0.49605500	-0.41677300
C	-0.45334000	1.46290400	-0.55084400
C	-1.00695600	2.85224500	-0.76719500
C	-2.51172200	2.74238600	-0.44111700
C	-2.68104800	1.40821400	0.34420600
C	-4.14097100	0.88678000	0.26229900
C	-4.35179200	-0.44830600	1.04645800
H	3.62572200	0.41130600	-1.72830400
O	4.51701300	-0.79811300	1.87623600
O	-1.00974400	-0.82276200	1.60309000
C	-2.11599000	0.16941600	-1.85492400
C	-5.18727400	1.91657000	0.70698800
C	-4.78510900	-1.55938700	0.12799900
O	-4.04799000	-2.39862300	-0.34854700
O	-6.08915800	-1.48507300	-0.16194700
C	-6.59976100	-2.44581500	-1.09198500
C	5.91286300	-0.42996100	-1.61588600
C	6.04231200	1.09064300	0.35283300
C	-2.27921200	1.69784700	1.80499800
H	3.16412500	-2.08595300	-1.65021600
H	2.32868300	-2.78443700	-0.27494700
H	5.09233900	-2.95890700	-0.65231900
H	4.31035400	-3.17681100	0.89771800
H	6.22407100	-1.50132600	0.92832400
H	3.35765700	1.89064900	0.92905700
H	4.03795800	2.54904600	-0.54566500
H	1.61859500	3.15171900	-0.25640700
H	2.00611800	2.36969100	-1.77714300
H	1.58923100	-1.32726800	1.77406800
H	1.98574800	0.47567000	1.80709900
H	0.07199500	-1.41047800	-1.52026900
H	0.42509100	-2.27427700	-0.02174700
H	-1.93437500	-1.60946400	-0.07334900
H	-0.82794600	3.20599700	-1.79642300
H	-0.49932700	3.57601800	-0.10926500
H	-2.86323700	3.59876400	0.14888000
H	-3.11270100	2.73174000	-1.36158200
H	-4.34514200	0.69054400	-0.80101800
H	-3.43130800	-0.76448400	1.54457600
H	-5.11924200	-0.31011200	1.82070200
H	4.60472100	-1.46176800	2.58228100
H	-2.90474800	-0.59401800	-1.83458700
H	-2.50513000	1.05495100	-2.37091400
H	-1.29541300	-0.21873100	-2.47312800
H	-5.07844300	2.17378400	1.77195700
H	-6.19528200	1.49788000	0.56738700
H	-5.12938300	2.84597500	0.12270100
H	-7.67081900	-2.23483000	-1.18958300
H	-6.09826200	-2.34566000	-2.06603500
H	-6.44125600	-3.46787500	-0.71870000
H	6.92782300	-0.81256400	-1.42569600
H	5.35658900	-1.19405600	-2.17755900
H	6.00869100	0.45113400	-2.26719200
H	5.61947000	1.42706200	1.30762500

H	7.06267400	0.72512300	0.54630800
H	6.13089900	1.96210800	-0.30889200
H	-2.84768700	2.56119800	2.18058900
H	-2.45296300	0.85056600	2.47441900
H	-1.21047400	1.94373400	1.88320300
H	-1.37811800	-1.63836300	1.96286100
H	3.37074700	-0.64511000	1.58401100

boat-19b

Thermal correction to Gibbs free energy (Hartree): 0.609498

Single point energy (Hartree): -1355.365563

Solvation Gibbs free energy (Hartree): -0.056827

G_{sol} (Hartree): -1354.812892

C	2.96824200	-2.02281500	0.06169300
C	4.43556400	-2.37178000	0.38038600
C	5.44340100	-1.21175800	0.23621300
C	5.00709300	-0.15602000	-0.80071500
C	3.52843000	0.35920600	-0.56094800
C	3.35681000	1.81491600	-0.13149600
C	1.89331400	2.24759100	-0.31175500
C	0.85522700	1.15154500	-0.15504700
C	1.19584500	-0.18436000	0.11881500
C	2.63005800	-0.54995200	0.34812300
C	2.74191000	-0.27288800	1.88968700
C	0.14348700	-1.23073400	0.23287000
C	-1.24340800	-0.71961900	0.64951000
C	-1.62916300	0.49889900	-0.21112800
C	-0.49136500	1.46316400	-0.32595000
C	-1.00742400	2.81612000	-0.67149100
C	-2.53935200	2.69373800	-0.66697000
C	-2.83287300	1.45588000	0.22836100
C	-4.23531900	0.85313800	-0.04658400
C	-4.54495300	-0.38459100	0.85687200
H	3.05430300	0.28797000	-1.55599100
O	5.68722600	-0.55348600	1.47811100
O	-1.19617200	-0.36267600	2.01782600
C	-1.84944600	-0.03686200	-1.66878800
C	-5.37076000	1.87796100	0.06917600
C	-4.78992900	-1.61148200	0.01706200
O	-3.91569200	-2.35851500	-0.37863600
O	-6.07520100	-1.75443900	-0.30568200
C	-6.41256900	-2.85436600	-1.16175100
C	5.06867900	-0.81872100	-2.19372600
C	6.03245900	0.98944000	-0.78915800
C	-2.71620400	1.92996000	1.69252400
H	2.75725400	-2.22015000	-1.00119700
H	2.31924200	-2.69995100	0.63356100
H	4.74006900	-3.20569400	-0.26941900
H	4.51635100	-2.75070300	1.41087600
H	6.39930200	-1.63045100	-0.12453000
H	3.68768900	1.94976400	0.90751400
H	3.98225900	2.47971200	-0.73786400
H	1.64846000	3.07093900	0.37934200
H	1.76719100	2.67267000	-1.32250000
H	2.16738000	-1.02627700	2.44752600
H	2.35601200	0.71424100	2.17389500
H	0.10548600	-1.75129000	-0.74302800
H	0.46714600	-2.00601400	0.94142100
H	-1.98039500	-1.51673200	0.47058500

H	-0.57313100	3.17052300	-1.62329000
H	-0.63721500	3.53405900	0.08233000
H	-3.01797300	3.60002300	-0.27651400
H	-2.92119400	2.55021400	-1.68772400
H	-4.23577100	0.51908200	-1.09524300
H	-3.71089300	-0.60299500	1.53247200
H	-5.42951000	-0.18710900	1.47637000
H	6.25070500	-1.11567200	2.02490900
H	-2.56996200	-0.86415700	-1.64437700
H	-2.22375500	0.74225600	-2.34136100
H	-0.91317400	-0.41418800	-2.10172800
H	-5.46298900	2.27172500	1.09271500
H	-6.32536500	1.39433000	-0.18620700
H	-5.23632000	2.72747200	-0.61597900
H	-7.49864600	-2.80859100	-1.29896900
H	-5.89716400	-2.76145000	-2.12885700
H	-6.12205100	-3.80675900	-0.69598100
H	6.08278200	-1.18911400	-2.40807700
H	4.37475500	-1.66568600	-2.29644200
H	4.81319500	-0.08531300	-2.97393200
H	6.05193300	1.51505600	0.17253000
H	7.04059100	0.58227800	-0.96221800
H	5.83235200	1.71386700	-1.59241400
H	-3.36274300	2.80616200	1.84317600
H	-3.00251700	1.16021200	2.41405800
H	-1.68901100	2.22353300	1.95149600
H	-1.23437300	-1.16677000	2.55147300
H	3.80189800	-0.33174100	2.16993800

chair-19b

Thermal correction to Gibbs free energy (Hartree): 0.609440

Single point energy (Hartree): -1355.376049

Solvation Gibbs free energy (Hartree): -0.059417

G_{sol} (Hartree): -1354.826026

C	2.89344200	-1.97792900	-0.05875600
C	4.37165900	-2.33222000	0.08153500
C	5.27311600	-1.36990300	-0.68529600
C	5.08426300	0.11169100	-0.24905300
C	3.56448800	0.45064500	-0.34106500
C	3.22486300	1.90145900	-0.00031500
C	1.82166800	2.25679500	-0.48200600
C	0.79762300	1.16584300	-0.25001700
C	1.15696800	-0.14481000	0.09444500
C	2.58711300	-0.52477200	0.39155700
C	2.62508400	-0.44213100	1.95384100
C	0.11167900	-1.20411000	0.20079800
C	-1.27816400	-0.70646400	0.62316900
C	-1.68554600	0.49135400	-0.25755300
C	-0.55939800	1.45688400	-0.42096500
C	-1.09115900	2.79143200	-0.80675900
C	-2.62192700	2.66319000	-0.76575000
C	-2.89115000	1.44972400	0.17011600
C	-4.29287700	0.82937400	-0.06766600
C	-4.58092200	-0.38815000	0.86936900
H	3.32248200	0.31598400	-1.41273500
O	6.62142700	-1.78009600	-0.64913200
O	-1.22618200	-0.33367100	1.98736200
C	-1.91716600	-0.07932400	-1.70354600
C	-5.43312300	1.84977800	0.04162800

C	-4.81554000	-1.64050300	0.06429600
O	-3.93189500	-2.37761000	-0.33018300
O	-6.10242100	-1.81989100	-0.22813500
C	-6.43321800	-2.94939900	-1.04842700
C	5.85620300	0.98152000	-1.25970600
C	5.69338700	0.35386800	1.14313900
C	-2.75382500	1.96418600	1.61861500
H	2.59962900	-2.08815500	-1.11644500
H	2.29414900	-2.69969900	0.51361300
H	4.54263100	-3.35127400	-0.29712400
H	4.66461600	-2.34837700	1.14540400
H	4.99091300	-1.42404700	-1.75188600
H	3.30556200	2.07261800	1.08328100
H	3.94291000	2.58563200	-0.46905700
H	1.47928900	3.19001800	-0.00851100
H	1.84633500	2.46770000	-1.56641000
H	1.69852500	-0.83401400	2.39797700
H	2.74112100	0.58929900	2.30586600
H	0.06636800	-1.70234600	-0.78555000
H	0.43395600	-1.99110700	0.89440100
H	-2.00533100	-1.51559500	0.46129200
H	-0.67477000	3.11347400	-1.77804900
H	-0.70976800	3.53763800	-0.08647000
H	-3.09488700	3.57850600	-0.38988300
H	-3.02561500	2.49107300	-1.77343400
H	-4.30699600	0.47038300	-1.10804100
H	-3.73965300	-0.57786900	1.54478900
H	-5.46359100	-0.18607600	1.48989100
H	6.88936300	-1.90230600	0.27144200
H	-2.62284300	-0.91783500	-1.64634600
H	-2.31696600	0.67867900	-2.38499700
H	-0.98265200	-0.45069100	-2.14518500
H	-5.51316900	2.26574700	1.05735700
H	-6.38819600	1.35479900	-0.18888500
H	-5.31446300	2.68447000	-0.66429200
H	-7.52264200	-2.93057700	-1.16307800
H	-5.94037800	-2.87027500	-2.02835600
H	-6.11171800	-3.88239500	-0.56426200
H	6.87135500	0.57873800	-1.37716100
H	5.37390400	0.97014100	-2.25060800
H	5.94472400	2.02729200	-0.93128000
H	5.32650300	-0.33644700	1.91378000
H	6.78676900	0.24455100	1.09279600
H	5.49525700	1.37692600	1.49425500
H	-3.40267400	2.84058700	1.75691800
H	-3.02393500	1.21278100	2.36537800
H	-1.72402700	2.27050200	1.85255500
H	-1.32172900	-1.12600500	2.53138600
H	3.45695900	-1.04046800	2.34261900

boat-20d

Thermal correction to Gibbs free energy (Hartree): 0.598005

Single point energy (Hartree): -1355.007399

Solvation Gibbs free energy (Hartree): 0.004539

G_{sol} (Hartree): -1354.404855

C	3.02100900	-2.02094100	-0.29686100
C	4.33016800	-2.19653200	-1.08242300
C	5.51535300	-1.48538200	-0.43914400
C	5.28755800	0.05673000	-0.41863600

C	3.75607600	0.39501200	-0.44255500
C	3.43718600	1.83852200	-0.05462200
C	2.01413700	2.19994100	-0.46625300
C	1.00356600	1.11555300	-0.17336100
C	1.36529100	-0.15307200	0.16130000
C	2.82518300	-0.59320900	0.31741100
C	3.11358000	-0.63872200	1.83885300
C	0.31358500	-1.20130300	0.46855500
C	-1.01267200	-0.59087500	0.93866000
C	-1.50783500	0.44067900	-0.10877200
C	-0.40879200	1.48617200	-0.28159800
C	-0.94149800	2.68526600	-0.58572300
C	-2.44319300	2.63696400	-0.59474700
C	-2.78905500	1.34300600	0.20899100
C	-4.13065200	0.72536000	-0.27426100
C	-4.53010500	-0.53501100	0.52447100
H	3.45133500	0.29641500	-1.49985600
O	5.75014100	-1.96766300	0.88037800
O	-0.82824000	-0.05802400	2.23816000
C	-1.67428900	-0.27642600	-1.47130900
C	-5.30377700	1.71519000	-0.28673900
C	-5.48583900	-1.39214200	-0.26715200
O	-5.21471300	-1.92948400	-1.31603400
O	-6.69920700	-1.48454500	0.30984600
C	-7.66706300	-2.26590500	-0.38940700
C	5.89952300	0.61689800	-1.71857700
C	6.03759100	0.69037500	0.76537400
C	-2.89604500	1.74559800	1.69025600
H	2.19346500	-2.25729300	-0.98039800
H	2.97087600	-2.76811100	0.50912700
H	4.21438700	-1.80896400	-2.10717400
H	4.55397400	-3.27191300	-1.19796000
H	6.42166800	-1.67595200	-1.04642100
H	3.55907700	1.97322700	1.03097200
H	4.14295100	2.53645000	-0.52979600
H	1.70195800	3.13194800	0.03283500
H	1.97931400	2.42185100	-1.54937800
H	2.34196300	-1.23056200	2.35371000
H	3.09261700	0.36775300	2.28064100
H	0.15391400	-1.85266700	-0.40519300
H	0.66943400	-1.86535800	1.26980600
H	-1.74928900	-1.39914800	1.05906500
H	-0.37659300	3.58761200	-0.82633900
H	-2.90476500	3.53347100	-0.14942100
H	-2.82444000	2.58219500	-1.63274600
H	-3.98637800	0.40172700	-1.31342900
H	-3.64744300	-1.15845700	0.71690700
H	-4.97481100	-0.27021400	1.49273400
H	5.84362300	-2.92760700	0.83394200
H	-2.36028800	-1.13554000	-1.41398600
H	-2.06833500	0.41599400	-2.22732500
H	-0.70635400	-0.63065200	-1.84850800
H	-5.54575800	2.08102500	0.72284000
H	-6.21069800	1.22821600	-0.67842600
H	-5.09895600	2.58707800	-0.92447200
H	-8.58402200	-2.22824000	0.21124200
H	-7.84915200	-1.85444500	-1.39375900
H	-7.32400000	-3.30567700	-0.50005000
H	6.99415600	0.49532500	-1.72125700
H	5.49896300	0.10472600	-2.60823300

H	5.68280300	1.69009200	-1.82914800
H	5.60103100	0.42257600	1.73357200
H	7.08442300	0.35112600	0.77442300
H	6.04262500	1.78672200	0.67813500
H	-3.73993500	2.43965200	1.82288500
H	-3.03535600	0.88779300	2.35662000
H	-1.98752200	2.26427800	2.02272800
H	-0.14411700	0.62357800	2.17399700
H	4.08584800	-1.10277600	2.03791000

chair-20d

Thermal correction to Gibbs free energy (Hartree): 0.597271

Single point energy (Hartree): -1355.011396

Solvation Gibbs free energy (Hartree): 0.001902

G_{sol} (Hartree): -1354.412224

C	3.00161700	-1.96984200	0.12781000
C	4.47310200	-2.37952400	0.09998800
C	5.30224600	-1.48641600	-0.81732900
C	5.20250900	0.02291200	-0.45697700
C	3.69103600	0.39398500	-0.35846700
C	3.41123000	1.87155700	-0.08135100
C	1.97124100	2.21341000	-0.45565300
C	0.96792700	1.14560600	-0.08815000
C	1.33089900	-0.08318500	0.36130100
C	2.79611900	-0.49684000	0.55874700
C	3.09161800	-0.36057800	2.07201200
C	0.28275900	-1.10600000	0.74329300
C	-1.08532500	-0.50040700	1.07886200
C	-1.53352700	0.44158300	-0.05978200
C	-0.44280700	1.48725500	-0.26465800
C	-0.97571900	2.64742600	-0.69022800
C	-2.47414100	2.57525000	-0.76401500
C	-2.84383000	1.34273200	0.12132600
C	-4.15010500	0.66738800	-0.38117900
C	-4.57295200	-0.53769200	0.48978200
H	3.30202900	0.19679600	-1.37516700
O	6.64324200	-1.93847200	-0.90775400
O	-0.98697300	0.21662300	2.29849900
C	-1.62222000	-0.38921800	-1.36407800
C	-5.33386200	1.63389500	-0.52462400
C	-5.46233500	-1.47532000	-0.28693300
O	-5.10540600	-2.12005700	-1.24578800
O	-6.72343300	-1.50546600	0.18589300
C	-7.63457500	-2.35093300	-0.51503800
C	5.84369000	0.80459100	-1.62047800
C	6.01407800	0.33744000	0.81286700
C	-3.03100800	1.85745600	1.55858100
H	2.57531600	-2.10242300	-0.88157300
H	2.44687500	-2.64878200	0.79258400
H	4.57358500	-3.42023800	-0.24659400
H	4.89808000	-2.35363800	1.11899700
H	4.90127600	-1.59446700	-1.84038200
H	3.58794800	2.09853800	0.98157800
H	4.09653700	2.51633700	-0.64875200
H	1.67131600	3.16537600	0.01274000
H	1.90121700	2.38841000	-1.54528600
H	2.28348900	-0.82641000	2.65604800
H	3.14707600	0.69101500	2.38240600
H	0.17908700	-1.86806500	-0.04644700

H	0.61725400	-1.67541200	1.62871500
H	-1.81000800	-1.33077500	1.18406800
H	-0.41176000	3.53632400	-0.97800600
H	-2.96736400	3.49569600	-0.41125800
H	-2.80561300	2.43457300	-1.81119400
H	-3.94846900	0.27079900	-1.38508100
H	-3.69119800	-1.12251200	0.78141900
H	-5.08110400	-0.20706900	1.40518500
H	7.00402800	-1.97914700	-0.01235300
H	-2.30724600	-1.24617500	-1.27474600
H	-1.97544200	0.23642400	-2.19442600
H	-0.63277300	-0.76442600	-1.65647800
H	-5.62600100	2.07276600	0.44167000
H	-6.21567900	1.10358000	-0.91704300
H	-5.10972000	2.45706700	-1.21808300
H	-8.60089200	-2.24967500	-0.00611200
H	-7.72150300	-2.04308200	-1.56804100
H	-7.29561600	-3.39758600	-0.48901100
H	6.82607400	0.36919000	-1.85234200
H	5.22268500	0.74628400	-2.52907600
H	5.99110300	1.86692000	-1.37656400
H	5.77491800	-0.31773900	1.66035400
H	7.09105900	0.23886900	0.60641000
H	5.84347100	1.37276500	1.14238600
H	-3.86918900	2.57011000	1.58865200
H	-3.23092900	1.05031600	2.27218200
H	-2.12884000	2.37260300	1.90885000
H	-0.45445800	-0.30847300	2.90771100
H	4.02395000	-0.85487700	2.37149900

TS9

Thermal correction to Gibbs free energy (Hartree): 0.607624

Single point energy (Hartree): -1355.341712

Solvation Gibbs free energy (Hartree): -0.062955

G_{sol} (Hartree): -1354.797042

C	-2.97002500	2.00534700	-0.27301600
C	-4.42831600	2.38159100	-0.01382300
C	-5.39557100	1.37496900	-0.63202400
C	-5.14321900	-0.08455200	-0.14308500
C	-3.65090800	-0.43573700	-0.44133300
C	-3.27633100	-1.87314900	-0.07477400
C	-1.84979000	-2.20229800	-0.49708200
C	-0.79689700	-1.19319500	-0.06777200
C	-1.19894700	0.19017200	0.34796400
C	-2.68056900	0.58020700	0.17317100
C	-2.14604800	0.32083900	1.54143000
C	-0.09679500	1.23770000	0.22405000
C	1.25815700	0.66720100	0.67056400
C	1.67409100	-0.50129900	-0.24441600
C	0.55178900	-1.48338700	-0.37252200
C	1.07899900	-2.79641400	-0.87790600
C	2.61557000	-2.65950000	-0.81580200
C	2.89719000	-1.45707100	0.13507100
C	4.28169500	-0.80877000	-0.13325000
C	4.59372700	0.37051600	0.84249200
H	-3.53506800	-0.34234500	-1.53838900
O	-6.73751100	1.77603300	-0.46590700
O	1.14104000	0.16503700	1.99606200
H	-0.10148000	-1.61894400	0.89135200

C	1.85238200	0.07371900	-1.68754100
C	5.44153900	-1.81274300	-0.12226900
C	4.82284300	1.65065800	0.07826200
O	3.93054000	2.33819100	-0.37913200
O	6.11601900	1.91918000	-0.09262300
C	6.44103400	3.09093200	-0.85398300
C	-6.07145100	-1.00815300	-0.94840000
C	-5.48637300	-0.21288900	1.35020100
C	2.82431600	-2.00613700	1.57318300
H	-2.76011600	2.08112100	-1.35445400
H	-2.30726600	2.72380200	0.22765800
H	-4.64378900	3.37846900	-0.42718300
H	-4.60652700	2.44390800	1.07403700
H	-5.23407500	1.37381200	-1.72495200
H	-3.40900000	-2.05277900	1.00210500
H	-3.94917800	-2.57667400	-0.58189500
H	-1.56597300	-3.21495700	-0.17463000
H	-1.79867900	-2.21548500	-1.60075200
H	-1.95322700	1.17472800	2.19560000
H	-2.44516500	-0.58112200	2.07642600
H	-0.03004700	1.63651500	-0.79761400
H	-0.32874800	2.10115300	0.86241900
H	2.02514900	1.45245500	0.59722900
H	0.69273200	-2.96654800	-1.89741400
H	0.69640700	-3.63502600	-0.27718700
H	3.08411400	-3.57934100	-0.44527500
H	3.02539400	-2.48131900	-1.81913300
H	4.24289500	-0.40199200	-1.15443300
H	3.76185300	0.54697600	1.53456100
H	5.48021300	0.14067100	1.44727900
H	-6.88528000	2.00299400	0.46171900
H	2.46880000	0.98109700	-1.62499600
H	2.34129700	-0.63566700	-2.36332400
H	0.88910400	0.34492900	-2.13869600
H	5.57637100	-2.27455500	0.86747100
H	6.37740500	-1.29015900	-0.37030500
H	5.30647200	-2.61556300	-0.86157800
H	7.53521200	3.14133300	-0.87852500
H	6.03440500	3.01225900	-1.87265900
H	6.02362200	3.98769800	-0.37439200
H	-7.09800000	-0.62052200	-0.90275400
H	-5.77537500	-1.04433400	-2.00962400
H	-6.07984100	-2.03608000	-0.55683000
H	-4.86444100	0.42615900	1.99288600
H	-6.53900100	0.06093900	1.51654800
H	-5.37666100	-1.24954200	1.70086300
H	3.57293900	-2.80174600	1.69246100
H	2.99751700	-1.24164300	2.33488800
H	1.84478600	-2.45469000	1.80068800
H	0.85698800	0.88113800	2.57926500

19i

Thermal correction to Gibbs free energy (Hartree): 0.610507

Single point energy (Hartree): -1355.361812

Solvation Gibbs free energy (Hartree): -0.061011

G_{sol} (Hartree): -1354.812316

C	-2.72749200	1.87798600	0.36753700
C	-4.19031800	2.33347000	0.36675000
C	-5.02352200	1.59081700	-0.67541200

C	-4.97021200	0.04199900	-0.49577500
C	-3.46620400	-0.38855300	-0.53211800
C	-3.25591300	-1.89803200	-0.41256800
C	-1.77990400	-2.25841700	-0.51245500
C	-0.78641100	-1.37242900	0.14305600
C	-1.13292800	-0.17959300	0.82022200
C	-2.64868900	0.36980600	0.51070700
C	-2.37846200	-0.24504300	1.79453500
C	-0.05253500	0.84879600	1.16262000
C	1.35030200	0.24094800	1.29628400
C	1.65442600	-0.62446700	0.06038600
C	0.62867900	-1.77845200	0.05813900
C	1.12225800	-2.77666700	-1.00162900
C	2.64084500	-2.49082200	-1.12532500
C	3.01594000	-1.43356300	-0.03644800
C	4.22623700	-0.56334000	-0.48776000
C	4.65709800	0.48678800	0.58771000
H	-3.08299600	-0.06986600	-1.51922200
O	-6.34178500	2.08299500	-0.73081600
O	1.39104800	-0.58006800	2.45629200
C	1.44594400	0.23905000	-1.20667400
C	5.44808800	-1.38339000	-0.92315400
C	4.44571000	1.89349500	0.09086100
O	3.43652100	2.54721500	0.26620600
O	5.48112300	2.32683900	-0.63204500
C	5.36518800	3.63011100	-1.21579200
C	-5.71946300	-0.59107300	-1.67838100
C	-5.65846500	-0.37005700	0.81525100
C	3.37570400	-2.20996900	1.24480600
H	-2.25641000	2.16655500	-0.58686400
H	-2.17930600	2.38896400	1.16882000
H	-4.24006600	3.41296200	0.16017700
H	-4.62672100	2.18088600	1.36890000
H	-4.59744500	1.80773500	-1.67133300
H	-3.68239000	-2.27548600	0.52700500
H	-3.79463500	-2.41889100	-1.21410300
H	-1.57827200	-3.30247900	-0.21437400
H	-1.45746000	-2.24080500	-1.57432900
H	-2.20508100	0.38810100	2.66705800
H	-2.75968000	-1.23753600	2.03052300
H	-0.03600700	1.64054000	0.40140300
H	-0.29581600	1.34630500	2.11178400
H	2.06998600	1.07036500	1.35412100
H	0.61802500	-2.60851200	-1.96511900
H	0.91307300	-3.81635900	-0.71386500
H	3.23506200	-3.40482200	-0.99924600
H	2.86905200	-2.11027900	-2.13085800
H	3.90358900	-0.01390400	-1.38436000
H	4.08844500	0.37086800	1.51645900
H	5.71897300	0.35450800	0.83427300
H	-6.70471200	2.12575600	0.16387700
H	1.95475300	1.20646100	-1.10692600
H	1.82631200	-0.25316800	-2.10944900
H	0.38011700	0.44427800	-1.38859300
H	5.88625000	-1.94583200	-0.08481100
H	6.22460300	-0.70381900	-1.30490600
H	5.20875000	-2.09592200	-1.72545500
H	6.30891200	3.81141100	-1.74236300
H	4.51990500	3.66412500	-1.91895800
H	5.20671500	4.38881400	-0.43615100

H	-6.71180000	-0.12877400	-1.76616300
H	-5.18608000	-0.41820500	-2.62716800
H	-5.85916000	-1.67453900	-1.55169500
H	-5.16300800	0.03015100	1.71228400
H	-6.69856200	-0.01167600	0.81884400
H	-5.70873200	-1.46366100	0.91889500
H	4.25607700	-2.83836600	1.04999500
H	3.59276700	-1.55959500	2.09795500
H	2.57040700	-2.88629100	1.56423700
H	1.49258800	-0.02181000	3.23697900
H	0.72930900	-2.25042900	1.06337700

19k

Thermal correction to Gibbs free energy (Hartree): 0.611007

Single point energy (Hartree): -1355.354693

Solvation Gibbs free energy (Hartree): -0.059540

G_{sol} (Hartree): -1354.803226

C	-2.50417300	1.90163900	-0.05705400
C	-3.69167800	2.38632700	-0.93250900
C	-4.98275200	1.73393000	-0.42682700
C	-5.00054500	0.20863700	-0.70753200
C	-3.51572900	-0.36200300	-0.53267100
C	-3.41995700	-1.83720200	-0.15575400
C	-1.96277900	-2.29886000	-0.18559700
C	-0.90050300	-1.42662000	0.42454000
C	-1.10787400	-0.33652500	1.24210100
C	-2.78777400	0.51548900	0.42477700
C	-2.50345700	0.07060300	1.77421900
C	0.00917000	0.59536800	1.66565800
C	1.42604400	0.01184800	1.51811800
C	1.54938800	-0.70064500	0.16252400
C	0.51521400	-1.84798600	0.14237000
C	0.85001800	-2.64050300	-1.13481100
C	2.35967400	-2.38097400	-1.37774000
C	2.88101500	-1.48190000	-0.20976700
C	4.03587900	-0.55049000	-0.68141300
C	4.60187100	0.34233700	0.47129800
H	-3.03854600	-0.21922600	-1.51767500
O	-5.06464100	1.90307800	0.98220600
O	1.65948600	-0.92318300	2.55874000
C	1.20818500	0.32855100	-0.94229100
C	5.18974000	-1.28998600	-1.37121500
C	4.41019300	1.80353500	0.16256500
O	3.44183700	2.46160200	0.48762500
O	5.40825200	2.29238800	-0.58041400
C	5.29743900	3.65781100	-0.99558300
C	-5.42418600	-0.04225900	-2.16232800
C	-5.99251800	-0.48320100	0.23627900
C	3.39472900	-2.42234700	0.89807500
H	-1.58431100	1.90307900	-0.66624300
H	-2.33096500	2.57150600	0.79449800
H	-3.53120500	2.14313300	-1.99276300
H	-3.75545400	3.48350300	-0.87373400
H	-5.86137400	2.18199000	-0.92421200
H	-3.87993500	-2.01918600	0.82335700
H	-3.99274200	-2.44232100	-0.87260700
H	-1.86427800	-3.30554300	0.26027900
H	-1.66491200	-2.44311500	-1.23742100
H	-2.41081600	0.87207800	2.51234300

H	-3.10064600	-0.75837500	2.15849200
H	-0.06153700	1.54226300	1.10557500
H	-0.13723800	0.86819100	2.72334900
H	2.13324500	0.85397000	1.56287100
H	0.26179900	-2.27342100	-1.98941000
H	0.62033900	-3.70981700	-1.02814500
H	2.92947800	-3.31806700	-1.42716300
H	2.50359000	-1.88333500	-2.34748000
H	3.61154500	0.11620700	-1.44648200
H	4.10408800	0.13351000	1.42376500
H	5.67306400	0.14323400	0.60883400
H	-5.17523300	2.84169300	1.18535900
H	1.74030000	1.27425300	-0.77575500
H	1.47034400	-0.03531300	-1.94271400
H	0.13089400	0.54870700	-0.96420300
H	5.71877500	-1.96238500	-0.67909500
H	5.92201400	-0.55737400	-1.74268000
H	4.84853400	-1.88426400	-2.23102700
H	6.20431800	3.87485100	-1.57136800
H	4.40279000	3.80088000	-1.61970900
H	5.22758000	4.32259200	-0.12256700
H	-6.47381300	0.25191900	-2.31192400
H	-4.80727900	0.52133800	-2.87898600
H	-5.34104100	-1.10994100	-2.41486400
H	-5.68036100	-0.42659000	1.28616400
H	-6.97295200	0.01096600	0.16436000
H	-6.13268200	-1.53683900	-0.04257100
H	4.22772300	-3.02118100	0.50309700
H	3.73909400	-1.88995800	1.79012200
H	2.62606100	-3.13134600	1.23313900
H	1.77953500	-0.44623300	3.38926700
H	0.75493700	-2.48456900	1.01408400

TS10

Thermal correction to Gibbs free energy (Hartree): 0.612582

Single point energy (Hartree): -1355.345549

Solvation Gibbs free energy (Hartree): -0.068233

G_{sol} (Hartree): -1354.801200

C	-2.73300800	2.04554000	-0.05819600
C	-4.02905700	2.56649600	-0.74692700
C	-5.13344800	1.61596500	-0.27875200
C	-5.06048600	0.20259000	-0.88016100
C	-3.62047100	-0.28432900	-0.42898900
C	-3.48313800	-1.72976300	0.04415800
C	-2.02460700	-2.20981800	-0.00283900
C	-0.91103500	-1.33118500	0.52566100
C	-1.05173700	-0.24916200	1.32686200
C	-3.09580800	0.72656300	0.58089100
C	-2.41637100	0.25494500	1.80833500
C	0.10847500	0.61054800	1.77653600
C	1.50527400	0.00165400	1.55895700
C	1.55371900	-0.68438500	0.18428000
C	0.48444500	-1.79870200	0.17324500
C	0.73410300	-2.52682500	-1.16051000
C	2.24829000	-2.33440900	-1.44142600
C	2.84515600	-1.49345900	-0.26485000
C	4.01155800	-0.58383100	-0.74842100
C	4.64920600	0.24340800	0.41569300
H	-2.96789000	-0.16352800	-1.30882900

O	-4.77010800	1.31131700	1.11410900
O	1.76989800	-0.95903800	2.56946700
C	1.21538000	0.39350200	-0.87484800
C	5.11410400	-1.32883500	-1.51188900
C	4.55260700	1.71858300	0.13481700
O	3.64221900	2.43792600	0.49294600
O	5.56560900	2.15011700	-0.62777500
C	5.53568800	3.52479600	-1.02093700
C	-5.19215200	0.20785400	-2.40556100
C	-6.18975600	-0.65169500	-0.27917700
C	3.37398300	-2.48461400	0.79097500
H	-1.92168000	1.87238000	-0.77970700
H	-2.35045200	2.75276800	0.69140100
H	-3.95867300	2.58035600	-1.84133900
H	-4.24451700	3.59813200	-0.43216900
H	-6.14566100	2.04124700	-0.30174600
H	-3.92955600	-1.85402400	1.04064800
H	-4.06494600	-2.38197700	-0.62233600
H	-1.94570600	-3.19554400	0.49041700
H	-1.78686700	-2.41490500	-1.05924300
H	-2.27183800	1.08385800	2.51442700
H	-2.99458300	-0.52843600	2.31257400
H	0.04830900	1.59670500	1.28016100
H	-0.00079200	0.82643000	2.85434000
H	2.23485000	0.82591500	1.59106300
H	0.13865900	-2.07604800	-1.96980600
H	0.45114200	-3.58796100	-1.11251600
H	2.77091900	-3.29624200	-1.53051600
H	2.39166400	-1.81928600	-2.40234600
H	3.57988800	0.12636700	-1.46859400
H	4.14517300	0.05146500	1.36794400
H	5.70542900	-0.03193400	0.53861600
H	-4.70694900	2.11683200	1.65776400
H	1.79482800	1.30993500	-0.70082500
H	1.42402600	0.05218800	-1.89581200
H	0.14892400	0.65825200	-0.84315200
H	5.64285500	-2.04941400	-0.86976500
H	5.85832700	-0.60508600	-1.87732900
H	4.72132200	-1.87251300	-2.38320300
H	6.43844400	3.68999800	-1.62026100
H	4.63541400	3.73832700	-1.61645500
H	5.53551700	4.18044900	-0.13803700
H	-6.16799900	0.61065700	-2.71812600
H	-4.40281200	0.79336800	-2.89911700
H	-5.12497900	-0.82208200	-2.78663500
H	-6.12945000	-0.71651600	0.81438700
H	-7.16520600	-0.21509700	-0.54316200
H	-6.17035800	-1.67106300	-0.68600000
H	4.17383900	-3.09320300	0.34489000
H	3.76735100	-1.99023900	1.68485200
H	2.59793600	-3.18112600	1.13325800
H	1.88775600	-0.49992400	3.41012000
H	0.75190400	-2.49064500	0.98864100

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Thermal correction to Gibbs free energy (Hartree): 0.613585

Single point energy (Hartree): -1355.349504

Solvation Gibbs free energy (Hartree): -0.072003

G_{sol} (Hartree): -1354.807922

C	-2.78695300	2.06738300	-0.10618900
C	-4.10572800	2.57498700	-0.75879900
C	-5.16712600	1.59027100	-0.26713900
C	-5.09038700	0.18133600	-0.87818500
C	-3.64709700	-0.28031200	-0.42364400
C	-3.49119300	-1.71413400	0.07892400
C	-2.03021100	-2.18745000	0.02225900
C	-0.91279400	-1.29904000	0.52991100
C	-1.04751200	-0.20844500	1.31612300
C	-3.18091200	0.77376500	0.59458700
C	-2.40240900	0.31285000	1.78669300
C	0.12295000	0.63480200	1.77252400
C	1.51461800	0.01450600	1.55833300
C	1.55813800	-0.67399800	0.18464500
C	0.47882000	-1.77820600	0.17471200
C	0.72004400	-2.50478800	-1.16131700
C	2.23690200	-2.33066600	-1.44076100
C	2.84204700	-1.49539000	-0.26413200
C	4.01706500	-0.59705400	-0.74748200
C	4.66244100	0.22276700	0.41752500
H	-2.98175800	-0.16604300	-1.29221800
O	-4.66433300	1.24753000	1.11091900
O	1.77171500	-0.94730600	2.57055100
C	1.23205800	0.40723500	-0.87499200
C	5.11251600	-1.35123000	-1.51210100
C	4.59091100	1.69822300	0.13155800
O	3.69471800	2.43508700	0.48903900
O	5.60989200	2.10913200	-0.63557300
C	5.60189900	3.48214300	-1.03447300
C	-5.22476900	0.19701800	-2.40353200
C	-6.21657500	-0.67804000	-0.27851300
C	3.36192200	-2.49069800	0.79224400
H	-1.99571700	1.86019000	-0.83787700
H	-2.38124900	2.79472200	0.61250400
H	-4.06885800	2.59065700	-1.85462500
H	-4.34310300	3.59856600	-0.43467400
H	-6.18465000	1.98665200	-0.16552600
H	-3.92321800	-1.82174800	1.08408800
H	-4.07643300	-2.38540000	-0.56571500
H	-1.94512700	-3.16687000	0.52698300
H	-1.80559300	-2.40507700	-1.03450300
H	-2.24676500	1.15741200	2.47497000
H	-2.96691800	-0.45419300	2.33364100
H	0.07394800	1.62446100	1.28095000
H	0.01331400	0.84833300	2.85127500
H	2.25202500	0.83192400	1.59031600
H	0.13016600	-2.04364200	-1.96907500
H	0.42426800	-3.56269300	-1.11753200
H	2.74845600	-3.29871300	-1.52796100
H	2.38792100	-1.81844100	-2.40210400
H	3.59189300	0.11805400	-1.46657600
H	4.15035800	0.04220800	1.36759300
H	5.71344800	-0.06955500	0.54650500
H	-4.60720900	2.02440800	1.69983900
H	1.82182000	1.31716300	-0.70095800
H	1.43773600	0.06350300	-1.89581300
H	0.16881800	0.68360500	-0.84311500
H	5.63363100	-2.07862700	-0.87137100
H	5.86417100	-0.63412600	-1.87548400
H	4.71461100	-1.88904200	-2.38475800

H	6.50476900	3.62944000	-1.63832800
H	4.70288400	3.70886900	-1.62703100
H	5.61676000	4.14170300	-0.15457300
H	-6.19830000	0.60573800	-2.71594600
H	-4.43049800	0.77785700	-2.89424700
H	-5.16266000	-0.83242000	-2.78644400
H	-6.16270200	-0.73542400	0.81657600
H	-7.19554800	-0.25639800	-0.55347300
H	-6.18118500	-1.70133000	-0.67387300
H	4.15743100	-3.10593900	0.34733400
H	3.75796000	-1.99895100	1.68643900
H	2.57973600	-3.18056700	1.13377600
H	1.88055700	-0.48774300	3.41213000
H	0.74288700	-2.47508800	0.98671200

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Thermal correction to Gibbs free energy (Hartree): 0.599140

Single point energy (Hartree): -1355.003581

Solvation Gibbs free energy (Hartree): 0.004849

G_{sol} (Hartree): -1354.399592

C	-3.00102200	2.16026600	-0.05526700
C	-4.34312000	2.70098900	-0.62041000
C	-5.34450500	1.65512800	-0.07961700
C	-5.30965800	0.31064700	-0.86284500
C	-3.85884500	-0.16245500	-0.48121200
C	-3.67334500	-1.61735500	-0.05898100
C	-2.20939200	-2.06627100	-0.16200300
C	-1.10644100	-1.22958300	0.45481200
C	-1.26991000	-0.19918200	1.31174000
C	-3.47715200	0.86377900	0.63616700
C	-2.61677400	0.33171000	1.76322600
C	-0.09388500	0.56711900	1.87889800
C	1.28891300	-0.06369800	1.67315600
C	1.38989000	-0.61679400	0.23745800
C	0.29481000	-1.70278000	0.11559200
C	0.56748700	-2.33690500	-1.25506700
C	2.10141800	-2.23025200	-1.43830300
C	2.68609800	-1.40720100	-0.23744400
C	3.84588500	-0.49554900	-0.74010700
C	4.47710000	0.37166400	0.36830300
H	-3.20460500	0.00343900	-1.35167200
O	-4.75266500	1.27455300	1.16213000
O	1.48685000	-1.11736700	2.60482000
C	1.11293000	0.54904000	-0.73756100
C	4.96203600	-1.25778900	-1.47033500
C	5.23324000	1.53555000	-0.22349100
O	4.74596100	2.37154500	-0.94838900
O	6.53082300	1.54615500	0.13708300
C	7.31684400	2.61593400	-0.38599100
C	-5.50315400	0.43674300	-2.37439300
C	-6.40906600	-0.59364800	-0.28576900
C	3.22455300	-2.38775800	0.82013800
H	-2.24006500	1.97242300	-0.82537600
H	-2.57465000	2.84913200	0.68884200
H	-4.35603400	2.78853300	-1.71491700
H	-4.58040100	3.69101500	-0.20654300
H	-6.35983300	2.03904800	0.09085500
H	-4.07750500	-1.78176600	0.95056300
H	-4.25830900	-2.27467000	-0.72165600

H	-2.11185500	-3.09758600	0.22857400
H	-1.97926700	-2.15840900	-1.23724100
H	-2.47317500	1.15079300	2.48411500
H	-3.18789300	-0.44023100	2.30041800
H	-0.10638400	1.59438100	1.47038200
H	-0.24425500	0.70853100	2.96696000
H	2.04686600	0.72480400	1.83831700
H	0.04785800	-1.78053300	-2.05044600
H	0.21165700	-3.37569000	-1.31213300
H	2.57569100	-3.22120400	-1.48575200
H	2.33219700	-1.73538200	-2.39325000
H	3.41661000	0.20439100	-1.46923000
H	3.69531000	0.81084300	1.00126200
H	5.14161600	-0.21697900	1.01437500
H	1.77051200	1.40817600	-0.53725400
H	1.28172600	0.25529800	-1.78136100
H	0.07240600	0.88956900	-0.66686400
H	5.50883100	-1.93348200	-0.79494500
H	5.69797800	-0.55113900	-1.88568300
H	4.57653200	-1.85521700	-2.30845500
H	8.33280100	2.46779900	-0.00002100
H	7.31838300	2.59751800	-1.48639200
H	6.92075600	3.58916000	-0.05866400
H	-6.47696000	0.89472100	-2.61602800
H	-4.71573900	1.04073300	-2.84917000
H	-5.48207700	-0.55871500	-2.84708200
H	-6.31536400	-0.67838000	0.80497600
H	-7.40162400	-0.17106800	-0.51202300
H	-6.37580500	-1.60390600	-0.71944600
H	4.03909400	-2.98835200	0.38811000
H	3.60046200	-1.87371600	1.71259100
H	2.45098300	-3.08576400	1.16316500
H	1.15041100	-0.82395700	3.46001600
H	0.53578000	-2.46134000	0.87876000

Py

Thermal correction to Gibbs free energy (Hartree): 0.064682

Single point energy (Hartree): -248.266786

Solvation Gibbs free energy (Hartree): -0.004349

G_{sol} (Hartree): -248.206453

C	0.00000000	0.00000000	-1.38623400
C	0.00000000	1.20002400	-0.67246100
C	0.00000000	1.14303900	0.72505200
C	0.00000000	-1.14303900	0.72505200
C	0.00000000	-1.20002400	-0.67246100
H	0.00000000	0.00000000	-2.47918100
H	0.00000000	2.16445200	-1.18515300
H	0.00000000	2.06871000	1.31300900
H	0.00000000	-2.06871000	1.31300900
H	0.00000000	-2.16445200	-1.18515300
N	0.00000000	0.00000000	1.41568400

PyH⁺

Thermal correction to Gibbs free energy (Hartree): 0.078652

Single point energy (Hartree): -248.631613

Solvation Gibbs free energy (Hartree): -0.087629

G_{sol} (Hartree): -248.640590

C	-1.41767500	0.00000000	0.00000000
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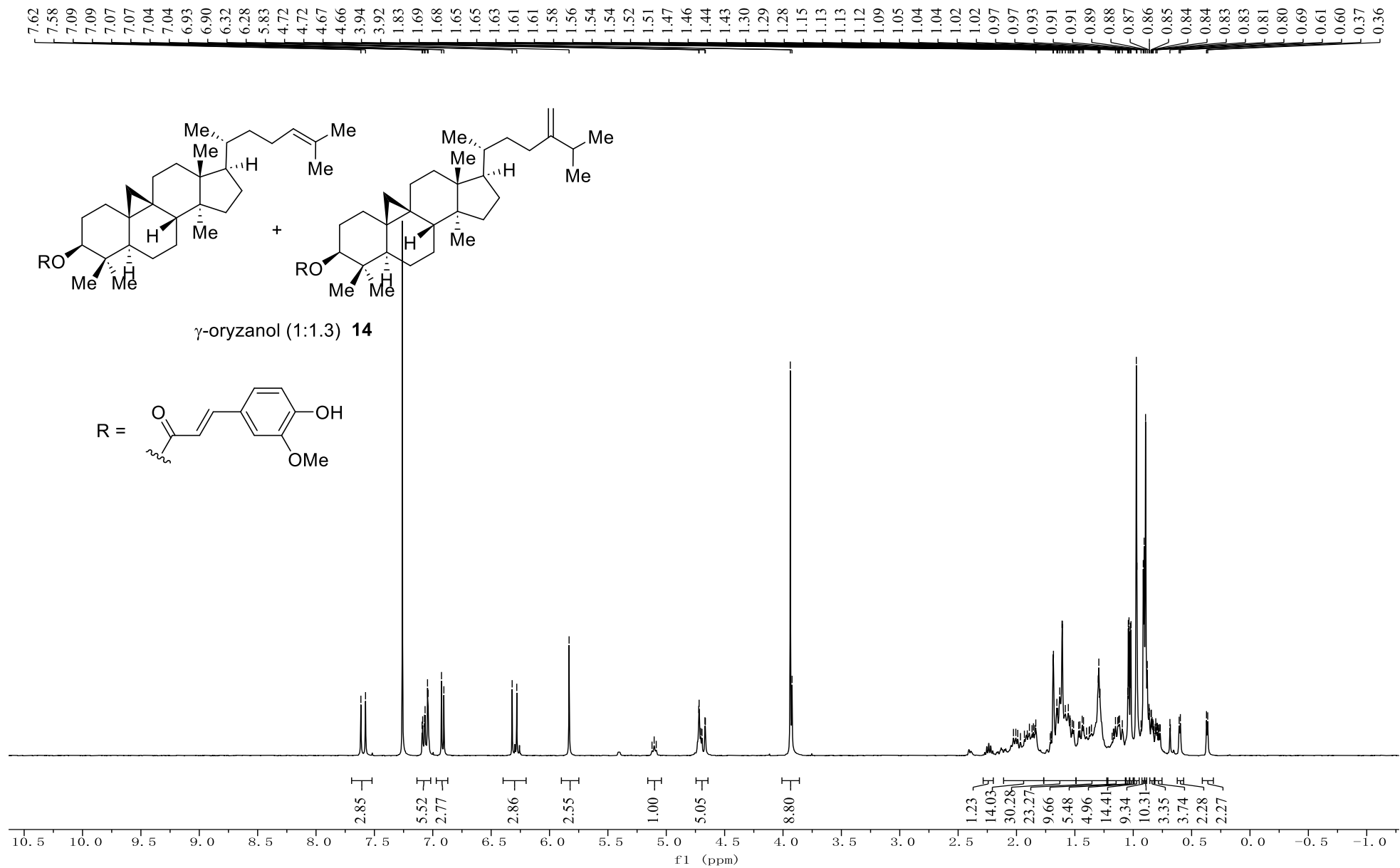
C	-0.71739600	-1.21271500	0.00000000
C	0.66864900	-1.18900700	0.00000000
C	0.66864900	1.18900700	0.00000000
C	-0.71739600	1.21271500	0.00000000
H	-2.51022500	0.00000000	0.00000000
H	-1.23810200	-2.17139100	0.00000000
H	1.28952400	-2.08639400	0.00000000
H	1.28952400	2.08639400	0.00000000
H	-1.23810200	2.17139100	0.00000000
N	1.30961200	0.00000000	0.00000000
H	2.33110500	0.00000000	0.00000000

VI References

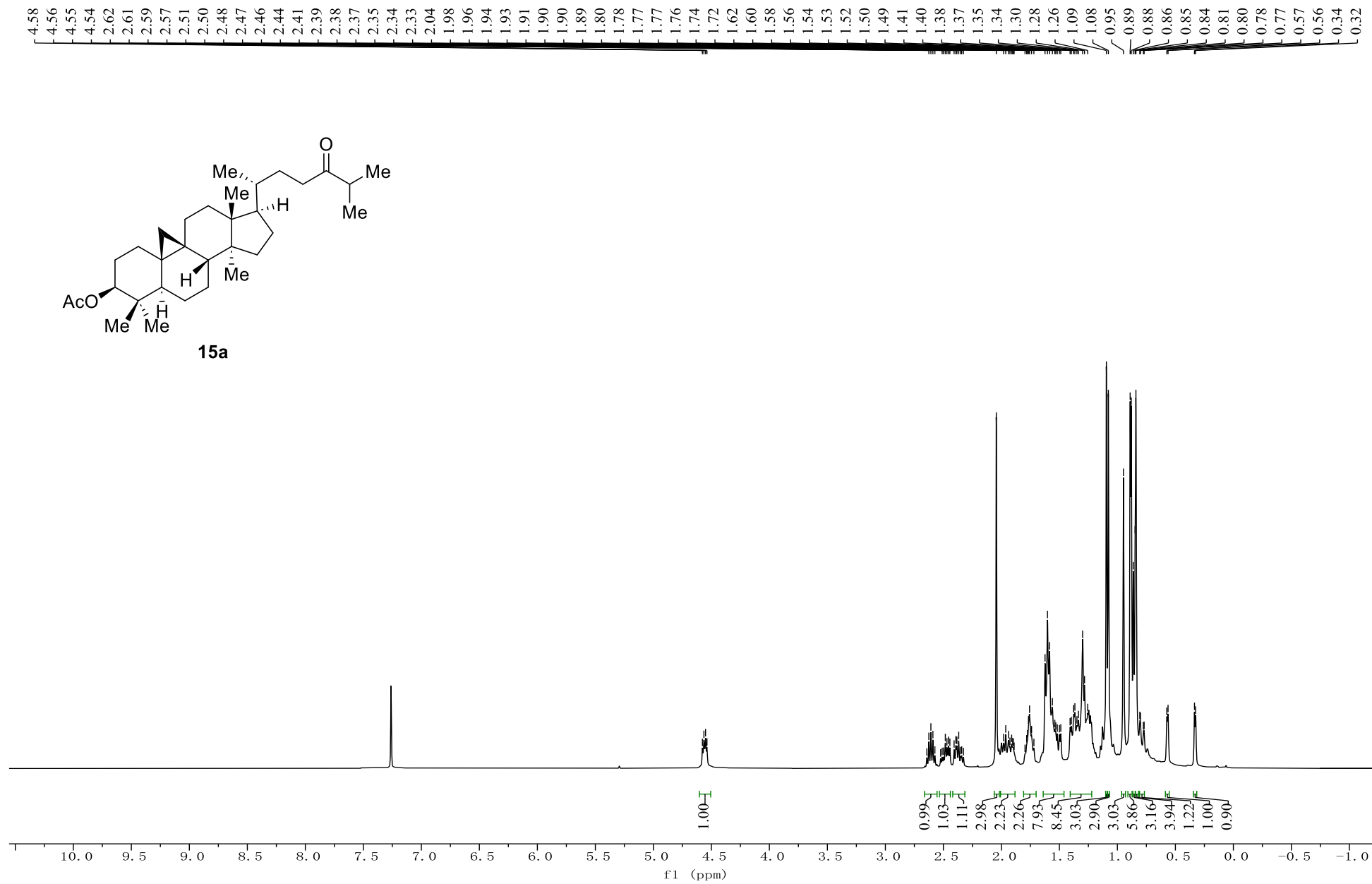
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VII ¹H and ¹³C NMR Spectra of Compounds

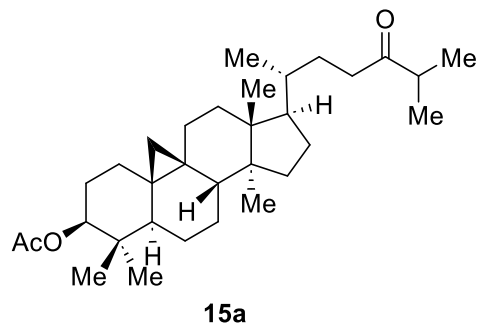
¹H NMR Spectra of 14 (400 MHz, CDCl₃)



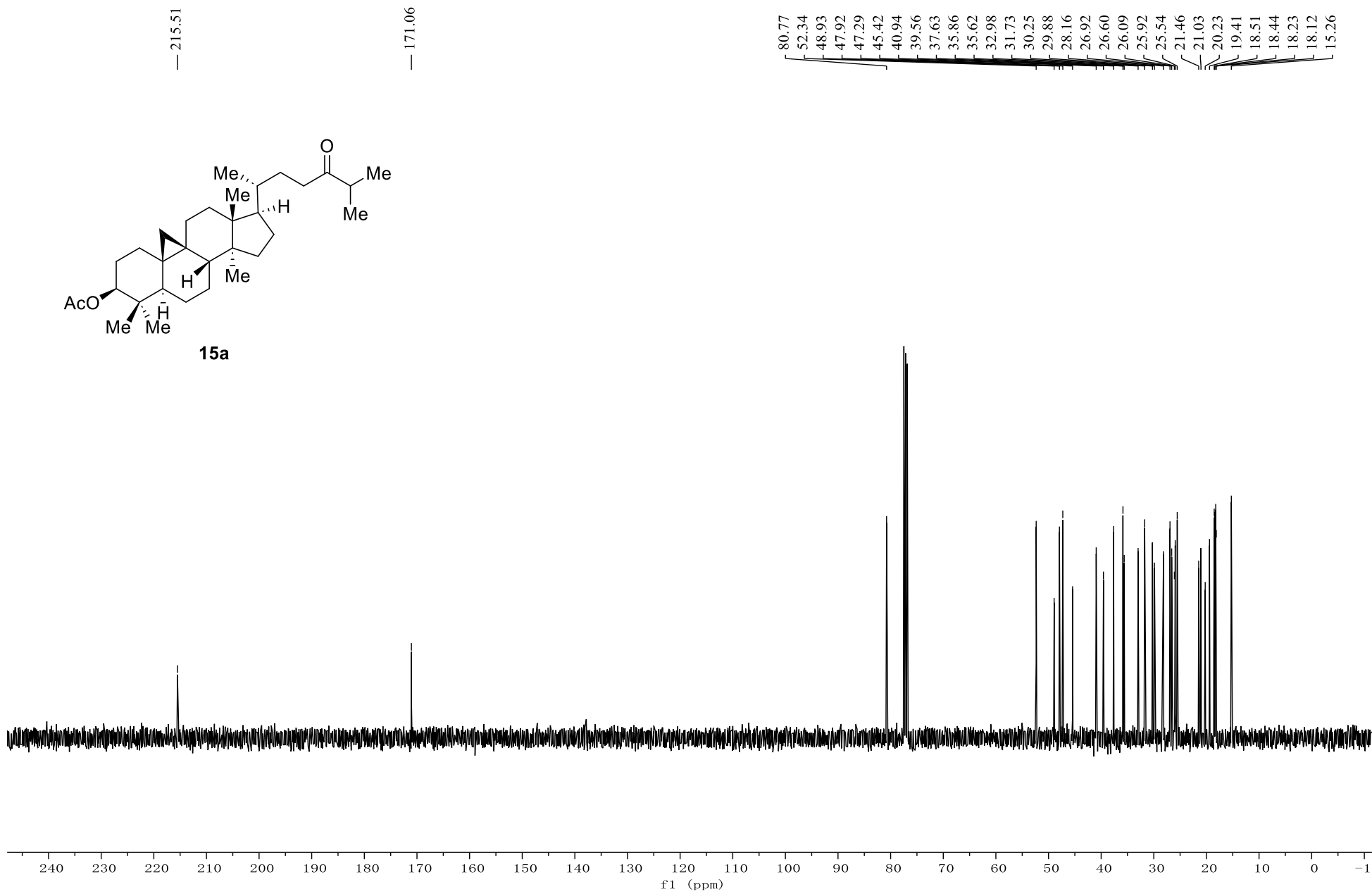
¹H NMR Spectra of 15a (400 MHz, CDCl₃)



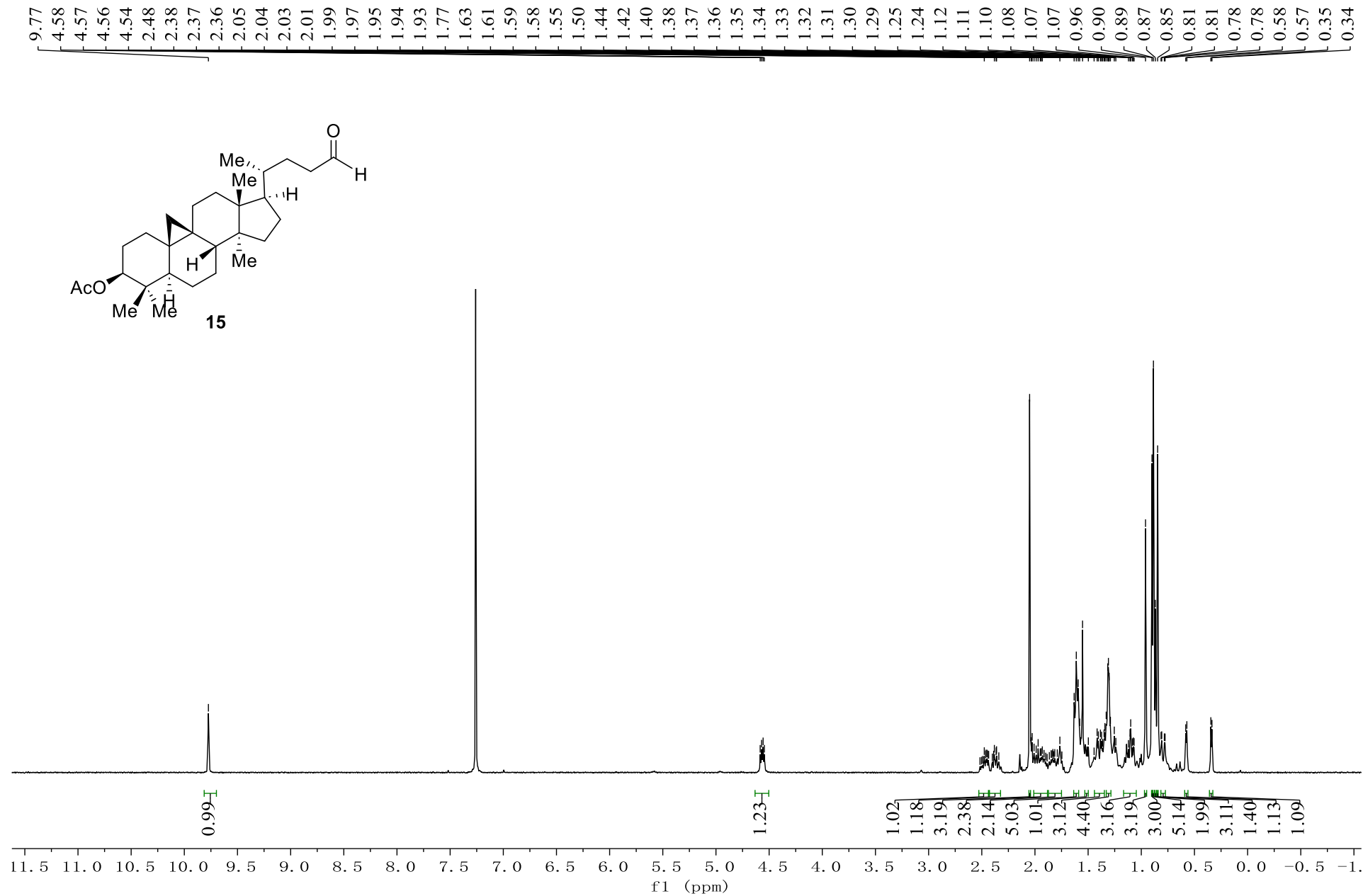
¹³C NMR Spectrum of 15a (101 MHz, CDCl₃)



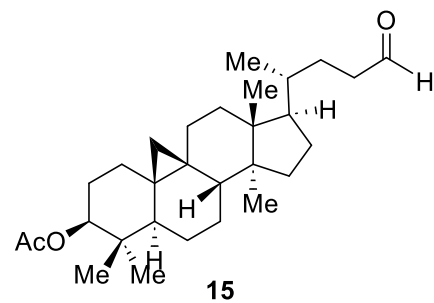
80.77
52.34
48.93
47.92
47.29
45.42
40.94
39.56
37.63
35.86
35.62
32.98
31.73
30.25
29.88
28.16
26.92
26.60
26.09
25.92
25.54
21.46
21.03
20.23
19.41
18.51
18.44
18.23
18.12
15.26



¹H NMR Spectrum of 15 (400 MHz, CDCl₃)



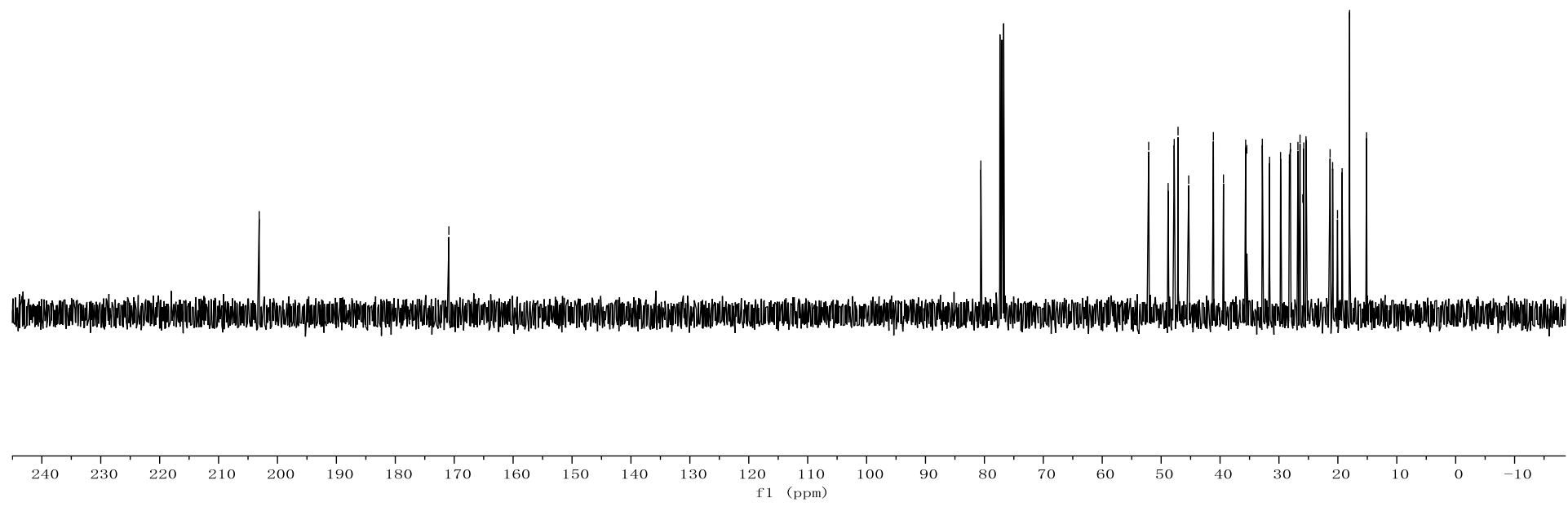
¹³C NMR Spectrum of 15 (101 MHz, CDCl₃)



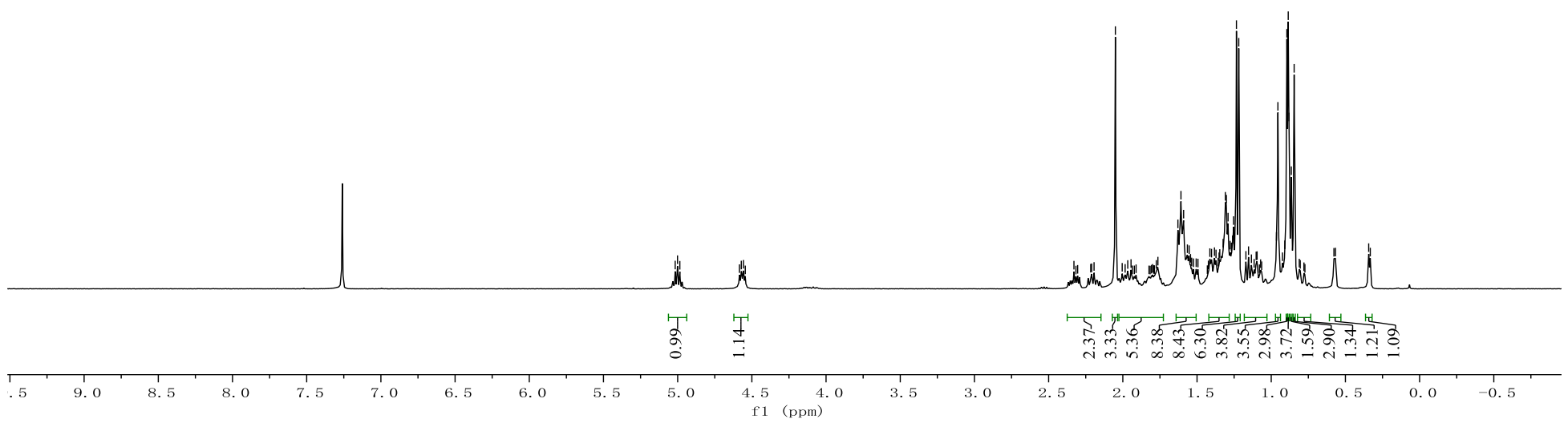
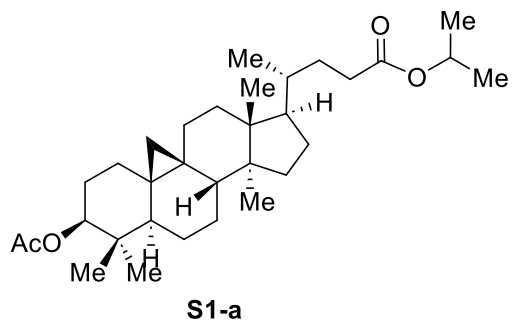
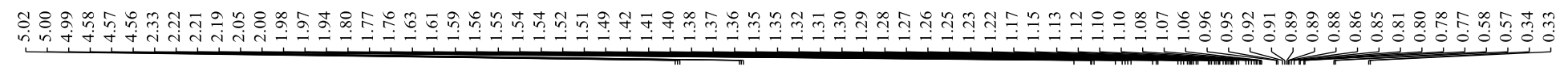
203.10

170.91

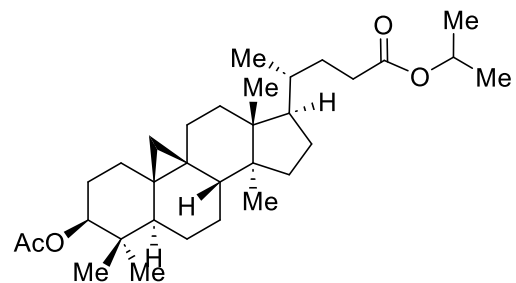
80.60
52.12
48.81
47.78
47.13
45.32
41.13
39.42
35.65
35.46
32.82
31.59
29.73
28.23
28.07
26.78
26.42
25.96
25.78
25.41
21.32
20.89
20.06
19.28
18.00
15.13



¹H NMR Spectrum of S1-a (400 MHz, CDCl₃)



¹³C NMR Spectrum of S1-a (101 MHz, CDCl₃)



S1-a

173.93
171.06

80.77
67.43
52.22
48.94
47.94
47.28
45.45
39.57
35.76
35.62
32.97
32.00
31.73
31.42
28.14
26.93
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21.47
21.04
20.23
19.42
18.12
18.04
15.27

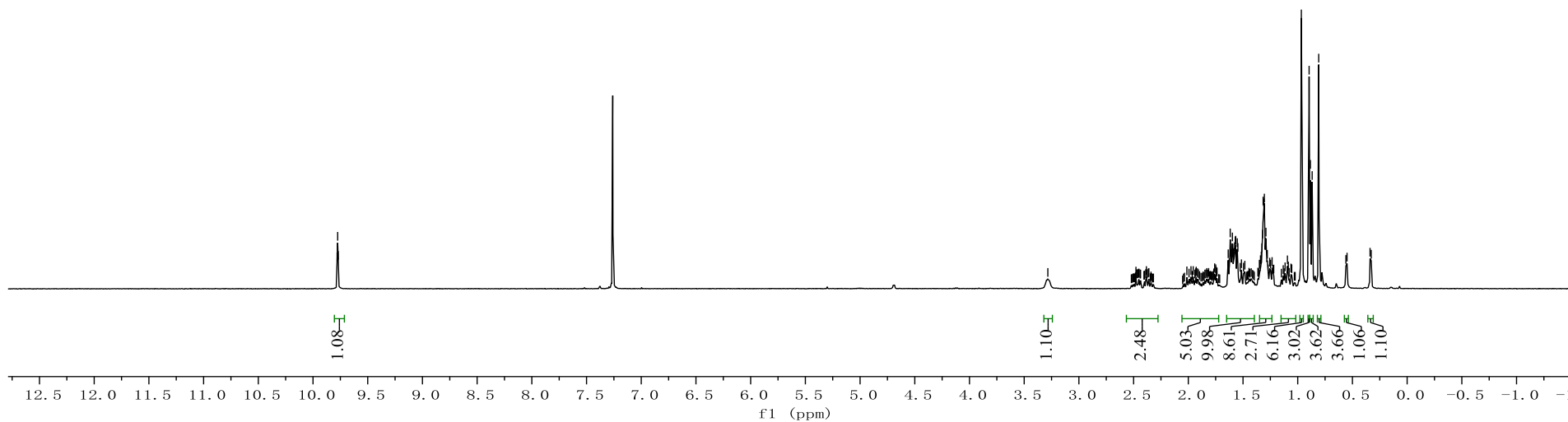
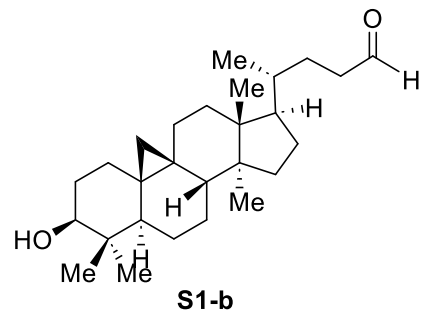


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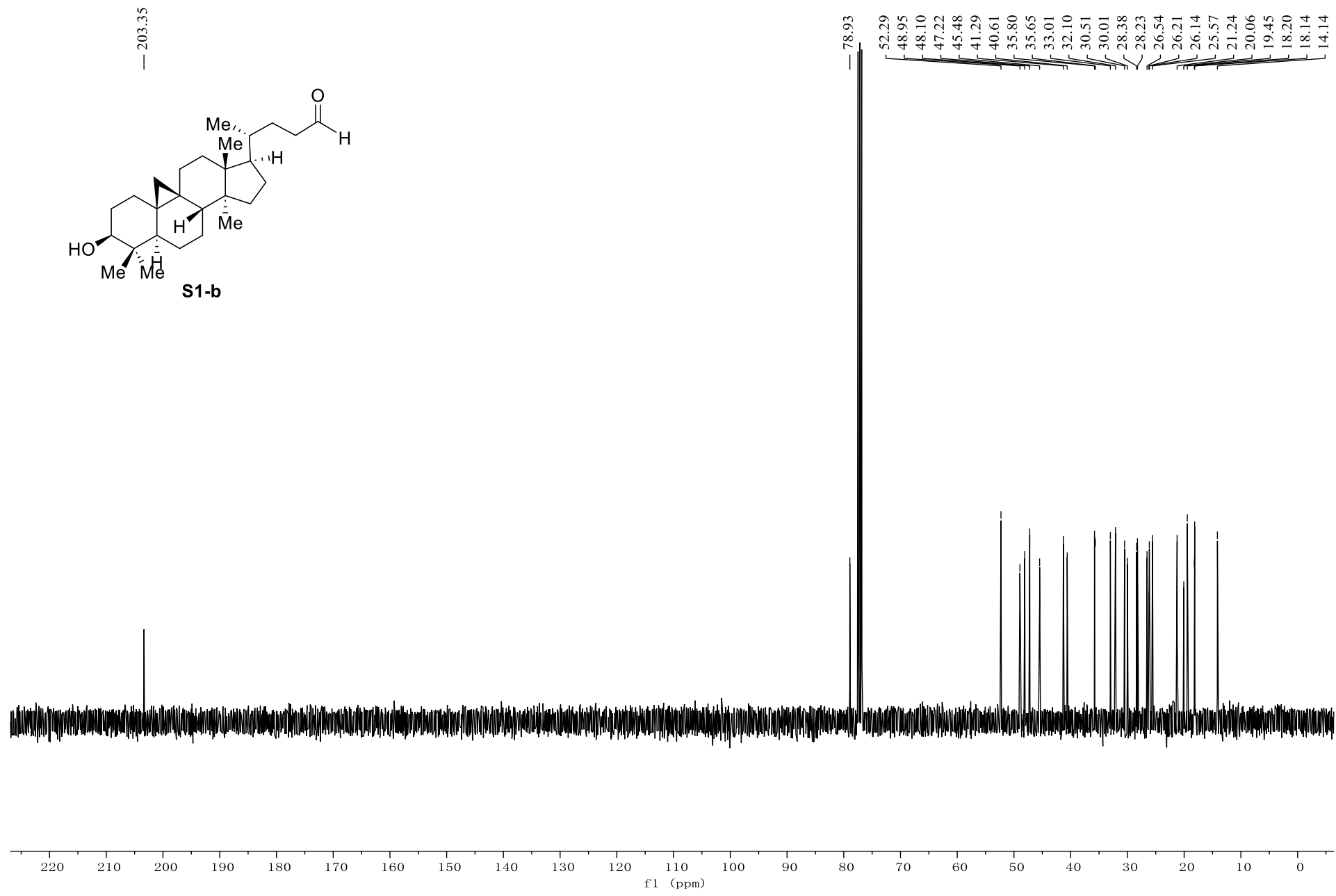
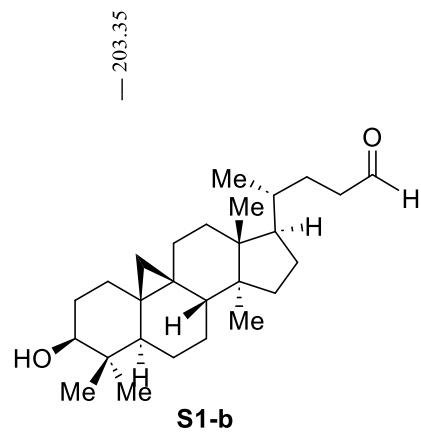
f1 (ppm)

¹H NMR Spectrum of S1-b (400 MHz, CDCl₃)

9.78
9.77
9.77
3.28
2.48
2.38
2.36
2.01
1.98
1.96
1.93
1.83
1.81
1.76
1.75
1.75
1.74
1.64
1.63
1.62
1.61
1.60
1.60
1.59
1.59
1.58
1.58
1.57
1.57
1.56
1.55
1.55
1.53
1.51
1.50
1.48
1.45
1.43
1.36
1.35
1.35
1.34
1.33
1.33
1.32
1.32
1.31
1.31
1.29
1.28
1.27
1.26
1.25
1.23
1.23
1.22
1.13
1.12
1.09
1.09
1.08
1.06
1.05
0.97
0.90
0.88
0.87
0.81
0.56
0.55
0.34
0.33

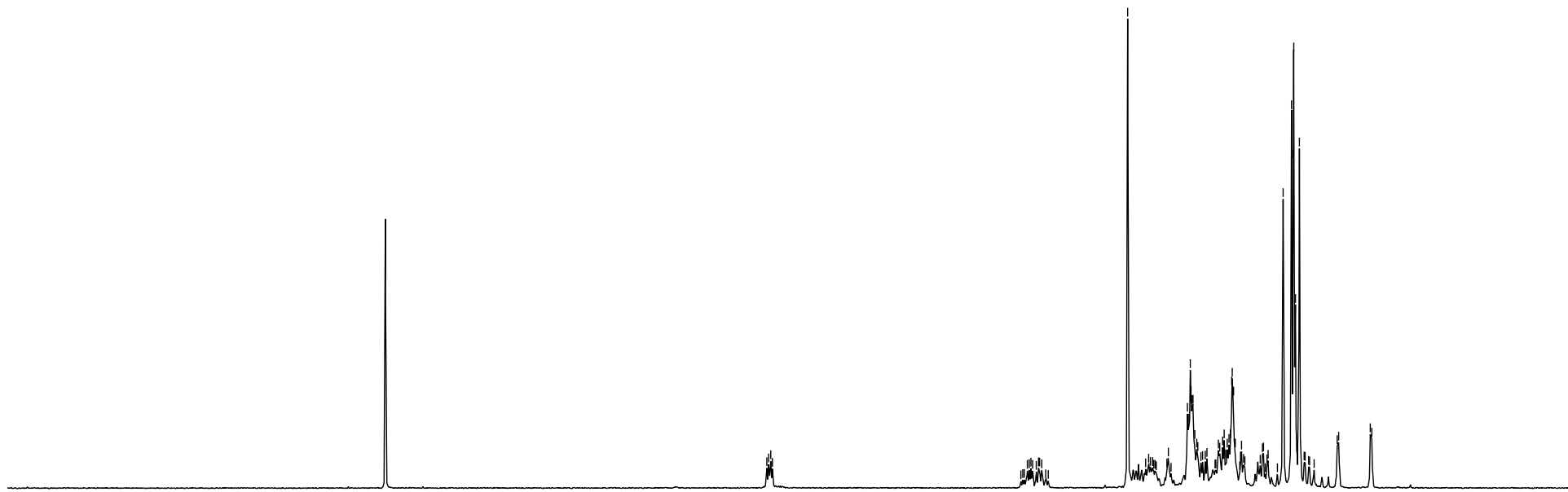
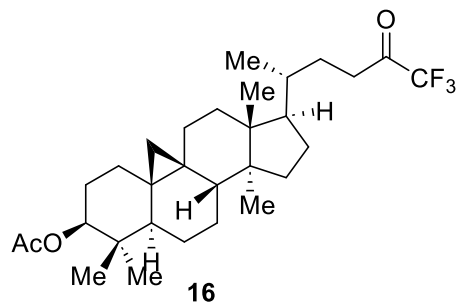


¹³C NMR Spectrum of S1-b (101 MHz, CDCl₃)



¹H NMR Spectrum of 16 (400 MHz, CDCl₃)

4.52
4.50
4.49
4.48
2.69
2.68
2.66
2.65
2.61
2.60
2.59
1.98
1.86
1.84
1.83
1.81
1.80
1.79
1.71
1.70
1.57
1.55
1.55
1.54
1.53
1.53
1.51
1.50
1.49
1.47
1.46
1.44
1.43
1.37
1.37
1.35
1.34
1.32
1.31
1.30
1.29
1.27
1.26
1.25
1.25
1.24
1.23
1.19
1.19
1.17
1.16
1.05
1.04
1.03
1.01
1.00
0.89
0.84
0.82
0.82
0.81
0.80
0.78
0.75
0.74
0.71
0.71
0.68
0.51
0.50
0.28
0.27



1.00

2.05

3.09

3.24

0.99

5.65

1.11

4.07

1.06

2.03

2.91

3.02

5.82

2.92

0.83

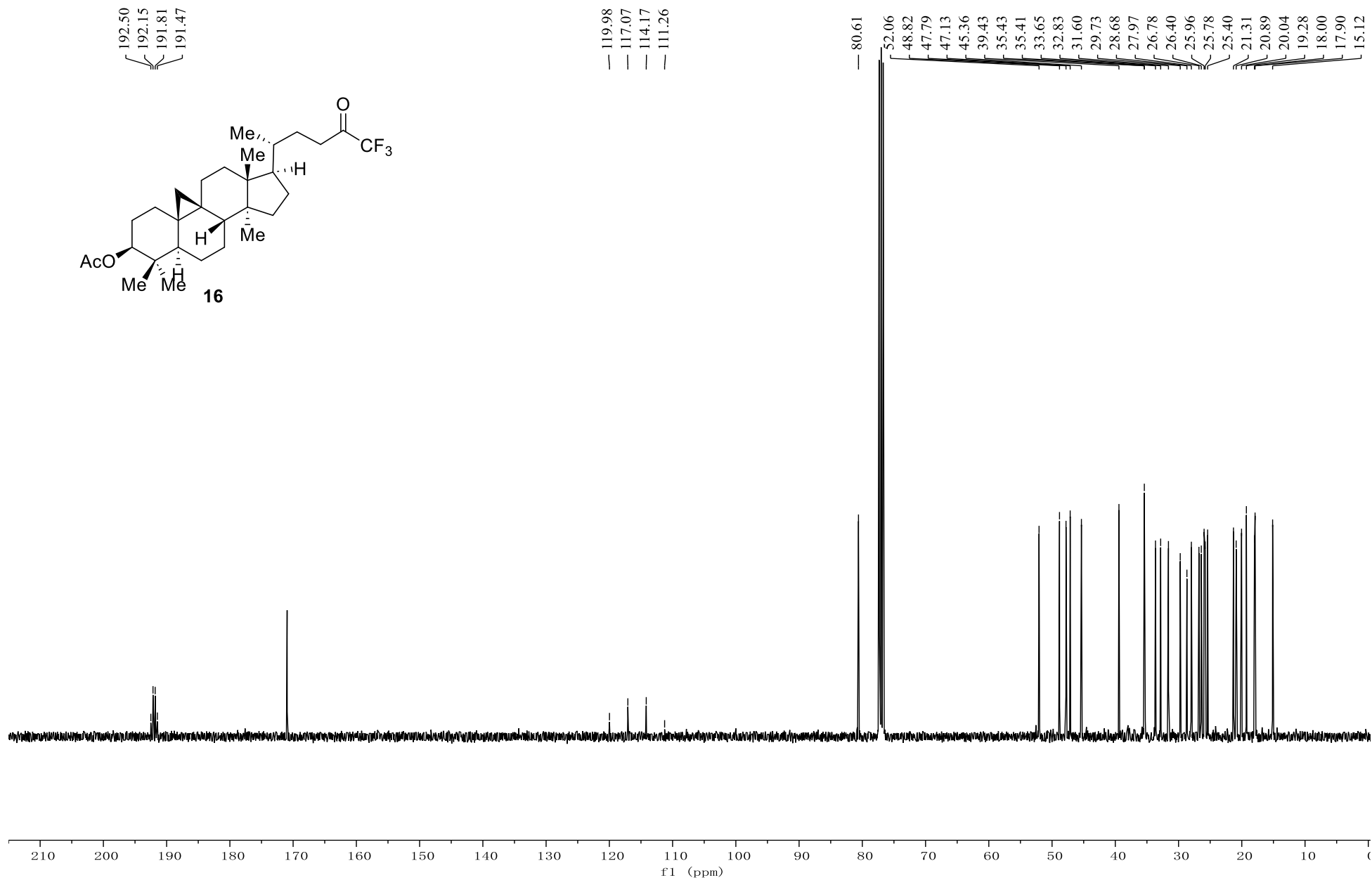
0.95

0.97

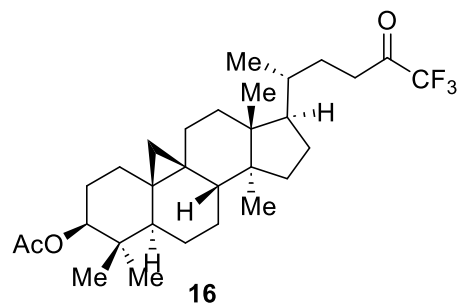
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0

f1 (ppm)

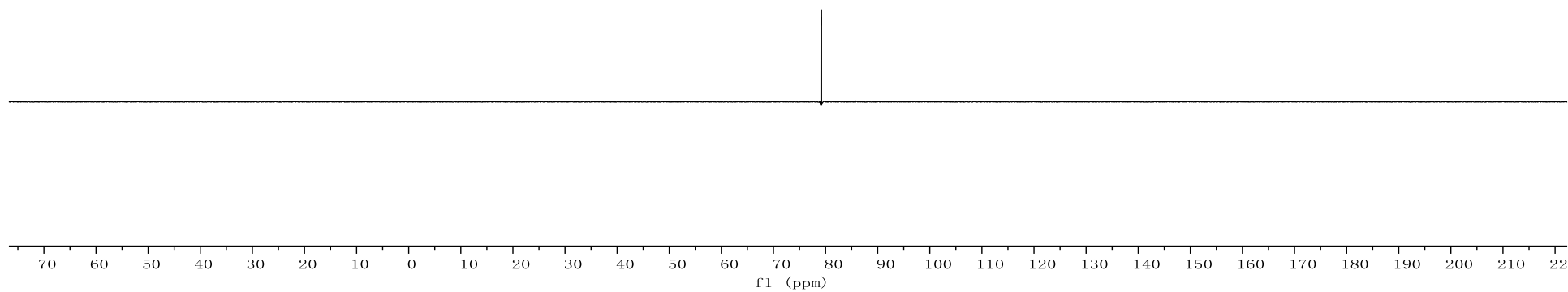
¹³C NMR Spectrum of 16 (101 MHz, CDCl₃)



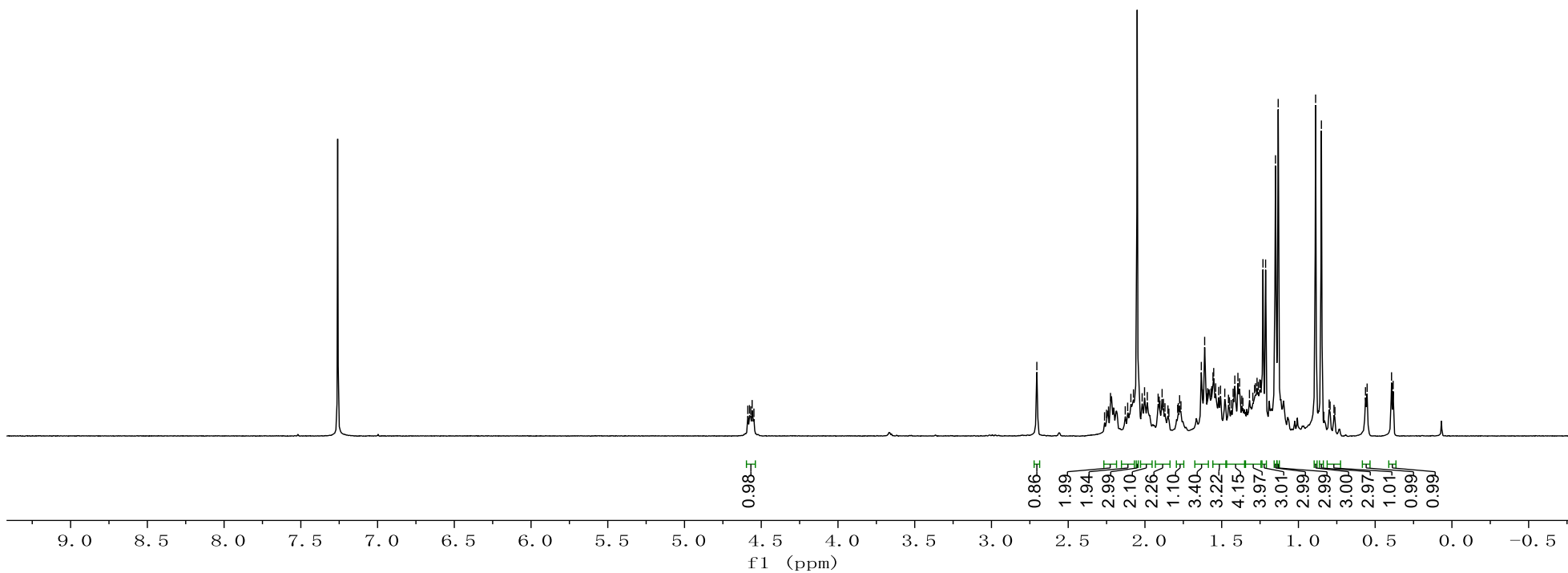
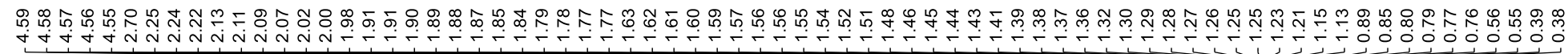
¹⁹F -NMR Spectrum of 16 (376 MHz, CDCl₃)



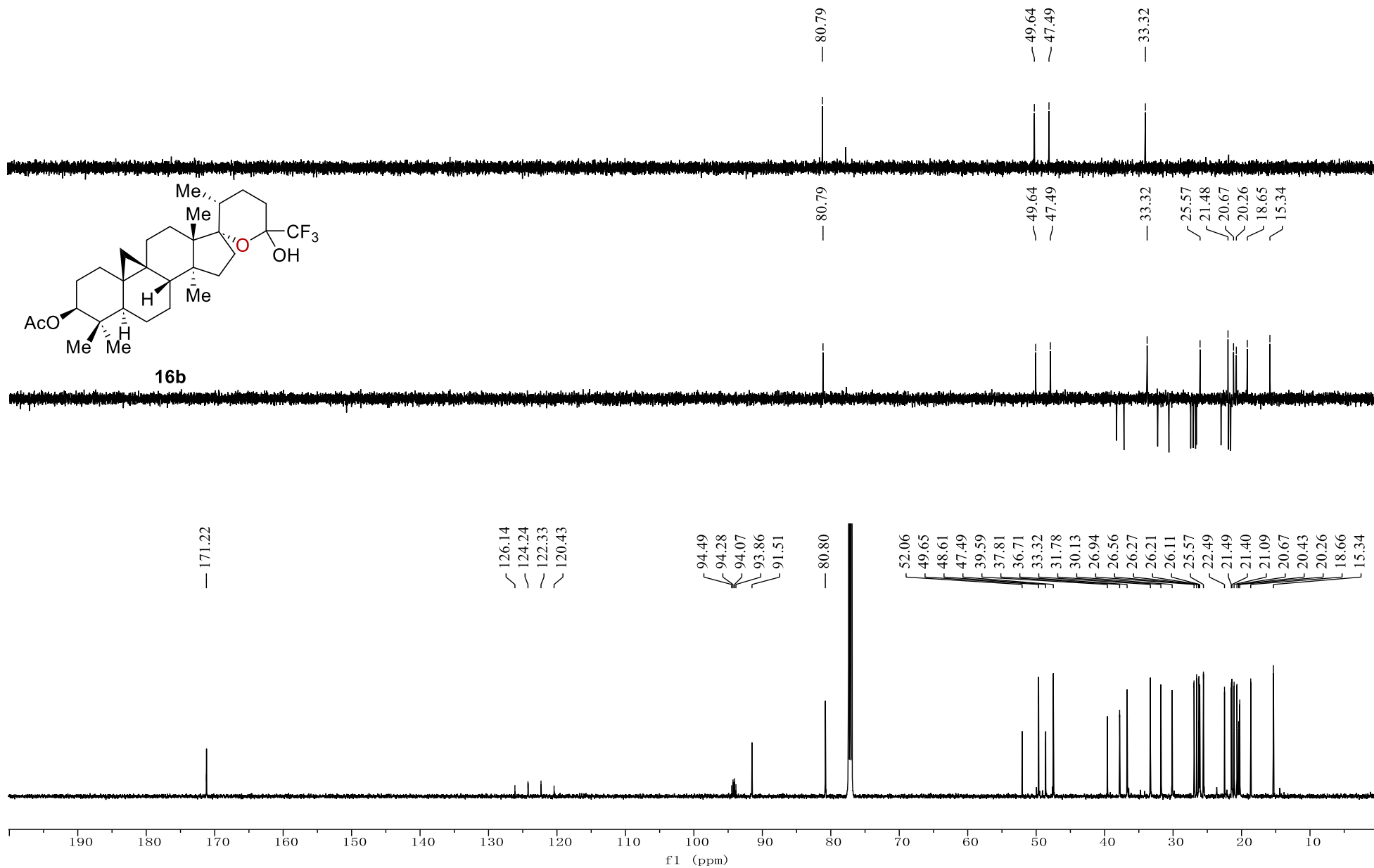
— -79.14



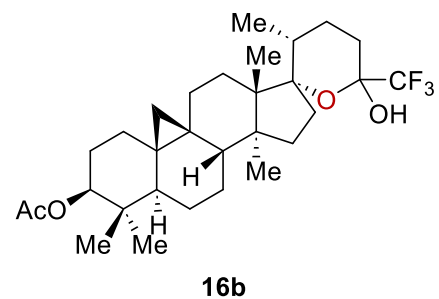
¹H NMR Spectrum of 16b(400 MHz, CDCl₃)



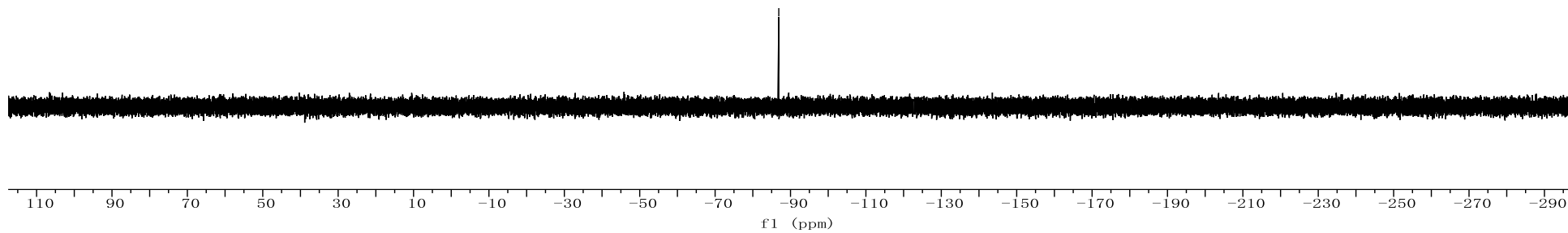
DEPT and ¹³C NMR Spectrum of 16b (151 MHz, CDCl₃)



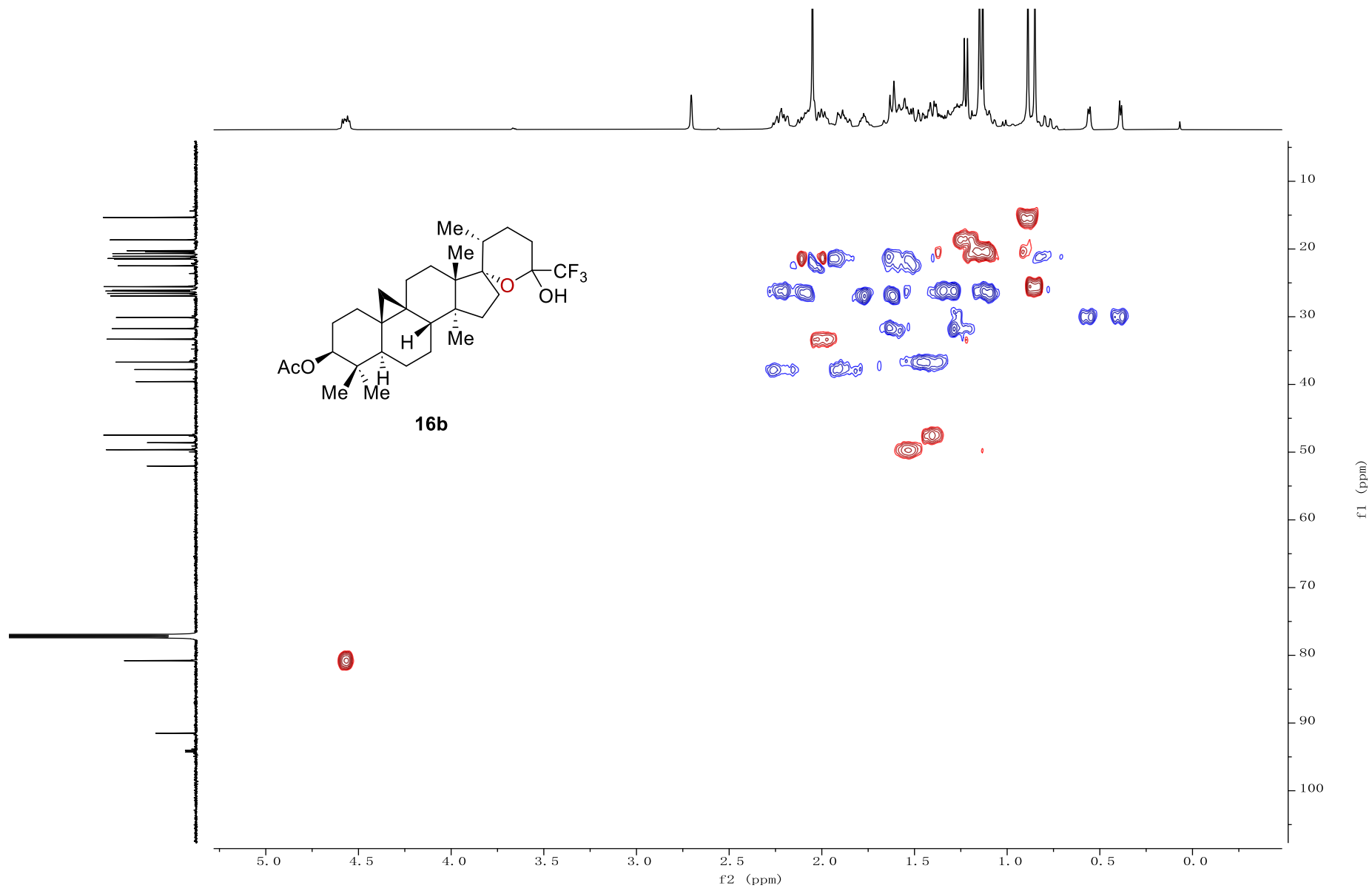
¹⁹F -NMR Spectrum of 16b (376 MHz, CDCl₃)



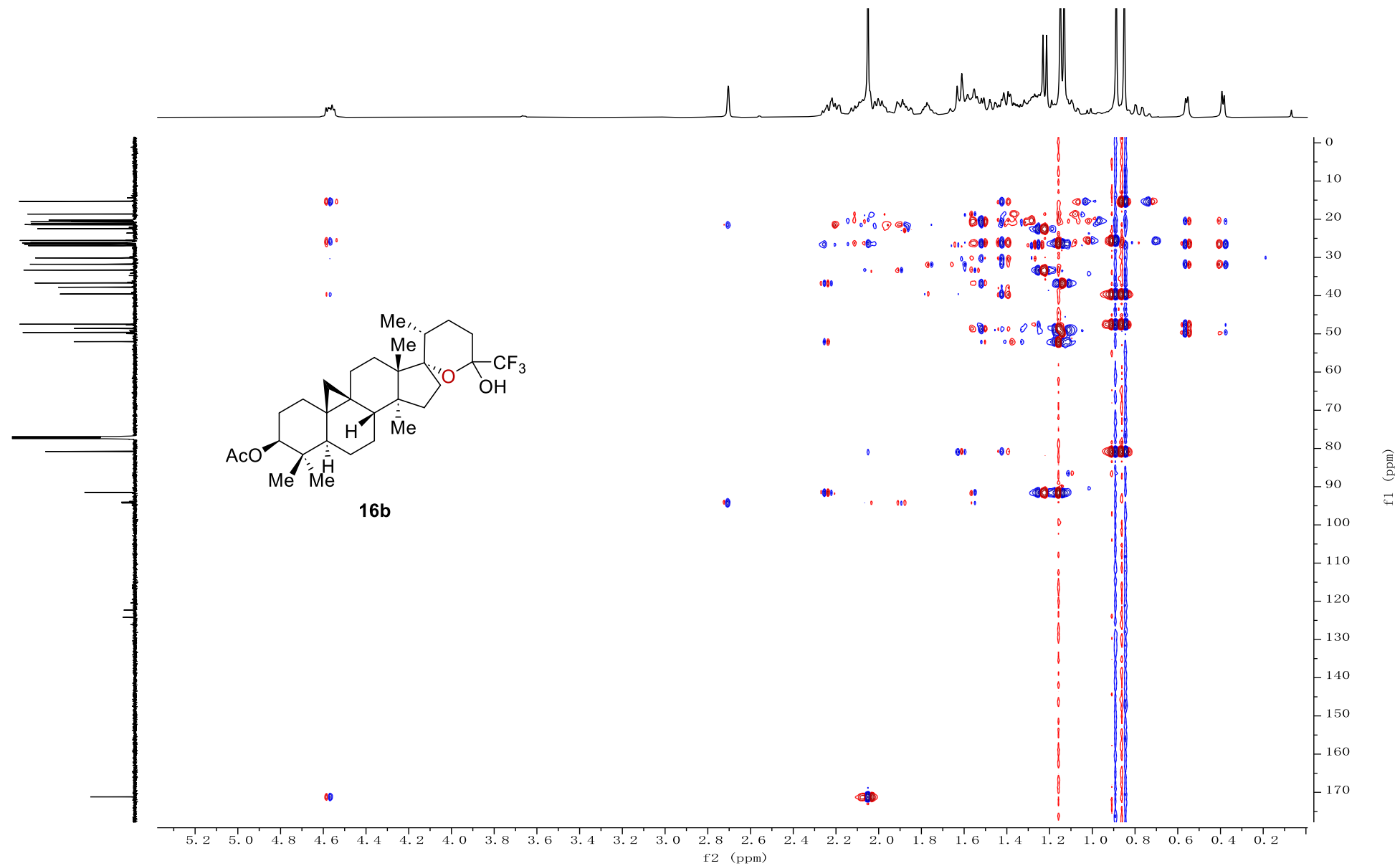
68.89



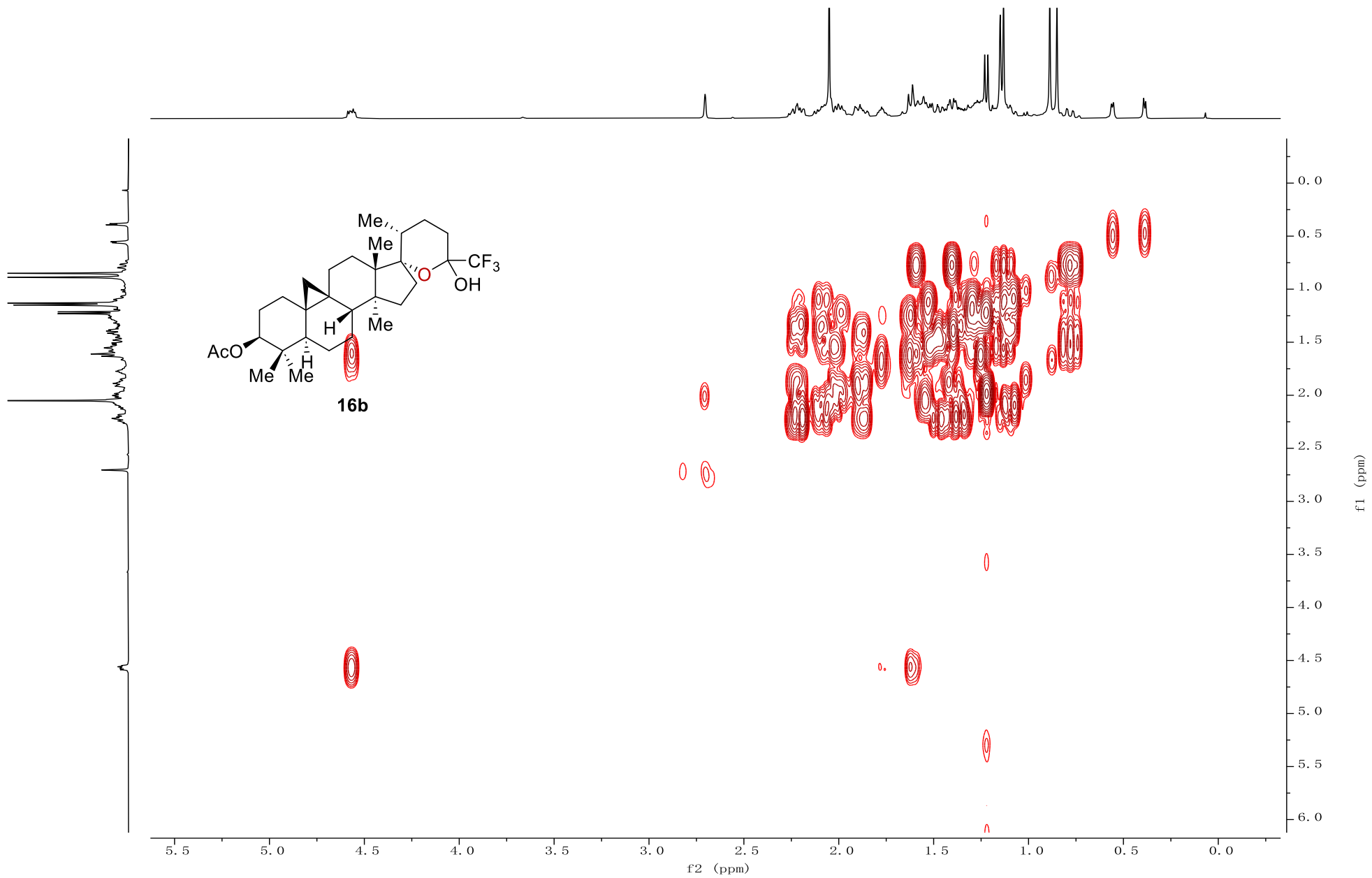
HSQC Spectrum of 16b



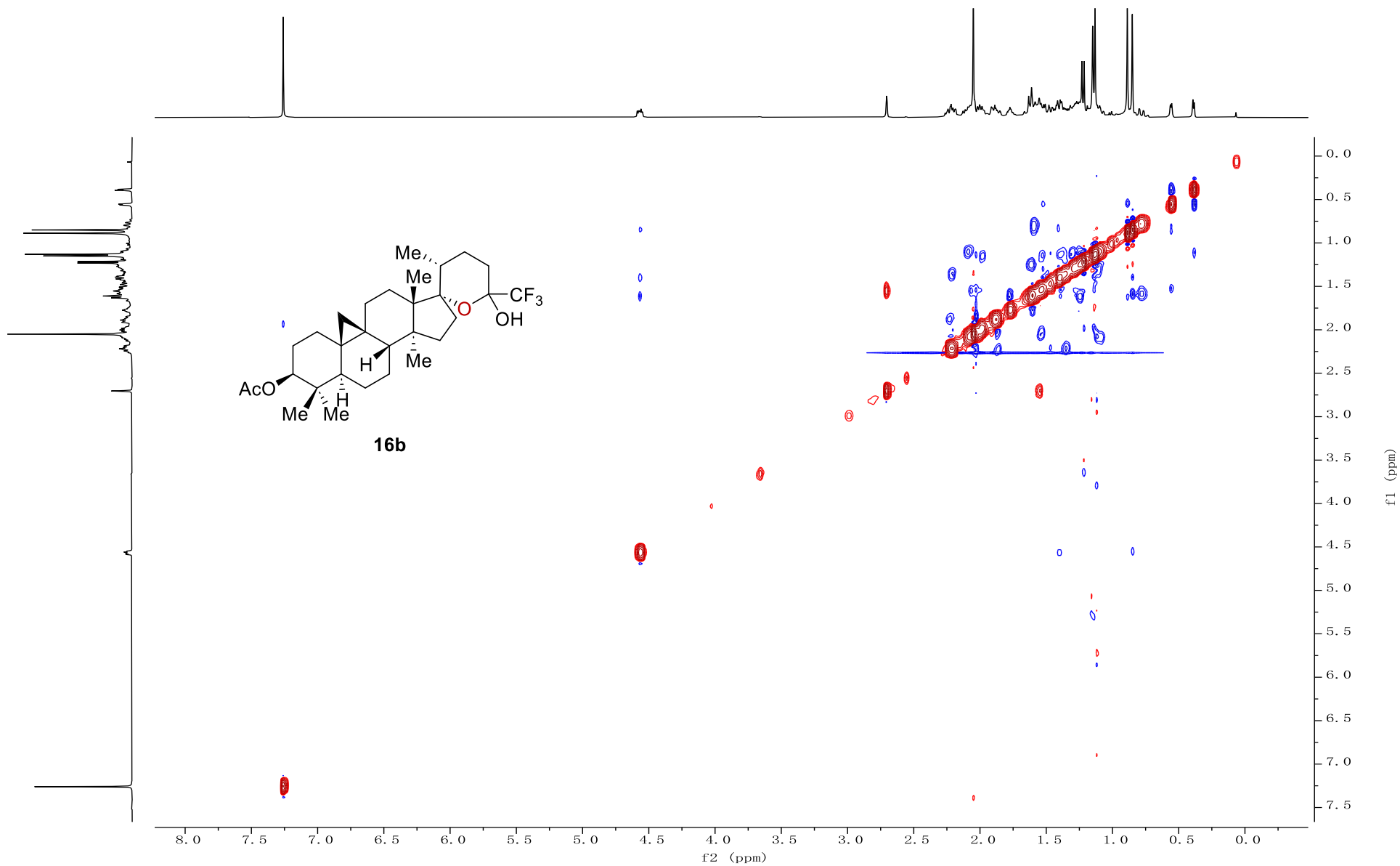
HMBC Spectrum of 16b



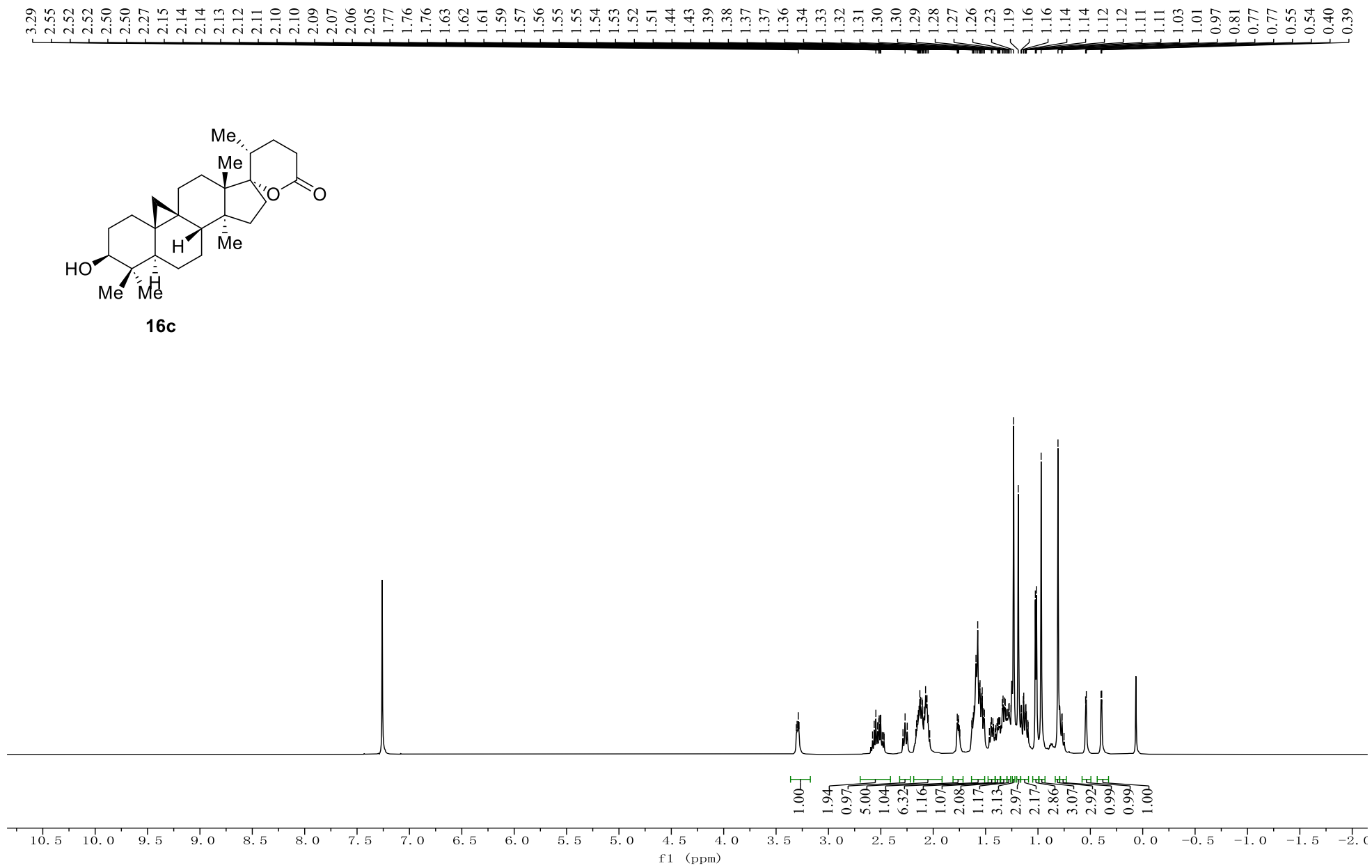
^1H - ^1H COSY Spectrum of 16b



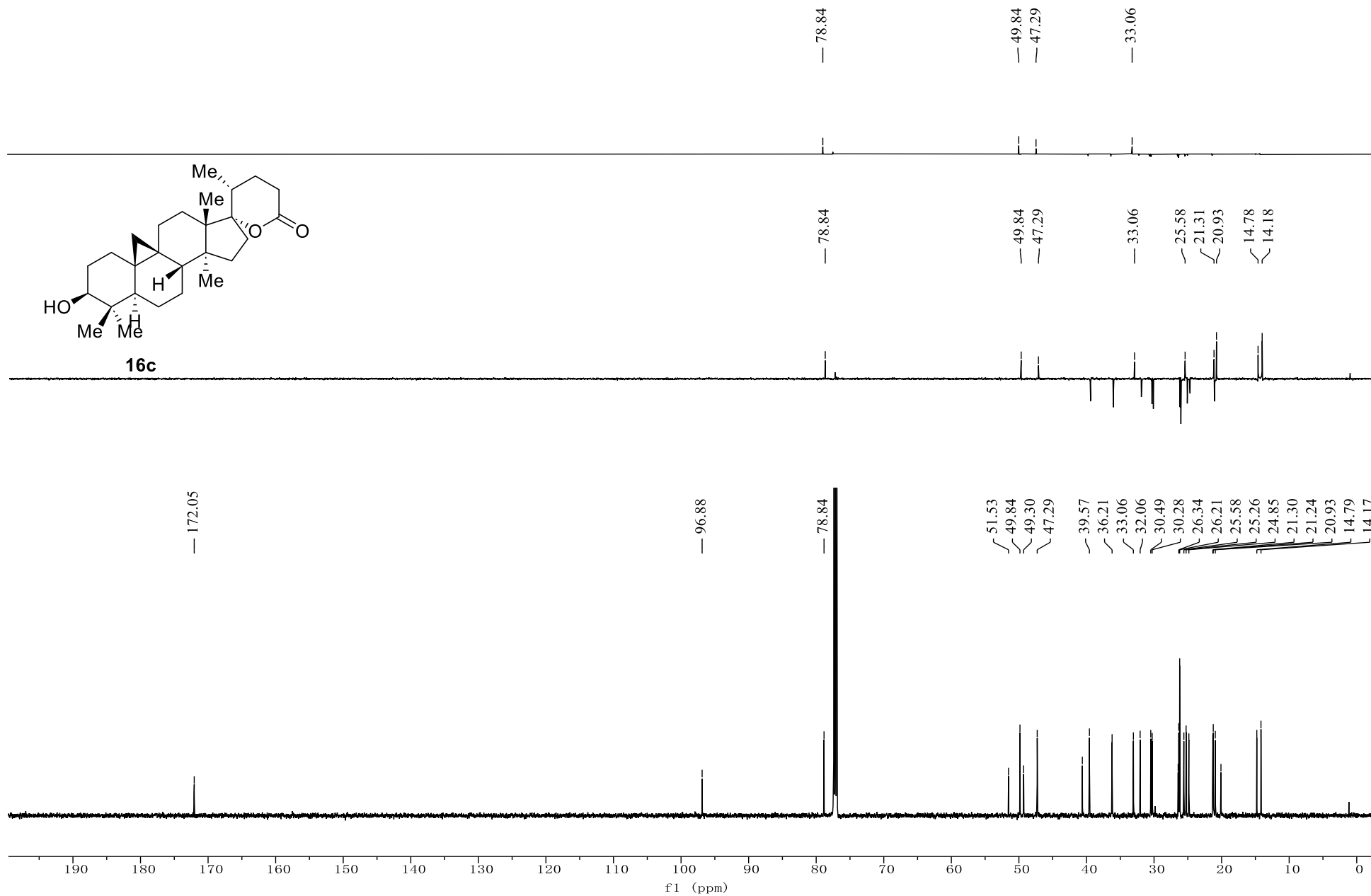
NOESY Spectrum of 16b



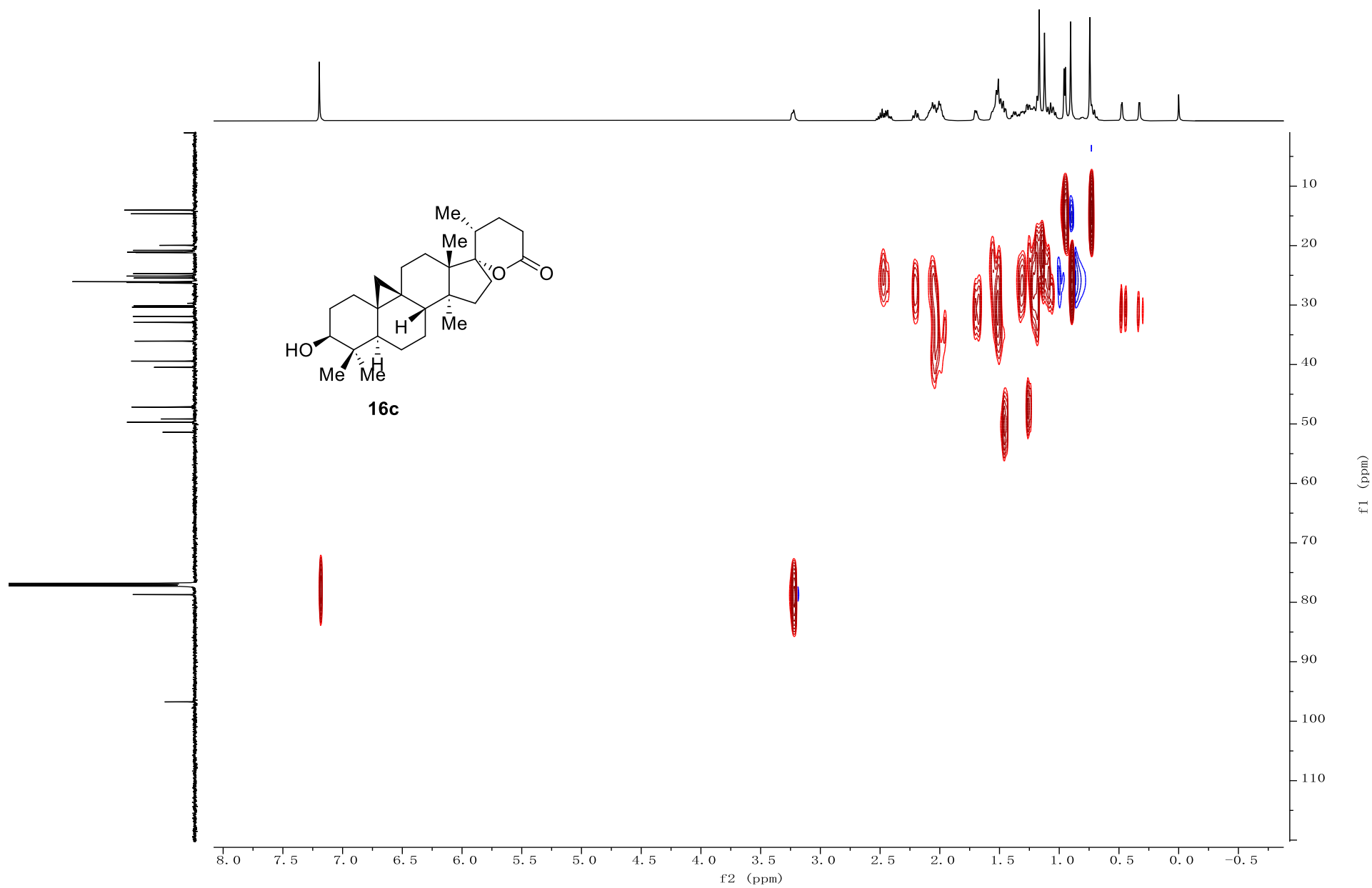
¹H NMR Spectrum of 16c (600 MHz, CDCl₃)



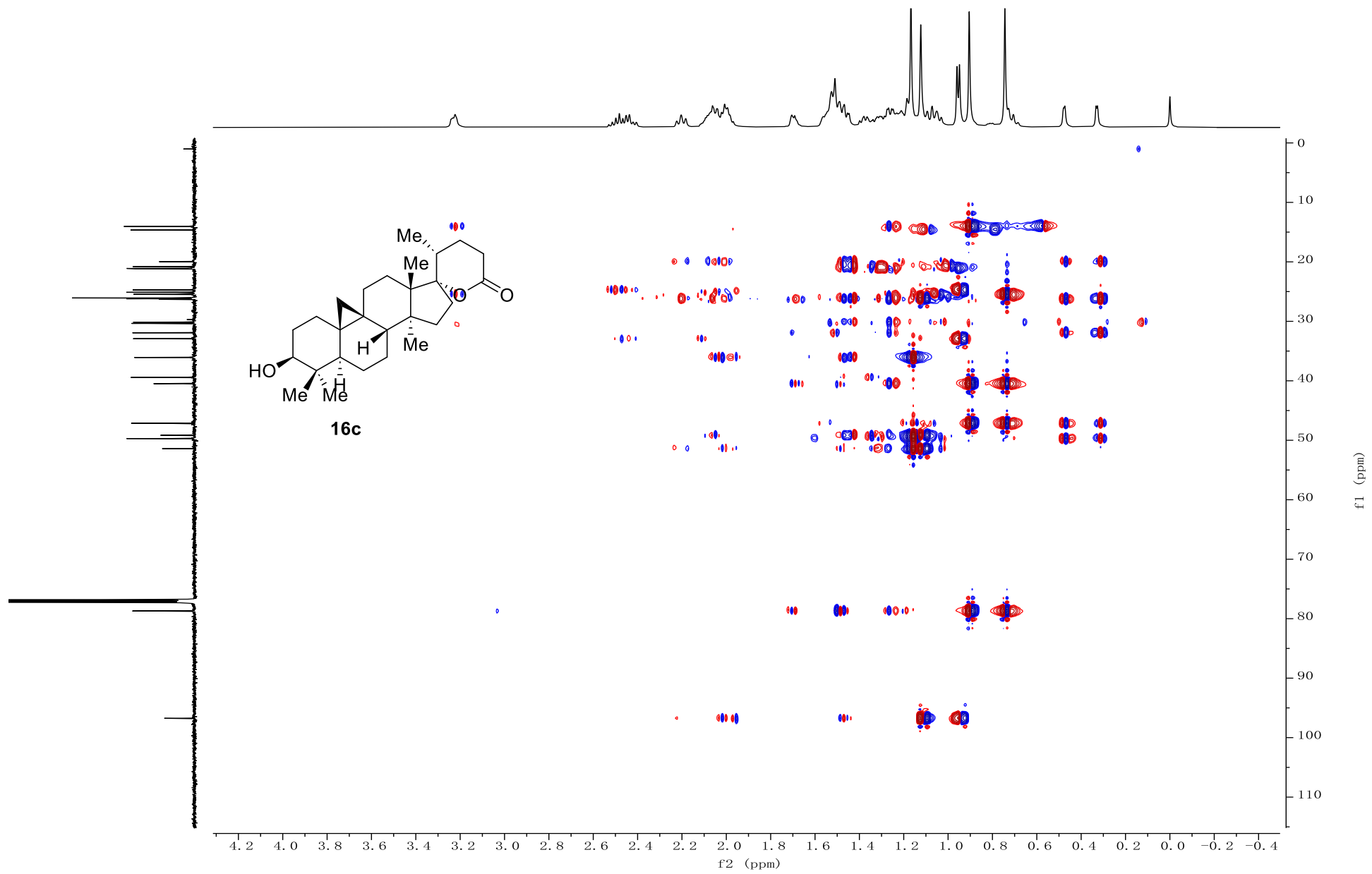
DEPT and ¹³C NMR Spectrum of 16c (151 MHz, CDCl₃)



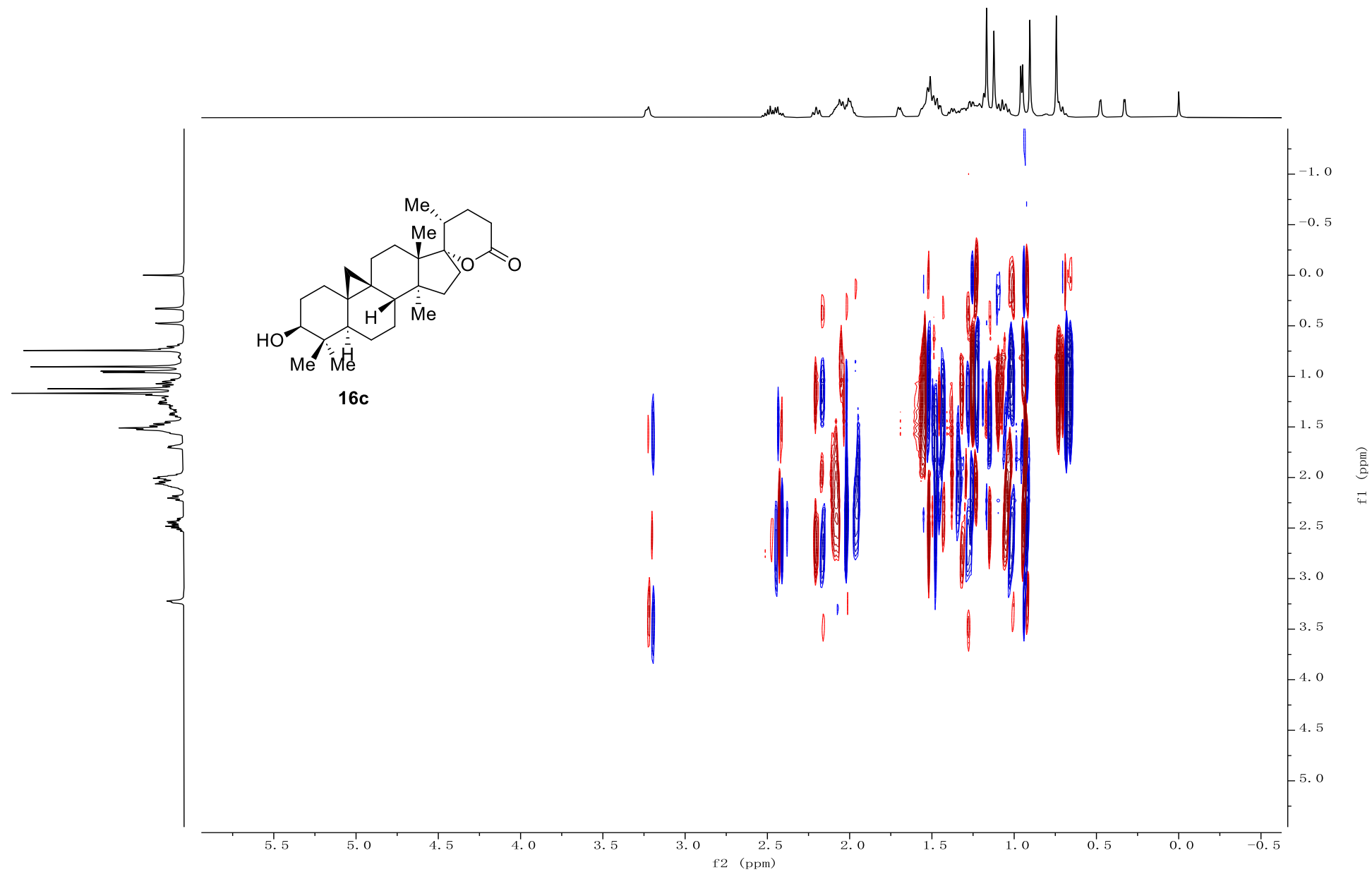
HSQC Spectrum of 16c



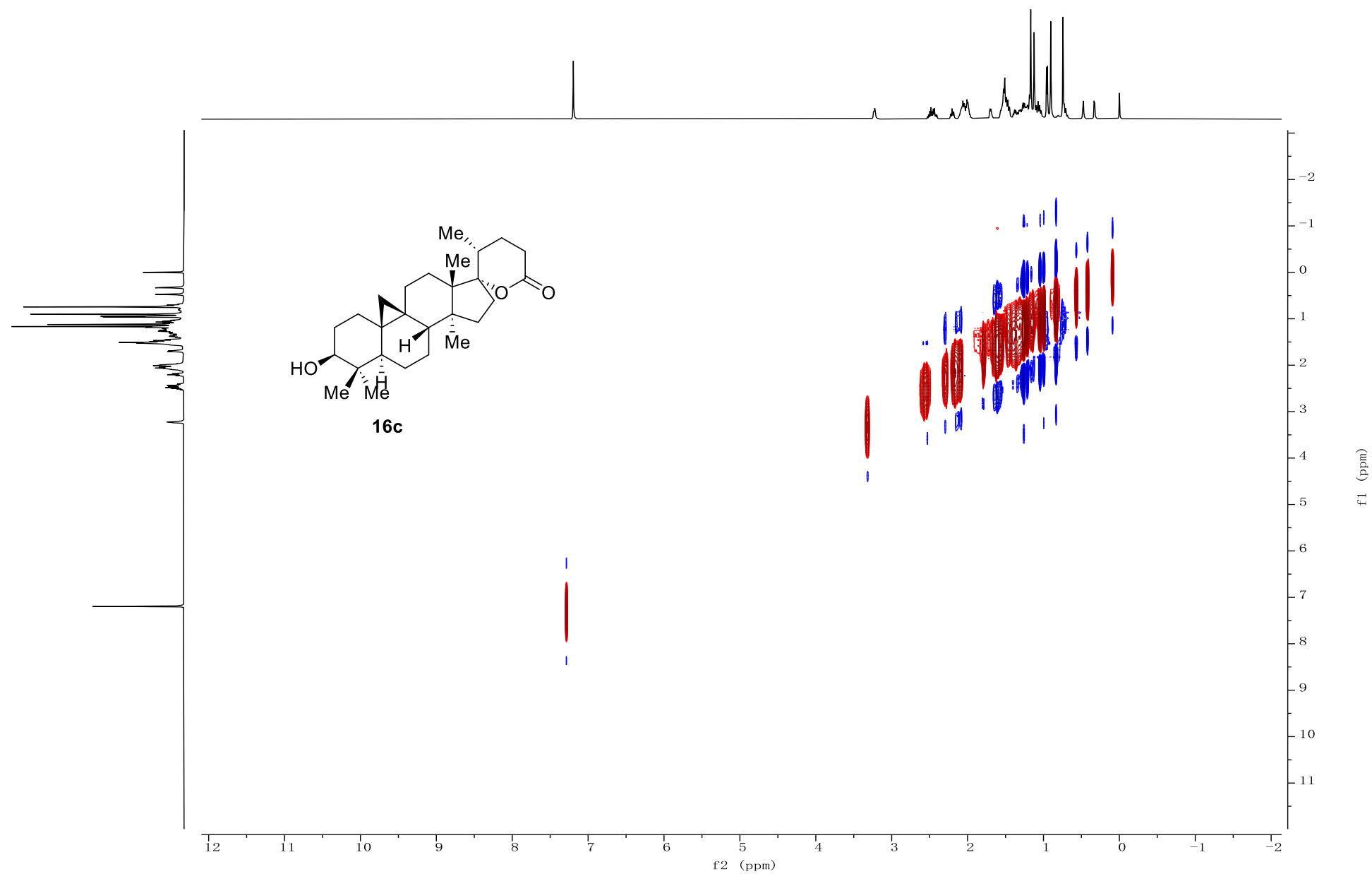
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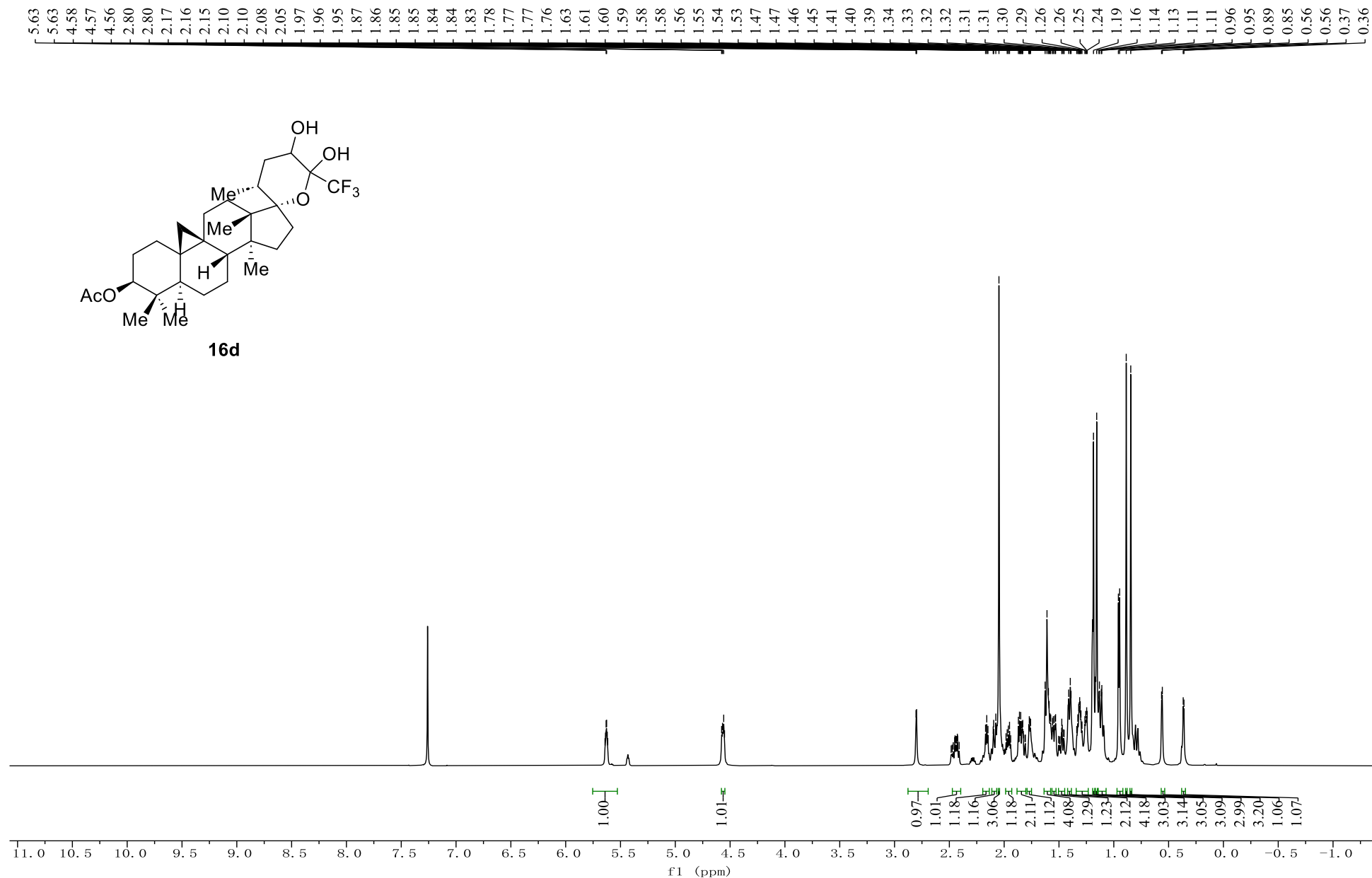
^1H - ^1H COSY Spectrum of 16c



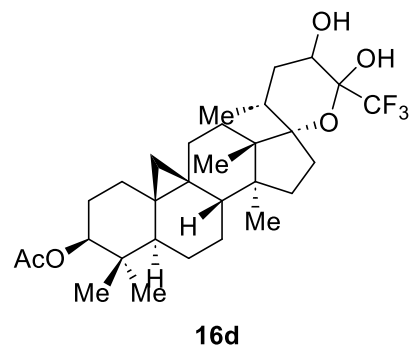
NOESY Spectrum of 16c



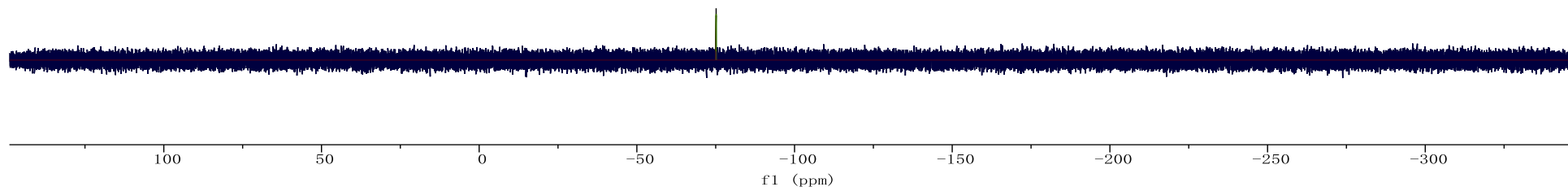
¹H NMR Spectrum of 16d (400 MHz, CDCl₃)



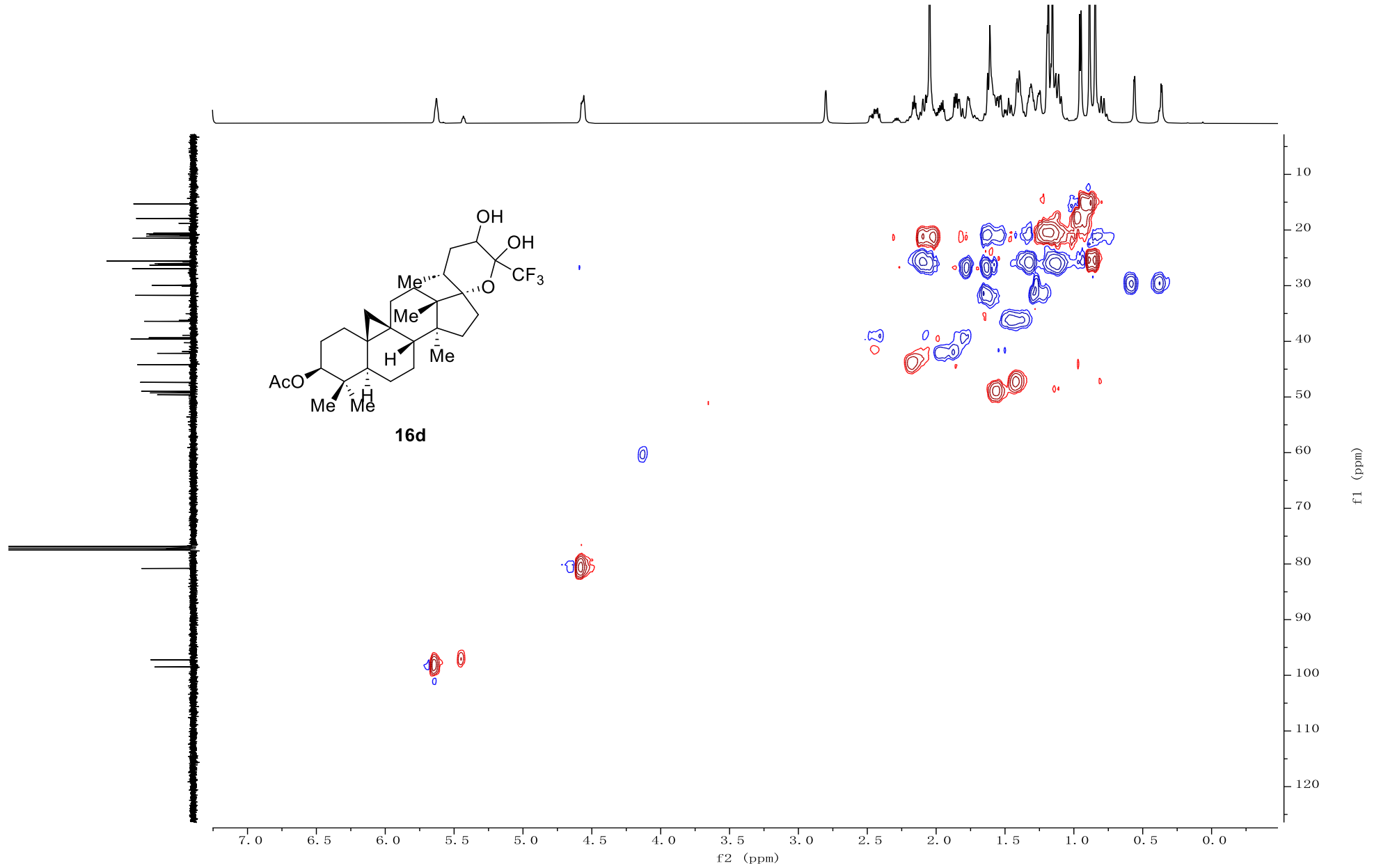
¹⁹F -NMR Spectrum of 16d (376 MHz, CDCl₃)



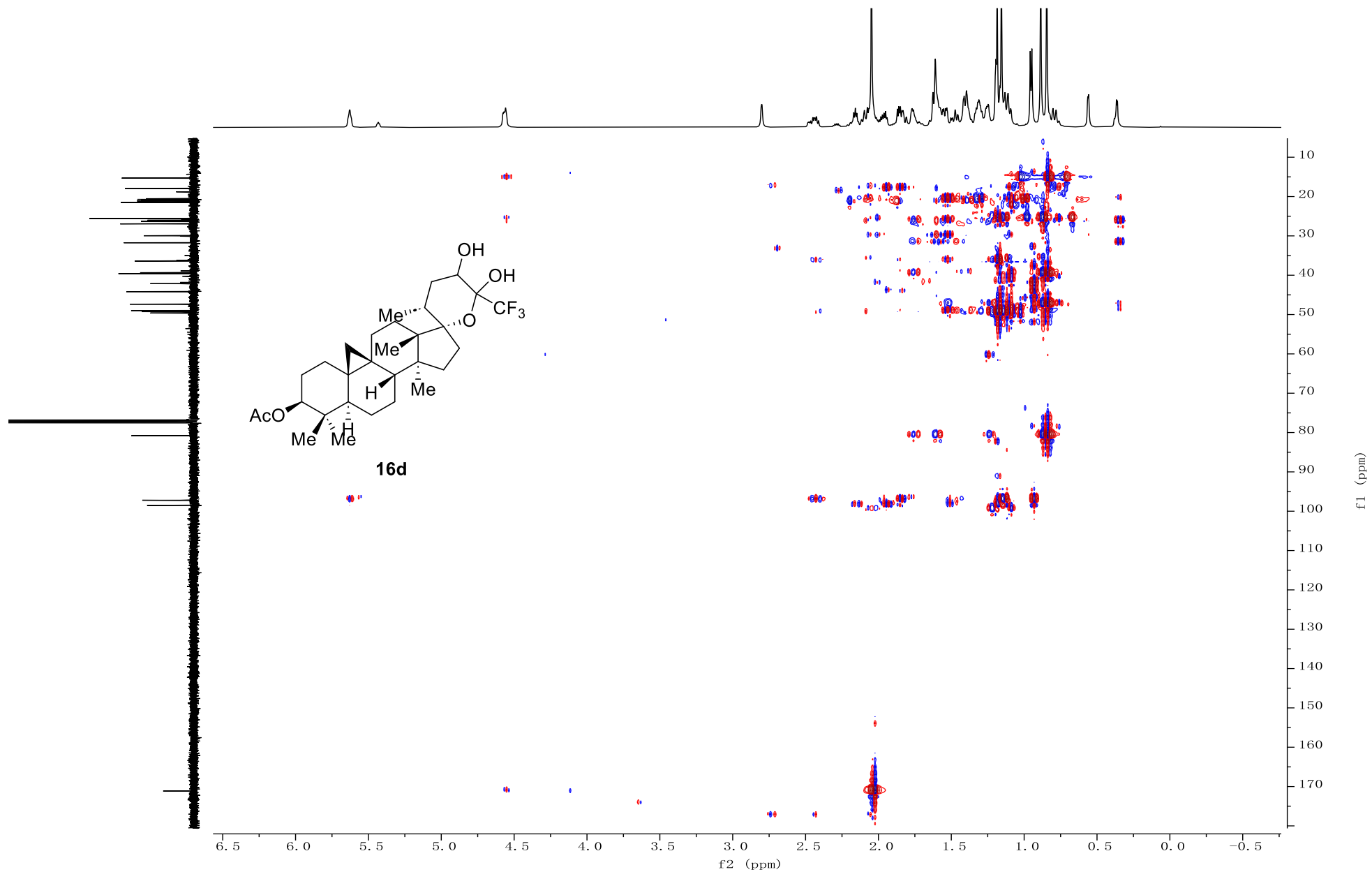
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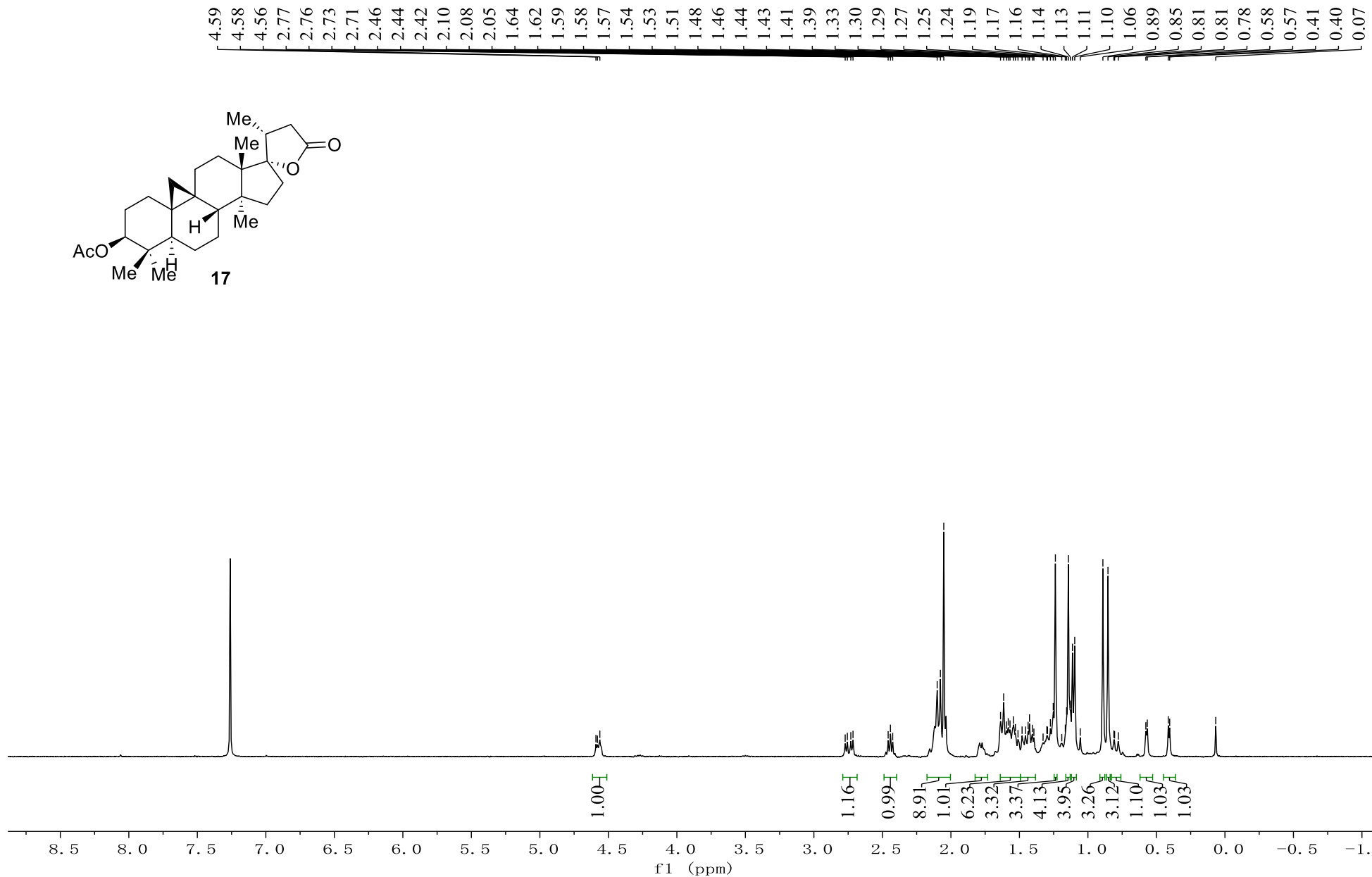
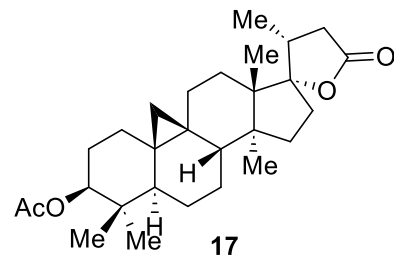
HSQC Spectrum of 16d



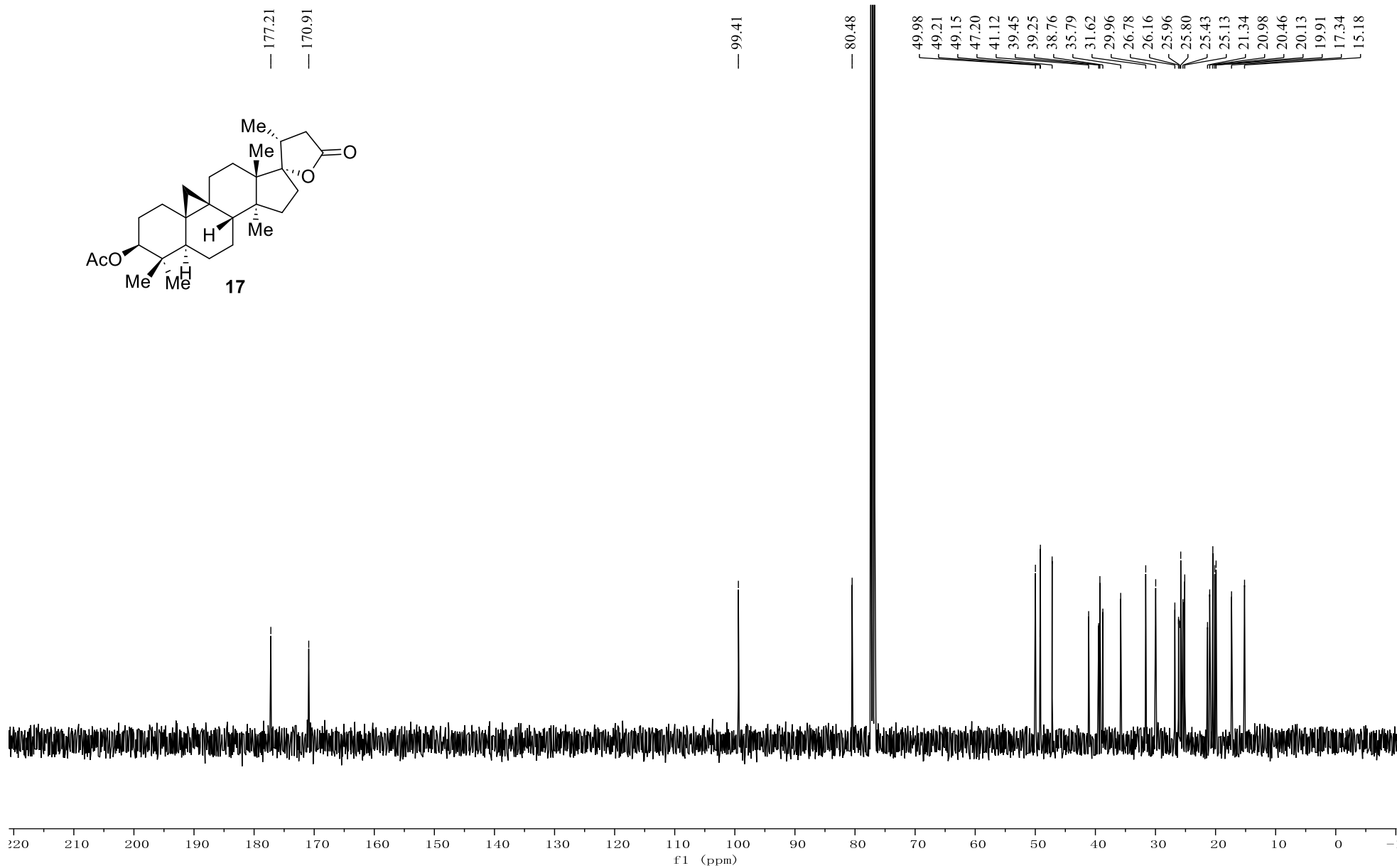
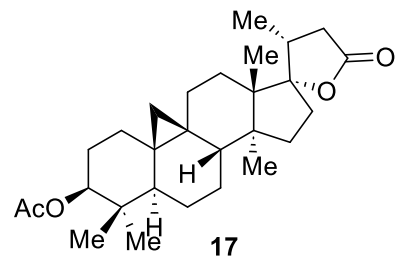
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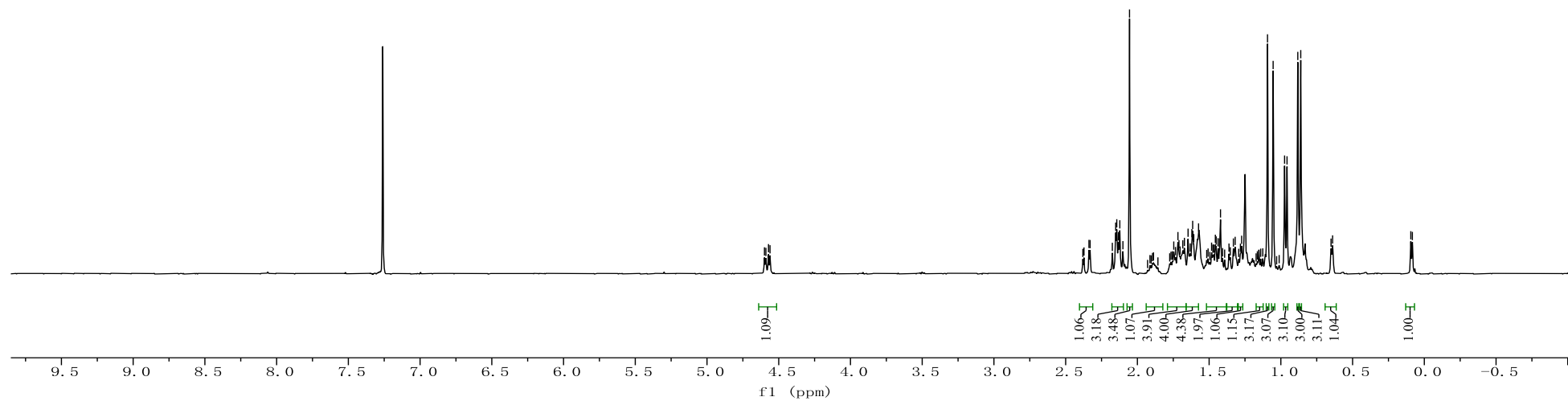
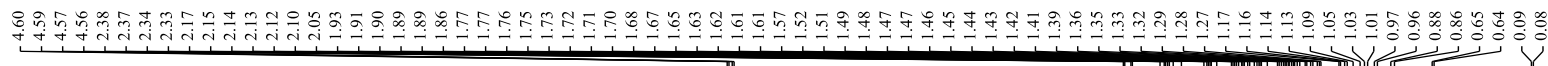
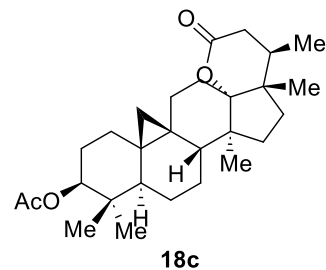
¹H NMR Spectrum of 17 (400 MHz, CDCl₃)



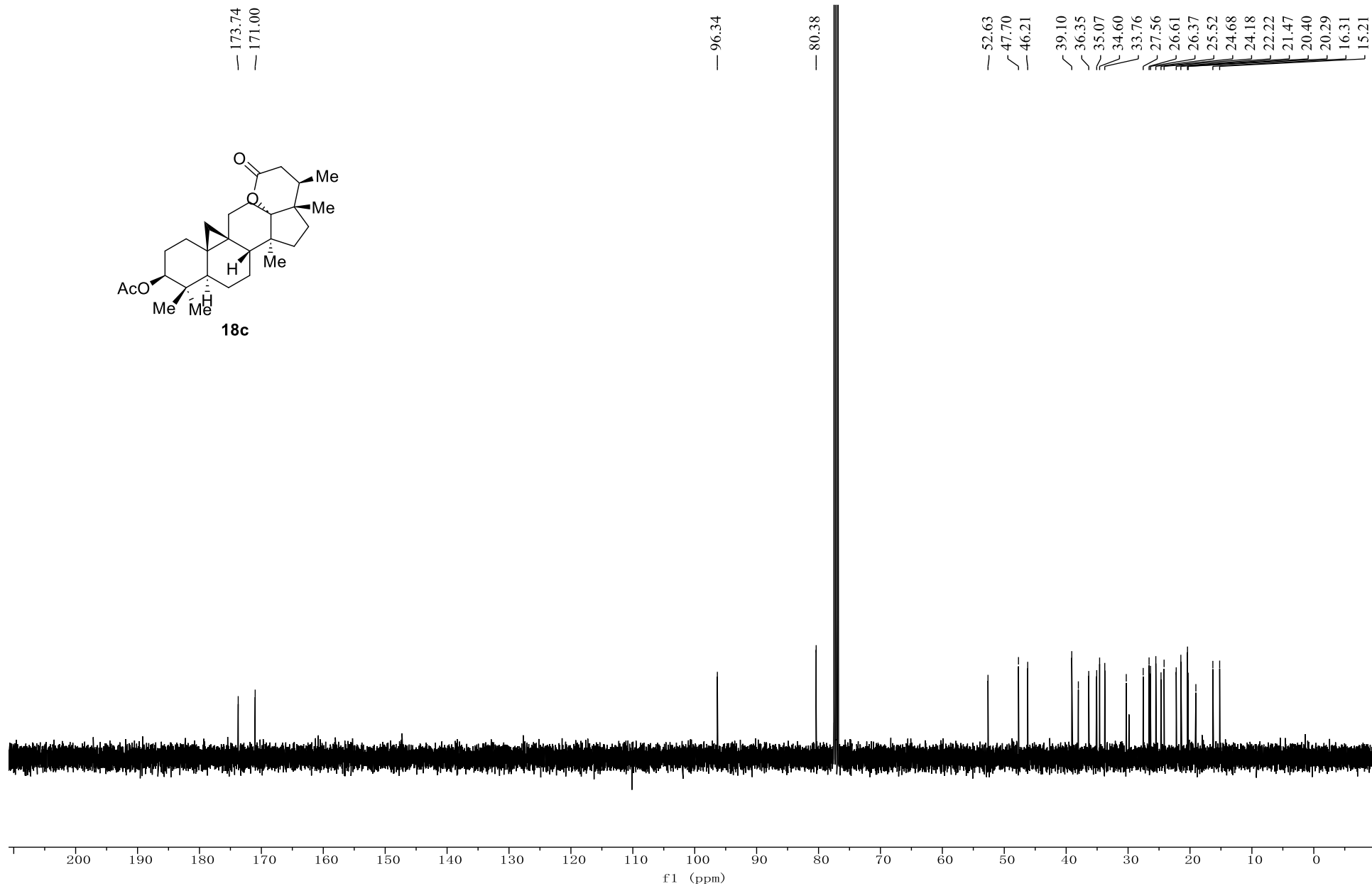
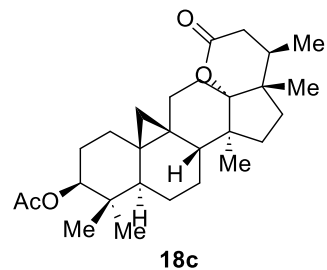
¹³C NMR Spectrum of 17 (101 MHz, CDCl₃)



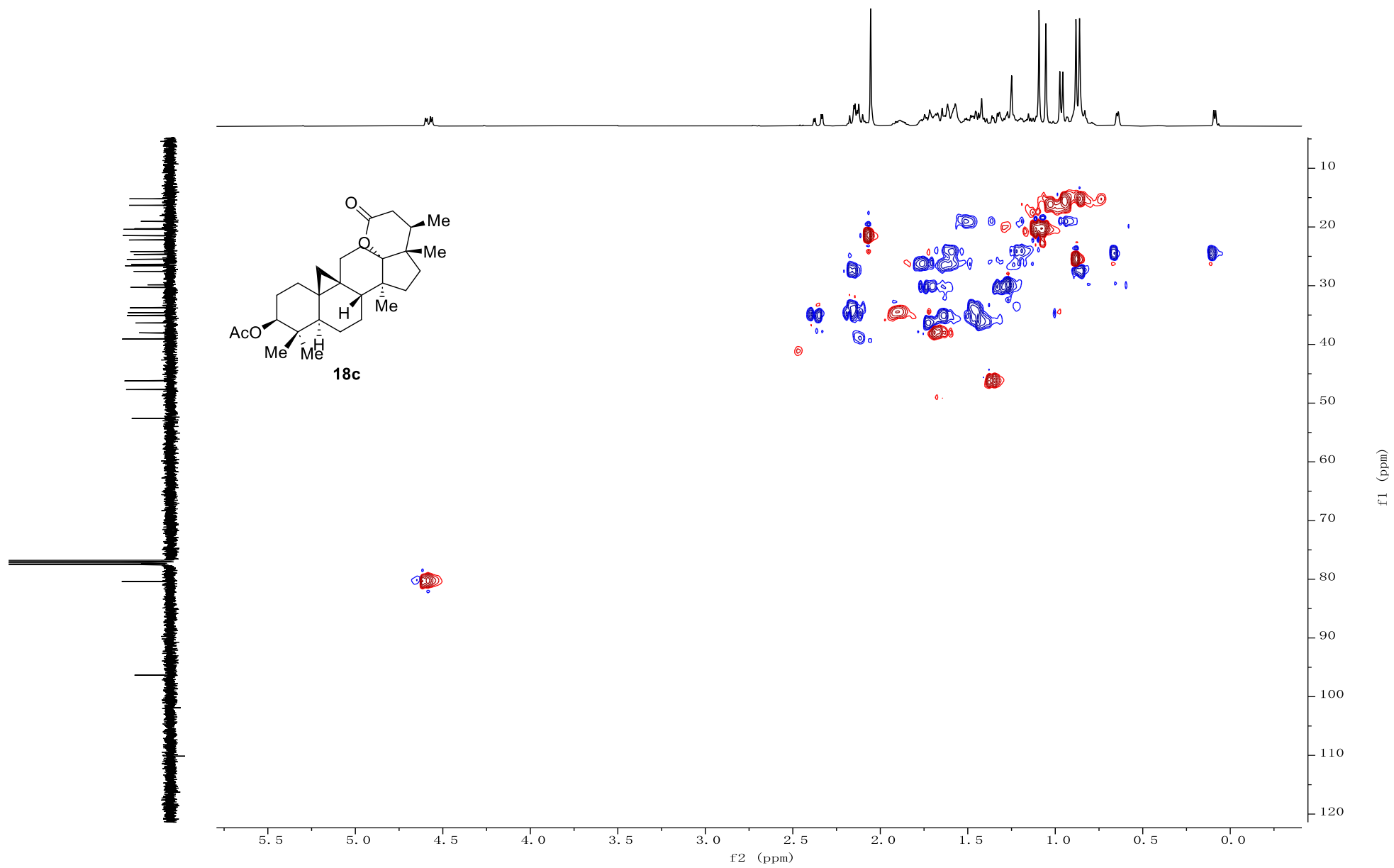
¹H NMR Spectrum of 18c (400 MHz, CDCl₃)



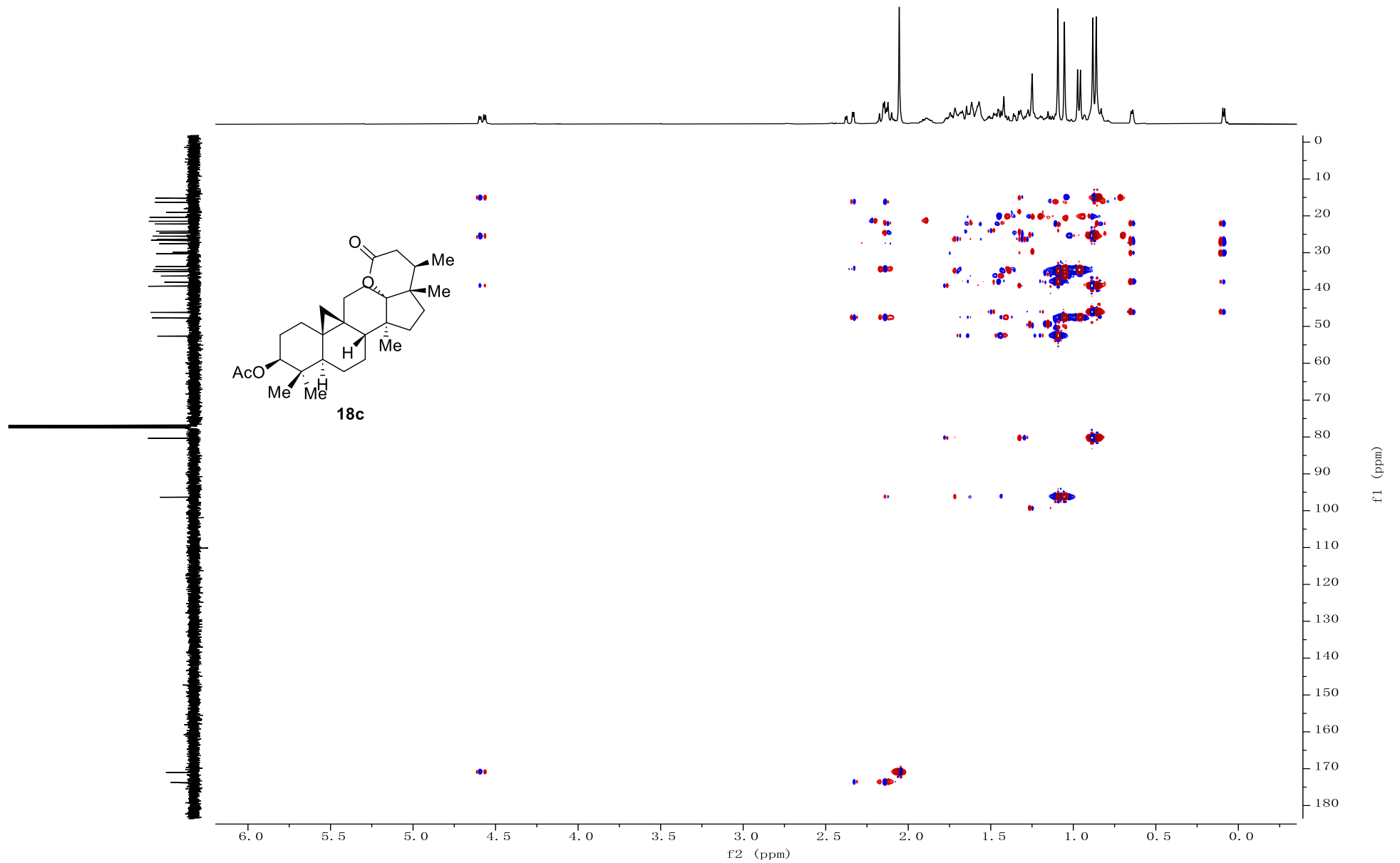
¹³C NMR Spectrum of 18c (101 MHz, CDCl₃)



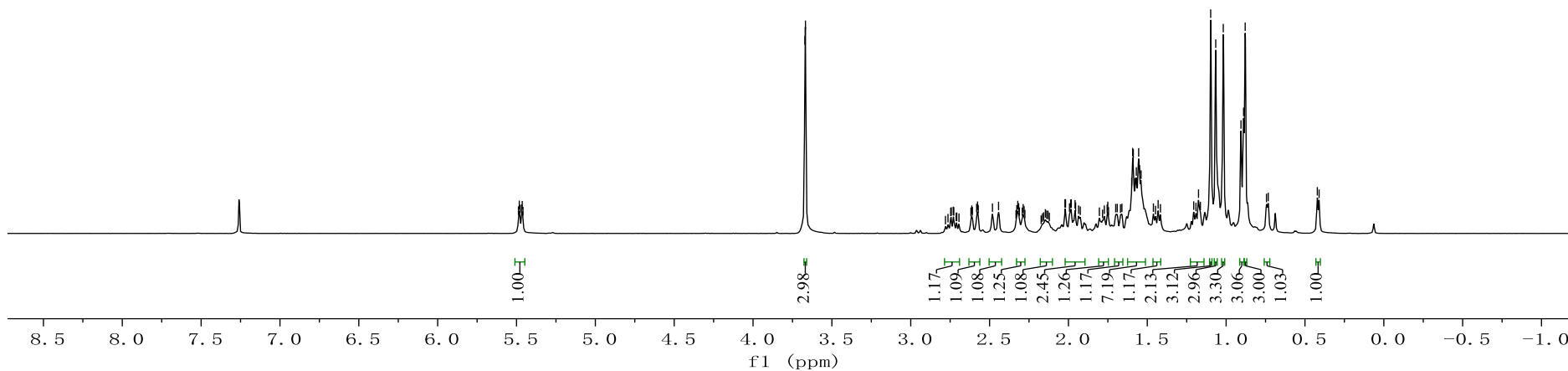
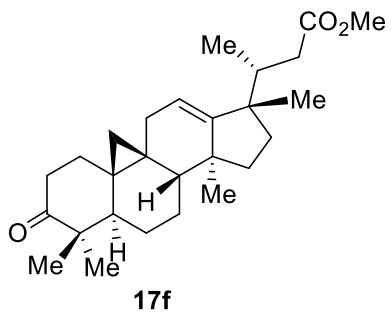
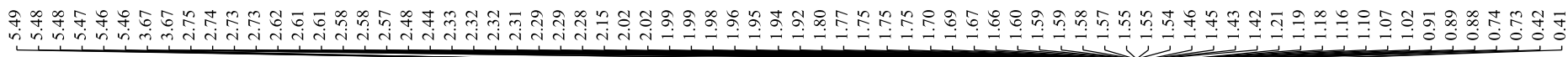
HSQC Spectrum of 18c



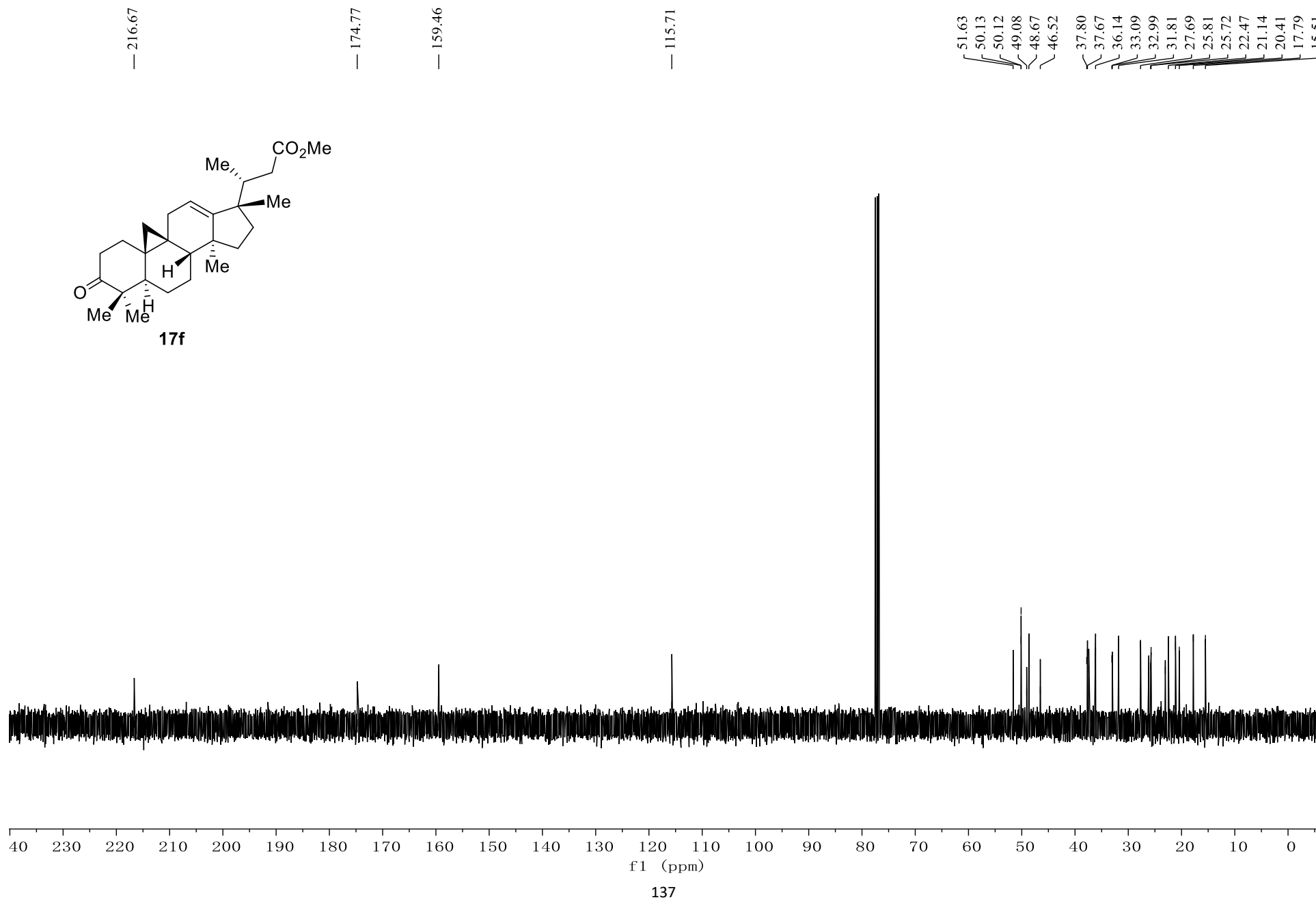
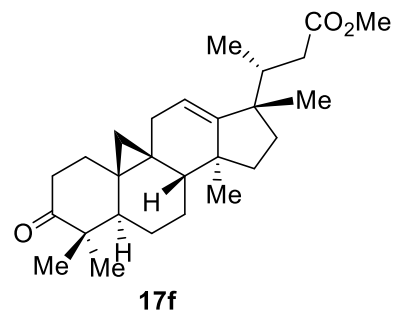
HMBC Spectrum of 18c



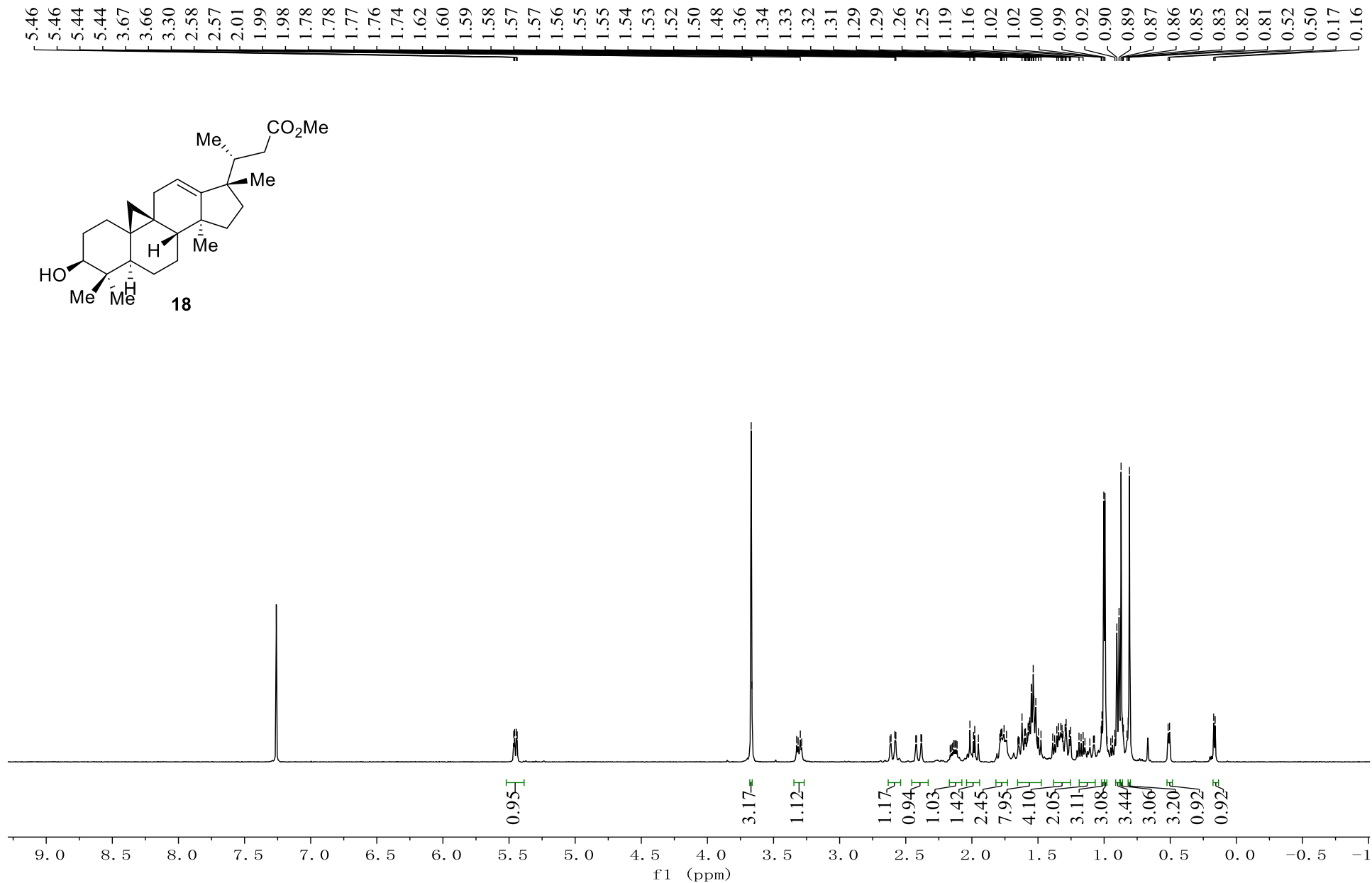
¹H NMR Spectrum of 17f (400 MHz, CDCl₃)



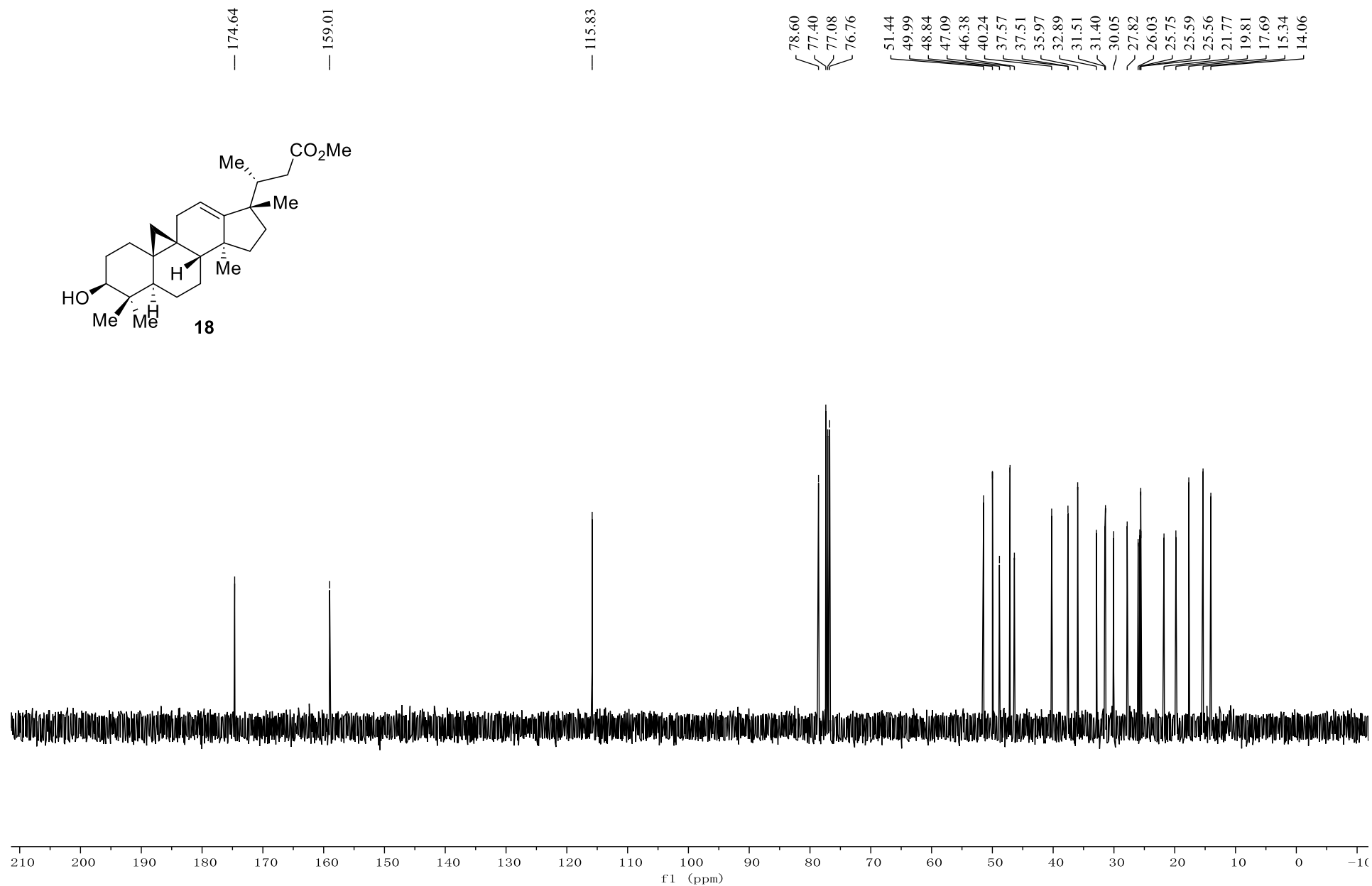
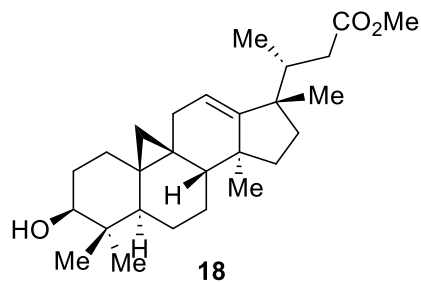
¹³C NMR Spectrum of 17f (101 MHz, CDCl₃)



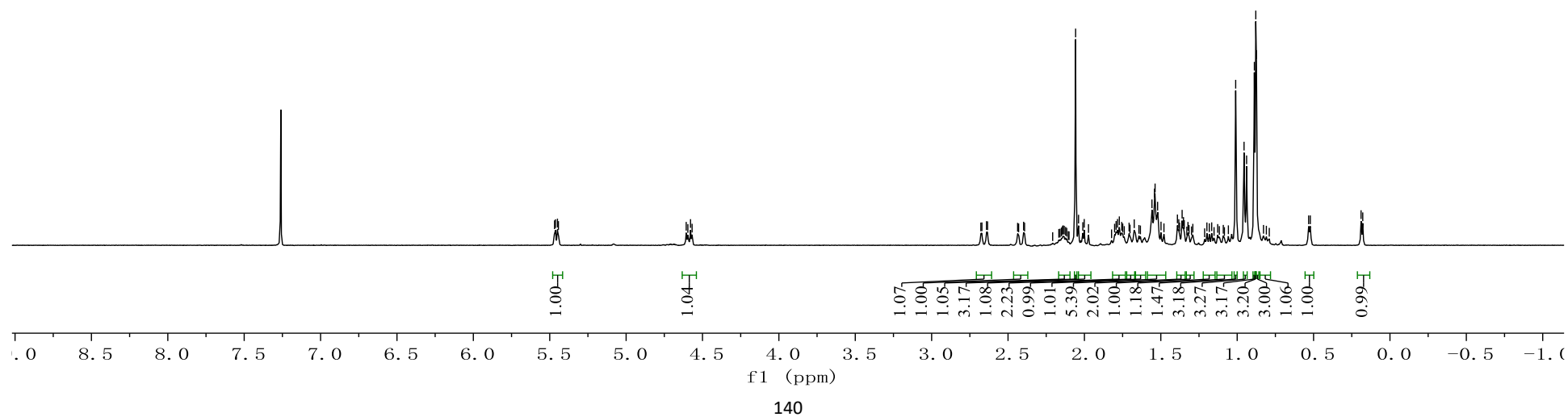
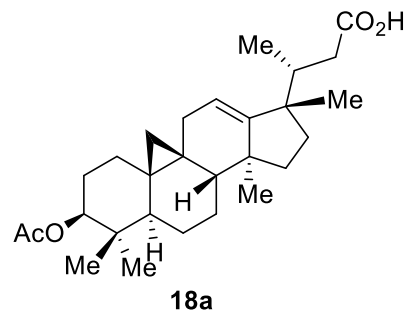
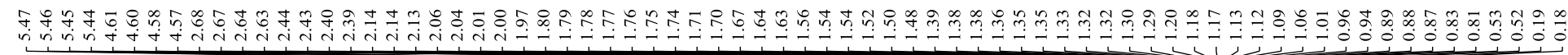
¹H NMR Spectrum of 18 (400 MHz, CDCl₃)



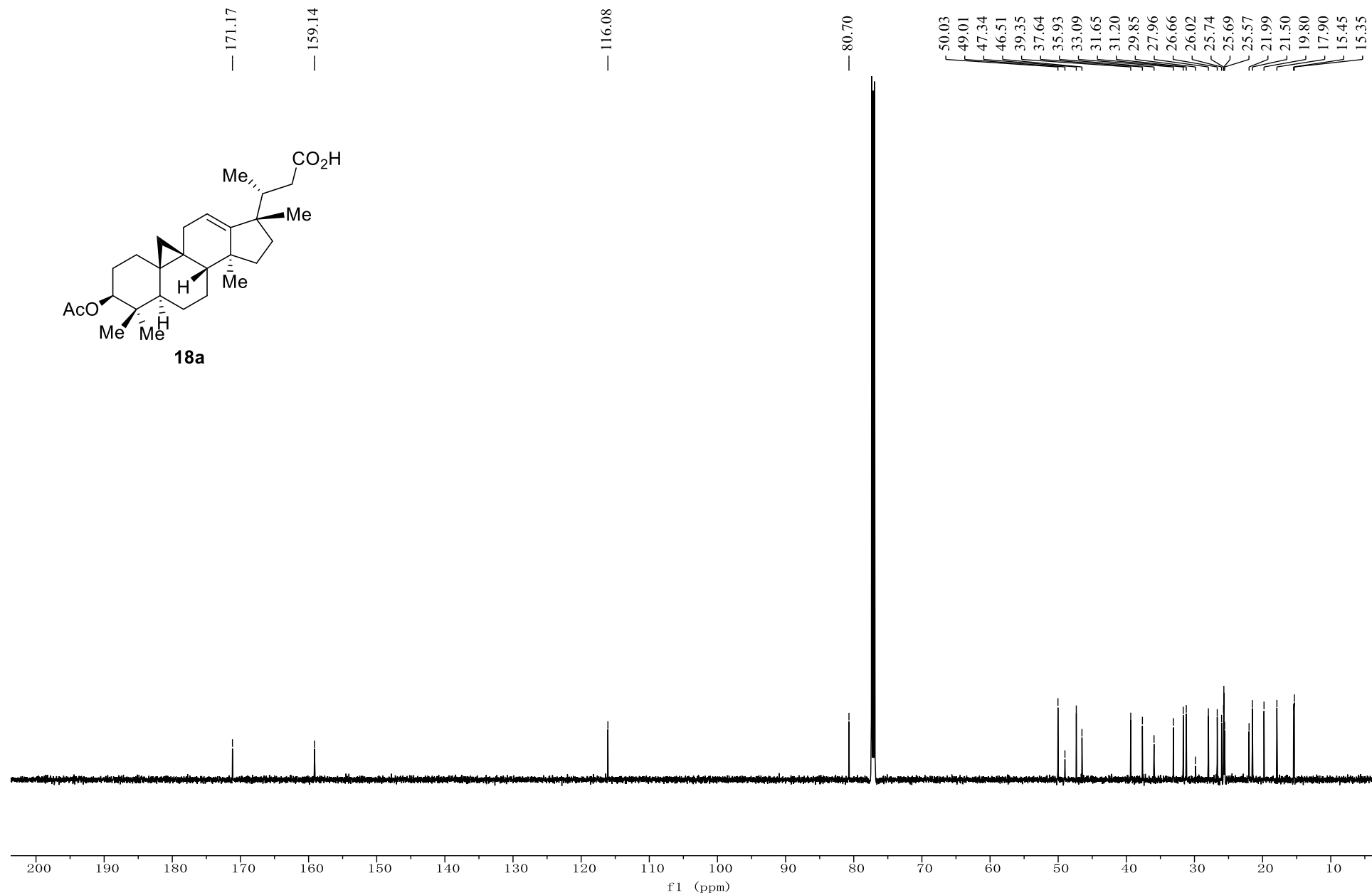
¹³C NMR Spectrum of 18 (101 MHz, CDCl₃)



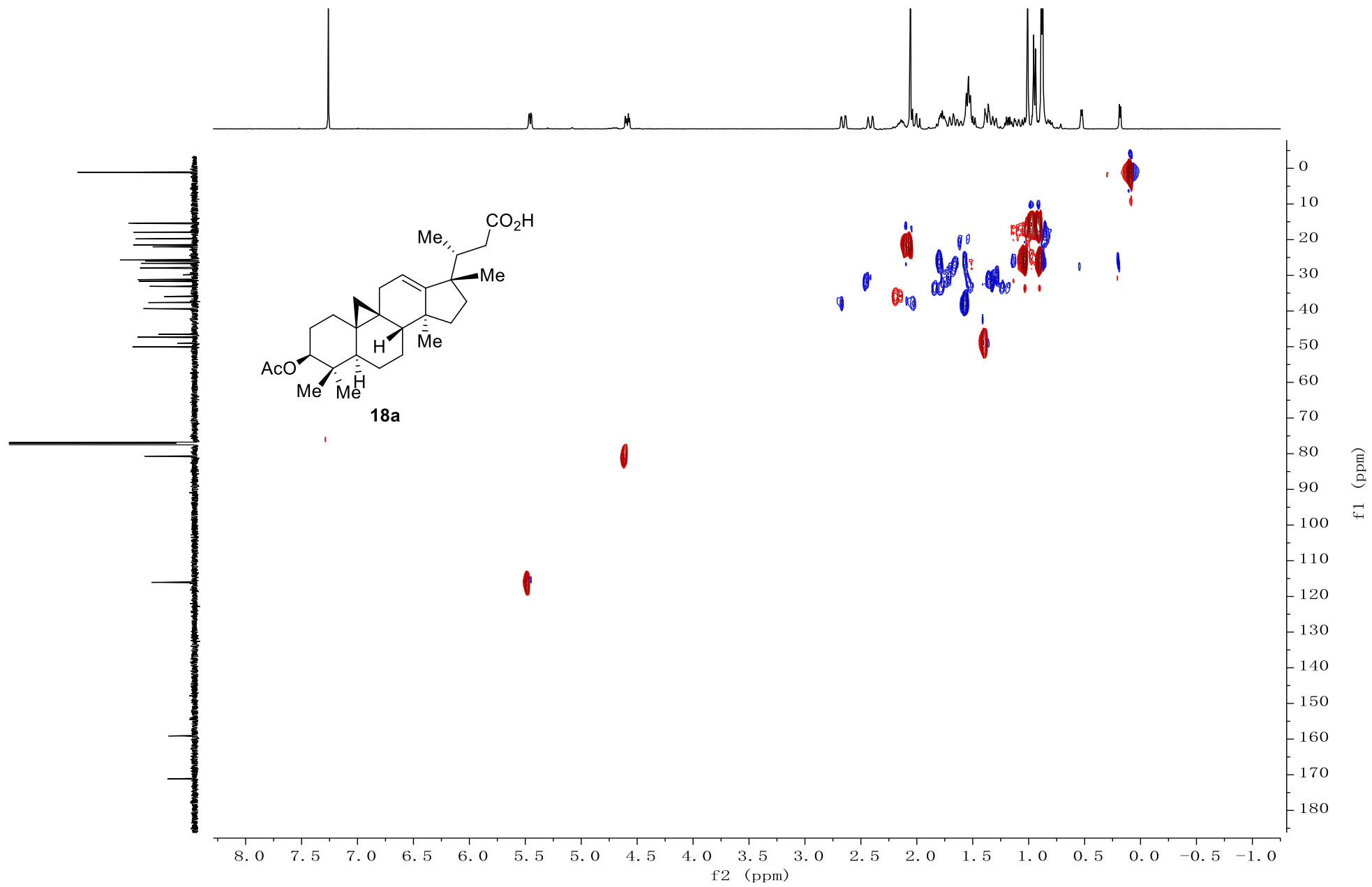
¹H NMR Spectrum of 18a (400 MHz, CDCl₃)



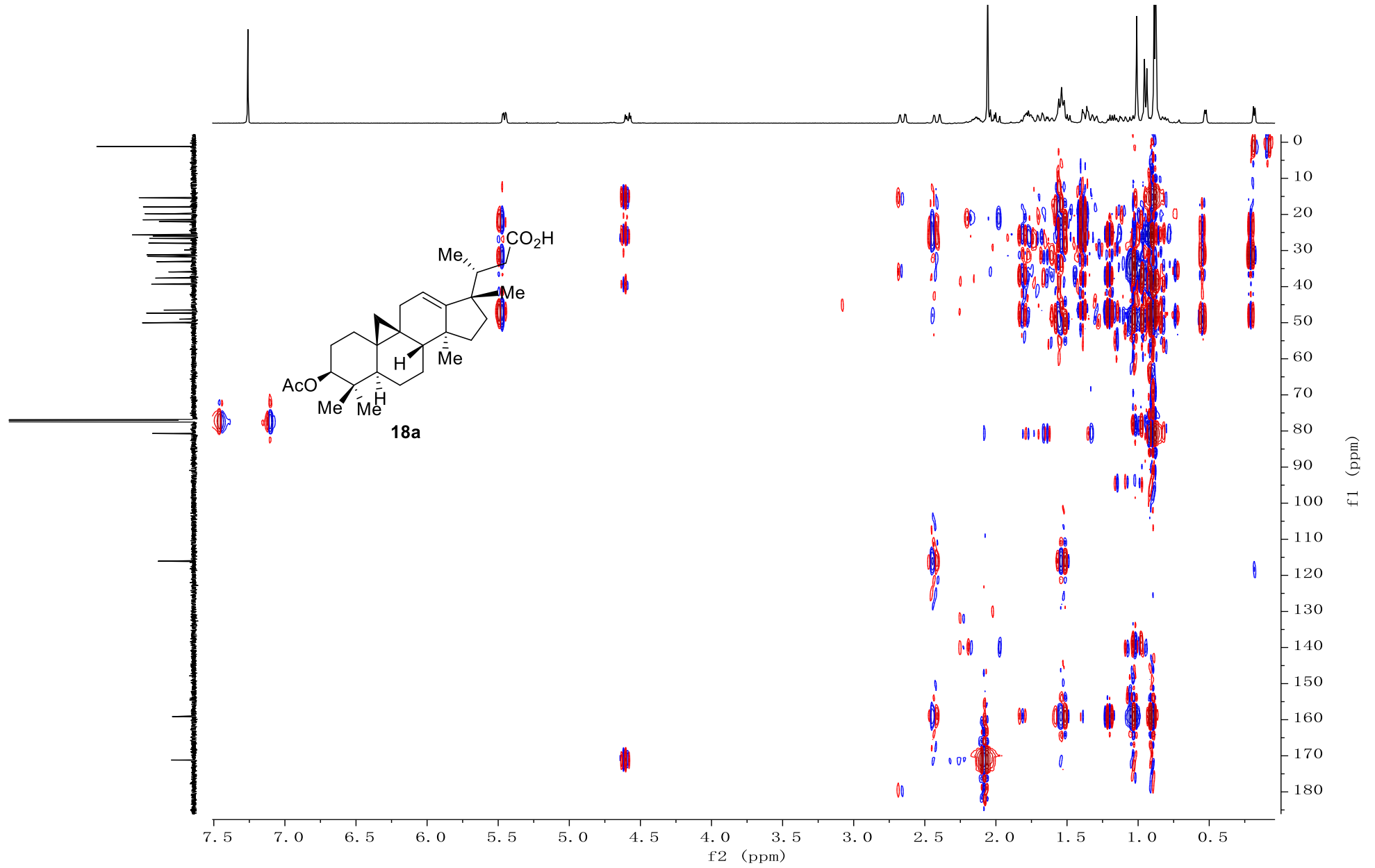
¹³C NMR Spectrum of 18a (151 MHz, CDCl₃)



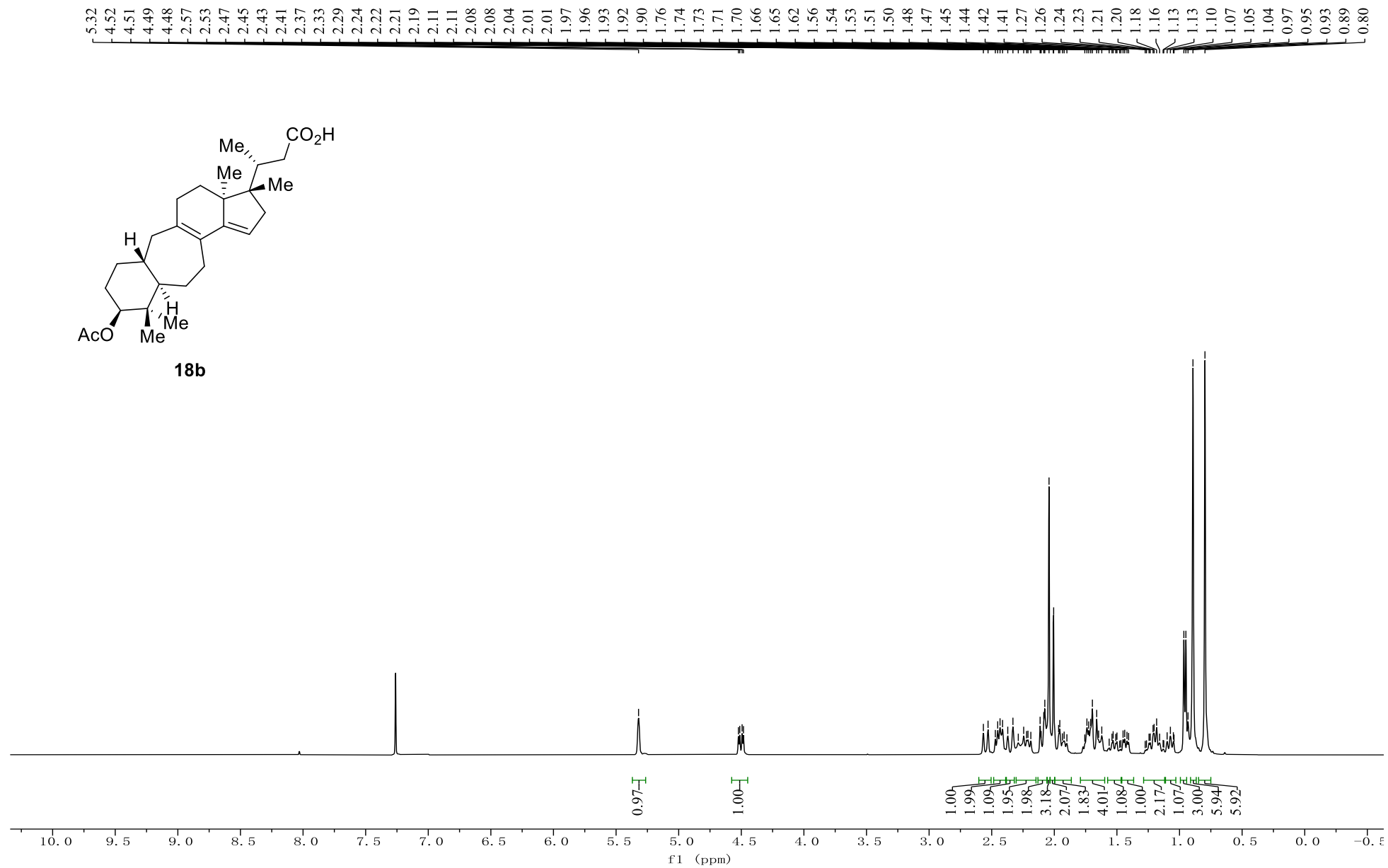
HSQC Spectrum of 18a



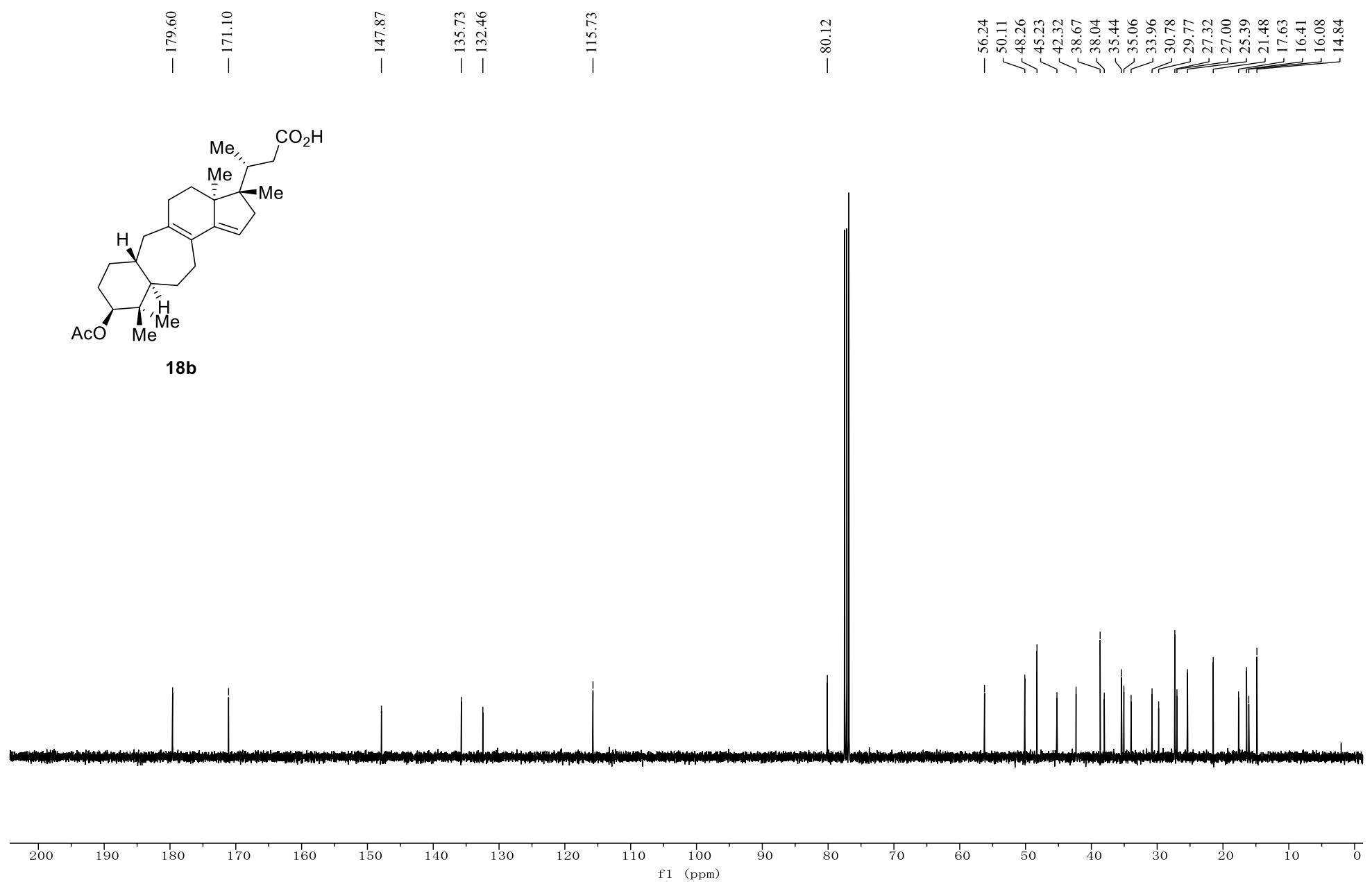
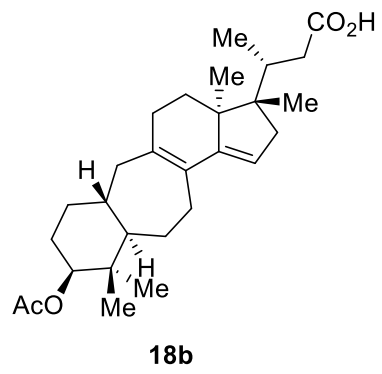
HMBC Spectrum of 18a



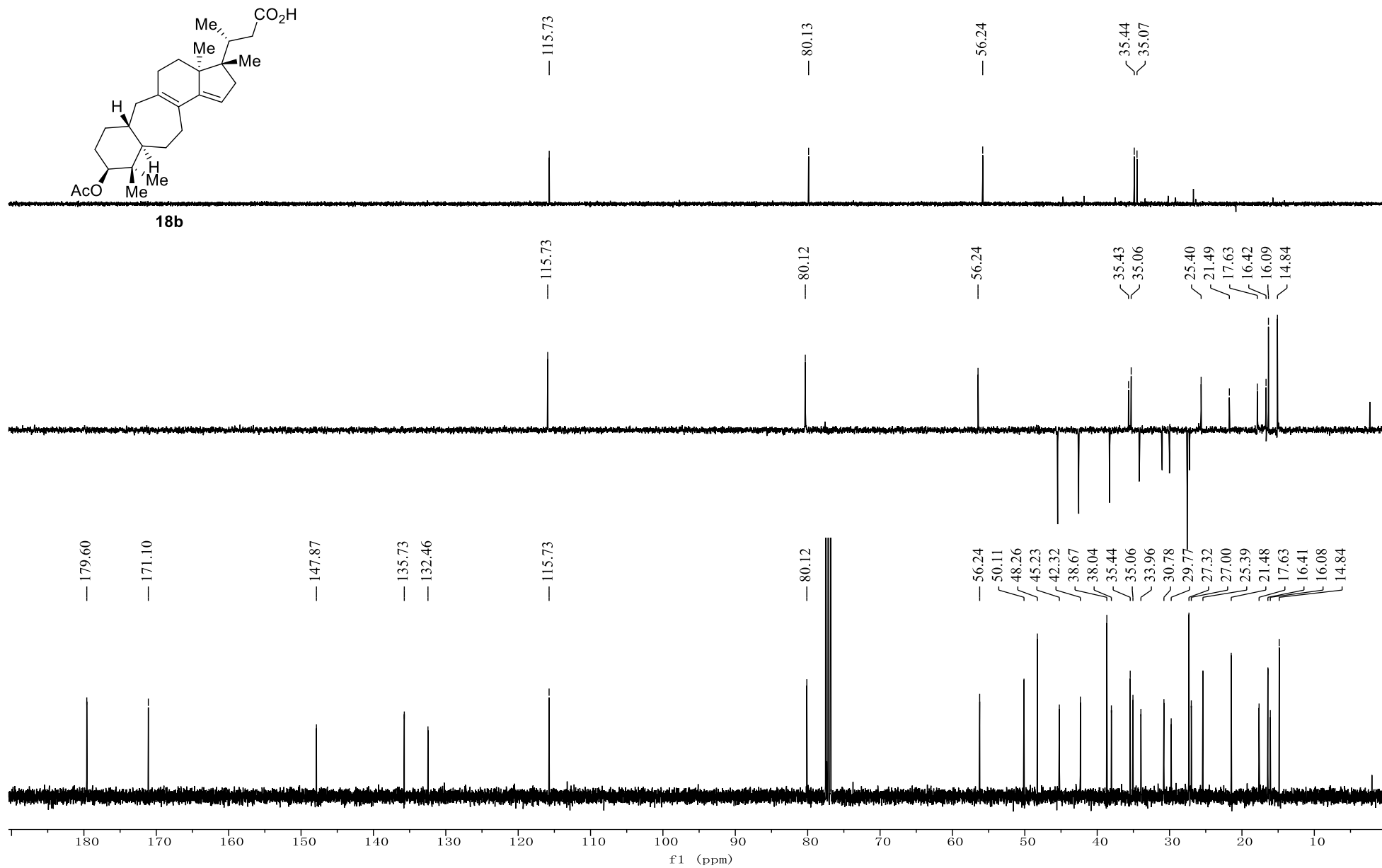
¹H NMR Spectrum of 18b (400 MHz, CDCl₃)



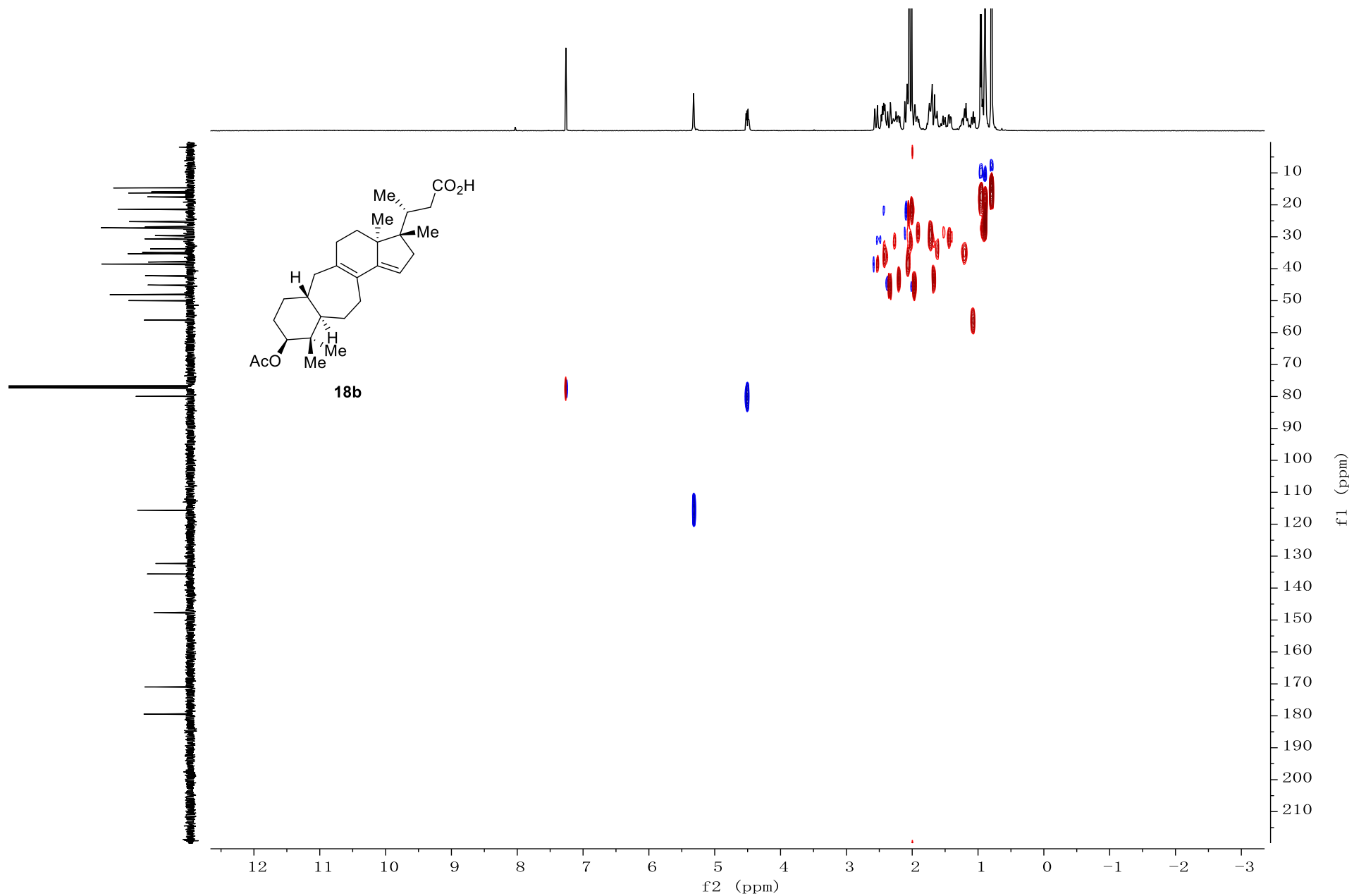
¹³C NMR Spectrum of 18b (151 MHz, CDCl₃)



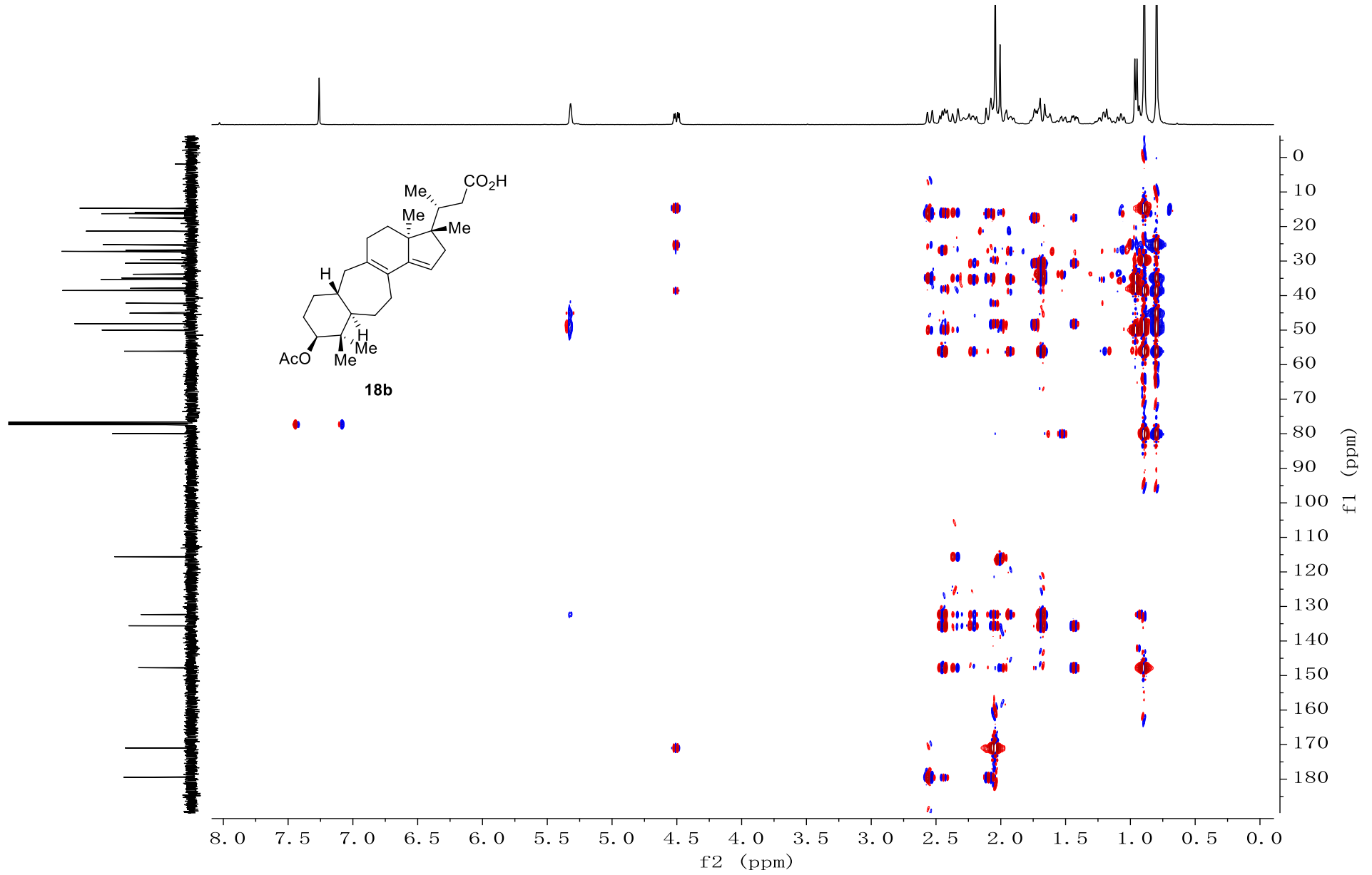
DEPT and ¹³C NMR Spectrum of 18b (151 MHz, CDCl₃)



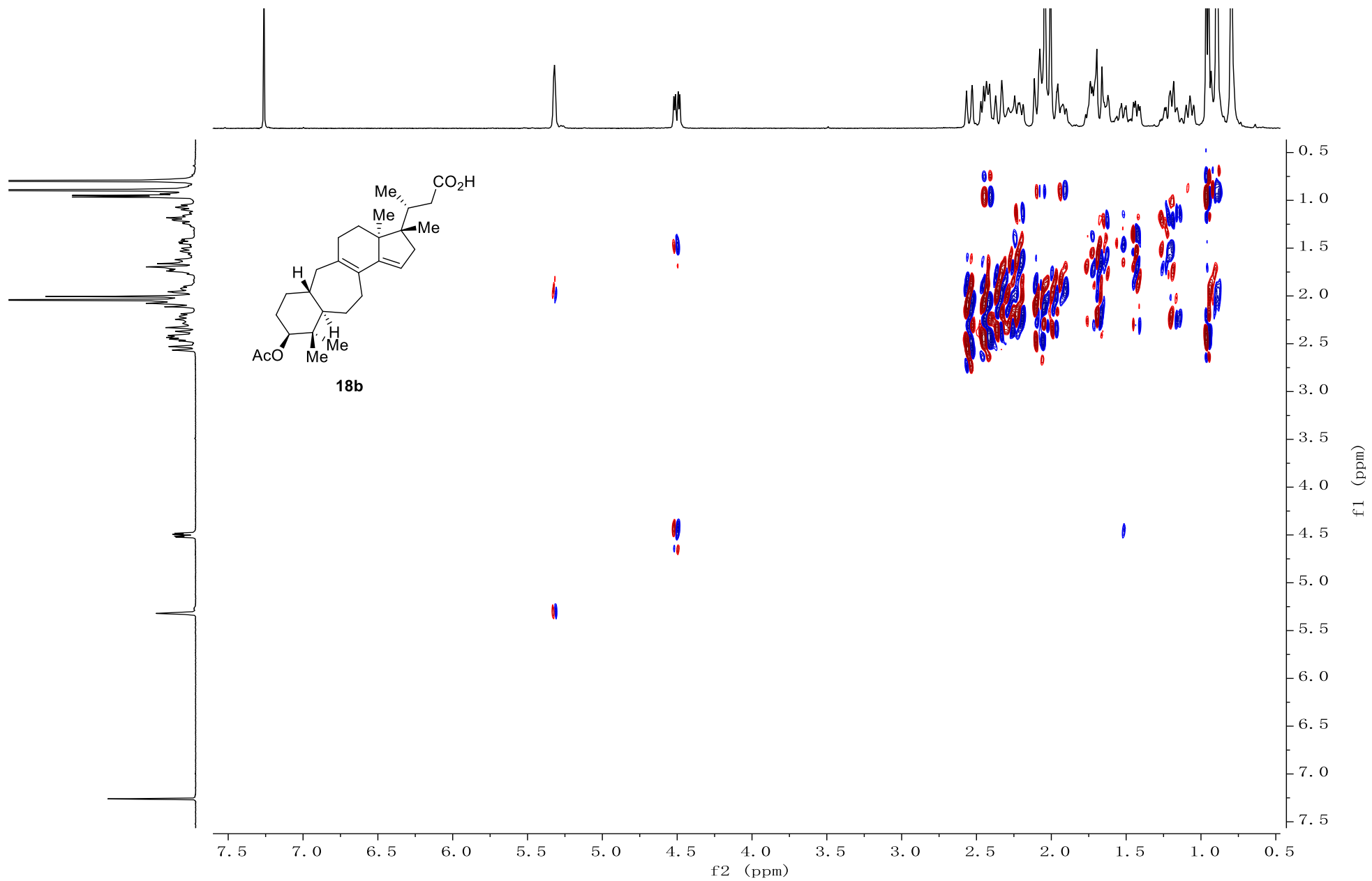
HSQC Spectrum of 18b



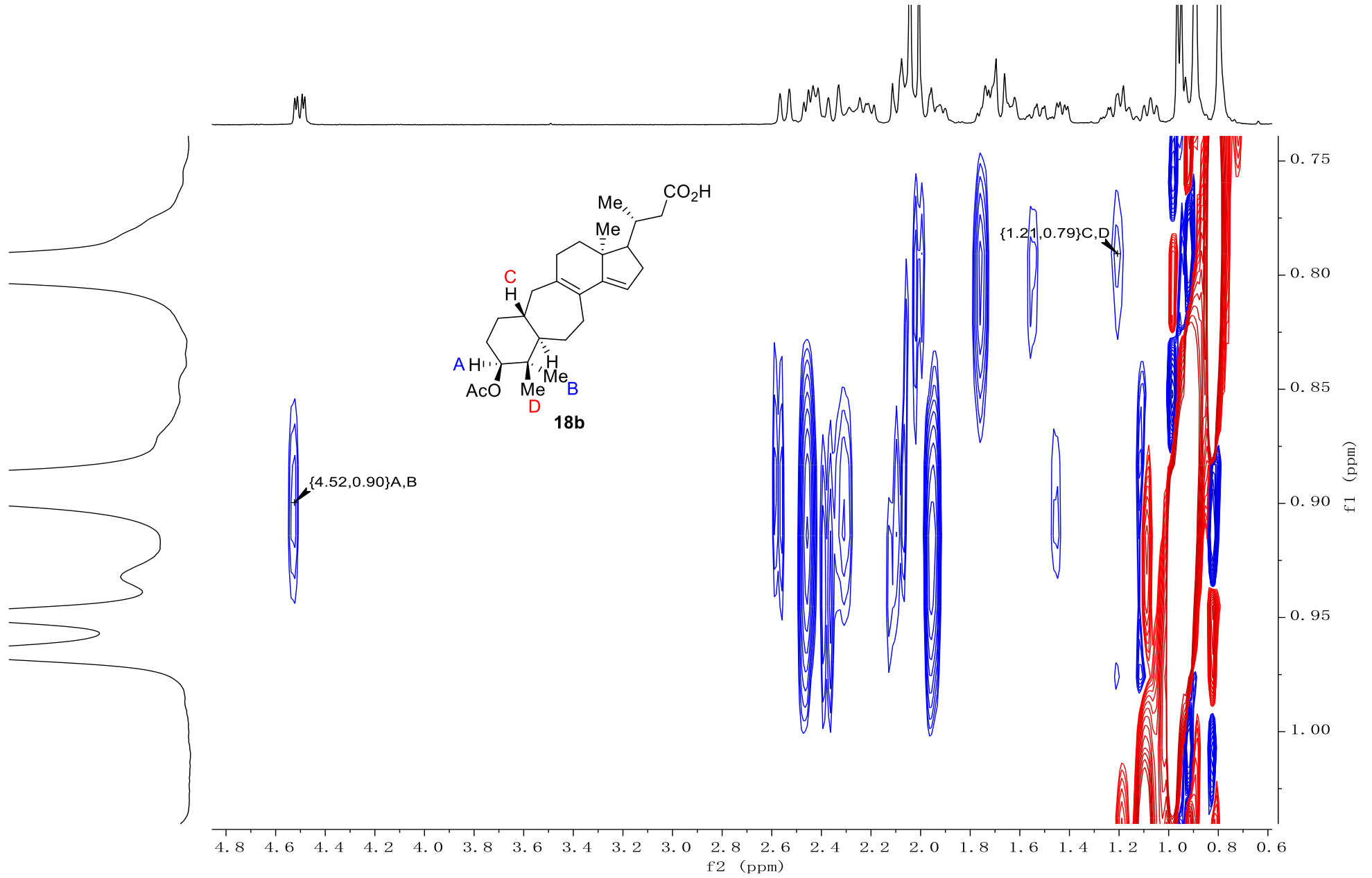
HMBC Spectrum of 18b



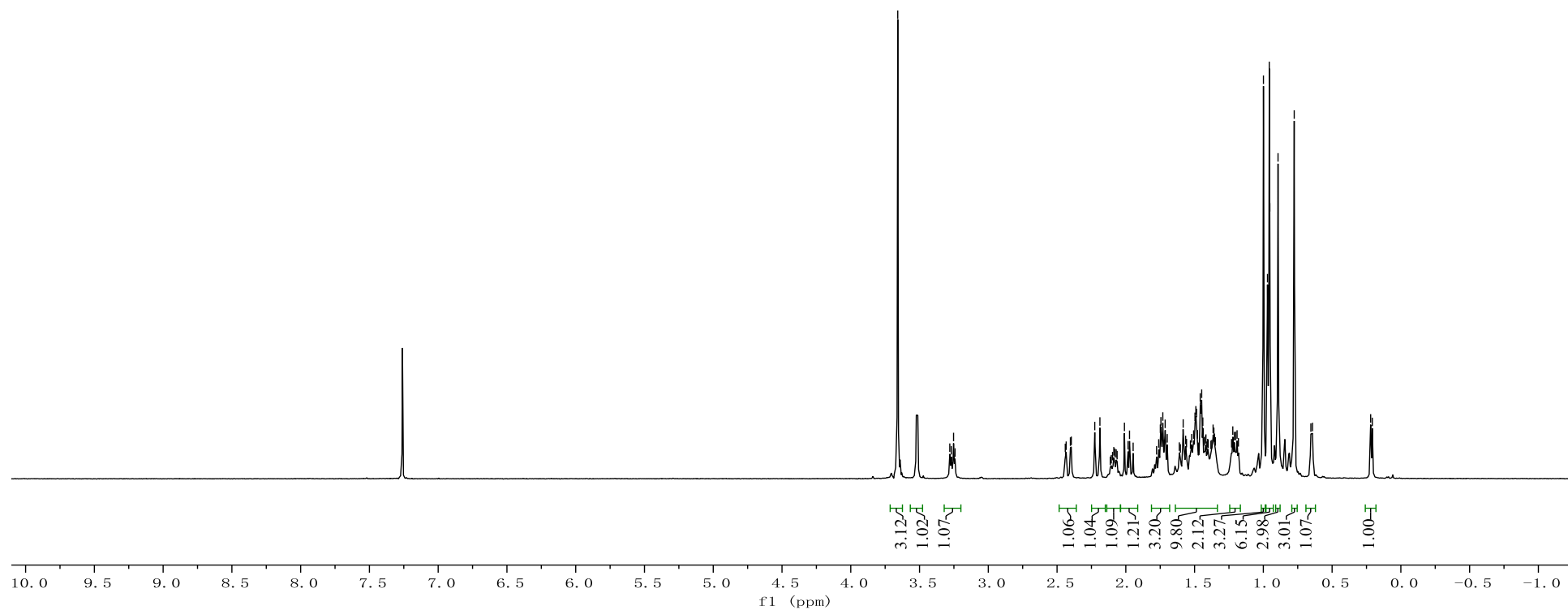
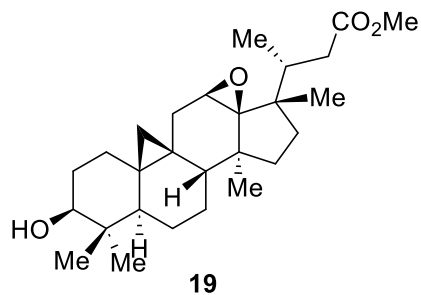
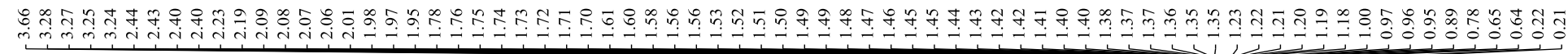
^1H - ^1H COSY Spectrum of 18b



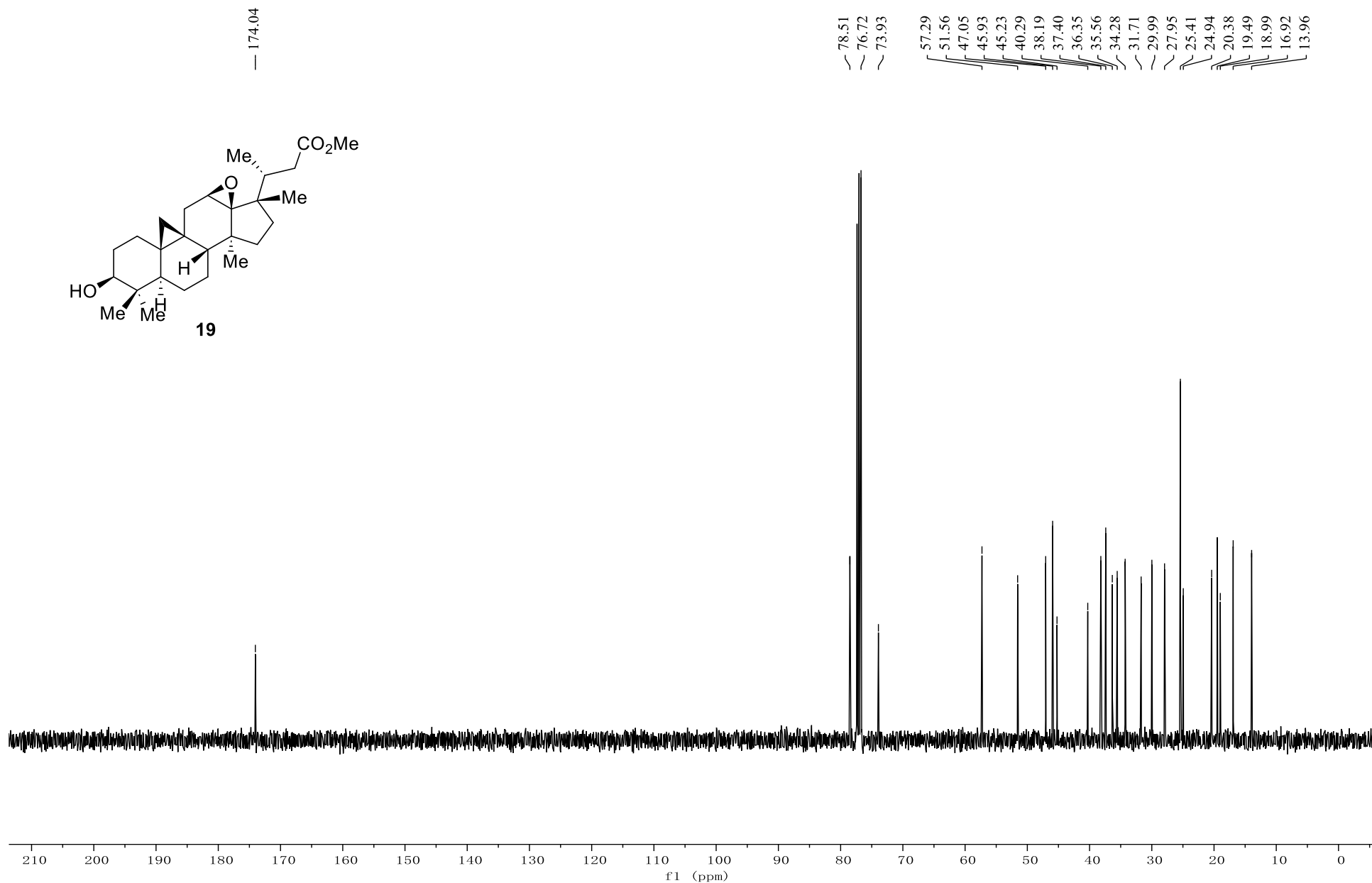
NOESY Spectrum of 18b



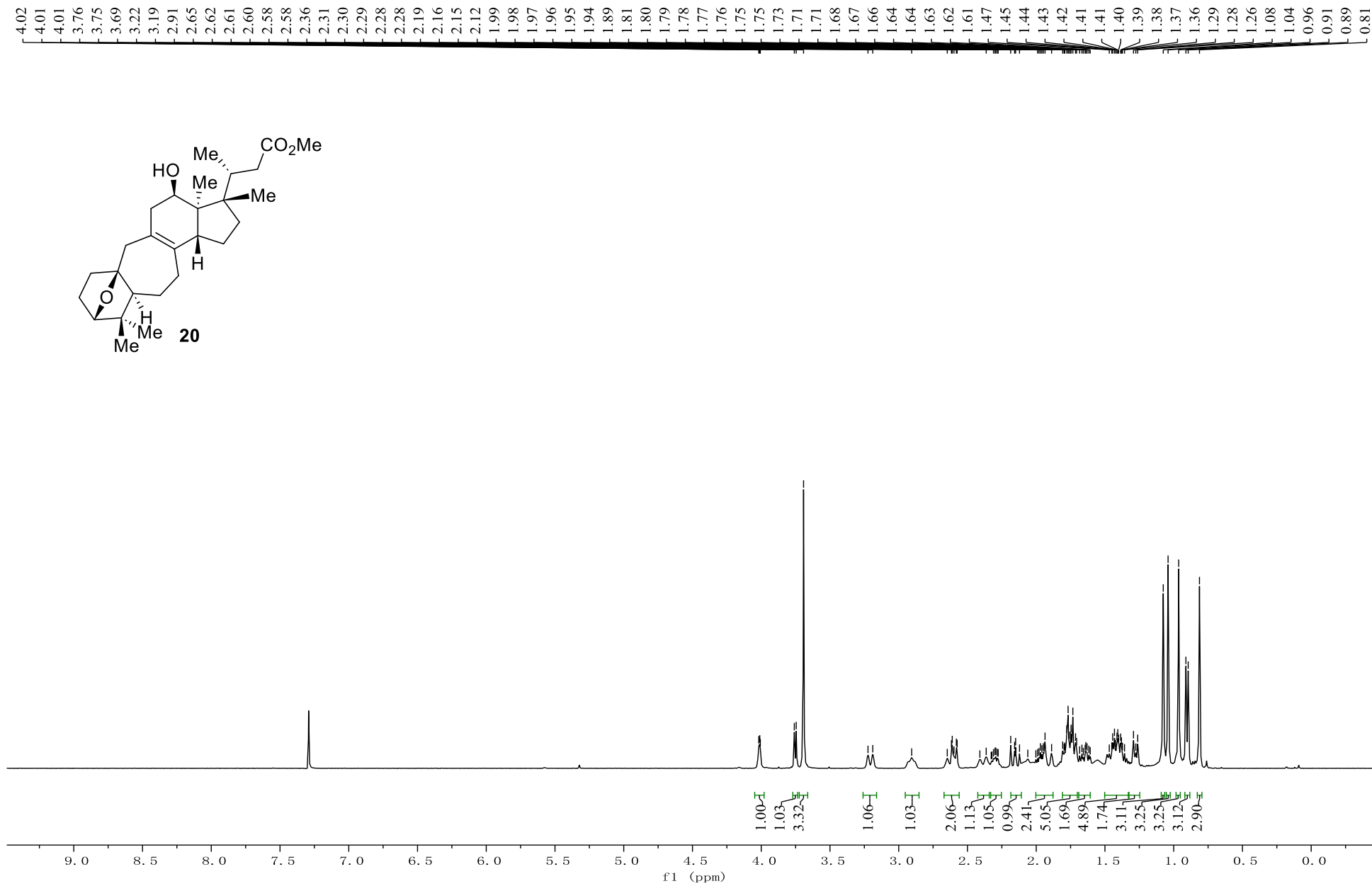
¹H NMR Spectrum of 19 (400 MHz, CDCl₃)



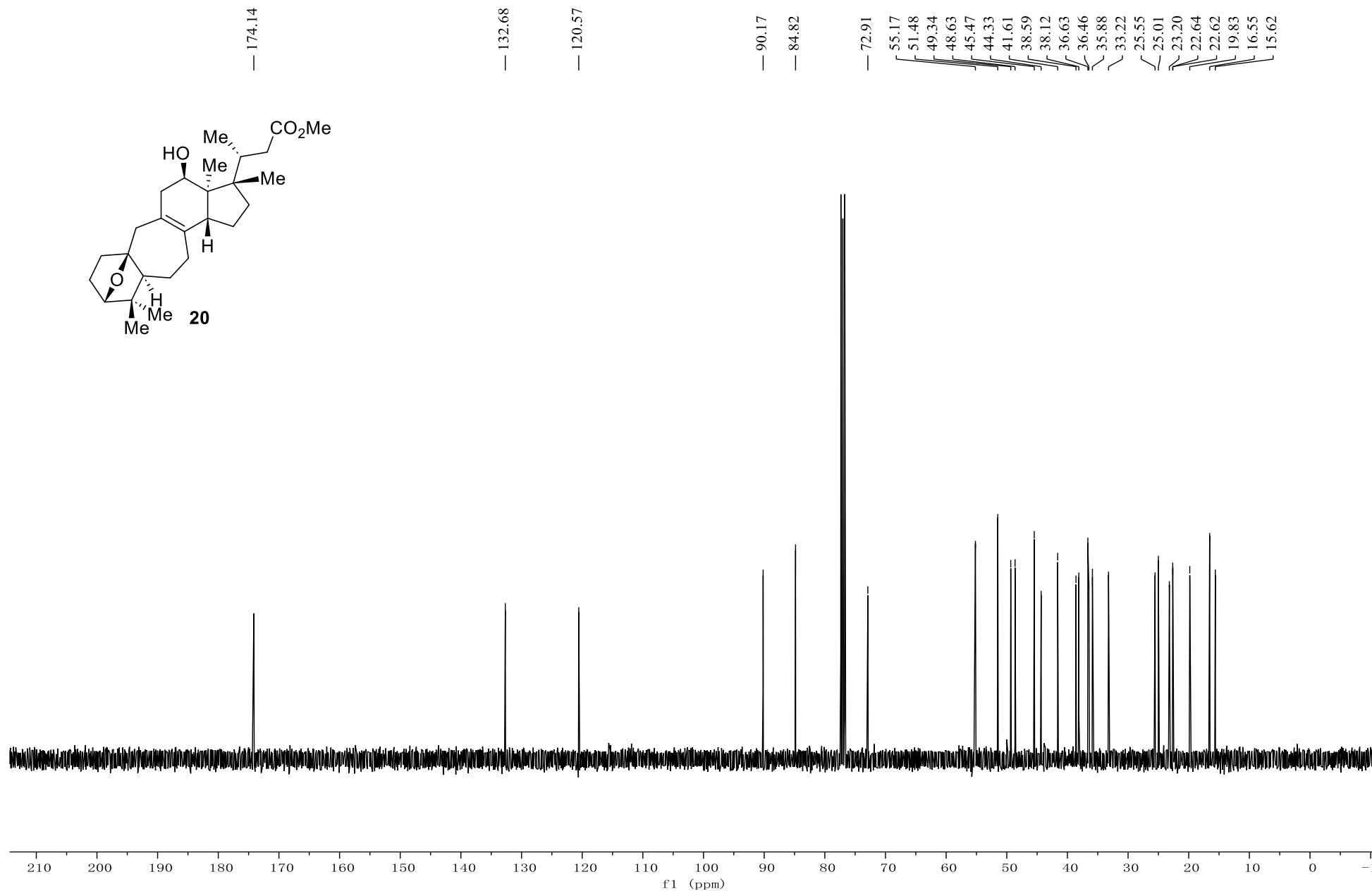
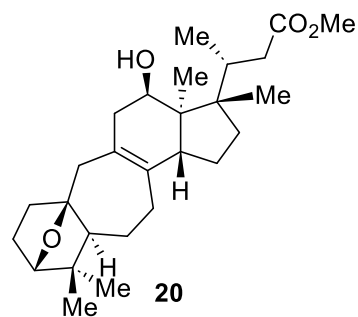
¹³C NMR Spectrum of 19 (101 MHz, CDCl₃)



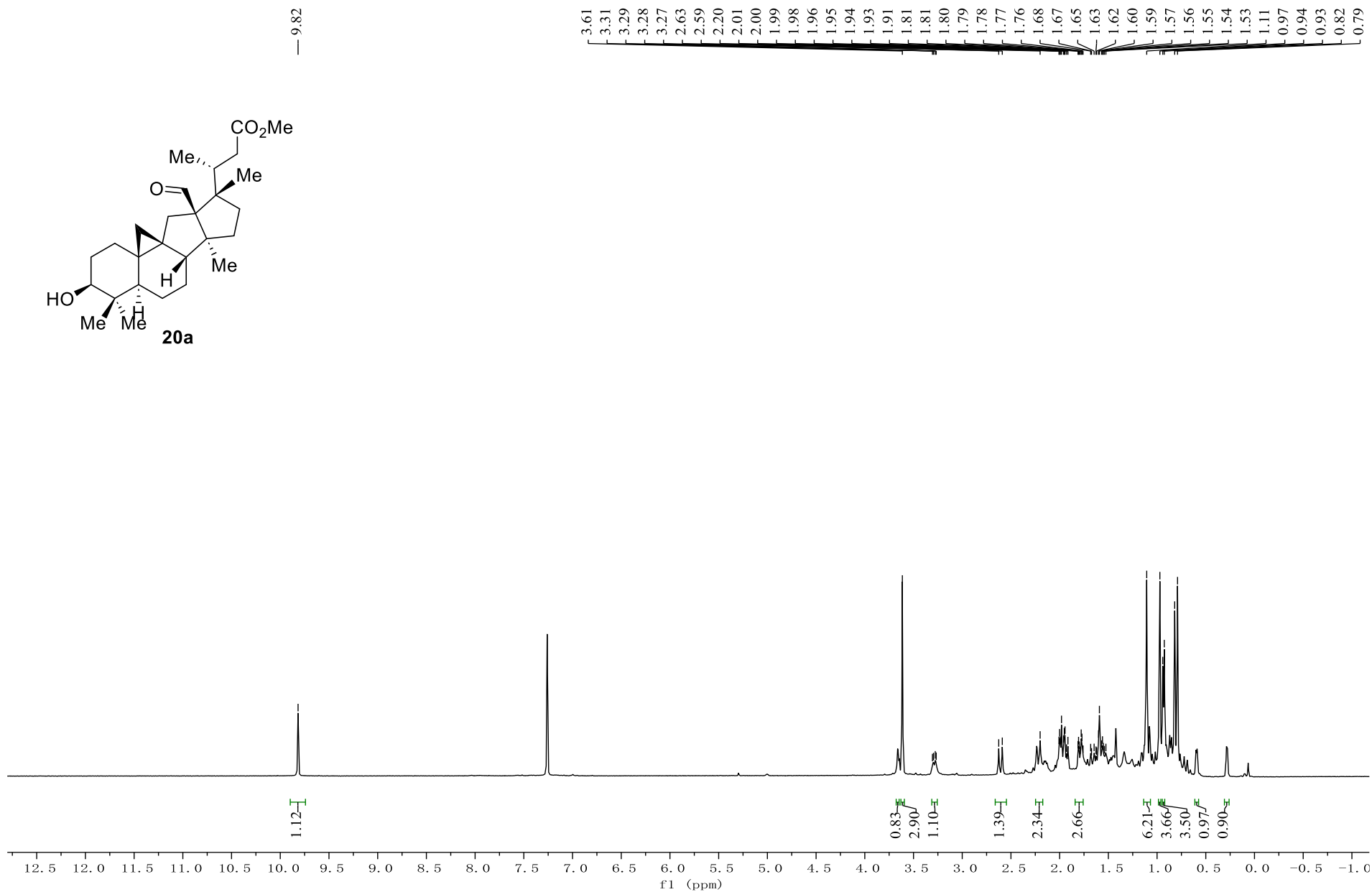
¹H NMR Spectrum of 20 (400 MHz, CDCl₃)



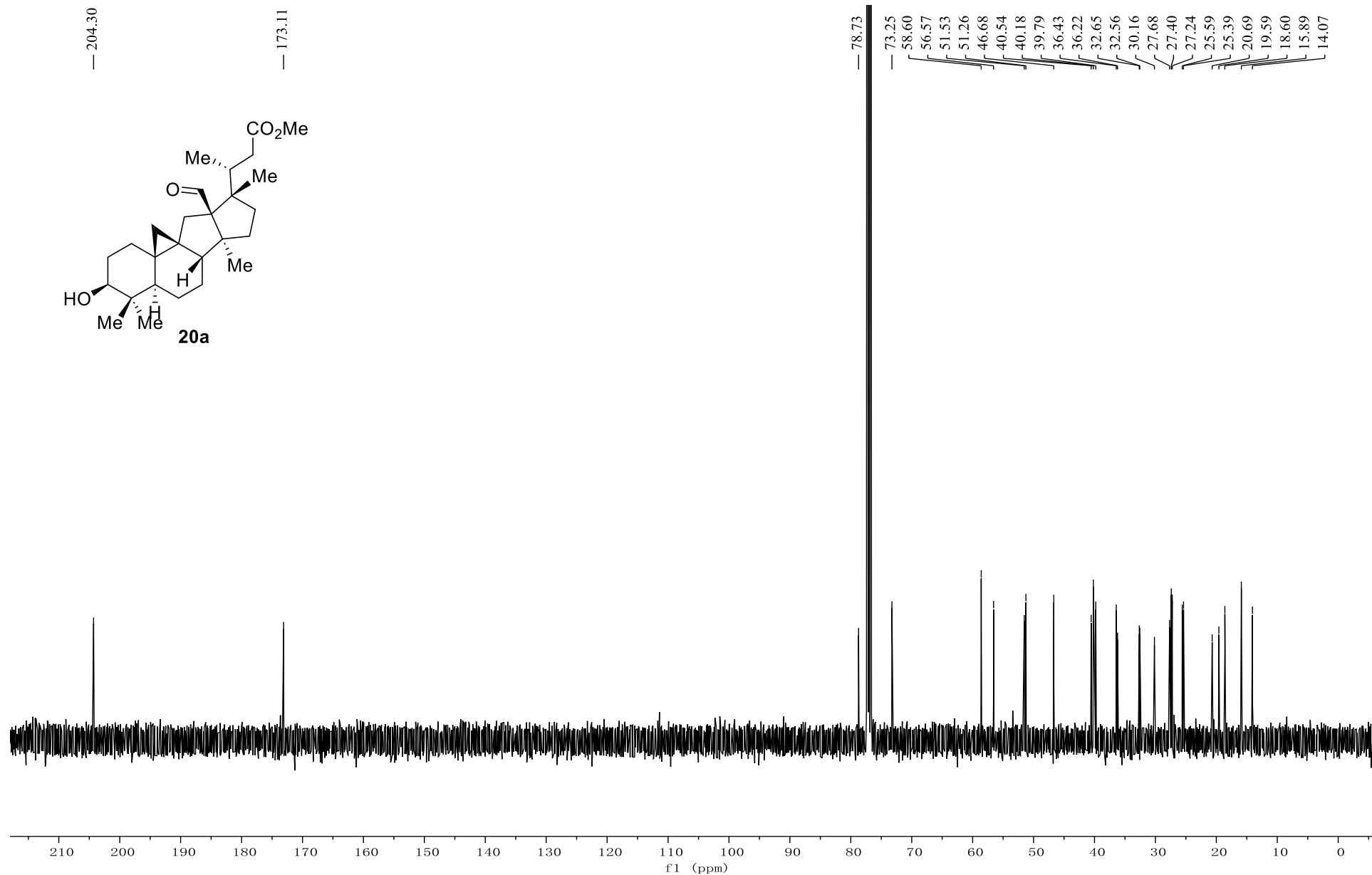
¹³C NMR Spectrum of 20 (101 MHz, CDCl₃)



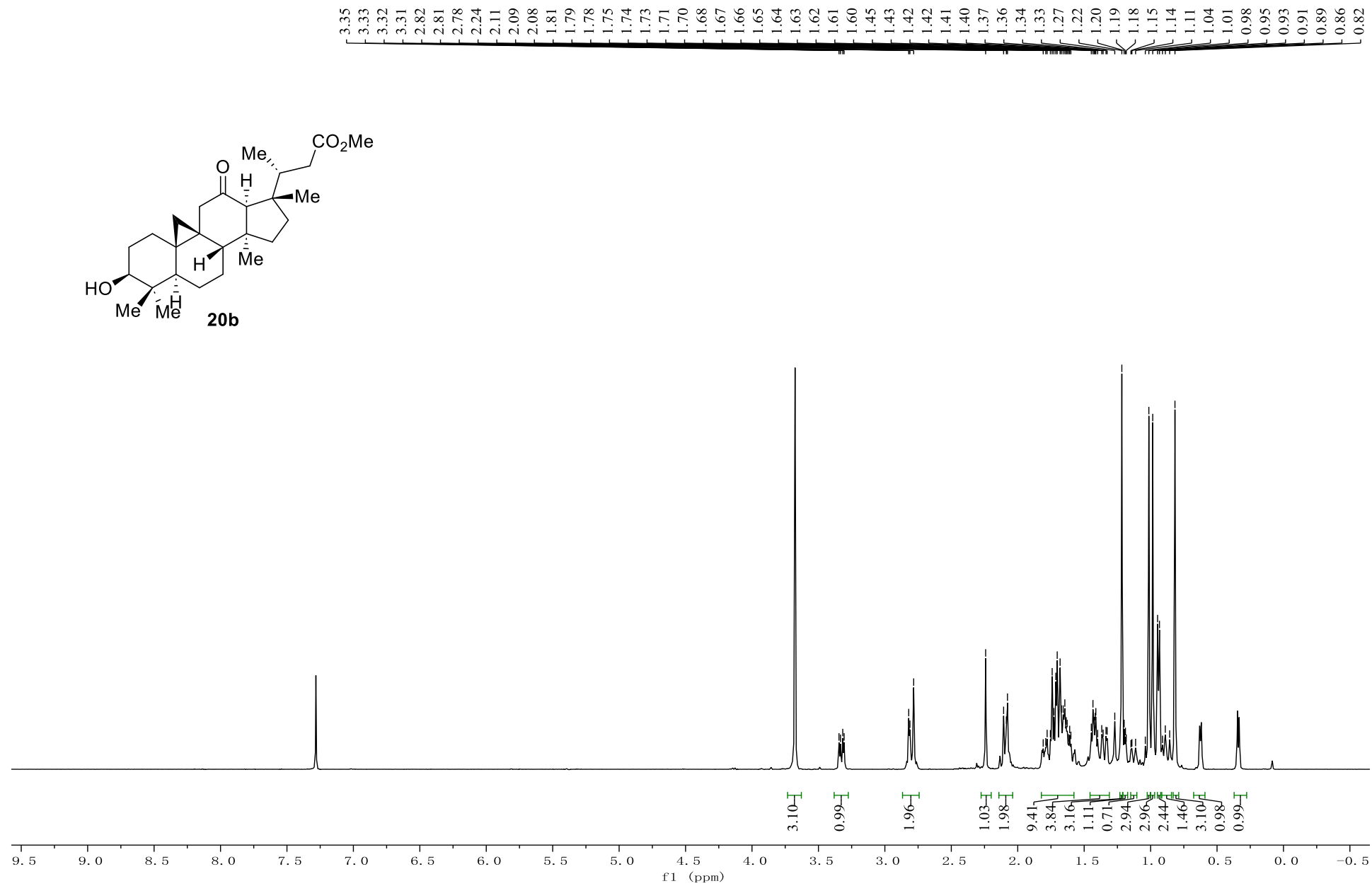
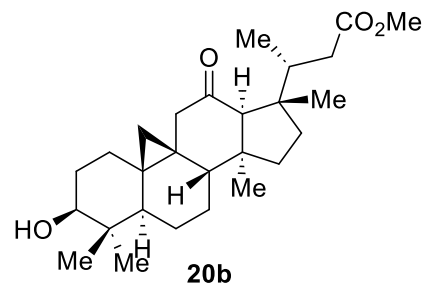
¹H NMR Spectrum of 20a (400 MHz, CDCl₃)



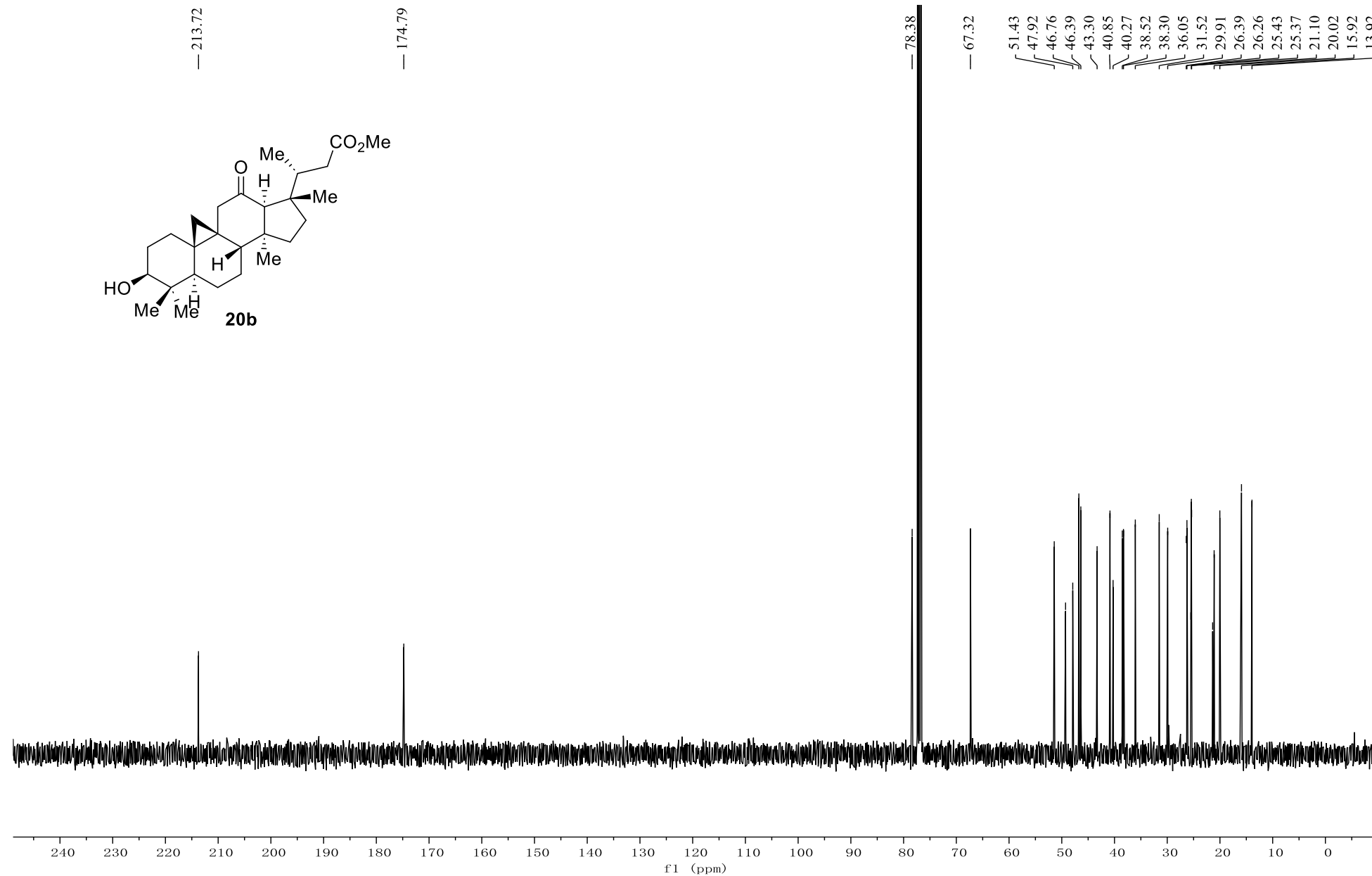
¹³C NMR Spectrum of 20a (101 MHz, CDCl₃)



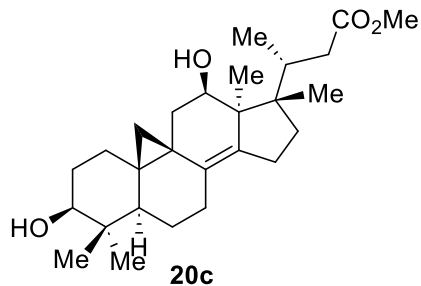
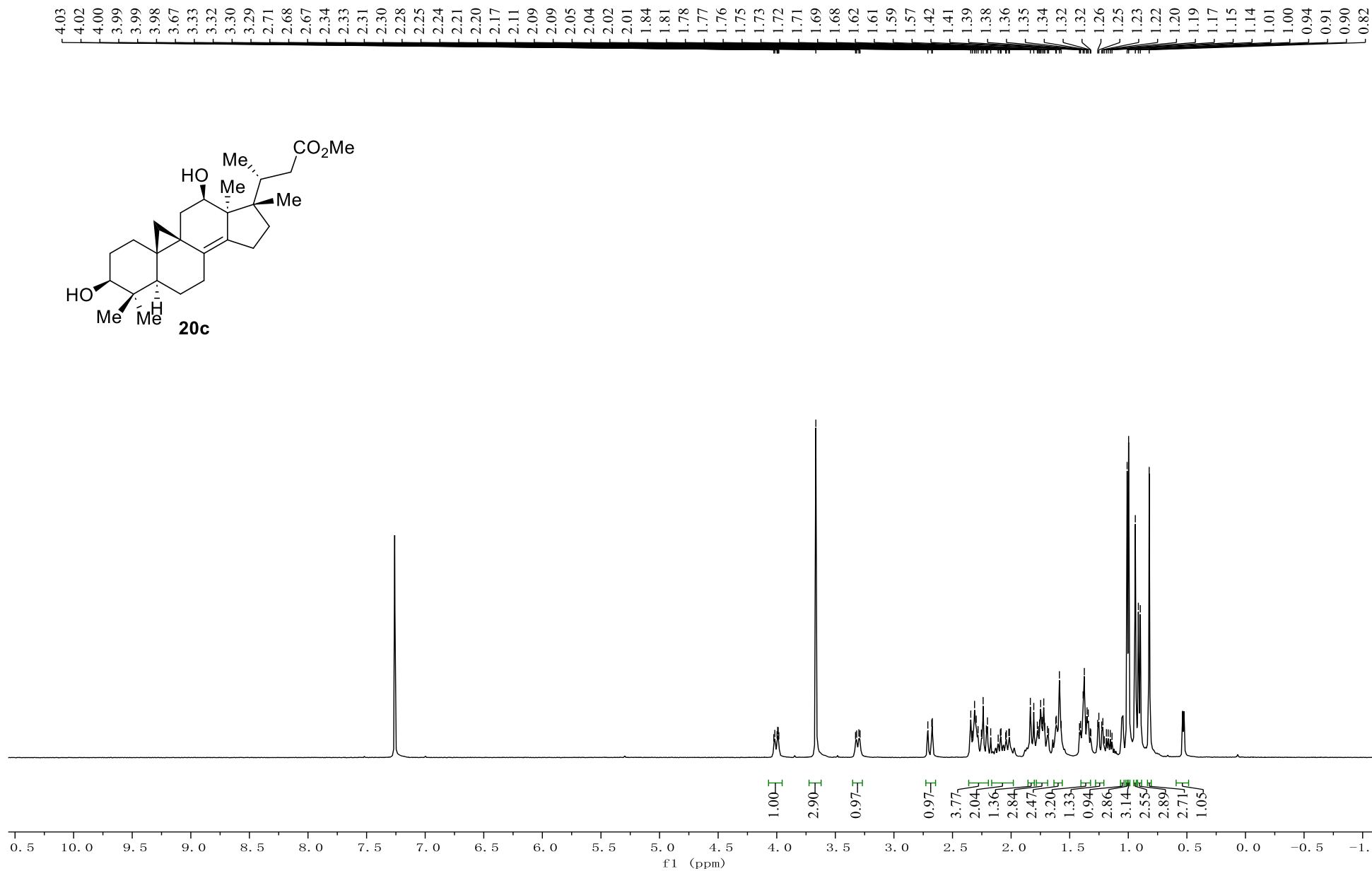
¹H NMR Spectrum of 20b (400 MHz, CDCl₃)



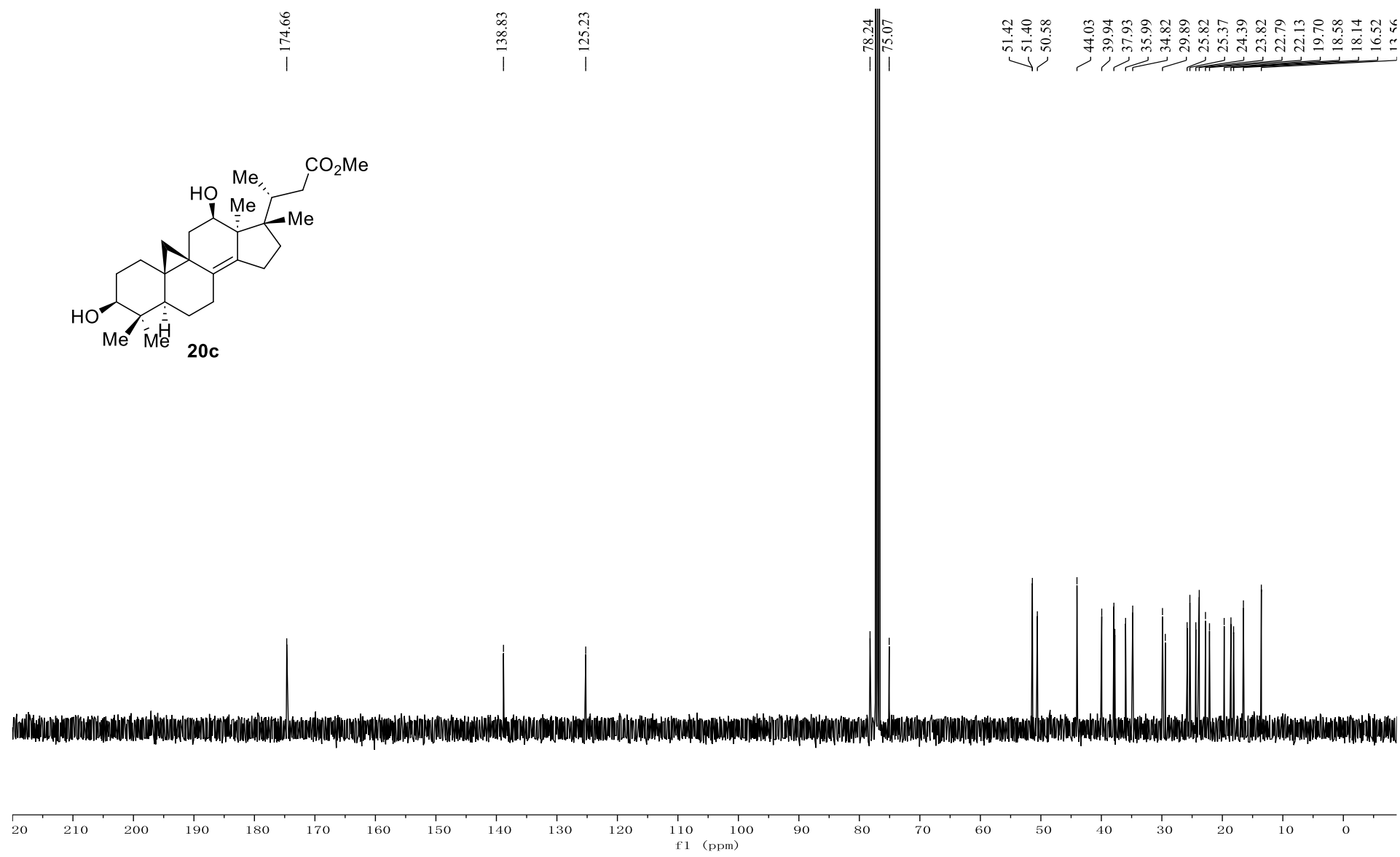
¹³C NMR Spectrum of 20b (101 MHz, CDCl₃)



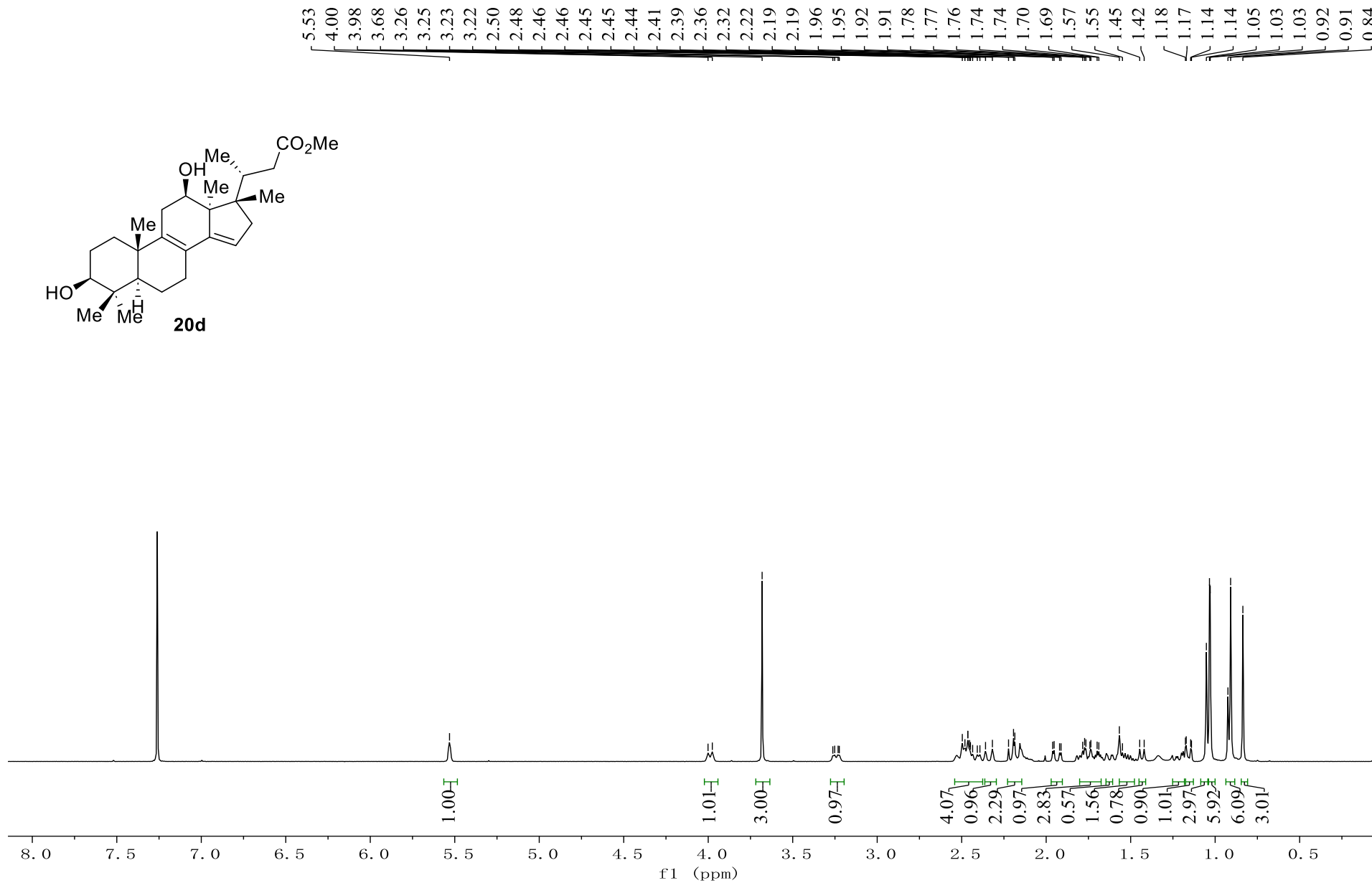
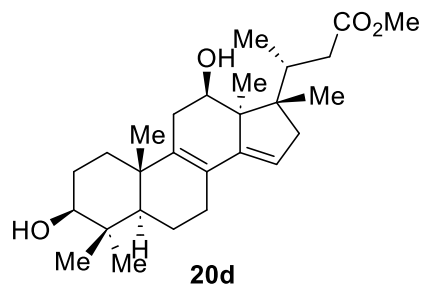
¹H NMR Spectrum of 20c (400 MHz, CDCl₃)



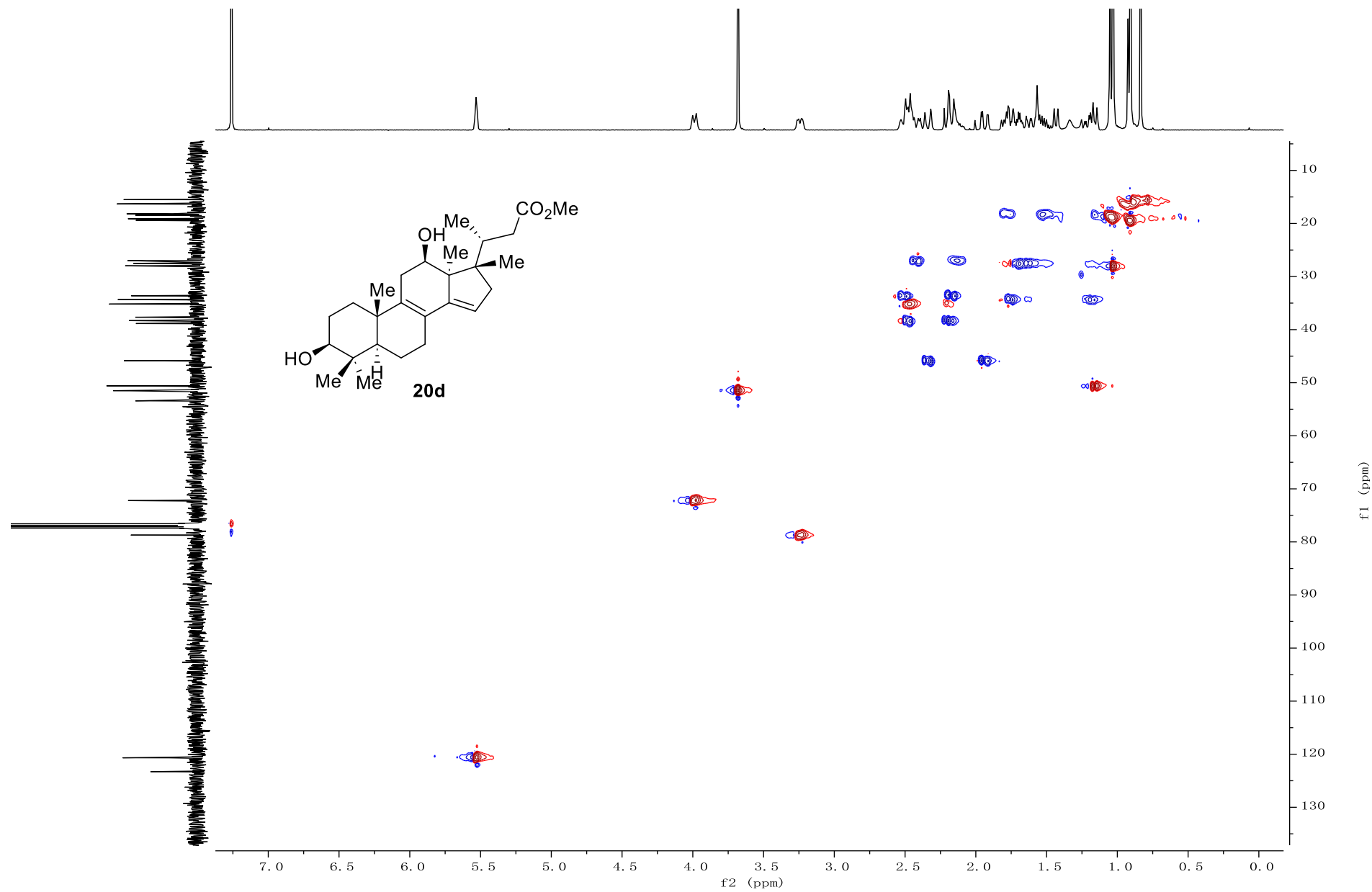
¹³C NMR Spectrum of 20c (101 MHz, CDCl₃)



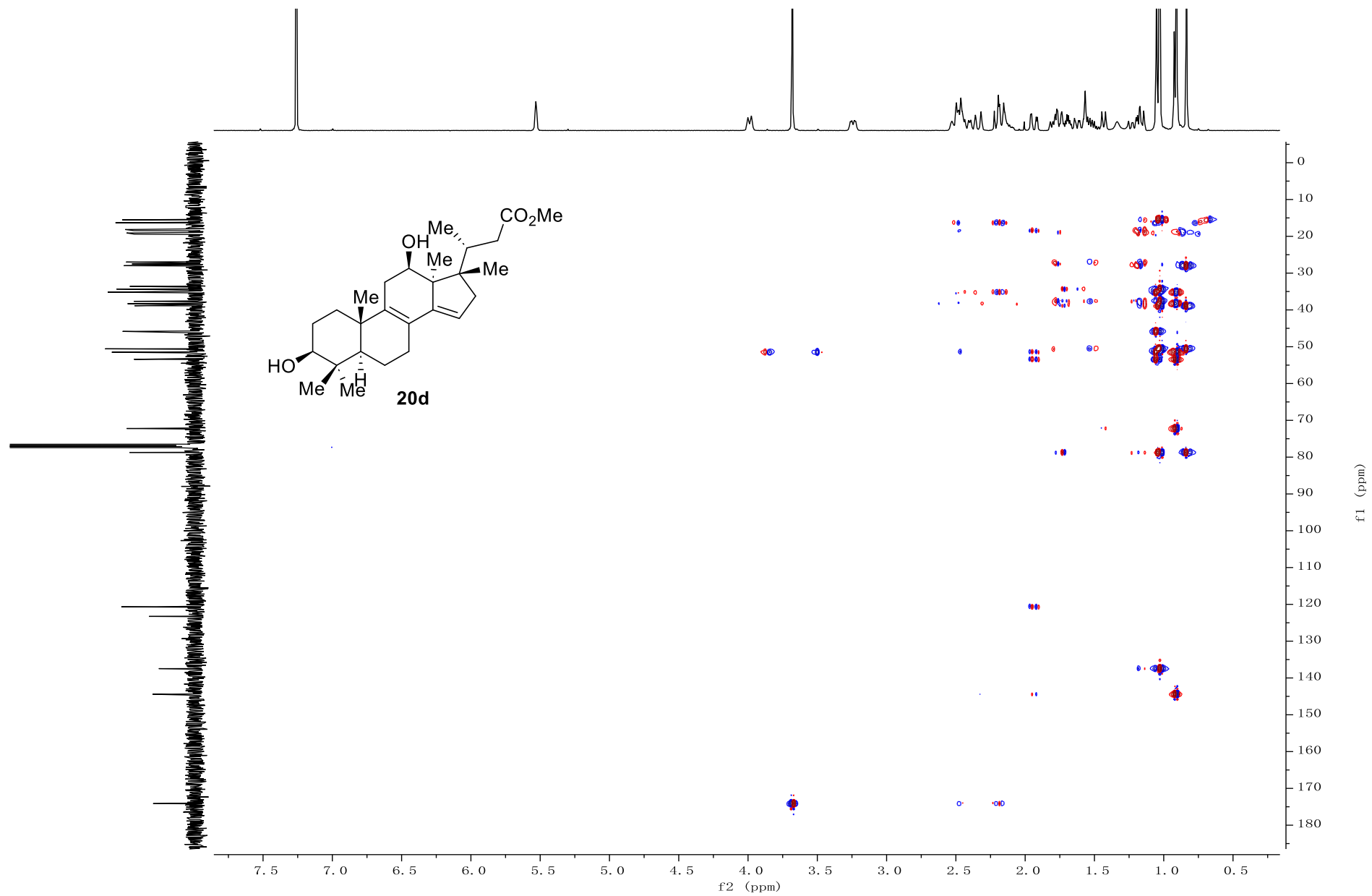
¹H NMR Spectrum of 20d (400 MHz, CDCl₃)



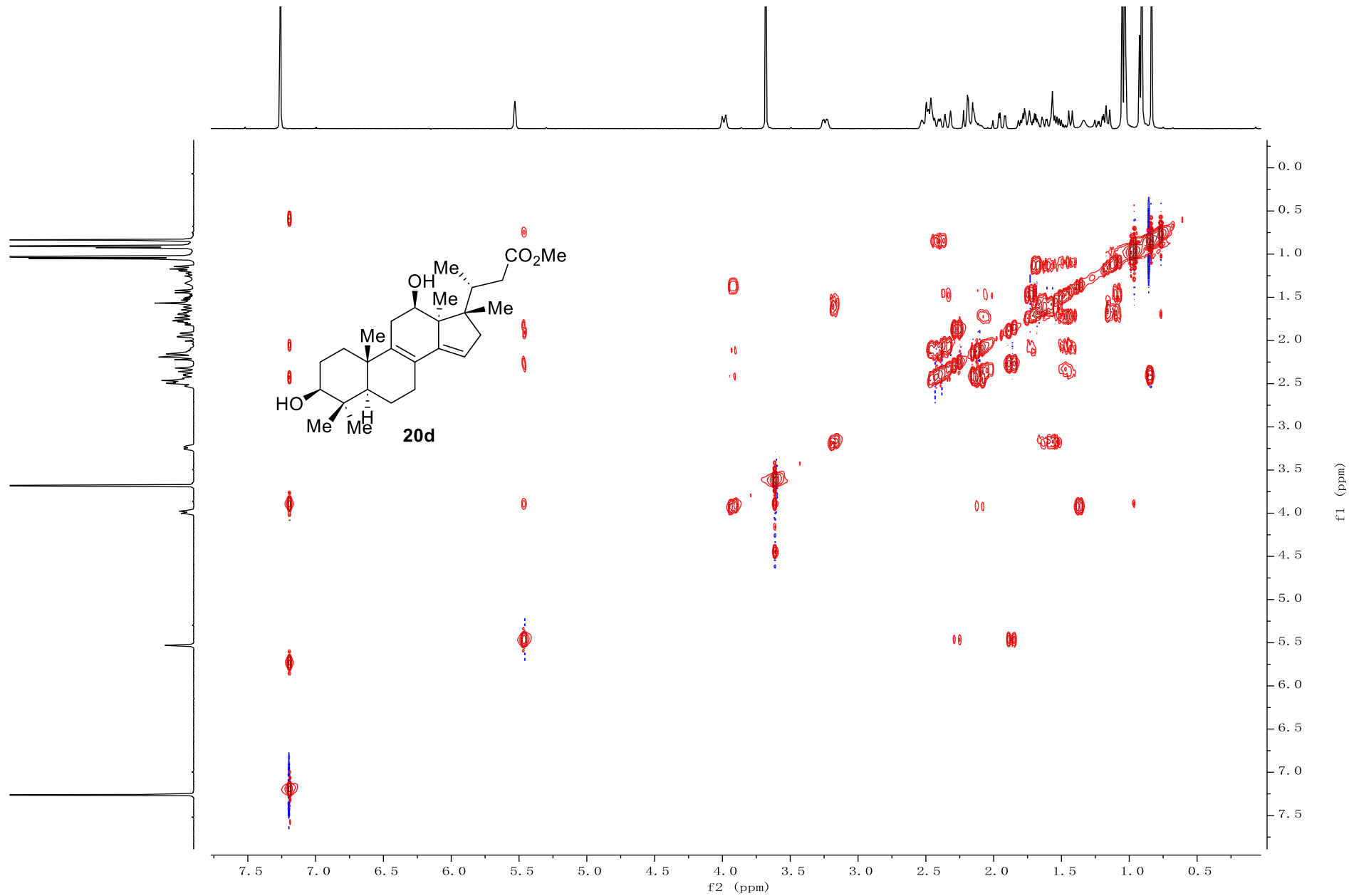
HSQC Spectrum of 20d



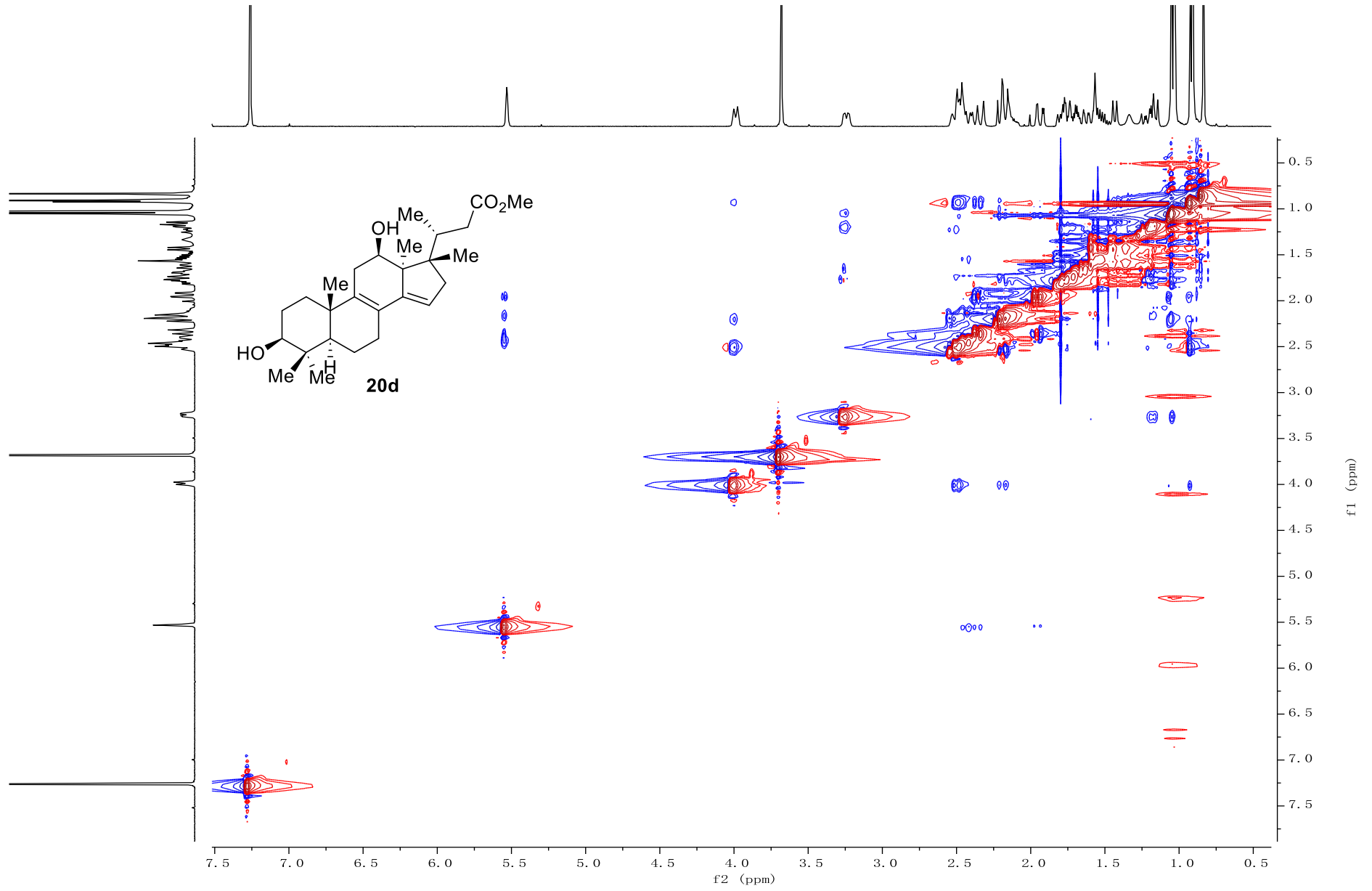
HMBC Spectrum of 20d



^1H - ^1H COSY Spectrum of 20d

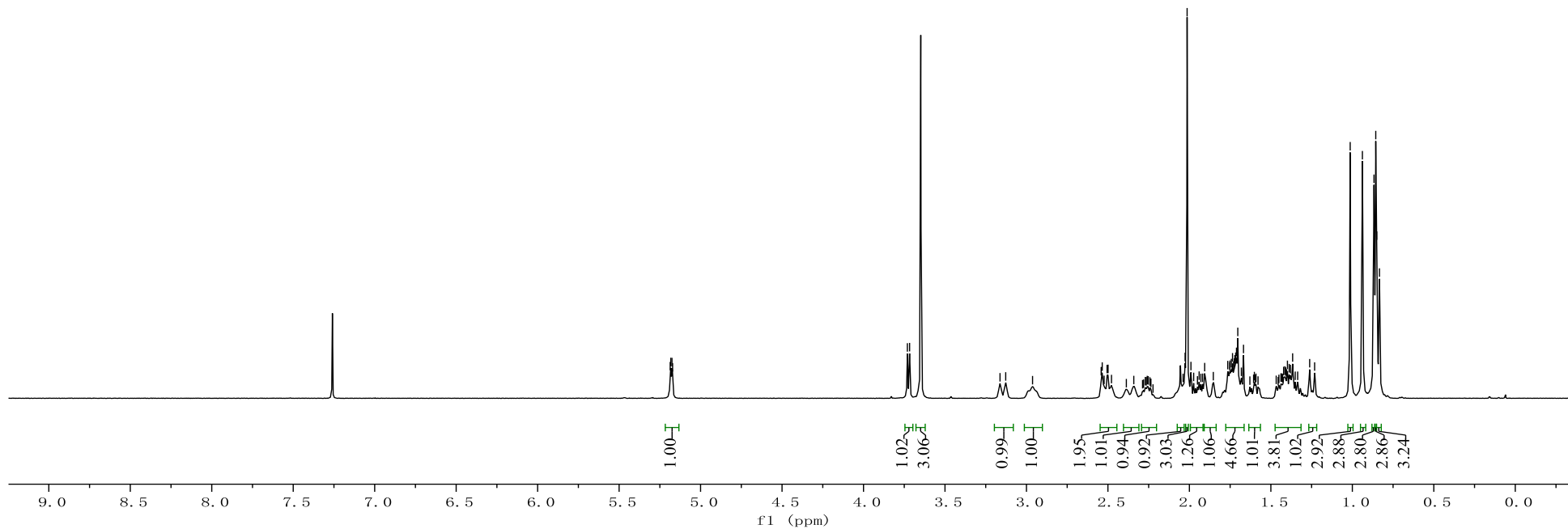
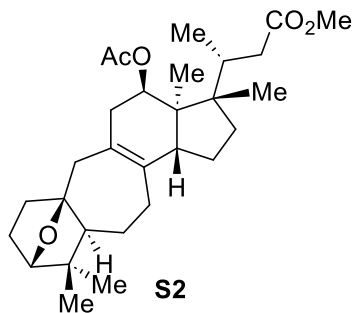


NOESY Spectrum of 20d

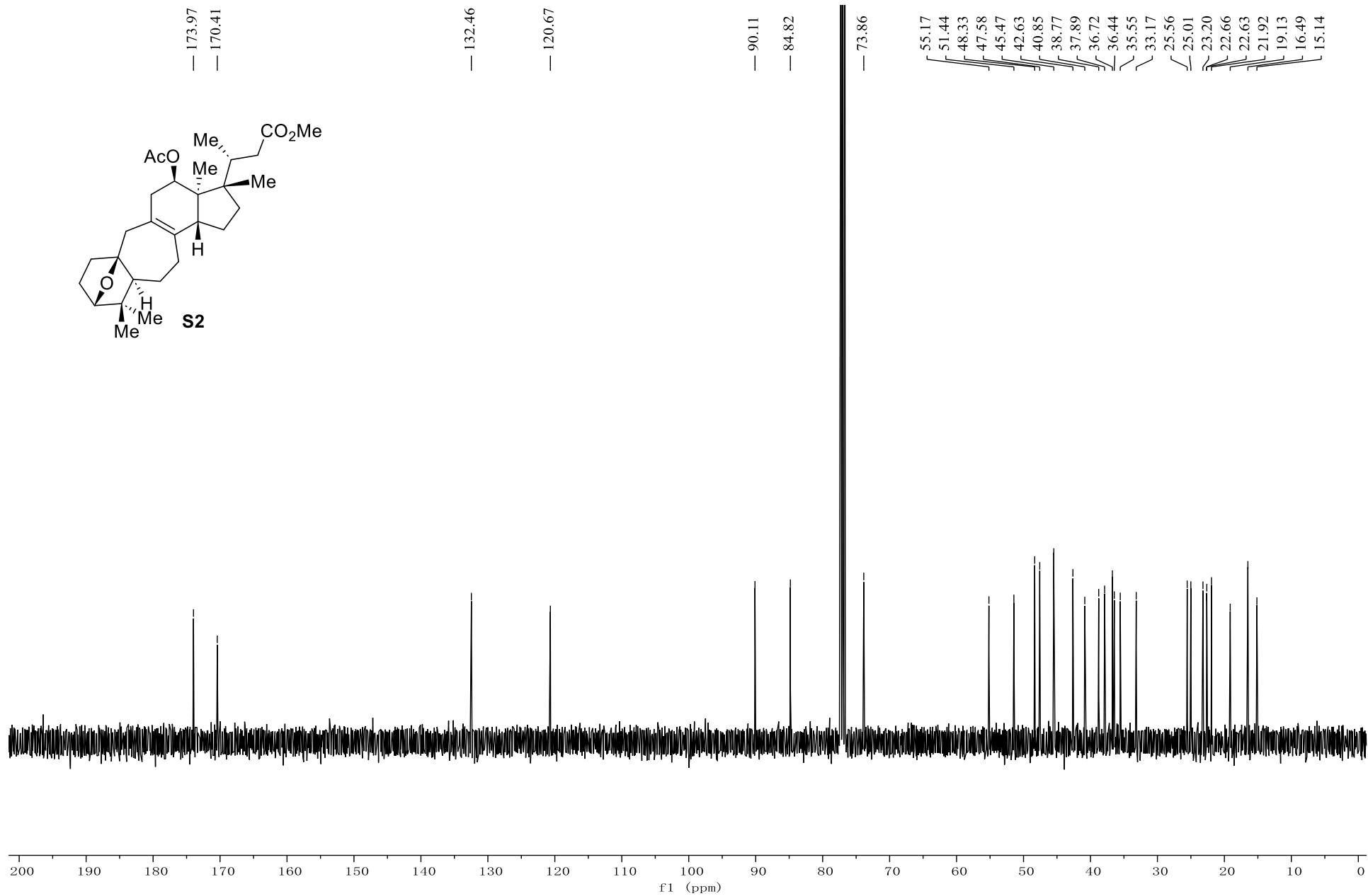


¹H NMR Spectrum of S2 (101 MHz, CDCl₃)

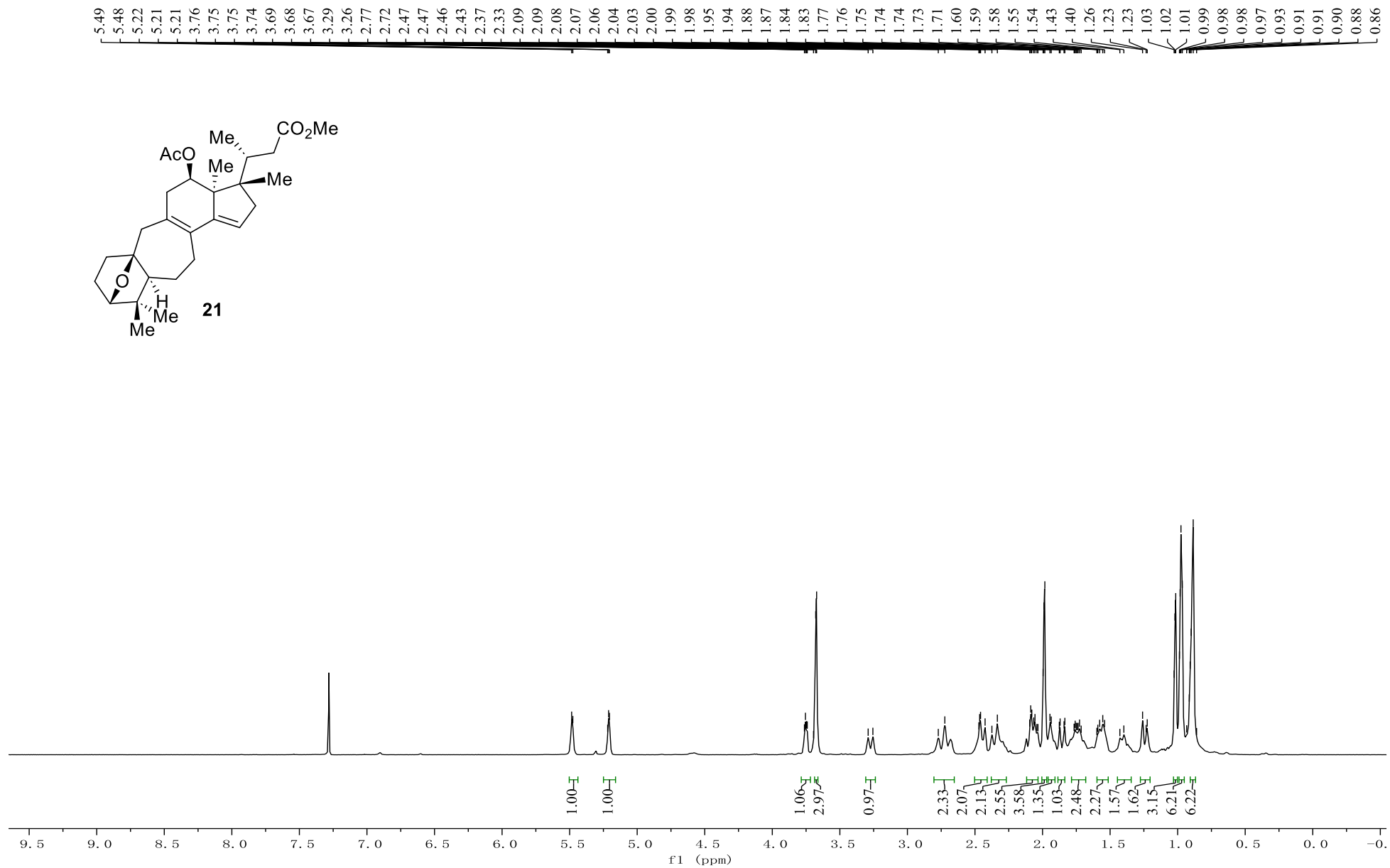
5.19
5.18
5.18
5.17
3.73
3.72
3.16
3.13
2.96
2.54
2.53
2.52
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2.50
2.48
2.34
2.27
2.26
2.25
2.04
2.03
2.01
1.99
1.97
1.95
1.94
1.93
1.92
1.91
1.85
1.76
1.75
1.75
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1.72
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0.85
0.83



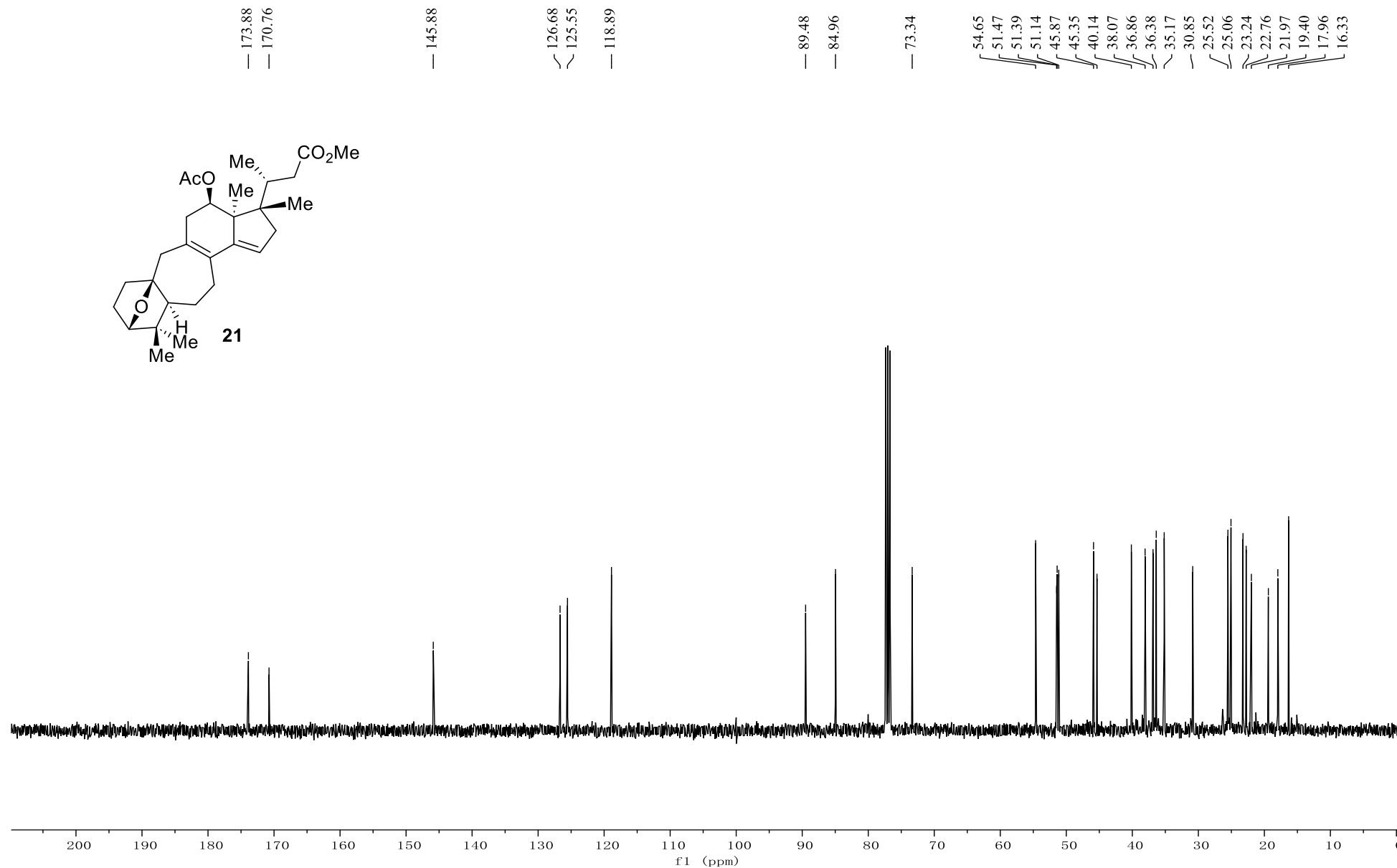
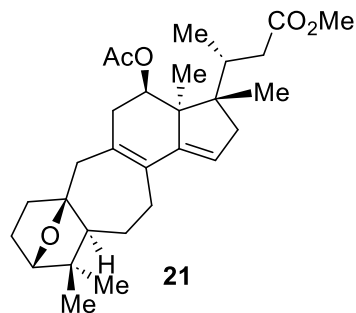
¹³C NMR Spectrum of S2 (101 MHz, CDCl₃)



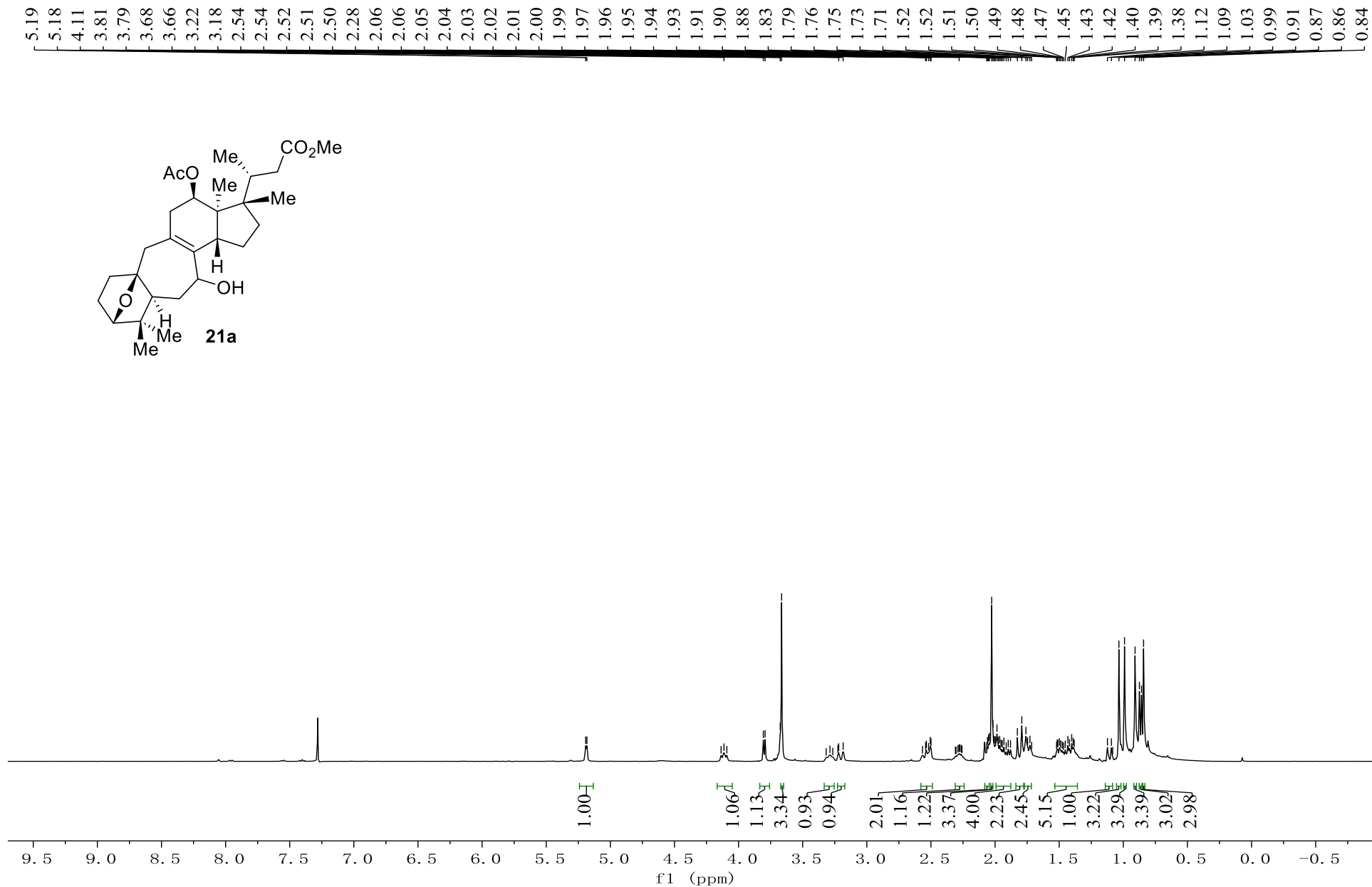
¹H NMR Spectrum of 21 (400 MHz, CDCl₃)



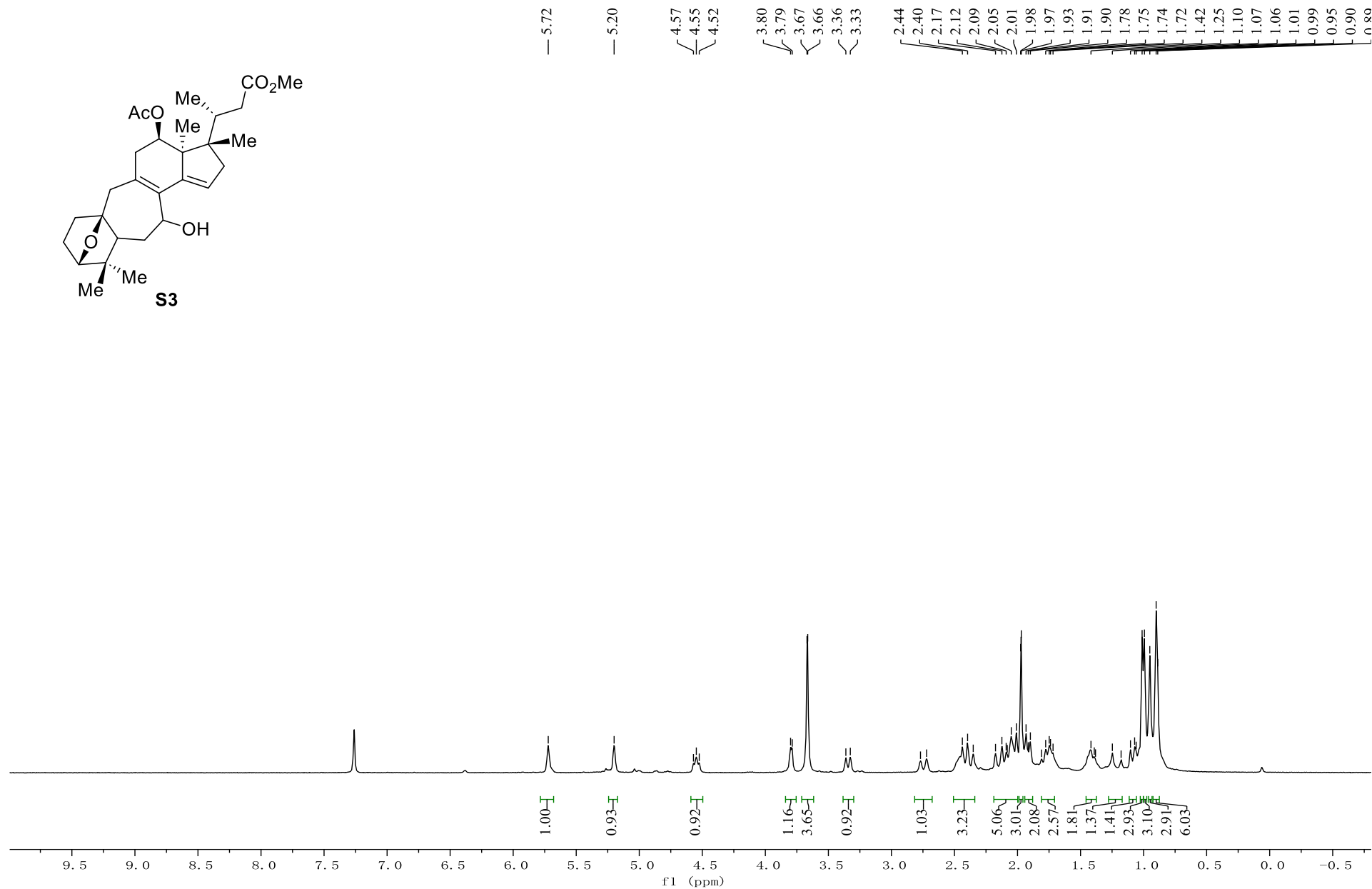
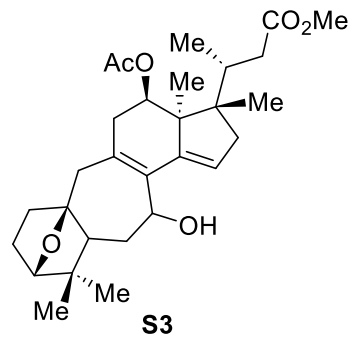
¹³C NMR Spectrum of 21 (101 MHz, CDCl₃)



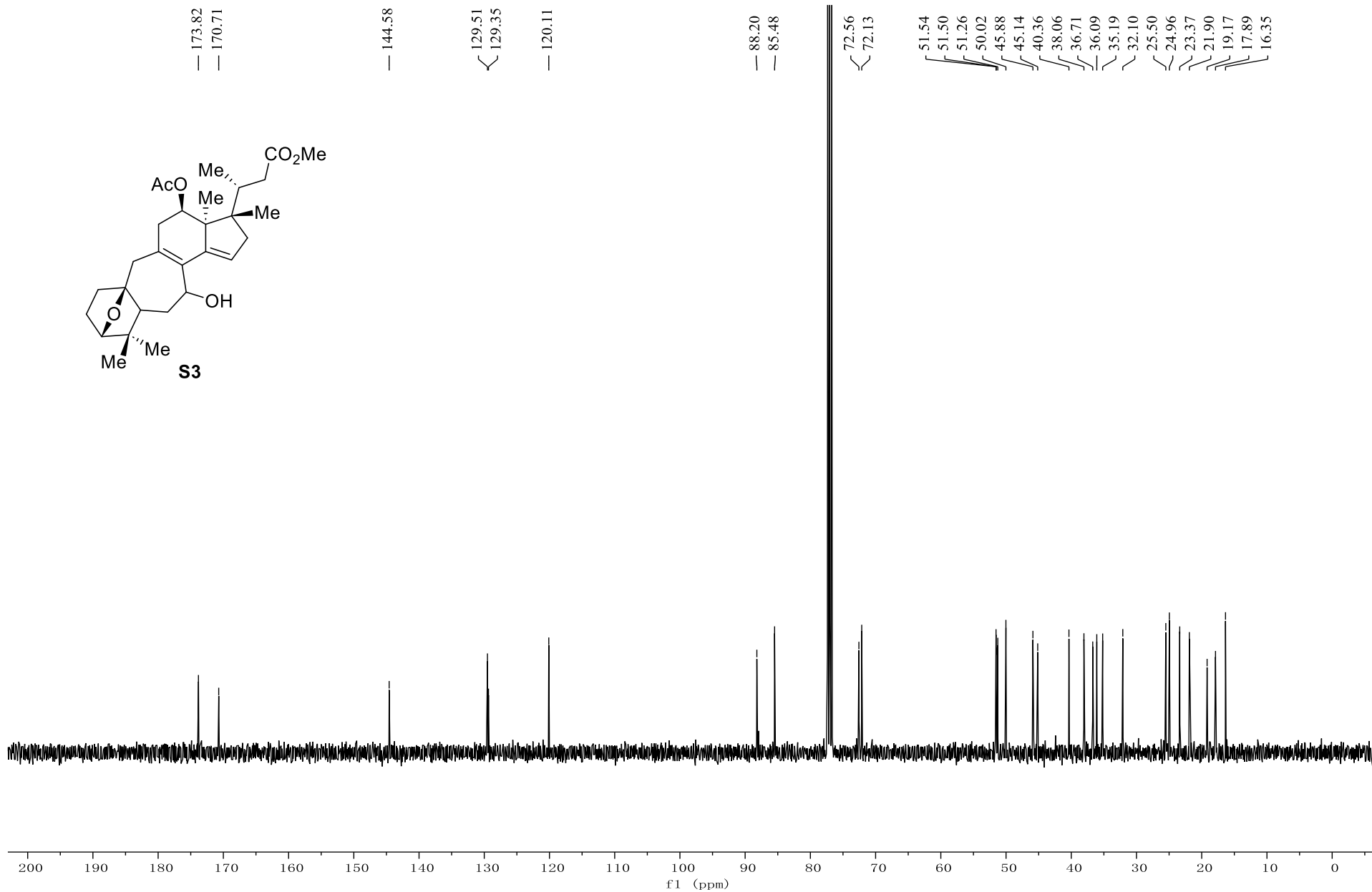
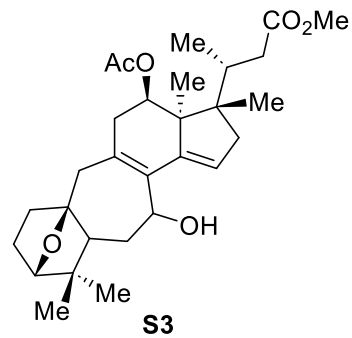
¹H NMR Spectrum of 21a (400 MHz, CDCl₃)



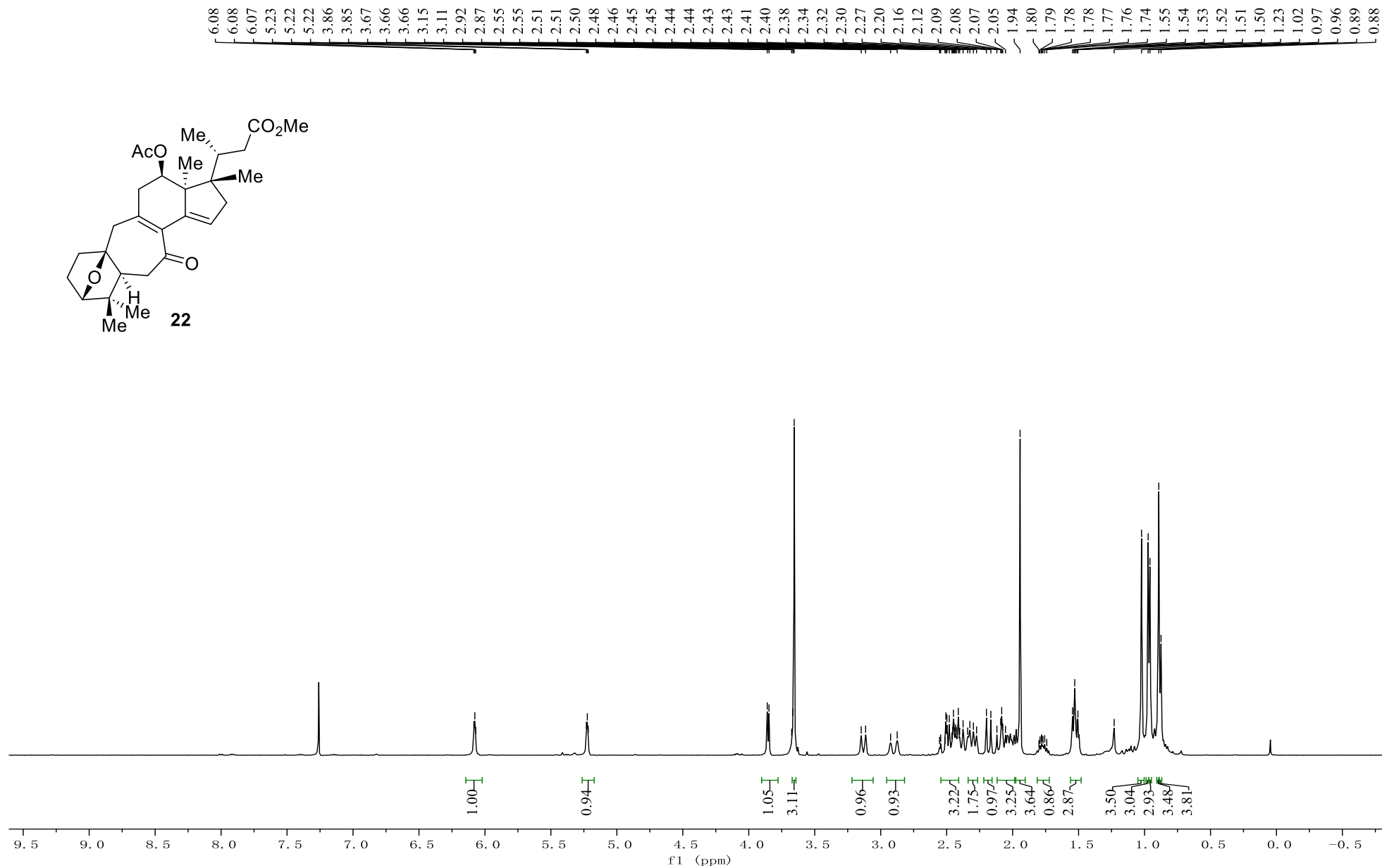
¹H NMR Spectrum of S3 (400 MHz, CDCl₃)



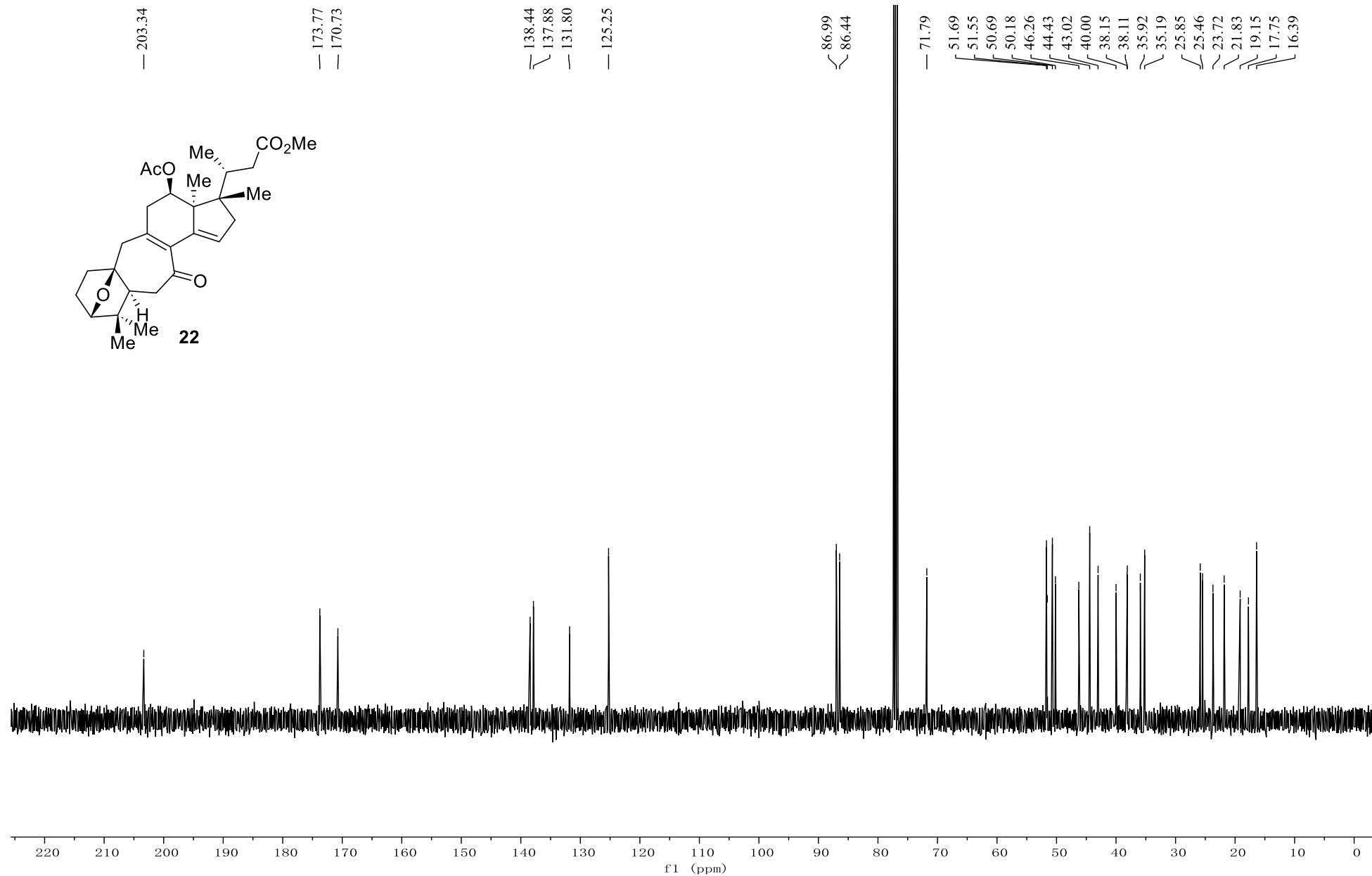
¹³C NMR Spectrum of S3 (101 MHz, CDCl₃)



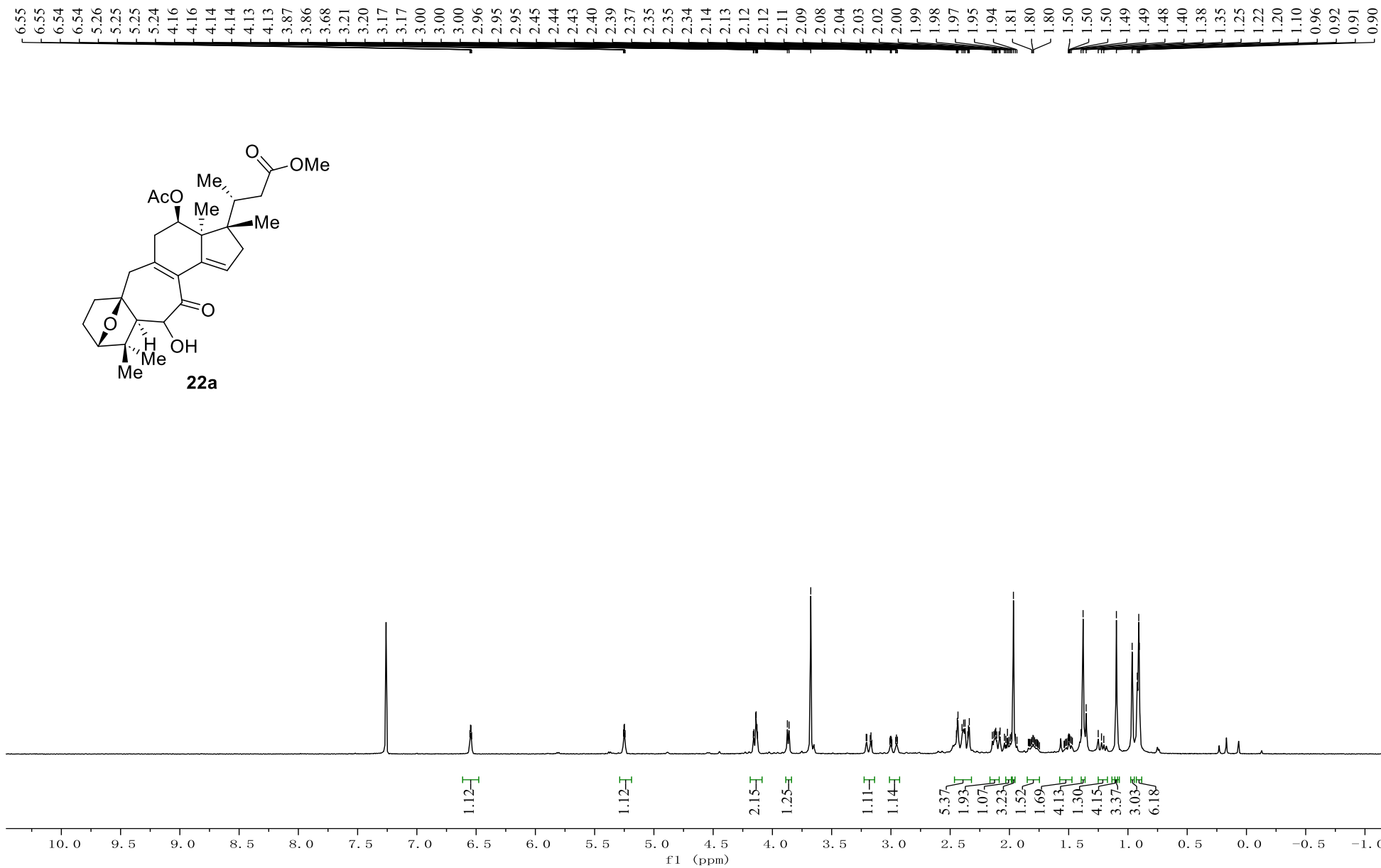
¹H NMR Spectrum of 22 (400 MHz, CDCl₃)



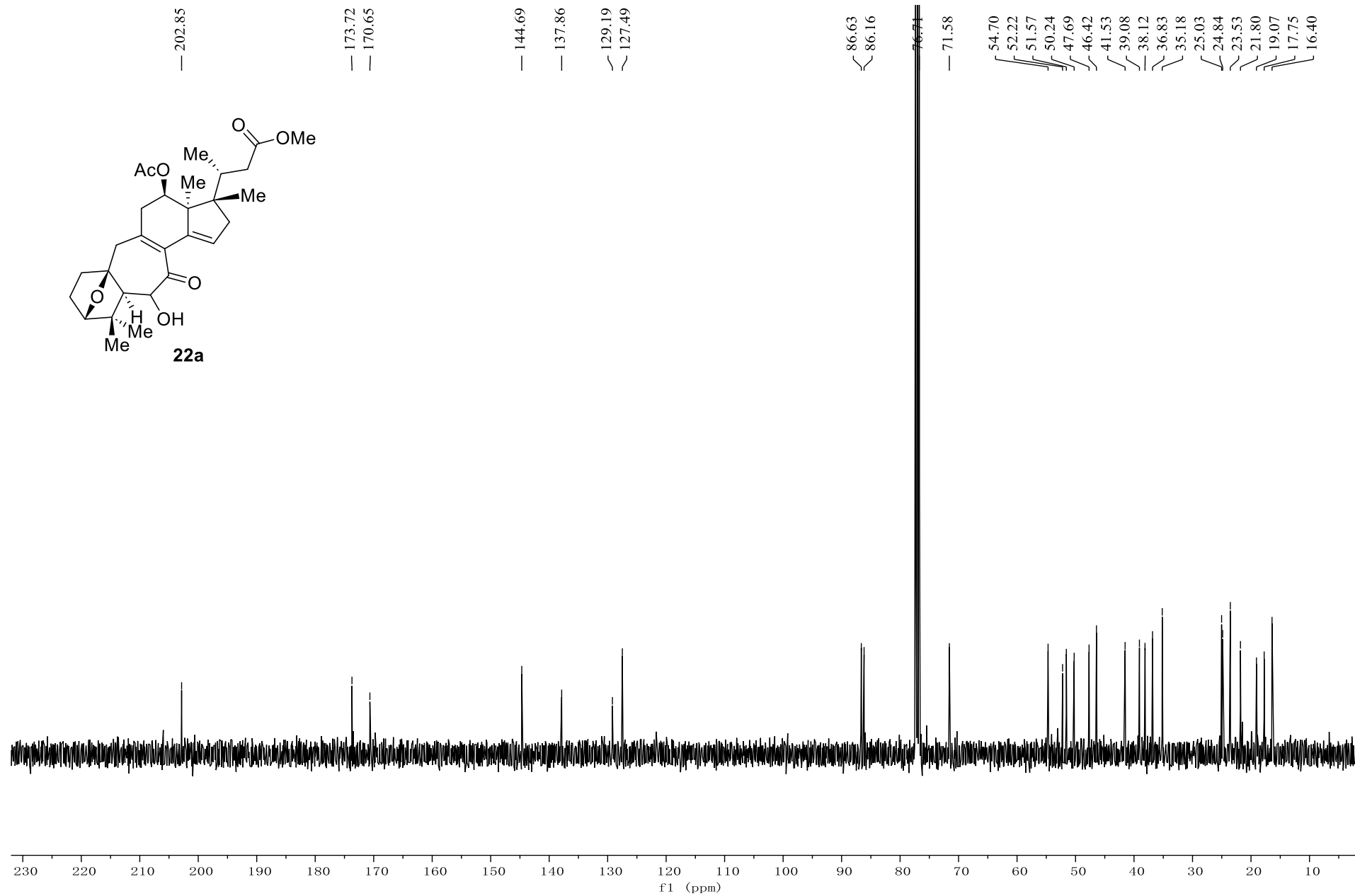
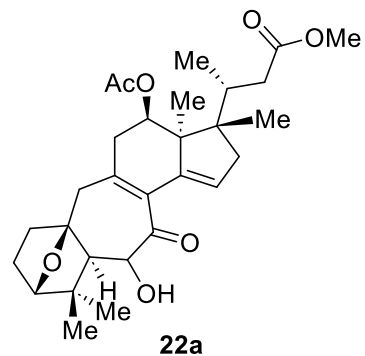
¹³C NMR Spectrum of 22 (101 MHz, CDCl₃)



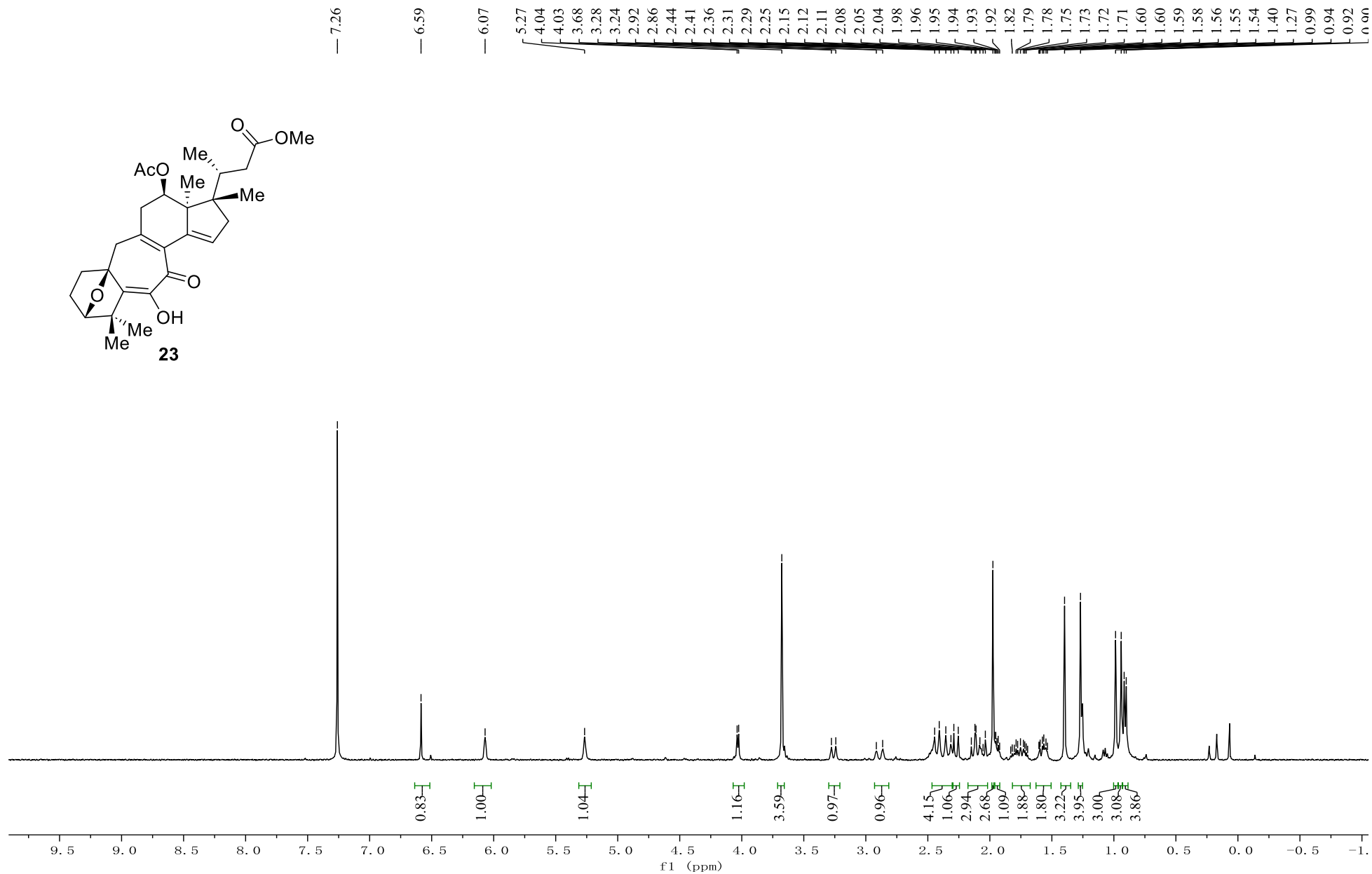
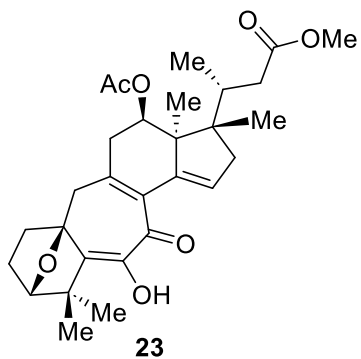
¹H NMR Spectrum of 22a (400 MHz, CDCl₃)



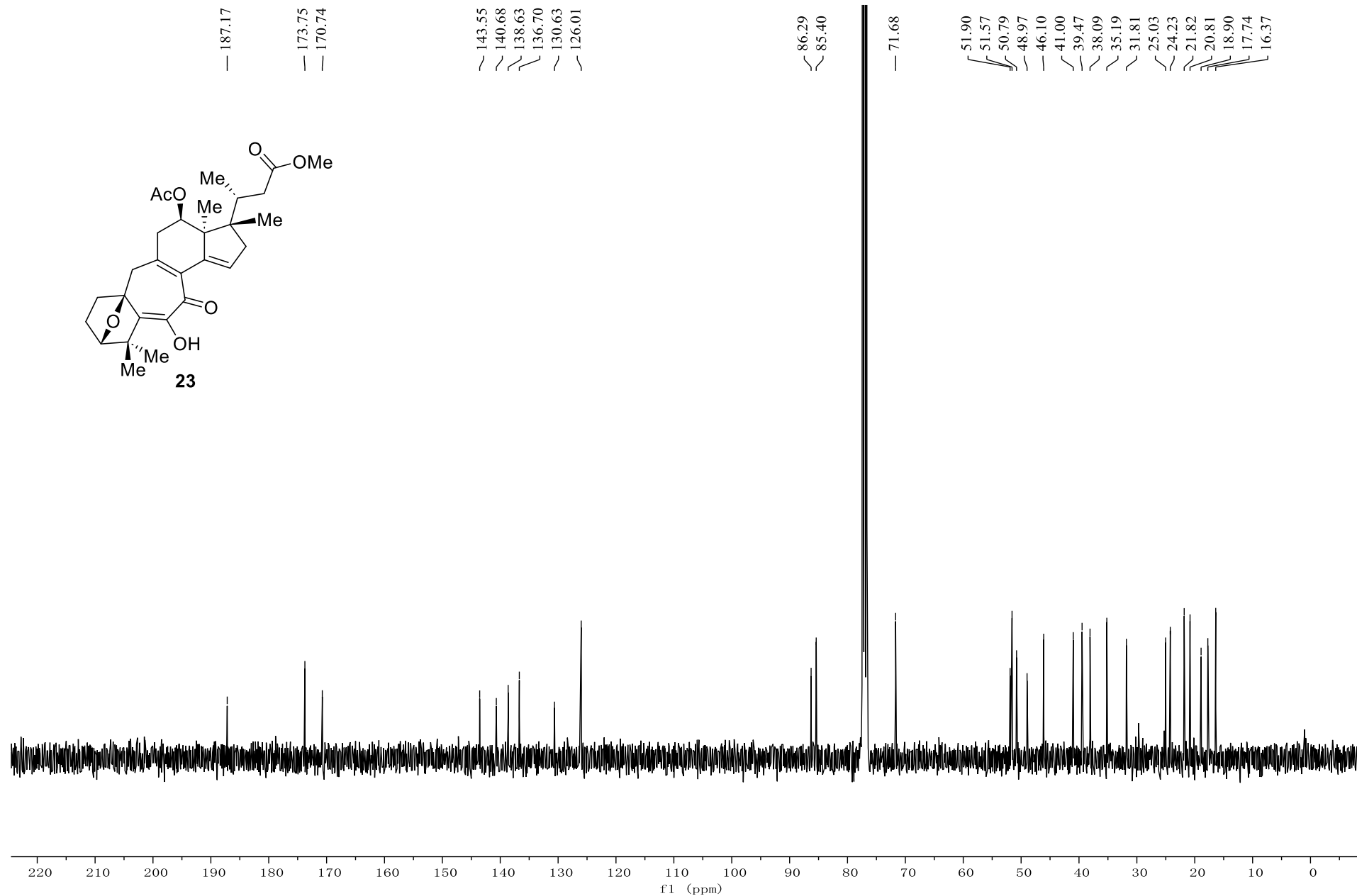
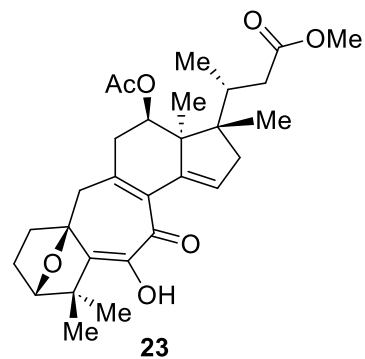
¹³C NMR Spectrum of 22a (101 MHz, CDCl₃)



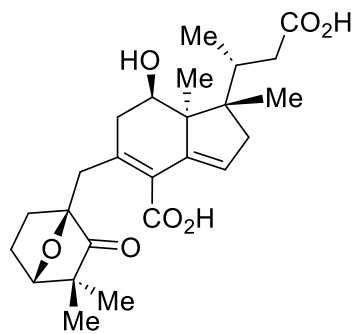
¹H NMR Spectrum of 23 (400 MHz, CDCl₃)



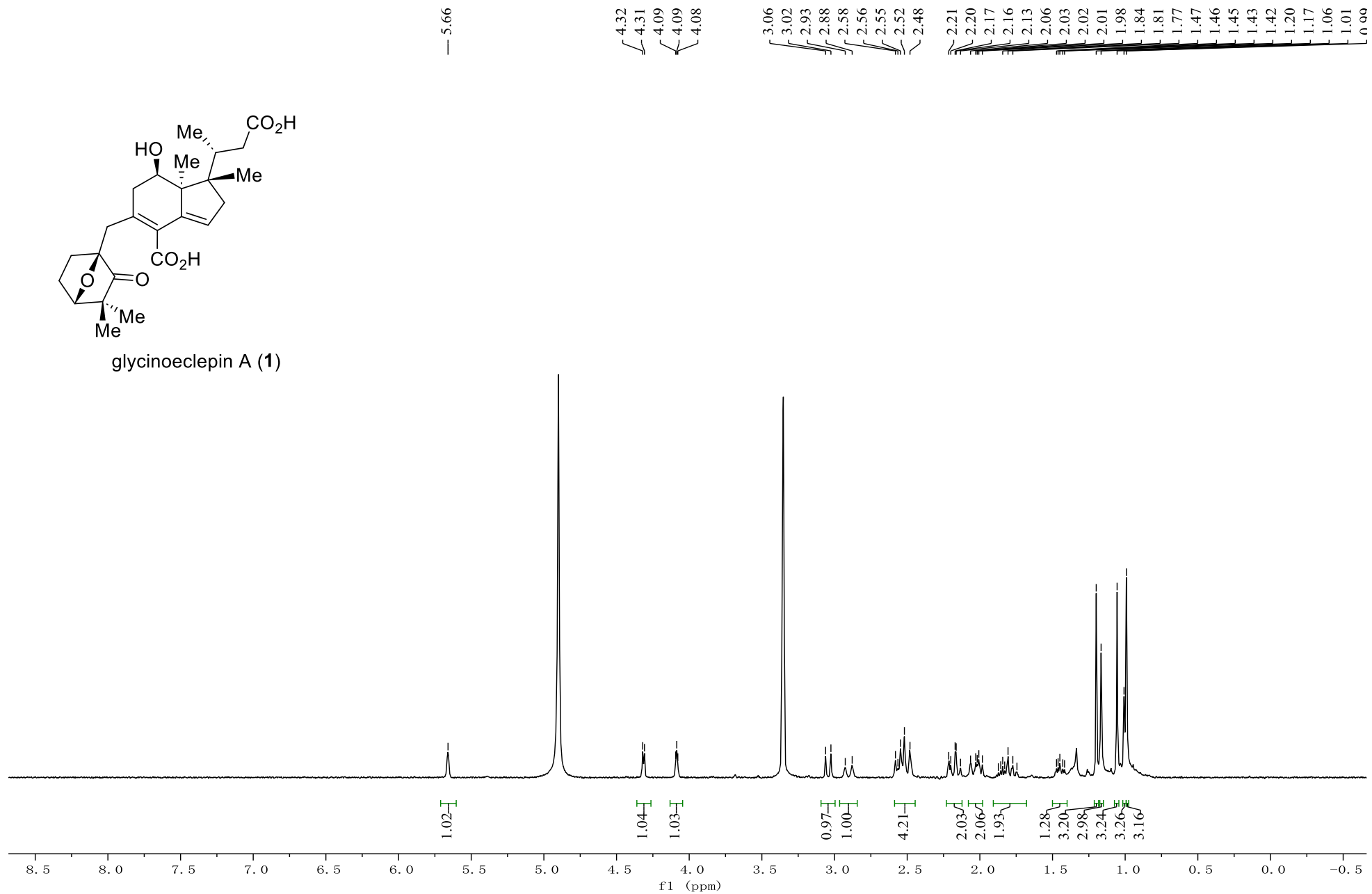
¹³C NMR Spectrum of 23 (101 MHz, CDCl₃)



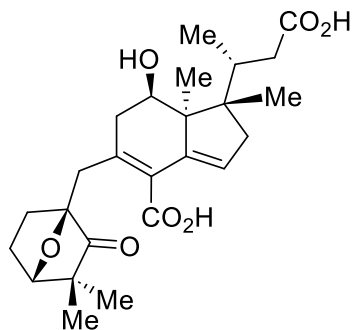
¹H NMR Spectrum of glycinoclepin A (1) (400 MHz, Methanol-d₄)



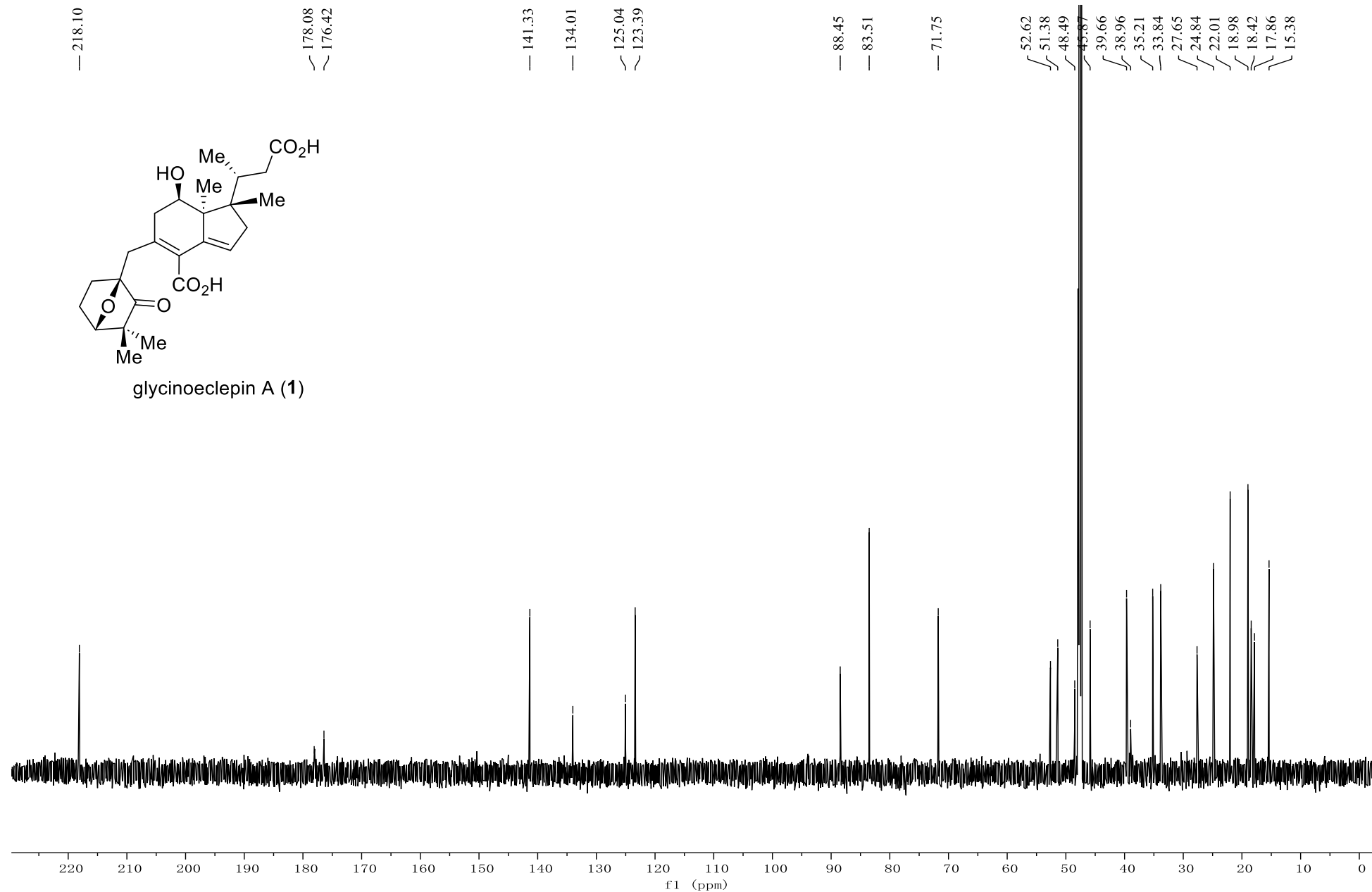
glycinoclepin A (1)



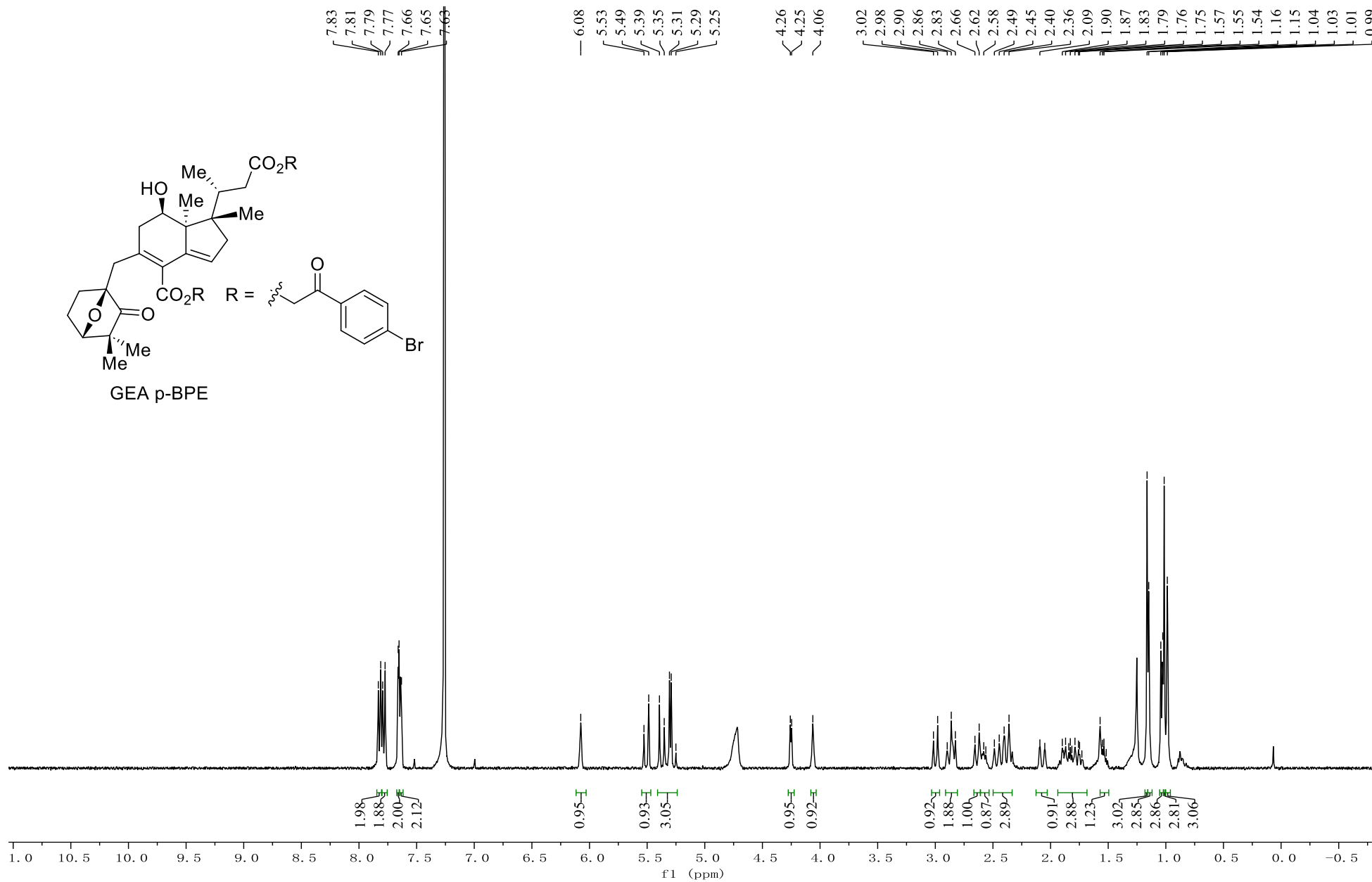
¹³C NMR Spectrum of glycinoclepin A (1) (200 MHz, Methanol-d₄)



glycinoclepin A (1)



¹H NMR Spectrum of GEA p-BPE (S4) (400 MHz, CDCl₃)



¹³C NMR Spectrum of GEA p-BPE (S4) (200 MHz, CDCl₃)

