

Supplementary Information for

Enantiodivergent dearomative skeletal ring expansion of indoles through
carbon atom insertion

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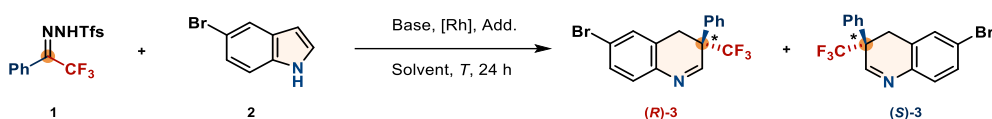
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1. Materials and Methods

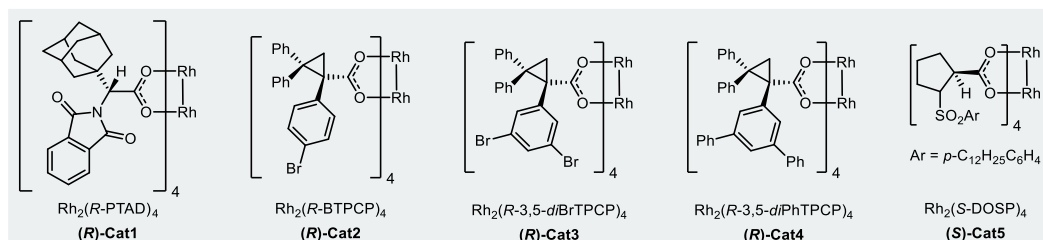
All reagents were purchased from commercial sources and used without treatment, unless otherwise indicated. The products were purified by column chromatography over silica gel. NMR spectra were recorded on a Bruker Advance 600 (^1H : 600 MHz, ^{13}C : 150 MHz, ^{19}F : 564 MHz) and Bruker Advance 500 (^1H : 500 MHz, ^{13}C : 125 MHz, ^{19}F : 470 MHz) at ambient temperature. ^1H and ^{13}C NMR spectra were reported as chemical shifts in parts per million (ppm) downfield from tetramethylsilane, using the residual undeuterated solvent (CHCl_3 at 7.26 ppm ^1H NMR, 77.00 ppm ^{13}C NMR) or tetramethylsilane as reference. ^{19}F NMR spectra were reported as chemical shifts in parts per million (ppm) using CFCl_3 (0 ppm) in CDCl_3 as reference. Coupling constants were reported in hertz (Hz). The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. High-resolution mass spectra (HRMS) were recorded on Bruker microTof by using ESI method. Enantiomeric excess (% ee) data were obtained on an Agilent 1260 HPLC, eluting the purified products using a mixed solution of HPLC-grade 2-propanol (i-PrOH) and n-hexane.

2. Optimization of the Reaction Conditions

Supplementary Table S1. Reaction Optimization Studies



Entry	[Rh] cat (1 mol%)	Base (4 equiv)	Additive (5 mol%)	Solvent (4 mL)	T (°C)	3 yield (%) ^a	e.r. (R:S)
1	(R)-Cat1	NaH	NaBARf	PhCF ₃	40	74	18.3:81.7
2	(R)-Cat2	NaH	NaBARf	PhCF ₃	40	92	12.0:88.0
3	(R)-Cat3	NaH	NaBARf	PhCF ₃	40	92	5.0:95.0
4	(R)-Cat4	NaH	NaBARf	PhCF ₃	40	92	4.1:95.9
5	(S)-Cat5	NaH	NaBARf	PhCF ₃	40	64	78.4:21.6
6	(S)-Cat4	NaH	NaBARf	PhCF ₃	40	94	94.1:5.9
7	(R)-Cat4	NaH	NaBARf	PhCF ₃	60	86	3.8:96.2
8	(R)-Cat4	NaH	NaBARf	PhCF ₃	80	60	3.5:96.5
9	(R)-Cat4	NaH	none	PhCF ₃	40	34 ^b	-
10	(R)-Cat4	K ₂ CO ₃	NaBARf	PhCF ₃	40	n.d.	-
11	(R)-Cat4	DIPEA	NaBARf	PhCF ₃	40	11 ^b	-
12	(R)-Cat4	NaH	NaBARf	DCM	40	87	4.3:95.7
13	(R)-Cat4	NaH	NaBARf	1,4-dioxane	40	9 ^b	-

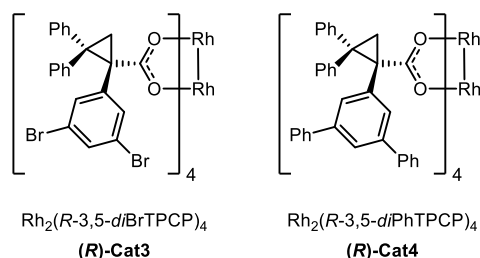


Reaction conditions: **1** (0.2 mmol), **2** (0.3 mmol), Rh catalyst (1 mol%), additive (5 mol%), and solvent (1.0 mL). ^aIsolated yields are given. The ee values were determined by HPLC equipped with chiral column. ^bYield of the product was determined by ¹H-NMR with CH₂Br₂ as an internal standard.

General Procedure: To an oven-dried screw-cap reaction tube equipped with a Teflon-coated magnetic stir bar were added Rh catalyst (1 mol%), additive (5 mol%), and solvent (1.0 mL) inside a glove box with nitrogen atmosphere. After the mixture was stirred for 5 min, trifluoromethyl phenyl *N*-triflylhydrazone **1** (0.2 mmol), base (0.8 mmol, 4.0 equiv), 5-bromo-1*H*-indole **2** (0.3 mmol, 1.5 equiv), and dry solvent (3 mL) were added. After transfer out of the glove box, the reaction was continued for an additional 24 h at T °C. When the reaction was completed, and filtered through a short pad of silica gel with DCM as an eluent. After removal of the solvent under vacuum, the yields of product were determined by isolated.

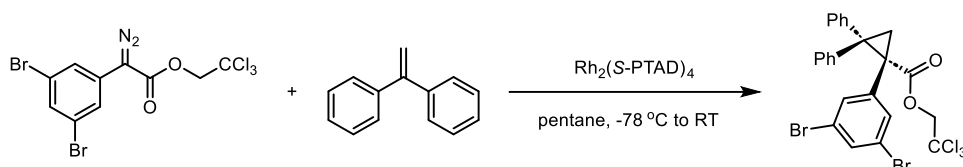
3. Preparation of Starting Materials

3.1 Preparation of Catalysts:



Catalysts **(R)-Cat1**, **(R)-Cat2**, and **(S)-Cat5** are commercially available. **(R)-Cat3** and **(R)-Cat4** are prepared according to the established literature (1).

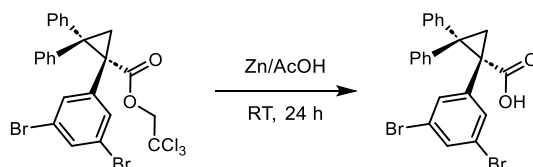
Preparation of (R)-1-(3,5-dibromophenyl)-2,2-diphenylcyclopropane-1-carboxylate.



A flame-dried round bottom flask was kept under a dry atmosphere of nitrogen. $\text{Rh}_2(\text{S-PTAD})_4$ (94 mg, 0.06 mmol, 0.005 equiv), 1,1-diphenylethylene (5.04 g, 27.6 mmol, 2.3 equiv), and dry degassed pentane (30 mL) were added. A solution of 2,2,2-trichloroethyl 2-diazo-2-(3,5-dibromophenyl)acetate (2.16 g, 12 mmol, 1.0 equiv) in dry degassed pentane (30 mL) was added to the former solution drop-wise over 30 min at -78°C . The mixture was allowed to warm up to RT and stir overnight, and then concentrated in vacuum. The crude product was purified by flash column chromatography to provide the ester as white foam in 95% yield (6.84 g).

^1H NMR (500 MHz, CDCl_3) δ 7.55 (d, $J = 8.0$ Hz, 2H), 7.48 (d, $J = 1.5$ Hz, 2H), 7.44-7.41 (m, 1H), 7.35 (t, $J = 7.5$ Hz, 2H), 7.30-7.26 (m, 1H), 7.15-7.09 (m, 4H), 7.08-7.03 (m, 1H), 4.57 (d, $J = 11.5$ Hz, 1H), 4.23 (d, $J = 11.5$ Hz, 1H), 2.77 (d, $J = 6.0$ Hz, 1H), 2.53 (d, $J = 6.0$ Hz, 1H). **^{13}C NMR** (125 MHz, CDCl_3) δ 168.4, 140.9, 138.8, 138.3, 133.9, 133.0, 129.8, 128.73, 128.66, 128.2, 127.6, 127.1, 121.8, 94.2, 75.4, 46.3, 41.8, 22.8. Datas consistent with reported spectra (1).

Preparation of (R)-1-(3,5-dibromophenyl)-2,2-diphenylcyclopropane-1-carboxylic acid.

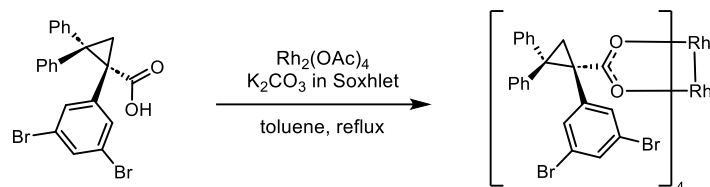


The 2,2,2-trichloroethyl (R)-1-(3,5-dibromophenyl)-2,2-diphenylcyclopropane-1-carboxylate (6 g, 10 mmol, 1.0 equiv) was dissolved in 30 mL of glacial acetic acid, and zinc powder (3.27 g, 50 mmol, 5.0 equiv) was added. The solution was allowed to stir at room temperature for 24 h. The starting material had been fully consumed as indicated by TLC analysis. The solution was diluted with H_2O (50 mL) and extracted with ethyl acetate (3x50 mL). The organic extracts were washed with H_2O and brine, dried over MgSO_4 and filtered. Then the filtrate was concentrated to give the crude product. The crude product was purified by flash column chromatography to provide the acid as white solid in 98% yield

(4.61 g).

¹H NMR (500 MHz, CDCl₃) δ 7.48-7.44 (m, 2H), 7.38 (s, 1H), 7.35-7.28 (m, 5H), 7.10-7.05 (m, 2H), 7.02 (d, *J* = 7.5 Hz, 3H), 2.59 (d, *J* = 5.5 Hz, 1H), 2.44 (d, *J* = 5.5 Hz, 1H). **¹³C NMR** (125 MHz, CDCl₃) δ 175.8, 140.8, 139.2, 138.3, 133.7, 132.8, 129.6, 128.53, 128.49, 128.0, 127.3, 126.9, 121.7, 46.3, 41.5, 23.0. Datas consistent with reported spectra (1).

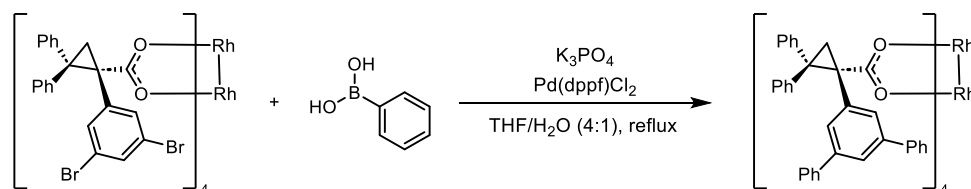
Preparation of dirhodium tetrakis((*R*)-1-(3,5-dibromophenyl)-2,2-diphenylcyclopropanecarboxylate) ((*R*)-Cat3)



A 50 mL round bottom flask, equipped with a Teflon-coated stirring bar and nitrogen inlet, was flushed with nitrogen and then charged with rhodium(II) acetate (0.5 mmol, 0.22 g, 1.0 equiv), (*R*)-1-(3,5-dibromophenyl)-2,2-diphenylcyclopropane-1-carboxylic acid (4 mmol, 1.88 g, 8.0 equiv), and 35 mL of toluene. The flask was fitted with a Soxhlet extraction apparatus into which was placed a thimble containing 15 g of an oven-dried mixture of 2 parts sodium carbonate and 1 part of sand. The solution was heated at reflux for 24 h; removal of the solvent under reduced pressure using a rotary evaporator and then purified by flash column chromatography (hexanes/diethyl ether = 80/1) to give green solid in 45% overall yield (470 mg).

¹H NMR (500 MHz, CDCl₃) δ 7.43-7.37 (m, 2H), 7.33 (t, *J* = 7.5 Hz, 2H), 7.18 (d, *J* = 7.5 Hz, 2H), 7.15 (d, *J* = 2.0 Hz, 2H), 7.10 (t, *J* = 7.5 Hz, 2H), 7.05-6.99 (m, 3H), 2.24 (d, *J* = 5.0 Hz, 1H), 2.18 (d, *J* = 5.0 Hz, 1H). **¹³C NMR** (125 MHz, CDCl₃) δ 188.7, 141.2, 140.7, 139.3, 133.4, 132.2, 129.8, 128.8, 128.1, 128.0, 126.9, 126.8, 121.5, 46.5, 43.3, 25.2. Datas consistent with reported spectra (1).

Preparation of dirhodium tetrakis((*R*)-1-([1,1':3',1''-terphenyl]-5'-yl)-2,2-diphenylcyclopropanecarboxylate) ((*R*)-Cat4)



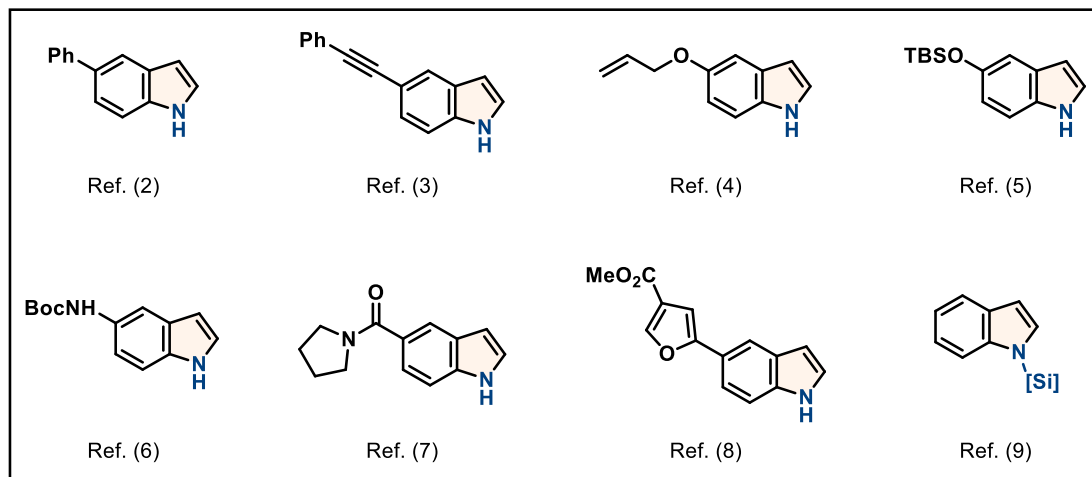
A 25 mL round bottom flask was charged with dirhodium tetrakis((*R*)-1-(3,5-dibromophenyl)-2,2-diphenylcyclopropanecarboxylate) (73 mg, 0.035 mmol, 1.0 equiv), boronic acid (68 mg, 0.56 mmol, 16 equiv). K₃PO₄ (178 mg, 0.84 mmol, 24 equiv) and THF:H₂O (4:1) (12 mL). The solution was heated to reflux for 10 min to degass and then [1,1'-Bis(diphenylphosphino)ferrocene]dichloropalladium(II) [Pd(dppf)Cl₂] (10 mg, 0.014 mmol, 0.4 equiv) was added. The resulting red solution was then remained reflux for 12 h. After the allotted time had passed, the solution was cooled to room temperature and concentrated under reduced pressure. The residue was redissolved in DCM, washed with water (3x15 mL) and brine (3x15 mL). The organic layer was dried over sodium sulfate and filtered. The filtrate was concentrated by rotary evaporation to afford the crude product. The crude product was purified by flash column chromatography (hexanes/diethyl ether = 30/1) to give a green solid in 93% yield (65 mg).

¹H NMR (500 MHz, CDCl₃) δ 7.47-7.41 (m, 9H), 7.38-7.33 (m, 2H), 7.21 (s, 2H), 7.06-6.91 (m, 8H), 6.87 (d, *J* = 7.5 Hz, 2H), 2.13-2.05 (m, 2H). **¹³C NMR** (150 MHz, CDCl₃) δ 189.9, 141.5, 141.3, 140.7,

140.5, 138.3, 130.0, 129.9, 129.0, 128.6, 127.9, 127.6, 127.4, 127.2, 126.1, 124.4, 45.6, 44.3, 29.7.
 Datas consistent with reported spectra (1).

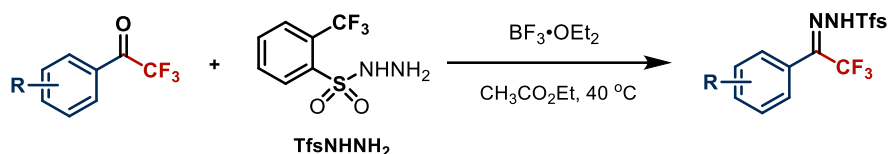
3.2 Preparation of Indoles:

Indoles employed in this work were either commercially available, (used as received from commercial sources) or prepared according to literature procedures as described below (2-9).



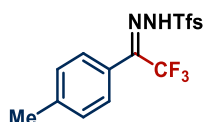
Supplementary Fig. S1. The list of functionalized indoles was prepared according to the corresponding literature.

3.3 Preparation of *N*-Triftosylhydrazones:



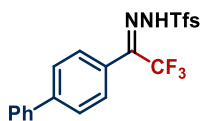
N-Triftosylhydrazones were prepared according to literature procedures (10). A 100 mL flask equipped with a magnetic stir bar was charged with fluoroalkyl ketones (1.2 equiv) and $\text{CH}_3\text{CO}_2\text{Et}$ (1 mmol/mL). Then 2-trifluoromethylbenzenesulfonylhydrazide (TfsNHNH_2) (1.0 equiv) and $\text{BF}_3 \cdot \text{Et}_2\text{O}$ (0.1 mL/mmol) were added and the mixture was stirred at 40 °C and monitored by TLC. After completion, the reaction mixture was concentrated under reduced pressure and the obtained crude product was purified by column chromatography using PE/EA (5:1 to 2:1) as eluent to afford the trifluoromethyl ketones *N*-triftosylhydrazones.

Characterization data of selected fluoroalkyl ketones *N*-triftosylhydrazones

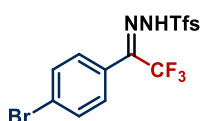


Yield: 85%, ^1H NMR (600 MHz, CDCl_3) δ 8.46-8.40 (m, 1H), 8.17 (s, 1H), 7.94-7.87 (m, 1H), 7.84-7.77 (m, 2H), 7.35 (d, $J = 7.8$ Hz, 2H), 7.13 (d, $J = 7.8$ Hz, 2H), 2.43 (s, 3H). ^{13}C NMR (150 MHz, CDCl_3) δ 142.9 (q, $J = 35.5$ Hz), 142.3, 135.9, 133.9, 133.8, 132.6, 130.7, 128.4 (q, $J = 6.3$

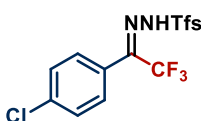
Hz), 127.8, 127.7 (q, $J = 33.0$ Hz), 121.7 (d, $J = 19.8$ Hz), 122.6 (q, $J = 271.5$ Hz), 119.8 (q, $J = 273.0$ Hz), 21.5. **^{19}F NMR** (564 MHz, CDCl_3) δ -58.33 (s, 3F), -68.66 (s, 3F).



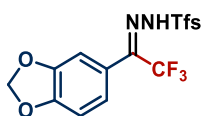
Yield: 83%, **^1H NMR** (500 MHz, CDCl_3) δ 8.49-8.42 (m, 1H), 8.25 (s, 1H), 7.98-7.89 (m, 1H), 7.86-7.79 (m, 2H), 7.79-7.73 (m, 2H), 7.67-7.60 (m, 2H), 7.53-7.47 (m, 2H), 7.47-7.41 (m, 1H), 7.33 (d, $J = 8.0$ Hz, 2H). **^{13}C NMR** (125 MHz, CDCl_3) δ 144.7, 142.4 (q, $J = 35.0$ Hz), 139.4, 135.9, 134.0, 133.9, 132.7, 129.1, 128.7, 128.43, 128.41, 128.1 (q, $J = 6.3$ Hz), 127.2, 123.4, 122.6 (q, $J = 271.3$ Hz), 119.8 (q, $J = 272.5$ Hz). **^{19}F NMR** (470 MHz, CDCl_3) δ -58.26 (s, 3F), -68.43 (s, 3F).



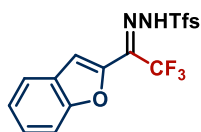
Yield: 78%, **^1H NMR** (500 MHz, CDCl_3) δ 8.45-8.39 (m, 1H), 8.14 (s, 1H), 7.96-7.87 (m, 1H), 7.85-7.77 (m, 2H), 7.74-7.64 (m, 2H), 7.19-7.07 (m, 2H). **^{13}C NMR** (125 MHz, CDCl_3) δ 141.2 (q, $J = 36.3$ Hz), 135.7, 134.2, 133.8, 133.4, 132.7, 129.6, 128.5 (q, $J = 6.3$ Hz), 127.7 (q, $J = 32.5$ Hz), 126.6, 123.6, 122.6 (q, $J = 272.5$ Hz), 119.5 (q, $J = 273.8$ Hz). **^{19}F NMR** (470 MHz, CDCl_3) δ -58.28 (s, 3F), -68.51 (s, 3F).



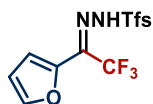
Yield: 85%, **^1H NMR** (500 MHz, CDCl_3) δ 8.07-8.02 (m, 1H), 8.03-7.98 (m, 1H), 7.98-7.88 (m, 2H), 7.68-7.61 (m, 2H), 7.44 (d, $J = 8.5$ Hz, 2H). **^{13}C NMR** (125 MHz, CDCl_3) δ 142.6 (q, $J = 35.5$ Hz), 141.9, 135.3, 133.1, 132.9, 132.6, 130.6, 128.2 (q, $J = 6.3$ Hz), 127.8, 127.7 (q, $J = 33.0$ Hz), 121.7 (q, $J = 20.0$ Hz), 122.6 (q, $J = 273.0$ Hz), 119.8 (q, $J = 275.0$ Hz). **^{19}F NMR** (470 MHz, CDCl_3) δ -58.12 (s, 3F), -68.46 (s, 3F).



Yield: 68%, **^1H NMR** (500 MHz, DMSO) δ 12.26 (s, 1H), 8.06-8.02 (m, 1H), 8.01-7.88 (m, 3H), 7.10 (d, $J = 8.0$ Hz, 1H), 6.98 (s, 1H), 6.88 (d, $J = 8.0$ Hz, 1H), 6.03 (s, 2H). **^{13}C NMR** (125 MHz, DMSO) δ 154.3, 152.9, 144.7 (q, $J = 32.5$ Hz), 142.4, 138.8, 138.4, 133.5 (q, $J = 6.0$ Hz), 131.5 (q, $J = 33.0$ Hz), 128.1, 127.6 (q, $J = 272.5$ Hz), 125.1 (q, $J = 273.0$ Hz), 124.7, 124.1, 114.2, 113.8, 106.7. **^{19}F NMR** (470 MHz, DMSO) δ -56.23 (s, 3F), -66.88 (s, 3F).



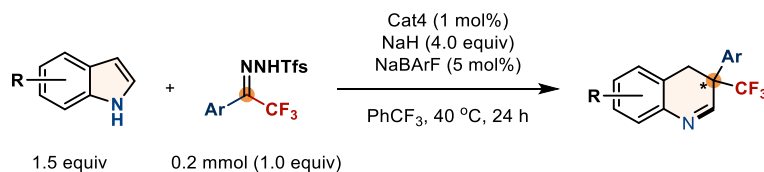
Yield: 71%, **¹H NMR** (500 MHz, CDCl₃) δ 10.74 (s, 1H), 8.46-8.41 (m, 1H), 7.93-7.88 (m, 1H), 7.84-7.74 (m, 2H), 7.72-7.66 (m, 1H), 7.66-7.61 (m, 1H), 7.55-7.49 (m, 1H), 7.41-7.35 (m, 1H), 7.23-7.18 (m, 1H). **¹³C NMR** (150 MHz, CDCl₃) δ 154.6, 144.3, 136.2, 133.9, 133.4, 132.6, 128.5 (q, *J* = 6.0 Hz), 128.2, 127.9 (q, *J* = 33.0 Hz), 125.9, 124.9, 122.9, 122.8 (q, *J* = 273.0 Hz), 119.9 (q, *J* = 273.0 Hz), 112.2, 111.7. **¹⁹F NMR** (564 MHz, CDCl₃) δ -58.29 (s, 3F), -65.99 (s, 3F).



Yield: 50%, **¹H NMR** (600 MHz, CDCl₃) δ 10.37 (s, 1H), 8.43-8.39 (m, 1H), 7.92-7.87 (m, 1H), 7.81-7.74 (m, 2H), 7.72 (d, *J* = 1.8 Hz, 1H), 6.88 (dd, *J* = 3.8, 1.9 Hz, 1H), 6.62 (dd, *J* = 3.8, 1.9 Hz, 1H). **¹³C NMR** (150 MHz, CDCl₃) δ 145.4, 143.9, 136.1, 133.8, 133.5, 132.5, 128.4 (q, *J* = 6.5 Hz), 127.8 (q, *J* = 33.0 Hz), 122.7 (q, *J* = 273.0 Hz), 119.8 (q, *J* = 273.0 Hz), 116.1, 116.0, 112.2. **¹⁹F NMR** (564 MHz, CDCl₃) δ -58.35 (s, 3F), -66.41 (s, 3F).

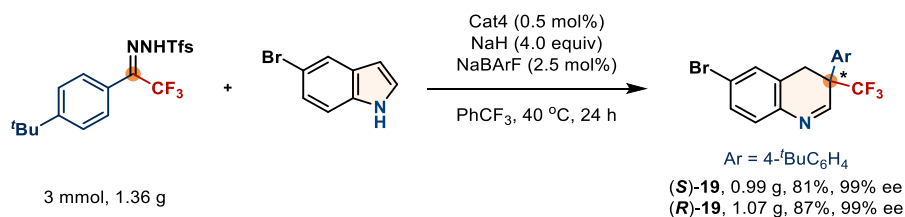
4. Experimental Procedure

4.1 General Procedure of Carbon-Atom Insertion into Indole Skeletons



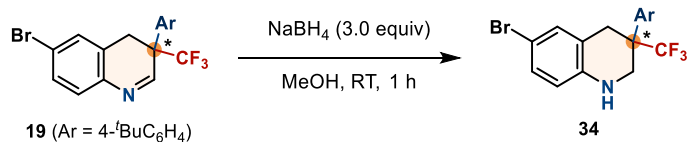
General Procedure A: To an oven-dried screw-cap reaction tube equipped with a Teflon-coated magnetic stir bar were added Rh catalyst (4 mg, 1 mol%), NaBARF (5 mol%), and PhCF₃ (1.0 mL). After the mixture was stirred for 5 min, *N*-triflylhydrazones (0.2 mmol, 1.0 equiv), NaH (32.0 mg, 0.8 mmol, 4.0 equiv, 60 wt% dispersion in mineral oil), indoles (0.3 mmol, 1.5 equiv), and dry PhCF₃ (3.0 mL) were added. After transfer out of the glove box, the reaction was continued for an additional 24 h at 40 °C. When the reaction was completed, and filtered through a short pad of silica gel with DCM as an eluent. After removal of the solvent under vacuum, the residue was purified by flash chromatography on silica gel (using petroleum ether/EtOAc as eluent) to obtain the quinolines products.

4.2 Gram-Scale Reaction and Synthetic Derivatization

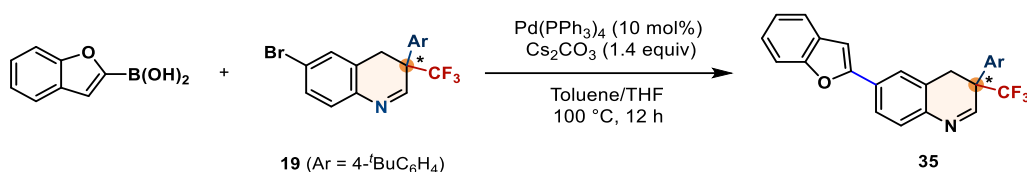


Gram-Scale Experiment:

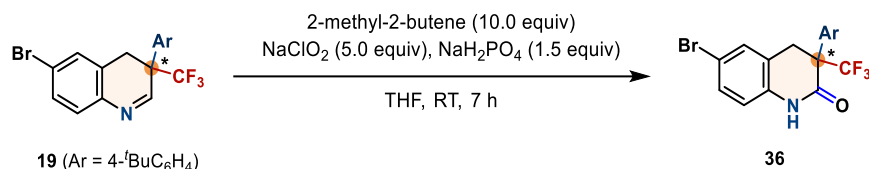
To an oven-dried 100 mL Schlenk tube equipped with a Teflon-coated magnetic stir bar were added Rh catalyst (30 mg, 0.5 mol%), NaBARF (68 mg, 2.5 mol%), and PhCF₃ (10 mL). After the mixture was stirred for 5 min, trifluoromethyl 4-(tert-butyl)phenyl *N*-triflylhydrazones (1.36 g, 3 mmol, 1.0 equiv), 5-bromo-1*H*-indole (0.878 g, 4.5 mmol, 1.5 equiv), and dry PhCF₃ (50 mL) were added, followed by the addition of NaH (0.48 g, 12 mmol, 4.0 equiv, 60 wt% dispersion in mineral oil) in batches. After transfer out of the glove box, the reaction was continued for an additional 24 h at 40 °C. When the reaction was completed, and filtered through a short pad of silica gel with DCM as an eluent. After removal of the solvent under vacuum, the residue was purified by flash chromatography on silica gel (using petroleum ether/EtOAc as eluent) to obtain the quinolines products **19**. The product was recrystallized from hexane to improve the enantio- purity to 99% ee.



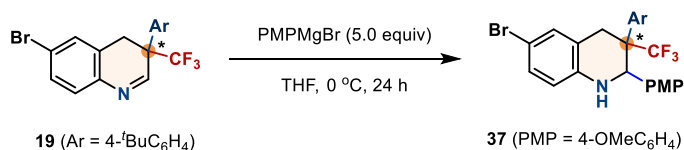
General Procedure B: **19** (82 mg, 0.2 mmol, 1.0 equiv) was solved in methanol (3.0 mL), then NaBH₄ (22.7 mg, 0.6 mmol, 3.0 equiv) was added in one portion. The mixture was stirred for 1 h. When the reaction was completed, a saturated aqueous solution of sodium bicarbonate was added and extracted with EtOAc. The combined organic layers were washed with brine, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (using petroleum ether/EtOAc as eluent) to afford the tetrahydroquinolines.



General Procedure C: According to literature procedure (11), a round bottom flask was filled with **19** (82 mg, 0.2 mmol, 1.0 equiv), benzofuran-2-ylboronic acid (49 mg, 0.3 mmol, 1.5 equiv), Pd(PPh₃)₄ (23 mg, 0.02 mmol, 10 mol%), and Cs₂CO₃ (92 mg, 0.28 mmol, 1.4 equiv), which toluene (2.0 mL) and THF (0.5 mL) were subsequently added into. Then, the reaction mixture was heated at 100 °C until the reaction was completed (12 h). The reaction mixture was then cooled to ambient temperature and quenched with saturated NH₄Cl solution. Aqueous phase was extracted with EtOAc (10 mL ×3), and the combined organic phases were washed with brine (10 mL), dried over Na₂SO₄, filtrated and concentrated under reduced pressure to afford the crude derivatives. The crude mixture was purified by flash chromatography on silica gel (pre-neutralized with trimethylamine, using petroleum ether/EtOAc as eluent) to obtain the product **35**.

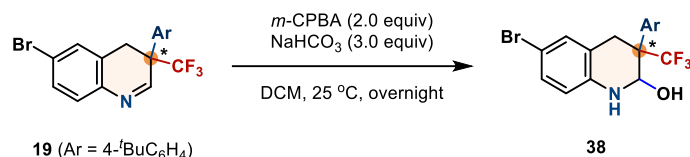


General Procedure D: According to literature procedure (12), 2-methyl-2-butene (220 µl, 2.0 mmol, 10.0 equiv) and sodium chlorite (113 mg, 1.0 mmol, 5.0 equiv) was added to a solution of compound **19** (82 mg, 0.2 mmol, 1.0 equiv) in THF (2.0 ml). The mixture was stirred for 10 min before an aqueous solution of sodium dihydrogen phosphate (1 M, 300 µl, 0.3 mmol, 1.5 equiv) was added dropwise at ambient temperature. When the reaction was completed, removing the solvent before EtOAc was added. The organic phase was washed with aqueous solution of sodium thiosulfate (10%) and brine, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (using petroleum ether/EtOAc as eluent) to afford the product **36**.

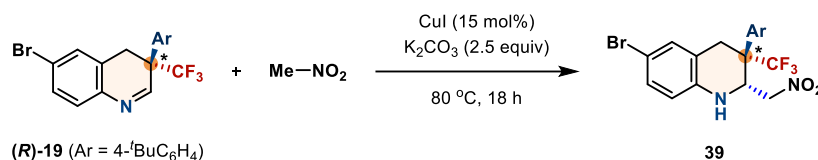


General Procedure E: According to literature procedure(13), to a flame dried 25 mL round bottom flask, a solution of compound **19** (82 mg, 0.2 mmol, 1.0 equiv) in THF (2.0 ml) were added under

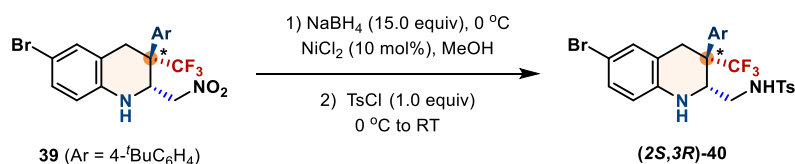
argon. Then PMPMgBr (1 mL, 1 M in THF, 5.0 equiv) was added to the system slowly at 0 °C . The mixture was stirred at 0 °C for 12 h. When the reaction was completed, saturated NH₄Cl solution (5 mL) was added to quench the reaction. Aqueous phase was extracted with EtOAc (3×5 mL), and the combined organic phases were washed with brine (10 mL), dried over Na₂SO₄, filtrated and concentrated under reduced pressure to afford the crude derivative. The mixture was purified by flash chromatography on silica gel to obtain the product **37**.



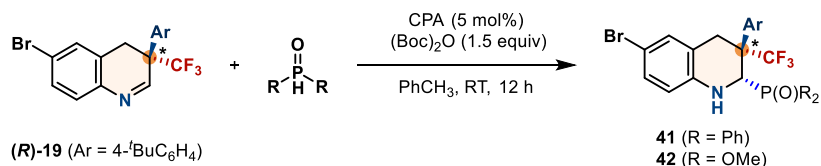
General Procedure F: According to literature procedure(14), to a flame dried 25 mL round bottom flask, *m*-CPBA (*m*-chloroperbenzoic acid, 70 mg, 0.4 mmol, 2.0 equiv), NaHCO₃ (50 mg, 0.6 mmol, 3.0 equiv) and **19** (82 mg, 0.2 mmol, 1.0 equiv) were added under argon, followed by 2.5 mL of anhydrous DCM (3.0 mL). The mixture was stirred at 25 °C overnight. When the reaction was completed, and filtered through a short pad of silica gel with DCM as an eluent. After removal of the solvent under vacuum, the residue was purified by flash chromatography on silica gel (using petroleum ether/EtOAc as eluent) to obtain the product **38**.



General Procedure G: According to literature procedure (15), a mixture of **(R)-19** (82 mg, 0.2 mmol, 1.0 equiv), K₂CO₃ (69 mg, 0.5 mmol, 2.5 equiv), and CuI (6.0 mg, 0.045 mmol, 15 mol%) in nitromethane (2.0 mL) was stirred at 80 °C under N₂ for 18 h. After cooling down to room temperature, the resulting mixture was concentrated by removing the solvent under vacuum, and the residue was purified by flash chromatography on silica gel (using petroleum ether/EtOAc as eluent) to afford **(2S,3R)-39**.

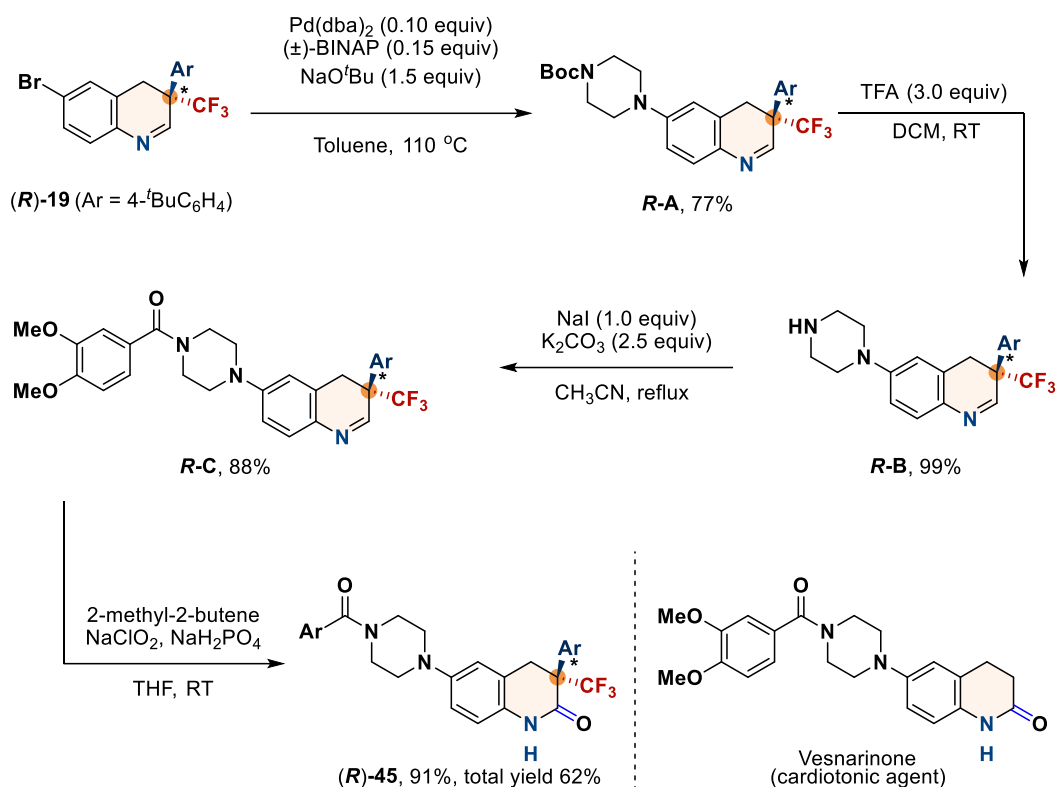


General Procedure H: In an oven-dried round bottomed flask, **39** (76 mg, 0.2 mmol, 1.0 equiv) and NiCl₂ (3 mg, 0.02 mmol, 0.1 equiv) were dissolved in anhydrous MeOH (3 mL). Then NaBH₄ (114 mg, 3 mmol, 15.0 equiv) was added at 0 °C, and the reaction was stirred at 0 °C for 3 h. The mixture was filtered and washed with DCM/acetone (1:1). The combined filtrate was removed under reduced pressure. The residue was directly dissolved in anhydrous DCM (3 mL). The mixture was cooled down to 0 °C and TsCl (76 mg, 0.4 mmol, 2 equiv) was slowly added at the same temperature. The mixture was allowed to warm up to room temperature. After being stirred for 2 h, water (3 mL) was added. The resulted mixture was extracted with DCM (5 mL x 3). The combined organics were washed with brine (15 mL), dried over Na₂SO₄, and concentrated. Purification by flash chromatography on silica gel (using petroleum ether/EtOAc as eluent) to afford **(2S,3R)-40**.



General Procedure I: According to literature procedure (16), a mixture of **(R)-19** (82 mg, 0.2 mmol, 1.0 equiv), CPA catalyst (5 mol%), (Boc)₂O (65 mg, 0.3 mmol, 1.5 equiv), and diphenylphosphine oxide or dimethyl phosphite (0.24 mmol, 1.2 equiv) in PhCH₃ (5 mL) was stirred at room temperature for 12 h. The reaction mixture was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (using petroleum ether/EtOAc as eluent) to afford the product **(2R,3S)-41** or **(2R,3S)-42**.

4.3. Preparation of Vesnarinone Analogue



Supplementary Fig. S2. Preparation of vesnarinone analogue (R)-45

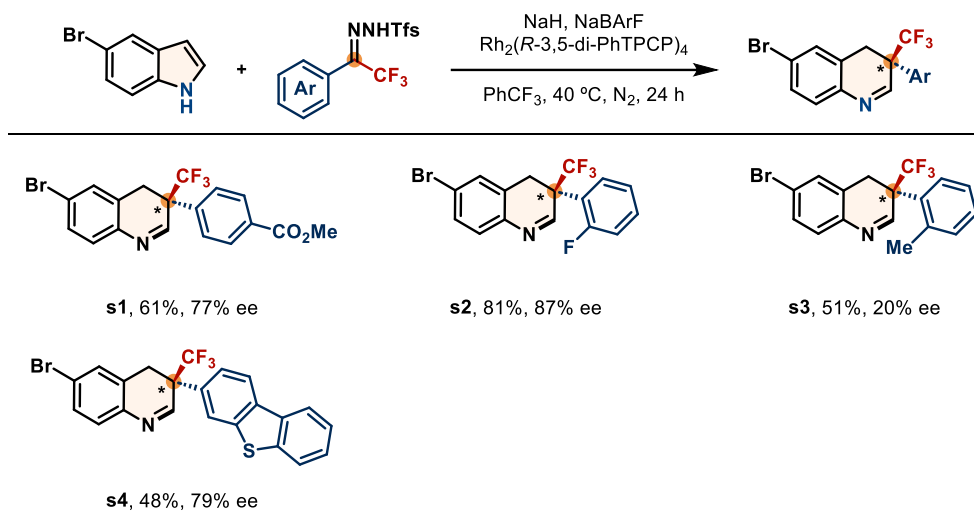
General Procedure J: A round bottom flask was charged with Pd(dba)₂ (12 mg, 0.02 mmol, 10 mol%), (±)-BINAP (18.6 mg, 0.03 mmol, 15 mol%) and NaO^tBu (29 mg, 0.3 mmol, 1.5 equiv) under N₂ atmosphere. A solution of **(R)-19** (82 mg, 0.2 mmol, 1.0 equiv) in dry toluene was added, followed by the 1-Boc-piperazine (22 mg, 0.22 mmol, 1.1 equiv). The resulting mixture was stirred at 110 °C until the reaction was completed (16 h). The reaction mixture was allowed to cool to ambient temperature and diluted with DCM (5 mL). The solids filtered off on celite and washed twice with DCM (2 × 5 mL). The combined filtrate was evaporated under reduced pressure to afford the crude product, which was purified by flash chromatography on silica gel (pre-neutralized with trimethylamine, using petroleum

ether/EtOAc as eluent) to obtain the product **R-A** in 77% yield. Then **R-A** was treated with acetic acid in dichloromethane to give **R-B** in quantitative yield.

General Procedure K: a round bottom flask was filled with NaI (30 mg, 0.2 mmol, 1.0 equiv), K₂CO₃ (69 mg, 0.5 mmol, 2.5 equiv) and **R-B** (83 mg, 0.2 mmol, 1.0 equiv) and placed under inert atmosphere. MeCN (1 mL) was added. Then a solution of 3,4-dimethoxybenzoyl chloride (48 mg, 0.24 mmol, 1.2 equiv) in MeCN was added dropwise at room temperature. The resulting mixture was then remained reflux for 12 h. After cooling down to room temperature, the resulting mixture was concentrated by removing the solvent under vacuum, and the residue was purified by flash chromatography on silica gel (using petroleum ether/EtOAc as eluent) to afford **R-C**.

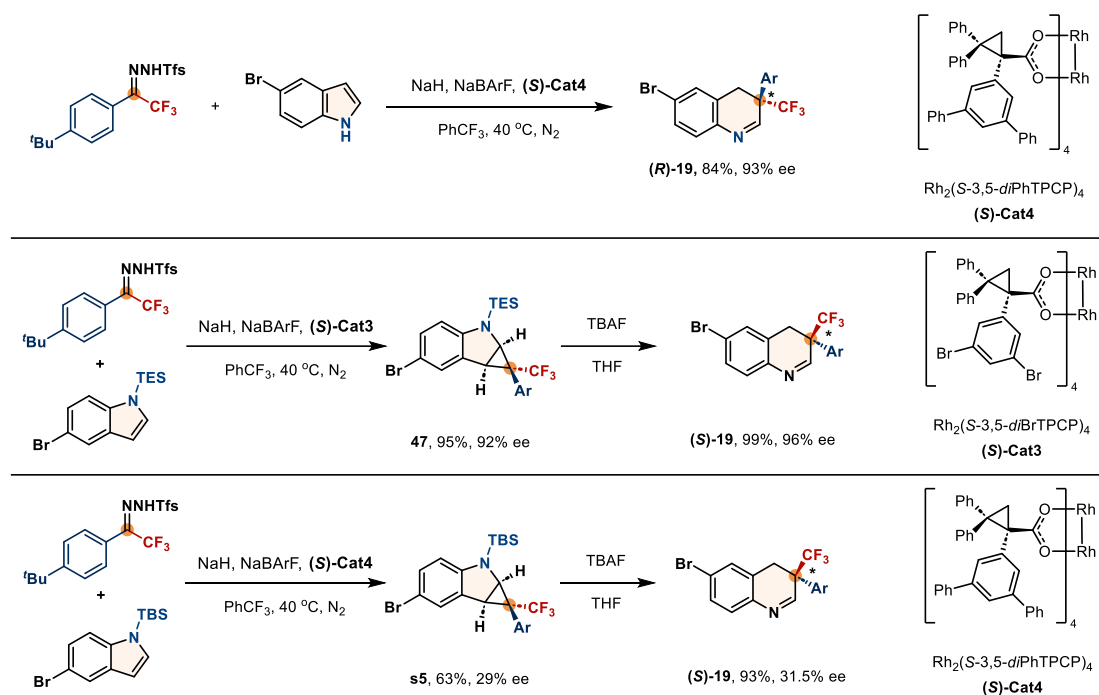
General Procedure L: 2-methyl-2-butene (220 μ L, 2.0 mmol, 10.0 equiv) and sodium chlorite (80%, 113 mg, 1.0 mmol, 5.0 equiv) was added to a solution of compound **R-C** (116 mg, 0.2 mmol, 1.0 equiv) in THF (2.0 mL). The mixture was stirred for 10 min before an aqueous solution of sodium dihydrogen phosphate (1 M, 300 μ L, 0.3 mmol, 1.5 equiv) was added dropwise at ambient temperature. When the reaction was completed, removing the solvent before EtOAc was added. The organic phase was washed with aqueous solution of sodium thiosulfate (10%) and brine, dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product was purified by flash chromatography on silica gel (using petroleum ether/EtOAc as eluent) to afford the product (**R**)-**45**.

4.4 Substrates Ineffective for One-Carbon Insertion of Indoles



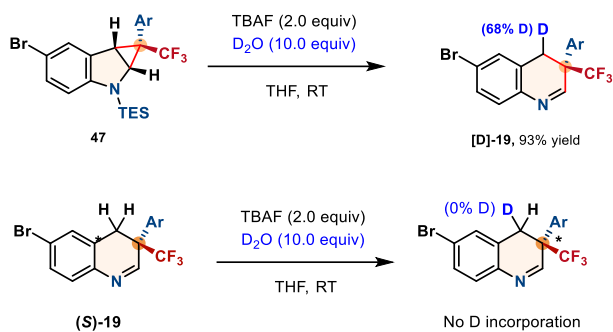
Supplementary Fig. S3. Ineffective examples

5. Mechanistic Considerations

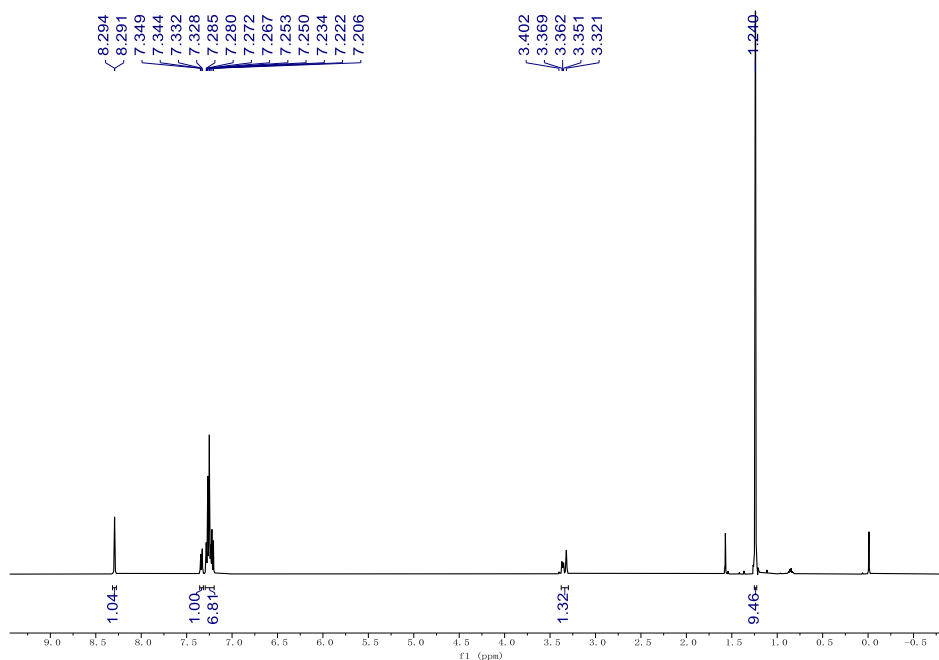


Supplementary Fig. S4. Reaction between *N*-protected indole and *N*-triftosylhydrazones. The reactions of *N*-triftosylhydrazone reacted with TES- and TBS-protected indoles yielded cyclopropanes in 92% ee and 29% ee, respectively. Deprotection of two cyclopropane intermediates gave configuration-preserved products with 96% and 31.5% ee.

General Procedure: To an oven-dried screw-cap reaction tube equipped with a Teflon-coated magnetic stir bar were added Rh catalyst (1 mol%), NaBARF (5 mol%), and PhCF₃ (1.0 mL) inside a glove box with nitrogen atmosphere. After the mixture was stirred for 5 min, trifluoromethyl 4-(tert-butyl)phenyl *N*-triftosylhydrazones (0.2 mmol, 1.0 equiv), NaH (4.0 equiv), *N*-protected indoles (0.3 mmol, 1.5 equiv), and PhCF₃ (3 mL) were added. The reaction was continued for an additional 24 h at 40 °C after transfer out of the glove box. When the reaction was completed, and filtered through a short pad of silica gel with DCM as an eluent. After removal of the solvent under vacuum, tetrabutylammonium fluoride (0.4 mmol, 2.0 equiv, 1M in THF) and dry THF (3 mL) were added and the mixture was stirred at room temperature for 1 hour. Then the yields of product were determined by isolated.



Supplementary Fig. S5. Deprotection of cyclopropene in presence of D₂O. The reaction of **47** with TBAF in D₂O yielded the C4-deuterated ring-expansion product **[D]-19**, implying that a carbanion intermediate may be involved in the ring-opening process. No D incorporation was detected when exposure of 3,4-dihydroquinoline **(S)-19** to TBAF and D₂O.

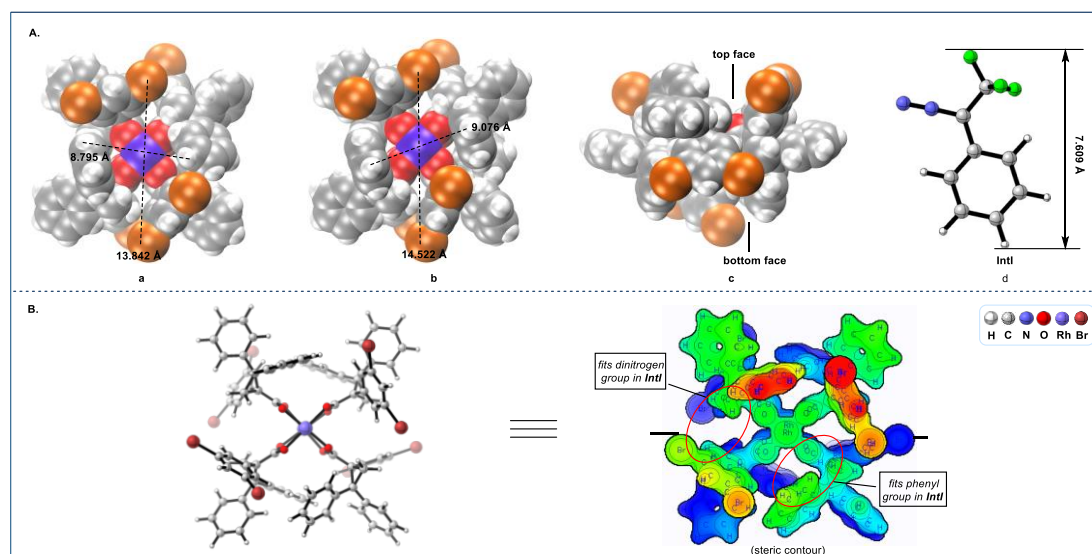


Supplementary Fig. S6. ¹H NMR spectrum of [D]-19

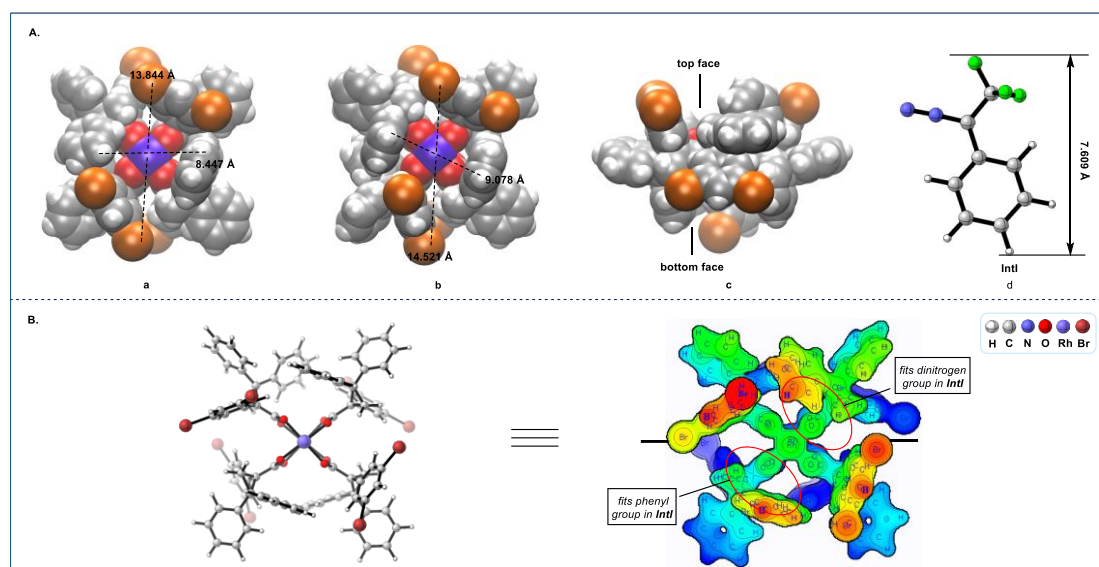
6. Computational Details

DFT Methods

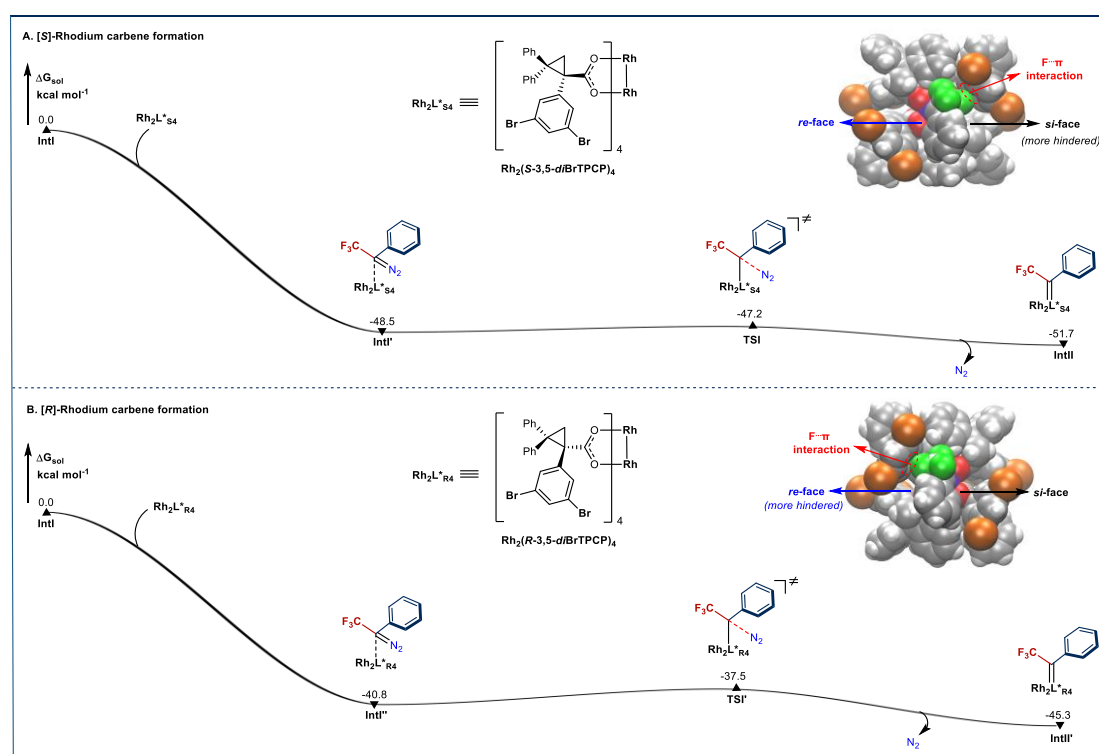
The quantum chemical calculations described in this work were carried out with Gaussian16 package (17). Due to the large reaction system, the density functional calculations (DFT) are highly time-consuming. Thus geometry optimizations were conducted at the BLYP (18,19) level. The effective core potential SDD (20,21) basis set was used to represent Rh and Br atoms, all the other atoms were described with 3-21G basis set (22). The nature of the local minima was established with analytical frequencies calculations and geometry optimizations were computed without any symmetry constraints. Intrinsic reaction coordinate (IRC) (23,24) calculations were carried out to ascertain the true nature of the transition states. Single-point solvation energies were calculated at the B3LYP (25,26) -GD3(BJ) (27)/6-31G(d,p) (28-30) level (SDD for Rh and Br) with the SMD (31) (solvation-model density) implicit continuum solvent model (CH₂Cl₂ solvent) on BLYP-optimized geometries. 3D structures of optimized geometries were generated using CYLview visualization software (32).



Supplementary Fig. S7. Structural information about the dirhodium catalyst $\text{Rh}_2(\text{S-diBrTPCP})_4$. (A) The calculated vDW structure of $\text{Rh}_2(\text{S-diBrTPCP})_4$. The atoms in the structure are colour-coded: rhodium (purple), oxygen (red), carbon (silver), hydrogen (white) and bromine (orange). Both faces of the dirhodium catalyst are the same, which limits the number of possible orientations of the diazo compound **IntI** when it binds to the dirhodium core. The length of the diazo compound **IntI** (7.609 Å) indicates that it can bind to the dirhodium core smoothly. (B) Steric environment of $\text{Rh}_2(\text{S-diBrTPCP})_4$ and favorable ligand-substrate arrangement in forming the carbene. The bulky benzene ring of diazo compound **IntI** is on the less encumbered face of catalyst.

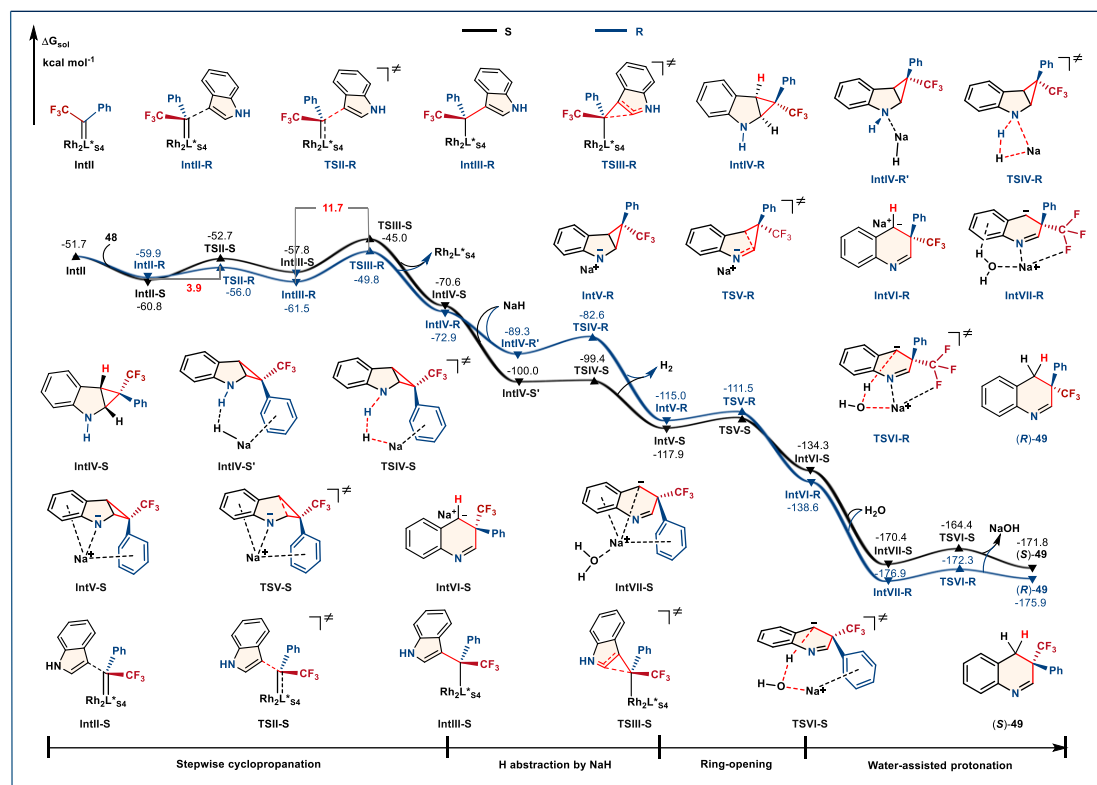


Supplementary Fig. S8. Structural information about the dirhodium catalyst $\text{Rh}_2(\text{R-diBrTPCP})_4$. (A) The calculated vDW structure of $\text{Rh}_2(\text{R-diBrTPCP})_4$. The atoms in the structure are colour-coded: rhodium (purple), oxygen (red), carbon (silver), hydrogen (white) and bromine (orange). Both faces of the dirhodium catalyst are the same, which limits the number of possible orientations of the diazo compound **IntI** when it binds to the dirhodium core. The length of the diazo compound **IntI** (7.609 Å) indicates that it can bind to the dirhodium core smoothly. (B) Steric environment of $\text{Rh}_2(\text{R-diBrTPCP})_4$ and favorable ligand-substrate arrangement in forming the carbene. The bulky benzene ring of diazo compound **IntI** is on the less encumbered face of catalyst.

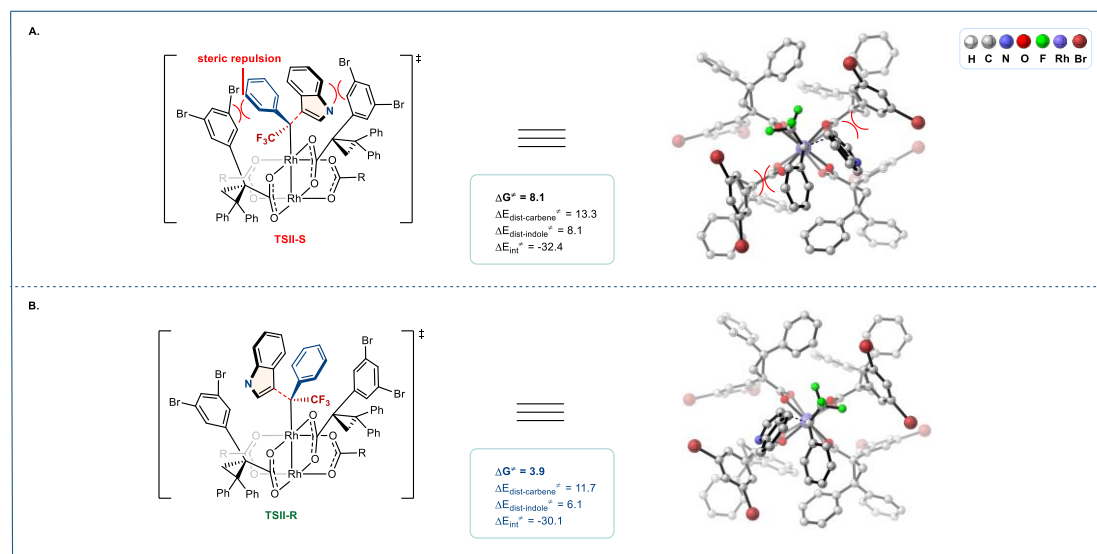


Supplementary Fig. S9. The generations of chiral Rh-carbenes. (A) The formation of (S)-rhodium carbene **IntII** from $\text{Rh}_2(\text{S-diBrTPCP})_4$. $\text{F}\cdots\pi$ interaction in *si*-face leads to a more hindered environment of *si*-face and the carbene *re*-face would be attacked predominantly. (B) The formation of (R)-rhodium carbene **IntII'** from $\text{Rh}_2(\text{R-diBrTPCP})_4$. $\text{F}\cdots\pi$ interaction in *re*-face leads to a more hindered environment of *re*-face and the carbene

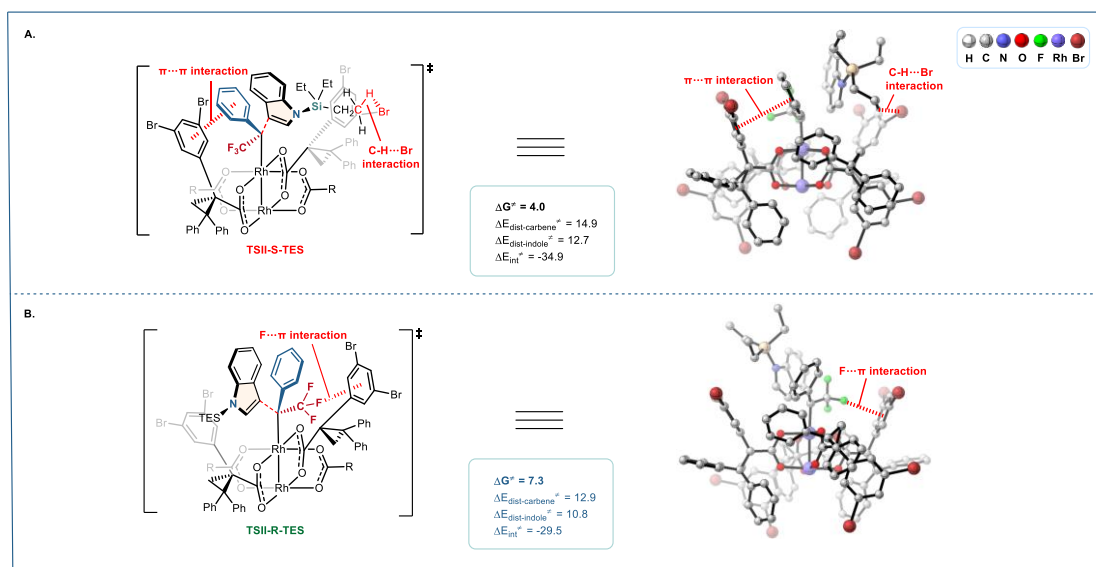
si-face would be attacked predominantly. The observed *re* attack is from the left, *si* attack from the right.



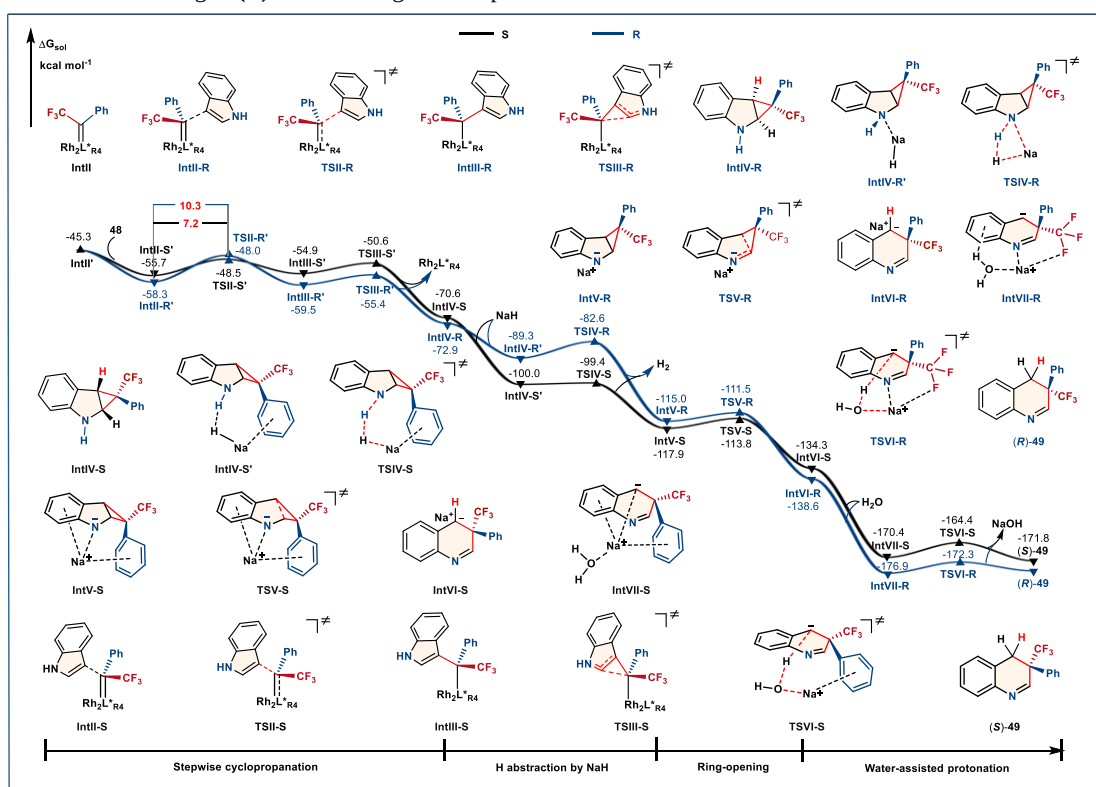
Supplementary Fig. S10. Energy profile for $\text{Rh}_2(\text{S-diBrTPCP})_4$ catalysed enantioselective dearomative one-carbon insertion of indole. In the process of $\text{Rh}_2(\text{S-diBrTPCP})_4$ catalysed enantioselective dearomative one-carbon insertion of indole, nucleophilic attack of C3-indole on [S]-rhodium carbene was entio-determining step. The Gibbs free energy barriers for this step leading to (R)-49 and (S)-49 are 3.9 kcal mol⁻¹ (TSII-R) and 8.1 kcal mol⁻¹ (TSII-S) respectively. Zwitterionic-type cyclopropanation was rate-determining step, Gibbs free energy barriers for this step are 11.7 kcal mol⁻¹ (TSIII-R) and 15.8 kcal mol⁻¹ (TSIII-S) respectively.



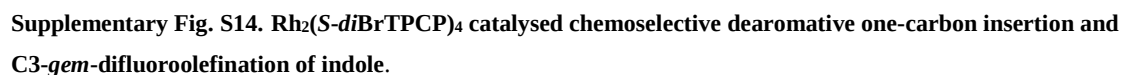
Supplementary Fig. S11. D/I analysis for optimized entio-determining transition states for the reaction of NH indoles with $\text{Rh}_2(\text{S-diBrTPCP})_4$ catalyst. (A) TSII-S leading to (S)-49. (B) TSII-R leading to (R)-49. All energies are reported in kcal mol⁻¹.



Supplementary Fig. S12. D/I analysis for optimized enantio-determining transition states for the reaction of *N*-TES protected indoles with $\text{Rh}_2(\text{S-diBrTPCP})_4$ catalyst. (A) TSII-S-TES leading to (*S*)-19. (B) TSII-R-TES leading to (*R*)-19. All energies are reported in kcal mol⁻¹.



Supplementary Fig. S13. Energy profile for $\text{Rh}_2(\text{R-diBrTPCP})_4$ catalysed enantioselective dearomative one-carbon insertion of indole. In the process of $\text{Rh}_2(\text{R-diBrTPCP})_4$ catalysed enantioselective dearomative one-carbon insertion of indole, nucleophilic attack of C3-indole on [R]-rhodium carbene was both the enantio-determining and rate-determining step. The Gibbs free energy barriers for this step leading to (*R*)-49 and (*S*)-49 are 10.3 kcal mol⁻¹ (TSII-R') and 7.2 kcal mol⁻¹ (TSII-S') respectively.



Cartesian coordinates are given in Å, self-consistent field (SCF) Gibbs free energies (G) are given in Hartrees, and imaginary vibrational frequencies (ν) are given in cm^{-1} .

IntI (G = -716.791764)

C	-0.72451100	0.46866500	0.07404900
N	-1.19583500	1.69642600	0.11946900
N	-1.57264800	2.80488400	0.16643700
C	0.72593200	0.20686100	0.04443900
C	1.21555000	-1.11777600	0.18864000
C	1.65762400	1.26305700	-0.12122100
C	2.59483700	-1.36863600	0.14426600
H	0.51384300	-1.92922100	0.35388500
C	3.03500500	1.00218200	-0.15399100
H	1.30069300	2.28823000	-0.23341100
C	3.51294700	-0.31613100	-0.02686500
H	2.95277800	-2.39362000	0.25319700
H	3.73530300	1.82853700	-0.28493000
H	4.58411200	-0.51845800	-0.05736100
C	-1.72121800	-0.63917800	-0.05802300
F	-3.01542700	-0.14275800	0.02853700
F	-1.59106600	-1.33291700	-1.25869400
F	-1.55843400	-1.61086900	0.94343700

IntI' (G = -5035.448688)

C	-2.50716800	-1.11485300	-0.15485600
C	-3.89954300	-1.68244700	-0.13392400
C	-4.75341900	-1.36514600	-1.38538800
H	-5.81364200	-1.18072000	-1.21917500
H	-4.26519700	-0.73121000	-2.12331000
C	-4.25221200	-2.79631700	-1.25331800
C	-3.18163700	-3.26950300	-2.22561800
C	-3.34868900	-3.00408500	-3.60390700
H	-4.20860700	-2.42011100	-3.93658000
C	-2.41894300	-3.47981100	-4.54436100
H	-2.55984900	-3.26282700	-5.60479600
C	-1.31107300	-4.23763900	-4.11867700
H	-0.58993000	-4.61152400	-4.84810700
C	-1.14315000	-4.51131400	-2.74880800
H	-0.29295700	-5.10078900	-2.40376300
C	-2.07084500	-4.03208800	-1.80627100
H	-1.91441800	-4.24279100	-0.74766800
C	-5.25683200	-3.86732100	-0.85228000
C	-4.86790600	-4.95918200	-0.04148100
H	-3.84332300	-5.02655700	0.32396100
C	-5.79029400	-5.96434700	0.29528800
H	-5.47573300	-6.79592300	0.92833600
C	-7.11443700	-5.90203000	-0.17953700
H	-7.82967100	-6.68255800	0.08413300
C	-7.50696300	-4.82930700	-0.99923400
H	-8.52761300	-4.77678400	-1.38180500
C	-6.58448900	-3.82029100	-1.33292000
H	-6.89477200	-2.99914100	-1.98067000
C	-4.56011100	-1.74612300	1.22458100
C	-3.97700400	-2.50922200	2.26877300
H	-3.05672200	-3.05820900	2.09249000
C	-4.58506500	-2.51131000	3.52607000
C	-5.76280100	-1.80327200	3.81493200
C	-6.31110600	-1.05990800	2.76300500
C	-5.73808500	-1.00964100	1.48641400
H	-6.19218800	-0.40048800	0.70872600
C	1.39507800	-2.17084300	-0.27797200
C	2.51978300	-3.18639000	-0.37734700
C	2.30631400	-4.71615400	0.18847400
C	3.10318400	-3.66116600	0.96063400
H	2.65959600	-3.20909800	1.84512400
H	4.17878400	-3.82533000	1.01696600
C	3.43126400	-2.99680500	-1.57798100

C	2.89551000	-2.93567200	-2.89318700
H	1.82163400	-2.98824200	-3.04243300
C	3.76409900	-2.77782000	-3.97504000
C	5.15813000	-2.67457500	-3.83813800
C	5.65359200	-2.72728200	-2.52960400
C	4.83168600	-2.87991300	-1.40669600
H	5.27388900	-2.90685000	-0.41466000
C	3.13841100	-5.77590300	-0.52027500
C	2.90182500	-6.12836100	-1.86893400
H	2.15042500	-5.58494000	-2.44182000
C	3.63931300	-7.15831900	-2.48028300
H	3.45102700	-7.41222500	-3.52475100
C	4.62130600	-7.85434200	-1.75031600
H	5.19645700	-8.65005300	-2.22593200
C	4.85637000	-7.51898700	-0.40410000
H	5.61054200	-8.05890000	0.17068700
C	4.11737700	-6.48949800	0.20682400
H	4.29209100	-6.24191700	1.25525200
C	0.95966300	-5.20130700	0.70366600
C	0.30885400	-4.58025600	1.79564300
H	0.73221300	-3.70088800	2.26376700
C	-0.89757100	-5.09408200	2.30436300
H	-1.36123300	-4.59794000	3.15657600
C	-1.48462000	-6.23959200	1.73574000
H	-2.40954200	-6.64724200	2.14783100
C	-0.85057000	-6.86614200	0.64621000
H	-1.28563900	-7.76089200	0.19799800
C	0.35827700	-6.35794000	0.14114600
H	0.85901100	-6.87847100	-0.67292800
C	2.33797500	1.14961400	-0.19325200
C	3.79059100	1.54675500	-0.21209800
C	4.63015000	0.82237300	-1.30964900
H	5.61215700	0.47202600	-0.99606000
H	4.06578400	0.15997400	-1.96325600
C	4.39467700	2.31410600	-1.49561900
C	3.45934300	2.72526700	-2.62482000
C	2.35229100	3.57212600	-2.41183500
H	2.10247900	3.87429200	-1.39488100
C	1.54732000	3.98720600	-3.48767600
H	0.68876000	4.63670200	-3.30402000
C	1.84049900	3.55698700	-4.79524500
H	1.21269600	3.87193000	-5.63043100
C	2.94814500	2.71617200	-5.01822900
H	3.18351600	2.37867200	-6.02904800

C	3.75516000	2.30851700	-3.94111800
H	4.61502600	1.65962500	-4.11715800
C	5.54705700	3.29286600	-1.26942500
C	5.30315000	4.68733800	-1.35015700
H	4.30511600	5.03950200	-1.61019200
C	6.33479700	5.61695900	-1.13805300
H	6.12183900	6.68513400	-1.20667100
C	7.64058900	5.17447900	-0.85292300
H	8.44409100	5.89477500	-0.69311400
C	7.90123700	3.79440400	-0.78968600
H	8.91142600	3.43692100	-0.58391100
C	6.86592900	2.86396100	-0.99522000
H	7.09957100	1.80134500	-0.94553500
C	4.41599500	1.69069800	1.15813000
C	4.74788200	2.94477400	1.71386600
H	4.58132400	3.85624100	1.14814500
C	5.33122600	2.98611900	2.98566200
C	5.59247300	1.84024000	3.74812000
C	5.23180600	0.61232200	3.17124100
C	4.65863700	0.50981100	1.90284200
H	4.37798900	-0.45822200	1.49103200
C	-1.59715900	2.26198700	-0.14582600
C	-2.72657400	3.26829500	-0.22354900
C	-2.55065700	4.77277300	0.30822200
C	-3.34687900	3.73368900	1.10245300
H	-2.87374500	3.33767000	1.99890000
H	-4.43129900	3.82655700	1.14245800
C	-3.62769300	3.04903700	-1.42476500
C	-4.94380900	2.56687200	-1.24767600
H	-5.32162600	2.35283600	-0.25016700
C	-5.75219000	2.36239900	-2.37332300
C	-5.31298100	2.60426900	-3.68081300
C	-3.99362000	3.06635000	-3.82039500
C	-3.14594200	3.29276300	-2.73379900
H	-2.12661700	3.63373300	-2.88513100
C	-3.29469500	5.84623900	-0.47507200
C	-4.62618900	6.21106200	-0.17935200
H	-5.15675100	5.72607800	0.64018300
C	-5.27890100	7.21231800	-0.92324900
H	-6.30704900	7.48272700	-0.67742300
C	-4.61010100	7.86384000	-1.97406700
H	-5.11725400	8.63732800	-2.55237800
C	-3.27701600	7.51745500	-2.26946200
H	-2.74606100	8.02503500	-3.07639700

C	-2.62507600	6.52236300	-1.52359500
H	-1.58460200	6.27561800	-1.73925400
C	-1.22685400	5.25998000	0.87140900
C	-1.26395500	6.12400700	1.99206100
H	-2.22321800	6.34333500	2.46385200
C	-0.08730700	6.71735700	2.47736000
H	-0.13231900	7.38978700	3.33568900
C	1.14765300	6.45321700	1.85049200
H	2.06230300	6.92181600	2.21797500
C	1.19410300	5.58372200	0.74643300
H	2.14854900	5.37228000	0.26192300
C	0.01334500	4.99138200	0.25480700
H	0.05300800	4.31848100	-0.60279000
O	1.12841200	-1.66083600	0.90931500
O	0.79850800	-1.79636400	-1.38979900
O	1.71386700	1.12137900	0.97312100
O	1.79658400	0.79992000	-1.34125700
O	-1.28315100	1.75040100	1.03243800
O	-1.03764200	1.90160400	-1.27980600
O	-1.86291600	-1.02111600	0.99756900
O	-2.01572800	-0.73343400	-1.31179400
Rh	-0.07903800	0.03985200	1.08720800
Rh	-0.11243500	0.05229100	-1.37006700
C	-0.10519400	0.08746900	3.46228900
N	-1.47545300	0.35797300	3.53654200
N	-2.57588300	0.68745000	3.43564300
C	0.71561700	1.20091400	4.08823100
C	1.49793300	0.96767300	5.24599300
C	0.64137300	2.50527400	3.54814800
C	2.22618700	2.01990600	5.82336400
H	1.51550800	-0.01723000	5.70256700
C	1.35612900	3.55482500	4.14668200
H	0.03561700	2.69054600	2.66326400
C	2.15517000	3.31580400	5.28003500
H	2.83163300	1.82744200	6.71061300
H	1.29227800	4.55151000	3.71245300
H	2.71683800	4.13248000	5.73596600
C	0.17138300	-1.33611800	3.89039100
F	-0.73154700	-2.22938600	3.29351800
F	1.47162900	-1.71212500	3.55627900
F	0.04546300	-1.55207900	5.27820700
H	5.81328700	-2.56132600	-4.69805900
Br	2.99470100	-2.70465200	-5.82469700
Br	7.63643000	-2.56908600	-2.25429200

Br	5.55866000	-1.06432700	4.22570300
Br	5.83564600	4.77033300	3.75801000
H	6.04935400	1.89778900	4.73255100
Br	-7.62818400	1.69851300	-2.10408600
Br	-3.31020400	3.42143000	-5.66900500
H	-5.95733300	2.44556100	-4.54189000
H	-6.21948900	-1.82850800	4.80102700
Br	-7.98459600	-0.00879600	3.11127900
Br	-3.73606300	-3.55240400	5.01855000

TSI (G = -5035.446538)

C	2.50165100	-1.14641800	0.17290900
C	3.88934000	-1.72245100	0.15619600
C	4.75810300	-1.38496600	1.39209300
H	5.81487400	-1.19915900	1.20551600
H	4.27885700	-0.74353100	2.12962200
C	4.25299100	-2.81759700	1.28673000
C	3.19133400	-3.26856400	2.27924900
C	3.41172400	-3.03920800	3.65644000
H	4.30727400	-2.50141200	3.97291900
C	2.48954000	-3.49203800	4.61536200
H	2.67123300	-3.30338400	5.67498300
C	1.33589600	-4.19009100	4.20904500
H	0.61969800	-4.54501700	4.95266300
C	1.11481900	-4.42776200	2.84017900
H	0.22781200	-4.96969300	2.51017300
C	2.03517600	-3.97127600	1.87914700
H	1.83592000	-4.14761800	0.82123300
C	5.24394200	-3.90216400	0.88685400
C	4.80934200	-5.04336500	0.17213600
H	3.76070300	-5.14084000	-0.10861900
C	5.71529500	-6.06041200	-0.17245100
H	5.36396200	-6.93066600	-0.72967800
C	7.07003000	-5.96142600	0.19899900
H	7.77253000	-6.75164200	-0.06995800
C	7.50892500	-4.83997000	0.92412800
H	8.55379800	-4.75851200	1.22819300
C	6.60237100	-3.81891300	1.26541000
H	6.95189700	-2.96110800	1.84130100
C	4.53656400	-1.80334300	-1.20735200
C	3.99550700	-2.64920200	-2.20769400
H	3.11870400	-3.25332300	-1.99269200
C	4.58792400	-2.66452500	-3.47247100
C	5.70499000	-1.88262500	-3.80949800

C	6.20943000	-1.05381600	-2.80011300
C	5.65301800	-0.99365000	-1.51665800
H	6.07051200	-0.32370400	-0.76859100
C	-1.41567200	-2.15695100	0.30077600
C	-2.55367300	-3.15748900	0.40457800
C	-2.34721200	-4.70023400	-0.12661500
C	-3.12319900	-3.65411100	-0.93143800
H	-2.66346600	-3.22317600	-1.81805100
H	-4.19941700	-3.80970200	-0.99933500
C	-3.47921900	-2.93225600	1.58820700
C	-2.96019400	-2.84237800	2.90853300
H	-1.88866800	-2.89773000	3.07256700
C	-3.84127400	-2.65181100	3.97491000
C	-5.23266300	-2.54223100	3.81727600
C	-5.71156900	-2.62381300	2.50401500
C	-4.87655000	-2.80999100	1.39593300
H	-5.30644000	-2.85922900	0.39935700
C	-3.19845400	-5.73785700	0.59201100
C	-2.98862200	-6.05987200	1.95265300
H	-2.24503700	-5.50707300	2.52682700
C	-3.74336000	-7.07108100	2.57424100
H	-3.57560000	-7.30149100	3.62761400
C	-4.71626700	-7.77825400	1.84289500
H	-5.30481800	-8.55935100	2.32629100
C	-4.92512900	-7.47284500	0.48524600
H	-5.67234900	-8.02149500	-0.09035800
C	-4.16887400	-6.46224100	-0.13591000
H	-4.32321800	-6.23783800	-1.19272700
C	-0.99755500	-5.20811900	-0.61161700
C	-0.33613900	-4.63030100	-1.72084100
H	-0.75630900	-3.77342800	-2.23178500
C	0.87412600	-5.16526300	-2.19805000
H	1.34786700	-4.70029400	-3.06214400
C	1.45239900	-6.29052900	-1.58212400
H	2.37960300	-6.71561300	-1.97085300
C	0.80699800	-6.87440400	-0.47551900
H	1.23509200	-7.75321400	0.00944800
C	-0.40394500	-6.34357500	0.00015400
H	-0.91295700	-6.83147400	0.82920700
C	-2.31616200	1.17546800	0.18404100
C	-3.76459500	1.58951700	0.19902000
C	-4.60566500	0.90532300	1.32018800
H	-5.59415100	0.55876500	1.02337200
H	-4.04437200	0.25360100	1.98709500

C	-4.35144500	2.39851600	1.46605700
C	-3.40145300	2.82748900	2.57593000
C	-2.28951800	3.65926600	2.33088300
H	-2.04894100	3.93554800	1.30426500
C	-1.46993100	4.09354300	3.38796100
H	-0.60851300	4.73190200	3.17999900
C	-1.75272200	3.69749900	4.70853200
H	-1.11328600	4.02693000	5.52917200
C	-2.86476900	2.87173900	4.96329100
H	-3.09187300	2.56033400	5.98430700
C	-3.68670200	2.44525100	3.90490800
H	-4.54988600	1.80808200	4.10567200
C	-5.49326900	3.38489100	1.21995600
C	-5.23632700	4.77815000	1.27860400
H	-4.23600200	5.12506500	1.53656400
C	-6.25829600	5.71406500	1.04770300
H	-6.03514700	6.78109100	1.09995400
C	-7.56727000	5.27973700	0.76515700
H	-8.36327500	6.00501200	0.59097800
C	-7.84094200	3.90131300	0.72320200
H	-8.85377600	3.55017800	0.51950300
C	-6.81548600	2.96450700	0.94755800
H	-7.05953900	1.90365400	0.91354700
C	-4.39740400	1.70911400	-1.16973900
C	-4.70490400	2.95535200	-1.75657800
H	-4.50964000	3.87748300	-1.21781100
C	-5.30170000	2.97614500	-3.02250100
C	-5.60084400	1.81632400	-3.74932400
C	-5.26294600	0.59616200	-3.14294900
C	-4.67695300	0.51457000	-1.87872800
H	-4.41643300	-0.44831600	-1.44232900
C	1.64048200	2.22978700	0.11618700
C	2.77969600	3.22411600	0.18448800
C	2.62439500	4.71755600	-0.38745800
C	3.42511700	3.65453300	-1.14218800
H	2.96830200	3.23796500	-2.03709800
H	4.51081300	3.73879800	-1.16312500
C	3.66000900	3.02859700	1.40523000
C	4.97642400	2.53639200	1.26046200
H	5.36914000	2.29833400	0.27423600
C	5.76613700	2.35401700	2.40302900
C	5.30778100	2.62862100	3.69736500
C	3.98909900	3.10081400	3.80533100
C	3.15948900	3.30566600	2.70057700

H	2.13973500	3.65489600	2.82846900
C	3.36408200	5.80421400	0.38173600
C	4.70017000	6.15686100	0.09189000
H	5.23668700	5.65195700	-0.71159200
C	5.34978800	7.17121400	0.82058500
H	6.38159600	7.43179300	0.57955500
C	4.67322500	7.84822400	1.85008800
H	5.17793400	8.63183200	2.41679100
C	3.33560400	7.51415000	2.13909300
H	2.79877100	8.04142200	2.92933700
C	2.68681000	6.50593800	1.40827000
H	1.64308100	6.26866400	1.61873900
C	1.31290300	5.20057300	-0.98174900
C	1.37138600	6.02495100	-2.13091900
H	2.33732200	6.21397800	-2.60219700
C	0.20739100	6.61921100	-2.64511800
H	0.26910300	7.26188800	-3.52494300
C	-1.03596600	6.39568300	-2.01901800
H	-1.94038100	6.86674100	-2.40814700
C	-1.10399900	5.56404800	-0.88711500
H	-2.06500800	5.38358500	-0.40293300
C	0.06394200	4.97081000	-0.36703700
H	0.00749800	4.32738500	0.51198400
O	-1.13744600	-1.66781000	-0.89373300
O	-0.82143500	-1.77567000	1.40995200
O	-1.69385800	1.12585300	-0.98350600
O	-1.77876300	0.83600000	1.33525800
O	1.31789400	1.70648100	-1.05822200
O	1.07266700	1.88978500	1.25029300
O	1.86555100	-1.05674200	-0.98583600
O	2.00809400	-0.75321300	1.32335400
Rh	0.09150000	0.01583800	-1.09940600
Rh	0.11787000	0.06042800	1.37345700
C	0.04959400	-0.01431900	-3.28247300
N	1.60829500	0.29627600	-3.59788900
N	2.55946300	0.90658500	-3.39518400
C	-0.72177600	1.05696600	-4.00357200
C	-1.52115200	0.78028100	-5.14649900
C	-0.62628200	2.39475500	-3.54012400
C	-2.23635000	1.81070200	-5.77345100
H	-1.56684500	-0.22561600	-5.55093300
C	-1.32495700	3.42144200	-4.18891300
H	0.00202500	2.61899700	-2.68050100
C	-2.13816300	3.13329000	-5.30211800

H	-2.85372500	1.58216100	-6.64362700
H	-1.23867500	4.43995800	-3.81339800
H	-2.68842100	3.93371900	-5.79910500
C	-0.10496400	-1.43195500	-3.80999600
F	0.79975300	-2.31288600	-3.20627500
F	-1.40471000	-1.89530900	-3.55461100
F	0.10237100	-1.57403800	-5.19370100
H	-5.89804700	-2.40313000	4.66548100
Br	-3.09443900	-2.53848300	5.83159600
Br	-7.68951800	-2.45855800	2.19921700
Br	-5.64302400	-1.09984600	-4.14708800
Br	-5.76950900	4.75033300	-3.83998000
H	-6.06936800	1.85797900	-4.72911100
Br	7.64242800	1.67465000	2.17930800
Br	3.27987300	3.50414100	5.63405400
H	5.93752900	2.48644100	4.57199800
H	6.15037600	-1.91793100	-4.80045100
Br	7.79146200	0.10696500	-3.22191600
Br	3.81141500	-3.84062900	-4.90128000

IntII (G = -5035.477644)

C	2.50729900	-1.05424300	0.18692900
C	3.90464600	-1.60598100	0.19304900
C	4.73889100	-1.24183500	1.44669000
H	5.79869000	-1.04960600	1.28712900
H	4.23413400	-0.59210900	2.15931500
C	4.25608800	-2.68176600	1.35092900
C	3.17970700	-3.14181300	2.32318600
C	3.32389300	-2.83369100	3.69508700
H	4.17120900	-2.22844300	4.02212700
C	2.38694500	-3.29362100	4.63629200
H	2.50992100	-3.04339600	5.69164400
C	1.29450700	-4.07752700	4.21794600
H	0.56678400	-4.43772800	4.94773100
C	1.14996800	-4.39405700	2.85464900
H	0.31034900	-5.00228100	2.51575100
C	2.08522900	-3.93153100	1.91142200
H	1.94645200	-4.17580000	0.85756400
C	5.27995600	-3.75105300	0.99670100
C	4.91903800	-4.86853900	0.20845500
H	3.90352400	-4.95564500	-0.17726100
C	5.85839200	-5.87262100	-0.08144100
H	5.56567800	-6.72418900	-0.69821400
C	7.17165600	-5.78317900	0.41858500

H	7.90016600	-6.56281900	0.19109300
C	7.53630500	-4.68407900	1.21596700
H	8.54837600	-4.60990000	1.61729600
C	6.59689800	-3.67626500	1.50263300
H	6.88542400	-2.83399900	2.13314100
C	4.58447300	-1.71001000	-1.15349800
C	4.02721800	-2.51734100	-2.17784600
H	3.09665100	-3.05032400	-2.00722000
C	4.67221800	-2.57998600	-3.41529600
C	5.85652700	-1.88252300	-3.70387000
C	6.37199000	-1.08534400	-2.67534800
C	5.76597300	-0.97986600	-1.41765400
H	6.19746000	-0.33345800	-0.65744800
C	-1.37370800	-2.21258000	0.25215100
C	-2.48740300	-3.24165600	0.32937500
C	-2.24049800	-4.76645900	-0.23390100
C	-3.03215200	-3.72236100	-1.02438100
H	-2.57412800	-3.25764700	-1.89489700
H	-4.10355300	-3.90271800	-1.10647700
C	-3.42551800	-3.06227100	1.51068600
C	-2.91641400	-2.96681000	2.83483000
H	-1.84416800	-2.98121700	3.00373600
C	-3.80970700	-2.82615500	3.89893800
C	-5.20371500	-2.77202700	3.73571700
C	-5.67289100	-2.85658500	2.41910500
C	-4.82599900	-2.99436600	1.31316300
H	-5.24907300	-3.04943200	0.31410200
C	-3.07339200	-5.84283400	0.44886200
C	-2.89290800	-6.17804700	1.81041500
H	-2.19076600	-5.60576000	2.41666900
C	-3.62746800	-7.22678500	2.39316100
H	-3.48303500	-7.46749100	3.44769800
C	-4.55033700	-7.95797300	1.62195000
H	-5.12297300	-8.76838300	2.07528100
C	-4.73012400	-7.63835500	0.26329900
H	-5.43870200	-8.20494600	-0.34298800
C	-3.99437100	-6.59043200	-0.31905800
H	-4.12520800	-6.35428600	-1.37650800
C	-0.87139700	-5.22922900	-0.70701700
C	-0.24498500	-4.66306400	-1.84091300
H	-0.71416400	-3.85856200	-2.39311700
C	0.99692100	-5.14525700	-2.29302500
H	1.45088700	-4.68491400	-3.17024600
C	1.63638300	-6.20920700	-1.63127100

H	2.58877800	-6.59425800	-2.00043900
C	1.02092300	-6.78632900	-0.50350400
H	1.49648300	-7.62010400	0.01557200
C	-0.21844900	-6.30498200	-0.04972300
H	-0.70278600	-6.78794400	0.79708800
C	-2.38634300	1.09777100	0.18136600
C	-3.84206500	1.47448600	0.15373900
C	-4.71936900	0.70279700	1.18653000
H	-5.68124800	0.34943500	0.81848500
H	-4.17565000	0.02597800	1.84300400
C	-4.51350100	2.19003300	1.43424900
C	-3.63483200	2.56701200	2.61946900
C	-2.52970100	3.43344200	2.49121200
H	-2.24027500	3.78443200	1.50103800
C	-1.77584200	3.80884600	3.61746300
H	-0.91604900	4.47160100	3.49901300
C	-2.12043600	3.32028800	4.89151400
H	-1.53158400	3.60367200	5.76538400
C	-3.22783600	2.46146700	5.03057300
H	-3.50303500	2.07902700	6.01494800
C	-3.98263800	2.09203000	3.90301800
H	-4.84138800	1.42748800	4.01410400
C	-5.66242900	3.16492500	1.17787500
C	-5.45133700	4.55451600	1.36482000
H	-4.48528700	4.90212500	1.72992800
C	-6.47843200	5.48251000	1.12393400
H	-6.29107200	6.54668500	1.27702600
C	-7.74718900	5.04259100	0.70199300
H	-8.54746000	5.76110500	0.51967700
C	-7.97650900	3.66592500	0.53075000
H	-8.95901900	3.30940400	0.21749500
C	-6.94575000	2.73768500	0.76522600
H	-7.15540400	1.67796400	0.62689400
C	-4.39880400	1.66715200	-1.23995200
C	-4.66450400	2.94502200	-1.77687500
H	-4.51640300	3.83453400	-1.17217900
C	-5.15185500	3.03874900	-3.08573300
C	-5.38293400	1.92205400	-3.90017000
C	-5.09452400	0.66842300	-3.33768000
C	-4.61579800	0.51499300	-2.03501100
H	-4.38245400	-0.47135100	-1.63683900
C	1.49295000	2.30374000	0.15682100
C	2.57134500	3.36281700	0.24827000
C	2.31699600	4.86781900	-0.25155400

C	3.16579700	3.88849700	-1.06576500
H	2.71723200	3.48723100	-1.97148400
H	4.24445900	4.03495800	-1.10069600
C	3.48413200	3.16044000	1.44336400
C	4.81264100	2.71892500	1.25256400
H	5.18904800	2.52712200	0.24986000
C	5.63288500	2.52509200	2.37147400
C	5.19355700	2.73817500	3.68421800
C	3.86183300	3.15879600	3.83666400
C	3.00182400	3.37312400	2.75729200
H	1.97386700	3.68262000	2.91753000
C	2.99881600	5.96305900	0.55722900
C	4.31927700	6.38718000	0.29202400
H	4.88526700	5.93544800	-0.52262400
C	4.91530000	7.40465800	1.06085200
H	5.93571700	7.72069800	0.83833500
C	4.20035800	8.01391400	2.10668700
H	4.66382200	8.80010500	2.70421700
C	2.87770300	7.60840800	2.37191800
H	2.31083000	8.08276900	3.17463900
C	2.28222100	6.59685600	1.60129200
H	1.24913800	6.30435000	1.79387500
C	0.97107100	5.29109600	-0.81394900
C	0.96579900	6.16332900	-1.92894300
H	1.91403900	6.43738600	-2.39433700
C	-0.23994800	6.69292200	-2.41793400
H	-0.22768500	7.37473200	-3.27025100
C	-1.46191400	6.35578000	-1.80024800
H	-2.39984800	6.77033200	-2.17333600
C	-1.46494500	5.48026600	-0.70046400
H	-2.40841100	5.21505800	-0.22091800
C	-0.25557500	4.95198900	-0.20519300
H	-0.26201500	4.27361700	0.64899400
O	-1.11834400	-1.68628500	-0.93437100
O	-0.78286000	-1.83807100	1.36227600
O	-1.73044900	1.11589500	-0.97215900
O	-1.86451700	0.72133800	1.32390600
O	1.22417900	1.78025000	-1.02920400
O	0.93193200	1.92177000	1.28123600
O	1.88133500	-0.97701400	-0.97588500
O	1.99258300	-0.67265000	1.33375000
Rh	0.06234100	0.03514500	-1.12139800
Rh	0.07402300	0.04335700	1.36885600
C	-0.17381300	-0.01115100	-3.12932900

C	-0.67114500	1.06730900	-3.94696800
C	-1.24908900	0.86194400	-5.25420500
C	-0.60006900	2.41774500	-3.46041600
C	-1.74545300	1.93533400	-5.99339500
H	-1.29436800	-0.13978700	-5.66730000
C	-1.08016300	3.48523900	-4.22428200
H	-0.13285400	2.60492800	-2.49911200
C	-1.66265100	3.25097900	-5.48608300
H	-2.18974000	1.75602200	-6.97363900
H	-1.00514300	4.49790000	-3.83036200
H	-2.04721200	4.08638300	-6.07380400
C	-0.09066800	-1.38950500	-3.73605400
F	0.82096700	-2.22352700	-3.07807700
F	-1.35227600	-2.05301400	-3.66930400
F	0.29658500	-1.42172300	-5.08589200
H	-5.87812600	-2.67192000	4.58229100
Br	-3.07795500	-2.70799200	5.76118600
Br	-7.65452800	-2.76921700	2.10611500
Br	-5.37961000	-0.96659900	-4.46388200
Br	-5.55459400	4.85630300	-3.83890500
H	-5.76526400	2.02014300	-4.91288100
Br	7.52586000	1.92007800	2.08499500
Br	3.17764800	3.46988800	5.69299100
H	5.84717200	2.58828000	4.53990000
H	6.34109200	-1.95428100	-4.67425400
Br	8.04812300	-0.03992300	-3.02926800
Br	3.88227500	-3.70475800	-4.87629600

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H	5.89801800	1.12225300	-1.11479700
H	4.37546400	0.92416600	-2.14792900
C	4.46765900	2.86747200	-1.04429500
C	3.46795500	3.50984600	-1.99463000
C	3.74803800	3.50086100	-3.37972500
H	4.64309400	2.99104100	-3.74101600
C	2.88505300	4.13599800	-4.28908000
H	3.11098500	4.11557700	-5.35676700
C	1.73411500	4.80058300	-3.82250300
H	1.06560000	5.29912800	-4.52716900
C	1.45385400	4.81859200	-2.44412400
H	0.56908400	5.33288500	-2.06699400

C	2.31208300	4.17522800	-1.53371500
H	2.06412400	4.17404600	-0.47101100
C	5.51139900	3.82864900	-0.48618400
C	5.10236500	5.01149300	0.17689000
H	4.04039700	5.23211300	0.28406200
C	6.05000500	5.91459000	0.68628100
H	5.71384700	6.81839600	1.19758600
C	7.42689600	5.66104600	0.53494200
H	8.16232300	6.36331000	0.93024700
C	7.84494700	4.50022500	-0.13808900
H	8.90878000	4.29908800	-0.27489000
C	6.89549300	3.59308400	-0.64457500
H	7.23966600	2.70699100	-1.17793000
C	4.59732600	1.52273200	1.29853800
C	4.29563800	2.43824400	2.33151100
H	3.63614000	3.27809100	2.13421100
C	4.84255000	2.23093000	3.59946000
C	5.68349500	1.15046400	3.90637900
C	5.95350800	0.25777300	2.86081700
C	5.43575400	0.41794900	1.57120500
H	5.66238400	-0.30061200	0.78646500
C	-1.29248000	2.37168100	-0.11799000
C	-2.34903600	3.46409200	-0.09808800
C	-2.01636500	4.95054800	0.50332300
C	-2.86501600	3.92293900	1.26664900
H	-2.41634700	3.44171700	2.13334900
H	-3.92749800	4.14430400	1.36266700
C	-3.31405100	3.38321400	-1.27083600
C	-2.83068000	3.41411600	-2.60606500
H	-1.76175300	3.45676700	-2.79119800
C	-3.74343400	3.35736900	-3.66152000
C	-5.13318800	3.26548100	-3.47466800
C	-5.57548900	3.21872200	-2.14687900
C	-4.70745500	3.27148200	-1.04954700
H	-5.10650600	3.22865300	-0.03946300
C	-2.77878600	6.08273900	-0.16665700
C	-2.44615400	6.51173600	-1.47271300
H	-1.66229700	5.99099800	-2.02340000
C	-3.11894800	7.59484000	-2.06509500
H	-2.85556100	7.90845400	-3.07657400
C	-4.13155100	8.27047800	-1.35710200
H	-4.65667300	9.10833700	-1.81795100
C	-4.45923100	7.86202600	-0.05146100
H	-5.23479900	8.38760200	0.50793500

C	-3.78435600	6.77800100	0.54043500
H	-4.03023400	6.47674600	1.55993800
C	-0.63719200	5.31521600	1.03693100
C	0.07256600	4.46094900	1.91576300
H	-0.30419700	3.47296300	2.15434700
C	1.28863000	4.86412200	2.49333200
H	1.78697300	4.18019600	3.17987200
C	1.83478400	6.12866900	2.20093100
H	2.76993400	6.44557800	2.66594000
C	1.15076300	6.98094500	1.31477500
H	1.55647000	7.96585800	1.07732800
C	-0.07148800	6.58306600	0.74381000
H	-0.60387900	7.26768200	0.08692100
C	-2.33985700	-0.91913200	-0.65585300
C	-3.77857200	-1.33035100	-0.83997100
C	-4.57355300	-0.45314600	-1.84915100
H	-5.59142000	-0.18777100	-1.56901700
H	-3.99012800	0.32834600	-2.33194500
C	-4.27434200	-1.87923000	-2.28325700
C	-3.28731900	-2.07045500	-3.42482400
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H	-1.91690200	-3.35779000	-2.35696100
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H	-0.42537100	-3.74319600	-4.31512500
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H	-0.91431800	-2.62263700	-6.49986900
C	-2.70955300	-1.64334200	-5.76459700
H	-2.92915800	-1.14908700	-6.71247300
C	-3.56022100	-1.44669700	-4.66260400
H	-4.43788200	-0.80479300	-4.75802300
C	-5.39852800	-2.91080800	-2.25807100
C	-5.08415000	-4.29045400	-2.31775500
H	-4.04211100	-4.59775900	-2.40846800
C	-6.09499600	-5.26520000	-2.29879300
H	-5.82863500	-6.32240400	-2.34741900
C	-7.44785400	-4.88046000	-2.22885000
H	-8.23462800	-5.63596300	-2.21684900
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H	-8.82063900	-3.20230300	-2.15383100
C	-6.76069100	-2.53889800	-2.20505000
H	-7.04070400	-1.48583700	-2.19199900
C	-4.50302700	-1.83188600	0.38595500
C	-4.25785900	-3.13526500	0.88406200
H	-3.52183600	-3.77469300	0.40259200

C	-4.98670500	-3.58708000	1.98962200
C	-5.95128700	-2.80080300	2.64470900
C	-6.15862900	-1.50864000	2.13770800
C	-5.45783700	-1.01158700	1.03164700
H	-5.64842100	-0.00467600	0.66653400
C	1.58688400	-2.10129500	-0.64573700
C	2.72328400	-3.09558500	-0.81888800
C	2.51424700	-4.66374800	-0.55238000
C	3.23569700	-3.77216800	0.46238000
H	2.68595000	-3.51095500	1.36534700
H	4.31198800	-3.88935800	0.58027700
C	3.70371300	-2.70452900	-1.91089100
C	5.05390900	-2.42437900	-1.60079000
H	5.40566700	-2.47485800	-0.57306500
C	5.93643400	-2.07914300	-2.63256500
C	5.54317200	-1.98619600	-3.97316900
C	4.19183900	-2.25651500	-4.24449300
C	3.27020500	-2.61176100	-3.25752800
H	2.22893300	-2.78876800	-3.50633400
C	3.33702100	-5.60161400	-1.42687500
C	4.59586900	-6.09347800	-1.01914000
H	5.00755100	-5.80161500	-0.05253500
C	5.32439600	-6.97334600	-1.84243300
H	6.29462900	-7.34536900	-1.50925800
C	4.80431500	-7.37331900	-3.08557100
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C	3.54323400	-6.89857600	-3.49672600
H	3.12780500	-7.21053900	-4.45633700
C	2.81511500	-6.02581100	-2.67221400
H	1.82929700	-5.67881900	-2.98480800
C	1.15373000	-5.23986100	-0.20313200
C	1.10017100	-6.28602900	0.74839400
H	2.01376400	-6.57979500	1.26759900
C	-0.10490400	-6.95899400	1.00598800
H	-0.12845900	-7.77177100	1.73405000
C	-1.27865200	-6.59695400	0.31445800
H	-2.21321600	-7.12863600	0.50045800
C	-1.23470900	-5.55060800	-0.62430100
H	-2.13660400	-5.27754300	-1.17529400
C	-0.02566600	-4.87370600	-0.88386800
H	0.00719300	-4.06162300	-1.61100900
O	-1.13197300	1.64829800	0.98187100
O	-0.66325900	2.15497000	-1.24648600
O	-1.77454400	-1.07798700	0.53641100

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O	1.25646200	-1.76211300	0.58648600
O	1.04880900	-1.59026500	-1.73200100
O	1.88472200	0.99865200	0.92442500
O	2.09659000	0.97151500	-1.39949400
Rh	0.07648400	-0.07050100	0.91339600
Rh	0.17808000	0.28937800	-1.56197900
C	0.19527100	-0.44885700	2.93980700
C	0.08468600	-1.77408900	3.52073200
C	0.68285900	-2.13180600	4.78091200
C	-0.62579500	-2.79895000	2.81222200
C	0.61687900	-3.44185200	5.25971000
H	1.18513100	-1.37005900	5.36576000
C	-0.69302500	-4.10438100	3.30993400
H	-1.11501400	-2.54445800	1.87631400
C	-0.06691400	-4.43485300	4.52857100
H	1.08732800	-3.69148000	6.21197600
H	-1.21598500	-4.87118900	2.73939800
H	-0.11468200	-5.45736400	4.90789300
C	1.03987100	0.56460900	3.67725200
F	0.82200800	1.88601800	3.23044800
F	0.87442800	0.65491000	5.08270200
F	2.39727800	0.26351600	3.48236000
C	-1.88216400	0.83194300	4.40440500
H	-1.31585900	1.74463400	4.27873600
C	-2.64085800	0.20175900	3.41175400
N	-3.24682500	-0.92998700	3.95099300
C	-2.89835600	-1.04903900	5.31079400
C	-2.03239300	0.05891400	5.62066700
H	-2.75261600	0.46575200	2.36945500
H	-3.83260400	-1.58292600	3.42944400
C	-3.25883000	-2.00061300	6.27775600
H	-3.91816600	-2.83530600	6.03614400
C	-2.73318400	-1.84765400	7.57169400
H	-2.99693300	-2.57138900	8.34426500
C	-1.85933600	-0.77498200	7.88961900
H	-1.46110400	-0.69507800	8.90220200
C	-1.49845500	0.17557700	6.92393800
H	-0.81275300	0.98851000	7.16369400
Br	-7.51565400	-0.34198100	3.02968900
Br	-4.69382300	-5.44982900	2.66447800
Br	7.12716600	-1.32704600	3.24335800
Br	4.39418300	3.51964000	5.07218100
Br	-3.04869000	3.42465000	-5.53855100

Br	-7.54868600	3.06103900	-1.80337200
Br	3.57007100	-2.13203400	-6.14497600
Br	7.85401100	-1.70019800	-2.17387300
H	6.09603800	1.01019200	4.90215000
H	6.24376700	-1.72114300	-4.76096200
H	-6.51960700	-3.18119600	3.48992000
H	-5.82422400	3.23408600	-4.31327000

TSII-R (G = -5290.122563)

C	2.51683000	1.22262200	-0.20989300
C	3.94376300	1.68791400	-0.09244800
C	4.81766400	1.46522400	-1.35072900
H	5.83778000	1.13124800	-1.16730300
H	4.30502200	1.00968200	-2.19611200
C	4.44057600	2.90587200	-1.02127300
C	3.43660900	3.58908300	-1.93794700
C	3.71484500	3.65256700	-3.32179100
H	4.61366200	3.16910200	-3.70912600
C	2.84463800	4.32528400	-4.19673200
H	3.06851800	4.36027200	-5.26447300
C	1.68883300	4.95560100	-3.69570400
H	1.01448000	5.48268500	-4.37355200
C	1.41071100	4.90195800	-2.31786300
H	0.52185600	5.38889200	-1.91466500
C	2.27564300	4.22005100	-1.44227600
H	2.03143600	4.16245600	-0.38015200
C	5.49533100	3.83791200	-0.43214100
C	5.10086800	5.07712200	0.13130200
H	4.04871000	5.36057000	0.12475000
C	6.05016000	5.95273100	0.68385600
H	5.72313600	6.90105200	1.11413800
C	7.41722300	5.61578100	0.67702500
H	8.15469700	6.29682500	1.10437700
C	7.82347500	4.39792300	0.10485200
H	8.88106700	4.12992800	0.08017200
C	6.87214500	3.51868500	-0.44484700
H	7.21402400	2.58729600	-0.89506800
C	4.56129700	1.46414600	1.26797500
C	4.40764600	2.40925100	2.30610400
H	3.88089600	3.33965400	2.11742800
C	4.93755400	2.11936500	3.56580400
C	5.62040500	0.92902100	3.85730100
C	5.74983200	0.01402600	2.80370500
C	5.24415100	0.25291300	1.52252900

H	5.35200000	-0.48507500	0.73046100
C	-1.31901500	2.39740300	0.02256700
C	-2.35479600	3.50693200	0.11987900
C	-1.97465400	4.96401900	0.75625200
C	-2.81395000	3.92524700	1.51702700
H	-2.33740500	3.41086600	2.34925500
H	-3.86819100	4.16002100	1.66113400
C	-3.36382000	3.47986500	-1.01779900
C	-2.92912300	3.55397400	-2.36791700
H	-1.86700900	3.59113700	-2.59001800
C	-3.88041300	3.54478200	-3.39036700
C	-5.26335500	3.45713100	-3.15564000
C	-5.65691500	3.36478000	-1.81509900
C	-4.74905700	3.37161700	-0.74930300
H	-5.11115300	3.29632500	0.27274100
C	-2.74073300	6.13035700	0.15200800
C	-2.43859600	6.60215900	-1.14666700
H	-1.67565600	6.09290900	-1.73612100
C	-3.11327700	7.71365500	-1.68128600
H	-2.87348300	8.06026900	-2.68785100
C	-4.09720100	8.37568500	-0.92173500
H	-4.62383900	9.23578400	-1.33771600
C	-4.39375000	7.92490200	0.37735600
H	-5.14634900	8.43973600	0.97674100
C	-3.71685100	6.81226700	0.91121600
H	-3.93801300	6.47831500	1.92619700
C	-0.57288700	5.28958600	1.25746700
C	0.17139000	4.38138200	2.05098000
H	-0.19191900	3.37665100	2.23738700
C	1.40916600	4.75021900	2.60509300
H	1.93596700	4.02424200	3.22340700
C	1.94348100	6.03212500	2.37378900
H	2.89800800	6.31902500	2.81823700
C	1.22572300	6.93783800	1.57181900
H	1.62206700	7.93686400	1.38192500
C	-0.01785700	6.57447500	1.02454700
H	-0.57405600	7.29798100	0.43243700
C	-2.38682800	-0.88824100	-0.64424500
C	-3.82997000	-1.29952400	-0.81544500
C	-4.66364100	-0.35314600	-1.72658300
H	-5.67270700	-0.11309100	-1.39563500
H	-4.09795500	0.46317700	-2.17175600
C	-4.37542300	-1.74333800	-2.27314900
C	-3.43622700	-1.84803300	-3.46560100

C	-2.28228500	-2.65651200	-3.45698900
H	-1.98677100	-3.15541300	-2.53514900
C	-1.47867500	-2.77197800	-4.60524000
H	-0.57917500	-3.39018700	-4.57686300
C	-1.82269500	-2.07938000	-5.78080200
H	-1.19542300	-2.16234700	-6.66978500
C	-2.97765100	-1.27382400	-5.80014700
H	-3.25220700	-0.73226200	-6.70698600
C	-3.78050500	-1.16183600	-4.65147500
H	-4.67617200	-0.53815500	-4.67003200
C	-5.49695000	-2.77836900	-2.28141400
C	-5.18061100	-4.14926800	-2.44234500
H	-4.14046500	-4.44393900	-2.58283300
C	-6.18778300	-5.12783100	-2.45939700
H	-5.92015000	-6.17816100	-2.58648700
C	-7.53913600	-4.75479500	-2.32480400
H	-8.32320400	-5.51305300	-2.34103700
C	-7.86935000	-3.39573600	-2.18476500
H	-8.91386000	-3.09184100	-2.09875000
C	-6.85780600	-2.41691900	-2.16429000
H	-7.13975800	-1.36809100	-2.07396300
C	-4.50476200	-1.89927900	0.39423400
C	-4.21564400	-3.22814600	0.79426900
H	-3.48340900	-3.81678900	0.24592000
C	-4.89281400	-3.76944700	1.89210300
C	-5.84518000	-3.04818700	2.63607800
C	-6.09793600	-1.72968400	2.22463500
C	-5.45085200	-1.14494900	1.12782900
H	-5.67833500	-0.12187800	0.83582000
C	1.53996300	-2.05132800	-0.73967000
C	2.67784600	-3.03724300	-0.96628700
C	2.45166700	-4.61756500	-0.82638700
C	3.15424800	-3.81221700	0.27144900
H	2.58532300	-3.61259800	1.17836500
H	4.22550200	-3.95257500	0.40787300
C	3.68440400	-2.57568300	-2.00780700
C	5.04924500	-2.41231200	-1.67546300
H	5.39837100	-2.59804000	-0.66280600
C	5.95334800	-2.00913300	-2.66673200
C	5.57115800	-1.74709500	-3.98808600
C	4.20689800	-1.90586400	-4.28148800
C	3.26290500	-2.31114000	-3.33610800
H	2.21264400	-2.39358800	-3.59574100
C	3.29208800	-5.49636300	-1.74456100

C	4.50695700	-6.07320800	-1.31570400
H	4.86961100	-5.88634400	-0.30427000
C	5.25231300	-6.90161700	-2.17664600
H	6.18817800	-7.34083400	-1.82718700
C	4.79284100	-7.16363100	-3.47907100
H	5.37235300	-7.80131500	-4.14815200
C	3.57573700	-6.60230400	-3.91311900
H	3.20810400	-6.80594300	-4.92018700
C	2.83052900	-5.78129000	-3.05144500
H	1.87922700	-5.36489100	-3.38545100
C	1.08185200	-5.21331700	-0.55531000
C	0.99822400	-6.30559500	0.34039900
H	1.89253100	-6.61864900	0.88130600
C	-0.21114500	-6.99682800	0.51706700
H	-0.25754100	-7.84504500	1.20249100
C	-1.35882500	-6.60758600	-0.20244400
H	-2.29556000	-7.15376700	-0.08059900
C	-1.28571800	-5.51519900	-1.08529100
H	-2.16681300	-5.22032600	-1.65785800
C	-0.07277600	-4.81863300	-1.26246700
H	-0.01756600	-3.96797700	-1.94269200
O	-1.14441200	1.62703000	1.08922400
O	-0.72624200	2.22005700	-1.13091600
O	-1.79973800	-1.09107000	0.53052300
O	-1.82490700	-0.30465700	-1.66795200
O	1.24814000	-1.74411400	0.50833300
O	0.96710800	-1.51812900	-1.80014000
O	1.85028600	1.01315900	0.91038700
O	2.03218700	1.03352200	-1.41578500
Rh	0.05903400	-0.08109800	0.91176500
Rh	0.10652700	0.36407800	-1.55448500
C	0.16360000	-0.52173800	3.00125500
C	0.19569700	-1.93736800	3.43386700
C	1.00768900	-2.39769000	4.51826000
C	-0.58517900	-2.90220500	2.73243700
C	1.07143600	-3.75896200	4.83990900
H	1.57720600	-1.68126600	5.10056900
C	-0.52691300	-4.26113900	3.07293600
H	-1.21218600	-2.57148600	1.90804600
C	0.30634500	-4.69755700	4.12072800
H	1.71061000	-4.08780700	5.66139800
H	-1.11098600	-4.98404200	2.50344500
H	0.35796500	-5.75795400	4.37493200
C	1.19030000	0.37965400	3.65353700

F	1.01279500	1.74127800	3.31317600
F	1.21752100	0.40651800	5.08103900
F	2.47860400	-0.01036700	3.27893800
C	-1.49661800	0.36411800	4.13491200
H	-1.05249700	1.34686300	4.02835500
C	-2.53202000	-0.10825500	3.27643900
N	-3.19716600	-1.13304400	3.88447100
C	-2.71019400	-1.32016600	5.20873800
C	-1.66642300	-0.36339000	5.40806500
H	-2.74308600	0.19352600	2.26077100
H	-3.93751300	-1.68940100	3.44562200
C	-3.13141200	-2.20337600	6.21034200
H	-3.92513900	-2.92994100	6.03484500
C	-2.49112200	-2.11381300	7.45902400
H	-2.79479000	-2.78185300	8.26565500
C	-1.46038400	-1.16962000	7.68160900
H	-0.98365000	-1.12270300	8.66154700
C	-1.03292600	-0.29899500	6.66393200
H	-0.22124500	0.40300800	6.83302300
Br	-7.44483800	-0.65478500	3.24255600
Br	-4.54122600	-5.66325600	2.43080100
Br	6.68825000	-1.72500200	3.16697500
Br	4.69603600	3.45084700	5.05012600
Br	-3.25501100	3.67965300	-5.28768600
Br	-7.61815100	3.20846700	-1.40425200
Br	3.59627300	-1.53741200	-6.15432600
Br	7.88862000	-1.79483500	-2.17564900
H	6.02031300	0.72512000	4.84725100
H	6.28866200	-1.43913900	-4.74439600
H	-6.37755300	-3.49918300	3.47006200
H	-5.98490400	3.46250600	-3.96871000

IntIII-R (G = -5290.131376)

C	2.48075200	1.24278400	-0.31773500
C	3.89525900	1.75386100	-0.23382600
C	4.78647700	1.44042900	-1.45960000
H	5.81271500	1.15108400	-1.23851400
H	4.29411900	0.89740900	-2.26437100
C	4.36882000	2.89505000	-1.26499800
C	3.35134100	3.46007900	-2.24512200
C	3.63620600	3.40643200	-3.62798200
H	4.55245200	2.91905000	-3.96652500
C	2.74985200	3.96706700	-4.56368800
H	2.97897200	3.91134800	-5.62945500

C	1.57085100	4.60179500	-4.12626300
H	0.88348700	5.04149100	-4.85176000
C	1.28619100	4.66515800	-2.75018500
H	0.37917200	5.15681300	-2.39610700
C	2.16737300	4.09511400	-1.81299400
H	1.91932700	4.12687300	-0.75070600
C	5.39176100	3.90850700	-0.75948900
C	4.96171200	5.19818900	-0.35800600
H	3.90647500	5.45950700	-0.43130800
C	5.87952600	6.14932200	0.11767400
H	5.52482000	7.13559700	0.42248000
C	7.25057000	5.83854100	0.19404600
H	7.96378400	6.57796500	0.56139500
C	7.69253800	4.56917000	-0.21729700
H	8.75388600	4.31858500	-0.17594800
C	6.77279700	3.61485400	-0.68985400
H	7.14331900	2.64309100	-1.01419300
C	4.50499900	1.66184700	1.14547600
C	4.36086700	2.70582600	2.08531300
H	3.85214700	3.62216000	1.80258000
C	4.88172600	2.53225400	3.37026900
C	5.54566000	1.36656600	3.78012800
C	5.66765000	0.35213900	2.82062800
C	5.17066900	0.47219300	1.51992900
H	5.26763400	-0.34154700	0.80417200
C	-1.38231900	2.29722800	-0.19250400
C	-2.44374100	3.38871400	-0.19326600
C	-2.09998200	4.90433500	0.31121400
C	-2.91842800	3.91715600	1.15992600
H	-2.43003100	3.49277400	2.03494800
H	-3.97845200	4.13815400	1.28243300
C	-3.44953500	3.23704800	-1.32376600
C	-3.01438800	3.20656400	-2.67536900
H	-1.95310600	3.25373900	-2.89968100
C	-3.96298800	3.08168800	-3.69275600
C	-5.34354600	2.97517100	-3.45073500
C	-5.73667700	2.98760200	-2.10709600
C	-4.83163700	3.11245500	-1.04631500
H	-5.19311500	3.11546700	-0.02124300
C	-2.88990600	5.99447700	-0.39581000
C	-2.58616500	6.36100400	-1.72772900
H	-1.80240900	5.82505400	-2.26372400
C	-3.28463000	7.40276400	-2.36267300
H	-3.04269600	7.66789500	-3.39320000

C	-4.29479700	8.10001700	-1.67221800
H	-4.83987800	8.90588700	-2.16581700
C	-4.59343200	7.75505200	-0.34162000
H	-5.36629800	8.29865600	0.20423900
C	-3.89257100	6.71206600	0.29261000
H	-4.11588700	6.46127200	1.33081600
C	-0.70873300	5.30498000	0.78741800
C	0.06149100	4.47609200	1.64083500
H	-0.27128700	3.47597900	1.89586200
C	1.28881400	4.91677900	2.16453000
H	1.83676100	4.24759900	2.82684100
C	1.78590800	6.19428600	1.84362000
H	2.73334000	6.53749200	2.26258600
C	1.04179600	7.02154300	0.98295700
H	1.40957900	8.01577800	0.72304200
C	-0.19099900	6.58590200	0.46455100
H	-0.76681800	7.24989000	-0.17656100
C	-2.34595500	-1.06623900	-0.63621400
C	-3.78747400	-1.50020800	-0.76388500
C	-4.62926800	-0.67085000	-1.77411900
H	-5.64166400	-0.40673200	-1.47270300
H	-4.07146700	0.09705700	-2.30693400
C	-4.32542500	-2.10986300	-2.16309000
C	-3.38247200	-2.33105400	-3.33652200
C	-2.20596000	-3.09939800	-3.23666700
H	-1.89638500	-3.47973300	-2.26458200
C	-1.39824600	-3.32489100	-4.36573200
H	-0.48115100	-3.90882900	-4.26678500
C	-1.76154700	-2.78477300	-5.61304500
H	-1.13164800	-2.95283600	-6.48799900
C	-2.93923400	-2.02032600	-5.72333300
H	-3.22861600	-1.59673900	-6.68657000
C	-3.74535200	-1.79735600	-4.59346300
H	-4.65810200	-1.20522500	-4.68200700
C	-5.43126500	-3.15451700	-2.05345200
C	-5.09255000	-4.52939700	-2.04043500
H	-4.04652800	-4.82216300	-2.13471100
C	-6.08498900	-5.51819300	-1.94248200
H	-5.80091300	-6.57185100	-1.93590800
C	-7.44289600	-5.15243000	-1.86480400
H	-8.21546700	-5.91916000	-1.79232600
C	-7.79469500	-3.79187900	-1.89696100
H	-8.84441700	-3.49646400	-1.85696200
C	-6.79798800	-2.80210000	-1.99109400

H	-7.09523400	-1.75431300	-2.03386400
C	-4.45812400	-1.96220200	0.50782700
C	-4.14717600	-3.22679700	1.06963000
H	-3.40827300	-3.86842200	0.59427000
C	-4.81087300	-3.63832200	2.23036500
C	-5.77205800	-2.84288200	2.88507600
C	-6.04168300	-1.58717200	2.31588600
C	-5.40777700	-1.13292500	1.15179400
H	-5.64610600	-0.15483000	0.73925700
C	1.62254600	-2.10518400	-0.54520900
C	2.78186300	-3.08507000	-0.67316800
C	2.58641100	-4.65290600	-0.40946400
C	3.25320400	-3.74514500	0.63055300
H	2.66395200	-3.48697700	1.50956800
H	4.32445700	-3.84985300	0.79594400
C	3.79715200	-2.68740300	-1.73291200
C	5.15466900	-2.47717200	-1.39597100
H	5.49248800	-2.58055300	-0.36779100
C	6.06622600	-2.13396200	-2.40279500
C	5.69929400	-1.97805400	-3.74510700
C	4.34193300	-2.18080700	-4.04322700
C	3.39072300	-2.52934600	-3.08279400
H	2.34505200	-2.64668600	-3.34772100
C	3.45882900	-5.58342600	-1.24247500
C	4.68085800	-6.09513300	-0.75530500
H	5.02676600	-5.81844700	0.24132100
C	5.45553100	-6.97260500	-1.53830800
H	6.39674600	-7.35978900	-1.14441600
C	5.01858900	-7.34990700	-2.81999500
H	5.62084900	-8.02567900	-3.42895200
C	3.79467700	-6.85420900	-3.31117500
H	3.44459000	-7.14694500	-4.30245400
C	3.02052100	-5.98384600	-2.52693800
H	2.06451500	-5.61738700	-2.90355300
C	1.22850900	-5.25992100	-0.10270200
C	1.16988400	-6.29098200	0.86507800
H	2.07177400	-6.54721100	1.42283200
C	-0.02423100	-6.99242800	1.09530300
H	-0.05070200	-7.79174300	1.83811200
C	-1.18273200	-6.67511100	0.35800400
H	-2.10798800	-7.23018400	0.52180800
C	-1.13447500	-5.64442800	-0.59749300
H	-2.02366000	-5.40770900	-1.18439800
C	0.06360000	-4.93748600	-0.82930200

H	0.09847900	-4.13324600	-1.56516300
O	-1.19283900	1.62676800	0.93763300
O	-0.78594800	2.03514400	-1.32773600
O	-1.75062500	-1.17360300	0.54967500
O	-1.78730700	-0.56323400	-1.69840100
O	1.32930800	-1.67939700	0.66477500
O	1.03647200	-1.69710000	-1.65635800
O	1.80055700	1.13887300	0.80703200
O	2.02057600	0.91349600	-1.50406300
Rh	0.07287300	-0.04407600	0.89941900
Rh	0.12063500	0.17754300	-1.60099500
C	0.05126700	-0.25816700	3.19469800
C	0.22647300	-1.70630600	3.65778700
C	1.02911300	-2.04443500	4.77932400
C	-0.45710800	-2.75509000	2.99271700
C	1.15686600	-3.37857500	5.20237000
H	1.53815700	-1.25493000	5.32340700
C	-0.34043800	-4.08749300	3.42905100
H	-1.04251900	-2.53480500	2.10145300
C	0.47118200	-4.40746700	4.53294300
H	1.78472500	-3.60860700	6.06582600
H	-0.85340700	-4.87751000	2.88005800
H	0.57077500	-5.44369400	4.86166000
C	1.18202000	0.63447700	3.59518600
F	0.97358500	1.97221800	3.17568500
F	1.40523400	0.80622800	5.02299500
F	2.41183500	0.17192900	3.13988400
C	-1.32348600	0.35331500	3.70658800
H	-1.39225100	1.35957500	3.24254800
C	-2.46977900	-0.45786000	3.17700200
N	-3.31736700	-0.77773600	4.14485600
C	-2.89434500	-0.26326100	5.42376500
C	-1.66941700	0.42185500	5.21986100
H	-2.57904800	-0.78571300	2.14047900
H	-4.16124500	-1.35035500	3.98731800
C	-3.53900400	-0.36242700	6.65937100
H	-4.48067200	-0.89924800	6.77612300
C	-2.91738400	0.27236700	7.75174100
H	-3.38090900	0.22275800	8.73710000
C	-1.70298200	0.96898800	7.57813700
H	-1.23600600	1.45032100	8.43818800
C	-1.06954100	1.05036400	6.31940100
H	-0.11674900	1.55402700	6.20474000
Br	-7.40283200	-0.41097400	3.20195300

Br	-4.43058200	-5.44410900	2.99428200
Br	6.58119200	-1.35475400	3.35685100
Br	4.65874500	4.00829800	4.71518100
Br	-3.33793900	3.06670800	-5.59471500
Br	-7.69416200	2.81050000	-1.68273800
Br	3.75260200	-1.96494800	-5.94723700
Br	7.99118300	-1.85108300	-1.90429600
H	5.93697000	1.25364200	4.78785400
H	6.42276500	-1.71593300	-4.51289500
H	-6.30857000	-3.20407900	3.75984200
H	-6.06317300	2.88950900	-4.26101800

TSIII-R (G = -5290.112806)

C	2.47557500	1.21379000	-0.12374000
C	3.91733600	1.62820200	-0.01403200
C	4.73796900	1.51574300	-1.32235600
H	5.75296100	1.13804600	-1.20927100
H	4.18428300	1.16275100	-2.19018300
C	4.41822500	2.92197400	-0.82926600
C	3.40272500	3.72846900	-1.62397400
C	3.62308200	3.92771800	-3.00542300
H	4.48257300	3.45406000	-3.48334100
C	2.74732000	4.72432600	-3.76288300
H	2.92680000	4.86433500	-4.83034300
C	1.64492300	5.34518400	-3.14387600
H	0.96794000	5.97075400	-3.72895800
C	1.42422400	5.15454900	-1.76772700
H	0.57874700	5.63482700	-1.27374800
C	2.29284500	4.34754400	-1.01038200
H	2.09253400	4.18632700	0.05033100
C	5.52763000	3.75660600	-0.19645000
C	5.19948100	4.90344300	0.56825000
H	4.15495100	5.18756900	0.69406100
C	6.20471600	5.68919400	1.15575300
H	5.92935800	6.56659500	1.74365700
C	7.56129500	5.35332600	0.98375600
H	8.34182600	5.96455200	1.43921700
C	7.90052200	4.22885500	0.21187500
H	8.94827500	3.96482500	0.05904800
C	6.89327900	3.43922900	-0.37328600
H	7.18041800	2.58098400	-0.98014400
C	4.58095300	1.24000800	1.28722400
C	4.48287400	2.05781100	2.43453900
H	3.95643400	3.00583900	2.38171100

C	5.06562500	1.61833500	3.62636200
C	5.74274000	0.39550000	3.74599600
C	5.81207200	-0.39202900	2.58896300
C	5.25611600	0.00086500	1.36800800
H	5.31631700	-0.64110600	0.49163600
C	-1.27637600	2.47402300	0.31918500
C	-2.23379200	3.62488000	0.56518200
C	-1.76962300	4.93727700	1.43657600
C	-2.69294000	3.85371700	2.00772200
H	-2.27684700	3.18354300	2.75684700
H	-3.73199300	4.13876700	2.16978100
C	-3.21651300	3.84228700	-0.57386400
C	-2.75101700	4.10790800	-1.88904600
H	-1.68470300	4.12741700	-2.09234400
C	-3.68118600	4.31125300	-2.91078100
C	-5.07086500	4.25885200	-2.70996600
C	-5.49632400	3.97601500	-1.40631300
C	-4.61040500	3.76574700	-0.34268100
H	-4.99570500	3.54400200	0.64913700
C	-2.45485400	6.23466700	1.03243900
C	-2.13765400	6.88767100	-0.18080700
H	-1.42382600	6.42899600	-0.86462700
C	-2.73736900	8.11503300	-0.51393300
H	-2.48694600	8.60139800	-1.45812100
C	-3.65961400	8.71293300	0.36607100
H	-4.12799200	9.66330900	0.10629000
C	-3.97018200	8.08030400	1.58361300
H	-4.67501200	8.54269600	2.27644900
C	-3.36892400	6.85201100	1.91518100
H	-3.59989500	6.37485000	2.86892300
C	-0.35546300	5.08610800	1.98618900
C	0.30629200	4.03532400	2.67112800
H	-0.13522600	3.04650800	2.73442500
C	1.56436100	4.23610800	3.26461700
H	2.02974800	3.40038000	3.78536100
C	2.19987600	5.48992100	3.18641800
H	3.16920600	5.64499500	3.66322700
C	1.56410600	6.53821400	2.49612400
H	2.03897000	7.51853600	2.42755700
C	0.30261400	6.34115200	1.90696600
H	-0.18829100	7.17116400	1.40348000
C	-2.48891100	-0.76345000	-0.53425300
C	-3.95070100	-1.09820900	-0.69028400
C	-4.78741600	0.05771900	-1.32356200

H	-5.76942800	0.24577100	-0.89226300
H	-4.21110000	0.93643400	-1.60713100
C	-4.59061000	-1.18978500	-2.17090100
C	-3.73150800	-1.07745600	-3.42297100
C	-2.66233500	-1.95599800	-3.69076900
H	-2.36656400	-2.68392000	-2.93655400
C	-1.93305700	-1.85418300	-4.88840300
H	-1.09692600	-2.53182700	-5.07257900
C	-2.26898100	-0.87186200	-5.83930400
H	-1.69971400	-0.78805700	-6.76638500
C	-3.34107900	0.00434700	-5.58352500
H	-3.60927800	0.76933300	-6.31427500
C	-4.06895600	-0.10005700	-4.38475900
H	-4.89813500	0.58247400	-4.18927800
C	-5.77703200	-2.13491600	-2.33912000
C	-5.55834600	-3.49979400	-2.64161300
H	-4.53831300	-3.87035400	-2.74363400
C	-6.63678700	-4.37909600	-2.83191300
H	-6.44587500	-5.42850500	-3.06249500
C	-7.96028700	-3.90758200	-2.73317100
H	-8.79875500	-4.58922600	-2.88251800
C	-8.19159200	-2.54989200	-2.45265400
H	-9.21234500	-2.16924600	-2.39052600
C	-7.10881700	-1.67125800	-2.25831700
H	-7.30727100	-0.61742700	-2.06098900
C	-4.58742800	-1.93708500	0.39310300
C	-4.28047100	-3.31862800	0.49909400
H	-3.53025000	-3.76474900	-0.15142400
C	-4.97424100	-4.09773300	1.43072100
C	-5.96376500	-3.57479800	2.28221200
C	-6.21499800	-2.19981500	2.18279700
C	-5.54821500	-1.37459000	1.26779300
H	-5.78657600	-0.31477100	1.21134200
C	1.38265200	-2.00090000	-0.92549300
C	2.47270200	-2.99483700	-1.29251300
C	2.16667400	-4.55667900	-1.46145600
C	2.85551000	-4.00758100	-0.20552400
H	2.25770300	-3.95412000	0.70338300
H	3.91142200	-4.22899500	-0.05783700
C	3.54057900	-2.40965500	-2.20568100
C	4.90732000	-2.43610100	-1.84184800
H	5.21878600	-2.84589300	-0.88440000
C	5.86379500	-1.93320600	-2.73412800
C	5.53368900	-1.38892500	-3.98192400

C	4.16713600	-1.36172600	-4.30416000
C	3.17213200	-1.85483100	-3.45823000
H	2.12347900	-1.79429100	-3.73149700
C	3.01040000	-5.29542300	-2.49347800
C	4.15705800	-6.03100500	-2.12370300
H	4.46328700	-6.06905900	-1.07757900
C	4.90516600	-6.72972400	-3.09078600
H	5.78752400	-7.29514400	-2.78639400
C	4.51664000	-6.70107400	-4.44148700
H	5.09865600	-7.23792500	-5.19196300
C	3.36698000	-5.97968800	-4.81925700
H	3.05426600	-5.95764800	-5.86451000
C	2.61827700	-5.28873600	-3.85274400
H	1.71857500	-4.74712000	-4.14766200
C	0.76307300	-5.12694600	-1.35855100
C	0.59730200	-6.34796400	-0.66213400
H	1.45062000	-6.77846500	-0.13629400
C	-0.64025500	-7.01104600	-0.65961100
H	-0.75036400	-7.95620900	-0.12491900
C	-1.73363300	-6.46605200	-1.36182900
H	-2.69168600	-6.98764700	-1.37646800
C	-1.57920400	-5.24837200	-2.04790300
H	-2.41793800	-4.83317800	-2.60924400
C	-0.33892900	-4.57639200	-2.04669600
H	-0.22488400	-3.62676400	-2.57111700
O	-1.08986800	1.59770300	1.29633800
O	-0.74295800	2.36170100	-0.87188800
O	-1.86420100	-1.09167900	0.59124000
O	-1.94436300	-0.09527800	-1.51795900
O	1.16437800	-1.78406400	0.35321600
O	0.77902800	-1.35277500	-1.90938900
O	1.82616300	0.93742800	0.98890200
O	1.95272000	1.12417100	-1.33120600
Rh	0.03194800	-0.14485100	0.94072700
Rh	0.00533600	0.51522200	-1.43942000
C	0.26914300	-1.04375500	3.49509300
C	0.43208300	-2.53909100	3.38455600
C	1.37472400	-3.19234100	4.22146600
C	-0.35300600	-3.32036600	2.50858700
C	1.54438000	-4.58418200	4.16048600
H	1.96638800	-2.59151600	4.90940200
C	-0.19587700	-4.71854600	2.46641400
H	-1.06620000	-2.83463400	1.84569100
C	0.75478400	-5.35466900	3.28573500

H	2.28343800	-5.06630500	4.80353000
H	-0.79929500	-5.30638200	1.77411900
H	0.87864900	-6.43849300	3.24349600
C	1.51411600	-0.26417700	3.72603700
F	1.27350500	1.13548000	3.61475800
F	2.00711000	-0.39869000	5.06959800
F	2.57517400	-0.63602100	2.91444700
C	-0.73893500	-0.56938800	4.68668400
H	-0.31504900	0.22178200	5.30676300
C	-1.57594600	-0.21225200	3.50709600
N	-2.61582100	-1.10594900	3.41988900
C	-2.60811500	-2.00757400	4.53756300
C	-1.50058100	-1.67823900	5.36198900
H	-1.54963900	0.70465800	2.93102900
H	-3.13538600	-1.25270600	2.54674600
C	-3.49848000	-3.03232700	4.86917200
H	-4.33571300	-3.28286500	4.22165800
C	-3.27100400	-3.72585600	6.07746000
H	-3.95273900	-4.52702600	6.36593000
C	-2.18510000	-3.39878800	6.91343900
H	-2.03230500	-3.95072800	7.84127000
C	-1.28533600	-2.36924700	6.55606700
H	-0.43433200	-2.12852500	7.19393500
Br	-7.46967200	3.86075300	-1.04898300
Br	-3.01285300	4.71432200	-4.75503100
Br	4.92072000	2.77160900	5.26431000
Br	6.73234800	-2.17227500	2.70774000
Br	-7.59634400	-1.39059900	3.38389000
Br	-4.58927900	-6.05582600	1.55648500
Br	3.62749700	-0.58802600	-6.07267500
Br	7.79913800	-1.99656900	-2.20756700
H	6.29186000	-1.01051100	-4.66297000
H	6.18172500	0.07345100	4.68680000
H	-5.77456300	4.43058900	-3.52054800
H	-6.51372000	-4.20904600	2.97348600

IntIV-R (G = -971.084715)

C	-1.70556700	1.91775100	4.01845600
C	-1.78348500	1.21258700	5.34093200
C	-1.48619500	1.90560100	6.53436200
C	-2.08280300	-0.16627600	5.39468000
C	-1.49033100	1.22979000	7.76654400
H	-1.25897100	2.97132300	6.49303500
C	-2.08992400	-0.84065900	6.62970500

H	-2.31049500	-0.70285800	4.47270000
C	-1.79265000	-0.14440600	7.81617900
H	-1.25977100	1.77263800	8.68437600
H	-2.33165000	-1.90411300	6.66300400
H	-1.79829200	-0.66848400	8.77324400
C	-0.36061800	1.90901600	3.40379000
F	-0.25027900	2.77487500	2.30083400
F	0.70653400	2.13543900	4.24029000
F	-0.08010600	0.56246100	2.82995700
C	-2.58467500	3.18175300	3.65232900
H	-2.08499500	4.01325500	3.16072300
C	-2.84968700	1.83379400	2.93832800
N	-4.14481600	1.39090200	3.40176800
C	-4.67528000	2.28106600	4.34287400
C	-3.79091400	3.39323100	4.50935800
H	-2.56834200	1.62370400	1.90718400
H	-4.54182900	0.48267600	3.15827200
C	-5.88580800	2.21984800	5.05714900
H	-6.55803700	1.36756400	4.95246400
C	-6.22009200	3.29762400	5.89999200
H	-7.16151900	3.26592000	6.45106100
C	-5.36982400	4.41409300	6.03901400
H	-5.65482900	5.23739700	6.69440400
C	-4.14480700	4.46194400	5.33887100
H	-3.47708300	5.31812100	5.45184800

IntIV-R' (G = -1133.201453)

F	1.73469100	-2.87483800	-0.80940500
F	2.87622500	-1.10063900	-1.61096300
C	2.14609200	-1.56043700	-0.53131900
C	1.28111400	0.73527300	0.09636300
C	0.95559800	-0.69795400	-0.22270600
C	0.93388400	1.80051400	-0.76073800
H	0.38768500	1.59645000	-1.68004100
C	1.27875400	3.12178300	-0.42307600
H	1.00545300	3.93893400	-1.09212300
C	1.99811600	1.00966100	1.28648800
H	2.32440700	0.17780400	1.90937000
C	1.97431600	3.39084800	0.77025900
H	2.23758500	4.41705800	1.03051400
C	2.33850800	2.33069100	1.62213600
H	2.89459100	2.53097100	2.53919700
F	3.00986100	-1.63156100	0.56713600
C	-3.60873600	1.55195500	-0.40507600

C	-3.29175400	1.19400600	-1.72959700
C	-2.23617800	0.29341600	-1.99655400
C	-1.50812300	-0.23615600	-0.92360900
C	-1.85747300	0.10667200	0.40684300
C	-2.89676000	1.00469300	0.68527600
H	-4.42538100	2.24825400	-0.21139600
H	-3.86455200	1.61526300	-2.55597900
H	-1.98525700	0.02478000	-3.02388300
H	-3.15748500	1.27309300	1.71082300
C	-0.35589900	-1.19450300	-0.90603900
C	-0.10064800	-1.48217600	0.59470200
N	-1.10210700	-0.69561200	1.36364000
H	0.13497400	-2.47635600	0.96701000
H	-0.26761900	-1.98162300	-1.65016200
H	-0.70404800	-0.16848200	2.16053500
Na	-3.03737800	-2.06661400	1.74687600
H	-4.34630800	-3.34049700	2.43400200

TSIV-R (G = -1133.190786)

F	2.07448400	-2.58194600	-1.06683000
F	2.99765400	-0.56958400	-1.47446500
C	2.26664000	-1.29527200	-0.52684300
C	1.08666200	0.73793800	0.35413600
C	0.95347700	-0.64460700	-0.22301900
C	1.55138300	1.77563300	-0.48804000
H	1.78885600	1.54478500	-1.52537800
C	1.73537800	3.07271600	0.01542000
H	2.09268000	3.86576400	-0.64382100
C	0.83669300	1.01438000	1.71420900
H	0.49236700	0.22269900	2.37916300
C	1.46400200	3.34857300	1.36991200
H	1.60333800	4.35772100	1.76166800
C	1.01966000	2.31709500	2.21598300
H	0.81642400	2.52080700	3.26870000
F	3.06904900	-1.43198600	0.59671500
C	-3.66785600	1.33669000	-0.73029600
C	-3.03828800	1.44342700	-1.98697700
C	-1.86746800	0.70147900	-2.25925500
C	-1.34884600	-0.14287600	-1.27153500
C	-2.00807300	-0.27710300	-0.01349600
C	-3.16229900	0.47726300	0.26542700
H	-4.56406100	1.92462800	-0.52325100
H	-3.44946300	2.10892400	-2.74691400
H	-1.36655300	0.79873000	-3.22420800

H	-3.65793600	0.40227100	1.23597500
C	-0.13689300	-1.02048300	-1.27923400
C	-0.15151200	-1.68482100	0.12674300
N	-1.38295800	-1.26240900	0.82716200
H	0.17483600	-2.71256000	0.26471000
H	0.18081400	-1.55506000	-2.17222200
H	-1.26513700	-1.00308400	2.05836100
Na	-2.56819200	-2.56862900	2.24377800
H	-1.38199600	-1.09240300	3.19793200

IntV-R (G = -1132.060471)

F	-2.06489200	-2.82890400	0.27651400
F	-2.96130700	-1.06151700	1.33828300
C	-2.29019800	-1.44426900	0.16237800
C	-1.16750400	0.77629500	-0.20493400
C	-1.00497300	-0.70705900	-0.01726000
C	-1.74658900	1.54440200	0.83267800
H	-2.06928900	1.03842300	1.74033700
C	-1.94506800	2.92518400	0.67156300
H	-2.39622600	3.50615000	1.47813700
C	-0.80094100	1.41491100	-1.40962900
H	-0.33338400	0.82253900	-2.19409800
C	-1.56848500	3.55816800	-0.52872200
H	-1.72054900	4.63197100	-0.65320600
C	-0.99945700	2.79878200	-1.56766500
H	-0.71210600	3.28339500	-2.50305500
F	-3.17769200	-1.25168300	-0.88765700
C	3.72140300	1.00367000	0.79552300
C	3.23034300	0.65558300	2.06688500
C	2.02785400	-0.09297000	2.18389100
C	1.35479500	-0.51368500	1.03914400
C	1.89826200	-0.23814200	-0.27584300
C	3.06605900	0.58092900	-0.38507600
H	4.60503600	1.64182300	0.71413600
H	3.74658700	0.99805200	2.96436400
H	1.62831100	-0.32325900	3.17449400
H	3.35026200	1.01799800	-1.35362100
C	0.13440200	-1.34128200	0.85863500
C	0.08961100	-1.56685800	-0.71307800
N	1.24556300	-0.91009400	-1.31371700
H	-0.23942000	-2.50814700	-1.14842100
H	-0.16168700	-2.09804400	1.58247800
Na	3.22013300	-1.40756900	-2.01824700

TSV-R (G = -1132.054915)

F	-1.69525800	-2.96326500	0.19346500
F	-2.65037800	-1.37149200	1.45815700
C	-2.08228100	-1.60695100	0.19348800
C	-1.24792700	0.74580400	-0.15254100
C	-0.90703900	-0.71895600	-0.06769000
C	-1.82547600	1.38770500	0.96845500
H	-2.02467800	0.80233200	1.86380100
C	-2.18100800	2.74452600	0.90579100
H	-2.63070200	3.22811300	1.77499300
C	-1.03790300	1.48389400	-1.33776200
H	-0.56334200	0.99137900	-2.18451900
C	-1.96320800	3.47826800	-0.27652200
H	-2.23689600	4.53393700	-0.32416800
C	-1.39361900	2.84393400	-1.39557400
H	-1.22439300	3.40741800	-2.31509900
F	-3.09390600	-1.46249600	-0.74153900
C	3.72383500	1.36936200	0.33424300
C	3.38028800	0.95759900	1.64589700
C	2.26176400	0.12012200	1.84887100
C	1.49692700	-0.30621000	0.75053700
C	1.86459900	0.08458600	-0.60813200
C	2.98714500	0.94670500	-0.78616400
H	4.57536000	2.03839700	0.18915900
H	3.96082800	1.31098600	2.49894000
H	1.97994500	-0.17950000	2.86194200
H	3.25039600	1.28278200	-1.79179100
C	0.35600000	-1.24683800	0.68396400
C	0.16013700	-1.40897900	-0.94787200
N	1.20247500	-0.63910900	-1.61810300
H	-0.14315900	-2.34654500	-1.41214800
H	0.20122400	-2.02927200	1.42720000
Na	2.89459500	-1.96712900	-0.90966100

IntVI-R (G = -1132.098066)

F	-0.11111500	-2.90977600	-0.11978900
F	-1.61990100	-2.16266800	1.36499900
C	-1.14748100	-1.91342100	0.07787500
C	-1.72203900	0.54555200	-0.08083000
C	-0.56890700	-0.50388000	-0.10903200
C	-2.78910000	0.46814400	0.84568300
H	-2.85965800	-0.38987500	1.50985600
C	-3.76017600	1.48142500	0.90383100
H	-4.58049800	1.40128800	1.61968400

C	-1.64508400	1.66936000	-0.93164700
H	-0.81619200	1.74841900	-1.63579000
C	-3.67977600	2.59361000	0.04463600
H	-4.43412700	3.38065700	0.09197300
C	-2.61670800	2.68419300	-0.87182500
H	-2.54029900	3.54492000	-1.53869300
F	-2.13110200	-2.22907800	-0.83498500
C	4.26596000	1.51730400	-0.02438600
C	3.82716400	1.46563100	1.33739600
C	2.59018100	0.94275600	1.68278500
C	1.68079200	0.43217000	0.67724300
C	2.14145500	0.51005500	-0.71426100
C	3.42158700	1.04310800	-1.02477500
H	5.24107100	1.93803900	-0.26978300
H	4.48167000	1.85393400	2.12141700
H	2.27086600	0.91810100	2.72810500
H	3.70986400	1.07478100	-2.07770800
C	0.47989300	-0.24762200	0.98189100
C	0.14888200	-0.52165700	-1.48857600
N	1.35274500	-0.03322700	-1.75032400
H	-0.43395000	-0.93245200	-2.31811100
H	0.11228700	-0.25224700	2.01015800
Na	1.94354100	-1.93996800	-0.13790100

IntVII-R (G = -1209.092369)

F	0.18145400	2.64771200	-0.10538300
F	-1.53682500	2.13837500	-1.46758100
C	-1.04562500	1.88409800	-0.20798800
C	-2.09911400	-0.42612400	-0.06902900
C	-0.76997300	0.39380400	0.06068700
C	-2.02183000	-1.73190100	-0.59763300
H	-1.05491200	-2.09435400	-0.94686600
C	-3.16306700	-2.54927000	-0.66832000
H	-3.08236600	-3.55610200	-1.08228800
C	-3.34774300	0.03897800	0.40820500
H	-3.42863100	1.04124900	0.81894600
C	-4.40317700	-2.07510000	-0.20285600
C	-4.48920900	-0.77814700	0.33555100
H	-5.44592300	-0.39936400	0.70026100
F	-1.88017900	2.48677000	0.73946300
C	3.88095900	-2.01487300	0.52245200
C	3.65059900	-1.86199800	-0.87832800
C	2.50064100	-1.24203100	-1.36980600
C	1.45730700	-0.75825500	-0.46983000

C	1.73102000	-0.91451000	0.96789600
C	2.92096400	-1.53521900	1.41739800
H	4.78959000	-2.49709000	0.88088500
H	4.39138000	-2.24442700	-1.58566100
H	2.32385500	-1.18056200	-2.44818400
H	3.06047800	-1.62266000	2.49712500
C	0.32724500	-0.06158700	-0.90038400
C	-0.24425200	0.27938900	1.51724900
N	0.85086000	-0.34650400	1.91398100
H	-0.89482500	0.71415400	2.28072400
H	0.12293900	0.05570600	-1.96735900
H	3.60384200	2.00255900	-1.75242700
H	-5.29002700	-2.70888100	-0.25497900
O	3.64922600	1.52515100	-0.87171800
H	3.64520400	0.52508600	-1.09722000
Na	1.99282300	1.53179800	0.53116600

TSVI-R (G = -1209.085092)

F	-0.05462700	2.71957200	-0.31603100
F	1.41155800	2.27742500	1.35066900
C	1.06187500	1.90994800	0.07777500
C	1.90911900	-0.53033000	0.02464500
C	0.68600900	0.42966200	-0.07312600
C	1.63745200	-1.89737500	0.27605500
H	0.60555500	-2.21545100	0.41837900
C	2.67538000	-2.84074200	0.34524900
H	2.43885700	-3.88862500	0.53748500
C	3.25577400	-0.14020500	-0.16904700
H	3.49427900	0.89529700	-0.38337800
C	4.01227400	-2.43710700	0.17375000
C	4.29447600	-1.08423100	-0.08129200
H	5.32666500	-0.75680200	-0.21802600
F	2.07354200	2.31760800	-0.80765700
C	-3.91677000	-2.02615200	-0.45381000
C	-3.56410800	-2.06970300	0.91676600
C	-2.39394700	-1.45359900	1.37858200
C	-1.51706300	-0.77058200	0.48819100
C	-1.86643900	-0.77562100	-0.90512200
C	-3.05900700	-1.38384600	-1.35719400
H	-4.83199600	-2.50370300	-0.80401600
H	-4.21460100	-2.58655400	1.62529300
H	-2.14631100	-1.47824200	2.44309700
H	-3.26912300	-1.36240500	-2.42809400
C	-0.42847500	0.10318700	0.97503800

C	0.13627100	0.33365800	-1.52203100
N	-1.00934100	-0.16940600	-1.89456700
H	0.80585800	0.73823600	-2.28755300
H	0.01968100	-0.24428200	1.91671000
H	-1.16992500	1.21409600	1.37397500
H	4.82094300	-3.16687100	0.23644000
O	-2.07323400	2.13846200	1.50680400
H	-2.68416200	1.78948300	2.22681200
Na	-2.17778500	1.78279500	-0.55081700

IntII-S (G = -5290.133893)

C	2.38570600	1.27250200	-0.33107600
C	3.76063100	1.87836300	-0.34545600
C	4.53399000	1.70667800	-1.67765100
H	5.60473300	1.52613000	-1.59438800
H	4.00800300	1.14251700	-2.44551300
C	4.01891800	3.10512500	-1.36845100
C	2.87727100	3.64840800	-2.21511200
C	2.97888500	3.56941000	-3.62261300
H	3.84343200	3.07587900	-4.07035000
C	1.97815800	4.11426100	-4.44533800
H	2.06798400	4.04081700	-5.53071500
C	0.86422800	4.75567800	-3.86982000
H	0.08667900	5.18111200	-4.50727600
C	0.76192500	4.84451500	-2.46950500
H	-0.09470000	5.33886100	-2.00938500
C	1.76059100	4.29549100	-1.64515200
H	1.65218800	4.35573900	-0.56143200
C	5.02919400	4.15711500	-0.92959900
C	4.64658700	5.20304900	-0.05686700
H	3.62584000	5.24754600	0.32221100
C	5.56830900	6.19349800	0.32187900
H	5.25736900	6.98909800	1.00130600
C	6.88676200	6.16374900	-0.17182700
H	7.60159600	6.93307700	0.12382600
C	7.27275400	5.13899000	-1.05324200
H	8.28808400	5.11279400	-1.45231900
C	6.35069500	4.14431600	-1.42899700
H	6.65821700	3.36353500	-2.12570600
C	4.51994400	1.82948900	0.95947900
C	4.07667600	2.58133200	2.07632300
H	3.17996300	3.19089500	2.00107800
C	4.80184900	2.50813200	3.26841700
C	5.95258600	1.71883100	3.42352900

C	6.35316800	0.97741800	2.30549600
C	5.66650400	1.01275000	1.08602800
H	6.01009400	0.41422600	0.24544800
C	-1.52812900	2.27110500	-0.01945300
C	-2.67646900	3.25504500	0.12196100
C	-2.42894900	4.69927100	0.86551900
C	-3.13804500	3.53358000	1.55958400
H	-2.61141200	2.97481600	2.32980500
H	-4.20524900	3.66526800	1.73478200
C	-3.69080700	3.20355200	-1.00860000
C	-3.27258700	3.29015700	-2.36483600
H	-2.21444100	3.34996800	-2.59959600
C	-4.23414400	3.26557800	-3.37718800
C	-5.61283500	3.15931100	-3.13107700
C	-5.99191200	3.06451500	-1.78629900
C	-5.07379000	3.07910500	-0.72991100
H	-5.42938400	2.99599600	0.29316500
C	-3.33121700	5.82828400	0.38759600
C	-3.24714500	6.34756600	-0.92473200
H	-2.56977200	5.88577800	-1.64317700
C	-4.04524400	7.43789100	-1.31598900
H	-3.97510400	7.82144400	-2.33521300
C	-4.93623600	8.02724300	-0.39942700
H	-5.55831000	8.86999500	-0.70436900
C	-5.02013700	7.52392700	0.91206300
H	-5.70348100	7.97971400	1.63038800
C	-4.22078600	6.43442800	1.30296400
H	-4.27757700	6.05531400	2.32478900
C	-1.04157700	5.13733200	1.30722300
C	-0.31946700	4.43276300	2.29787000
H	-0.72192800	3.53424500	2.74821500
C	0.93506600	4.89273800	2.73758800
H	1.46093600	4.32678700	3.50621000
C	1.49396400	6.06942400	2.20567400
H	2.45654900	6.43438200	2.56877700
C	0.78484700	6.78151400	1.21889900
H	1.19721400	7.70208200	0.80251100
C	-0.46787300	6.32314500	0.77788000
H	-1.02375600	6.90578300	0.04553400
C	-2.44671200	-1.02124600	-0.39839600
C	-3.89402500	-1.43313600	-0.34813900
C	-4.82929300	-0.55735800	-1.23667000
H	-5.77868700	-0.27479200	-0.78523900
H	-4.32555700	0.20909400	-1.82246100

C	-4.61153500	-1.99644200	-1.67955700
C	-3.77067300	-2.20785500	-2.93137900
C	-2.66801900	-3.08692200	-2.95113700
H	-2.35929900	-3.57464800	-2.02669400
C	-1.94600000	-3.30919800	-4.13720300
H	-1.08980400	-3.98741000	-4.13255300
C	-2.31951200	-2.65086500	-5.32371400
H	-1.75557600	-2.81504100	-6.24342600
C	-3.42430400	-1.77752600	-5.31549500
H	-3.72163300	-1.26371900	-6.23122700
C	-4.14814100	-1.56254500	-4.12907700
H	-5.00430900	-0.88560700	-4.12655400
C	-5.73945300	-3.01485700	-1.50985700
C	-5.51516900	-4.37131200	-1.85686000
H	-4.55391000	-4.66206900	-2.27941300
C	-6.52444300	-5.33607400	-1.69982600
H	-6.32689800	-6.37340500	-1.97542400
C	-7.78878200	-4.96604500	-1.20380300
H	-8.57506900	-5.71289300	-1.08588300
C	-8.03197400	-3.62091500	-0.87478800
H	-9.01163100	-3.31669500	-0.50292100
C	-7.01886700	-2.65649600	-1.02556100
H	-7.23963900	-1.62201300	-0.76656700
C	-4.37817900	-1.80771400	1.03575700
C	-4.65826900	-3.14032500	1.40642700
H	-4.57825800	-3.94015600	0.67648700
C	-5.07572800	-3.40289100	2.71669800
C	-5.22303500	-2.40577900	3.68949700
C	-4.92345700	-1.09359100	3.28877200
C	-4.51145400	-0.77236600	1.99414800
H	-4.26328900	0.25298000	1.72406200
C	1.48052400	-2.09628300	-0.81692700
C	2.56578200	-3.07768800	-1.21834700
C	2.38374800	-4.66235100	-1.01997600
C	3.34559200	-3.85175400	-0.14632800
H	3.04940900	-3.70431700	0.88835100
H	4.41721200	-3.96546100	-0.30410200
C	3.32661200	-2.61872800	-2.45247200
C	4.66101800	-2.17013400	-2.33183700
H	5.15200100	-2.15683700	-1.36080400
C	5.34218000	-1.73900100	-3.47782500
C	4.75529500	-1.71954400	-4.74906500
C	3.42207100	-2.15546300	-4.82867400
C	2.69741100	-2.60051200	-3.72063400

H	1.66321900	-2.91332200	-3.82195600
C	2.92690800	-5.55042500	-2.12896300
C	4.27081100	-5.98184000	-2.16422100
H	4.96052000	-5.68885600	-1.37255200
C	4.73331100	-6.80456900	-3.20865500
H	5.77460200	-7.13035100	-3.21735100
C	3.85922100	-7.20839700	-4.23295100
H	4.21898300	-7.84357400	-5.04348600
C	2.51297300	-6.79477200	-4.20100000
H	1.82469500	-7.11197500	-4.98605800
C	2.05108100	-5.97800600	-3.15650900
H	1.00208500	-5.67975500	-3.12251600
C	1.14206200	-5.22675100	-0.34954700
C	1.31127200	-6.31903600	0.53599200
H	2.31901000	-6.67866800	0.75182600
C	0.19747100	-6.95681600	1.10651100
H	0.34222500	-7.80321300	1.77981800
C	-1.10498800	-6.51198500	0.80073700
H	-1.97323400	-7.01207500	1.23360000
C	-1.27960700	-5.42273600	-0.07137600
H	-2.28539200	-5.07080800	-0.30606500
C	-0.16301900	-4.78430900	-0.64866200
H	-0.30474500	-3.94404600	-1.32888900
O	-1.19825200	1.56880300	1.05302900
O	-0.98133800	2.10788800	-1.20065400
O	-1.72300900	-1.19909900	0.69946000
O	-2.00180800	-0.46221400	-1.49838100
O	1.30158100	-1.78555300	0.46307100
O	0.80472900	-1.55985100	-1.80065000
O	1.84514500	0.98574000	0.84528900
O	1.81031000	1.04838900	-1.48886900
Rh	0.05122100	-0.10148700	0.92462900
Rh	-0.08698100	0.27889500	-1.54003200
C	-0.03933900	-0.36884000	2.96592100
C	2.87728500	-0.74562000	4.88683900
H	2.99549300	0.10532000	5.54774900
C	2.84361200	-2.13384900	5.26860200
C	-0.02765500	0.92532600	3.74264500
F	-1.32028500	1.52688200	3.74523700
F	0.35222300	0.86010400	5.09782400
F	0.84368000	1.87746300	3.18255700
C	-0.51820900	-1.56578200	3.61455900
C	-0.95595800	-1.60151100	4.98912700
C	-0.56996500	-2.79934900	2.87868000

C	-1.45904200	-2.77374400	5.55290000
H	-0.88223900	-0.70344800	5.59122200
C	-1.06199600	-3.96959500	3.46234300
H	-0.20555500	-2.82017700	1.85696100
C	-1.51710900	-3.96307000	4.79517600
H	-1.79204200	-2.77221000	6.59189300
H	-1.08519500	-4.88676000	2.87553800
H	-1.90419600	-4.87886900	5.24516400
C	2.72556500	-0.68586000	3.49980900
C	2.66126400	-2.90270100	4.05023300
N	2.62405000	-1.99688100	2.98937000
H	2.74040000	0.16090500	2.82463300
H	2.27537900	-2.16348200	2.03509300
C	2.95067300	-2.81621100	6.50742200
C	2.86189900	-4.21062300	6.52239400
C	2.66578300	-4.94892000	5.31879500
C	2.56613300	-4.30841400	4.07776700
H	3.09918100	-2.25574200	7.43204100
H	2.94274500	-4.74977000	7.46758700
H	2.59555600	-6.03690800	5.36742100
H	2.40649400	-4.88022100	3.16251300
Br	-7.94608100	2.89191100	-1.35770400
Br	-3.62802400	3.40054500	-5.28300100
Br	7.24637800	-1.13041000	-3.29560800
Br	2.53248400	-2.14070000	-6.62165200
Br	-5.09158000	0.37385000	4.64476900
Br	-5.49413200	-5.29831200	3.23393500
Br	4.18543200	3.57031500	4.85659700
Br	7.97735800	-0.18731900	2.46530000
H	-5.55029000	-2.63412300	4.70049600
H	-6.34209500	3.15245800	-3.93712400
H	5.30136300	-1.38749100	-5.62852300
H	6.49845200	1.68093100	4.36265000

TSII-S (G = -5290.120925)

C	2.39774600	1.25164700	-0.34458500
C	3.79861600	1.80444400	-0.35270200
C	4.59689900	1.58010700	-1.65976800
H	5.65335400	1.34081300	-1.54481100
H	4.06137900	1.04246400	-2.44004400
C	4.14018200	3.00561800	-1.37411800
C	3.04224600	3.58030600	-2.25726900
C	3.22255800	3.55350800	-3.65886100
H	4.11593900	3.08385200	-4.07488800

C	2.26238300	4.11928300	-4.51485200
H	2.41153100	4.08572400	-5.59564500
C	1.11134500	4.72859000	-3.97823300
H	0.36413000	5.16820800	-4.64178100
C	0.93080600	4.76578600	-2.58386300
H	0.04436000	5.23277800	-2.15345900
C	1.88930800	4.19546100	-1.72626500
H	1.71902700	4.20812800	-0.64871200
C	5.17278600	4.02327500	-0.90536200
C	4.76047000	5.16546700	-0.17718900
H	3.70343900	5.31434800	0.04310400
C	5.69721800	6.12069300	0.25098400
H	5.35986100	6.99266800	0.81426700
C	7.06397500	5.96032300	-0.04820700
H	7.79058600	6.70329200	0.28394700
C	7.48239100	4.84024900	-0.78706200
H	8.53654100	4.71254600	-1.03889300
C	6.54447300	3.88058200	-1.21206900
H	6.88455200	3.02736700	-1.79950800
C	4.52198300	1.71704700	0.96958000
C	4.16332200	2.56814700	2.04236500
H	3.38291000	3.31157900	1.90431900
C	4.81609400	2.42332600	3.26906800
C	5.81771300	1.46493600	3.49871900
C	6.13990200	0.63334200	2.41909000
C	5.52173100	0.73676200	1.16677700
H	5.80340500	0.07236800	0.35213300
C	-1.49118900	2.30135300	-0.05852100
C	-2.61979100	3.31471100	0.07801900
C	-2.33407700	4.80550600	0.69036300
C	-3.00421500	3.69292200	1.51072400
H	-2.43556400	3.18688600	2.28900900
H	-4.06000200	3.83760000	1.73806000
C	-3.68994100	3.19907900	-0.99571900
C	-3.33317500	3.20256700	-2.37162500
H	-2.28482600	3.22828600	-2.65317500
C	-4.34038400	3.14236100	-3.33656400
C	-5.70769300	3.07254500	-3.02225500
C	-6.02503500	3.05360700	-1.65823200
C	-5.05921300	3.11058900	-0.64671200
H	-5.36683800	3.08866000	0.39497800
C	-3.26625400	5.89129400	0.17127000
C	-3.20659900	6.33551900	-1.17006300
H	-2.52351100	5.84850100	-1.86646100

C	-4.03089900	7.38473700	-1.61464500
H	-3.97956300	7.70972300	-2.65515600
C	-4.92399900	8.00901400	-0.72301800
H	-5.56701700	8.81954600	-1.06920000
C	-4.98177900	7.58296300	0.61669100
H	-5.66542800	8.06725900	1.31588200
C	-4.15548500	6.53411900	1.06076200
H	-4.19226100	6.21621300	2.10406200
C	-0.93184800	5.28497300	1.03605000
C	-0.10736400	4.57671900	1.94136100
H	-0.42431200	3.62706100	2.35341200
C	1.14130300	5.09058700	2.33487600
H	1.73604000	4.53438900	3.06138300
C	1.60370100	6.31954300	1.82634500
H	2.56286600	6.72604900	2.15234700
C	0.80149400	7.02626500	0.91135000
H	1.13977500	7.98276100	0.50934100
C	-0.45238000	6.52035500	0.52692200
H	-1.07967200	7.10086500	-0.14654800
C	-2.43608400	-1.01302400	-0.38366200
C	-3.88037800	-1.44276400	-0.33134200
C	-4.84493700	-0.53143200	-1.14737200
H	-5.78699400	-0.28082300	-0.66254400
H	-4.36218700	0.26667600	-1.70749100
C	-4.62454600	-1.94346600	-1.67217600
C	-3.83167100	-2.07171500	-2.96609200
C	-2.70570200	-2.91273600	-3.07844500
H	-2.33422900	-3.42418600	-2.19156800
C	-2.03611100	-3.05966700	-4.30620500
H	-1.15889800	-3.70707100	-4.37169000
C	-2.48746100	-2.36371300	-5.44319200
H	-1.96494500	-2.46989100	-6.39538800
C	-3.61600800	-1.52735900	-5.34285400
H	-3.97342500	-0.98340200	-6.21891800
C	-4.28609800	-1.38725000	-4.11449200
H	-5.16019400	-0.73788900	-4.04005400
C	-5.73422100	-2.98480200	-1.52384200
C	-5.51689400	-4.30652000	-1.98906000
H	-4.57613000	-4.54898200	-2.48254900
C	-6.50756900	-5.29419500	-1.85762400
H	-6.31530700	-6.30355000	-2.22566500
C	-7.74692500	-4.98190600	-1.26814300
H	-8.51935500	-5.74596100	-1.16984800
C	-7.98353100	-3.67082000	-0.81841300

H	-8.94402400	-3.41056100	-0.37070600
C	-6.98874700	-2.68416200	-0.94412300
H	-7.20319800	-1.67778200	-0.58747200
C	-4.34123800	-1.90346300	1.03386500
C	-4.53754000	-3.26694200	1.34149400
H	-4.39019200	-4.02617000	0.57958700
C	-4.95937300	-3.61418500	2.62958600
C	-5.18930600	-2.67303300	3.64156000
C	-4.96949800	-1.32840800	3.30356300
C	-4.55735700	-0.92288500	2.03285900
H	-4.37733700	0.12754800	1.81036400
C	1.45936600	-2.08203800	-0.86713200
C	2.55464700	-3.07296200	-1.23641100
C	2.35352700	-4.65339900	-1.06956500
C	3.23657900	-3.85045600	-0.10451800
H	2.80902200	-3.68656200	0.88353700
H	4.31739200	-3.97999000	-0.14801700
C	3.39546700	-2.60216000	-2.41181600
C	4.75643200	-2.26751700	-2.23223400
H	5.22019300	-2.34428000	-1.25128600
C	5.50456400	-1.83114000	-3.33342000
C	4.96258800	-1.69799000	-4.61729300
C	3.60271200	-2.02350700	-4.75699600
C	2.81145200	-2.46854800	-3.69562800
H	1.75799800	-2.68646800	-3.83884100
C	3.00433000	-5.52764000	-2.13147400
C	4.32811300	-6.00361100	-2.01630300
H	4.92476600	-5.75364100	-1.13846500
C	4.88917100	-6.81593300	-3.02026600
H	5.91325600	-7.17702000	-2.91275800
C	4.13418300	-7.16317700	-4.15393900
H	4.57016500	-7.78938100	-4.93346800
C	2.80782300	-6.70355100	-4.27335800
H	2.21123000	-6.97562800	-5.14549000
C	2.24750000	-5.89782800	-3.26925300
H	1.21270100	-5.56286200	-3.35394200
C	1.06388400	-5.24009800	-0.51905700
C	1.16823900	-6.35831700	0.34371300
H	2.15762000	-6.72164700	0.62793400
C	0.01659900	-7.01420900	0.80791700
H	0.11145800	-7.88012700	1.46555000
C	-1.25959400	-6.56140700	0.41552400
H	-2.15710700	-7.06831500	0.77323300
C	-1.36957300	-5.44889200	-0.43554800

H	-2.35549900	-5.09301000	-0.73706600
C	-0.21521200	-4.79081600	-0.90627100
H	-0.30601900	-3.92547600	-1.56308800
O	-1.18754400	1.59115200	1.00994100
O	-0.94683200	2.13248600	-1.24214500
O	-1.70387400	-1.19916600	0.70447700
O	-2.01510400	-0.43550700	-1.48611500
O	1.32559900	-1.73585500	0.40269300
O	0.76594600	-1.57656000	-1.85644800
O	1.83889200	1.02218000	0.83876100
O	1.83588000	1.01130200	-1.50297600
Rh	0.06508900	-0.09331700	0.89860800
Rh	-0.09143800	0.28510000	-1.57112800
C	0.11034300	-0.45456300	3.02190400
C	2.09709100	-0.34754200	3.78938300
H	2.12526200	0.73040800	3.67196200
C	2.18814300	-1.05475300	5.09038900
C	-0.34484900	0.80261000	3.72586000
F	-1.70903300	1.04833300	3.51140500
F	-0.18576200	0.86139600	5.14297600
F	0.37483600	1.94400900	3.28399300
C	-0.42000200	-1.73253400	3.55955300
C	-1.11129800	-1.82229900	4.80776400
C	-0.22717200	-2.93758200	2.82369600
C	-1.60763800	-3.04772900	5.26949000
H	-1.24210600	-0.93049800	5.41078200
C	-0.71182900	-4.16343900	3.30139400
H	0.29031300	-2.89451200	1.86977900
C	-1.40682900	-4.22515100	4.52399700
H	-2.13983900	-3.08667700	6.22184300
H	-0.56465000	-5.06481100	2.70638500
H	-1.79226800	-5.17870800	4.88948700
C	2.76002800	-1.19632000	2.85027100
C	2.76616700	-2.33672600	4.83895000
N	3.08627900	-2.37711700	3.44882500
H	2.92996500	-1.01736800	1.79952900
H	3.50286000	-3.17687300	2.96738800
C	1.82801500	-0.72214000	6.40910600
C	2.06113500	-1.65986900	7.43180200
C	2.62515900	-2.92698800	7.15526300
C	2.98616900	-3.28529400	5.84354100
H	1.36471900	0.23616200	6.62378400
H	1.79497300	-1.40789800	8.45904500
H	2.78584600	-3.63637900	7.96762000

H	3.42572400	-4.25931300	5.62682100
Br	-7.96021400	2.93553500	-1.13316300
Br	-3.82034000	3.17923400	-5.27225600
Br	7.44215200	-1.37861000	-3.06104700
Br	2.77221000	-1.84291500	-6.56815800
Br	-5.26238400	0.06443100	4.71865800
Br	-5.27317700	-5.55362100	3.05377800
Br	4.30500200	3.62602000	4.79092900
Br	7.54321400	-0.78020400	2.68841400
H	-5.51983200	-2.96702900	4.63422900
H	-6.47399800	3.03711500	-3.79238600
H	5.55983500	-1.36203900	-5.46124400
H	6.31188800	1.37358300	4.46256500

IntIII-S (G = -5290.125194)

C	2.35981200	1.15294200	-0.44198300
C	3.78303600	1.64354900	-0.51257800
C	4.54153900	1.32517100	-1.82354500
H	5.58382300	1.02723700	-1.71611500
H	3.96088500	0.79231800	-2.57425600
C	4.16552500	2.78351100	-1.58476200
C	3.07482000	3.36963500	-2.46946000
C	3.24318100	3.31006400	-3.87155300
H	4.12136500	2.81000700	-4.28463800
C	2.29035900	3.88270300	-4.73108500
H	2.42920500	3.82344100	-5.81211400
C	1.15971300	4.53196900	-4.19768400
H	0.41810600	4.97667100	-4.86407600
C	0.99160000	4.60167300	-2.80317900
H	0.12079700	5.09953000	-2.37553900
C	1.94206800	4.02347700	-1.94147600
H	1.78181000	4.06137100	-0.86293200
C	5.25037800	3.77295300	-1.17343100
C	4.88293400	5.02438700	-0.61986100
H	3.82809800	5.27452700	-0.50745500
C	5.86126000	5.95498300	-0.23232900
H	5.55638300	6.91300900	0.19272500
C	7.22831900	5.66062500	-0.39865400
H	7.98770600	6.38499100	-0.10048500
C	7.60483900	4.43024800	-0.96449700
H	8.66019900	4.19657100	-1.11484100
C	6.62494900	3.49579900	-1.34873000
H	6.93961300	2.55611400	-1.80241700
C	4.53577100	1.55043200	0.79194300

C	4.40119600	2.54431900	1.78890800
H	3.77918500	3.41530200	1.60207900
C	5.07890700	2.38600200	3.00181900
C	5.88407500	1.26999100	3.29041000
C	5.97980200	0.30001200	2.28467800
C	5.33803200	0.41272500	1.04716100
H	5.44650000	-0.35599900	0.28401300
C	-1.46886600	2.31861200	-0.11330300
C	-2.54385400	3.39078600	0.00483400
C	-2.16810800	4.88859000	0.54358400
C	-2.87816300	3.84875800	1.42531100
H	-2.31866900	3.35059300	2.21514600
H	-3.92021900	4.05818400	1.66513100
C	-3.64299400	3.28174600	-1.03987000
C	-3.31983700	3.23375200	-2.42296800
H	-2.27851000	3.21573200	-2.72981200
C	-4.35172400	3.17878100	-3.36150000
C	-5.71231500	3.15988300	-3.01306900
C	-5.99667900	3.18873500	-1.64194500
C	-5.00500200	3.24538200	-0.65567800
H	-5.28607000	3.26012900	0.39370700
C	-3.05299900	5.99927800	-0.00422800
C	-2.99087700	6.38829700	-1.36254900
H	-2.34087000	5.84272000	-2.04711500
C	-3.76964200	7.45846300	-1.83808000
H	-3.71731800	7.74001000	-2.89114500
C	-4.61899700	8.15959900	-0.96091300
H	-5.22717400	8.98634200	-1.33094000
C	-4.67814200	7.78915200	0.39512300
H	-5.32769000	8.33287900	1.08306900
C	-3.89724100	6.71915300	0.86993500
H	-3.93474500	6.44409600	1.92529200
C	-0.73446000	5.30418200	0.84168800
C	0.08270700	4.56986800	1.73414400
H	-0.27173100	3.64713000	2.17683800
C	1.36663000	5.02885000	2.07942500
H	1.95735500	4.45542800	2.79617500
C	1.87171700	6.22624200	1.53722300
H	2.85965900	6.58973400	1.82589800
C	1.07572600	6.95775400	0.63646800
H	1.44580800	7.89171200	0.20995000
C	-0.21195400	6.50683100	0.29793300
H	-0.83045200	7.10573400	-0.36742300
C	-2.51169500	-1.00183300	-0.23207500

C	-3.96164000	-1.39778000	-0.10256400
C	-4.94648500	-0.45225300	-0.85280200
H	-5.85234000	-0.18130800	-0.31275400
H	-4.47640900	0.33832400	-1.43406300
C	-4.79457400	-1.86637900	-1.39909100
C	-4.08697400	-2.00728800	-2.74058900
C	-2.99194300	-2.87587000	-2.92751300
H	-2.57613500	-3.40019800	-2.06821300
C	-2.40523000	-3.03223700	-4.19582600
H	-1.54991400	-3.70019000	-4.31913900
C	-2.90998700	-2.31898300	-5.29931100
H	-2.45159700	-2.43279900	-6.28314600
C	-4.00830000	-1.45524600	-5.12430400
H	-4.40639700	-0.89736100	-5.97370900
C	-4.59534300	-1.30528600	-3.85522200
H	-5.44588300	-0.63421500	-3.72252700
C	-5.92272600	-2.87783100	-1.19117900
C	-5.77057500	-4.20106300	-1.67735700
H	-4.86813100	-4.46494400	-2.22806900
C	-6.77794100	-5.16290000	-1.49216500
H	-6.63564500	-6.17414900	-1.87738200
C	-7.97004600	-4.82248100	-0.82594300
H	-8.75533200	-5.56651500	-0.68497600
C	-8.14280700	-3.50926900	-0.35407100
H	-9.06648900	-3.22709200	0.15382900
C	-7.13102800	-2.54864900	-0.53408200
H	-7.29581400	-1.54008100	-0.15791200
C	-4.35179500	-1.86482000	1.28292000
C	-4.54209500	-3.23011400	1.58640300
H	-4.45107400	-3.98096700	0.80776500
C	-4.88289900	-3.59009100	2.89454500
C	-5.03891200	-2.65971300	3.93020700
C	-4.83149700	-1.31295200	3.59363600
C	-4.49606800	-0.89490100	2.30449900
H	-4.31647400	0.15595100	2.08578000
C	1.33623600	-2.17685000	-0.85730200
C	2.39106900	-3.20814300	-1.23111700
C	2.12979400	-4.77877900	-1.06373500
C	3.06356800	-4.01409200	-0.11317900
H	2.66952800	-3.85609100	0.89013900
H	4.13687500	-4.18832200	-0.18145200
C	3.23127800	-2.77328900	-2.42245600
C	4.61409600	-2.52146700	-2.27499200
H	5.09816700	-2.63794700	-1.30794300

C	5.35971100	-2.12007600	-3.39091600
C	4.79616700	-1.94340200	-4.66007900
C	3.41629600	-2.18698900	-4.76844200
C	2.62612700	-2.59437200	-3.69115000
H	1.55826700	-2.74804500	-3.80875900
C	2.72101600	-5.67727800	-2.13931200
C	4.02057900	-6.21965900	-2.04456200
H	4.64012900	-6.00430900	-1.17333400
C	4.52620500	-7.05441800	-3.05956600
H	5.53202000	-7.46758500	-2.96784600
C	3.73906700	-7.35755700	-4.18400400
H	4.13202900	-8.00125100	-4.97214700
C	2.43601200	-6.83111900	-4.28296200
H	1.81451700	-7.06869100	-5.14776600
C	1.93073500	-6.00314800	-3.26775100
H	0.91313800	-5.61580100	-3.33644200
C	0.83406400	-5.31506900	-0.47603700
C	0.92498100	-6.42704000	0.39651000
H	1.90902900	-6.82284800	0.65462600
C	-0.23429300	-7.03156600	0.90869100
H	-0.15029500	-7.89138400	1.57576600
C	-1.50458100	-6.53331100	0.55487300
H	-2.40784100	-6.99651100	0.95446100
C	-1.60050500	-5.42951000	-0.30847100
H	-2.58158900	-5.03859200	-0.58046800
C	-0.43905400	-4.82235700	-0.82788500
H	-0.52025200	-3.96095200	-1.49094200
O	-1.16933400	1.63773100	0.97186600
O	-0.96387900	2.08271300	-1.30449100
O	-1.74012100	-1.17359800	0.82880700
O	-2.12739300	-0.46359700	-1.36928000
O	1.27334400	-1.76229600	0.39851200
O	0.60198400	-1.70048600	-1.82872500
O	1.82510600	1.00397100	0.76594300
O	1.76495400	0.87264400	-1.57397900
Rh	0.03596800	-0.08650500	0.90642900
Rh	-0.18708200	0.19854500	-1.57129800
C	0.24844000	-0.38914000	3.19533000
C	1.79330100	-0.24054200	3.52426900
H	2.11676000	0.71199000	3.04827700
C	2.33069600	-0.30530000	4.98028900
C	-0.47909300	0.80609900	3.71306200
F	-1.82227000	0.86073800	3.33878900
F	-0.54456500	0.98529900	5.15567600

F	0.17420900	2.00596200	3.31462700
C	-0.28458800	-1.73087100	3.71319200
C	-0.92028000	-1.84828100	4.97721300
C	-0.06538900	-2.92005800	2.97370500
C	-1.32251900	-3.10058800	5.47316400
H	-1.08411400	-0.95609600	5.57222200
C	-0.45440000	-4.17415400	3.47921200
H	0.37061400	-2.85996300	1.97949400
C	-1.08582500	-4.27162600	4.73214800
H	-1.80903900	-3.15779800	6.44936400
H	-0.29235700	-5.06655100	2.87347000
H	-1.39828200	-5.24334000	5.11918700
C	2.59491200	-1.32234700	2.86103500
C	3.35909700	-1.27859600	5.02854500
N	3.45984500	-1.86063400	3.71338800
H	2.47371000	-1.64269500	1.82404100
H	4.14127000	-2.59013200	3.46992700
C	2.05164400	0.42355100	6.14440800
C	2.80157500	0.15628000	7.30986200
C	3.81878300	-0.82177400	7.32743300
C	4.11490100	-1.56488700	6.16869400
H	1.24630500	1.14863100	6.15001800
H	2.58236900	0.71465100	8.22066200
H	4.37907400	-1.00863200	8.24359200
H	4.89921700	-2.32227100	6.16559200
Br	-7.92127000	3.14446600	-1.06807000
Br	-3.87848500	3.14856800	-5.30957900
Br	7.32700900	-1.78370600	-3.16173000
Br	2.55353200	-1.94169200	-6.55614400
Br	-5.02232600	0.06504100	5.04058900
Br	-5.18592500	-5.53230300	3.31470700
Br	4.90299300	3.80306100	4.40568800
Br	7.08171800	-1.35086800	2.65084900
H	-5.30435500	-2.96347400	4.93926400
H	-6.49797700	3.12676400	-3.76352800
H	5.39175600	-1.63562200	-5.51586700
H	6.40210100	1.16985000	4.24061900

TSIII-S (G = -5290.104785)

C	2.38035800	1.42125100	-0.52987900
C	3.67953600	2.17574400	-0.58867400
C	4.56167400	1.88406700	-1.82649700
H	5.63810100	1.85237200	-1.66066700
H	4.15623000	1.14682400	-2.51745800

C	3.87511900	3.24305000	-1.78571200
C	2.74767100	3.49803500	-2.77504500
C	2.96680400	3.20703300	-4.14087400
H	3.91198900	2.75562600	-4.44805700
C	1.98049800	3.49059900	-5.10093500
H	2.16218200	3.25596900	-6.15132600
C	0.76368800	4.08080300	-4.70810700
H	-0.00155500	4.30633600	-5.45337400
C	0.54291800	4.37935700	-3.35122900
H	-0.39128200	4.84157600	-3.03099500
C	1.52654000	4.08946300	-2.38817900
H	1.32705500	4.30794600	-1.33822600
C	4.72613600	4.46565400	-1.46829900
C	4.16243000	5.58055500	-0.80368200
H	3.11445600	5.56293300	-0.50479500
C	4.93778200	6.72103100	-0.53503200
H	4.48770000	7.56942600	-0.01656300
C	6.28719100	6.77380100	-0.93412900
H	6.88781200	7.66014400	-0.72461300
C	6.85199600	5.67918000	-1.61152200
H	7.89249900	5.71461100	-1.93858700
C	6.07686200	4.53469900	-1.87642800
H	6.52200900	3.69912700	-2.41813500
C	4.33256000	2.42089100	0.75169500
C	3.69613000	3.24323800	1.71549800
H	2.74744100	3.71891700	1.48285800
C	4.29219700	3.40212200	2.96842000
C	5.50473200	2.79005100	3.32817700
C	6.10385200	1.98116400	2.35478400
C	5.54768300	1.78108900	1.08498400
H	6.04337200	1.13420100	0.36485900
C	-1.61416600	1.96724600	-0.64540100
C	-2.87938500	2.78815400	-0.79553900
C	-2.89459300	4.38750900	-0.44200100
C	-3.50003500	3.33348200	0.49323300
H	-2.97712500	3.08378500	1.41343100
H	-4.58728400	3.32637500	0.56416900
C	-3.77904800	2.27988300	-1.91037100
C	-3.31460000	2.23950000	-3.25144600
H	-2.30234000	2.55480800	-3.48442500
C	-4.16314300	1.75545500	-4.24795100
C	-5.46756200	1.30043600	-3.99659800
C	-5.88876000	1.33781800	-2.66116400
C	-5.07893900	1.80544800	-1.61827000

H	-5.44311000	1.78676400	-0.59416200
C	-3.89241900	5.20628300	-1.24744900
C	-3.70064100	5.45863400	-2.62577000
H	-2.84948400	5.01132000	-3.13928100
C	-4.60177500	6.26897400	-3.33938300
H	-4.44413200	6.44592500	-4.40464400
C	-5.70691900	6.84408300	-2.68383000
H	-6.40909100	7.46836100	-3.23835700
C	-5.90008200	6.61013800	-1.31002900
H	-6.74979200	7.05852400	-0.79268300
C	-4.99705600	5.80027200	-0.59712400
H	-5.14281100	5.63282900	0.47119900
C	-1.62661600	5.12582300	-0.03520100
C	-0.81287800	4.67531000	1.03207800
H	-1.03439200	3.75102900	1.54852100
C	0.30647500	5.41599000	1.45106400
H	0.88904800	5.04570100	2.29537100
C	0.64601700	6.62438100	0.81346900
H	1.50206000	7.20889900	1.15597000
C	-0.14923300	7.08118400	-0.25398400
H	0.09237700	8.01968400	-0.75583300
C	-1.27396100	6.34630000	-0.66863200
H	-1.90137900	6.73415900	-1.46878000
C	-2.20101600	-1.35310900	-0.24372400
C	-3.58478900	-1.95672400	-0.20825900
C	-4.18911500	-2.26054400	-1.59770700
H	-5.27136100	-2.16146000	-1.67314500
H	-3.62962300	-1.85884200	-2.43863300
C	-3.63316200	-3.47246600	-0.86057800
C	-2.36946900	-4.14591200	-1.39646600
C	-1.77555600	-5.20646200	-0.66713100
H	-2.19549200	-5.48830500	0.29816700
C	-0.70364400	-5.94295700	-1.20006700
H	-0.28235400	-6.77160300	-0.62805800
C	-0.19582500	-5.63350900	-2.47721300
H	0.61593700	-6.22260200	-2.90872900
C	-0.76782800	-4.57632900	-3.20779200
H	-0.38575200	-4.32816400	-4.19944600
C	-1.84408000	-3.84365300	-2.67572000
H	-2.28028800	-3.04738800	-3.27451300
C	-4.59014100	-4.46865800	-0.22830400
C	-4.52492500	-4.78534500	1.14820600
H	-3.83472300	-4.23788900	1.79271400
C	-5.37349300	-5.76736100	1.69170600

H	-5.32260000	-5.99759900	2.75719300
C	-6.29867200	-6.43881600	0.86989000
H	-6.96030800	-7.19533900	1.29429700
C	-6.37193400	-6.12442100	-0.50064700
H	-7.08812800	-6.64000800	-1.14241600
C	-5.52068200	-5.14686300	-1.04729600
H	-5.56892100	-4.91022200	-2.11175900
C	-4.56943000	-1.51372300	0.87174000
C	-4.23892900	-0.54263900	1.86128700
H	-3.22158700	-0.17885700	1.96322200
C	-5.24991500	-0.06271800	2.70614700
C	-6.57822800	-0.50660800	2.66788300
C	-6.86730400	-1.47818100	1.70385400
C	-5.91625600	-1.97350000	0.81311200
H	-6.21548100	-2.72434600	0.09157700
C	1.96208600	-1.99658900	-0.35785000
C	3.28459000	-2.72403300	-0.53784200
C	3.73996200	-3.94022200	0.39411200
C	4.34303500	-2.54762000	0.57549000
H	4.03014300	-1.97310100	1.44443400
H	5.37133000	-2.38626000	0.25529500
C	3.76728200	-2.74103000	-1.97752600
C	4.86320000	-1.94432700	-2.37403100
H	5.37134400	-1.30834500	-1.65288100
C	5.28285400	-1.97385800	-3.71025200
C	4.65844800	-2.75928700	-4.68591200
C	3.56343900	-3.52860100	-4.25862100
C	3.10313500	-3.53779300	-2.94054500
H	2.23665500	-4.12755000	-2.65438500
C	4.57980700	-5.02110600	-0.27854500
C	5.99059700	-4.98324600	-0.28699900
H	6.51847700	-4.15919900	0.19400300
C	6.73252300	-6.01095100	-0.90049300
H	7.82270800	-5.96588400	-0.89560600
C	6.07370600	-7.09112600	-1.51252800
H	6.64831100	-7.88553800	-1.99064600
C	4.66591400	-7.14526300	-1.49779700
H	4.14676100	-7.98488300	-1.96285000
C	3.92687100	-6.12249800	-0.88207700
H	2.83777600	-6.17700900	-0.85655000
C	2.83686900	-4.50713800	1.47701200
C	3.45588400	-4.98179400	2.66085500
H	4.53153300	-4.84816900	2.78961800
C	2.70914300	-5.66881300	3.63354400

H	3.20624100	-6.06032400	4.52343800
C	1.32745900	-5.87572700	3.44642800
H	0.74596100	-6.40924700	4.19943300
C	0.70672800	-5.40012200	2.27827700
H	-0.35955700	-5.56460300	2.11778300
C	1.45485400	-4.72479900	1.29311500
H	0.96124200	-4.39930900	0.37781600
O	-1.25169600	1.59106800	0.56447200
O	-0.99568700	1.59473800	-1.74583700
O	-1.55953900	-1.15922800	0.89546900
O	-1.70009400	-1.07632400	-1.43142400
O	1.60999500	-1.53125300	0.82930100
O	1.27494000	-1.80327700	-1.45875000
O	1.80434400	1.29989800	0.65948500
O	1.90607900	0.91339100	-1.64104600
Rh	0.14396500	0.06222900	0.88207500
Rh	0.11579400	-0.11705600	-1.58492200
C	0.09219400	0.34272600	3.59477600
C	1.49038700	0.53744300	4.44798600
H	1.73878600	1.58708700	4.60708600
C	1.68333500	-0.43174000	5.58081700
C	-0.48346200	1.70912500	3.56488900
F	-1.77131300	1.79372600	3.03152400
F	-0.59369200	2.30184500	4.86875300
F	0.35758900	2.62301700	2.86678400
C	-0.79960500	-0.74709700	4.13715900
C	-1.62519100	-0.48059400	5.26093700
C	-0.80381500	-2.05035500	3.59209900
C	-2.45706200	-1.47599200	5.79521600
H	-1.60773600	0.51731500	5.69375000
C	-1.62399500	-3.05150200	4.14369800
H	-0.18121200	-2.27358300	2.72909900
C	-2.45887100	-2.76903400	5.23923100
H	-3.09844800	-1.24344600	6.64725700
H	-1.61041700	-4.05347400	3.71103700
H	-3.10186600	-3.54554500	5.65774800
C	2.05544000	-0.15572500	3.26315400
C	2.15855700	-1.64827000	5.02611700
N	2.35229400	-1.44536400	3.61394700
H	2.36395800	0.31299000	2.33741500
H	2.46033800	-2.19362200	2.92051900
C	1.46580100	-0.32513800	6.95593600
C	1.72314000	-1.45202700	7.76907000
C	2.17472500	-2.65992800	7.20128900

C	2.39764500	-2.77762400	5.81215400
H	1.09557400	0.60373100	7.39090000
H	1.56105600	-1.38881500	8.84549600
H	2.35852200	-3.52214200	7.84370700
H	2.73295800	-3.71186400	5.36751600
Br	-4.83797400	1.37212900	4.04726300
Br	-8.74686400	-2.17395600	1.58834500
Br	-7.73423300	0.68195500	-2.22737100
Br	-3.49640500	1.70373600	-6.14064800
Br	2.63969700	-4.67404800	-5.62204400
Br	6.85735500	-0.85255300	-4.25302500
Br	7.82859000	1.05934600	2.80717300
Br	3.37471600	4.53979500	4.34347300
H	5.95126500	2.93592800	4.30847800
H	5.00138000	-2.77509100	-5.71723400
H	-6.11275100	0.93852600	-4.79318700
H	-7.33584300	-0.11697300	3.34257000

IntIV-S (G = -971.080620)

C	-1.08060600	-0.68922600	-0.00743700
C	-0.03525800	-1.83975600	-0.21520200
H	-0.40880000	-2.76203500	-0.65326500
C	1.40308900	-1.44319900	-0.35274700
C	-2.49248700	-1.14618900	-0.19805100
F	-3.37335600	-0.49935500	0.68734100
F	-2.96805300	-0.91273200	-1.48064900
F	-2.60723700	-2.51802200	0.06520600
C	-0.84450700	0.76466000	-0.30483900
C	0.10118800	1.20681100	-1.26418100
C	-1.58067400	1.73927000	0.42393400
C	0.32689000	2.58619300	-1.46624700
H	0.67292500	0.47537400	-1.83028900
C	-1.36527000	3.11462100	0.20890400
H	-2.33160800	1.40369500	1.13406200
C	-0.40044800	3.54551000	-0.72711700
H	1.05718200	2.90795600	-2.21066100
H	-1.94141800	3.84493600	0.77841300
H	-0.22882600	4.61044700	-0.88987500
C	-0.41192100	-1.41119300	1.22880700
C	1.81883700	-0.81351600	0.86479100
N	0.77949900	-0.81863900	1.80657600
H	-1.05744500	-2.00493400	1.87136200
H	0.78708600	-0.15625200	2.63713000
C	2.30167800	-1.60463900	-1.41035400

C	3.60902600	-1.07401300	-1.29336400
C	3.99795800	-0.40540900	-0.11480900
C	3.11835800	-0.26828600	0.98199800
H	1.99494000	-2.11692100	-2.32483900
H	4.31709100	-1.18750100	-2.11469400
H	5.01130500	-0.00769700	-0.03059500
H	3.44339200	0.19354200	1.91487500

IntIV-S' (G = -1133.214941)

C	-1.08060600	-0.68922600	-0.00743700
C	-0.03525800	-1.83975600	-0.21520200
H	-0.40880000	-2.76203500	-0.65326500
C	1.40308900	-1.44319900	-0.35274700
C	-2.49248700	-1.14618900	-0.19805100
F	-3.37335600	-0.49935500	0.68734100
F	-2.96805300	-0.91273200	-1.48064900
F	-2.60723700	-2.51802200	0.06520600
C	-0.84450700	0.76466000	-0.30483900
C	0.10118800	1.20681100	-1.26418100
C	-1.58067400	1.73927000	0.42393400
C	0.32689000	2.58619300	-1.46624700
H	0.67292500	0.47537400	-1.83028900
C	-1.36527000	3.11462100	0.20890400
H	-2.33160800	1.40369500	1.13406200
C	-0.40044800	3.54551000	-0.72711700
H	1.05718200	2.90795600	-2.21066100
H	-1.94141800	3.84493600	0.77841300
H	-0.22882600	4.61044700	-0.88987500
C	-0.41192100	-1.41119300	1.22880700
C	1.81883700	-0.81351600	0.86479100
N	0.77949900	-0.81863900	1.80657600
H	-1.05744500	-2.00493400	1.87136200
H	0.78708600	-0.15625200	2.63713000
C	2.30167800	-1.60463900	-1.41035400
C	3.60902600	-1.07401300	-1.29336400
C	3.99795800	-0.40540900	-0.11480900
C	3.11835800	-0.26828600	0.98199800
H	1.99494000	-2.11692100	-2.32483900
H	4.31709100	-1.18750100	-2.11469400
H	5.01130500	-0.00769700	-0.03059500
H	3.44339200	0.19354200	1.91487500
Na	1.08005100	1.89773100	1.29315900
H	1.08980800	1.45596100	3.27599700

TSIV-S (G = -1133.215955)

C	-1.10402900	-0.66292100	-0.02071000
C	-0.09334100	-1.83217800	-0.26813800
H	-0.48523000	-2.72723500	-0.74613300
C	1.35115300	-1.45182200	-0.38492000
C	-2.53089800	-1.05776200	-0.21611300
F	-3.38083500	-0.39680700	0.69000000
F	-3.00554300	-0.76755500	-1.48999700
F	-2.70109500	-2.42991800	0.00581300
C	-0.82300100	0.78803400	-0.28199500
C	0.08402900	1.22418600	-1.28174300
C	-1.47301000	1.76587400	0.52039500
C	0.36609000	2.59846000	-1.44510900
H	0.58457300	0.48888800	-1.90729200
C	-1.19961700	3.13723000	0.34769000
H	-2.19745300	1.43477200	1.25996000
C	-0.26604400	3.55967600	-0.62414500
H	1.06534000	2.91618000	-2.22044400
H	-1.70732000	3.87102400	0.97518300
H	-0.05005600	4.62102800	-0.75484300
C	-0.45372100	-1.44531000	1.19730900
C	1.76694800	-0.89163900	0.87488500
N	0.74363000	-0.90762900	1.82831500
H	-1.13220200	-2.03703300	1.80688600
H	0.74258900	-0.00551500	2.64951200
C	2.25091500	-1.57119000	-1.44445100
C	3.56503400	-1.05722900	-1.30289100
C	3.95896100	-0.45295200	-0.09219600
C	3.08107200	-0.36615700	1.01275000
H	1.94344500	-2.03689200	-2.38393500
H	4.27305200	-1.13859600	-2.12813900
H	4.97866300	-0.07573100	0.01359700
H	3.42702400	0.00926200	1.97766000
Na	1.21640800	1.69124800	1.19030100
H	0.87569700	1.07224500	3.17042700

IntV-S (G = -1132.083304)

C	-1.28069500	-0.46424200	0.20681300
C	-0.45907000	-1.68462700	-0.39123600
H	-0.99903000	-2.34122700	-1.07089700
C	1.00629400	-1.47462600	-0.47416700
C	-2.71803600	-0.55777500	-0.15371600
F	-3.53516600	0.23681100	0.63971700
F	-2.94861900	-0.15068600	-1.49196000

F	-3.16957100	-1.87842300	-0.06325600
C	-0.71258700	0.91972800	0.19768200
C	-0.69599800	1.66231200	-1.01532800
C	-0.10990400	1.47807600	1.35610800
C	-0.07066100	2.92767700	-1.07600800
H	-1.21520800	1.24975600	-1.87814600
C	0.52385200	2.74008500	1.28958700
H	-0.07948000	0.87387400	2.26209900
C	0.55714400	3.46374200	0.07293100
H	-0.08564000	3.49691800	-2.00728300
H	0.97617100	3.16443700	2.18764900
H	1.03690100	4.44305900	0.02957800
C	-0.74078000	-1.58927900	1.15492000
C	1.47970100	-1.25639600	0.91026500
N	0.51368500	-1.32978400	1.86538700
H	-1.49059200	-2.20453800	1.64798200
C	1.87690900	-1.43473100	-1.56778500
C	3.25781500	-1.12738800	-1.36455000
C	3.73290000	-0.90346300	-0.03735700
C	2.87859600	-0.94495900	1.08343100
H	1.50529700	-1.61984700	-2.57996000
H	3.95104200	-1.12064700	-2.20571200
H	4.79662700	-0.70350700	0.11618400
H	3.27023300	-0.79623100	2.09081600
Na	1.86047500	0.95202900	-0.41455100

TSV-S (G = -1132.076730)

C	1.23483400	-0.51978600	-0.17416600
C	0.42825600	-1.53872300	0.64219800
H	0.92930800	-2.09036300	1.43701200
C	-1.00825500	-1.41254900	0.52831300
C	2.69657200	-0.60891900	0.14780000
F	3.47279600	0.19775300	-0.67111900
F	2.94067800	-0.20355800	1.47824000
F	3.16032200	-1.91789200	0.04059800
C	0.73648300	0.91434300	-0.18679400
C	0.70656800	1.64338700	1.03224600
C	0.16252900	1.49015400	-1.34791300
C	0.09737700	2.91409500	1.09620500
H	1.19284000	1.20903900	1.90403200
C	-0.45979600	2.75975100	-1.28046400
H	0.15726900	0.91083600	-2.26962100
C	-0.50694900	3.46984200	-0.05931700
H	0.10605700	3.47556700	2.03233000

H	-0.89798600	3.19427500	-2.18072100
H	-0.97713100	4.45358300	-0.01316300
C	0.78927100	-1.51080300	-1.24784600
C	-1.43958400	-1.23072100	-0.88555700
N	-0.46942500	-1.41640200	-1.82621900
H	1.55415400	-2.13830200	-1.70290300
C	-1.97989300	-1.42634300	1.55790300
C	-3.34056100	-1.15120300	1.27278000
C	-3.74719800	-0.89629500	-0.07366300
C	-2.82152800	-0.93609700	-1.13444000
H	-1.66755400	-1.60402700	2.59130300
H	-4.07992200	-1.15340300	2.07482300
H	-4.80024700	-0.70006800	-0.28742700
H	-3.14859400	-0.79392900	-2.16596000
Na	-1.86683000	0.97309800	0.40096800

IntVI-S (G = -1132.093302)

C	-1.15298600	-0.62332200	0.15694600
C	-0.25436200	-1.18243300	-0.93620200
H	-0.65838300	-1.30699100	-1.93980500
C	1.10373000	-1.26456600	-0.63675700
C	-2.61630600	-0.85625800	-0.15258600
F	-3.44444500	-0.08465900	0.65335000
F	-2.90362300	-0.52039900	-1.49317300
F	-2.97143300	-2.18573900	0.02159200
C	-0.86449400	0.91946000	0.23550000
C	-0.99901400	1.69476100	-0.94866600
C	-0.20959100	1.49919700	1.35165300
C	-0.46573800	2.99369200	-1.03040800
H	-1.53029000	1.25486000	-1.79091600
C	0.34298300	2.80467900	1.26738600
H	-0.11669300	0.92228700	2.27058700
C	0.23637900	3.54776400	0.07435200
H	-0.60115300	3.58182900	-1.93997900
H	0.84834700	3.23237700	2.13604500
H	0.65609100	4.55304500	0.01052000
C	-0.73369500	-1.35849500	1.43943700
C	1.50236100	-1.20685400	0.79322100
N	0.53368400	-1.49346300	1.77084300
H	-1.50603300	-1.74503600	2.10780700
C	2.18203000	-1.27546600	-1.61487900
C	3.49790200	-1.01429800	-1.23110200
C	3.84654800	-0.81168700	0.14858700
C	2.85928300	-0.98550600	1.13654200

H	1.93072000	-1.42528500	-2.66866200
H	4.28326000	-0.97595400	-1.98968900
H	4.88328400	-0.62431500	0.42824200
H	3.11711200	-0.95224500	2.19732500
Na	1.74393500	1.07025700	-0.37922200

IntVII-S (G = -1209.085631)

C	-1.26342800	-0.68979700	0.15842100
C	-0.28377300	-1.13010200	-0.92664600
H	-0.65638300	-1.22987300	-1.94632100
C	1.06135900	-1.27784900	-0.59590200
C	-2.67591600	-1.13400500	-0.17526800
F	-3.61271100	-0.51955000	0.64834000
F	-3.00793100	-0.81178900	-1.50957200
F	-2.82507500	-2.50487700	-0.04086700
C	-1.20732900	0.87783000	0.24735300
C	-1.53844800	1.65442400	-0.89847200
C	-0.58081600	1.52551600	1.34258700
C	-1.22024000	3.02175000	-0.95978700
H	-2.04919400	1.16346200	-1.72445700
C	-0.24833900	2.90069800	1.27367000
H	-0.33126000	0.94582600	2.23084500
C	-0.54787500	3.64821300	0.11930600
H	-1.49600200	3.60321100	-1.84176100
H	0.25410500	3.37485900	2.11881300
H	-0.28362100	4.70514400	0.06319100
C	-0.80826600	-1.34114600	1.47627500
C	1.44694200	-1.26475200	0.83205100
N	0.45260200	-1.47682200	1.81139900
H	-1.58102800	-1.63583800	2.19182500
C	2.14838700	-1.39805700	-1.55985400
C	3.47443800	-1.34028300	-1.15676000
C	3.83441700	-1.18208900	0.22895300
C	2.80801000	-1.22397900	1.19708700
H	1.89391300	-1.51854900	-2.61733600
H	4.26792600	-1.42036800	-1.90477300
H	4.88155100	-1.22998900	0.53297100
H	3.04499400	-1.24404300	2.26315100
Na	1.23109200	1.15964600	-0.49627600
O	3.29222600	1.72457300	-0.17237200
H	3.95562800	2.11654900	-0.81199800
H	3.66805400	0.80237500	0.10488300

TSVI-S (G = -1209.076055)

C	1.00529900	-0.80156100	-0.21553000
C	-0.01319000	-1.14280400	0.91455000
H	0.30794800	-1.92190000	1.61813000
C	-1.39534300	-1.13912800	0.47342500
C	2.37687000	-1.34002300	0.14359300
F	3.33566300	-0.96023800	-0.78832600
F	2.80943600	-0.91155800	1.40844300
F	2.35369100	-2.73227900	0.18275100
C	1.05328600	0.75022700	-0.42651300
C	1.61918000	1.58665600	0.56896900
C	0.38841900	1.36887000	-1.51794700
C	1.49253300	2.98443900	0.49955100
H	2.15008300	1.12783400	1.39673600
C	0.22924500	2.77376800	-1.56802100
H	-0.00398900	0.75225600	-2.32412900
C	0.76940100	3.58585300	-0.55047300
H	1.93611300	3.60143600	1.28243000
H	-0.29297400	3.22518600	-2.41424900
H	0.65130300	4.66994700	-0.58942500
C	0.53436500	-1.50146800	-1.50023800
C	-1.68673100	-1.02895200	-0.94812500
N	-0.71656000	-1.48365700	-1.87834700
H	1.27533300	-2.00520100	-2.12727400
C	-2.51650700	-1.06162900	1.36947500
C	-3.77894400	-0.66691200	0.91545900
C	-4.00071700	-0.38177500	-0.46368000
C	-2.97141200	-0.61708100	-1.38639100
H	-2.34886100	-1.23412100	2.43646800
H	-4.60356500	-0.56891900	1.62480600
H	-4.98291400	-0.05170200	-0.80382900
H	-3.14428300	-0.52130700	-2.46015000
Na	-1.39180900	1.35141900	0.47779400
O	-0.56534800	1.08849200	2.48122500
H	-0.16211500	0.16625700	2.02117500
H	-1.05710400	0.79808200	3.30777300

(S)-49 (G = -971.101719)

C	0.85312000	-0.90267300	-0.13975400
C	-0.15794000	-0.93818400	1.05977000
H	-0.08849000	-1.94767500	1.50599600
C	-1.57690200	-0.71453300	0.54379500
C	2.14430100	-1.58100500	0.29102000
F	3.08821800	-1.56890500	-0.73087500
F	2.72001900	-0.99262300	1.42570600

F	1.89018800	-2.91251700	0.61796300
C	1.08532500	0.55607600	-0.60965900
C	1.96347300	1.42123700	0.09628200
C	0.28730100	1.11030400	-1.64341500
C	2.03561300	2.79199000	-0.22021500
H	2.57575600	1.01616100	0.89460600
C	0.34706200	2.48854600	-1.94701900
H	-0.37864400	0.46423400	-2.21196200
C	1.21848500	3.33748300	-1.23237900
H	2.71845600	3.43353600	0.33835800
H	-0.27557000	2.88927300	-2.74875100
H	1.26901900	4.40115300	-1.46894300
C	0.27970800	-1.77203200	-1.28991900
C	-1.94220500	-1.24503900	-0.71951400
N	-0.98145700	-1.92378500	-1.55628700
H	1.01980500	-2.26056000	-1.93303900
C	-2.51897700	0.01059600	1.30552100
C	-3.82841400	0.18533800	0.80701800
C	-4.20244000	-0.37601700	-0.43191600
C	-3.25947300	-1.08785700	-1.19545500
H	-2.13275500	0.49329700	2.22318600
H	-4.55684800	0.75481800	1.38850900
H	-5.22106000	-0.25398300	-0.80407100
H	-3.51523900	-1.51876000	-2.16387000
H	0.04076600	-0.15048800	1.83925400

(R)-49 (G = -971.089654)

F	0.00353800	2.75720300	0.30015700
F	-1.44159800	2.27484500	-1.37488800
C	-1.08726500	1.92405900	-0.09960900
C	-1.87365400	-0.54135000	-0.02617100
C	-0.67959800	0.45314100	0.05830300
C	-1.57139000	-1.90299900	-0.27530000
H	-0.53450100	-2.19998000	-0.42456200
C	-2.58683200	-2.87116700	-0.33265400
H	-2.32605400	-3.91333800	-0.52422300
C	-3.22797600	-0.18400200	0.17757500
H	-3.49066900	0.84599300	0.38846200
C	-3.93149100	-2.49989100	-0.15063100
C	-4.24383500	-1.15341900	0.10208400
H	-5.28223900	-0.85005600	0.24629700
F	-2.11417400	2.30567700	0.78155200
C	3.83743100	-2.13226700	0.45256900
C	3.49798200	-2.16025300	-0.91824900

C	2.35819800	-1.48664900	-1.38724400
C	1.51503700	-0.77362500	-0.50066500
C	1.85290400	-0.77928100	0.88764000
C	3.00920200	-1.44301900	1.35078900
H	4.72639700	-2.65174600	0.81104900
H	4.12974500	-2.70464100	-1.62246200
H	2.11815000	-1.49492900	-2.45331400
H	3.21860900	-1.42313900	2.42138700
C	0.43971800	0.14705000	-1.00141200
C	-0.12038400	0.38239200	1.50313700
N	1.02071600	-0.12693300	1.87578200
H	-0.77698100	0.81557200	2.26445300
H	-0.02590200	-0.22621800	-1.92535700
H	1.07859300	1.15135100	-1.31605300
H	-4.72261400	-3.24926200	-0.20388800

Rh₂(*R*-diBrTPCP)₄-catalysed pathway:

IntI'' (G = -5035.450076)

O	1.59044300	1.18215800	-0.96492600
C	2.22746600	1.36542100	0.17588900
C	3.64958300	1.85920800	0.09563700
C	4.50206600	1.62811900	1.36399900
H	3.97065800	1.15943900	2.19043800
H	5.53209800	1.30782600	1.21487500
C	4.12919300	3.07396700	1.05031200
C	1.25196200	5.07209200	3.62561600
H	0.53920300	5.58329600	4.27388500
C	1.07253400	5.08609800	2.22952400
H	0.22650600	5.62227600	1.79328400
C	1.98129900	4.41309500	1.39317900
H	1.83307100	4.40774900	0.31194200
C	3.08639000	3.72616300	1.94055800
C	3.26615300	3.72624500	3.34072900
H	4.12241000	3.20361800	3.77052600
C	2.35052100	4.38742100	4.17863600
H	2.49550700	4.37078500	5.26011800
C	4.27349600	1.66942600	-1.26695500
C	4.12265800	2.64175700	-2.28013600
H	3.59294900	3.56715300	-2.07173400
C	4.66416400	2.39061000	-3.54351900
C	5.35439300	1.21007600	-3.85969500
H	5.76494000	1.03543500	-4.85106700
C	5.47825000	0.26603700	-2.83103900

C	4.96278300	0.46725500	-1.54674100
H	5.06418200	-0.29243200	-0.77359700
Rh	-0.06876700	-0.08628400	-1.02380800
Rh	-0.11824500	0.18320300	1.41823900
O	-1.20352700	1.92243000	1.17200900
O	0.94095400	-1.58197600	1.58580000
O	-1.75150600	-1.32655900	-0.86247900
O	-1.44410700	1.47039600	-1.10347000
O	1.29038700	-1.64965000	-0.72236200
C	-1.78549100	2.10335100	0.00564400
C	1.55301800	-2.03645500	0.51330300
C	-2.41536800	-1.27526000	0.28600700
C	-2.95151200	3.05831100	-0.05470700
C	2.68943900	-3.01883300	0.72502400
C	-3.81669000	-1.82147900	0.32849300
C	-3.82940900	2.98431100	-1.32661600
C	3.06238900	-3.92724300	-0.44356500
C	-4.74794500	-1.11086100	1.35561400
H	-3.51105700	2.25766200	-2.07089100
H	2.47200300	-3.80832700	-1.35037400
H	-4.27538600	-0.32524200	1.94361300
H	-4.90357100	3.09443400	-1.18292700
H	4.11777300	-4.14265700	-0.60727400
H	-5.76510600	-0.91852900	1.01617800
C	-2.95398800	4.22219300	-1.16720500
C	2.39214100	-4.61936500	0.75753500
C	-4.33383400	-2.54091800	1.67804100
C	0.35589400	4.81862900	-3.92228700
C	-1.56015900	-6.40393500	0.19937800
C	-1.64482600	-3.14587400	5.04467400
H	1.17949300	4.98124300	-4.61888200
H	-2.52774700	-6.88080500	0.03341400
H	-0.98273600	-3.30013100	5.89874900
C	0.59753200	4.80413600	-2.53693800
C	-1.17633300	-5.28687600	-0.56635200
C	-1.31443700	-3.68092300	3.78583400
H	1.61020400	4.95887200	-2.16007000
H	-1.83675900	-4.88730400	-1.33555000
H	-0.39548400	-4.25293000	3.65067100
C	-0.45716800	4.57959300	-1.63441600
C	0.07647100	-4.67900900	-0.37412200
C	-2.16297000	-3.47615800	2.68214100
H	-0.25829800	4.53992600	-0.56244800
H	0.33177600	-3.81983200	-0.98924600

H	-1.88159000	-3.87301700	1.70607700
C	-1.76927400	4.37062600	-2.10687100
C	0.98293400	-5.17607400	0.59719000
C	-3.35465500	-2.73484300	2.82863200
C	-2.00683500	4.38855000	-3.50006300
C	0.57795000	-6.29639800	1.36857800
C	-3.68848100	-2.21131900	4.09725700
H	-3.02238500	4.23866300	-3.87131400
H	1.26114900	-6.70894000	2.10761600
H	-4.61320400	-1.64345200	4.21770300
C	-0.95095100	4.60847100	-4.40205000
C	-0.67677700	-6.90023200	1.17394000
C	-2.83646200	-2.41015800	5.19779400
H	-1.14748400	4.61910900	-5.47563200
H	-0.95328000	-7.76714600	1.77660700
H	-3.10216300	-1.99418100	6.17131800
C	-3.62756600	3.31380000	1.27630100
C	3.77688900	-2.48681100	1.64798200
C	-4.40056900	-2.17914500	-1.01961000
C	-2.96411100	4.03101500	2.30130100
C	3.44372900	-2.00712100	2.94227100
C	-4.49445500	-3.51586200	-1.46636700
H	-1.95188700	4.39305300	2.14723500
H	2.40307500	-1.97640500	3.25022300
H	-4.17732600	-4.32791000	-0.81944400
C	-3.62241900	4.24085200	3.51578200
C	4.46128800	-1.55620300	3.78482700
C	-5.03926700	-3.77164700	-2.73073300
C	-4.91504600	3.76118600	3.78317000
C	5.81744500	-1.54914000	3.41944600
C	-5.49827100	-2.75969900	-3.58651700
H	-5.40648900	3.94207000	4.73563400
H	6.59364700	-1.20457300	4.09816100
H	-5.92588800	-2.98284800	-4.56073500
C	-5.53422500	3.03931500	2.75615500
C	6.11250200	-2.01268800	2.13070400
C	-5.38626700	-1.44230700	-3.11319900
C	-4.92463600	2.80617900	1.51769600
C	5.13289600	-2.47295700	1.24079100
C	-4.85480100	-1.13087500	-1.85798200
H	-5.44316200	2.23667200	0.75004100
H	5.42012500	-2.81958000	0.25137300
H	-4.78001100	-0.09791300	-1.52194700
C	-3.60557600	5.54035600	-0.77104900

C	-4.95988000	5.81463300	-1.06298200
C	-2.83926600	6.54054600	-0.12618700
C	-5.53891200	7.04636200	-0.70380000
H	-5.56435500	5.07323000	-1.58618100
C	-3.41656400	7.76821400	0.23669200
H	-1.78313500	6.36037700	0.07683900
C	-4.77208900	8.02447900	-0.04739000
H	-6.58614300	7.23993400	-0.94156400
H	-2.81016100	8.52504300	0.73692000
H	-5.22115800	8.97794100	0.23403500
C	3.30433200	-5.40382800	1.68613400
C	4.28511500	-6.27381200	1.16256000
C	3.14054300	-5.32807900	3.08954300
C	5.10137600	-7.03474400	2.02080600
H	4.40314600	-6.36220000	0.08142000
C	3.95455300	-6.08789800	3.94751300
H	2.37575400	-4.66978600	3.50395900
C	4.94120700	-6.94054100	3.41505600
H	5.85679000	-7.70062600	1.60051400
H	3.82218300	-6.01211800	5.02806900
H	5.57627300	-7.52646100	4.08106800
O	1.72254000	1.10343600	1.36360200
O	-1.95288500	-0.73454000	1.38803600
C	5.19231500	4.01767300	0.49133600
C	6.46658500	3.56140600	0.07132100
C	4.92055500	5.40493900	0.38653300
C	7.42296700	4.45317500	-0.44351600
H	6.72397200	2.50553500	0.13470900
C	5.87610700	6.29604100	-0.13172400
H	3.96178200	5.78712200	0.73224700
C	7.13248800	5.82529700	-0.55214800
H	8.39604900	4.07245100	-0.75794900
H	5.63888000	7.35920500	-0.19841200
H	7.87612700	6.51597900	-0.95214800
C	-5.35636200	-3.66756000	1.53470900
C	-6.71866200	-3.42604400	1.24379900
C	-4.94080100	-5.01119800	1.71681900
C	-7.63216400	-4.48928000	1.12022800
H	-7.08285300	-2.40685100	1.12064100
C	-5.85160400	-6.07291300	1.58698700
H	-3.90414300	-5.21805600	1.97986100
C	-7.20287300	-5.81777600	1.28463400
H	-8.67950100	-4.27543600	0.90094600
H	-5.50878200	-7.09869100	1.73371200

H	-7.91176700	-6.64150400	1.18966800
Br	6.42173300	-1.45936500	-3.23875900
Br	4.44693400	3.76761300	-4.98531600
Br	-2.70572800	5.28977400	4.95700500
Br	-7.37863000	2.31349000	3.07499300
Br	-6.03788500	0.04428700	-4.29199100
Br	-5.19154800	-5.67309200	-3.35212300
Br	3.97187300	-0.89889200	5.61401800
Br	8.02979400	-2.02178100	1.54073100
C	0.00952800	-0.48522800	-3.32303000
N	-1.19673600	0.15082200	-3.56664400
N	-2.21071900	0.70025200	-3.64293600
C	0.01611900	-1.95991600	-3.63666200
C	1.24326400	-2.64113600	-3.84068200
C	-1.19623800	-2.68295000	-3.74931000
C	1.24501900	-4.00816700	-4.16537000
H	2.18251600	-2.10459400	-3.75089700
C	-1.18169500	-4.04850300	-4.07741200
H	-2.15043500	-2.18794600	-3.57238200
C	0.03768500	-4.71825700	-4.28997200
H	2.19842300	-4.51296500	-4.33133400
H	-2.12638300	-4.58585200	-4.17079800
H	0.04486500	-5.77790400	-4.54789400
C	1.14806200	0.37666900	-3.85612800
F	1.29167300	0.28828600	-5.24210400
F	0.92709000	1.71999400	-3.55180100
F	2.36350200	-0.03043700	-3.29992000

TSI' (G = -5035.444769)

O	-1.59870900	1.17691100	0.97013400
C	-2.23108100	1.35022200	-0.17646300
C	-3.65962900	1.83022900	-0.10783800
C	-4.49307600	1.58885700	-1.38714900
H	-3.94713700	1.11904000	-2.20335600
H	-5.52398600	1.26484100	-1.25219500
C	-4.13723300	3.03941400	-1.07471500
C	-1.21978500	5.04436500	-3.60003900
H	-0.49635600	5.55620100	-4.23578600
C	-1.09820400	5.10775100	-2.19884400
H	-0.28775100	5.68361500	-1.74600300
C	-2.02107600	4.43389400	-1.37875900
H	-1.92129000	4.47328600	-0.29273100
C	-3.08234600	3.69616300	-1.94733100
C	-3.20469300	3.64821400	-3.35265000

H	-4.02669900	3.08684400	-3.79994800
C	-2.27474700	4.31037900	-4.17405300
H	-2.37479300	4.25575900	-5.25937900
C	-4.29767200	1.63685600	1.24715300
C	-4.17065100	2.61290400	2.25962800
H	-3.64807000	3.54329500	2.05586100
C	-4.72792400	2.36068100	3.51587000
C	-5.41354300	1.17563600	3.82455400
H	-5.83664300	0.99975300	4.81041400
C	-5.51560900	0.22846300	2.79627700
C	-4.98213600	0.43019300	1.51954100
H	-5.06617300	-0.33203200	0.74683400
Rh	0.07713100	-0.08409300	1.05323500
Rh	0.12555800	0.18170800	-1.41031700
O	1.20027800	1.91882500	-1.13366300
O	-0.92882600	-1.58741500	-1.58512200
O	1.77709400	-1.30790500	0.87147900
O	1.44214400	1.46960500	1.13984000
O	-1.26734200	-1.65774700	0.72429900
C	1.78140200	2.11150300	0.02871100
C	-1.53156000	-2.04629900	-0.51188200
C	2.43325200	-1.25790100	-0.28264000
C	2.92935700	3.08495900	0.08079900
C	-2.66372900	-3.03712800	-0.70739400
C	3.83730400	-1.79801600	-0.32911700
C	3.81110600	3.06863000	1.35077200
C	-3.03042800	-3.92293600	0.48125900
C	4.75715900	-1.09034000	-1.36868600
H	3.51233500	2.36432500	2.12292800
H	-2.44259700	-3.77731300	1.38599900
H	4.27606800	-0.31140200	-1.95858800
H	4.88239900	3.19158600	1.19630300
H	-4.08443500	-4.14081800	0.64997600
H	5.77582700	-0.89020400	-1.03862700
C	2.90904800	4.28299100	1.15984600
C	-2.35925900	-4.63817800	-0.70473300
C	4.34801600	-2.52446100	-1.67809100
C	-0.39909900	4.86763700	3.91782200
C	1.60860800	-6.38841900	-0.14853800
C	1.63848800	-3.17106000	-5.02035600
H	-1.22286600	5.02642200	4.61518500
H	2.58124000	-6.85556800	0.01547400
H	0.97153400	-3.33636400	-5.86855000
C	-0.65608000	4.74449800	2.54099500

C	1.21663700	-5.27321700	0.61569100
C	1.32117100	-3.69971000	-3.75549900
H	-1.68122500	4.80698500	2.17246300
H	1.87684100	-4.86539400	1.38066300
H	0.40772400	-4.27792200	-3.60989300
C	0.39851900	4.52365700	1.63733500
C	-0.04248400	-4.67747100	0.42620100
C	2.17595400	-3.48072100	-2.65938900
H	0.18844200	4.39725500	0.57418800
H	-0.30404600	-3.81875800	1.03955800
H	1.90491100	-3.87331300	-1.67865200
C	1.72608900	4.42656200	2.10208000
C	-0.94653400	-5.18458500	-0.54223300
C	3.36099400	-2.73163300	-2.81966000
C	1.97967700	4.55190300	3.48716600
C	-0.53355900	-6.30341500	-1.31166600
C	3.68162200	-2.21435900	-4.09422500
H	3.00695700	4.48676900	3.85055500
H	-1.21512800	-6.72408600	-2.04760400
H	4.60123600	-1.64059300	-4.22535500
C	0.92381700	4.76875500	4.38950500
C	0.72689700	-6.89558800	-1.11894800
C	2.82322400	-2.42729200	-5.18713600
H	1.13221100	4.86174400	5.45676500
H	1.00943600	-7.76164200	-1.72003000
H	3.07868700	-2.01603500	-6.16538900
C	3.60385600	3.32235800	-1.25524300
C	-3.75314900	-2.52745900	-1.64027400
C	4.43303300	-2.14290100	1.01704900
C	2.95054800	4.04535600	-2.28207400
C	-3.42042800	-2.05822300	-2.93871800
C	4.55234800	-3.47686800	1.46646900
H	1.94705700	4.43028200	-2.12588000
H	-2.37908800	-2.01887000	-3.24342300
H	4.24467900	-4.29588800	0.82372200
C	3.61055700	4.23672000	-3.49894700
C	-4.43981400	-1.62739600	-3.78959000
C	5.11107000	-3.72028800	2.72741200
C	4.89384900	3.73216000	-3.76570000
C	-5.79729300	-1.63141600	-3.42941400
C	5.55812900	-2.69856700	3.57769400
H	5.38674900	3.89938000	-4.71992800
H	-6.57462800	-1.30224700	-4.11444700
H	5.99480000	-2.91185700	4.55008300

C	5.50267600	3.00529200	-2.73594800
C	-6.09223500	-2.08505600	-2.13710000
C	5.41907600	-1.38443900	3.10285300
C	4.89137600	2.79032500	-1.49504800
C	-5.11099900	-2.52472900	-1.23866400
C	4.87441400	-1.08502200	1.85046200
H	5.40101300	2.21801300	-0.72324700
H	-5.39875400	-2.86416400	-0.24697100
H	4.77850100	-0.05403000	1.51354600
C	3.51602000	5.60531900	0.71158400
C	4.88701700	5.89687900	0.88503100
C	2.68642100	6.59220800	0.12604900
C	5.41915600	7.13139600	0.46776500
H	5.54369500	5.16846700	1.36090400
C	3.21681400	7.82246600	-0.29465700
H	1.61821900	6.39947900	0.02037500
C	4.58867200	8.09551500	-0.12930900
H	6.48042400	7.33825900	0.61469500
H	2.56124400	8.56905300	-0.74589300
H	5.00149200	9.05131000	-0.45483100
C	-3.27300800	-5.44656600	-1.61143600
C	-4.23701800	-6.31916000	-1.06151300
C	-3.12718400	-5.39177900	-3.01767800
C	-5.05447600	-7.10359300	-1.89706200
H	-4.34084200	-6.39065700	0.02235500
C	-3.94257400	-6.17508500	-3.85300100
H	-2.37621500	-4.73074000	-3.45234600
C	-4.91234400	-7.03042500	-3.29458200
H	-5.79684100	-7.77116400	-1.45670100
H	-3.82449400	-6.11529300	-4.93620100
H	-5.54848400	-7.63454500	-3.94307300
O	-1.71770500	1.09338700	-1.35962300
O	1.96140900	-0.72802400	-1.38372000
C	-5.22283700	3.97335000	-0.54216300
C	-6.47866000	3.49545000	-0.08981400
C	-4.99762100	5.37231800	-0.50312400
C	-7.46039300	4.37777100	0.39197100
H	-6.70065100	2.42988500	-0.09990900
C	-5.97898200	6.25422600	-0.01812100
H	-4.05457400	5.77043500	-0.87248600
C	-7.21562000	5.76247600	0.43454100
H	-8.41746200	3.97958800	0.73282600
H	-5.77660400	7.32652700	-0.00258900
H	-7.97905900	6.44580600	0.80905700

C	5.37834400	-3.64439300	-1.53666100
C	6.74065700	-3.39359300	-1.25351100
C	4.97041900	-4.99117000	-1.71300600
C	7.66152500	-4.45069100	-1.13220700
H	7.09910400	-2.37191600	-1.13426900
C	5.88861900	-6.04676400	-1.58530100
H	3.93377700	-5.20524600	-1.97014100
C	7.23984100	-5.78231300	-1.29094900
H	8.70860600	-4.22962500	-0.91897600
H	5.55151100	-7.07505700	-1.72754500
H	7.95446800	-6.60126300	-1.19771400
Br	-6.45404400	-1.50204200	3.19337900
Br	-4.54036900	3.74292600	4.95623900
Br	2.71323800	5.29676200	-4.94376000
Br	7.33446500	2.24792200	-3.05387000
Br	6.04649700	0.11619200	4.27626200
Br	5.30061900	-5.61750700	3.35124400
Br	-3.95081900	-0.98335200	-5.62373300
Br	-8.01133300	-2.11004900	-1.55454700
C	-0.08552900	-0.45025200	3.13018100
N	1.27575400	0.34168700	3.78879700
N	2.23430900	0.94007500	3.59753000
C	-0.00043300	-1.87266000	3.59843100
C	-1.17292000	-2.56646300	4.00600400
C	1.23914000	-2.56107900	3.61273800
C	-1.09669900	-3.90870000	4.41187700
H	-2.13228800	-2.05730400	3.99423500
C	1.30829500	-3.89255300	4.05071800
H	2.14010500	-2.05435700	3.27424400
C	0.14157400	-4.57461400	4.44815300
H	-2.00724000	-4.42562400	4.71987000
H	2.27436600	-4.39793700	4.08091800
H	0.19975800	-5.61124900	4.78272300
C	-1.18288400	0.38336600	3.79493800
F	-1.23680000	0.24396400	5.18197200
F	-1.01967200	1.74121300	3.52686000
F	-2.42968200	-0.03290300	3.29597400

IntII' (G = -5035.472014)

O	1.77380400	1.05492100	-0.97627000
C	2.39599500	1.17072600	0.18765900
C	3.80696700	1.67974700	0.16126800
C	4.66473300	1.32173100	1.40042500
H	4.14897800	0.75375500	2.17261500

H	5.69417900	1.03149500	1.19637200
C	4.25905500	2.78320600	1.25180900
C	1.39090900	4.37619500	4.10783900
H	0.68563000	4.78632800	4.83330300
C	1.14455200	4.50415600	2.72878700
H	0.25046400	5.01647900	2.37193900
C	2.04930800	3.97234500	1.79133500
H	1.83321500	4.05779900	0.72496300
C	3.21747900	3.31096800	2.22699500
C	3.46486900	3.19424400	3.61319600
H	4.37019400	2.68921700	3.95519600
C	2.55525500	3.71723000	4.54850600
H	2.75574200	3.61389500	5.61641900
C	4.44826200	1.64523500	-1.20573200
C	4.33425900	2.73594500	-2.09522300
H	3.82018400	3.64011500	-1.78187800
C	4.88910000	2.62346200	-3.37285700
C	5.55737800	1.47378900	-3.82026100
H	5.97919200	1.40990400	-4.82011100
C	5.64470200	0.40973200	-2.91170000
C	5.11339300	0.46793700	-1.61972700
H	5.19003400	-0.38000500	-0.94119900
Rh	-0.00358800	-0.04630300	-1.11756800
Rh	-0.04471700	0.12347500	1.36365900
O	-0.89427800	1.99025600	1.16118800
O	0.83423700	-1.74809900	1.46985900
O	-1.79705100	-1.13300700	-0.95189100
O	-1.24769100	1.64644200	-1.11572700
O	1.18376300	-1.75870200	-0.83682500
C	-1.48291300	2.27948000	0.02419500
C	1.42486300	-2.19810800	0.38969700
C	-2.46149800	-1.07286100	0.19941800
C	-2.56952400	3.33696300	0.04996500
C	2.53093200	-3.22491200	0.55499900
C	-3.87832500	-1.56343500	0.22576500
C	-3.02585700	3.92793400	-1.28476000
C	2.89430600	-4.06206100	-0.66938600
C	-4.76832000	-0.92651100	1.32775400
H	-2.54444100	3.53576100	-2.17670000
H	2.32143700	-3.86185300	-1.57302800
H	-4.26289700	-0.20822000	1.97087300
H	-4.08752500	4.14553200	-1.39891400
H	3.94597600	-4.29166700	-0.83629200
H	-5.78455600	-0.67297700	1.02999100

C	-2.23409800	4.88198800	-0.38130200
C	2.20306900	-4.81798000	0.47897200
C	-4.39170900	-2.38855000	1.52463800
C	1.73433300	6.19340700	-1.65940100
C	-1.79705200	-6.47017700	-0.14243500
C	-1.65194600	-3.32316100	4.77238600
H	2.70997900	6.54035800	-2.00385900
H	-2.77935700	-6.90979000	-0.32196900
H	-0.97690900	-3.56022000	5.59690200
C	1.00743800	6.93256900	-0.70774300
C	-1.35770800	-5.37484600	-0.90957500
C	-1.36580400	-3.77320600	3.47045300
H	1.41575700	7.86157000	-0.30582300
H	-1.99764900	-4.96599300	-1.69196900
H	-0.46963200	-4.36264000	3.27283200
C	-0.25798500	6.49341900	-0.27901000
C	-0.08826300	-4.80862100	-0.69825600
C	-2.23087000	-3.46154500	2.40507300
H	-0.81926400	7.09144100	0.43608500
H	0.21300300	-3.96335400	-1.31288300
H	-1.98398300	-3.79560000	1.39626100
C	-0.82836800	5.29910300	-0.79023600
C	0.78198400	-5.33199300	0.29178800
C	-3.39573600	-2.69833000	2.63314000
C	-0.08487300	4.56616900	-1.74692600
C	0.32397100	-6.43333400	1.06057900
C	-3.68414000	-2.25979000	3.94476600
H	-0.47693500	3.64885100	-2.17082700
H	0.98105000	-6.86831000	1.81039600
H	-4.58737600	-1.67496600	4.12871900
C	1.18054900	5.00532800	-2.17283700
C	-0.94894200	-6.99135900	0.84979000
C	-2.81564700	-2.56493300	5.00728000
H	1.71451700	4.40902100	-2.91253000
H	-1.26739100	-7.84295700	1.45329300
H	-3.04675600	-2.21305100	6.01429300
C	-3.59335100	3.10537200	1.15141500
C	3.62193600	-2.77065000	1.51481200
C	-4.48963700	-1.82372700	-1.13037800
C	-3.18969400	3.01888600	2.51007400
C	3.29102500	-2.37266900	2.83688100
C	-4.44581900	-3.10653500	-1.72092400
H	-2.13678200	3.08624400	2.76534600
H	2.25004200	-2.34036500	3.14390900

H	-4.00968200	-3.93818900	-1.17518200
C	-4.15730800	2.81468400	3.49587300
C	4.31314700	-1.99931900	3.71172000
C	-5.00620600	-3.28656700	-2.98964000
C	-5.52793500	2.68555900	3.21538700
C	5.67070200	-1.99307400	3.35078000
C	-5.61787400	-2.25068100	-3.71081300
H	-6.26338600	2.53796800	4.00219400
H	6.45019700	-1.71031900	4.05388500
H	-6.05159500	-2.41567800	-4.69375800
C	-5.89156800	2.75863700	1.86486900
C	5.96297900	-2.37164800	2.03402400
C	-5.64594100	-0.99096600	-3.09333100
C	-4.96501100	2.95907500	0.83416500
C	4.97880300	-2.75212700	1.11227400
C	-5.09969000	-0.75448200	-1.82739200
H	-5.30239700	3.00244900	-0.19831700
H	5.26297700	-3.03417500	0.10167500
H	-5.13500600	0.23645900	-1.37741200
C	-3.04371800	5.93351600	0.35953000
C	-4.01037700	6.69754500	-0.33108100
C	-2.79713100	6.22095700	1.72230500
C	-4.72970200	7.71096600	0.32914800
H	-4.19080600	6.50431100	-1.38969100
C	-3.51472600	7.23368900	2.38304900
H	-2.04604700	5.64483200	2.26349500
C	-4.48679100	7.97903000	1.68863800
H	-5.47430100	8.29099700	-0.21836600
H	-3.31828700	7.43748600	3.43696200
H	-5.04688400	8.76186600	2.20208200
C	3.10213100	-5.68784300	1.34356600
C	4.02781400	-6.56873400	0.74278300
C	2.97814100	-5.68739600	2.75275600
C	4.82914700	-7.41500100	1.53192500
H	4.11403900	-6.59729100	-0.34460600
C	3.77749400	-6.53307800	3.54191000
H	2.25859400	-5.01923000	3.22733700
C	4.70889400	-7.39650200	2.93339000
H	5.54194300	-8.08788800	1.05262100
H	3.67677000	-6.51486700	4.62832300
H	5.33261600	-8.04888700	3.54614900
O	1.87372100	0.84389000	1.34736300
O	-1.96701000	-0.58291900	1.30883100
C	5.29351500	3.81088300	0.80075200

C	6.66163200	3.48898500	0.64342800
C	4.88672100	5.14288500	0.53638700
C	7.58929000	4.45844700	0.22112800
H	7.01807000	2.48197600	0.85614100
C	5.81284100	6.10980800	0.11088700
H	3.84382200	5.42277500	0.67913400
C	7.16950900	5.77206000	-0.05213600
H	8.63984400	4.18482000	0.11062600
H	5.47583800	7.12909500	-0.08594300
H	7.88940200	6.52347000	-0.37970000
C	-5.43680900	-3.47527500	1.28328700
C	-6.78123500	-3.17808400	0.95856300
C	-5.06503700	-4.83881200	1.39828900
C	-7.71726400	-4.20503600	0.73986400
H	-7.11388000	-2.14395800	0.88011200
C	-5.99932700	-5.86426200	1.17546000
H	-4.04446100	-5.09178900	1.68224500
C	-7.33079000	-5.55307800	0.84169700
H	-8.74912100	-3.94804400	0.49514100
H	-5.68970500	-6.90632800	1.27368500
H	-8.05789700	-6.34873000	0.67332200
Br	6.56265300	-1.27447900	-3.50747300
Br	4.71356700	4.16523300	-4.64440900
Br	-3.57297300	2.71309700	5.40920700
Br	-7.83195800	2.56071600	1.38839300
Br	-6.51472100	0.52654100	-4.07393500
Br	-4.95320900	-5.11408200	-3.81912600
Br	3.82924500	-1.46225100	5.57975100
Br	7.88114200	-2.37156900	1.44827700
C	0.33076500	-0.27182400	-3.07586000
C	0.31858300	-1.52919400	-3.79632100
C	1.26515400	-1.81674900	-4.83874100
C	-0.69004200	-2.50197600	-3.50585000
C	1.20341400	-3.02232700	-5.54090200
H	2.04823000	-1.09371600	-5.05049700
C	-0.76524800	-3.68512200	-4.25092300
H	-1.41707700	-2.27797800	-2.72676900
C	0.18194400	-3.95531500	-5.26036700
H	1.94058700	-3.23636400	-6.31613000
H	-1.56356800	-4.40128800	-4.05283700
H	0.12301800	-4.88590300	-5.82723900
C	0.96153900	0.88509600	-3.80612800
F	0.49023500	0.97682700	-5.12313400
F	0.71370300	2.13063400	-3.22121900

F	2.36791800	0.74578700	-3.88069700
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IntII-R' (G = -5290.122420)

O	-1.76380600	0.99975600	0.75161300
C	-2.30839900	1.10740300	-0.45989100
C	-3.71770000	1.60984900	-0.59600700
C	-4.42791900	1.18181400	-1.90986400
H	-3.83094200	0.56217000	-2.57573500
H	-5.47908000	0.91430400	-1.81446500
C	-4.03815300	2.64809400	-1.80301100
C	-0.91429600	4.16820700	-4.42070500
H	-0.14575200	4.56023900	-5.08961900
C	-0.83516600	4.40043900	-3.03556100
H	-0.00556100	4.97305600	-2.61859800
C	-1.82140300	3.89241200	-2.17068600
H	-1.72785700	4.05635700	-1.09600200
C	-2.90377600	3.14769400	-2.68526100
C	-2.98220100	2.92318000	-4.07824500
H	-3.81928600	2.35155100	-4.48338500
C	-1.99193000	3.42473600	-4.94033400
H	-2.06229500	3.23834100	-6.01347200
C	-4.55177100	1.69695500	0.65875300
C	-4.41544400	2.78983000	1.54750600
H	-3.67571700	3.56031700	1.34732200
C	-5.25626400	2.86666100	2.66277600
C	-6.24107800	1.90697400	2.94718500
H	-6.89101400	1.99567600	3.81401200
C	-6.34094100	0.82930900	2.05656000
C	-5.51699000	0.69606300	0.93117900
H	-5.63233500	-0.14864900	0.25435600
Rh	0.06082500	-0.05813200	0.91848500
Rh	0.22442300	0.10603600	-1.56096900
O	1.03182100	1.99973800	-1.36647000
O	-0.57415200	-1.79405800	-1.67295600
O	1.86082700	-1.14936300	0.76663200
O	1.19602100	1.68704800	0.93415100
O	-1.11780300	-1.77920400	0.60043000
C	1.51527500	2.30530100	-0.18605700
C	-1.22267600	-2.25478200	-0.63081900
C	2.59618000	-1.03743800	-0.33216400
C	2.57306800	3.38782600	-0.08894500
C	-2.23242500	-3.35948100	-0.88082300
C	4.03352300	-1.47003100	-0.27193100
C	2.90405600	3.87039100	1.32719200

C	-2.64094600	-4.24792800	0.29116200
C	4.95368300	-0.77975700	-1.31914400
H	2.37596800	3.36430300	2.13238500
H	-2.16184500	-4.04288700	1.24630100
H	4.45269000	-0.07996800	-1.98586400
H	3.94197900	4.12216100	1.54316500
H	-3.68320500	-4.56001400	0.35240100
H	5.93668000	-0.48261300	-0.95687400
C	2.14953900	4.87252100	0.44275700
C	-1.78185800	-4.91892400	-0.79700600
C	4.65634300	-2.25719800	-1.53922300
C	-1.92689700	6.08498000	1.45454500
C	2.23395400	-6.25345300	0.30670900
C	2.13169100	-3.32434500	-4.91836800
H	-2.92054300	6.42564600	1.75058400
H	3.21730200	-6.61761800	0.60889600
H	1.51195600	-3.59647100	-5.77497200
C	-1.18627500	6.78793300	0.48611400
C	1.65954500	-5.14007100	0.94922100
C	1.80227900	-3.78409700	-3.63010200
H	-1.60542000	7.67747900	0.01270700
H	2.18576100	-4.63117800	1.75724500
H	0.92726700	-4.41692000	-3.47540100
C	0.11152700	6.37014800	0.14457900
C	0.38587800	-4.67664600	0.57647600
C	2.59529200	-3.42846800	-2.52345200
H	0.69009900	6.95295100	-0.56948400
H	-0.01867000	-3.81483500	1.09956000
H	2.31347400	-3.76906000	-1.52601300
C	0.70022500	5.22927500	0.74989900
C	-0.35187300	-5.31967200	-0.45058600
C	3.73291100	-2.61136600	-2.69690500
C	-0.06477400	4.51730400	1.70816900
C	0.24293200	-6.43582900	-1.09320100
C	4.06604900	-2.16252400	-3.99410500
H	0.33994000	3.64049600	2.20145100
H	-0.30799300	-6.95975900	-1.87122600
H	4.94829700	-1.53508500	-4.13461700
C	-1.35725800	4.94798200	2.05942800
C	1.51981800	-6.89346900	-0.72172700
C	3.26768700	-2.51081700	-5.09762000
H	-1.90753400	4.40706400	2.83169900
H	1.94585400	-7.76075800	-1.22920500
H	3.53193400	-2.15004400	-6.09331500

C	3.67340500	3.25819300	-1.12906300
C	-3.27376000	-2.96805300	-1.91975300
C	4.57925400	-1.68319000	1.12182700
C	3.35631600	3.18717000	-2.51219000
C	-2.87403800	-2.57866600	-3.22489500
C	4.70656000	-2.97196500	1.68629700
H	2.31783300	3.19449700	-2.82850900
H	-1.81770600	-2.52689100	-3.47056500
H	4.44501400	-3.84878200	1.10222900
C	4.39100500	3.06844800	-3.44213000
C	-3.85130100	-2.23683400	-4.16188300
C	5.20522400	-3.09233200	2.98792400
C	5.74779800	3.01154000	-3.08329800
C	-5.22759800	-2.25287500	-3.87927200
C	5.58306400	-1.99066500	3.76981000
H	6.53561000	2.92704900	-3.82752900
H	-5.97047400	-1.99439000	-4.62985600
H	5.97501600	-2.10951600	4.77681700
C	6.02633900	3.06816200	-1.71180700
C	-5.58772700	-2.62137000	-2.57666400
C	5.43894000	-0.72584200	3.17812500
C	5.03077200	3.18456800	-0.73407300
C	-4.65106300	-2.97248900	-1.59604100
C	4.95350700	-0.54812200	1.87964000
H	5.30530900	3.21626000	0.31703600
H	-4.98466200	-3.24727500	-0.59846700
H	4.84717900	0.44706900	1.45219200
C	2.98641800	6.01296400	-0.11867100
C	3.77807900	6.79152500	0.75483700
C	2.93296900	6.36770900	-1.48641800
C	4.51456100	7.88796100	0.27041300
H	3.80883700	6.54045500	1.81639900
C	3.66786900	7.46455600	-1.97150300
H	2.32545900	5.77564400	-2.17127700
C	4.46363100	8.22577000	-1.09458800
H	5.12355800	8.47750700	0.95759300
H	3.62322000	7.71990300	-3.03151700
H	5.03754800	9.07346900	-1.47169400
C	-2.50685700	-5.83452200	-1.76920900
C	-3.46588100	-6.76141800	-1.30631900
C	-2.18495200	-5.81996700	-3.14700800
C	-4.10738400	-7.63826000	-2.20150600
H	-3.70258700	-6.80419100	-0.24207400
C	-2.82395500	-6.69564100	-4.04193500

H	-1.43311100	-5.11944100	-3.51288700
C	-3.79166200	-7.60459400	-3.57173000
H	-4.84774100	-8.34745800	-1.82790800
H	-2.56993400	-6.66676400	-5.10281700
H	-4.29116400	-8.28111400	-4.26666300
O	-1.70061700	0.78097900	-1.57330900
O	2.16008700	-0.54293300	-1.46717600
C	-5.13394400	3.67848100	-1.54982000
C	-6.48868600	3.40885100	-1.84841900
C	-4.80009000	4.95864100	-1.04385100
C	-7.48400800	4.37950000	-1.62927600
H	-6.77343400	2.44551800	-2.27104400
C	-5.79386900	5.92610900	-0.82132000
H	-3.75862200	5.20297700	-0.83679600
C	-7.14226400	5.63954500	-1.10879500
H	-8.52286600	4.15004900	-1.87191000
H	-5.51546500	6.90582300	-0.42911700
H	-7.91328200	6.39210500	-0.93760100
C	5.74518700	-3.29247400	-1.26351600
C	7.06898000	-2.92895600	-0.92393500
C	5.43811000	-4.67311000	-1.36607300
C	8.04839400	-3.90863600	-0.67819900
H	7.35119600	-1.87918700	-0.85572300
C	6.41504200	-5.65113200	-1.11538900
H	4.43399400	-4.97686800	-1.65896600
C	7.72594300	-5.27416500	-0.76711600
H	9.06357100	-3.60106200	-0.42218900
H	6.15501800	-6.70762300	-1.20233100
H	8.48622900	-6.03320400	-0.57738100
Br	-7.74475400	-0.56157000	2.39228000
Br	-5.07894500	4.42268700	3.90968300
Br	3.92769100	2.98014500	-5.39010800
Br	7.94361900	2.97167100	-1.12512700
Br	5.94983900	0.88632000	4.25499900
Br	5.40880700	-4.92608100	3.78203300
Br	-3.27197700	-1.70973300	-6.00520800
Br	-7.53595900	-2.64323300	-2.09560800
C	0.28813700	-0.32321400	2.92738800
C	0.24772400	-1.65645400	3.52106000
C	1.39077700	-2.21791700	4.17826000
C	-0.93838100	-2.44387500	3.43427400
C	1.34313500	-3.51697800	4.69722500
H	2.31353600	-1.64413700	4.23165500
C	-0.98940400	-3.72049900	4.00930900

H	-1.80643400	-2.01824400	2.94200600
C	0.15055200	-4.26725000	4.63126200
H	2.23163200	-3.94388000	5.16504700
H	-1.91995700	-4.28967600	3.98053500
H	0.11162700	-5.26867400	5.06263700
C	1.19584200	0.66845100	3.62640000
F	0.73677900	2.00339400	3.52009400
F	1.34395300	0.45193100	5.00772400
F	2.50381700	0.64713000	3.09774100
C	-1.63598600	0.70549700	5.21164400
H	-0.78643400	1.12748800	5.73132700
C	-1.98202700	0.95465000	3.87728500
N	-3.10117400	0.17772600	3.54432200
C	-3.48039900	-0.59178900	4.65153600
C	-2.55497400	-0.27908800	5.72110700
H	-1.57651600	1.65740600	3.16559700
H	-3.54276500	0.19764300	2.62358500
C	-4.52034200	-1.52275600	4.82724000
H	-5.22433400	-1.74572700	4.02507300
C	-4.63491200	-2.14757100	6.07850900
H	-5.43636900	-2.86992100	6.24200100
C	-3.73206200	-1.85685100	7.13930800
H	-3.85573200	-2.36508600	8.09660000
C	-2.69704100	-0.93129200	6.97160000
H	-2.00721500	-0.70956600	7.78737600

TSII-R' (G = -5290.115563)

O	-1.79800500	1.01663300	0.79527800
C	-2.37502100	1.16166100	-0.39623700
C	-3.80166000	1.64141500	-0.45975900
C	-4.55808700	1.27809500	-1.76446300
H	-3.97178300	0.72916400	-2.49846800
H	-5.59391100	0.96463500	-1.64195600
C	-4.20115300	2.74625600	-1.57251000
C	-1.20862200	4.47477000	-4.21309300
H	-0.47215600	4.91801500	-4.88611000
C	-1.05345500	4.58653300	-2.81962700
H	-0.19755600	5.11642500	-2.39999200
C	-1.99734300	4.01074300	-1.94944900
H	-1.84795400	4.08117200	-0.87086900
C	-3.11249600	3.31921900	-2.46792900
C	-3.26833900	3.21705700	-3.86861500
H	-4.13183300	2.68709200	-4.27512400
C	-2.32018500	3.78568300	-4.73633300

H	-2.44908700	3.69310100	-5.81621400
C	-4.57568200	1.58250900	0.83389600
C	-4.59598300	2.67311100	1.73282000
H	-4.05498000	3.58279000	1.48905000
C	-5.33789800	2.56701100	2.91463700
C	-6.06092000	1.41411200	3.26175500
H	-6.63442000	1.35566500	4.18356000
C	-5.99971300	0.34496000	2.35659900
C	-5.28631200	0.39932100	1.15483700
H	-5.27206400	-0.44464600	0.46652000
Rh	0.02497700	-0.07160800	0.90246500
Rh	0.12668700	0.20256900	-1.58029300
O	0.93316200	2.09005600	-1.32821900
O	-0.68552200	-1.68776100	-1.75426700
O	1.80559900	-1.17800900	0.68431400
O	1.19830800	1.64802700	0.94306800
O	-1.19932700	-1.75999500	0.52642500
C	1.45422000	2.33750300	-0.14955800
C	-1.32082600	-2.18487800	-0.72063700
C	2.51626200	-1.00785200	-0.42220200
C	2.48708100	3.44397000	-0.02996900
C	-2.33872400	-3.27699500	-1.00611600
C	3.96039700	-1.43309300	-0.42446600
C	2.82675800	3.89828500	1.39159100
C	-2.68194400	-4.26274300	0.10671700
C	4.85237100	-0.64207800	-1.42590800
H	2.31099100	3.37269200	2.19222800
H	-2.14819900	-4.13565200	1.04649400
H	4.32981100	0.10438900	-2.02141200
H	3.86259900	4.16220900	1.60352700
H	-3.71659700	-4.59181000	0.20057200
H	5.83880400	-0.36424800	-1.05760800
C	2.04124400	4.90714000	0.53892000
C	-1.87552500	-4.83023500	-1.07894200
C	4.56776300	-2.09946600	-1.76493700
C	-2.03872800	6.00477400	1.67171400
C	2.18987600	-6.22111400	-0.27118200
C	2.01297900	-2.91700300	-5.19158200
H	-3.03519700	6.31066200	1.99535800
H	3.18698900	-6.60146700	-0.04310200
H	1.38571800	-3.12510100	-6.06059300
C	-1.29351200	6.81008700	0.79123300
C	1.65449900	-5.14479700	0.46176600
C	1.70245700	-3.48202700	-3.94095100

H	-1.71043800	7.74683100	0.41710500
H	2.22402100	-4.68103800	1.26764800
H	0.83391000	-4.13247300	-3.82766600
C	0.00454700	6.43059000	0.40778100
C	0.36448200	-4.66112500	0.18298400
C	2.50495600	-3.20839000	-2.81789500
H	0.58227200	7.08463600	-0.24205600
H	-0.00886200	-3.83142900	0.77663200
H	2.23695400	-3.62970500	-1.84822600
C	0.59183400	5.22948900	0.88462200
C	-0.42900300	-5.24630700	-0.83632300
C	3.63232700	-2.36795300	-2.93659900
C	-0.17738800	4.41788500	1.75795200
C	0.12738100	-6.32404900	-1.57219800
C	3.94688900	-1.81365400	-4.19703200
H	0.22333800	3.49131800	2.15417100
H	-0.46488100	-6.80227600	-2.34929300
H	4.82152800	-1.16783800	-4.29591400
C	-1.47170700	4.80703300	2.14747700
C	1.42070400	-6.80191400	-1.29502300
C	3.13953700	-2.08052800	-5.31663600
H	-2.02702200	4.17666400	2.84461100
H	1.81728000	-7.63859000	-1.87293200
H	3.38957800	-1.63843300	-6.28285400
C	3.57707500	3.36798200	-1.08642900
C	-3.43111300	-2.82026600	-1.96331500
C	4.54601600	-1.74954200	0.93328000
C	3.24182100	3.33543700	-2.46659100
C	-3.08960100	-2.29871400	-3.23880300
C	4.74533000	-3.07682100	1.37434400
H	2.19840400	3.33138900	-2.76672200
H	-2.04362800	-2.18358500	-3.50727300
H	4.50111800	-3.90874600	0.72139300
C	4.26542600	3.26764700	-3.41356000
C	-4.10868600	-1.91598100	-4.11305100
C	5.29884500	-3.29229500	2.64114600
C	5.62793600	3.22439200	-3.07485500
C	-5.47381300	-2.01335600	-3.79404200
C	5.66305300	-2.25086100	3.50675400
H	6.40682800	3.17945700	-3.83177100
H	-6.24984300	-1.72109000	-4.49714200
H	6.09977100	-2.44252000	4.48362500
C	5.92411000	3.24033700	-1.70599000
C	-5.77696600	-2.50994900	-2.52002600

C	5.44368000	-0.94569900	3.03848600
C	4.94056200	3.30639800	-0.71169400
C	-4.79665700	-2.90929900	-1.60223800
C	4.90266300	-0.67217500	1.77972800
H	5.22831500	3.30704300	0.33633300
H	-5.08939900	-3.29220000	-0.62786200
H	4.74224300	0.35192500	1.44882900
C	2.84767800	6.07268000	-0.01458000
C	3.67257900	6.82862000	0.84763800
C	2.73310800	6.47032900	-1.36687500
C	4.38331900	7.94355100	0.36625800
H	3.75009400	6.54568300	1.89870200
C	3.44203000	7.58512000	-1.84907500
H	2.09574100	5.89810200	-2.04157800
C	4.27256500	8.32284900	-0.98408800
H	5.01894000	8.51493900	1.04467400
H	3.35012600	7.87322100	-2.89761400
H	4.82668600	9.18453400	-1.35918500
C	-2.64047200	-5.66770000	-2.08971000
C	-3.57628100	-6.63611700	-1.66678900
C	-2.37703900	-5.53470000	-3.47367700
C	-4.25330400	-7.43824700	-2.60512300
H	-3.76706700	-6.77041000	-0.60086300
C	-3.05148900	-6.33553400	-4.41153600
H	-1.64215200	-4.80163600	-3.80940300
C	-3.99624600	-7.28686700	-3.97961100
H	-4.97511200	-8.18125800	-2.26205900
H	-2.84261100	-6.21603200	-5.47593900
H	-4.52300100	-7.90539100	-4.70770800
O	-1.79969300	0.89092000	-1.53872100
O	2.05942600	-0.45626700	-1.52263000
C	-5.29893100	3.73946900	-1.20038700
C	-6.67138500	3.40589500	-1.26248100
C	-4.94757600	5.05327300	-0.80028400
C	-7.66064800	4.34554800	-0.91809700
H	-6.98104400	2.41537200	-1.59395200
C	-5.93508600	5.98957600	-0.45166800
H	-3.89802000	5.34464300	-0.77880800
C	-7.29780300	5.63939700	-0.50530100
H	-8.71350800	4.06538500	-0.98005000
H	-5.64107700	6.99568300	-0.14743600
H	-8.06489100	6.36809800	-0.23931000
C	5.67797100	-3.13742100	-1.60673700
C	7.00648900	-2.78443500	-1.27531100

C	5.38541700	-4.50901400	-1.81737700
C	8.00475000	-3.76689000	-1.14068000
H	7.27732600	-1.73993300	-1.12679700
C	6.38089100	-5.49032500	-1.67714000
H	4.37713000	-4.80074000	-2.10847800
C	7.69674700	-5.12473900	-1.33496000
H	9.02317300	-3.46693100	-0.88834100
H	6.13152400	-6.53953500	-1.84575900
H	8.47150400	-5.88580700	-1.23110000
Br	-6.96093000	-1.36045700	2.83547500
Br	-5.38275500	4.11954100	4.17712300
Br	3.77690000	3.23810500	-5.35752400
Br	7.85143400	3.15911400	-1.14826000
Br	5.92905700	0.58507100	4.24171900
Br	5.60995700	-5.18021100	3.25427000
Br	-3.60969500	-1.20841400	-5.91866800
Br	-7.70770800	-2.66117900	-1.99068200
C	0.21100500	-0.38162500	2.99664300
C	0.36203100	-1.79120700	3.44398700
C	1.56787000	-2.27755000	4.03415100
C	-0.69925500	-2.71893800	3.24752600
C	1.69523300	-3.62561200	4.40053800
H	2.41367500	-1.60988100	4.16669400
C	-0.57625100	-4.05514500	3.65086600
H	-1.60840300	-2.37270100	2.76683200
C	0.62220200	-4.51889600	4.22818500
H	2.63519400	-3.97703800	4.82879700
H	-1.41216600	-4.74345300	3.50834900
H	0.71941000	-5.56188600	4.53333200
C	1.21818600	0.57085300	3.62691400
F	0.86326800	1.94423200	3.51834400
F	1.43319200	0.38579900	5.01112000
F	2.49087000	0.44713700	3.03996300
C	-1.43785300	0.40172600	4.29250100
H	-0.95927500	1.36836100	4.20075900
C	-2.57633400	0.05654200	3.50925300
N	-3.31197200	-0.89431900	4.16483400
C	-2.73429200	-1.17567400	5.43627700
C	-1.56716300	-0.35633400	5.55218700
H	-2.82727800	0.42343700	2.52053100
H	-4.17000500	-1.31820700	3.79999100
C	-3.15964600	-2.03549100	6.45616800
H	-4.05314500	-2.65195500	6.35056200
C	-2.38741400	-2.07215300	7.63125600

H	-2.68834400	-2.72800300	8.44890200
C	-1.22556000	-1.27448000	7.76498000
H	-0.64423900	-1.33084100	8.68606900
C	-0.80222900	-0.42027700	6.73208500
H	0.10738400	0.16665700	6.82309600

IntIII-R' (G = -5290.120615)

O	-1.82141800	1.01882500	0.62693200
C	-2.34353200	1.03811400	-0.59710300
C	-3.75257100	1.55085100	-0.77153600
C	-4.46755700	1.07985100	-2.06332200
H	-3.87659900	0.42857000	-2.70391900
H	-5.52496600	0.83589800	-1.96659200
C	-4.05693100	2.54592400	-2.00721600
C	-0.92010100	3.92921900	-4.68339500
H	-0.14695700	4.28519200	-5.36695500
C	-0.83621100	4.21251200	-3.30822000
H	0.00170000	4.78908100	-2.91431700
C	-1.82704900	3.74996200	-2.42344900
H	-1.72961100	3.95461300	-1.35632000
C	-2.91789700	2.99843900	-2.90843500
C	-3.00100900	2.72187400	-4.29183300
H	-3.84434900	2.14335600	-4.67355400
C	-2.00678600	3.17916100	-5.17347800
H	-2.08015800	2.95228100	-6.23860000
C	-4.57310600	1.68494900	0.48663000
C	-4.35779900	2.76008000	1.38340700
H	-3.58516200	3.49481500	1.17050600
C	-5.15537500	2.86015400	2.52756500
C	-6.15701700	1.92738800	2.84773700
H	-6.77053400	2.03301100	3.73896700
C	-6.31815400	0.85965700	1.95588800
C	-5.56391900	0.71867700	0.78564700
H	-5.73134300	-0.11801200	0.10939600
Rh	-0.00289700	-0.05589500	0.91544100
Rh	0.19546300	-0.05608400	-1.57717000
O	0.98638300	1.84841300	-1.49854200
O	-0.58917400	-1.97793300	-1.54927800
O	1.81870600	-1.10728700	0.92528700
O	1.13953700	1.69874900	0.82284500
O	-1.16054200	-1.79569400	0.71016500
C	1.46863700	2.22917000	-0.33602200
C	-1.23066800	-2.37624500	-0.48289600
C	2.55860500	-1.05886700	-0.17249700

C	2.53978300	3.31025700	-0.32991300
C	-2.20624700	-3.52963800	-0.63505400
C	4.01895400	-1.42693400	-0.07971400
C	2.91118300	3.86533700	1.04848200
C	-2.51633000	-4.37887500	0.59707000
C	4.91752700	-0.70073700	-1.12716200
H	2.39625800	3.40267600	1.88782100
H	-1.98840300	-4.11751000	1.51364300
H	4.38896300	-0.04122400	-1.81257300
H	3.95425700	4.12132500	1.23141000
H	-3.53811700	-4.73433500	0.73085700
H	5.87658100	-0.34590400	-0.75273500
C	2.14133800	4.82579800	0.13156900
C	-1.68945700	-5.05851500	-0.51310300
C	4.70234900	-2.19517500	-1.32237000
C	-1.91212700	6.09997300	1.15449600
C	2.42379600	-6.19656000	0.43242900
C	2.32313600	-3.46176100	-4.74035900
H	-2.90166400	6.45600700	1.44707900
H	3.43493900	-6.51024300	0.69729700
H	1.74025700	-3.78179900	-5.60627300
C	-1.19874700	6.73530300	0.12038500
C	1.85977100	-5.04807200	1.01927400
C	1.98369700	-3.91155800	-3.45104100
H	-1.63542300	7.58542400	-0.40670200
H	2.42037500	-4.45853800	1.74425000
H	1.13617700	-4.58287000	-3.30396200
C	0.09326700	6.29999100	-0.22111400
C	0.55024700	-4.64882100	0.69983200
C	2.72873200	-3.49326700	-2.33297600
H	0.65064100	6.83101100	-0.99046000
H	0.15745700	-3.75761500	1.18399600
H	2.43776000	-3.82587400	-1.33627800
C	0.70320300	5.20924000	0.45201900
C	-0.22915700	-5.38972200	-0.22543900
C	3.82575300	-2.62099900	-2.49455800
C	-0.03144600	4.56820900	1.47941700
C	0.35775700	-6.53683700	-0.81897100
C	4.17054900	-2.18306900	-3.79223400
H	0.39006500	3.73170500	2.02458600
H	-0.22319300	-7.13057800	-1.52130200
H	5.02196800	-1.51244000	-3.92375700
C	-1.31927800	5.01432500	1.82754500
C	1.66695800	-6.93429200	-0.49451800

C	3.42108800	-2.59514500	-4.90802600
H	-1.84569300	4.52534500	2.64930400
H	2.08628400	-7.82787000	-0.96030800
H	3.69338800	-2.24160400	-5.90428000
C	3.61154000	3.13579100	-1.39303200
C	-3.31138400	-3.22035200	-1.63517300
C	4.56295400	-1.54647500	1.32684700
C	3.25754200	2.98063300	-2.76086000
C	-2.98366100	-2.81257600	-2.95519000
C	4.95410400	-2.78016500	1.89273300
H	2.21032200	2.94089800	-3.04381800
H	-1.94099300	-2.68986800	-3.23404200
H	4.88837600	-3.69285400	1.30918200
C	4.26840500	2.84106600	-3.71358300
C	-4.01258300	-2.54472400	-3.86012500
C	5.46636700	-2.79469500	3.19622300
C	5.63624300	2.83994600	-3.39467300
C	-5.37484200	-2.65095600	-3.53096200
C	5.60272600	-1.64158200	3.98098200
H	6.40430000	2.73641700	-4.15684600
H	-6.15834600	-2.44861000	-4.25704500
H	6.00505000	-1.67733100	4.99012300
C	5.95135100	2.97797400	-2.03724900
C	-5.66425500	-3.03523400	-2.21574000
C	5.19288100	-0.43442300	3.39081900
C	4.98191900	3.12084500	-1.03759500
C	-4.67400600	-3.31759600	-1.26644500
C	4.68508200	-0.35882100	2.09200400
H	5.28730600	3.21572900	0.00080800
H	-4.95666900	-3.61782100	-0.26078100
H	4.36863600	0.59203900	1.66765900
C	2.97045600	5.93415300	-0.50189600
C	3.77289600	6.75748200	0.31946200
C	2.89858600	6.21819300	-1.88514100
C	4.50104900	7.82825500	-0.23028200
H	3.81894700	6.56030700	1.39183400
C	3.62502500	7.28962800	-2.43574600
H	2.28587700	5.58912400	-2.53109100
C	4.43104200	8.09580300	-1.61003900
H	5.11887600	8.45247300	0.41735700
H	3.56621400	7.48954500	-3.50695300
H	4.99868400	8.92345100	-2.03790000
C	-2.42388400	-6.03933000	-1.41149000
C	-3.31861000	-6.98728000	-0.87015400

C	-2.17084000	-6.05870300	-2.80353000
C	-3.96729400	-7.91907600	-1.70285400
H	-3.49826700	-7.00378500	0.20604200
C	-2.81714200	-6.98894500	-3.63580300
H	-1.46574000	-5.34262400	-3.22813300
C	-3.72205500	-7.91909400	-3.08784800
H	-4.65728200	-8.64495700	-1.26944200
H	-2.61727800	-6.98674200	-4.70859500
H	-4.22681100	-8.63843100	-3.73436800
O	-1.74277400	0.61488700	-1.67816900
O	2.12903200	-0.67139700	-1.35176800
C	-5.14109000	3.59598500	-1.79118200
C	-6.48566100	3.35434300	-2.15191900
C	-4.80500300	4.86409800	-1.25806600
C	-7.47151000	4.34194800	-1.96755200
H	-6.76617400	2.39952800	-2.59690300
C	-5.78968400	5.84832700	-1.06974200
H	-3.76888300	5.08634000	-1.00341600
C	-7.12921200	5.59020500	-1.41953600
H	-8.50275300	4.13564100	-2.25894000
H	-5.51064600	6.81892400	-0.65576600
H	-7.89268500	6.35606700	-1.27530500
C	5.85483400	-3.15954100	-1.04393200
C	7.17056000	-2.71348200	-0.78356500
C	5.61686400	-4.55739900	-1.07190200
C	8.21049900	-3.62983400	-0.53894300
H	7.39775900	-1.64816000	-0.77819300
C	6.65344800	-5.47172500	-0.82116100
H	4.61845700	-4.92369600	-1.30811900
C	7.95679600	-5.01233700	-0.54973700
H	9.21846100	-3.25949200	-0.34467000
H	6.44650800	-6.54317000	-0.84818200
H	8.76328700	-5.72213100	-0.35990000
Br	-7.66325000	-0.56983300	2.41562800
Br	-4.88443700	4.39623800	3.78330900
Br	3.75319200	2.64164800	-5.64129900
Br	7.88762400	2.96461200	-1.50318700
Br	5.34930700	1.24565500	4.47526500
Br	6.04790500	-4.54813700	3.98683600
Br	-3.53333900	-1.99302700	-5.72442600
Br	-7.59038200	-3.19032500	-1.66762100
C	-0.22019200	-0.17530600	3.19234800
C	0.13294600	-1.56260400	3.67332200
C	1.48922800	-1.96655200	3.83870100

C	-0.86466600	-2.52145400	3.98744000
C	1.81074200	-3.25211000	4.29975100
H	2.28556900	-1.26725800	3.60792200
C	-0.54111000	-3.81581100	4.43094700
H	-1.91739300	-2.25395700	3.91213800
C	0.80293800	-4.18986800	4.59610200
H	2.86016400	-3.52008100	4.42872700
H	-1.34129700	-4.51990800	4.67014400
H	1.06115500	-5.18807700	4.95237500
C	0.70880900	0.88633400	3.71030700
F	0.19546700	2.18799700	3.47126100
F	0.93700300	0.84894400	5.12134100
F	2.00962000	0.85366700	3.17540000
C	-1.69611100	0.25979600	3.48916500
H	-1.78240000	1.26354700	3.01095000
C	-2.77207000	-0.52979300	2.79561300
N	-3.84884800	-0.63239100	3.57338400
C	-3.62327500	-0.07864300	4.88500500
C	-2.29291100	0.40787000	4.91542800
H	-2.70437600	-0.95352300	1.79847600
H	-4.74287000	-1.04579800	3.27780900
C	-4.49722800	-0.02007600	5.97494400
H	-5.51521600	-0.40680600	5.91952200
C	-3.99741300	0.56042600	7.15634700
H	-4.63886600	0.62452300	8.03537700
C	-2.67350700	1.04870700	7.21418700
H	-2.30421400	1.47968300	8.14533600
C	-1.81216000	0.98282100	6.09870500
H	-0.78571400	1.32930900	6.15206100

TSIII-R' (G = -5290.113985)

O	-1.81484900	1.02293800	0.82357900
C	-2.40487000	1.21025300	-0.35121100
C	-3.82061000	1.71337300	-0.36231800
C	-4.61540600	1.43188900	-1.66183900
H	-4.06189700	0.90436200	-2.43596400
H	-5.65598300	1.13941800	-1.52931200
C	-4.22072800	2.88056600	-1.40881600
C	-1.25245200	4.66773700	-4.03886200
H	-0.52162100	5.12513300	-4.70850700
C	-1.06148800	4.70947700	-2.64595700
H	-0.18301000	5.19949700	-2.22415600
C	-1.99860500	4.11599200	-1.78029700
H	-1.82166800	4.13390300	-0.70370600

C	-3.14240300	3.47557500	-2.30200500
C	-3.33358300	3.44380800	-3.70191700
H	-4.21939900	2.95422200	-4.11088100
C	-2.39313300	4.03098300	-4.56558900
H	-2.55057200	3.99373900	-5.64497400
C	-4.54735300	1.61899900	0.95766300
C	-4.36918500	2.60200800	1.95922100
H	-3.71476700	3.45006900	1.77551900
C	-5.05435000	2.46456200	3.17039100
C	-5.91835600	1.39247600	3.44607400
H	-6.44738500	1.31381500	4.39254400
C	-6.06367900	0.43100900	2.43661200
C	-5.39860000	0.51502200	1.20641300
H	-5.54041400	-0.24639100	0.44097400
Rh	0.01410100	-0.05195500	0.90557900
Rh	0.07808700	0.24179500	-1.53682000
O	0.91801900	2.10955600	-1.28261700
O	-0.76559700	-1.63250800	-1.73529200
O	1.79431200	-1.15296300	0.70260900
O	1.13905800	1.68343500	0.99306400
O	-1.19083700	-1.74854900	0.55812200
C	1.43426200	2.35879800	-0.09739400
C	-1.36841000	-2.15186000	-0.68991200
C	2.47764600	-1.00427600	-0.42057000
C	2.49207300	3.43801700	0.01875200
C	-2.41149200	-3.22125300	-0.95954100
C	3.90983100	-1.45848300	-0.48824000
C	2.90455700	3.80757900	1.44833000
C	-2.70942700	-4.23583600	0.14049100
C	4.78195500	-0.63514300	-1.48600500
H	2.42652900	3.23459400	2.23975300
H	-2.11877700	-4.14926700	1.05113200
H	4.25477500	0.14785300	-2.02787400
H	3.95385200	4.04639000	1.62015200
H	-3.74378900	-4.54371100	0.29064200
H	5.78398100	-0.39149100	-1.13617700
C	2.10174000	4.87522600	0.69346500
C	-1.98963400	-4.78151000	-1.11037600
C	4.46125800	-2.06930000	-1.88180500
C	-1.92165300	5.98907200	1.99376400
C	2.07589600	-6.30114100	-0.59284600
C	1.78241100	-2.67701600	-5.25864100
H	-2.90294800	6.29955500	2.35659900
H	3.07299300	-6.71459600	-0.43314800

H	1.12342000	-2.83123400	-6.11534400
C	-1.23805200	6.75497900	1.03117500
C	1.63201500	-5.20277600	0.16774600
C	1.51060500	-3.30937500	-4.03122700
H	-1.68854400	7.66559800	0.63245500
H	2.27047200	-4.75754400	0.93121700
H	0.63954000	-3.95763200	-3.92350100
C	0.04275600	6.37122700	0.59811300
C	0.34280400	-4.67638500	-0.02338500
C	2.35468500	-3.10545500	-2.92398800
H	0.57776200	7.00015300	-0.11079300
H	0.04444400	-3.82581100	0.58339700
H	2.11509500	-3.57715600	-1.97040000
C	0.67202200	5.20422100	1.10483600
C	-0.54310700	-5.24096100	-0.97468200
C	3.48518500	-2.26826800	-3.03483800
C	-0.03316600	4.43432600	2.06414000
C	-0.07829000	-6.34135700	-1.73998700
C	3.76144200	-1.64729000	-4.27297400
H	0.41241000	3.54316900	2.49198000
H	-0.74119300	-6.80371300	-2.46789100
H	4.63852400	-1.00401300	-4.36691600
C	-1.31025800	4.82805000	2.50426300
C	1.21547500	-6.86044100	-1.55390800
C	2.91274600	-1.84431500	-5.37651000
H	-1.81638100	4.23909600	3.27177000
H	1.54071600	-7.71323900	-2.15234400
H	3.13389300	-1.35134300	-6.32503600
C	3.53047600	3.39782700	-1.08926900
C	-3.54243600	-2.71995000	-1.84802800
C	4.54691500	-1.83823000	0.82990200
C	3.13678800	3.45538300	-2.45310000
C	-3.25213700	-2.17359700	-3.12552100
C	4.77639700	-3.18320000	1.19502200
H	2.08305700	3.50180100	-2.70991600
H	-2.21833300	-2.06652900	-3.44026400
H	4.50470300	-3.98536100	0.51650600
C	4.11724200	3.41232300	-3.44627300
C	-4.30468300	-1.76228000	-3.94540400
C	5.40440900	-3.45561300	2.41543800
C	5.49059800	3.31030500	-3.17034300
C	-5.65501100	-1.85771400	-3.56943800
C	5.81183800	-2.45445700	3.30767000
H	6.23507800	3.28588300	-3.96204200

H	-6.45866400	-1.54591000	-4.23202900
H	6.30344000	-2.68955900	4.24817500
C	5.84480200	3.23973600	-1.81708800
C	-5.90747200	-2.38085800	-2.29456500
C	5.55700100	-1.13071700	2.91794200
C	4.90591600	3.27628100	-0.77894400
C	-4.89111200	-2.80639100	-1.42853700
C	4.94435900	-0.80053500	1.70722100
H	5.23688300	3.20687400	0.25393800
H	-5.14411600	-3.20867000	-0.45078900
H	4.76492200	0.23727100	1.43544600
C	2.90909600	6.06136400	0.18431700
C	3.74036400	6.77027800	1.08035900
C	2.79008900	6.52733000	-1.14530500
C	4.45060600	7.90717200	0.65385600
H	3.82270800	6.43239500	2.11473400
C	3.49881800	7.66488700	-1.57252600
H	2.15311400	5.99002000	-1.84813100
C	4.33385800	8.35610400	-0.67464900
H	5.09080100	8.44148000	1.35765300
H	3.40334600	8.00597700	-2.60470200
H	4.88752700	9.23528600	-1.00732800
C	-2.83580900	-5.56409800	-2.10058100
C	-3.78708100	-6.50706600	-1.65555100
C	-2.63361700	-5.40572700	-3.49221800
C	-4.53918400	-7.25842200	-2.57880700
H	-3.93139000	-6.66284400	-0.58532000
C	-3.38325100	-6.15545700	-4.41488200
H	-1.88610000	-4.69412700	-3.84588500
C	-4.34296700	-7.08101100	-3.96012600
H	-5.27161900	-7.98262900	-2.21862600
H	-3.22080900	-6.01688100	-5.48503800
H	-4.92778300	-7.66011600	-4.67618400
O	-1.84553000	0.95715800	-1.50875400
O	1.99813200	-0.43479200	-1.50938300
C	-5.28620200	3.87146000	-0.95183400
C	-6.66725000	3.59880800	-1.07819600
C	-4.89620600	5.11947100	-0.40626900
C	-7.63000300	4.53382500	-0.65481200
H	-7.00213800	2.66202100	-1.52265500
C	-5.85725500	6.05103900	0.02008500
H	-3.83765000	5.36594200	-0.32971200
C	-7.23003700	5.76095800	-0.09810700
H	-8.69056900	4.30278100	-0.76692800

H	-5.53493400	7.00637100	0.43809000
H	-7.97623400	6.48571100	0.23059500
C	5.56216700	-3.12757600	-1.81755500
C	6.91128500	-2.80302700	-1.54653300
C	5.23974800	-4.48650400	-2.06355300
C	7.90181300	-3.80154400	-1.50349200
H	7.20408800	-1.76810100	-1.37473500
C	6.22771300	-5.48397800	-2.01485200
H	4.21366200	-4.75619300	-2.31033600
C	7.56509000	-5.14715600	-1.73145500
H	8.93640100	-3.52338000	-1.29602500
H	5.95517800	-6.52298400	-2.20884600
H	8.33368100	-5.92072200	-1.69854900
Br	-7.29058300	-1.12029700	2.76913900
Br	-4.81521000	3.86081700	4.58882000
Br	3.54706700	3.50656800	-5.36584500
Br	7.78938800	3.07165800	-1.34920600
Br	6.09763600	0.34615900	4.16449400
Br	5.76829500	-5.36712100	2.91098000
Br	-3.87777800	-1.01856600	-5.75522100
Br	-7.81394200	-2.53525800	-1.69008200
C	0.45947600	-0.44211200	3.71721400
C	0.85735000	-1.89477200	3.79532600
C	1.97001900	-2.27333700	4.59298600
C	0.06609200	-2.91483900	3.22254400
C	2.28543300	-3.62719700	4.78962100
H	2.56376800	-1.50142400	5.07441600
C	0.37300900	-4.27000600	3.44310700
H	-0.77372700	-2.64507700	2.58737300
C	1.48480700	-4.63487500	4.22249400
H	3.14957600	-3.89355700	5.40099000
H	-0.25096300	-5.04324100	2.99158300
H	1.72360600	-5.68697000	4.38627100
C	1.54401700	0.57205200	3.82430200
F	1.02463800	1.90114600	3.71158900
F	2.15651200	0.59058700	5.11702300
F	2.59175400	0.44474200	2.92321000
C	-0.66713900	-0.00871400	4.76444900
H	-0.34073400	0.73422500	5.49861400
C	-1.34008900	0.43076400	3.49786200
N	-2.45436700	-0.34780600	3.28409600
C	-2.61416000	-1.30687300	4.32863300
C	-1.55907900	-1.12549600	5.26405300
H	-1.19783300	1.37251500	2.98886400

H	-2.96485700	-0.32369400	2.39719600
C	-3.59980700	-2.28468500	4.50383000
H	-4.40878500	-2.41510900	3.78514900
C	-3.52486300	-3.08263100	5.66636700
H	-4.28384900	-3.84797200	5.83456700
C	-2.49476600	-2.90188200	6.61036000
H	-2.45952700	-3.53257100	7.49901000
C	-1.50054500	-1.91654200	6.41245100
H	-0.69228300	-1.79207300	7.13358300

IntII-S' (G = -5290.130913)

O	-1.75167600	0.98281600	0.86417000
C	-2.30835100	1.25378400	-0.31106700
C	-3.71163400	1.79344800	-0.33906500
C	-4.43448900	1.63817600	-1.70234300
H	-3.85981300	1.13093000	-2.47366100
H	-5.49601100	1.39975700	-1.65492900
C	-4.00072000	3.04693000	-1.32752100
C	-0.86345200	4.97032000	-3.64853300
H	-0.09395000	5.46972800	-4.24040900
C	-0.80305800	4.99044700	-2.24314300
H	0.01167700	5.50727900	-1.73399300
C	-1.79153200	4.34646300	-1.47717600
H	-1.71429600	4.35357000	-0.38917000
C	-2.85882700	3.67627300	-2.11179600
C	-2.91776700	3.66416900	-3.52382900
H	-3.74247100	3.15100500	-4.02167500
C	-1.92488000	4.30113300	-4.28791100
H	-1.98146800	4.27882400	-5.37776500
C	-4.52884100	1.66976600	0.92550400
C	-4.23572600	2.47161100	2.05520300
H	-3.38707100	3.14993600	2.03177900
C	-5.05746300	2.37796800	3.18126700
C	-6.16254000	1.51588000	3.25731300
H	-6.79540900	1.47411500	4.14018800
C	-6.40631700	0.71625400	2.13382200
C	-5.62002900	0.77094200	0.97721300
H	-5.84659700	0.13301700	0.12568700
Rh	0.05188500	-0.10738600	0.90284500
Rh	0.20733900	0.38513100	-1.53550300
O	1.02908000	2.22782400	-1.10352600
O	-0.61103600	-1.48116800	-1.89500400
O	1.81689400	-1.22089900	0.61590300
O	1.16361900	1.62629600	1.13918500

O	-1.06008600	-1.84145300	0.36390700
C	1.50230000	2.38115300	0.10998400
C	-1.21884100	-2.11821200	-0.93031400
C	2.57132600	-0.93992700	-0.44094500
C	2.56344600	3.43145500	0.36235000
C	-2.25872300	-3.15602900	-1.32052600
C	4.00590900	-1.38132900	-0.43124000
C	2.95026700	3.64393700	1.83318900
C	-2.56212300	-4.27849100	-0.32819700
C	4.96976700	-0.42421000	-1.19324200
H	2.45142700	3.00001100	2.55451000
H	-2.01319600	-4.26861000	0.60905700
H	4.49124300	0.42997300	-1.66928500
H	3.99842000	3.85223500	2.04692600
H	-3.59236000	-4.62249700	-0.24527400
H	5.92998500	-0.23283500	-0.71641100
C	2.17131000	4.79368300	1.18504600
C	-1.81524400	-4.69064100	-1.60616700
C	4.71339900	-1.78250700	-1.83245700
C	-1.85264600	5.81973700	2.54653900
C	2.31844400	-6.10611100	-1.43449300
C	2.39013800	-1.80928700	-5.51162700
H	-2.83240200	6.10522300	2.93364300
H	3.33669200	-6.49550900	-1.39073600
H	1.81439300	-1.80938300	-6.43899700
C	-1.14798900	6.67255400	1.67644800
C	1.69500800	-5.61690900	-0.27260000
C	2.00790300	-2.63793300	-4.44001800
H	-1.58150200	7.62615700	1.37035400
H	2.21995400	-5.63498100	0.68352300
H	1.13450700	-3.28574100	-4.52730300
C	0.13273600	6.31728900	1.21973400
C	0.37598800	-5.12749000	-0.32074600
C	2.74192200	-2.63113000	-3.23978300
H	0.68578400	7.01012700	0.58847600
H	-0.06940200	-4.78819100	0.61150900
H	2.42292400	-3.26215300	-2.40915300
C	0.73834900	5.09290900	1.60650400
C	-0.35364700	-5.11975800	-1.53394300
C	3.86805900	-1.79258000	-3.09829800
C	0.00947800	4.23352100	2.46667700
C	0.28759100	-5.62042400	-2.69666800
C	4.25769300	-0.97672400	-4.18312900
H	0.42617000	3.28918300	2.79824600

H	-0.26671000	-5.67080200	-3.63221300
H	5.13301900	-0.33218500	-4.08265300
C	-1.26494400	4.60056300	2.93541600
C	1.60634400	-6.10213900	-2.64890300
C	3.52117900	-0.98020700	-5.38089000
H	-1.78579900	3.93879100	3.62910200
H	2.06955700	-6.48956400	-3.55789700
H	3.82823900	-0.33721400	-6.20772300
C	3.62175100	3.50842400	-0.72388300
C	-3.38441200	-2.56514800	-2.16094000
C	4.47617600	-1.99527400	0.86637600
C	3.25445400	3.71297600	-2.08123100
C	-3.08643900	-1.85565600	-3.35451000
C	4.49840800	-3.39649300	1.04753500
H	2.20591100	3.78457600	-2.35360900
H	-2.05076500	-1.68206600	-3.63213800
H	4.20463300	-4.05235500	0.23312000
C	4.25537400	3.78486500	-3.05226600
C	-4.13538200	-1.37548700	-4.14089300
C	4.92703500	-3.91273500	2.27531500
C	5.62373200	3.65897500	-2.76129700
C	-5.48882200	-1.55156700	-3.80824500
C	5.32886600	-3.10139700	3.34724200
H	6.38403200	3.72699700	-3.53520000
H	-6.28913900	-1.18271900	-4.44512700
H	5.66101300	-3.52491200	4.29175000
C	5.95131300	3.44076000	-1.41727900
C	-5.74956300	-2.23096600	-2.61092100
C	5.28542700	-1.71506300	3.13423900
C	4.99174300	3.35924600	-0.40115700
C	-4.73700100	-2.73246300	-1.78226400
C	4.87695300	-1.14622500	1.92431900
H	5.30265100	3.17975100	0.62449700
H	-4.99740800	-3.25044700	-0.86305000
H	4.84694800	-0.06628600	1.79629900
C	2.99992200	6.01776100	0.81941300
C	3.81963600	6.61684700	1.80217000
C	2.91172600	6.62517800	-0.45416000
C	4.54896800	7.78464100	1.51382500
H	3.87707500	6.16985700	2.79605500
C	3.63979100	7.79354600	-0.74329800
H	2.28350100	6.17384300	-1.22205600
C	4.46333900	8.37466400	0.23920100
H	5.17933000	8.23337800	2.28320200

H	3.56761000	8.24483500	-1.73423600
H	5.03164800	9.27814400	0.01356700
C	-2.64711000	-5.44361000	-2.63620900
C	-3.36724000	-6.59055500	-2.23250400
C	-2.65628100	-5.08036400	-4.00247100
C	-4.09467400	-7.34756000	-3.16839000
H	-3.34713000	-6.89391600	-1.18434200
C	-3.38265700	-5.83835900	-4.93925200
H	-2.10690600	-4.19803600	-4.33021500
C	-4.10666400	-6.97164400	-4.52449200
H	-4.64665300	-8.22966800	-2.84008000
H	-3.38652400	-5.54015300	-5.98895600
H	-4.67317600	-7.55622500	-5.25073200
O	-1.72239700	1.07049600	-1.47152600
O	2.14769500	-0.26642800	-1.48204700
C	-5.07423500	4.03570100	-0.88957500
C	-6.39246100	3.94638100	-1.39030100
C	-4.75623000	5.10151500	-0.01449300
C	-7.37247100	4.88374000	-1.01384600
H	-6.65375900	3.15216100	-2.09019700
C	-5.73541000	6.03489300	0.36476100
H	-3.74056800	5.20723200	0.36559700
C	-7.04941100	5.92799300	-0.13014900
H	-8.38363000	4.79835100	-1.41520700
H	-5.47228900	6.84706000	1.04473900
H	-7.80873800	6.65357200	0.16510900
C	5.80414100	-2.85155400	-1.78407800
C	7.03820800	-2.65361300	-1.11976200
C	5.59405600	-4.09215900	-2.43743700
C	8.01942500	-3.66067300	-1.09800800
H	7.24801200	-1.71304000	-0.61271100
C	6.57293500	-5.10015400	-2.41180100
H	4.66591100	-4.25424200	-2.98291700
C	7.79122800	-4.89096800	-1.73982000
H	8.96321200	-3.47927700	-0.58126000
H	6.38780600	-6.04444000	-2.92704800
H	8.55400600	-5.67069900	-1.72340900
Br	-7.95761700	-0.55644300	2.19220400
Br	-4.68199500	3.53984100	4.77456900
Br	3.72619600	4.09522800	-4.96057400
Br	7.88714200	3.22896100	-0.92986900
Br	5.82036800	-0.50475100	4.64041000
Br	4.98922900	-5.90198000	2.52283600
Br	-3.69744700	-0.40661200	-5.83830900

Br	-7.65860500	-2.50483700	-2.06764500
C	-0.04218500	-0.30804600	2.93442900
C	1.24466100	-3.46548600	4.36318200
H	2.17706400	-3.31928700	4.89694900
C	0.05519600	-4.11181700	4.86761400
C	1.18762600	0.19964500	3.65941200
F	1.05263300	1.58847400	3.95577400
F	1.46404600	-0.42134200	4.89302500
F	2.37233200	0.07616500	2.92759000
C	-1.24279700	-0.53508600	3.70767900
C	-1.30841000	-0.35398600	5.13736300
C	-2.44218500	-0.97733200	3.04815300
C	-2.49839200	-0.56223800	5.83566600
H	-0.41327400	-0.06715900	5.67712600
C	-3.62026100	-1.19972800	3.76480900
H	-2.41835100	-1.15106100	1.97733800
C	-3.65979200	-0.98721500	5.15743300
H	-2.52295700	-0.41203600	6.91582600
H	-4.51739600	-1.53077100	3.24100400
H	-4.58405100	-1.15979800	5.71113200
C	0.98822600	-3.06613900	3.05526000
C	-0.92768000	-4.07712200	3.80371900
N	-0.32509300	-3.45882200	2.70045100
H	1.62379400	-2.57636000	2.32581900
H	-0.80125700	-3.03863700	1.89185500
C	-0.28378200	-4.71961000	6.10196500
C	-1.56442400	-5.25840500	6.26349900
C	-2.52124500	-5.20845600	5.21042500
C	-2.21366700	-4.62316400	3.97484400
H	0.44670800	-4.76401100	6.91153500
H	-1.83964200	-5.72925100	7.20852400
H	-3.51111600	-5.63995300	5.36742000
H	-2.95025600	-4.59400700	3.17062700

TSII-S' (G = -5290.116015)

O	-1.82707700	0.89203400	0.83848600
C	-2.41428600	1.05800700	-0.33749800
C	-3.82957600	1.57183600	-0.36670300
C	-4.61384600	1.22841000	-1.65919000
H	-4.06308200	0.63151400	-2.38309800
H	-5.66858700	0.98762900	-1.53670400
C	-4.18780500	2.67992300	-1.49421300
C	-1.22182900	4.31484600	-4.22686100
H	-0.49407600	4.73627400	-4.92324800

C	-1.09511700	4.54096000	-2.84414800
H	-0.26940100	5.13848100	-2.45559600
C	-2.02982100	3.99793200	-1.94425900
H	-1.90064000	4.16387400	-0.87405100
C	-3.10651800	3.21962400	-2.41912200
C	-3.23322800	3.00296200	-3.81001000
H	-4.06683200	2.40673300	-4.18569000
C	-2.29587100	3.54126800	-4.70819600
H	-2.40463800	3.35986300	-5.77917400
C	-4.56994100	1.62397200	0.94879800
C	-4.12722800	2.48823700	1.98106000
H	-3.22555500	3.07836300	1.84250300
C	-4.86623300	2.56300800	3.16295900
C	-6.03052300	1.81352000	3.39316600
H	-6.59393500	1.89974600	4.31859500
C	-6.42378300	0.95144900	2.36341300
C	-5.72629300	0.83717500	1.15603200
H	-6.07141600	0.15023200	0.38708400
Rh	0.03590600	-0.06717000	0.89868400
Rh	0.09622400	0.19604800	-1.59770600
O	0.84348800	2.09993600	-1.38668400
O	-0.64575600	-1.71662400	-1.80023200
O	1.88622100	-1.03085100	0.69991900
O	1.07090300	1.75856900	0.90350400
O	-0.94190500	-1.92193800	0.50204300
C	1.36803900	2.38360000	-0.21670000
C	-1.17634800	-2.28500900	-0.75155300
C	2.56543700	-0.89300000	-0.43588200
C	2.46428700	3.43702900	-0.16204500
C	-2.20540000	-3.38127600	-1.00323600
C	4.00885000	-1.31979000	-0.42068200
C	2.87777200	3.89777100	1.23900000
C	-2.59940700	-4.29564100	0.15147000
C	4.90657700	-0.59805100	-1.46160900
H	2.36340700	3.40085800	2.05873300
H	-2.04817400	-4.15650300	1.08045900
H	4.38551500	0.11369400	-2.09972400
H	3.93285300	4.10370400	1.41692600
H	-3.65247700	-4.54748800	0.27240900
H	5.89571700	-0.30191900	-1.11630500
C	2.12949700	4.93669100	0.39319500
C	-1.83765400	-4.96629300	-1.01095700
C	4.61293500	-2.07172400	-1.71571600
C	-1.85433100	6.29702900	1.55923700

C	2.10263900	-6.63844300	-0.10275400
C	2.02878700	-3.07351600	-5.07164900
H	-2.82684000	6.66871700	1.88722200
H	3.07218000	-7.07326900	0.14373400
H	1.39302700	-3.32737900	-5.92194900
C	-1.13295500	6.96869600	0.55505300
C	1.72892800	-5.38946700	0.42849100
C	1.73760600	-3.58012900	-3.79174500
H	-1.54725100	7.86216800	0.08503800
H	2.41661200	-4.84968100	1.08220000
H	0.87469000	-4.23057600	-3.63812800
C	0.13753300	6.50944800	0.16741900
C	0.47826400	-4.82395200	0.11665300
C	2.55112400	-3.24498100	-2.69405000
H	0.70382400	7.06726700	-0.57594800
H	0.21884500	-3.84538900	0.51198700
H	2.29880100	-3.62565600	-1.70339600
C	0.71331700	5.35583300	0.76084600
C	-0.43415100	-5.49309700	-0.73877700
C	3.67008400	-2.40180300	-2.86487300
C	-0.02986300	4.67982700	1.75861000
C	-0.03999900	-6.74798900	-1.26830500
C	3.96446000	-1.90691200	-4.15433900
H	0.36617500	3.79546000	2.24417100
H	-0.72246300	-7.28803600	-1.92040800
H	4.83110300	-1.25837900	-4.29512900
C	-1.29427600	5.15112800	2.15586800
C	1.21056500	-7.31063300	-0.95486900
C	3.14616300	-2.23467000	-5.24974100
H	-1.82868800	4.63158400	2.95231400
H	1.48115400	-8.28007300	-1.37647300
H	3.37991000	-1.83650900	-6.23869600
C	3.51254800	3.28963300	-1.25307100
C	-3.28584900	-2.92535600	-1.97611400
C	4.54592400	-1.57825900	0.96904300
C	3.13180000	3.23131200	-2.62126700
C	-2.94504100	-2.56716000	-3.30525400
C	4.72403600	-2.88695200	1.47148900
H	2.07942700	3.24817900	-2.88747000
H	-1.90591200	-2.57824700	-3.61865000
H	4.56081500	-3.74440300	0.82478100
C	4.12169200	3.11642600	-3.59892900
C	-3.95656800	-2.16625900	-4.18026400
C	5.15139400	-3.05234400	2.79442800

C	5.49413300	3.05165600	-3.30536800
C	-5.30950300	-2.09069100	-3.80810600
C	5.41607800	-1.97711000	3.65378400
H	6.24601300	2.97267200	-4.08639900
H	-6.08071600	-1.78463700	-4.51069300
H	5.74925100	-2.12954600	4.67723700
C	5.83517500	3.09570800	-1.94803100
C	-5.60779500	-2.42800600	-2.48193900
C	5.23001000	-0.69037900	3.12096500
C	4.88721300	3.20768100	-0.92404300
C	-4.63403200	-2.83634700	-1.56147000
C	4.80711800	-0.46712900	1.80752300
H	5.21234500	3.23347200	0.11246100
H	-4.91684800	-3.07351600	-0.53877800
H	4.65070400	0.54301600	1.43280200
C	2.99019300	6.04346800	-0.19954900
C	3.85323100	6.78125900	0.64101800
C	2.88984800	6.41056900	-1.56148200
C	4.61350200	7.84894200	0.12969900
H	3.92063800	6.52159000	1.69884600
C	3.64819500	7.47900400	-2.07327400
H	2.22692400	5.85013400	-2.22107800
C	4.51516300	8.19896000	-1.22964200
H	5.27748100	8.40718300	0.79174300
H	3.56577900	7.74435500	-3.12859900
H	5.10692900	9.02452100	-1.62782700
C	-2.65572500	-5.78765300	-1.99379400
C	-3.72164400	-6.60434400	-1.55983100
C	-2.31199600	-5.79029700	-3.36679400
C	-4.44565100	-7.38812600	-2.47891000
H	-3.98131600	-6.63676100	-0.50072000
C	-3.03284600	-6.57219400	-4.28498200
H	-1.47677000	-5.17739000	-3.70914400
C	-4.10662800	-7.37043000	-3.84350600
H	-5.26885800	-8.01209600	-2.12746700
H	-2.76064100	-6.55673100	-5.34152800
H	-4.66992800	-7.97373800	-4.55669900
O	-1.86332600	0.79288700	-1.50178700
O	2.07702500	-0.39191600	-1.53913800
C	-5.25915100	3.70103500	-1.13320800
C	-6.58542400	3.55466700	-1.59763600
C	-4.93290100	4.84981600	-0.37435300
C	-7.56560000	4.51925700	-1.29803000
H	-6.85213000	2.69131700	-2.20836700

C	-5.91198100	5.81115500	-0.07209800
H	-3.91129200	4.99802900	-0.02557200
C	-7.23392900	5.64837300	-0.52912300
H	-8.58365100	4.38824600	-1.66874600
H	-5.64245000	6.68820600	0.51918600
H	-7.99327900	6.39528000	-0.29262200
C	5.71413500	-3.10651900	-1.48634200
C	7.02576000	-2.74672800	-1.09700500
C	5.43100500	-4.48337300	-1.67623600
C	8.01424400	-3.72570600	-0.88893300
H	7.29135800	-1.69972400	-0.95804800
C	6.41719000	-5.46134500	-1.46293000
H	4.43943600	-4.78264100	-2.01350700
C	7.71468600	-5.08811400	-1.06494200
H	9.01911200	-3.41967400	-0.59353600
H	6.17501400	-6.51401700	-1.61985600
H	8.48246300	-5.84630300	-0.90444200
Br	-8.07182700	-0.16649400	2.63691700
Br	-4.27044300	3.81631400	4.61603100
Br	3.56912300	3.05166600	-5.52491700
Br	7.77894400	2.98695500	-1.45053000
Br	5.57514300	0.88392500	4.31205300
Br	5.39620500	-4.91505700	3.50342800
Br	-3.46562800	-1.68364100	-6.06041800
Br	-7.51522800	-2.31220200	-1.87083900
C	-0.06066100	-0.23052600	3.05845500
C	1.23426900	-1.72843000	3.87888900
H	2.09711500	-1.07299800	3.83770200
C	0.66612700	-2.28544900	5.12468400
C	0.75237100	0.88273900	3.67853600
F	0.10169900	2.11999400	3.49649300
F	0.98105000	0.80143500	5.09010500
F	2.05488400	0.99565800	3.15441800
C	-1.36979400	-0.49702100	3.71543100
C	-1.77307100	0.12901200	4.93636900
C	-2.27558000	-1.42402300	3.12300400
C	-3.02636000	-0.13638700	5.50375200
H	-1.09983700	0.81518700	5.43799500
C	-3.51721900	-1.70078500	3.71084400
H	-1.99708800	-1.89497800	2.18532900
C	-3.90391800	-1.05671300	4.90149600
H	-3.31388100	0.36951900	6.42712600
H	-4.19599100	-2.41035300	3.23240400
H	-4.87543700	-1.26779900	5.35167800

C	1.06473200	-2.74796900	2.89589900
C	0.08579100	-3.55147400	4.80233600
N	0.34743200	-3.78261700	3.41553400
H	1.41192900	-2.70464300	1.87250900
H	0.07224800	-4.61303700	2.88203100
C	0.58087000	-1.80975800	6.44407900
C	-0.05135600	-2.61326800	7.41064300
C	-0.61479200	-3.86546700	7.07102300
C	-0.55735700	-4.35306700	5.75147900
H	0.98462500	-0.83241800	6.69440800
H	-0.11656000	-2.26188500	8.44107200
H	-1.10328500	-4.46394200	7.84059500
H	-0.99262200	-5.31768500	5.48902200

IntIII-S' (G = -5290.124087)

O	-1.90485500	0.94889200	0.84188300
C	-2.53622100	1.04772900	-0.31127300
C	-3.96584700	1.53138400	-0.32517300
C	-4.77626300	1.10123300	-1.57462900
H	-4.23146000	0.47355300	-2.27715000
H	-5.82391700	0.85039300	-1.41571700
C	-4.37399900	2.56821700	-1.49974900
C	-1.49841800	4.10478700	-4.38130600
H	-0.79179500	4.49858500	-5.11471800
C	-1.33769100	4.39420000	-3.01388400
H	-0.50577500	5.01215900	-2.67365700
C	-2.24506800	3.88661700	-2.06674600
H	-2.08929600	4.09958800	-1.00835800
C	-3.32655400	3.07945200	-2.47806200
C	-3.48804900	2.79941200	-3.85372800
H	-4.32505500	2.17908100	-4.17958300
C	-2.57872500	3.30359900	-4.79942200
H	-2.71321000	3.07300800	-5.85794900
C	-4.66973700	1.64737100	1.00546800
C	-4.18446900	2.54335300	1.99154200
H	-3.27943400	3.11329100	1.80503100
C	-4.87626900	2.66160600	3.19934300
C	-6.04173700	1.93545000	3.49440200
H	-6.56811200	2.05579400	4.43776900
C	-6.48523200	1.04942500	2.50461700
C	-5.82872100	0.88501900	1.27928500
H	-6.20590700	0.17345800	0.54918100
Rh	-0.00889900	0.02643900	0.92456200
Rh	-0.08259900	0.12384800	-1.57973800

O	0.72000400	2.03923500	-1.44889800
O	-0.86330400	-1.78846500	-1.55855200
O	1.85547900	-0.99223900	0.60638700
O	1.12291600	1.77165600	0.83336900
O	-1.08389100	-1.76919400	0.76865600
C	1.32970100	2.35847900	-0.33051900
C	-1.36884400	-2.23720200	-0.43033900
C	2.43614600	-0.95510500	-0.58906400
C	2.41971800	3.41880700	-0.38774700
C	-2.41112100	-3.33948000	-0.53631300
C	3.86072900	-1.43311600	-0.71328100
C	2.88719500	3.98223800	0.95655400
C	-2.81348900	-4.02725900	0.76660700
C	4.63982500	-0.84987100	-1.92199200
H	2.40750300	3.55621500	1.83518200
H	-2.36010300	-3.63836500	1.67532300
H	4.06300800	-0.17838000	-2.55569000
H	3.94547600	4.21440900	1.07345000
H	-3.85464400	-4.33195000	0.86970900
H	5.67381100	-0.56536000	-1.73221900
C	2.08423400	4.94829300	0.07358000
C	-1.97457500	-4.87267900	-0.20503500
C	4.27517300	-2.32815600	-1.99263600
C	-1.88296400	6.28361600	1.33095100
C	2.11550300	-6.03860000	0.82567200
C	1.29678800	-3.56229200	-4.91182500
H	-2.85403200	6.64658800	1.67271900
H	3.11905600	-6.36349000	1.10604600
H	0.56210500	-3.87802300	-5.65490900
C	-1.21331900	6.92171600	0.27009000
C	1.46140900	-5.02757800	1.55373800
C	1.13018900	-3.90863000	-3.55868300
H	-1.66617000	7.78058500	-0.22808000
H	1.95702000	-4.56943600	2.41177600
H	0.26601500	-4.49431700	-3.24224700
C	0.05219300	6.47105400	-0.14331100
C	0.15973700	-4.61611500	1.21645100
C	2.06985600	-3.49430300	-2.59721500
H	0.57506600	6.99960200	-0.93819200
H	-0.31292200	-3.82944600	1.79897400
H	1.91118500	-3.74441700	-1.54686200
C	0.67830600	5.36325000	0.48560500
C	-0.53101700	-5.22072000	0.13424900
C	3.19259800	-2.73154100	-2.98282700

C	-0.01074500	4.72561300	1.54550000
C	0.13967000	-6.23983300	-0.59100200
C	3.36006000	-2.39399800	-4.34430600
H	0.42184800	3.88238200	2.07049100
H	-0.38065400	-6.74232400	-1.40401500
H	4.22878000	-1.80714800	-4.64858000
C	-1.27394100	5.18270600	1.96152500
C	1.44481900	-6.63891000	-0.25554600
C	2.41551000	-2.80083900	-5.30242700
H	-1.76454500	4.67536000	2.79190800
H	1.92692900	-7.43364000	-0.82750600
H	2.55194700	-2.52502400	-6.34952100
C	3.42389200	3.20147200	-1.50817000
C	-3.45974800	-3.08067700	-1.60611200
C	4.59963000	-1.59322800	0.59224000
C	2.98410900	3.02951800	-2.84892500
C	-3.08293300	-2.86644200	-2.95864800
C	4.70979700	-2.85067200	1.23304200
H	1.92009800	3.01555200	-3.06527300
H	-2.03206800	-2.85312500	-3.22970300
H	4.28179700	-3.73559500	0.76976000
C	3.93089200	2.84251200	-3.85760400
C	-4.07545400	-2.62816700	-3.91090600
C	5.40436800	-2.92482400	2.44495400
C	5.31576000	2.81061500	-3.62144000
C	-5.44502100	-2.57942700	-3.60278600
C	6.00429000	-1.81936000	3.06476900
H	6.03320000	2.67421500	-4.42666300
H	-6.19912900	-2.39840400	-4.36461500
H	6.55382600	-1.90943100	3.99862100
C	5.71578600	2.96680200	-2.28882400
C	-5.78114500	-2.77285700	-2.25705400
C	5.86108600	-0.58502900	2.40905000
C	4.81303200	3.15621300	-1.23548600
C	-4.82993200	-3.01612400	-1.25895100
C	5.17912700	-0.44976900	1.19491900
H	5.18370400	3.27460400	-0.22075700
H	-5.14435400	-3.14181500	-0.22616900
H	5.08959500	0.51935500	0.70608700
C	2.89174000	6.02357700	-0.63777600
C	3.78475100	6.83166800	0.10051000
C	2.71377700	6.28970000	-2.01520500
C	4.49882900	7.86962800	-0.52581100
H	3.91142300	6.65036500	1.16921700

C	3.42593400	7.32824900	-2.64195300
H	2.02542300	5.67484900	-2.59562700
C	4.32351200	8.11884700	-1.89956700
H	5.18663300	8.48356000	0.05806400
H	3.28356300	7.51575800	-3.70754100
H	4.87923800	8.92136900	-2.38685400
C	-2.73300600	-5.95085300	-0.96553900
C	-3.54274600	-6.86509900	-0.25482600
C	-2.59061000	-6.11518700	-2.36286300
C	-4.20866700	-7.90730400	-0.92511600
H	-3.64473300	-6.75951800	0.82651000
C	-3.25456200	-7.15791100	-3.03431900
H	-1.96988900	-5.41723400	-2.92484700
C	-4.06831800	-8.05519500	-2.31742600
H	-4.83357400	-8.60207300	-0.36155300
H	-3.14163000	-7.26437600	-4.11451500
H	-4.58799200	-8.86031300	-2.83893400
O	-2.01731600	0.74794200	-1.48111000
O	1.86513200	-0.50626000	-1.66993100
C	-5.45498000	3.58793200	-1.16551600
C	-6.78557700	3.40284400	-1.60242300
C	-5.13431000	4.77171400	-0.45991700
C	-7.77548400	4.36495800	-1.32750700
H	-7.04778100	2.51026800	-2.17181800
C	-6.12300800	5.73047600	-0.18172800
H	-4.10924400	4.94715700	-0.13403700
C	-7.44906900	5.52962400	-0.61109700
H	-8.79707200	4.20401300	-1.67608000
H	-5.85849500	6.63474000	0.36945300
H	-8.21602200	6.27448500	-0.39333300
C	5.36470000	-3.37934000	-1.78807300
C	6.73429500	-3.04255600	-1.68440200
C	5.00751200	-4.74980500	-1.71294600
C	7.71206000	-4.03627100	-1.49347900
H	7.05274200	-2.00389200	-1.76416700
C	5.98336400	-5.74139500	-1.51691700
H	3.96293000	-5.03622900	-1.82955000
C	7.34193700	-5.38960900	-1.40259700
H	8.76278500	-3.74998900	-1.42406200
H	5.68447300	-6.78999700	-1.46678000
H	8.10086700	-6.15987800	-1.25797700
Br	-8.14079700	-0.02837700	2.86559000
Br	-4.19537500	3.92894300	4.59962700
Br	3.29495100	2.61608400	-5.74469400

Br	7.68168400	2.91434000	-1.87275100
Br	6.67105100	1.03481000	3.25979200
Br	5.52327500	-4.70829300	3.38505100
Br	-3.52984800	-2.34189900	-5.81942300
Br	-7.71878500	-2.68498100	-1.73653300
C	-0.00694000	0.03792500	3.26725800
C	1.37242500	-0.41903700	3.87824100
H	2.06339400	0.41858000	3.62186000
C	1.56216500	-0.70497000	5.39511800
C	-0.18761700	1.48614600	3.65924300
F	-1.13771100	2.21090700	2.92416400
F	-0.60454600	1.69738500	5.01117900
F	1.02840700	2.22496900	3.54170700
C	-1.16256500	-0.85027200	3.65572100
C	-2.50591300	-0.38502900	3.60141600
C	-0.95934200	-2.19848400	4.04607400
C	-3.57678000	-1.22838200	3.93364100
H	-2.70917200	0.63030900	3.27830400
C	-2.03400100	-3.04577600	4.36963600
H	0.05081300	-2.60234900	4.10117100
C	-3.35411200	-2.56348700	4.32202800
H	-4.59290800	-0.83475500	3.88415800
H	-1.83425100	-4.07586500	4.67418600
H	-4.19145500	-3.21109900	4.58737400
C	2.03776100	-1.61271200	3.26065400
C	2.36691400	-1.86369600	5.52460200
N	2.62273900	-2.35858000	4.19506200
H	2.13918200	-1.76626400	2.18110400
H	3.21988500	-3.17318500	3.99299600
C	1.16265600	-0.03102800	6.55584000
C	1.57440900	-0.53810000	7.80601600
C	2.37898900	-1.69416300	7.90713500
C	2.79180200	-2.38354600	6.75122800
H	0.53016700	0.84596200	6.47621800
H	1.25788300	-0.02726800	8.71599000
H	2.68131500	-2.06169200	8.88779500
H	3.41140500	-3.27847400	6.81451200

TSHI-S' (G = -5290.117321)

O	-1.89904400	0.96146800	0.74378200
C	-2.45514000	1.01466200	-0.45423700
C	-3.86155200	1.52848100	-0.60314100
C	-4.57712900	1.04161200	-1.89280100
H	-3.99809100	0.34880500	-2.49996700

H	-5.64308900	0.83478600	-1.81494700
C	-4.13700600	2.49713500	-1.88035200
C	-0.98437800	3.78527500	-4.59015600
H	-0.20815800	4.11799400	-5.28225000
C	-0.98884300	4.23601400	-3.25723400
H	-0.21631900	4.91962000	-2.90233800
C	-1.98727200	3.80884200	-2.36378800
H	-1.96216000	4.15412100	-1.32973100
C	-2.99655800	2.92131600	-2.79394200
C	-2.99245500	2.47966900	-4.13651100
H	-3.77280500	1.79770400	-4.47923600
C	-1.99154900	2.90319300	-5.02789700
H	-1.99936600	2.54920700	-6.06063600
C	-4.66942500	1.76327700	0.65147100
C	-4.19508100	2.65228700	1.64973600
H	-3.21335100	3.10573000	1.54848000
C	-5.00683500	2.92638500	2.75216600
C	-6.27535900	2.35535500	2.93801600
H	-6.88992900	2.59357400	3.80199100
C	-6.69973800	1.46125900	1.94962100
C	-5.93297300	1.15141300	0.82184200
H	-6.31164100	0.44835200	0.08493200
Rh	-0.05675200	-0.02127400	0.92542600
Rh	0.08577900	0.03279900	-1.53761000
O	0.84435000	1.95190600	-1.46063600
O	-0.65248900	-1.88984500	-1.56911100
O	1.81688400	-1.00498500	0.82978900
O	1.06393300	1.74387400	0.84583700
O	-1.10327700	-1.84072300	0.71870100
C	1.36394500	2.31070000	-0.30431100
C	-1.25348200	-2.34454900	-0.49126000
C	2.53822600	-0.92819400	-0.28038000
C	2.45612400	3.36916100	-0.29919800
C	-2.21275500	-3.50059900	-0.70120600
C	4.01166100	-1.22976900	-0.17936600
C	2.80341000	3.94606000	1.07830700
C	-2.91191500	-4.10323700	0.52319100
C	4.88291100	-0.48256300	-1.22804600
H	2.23971300	3.52366300	1.90845800
H	-2.61132100	-3.70209200	1.48982100
H	4.32323000	0.13574000	-1.92714500
H	3.84869800	4.16083200	1.29817100
H	-3.96760300	-4.35296500	0.42245600
H	5.82267400	-0.06866100	-0.86797100

C	2.10759600	4.91407100	0.11285200
C	-1.87887200	-4.98590500	-0.19482500
C	4.75376400	-1.98907600	-1.40331600
C	-1.91459700	6.39266600	0.94891900
C	1.70049400	-6.08029000	2.03896200
C	2.36937200	-3.41909900	-4.75503500
H	-2.89906900	6.79641600	1.19239300
H	2.58646500	-6.36863300	2.60616300
H	1.77601300	-3.77442100	-5.59916900
C	-1.14042700	6.96507100	-0.07757200
C	1.76073700	-5.00838300	1.13156800
C	2.15106400	-3.94138300	-3.46634900
H	-1.52495400	7.81167100	-0.64877200
H	2.69527600	-4.46390800	0.99286800
H	1.38937900	-4.70802500	-3.30712900
C	0.14402600	6.46818800	-0.35761700
C	0.61977500	-4.62799400	0.39052000
C	2.90726500	-3.47201900	-2.37758900
H	0.75044300	6.95280400	-1.12036400
H	0.69493400	-3.81723800	-0.33253000
H	2.72416400	-3.87131200	-1.37959100
C	0.68072500	5.37310900	0.36906900
C	-0.60268400	-5.30978600	0.56649900
C	3.89151100	-2.47645100	-2.55907400
C	-0.11476600	4.79670400	1.38644600
C	-0.65300900	-6.39316500	1.47960600
C	4.11707100	-1.97123100	-3.85758600
H	0.24126600	3.95317400	1.96586300
H	-1.58860500	-6.94177500	1.59912400
H	4.87908700	-1.20528600	-4.01102400
C	-1.39304400	5.30604100	1.67616400
C	0.48721400	-6.77812100	2.20499700
C	3.35711600	-2.43404300	-4.94685100
H	-1.96702000	4.86174400	2.48947800
H	0.43194600	-7.62144600	2.89546700
H	3.53433300	-2.02409200	-5.94256200
C	3.54521200	3.15218300	-1.33677700
C	-3.00351900	-3.36367900	-1.99093000
C	4.50523200	-1.34832700	1.24511500
C	3.20998600	2.93782000	-2.70192500
C	-2.36943700	-3.53313700	-3.24509700
C	4.82476100	-2.59491400	1.82700900
H	2.16590600	2.87549100	-2.99376800
H	-1.31131300	-3.77026100	-3.29439600

H	4.80481700	-3.49857100	1.22455200
C	4.23410700	2.78715400	-3.63903400
C	-3.12191700	-3.36672600	-4.40988900
C	5.20172000	-2.63823800	3.17498900
C	5.59846700	2.83516700	-3.30785000
C	-4.48626600	-3.03161700	-4.40157700
C	5.28169500	-1.49589100	3.98316500
H	6.37708600	2.72709800	-4.05865700
H	-5.05187300	-2.91532500	-5.32266000
H	5.57925600	-1.55265600	5.02724300
C	5.89548000	3.03305400	-1.95351600
C	-5.07693200	-2.85677100	-3.14390400
C	4.95952900	-0.27193800	3.37292900
C	4.91243300	3.18658200	-0.96894600
C	-4.37015400	-3.00940900	-1.94395500
C	4.57814200	-0.17140300	2.03173600
H	5.20593600	3.33781500	0.06597000
H	-4.86480900	-2.84923800	-0.98813600
H	4.30859400	0.78969200	1.59660800
C	3.00698800	5.96193200	-0.52807200
C	3.83156000	6.76522500	0.29064900
C	2.97737600	6.21355000	-1.91931100
C	4.62368600	7.78451000	-0.26903900
H	3.84334300	6.59576400	1.36868500
C	3.76777600	7.23328600	-2.47948200
H	2.34532500	5.60056600	-2.56228700
C	4.59611300	8.01942500	-1.65613800
H	5.25680800	8.39502200	0.37685500
H	3.74018200	7.40973200	-3.55605500
H	5.21233600	8.80747400	-2.09144900
C	-2.34204300	-6.11814200	-1.09796800
C	-3.63877000	-6.67096600	-1.02617000
C	-1.42773600	-6.65336600	-2.03824400
C	-4.01907200	-7.72128000	-1.88336300
H	-4.35501400	-6.29237100	-0.29671800
C	-1.80743500	-7.69788300	-2.89594000
H	-0.41380600	-6.25165900	-2.08314900
C	-3.10839100	-8.23408000	-2.82348800
H	-5.02514800	-8.13758500	-1.81253500
H	-1.09160700	-8.09534000	-3.61723300
H	-3.40496600	-9.04559800	-3.48930700
O	-1.86248900	0.63263000	-1.56965200
O	2.05815500	-0.55752800	-1.44118500
C	-5.21924000	3.55579600	-1.71493300

C	-6.47049000	3.40041000	-2.35268400
C	-4.97494200	4.74103600	-0.98322000
C	-7.46063900	4.39492700	-2.24894000
H	-6.66648300	2.50402700	-2.94300400
C	-5.96520200	5.73241700	-0.87589600
H	-4.01111200	4.89081400	-0.49784300
C	-7.21319200	5.56234800	-1.50527900
H	-8.42019700	4.25733500	-2.75022900
H	-5.76263300	6.63735400	-0.30023100
H	-7.98134000	6.33236700	-1.41918900
C	5.95190700	-2.88088600	-1.07170100
C	7.14781200	-2.36754300	-0.51251800
C	5.88948000	-4.27298300	-1.33395100
C	8.23075300	-3.21289700	-0.21423900
H	7.24749800	-1.30392300	-0.30230900
C	6.97010600	-5.11904400	-1.02988600
H	4.99921900	-4.68759900	-1.80375600
C	8.14674500	-4.59424300	-0.46551500
H	9.14076700	-2.78807900	0.21235600
H	6.89456700	-6.18621800	-1.24530000
H	8.98806600	-5.24870200	-0.23363500
Br	-8.49887500	0.59040100	2.16064600
Br	-4.36656300	4.21980600	4.14861500
Br	3.74417600	2.50653800	-5.56306800
Br	7.82545700	3.09348800	-1.40169700
Br	5.04092700	1.38953300	4.48848000
Br	5.65145200	-4.41323600	3.99363600
Br	-2.22693900	-3.61871900	-6.18414100
Br	-7.02307400	-2.37250700	-3.06091300
C	-0.44098200	0.02909600	3.74717000
C	0.45691100	-0.86696000	4.74248900
H	1.12586500	-0.28086500	5.37895900
C	-0.26688700	-2.03567900	5.37421600
C	0.10769300	1.40113400	3.82183700
F	-0.61086500	2.33710600	3.06114500
F	0.12561400	1.94169300	5.14928600
F	1.47495100	1.45685500	3.43993500
C	-1.92512900	-0.12328100	4.00068700
C	-2.49214300	0.55293000	5.11365900
C	-2.74065200	-0.99949700	3.25615700
C	-3.83663400	0.35660300	5.46384200
H	-1.86383000	1.23106500	5.68748700
C	-4.08611900	-1.20154300	3.61776300
H	-2.32540800	-1.50364200	2.38814700

C	-4.63939300	-0.53078900	4.72215300
H	-4.25453400	0.89170100	6.31895100
H	-4.70576600	-1.88244200	3.02961700
H	-5.68253400	-0.69307400	4.99923300
C	0.95498400	-1.42220500	3.44894100
C	-0.24053000	-3.11873000	4.45562600
N	0.50782700	-2.71011100	3.30649300
H	1.72749400	-1.01636300	2.81125200
H	0.58577000	-3.24554900	2.43411600
C	-0.89601500	-2.18827800	6.61109400
C	-1.50931900	-3.42566200	6.91323700
C	-1.48861900	-4.48458700	5.98424000
C	-0.85004600	-4.34640400	4.73311600
H	-0.93049300	-1.36481100	7.32431900
H	-2.00940400	-3.55868600	7.87301600
H	-1.96848200	-5.43169200	6.23519800
H	-0.81426000	-5.16606900	4.01725800

Rh₂(S-*di*BrTPCP)₄-catalysed C3-*gem*-difluoroolefination:

IntIV' (G = -1133.201453)

F	-1.73446500	-2.87473400	0.80978900
F	-2.87604700	-1.10054300	1.61128900
C	-2.14595400	-1.56037700	0.53163900
C	-1.28111400	0.73533000	-0.09638100
C	-0.95554700	-0.69784500	0.22286000
C	-0.93357800	1.80071800	0.76040400
H	-0.38714900	1.59681500	1.67960300
C	-1.27844700	3.12195800	0.42257100
H	-1.00489500	3.93920500	1.09139800
C	-1.99842800	1.00953800	-1.28637500
H	-2.32493700	0.17757300	-1.90899200
C	-1.97432400	3.39083000	-0.77060600
H	-2.23762000	4.41699500	-1.03101100
C	-2.33882400	2.33051500	-1.62217800
H	-2.89515600	2.53067200	-2.53911400
F	-3.00981800	-1.63165900	-0.56676200
C	3.60884200	1.55209700	0.40503500
C	3.29189400	1.19420600	1.72957700
C	2.23633100	0.29361000	1.99660500
C	1.50825900	-0.23599400	0.92369600
C	1.85758300	0.10676500	-0.40676600
C	2.89684400	1.00476400	-0.68527800
H	4.42546200	2.24841000	0.21129800

H	3.86471100	1.61549200	2.55593100
H	1.98545200	0.02500700	3.02395100
H	3.15754500	1.27312200	-1.71084300
C	0.35603200	-1.19431800	0.90619300
C	0.10074000	-1.48211300	-0.59447300
N	1.10215600	-0.69556600	-1.36358000
H	-0.13477000	-2.47635700	-0.96667700
H	0.26767100	-1.98139500	1.65035200
H	0.70378000	-0.16820300	-2.16019200
Na	3.03653500	-2.06727200	-1.74785400
H	4.34406600	-3.34405600	-2.43224100

TSIV' (G = -1133.163301)

F	-1.73482700	-2.87727300	0.32588100
F	-2.61095100	-1.28698800	1.66299800
C	-2.07411400	-1.52224200	0.40854400
C	-1.20673900	0.82298100	0.03682300
C	-0.88797700	-0.65093700	0.10241200
C	-0.72281500	1.73248200	1.00054800
H	-0.08534400	1.36730400	1.80388000
C	-1.04680800	3.09910300	0.91839200
H	-0.66450200	3.79169600	1.67020100
C	-2.04422600	1.30436900	-0.99889900
H	-2.47159300	0.59176100	-1.70242600
C	-1.86056900	3.57320200	-0.12701600
H	-2.10785500	4.63424900	-0.19165900
C	-2.36295300	2.67016700	-1.08353100
H	-3.01006800	3.02808100	-1.88658900
F	-3.10691500	-1.32185500	-0.52761600
C	3.77204300	1.43858700	0.00343000
C	3.57836400	0.91140900	1.29538800
C	2.51411400	0.01721800	1.55428000
C	1.62792800	-0.33323700	0.51754600
C	1.88025800	0.16925500	-0.80191000
C	2.92602700	1.06530200	-1.06593500
H	4.58983500	2.13667000	-0.18250000
H	4.24832500	1.20392900	2.10534100
H	2.34606100	-0.37616500	2.55874400
H	3.08585800	1.47064400	-2.06721800
C	0.46354900	-1.28650600	0.55090600
C	0.01155000	-1.28772200	-0.97429600
N	0.98886400	-0.46924100	-1.74599100
H	-0.32891700	-2.19745700	-1.48246100
H	0.97729800	-2.86233800	0.96362200

H	0.63474600	0.10951600	-2.52373100
Na	2.18944700	-2.45178200	-0.80969300
H	1.44864200	-3.60915700	0.89188800

IntV' (G = -1132.053559)

F	2.79281800	-1.65820100	0.69638000
F	2.64358100	-0.83348000	-1.38105200
C	2.34134300	-0.46643400	0.01056900
C	0.50115900	1.21687600	-0.05645600
C	0.92191900	-0.19574100	0.25191300
C	-0.35194100	1.52147500	-1.13982000
H	-0.75885000	0.70957300	-1.73980900
C	-0.70140100	2.85499400	-1.42096400
H	-1.36553600	3.07406300	-2.25888300
C	1.00343600	2.27981400	0.73451400
H	1.68667200	2.05407200	1.55371500
C	-0.20159300	3.90286500	-0.62599200
H	-0.47529700	4.93657300	-0.84466300
C	0.65480200	3.61146700	0.45302000
H	1.05185900	4.41978900	1.07015500
F	3.24317800	0.53216800	0.31271400
C	-4.14886300	-0.49005600	0.03728300
C	-3.66080300	-1.19943800	-1.07810000
C	-2.30347700	-1.59263600	-1.12947200
C	-1.44204600	-1.26717400	-0.07426100
C	-1.96330900	-0.57633800	1.06923800
C	-3.30694400	-0.16923700	1.12366600
H	-5.19761800	-0.18847000	0.07051000
H	-4.33164600	-1.44375000	-1.90331400
H	-1.91595100	-2.13986800	-1.99381300
H	-3.69760200	0.37837500	1.98306000
C	0.01891600	-1.56680000	0.10582000
C	0.30461700	-0.96048400	1.49900100
N	-0.94227700	-0.43071400	2.02064800
H	0.99269700	-1.38420900	2.23029300
H	-0.98849100	0.23710800	2.79358800
Na	1.58951200	-2.85650600	-0.93795500

TSV' (G = -1132.045709)

F	-2.67383800	-1.69567100	-0.81954000
F	-2.68876100	-1.28123900	1.38671400
C	-2.33540700	-0.55438500	0.07391800
C	-0.61075900	1.29059000	0.11836400
C	-0.97609800	-0.14410500	-0.03552700

C	0.52741500	1.70062600	0.86325500
H	1.15358400	0.94702000	1.33247400
C	0.85918500	3.05957300	0.99643700
H	1.74159900	3.33961900	1.57568400
C	-1.40630200	2.31491800	-0.47668700
H	-2.29186800	2.03449800	-1.04162300
C	0.06255900	4.05511500	0.40236700
H	0.32166600	5.10987200	0.50903100
C	-1.07659600	3.67016700	-0.33080300
H	-1.70739400	4.42956400	-0.79826400
F	-3.35637900	0.35804000	-0.05059700
C	4.21759700	-0.50004600	0.08945700
C	3.63037300	-1.05153000	1.24738100
C	2.26014700	-1.39162300	1.26832500
C	1.47014500	-1.16154400	0.13101200
C	2.09147200	-0.60574500	-1.03508400
C	3.45009200	-0.27112700	-1.07308700
H	5.27973600	-0.25052400	0.08612100
H	4.24352200	-1.21870200	2.13447100
H	1.80759800	-1.81650900	2.16789500
H	3.90737700	0.16012400	-1.96487600
C	0.02094400	-1.41535700	-0.14586500
C	-0.12086200	-0.97673100	-1.55320300
N	1.09341400	-0.48800300	-2.04120200
H	-0.93908600	-1.20132600	-2.22752100
H	1.21793300	0.02908100	-2.91509300
Na	-1.48192600	-2.97178600	0.68539700

49' (G = -865.492295)

F	-0.67568400	3.35505300	-0.37047500
C	-1.37237000	2.17476200	-0.29573800
C	-1.67108500	-0.24445300	0.12772800
C	-0.81761400	0.97973300	-0.00351600
C	-1.31181500	-1.24895700	1.06223400
H	-0.41124300	-1.11642500	1.66026000
C	-2.09969900	-2.40153300	1.21598700
H	-1.80607000	-3.16135900	1.94228700
C	-2.85192500	-0.42736000	-0.63808900
H	-3.15663900	0.34568300	-1.33897400
C	-3.26161500	-2.57741200	0.44165200
H	-3.87063300	-3.47509700	0.55883400
C	-3.63286000	-1.58360500	-0.48370200
H	-4.53339100	-1.70849500	-1.08758400
F	-2.70327200	2.40054700	-0.53670100

C	3.82767400	-1.79529900	-0.60578300
C	2.53667200	-2.21052700	-1.02727400
C	1.40668300	-1.41293300	-0.80353000
C	1.56128700	-0.17140900	-0.14175400
C	2.88265100	0.23962000	0.26291300
C	4.01428500	-0.56611700	0.04107800
H	4.68793000	-2.43973500	-0.79248100
H	2.42573100	-3.16895700	-1.53670300
H	0.42035000	-1.74071500	-1.12688300
H	5.00803300	-0.24331300	0.35552700
C	0.64304800	0.90868600	0.23385100
C	1.42262100	1.90801300	0.81653300
N	2.76350100	1.50601600	0.84491000
H	1.11278600	2.87701400	1.18411800
H	3.53360900	2.06163700	1.21626900

TSII-S-TES (G = -5816.583955)

C	1.84908500	-1.89668400	0.33255000
C	3.14715000	-2.65678000	0.33120500
C	3.71809700	-2.97617300	1.73803100
H	4.79565200	-2.86868100	1.85234900
H	3.10862300	-2.63141600	2.57123700
C	3.16969900	-4.15474400	0.94352600
C	1.86536100	-4.76976100	1.42956000
C	1.78734100	-5.22380400	2.76528400
H	2.64157800	-5.08186500	3.43022000
C	0.62107000	-5.84758300	3.24103000
H	0.57101700	-6.18654200	4.27743600
C	-0.47906600	-6.03614400	2.38146600
H	-1.38544000	-6.52066700	2.74983700
C	-0.40285400	-5.59543200	1.04785900
H	-1.24740600	-5.73168500	0.37134900
C	0.76105700	-4.96337300	0.57292400
H	0.79535900	-4.60033600	-0.45555900
C	4.14146500	-5.15014200	0.31343500
C	3.64424200	-6.16646400	-0.54093100
H	2.57261200	-6.23500200	-0.72332000
C	4.51102400	-7.09705500	-1.13785900
H	4.10388200	-7.87133700	-1.79063800
C	5.89534800	-7.04161700	-0.88834500
H	6.56824200	-7.76694100	-1.34813200
C	6.40027200	-6.04890200	-0.03044700
H	7.46932700	-6.00195600	0.18367000
C	5.53285300	-5.11434100	0.56426100

H	5.95191900	-4.36439400	1.23395400
C	4.11709700	-2.27998100	-0.76232600
C	4.49722179	-3.20584774	-1.75998187
H	4.10247634	-4.21731590	-1.73758335
C	5.40361692	-2.80412236	-2.74614696
C	5.94861595	-1.51197647	-2.80650940
C	5.53861963	-0.61716707	-1.80819836
C	4.64770691	-0.96828924	-0.78940651
H	4.35936215	-0.25088112	-0.02298566
C	-1.99881800	-2.08370300	-0.81609000
C	-3.16706800	-2.78785000	-1.49165000
C	-2.89260300	-3.99792400	-2.55509300
C	-3.28247100	-2.58099600	-3.00389700
H	-2.52832000	-1.92883300	-3.44056600
H	-4.27960400	-2.47631500	-3.43076200
C	-4.41736000	-2.87296500	-0.63202900
C	-4.35336700	-3.41520800	0.68026100
H	-3.39369000	-3.71701500	1.08905200
C	-5.52585600	-3.52131200	1.43080200
C	-6.78375900	-3.10981000	0.95997100
C	-6.80948000	-2.56169700	-0.32872100
C	-5.66772400	-2.43105800	-1.12787300
H	-5.74848500	-1.99384300	-2.11922100
C	-4.00056600	-5.03862700	-2.63291300
C	-4.26208700	-5.92053100	-1.55868300
H	-3.70159300	-5.81516900	-0.62938900
C	-5.24680000	-6.91812000	-1.67404500
H	-5.44285900	-7.58501200	-0.83275800
C	-5.98168700	-7.05201600	-2.86746800
H	-6.74896300	-7.82268400	-2.95504700
C	-5.72052900	-6.18760700	-3.94650100
H	-6.28028700	-6.29010200	-4.87761700
C	-4.73411000	-5.19089400	-3.83041300
H	-4.52388200	-4.53156000	-4.67419900
C	-1.49224400	-4.53551800	-2.81162600
C	-0.43417800	-3.69101200	-3.22411400
H	-0.57695000	-2.62087200	-3.31059500
C	0.82951100	-4.22079100	-3.54069200
H	1.61781400	-3.54317300	-3.87252600
C	1.07114900	-5.60472100	-3.45190600
H	2.04875800	-6.01251300	-3.71471300
C	0.02996400	-6.45481500	-3.03498500
H	0.19393700	-7.53185600	-2.96823900
C	-1.23573000	-5.92880900	-2.72327700

H	-2.04055300	-6.60374900	-2.43910500
C	-2.62322300	1.00960500	0.63321800
C	-3.97565800	1.67131000	0.56198000
C	-5.16942600	0.70656900	0.83112500
H	-6.02682100	0.81718300	0.16921300
H	-4.89070100	-0.31151600	1.09560600
C	-4.89257700	1.77143100	1.88381300
C	-4.33951400	1.28597200	3.21738500
C	-3.15863500	1.81325000	3.77906400
H	-2.57081400	2.52865700	3.20531900
C	-2.71104400	1.38949200	5.04297000
H	-1.78772600	1.80012200	5.45739700
C	-3.44361100	0.42857200	5.76468600
H	-3.09393500	0.09213100	6.74217500
C	-4.62842200	-0.09822200	5.21527200
H	-5.20291300	-0.84429600	5.76704100
C	-5.07557300	0.33185600	3.95328500
H	-5.99424000	-0.07851000	3.53028500
C	-5.83315800	2.97001500	2.01005600
C	-5.54203900	3.98716800	2.95417100
H	-4.67399300	3.87733600	3.60385700
C	-6.37405500	5.11118300	3.08906900
H	-6.12847700	5.87947700	3.82434800
C	-7.52671600	5.24030300	2.29139100
H	-8.17686400	6.10978200	2.39818500
C	-7.83840700	4.23011900	1.36437600
H	-8.73566800	4.31010300	0.74855500
C	-7.00098900	3.10822800	1.22490700
H	-7.27024400	2.34128700	0.50008100
C	-4.11795400	2.66664500	-0.56879900
C	-4.12098000	4.06113500	-0.35017300
H	-4.05959200	4.45707200	0.65882100
C	-4.24095200	4.91579500	-1.45162000
C	-4.34832100	4.45796700	-2.77097600
C	-4.32591900	3.06573600	-2.95136100
C	-4.21791000	2.16522900	-1.88997800
H	-4.18028800	1.09179000	-2.06780800
C	1.25103500	1.15005900	1.92433500
C	2.36878100	1.71223900	2.78796500
C	2.38161300	3.25318600	3.23018200
C	3.32773700	2.71715100	2.14805600
H	3.08642200	2.99760800	1.12601100
H	4.38909200	2.63294800	2.37537100
C	2.91650400	0.70390700	3.78533400

C	4.25525300	0.25978800	3.69337800
H	4.90713700	0.62804600	2.90447100
C	4.73674000	-0.66302100	4.63094500
C	3.94644900	-1.18353100	5.66274800
C	2.61650100	-0.73330800	5.71572900
C	2.08566200	0.18970000	4.81200300
H	1.04582200	0.49409600	4.87152700
C	2.92813500	3.54868200	4.61935200
C	4.29047600	3.83971900	4.84737600
H	4.99106100	3.85934400	4.01190800
C	4.75735700	4.12107500	6.14565200
H	5.81352200	4.34618300	6.30264400
C	3.86805900	4.11498400	7.23425300
H	4.23034000	4.32886000	8.24072400
C	2.50406700	3.83774700	7.01623200
H	1.80509400	3.83919400	7.85414100
C	2.03864200	3.56228300	5.72044900
H	0.97808300	3.36919200	5.55260900
C	1.28351500	4.21553900	2.80794000
C	1.66390000	5.53293000	2.45427300
H	2.72397000	5.79161800	2.42941300
C	0.69405500	6.50584100	2.16373900
H	1.00189000	7.51948300	1.90097700
C	-0.67541700	6.17592700	2.22118400
H	-1.43289000	6.92989000	2.00067100
C	-1.05998800	4.86802700	2.56362400
H	-2.11860000	4.60818700	2.60511000
C	-0.08812700	3.89073800	2.86047700
H	-0.39089100	2.87658500	3.12214600
O	-1.43337200	-1.09588900	-1.47943500
O	-1.67705400	-2.44099900	0.40611200
O	-1.68629000	1.44944700	-0.19419600
O	-2.47541800	0.01008900	1.47056100
O	1.30722000	1.32210300	0.61302500
O	0.32396200	0.46585300	2.55207200
O	1.54074300	-1.17003000	-0.73655100
O	1.11310600	-1.97885800	1.41344200
Rh	-0.04737200	0.20717900	-0.59050800
Rh	-0.68705600	-1.00260900	1.50541900
C	0.37244400	1.30465800	-2.37203100
C	2.56752300	0.95857300	-2.67840700
H	2.46031200	0.05221200	-2.08718000
C	2.94251500	0.99001300	-4.10285200
C	-0.08384800	0.50119400	-3.56758800

F	-1.49150800	0.39365400	-3.57995600
F	0.24164700	0.95579900	-4.86712600
F	0.44430700	-0.81695600	-3.53337500
C	0.13204900	2.77375500	-2.44365700
C	-0.12870500	3.46208000	-3.66912200
C	0.15494000	3.55379200	-1.24881200
C	-0.39396800	4.84076900	-3.68615100
H	-0.13159400	2.90714300	-4.59961800
C	-0.10092400	4.93145800	-1.27387600
H	0.37460200	3.06790800	-0.30366000
C	-0.38484700	5.58375800	-2.49143700
H	-0.61174700	5.33176700	-4.63690000
H	-0.09763800	5.49014000	-0.33819000
H	-0.60482600	6.65288300	-2.50417400
C	3.04612900	2.18862700	-2.14318000
C	3.51182800	2.27239400	-4.37061600
N	3.56334100	3.01032800	-3.12813500
H	2.96947200	2.51041500	-1.11176500
C	2.85434100	0.03736500	-5.13680700
C	3.32202400	0.37873900	-6.41534500
C	3.85220500	1.66483300	-6.67613200
C	3.95012500	2.62867800	-5.65682900
H	2.40220900	-0.93286300	-4.94532700
H	3.26185700	-0.35079000	-7.22403700
H	4.19080300	1.91564700	-7.68225200
H	4.35633600	3.61416900	-5.87218700
Br	-8.57134900	-1.93206500	-1.05952200
Br	-5.42371800	-4.32048500	3.26663000
Br	6.64698500	-1.26753600	4.49282200
Br	1.43660800	-1.44916500	7.16534600
Br	-4.45041400	2.35184300	-4.82177200
Br	-4.27867400	6.90108200	-1.13479200
Br	5.97671472	-4.13514658	-4.13281438
Br	6.27654203	1.25277085	-1.84488010
H	-4.44310400	5.14189100	-3.61022200
H	-7.68415000	-3.21208700	1.56030400
H	4.33888800	-1.89580800	6.38416500
H	6.64951967	-1.22211926	-3.58487626
Si	4.26093400	4.73123800	-2.90684200
C	6.18360900	4.67912600	-3.14737100
H	6.56812200	5.59164000	-2.65169600
H	6.57415000	3.82264600	-2.56813000
C	6.73609300	4.61898400	-4.60566300
H	7.83620400	4.70358600	-4.59999500

H	6.47332000	3.66578300	-5.08868600
H	6.33800200	5.44497900	-5.21957800
C	3.35924800	5.88912300	-4.16025300
H	2.27985000	5.85478700	-3.92935300
H	3.47292400	5.50885700	-5.18908300
C	3.88023100	7.36306100	-4.08725200
H	4.94655000	7.42358500	-4.36349100
H	3.31296900	8.00668700	-4.78040600
H	3.76346100	7.77863700	-3.07185000
C	3.86876700	5.27908200	-1.09486200
H	2.89990000	4.85436200	-0.77961900
H	3.71449500	6.37422900	-1.12766000
C	4.98460800	4.95699400	-0.04910400
H	4.67592900	5.28783300	0.95687200
H	5.19698900	3.87587300	-0.00080100
H	5.92446600	5.47320800	-0.30314600

TSII-R-TES (G = -5816.582384)

C	-2.85991700	0.95094600	-0.31837300
C	-4.27891600	1.10246300	-0.79883300
C	-5.35095200	1.18420400	0.31440400
H	-6.27616200	0.64279800	0.12279700
H	-4.96728600	1.14005100	1.33211900
C	-5.06825700	2.46498900	-0.46443400
C	-4.33312800	3.57681800	0.26924100
C	-4.87619800	4.06930100	1.47709500
H	-5.77894500	3.60977100	1.88395500
C	-4.26209100	5.13620300	2.15538500
H	-4.68841100	5.50166300	3.09139800
C	-3.10169000	5.73419400	1.62608500
H	-2.62635200	6.56615100	2.14951100
C	-2.56071300	5.25246500	0.42032200
H	-1.66463800	5.70750400	-0.00355900
C	-3.16819300	4.17740400	-0.25410000
H	-2.71989500	3.79515900	-1.17280000
C	-6.07989700	2.95069300	-1.49845000
C	-5.71767100	3.97697200	-2.40648500
H	-4.72467300	4.42170700	-2.34675100
C	-6.62714500	4.44011800	-3.37164000
H	-6.32554300	5.23023600	-4.06168000
C	-7.92380000	3.89641700	-3.44567100
H	-8.63091200	4.25768000	-4.19388400
C	-8.30158400	2.89080300	-2.53920900
H	-9.30772600	2.46976300	-2.57604000

C	-7.38917400	2.42365900	-1.57515300
H	-7.71117000	1.65325900	-0.87530900
C	-4.59295000	0.32290200	-2.05420100
C	-4.35307700	0.86799100	-3.33460200
H	-3.98727300	1.88573600	-3.42960500
C	-4.58624800	0.07417900	-4.46018800
C	-5.05235100	-1.24686000	-4.38590400
C	-5.27687400	-1.75403200	-3.09890900
C	-5.06381500	-1.00493800	-1.93810200
H	-5.23461500	-1.43521200	-0.95348600
C	0.81100200	2.59482600	-0.39618500
C	1.72503000	3.75930000	-0.74333800
C	1.33217400	4.82656800	-1.91916200
C	2.40853800	3.74522100	-2.11033800
H	2.16457600	2.90836900	-2.76153300
H	3.44152700	4.08676200	-2.16942900
C	2.48061200	4.30307400	0.45964100
C	1.77548500	4.76984400	1.60058500
H	0.69255500	4.69730500	1.63127100
C	2.49528900	5.28807800	2.67927200
C	3.89799500	5.36817300	2.70285700
C	4.56317800	4.88092300	1.57107000
C	3.89480300	4.35175500	0.46044200
H	4.46263800	3.98355900	-0.39006100
C	1.83548000	6.24061900	-1.67724000
C	1.21741100	7.07576500	-0.71743400
H	0.39807500	6.68230300	-0.11516500
C	1.65157900	8.39994500	-0.53243400
H	1.16907400	9.02842500	0.21791700
C	2.70749900	8.91284400	-1.31056700
H	3.04746600	9.93911800	-1.16441600
C	3.31794900	8.09639100	-2.27974700
H	4.12885800	8.48993100	-2.89479400
C	2.88172600	6.77080600	-2.46372600
H	3.34735300	6.14802300	-3.22914100
C	0.03396800	4.71867600	-2.70873200
C	-0.45839200	3.47384100	-3.17349100
H	0.02021300	2.54491700	-2.88344800
C	-1.58927800	3.40585800	-4.00565600
H	-1.91534600	2.42600100	-4.35263200
C	-2.26785400	4.57939900	-4.38634900
H	-3.13801000	4.52394400	-5.04266400
C	-1.80334600	5.82095800	-3.91591800
H	-2.31509000	6.74207600	-4.20044500

C	-0.66497300	5.89192600	-3.09225400
H	-0.30268400	6.86295100	-2.76167300
C	2.06581500	-0.07015500	1.49841000
C	3.48866800	-0.15001200	1.98813900
C	4.04915800	1.19347500	2.54137100
H	5.06885200	1.44671300	2.25550000
H	3.33614600	2.01550600	2.55573600
C	3.81209500	0.08702600	3.55930300
C	2.67916200	0.29621100	4.55419800
C	1.65102500	-0.65010500	4.74124500
H	1.60380100	-1.52199100	4.09015200
C	0.65800900	-0.44978800	5.71638500
H	-0.13986100	-1.18544700	5.83650800
C	0.68276300	0.70412800	6.52178800
H	-0.09211900	0.86551000	7.27297900
C	1.71052600	1.65102100	6.34790900
H	1.73791200	2.54911700	6.96742500
C	2.70404800	1.44579900	5.37413600
H	3.49970300	2.18135200	5.24235600
C	5.00830000	-0.66887800	4.13682800
C	4.78372000	-1.76982300	5.00116200
H	3.76158000	-2.03431000	5.27161300
C	5.85610600	-2.49585900	5.54566800
H	5.65578300	-3.33688800	6.21179700
C	7.18281600	-2.13163700	5.24748100
H	8.01707800	-2.69047900	5.67389000
C	7.42152000	-1.02981100	4.40726100
H	8.44468600	-0.72511000	4.18114600
C	6.34659700	-0.30625800	3.85902000
H	6.56417900	0.54892600	3.22062500
C	4.43267300	-1.01608100	1.18830100
C	4.60884600	-2.38309500	1.50536500
H	4.03012000	-2.83502100	2.30567700
C	5.56929400	-3.12327000	0.80947900
C	6.36468300	-2.57687400	-0.21089300
C	6.13661400	-1.22866200	-0.52730000
C	5.19866900	-0.43964500	0.14690900
H	5.06487100	0.60992600	-0.10899900
C	-1.67270100	-1.72829400	1.52891700
C	-2.70906000	-2.74926700	1.97564700
C	-2.29166700	-4.20691300	2.49664700
C	-2.87524600	-3.99333400	1.09372700
H	-2.17872900	-4.05868100	0.25899400
H	-3.88502200	-4.34884900	0.89371700

C	-3.93025200	-2.11535500	2.62317100
C	-5.21733500	-2.28720700	2.06364100
H	-5.35151400	-2.86521900	1.15250000
C	-6.32309900	-1.70514300	2.69686300
C	-6.21903800	-0.94349000	3.86722000
C	-4.92491400	-0.78080600	4.38844300
C	-3.78841800	-1.34257600	3.80365200
H	-2.80188200	-1.17035500	4.22147900
C	-3.17520700	-4.80224100	3.58463600
C	-4.26341300	-5.65085000	3.28786400
H	-4.49684000	-5.89380700	2.25067300
C	-5.04708200	-6.20158500	4.32024300
H	-5.88313500	-6.85758200	4.07208800
C	-4.75352700	-5.91025100	5.66370200
H	-5.36335700	-6.33302400	6.46340200
C	-3.66245200	-5.07364600	5.97149200
H	-3.42281500	-4.84822700	7.01196700
C	-2.87829400	-4.52985000	4.94144700
H	-2.02163100	-3.89927600	5.18402300
C	-0.84003700	-4.63424600	2.63041400
C	-0.52178500	-5.98033900	2.32793600
H	-1.30432800	-6.63797000	1.94624300
C	0.77664900	-6.47382900	2.53155600
H	1.00494900	-7.51603100	2.30082400
C	1.78102800	-5.62827500	3.04549900
H	2.78930600	-6.01007400	3.21406900
C	1.47171000	-4.29034200	3.34665900
H	2.24089900	-3.63636900	3.76150400
C	0.16821500	-3.79253800	3.14301800
H	-0.06686100	-2.75323300	3.37345400
O	0.93148500	1.48057100	-1.10817300
O	0.01560200	2.73072000	0.63333500
O	1.71144700	-0.78155600	0.43350800
O	1.27668100	0.74983300	2.14298600
O	-1.22297900	-1.81940300	0.29331000
O	-1.34506300	-0.77830000	2.38140800
O	-1.97067600	0.49716900	-1.18314900
O	-2.60093300	1.25845700	0.93246600
Rh	-0.12016800	-0.24347100	-0.52262600
Rh	-0.67110900	1.01355900	1.56941000
C	0.24117900	-1.37650400	-2.27757600
C	0.36306300	-2.86163800	-2.15593100
C	-0.12233200	-3.76068000	-3.15440900
C	0.93804600	-3.43101000	-0.98142400

C	-0.08078900	-5.15133100	-2.95929800
H	-0.53544500	-3.36408900	-4.07542900
C	0.99466000	-4.82087400	-0.80234700
H	1.33429500	-2.77092900	-0.21286200
C	0.47404700	-5.69009800	-1.78416400
H	-0.48777000	-5.81201800	-3.72767000
H	1.41408600	-5.22553600	0.11879100
H	0.49937800	-6.77047000	-1.63044900
C	-0.65636000	-0.91438400	-3.40130500
F	-0.66639600	0.48842200	-3.54533700
F	-0.37039100	-1.40438600	-4.69924000
F	-1.97385200	-1.32945000	-3.14029200
C	2.15193500	-0.51760400	-3.06418400
H	2.19074360	0.11212210	-2.18121426
C	2.84288549	-1.75845603	-3.20257824
N	3.05518487	-2.07962519	-4.52667296
C	2.60214546	-0.96166562	-5.31997610
C	2.06069496	0.02209152	-4.43639215
H	3.12505177	-2.43693510	-2.40720348
C	2.67977532	-0.75279223	-6.70521580
H	3.10282791	-1.49994093	-7.37523432
C	2.21392745	0.47509551	-7.21021129
H	2.26666466	0.66684737	-8.28265956
C	1.68879846	1.46430997	-6.34665363
H	1.33855501	2.40910114	-6.76453993
C	1.60415870	1.24683661	-4.96056728
H	1.17473170	2.00559259	-4.30973076
Br	7.23444800	-0.39567400	-1.98542600
Br	5.87359800	-5.03914900	1.31596100
Br	-5.91107400	-3.65286300	-2.92483100
Br	-4.21205900	0.83769600	-6.27979100
Br	1.48701200	5.97281800	4.26848200
Br	6.57120600	4.94151100	1.54447300
Br	-4.71142500	0.30509800	6.05889800
Br	-8.14431400	-1.97215800	1.89357800
H	-5.22110600	-1.84615400	-5.27684900
H	-7.08980700	-0.50337600	4.34650100
H	7.13028600	-3.16176600	-0.71439400
H	4.43488200	5.78615100	3.55065000
Si	3.73227658	-3.68223203	-5.21442863
C	2.37133985	-4.34643264	-6.41927390
H	1.59147955	-4.82042784	-5.79679606
H	1.88925393	-3.48846042	-6.91881742
C	2.88779231	-5.35434118	-7.49788790

H	2.05534300	-5.68788276	-8.14060446
H	3.64923192	-4.88924182	-8.14614277
H	3.33359102	-6.24878014	-7.03270850
C	5.38954241	-3.17770742	-6.08337586
H	5.89587594	-2.45503711	-5.41693391
H	5.15932490	-2.63219328	-7.01609605
C	6.36147543	-4.36257596	-6.39675401
H	5.90312980	-5.08893407	-7.08722390
H	7.28551066	-3.98454623	-6.86615548
H	6.64530505	-4.89615385	-5.47495485
C	3.97771060	-4.83422890	-3.69065468
H	4.82183613	-4.46567666	-3.08275207
H	3.07472100	-4.76618356	-3.05870690
C	4.20890279	-6.33832625	-4.05953938
H	4.32662934	-6.93411552	-3.13887850
H	3.34960567	-6.74299232	-4.61908138
H	5.11646297	-6.47486058	-4.66935113

7. Crystal Data

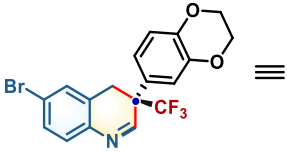
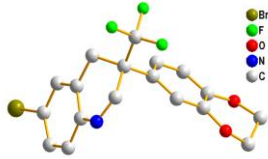
 (S)-31  CCDC 2261312	
Identification code	2261312
Empirical formula	C ₁₈ H ₁₃ BrF ₃ NO ₂
Formula weight	412.20
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	6.3080(5)
b/Å	14.5920(11)
c/Å	17.5297(13)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	1613.5(2)
Z	4
ρ _{calc} /g/cm ³	1.697
μ/mm ⁻¹	2.592
F(000)	824.0
Crystal size/mm ³	0.2 × 0.15 × 0.13
Radiation	Mo Kα (λ = 0.71073)
2θ range for data collection/°	6.864 to 58.424
Index ranges	-6 ≤ h ≤ 8, -18 ≤ k ≤ 14, -23 ≤ l ≤ 22
Reflections collected	7321
Independent reflections	3598 [R _{int} = 0.0402, R _{sigma} = 0.0696]
Data/restraints/parameters	3598/0/226
Goodness-of-fit on F ²	1.007
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0433, wR ₂ = 0.0673
Final R indexes [all data]	R ₁ = 0.0806, wR ₂ = 0.0793
Largest diff. peak/hole / e Å ⁻³	0.25/-0.32
Flack parameter	-0.012(7)

Table S2. X-Ray data of (S)-31

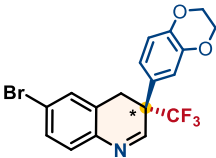
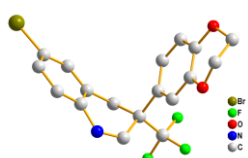
 (<i>R</i>)-31  CCDC 2266339	
Identification code	2266339
Empirical formula	C ₁₈ H ₁₃ BrF ₃ NO ₂
Formula weight	412.20
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
<i>a</i> /Å	6.3206(4)
<i>b</i> /Å	14.6110(10)
<i>c</i> /Å	17.5392(12)
α /°	90
β /°	90
γ /°	90
Volume/Å ³	1619.75(19)
<i>Z</i>	4
ρ_{calc} /g/cm ³	1.690
μ /mm ⁻¹	2.582
<i>F</i> (000)	824.0
Crystal size/mm ³	0.08 × 0.12 × 0.09
Radiation	Mo K α (λ = 0.71073)
2 Θ range for data collection/°	6.852 to 58.774
Index ranges	-7 ≤ <i>h</i> ≤ 8, -20 ≤ <i>k</i> ≤ 14, -22 ≤ <i>l</i> ≤ 16
Reflections collected	7354
Independent reflections	3754 [<i>R</i> _{int} = 0.0336, <i>R</i> _{sigma} = 0.0595]
Data/restraints/parameters	3754/0/226
Goodness-of-fit on <i>F</i> ²	1.027
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0414, <i>wR</i> ₂ = 0.0700
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0790, <i>wR</i> ₂ = 0.0841
Largest diff. peak/hole / e Å ⁻³	0.35/-0.39
Flack parameter	-0.018(6)

Table S3. X-Ray data of (*R*)-31.

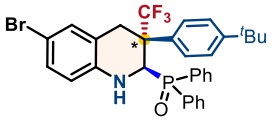
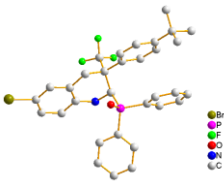
 (2<i>R</i>,3<i>S</i>)-41  CCDC 2281736	
CCDC NO.	2281736
Empirical formula	C ₆₄ H ₆₀ Br ₂ F ₆ N ₂ O ₂ P ₂
Formula weight	1224.90
Temperature/K	173.01
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	15.2025(7)
b/Å	18.6725(9)
c/Å	20.0559(10)
α/°	90
β/°	90
γ/°	90
Volume/Å ³	5693.2(5)
Z	4
ρ _{calc} /g/cm ³	1.429
μ/mm ⁻¹	2.887
F(000)	2512.0
Crystal size/mm ³	0.24 × 0.22 × 0.20
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	6.468 to 127.632
Index ranges	-17 ≤ h ≤ 16, -21 ≤ k ≤ 21, -23 ≤ l ≤ 22
Reflections collected	35402
Independent reflections	9218 [R _{int} = 0.0614, R _{sigma} = 0.0666]
Data/restraints/parameters	9218/1748/740
Goodness-of-fit on F ²	1.016
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0380, wR ₂ = 0.0539
Final R indexes [all data]	R ₁ = 0.0593, wR ₂ = 0.0585
Largest diff. peak/hole / e Å ⁻³	0.27/-0.23
Flack parameter	-0.011(8)

Table S4. X-Ray data of (2*R*,3*S*)-41.

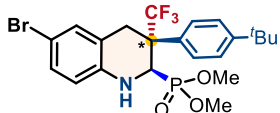
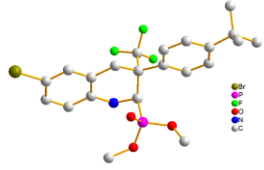
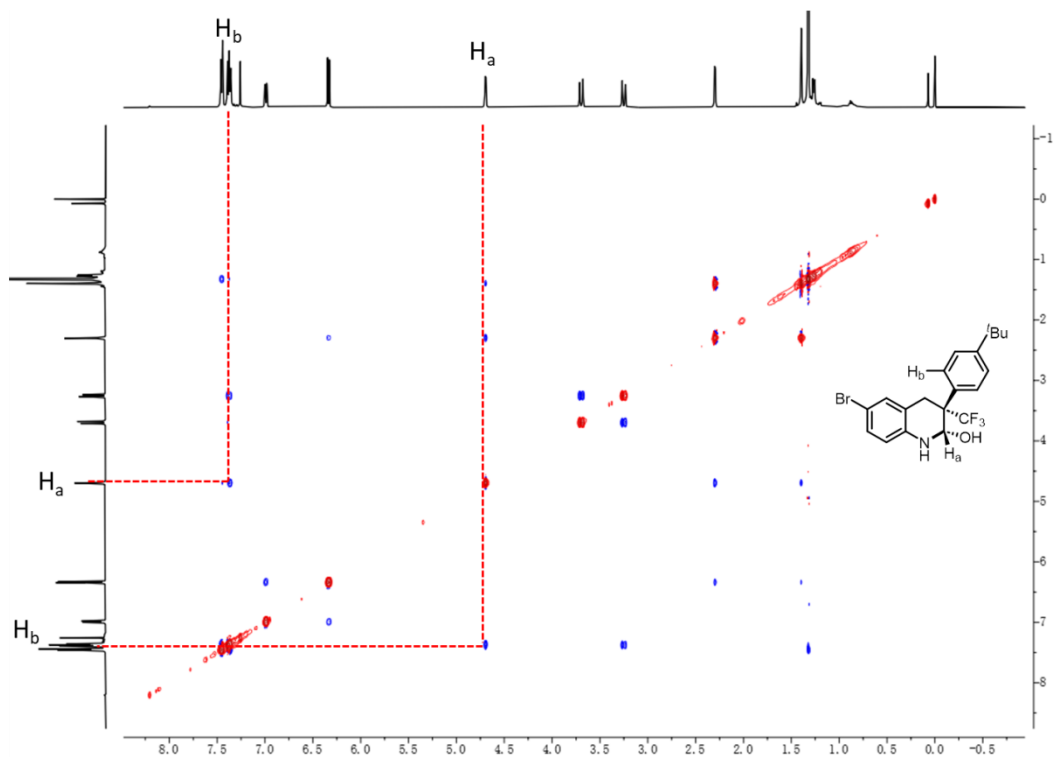
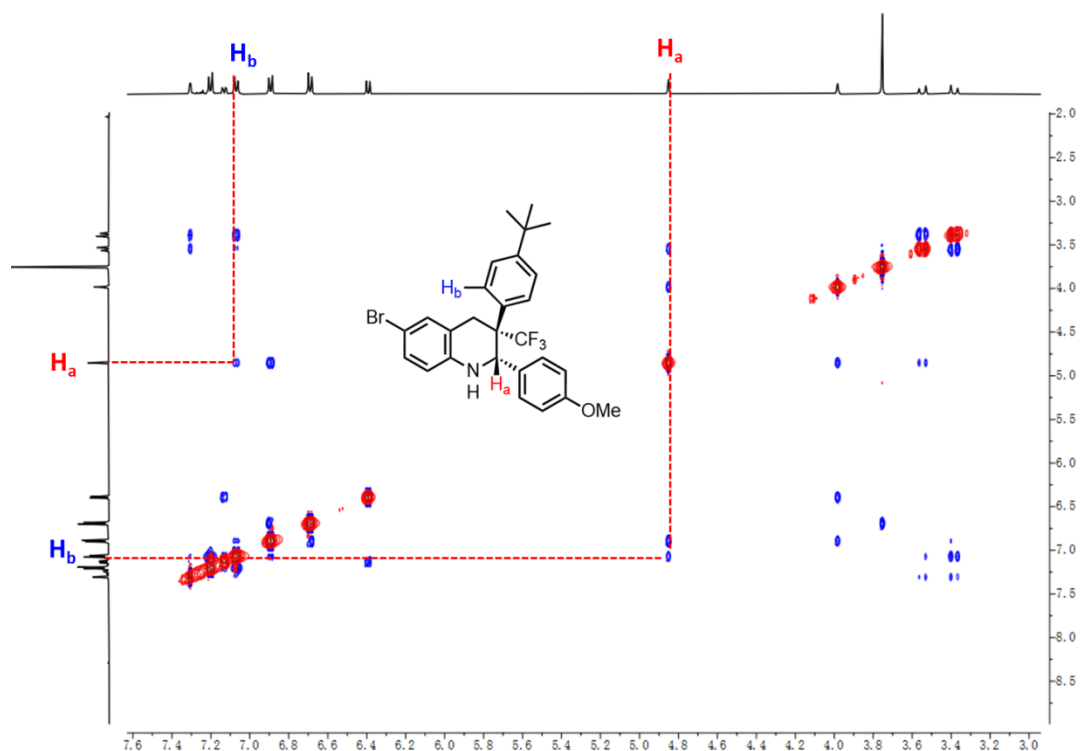
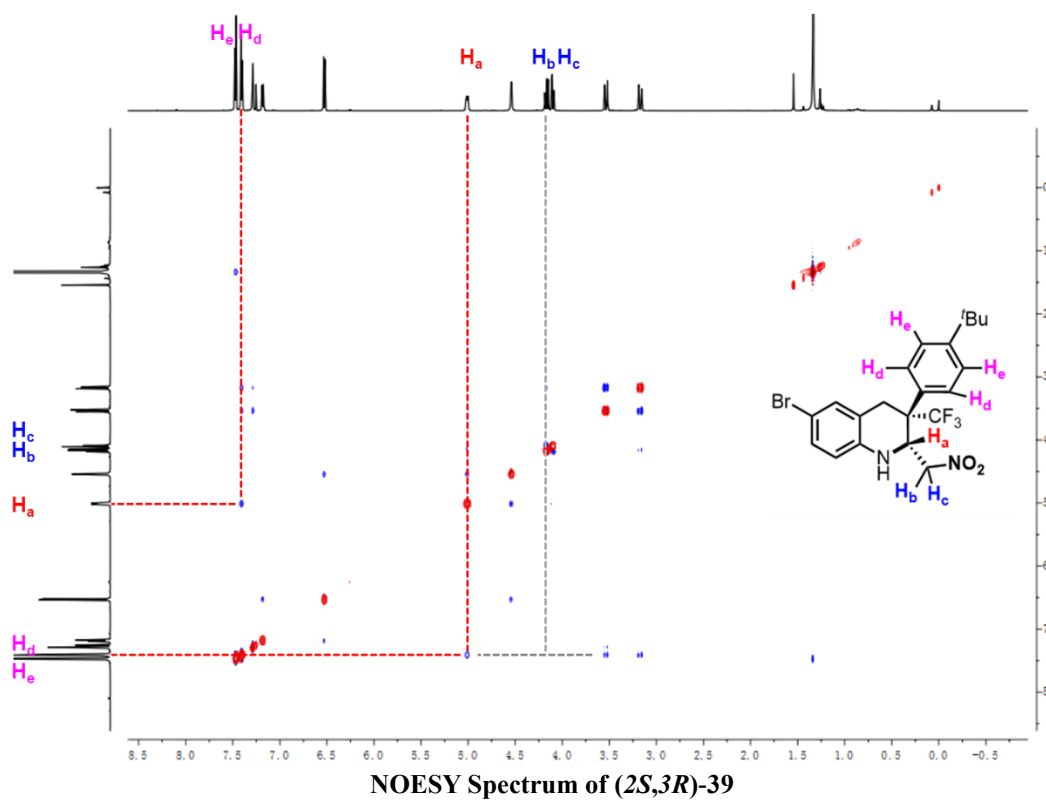
 (2<i>R</i>,3<i>S</i>)-42 ≡  CCDC 2281629	
CCDC NO.	2281629
Empirical formula	C ₂₂ H ₂₆ BrF ₃ NO ₃ P
Formula weight	520.32
Temperature/K	173.0
Crystal system	monoclinic
Space group	P2 ₁
a/Å	9.7513(6)
b/Å	10.5804(6)
c/Å	22.4441(14)
α/°	90
β/°	94.930(2)
γ/°	90
Volume/Å ³	2307.1(2)
Z	4
ρ _{calc} /g/cm ³	1.498
μ/mm ⁻¹	3.512
F(000)	1064.0
Crystal size/mm ³	0.18 × 0.20 × 0.17
Radiation	CuKα (λ = 1.54178)
2θ range for data collection/°	3.952 to 127.628
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -23 ≤ l ≤ 26
Reflections collected	22233
Independent reflections	7419 [R _{int} = 0.0299, R _{sigma} = 0.0370]
Data/restraints/parameters	7419/1/569
Goodness-of-fit on F ²	1.074
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0264, wR ₂ = 0.0638
Final R indexes [all data]	R ₁ = 0.0269, wR ₂ = 0.0640
Largest diff. peak/hole / e Å ⁻³	0.26/-0.64
Flack parameter	0.025(5)

Table S5. X-Ray data of (2*R*,3*S*)-42

8. 2D NMR spectrum

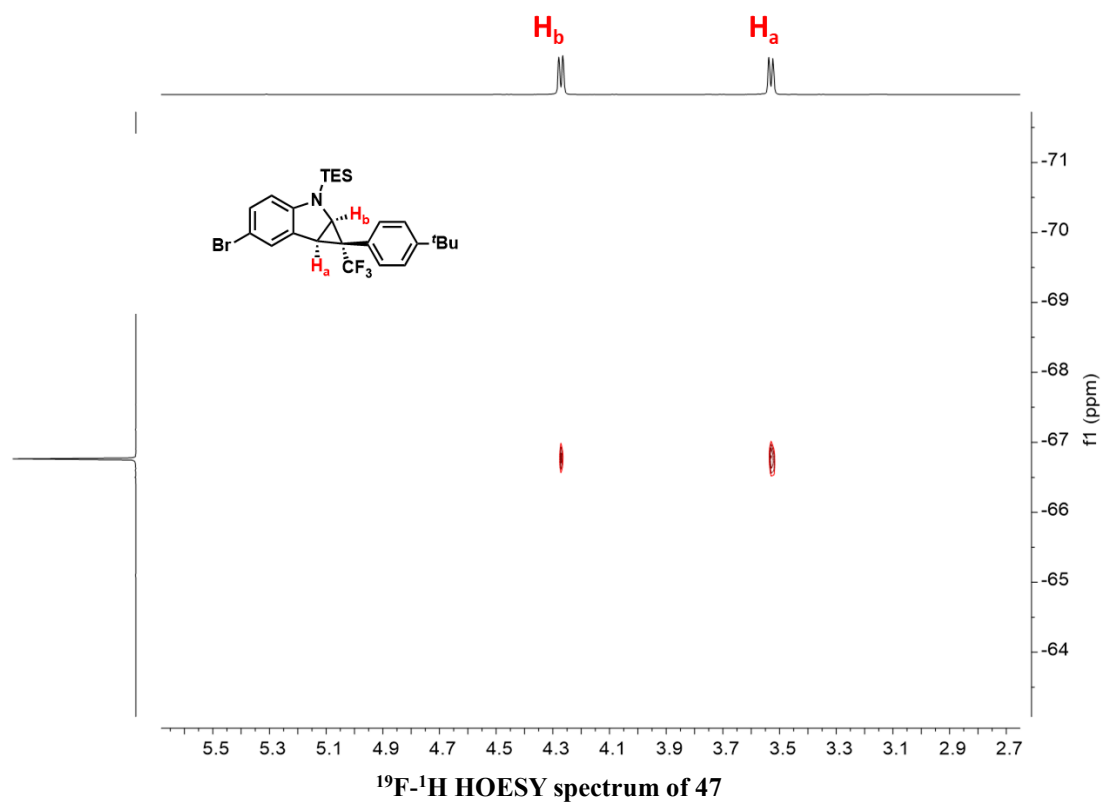


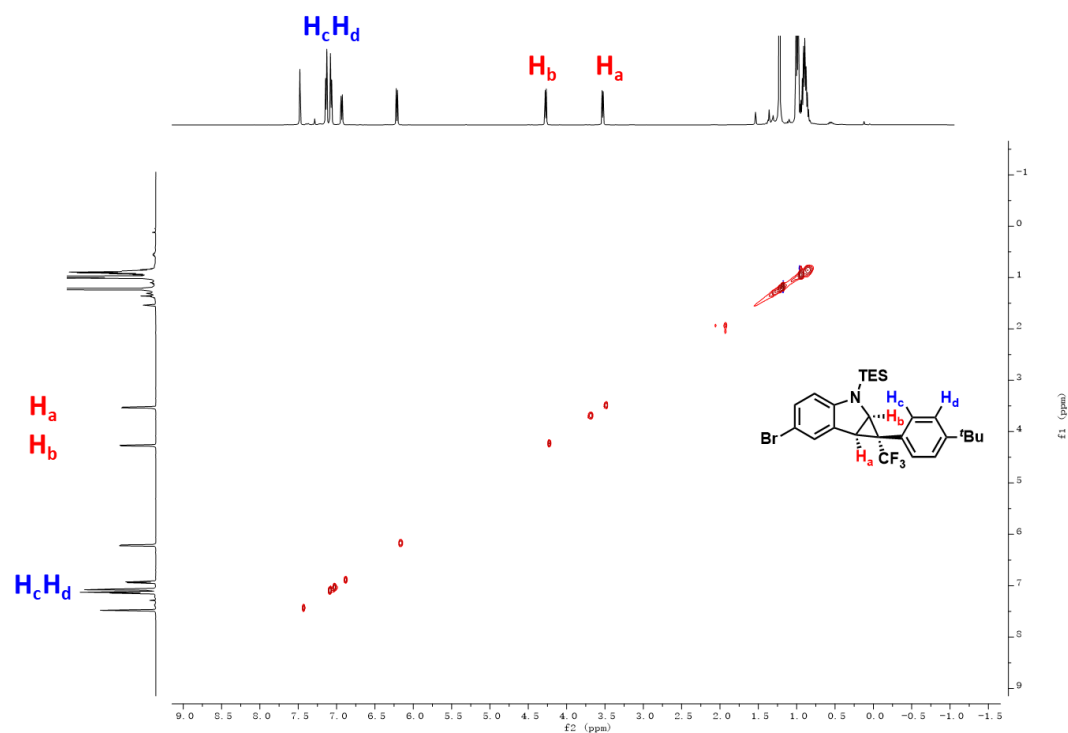
The correlation between H_a and H_b is evident from the detection of a strong cross peak.



The correlation between H_a and H_d is evident from the detection of a strong cross peak.

NingYQ_4519.ser

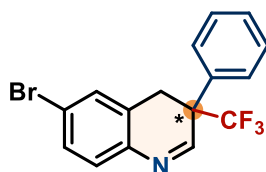




NOESY Spectrum of 47

There is no correlation between H_a , H_b and H_c , H_d .

9. Characterization Data of Products



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (80 mg) *N*-trifosylhydrazone provide **3** as a white solid, mp 103.5-104.7 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.33 (s, 1H), 7.38-7.32 (m, 3H), 7.31-7.24 (m, 4H), 7.21 (d, J = 8.0 Hz, 1H), 3.43-3.33 (m, 2H).

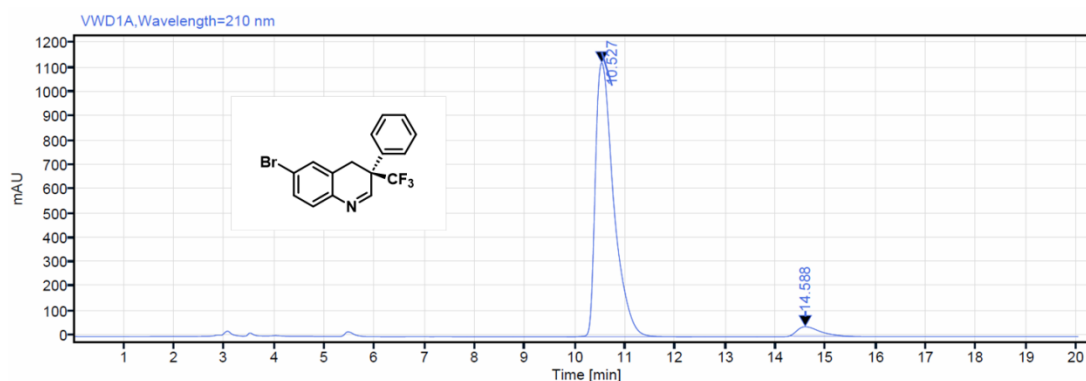
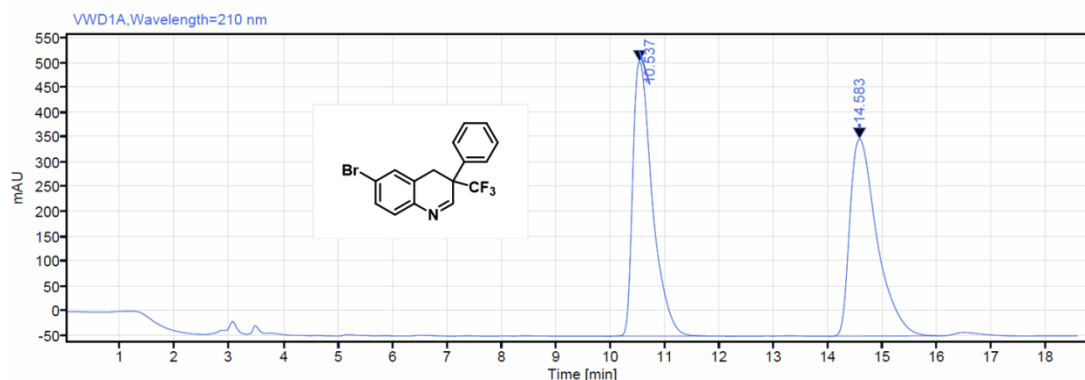
^{13}C NMR (125 MHz, CDCl_3) δ 158.1 (q, J = 2.5 Hz), 140.9, 132.5, 131.3, 130.9, 128.9, 128.8, 128.6, 127.7, 126.5 (q, J = 281.3 Hz), 125.6, 121.9, 49.3 (q, J = 25.0 Hz), 29.7 (q, J = 2.5 Hz).

^{19}F NMR (564 MHz, CDCl_3) δ -71.81.

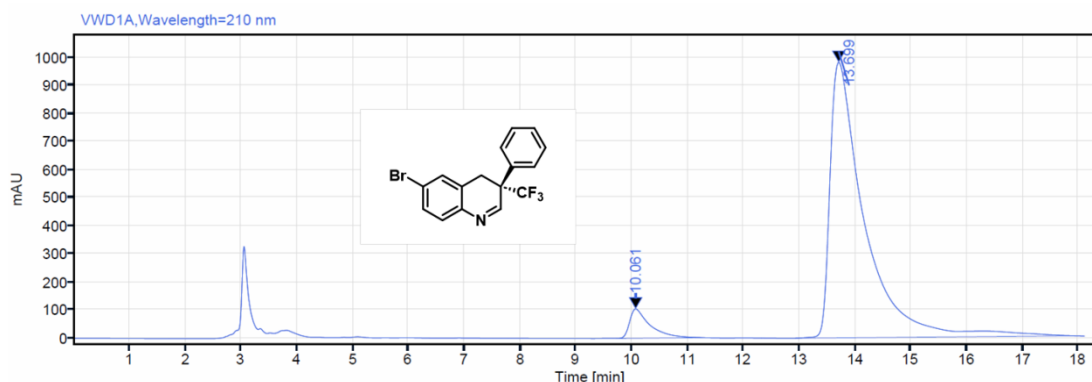
HRMS (ESI $^+$) m/z calcd for $\text{C}_{16}\text{H}_{12}\text{BrF}_3\text{N}^+$ $[\text{M}+\text{H}]^+$ 354.0100, found 354.0093.

(*S*)-6-bromo-3-phenyl-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 92% yield, 92% e.e. (Chiracel AD-H, 3.0% IPA/Hexanes, 1.0 mL/min, λ =210 nm, RT: Major: 10.527 min, Minor: 14.588 min).

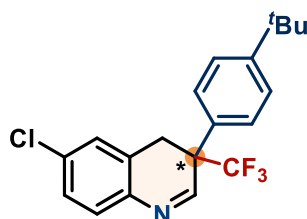
(*R*)-6-bromo-3-phenyl-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 94% yield, 88% e.e. (Chiracel AD-H, 3.0% IPA/Hexanes, 1.0 mL/min, λ =210 nm, RT: Major: 13.699 min, Minor: 10.061 min).



RT [min]	Width [min]	Area	Height	Area%
10.527	2.49	28551.92	1125.89	95.86
14.588	1.31	1233.40	38.70	4.14



RT [min]	Width [min]	Area	Height	Area%
10.061	1.54	2651.07	104.94	5.91
13.699	5.02	42237.83	984.47	94.09



Following General Procedure A, 0.3 mmol (46 mg) indole and 0.2 mmol (91 mg) *N*-trifosylhydrazone provide **4** as a white solid, mp 183.8-185.0 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.29 (s, 1H), 7.31-7.23 (m, 5H), 7.19 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.11 (d, *J* = 2.0 Hz, 1H), 3.42-3.32 (m, 2H), 1.25 (s, 9H).

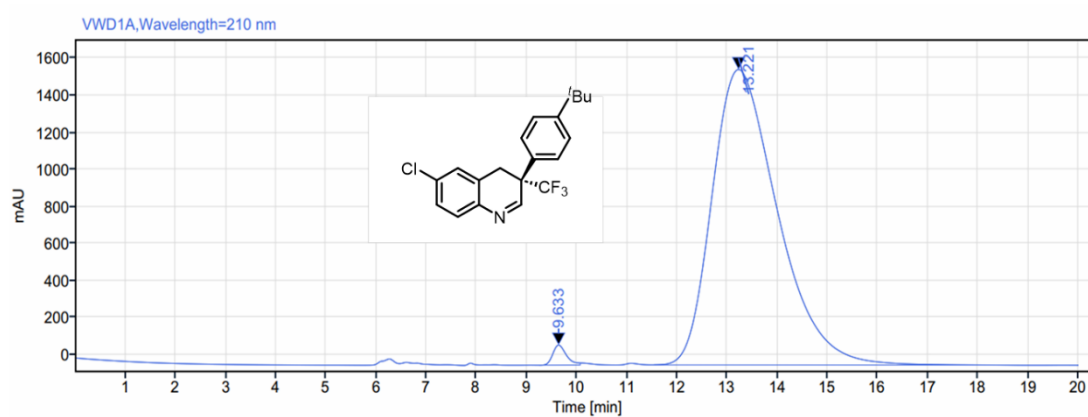
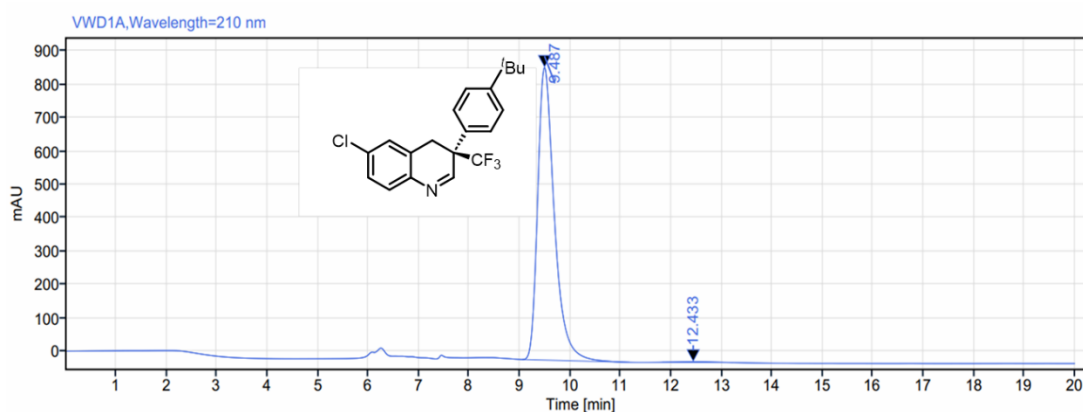
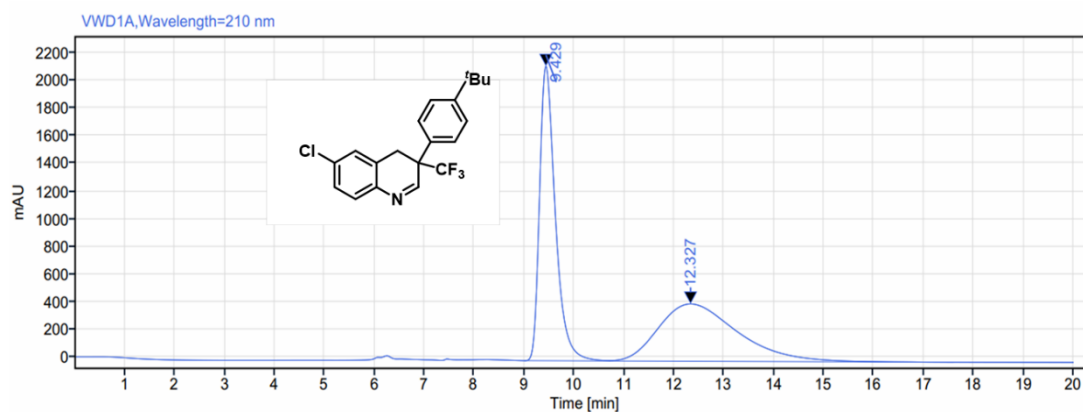
¹³C NMR (125 MHz, CDCl₃) δ 158.0 (q, *J* = 2.5 Hz), 151.8, 140.5, 133.6, 129.3, 128.4, 128.2, 128.1, 127.2, 126.6 (q, *J* = 281.3 Hz), 125.7, 125.5, 49.0 (q, *J* = 25.0 Hz), 34.5, 31.1, 29.7 (q, *J* = 2.5 Hz).

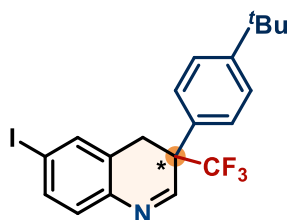
¹⁹F NMR (470 MHz, CDCl₃) δ -71.80.

HRMS (ESI⁺) *m/z* calcd for C₂₀H₂₀ClF₃N⁺ [M+H]⁺ 366.1231, found 366.1226.

(*S*)-3-(4-(tert-butyl)phenyl)-6-chloro-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 96% yield, 99% e.e. (Chiracel OJ-H, Hexanes/*i*-PrOH = 98/2, 0.5 mL/min, λ=210 nm, RT: Major: 9.487 min, Minor: 12.433 min).

(*R*)-3-(4-(tert-butyl)phenyl)-6-chloro-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 86% yield, 97% e.e. (Chiracel OJ-H, Hexanes/*i*-PrOH = 98/2, 0.5 mL/min, λ=210 nm, RT: Major: 13.221 min, Minor: 9.633 min).





Following General Procedure A, 0.3 mmol (73 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **5** as a white solid, mp 186.0-187.1 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.30 (s, 1H), 7.55 (dd, J = 8.5, 2.0 Hz, 1H), 7.46 (s, 1H), 7.31-7.22 (m, 4H), 7.08 (d, J = 8.0 Hz, 1H), 3.41-3.30 (m, 2H), 1.25 (s, 9H).

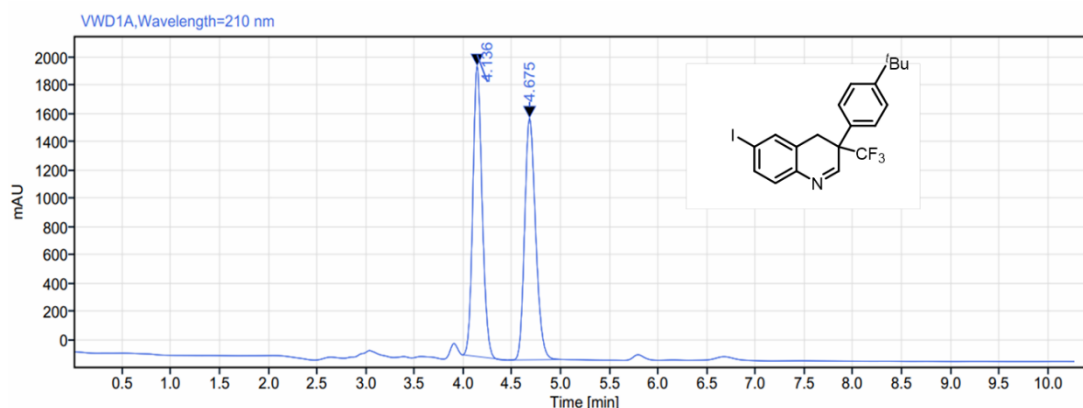
^{13}C NMR (150 MHz, CDCl_3) δ 158.3 (q, J = 3.0 Hz), 151.8, 141.5, 137.3, 136.8, 129.3, 128.9, 127.2, 126.5 (q, J = 280.5 Hz), 125.9, 125.8, 93.5, 49.0 (q, J = 25.5 Hz), 34.5, 31.1, 29.3.

^{19}F NMR (564 MHz, CDCl_3) δ -71.79.

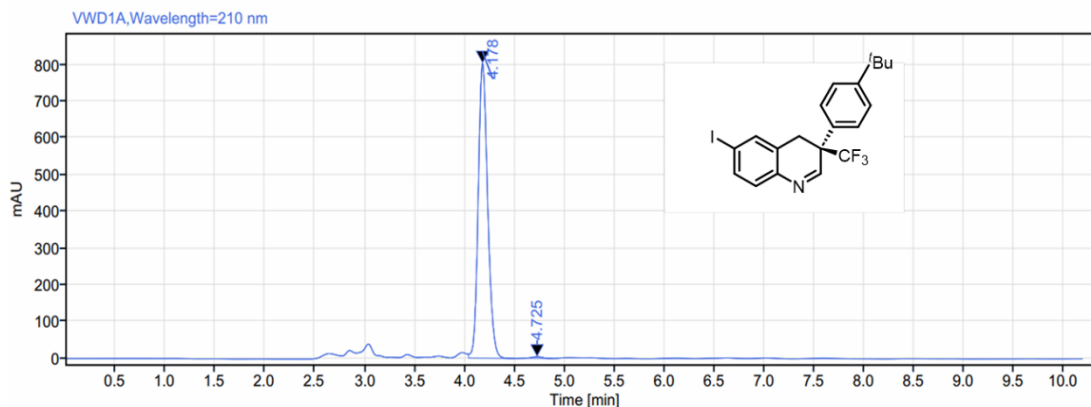
HRMS (ESI $^+$) m/z calcd for $\text{C}_{20}\text{H}_{20}\text{F}_3\text{IN}^+$ $[M+H]^+$ 458.0587, found 458.0574.

(*S*)-3-(4-(tert-butyl)phenyl)-6-iodo-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 91% yield, 99% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 4.178 min, Minor: 4.725 min).

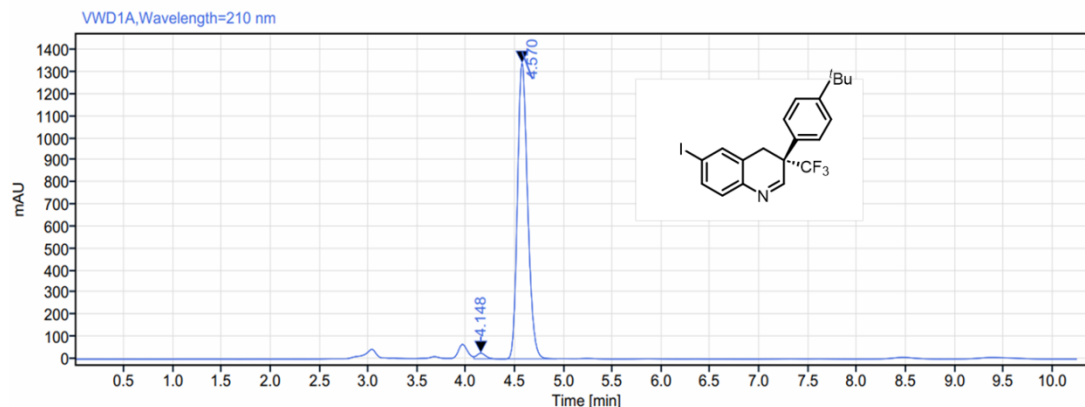
(*R*)-3-(4-(tert-butyl)phenyl)-6-iodo-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 98% yield, 96% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 4.570 min, Minor: 4.148 min).



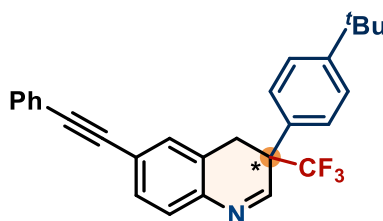
RT [min]	Width [min]	Area	Height	Area%
4.136	0.45	13573.09	2049.23	50.28
4.675	0.57	13424.45	1704.76	49.72



RT [min]	Width [min]	Area	Height	Area%
4.178	0.46	5288.02	803.78	99.39
4.725	0.30	32.38	4.49	0.61



RT [min]	Width [min]	Area	Height	Area%
4.148	0.30	171.03	26.29	1.72
4.570	0.55	9759.56	1340.33	98.28



Following General Procedure A, 0.3 mmol (66 mg) indole and 0.2 mmol (91 mg) *N*-trifosylhydrazone provide **6** as a red solid, mp 103.1-103.9 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.32 (s, 1H), 7.52-7.47 (m, 2H), 7.41-7.37 (m, 1H), 7.36-7.31 (m, 4H), 7.31-7.24 (m, 5H), 3.43-3.35 (m, 2H), 1.24 (s, 9H).

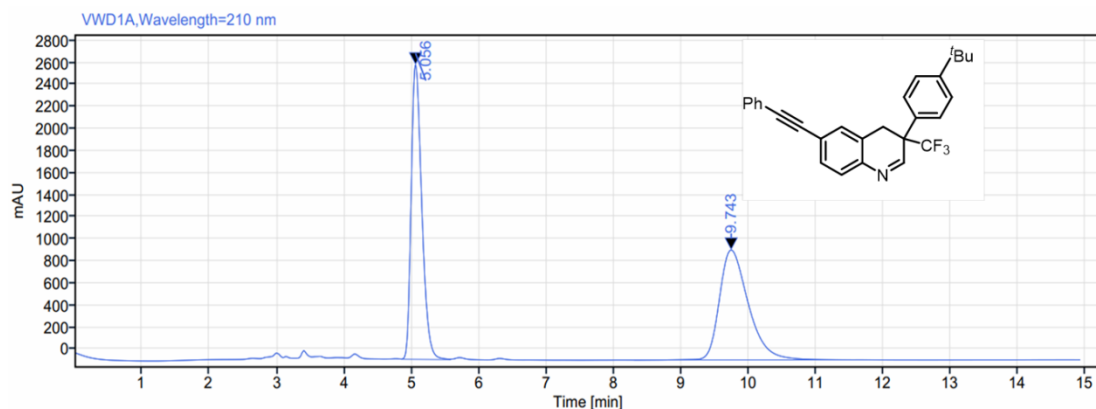
^{13}C NMR (150 MHz, CDCl_3) δ 158.4 (q, $J = 1.5$ Hz), 151.7, 141.7, 131.6, 131.4, 131.2, 129.4, 128.5, 128.4, 127.3, 127.2, 126.7 (q, $J = 280.5$ Hz), 125.7, 124.0, 123.2, 122.9, 90.6, 88.9, 49.2 (q, $J = 25.5$ Hz), 34.5, 31.1, 29.7.

^{19}F NMR (564 MHz, CDCl_3) δ -71.80.

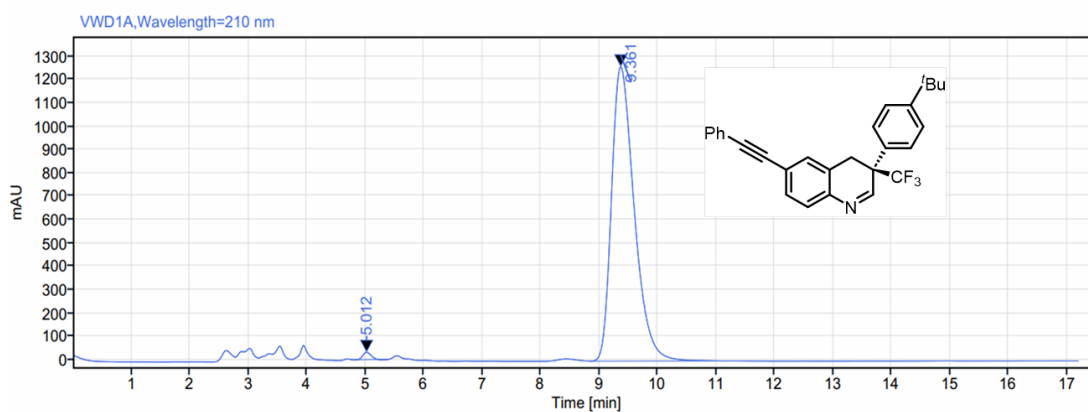
HRMS (ESI $^+$) m/z calcd for $\text{C}_{28}\text{H}_{25}\text{F}_3\text{N}^+$ $[\text{M}+\text{H}]^+$ 432.1934, found 432.1923.

(*S*)-3-(4-(tert-butyl)phenyl)-6-(phenylethynyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 92% yield, 98% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 9.361 min, Minor: 5.012 min).

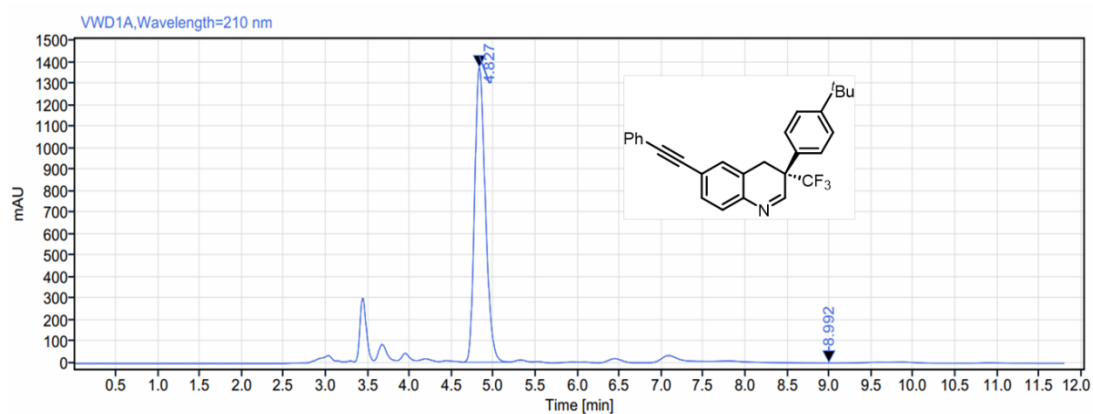
(*R*)-3-(4-(tert-butyl)phenyl)-6-(phenylethynyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 85% yield, 99% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 4.827 min, Minor: 8.992 min).



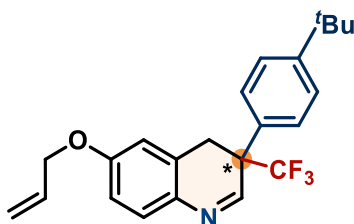
RT [min]	Width [min]	Area	Height	Area%
5.056	0.74	29118.51	2669.76	49.48
9.743	3.21	29724.67	996.94	50.52



RT [min]	Width [min]	Area	Height	Area%
5.012	0.74	290.50	31.09	0.85
9.361	2.33	33986.12	1259.58	99.15



RT [min]	Width [min]	Area	Height	Area%
4.827	0.54	12291.43	1372.15	99.83
8.992	0.58	20.74	0.70	0.17



Following General Procedure A, 0.3 mmol (52 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **7** as a red solid, mp 93.7-95.0 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.16 (s, 1H), 7.31-7.24 (m, 5H), 6.73 (dd, J = 8.5, 3.0 Hz, 1H), 6.66 (d, J = 2.5 Hz, 1H), 6.07-5.96 (m, 1H), 5.43-5.35 (m, 1H), 5.31-5.25 (m, 1H), 4.53-4.46 (m, 2H), 3.43-3.29 (m, 2H), 1.24 (s, 9H).

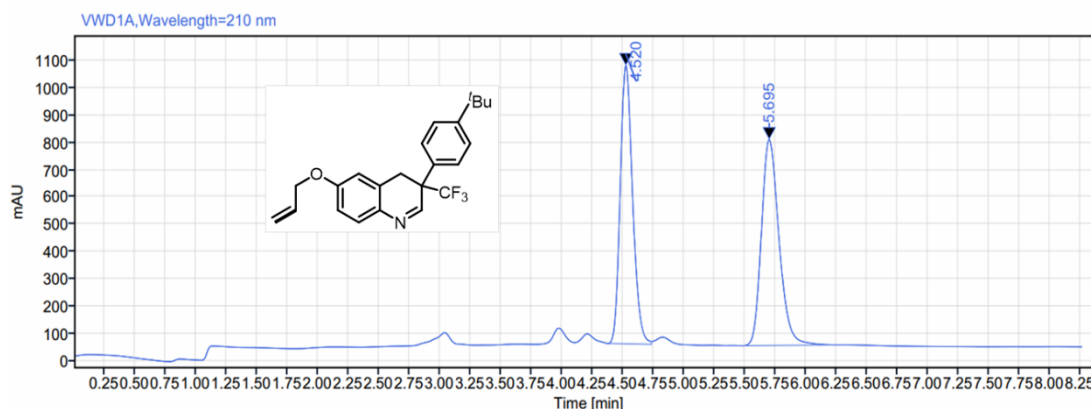
^{13}C NMR (125 MHz, CDCl_3) δ 158.4, 155.0 (q, J = 2.5 Hz), 151.5, 136.1, 132.9, 130.0, 128.5, 127.3, 126.8 (q, J = 281.3 Hz), 125.6, 125.3, 117.9, 114.8, 113.0, 68.9, 49.1 (q, J = 25.0 Hz), 34.4, 31.1, 30.3 (q, J = 2.5 Hz).

^{19}F NMR (470 MHz, CDCl_3) δ -71.80.

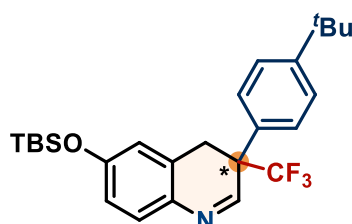
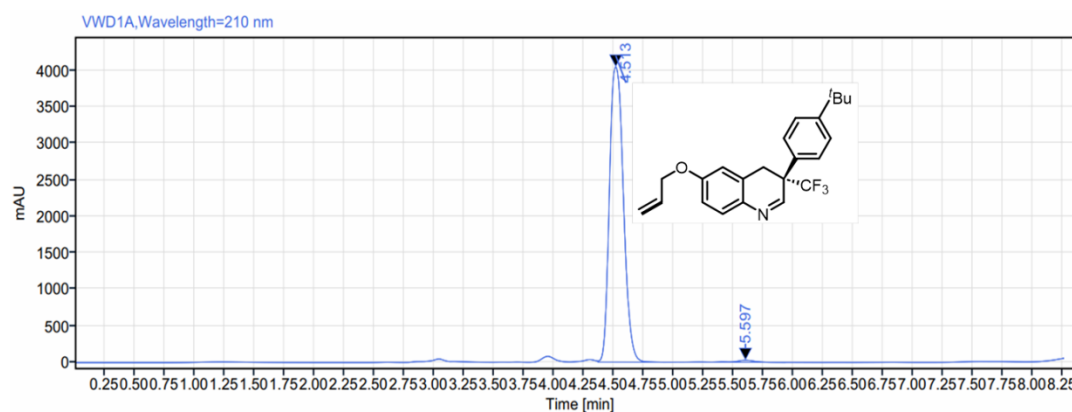
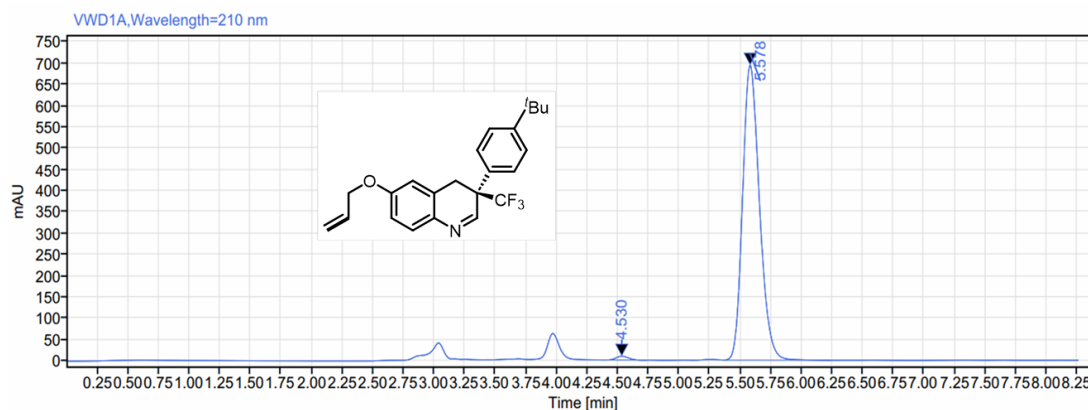
HRMS (ESI $^+$) m/z calcd for $\text{C}_{23}\text{H}_{25}\text{F}_3\text{NO}^+$ $[\text{M}+\text{H}]^+$ 388.1883, found 388.1883.

(*S*)-6-(allyloxy)-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a red solid: 71% yield, 98% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 5.578 min, Minor: 4.530 min).

(*R*)-6-(allyloxy)-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a red solid: 90% yield, 98% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 4.513 min, Minor: 5.597 min).



RT [min]	Width [min]	Area	Height	Area%
4.520	0.36	7197.91	1020.97	48.73
5.695	0.80	7573.52	755.59	51.27



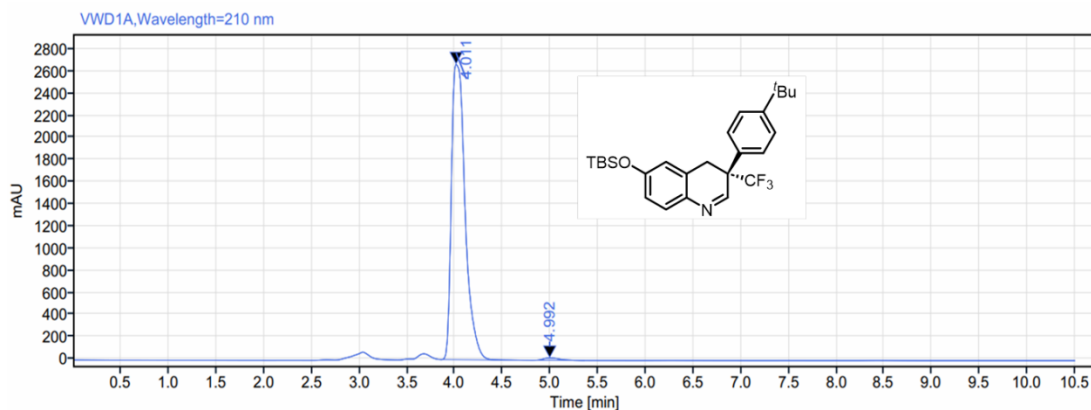
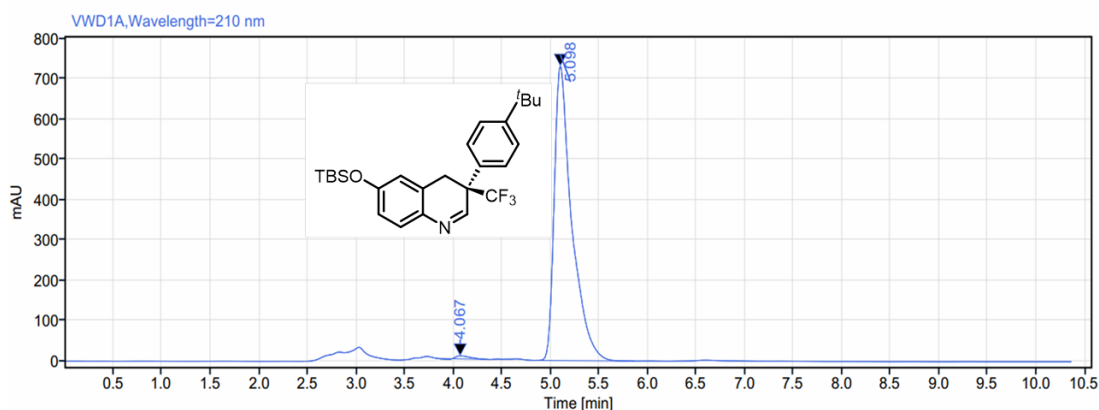
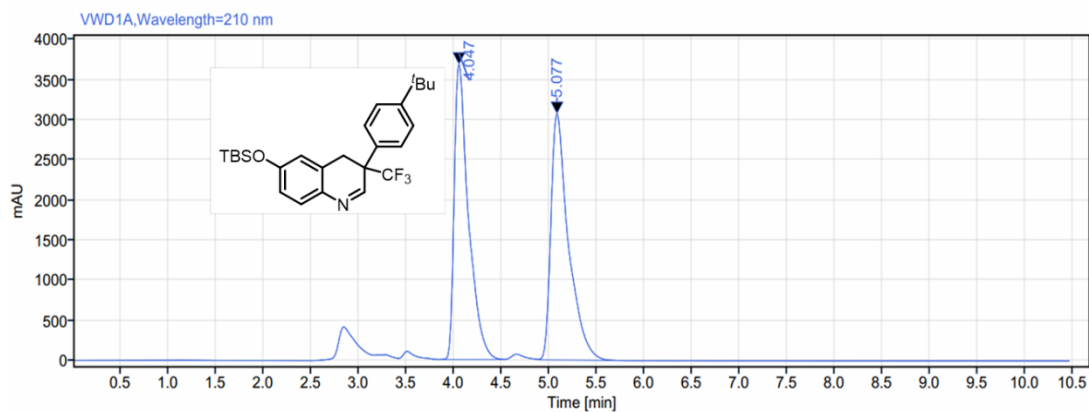
Following General Procedure A, 0.3 mmol (75 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **8** as a yellow solid, mp 87.8-88.3 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.17 (s, 1H), 7.30-7.23 (m, 4H), 7.21 (d, *J* = 8.5 Hz, 1H), 6.66 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.58 (d, *J* = 2.5 Hz, 1H), 3.38 (d, *J* = 16.0 Hz, 1H), 3.29 (d, *J* = 16.0 Hz, 1H), 1.24 (s, 9H), 0.94 (s, 9H), 0.16 (s, 3H), 0.15 (s, 3H).

¹³C NMR (150 MHz, CDCl₃) δ 155.6, 155.3 (q, *J* = 3.0 Hz), 151.4, 136.6, 129.9, 128.3, 127.3, 126.8 (q, *J* = 280.5 Hz), 125.5, 125.2, 119.8, 119.1, 49.0 (q, *J* = 25.5 Hz), 34.4, 31.1, 30.1, 25.6, 18.2, -4.45, -4.47.

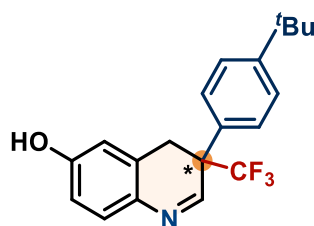
¹⁹F NMR (564 MHz, CDCl₃) δ -71.84.

HRMS (ESI⁺) *m/z* calcd for C₂₆H₃₅F₃NOSi⁺ [M+H]⁺ 462.2435, found 462.2434.

(S)-3-(4-(tert-butyl)phenyl)-6-((tert-butyldimethylsilyl)oxy)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a yellow solid: 70% yield, 98% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 5.098 min, Minor: 4.067 min).
 (R)-3-(4-(tert-butyl)phenyl)-6-((tert-butyldimethylsilyl)oxy)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a yellow solid: 92% yield, 98% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 4.011 min, Minor: 4.992 min).



RT [min]	Width [min]	Area	Height	Area%
4.011	0.78	26691.41	2668.58	99.11
4.992	0.72	238.38	20.33	0.89



Following General Procedure A, 0.3 mmol (40 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **9** as a colorless oil, ^1H NMR (500 MHz, DMSO- d_6) δ 9.71 (s, 1H), 8.23 (s, 1H), 7.42 (d, J = 8.5 Hz, 2H), 7.34 (d, J = 8.5 Hz, 2H), 7.07 (d, J = 8.5 Hz, 1H), 6.70 (d, J = 3.0 Hz, 1H), 6.58 (dd, J = 8.5, 2.5 Hz, 1H), 3.61 (d, J = 16.0 Hz, 1H), 3.19 (d, J = 16.0 Hz, 1H), 1.21 (s, 9H).

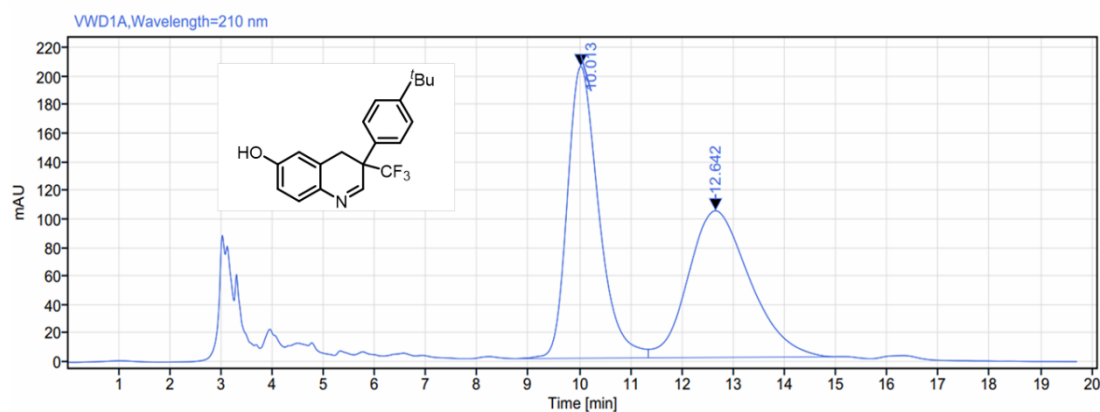
^{13}C NMR (125 MHz, DMSO- d_6) δ 157.9, 154.0, 151.5, 134.8, 130.6, 128.5, 128.2, 127.4 (q, J = 280.0 Hz), 126.0, 125.8, 115.6, 114.6, 48.5 (q, J = 25.0 Hz), 34.7, 31.4, 28.5.

^{19}F NMR (470 MHz, DMSO- d_6) δ -71.18.

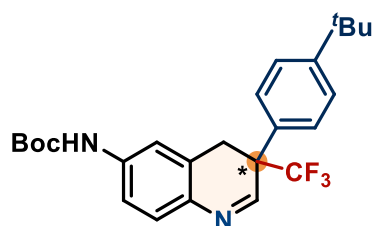
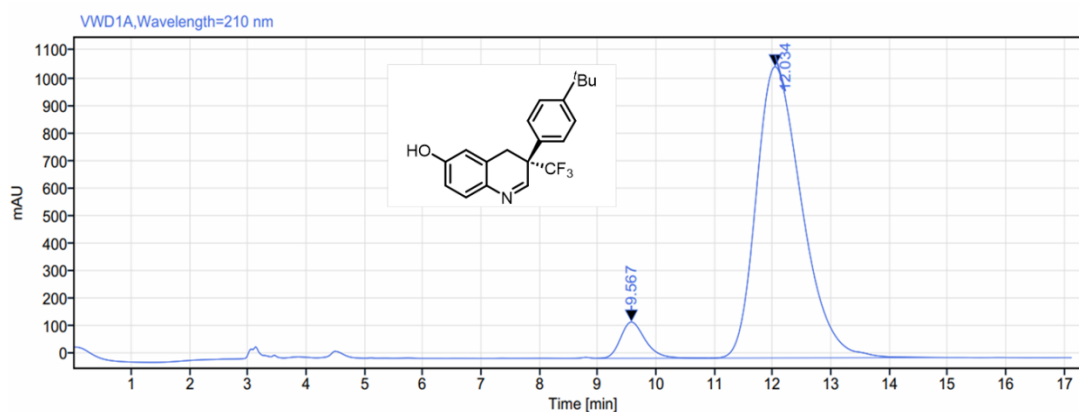
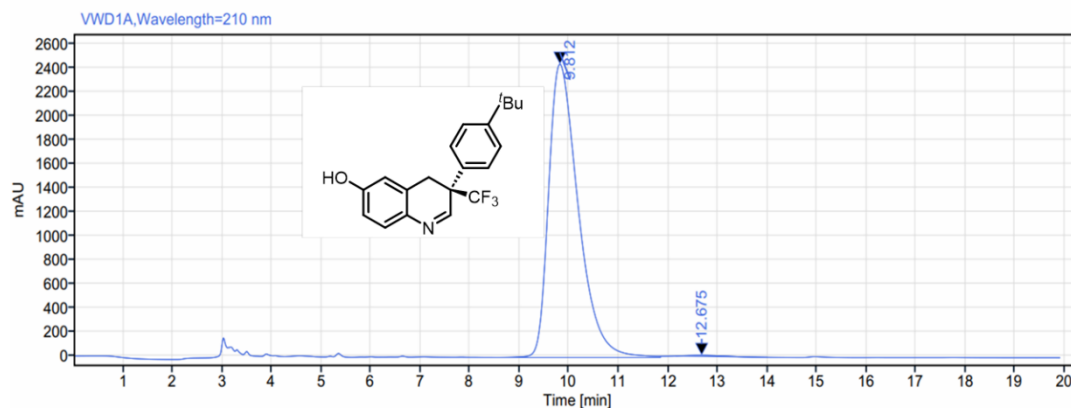
HRMS (ESI $^+$) m/z calcd for $\text{C}_{20}\text{H}_{21}\text{F}_3\text{NO}^+$ $[\text{M}+\text{H}]^+$ 348.1576, found 348.1580.

(*S*)-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinolin-6-ol was prepared following the general procedure as a colorless oil: 44% yield, 99% e.e. (Chiracel OJ-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 9.812 min, Minor: 12.675 min).

(*R*)-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinolin-6-ol was prepared following the general procedure as a colorless oil: 34% yield, 87% e.e. (Chiracel OJ-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 12.034 min, Minor: 9.567 min).



RT [min]	Width [min]	Area	Height	Area%
10.013	2.59	8698.72	204.38	50.37
12.642	3.60	8569.81	102.79	49.63



Following General Procedure A, 0.3 mmol (70 mg) indole and 0.2 mmol (91 mg) *N*-trifosylhydrazone provide **10** as a white solid, mp 173.7-174.9 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.19 (s, 1H), 7.33 (s, 1H), 7.30-7.23 (m, 5H), 7.03 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.64-6.51 (m, 1H), 3.42-3.31 (m, 2H), 1.50 (s, 9H), 1.24 (s, 9H).

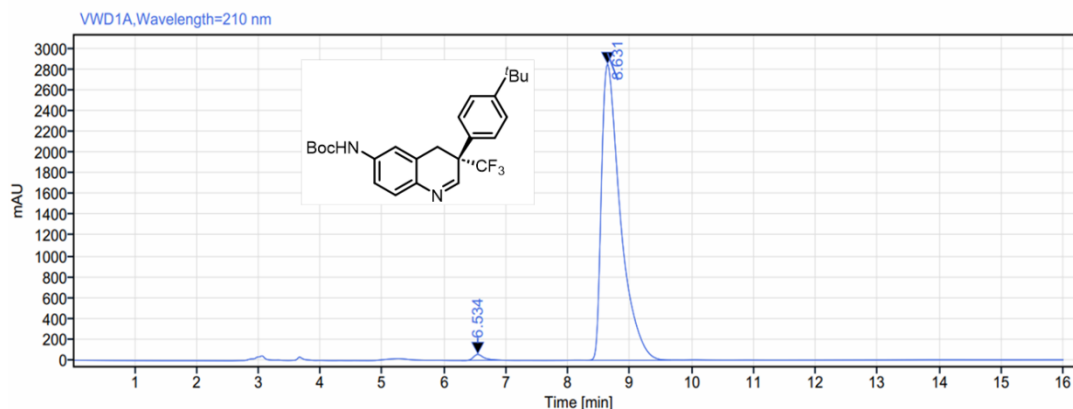
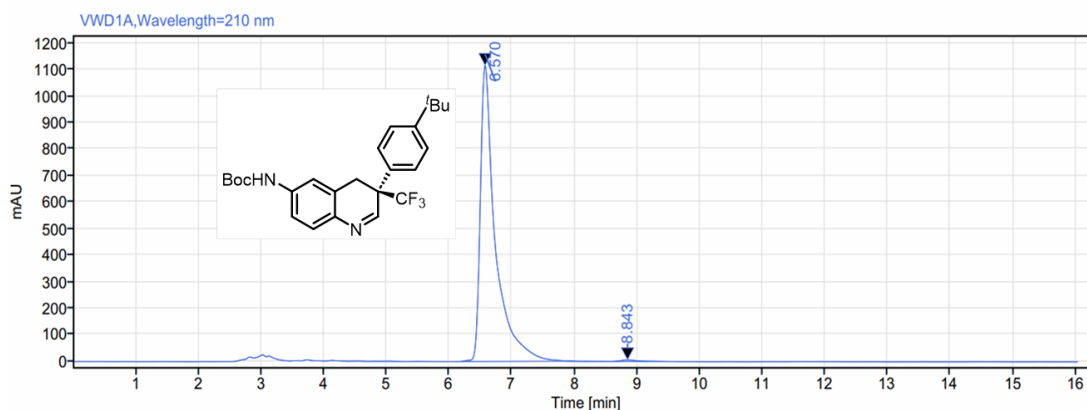
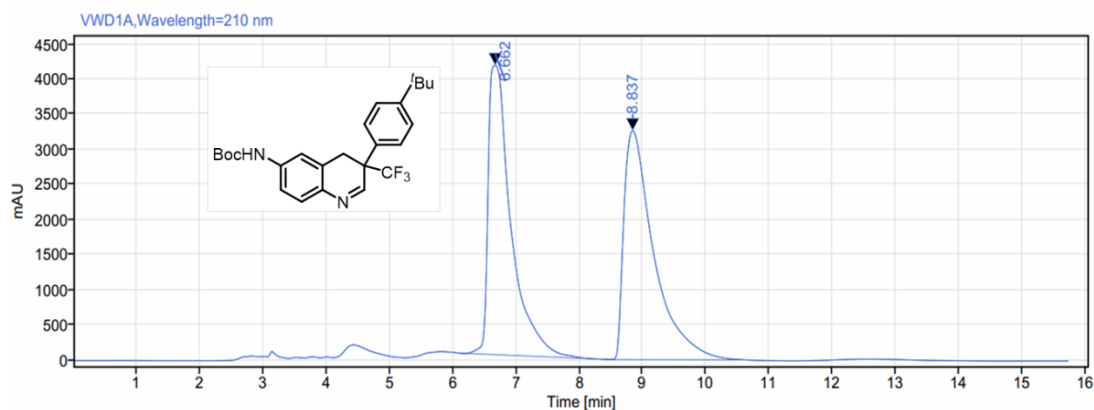
¹³C NMR (150 MHz, CDCl₃) δ 159.6, 144.8, 139.7, 138.3, 134.9, 129.3, 128.9, 128.3, 127.8 (q, *J* = 3.0 Hz), 127.76, 127.74, 124.9 (q, *J* = 294.0 Hz), 123.96 (q, *J* = 2.0 Hz), 117.3, 114.3, 110.0, 82.8 (q, *J* = 25.5 Hz), 34.28 (q, *J* = 1.7 Hz), 21.6.

¹⁹F NMR (564 MHz, CDCl₃) δ -74.63.

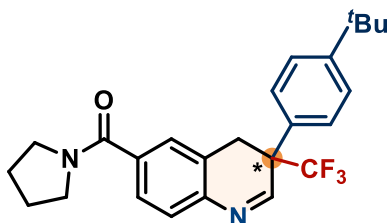
HRMS (ESI⁺) *m/z* calcd for C₂₅H₃₀F₃N₂O₂⁺ [M+H]⁺ 447.2259, found 447.2258.

(*S*)-*tert*-butyl (3-(4-(*tert*-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinolin-6-yl)carbamate was prepared following the general procedure A as a white solid: 97% yield, 99% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 6.570 min, Minor: 8.843 min).

(*R*)-*tert*-butyl (3-(4-(*tert*-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinolin-6-yl)carbamate was prepared following the general procedure A as a white solid: 97% yield, 98% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 8.631 min, Minor: 6.534 min).



RT [min]	Width [min]	Area	Height	Area%
6.534	0.63	679.14	57.91	1.10
8.631	1.37	60850.60	2859.52	98.90



Following General Procedure A, 0.3 mmol (65 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **11** as a white solid, mp 209.1-209.9 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.35 (s, 1H), 7.39-7.35 (m, 2H), 7.30 (s, 1H), 7.28-7.23 (m, 4H), 3.61 (t, $J = 7.0$ Hz, 2H), 3.45-3.39 (m, 2H), 3.36 (t, $J = 6.5$ Hz, 2H), 1.99-1.91 (m, 2H), 1.89-1.82 (m, 2H), 1.24 (s, 9H).

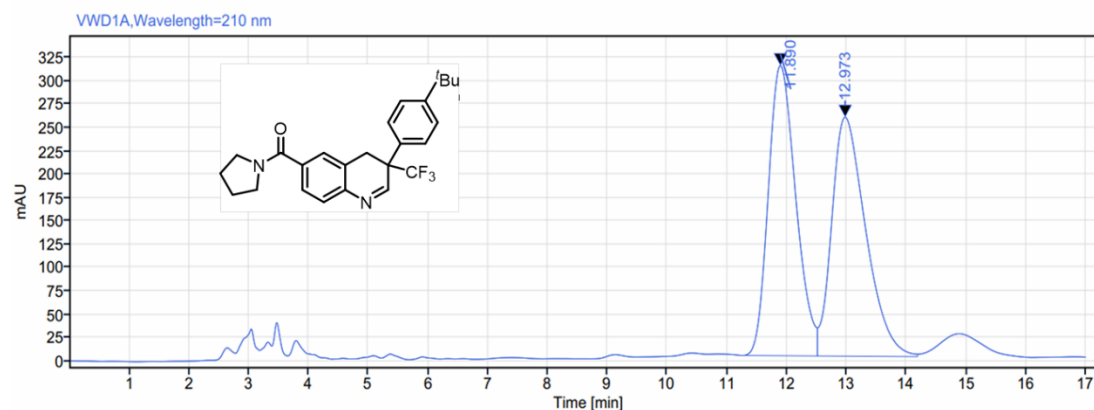
^{13}C NMR (150 MHz, CDCl_3) δ 168.8, 159.1, 151.7, 142.8, 136.9, 129.3, 127.24, 127.19, 126.92, 126.86, 126.6 (q, $J = 280.5$ Hz), 125.7, 123.8, 49.5, 49.3 (q, $J = 25.5$ Hz), 46.2, 34.4, 31.1, 29.9, 26.4, 24.4.

^{19}F NMR (564 MHz, CDCl_3) δ -71.78.

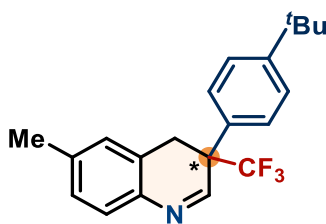
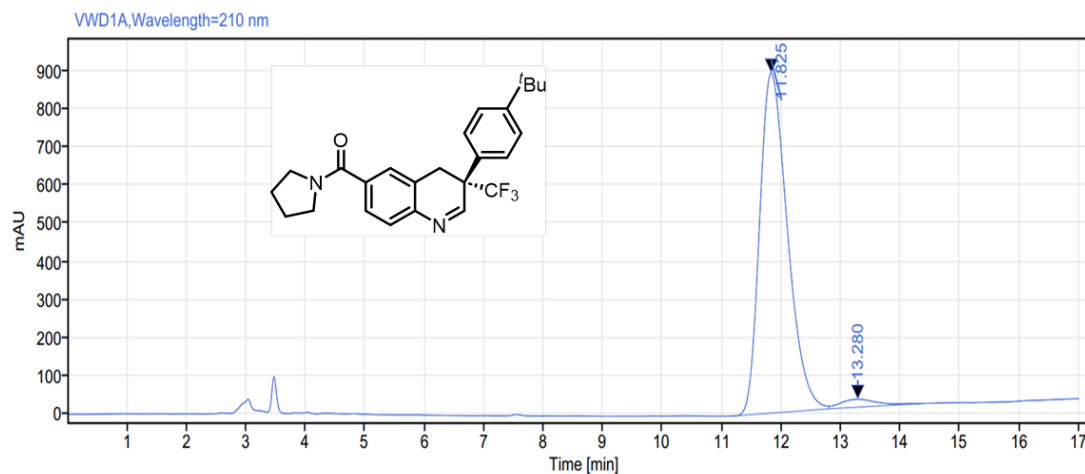
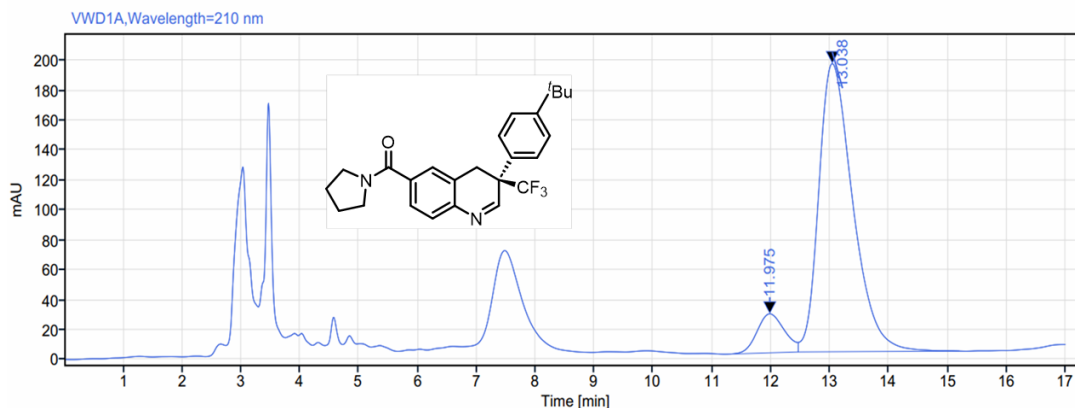
HRMS (ESI $^+$) m/z calcd for $\text{C}_{25}\text{H}_{28}\text{F}_3\text{N}_2\text{O}^+$ $[\text{M}+\text{H}]^+$ 429.2148, found 429.2150.

(*S*)-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinolin-6-yl(pyrrolidin-1-yl)methanone was prepared following the general procedure A as a white solid: 39% yield, 80% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, $\lambda=210$ nm, RT: Major: 13.038 min, Minor: 11.975 min).

(*R*)-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinolin-6-yl(pyrrolidin-1-yl)methanone was prepared following the general procedure A as a white solid: 38% yield, 94% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, $\lambda=210$ nm, RT: Major: 11.825 min, Minor: 13.280 min).



RT [min]	Width [min]	Area	Height	Area%
11.890	1.25	9956.04	310.76	49.60
12.973	1.68	10116.96	256.02	50.40



Following General Procedure A, 0.3 mmol (40 mg) indole and 0.2 mmol (91 mg) *N*-trifosylhydrazone provide **12** as a white solid, mp 153.1-154.3 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.23 (s, 1H), 7.31-7.22 (m, 5H), 7.01 (d, *J* = 7.5 Hz, 1H), 6.91 (s, 1H), 3.42-3.30 (m, 2H), 2.28 (s, 3H), 1.24 (s, 9H).

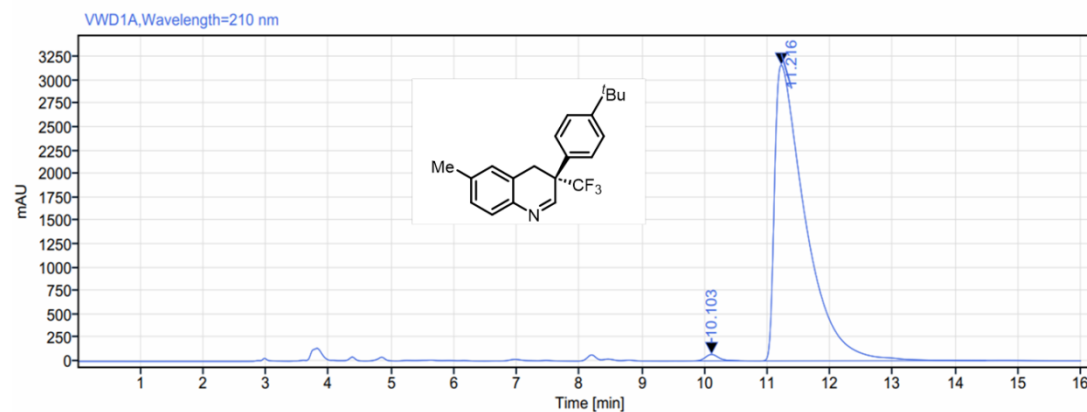
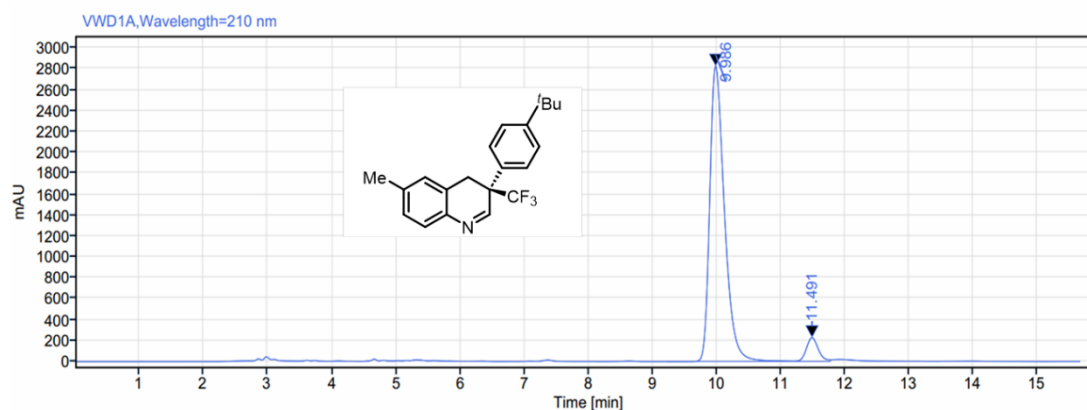
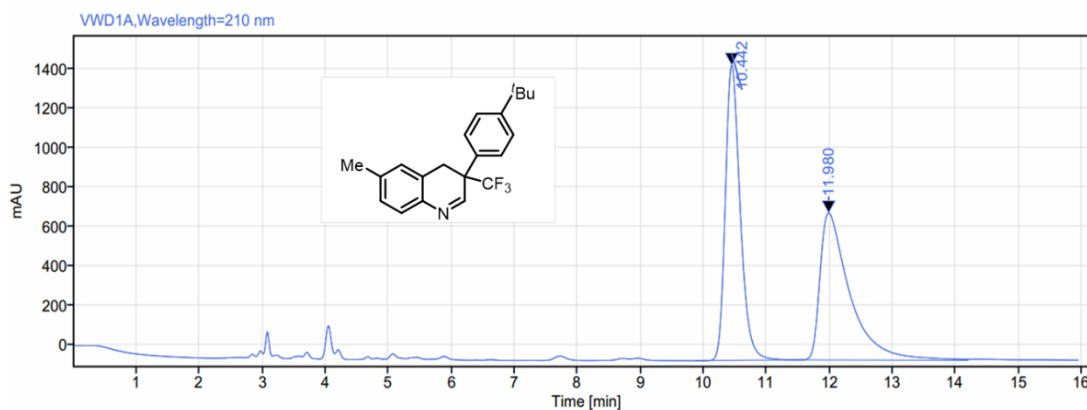
¹³C NMR (150 MHz, CDCl₃) δ 156.4 (q, *J* = 1.5 Hz), 151.4, 139.8, 138.5, 130.0, 128.8, 128.6, 127.3, 127.1, 126.8 (q, *J* = 280.5 Hz), 125.6, 123.3, 49.2 (q, *J* = 25.5 Hz), 34.4, 31.1, 29.8 (q, *J* = 3.0 Hz), 21.2.

¹⁹F NMR (564 MHz, CDCl₃) δ -71.79.

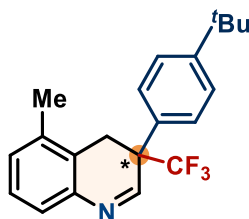
HRMS (ESI⁺) *m/z* calcd for C₂₁H₂₃F₃N⁺ [M+H]⁺ 346.1777, found 346.1783.

(S)-3-(4-(tert-butyl)phenyl)-6-methyl-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 74% yield, 88% e.e. (Chiracel IF, Hexanes/*i*-PrOH = 99/1, 1.0 mL/min, λ =210 nm, RT: Major: 9.986 min, Minor: 11.491 min).

(R)-3-(4-(tert-butyl)phenyl)-6-methyl-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 65% yield, 98% e.e. (Chiracel IF, Hexanes/*i*-PrOH = 99/1, 1.0 mL/min, λ =210 nm, RT: Major: 11.216 min, Minor: 10.103 min).



RT [min]	Width [min]	Area	Height	Area%
10.103	0.79	1041.84	69.57	0.96
11.216	3.64	107317.25	3162.91	99.04



Following General Procedure A, 0.3 mmol (40 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **13** as a white solid, mp 105.2-106.7 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.29 (s, 1H), 7.28-7.25 (m, 4H), 7.21 (d, *J* = 8.0 Hz, 1H), 7.12 (t, *J* = 7.5 Hz, 1H), 7.03 (d, *J* = 7.5 Hz, 1H), 3.52 (dd, *J* = 16.4, 1.6 Hz, 1H), 3.15 (d, *J* = 16.4 Hz, 1H), 2.32 (s, 3H), 1.23 (s, 9H).

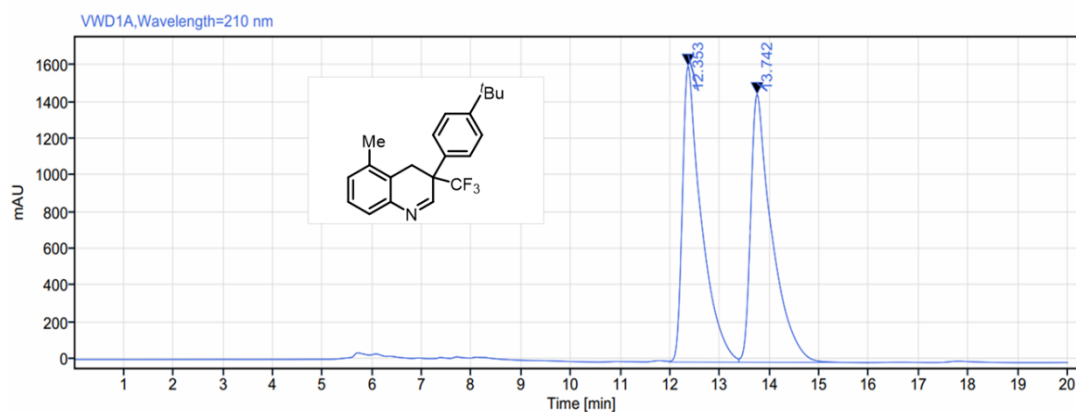
¹³C NMR (125 MHz, CDCl₃) δ 157.0 (q, *J* = 2.5 Hz), 151.5, 141.8, 135.3, 130.3, 130.2, 127.1, 127.0, 126.8 (q, *J* = 281.3 Hz), 125.6, 125.2, 122.0, 49.1 (q, *J* = 25.0 Hz), 34.4, 31.1, 26.3 (q, *J* = 2.5 Hz), 18.8.

¹⁹F NMR (470 MHz, CDCl₃) δ -71.81.

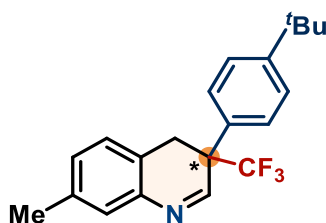
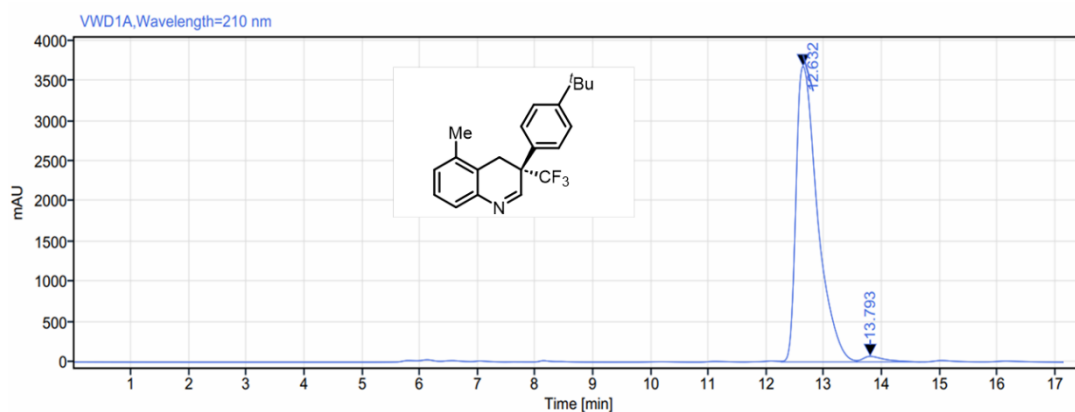
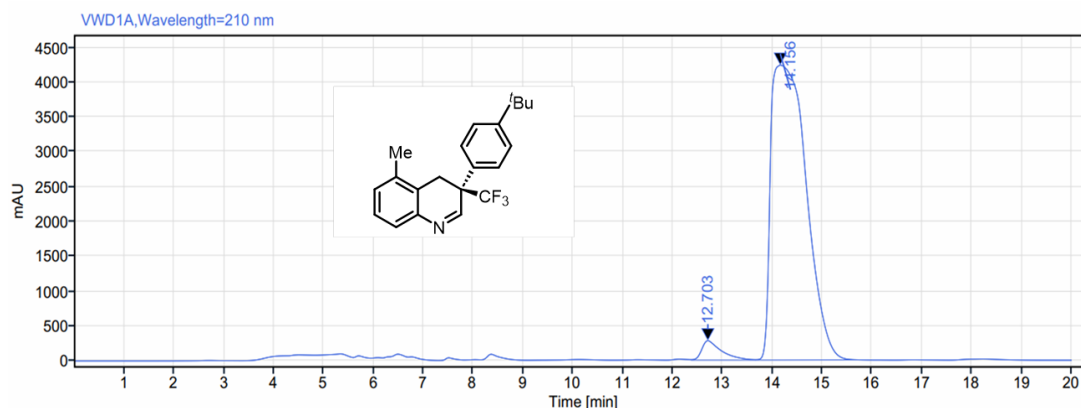
HRMS (ESI⁺) *m/z* calcd for C₂₁H₂₃F₃N⁺ [M+H]⁺ 346.1777, found 346.1783.

(*S*)-3-(4-(tert-butyl)phenyl)-5-methyl-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 58% yield, 93% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 98/2, 0.5 mL/min, λ=210 nm, RT: Major: 14.156 min, Minor: 12.703 min).

(*R*)-3-(4-(tert-butyl)phenyl)-5-methyl-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 67% yield, 96% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 98/2, 0.5 mL/min, λ=210 nm, RT: Major: 12.632 min, Minor: 13.793 min).



RT [min]	Width [min]	Area	Height	Area%
12.353	1.41	42738.23	1608.56	49.76
13.742	2.62	43144.51	1455.50	50.24



Following General Procedure A, 0.3 mmol (40 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **14** as a red solid, mp 129.1-130.8 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.28 (s, 1H), 7.31-7.23 (m, 4H), 7.17 (s, 1H), 7.01-6.94 (m, 2H), 3.40-3.31 (m, 2H), 2.29 (s, 3H), 1.23 (s, 9H).

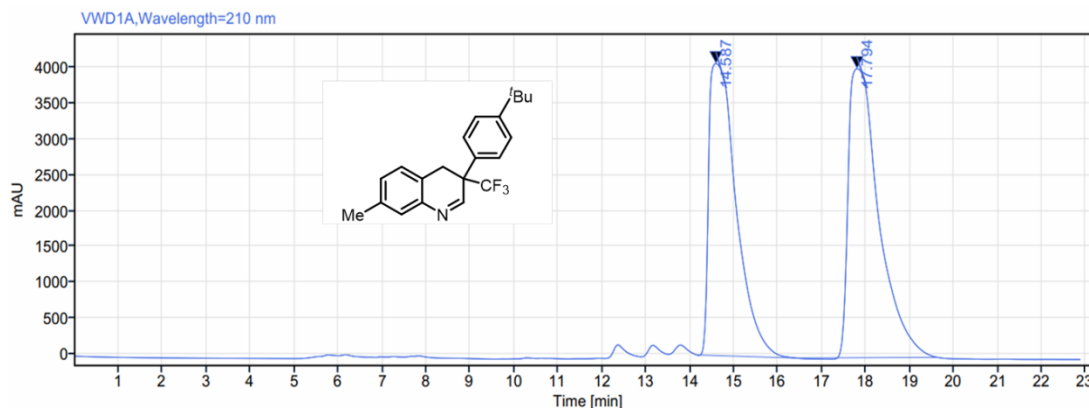
¹³C NMR (150 MHz, CDCl₃) δ 157.5 (q, *J* = 1.5 Hz), 151.4, 141.7, 137.7, 129.9, 129.1, 127.9, 127.8, 127.3, 126.8 (q, *J* = 282.0 Hz), 125.5, 120.4, 49.3 (q, *J* = 25.5 Hz), 34.4, 31.1, 29.4, 21.0.

¹⁹F NMR (564 MHz, CDCl₃) δ -71.82.

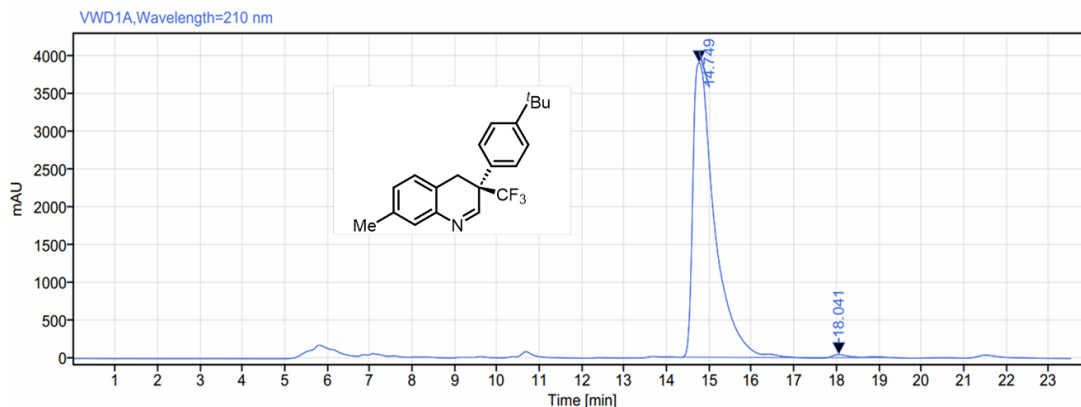
HRMS (ESI⁺) *m/z* calcd for C₂₁H₂₃F₃N⁺ [M+H]⁺ 346.1777, found 346.1783.

(*S*)-3-(4-(tert-butyl)phenyl)-7-methyl-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a red solid: 77% yield, 98% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 99/1, 0.5 mL/min, λ=210 nm, RT: Major: 14.749 min, Minor: 18.041 min).

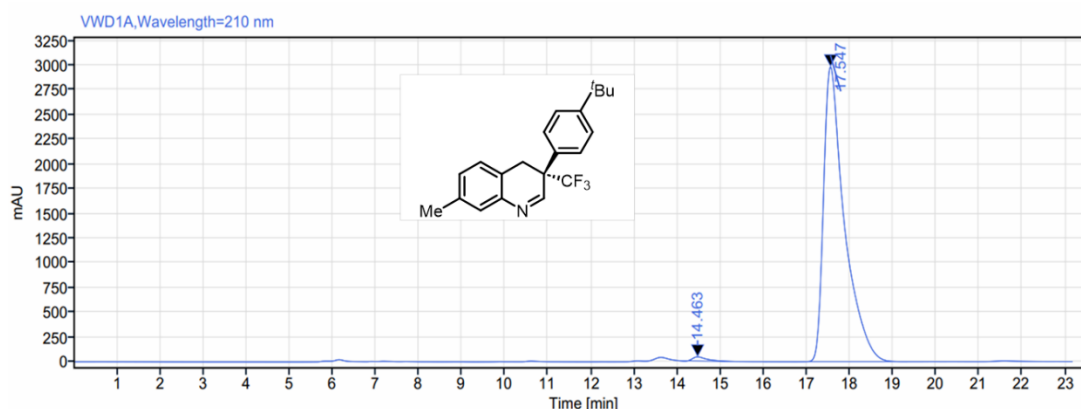
(*R*)-3-(4-(*tert*-butyl)phenyl)-7-methyl-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a red solid: 83% yield, 98% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 99/1, 0.5 mL/min, λ =210 nm, RT: Major: 17.547 min, Minor: 14.463 min).



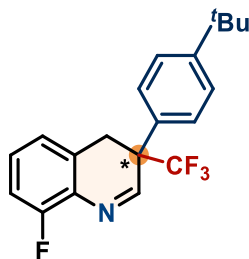
RT [min]	Width [min]	Area	Height	Area%
14.587	2.23	176159.99	4068.51	47.68
17.794	3.24	193287.64	4028.71	52.32



RT [min]	Width [min]	Area	Height	Area%
14.749	2.84	137262.67	3889.15	99.13
18.041	2.11	1198.57	40.34	0.87



RT [min]	Width [min]	Area	Height	Area%
14.463	2.84	915.46	41.46	0.90
17.547	3.32	100349.16	2987.54	99.10



Following General Procedure A, 0.3 mmol (41 mg) indole and 0.2 mmol (91 mg) *N*-trifosylhydrazone provide **15** as a white solid, mp 125.2–126.3 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.36 (s, 1H), 7.32–7.26 (m, 4H), 7.15–7.09 (m, 1H), 6.99–6.89 (m, 2H), 3.42 (ABq, J = 16.5 Hz, 2H), 1.24 (s, 9H).

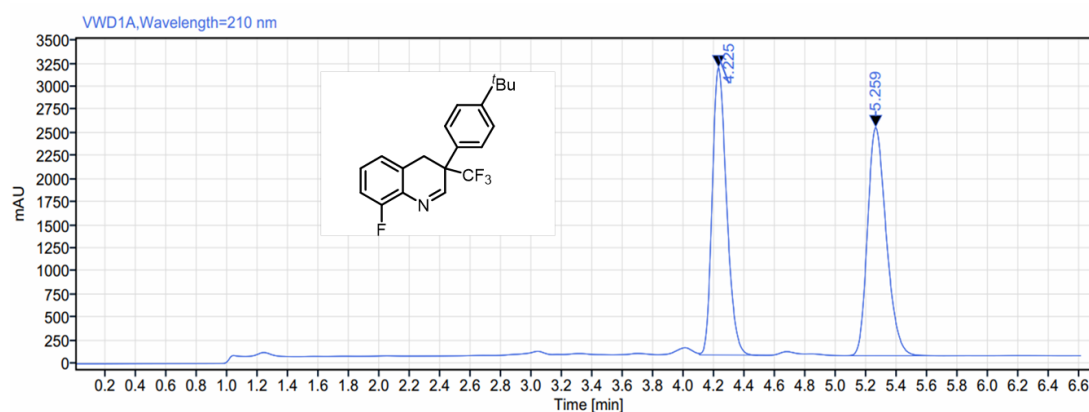
^{13}C NMR (150 MHz, CDCl_3) δ 158.5, 157.5 (d, J = 253.5 Hz), 151.8, 130.2 (d, J = 9.0 Hz), 129.291 (d, J = 9.0 Hz), 129.289, 127.3, 126.5 (q, J = 280.5 Hz), 126.1, 125.7, 123.4 (d, J = 3.0 Hz), 115.4 (d, J = 19.5 Hz), 49.1 (q, J = 25.5 Hz), 34.5, 31.1, 29.4.

^{19}F NMR (564 MHz, CDCl_3) δ -71.92, -125.37 (dd, J = 10.2, 5.6 Hz).

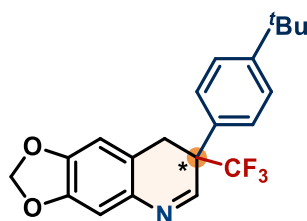
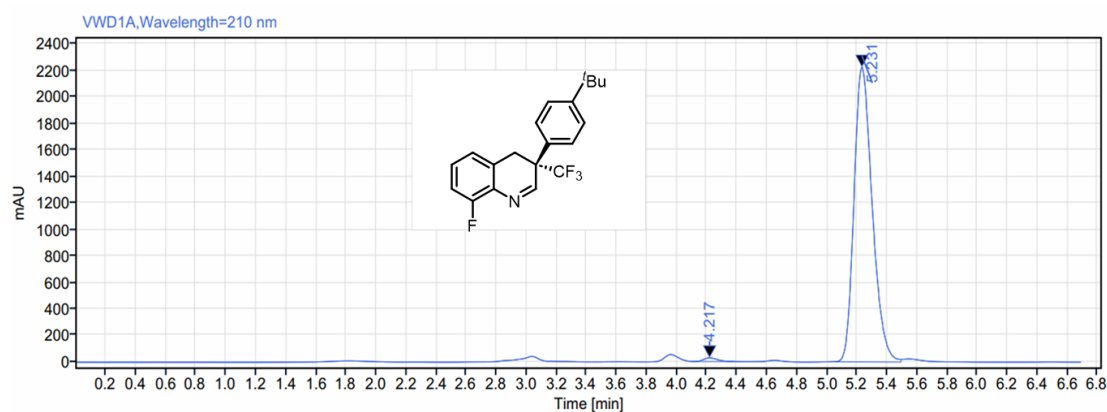
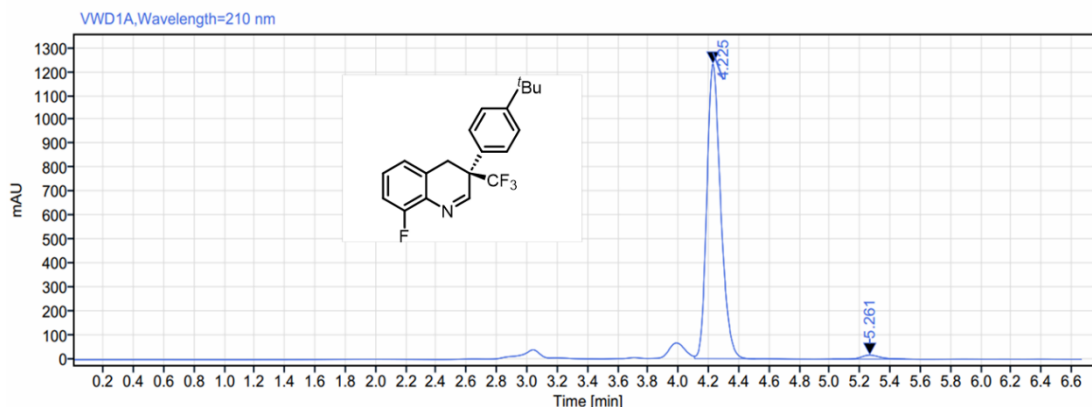
HRMS (ESI $^+$) m/z calcd for $\text{C}_{20}\text{H}_{20}\text{F}_4\text{N}^+$ $[\text{M}+\text{H}]^+$ 350.1526, found 350.1530.

(*S*)-3-(4-(tert-butyl)phenyl)-8-fluoro-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 80% yield, 96% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 4.225 min, Minor: 5.261 min).

(*R*)-3-(4-(tert-butyl)phenyl)-8-fluoro-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 78% yield, 98% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 5.231 min, Minor: 4.217 min).



RT [min]	Width [min]	Area	Height	Area%
4.225	0.39	20512.56	3116.81	49.24
5.259	0.65	21145.13	2474.40	50.76



Following General Procedure A, 0.3 mmol (49 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **16** as a white solid, mp 119.6-121.7 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.21 (s, 1H), 7.32-7.29 (m, 4H), 6.89 (s, 1H), 6.60 (s, 1H), 5.94 (d, *J* = 5.0 Hz, 2H), 3.41-3.25 (m, 2H), 1.28 (s, 9H).

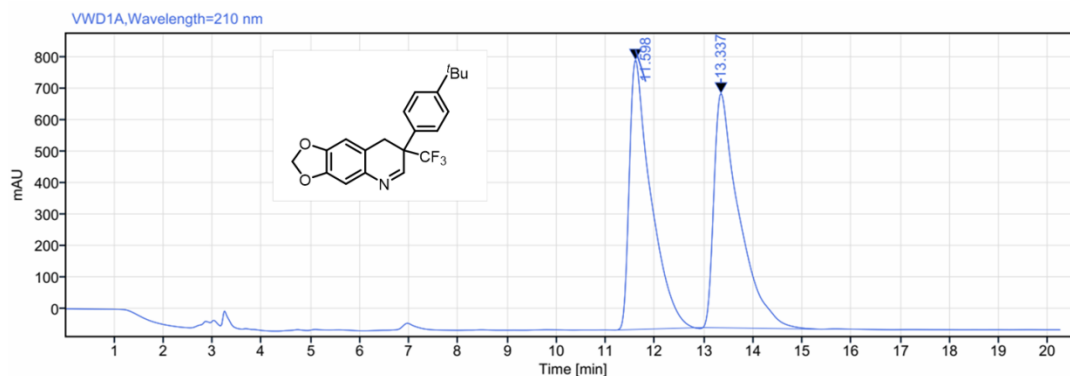
¹³C NMR (150 MHz, CDCl₃) δ 155.5, 151.5, 147.2, 147.0, 136.7, 129.7, 127.3, 126.8 (q, *J* = 280.5 Hz), 125.5, 117.3, 108.2, 107.9, 101.4, 49.0 (q, *J* = 24.0 Hz), 34.5, 31.1, 29.9.

¹⁹F NMR (564 MHz, CDCl₃) δ -71.71.

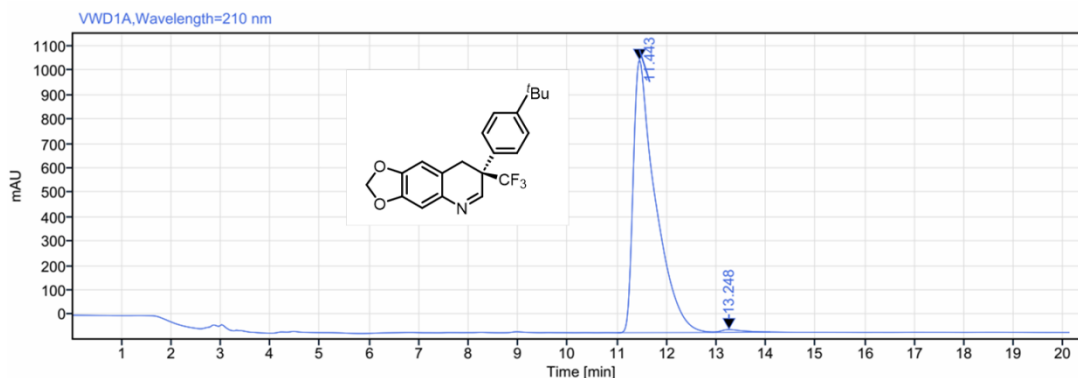
HRMS (ESI⁺) *m/z* calcd for C₂₁H₂₁F₃NO₂⁺ [M+H]⁺ 376.1519, found 376.1514.

(*S*)-7-(4-(tert-butyl)phenyl)-7-(trifluoromethyl)-7,8-dihydro-[1,3]dioxolo[4,5-*g*]quinoline was prepared following the general procedure A as a white solid: 68% yield, 98% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 99/1, 1.0 mL/min, λ=210 nm, RT: Major: 11.443 min, Minor: 13.248 min).

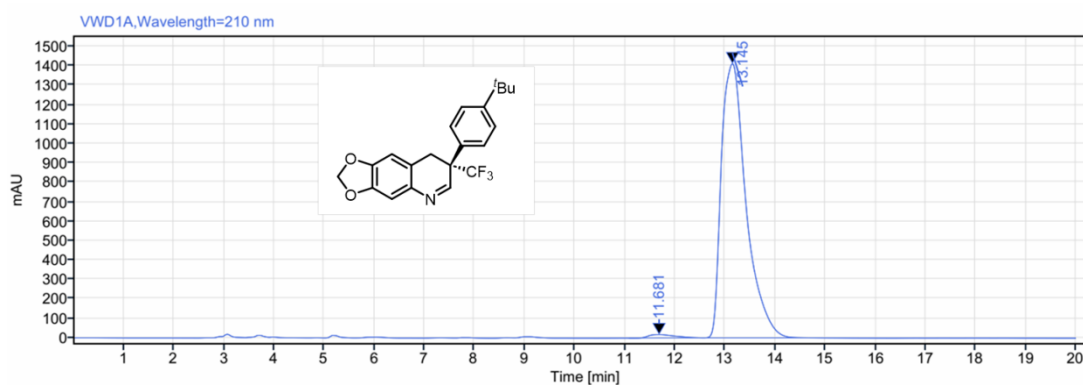
(*R*)-7-(4-(*tert*-butyl)phenyl)-7-(trifluoromethyl)-7,8-dihydro-[1,3]dioxolo[4,5-*g*]quinoline was prepared following the general procedure A as a white solid: 88% yield, 97% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 99/1, 1.0 mL/min, λ =210 nm, RT: Major: 13.145 min, Minor: 11.681 min).



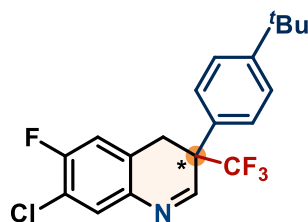
RT [min]	Width [min]	Area	Height	Area%
11.598	1.80	26203.31	859.26	49.50
13.337	2.41	26737.81	747.18	50.50



RT [min]	Width [min]	Area	Height	Area%
11.443	1.93	34717.05	1114.79	99.02
13.248	1.16	344.22	11.39	0.98



RT [min]	Width [min]	Area	Height	Area%
11.681	1.48	645.24	17.71	1.31
13.145	2.15	48423.71	1413.81	98.69



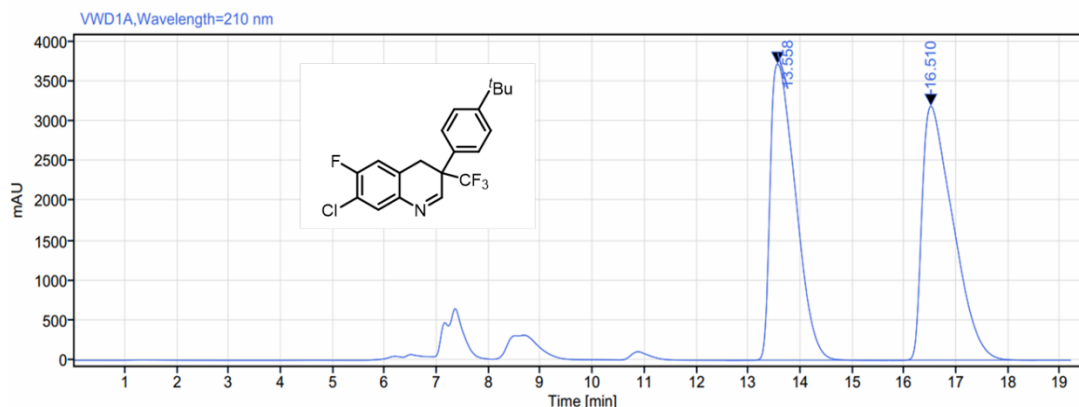
Following General Procedure A, 0.3 mmol (51 mg) indole and 0.2 mmol (91 mg) *N*-trifosylhydrazone provide **17** as a white solid, mp 129.0-129.7 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.29 (s, 1H), 7.42 (d, J = 7.0 Hz, 1H), 7.29 (d, J = 8.0 Hz, 2H), 7.24 (d, J = 8.0 Hz, 2H), 6.92 (d, J = 9.0 Hz, 1H), 3.35 (s, 2H), 1.25 (s, 9H).

^{13}C NMR (125 MHz, CDCl_3) δ 158.5 (q, J = 2.5 Hz), 157.2 (d, J = 250.0 Hz), 152.0, 138.7 (d, J = 3.8 Hz), 129.3, 129.1, 127.2, 126.5 (q, J = 280.0 Hz), 125.8, 124.3 (d, J = 7.5 Hz), 119.8 (d, J = 18.8 Hz), 116.1 (d, J = 22.5 Hz), 48.9 (q, J = 25.0 Hz), 34.5, 31.1, 29.6.

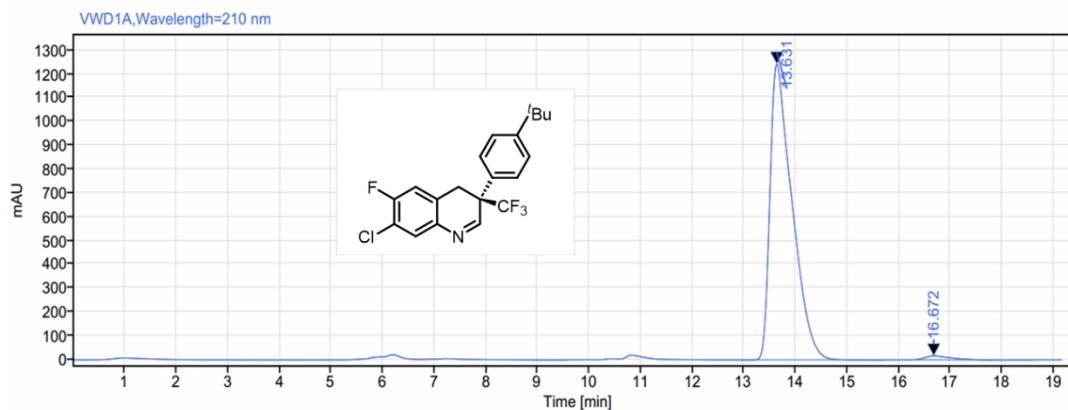
^{19}F NMR (470 MHz, CDCl_3) δ -71.86, -114.84 (t, J = 8.0 Hz).

(*S*)-3-(4-(tert-butyl)phenyl)-7-chloro-6-fluoro-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 98% yield, 96% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 99/1, 0.5 mL/min, λ =210 nm, RT: Major: 13.631 min, Minor: 16.672 min).

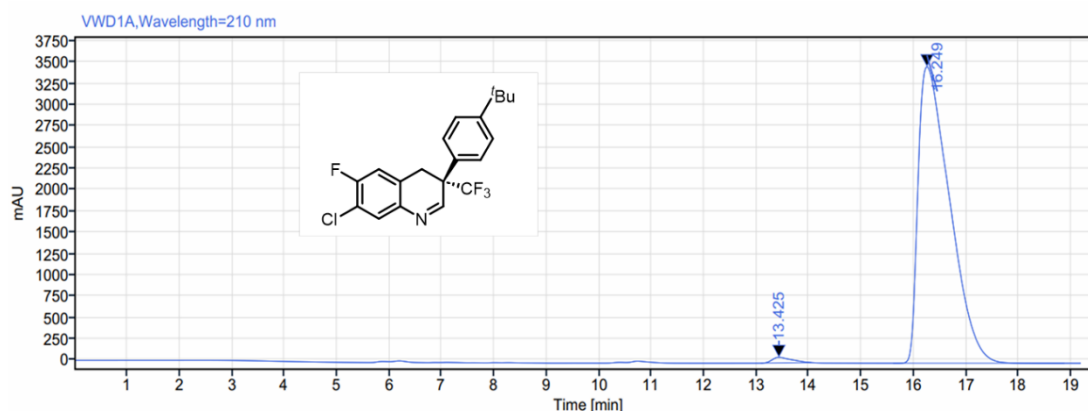
(*R*)-3-(4-(tert-butyl)phenyl)-7-chloro-6-fluoro-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 98% yield, 97% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 16.249 min, Minor: 13.425 min).



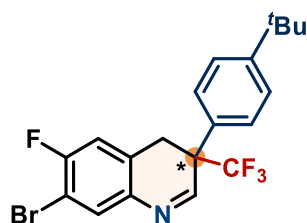
RT [min]	Width [min]	Area	Height	Area%
13.558	3.13	126005.16	3721.57	48.86
16.510	2.82	131875.71	3192.72	51.14



RT [min]	Width [min]	Area	Height	Area%
13.631	2.77	36833.96	1242.96	98.38
16.672	1.68	605.35	16.86	1.62



RT [min]	Width [min]	Area	Height	Area%
13.425	0.96	1684.73	65.82	1.15
16.249	3.26	145220.93	3481.97	98.85



Following General Procedure A, 0.3 mmol (65 mg) indole and 0.2 mmol (91 mg) *N*-trifosylhydrazone provide **18** as a white solid, mp 124.3–126.0 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.29 (s, 1H), 7.56 (d, J = 6.5 Hz, 1H), 7.29 (d, J = 8.5 Hz, 2H), 7.24 (d, J = 8.5 Hz, 2H), 6.90 (d, J = 8.0 Hz, 1H), 3.39–3.29 (m, 2H), 1.25 (s, 9H).

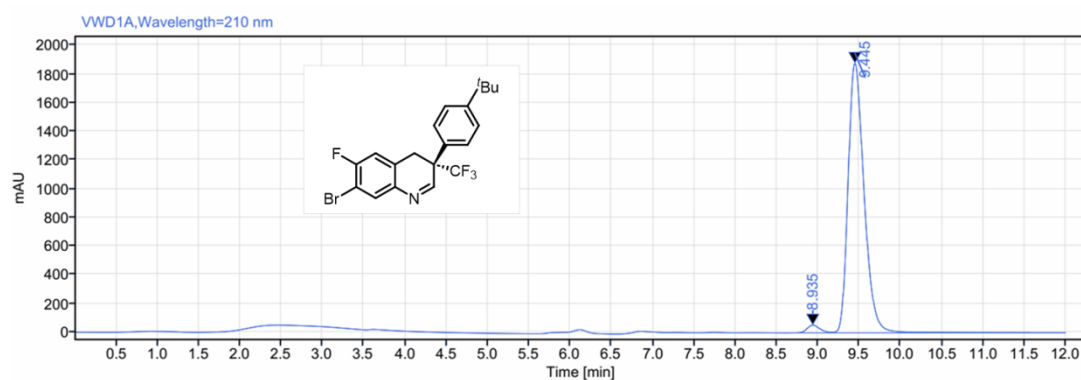
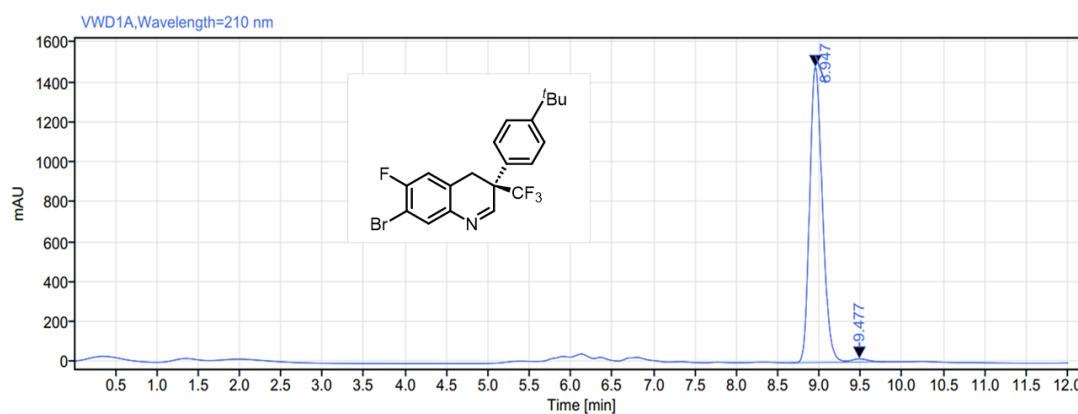
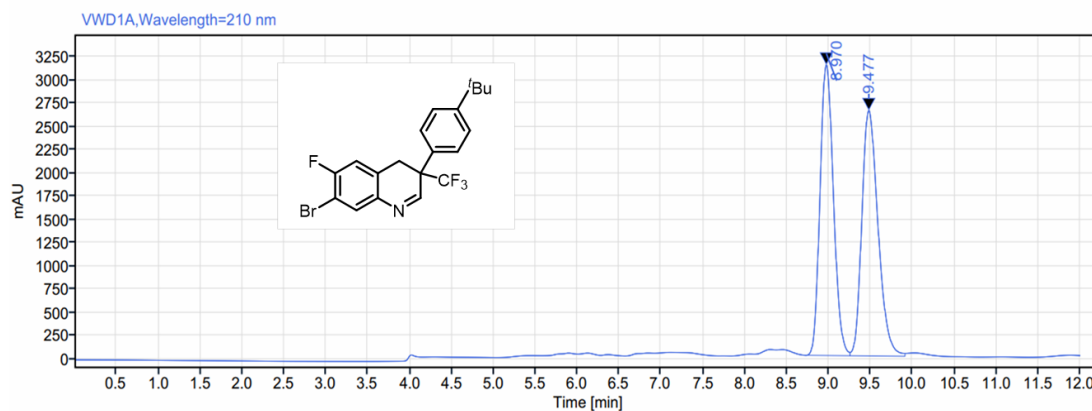
^{13}C NMR (150 MHz, CDCl_3) δ 158.5 (q, J = 3.0 Hz), 158.2 (d, J = 247.5 Hz), 152.0, 139.1 (d, J = 3.0 Hz), 132.1, 129.0, 127.2, 126.5 (q, J = 280.5 Hz), 125.8, 125.1 (d, J = 7.5 Hz), 115.9 (d, J = 24.0 Hz), 107.5 (d, J = 22.5 Hz), 48.8 (d, J = 25.5 Hz), 34.5, 31.1, 29.6.

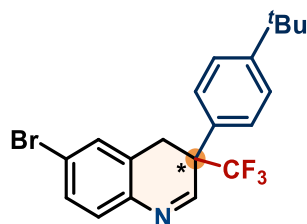
^{19}F NMR (564 MHz, CDCl_3) δ -71.86, -106.90 (t, J = 7.5 Hz).

HRMS (ESI $^+$) m/z calcd for $\text{C}_{20}\text{H}_{19}\text{BrF}_4\text{N}^+$ $[\text{M}+\text{H}]^+$ 428.0632, found 428.0625.

(*S*)-7-bromo-3-(4-(tert-butyl)phenyl)-6-fluoro-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 73% yield, 97% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 99/1, 0.5 mL/min, λ =210 nm, RT: Major: 8.947 min, Minor: 9.477 min).

(*R*)-7-bromo-3-(4-(tert-butyl)phenyl)-6-fluoro-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 90% yield, 95% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 99/1, 0.5 mL/min, λ =210 nm, RT: Major: 9.445 min, Minor: 8.935 min).





Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **19** as a white solid, mp 194.5-196.2 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.30 (s, 1H), 7.34 (dd, J = 8.0, 2.0 Hz, 1H), 7.30-7.24 (m, 5H), 7.22 (d, J = 8.5 Hz, 1H), 3.42-3.32 (m, 2H), 1.25 (s, 9H).

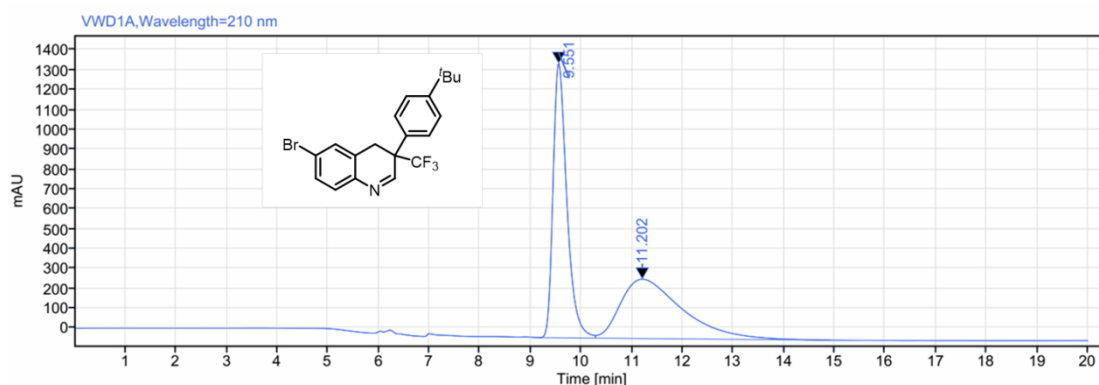
^{13}C NMR (125 MHz, CDCl_3) δ 158.2 (q, J = 2.5 Hz), 151.8, 140.9, 131.2, 131.0, 129.3, 128.7, 127.2, 126.5 (q, J = 281.3 Hz), 125.7, 121.8, 49.0 (q, J = 25.0 Hz), 34.5, 31.1, 29.6 (q, J = 2.5 Hz).

^{19}F NMR (470 MHz, CDCl_3) δ -71.80

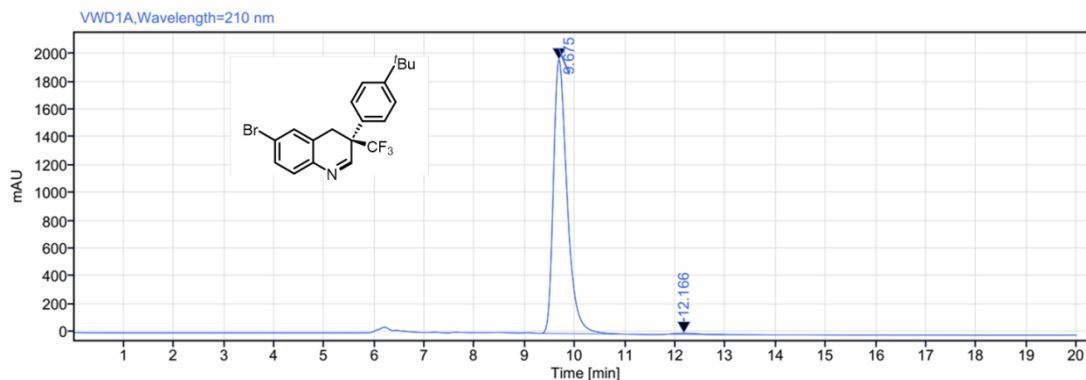
HRMS (ESI $^+$) m/z calcd for $\text{C}_{20}\text{H}_{20}\text{BrF}_3\text{N}^+$ $[\text{M}+\text{H}]^+$ 410.0726, found 410.0718.

(*S*)-6-bromo-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 86% yield, 99% e.e. (Chiracel OJ-H, Hexanes/*i*-PrOH = 98/2, 0.5 mL/min, λ =210 nm, RT: Major: 9.675 min, Minor: 12.166 min).

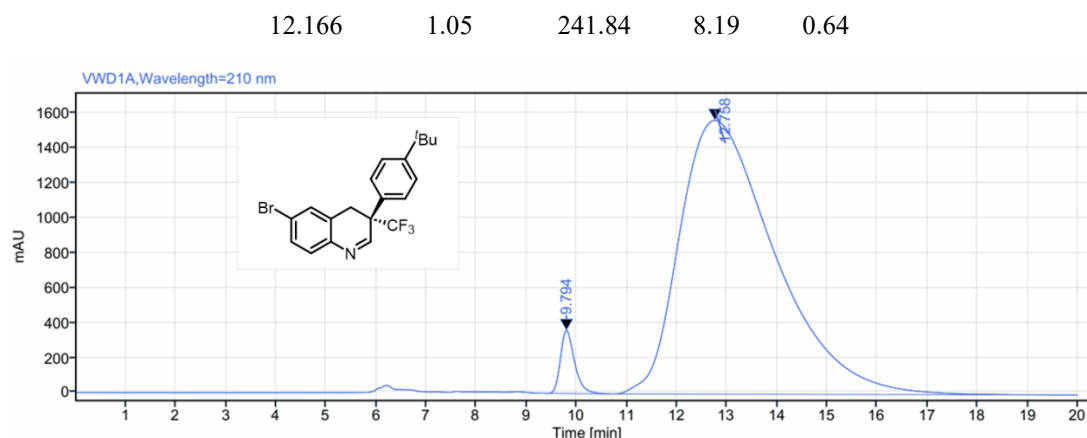
(*R*)-6-bromo-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 84% yield, 93% e.e. (Chiracel OJ-H, Hexanes/*i*-PrOH = 98/2, 0.5 mL/min, λ =210 nm, RT: Major: 12.758 min, Minor: 9.794 min).



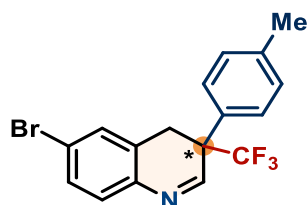
RT [min]	Width [min]	Area	Height	Area%
9.551	1.12	26039.37	1380.81	50.75
11.202	4.65	25272.68	298.71	49.25



RT [min]	Width [min]	Area	Height	Area%
9.675	1.58	37298.46	1967.99	99.36



RT [min]	Width [min]	Area	Height	Area%
9.794	1.30	7076.82	360.67	3.32
12.758	8.26	206382.30	1566.35	96.68



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (83 mg) *N*-trifosylhydrazone provide **20** as a white solid, mp 103.5-104.7 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.32 (s, 1H), 7.37-7.30 (m, 1H), 7.25-7.17 (m, 4H), 7.08 (d, *J* = 8.0 Hz, 2H), 3.41-3.30 (m, 2H), 2.27 (s, 3H).

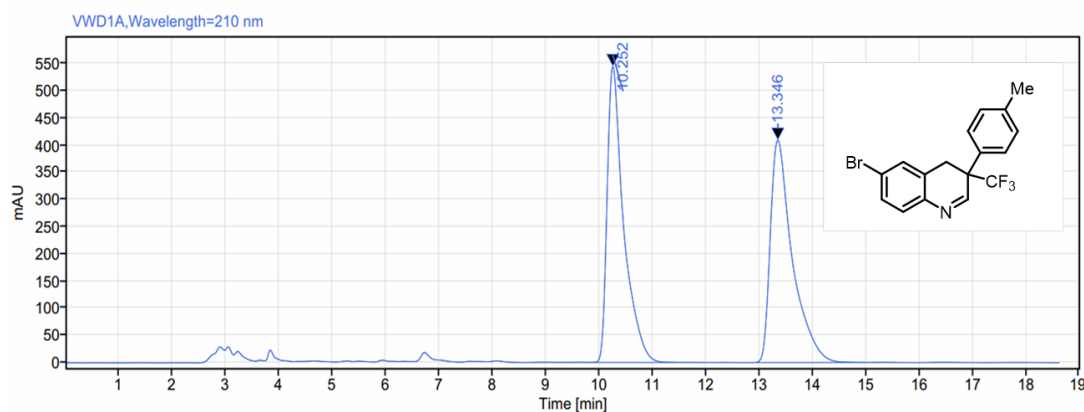
¹³C NMR (125 MHz, CDCl₃) δ 158.4 (q, *J* = 2.5 Hz), 141.0, 138.9, 131.2, 130.9, 129.5, 129.3, 128.6, 127.5, 126.5 (q, *J* = 281.3 Hz), 125.7, 121.8, 49.0 (q, *J* = 25.0 Hz), 29.7 (q, *J* = 2.5 Hz), 21.0.

¹⁹F NMR (470 MHz, CDCl₃) δ -71.79.

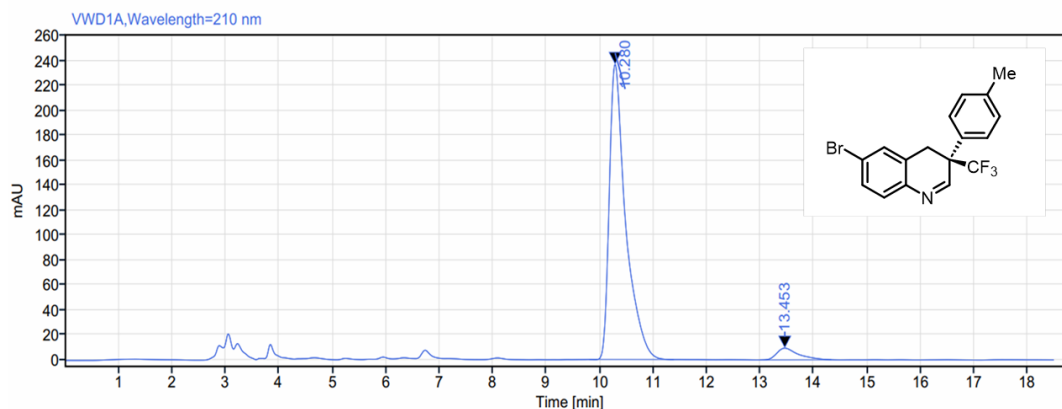
HRMS (ESI⁺) *m/z* calcd for C₁₇H₁₄BrF₃N⁺ [M+H]⁺ 368.0256, found 368.0254.

(*S*)-6-bromo-3-(*p*-tolyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 97% yield, 90% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 98/2, 1.0 mL/min, λ=210 nm, RT: Major: 10.280 min, Minor: 13.453 min).

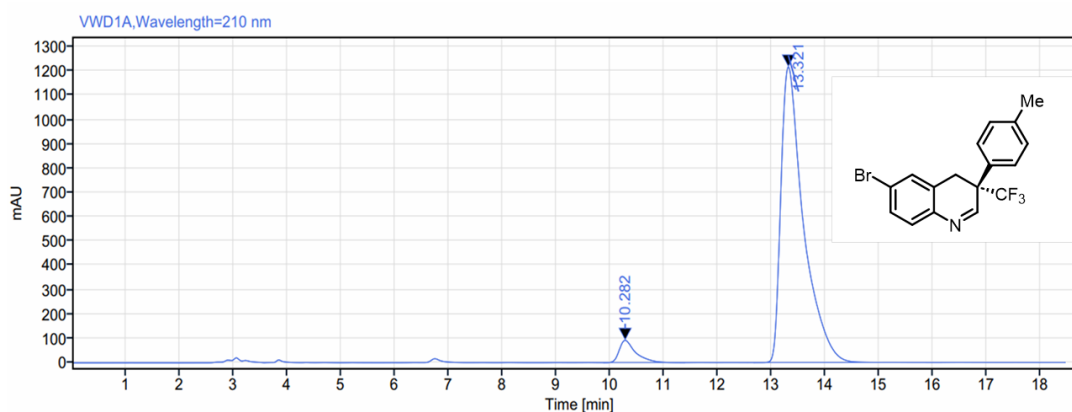
(*R*)-6-bromo-3-(*p*-tolyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 98% yield, 90% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 98/2, 1.0 mL/min, λ=210 nm, RT: Major: 13.321 min, Minor: 10.282 min).



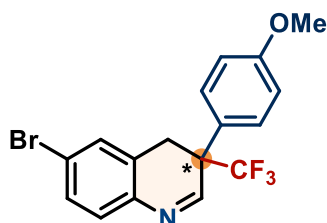
RT [min]	Width [min]	Area	Height	Area%
10.252	1.61	11700.13	544.42	49.95
13.346	2.15	11723.26	409.20	50.05



RT [min]	Width [min]	Area	Height	Area%
10.280	1.58	5038.41	236.41	95.01
13.453	1.34	264.37	9.40	4.99



RT [min]	Width [min]	Area	Height	Area%
10.282	1.52	1942.64	91.81	5.20
13.321	2.31	35423.00	1217.11	94.80



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (86 mg) *N*-trifosylhydrazone provide **21** as a white solid, mp 123.1-124.5 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.31 (s, 1H), 7.34 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.29-7.23 (m, 3H), 7.21 (d, *J* = 8.5 Hz, 1H), 6.82-6.77 (m, 2H), 3.74 (s, 3H), 3.40-3.28 (m, 2H).

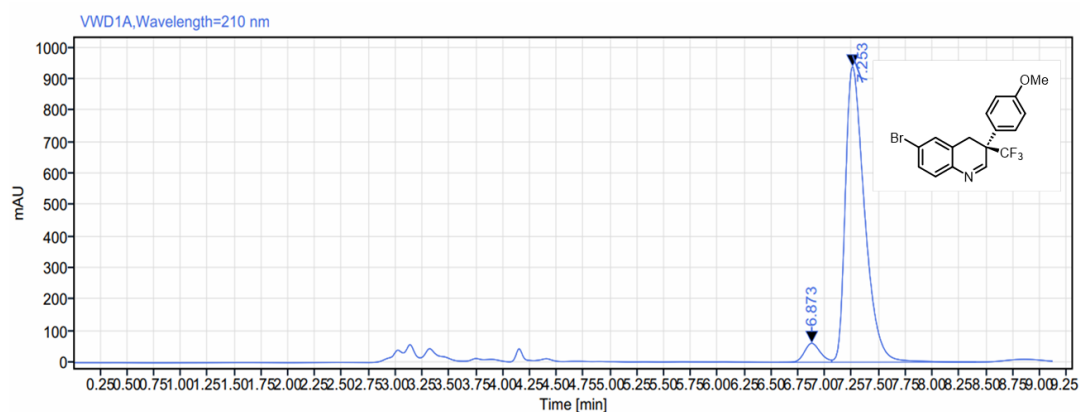
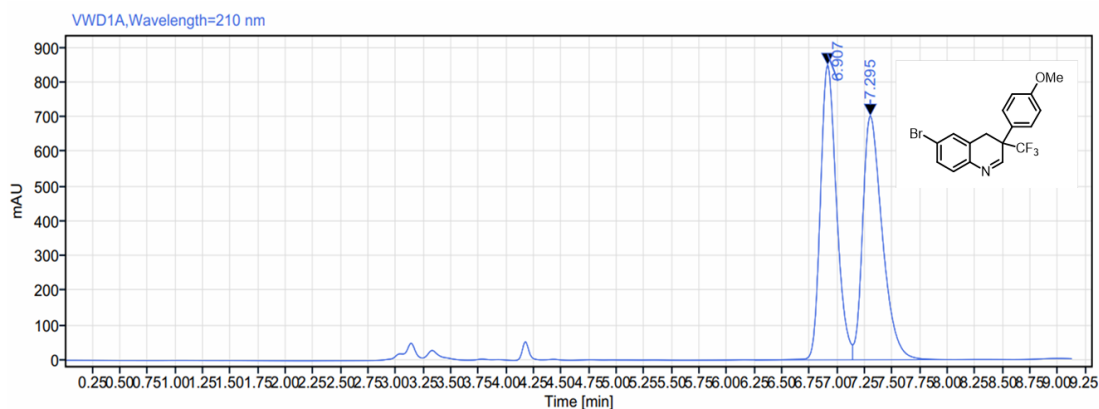
¹³C NMR (150 MHz, CDCl₃) δ 159.7, 158.4 (q, *J* = 1.5 Hz), 140.9, 131.2, 130.9, 128.9, 128.6, 126.5 (q, *J* = 280.5 Hz), 125.8, 124.0, 121.8, 114.1, 55.2, 48.8 (q, *J* = 25.5 Hz), 29.7 (q, *J* = 3.0 Hz).

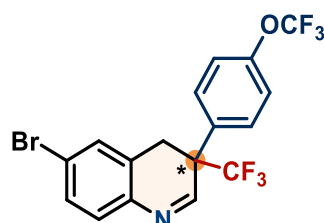
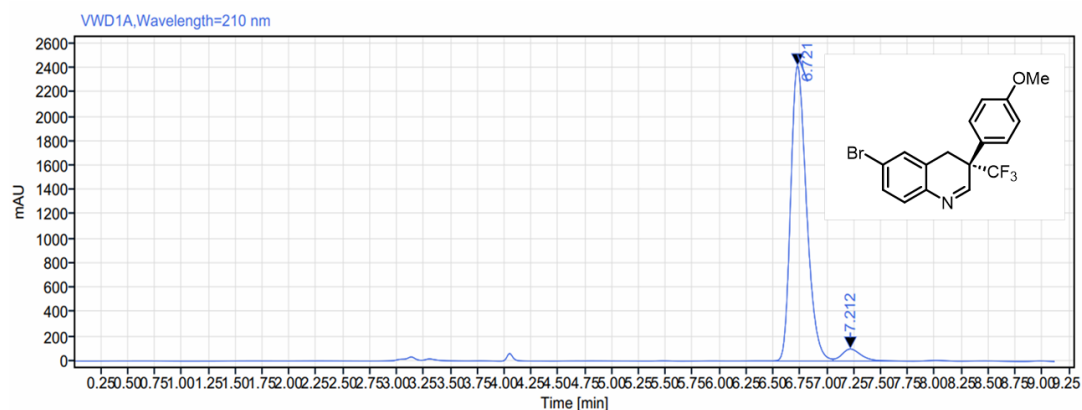
¹⁹F NMR (564 MHz, CDCl₃) δ -72.23.

HRMS (ESI⁺) m/z calcd for C₁₇H₁₄BrF₃NO⁺ [M+H]⁺ 384.0205, found 384.0201.

(S)-6-bromo-3-(4-methoxyphenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 90% yield, 90% e.e. (Chiracel OZ-H, Hexanes/*i*-PrOH = 99/1, 1.0 mL/min, λ =210 nm, RT: Major: 7.253 min, Minor: 6.873 min).

(R)-6-bromo-3-(4-methoxyphenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 97% yield, 90% e.e. (Chiracel OZ-H, Hexanes/*i*-PrOH = 99/1, 1.0 mL/min, λ =210 nm, RT: Major: 6.721 min, Minor: 7.212 min).





Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (97 mg) *N*-triftosylhydrazone provide **22** as a white solid, mp 68.4–71.3 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.30 (d, J = 1.5 Hz, 1H), 7.41–7.35 (m, 3H), 7.27–7.22 (m, 2H), 7.13 (d, J = 8.5 Hz, 2H), 3.43 (d, J = 16.5 Hz, 1H), 3.32 (dd, J = 16.5, 1.5 Hz, 1H).

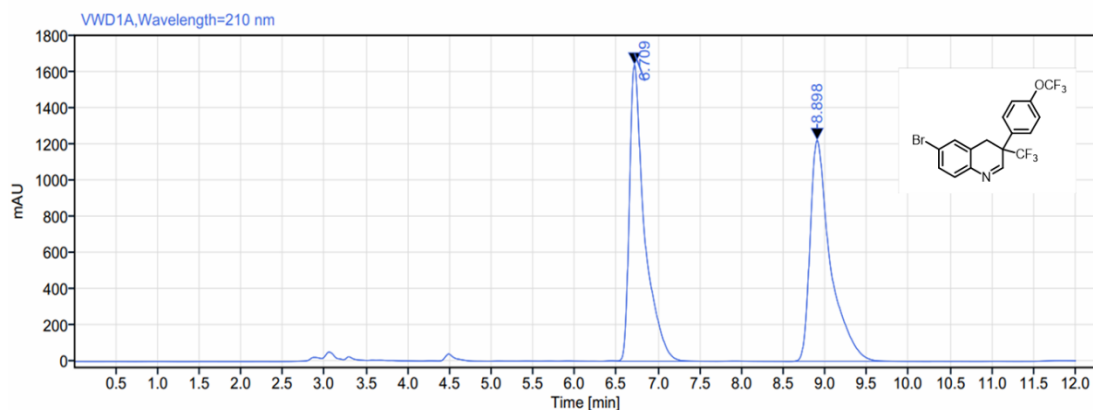
^{13}C NMR (125 MHz, CDCl_3) δ 157.2 (q, J = 2.5 Hz), 149.5, 140.8, 131.6, 131.0, 130.9, 129.3, 128.8, 126.2 (q, J = 281.3 Hz), 125.1, 122.2, 120.9, 120.3 (q, J = 257.5 Hz), 48.9 (q, J = 25.0 Hz), 29.8 (q, J = 2.5 Hz).

^{19}F NMR (564 MHz, CDCl_3) δ -57.79, -71.88.

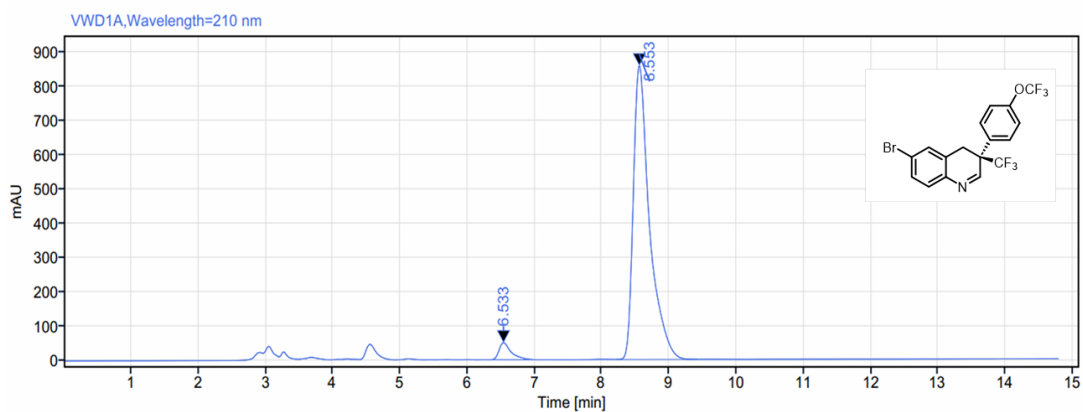
HRMS (ESI $^+$) m/z calcd for $\text{C}_{17}\text{H}_{11}\text{BrF}_6\text{NO}^+$ $[\text{M}+\text{H}]^+$ 437.9923, found 437.9925.

(*S*)-6-bromo-3-(4-(trifluoromethoxy)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 78% yield, 91% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 8.553 min, Minor: 6.533 min).

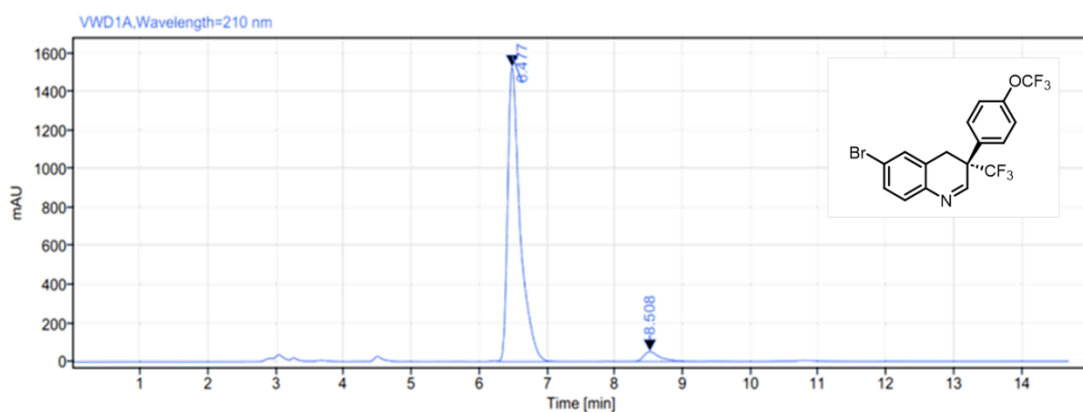
(*R*)-6-bromo-3-(4-(trifluoromethoxy)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 78% yield, 92% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 6.477 min, Minor: 8.508 min).



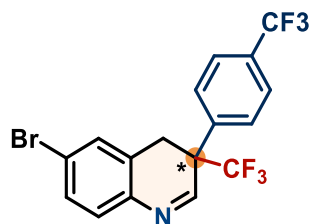
RT [min]	Width [min]	Area	Height	Area%
6.709	1.21	20550.51	1637.24	49.86
8.898	1.75	20668.83	1220.66	50.14



RT [min]	Width [min]	Area	Height	Area%
6.533	0.94	618.27	49.58	4.15
8.553	1.21	14290.76	855.97	95.85



RT [min]	Width [min]	Area	Height	Area%
6.477	1.32	19418.89	1527.27	95.91
8.508	1.10	828.72	50.74	4.09



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (93 mg) *N*-triftosylhydrazone provide **23** as a white solid, mp 94.3-96.4 °C, $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.33 (d, $J = 1.5$ Hz, 1H), 7.56 (d, $J = 8.5$ Hz, 2H), 7.49 (d, $J = 8.5$ Hz, 2H), 7.37 (dd, $J = 8.5$, 2.0 Hz, 1H), 7.28-7.22 (m, 2H), 3.45 (d, $J = 16.5$ Hz, 1H), 3.35 (dd, $J = 16.5$, 1.5 Hz, 1H).

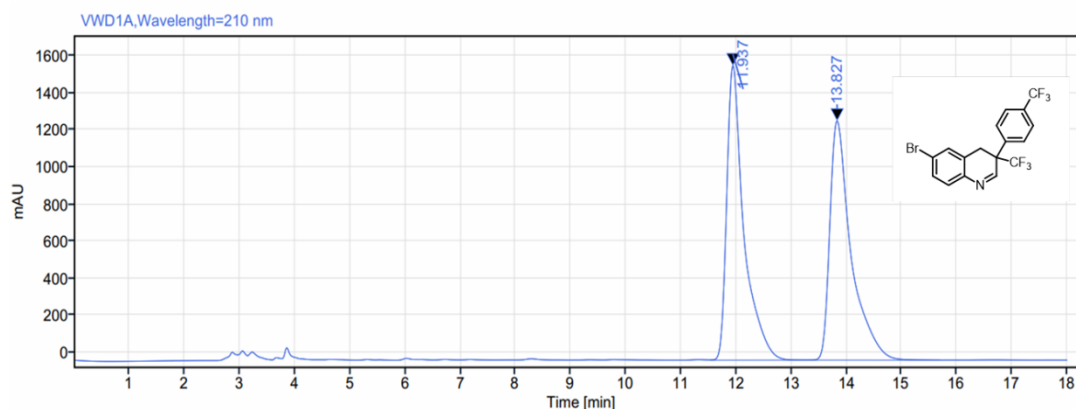
$^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 156.9 (q, $J = 1.5$ Hz), 140.8, 136.5, 131.6, 131.2 (q, $J = 31.5$ Hz), 130.9, 128.8, 128.2, 126.1 (q, $J = 280.5$ Hz), 125.8 (q, $J = 3.0$ Hz), 125.0, 123.5 (q, $J = 271.5$ Hz), 122.3, 49.3 (q, $J = 24.0$ Hz), 29.7 (q, $J = 1.5$ Hz).

$^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -63.03, -71.62.

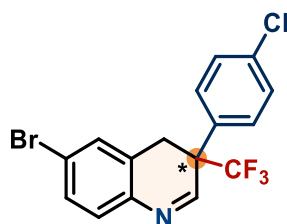
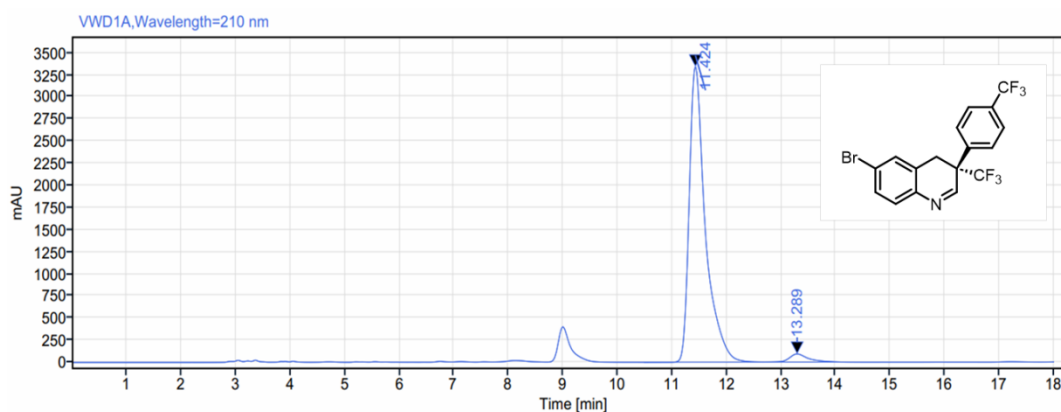
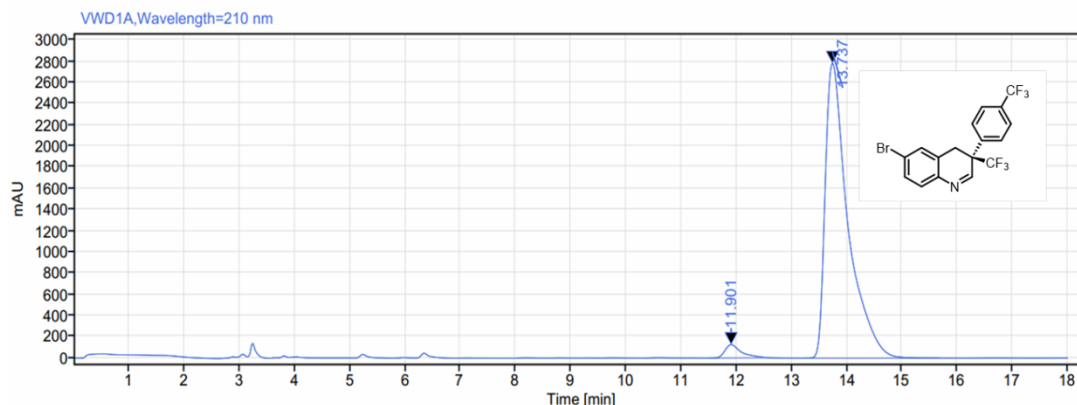
HRMS (ESI^+) m/z calcd for $\text{C}_{17}\text{H}_{11}\text{BrF}_6\text{N}^+$ $[\text{M}+\text{H}]^+$ 421.9974, found 421.9972.

(*S*)-6-bromo-3-(trifluoromethyl)-3-(4-(trifluoromethyl)phenyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 81% yield, 94% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 98/2, 1.0 mL/min, $\lambda=210$ nm, RT: Major: 13.737 min, Minor: 11.901 min).

(*R*)-6-bromo-3-(trifluoromethyl)-3-(4-(trifluoromethyl)phenyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 70% yield, 94% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 98/2, 1.0 mL/min, $\lambda=210$ nm, RT: Major: 11.424 min, Minor: 13.289 min).



RT [min]	Width [min]	Area	Height	Area%
11.937	1.72	34378.55	1594.45	49.86
13.827	2.45	34577.12	1295.08	50.14



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (87 mg) *N*-trifosylhydrazone provide **24** as a white solid, mp 123.3-125.1 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.30 (s, 1H), 7.36 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.30-7.24 (m, 5H), 7.22 (d, *J* = 8.5 Hz, 1H), 3.40 (d, *J* = 16.0 Hz, 1H), 3.30 (dd, *J* = 16.0, 1.5 Hz, 1H).

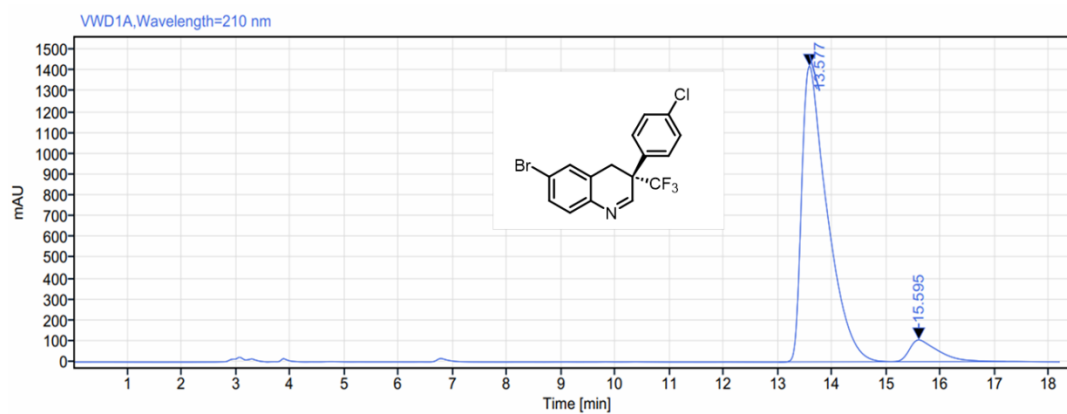
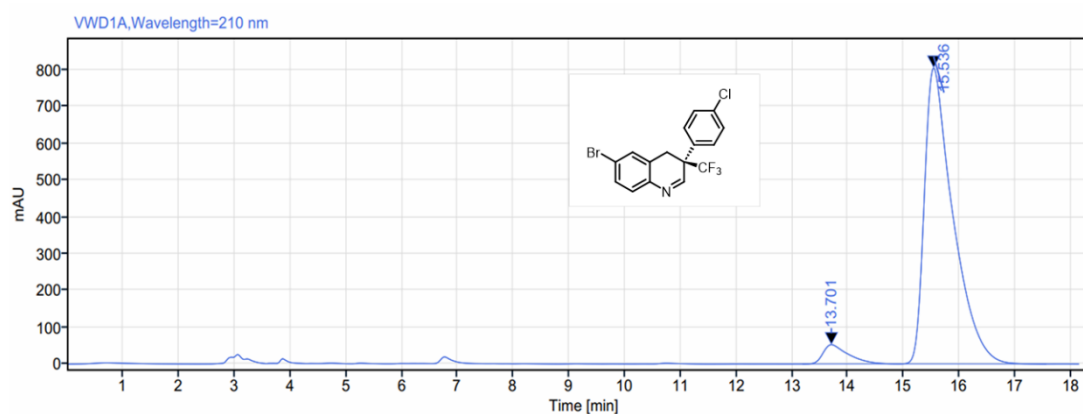
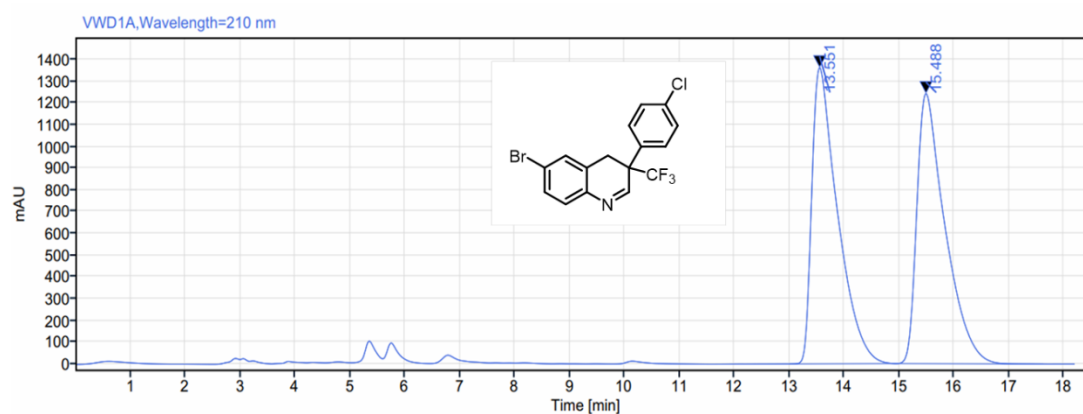
¹³C NMR (150 MHz, CDCl₃) δ 157.4 (q, *J* = 3.0 Hz), 140.8, 135.2, 131.50, 130.92, 130.88, 129.1, 128.7, 126.2 (q, *J* = 280.5 Hz), 125.2, 122.1, 48.9 (q, *J* = 25.5 Hz), 29.7 (q, *J* = 3.0 Hz).

¹⁹F NMR (564 MHz, CDCl₃) δ -71.94.

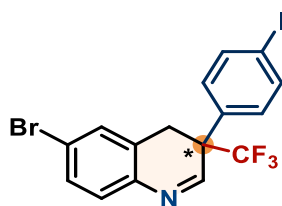
HRMS (ESI⁺) *m/z* calcd for C₁₆H₁₁BrClF₃N⁺ [M+H]⁺ 387.9710, found 387.9702.

(*S*)-6-bromo-3-(4-chlorophenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 86% yield, 89% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 98/2, 1.0 mL/min, λ=210 nm, RT: Major: 15.536 min, Minor: 13.701 min).

(*R*)-6-bromo-3-(4-chlorophenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 91% yield, 85% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 98/2, 1.0 mL/min, λ =210 nm, RT: Major: 13.577 min, Minor: 15.595 min).



15.595 2.11 3855.00 104.62 7.64



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (105 mg) *N*-triftosylhydrazone provide **25** as a white solid, mp 97.6-99.1 °C, $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.28 (s, 1H), 7.62 (d, $J = 8.5$ Hz, 2H), 7.39-7.33 (m, 1H), 7.25-7.19 (m, 2H), 7.08 (d, $J = 8.5$ Hz, 2H), 3.39 (d, $J = 16.0$ Hz, 1H), 3.29 (dd, $J = 16.0, 1.5$ Hz, 1H).

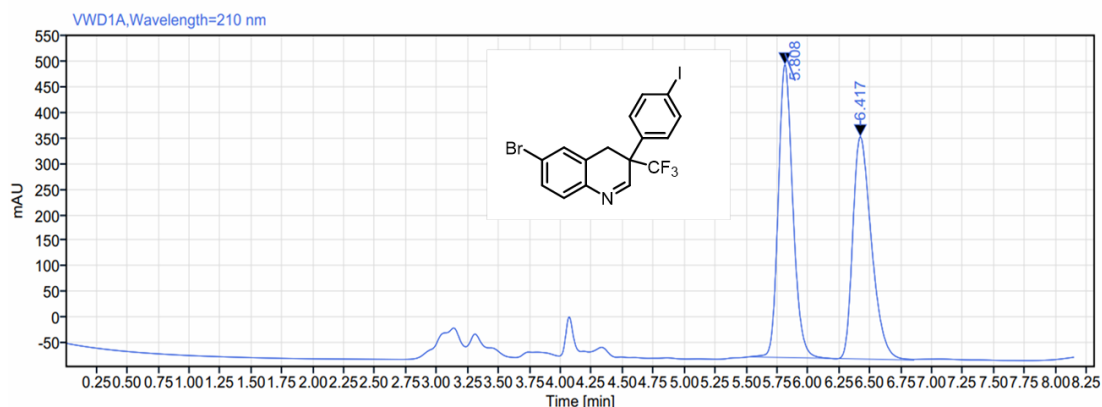
$^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 157.3 (d, $J = 2.5$ Hz), 140.8, 137.9, 132.2, 131.5, 130.9, 129.5, 128.7, 126.1 (q, $J = 280.0$ Hz), 125.2, 122.1, 95.2, 49.1 (q, $J = 25.0$ Hz), 29.6 (q, $J = 2.5$ Hz).

$^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -71.88.

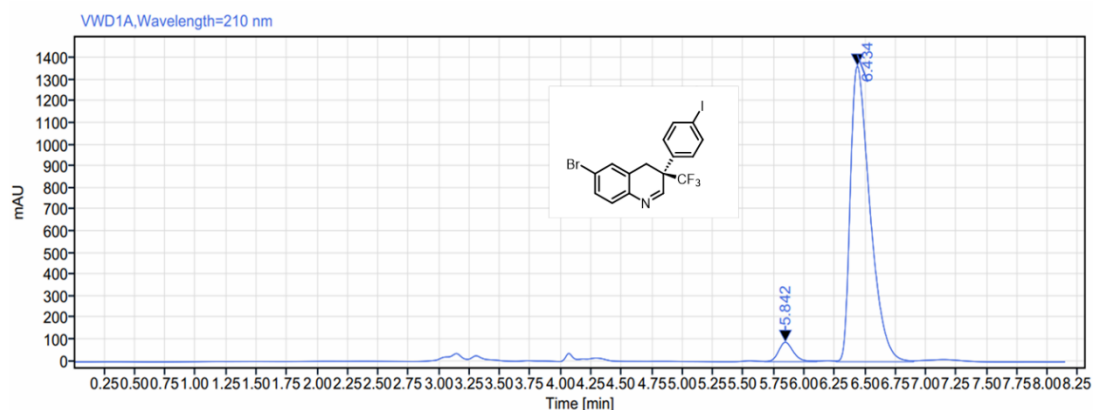
HRMS (ESI^+) m/z calcd for $\text{C}_{16}\text{H}_{11}\text{BrF}_3\text{IN}^+$ $[\text{M}+\text{H}]^+$ 479.9066, found 479.9070.

(*S*)-6-bromo-3-(4-iodophenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 91% yield, 90% e.e. (Chiracel OZ-H, Hexanes/*i*-PrOH = 99/1, 1.0 mL/min, $\lambda=210$ nm, RT: Major: 6.434 min, Minor: 5.842 min).

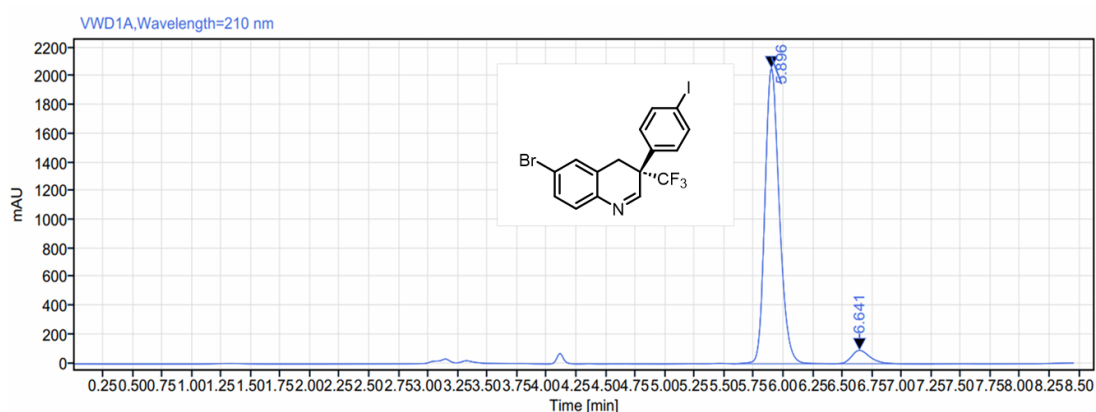
(*R*)-6-bromo-3-(4-iodophenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 95% yield, 89% e.e. (Chiracel OZ-H, Hexanes/*i*-PrOH = 99/1, 1.0 mL/min, $\lambda=210$ nm, RT: Major: 5.896 min, Minor: 6.641 min).



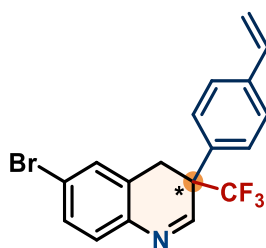
RT [min]	Width [min]	Area	Height	Area%
5.808	0.65	4698.98	573.24	50.71
6.417	0.69	4566.88	435.13	49.29



RT [min]	Width [min]	Area	Height	Area%
5.842	0.43	777.58	90.17	4.82
6.434	0.64	15341.35	1365.74	95.18



RT [min]	Width [min]	Area	Height	Area%
5.896	0.85	17466.44	2057.53	94.37
6.641	0.85	1041.56	93.85	5.63



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (85 mg) *N*-trifosylhydrazone provide **26** as a white solid, mp 114.8-116.3 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.32 (s, 1H), 7.37-7.28 (m, 4H), 7.27-7.24 (m, 2H), 7.21 (d, *J* = 8.5 Hz, 1H), 6.62 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.71 (d, *J* = 17.5 Hz, 1H), 5.26 (d, *J* = 11.0 Hz, 1H), 3.40 (d, *J* = 16.0 Hz, 1H), 3.34 (d, *J* = 16.0 Hz, 1H).

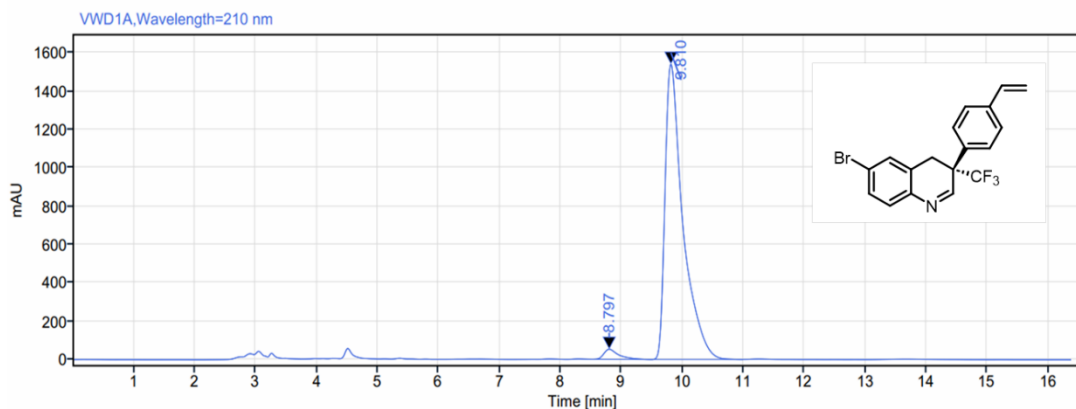
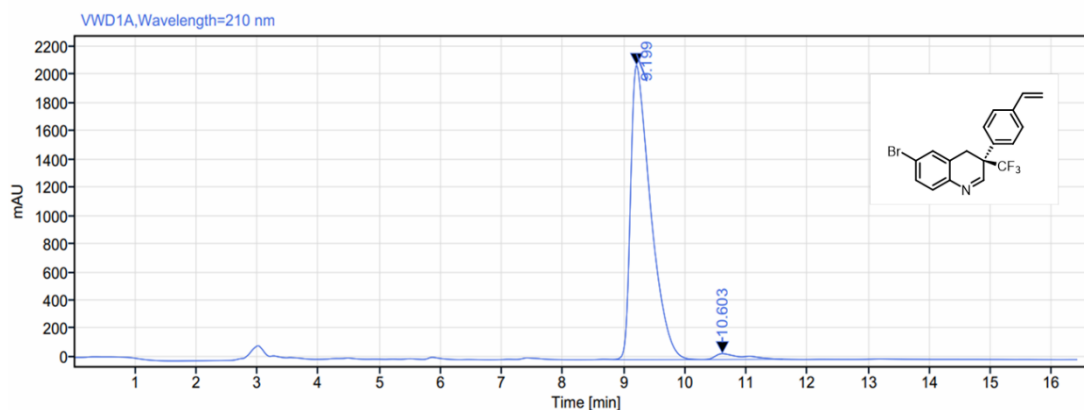
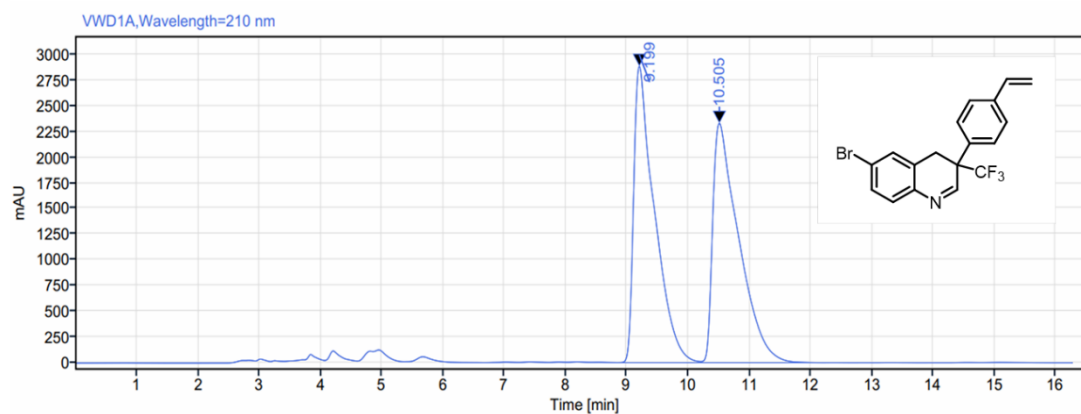
¹³C NMR (125 MHz, CDCl₃) δ 158.0 (q, *J* = 2.5 Hz), 141.0, 138.2, 135.7, 131.7, 131.4, 131.0, 128.6, 127.9, 126.5, 126.4 (q, *J* = 281.3 Hz), 125.6, 121.9, 115.3, 49.2 (q, *J* = 25.0 Hz), 29.7 (q, *J* = 2.5 Hz).

¹⁹F NMR (470 MHz, CDCl₃) δ -71.85.

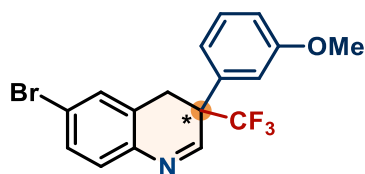
HRMS (ESI⁺) *m/z* calcd for C₁₈H₁₄BrF₃N⁺ [M+H]⁺ 380.0256, found 380.0253.

(S)-6-bromo-3-(trifluoromethyl)-3-(4-vinylphenyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 96% yield, 95% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 9.199 min, Minor: 10.603 min).

(R)-6-bromo-3-(trifluoromethyl)-3-(4-vinylphenyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 80% yield, 94% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 9.810 min, Minor: 8.797 min).



RT [min]	Width [min]	Area	Height	Area%
8.797	0.93	893.77	53.10	2.76
9.810	1.51	31435.26	1542.34	97.24



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (86 mg) *N*-triftosylhydrazone provide **27** as a white solid, mp 77.6-79.1 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.29 (s, 1H), 7.34 (d, *J* = 8.5 Hz, 1H), 7.27-7.17 (m, 3H), 6.93 (d, *J* = 7.5 Hz, 1H), 6.90-6.87 (m, 1H), 6.83-6.78 (m, 1H), 3.74 (s, 3H), 3.42-3.29 (m, 2H).

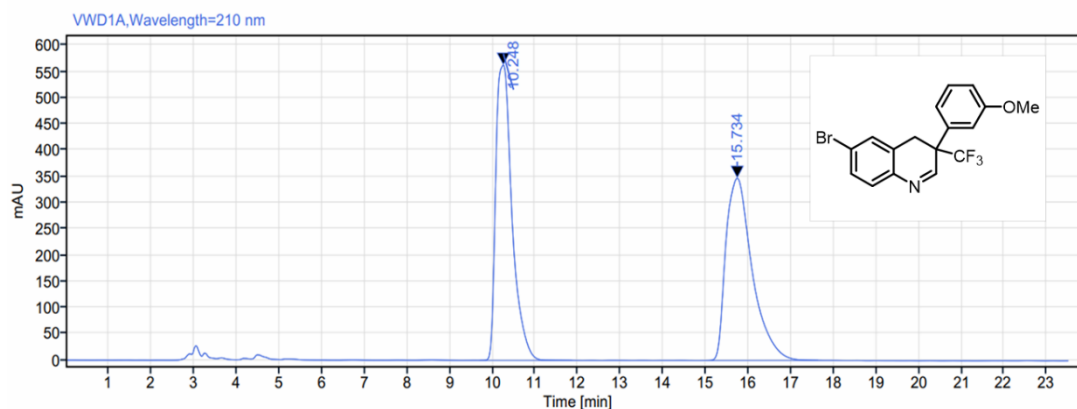
¹³C NMR (150 MHz, CDCl₃) δ 159.6, 157.9 (q, *J* = 3.0 Hz), 140.9, 133.9, 131.3, 130.9, 129.7, 128.6, 126.4 (q, *J* = 282.0 Hz), 125.6, 121.9, 120.0, 114.5, 113.6, 55.2, 49.3 (q, *J* = 25.5 Hz), 29.9 (q, *J* = 1.5 Hz).

¹⁹F NMR (564 MHz, CDCl₃) δ -71.65.

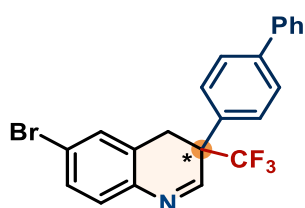
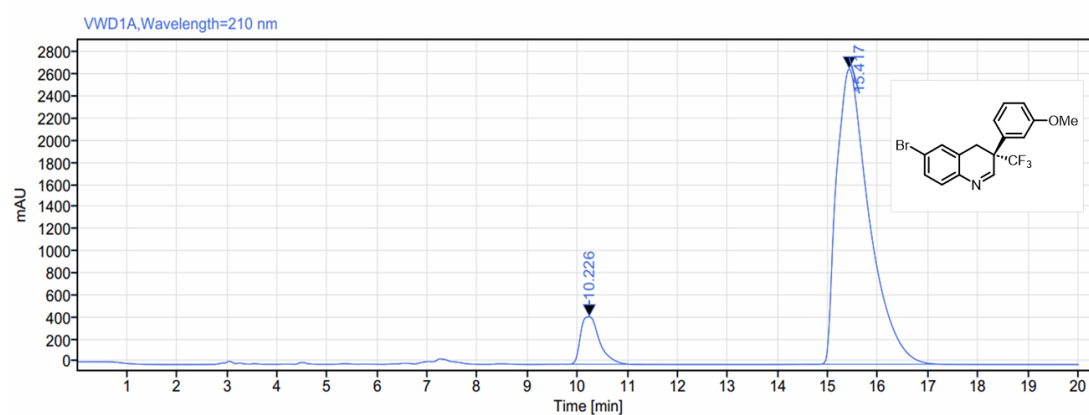
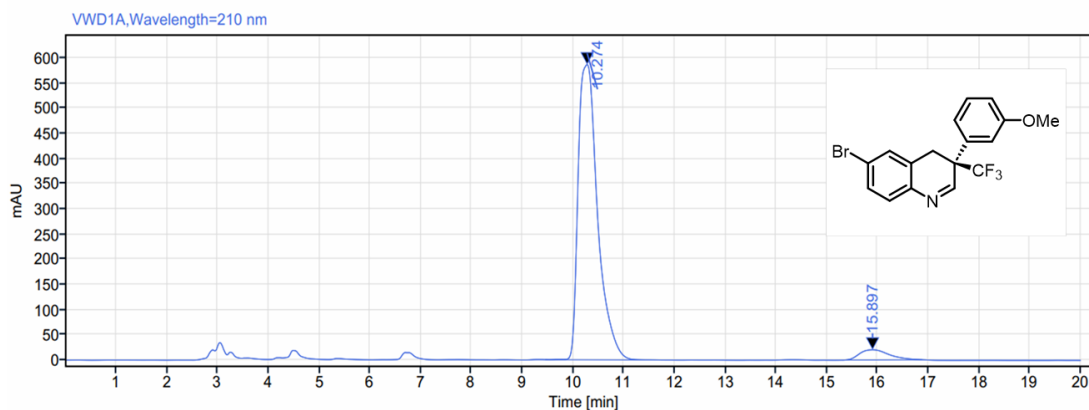
HRMS (ESI⁺) *m/z* calcd for C₁₇H₁₄BrF₃NO⁺ [M+H]⁺ 384.0205, found 384.0209.

(*S*)-6-bromo-3-(3-methoxyphenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 92% yield, 90% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ=210 nm, RT: Major: 10.274 min, Minor: 15.897 min).

(*R*)-6-bromo-3-(3-methoxyphenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 90% yield, 83% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ=210 nm, RT: Major: 15.417 min, Minor: 10.226 min).



RT [min]	Width [min]	Area	Height	Area%
10.248	2.16	14931.71	562.94	50.07
15.734	2.99	14890.73	347.54	49.93



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (95 mg) *N*-trifosylhydrazone provide **28** as a white solid, mp 153.2-154.3 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.36 (s, 1H), 7.53-7.48 (m, 4H), 7.43-7.38 (m, 4H), 7.38-7.31 (m, 2H), 7.28 (s, 1H), 7.24 (d, *J* = 8.5 Hz, 1H), 3.46-3.36 (m, 2H).

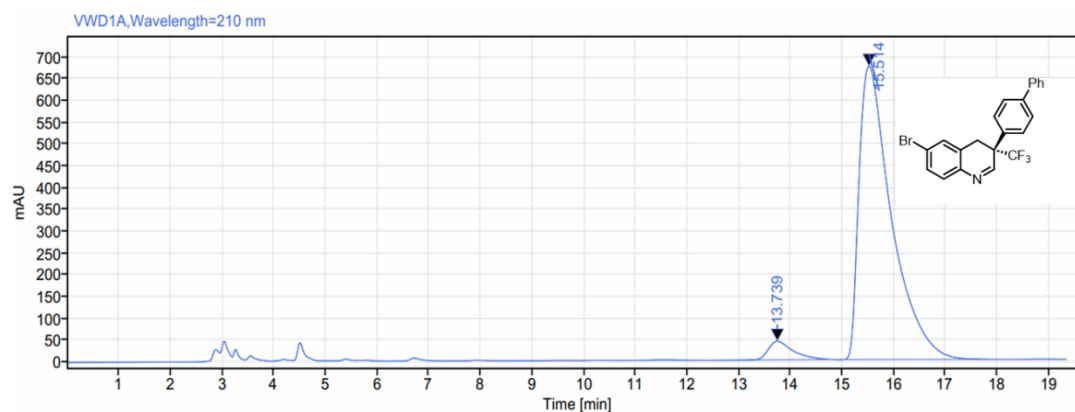
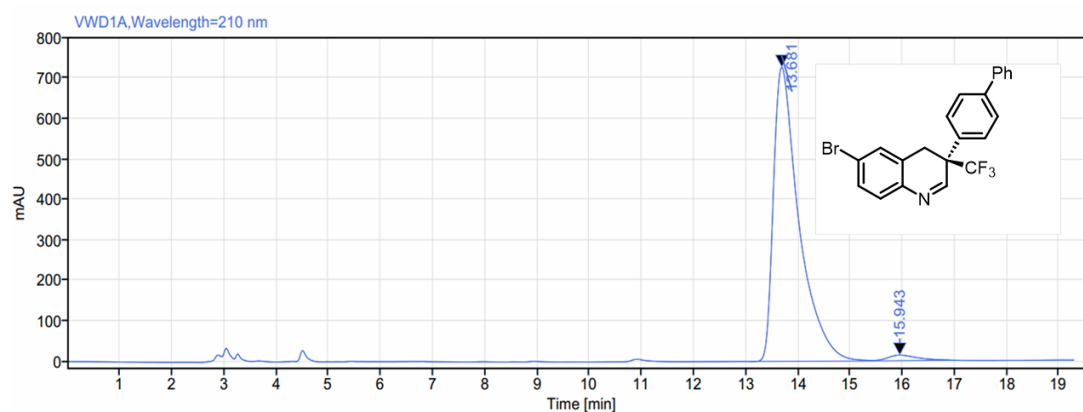
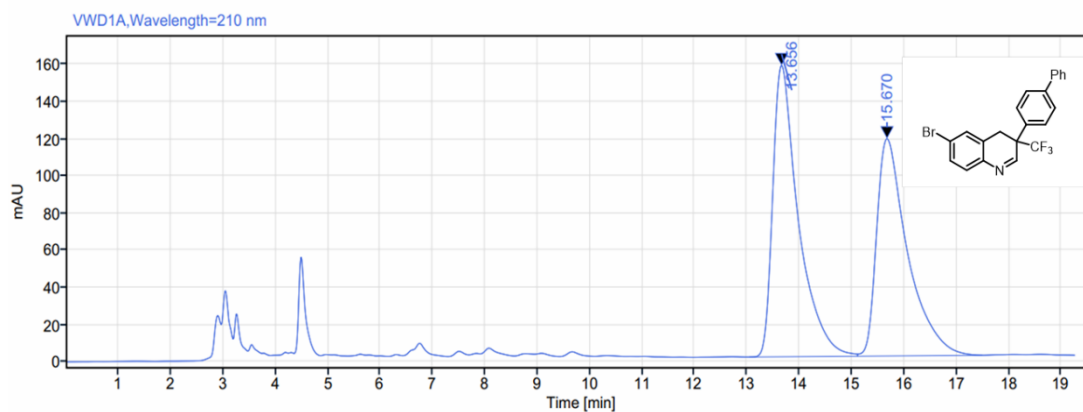
¹³C NMR (125 MHz, CDCl₃) δ 158.0 (q, *J* = 3.8 Hz), 141.7, 140.9, 139.8, 131.4, 131.3, 131.0, 128.8, 128.7, 128.1, 127.7, 127.4, 127.0, 126.5 (q, *J* = 281.3 Hz), 125.6, 121.9, 49.1 (q, *J* = 25.0 Hz), 29.7 (q, *J* = 2.5 Hz).

¹⁹F NMR (564 MHz, CDCl₃) δ -71.77.

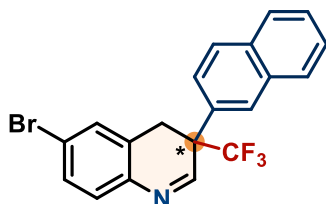
HRMS (ESI⁺) *m/z* calcd for C₂₂H₁₆BrF₃N⁺ [M+H]⁺ 430.0413, found 430.0408.

(S)-3-([1,1'-biphenyl]-4-yl)-6-bromo-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 87% yield, 96% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 13.681 min, Minor: 15.943 min).

(R)-3-([1,1'-biphenyl]-4-yl)-6-bromo-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 80% yield, 91% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 15.514 min, Minor: 13.739 min).



RT [min]	Width [min]	Area	Height	Area%
13.739	1.65	1416.48	42.78	4.61
15.514	2.88	29292.49	673.22	95.39



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (90 mg) *N*-triftosylhydrazone provide **29** as a white solid, mp 168.7-170.6 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.44 (s, 1H), 7.80-7.73 (m, 4H), 7.50-7.44 (m, 3H), 7.30 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.27-7.21 (m, 2H), 3.52-3.44 (m, 2H).

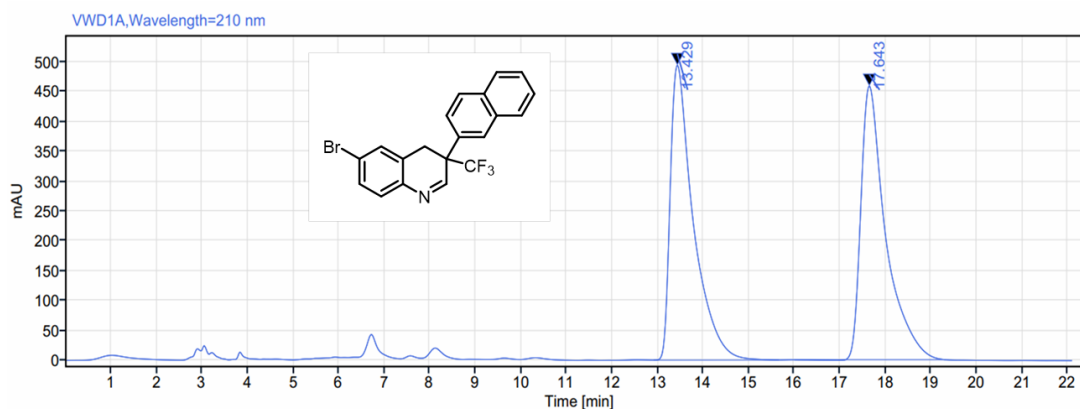
¹³C NMR (150 MHz, CDCl₃) δ 158.2, 140.9, 133.0, 132.7, 131.3, 130.9, 129.7, 128.7, 128.6, 128.2, 127.8, 127.4, 127.0, 126.61, 126.57 (q, *J* = 280.5 Hz), 125.5, 124.3, 122.0, 49.5 (q, *J* = 25.5 Hz), 29.8 (q, *J* = 3.0 Hz).

¹⁹F NMR (564 MHz, CDCl₃) δ -71.45.

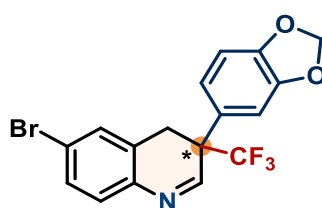
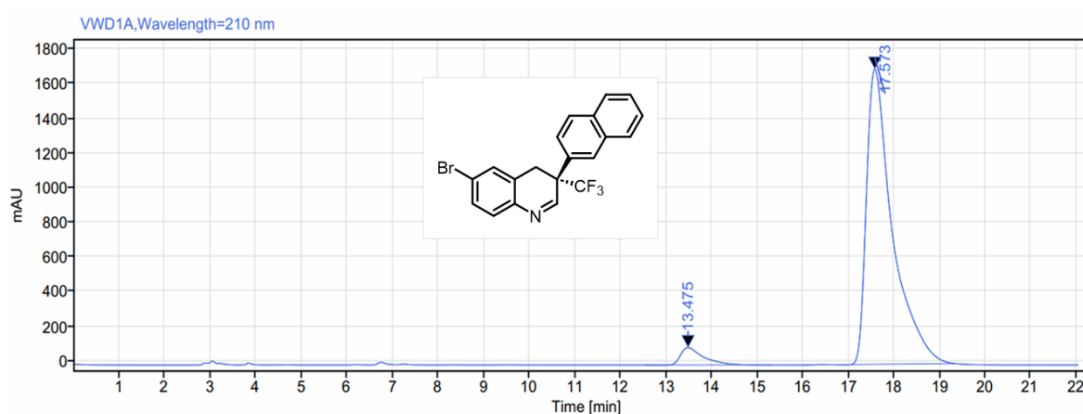
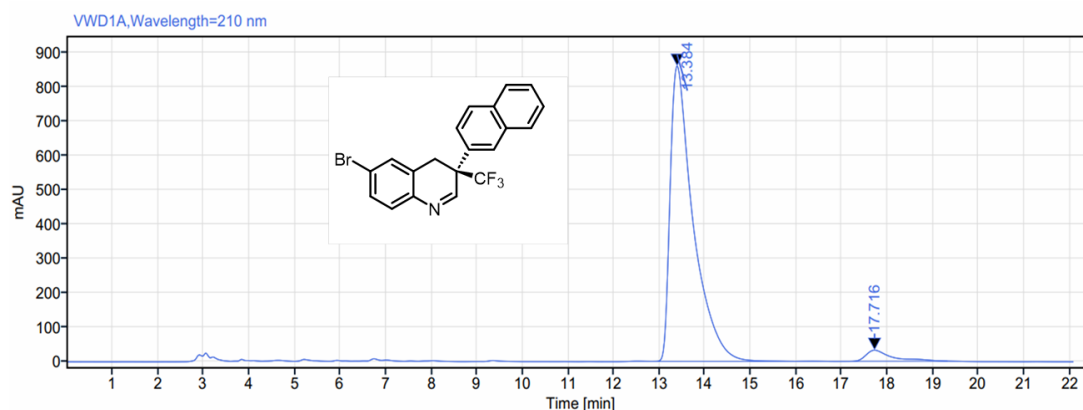
HRMS (ESI⁺) *m/z* calcd for C₂₀H₁₄BrF₃N⁺ [M+H]⁺ 404.0256, found 404.0254.

(*S*)-6-bromo-3-(naphthalen-2-yl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 73% yield, 92% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 98/2, 1.0 mL/min, λ=210 nm, RT: Major: 13.384 min, Minor: 17.716 min).

(*R*)-6-bromo-3-(naphthalen-2-yl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 84% yield, 90% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 98/2, 1.0 mL/min, λ=210 nm, RT: Major: 17.573 min, Minor: 13.475 min).



RT [min]	Width [min]	Area	Height	Area%
13.429	2.75	17362.98	494.17	50.08
17.643	3.32	17305.36	458.73	49.92



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (89 mg) *N*-trifosylhydrazone provide **30** as a white solid, mp 112.1-113.3 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.27 (s, 1H), 7.35 (dd, J = 8.5, 2.5 Hz, 1H), 7.25-7.19 (m, 2H), 6.83 (s, 1H), 6.78 (dd, J = 8.0, 2.0 Hz, 1H), 6.67 (d, J = 8.0 Hz, 1H), 5.91 (s, 2H), 3.35 (d, J = 16.0 Hz, 1H), 3.25 (d, J = 16.0 Hz, 1H).

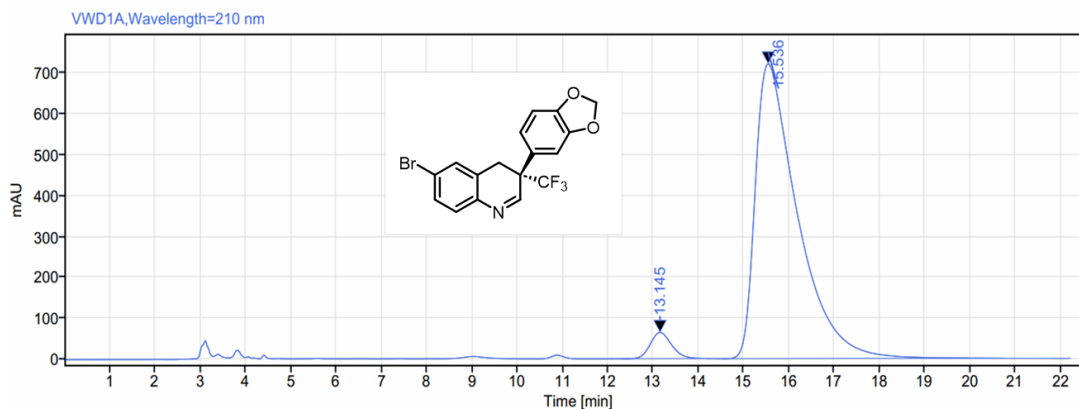
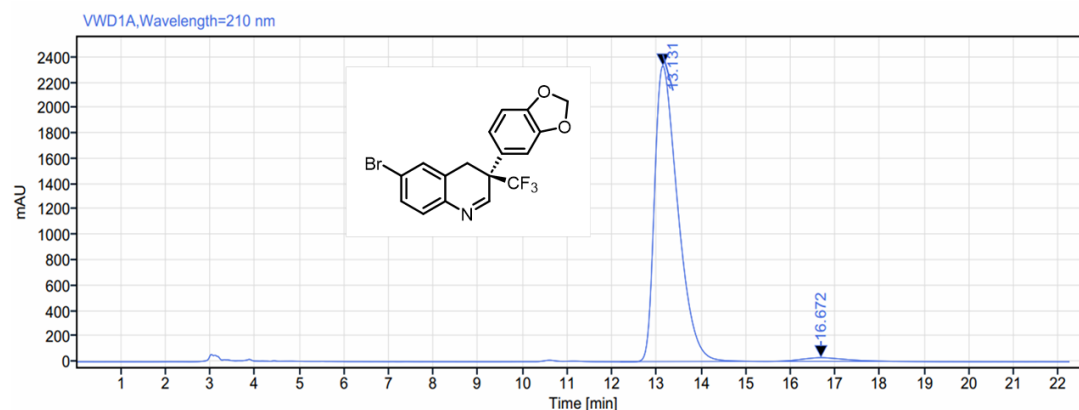
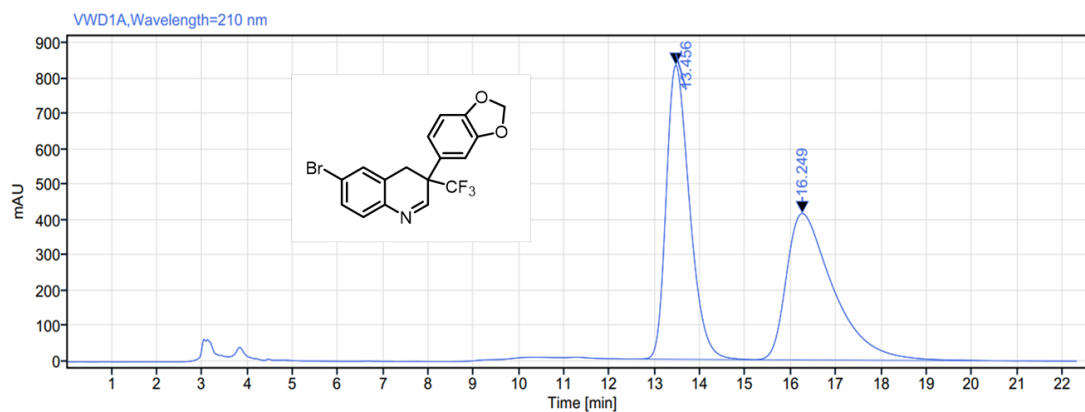
^{13}C NMR (150 MHz, CDCl_3) δ 158.0 (q, J = 1.5 Hz), 148.2, 148.1, 141.0, 131.3, 131.0, 128.6, 126.5 (q, J = 280.5 Hz), 125.7, 125.6, 121.9, 121.7, 108.3, 108.1, 101.5, 49.0 (q, J = 25.5 Hz), 30.0 (q, J = 1.5 Hz).

^{19}F NMR (564 MHz, CDCl_3) δ -72.08.

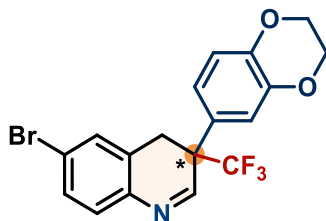
HRMS (ESI $^+$) m/z calcd for $\text{C}_{17}\text{H}_{12}\text{BrF}_3\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 397.9998, found 397.9992.

(S)-3-(benzo[d][1,3]dioxol-5-yl)-6-bromo-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 84% yield, 95% e.e. (Chiracel OJ-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 13.131 min, Minor: 16.672 min).

(R)-3-(benzo[d][1,3]dioxol-5-yl)-6-bromo-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 75% yield, 91% e.e. (Chiracel OJ-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 15.536 min, Minor: 13.145 min).



RT [min]	Width [min]	Area	Height	Area%
13.145	1.99	2099.50	63.94	4.31
15.536	5.45	46573.77	720.34	95.69



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **31** as a white solid, mp 113.5-115.0 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.26 (s, 1H), 7.37-7.32 (m, 1H), 7.26-7.20 (m, 2H), 6.86 (d, J = 2.5 Hz, 1H), 6.79 (dd, J = 8.5, 2.5 Hz, 1H), 6.74 (d, J = 8.5 Hz, 1H), 4.20 (s, 4H), 3.35 (d, J = 16.0 Hz, 1H), 3.26 (dd, J = 16.0, 1.5 Hz, 1H).

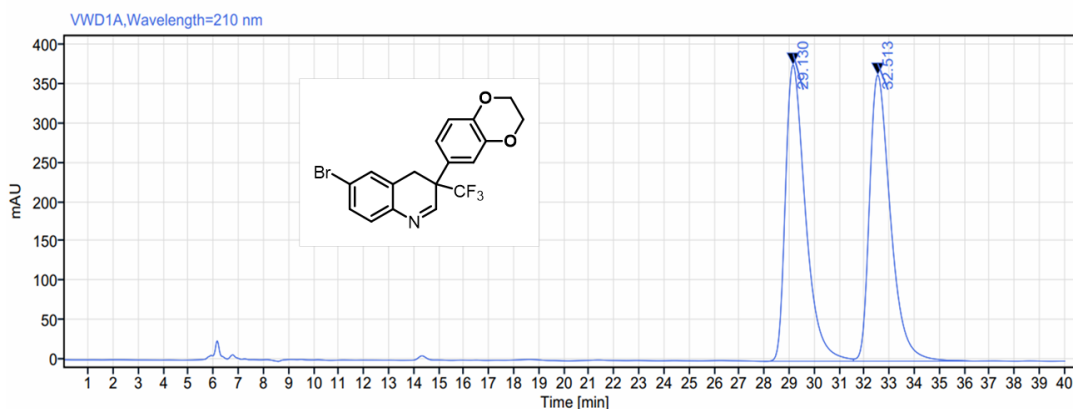
^{13}C NMR (150 MHz, CDCl_3) δ 158.0 (q, J = 3.0 Hz), 144.1, 143.5, 140.9, 131.2, 131.0, 128.6, 126.5 (q, J = 282.0 Hz) 125.7, 125.1, 121.8, 120.8, 117.4, 116.9, 64.24, 64.18, 48.8 (q, J = 25.5 Hz), 29.8 (q, J = 3.0 Hz).

^{19}F NMR (564 MHz, CDCl_3) δ -72.08.

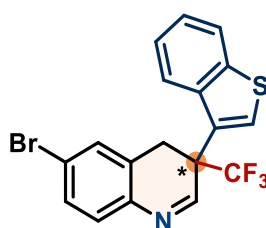
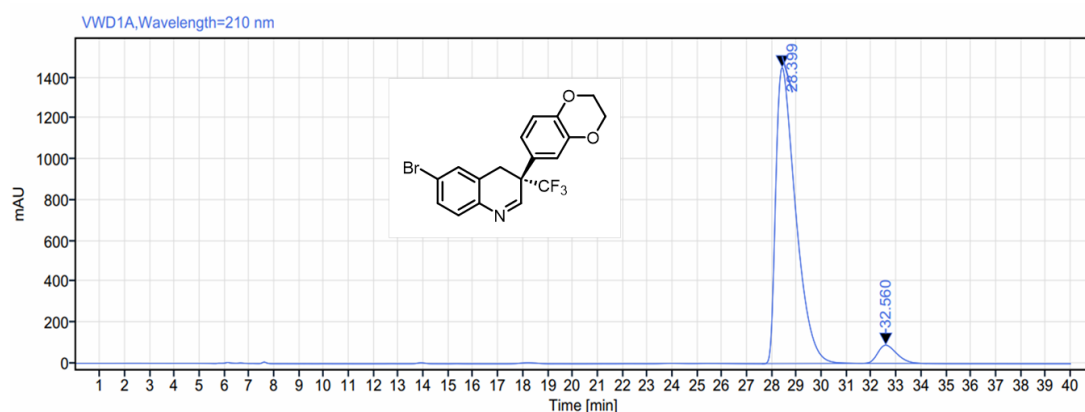
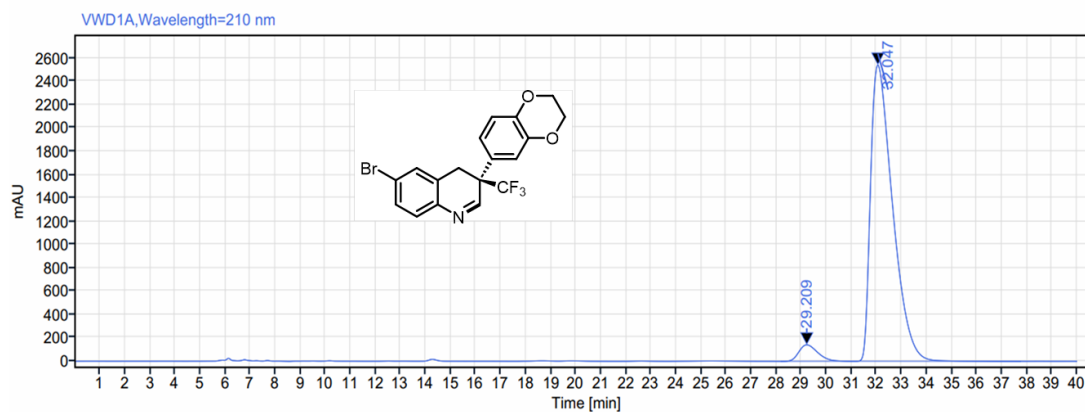
HRMS (ESI $^+$) m/z calcd for $\text{C}_{18}\text{H}_{14}\text{BrF}_3\text{NO}_2^+$ $[\text{M}+\text{H}]^+$ 412.0155, found 412.0160.

(*S*)-6-bromo-3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 95% yield, 91% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 99/1, 0.5 mL/min, λ =210 nm, RT: Major: 32.047 min, Minor: 29.209 min).

(*R*)-6-bromo-3-(2,3-dihydrobenzo[b][1,4]dioxin-6-yl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 96% yield, 89% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 99/1, 0.5 mL/min, λ =210 nm, RT: Major: 28.399 min, Minor: 32.560 min).



RT [min]	Width [min]	Area	Height	Area%
29.130	3.58	20971.06	376.79	49.74
32.513	4.83	21186.68	364.01	50.26



Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (91 mg) *N*-trifosylhydrazone provide **32** as a white solid, mp 128.4-129.5 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.40 (s, 1H), 7.92-7.87 (m, 1H), 7.86-7.80 (m, 1H), 7.45 (s, 1H), 7.42-7.32 (m, 3H), 7.29-7.26 (m, 1H), 7.24 (d, *J* = 8.5 Hz, 1H), 3.65 (d, *J* = 16.5 Hz, 1H), 3.45 (d, *J* = 16.5 Hz, 1H).

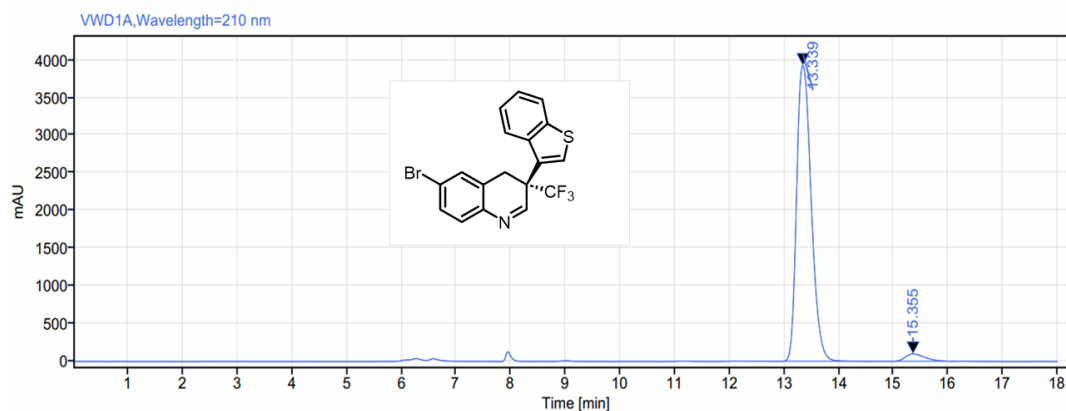
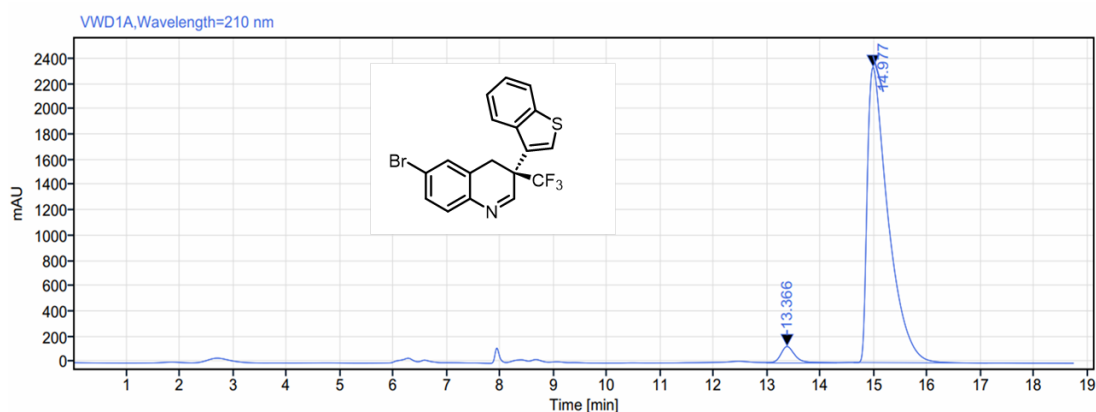
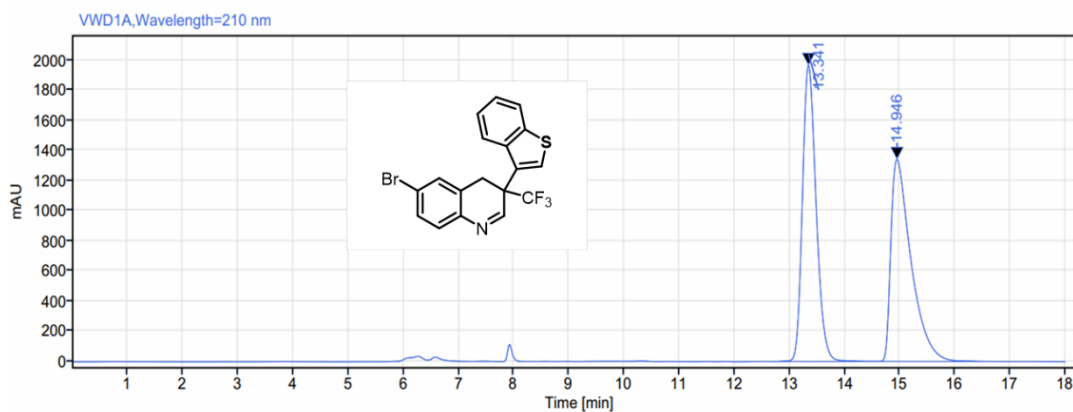
¹³C NMR (125 MHz, CDCl₃) δ 156.4, 140.6, 140.2, 136.7, 131.3, 130.7, 129.1, 127.9, 126.7, 126.4 (q, *J* = 281.3 Hz), 125.6, 124.6, 124.5, 123.6 (q, *J* = 1.3 Hz), 123.3, 122.1, 48.6 (q, *J* = 26.3 Hz), 29.4 (q, *J* = 2.5 Hz).

¹⁹F NMR (470 MHz, CDCl₃) δ -70.95.

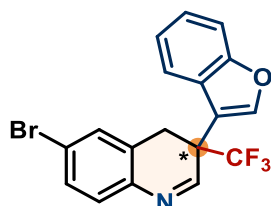
HRMS (ESI⁺) *m/z* calcd for C₁₈H₁₂BrF₃NS⁺ [M+H]⁺ 409.9820, found 409.9811.

(S)-3-(benzo[b]thiophen-3-yl)-6-bromo-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 89% yield, 92% e.e. (Chiracel OZ-H, Hexanes/*i*-PrOH = 99/1, 0.5 mL/min, λ =210 nm, RT: Major: 14.977 min, Minor: 13.366 min).

(R)-3-(benzo[b]thiophen-3-yl)-6-bromo-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 83% yield, 93% e.e. (Chiracel OZ-H, Hexanes/*i*-PrOH = 99/1, 0.5 mL/min, λ =210 nm, RT: Major: 13.339 min, Minor: 15.355 min).



RT [min]	Width [min]	Area	Height	Area%
13.339	1.88	72778.04	3926.37	96.73
15.355	1.22	2463.97	98.50	3.27



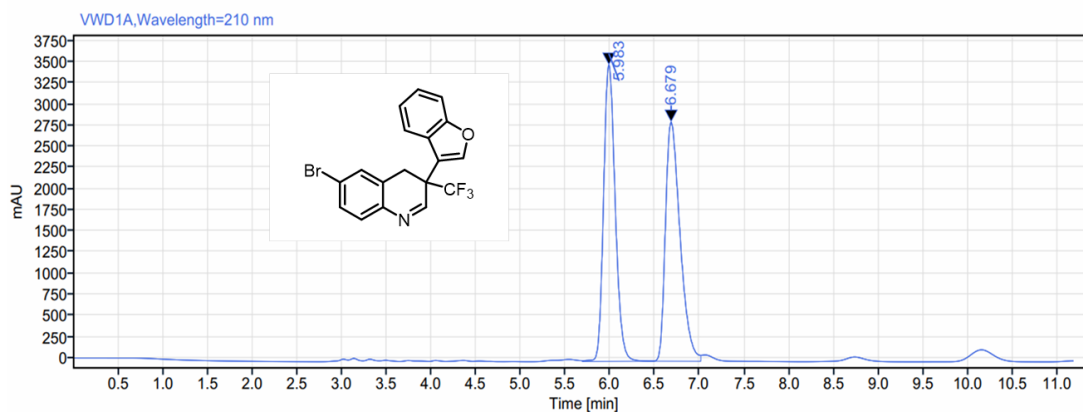
Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (88 mg) *N*-triftosylhydrazone provide **33** as a white solid, mp 119.6-121.7 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.24 (s, 1H), 7.60 (d, J = 7.5 Hz, 1H), 7.46-7.35 (m, 2H), 7.34-7.28 (m, 1H), 7.26-7.12 (m, 4H), 3.336 (s, 2H).

^{13}C NMR (150 MHz, CDCl_3) δ 155.6, 155.3 (q, J = 3.0 Hz), 144.8, 140.2, 131.5, 130.9, 129.1, 126.5 (q, J = 282.0 Hz), 125.3, 125.03, 125.01, 123.3, 122.2, 121.2 (q, J = 3.0 Hz), 112.6, 112.1, 45.7 (q, J = 27.0 Hz), 28.7 (q, J = 3.0 Hz).

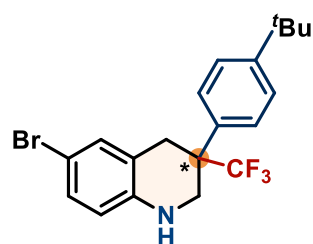
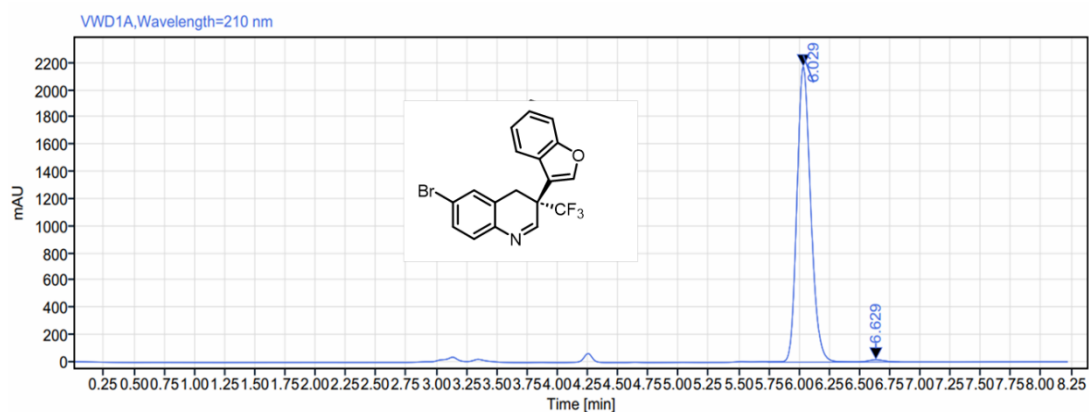
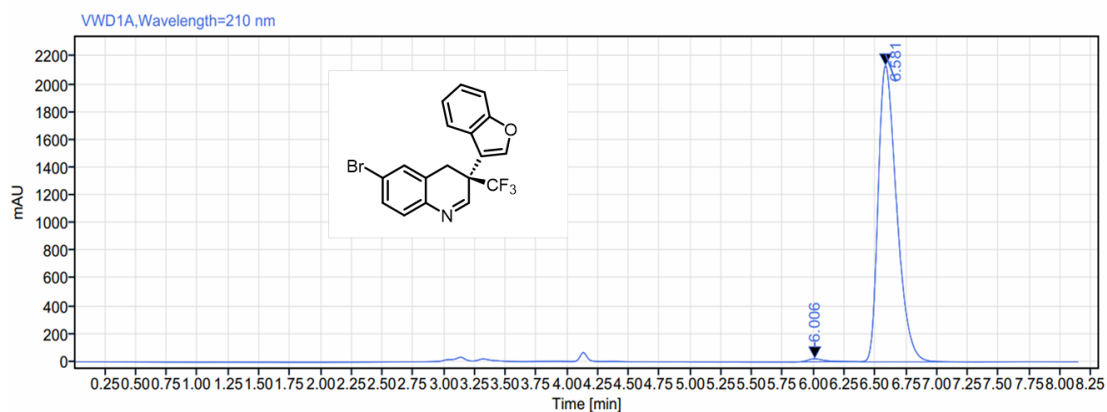
^{19}F NMR (564 MHz, CDCl_3) δ -71.84.

(*S*)-3-(benzofuran-3-yl)-6-bromo-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 98% yield, 98% e.e. (Chiracel OZ-H, Hexanes/*i*-PrOH = 99/1, 1.0 mL/min, λ =210 nm, RT: Major: 6.581 min, Minor: 6.006 min).

(*R*)-3-(benzofuran-3-yl)-6-bromo-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 81% yield, 98% e.e. (Chiracel OZ-H, Hexanes/*i*-PrOH = 99/1, 1.0 mL/min, λ =210 nm, RT: Major: 6.029 min, Minor: 6.629 min).



RT [min]	Width [min]	Area	Height	Area%
5.983	0.78	31752.46	3507.22	49.71
6.679	0.55	32128.55	2829.81	50.29



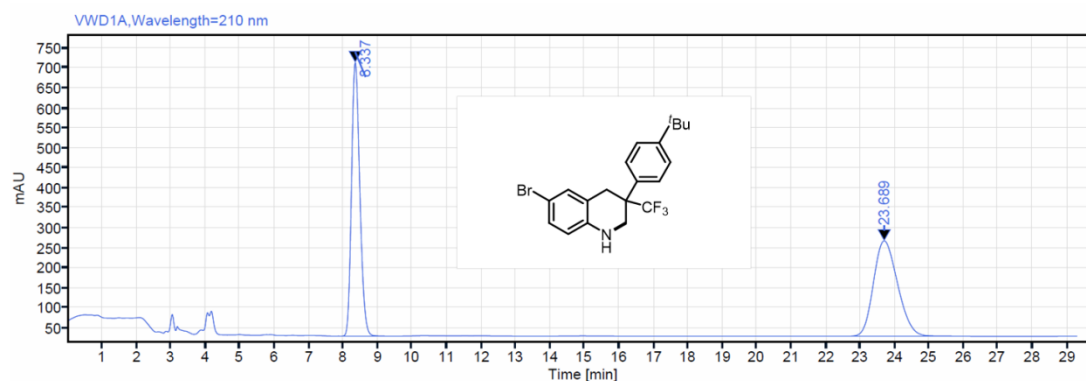
Following General Procedure B, 0.2 mmol (82 mg) **19** provides **34** as a white solid, mp 122.8-123.5 °C, ^1H NMR (500 MHz, CDCl_3) δ 7.35 (d, J = 8.5 Hz, 2H), 7.31 (d, J = 8.5 Hz, 2H), 7.20 (d, J = 2.0 Hz, 1H), 7.00 (dd, J = 8.5, 2.0 Hz, 1H), 6.25 (d, J = 8.5 Hz, 1H), 3.90 (d, J = 15.0 Hz, 1H), 3.83 (s, 1H), 3.65 (d, J = 12.5 Hz, 1H), 3.43 (dd, J = 16.5, 2.5 Hz, 1H), 3.38 (d, J = 16.5 Hz, 1H), 1.28 (s, 9H).

^{13}C NMR (150 MHz, CDCl_3) δ 150.8, 141.6, 131.9, 130.6, 129.9, 127.8, 127.0 (q, J = 280.5 Hz), 125.4, 120.2, 116.1, 109.3, 44.5 (q, J = 3.0 Hz), 44.4 (q, J = 24.0 Hz), 34.4, 31.2, 30.8 (q, J = 3.0 Hz).

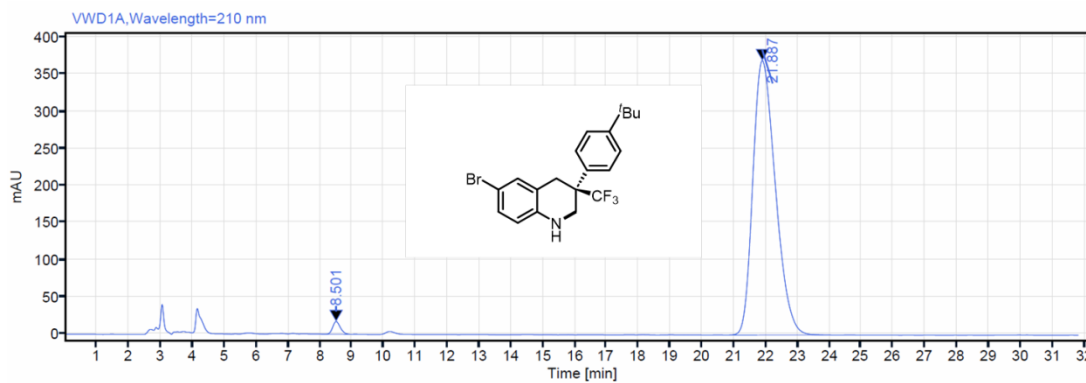
^{19}F NMR (564 MHz, CDCl_3) δ -74.03.

(S)-6-bromo-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-1,2,3,4-tetrahydroquinoline was prepared following the general procedure B as a white solid: 90% yield, 97% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 97/3, 1.0 mL/min, λ =210 nm, RT: Major: 21.887 min, Minor: 8.501 min).

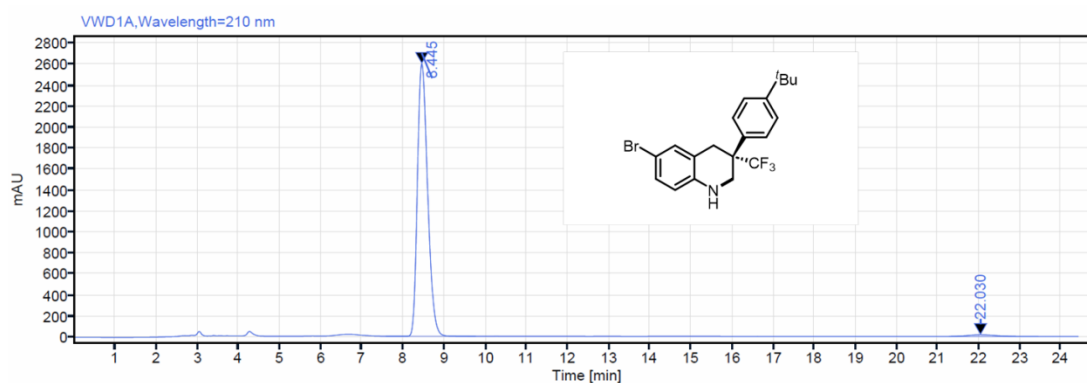
(*R*)-6-bromo-3-(4-(*tert*-butyl)phenyl)-3-(trifluoromethyl)-1,2,3,4-tetrahydroquinoline was prepared following the general procedure B as a white solid: 83% yield, 97% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 97/3, 1.0 mL/min, λ =210 nm, RT: Major: 8.445 min, Minor: 22.030 min).



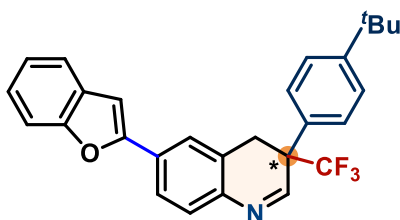
RT [min]	Width [min]	Area	Height	Area%
8.337	1.74	11417.00	684.11	49.66
23.689	3.41	11575.40	238.47	50.34



RT [min]	Width [min]	Area	Height	Area%
8.501	1.46	285.14	17.12	1.55
21.887	3.04	18160.10	369.53	98.45



RT [min]	Width [min]	Area	Height	Area%
8.445	2.18	44876.70	2600.21	98.45
22.030	2.17	706.36	15.42	1.55



Following General Procedure C, 0.2 mmol (82 mg) **19** and 0.3 mmol (49 mg) benzofuran-2-ylboronic provide **35** as a white solid, mp 155.5-157.3 °C, $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.33 (s, 1H), 7.70 (dd, J = 8.0, 2.0 Hz, 1H), 7.63 (s, 1H), 7.56 (d, J = 7.5 Hz, 1H), 7.49 (d, J = 8.0 Hz, 1H), 7.42 (d, J = 8.0 Hz, 1H), 7.34-7.20 (m, 6H), 7.00 (s, 1H), 3.51-3.43 (m, 2H), 1.22 (s, 9H).

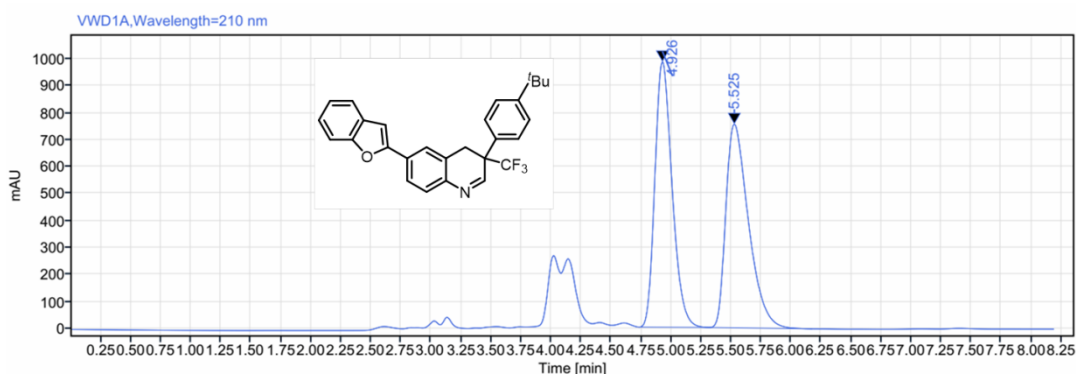
$^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 158.0 (q, J = 2.5 Hz), 155.0, 154.9, 151.7, 142.0, 130.3, 129.6, 129.0, 127.7, 127.3, 126.7 (q, J = 281.3 Hz), 125.7, 124.6, 124.50, 124.45, 124.3, 123.1, 121.0, 111.1, 102.0, 49.3 (q, J = 25.0 Hz), 34.4, 31.1, 29.9 (q, J = 2.5 Hz).

$^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -71.78.

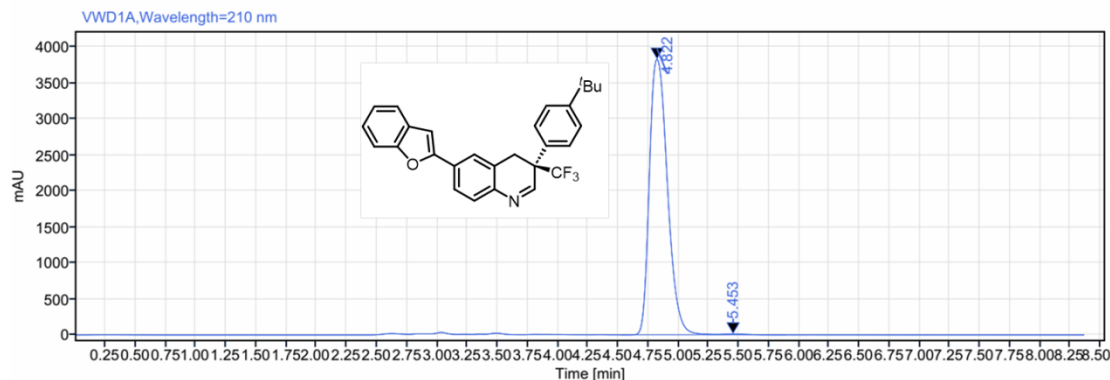
HRMS (ESI^+) m/z calcd for $\text{C}_{28}\text{H}_{25}\text{F}_3\text{NO}^+$ $[\text{M}+\text{H}]^+$ 448.1883, found 448.1887.

(*S*)-6-(benzofuran-2-yl)-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure C as a white solid: 84% yield, 99% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 4.822 min, Minor: 5.453 min).

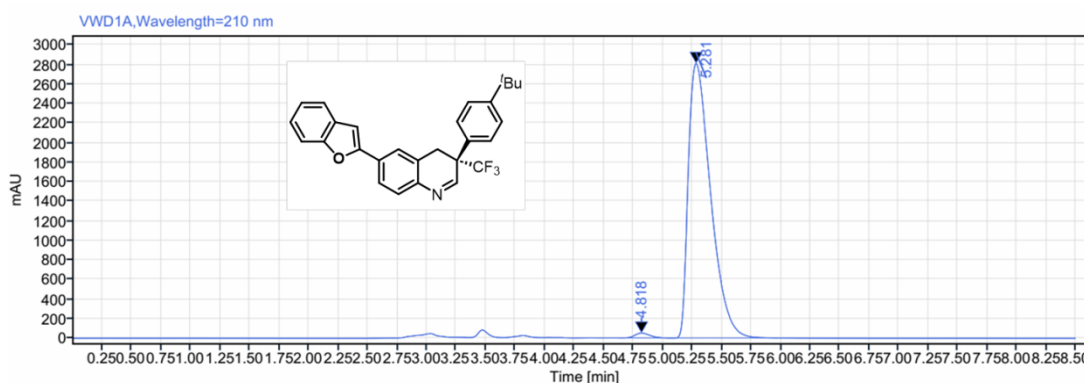
(*R*)-6-(benzofuran-2-yl)-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure C as a white solid: 90% yield, 98% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 5.281 min, Minor: 4.818 min).



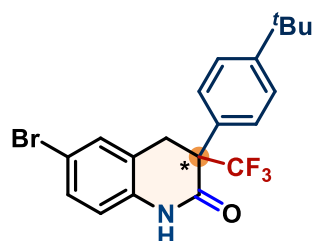
RT [min]	Width [min]	Area	Height	Area%
4.926	0.58	9815.95	983.87	49.79
5.525	0.86	9900.28	754.52	50.21



RT [min]	Width [min]	Area	Height	Area%
4.822	0.79	39828.39	3828.48	99.56
5.453	0.58	175.04	12.48	0.44



RT [min]	Width [min]	Area	Height	Area%
4.818	0.47	440.14	49.87	1.18
5.281	0.88	36941.09	2811.56	98.82



Following General Procedure D, 0.2 mmol (82 mg) **19** provides **36** as a white solid, mp 221.0-222.7 °C, ¹H NMR (500 MHz, CDCl₃) δ 9.37 (s, 1H), 7.41-7.34 (m, 3H), 7.32-7.27 (m, 2H), 7.21 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.65 (d, *J* = 8.5 Hz, 1H), 3.69-3.57 (m, 2H), 1.25 (s, 9H).

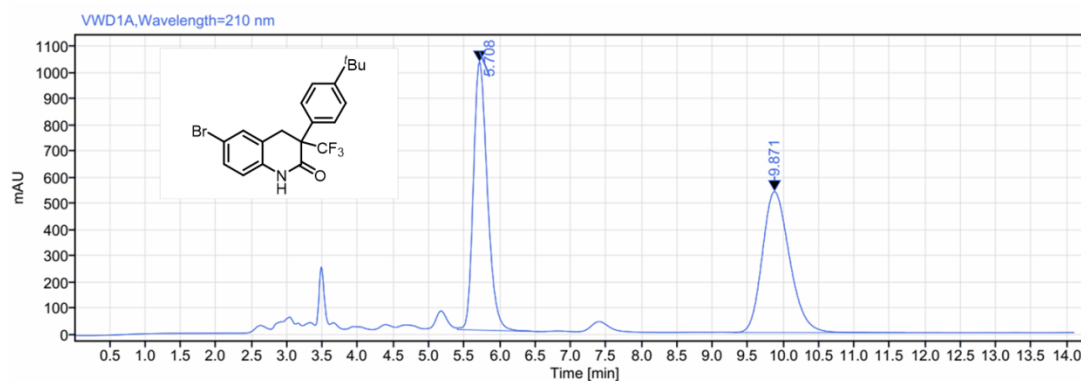
¹³C NMR (150 MHz, CDCl₃) δ 167.2, 152.2, 134.7, 131.0, 130.9, 127.8, 126.2, 125.8, 125.0 (q, *J* = 280.5 Hz), 122.8, 117.0, 116.1, 54.3 (q, *J* = 25.5 Hz), 34.5, 31.1, 30.5.

¹⁹F NMR (564 MHz, CDCl₃) δ -70.90.

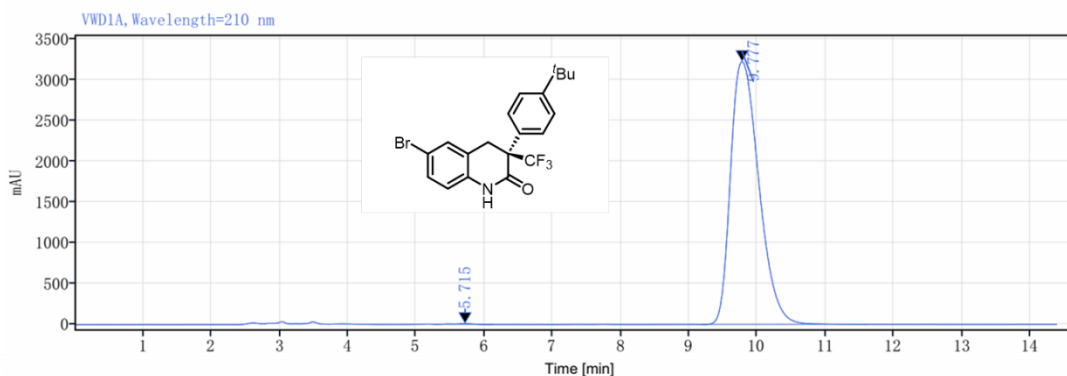
HRMS (ESI⁺) *m/z* calcd for C₂₀H₂₀BrF₃NO⁺ [M+H]⁺ 426.0675, found 426.0669.

(*S*)-6-bromo-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinolin-2(1H)-one was prepared following the general procedure D as a white solid: 91% yield, 99% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ=210 nm, RT: Major: 9.777 min, Minor: 5.715 min).

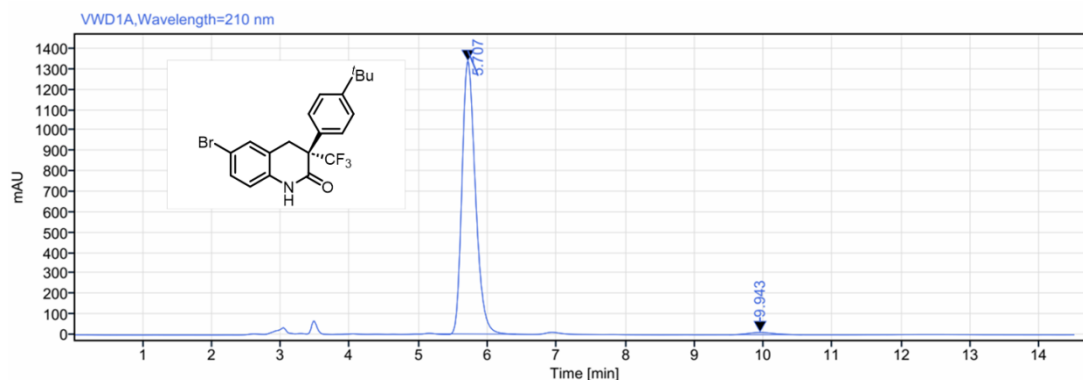
(*R*)-6-bromo-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinolin-2(1H)-one was prepared following the general procedure D as a white solid: 89% yield, 98% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ=210 nm, RT: Major: 5.707 min, Minor: 9.943 min).



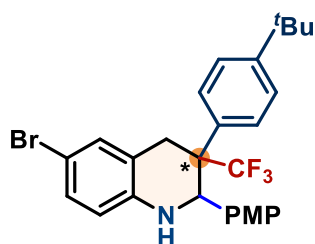
RT [min]	Width [min]	Area	Height	Area%
5.708	1.15	14071.25	1024.08	49.50
9.871	2.42	14358.38	538.34	50.50



RT [min]	Width [min]	Area	Height	Area%
5.715	0.88	156.46	8.83	0.17
9.777	2.44	93067.66	3227.90	99.83



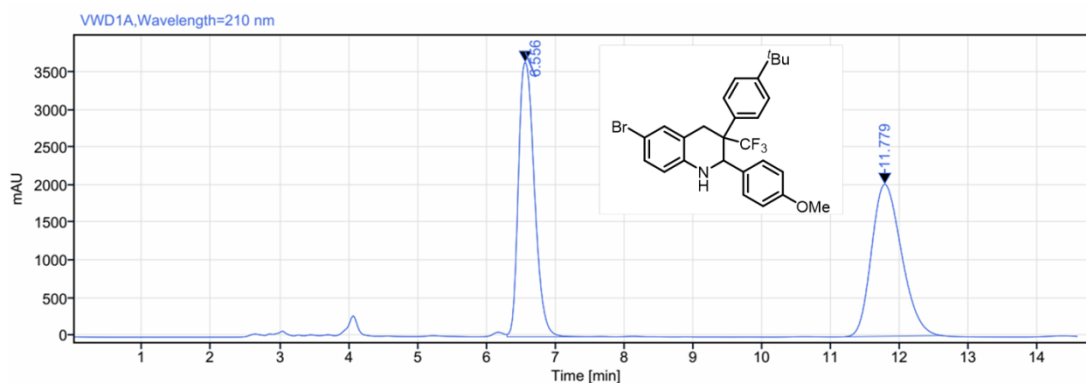
RT [min]	Width [min]	Area	Height	Area%
5.707	1.17	18069.86	1335.01	98.40
9.943	1.05	294.43	11.15	1.60



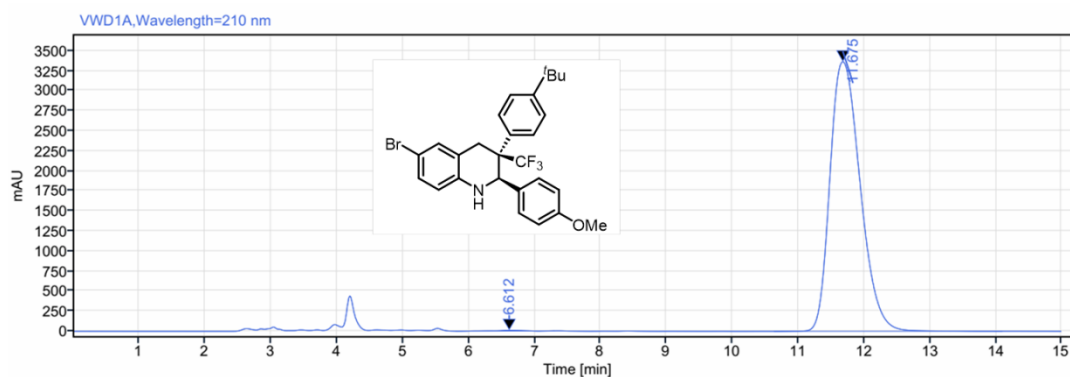
Following General Procedure E, 0.2 mmol (82 mg) **19** provides **37** as a white solid, mp 159.1-160.6 °C, ¹H NMR (500 MHz, CDCl₃) δ 7.32 (d, *J* = 2.0 Hz, 1H), 7.23-7.19 (m, 2H), 7.15 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.10-7.05 (m, 2H), 6.92-6.87 (m, 2H), 6.73-6.68 (m, 2H), 6.41 (d, *J* = 8.5 Hz, 1H), 4.86 (s, 1H), 4.00 (s, 1H), 3.77 (s, 3H), 3.56 (d, *J* = 17.0 Hz, 1H), 3.39 (d, *J* = 17.0 Hz, 1H), 1.28 (s, 9H). ¹³C NMR (150 MHz, CDCl₃) δ 159.4, 150.8, 142.9, 131.5, 131.3, 131.0, 130.0, 129.9, 128.4, 127.6 (q, *J* = 283.5 Hz), 124.6, 121.6, 115.6, 113.0, 109.9, 58.7, 55.2, 50.2 (q, *J* = 22.5 Hz), 34.4, 32.0 (q, *J* = 3.0 Hz), 31.2. ¹⁹F NMR (564 MHz, CDCl₃) δ -68.17.

(2*R*,3*S*)-6-bromo-3-(4-(tert-butyl)phenyl)-2-(4-methoxyphenyl)-3-(trifluoromethyl)-1,2,3,4-tetrahydroquinoline was prepared following the general procedure E as a white solid: 88% yield, >20:1 d.r., 98% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 11.675 min, Minor: 6.612 min).

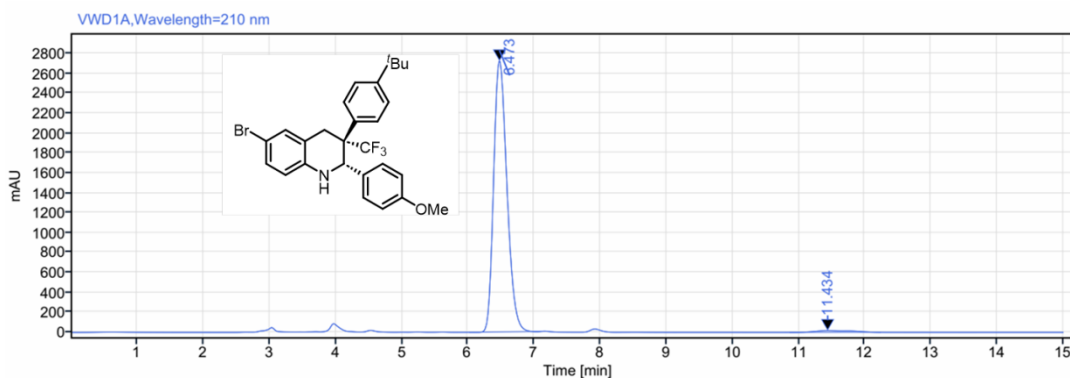
(2*S*,3*R*)-6-bromo-3-(4-(tert-butyl)phenyl)-2-(4-methoxyphenyl)-3-(trifluoromethyl)-1,2,3,4-tetrahydroquinoline was prepared following the general procedure E as a white solid: 79% yield, >20:1 d.r., 96% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 6.473 min, Minor: 11.434 min).



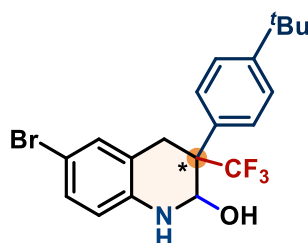
RT [min]	Width [min]	Area	Height	Area%
6.556	1.11	58695.91	3642.53	49.01
11.779	1.44	61069.82	2016.94	50.99



RT [min]	Width [min]	Area	Height	Area%
6.612	1.51	198.44	9.94	0.18
11.675	3.46	107187.31	3363.67	99.82



RT [min]	Width [min]	Area	Height	Area%
6.473	1.18	37988.96	2719.88	98.22
11.434	1.38	687.79	17.31	1.78



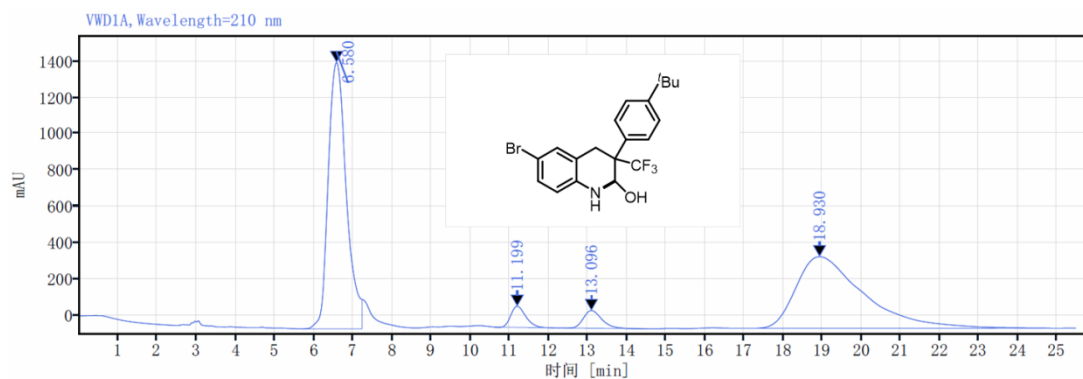
Following General Procedure F, 0.2 mmol (82 mg) **19** provides **38** as colorless oil, $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.45 (d, $J = 8.0$ Hz, 2H), 7.41-7.38 (m, 1H), 7.36 (d, $J = 8.0$ Hz, 2H), 7.00 (dd, $J = 8.5$, 2.0 Hz, 1H), 6.34 (d, $J = 9.0$ Hz, 1H), 4.68 (d, $J = 4.0$ Hz, 1H), 3.69 (d, $J = 16.5$ Hz, 1H), 3.25 (d, $J = 16.5$ Hz, 1H), 2.16 (d, $J = 4.0$ Hz, 1H), 1.37 (s, 1H), 1.32 (s, 9H).

$^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 152.2, 138.5, 131.27, 131.26, 130.1, 126.7, 126.2 (q, $J = 282.0$ Hz), 125.6, 120.9, 114.8, 112.1, 84.8, 50.4 (q, $J = 25.5$ Hz), 34.6, 31.1, 24.8 (q, $J = 3.0$ Hz).

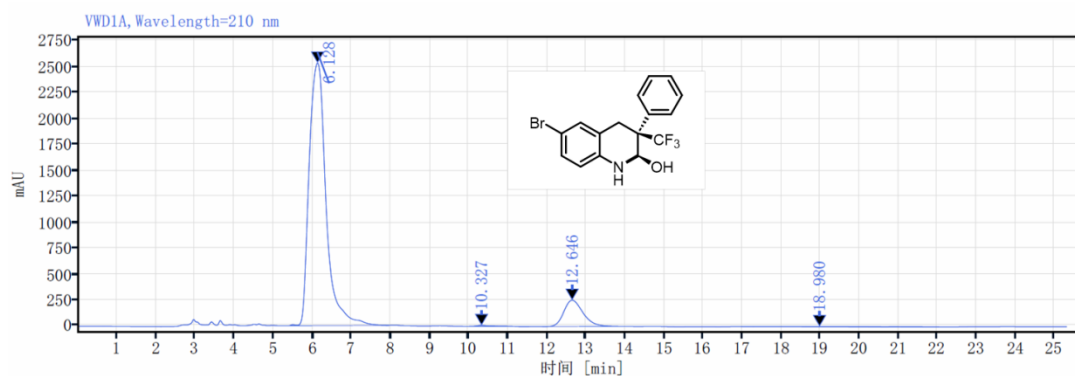
$^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -67.89.

(2*R*,3*S*)-6-bromo-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-1,2,3,4-tetrahydroquinolin-2-ol was prepared following the general procedure F as colorless oil: 36% yield, 9:1 d.r., 99% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 99.5/0.5, 1.0 mL/min, λ =210 nm, RT: Major: 6.128, 12.646 min, Minor: 18.980, 10.327 min).

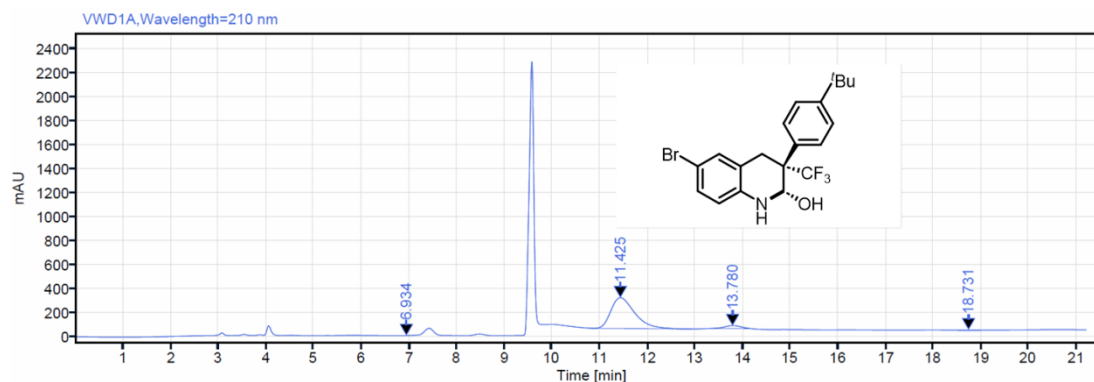
(2*S*,3*R*)-6-bromo-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-1,2,3,4-tetrahydroquinolin-2-ol was prepared following the general procedure F as colorless oil: 40% yield, >20:1 d.r., 90% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 99.5/0.5, 1.0 mL/min, λ =210 nm, RT: Major: 11.425, 18.731 min, Minor: 13.780, 6.934 min).



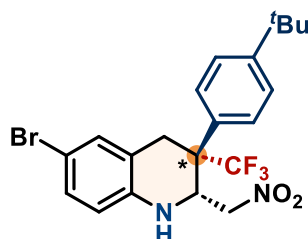
RT [min]	Width [min]	Area	Height	Area%
6.580	1.51	47142.78	1465.65	46.84
11.199	1.53	3070.74	116.32	3.05
13.096	2.09	3187.05	97.87	3.17
18.930	7.52	47250.78	394.46	46.95



RT [min]	Width [min]	Area	Height	Area%
6.128	2.66	76075.70	2533.91	89.20
10.327	1.56	303.21	9.94	0.36
12.646	2.09	8703.86	254.32	10.20
18.980	5.07	207.84	2.01	0.24



RT [min]	Width [min]	Area	Height	Area%
6.934	0.25	1.60	0.18	0.02
11.425	2.12	8918.58	256.66	92.88
13.780	0.78	532.44	23.01	5.55
18.731	2.04	149.20	2.39	1.55



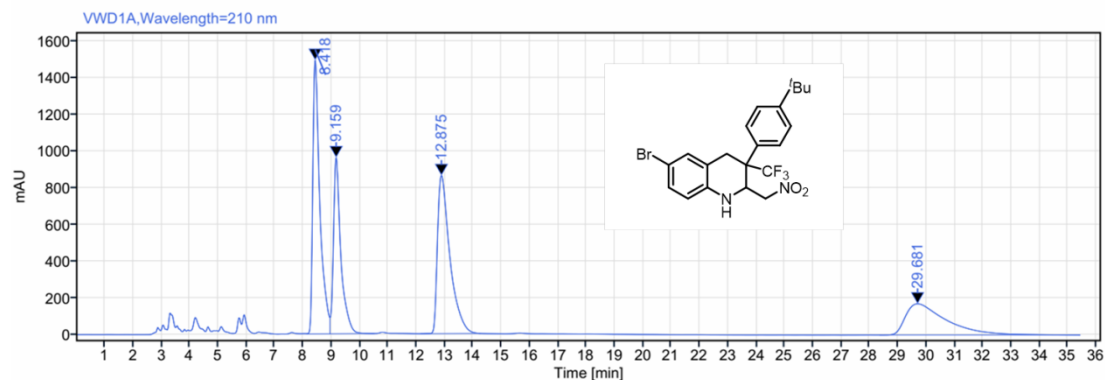
Following General Procedure G, 0.2 mmol (82 mg) **19** provides **39** as a yellow solid, mp 147.2-148.1 °C, ¹H NMR (600 MHz, CDCl₃) δ 7.50-7.46 (m, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.31-7.28 (m, 1H), 7.19 (dd, *J* = 8.4, 1.8 Hz, 1H), 6.53 (d, *J* = 8.4 Hz, 1H), 5.05-4.99 (m, 1H), 4.55 (d, *J* = 4.2 Hz, 1H), 4.20-4.14 (m, 1H), 4.10 (dd, *J* = 13.8, 2.4 Hz, 1H), 3.54 (d, *J* = 17.4 Hz, 1H), 3.18 (d, *J* = 17.4 Hz, 1H), 1.34 (s, 9H).

¹³C NMR (150 MHz, CDCl₃) δ 152.3, 139.0, 132.2, 131.6, 130.7, 126.51 (q, *J* = 283.5 Hz), 126.46, 126.3, 119.9, 117.3, 110.9, 75.7, 51.6, 46.2 (q, *J* = 25.5 Hz), 34.6, 31.2, 28.8.

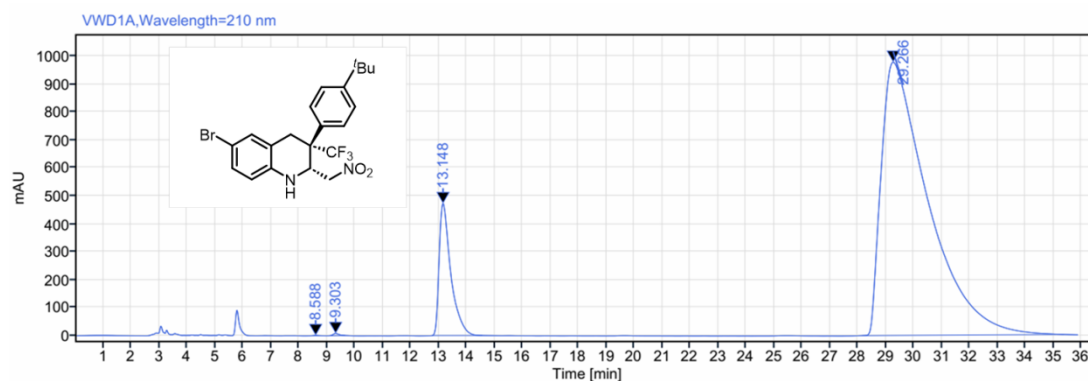
¹⁹F NMR (564 MHz, CDCl₃) δ -71.38.

HRMS (ESI⁺) *m/z* calcd for C₂₁H₂₃BrF₃N₂O₂⁺ [M+H]⁺ 471.0890, found 471.0883.

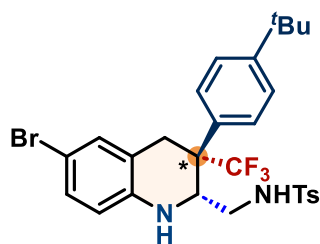
(2*S*,3*R*)-6-bromo-3-(4-(*tert*-butyl)phenyl)-2-(nitromethyl)-3-(trifluoromethyl)-1,2,3,4-tetrahydroquinoline was prepared following the general procedure G as a yellow solid: 69% yield, 9:1 d.r., 99% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ=210 nm, RT: Major: 13.148, 29.266 min, Minor: 8.588, 9.303min).



RT [min]	Width [min]	Area	Height	Area%
8.418	0.82	26080.43	1497.11	29.99
9.159	1.57	17520.52	963.72	20.15
12.875	2.13	26267.74	865.24	30.21
29.681	7.08	17084.60	170.88	19.65



RT [min]	Width [min]	Area	Height	Area%
8.588	0.57	18.80	1.38	0.01
9.303	0.71	112.56	7.83	0.09
13.148	1.79	13687.20	472.00	10.75
29.266	7.22	113517.26	977.35	89.15



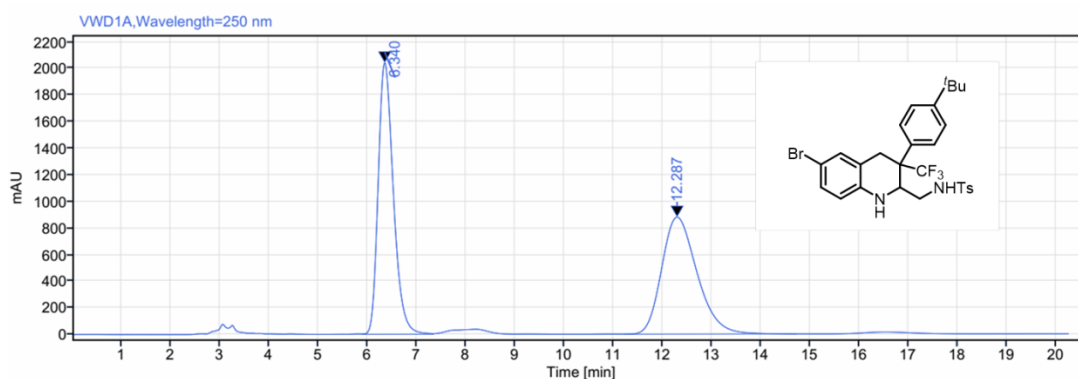
Following General Procedure H, 0.2 mmol (94 mg) **39** provides **40** as a yellow solid, mp 173.2-174.1 °C, ¹H NMR (500 MHz, CDCl₃) δ 7.52 (d, *J* = 8.0 Hz, 2H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.5 Hz, 2H), 7.20-7.15 (m, 3H), 7.13 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.51 (d, *J* = 8.5 Hz, 1H), 4.84 (t,

$J = 6.5$ Hz, 1H), 4.61 (d, $J = 4.5$ Hz, 1H), 4.34 (d, $J = 10.0$ Hz, 1H), 3.40 (d, $J = 17.5$ Hz, 1H), 3.10 (d, $J = 17.5$ Hz, 1H), 2.73-2.66 (m, 1H), 2.49-2.42 (m, 1H), 2.38 (s, 3H), 1.35 (s, 9H).

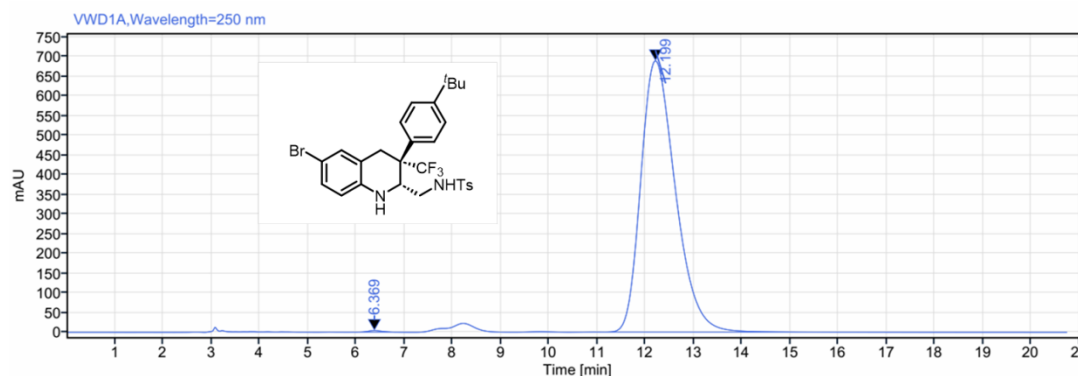
^{13}C NMR (150 MHz, CDCl_3) δ 151.5, 143.8, 139.9, 135.9, 132.8, 131.4, 130.2, 129.7, 127.1, 126.90, 126.86 (q, $J = 283.5$ Hz), 125.7, 120.9, 117.5, 110.3, 58.5, 52.9, 46.3 (q, $J = 24.0$ Hz), 42.6, 34.5, 31.2, 28.7, 21.5, 18.4.

^{19}F NMR (564 MHz, CDCl_3) δ -71.51.

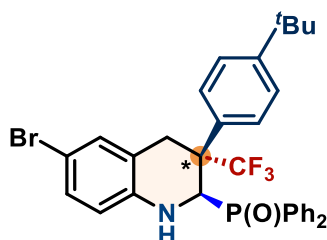
N-(((2*S*,3*R*)-6-bromo-3-(4-(*tert*-butyl)phenyl)-3-(trifluoromethyl)-1,2,3,4-tetrahydroquinolin-2-yl)methyl)-4-methylbenzenesulfonamide was prepared following the general procedure H as a yellow solid: 77% yield, 20:1 d.r., 99% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 80/20, 1.0 mL/min, $\lambda = 210$ nm, RT: Major: 12.199 min, Minor: 6.369 min).



RT [min]	Width [min]	Area	Height	Area%
6.340	1.46	43833.79	2040.19	49.95
12.287	3.50	43919.58	879.57	50.05



RT [min]	Width [min]	Area	Height	Area%
6.369	0.85	83.72	4.05	0.24
12.199	4.27	34377.33	690.08	99.76



Following General Procedure I, 0.2 mmol (82 mg) **19** provides **41** as a white solid, mp 158.3-159.8°C, ^1H NMR (500 MHz, CDCl_3) δ 7.65-7.56 (m, 2H), 7.51-7.45 (m, 1H), 7.45-7.35 (m, 4H), 7.34-7.27 (m,

2H), 7.25-7.18 (m, 4H), 6.99 (d, $J = 8.5$ Hz, 1H), 6.89 (d, $J = 8.0$ Hz, 2H), 5.86 (d, $J = 8.5$ Hz, 1H), 4.88 (s, 1H), 4.77 (d, $J = 16.5$ Hz, 1H), 4.03 (s, 1H), 3.21 (d, $J = 16.5$ Hz, 1H), 1.17 (s, 9H).

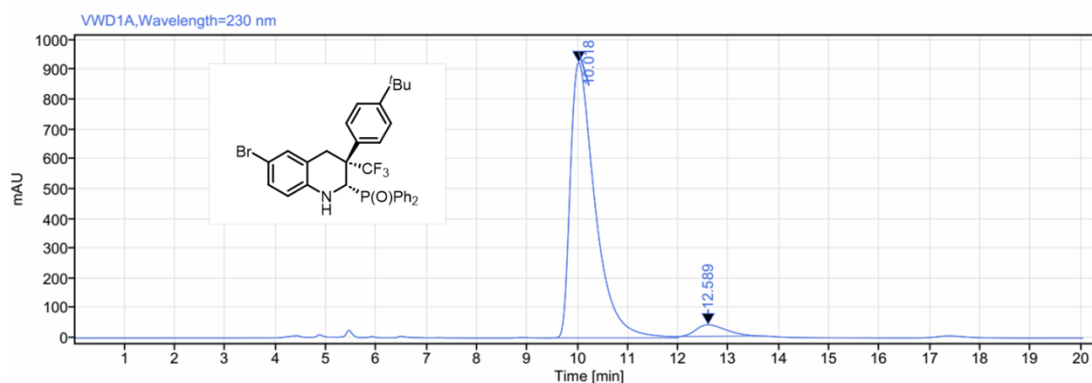
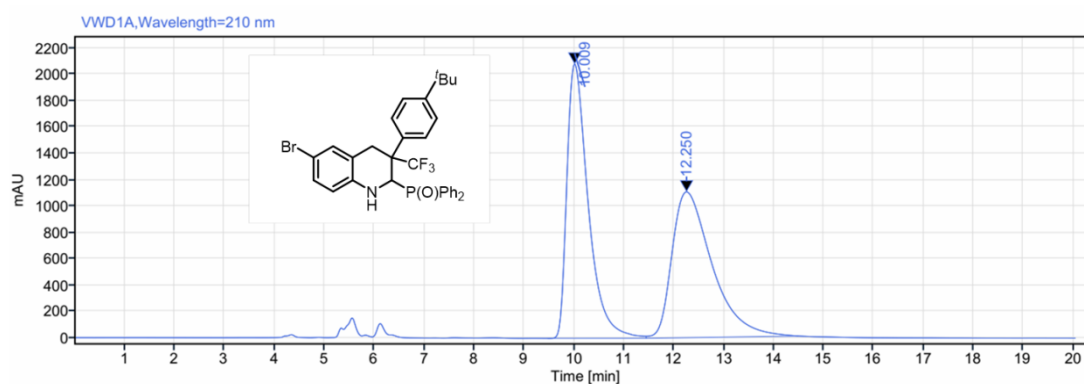
^{13}C NMR (150 MHz, CDCl_3) δ 151.0, 139.5, 132.7, 132.4, 132.1, 131.5 (d, $J = 1.5$ Hz), 131.3, 131.0 (d, $J = 3.0$ Hz), 130.9 (d, $J = 9.0$ Hz), 130.2 (d, $J = 9.0$ Hz), 129.5, 129.1, 128.6 (d, $J = 12.0$ Hz), 128.1 (d, $J = 12.0$ Hz), 127.7, 127.0 (qd, $J = 285.0, 16.5$ Hz), 124.6, 123.2, 115.5, 110.5, 54.5 (d, $J = 67.5$ Hz), 47.7 (qd, $J = 24.0, 6.0$ Hz), 34.2, 31.1, 28.5.

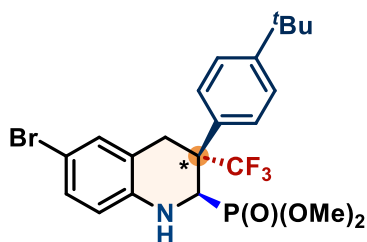
^{19}F NMR (470 MHz, CDCl_3) δ -70.83 (d, $J = 5.1$ Hz).

^{31}P NMR (202 MHz, CDCl_3) δ 31.54 (q, $J = 5.1$ Hz).

HRMS (ESI $^+$) m/z calcd for $\text{C}_{32}\text{H}_{31}\text{BrF}_3\text{NOP}^+$ $[\text{M}+\text{H}]^+$ 612.1273, found 612.1280.

((2*R*,3*S*)-6-bromo-3-(4-(*tert*-butyl)phenyl)-3-(trifluoromethyl)-1,2,3,4-tetrahydroquinolin-2-yl)diphenyl phosphine oxide was prepared following the general procedure I as a white solid: 82% yield, >20:1 d.r., 90% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 90/10, 0.7 mL/min, λ =230 nm, RT: Major: 10.018 min, Minor: 12.589 min).





Following General Procedure I, 0.2 mmol (82 mg) **19** provides **42** as a white solid, mp 191.5-192.6 °C, $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.49 (d, J = 8.5 Hz, 2H), 7.44 (d, J = 8.5 Hz, 2H), 7.26 (s, 1H), 7.12 (d, J = 8.5 Hz, 1H), 6.51 (d, J = 8.5 Hz, 1H), 4.59-4.52 (m, 1H), 4.51-4.45 (m, 1H), 4.13 (d, J = 17.0 Hz, 1H), 3.42 (d, J = 10.5 Hz, 3H), 3.28 (d, J = 17.0 Hz, 1H), 2.90 (d, J = 10.5 Hz, 3H), 1.32 (s, 9H).

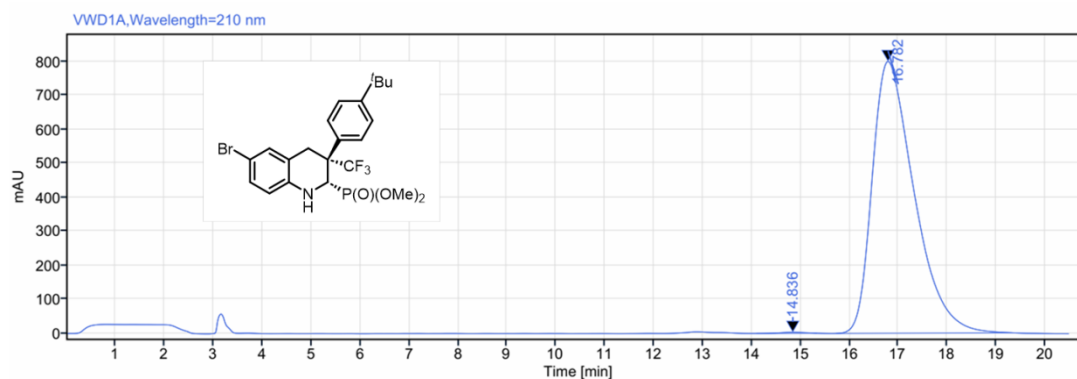
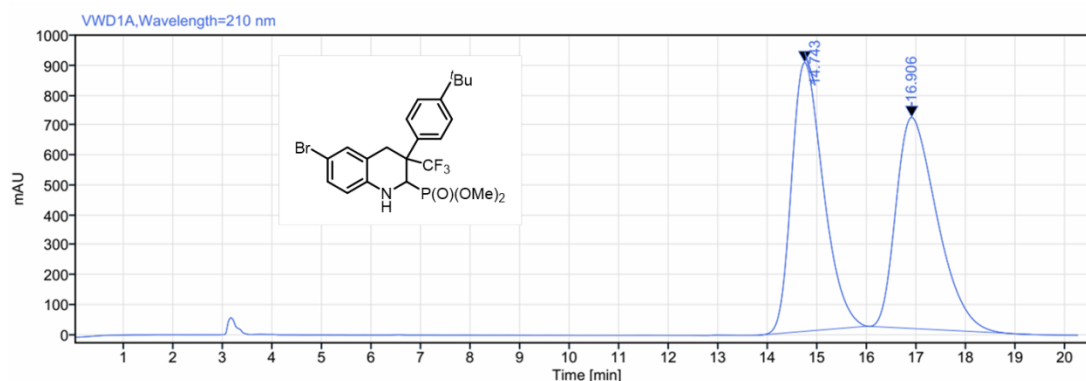
$^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 151.7, 140.3, 131.5, 131.3, 129.6, 127.4, 127.0 (qd, J = 285.0, 24.0 Hz), 125.2, 122.0, 115.6, 110.4, 53.1 (d, J = 151.5 Hz), 52.8 (dd, J = 7.5, 1.5 Hz), 52.2 (dd, J = 7.5, 1.5 Hz), 46.1 (qd, J = 24.0, 9.0 Hz), 34.5, 31.1, 28.5.

$^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -70.83 (d, J = 8.0 Hz).

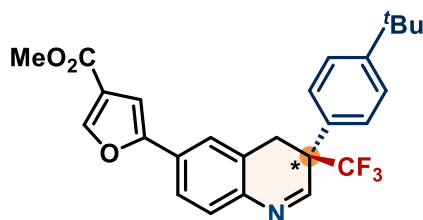
$^{31}\text{P NMR}$ (243 MHz, CDCl_3) δ 23.58 (q, J = 6.1 Hz).

HRMS (ESI $^+$) m/z calcd for $\text{C}_{22}\text{H}_{27}\text{BrF}_3\text{NO}_3\text{P}^+$ $[\text{M}+\text{H}]^+$ 520.0859, found 520.0852.

Dimethyl((2*R*,3*S*)-6-bromo-3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-1,2,3,4-tetrahydroquinolin-2-yl)phosphonate was prepared following the general procedure I as a white solid: 79% yield, >20:1 d.r., 99% e.e. (Chiracel OZ-H, Hexanes/*i*-PrOH = 95/5, 1.0 mL/min, λ =210 nm, RT: Major: 16.782 min, Minor: 14.836 min).



14.836	1.24	101.56	2.97	0.21
16.782	3.60	47478.48	798.96	99.79

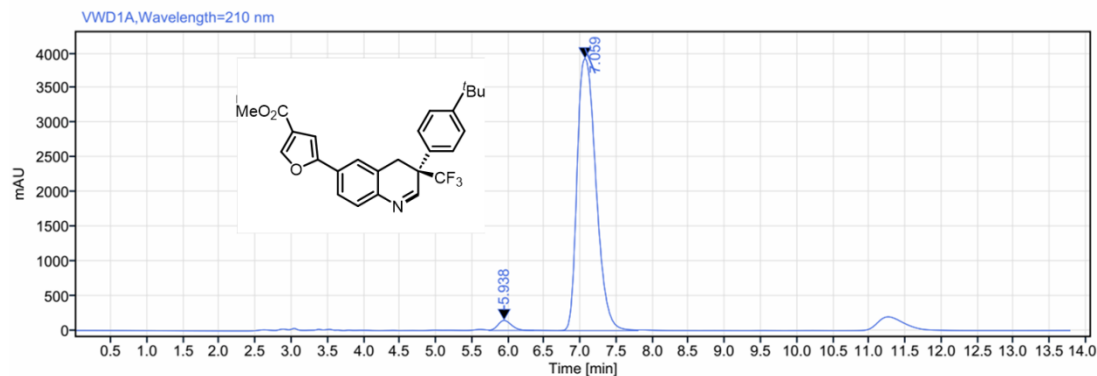
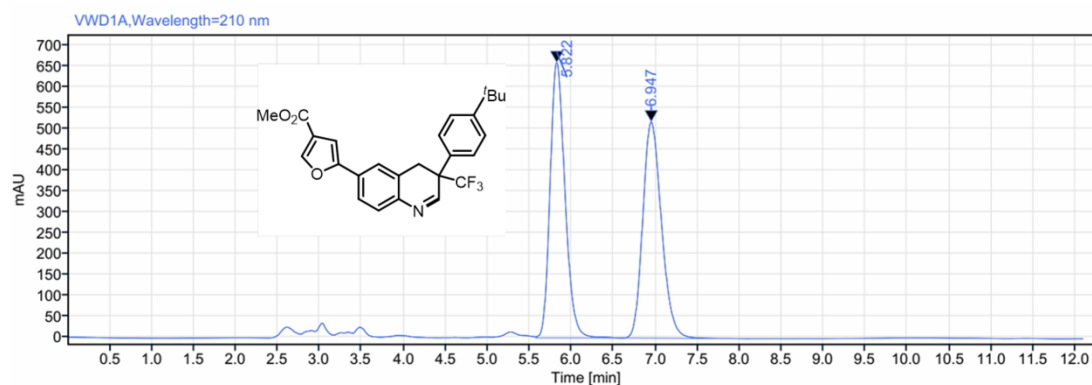


Following General Procedure A, 0.3 mmol (73 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **44** as a yellow solid, mp 141.4-142.3 °C, ^1H NMR (500 MHz, CDCl_3) δ 8.31 (s, 1H), 8.00 (s, 1H), 7.51 (dd, J = 8.5, 2.0 Hz, 1H), 7.43 (s, 1H), 7.38 (d, J = 8.5 Hz, 1H), 7.31-7.24 (m, 4H), 6.95 (s, 1H), 3.85 (s, 3H), 3.43 (s, 2H), 1.22 (s, 9H).

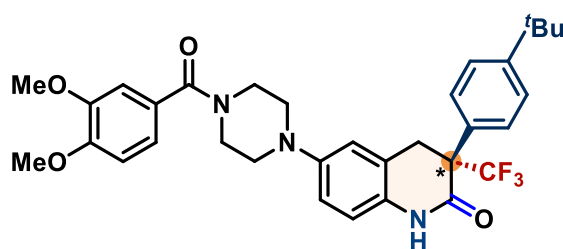
^{13}C NMR (150 MHz, CDCl_3) δ 163.3, 158.0 (q, J = 3.0 Hz), 154.4, 151.7, 147.0, 141.7, 129.7, 129.6, 127.7, 127.3, 126.7 (q, J = 282.0 Hz), 125.7, 124.4, 123.6, 121.1, 105.2, 51.7, 49.3 (q, J = 25.5 Hz), 34.4, 31.1, 29.9.

^{19}F NMR (564 MHz, CDCl_3) δ -71.81.

Methyl(*S*)-5-(3-(4-(tert-butyl)phenyl)-3-(trifluoromethyl)-3,4-dihydroquinolin-6-yl)furan-3-carboxylate was prepared following the general procedure A as a yellow solid: 83% yield, 95% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 7.059 min, Minor: 5.938 min).



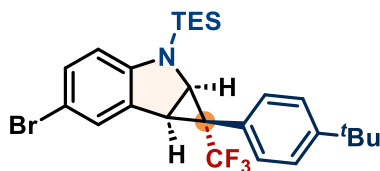
7.059 1.10 71243.08 3928.72 97.41



(**45**), white solid, mp 191.7-192.5 °C, $^1\text{H NMR}$ (500 MHz, DMSO- d_6) δ 10.83 (s, 1H), 7.45-7.40 (m, 3H), 7.36 (d, J = 8.0 Hz, 2H), 7.12-7.06 (m, 3H), 7.03 (d, J = 9.0 Hz, 1H), 6.75 (d, J = 8.5 Hz, 1H), 4.24 (s, 2H), 3.95-3.70 (m, 10H), 3.66-3.58 (m, 1H), 3.50 (d, J = 16.0 Hz, 1H), 1.21 (s, 9H).
 $^{13}\text{C NMR}$ (125 MHz, DMSO- d_6) δ 169.3, 165.7, 165.1, 151.8, 150.7, 148.9, 137.1, 135.1, 130.1, 128.4, 127.7, 127.6, 126.0, 125.9 (q, J = 281.3 Hz), 125.6, 121.4, 120.8, 115.4, 111.6, 56.1, 54.3 (q, J = 23.8 Hz), 34.7, 34.2, 31.7, 31.4, 29.8.

$^{19}\text{F NMR}$ (470 MHz, DMSO- d_6) δ -69.73.

HRMS (ESI $^+$) m/z calcd for $\text{C}_{33}\text{H}_{37}\text{F}_3\text{N}_3\text{O}_4$ $[\text{M}+\text{H}]^+$ 596.2703, found 596.2780.

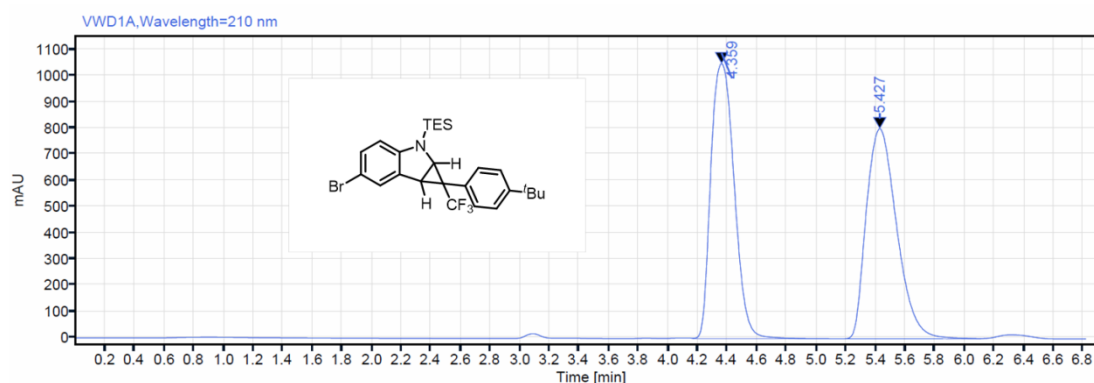


Following General Procedure A, 0.3 mmol (93 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **47** as a colorless oil, $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.45 (d, J = 2.0 Hz, 1H), 7.11 (d, J = 8.5 Hz, 2H), 7.04 (d, J = 8.5 Hz, 2H), 6.91 (dd, J = 8.5, 2.5 Hz, 1H), 6.19 (d, J = 8.5 Hz, 1H), 4.24 (d, J = 7.0 Hz, 1H), 3.50 (d, J = 7.0 Hz, 1H), 1.20 (s, 9H), 1.00-0.92 (m, 9H), 0.91-0.80 (m, 6H).

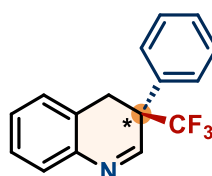
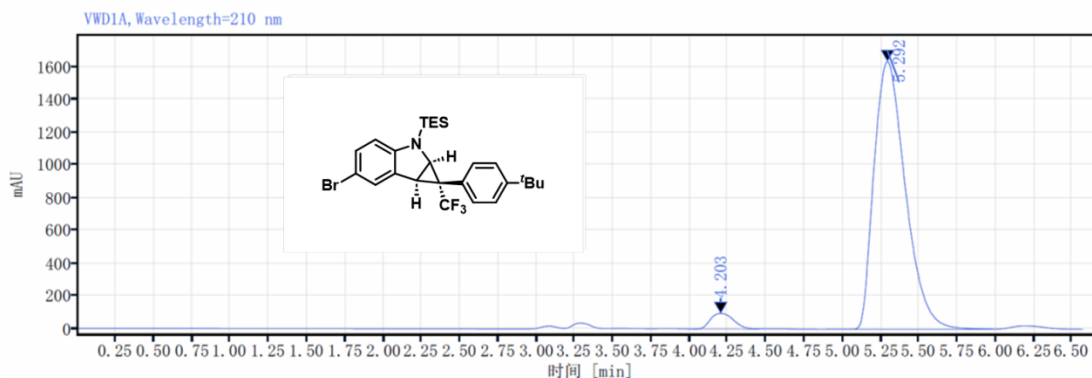
$^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 150.7, 149.8, 132.9, 130.6, 129.7, 128.1, 126.4 (q, J = 273.0 Hz), 124.4, 124.3, 111.1, 109.5, 49.1 (q, J = 4.5 Hz), 34.4, 31.1, 30.6 (d, J = 3.0 Hz), 25.7 (q, J = 30.0 Hz), 7.0, 4.4.

$^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -66.77.

47 was prepared following the general procedure as a white solid: 95% yield, 92% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 100/0, 1.0 mL/min, λ =210 nm, RT: Major: 5.292 min, Minor: 4.203 min).



RT [min]	Width [min]	Area	Height	Area%
4.359	1.00	11489.34	1049.52	50.10
5.427	0.94	11445.44	801.89	49.90

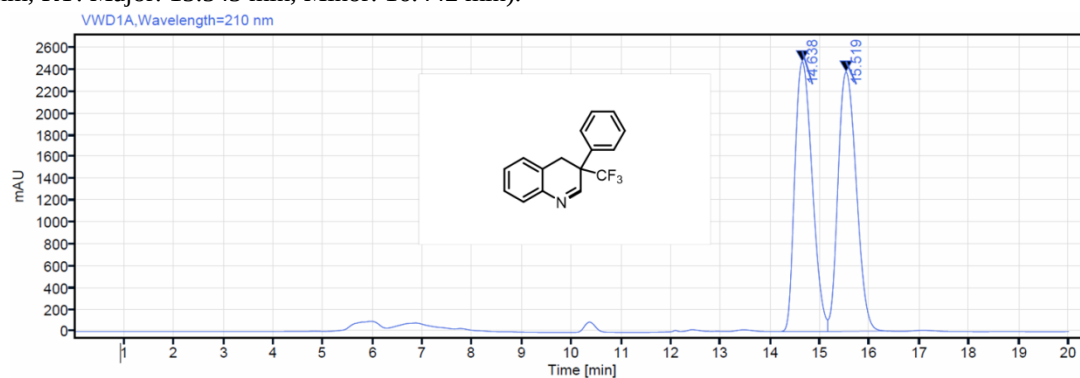


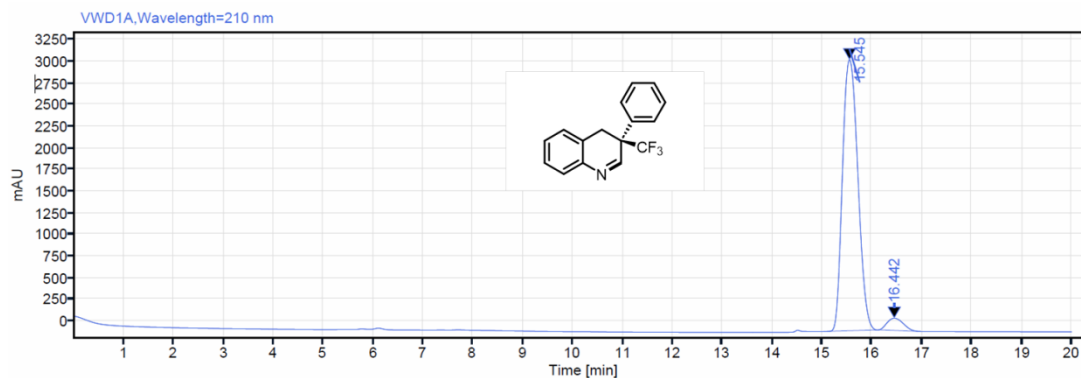
Following General Procedure A, 0.3 mmol (36 mg) indole and 0.2 mmol (80 mg) *N*-triftosylhydrazone provide **49** as a white solid, mp 91.8-92.5 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.33 (s, 1H), 7.41-7.36 (m, 2H), 7.34 (d, *J* = 7.5 Hz, 1H), 7.28-7.17 (m, 4H), 7.15-7.06 (m, 2H), 3.46-3.36 (m, 2H).

¹³C NMR (150 MHz, CDCl₃) δ 157.6 (q, *J* = 3.0 Hz), 141.9, 132.9, 128.7, 128.6, 128.5, 128.1, 128.0, 127.7, 127.1, 126.7 (d, *J* = 280.5 Hz), 123.5, 49.5 (q, *J* = 25.5 Hz), 29.9 (d, *J* = 3.0 Hz).

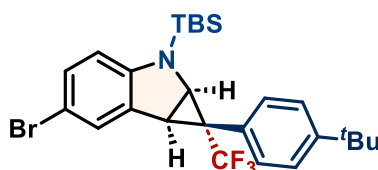
¹⁹F NMR (564 MHz, CDCl₃) δ -71.82.

(*S*)-3-phenyl-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 90% yield, 91% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 99.5/0.5, 0.5 mL/min, λ=210 nm, RT: Major: 15.545 min, Minor: 16.442 min).





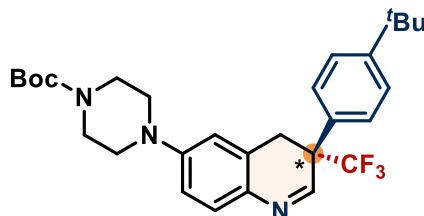
RT [min]	Width [min]	Area	Height	Area%
15.545	1.14	67000.45	3129.60	95.49
16.442	0.83	3165.97	140.45	4.51



Following General Procedure A, 0.3 mmol (93 mg) indole and 0.2 mmol (91 mg) *N*-triftosylhydrazone provide **s5** as a colorless oil, $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 7.39 (d, J = 2.5 Hz, 1H), 7.10 (d, J = 8.0 Hz, 2H), 7.02 (d, J = 8.0 Hz, 2H), 6.84 (dd, J = 8.5, 2.0 Hz, 1H), 6.15 (d, J = 8.5 Hz, 1H), 4.22 (d, J = 7.0 Hz, 1H), 3.49 (d, J = 7.0 Hz, 1H), 1.19 (s, 9H), 0.92 (s, 9H), 0.56 (s, 3H), 0.27 (s, 3H).

$^{13}\text{C NMR}$ (150 MHz, CDCl_3) δ 150.8, 149.7, 132.8, 130.8, 129.5, 128.0, 126.4 (q, J = 271.5 Hz), 124.4, 124.3, 112.1, 109.4, 49.5 (q, J = 3.0 Hz), 34.4, 31.2, 30.4 (q, J = 3.0 Hz), 26.7, 20.6, 1.0, -3.8, -4.3

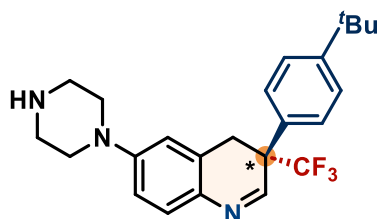
$^{19}\text{F NMR}$ (564 MHz, CDCl_3) δ -66.67.



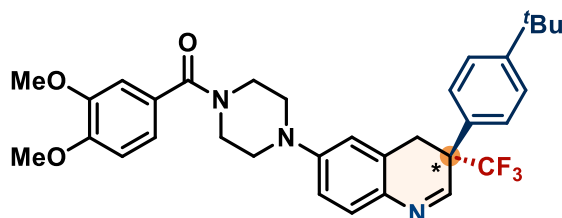
(**R-A**), $^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.11 (s, 1H), 7.33-7.21 (m, 5H), 6.70 (d, J = 8.5 Hz, 1H), 6.62 (s, 1H), 3.59-3.50 (m, 4H), 3.39 (d, J = 16.0 Hz, 2H), 3.30 (d, J = 16.0 Hz, 1H), 3.18-3.08 (m, 4H), 1.47 (s, 9H), 1.23 (s, 9H).

$^{13}\text{C NMR}$ (125 MHz, CDCl_3) δ 154.6, 154.0, 151.3, 150.8, 135.1, 130.2, 128.2, 127.2, 126.8 (q, J = 280.0 Hz), 125.5, 124.7, 115.3, 114.5, 79.9, 49.2 (q, J = 25.0 Hz), 48.6, 34.4, 31.0, 30.5, 28.3.

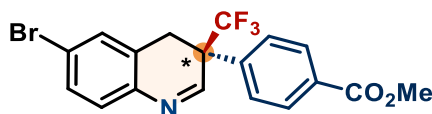
$^{19}\text{F NMR}$ (470 MHz, CDCl_3) δ -71.70.



(R-B), ^1H NMR (500 MHz, CDCl_3) δ 8.09 (s, 1H), 7.33-7.24 (m, 5H), 6.72 (dd, J = 9.0, 3.0 Hz, 1H), 6.63 (s, 1H), 3.39 (d, J = 16.0 Hz, 1H), 3.30 (d, J = 16.0 Hz, 1H), 3.19-3.10 (m, 4H), 3.03-2.94 (m, 4H), 2.10 (s, 1H), 1.24 (s, 9H).
 ^{13}C NMR (150 MHz, CDCl_3) δ 153.7, 151.4, 151.3, 134.8, 130.3, 128.2, 127.2, 126.9 (q, J = 280.5 Hz), 125.5, 124.6, 115.0, 114.1, 49.6, 49.3 (d, J = 25.5 Hz), 45.9, 34.4, 31.1, 30.6.
 ^{19}F NMR (564 MHz, CDCl_3) δ -71.72.



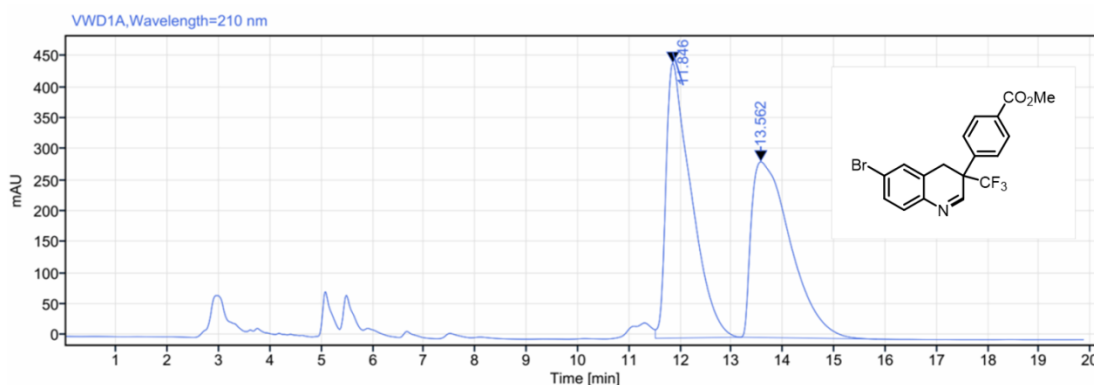
(R-C), ^1H NMR (500 MHz, CDCl_3) δ 8.13 (s, 1H), 7.32-7.25 (m, 5H), 7.04-6.99 (m, 2H), 6.87 (d, J = 8.0 Hz, 1H), 6.72 (dd, J = 8.5, 2.5 Hz, 1H), 6.65 (d, J = 3.0 Hz, 1H), 3.90 (s, 3H), 3.89 (s, 3H), 3.87-3.62 (m, 4H), 3.40 (d, J = 16.0 Hz, 1H), 3.32 (d, J = 16.0 Hz, 1H), 3.27-3.12 (m, 4H), 1.24 (s, 9H).
 ^{13}C NMR (150 MHz, CDCl_3) δ 170.3, 154.3, 151.4, 150.5, 150.4, 149.0, 135.2, 130.1, 128.2, 127.5, 127.1, 126.7 (q, J = 280.5 Hz), 125.5, 124.8, 120.1, 115.4, 114.6, 110.9, 110.4, 55.89, 55.88, 49.1 (q, J = 24.0 Hz), 48.9, 34.3, 31.0, 30.4.
 ^{19}F NMR (564 MHz, CDCl_3) δ -71.71.



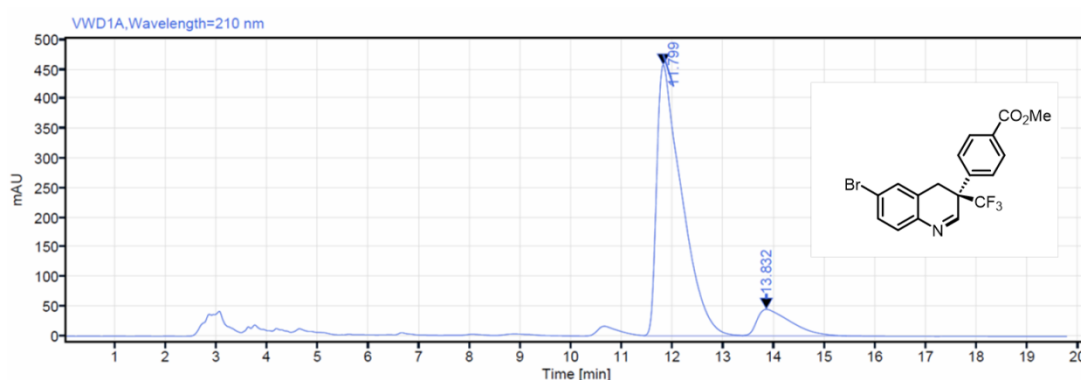
Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (91 mg) *N*-trifosylhydrazone provide **s1** as a white solid; mp: 160-161 °C, **^1H NMR** (500 MHz, CDCl_3) δ 8.33 (d, J = 1.5 Hz, 1H), 7.97-7.92 (m, 2H), 7.43 (d, J = 8.5 Hz, 2H), 7.35 (ddd, J = 8.5, 2.5, 1.0 Hz, 1H), 7.25-7.23 (m, 1H), 7.22 (d, J = 8.5 Hz, 1H), 3.87 (s, 3H), 3.43 (d, J = 16.0 Hz, 1H), 3.36 (dd, J = 16.0, 1.5 Hz, 1H).
 ^{13}C NMR (125 MHz, CDCl_3) δ 166.2, 157.3 (q, J = 2.5 Hz), 140.9, 137.4, 131.5, 130.9, 130.8, 129.9, 128.7, 127.8, 126.2 (q, J = 280.0 Hz), 125.1, 122.1, 52.3, 49.4 (q, J = 26.3 Hz), 29.8.
 ^{19}F NMR (470 MHz, CDCl_3) δ -71.56.

HRMS (ESI^+) m/z calcd for $\text{C}_{18}\text{H}_{14}\text{BrF}_3\text{NO}_2^+$ [$\text{M}+\text{H}$] $^+$ 412.0155, found 412.0148.

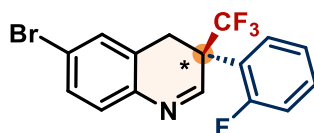
methyl (S)-4-(6-bromo-3-(trifluoromethyl)-3,4-dihydroquinolin-3-yl)benzoate was prepared following the general procedure A as a white solid: 61% yield, 77% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ =210 nm, RT: Major: 11.799 min, Minor: 13.832 min).



RT [min]	Width [min]	Area	Height	Area%
11.846	1.65	15172.81	443.09	50.19
13.562	2.67	15060.17	283.23	49.81



RT [min]	Width [min]	Area	Height	Area%
11.799	1.96	15742.87	457.65	88.39
13.832	2.06	2068.72	44.91	11.61



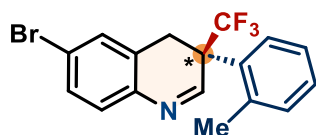
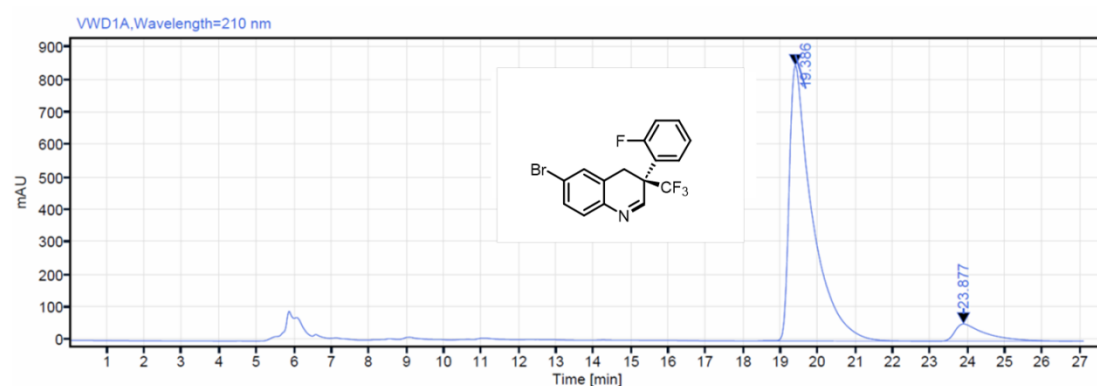
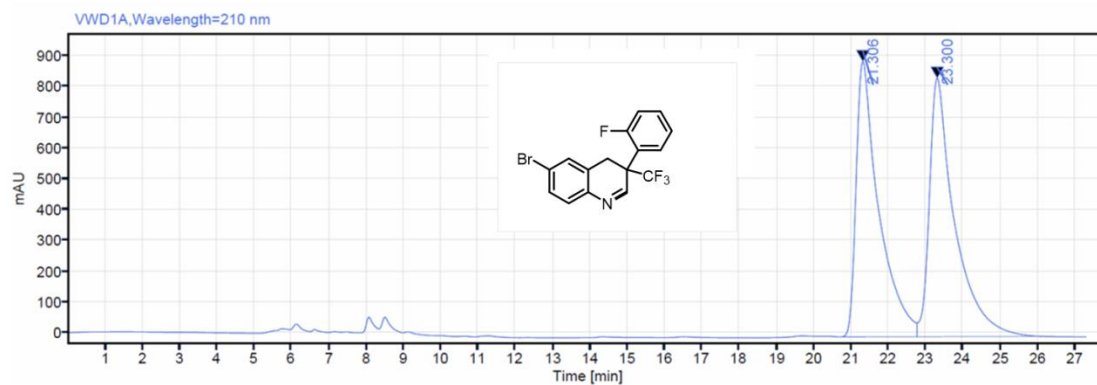
Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (83 mg) *N*-trifosylhydrazone provide **s2** as a white solid; mp: 149-151 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.43 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.37-7.32 (m, 2H), 7.30-7.24 (m, 2H), 7.21-7.16 (m, 1H), 7.06 (td, *J* = 8.0, 1.5 Hz, 1H), 7.01 (ddd, *J* = 12.0, 8.5, 1.5 Hz, 1H), 3.57 (d, *J* = 16.5, 1H), 3.32 (d, *J* = 16.5 Hz, 1H).

¹³C NMR (125 MHz, CDCl₃) δ 161.7 (d, *J* = 248.8 Hz), 157.65 (q, *J* = 5.0 Hz), 141.0, 131.4, 131.1 (d, *J* = 10.0 Hz), 130.7, 130.0 (d, *J* = 3.8 Hz), 128.3, 126.2 (q, *J* = 281.3 Hz), 125.7, 124.2 (d, *J* = 3.8 Hz), 121.5, 119.0 (d, *J* = 11.3 Hz), 117.1 (d, *J* = 22.5 Hz), 47.9 (d, *J* = 27.5 Hz), 28.1.

¹⁹F NMR (470 MHz, CDCl₃) δ -72.60 (d, *J* = 12.0 Hz), (-105.34)-(-105.48) (m).

HRMS (ESI⁺) *m/z* calcd for C₁₆H₁₁BrF₄N⁺ [M+H]⁺ 372.0006, found 372.0001.

(*S*)-6-bromo-3-(2-fluorophenyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 81% yield, 87% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 95/5, 0.5 mL/min, λ=210 nm, RT: Major: 19.386 min, Minor: 23.877 min).



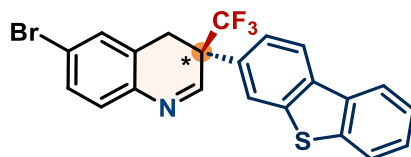
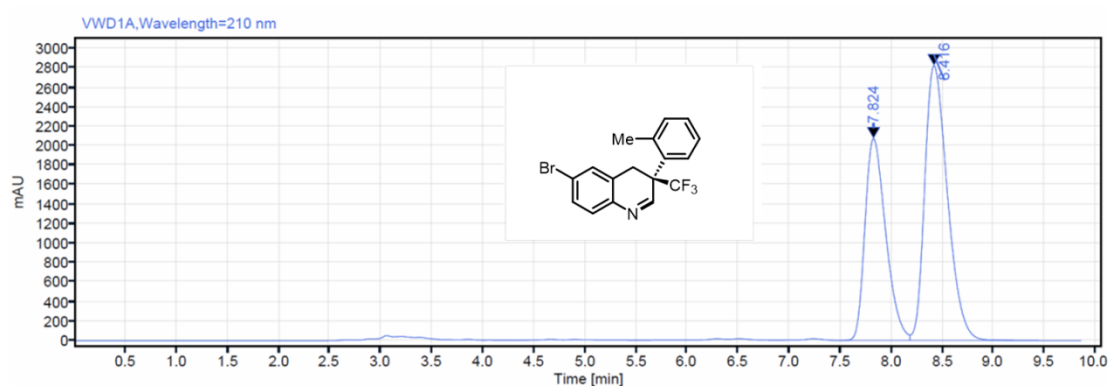
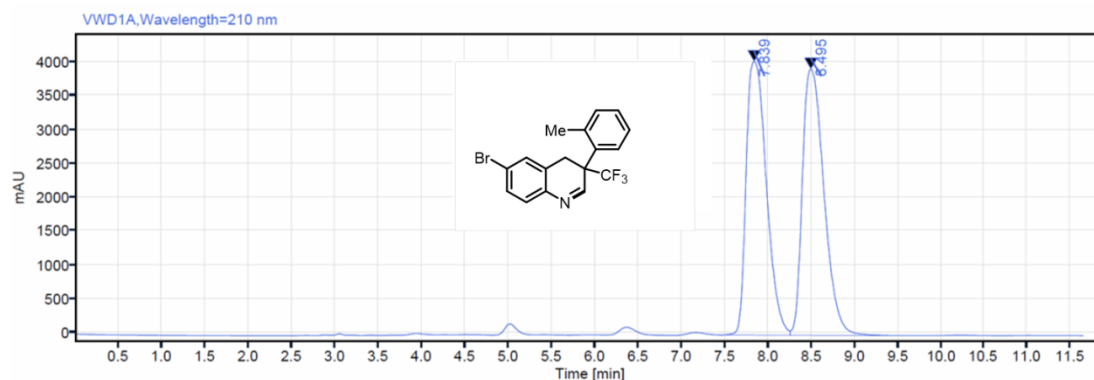
Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (82 mg) *N*-trifosylhydrazone provide **s3** as a white solid; mp: 103-105 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.45 (s, 1H), 7.40-7.35 (m, 1H), 7.34-7.28 (m, 2H), 7.18-7.11 (m, 3H), 7.10-7.05 (m, 1H), 3.55 (dd, *J* = 16.5, 1.5 Hz, 1H), 3.33 (d, *J* = 16.5 Hz, 1H), 2.42 (s, 3H).

¹³C NMR (125 MHz, CDCl₃) δ 158.9, 141.3, 138.1, 133.3, 131.2, 130.6, 130.4, 129.2, 128.8, 127.9, 126.9 (q, *J* = 281.3 Hz), 126.2, 126.0, 121.4, 50.0 (q, *J* = 25.0 Hz), 30.0 (q, *J* = 2.5 Hz), 24.2 (q, *J* = 2.5 Hz).

¹⁹F NMR (470 MHz, CDCl₃) δ -71.73.

HRMS (ESI⁺) *m/z* calcd for C₁₇H₁₄BrF₃N⁺ [M+H]⁺ 368.0256, found 368.0250.

(*S*)-6-bromo-3-(*o*-tolyl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 51% yield, 20% e.e. (Chiracel OD-H, Hexanes/*i*-PrOH = 99/1, 1.0 mL/min, λ=210 nm, RT: Major: 8.416 min, Minor: 7.824 min).



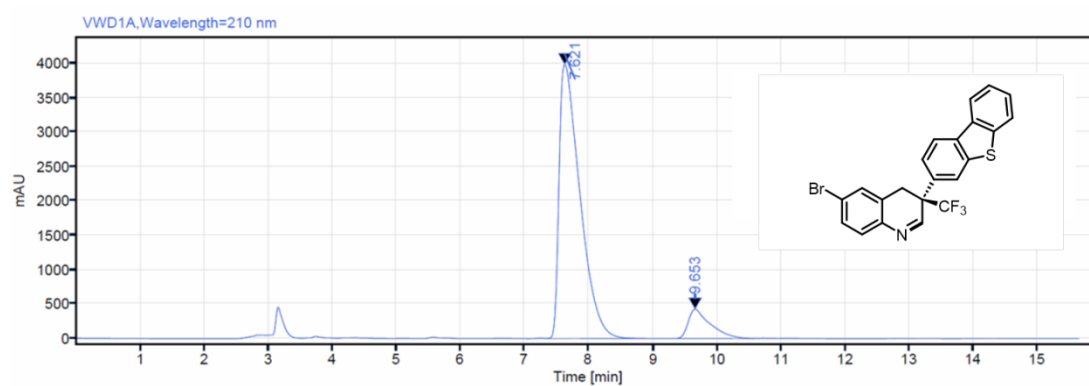
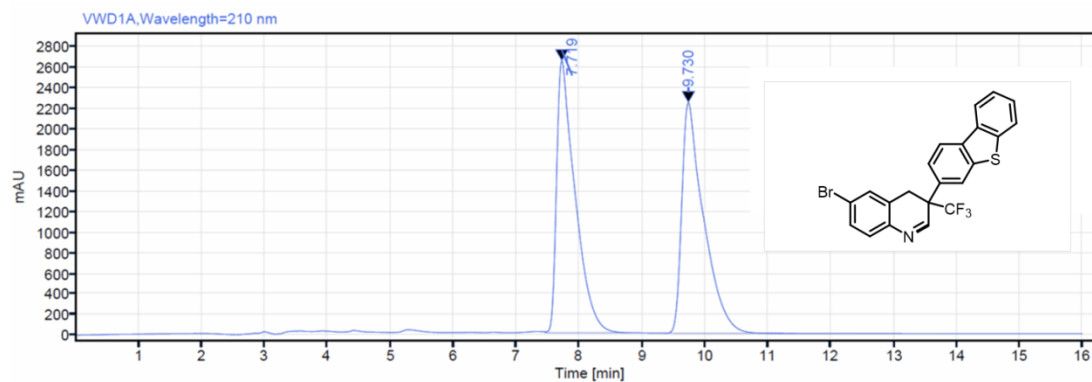
Following General Procedure A, 0.3 mmol (59 mg) indole and 0.2 mmol (101 mg) *N*-trifosylhydrazone provide **s4** as a white solid; mp: 136-138 °C, ¹H NMR (500 MHz, CDCl₃) δ 8.46 (s, 1H), 8.14-8.07 (m, 2H), 7.83-7.78 (m, 1H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.49-7.41 (m, 3H), 7.31 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.28-7.21 (m, 2H), 3.53 – 3.43 (m, 2H).

¹³C NMR (125 MHz, CDCl₃) δ 158.1 (q, *J* = 2.5 Hz), 140.9, 140.1, 139.8, 135.8, 134.8, 131.4, 130.9, 128.6, 127.2, 126.6 (q, *J* = 280.0 Hz), 125.6, 125.5, 124.6, 123.2, 122.9, 122.0, 121.6, 120.9, 49.4 (q, *J* = 25.0 Hz), 30.2 (q, *J* = 2.5 Hz).

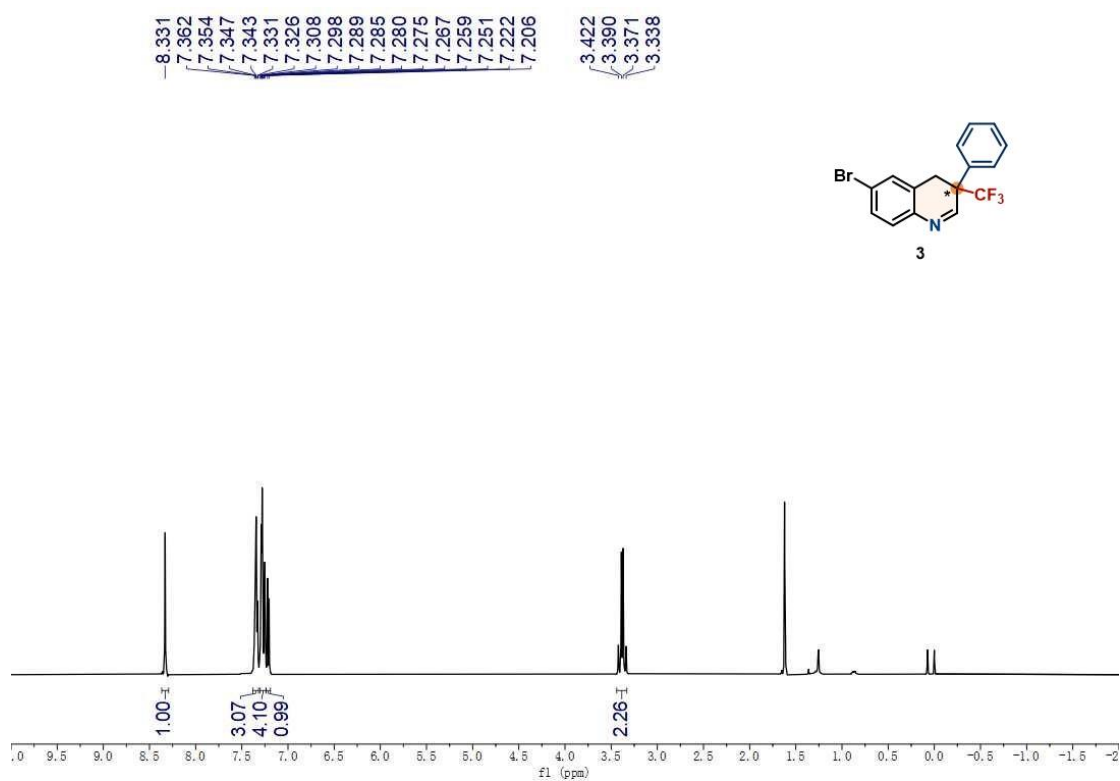
¹⁹F NMR (470 MHz, CDCl₃) δ -71.62.

HRMS (ESI) *m/z* calcd. for C₂₂H₁₄BrF₃NS⁺ [*M*+H]⁺ 459.9977, found 459.9973

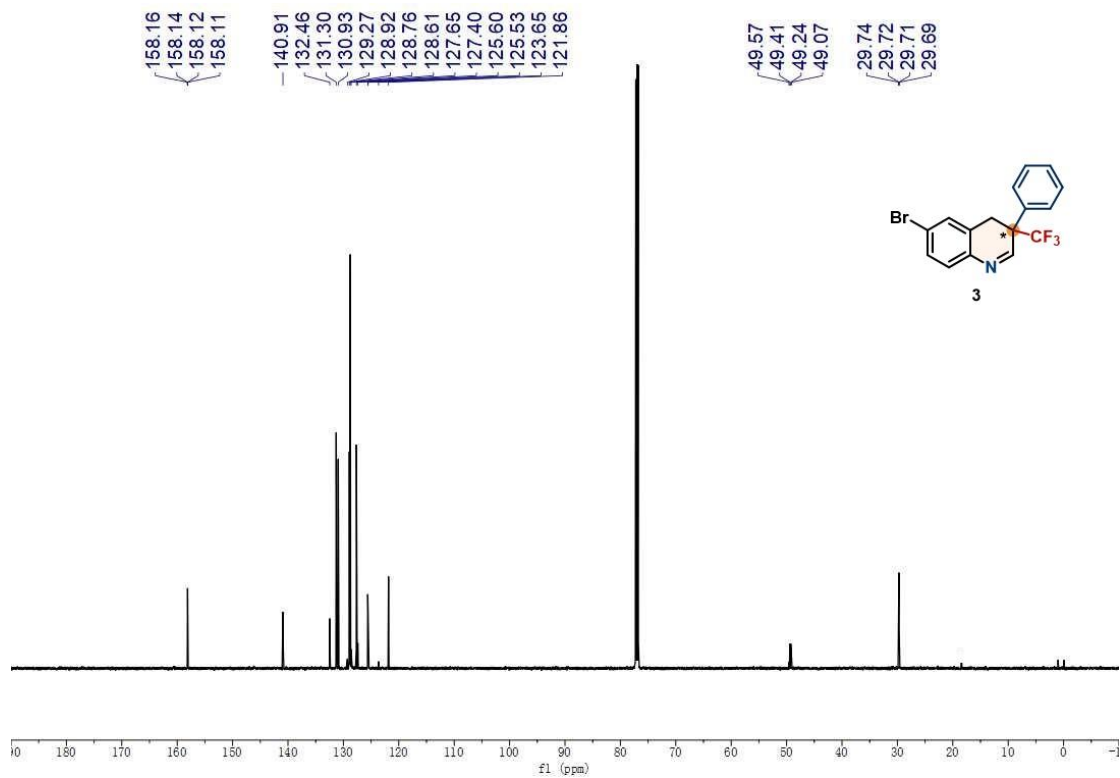
(*S*)-6-bromo-3-(dibenzo[*b,d*]thiophen-3-yl)-3-(trifluoromethyl)-3,4-dihydroquinoline was prepared following the general procedure A as a white solid: 48% yield, 79% e.e. (Chiracel AD-H, Hexanes/*i*-PrOH = 90/10, 1.0 mL/min, λ=210 nm, RT: Major: 7.621 min, Minor: 9.653 min).



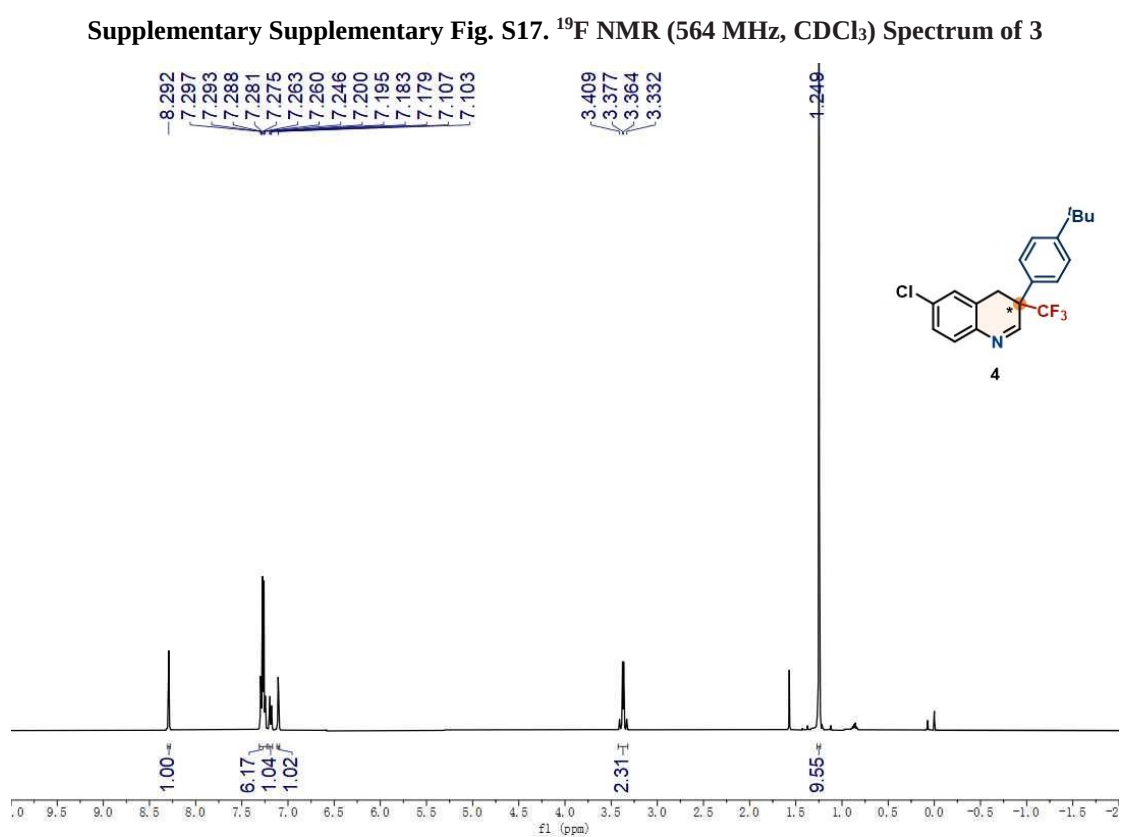
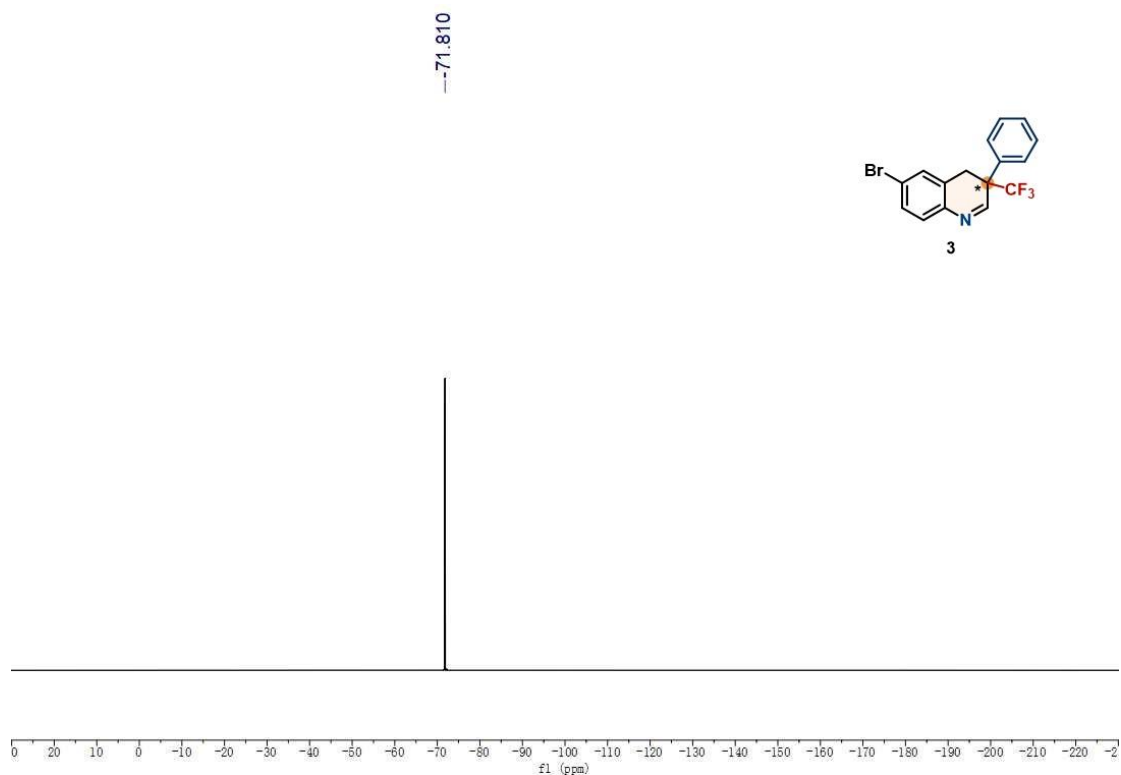
10. NMR Spectra for New Compounds



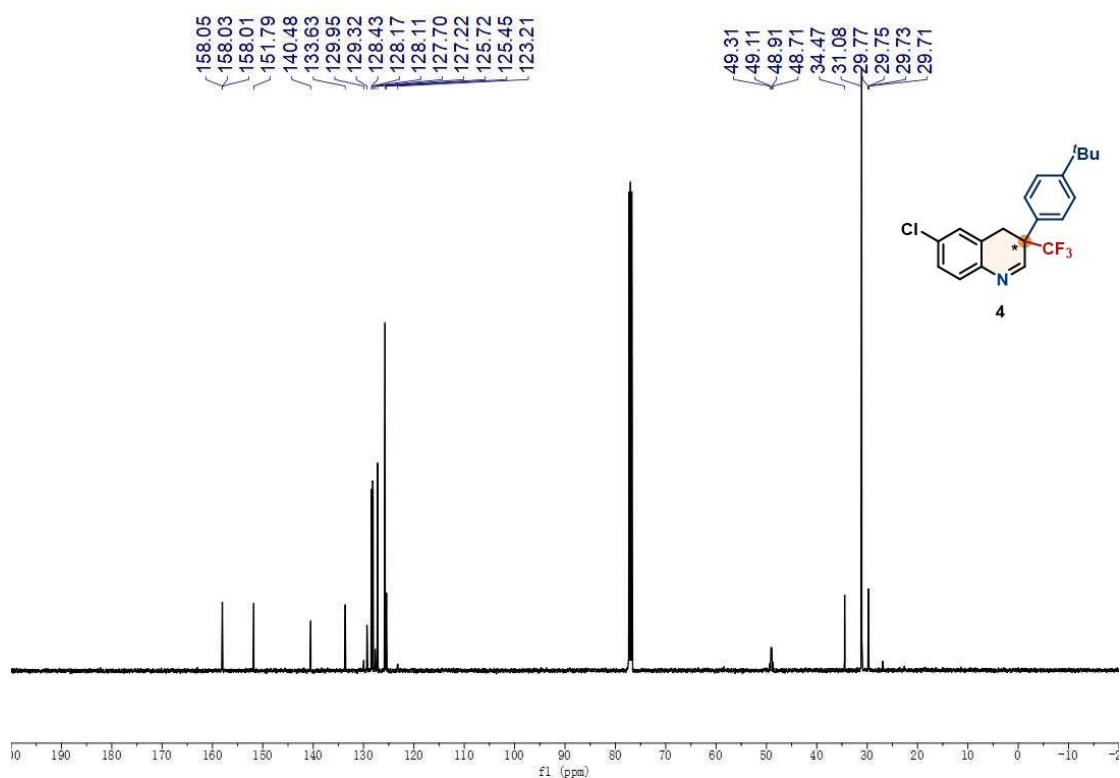
Supplementary Supplementary Fig. S15. ¹H NMR (500 MHz, CDCl₃) Spectrum of 3



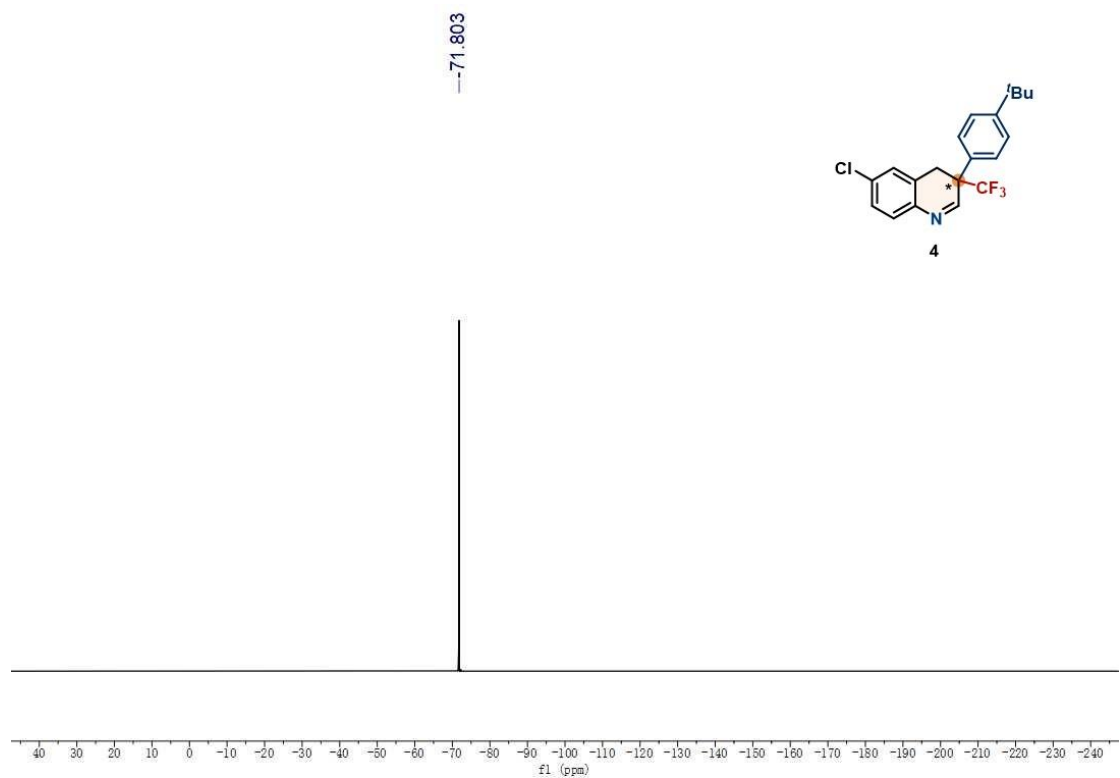
Supplementary Fig. S16. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 3



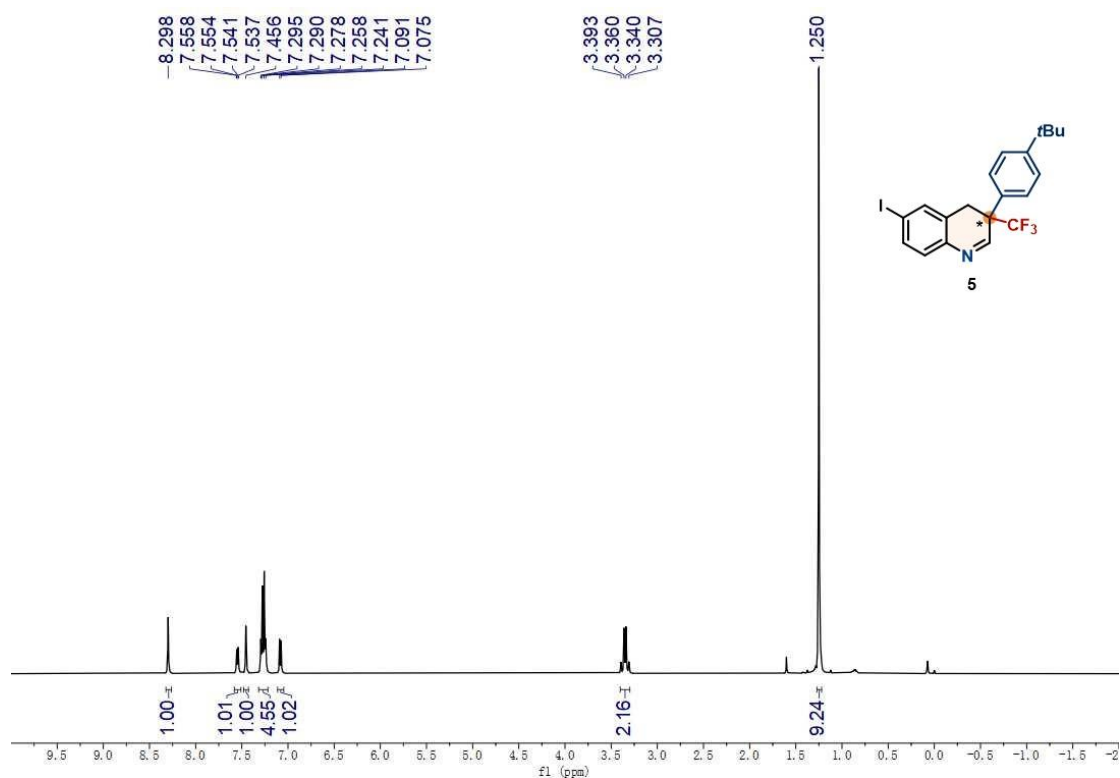
Supplementary Fig. S18. ^1H NMR (500 MHz, CDCl_3) Spectrum of 4



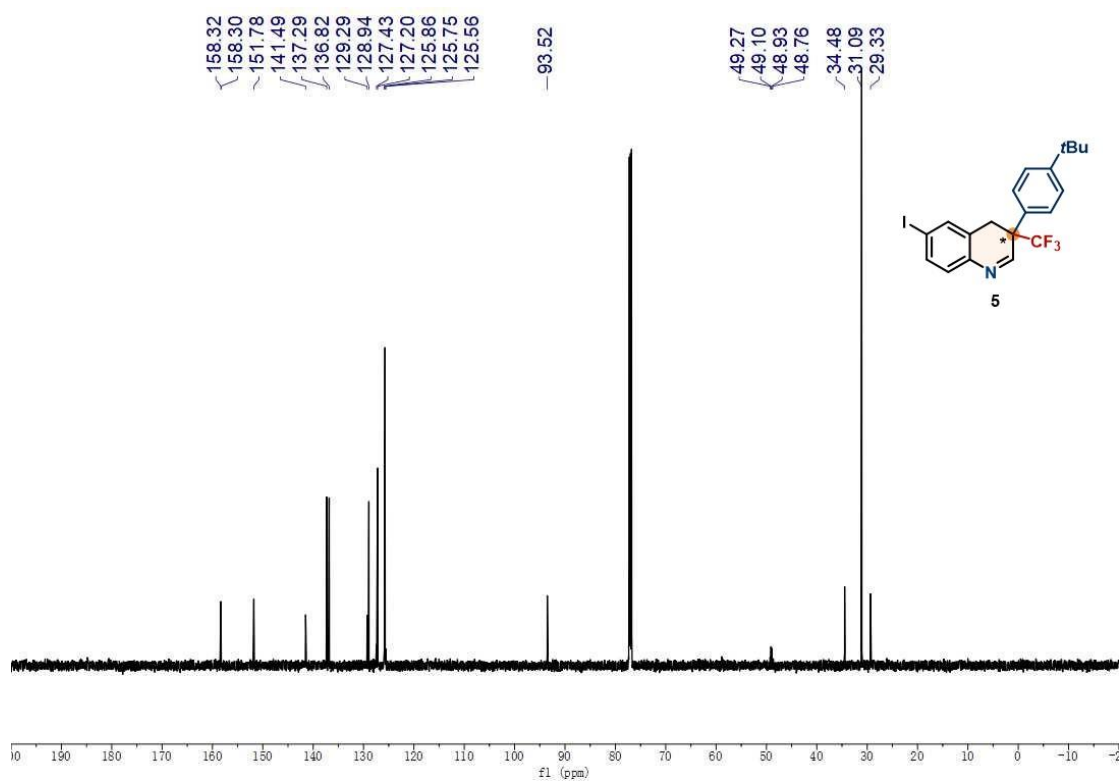
Supplementary Fig. S19. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 4



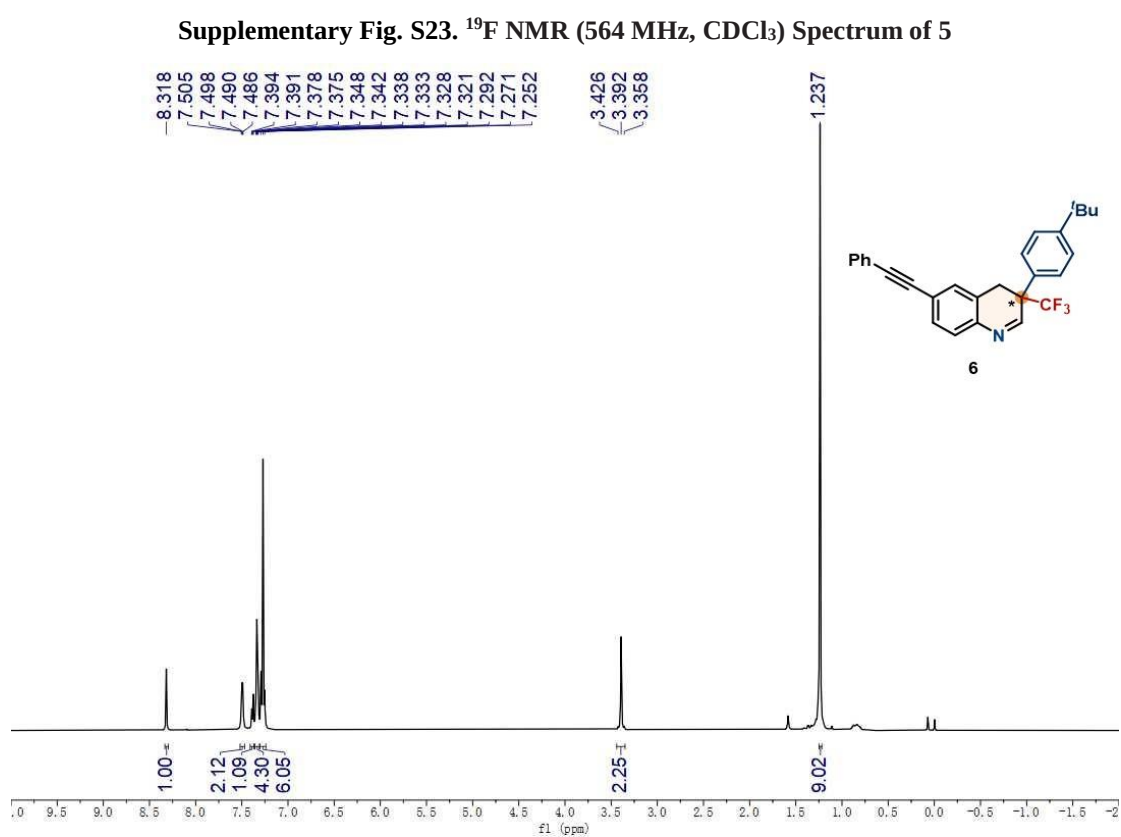
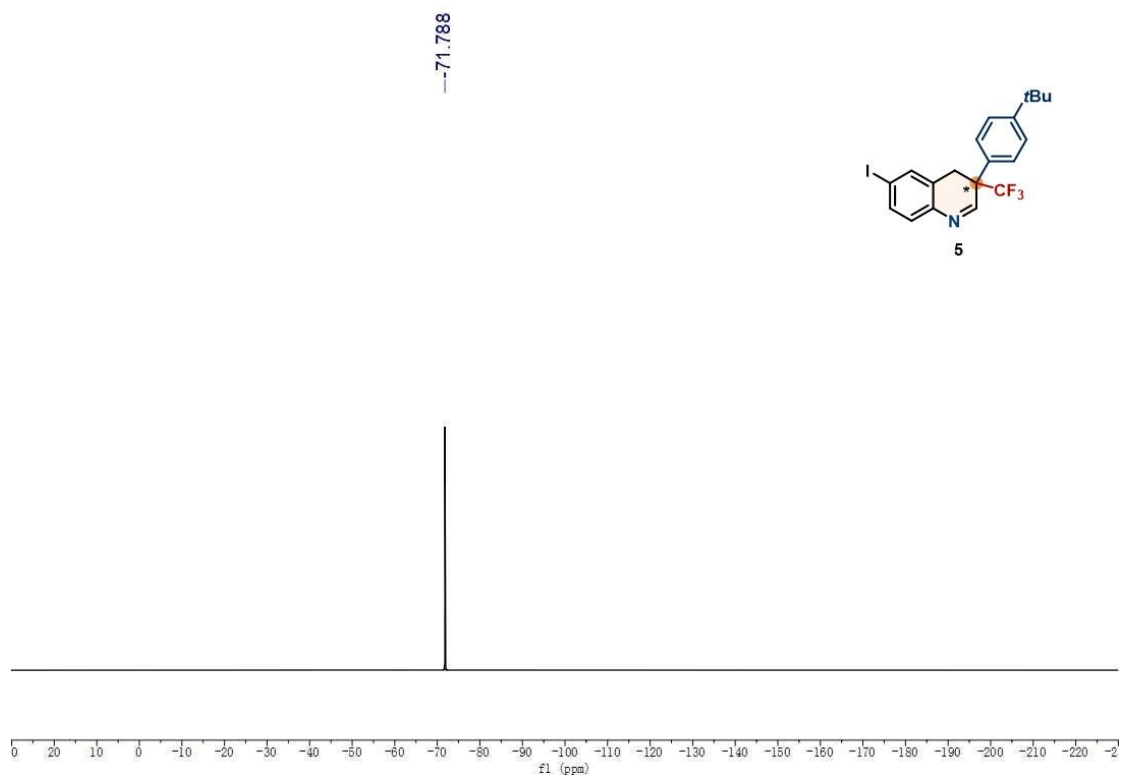
Supplementary Fig. S20. ¹⁹F NMR (470 MHz, CDCl₃) Spectrum of 4



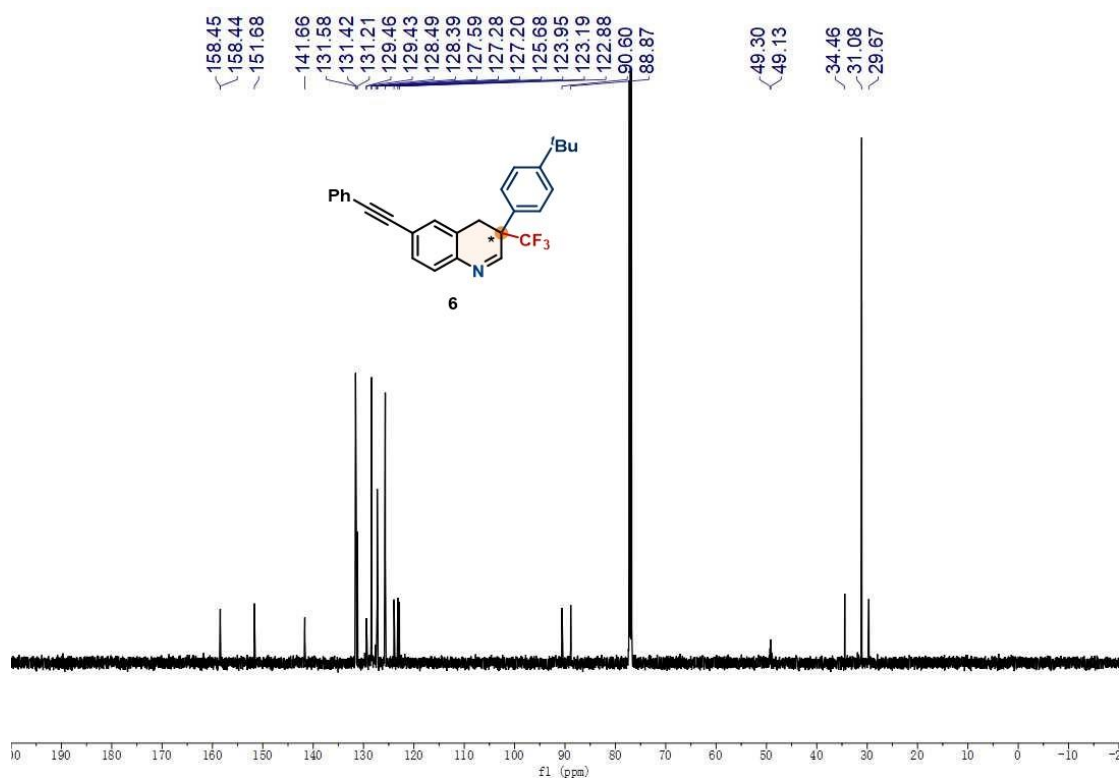
Supplementary Fig. S21. ¹H NMR (500 MHz, CDCl₃) Spectrum of 5



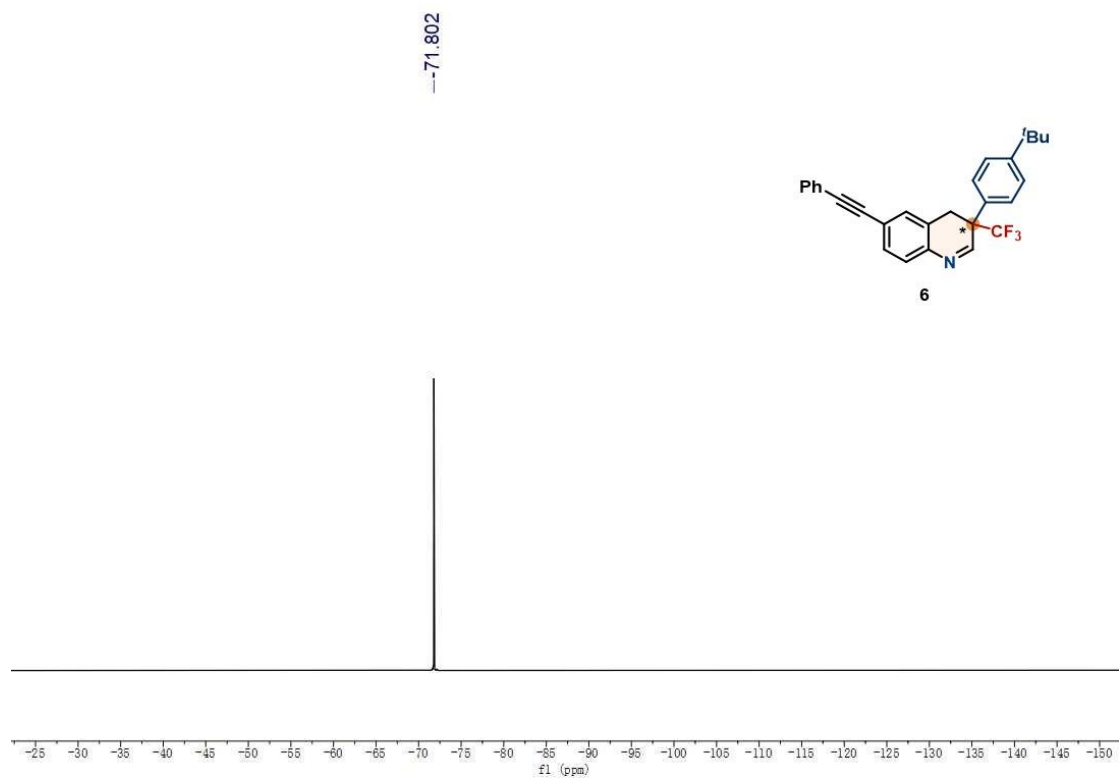
Supplementary Fig. S22. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 5



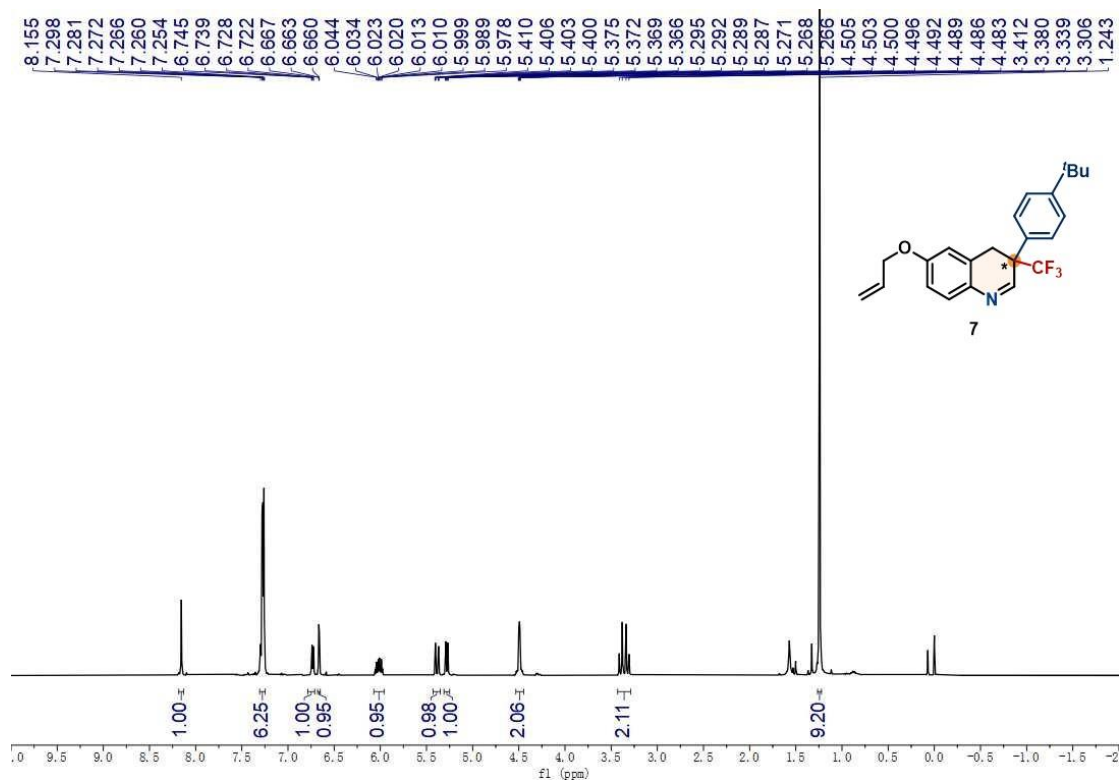
Supplementary Fig. S24. ^1H NMR (500 MHz, CDCl_3) Spectrum of 6



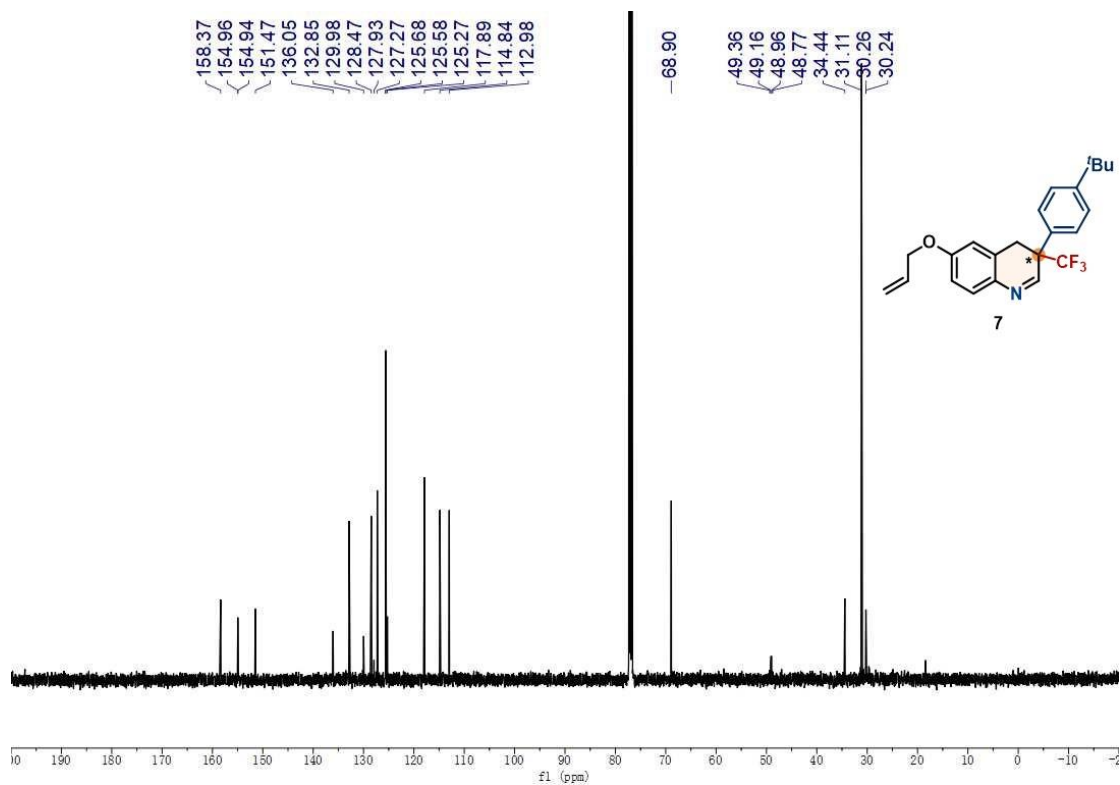
Supplementary Fig. S25. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 6



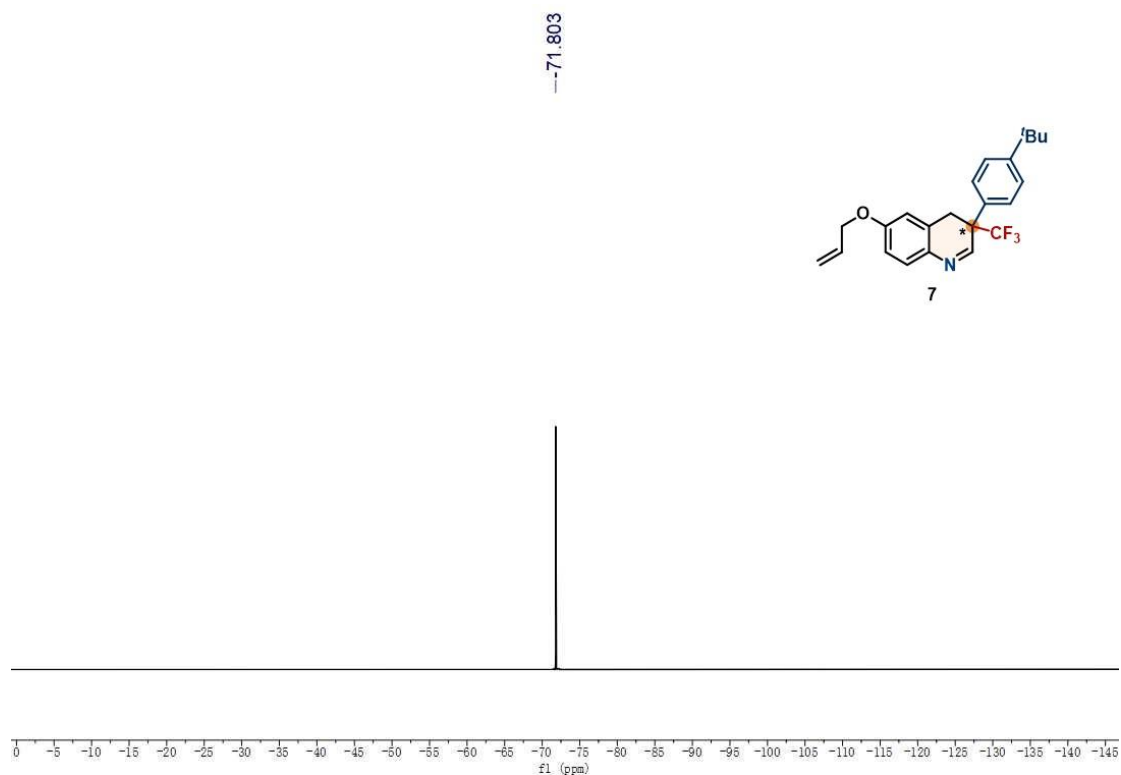
Supplementary Fig. S26. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 6



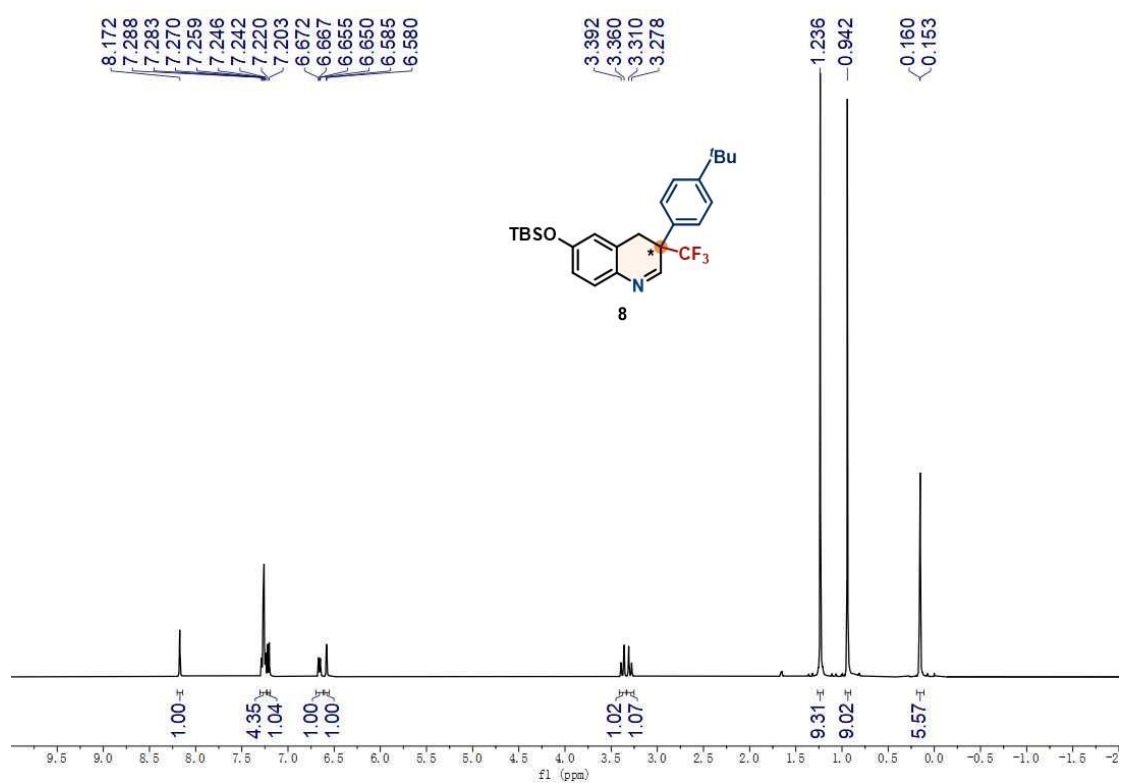
Supplementary Fig. S27. ¹H NMR (500 MHz, CDCl₃) Spectrum of 7



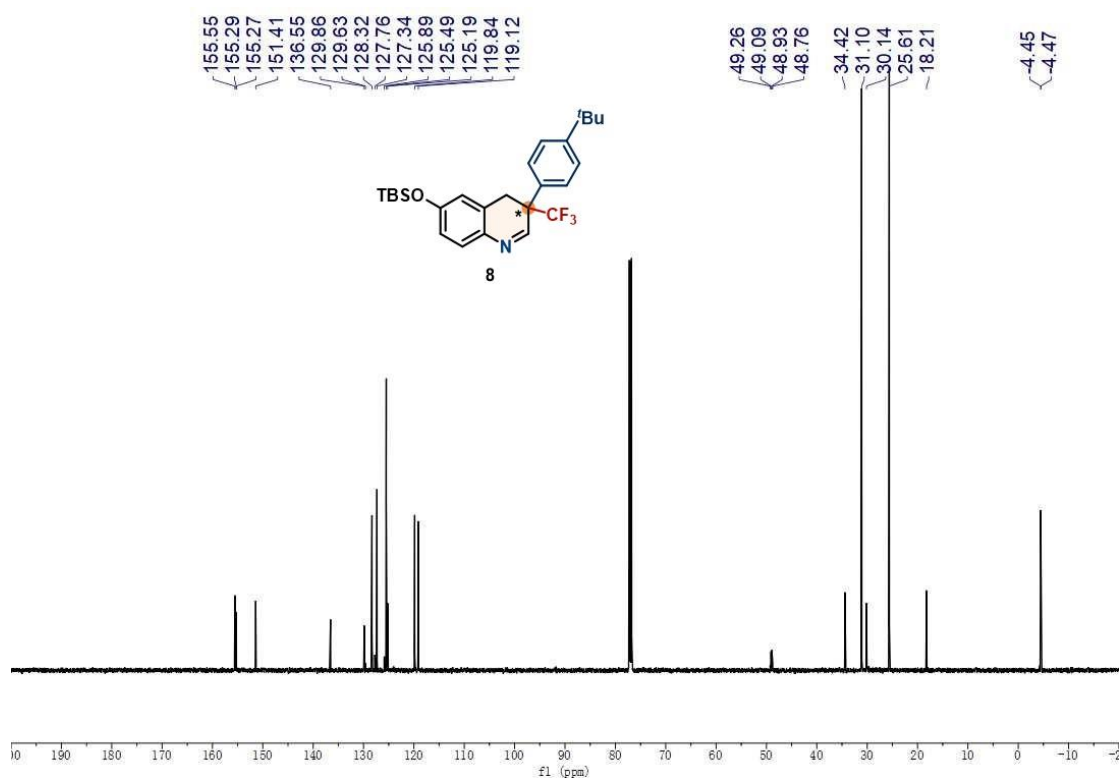
Supplementary Fig. S28. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 7



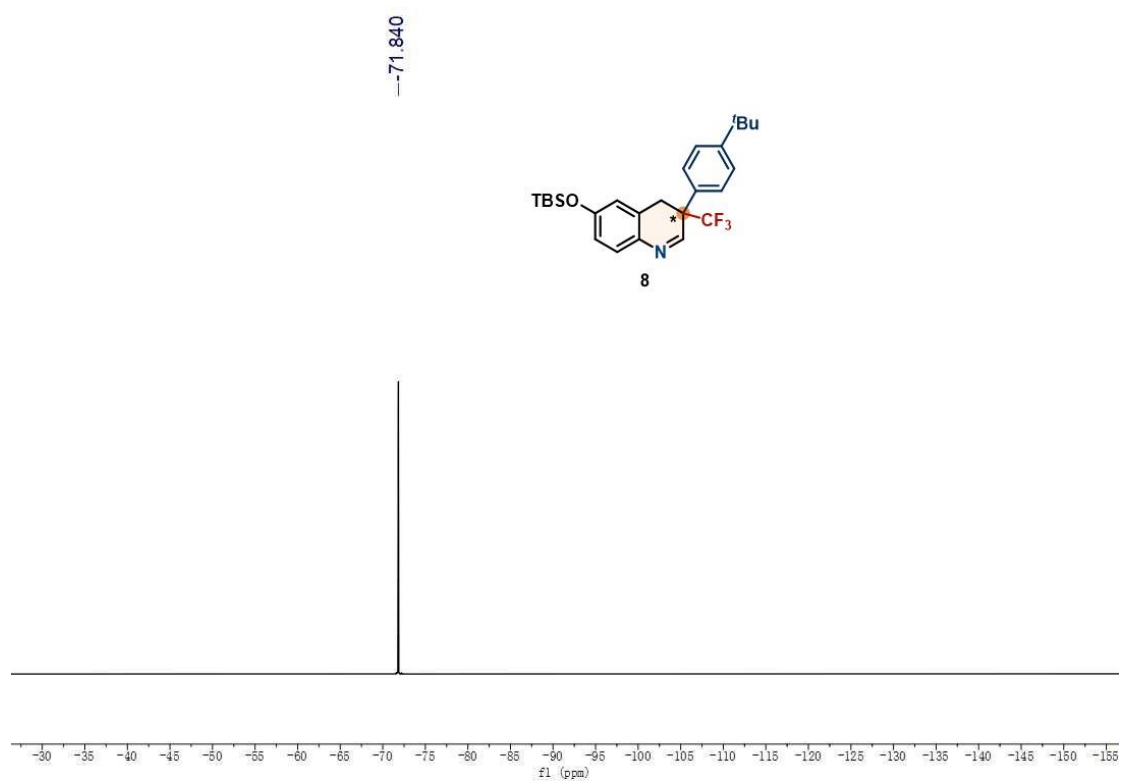
Supplementary Fig. S29. ¹⁹F NMR (470 MHz, CDCl₃) Spectrum of 7



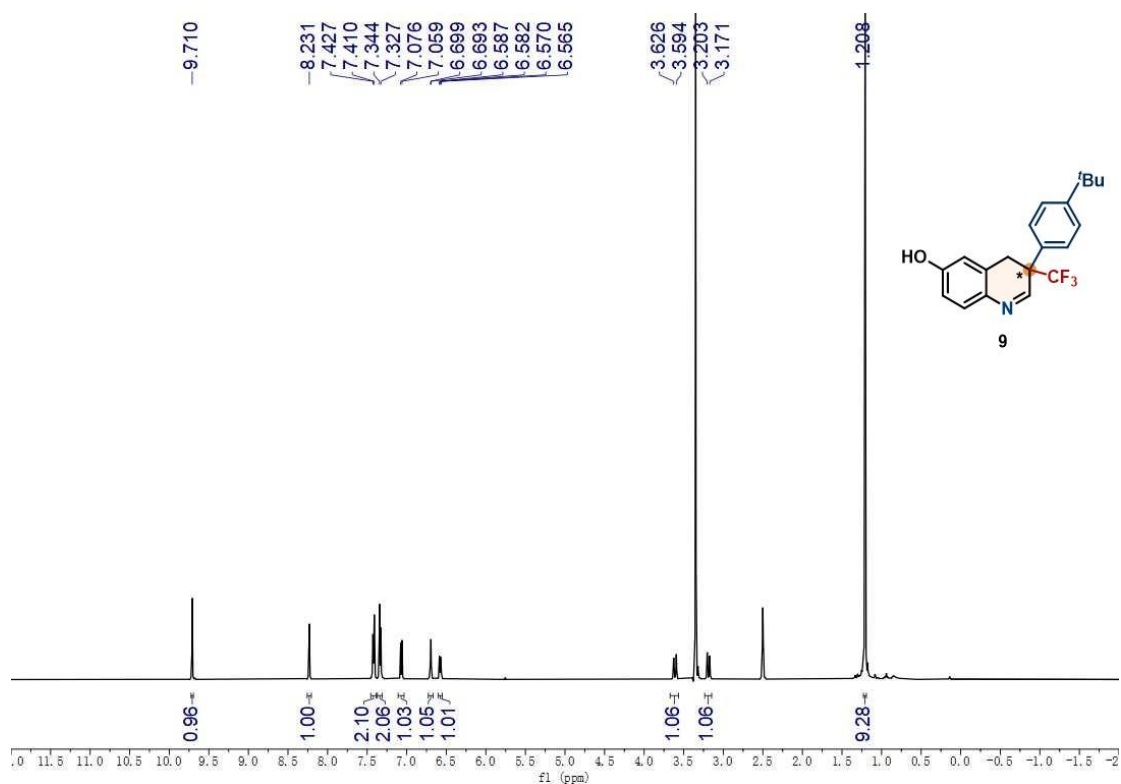
Supplementary Fig. S30. ¹H NMR (500 MHz, CDCl₃) Spectrum of 8



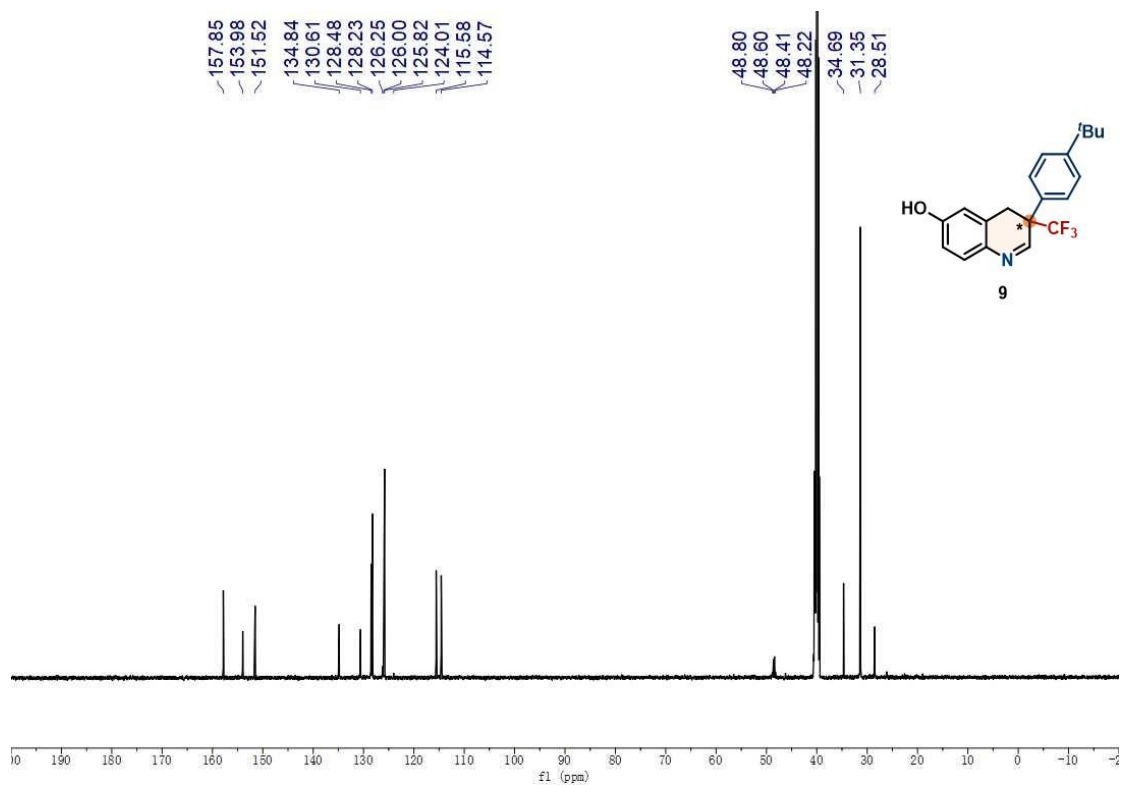
Supplementary Fig. S31. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 8



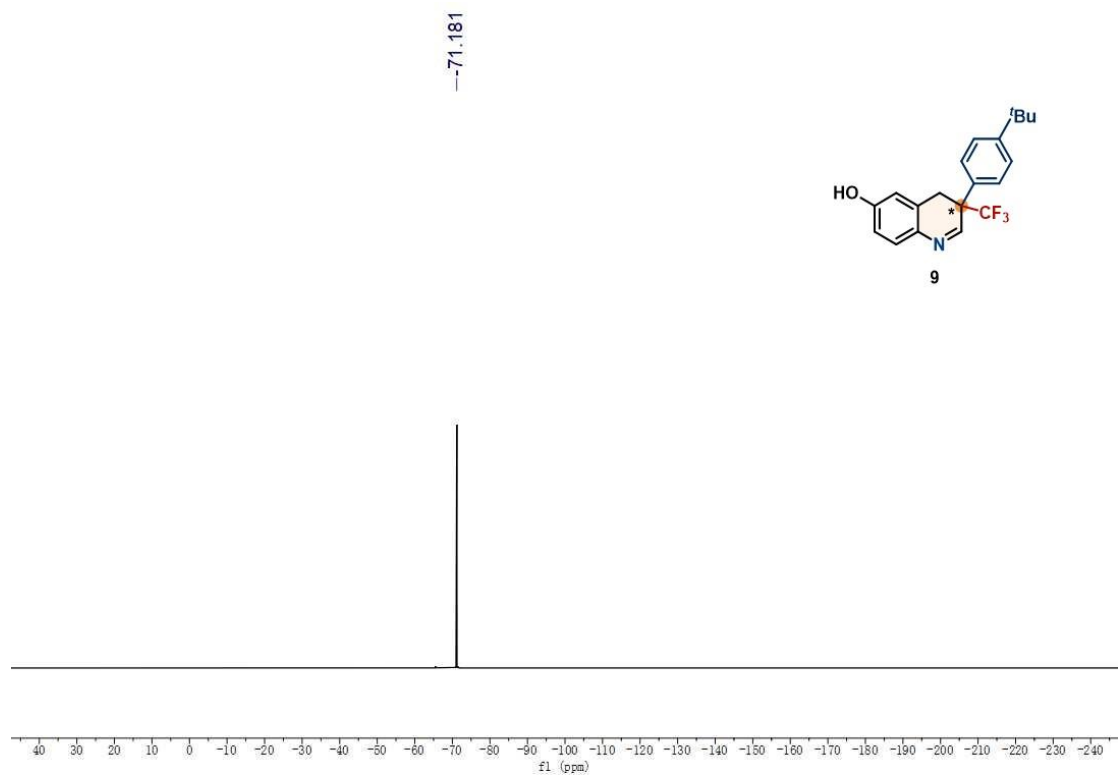
Supplementary Fig. S32. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 8



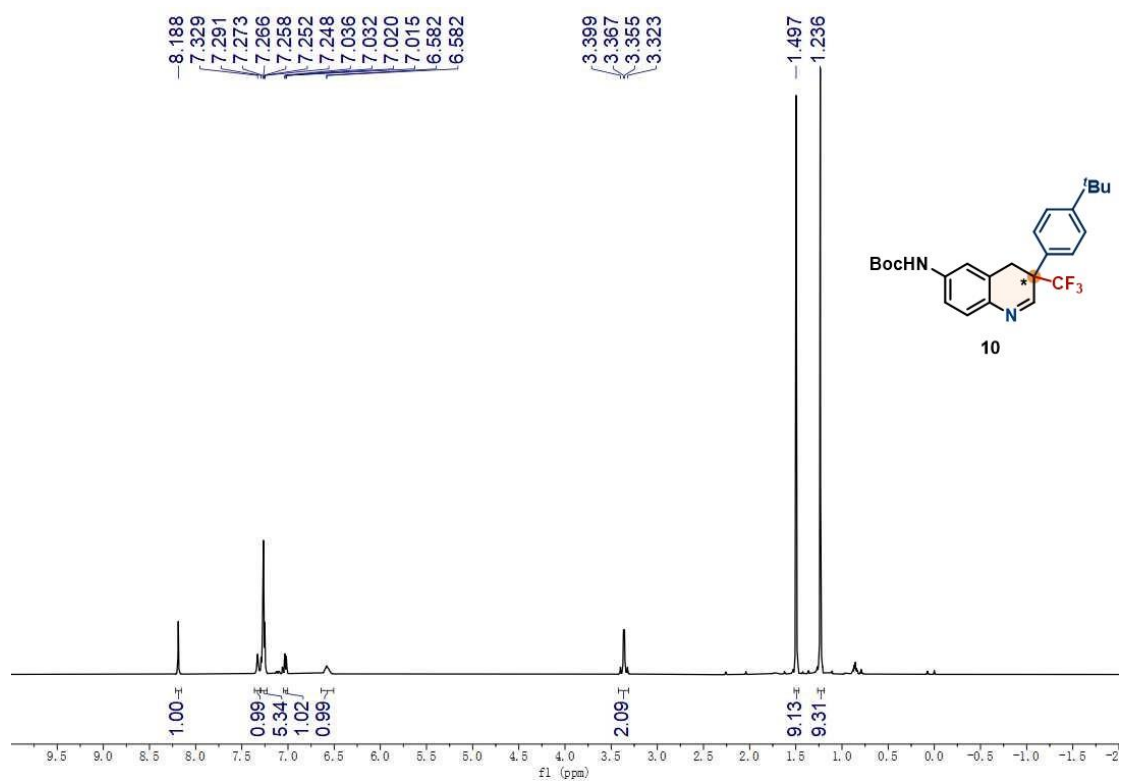
Supplementary Fig. S33. ¹H NMR (500 MHz, DMSO-*d*₆) Spectrum of 9



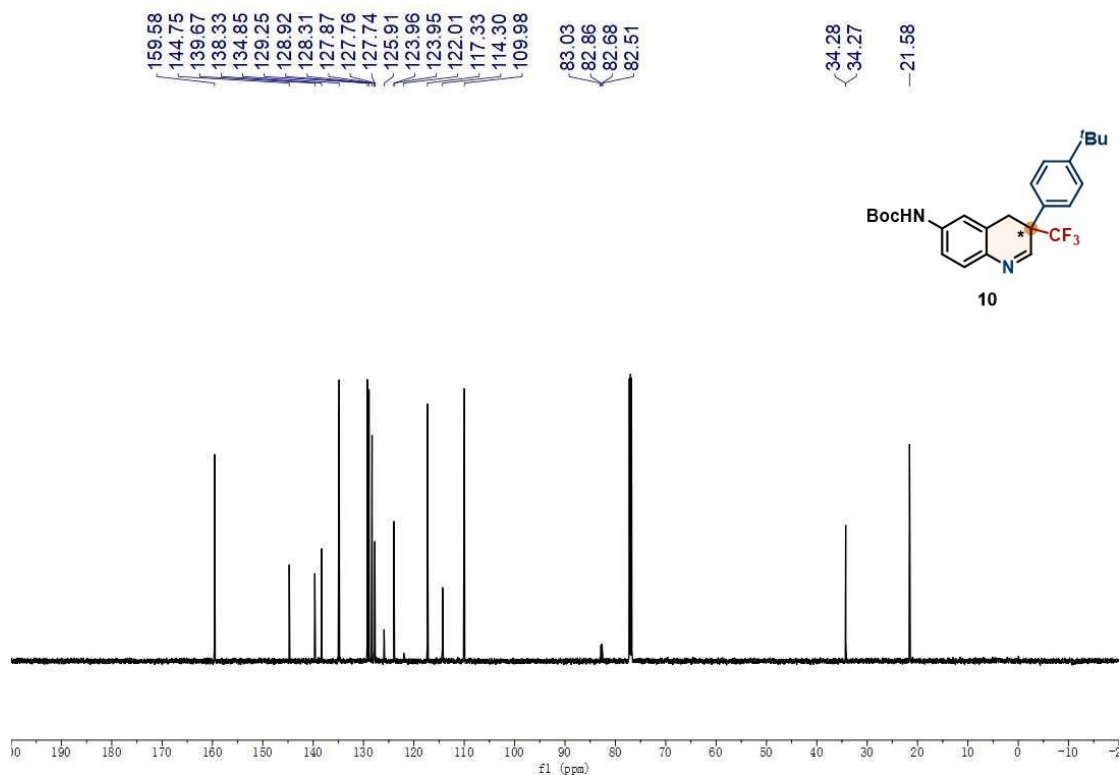
Supplementary Fig. S34. ¹³C NMR (125 MHz, DMSO-*d*₆) Spectrum of 9



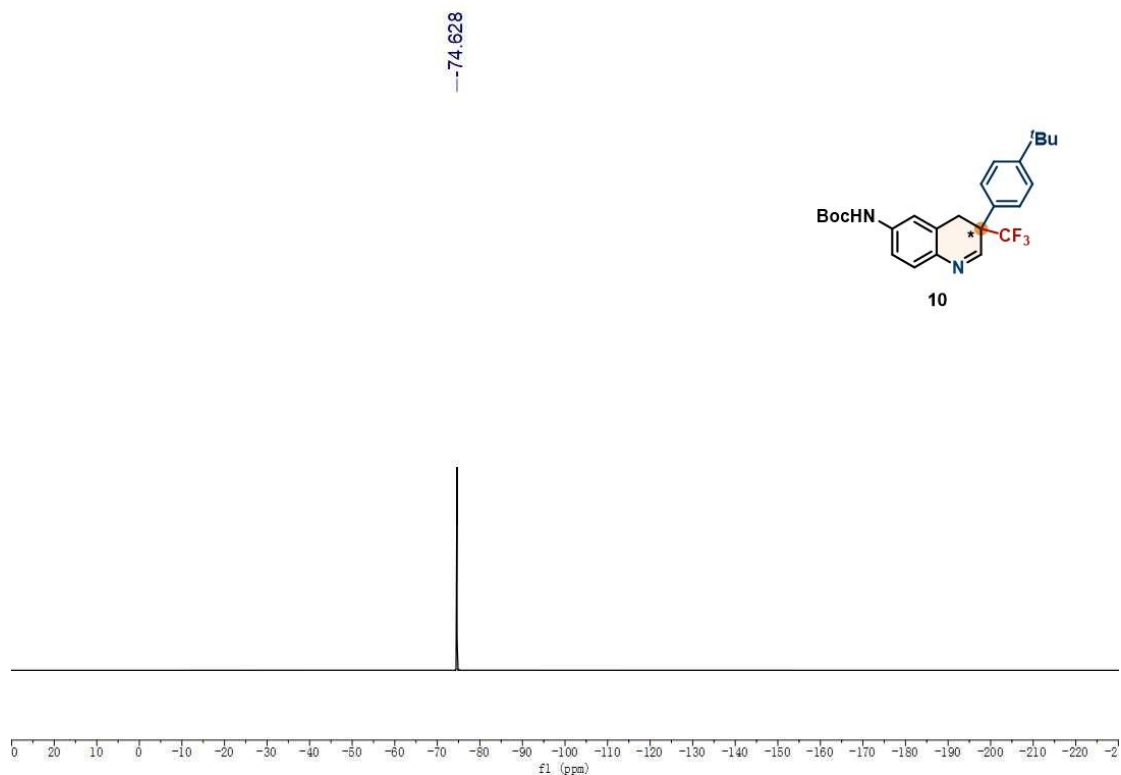
Supplementary Fig. S35. ¹⁹F NMR (471 MHz, DMSO-*d*₆) Spectrum of 9



Supplementary Fig. S36. ¹H NMR (500 MHz, CDCl₃) Spectrum of 10



Supplementary Fig. S37. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 10



Supplementary Fig. S38. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 10

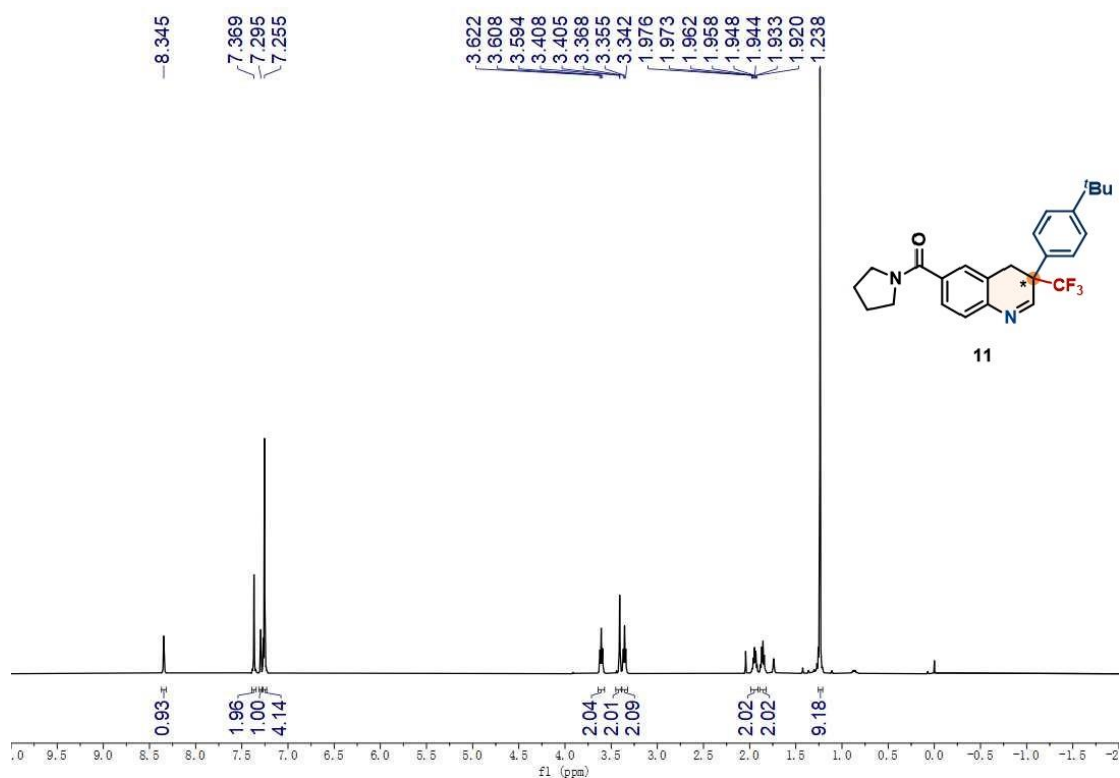
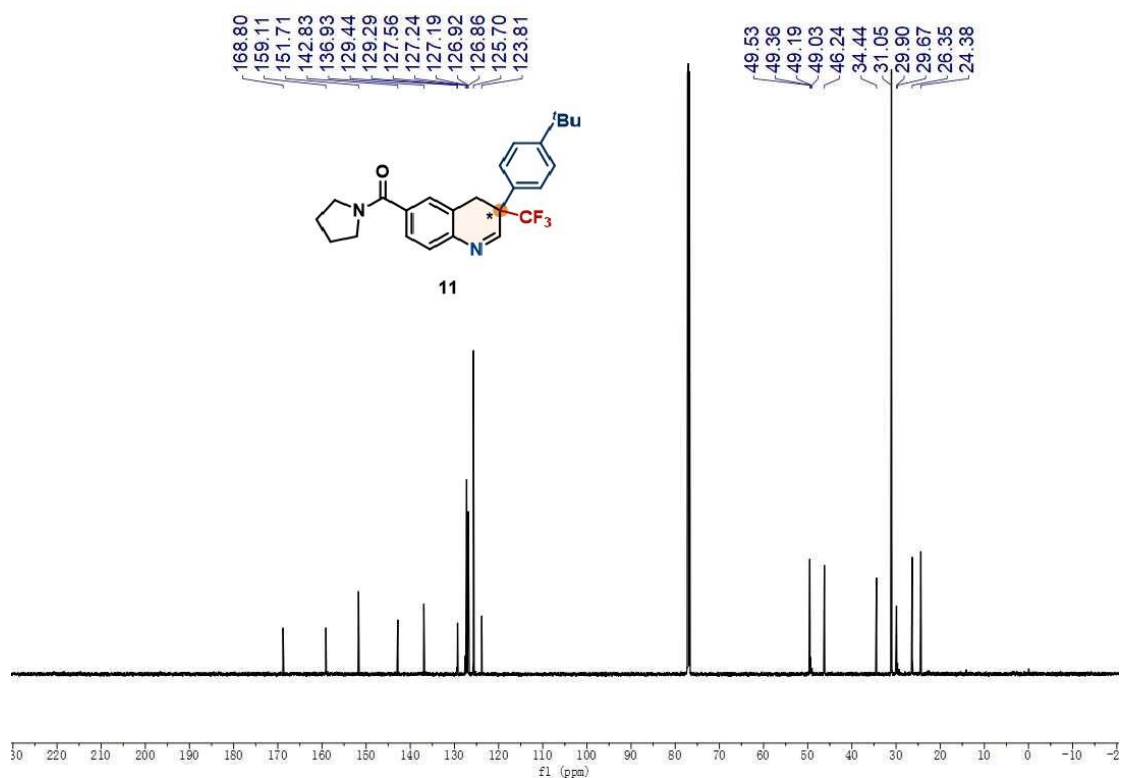
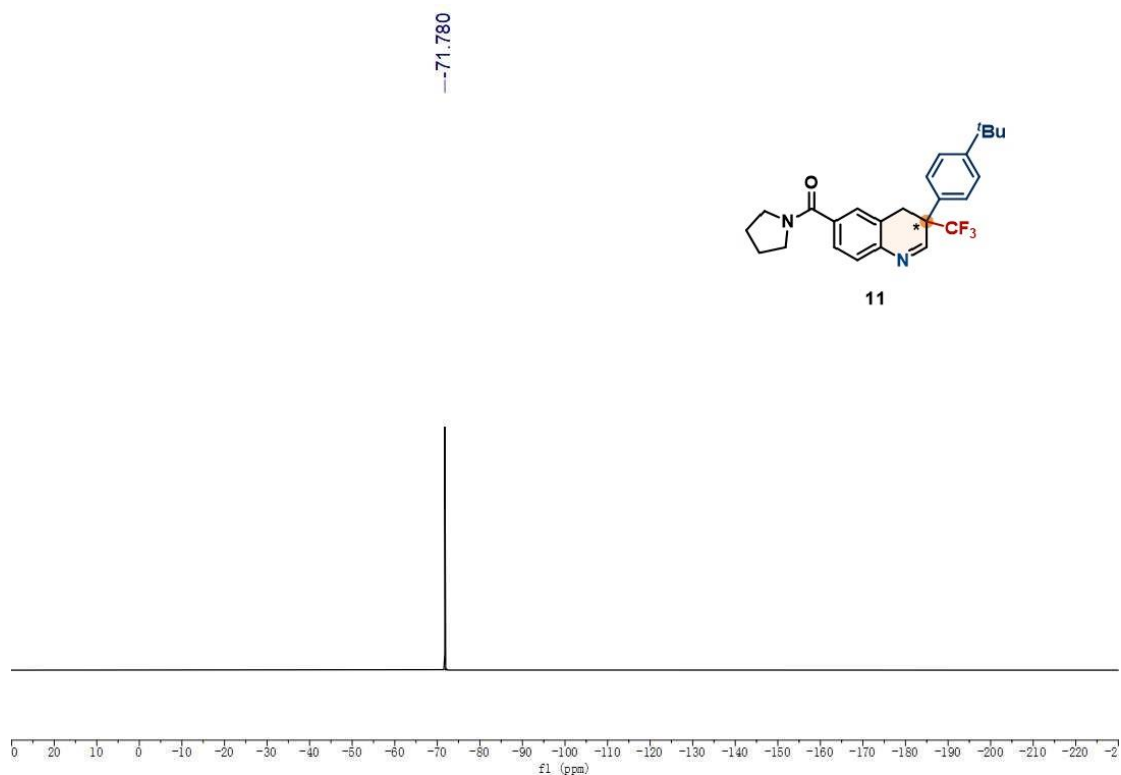


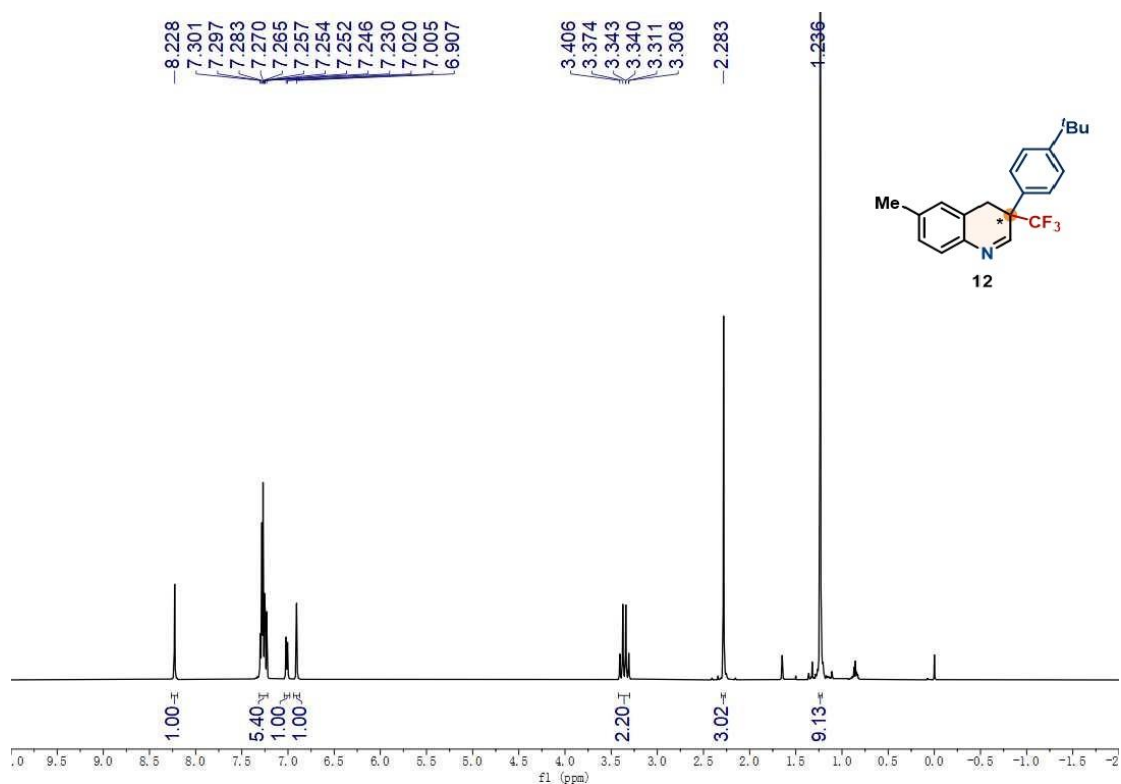
Fig S39. ¹H NMR (500 MHz, CDCl₃) Spectrum of 11



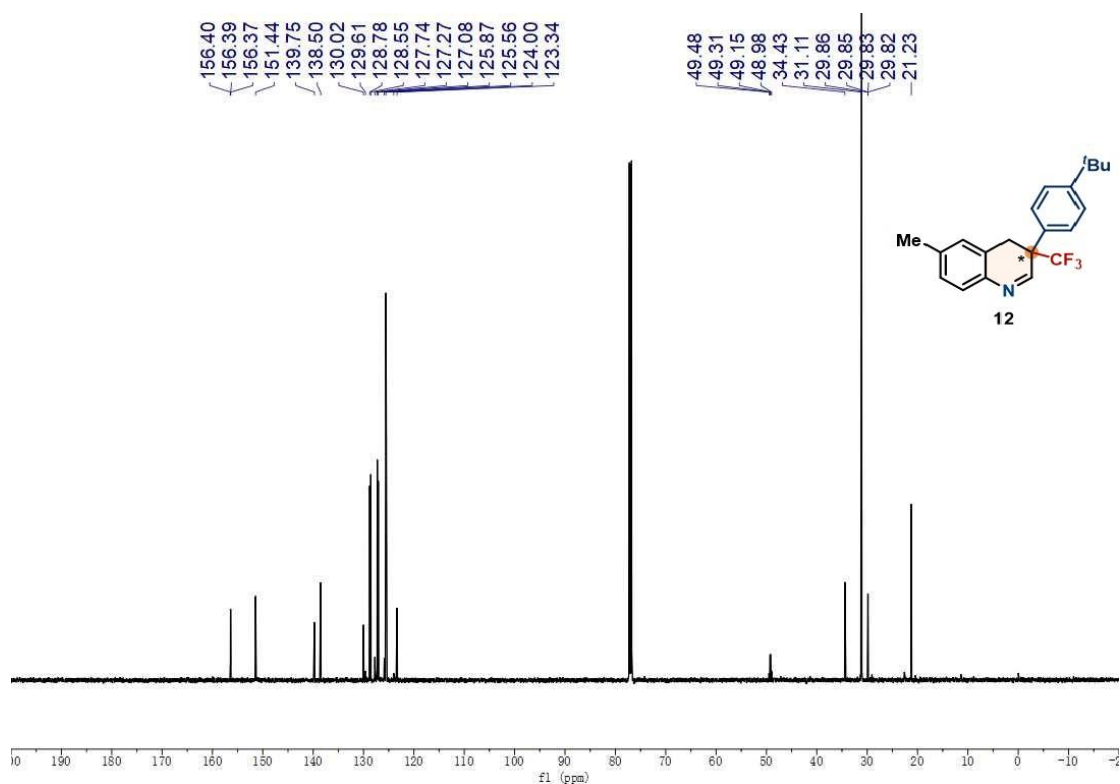
Supplementary Fig. S40. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 11



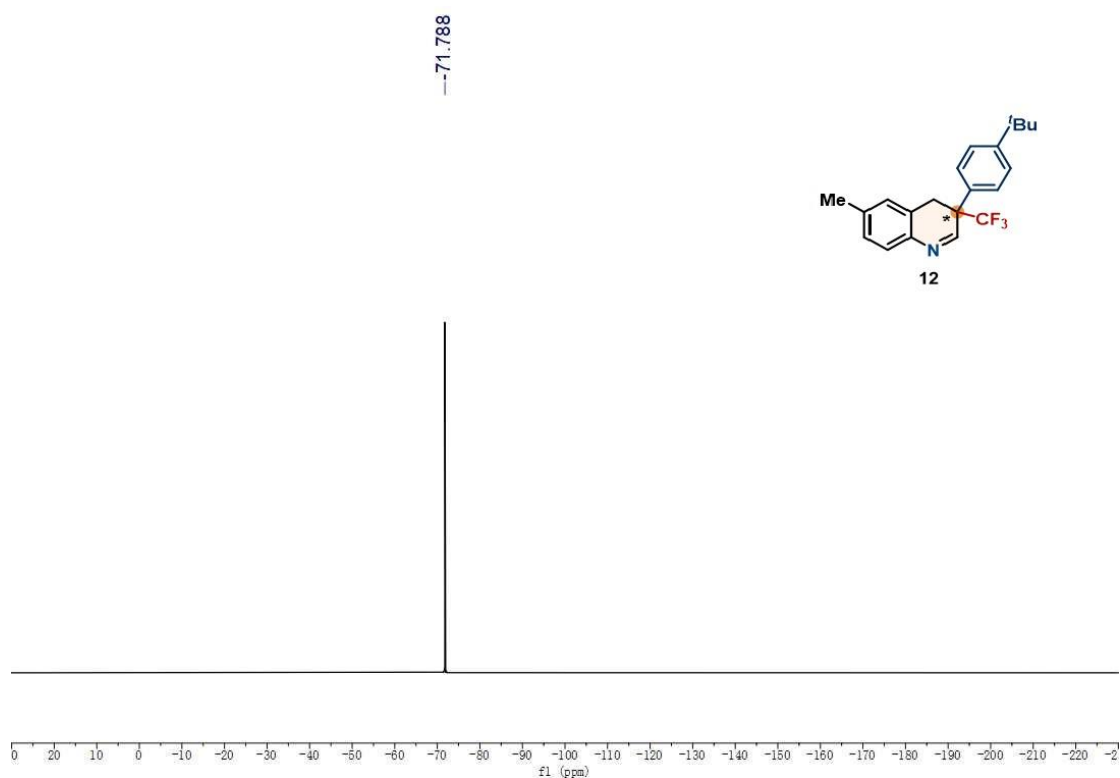
Supplementary Fig. S41. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 11



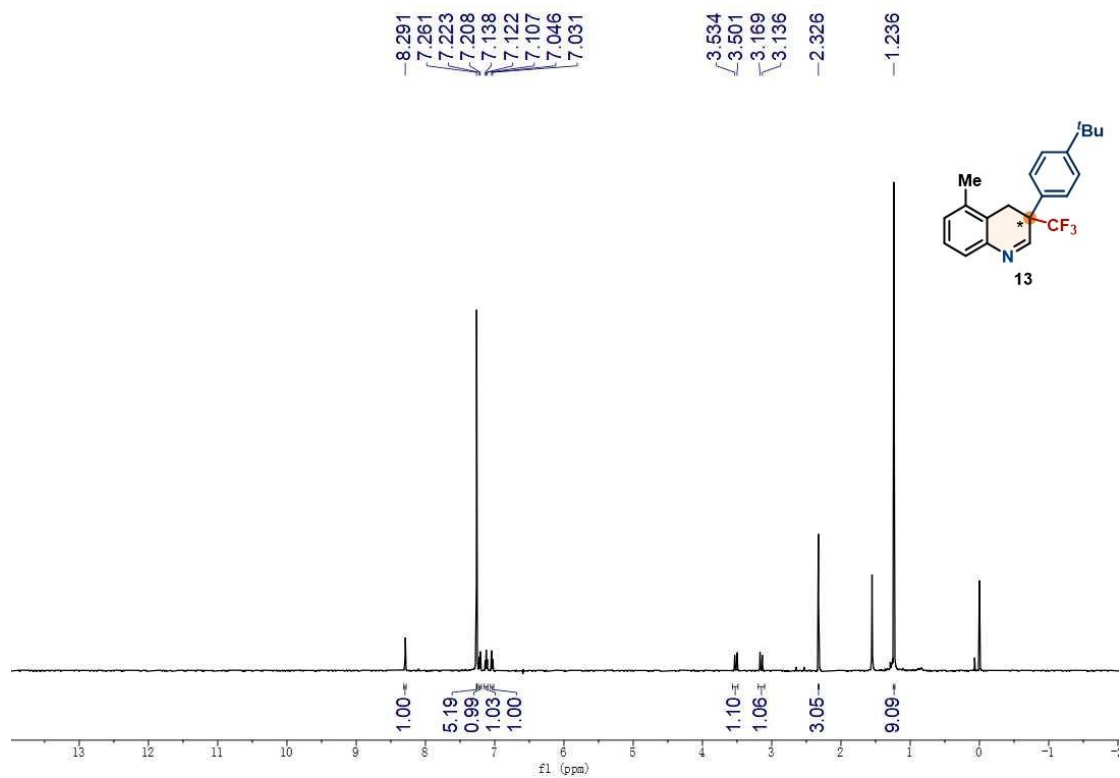
Supplementary Fig. S42. ¹H NMR (500 MHz, CDCl₃) Spectrum of 12



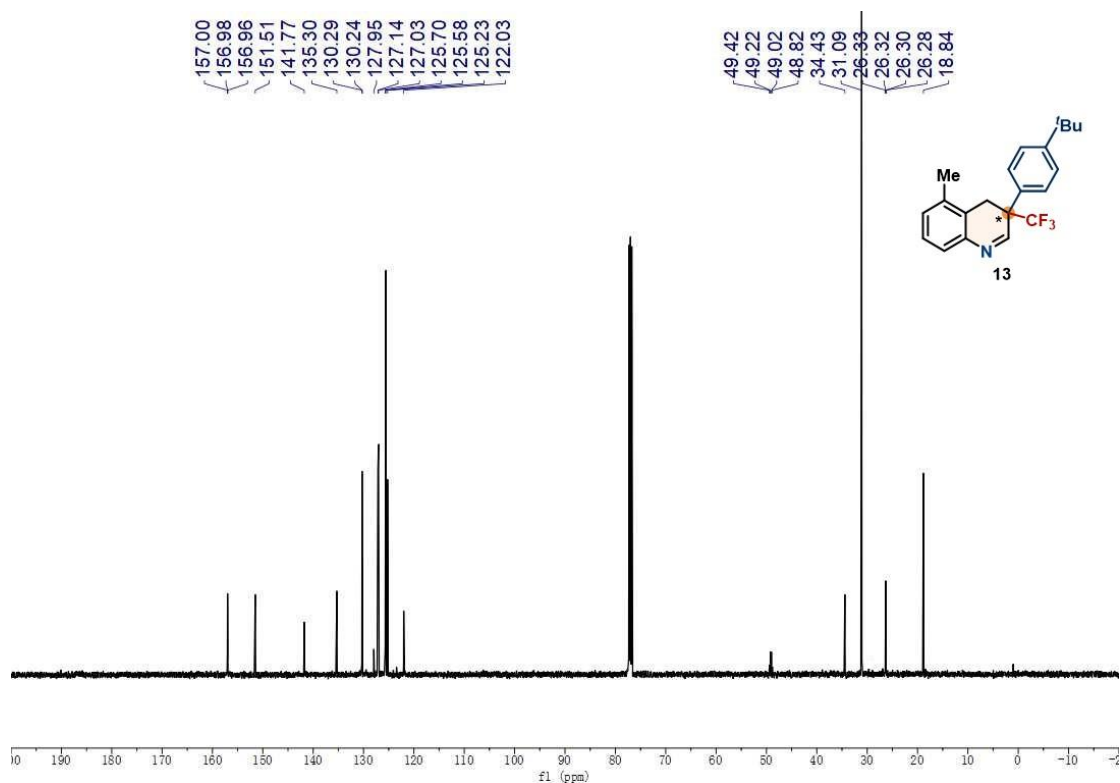
Supplementary Fig. S43. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 12



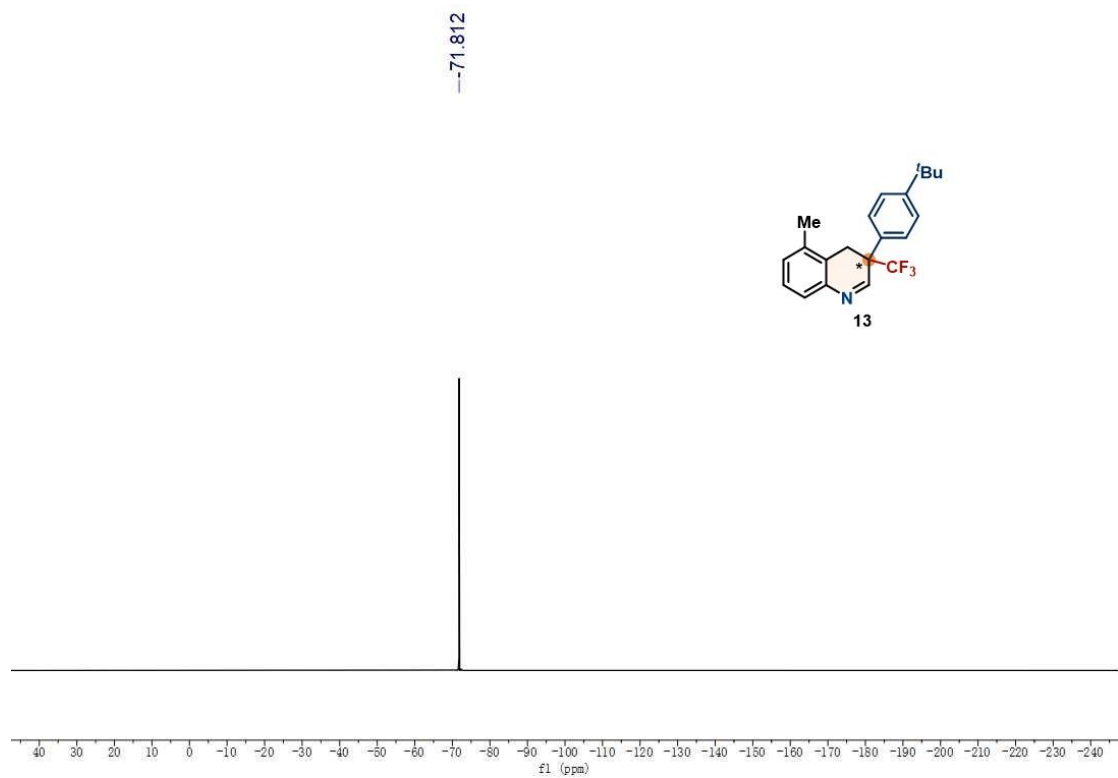
Supplementary Fig. S44. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 12



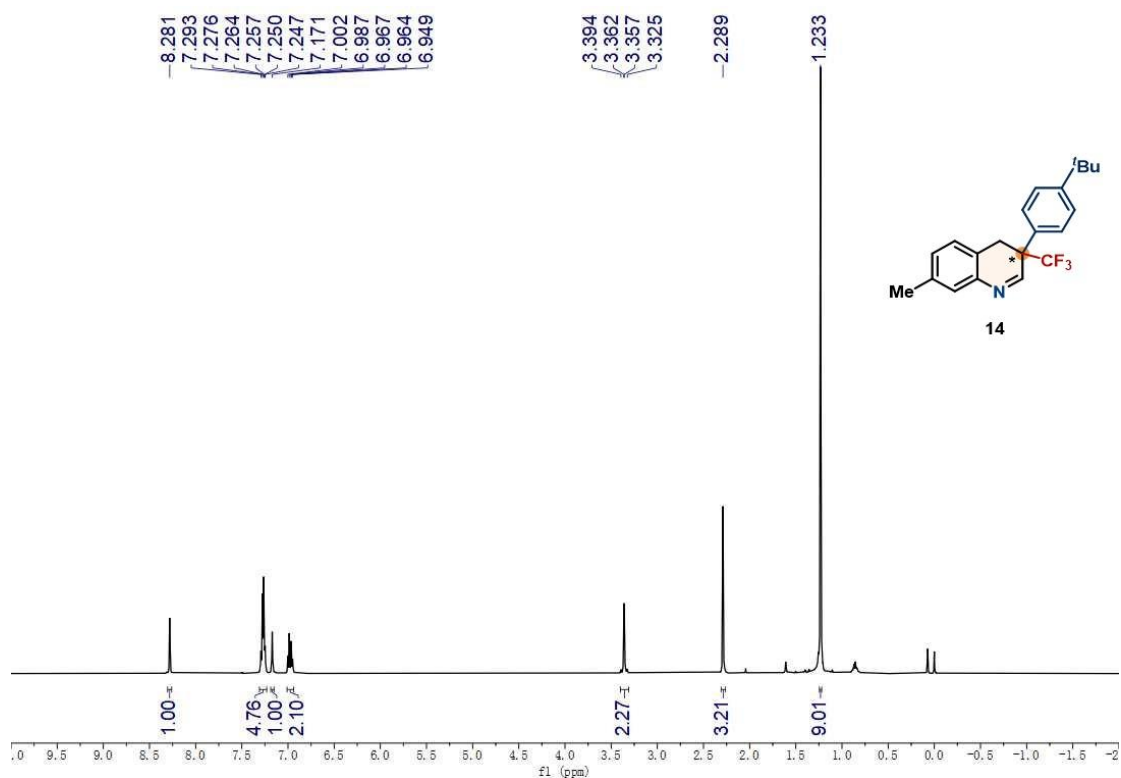
Supplementary Fig. S45. ¹H NMR (500 MHz, CDCl₃) Spectrum of 13



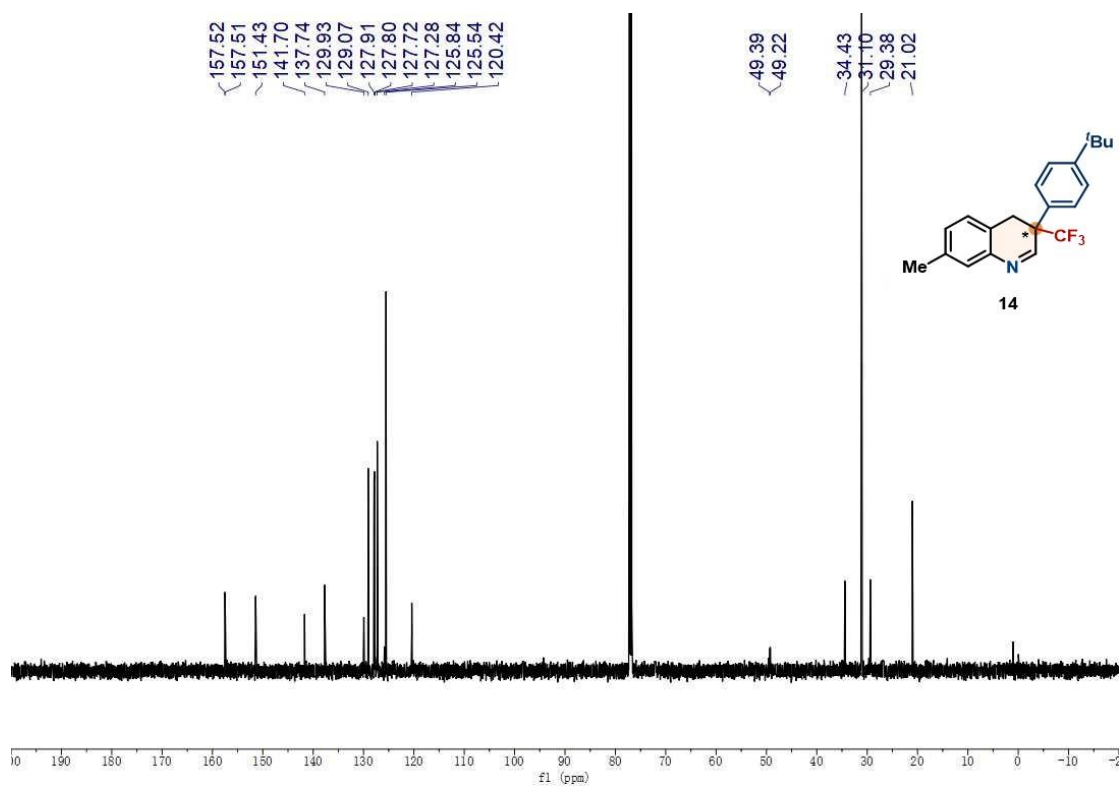
Supplementary Fig. S46. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 13



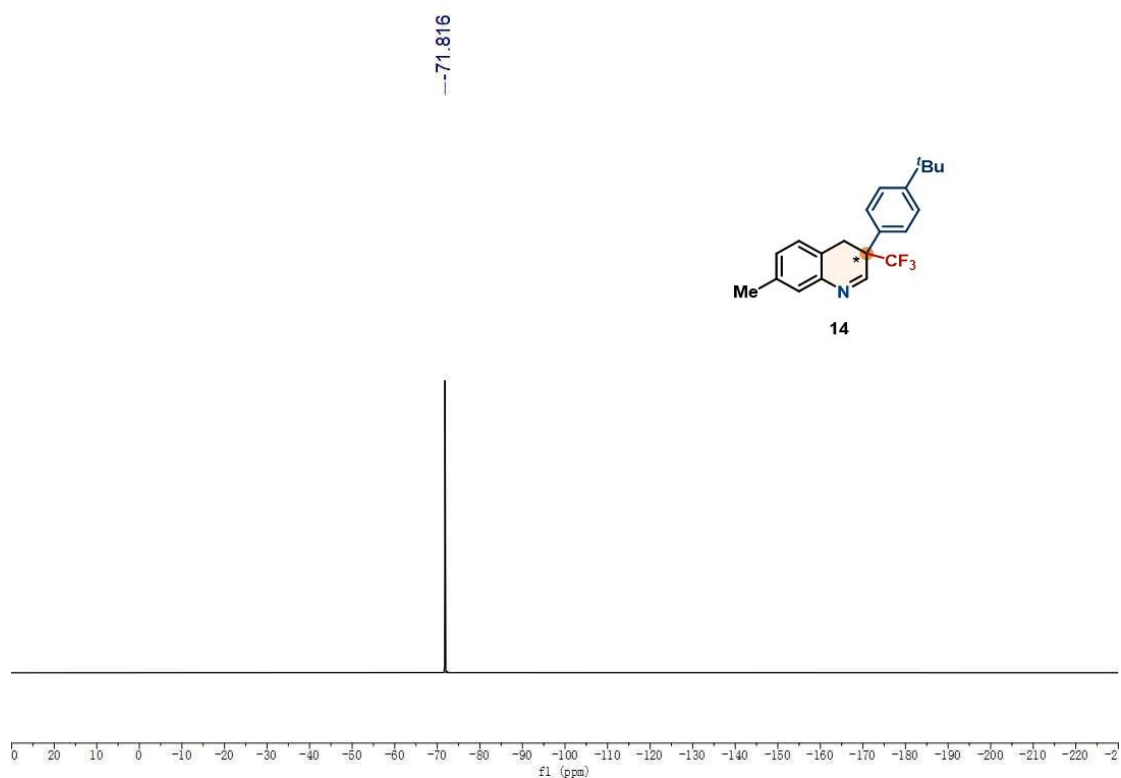
Supplementary Fig. S47. ^{19}F NMR (471 MHz, CDCl_3) Spectrum of 13



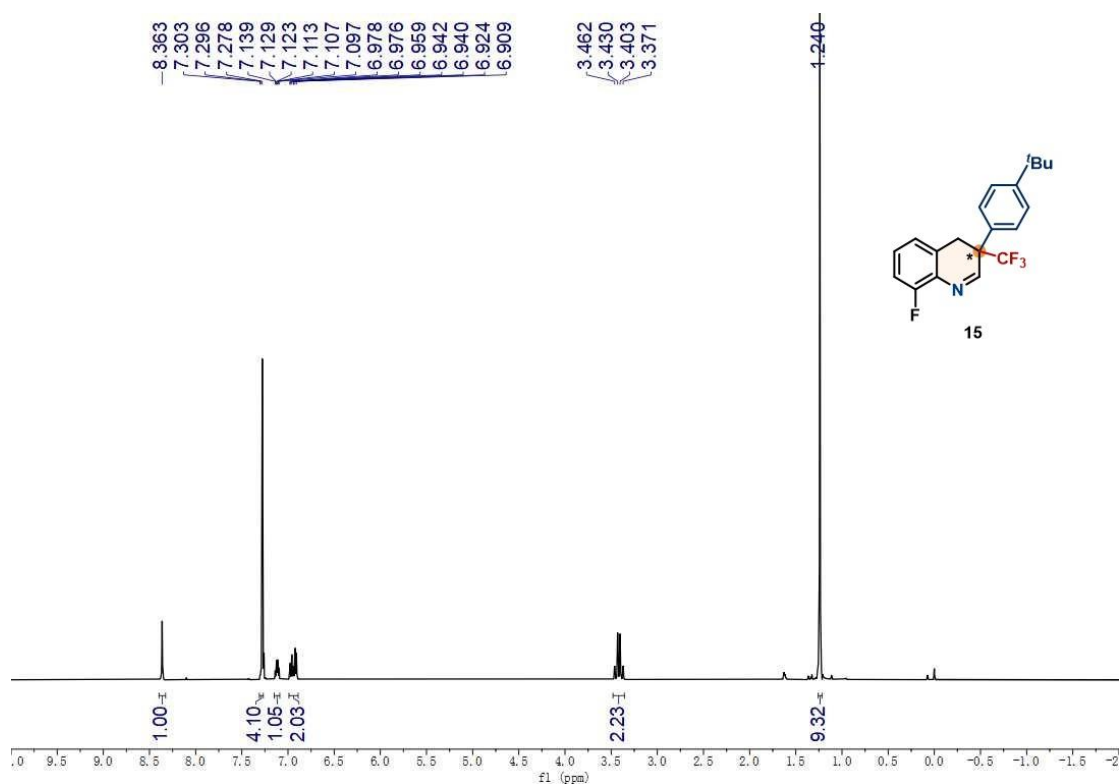
Supplementary Fig. S48. ^1H NMR (500 MHz, CDCl_3) Spectrum of 14



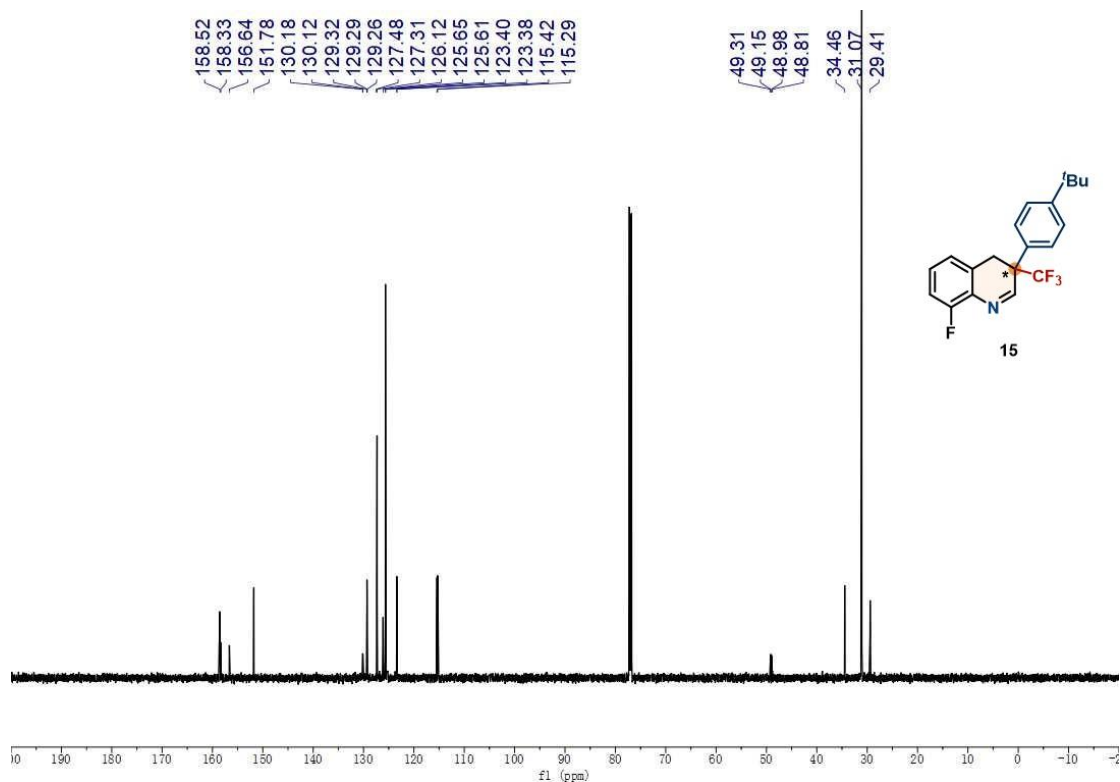
Supplementary Fig. S49. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 14



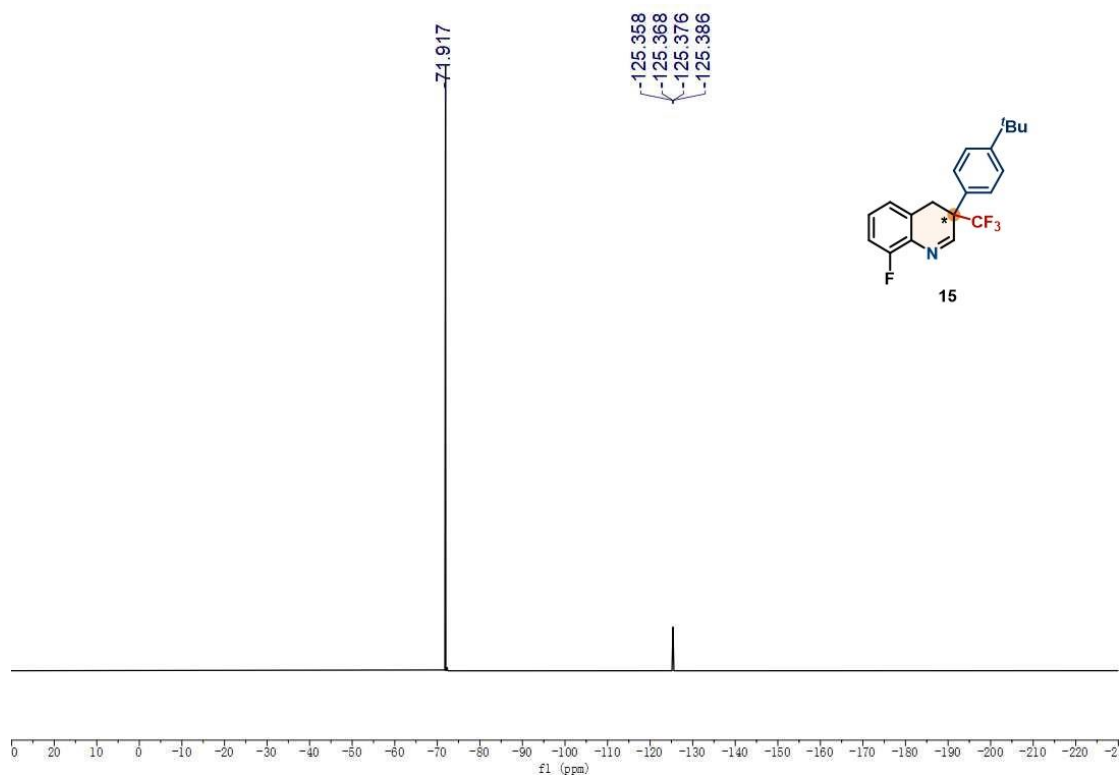
Supplementary Fig. S50. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 14



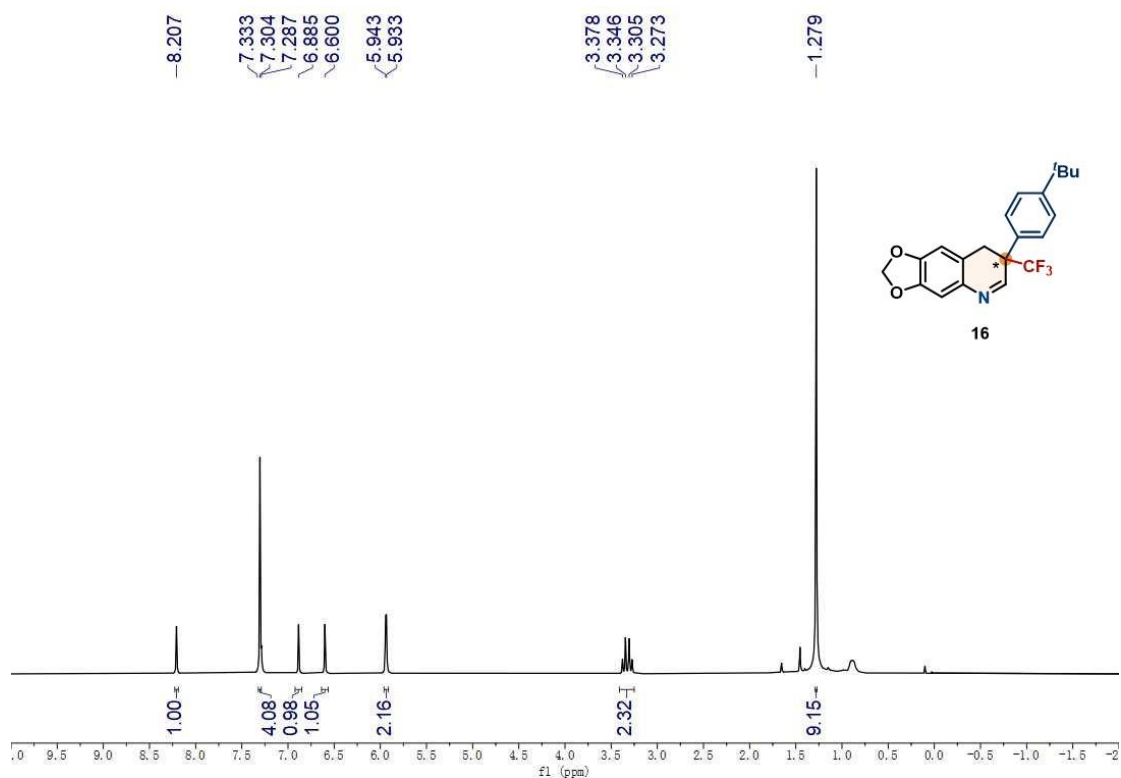
Supplementary Fig. S51. ¹H NMR (500 MHz, CDCl₃) Spectrum of 15



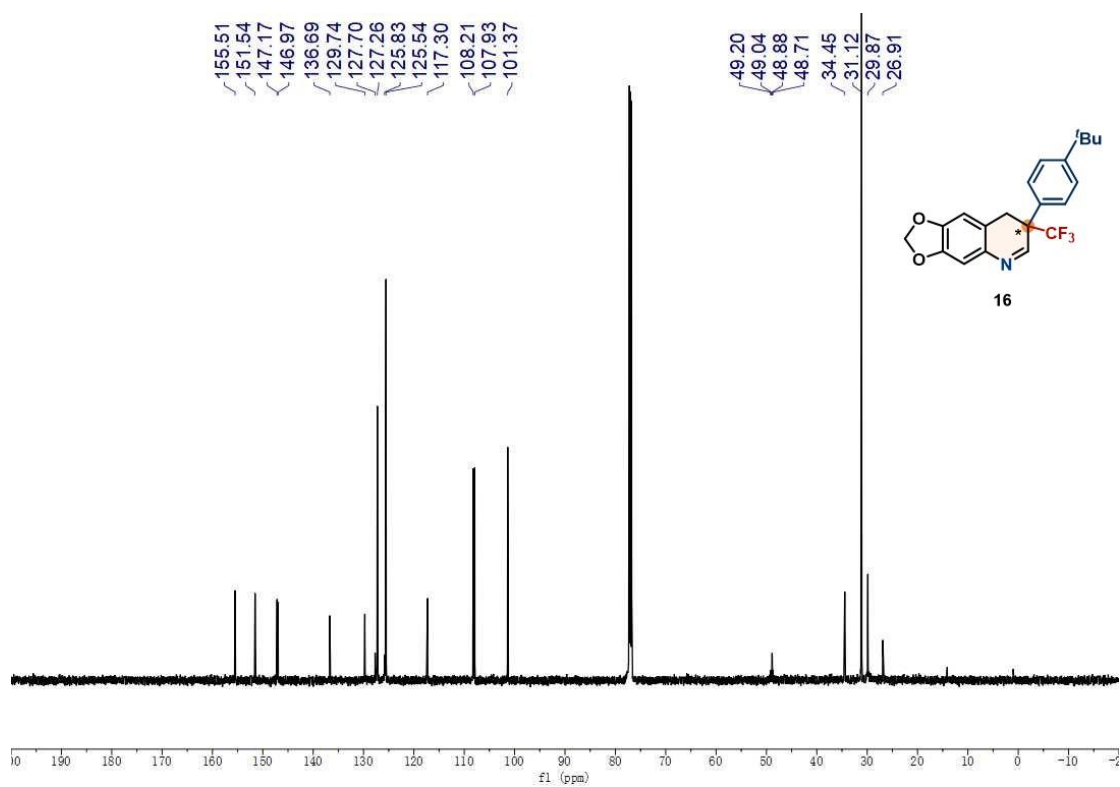
Supplementary Fig. S52. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 15



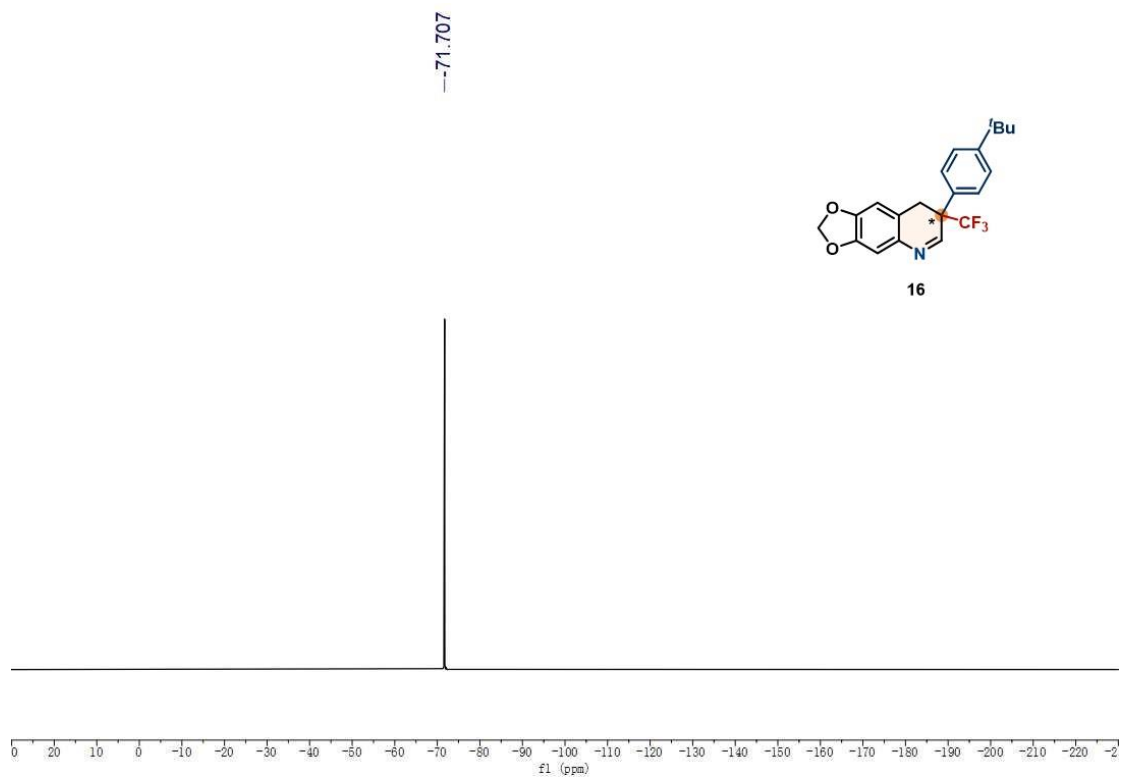
Supplementary Fig. S53. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 15



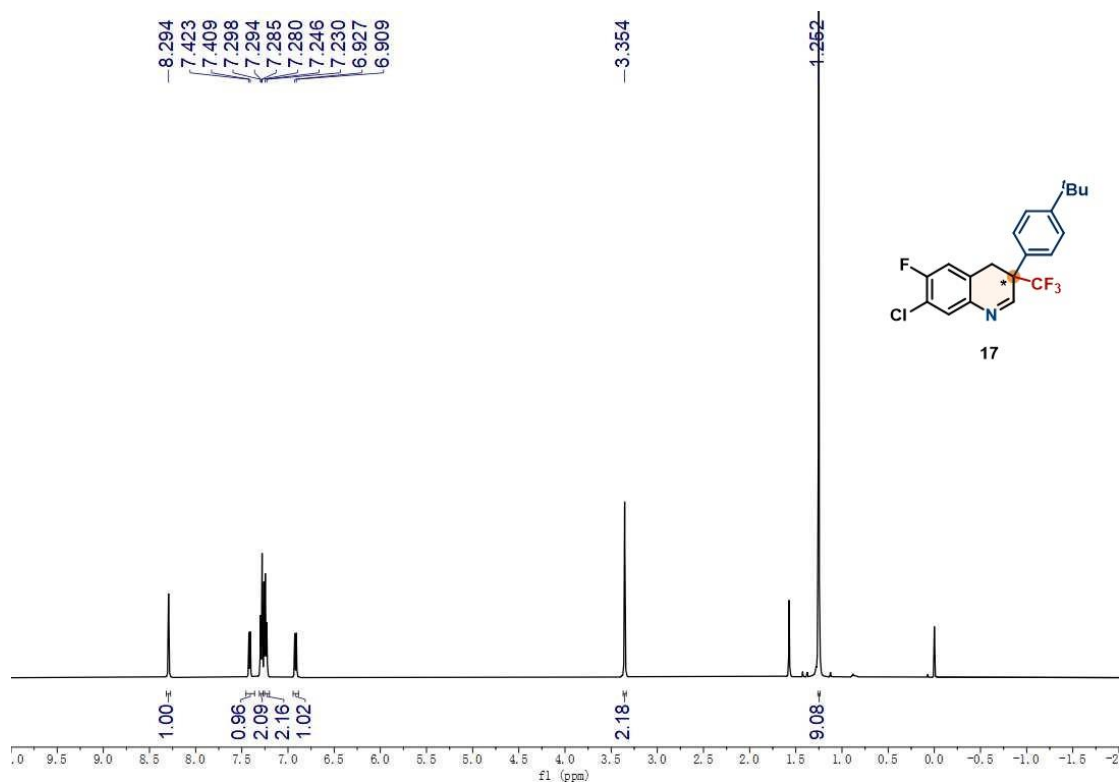
Supplementary Fig. S54. ¹H NMR (500 MHz, CDCl₃) Spectrum of 16



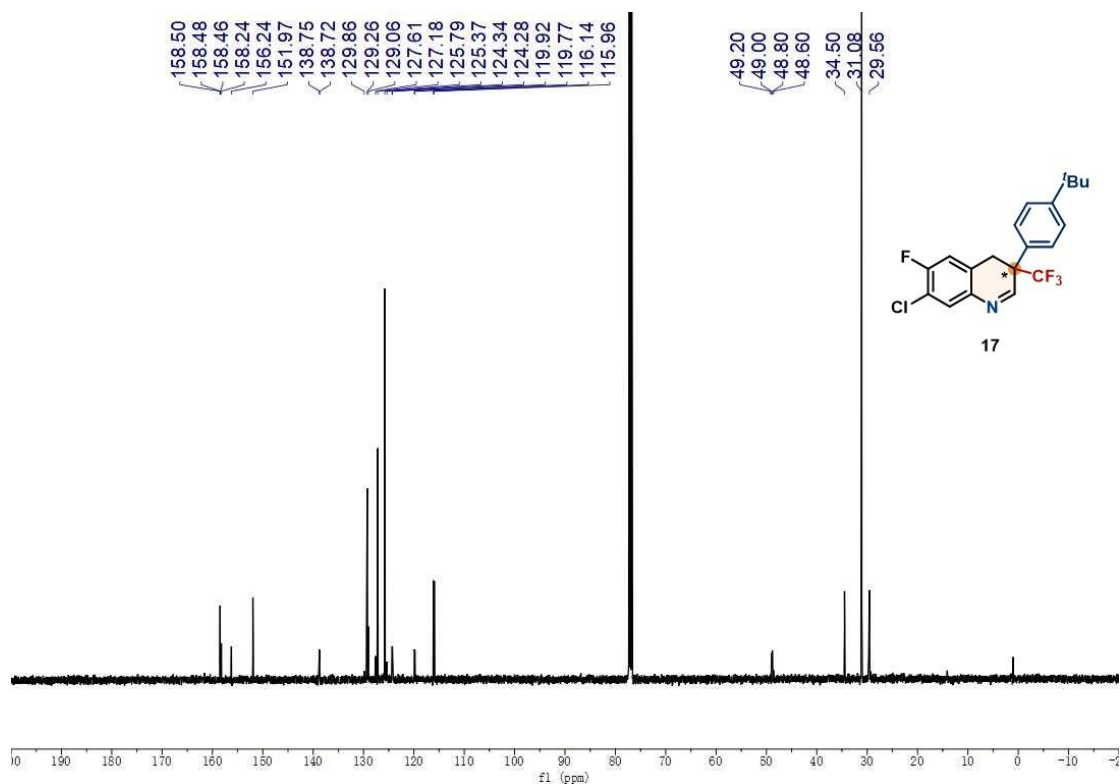
Supplementary Fig. S55. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 16



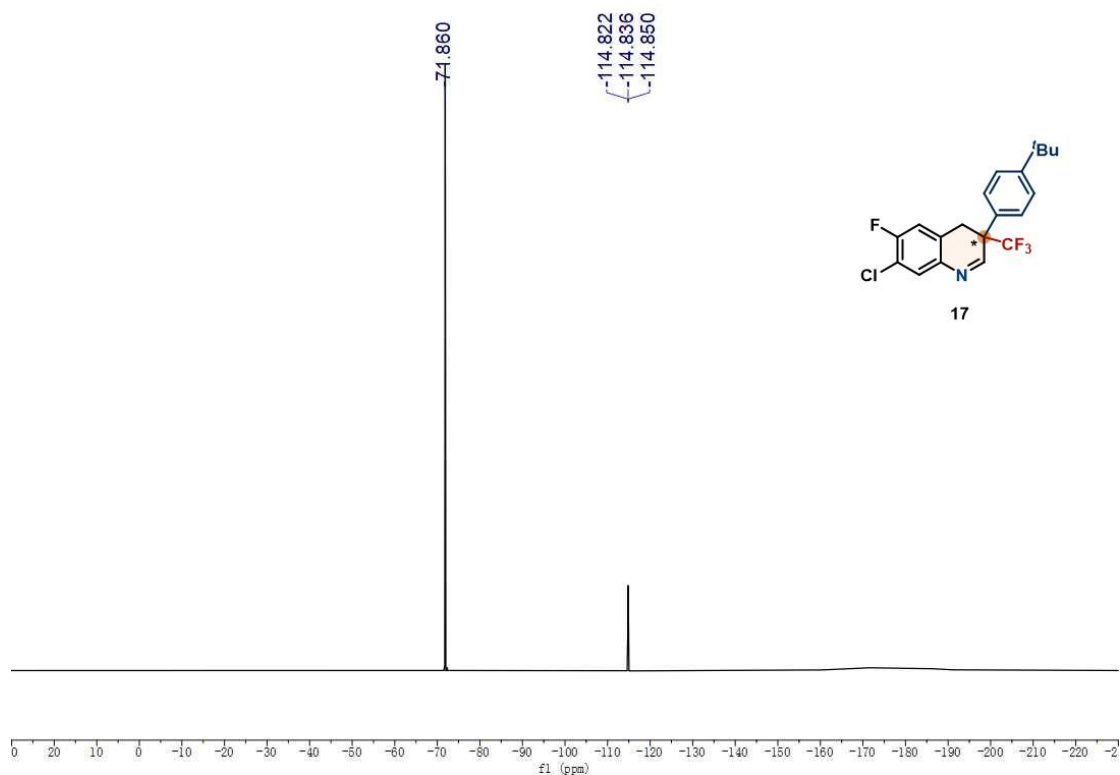
Supplementary Fig. S56. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 16



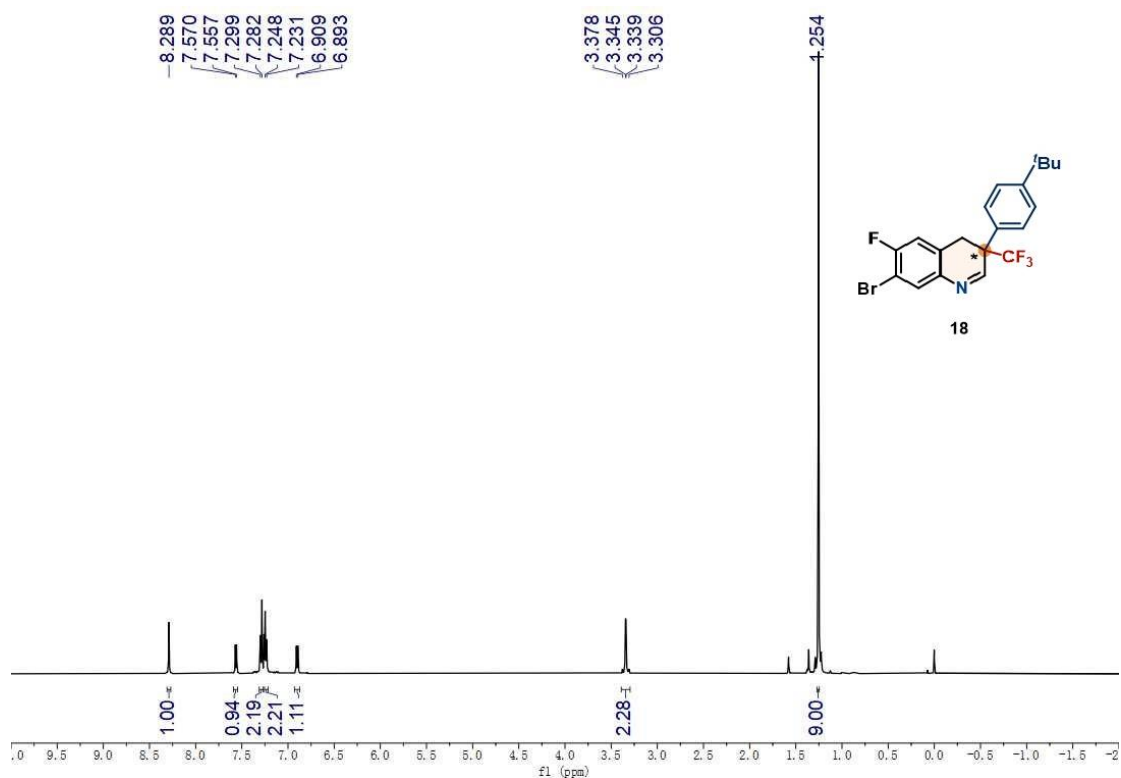
Supplementary Fig. S57. ¹H NMR (500 MHz, CDCl₃) Spectrum of 17



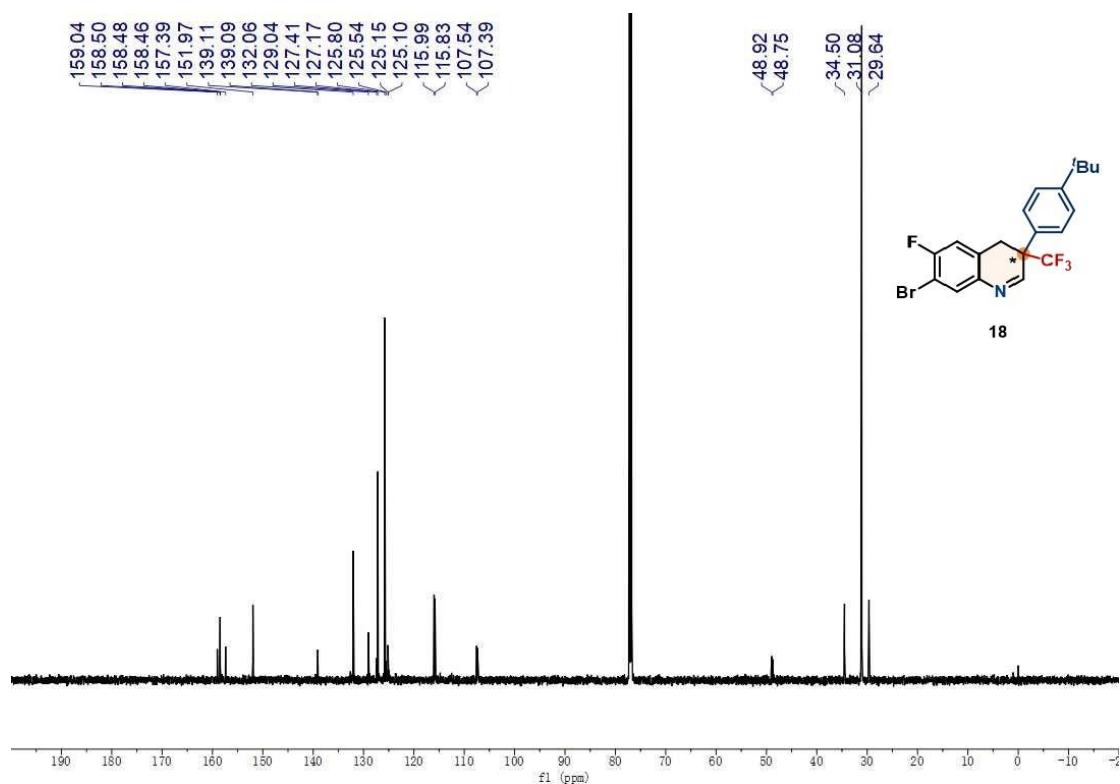
Supplementary Fig. S58. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 17



Supplementary Fig. S59. ¹⁹F NMR (470 MHz, CDCl₃) Spectrum of 17



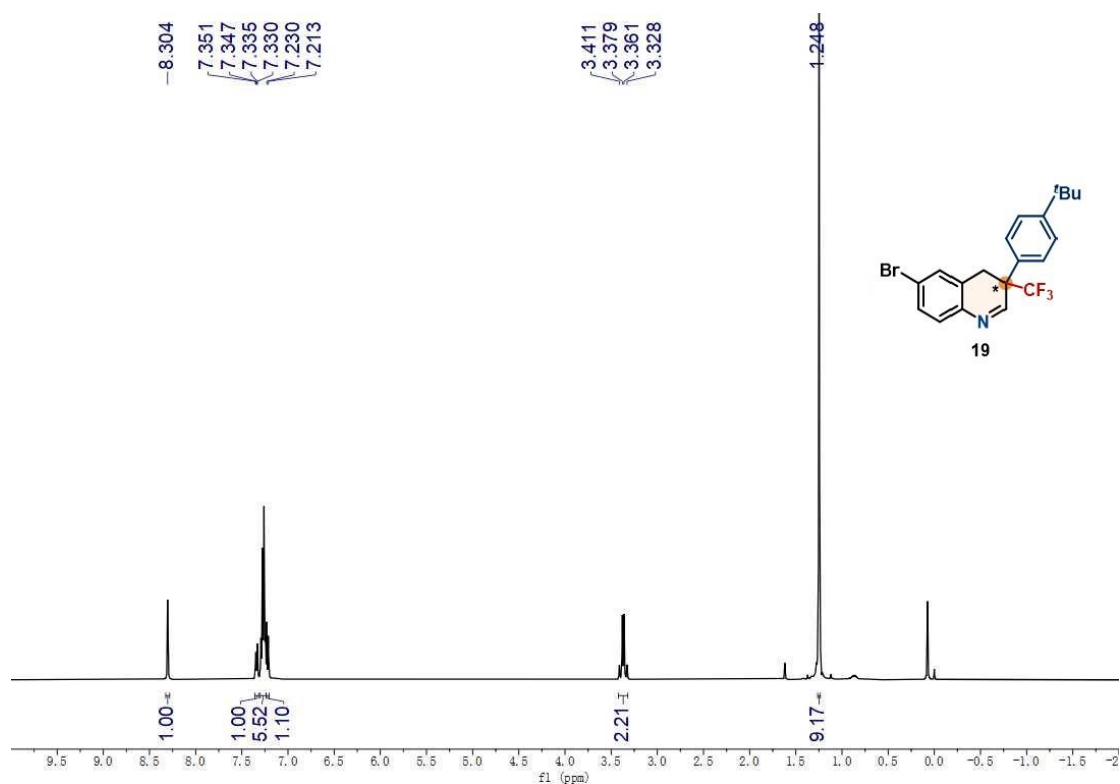
Supplementary Fig. S60. ¹H NMR (500 MHz, CDCl₃) Spectrum of 18



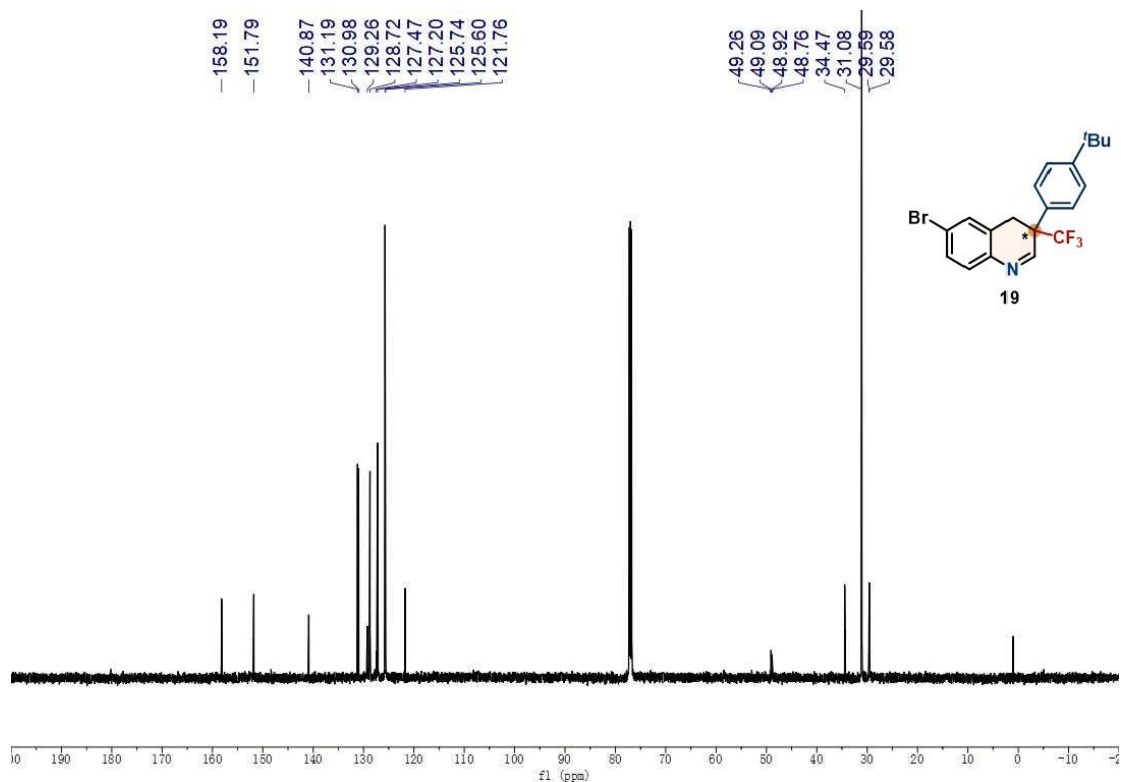
Supplementary Fig. S61. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 18



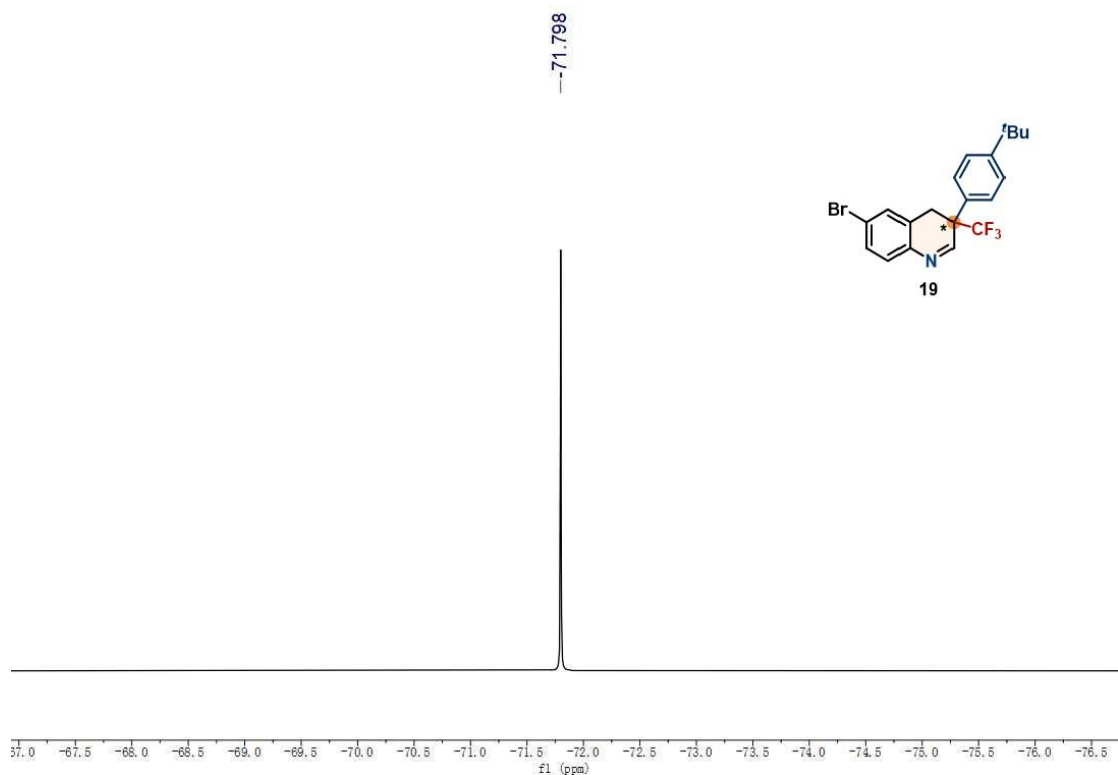
Supplementary Fig. S62. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 18



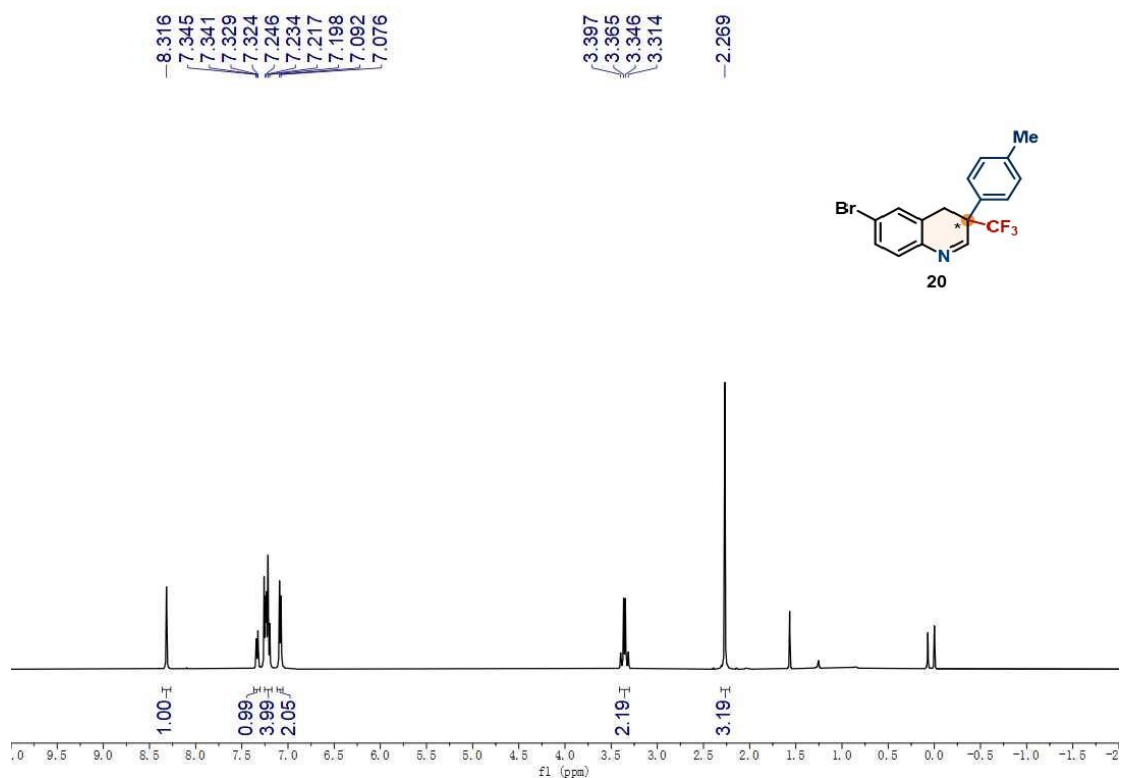
Supplementary Fig. S63. ¹H NMR (500 MHz, CDCl₃) Spectrum of 19



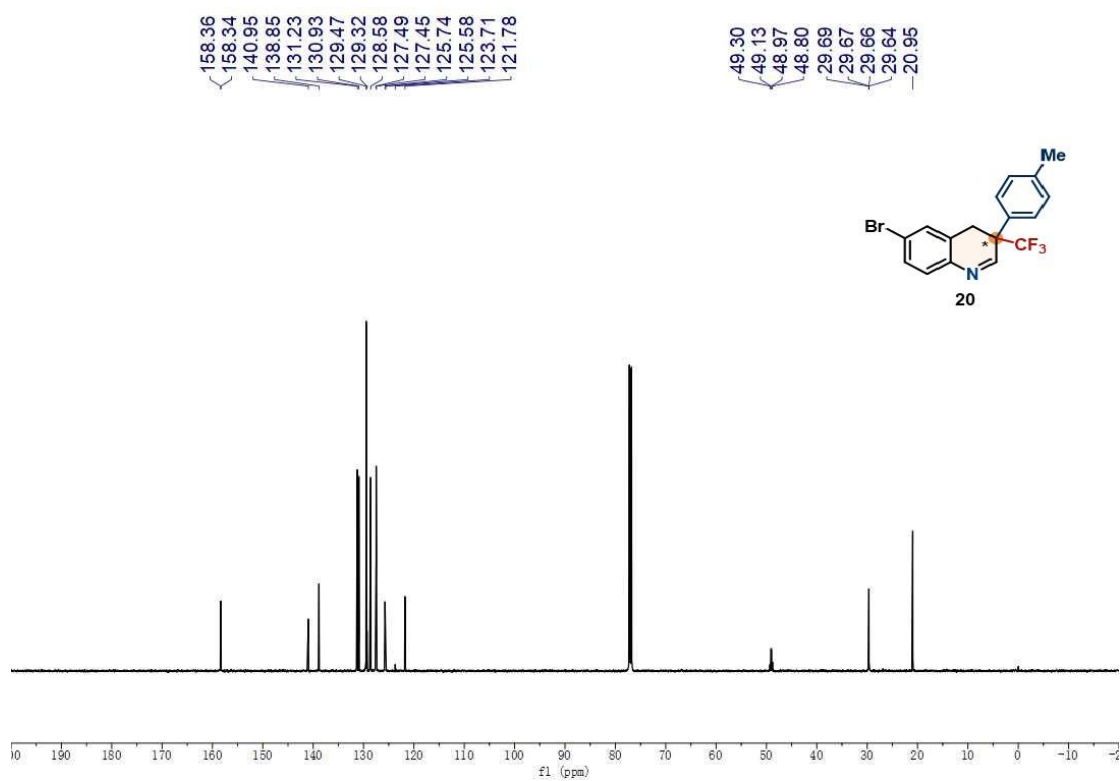
Supplementary Fig. S64. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 19



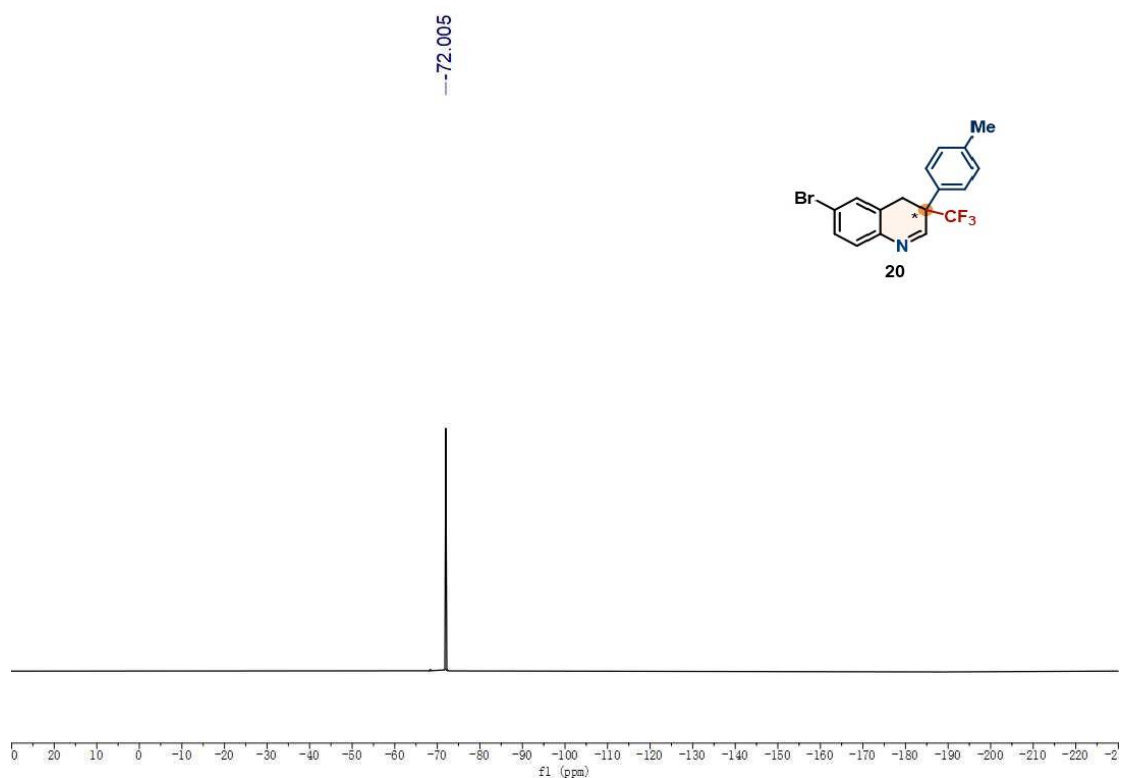
Supplementary Fig. S65. ¹⁹F NMR (470 MHz, CDCl₃) Spectrum of 19



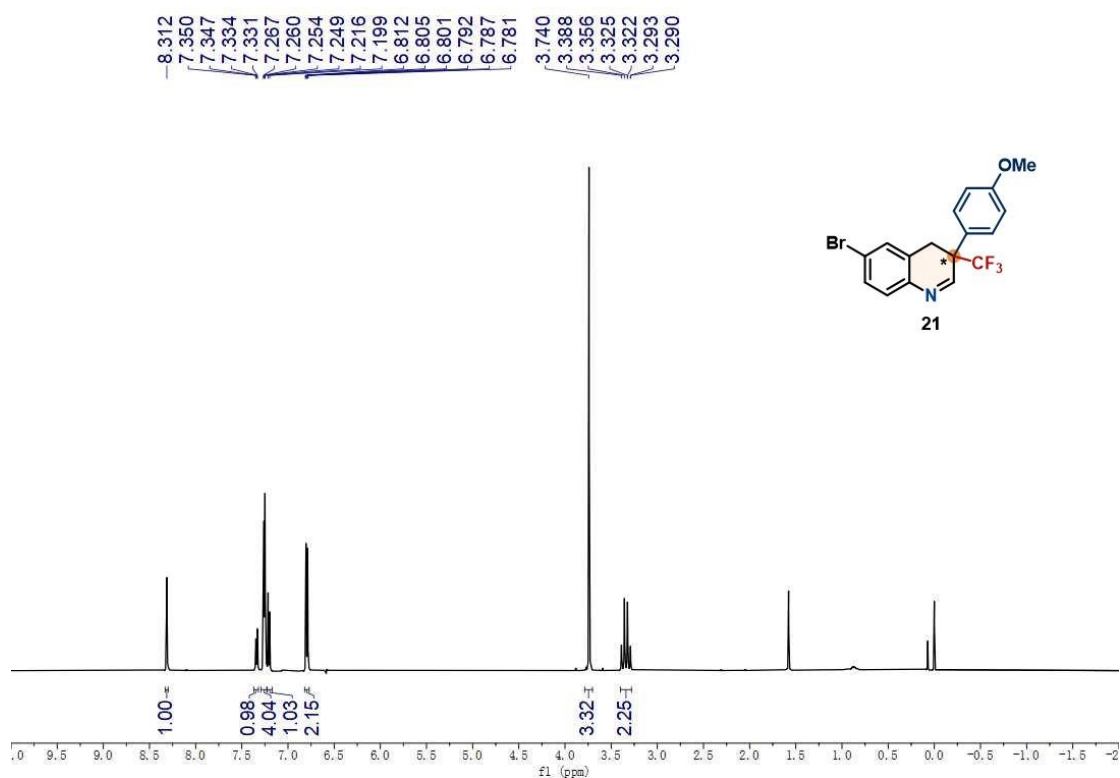
Supplementary Fig. S66. ¹H NMR (500 MHz, CDCl₃) Spectrum of 20



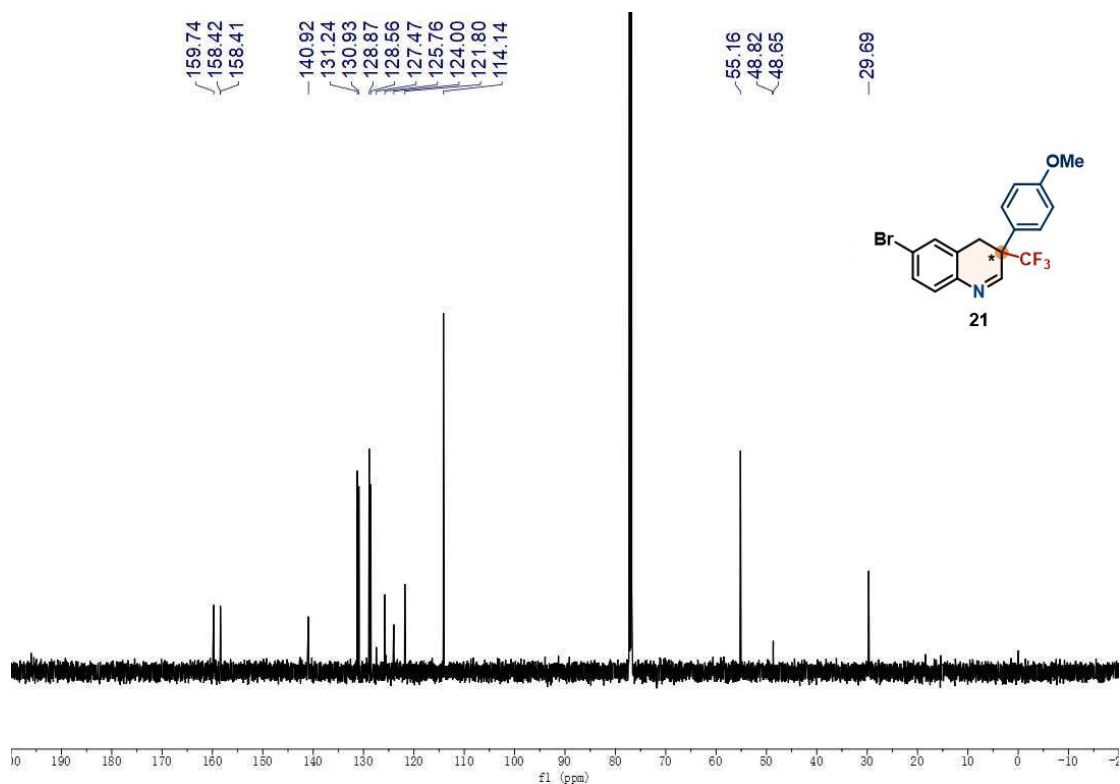
Supplementary Fig. S67. ^{13}C NMR (125 MHz, CDCl_3) Spectrum of 20



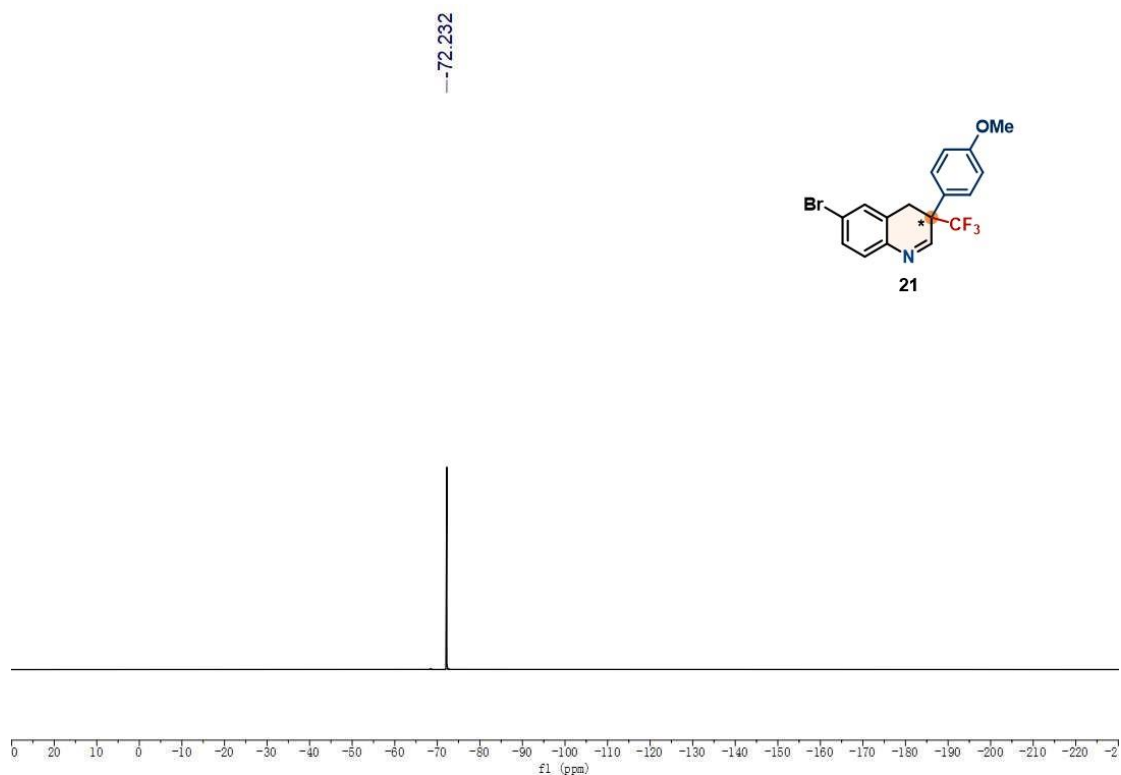
Supplementary Fig. S68. ^{19}F NMR (470 MHz, CDCl_3) Spectrum of 20



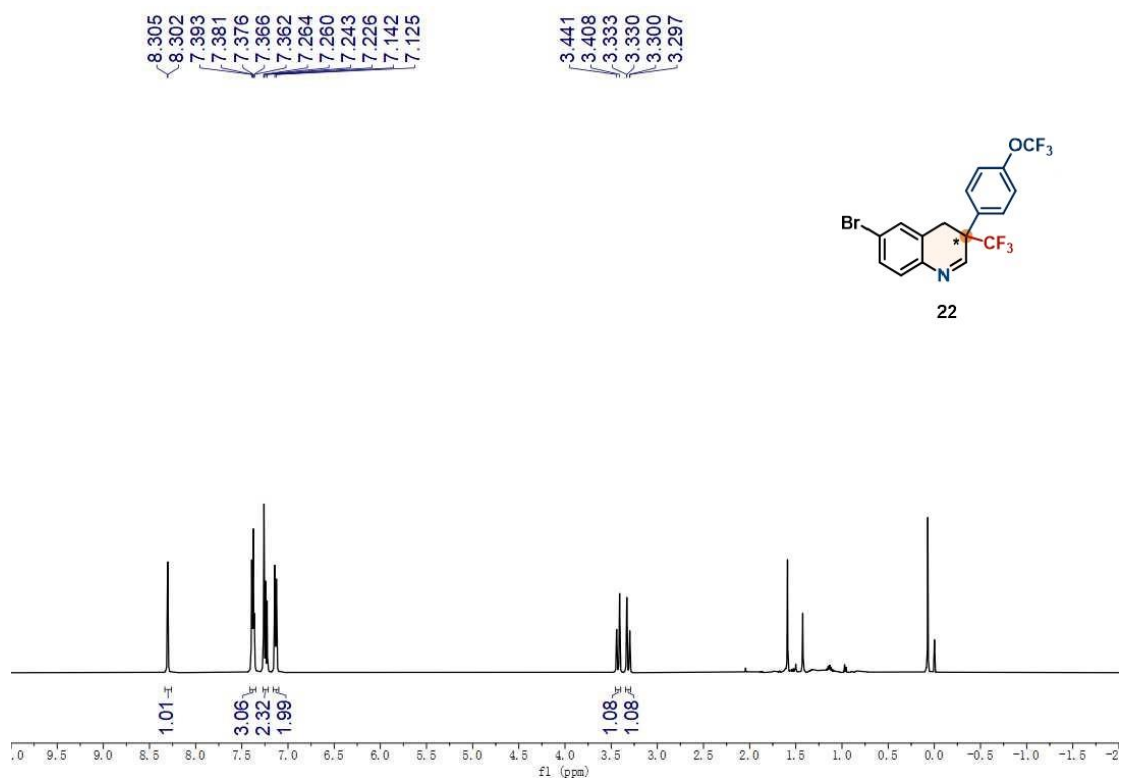
Supplementary Fig. S69. ¹H NMR (500 MHz, CDCl₃) Spectrum of 21



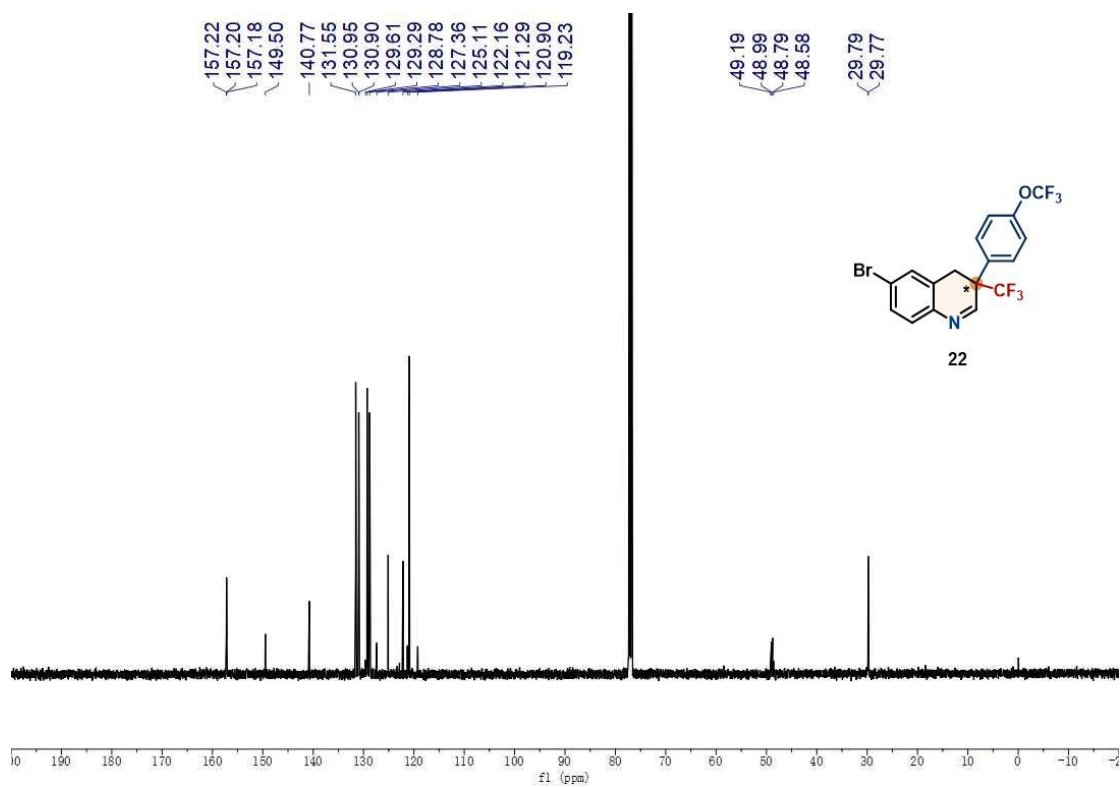
Supplementary Fig. S70. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 21



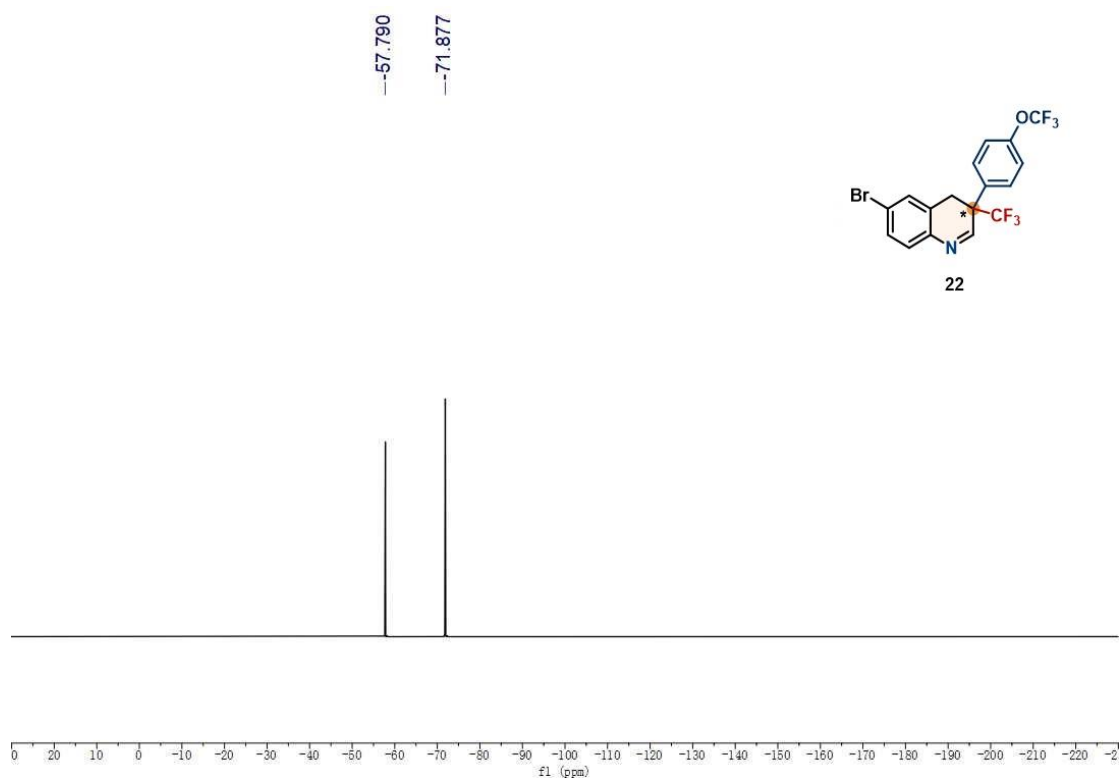
Supplementary Fig. S71. ^{19}F NMR (564 MHz, CDCl_3) Spectrum of 21



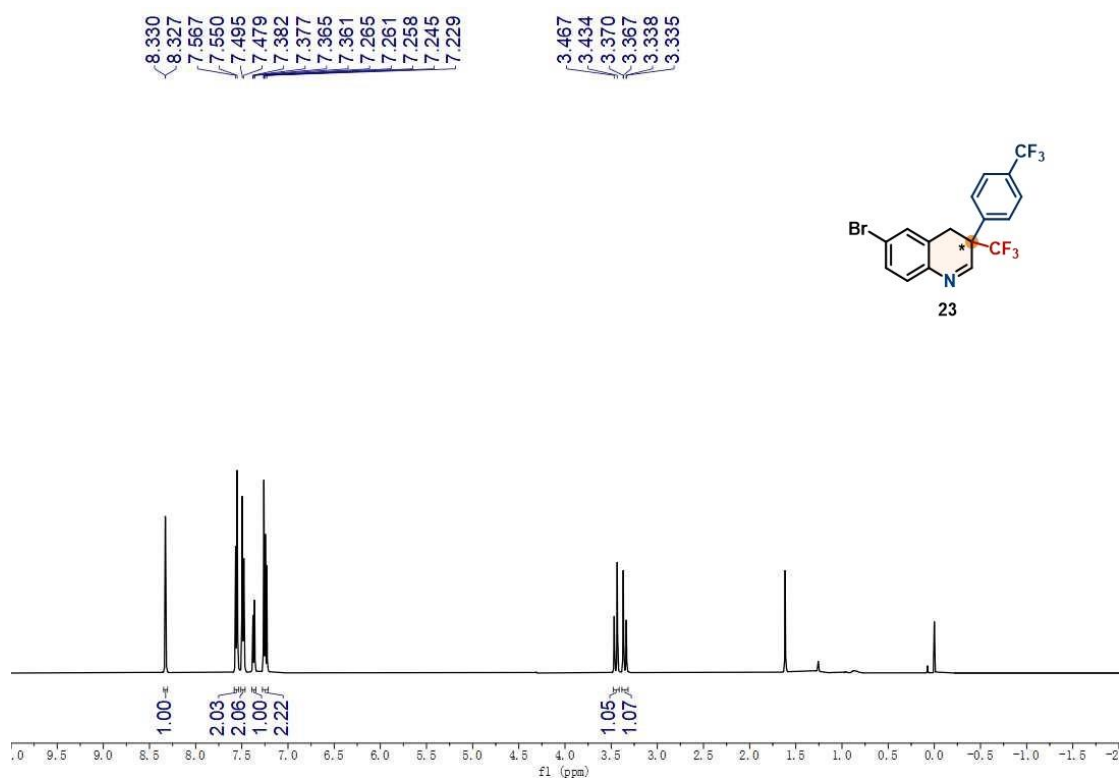
Supplementary Fig. S72. ^1H NMR (500 MHz, CDCl_3) Spectrum of 22



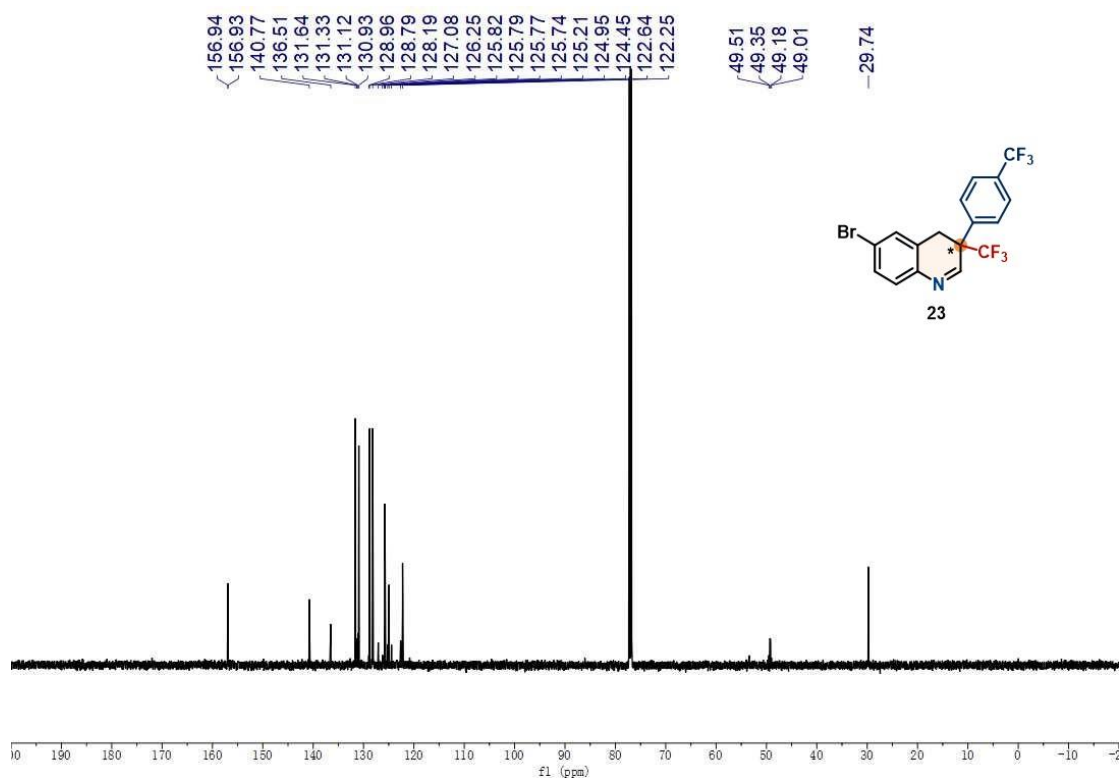
Supplementary Fig. S73. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 22



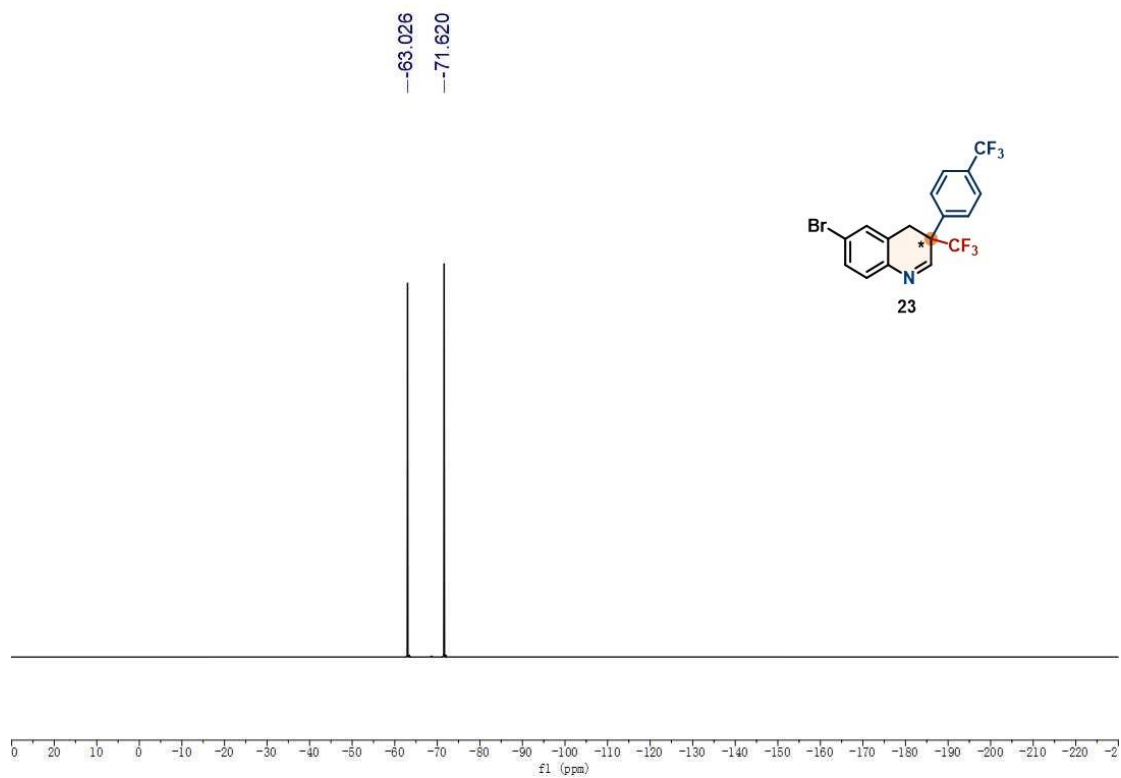
Supplementary Fig. S74. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 22



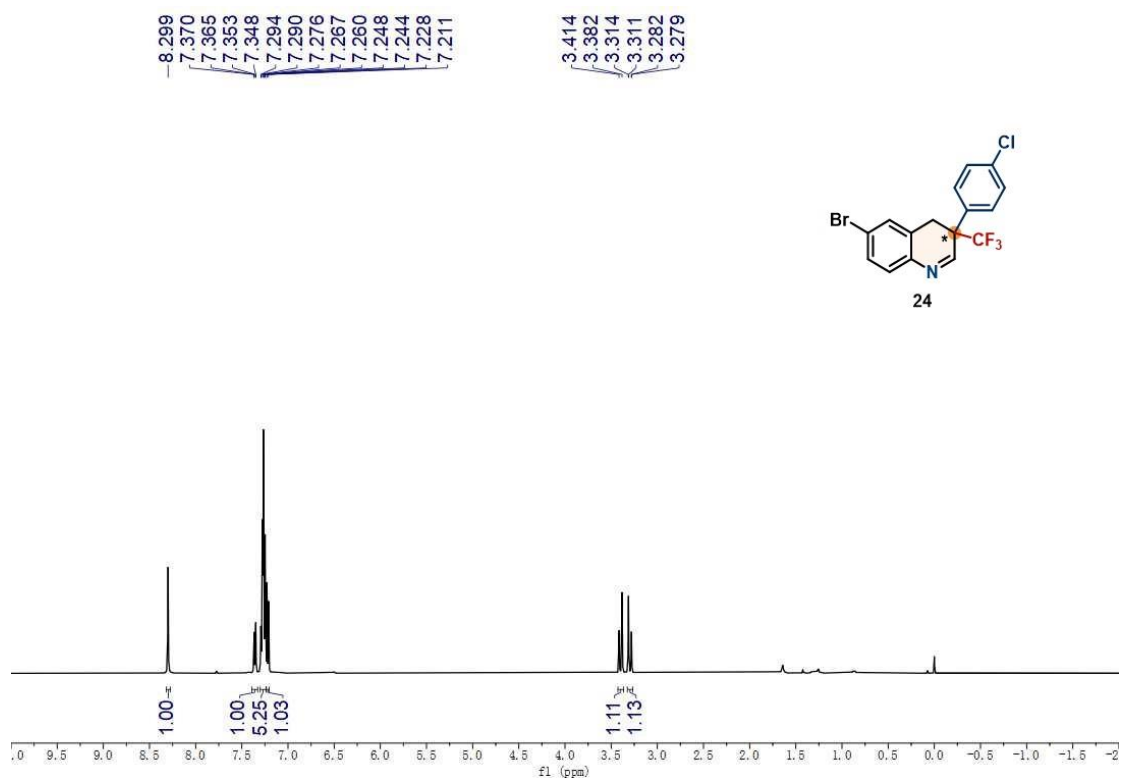
Supplementary Fig. S75. ¹H NMR (500 MHz, CDCl₃) Spectrum of 23



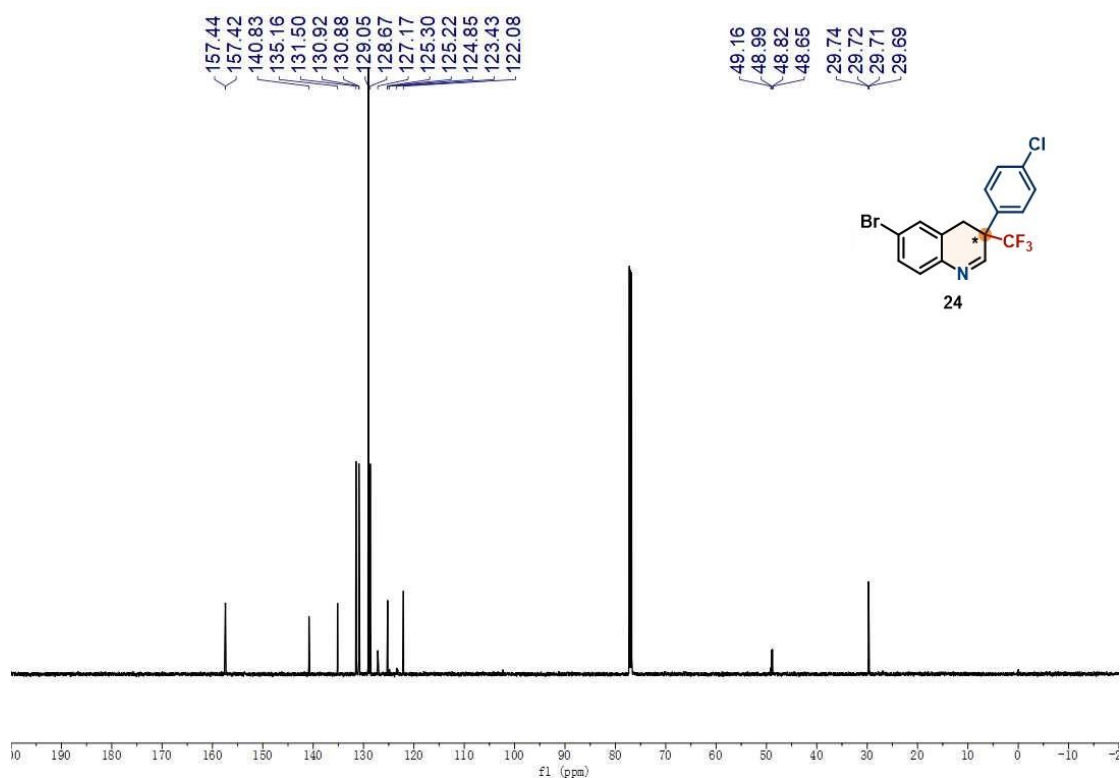
Supplementary Fig. S76. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 23



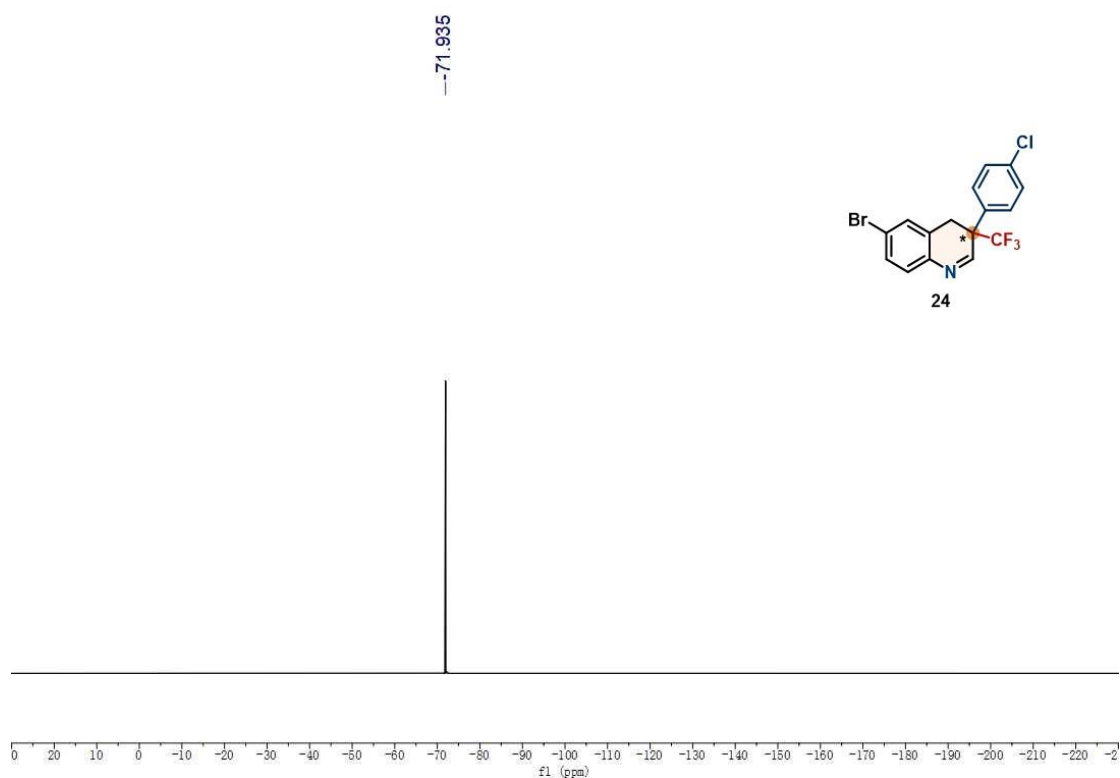
Supplementary Fig. S77. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 23



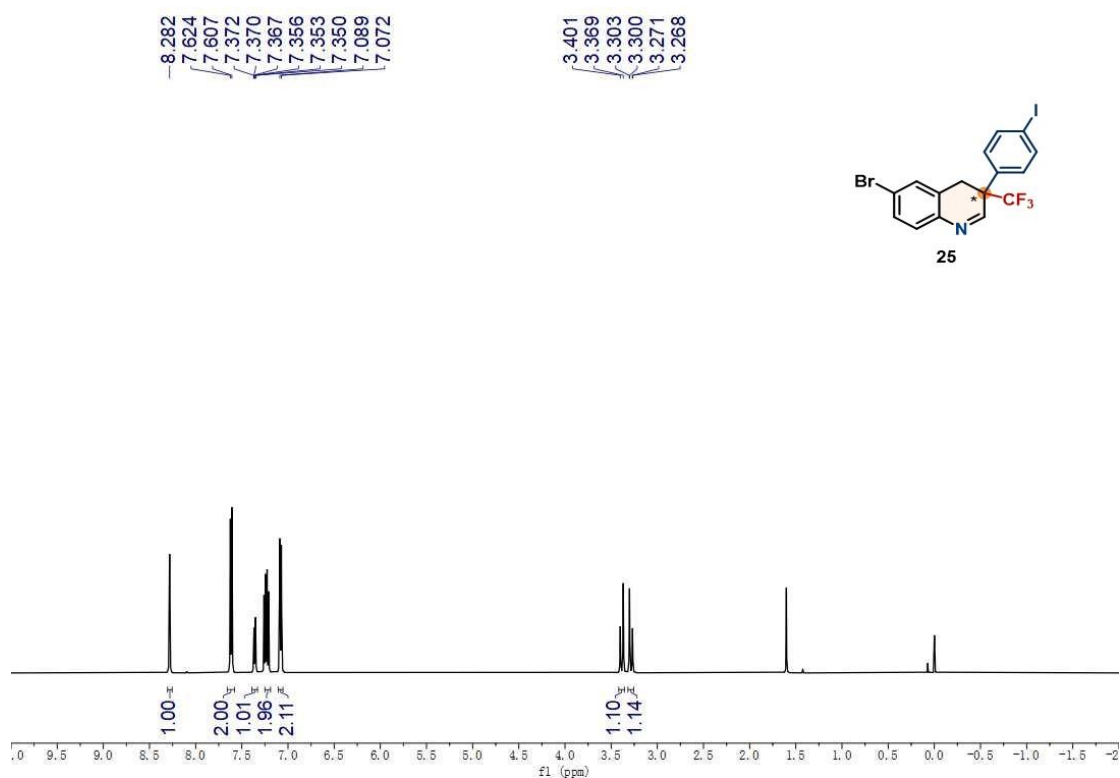
Supplementary Fig. S78. ¹H NMR (500 MHz, CDCl₃) Spectrum of 24



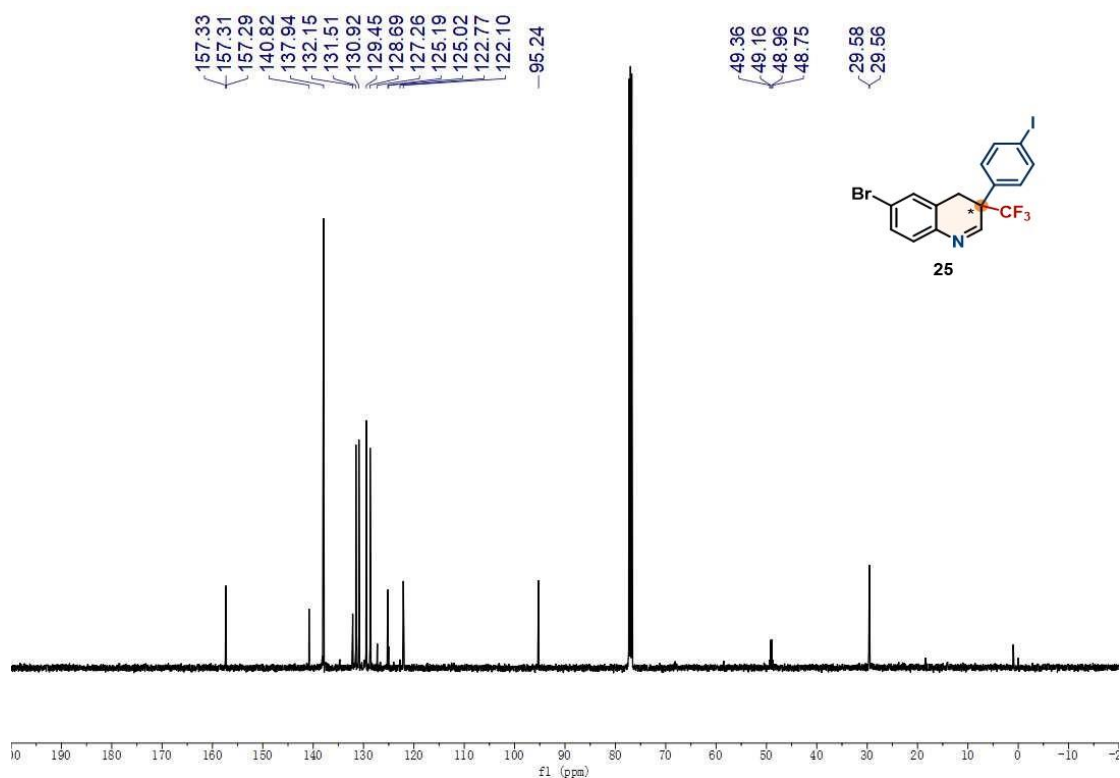
Supplementary Fig. S79. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 24



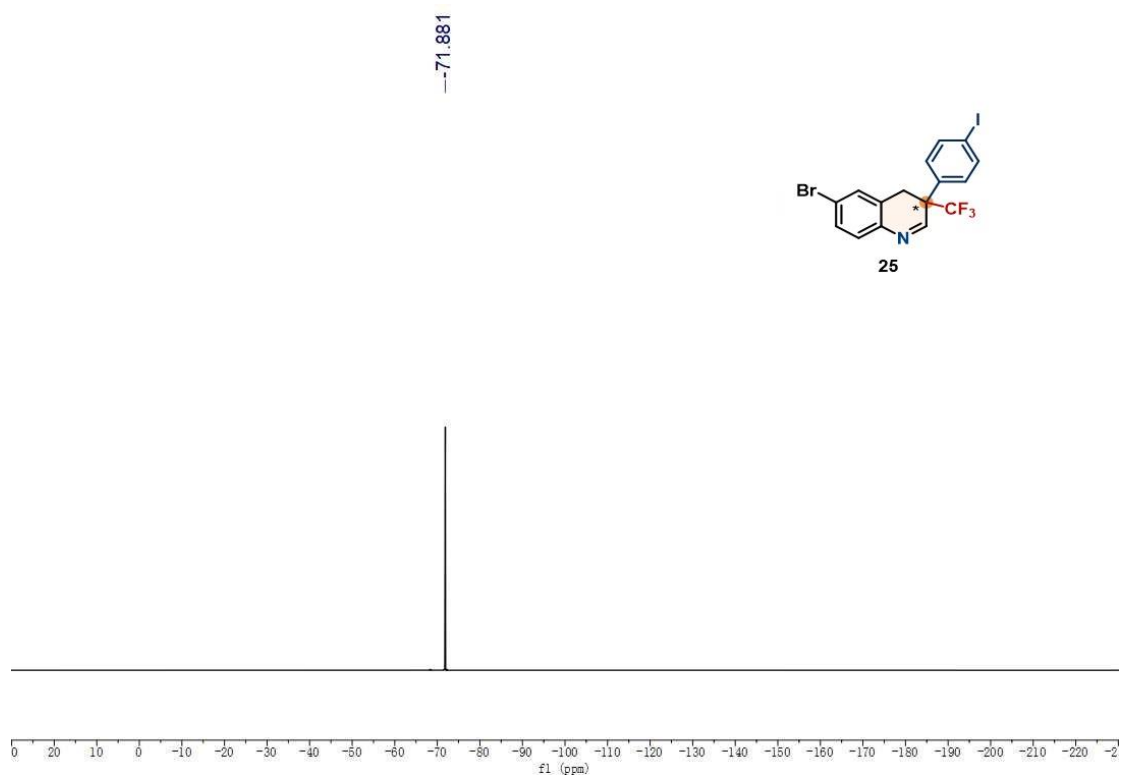
Supplementary Fig. S80. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 24



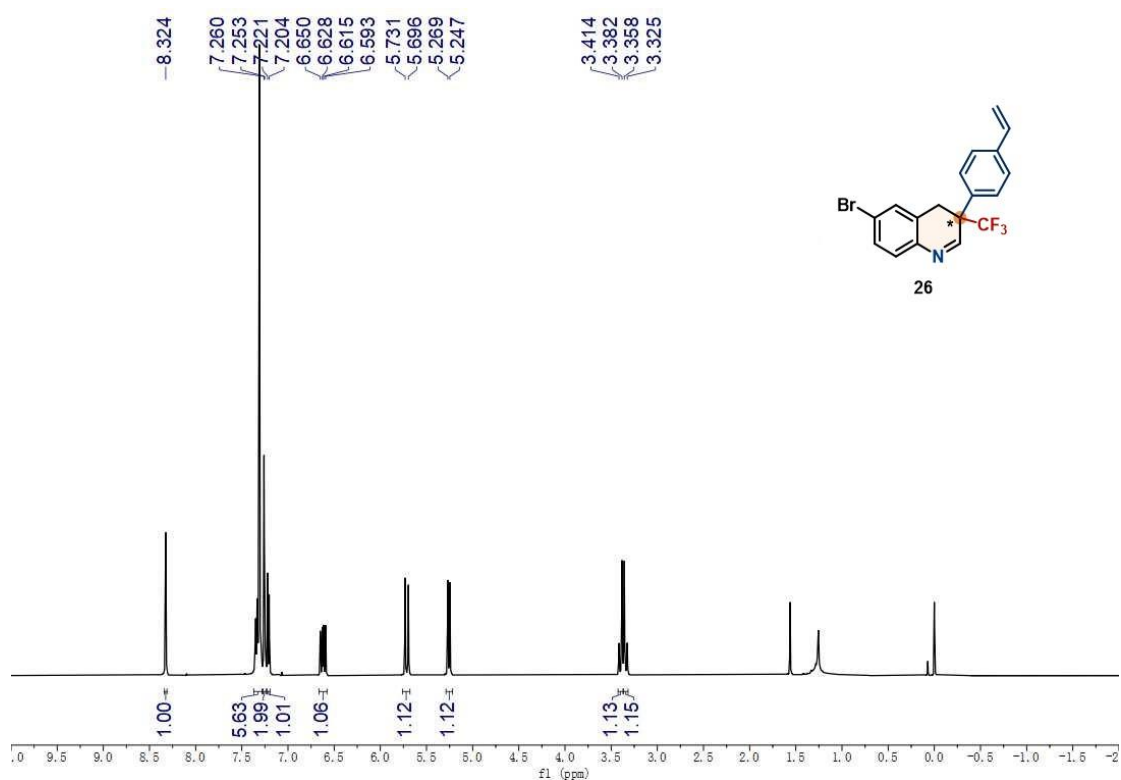
Supplementary Fig. S81. ¹H NMR (500 MHz, CDCl₃) Spectrum of 25



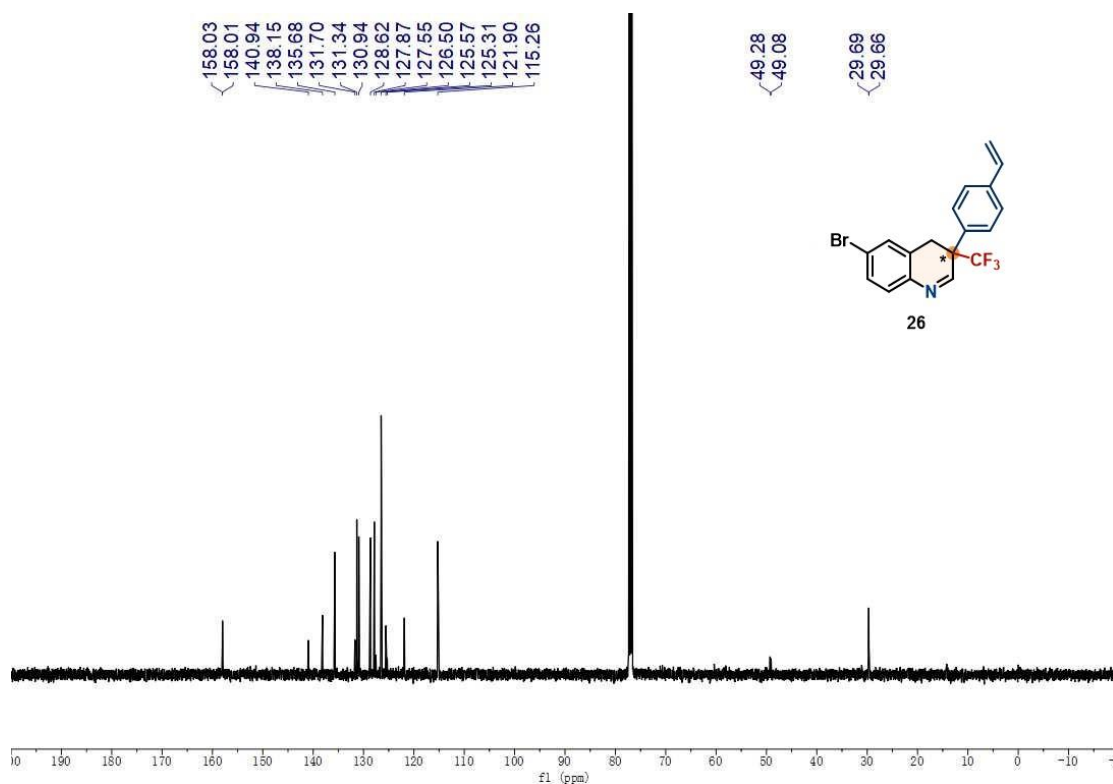
Supplementary Fig. S82. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 25



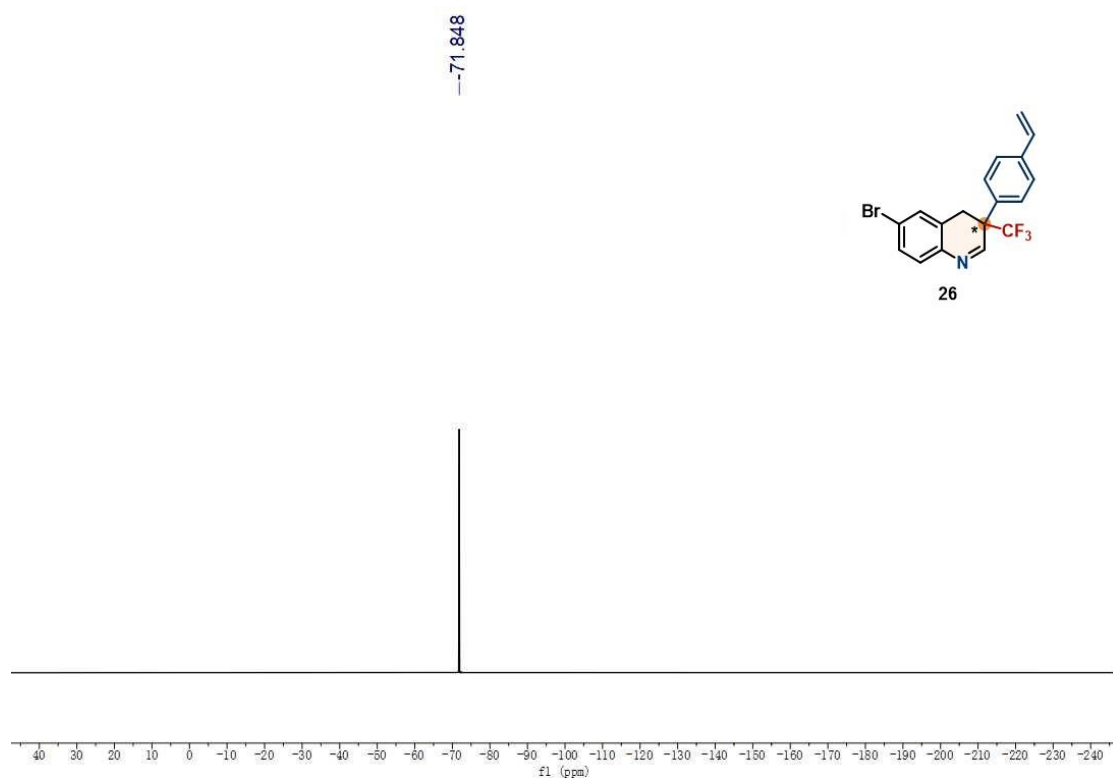
Supplementary Fig. S83. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 25



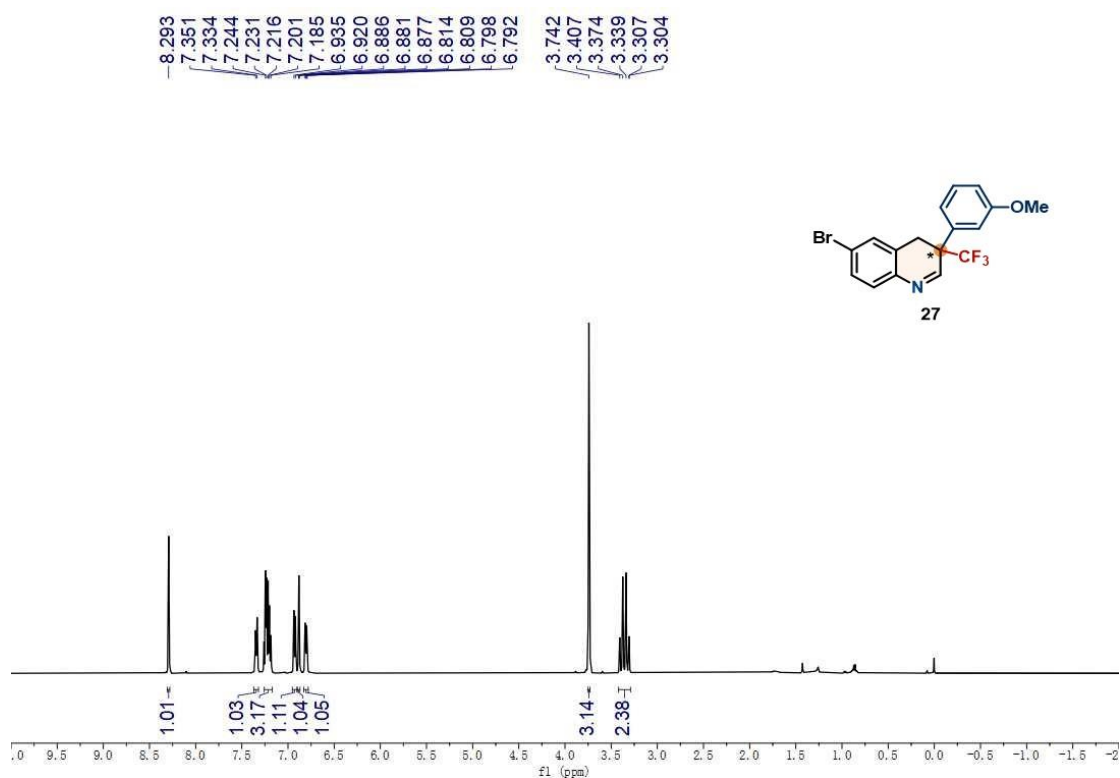
Supplementary Fig. S84. ¹H NMR (500 MHz, CDCl₃) Spectrum of 26



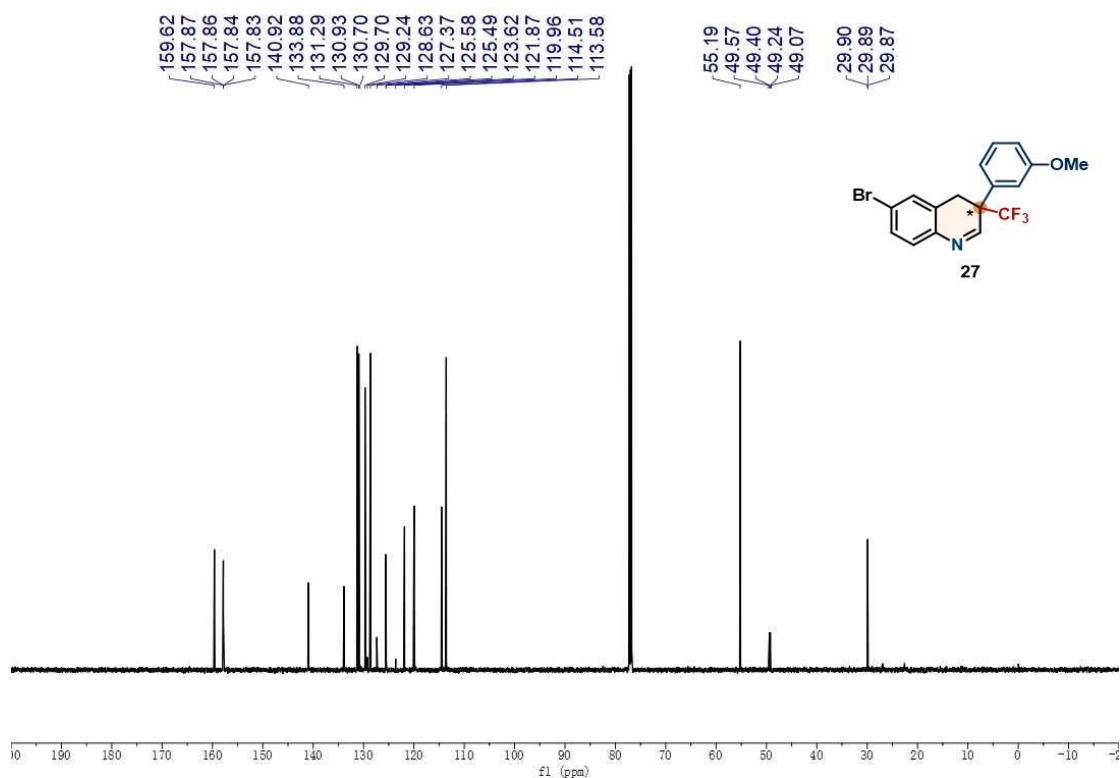
Supplementary Fig. S85. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 26



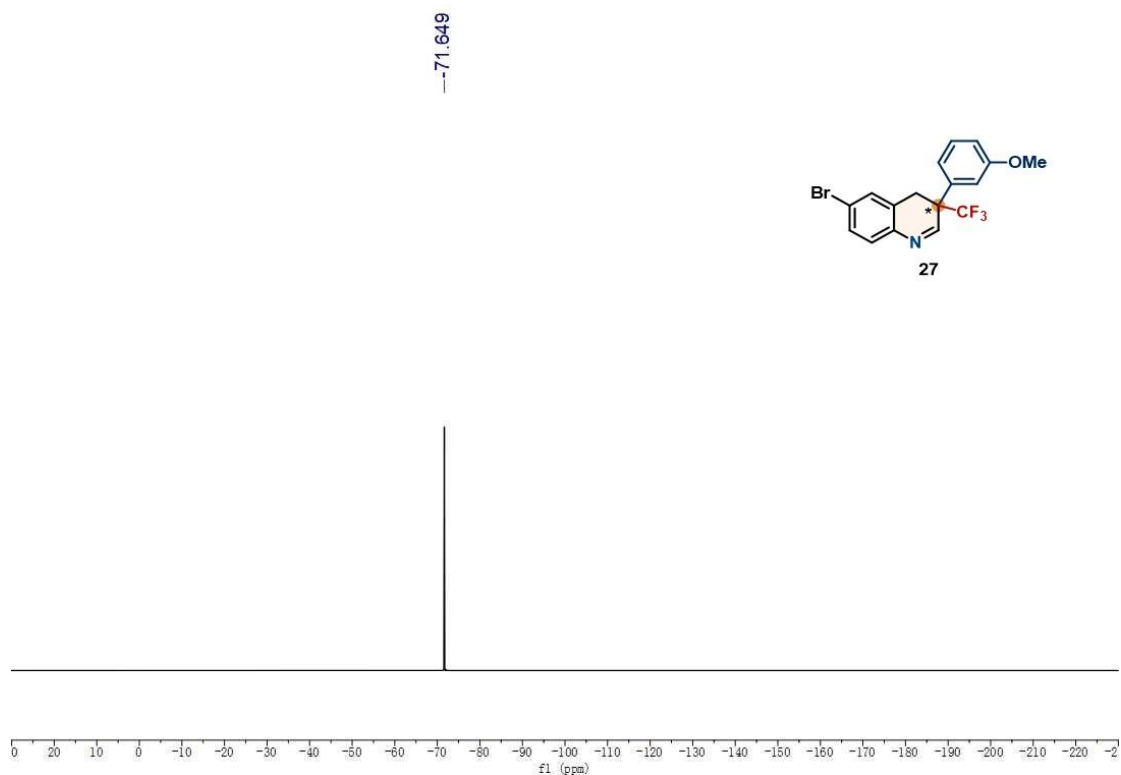
Supplementary Fig. S86. ¹⁹F NMR (470 MHz, CDCl₃) Spectrum of 26



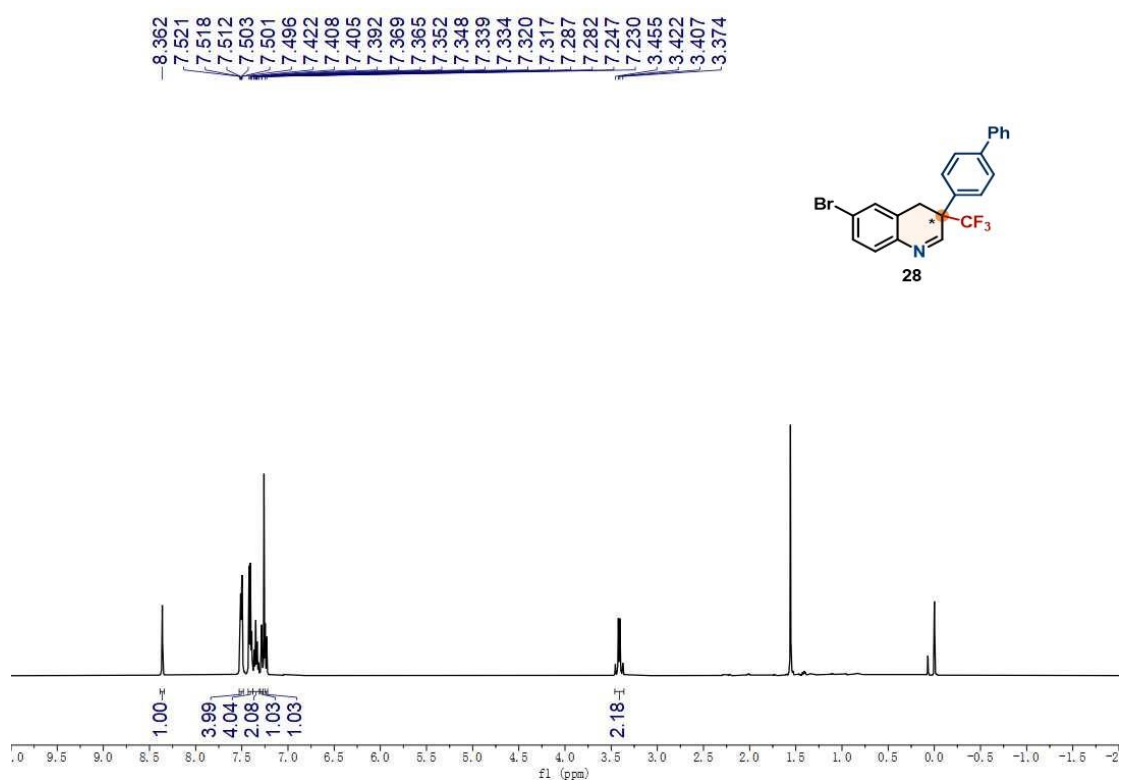
Supplementary Fig. S87. ¹H NMR (500 MHz, CDCl₃) Spectrum of 27



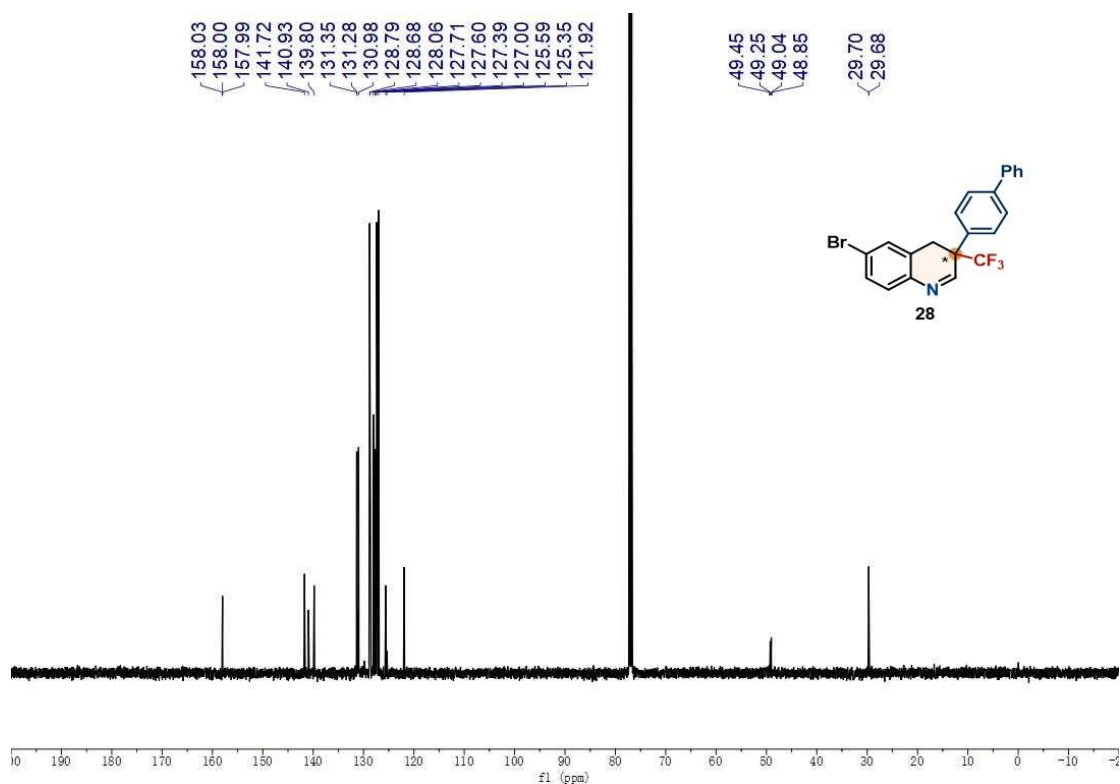
Supplementary Fig. S88. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 27



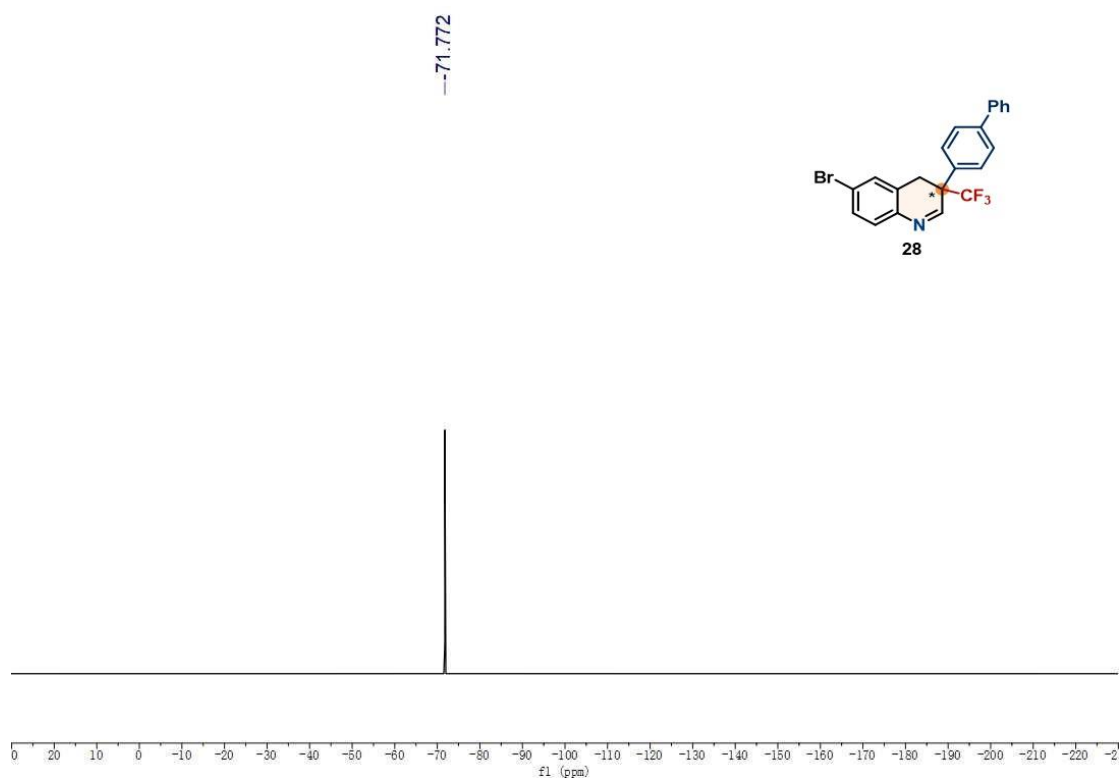
Supplementary Fig. S89. ^{19}F NMR (564 MHz, CDCl_3) Spectrum of 27



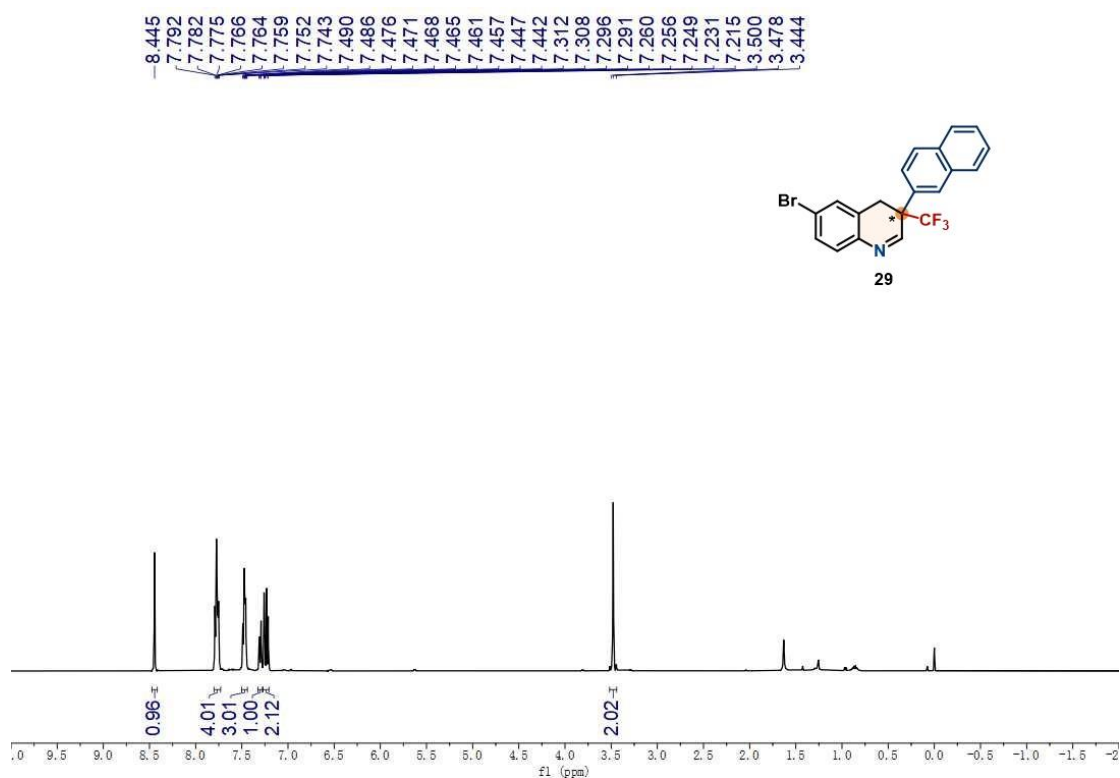
Supplementary Fig. S90. ^1H NMR (500 MHz, CDCl_3) Spectrum of 28



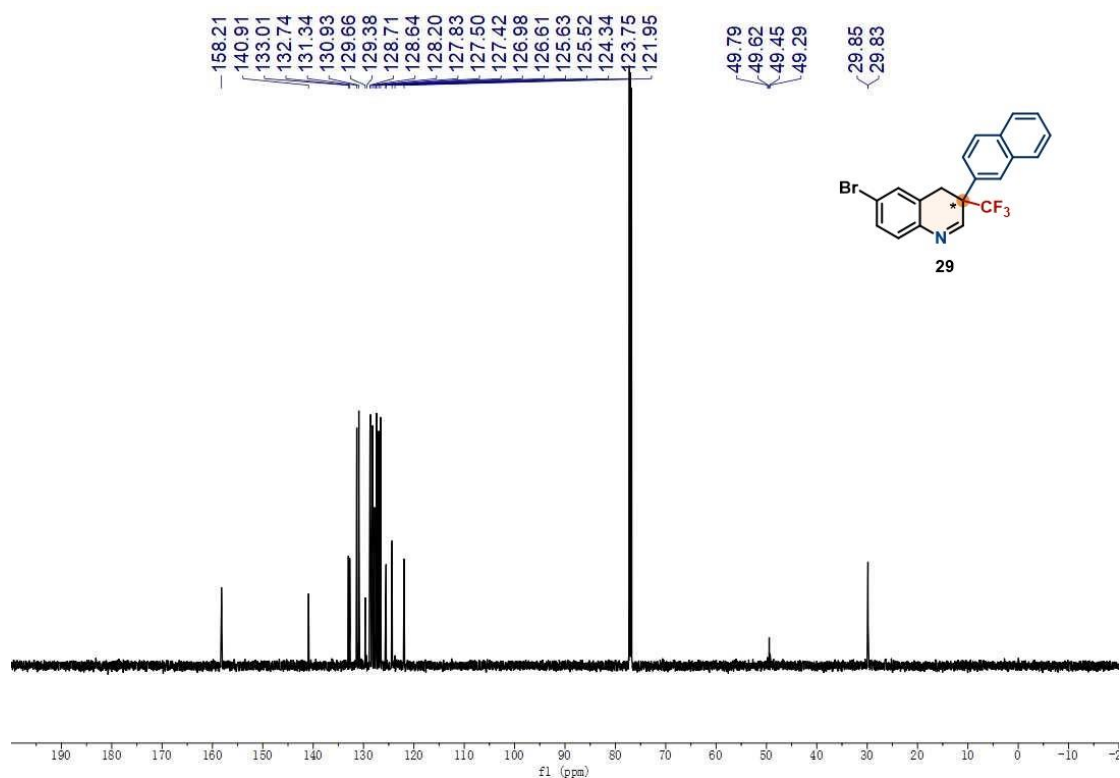
Supplementary Fig. S91. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 28



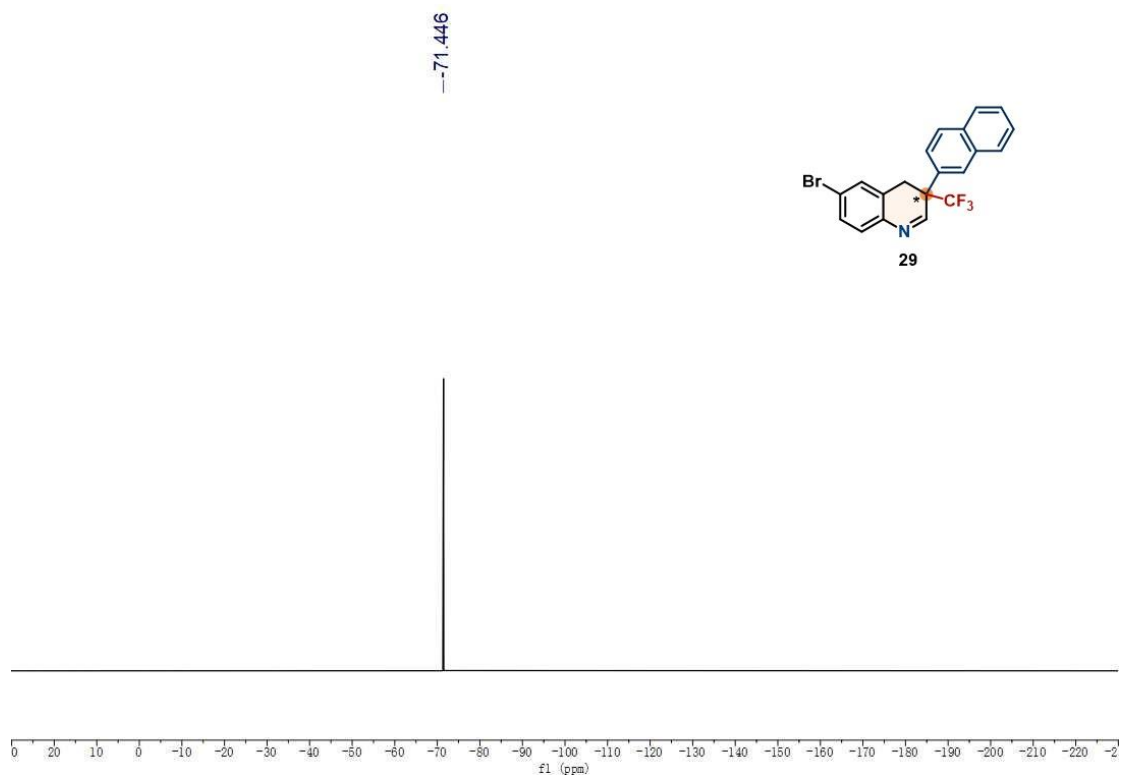
Supplementary Fig. S92. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 28



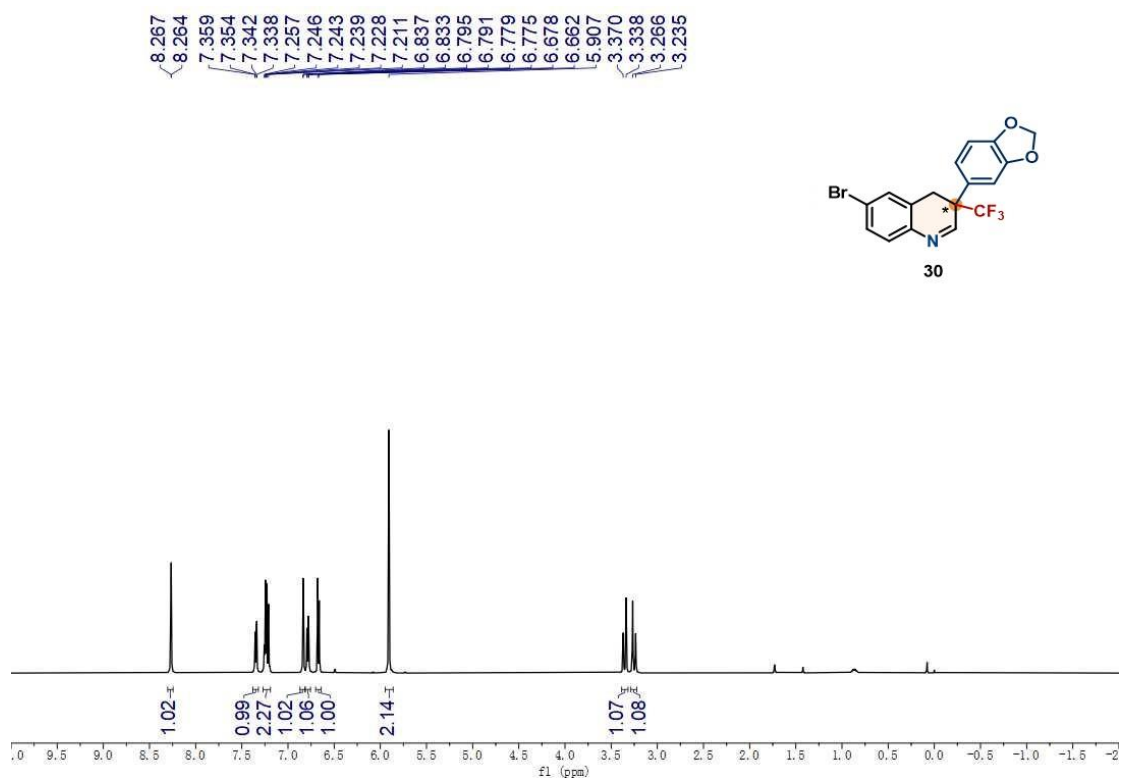
Supplementary Fig. S93. ¹H NMR (500 MHz, CDCl₃) Spectrum of 29



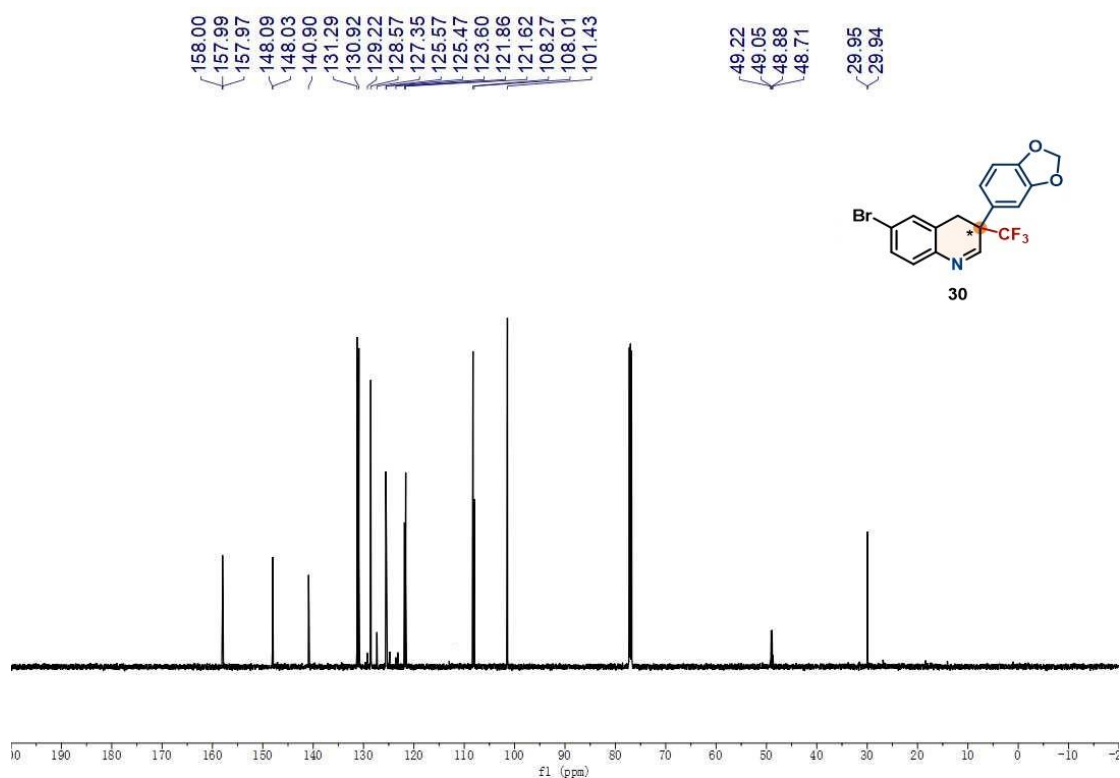
Supplementary Fig. S94. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 29



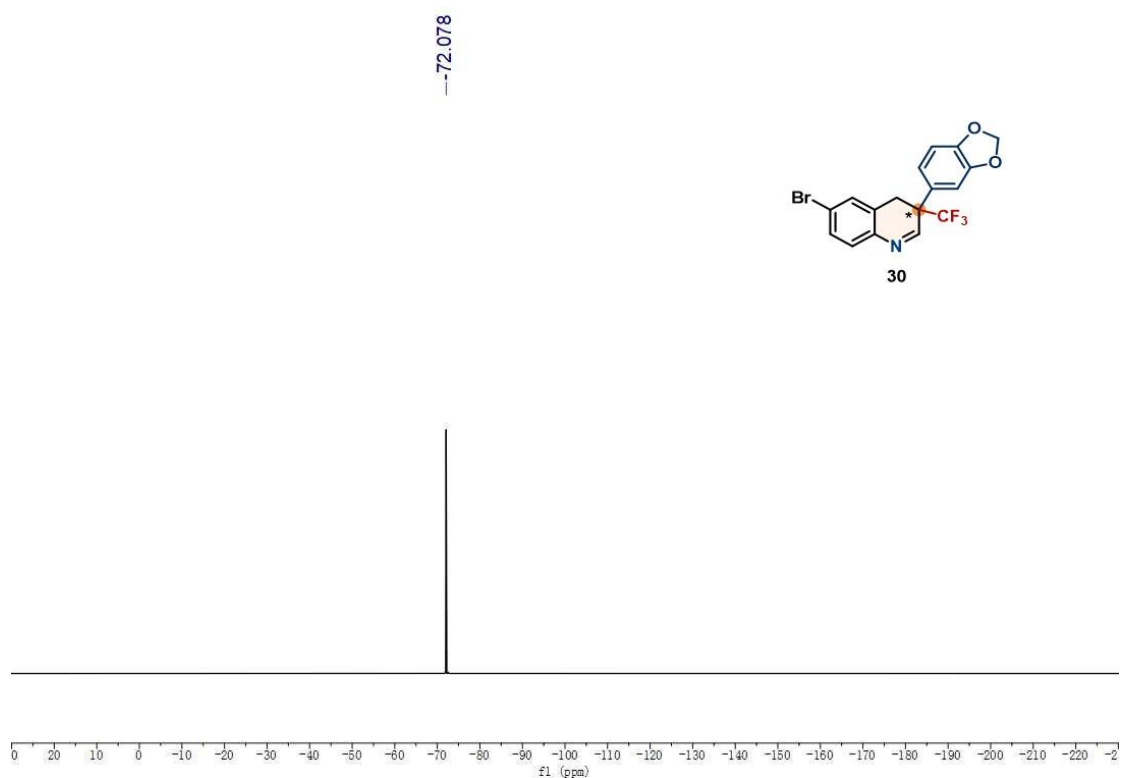
Supplementary Fig. S95. ^{19}F NMR (564 MHz, CDCl_3) Spectrum of 29



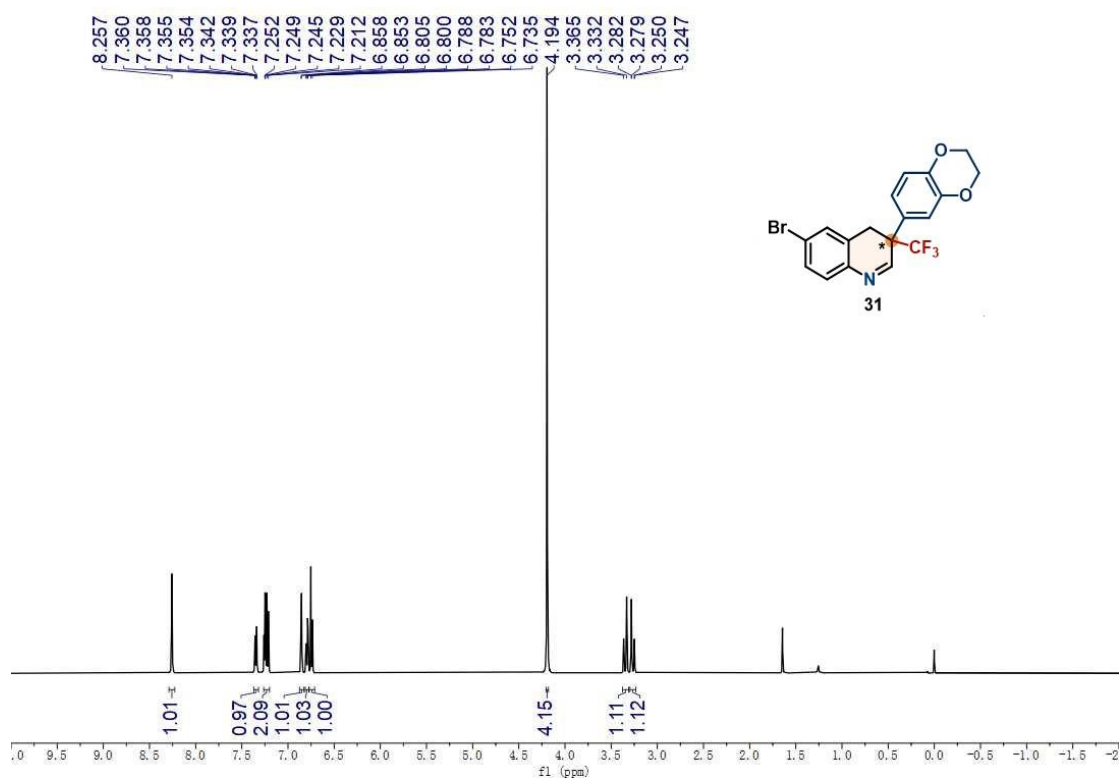
Supplementary Fig. S96. ^1H NMR (500 MHz, CDCl_3) Spectrum of 30



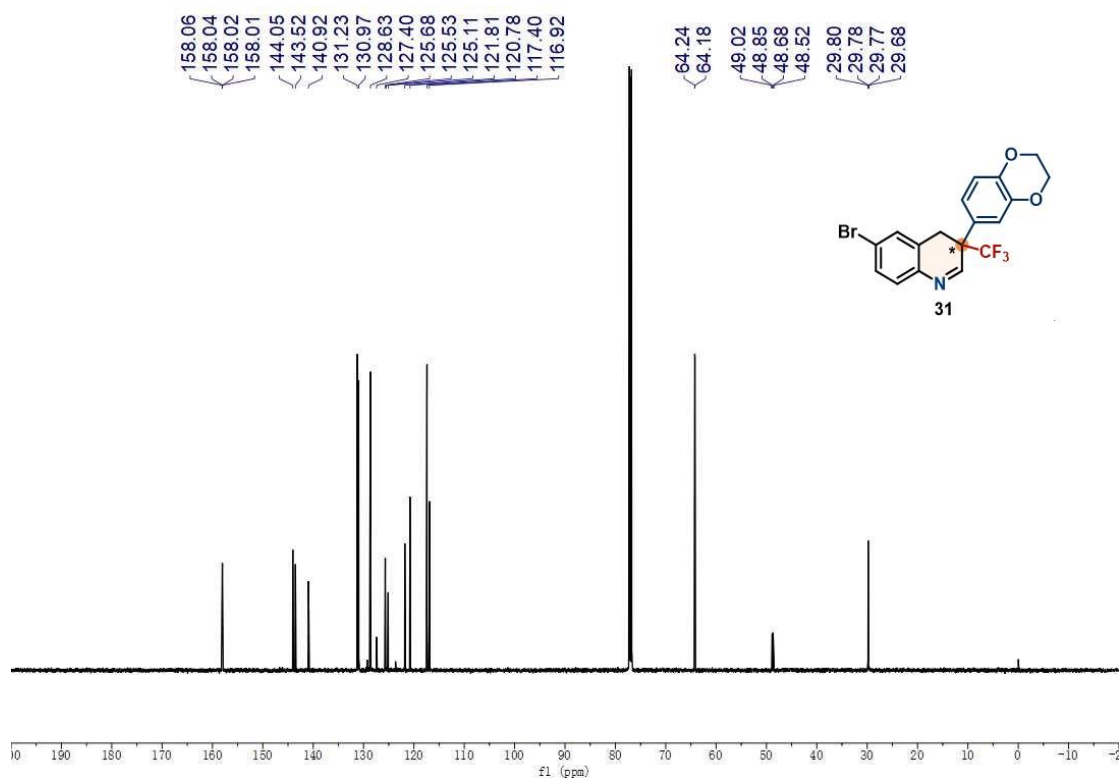
Supplementary Fig. S97. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 30



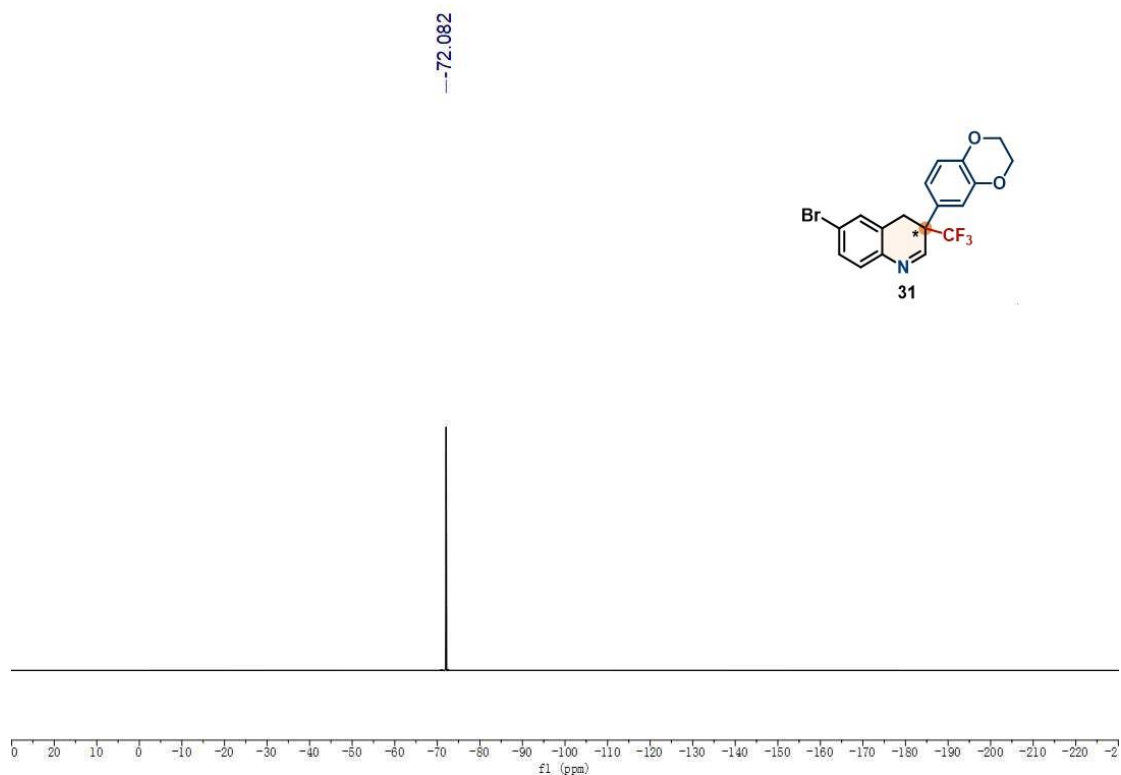
Supplementary Fig. S98. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 30



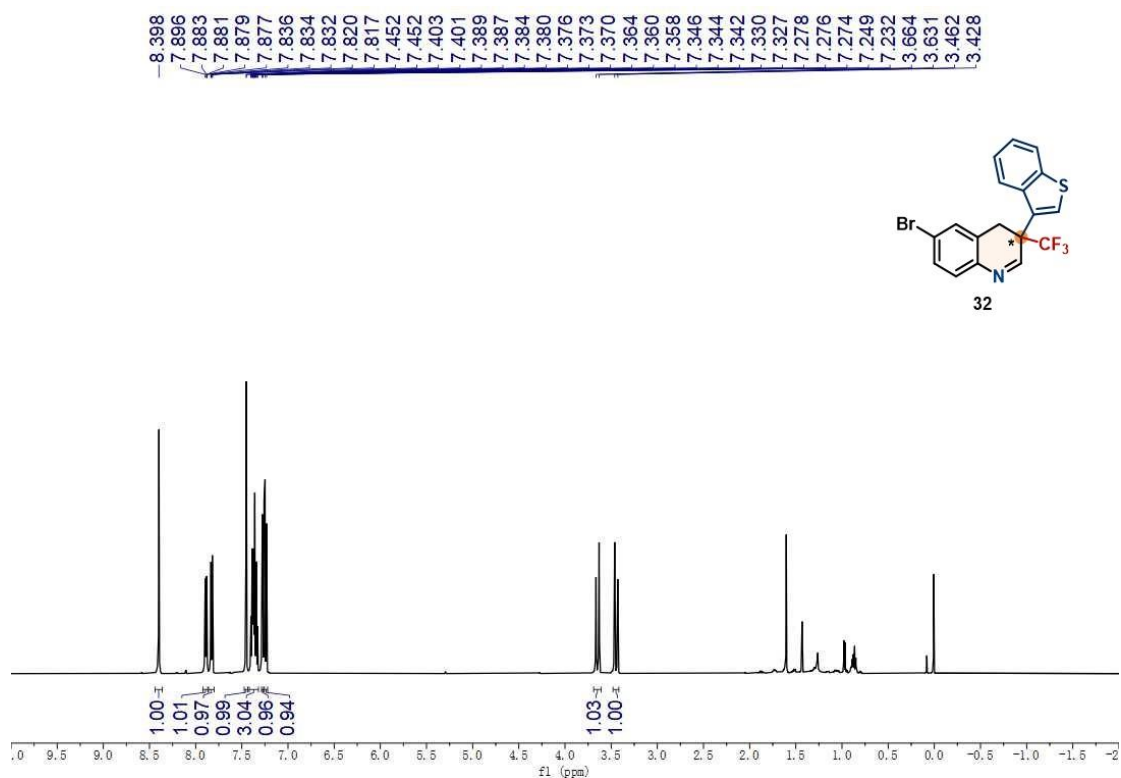
Supplementary Fig. S99. ¹H NMR (500 MHz, CDCl₃) Spectrum of 31



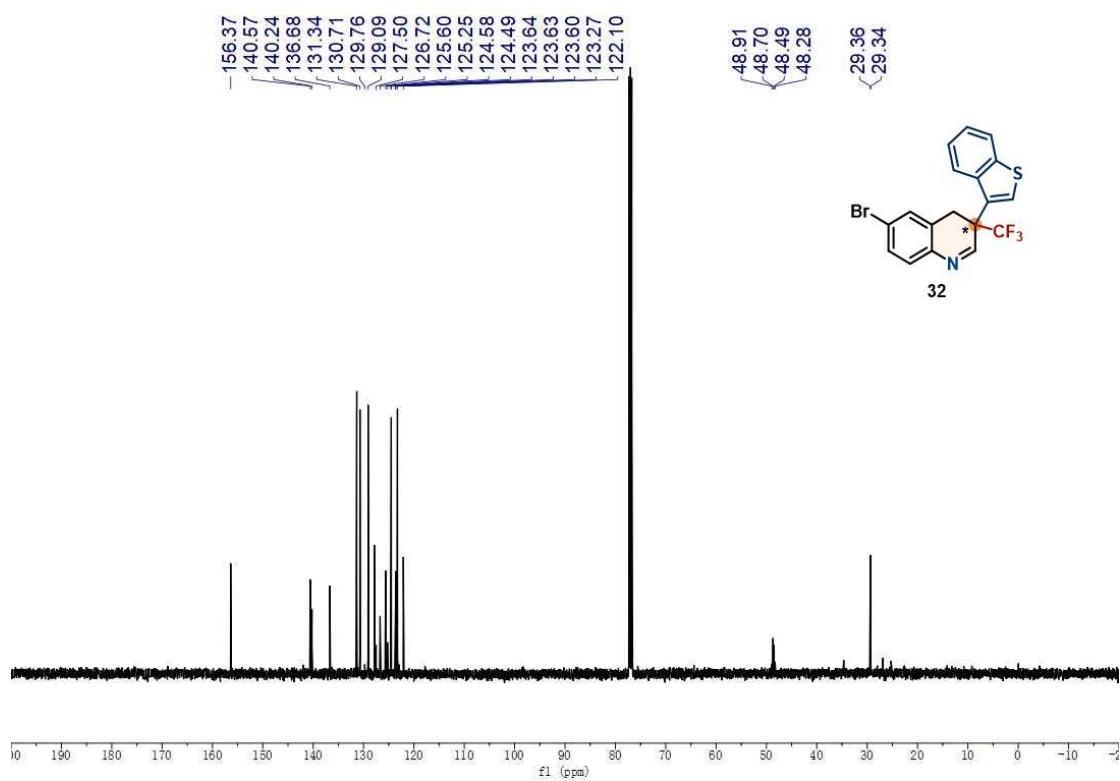
Supplementary Fig. S100. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 31



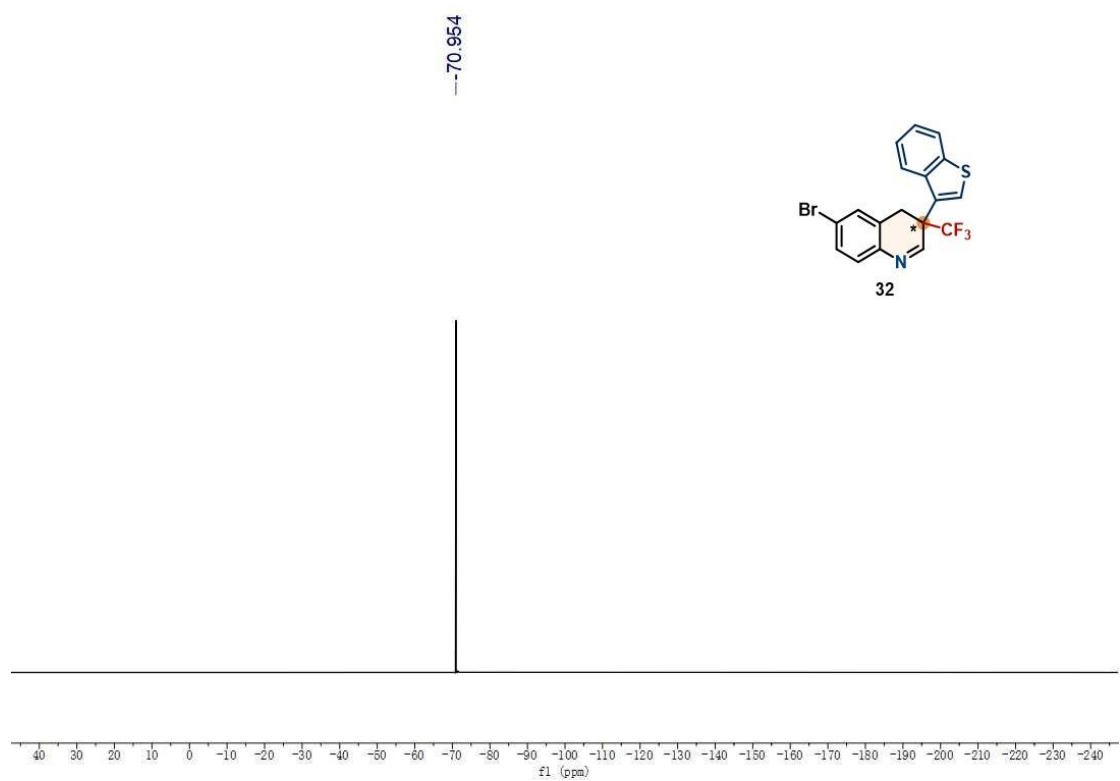
Supplementary Fig. S101. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 31



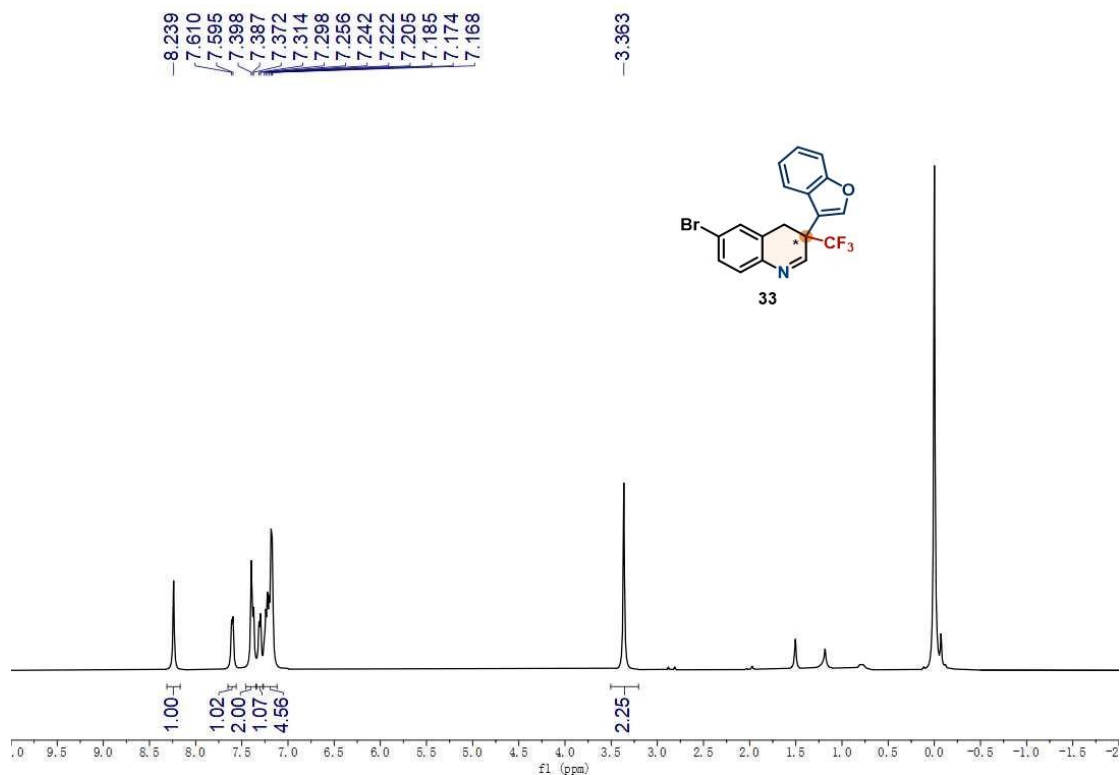
Supplementary Fig. S102. ¹H NMR (500 MHz, CDCl₃) Spectrum of 32



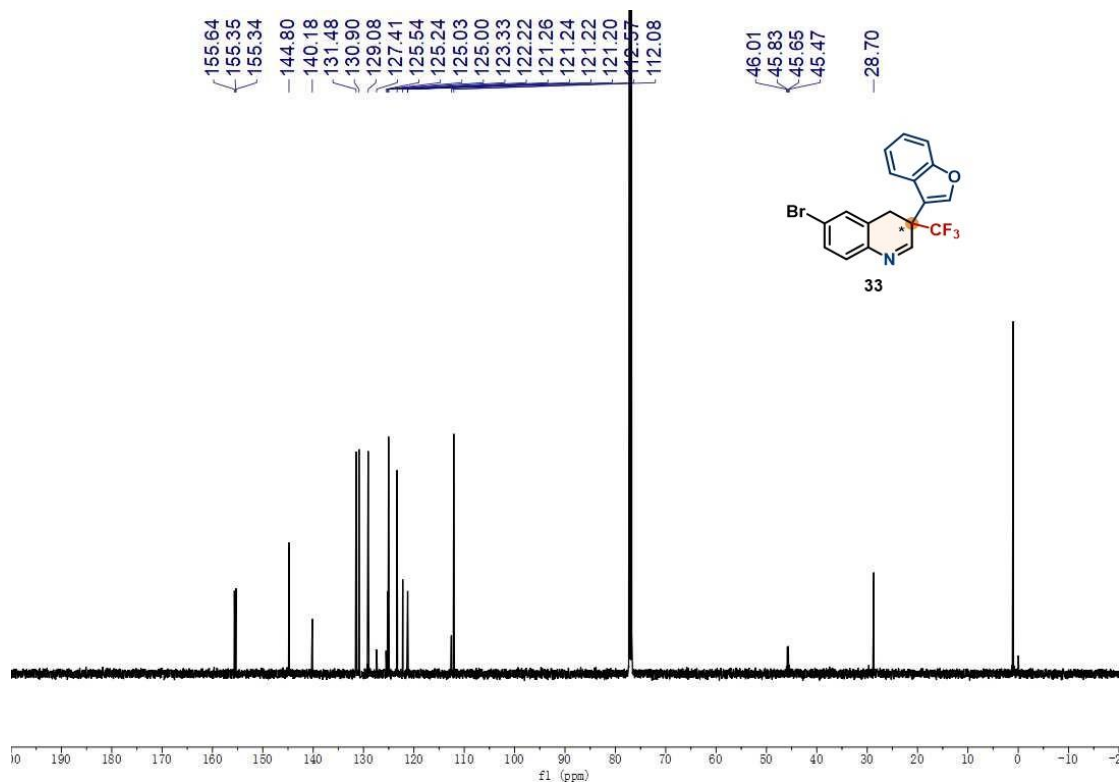
Supplementary Fig. S103. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 32



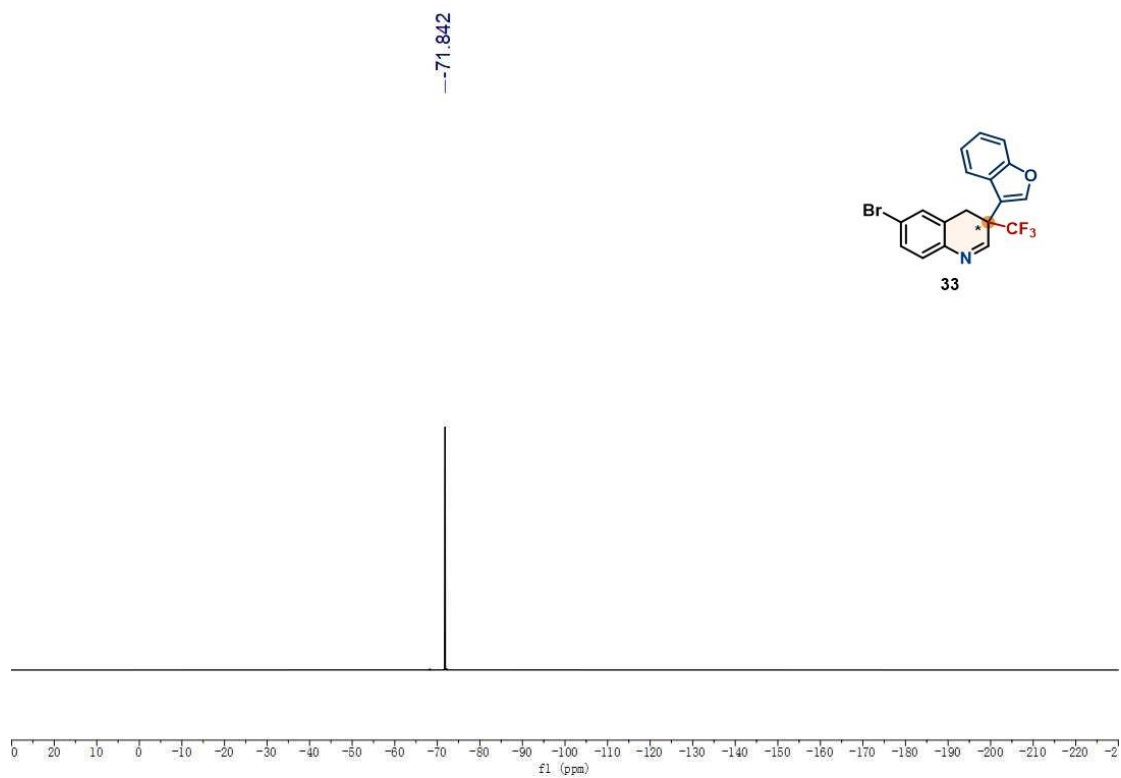
Supplementary Fig. S104. ¹⁹F NMR (470 MHz, CDCl₃) Spectrum of 32



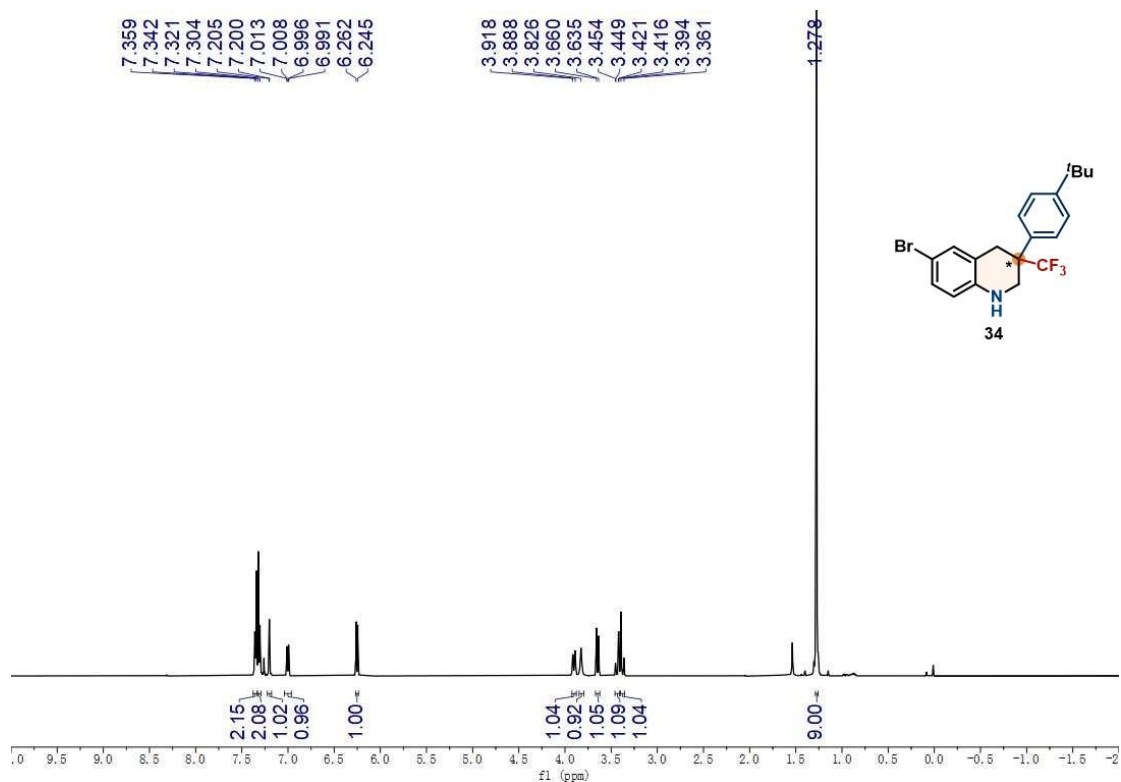
Supplementary Fig. S105. ¹H NMR (500 MHz, CDCl₃) Spectrum of 33



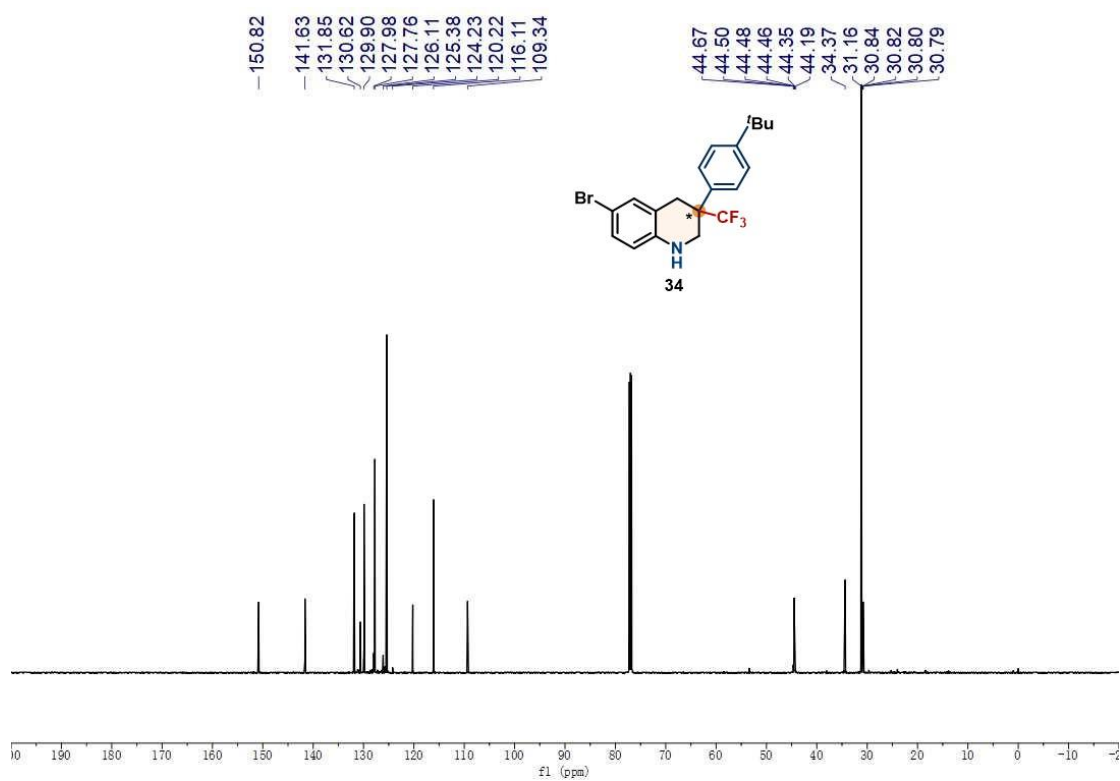
Supplementary Fig. S106. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 33



Supplementary Fig. S107. ^{19}F NMR (564 MHz, CDCl_3) Spectrum of 33



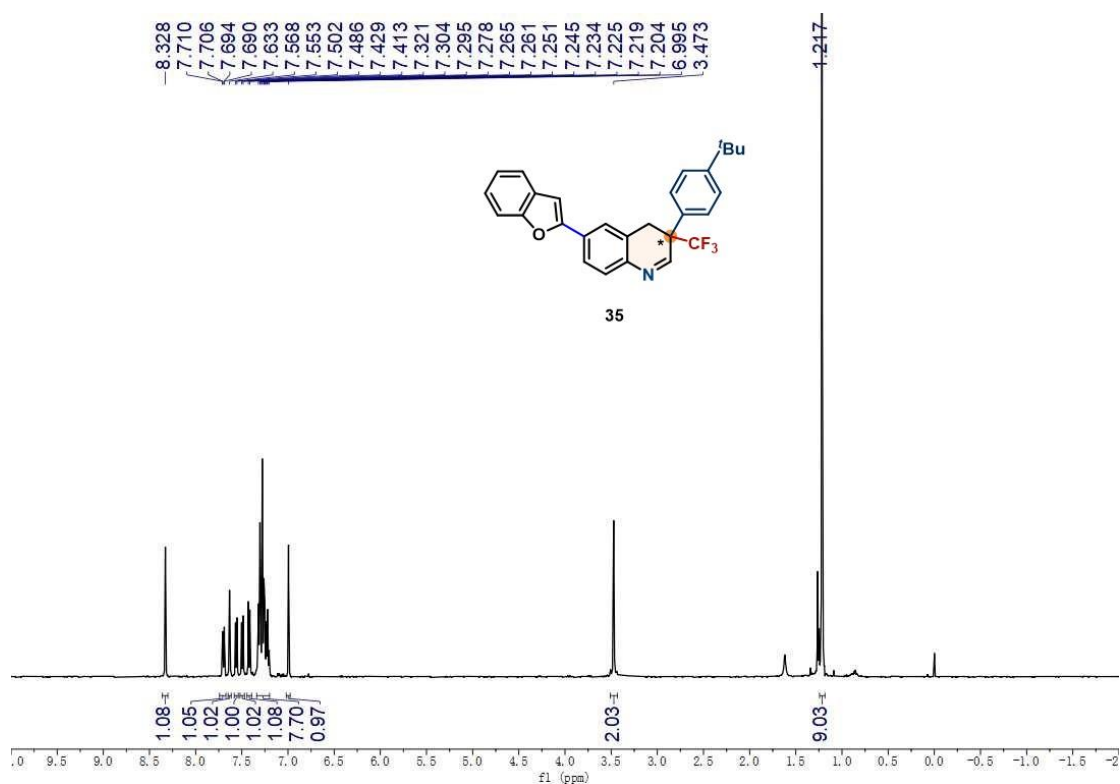
Supplementary Fig. S108. ^1H NMR (500 MHz, CDCl_3) Spectrum of 34



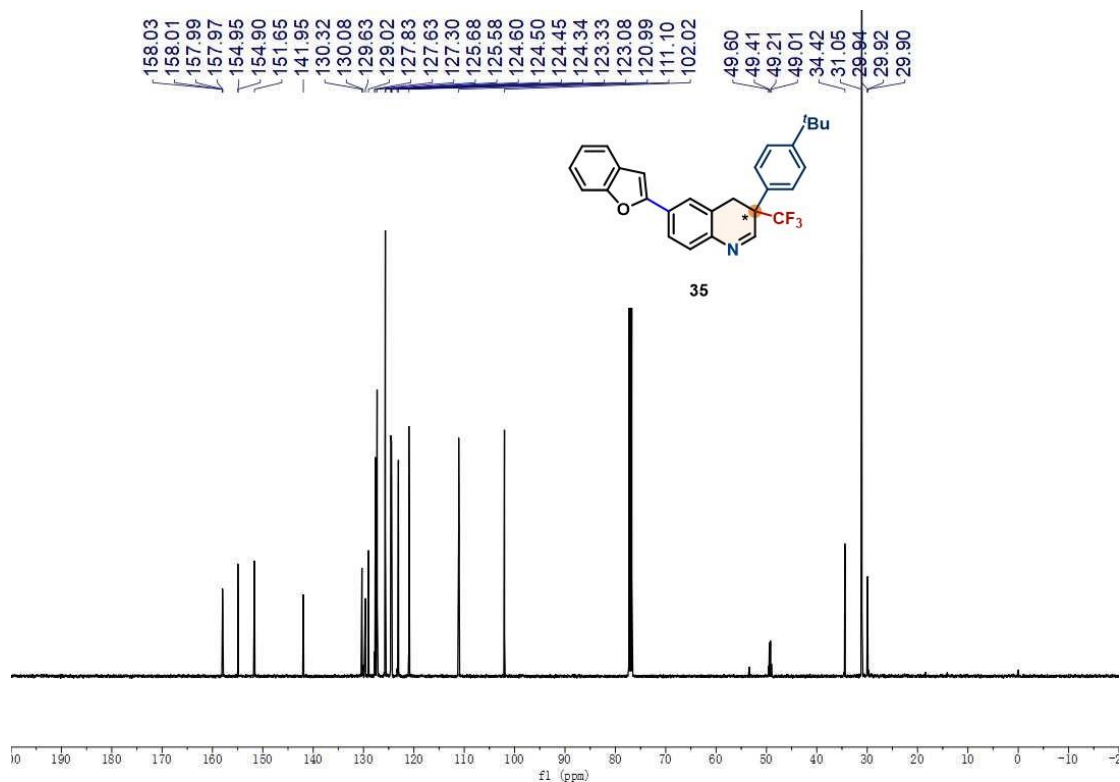
Supplementary Fig. S109. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 34



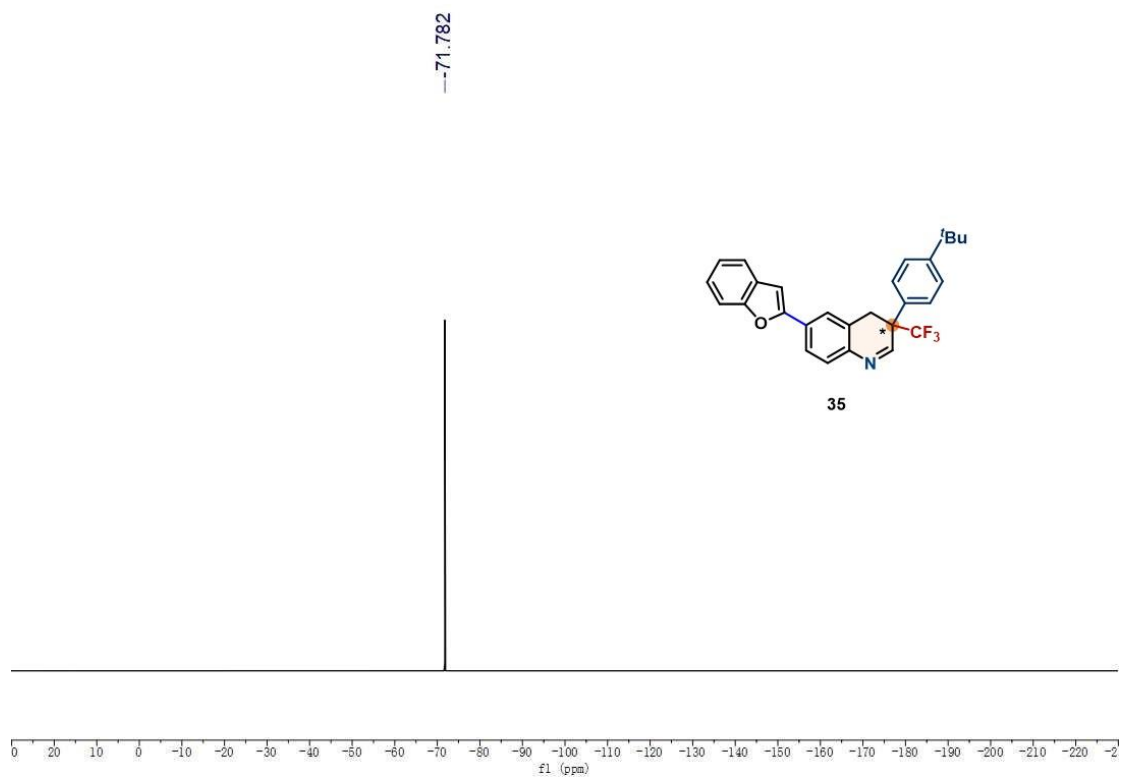
Supplementary Fig. S110. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 34



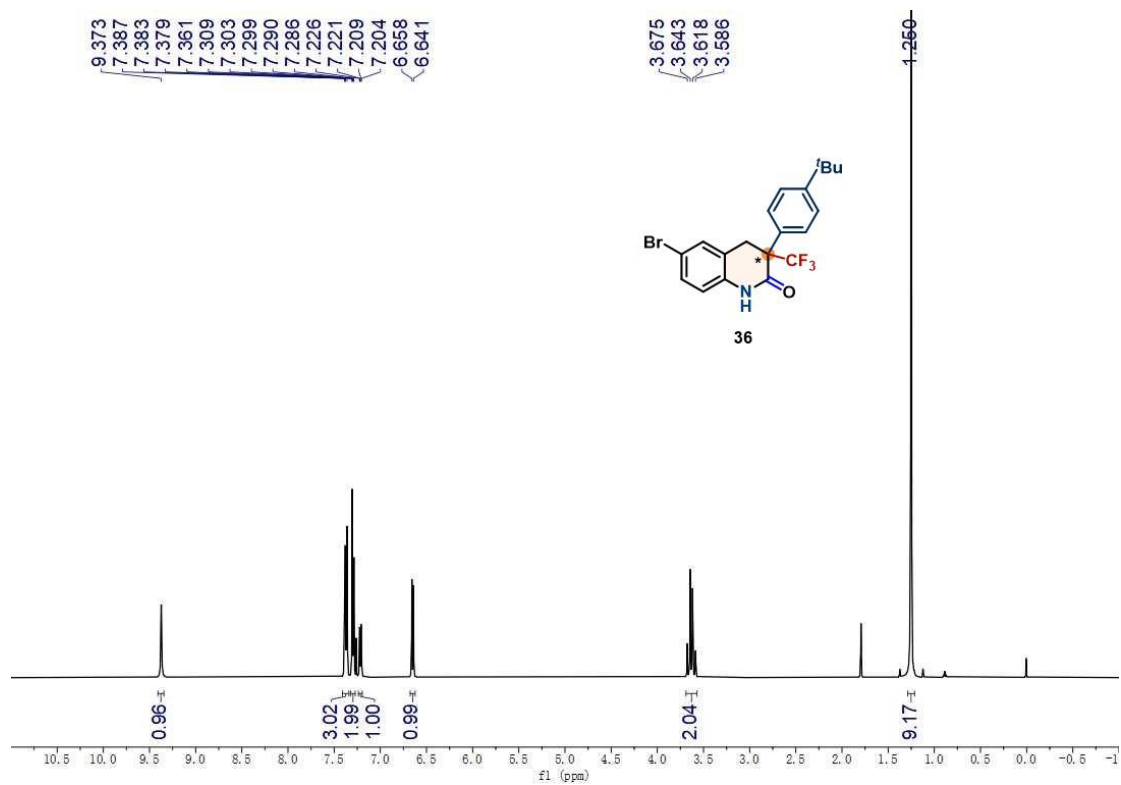
Supplementary Fig. S111. ¹H NMR (500 MHz, CDCl₃) Spectrum of 35



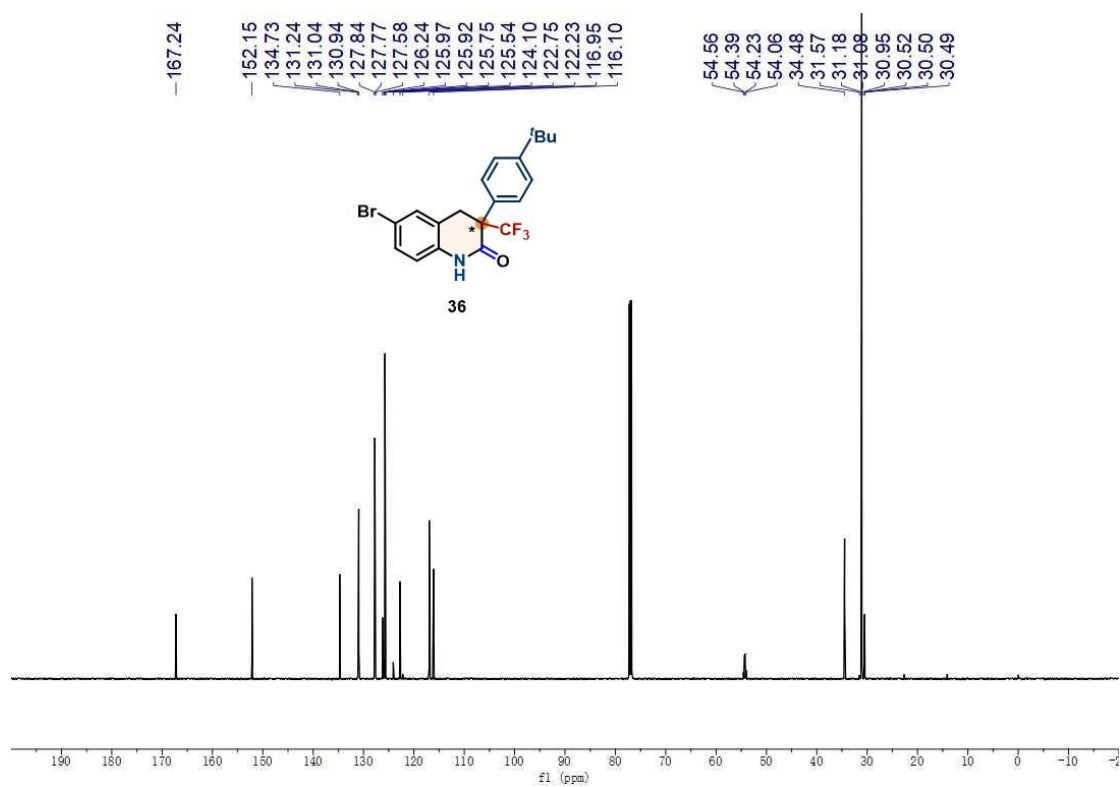
Supplementary Fig. S112. ¹³C NMR (125 MHz, CDCl₃) Spectrum of 35



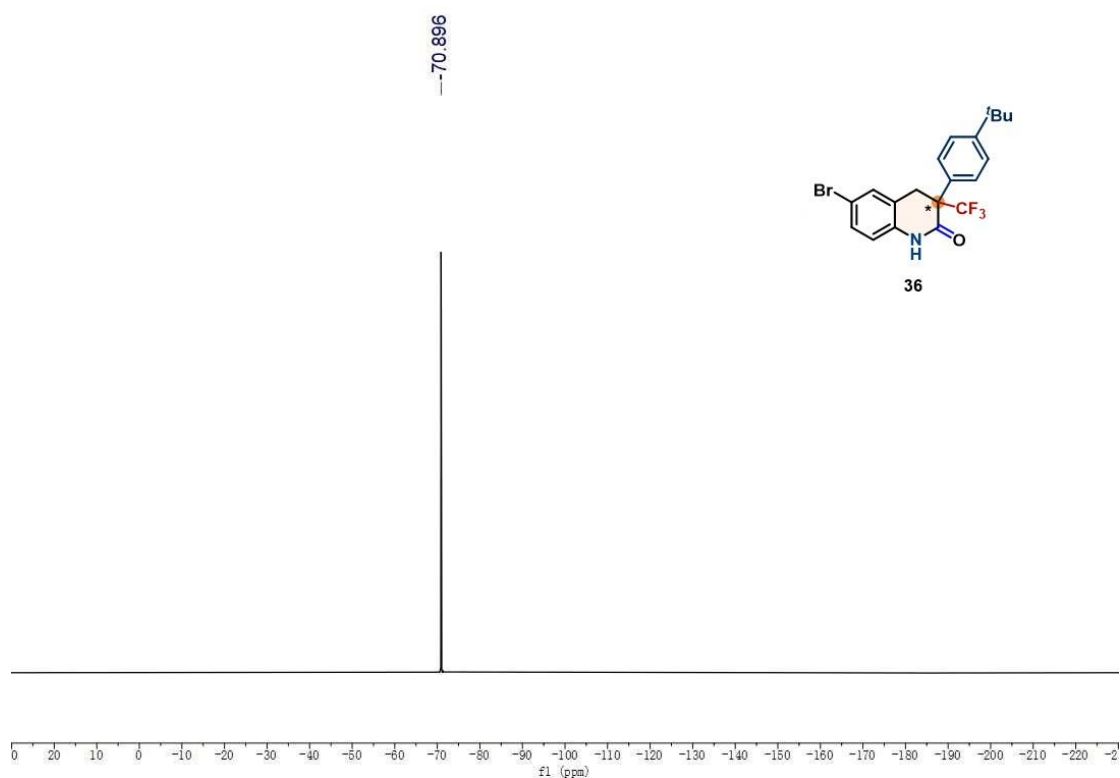
Supplementary Fig. S113. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 35



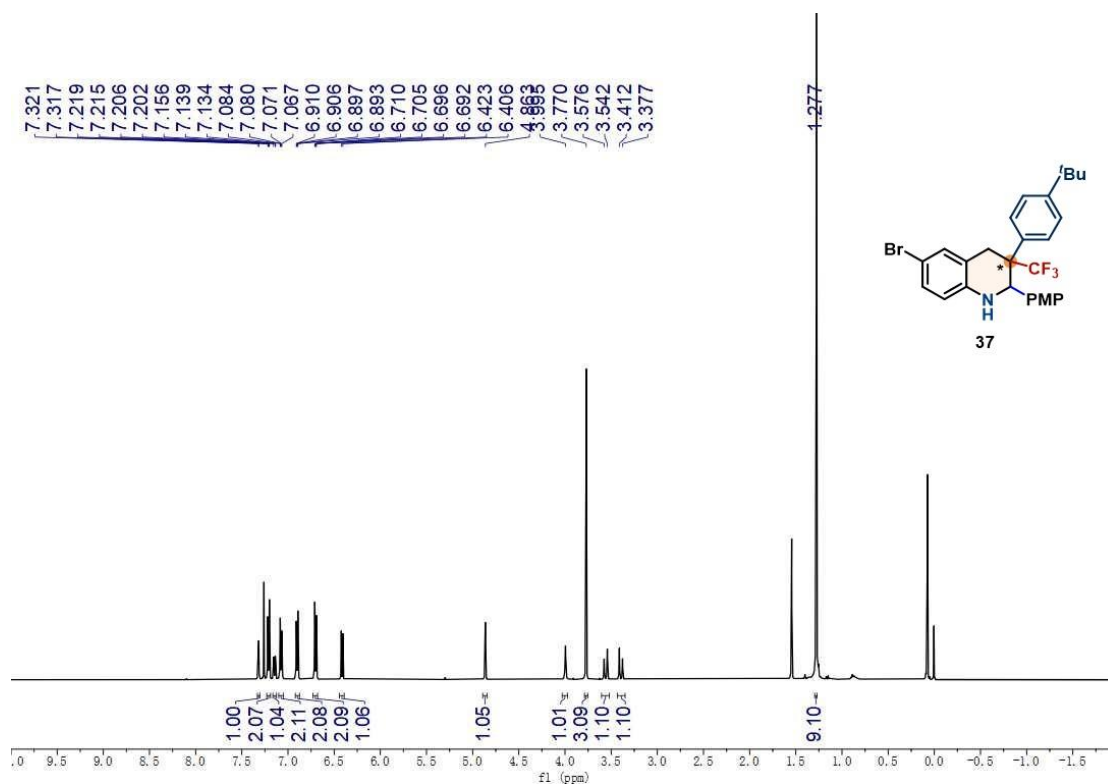
Supplementary Fig. S114. ¹H NMR (500 MHz, CDCl₃) Spectrum of 36



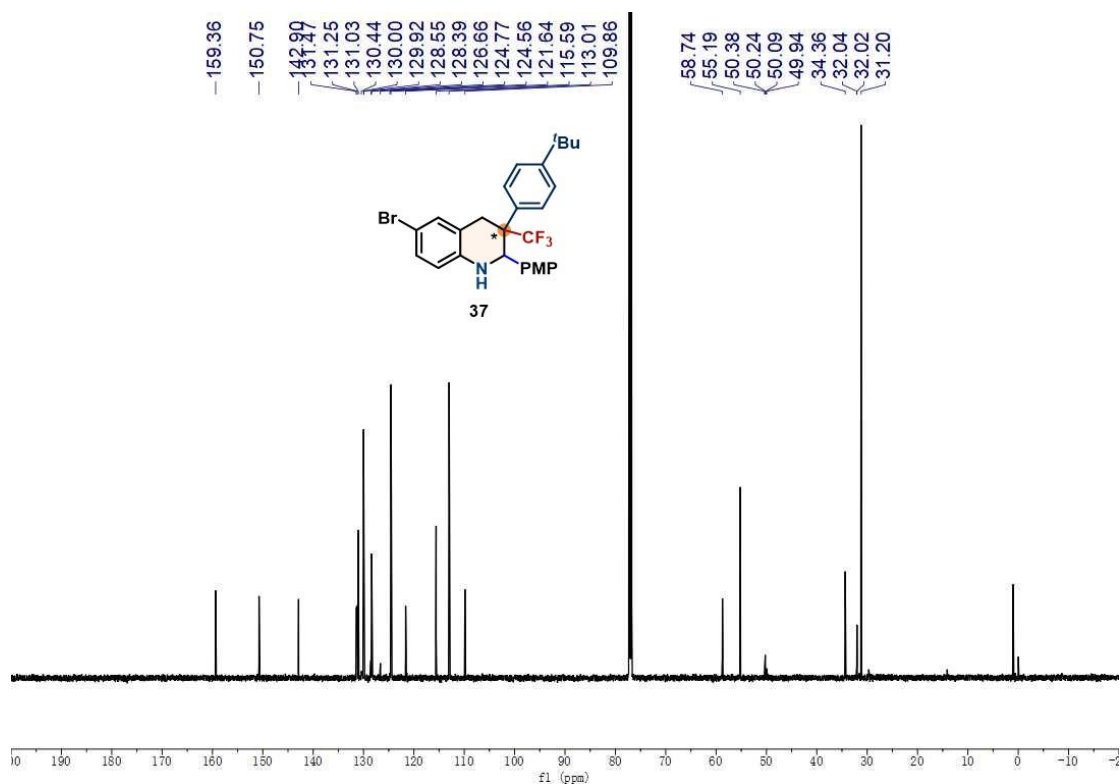
Supplementary Fig. S115. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 36



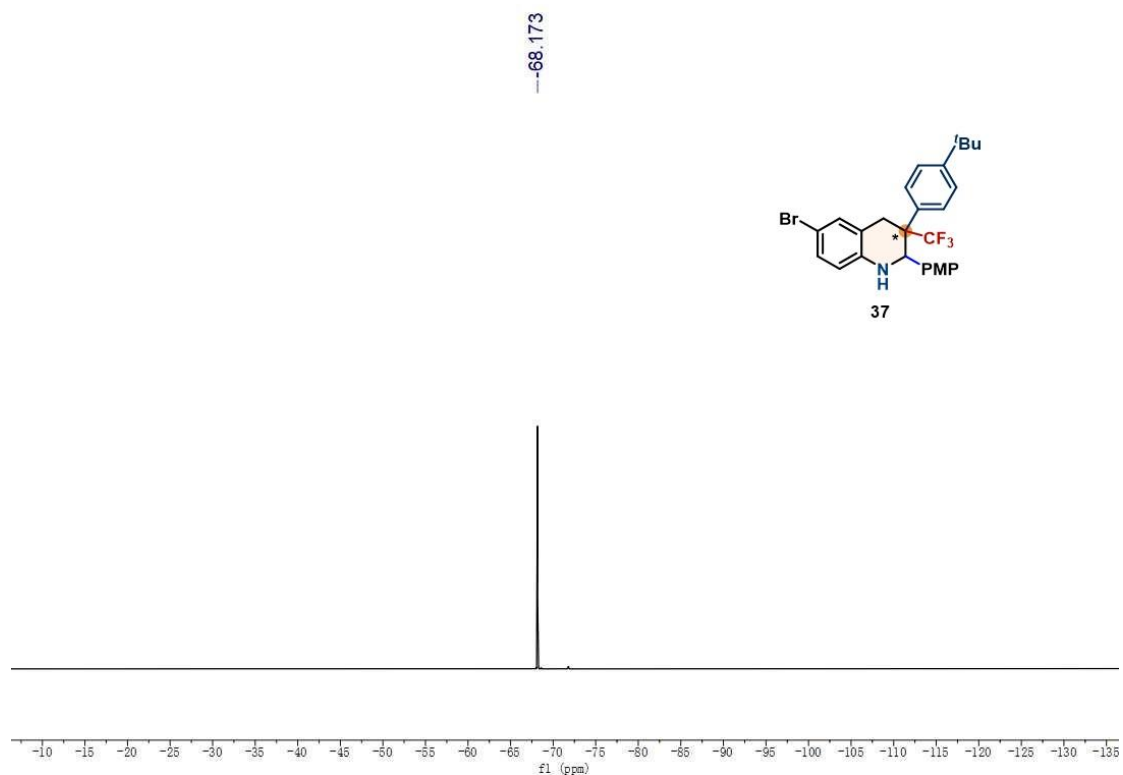
Supplementary Fig. S116. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 36



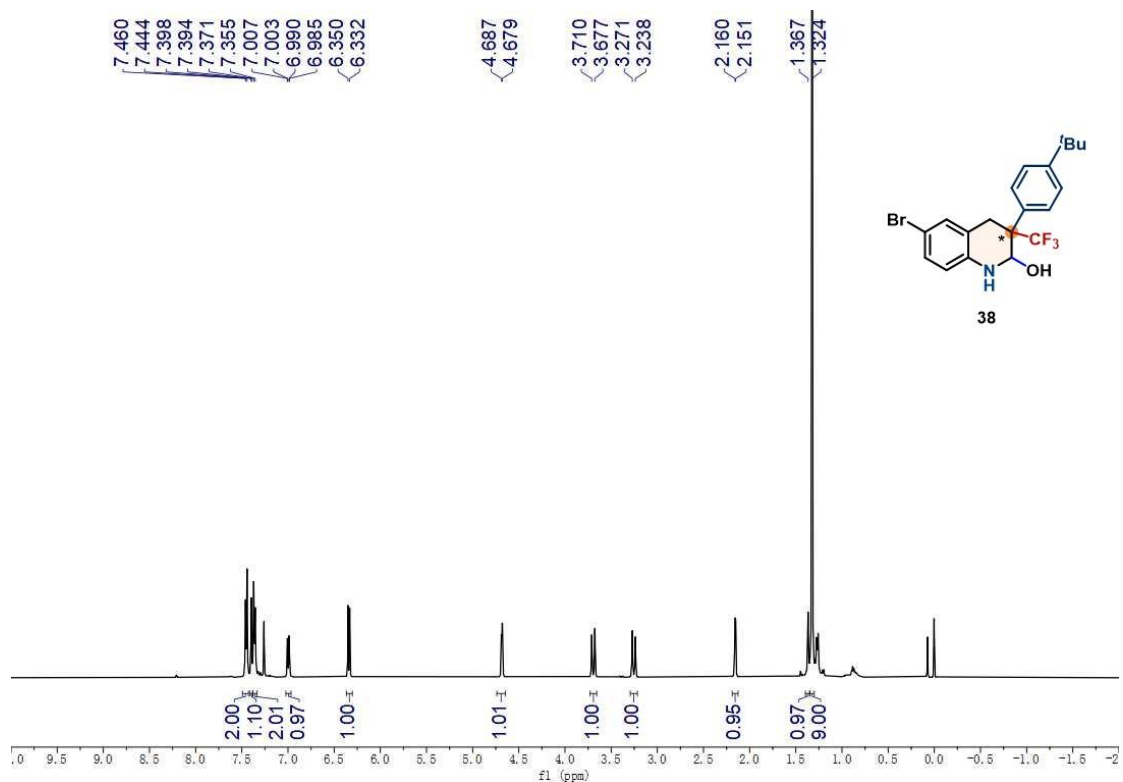
Supplementary Fig. S117. ¹H NMR (500 MHz, CDCl₃) Spectrum of 37



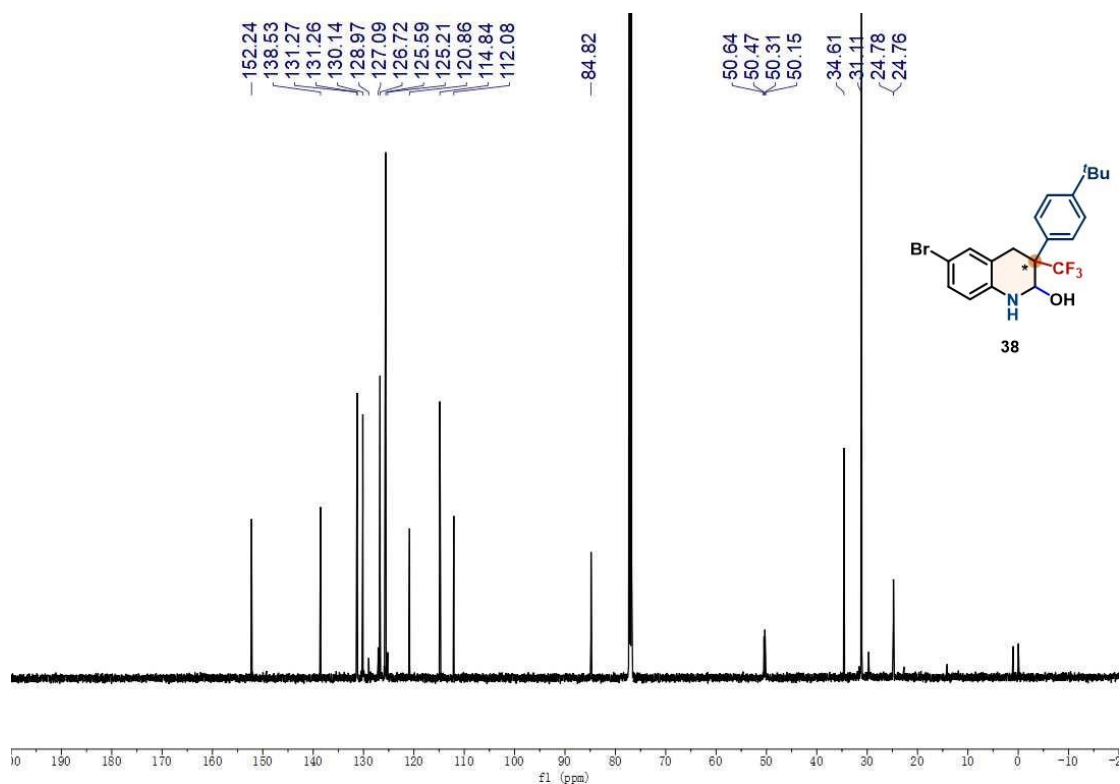
Supplementary Fig. S118. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 37



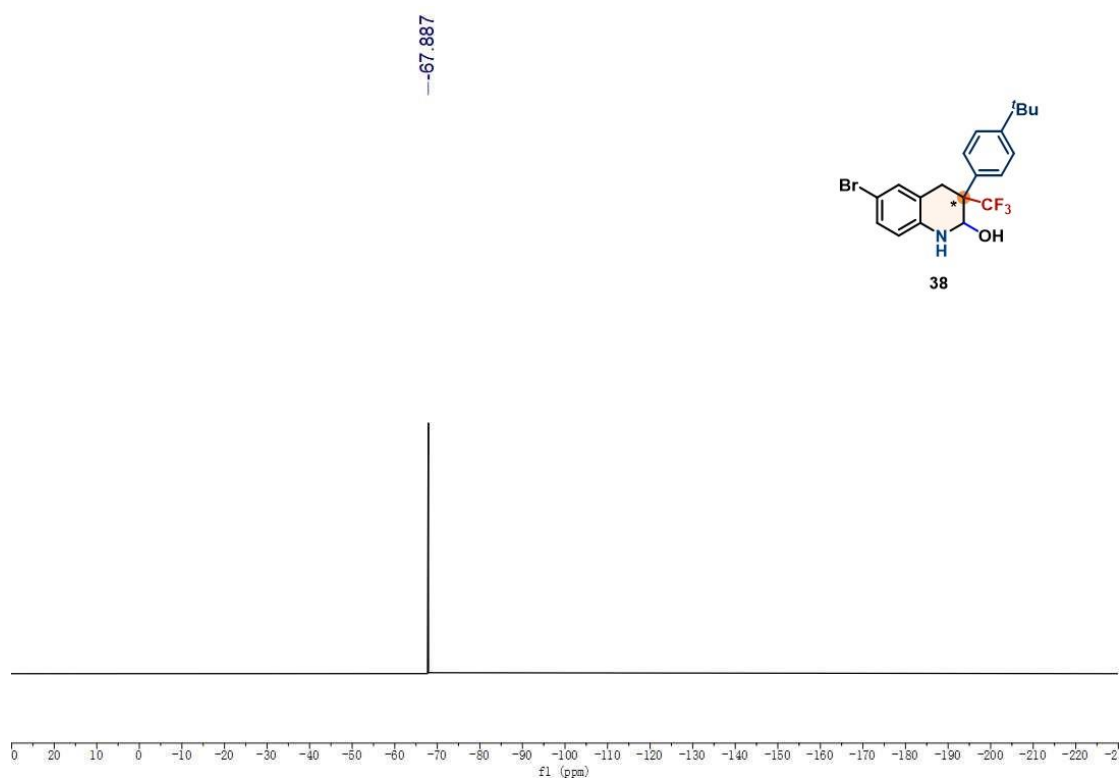
Supplementary Fig. S119. ^{19}F NMR (564 MHz, CDCl_3) Spectrum of 37



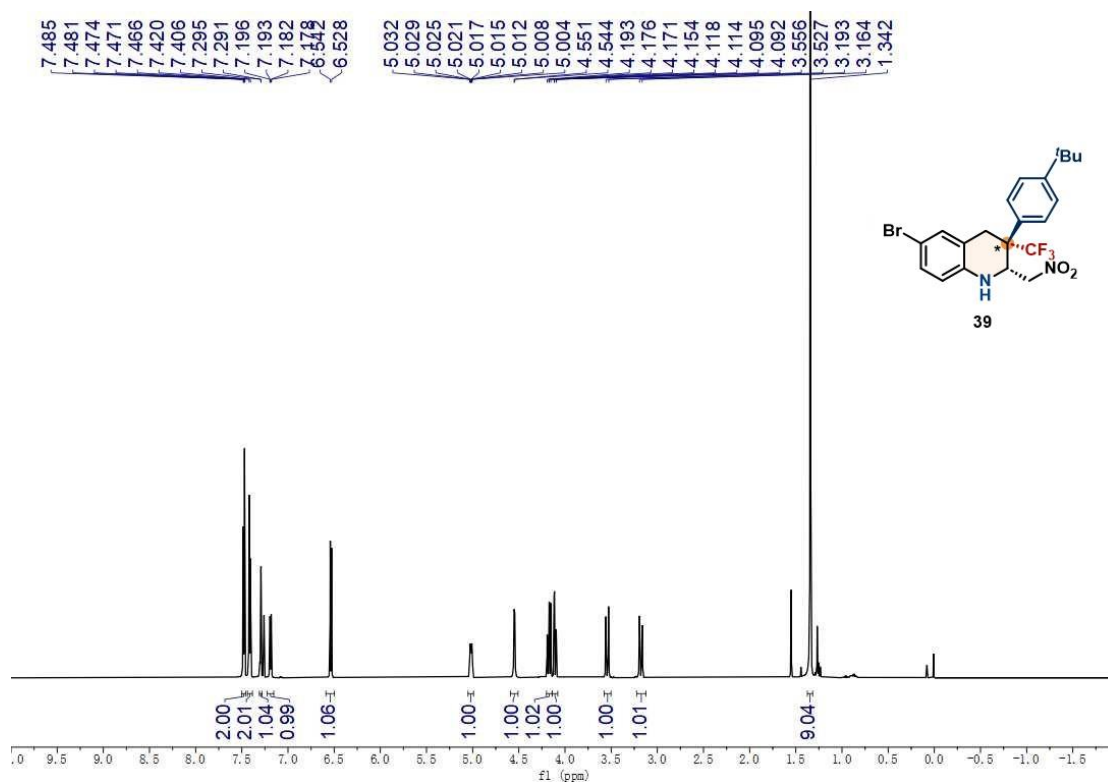
Supplementary Fig. S120. ^1H NMR (500 MHz, CDCl_3) Spectrum of 38



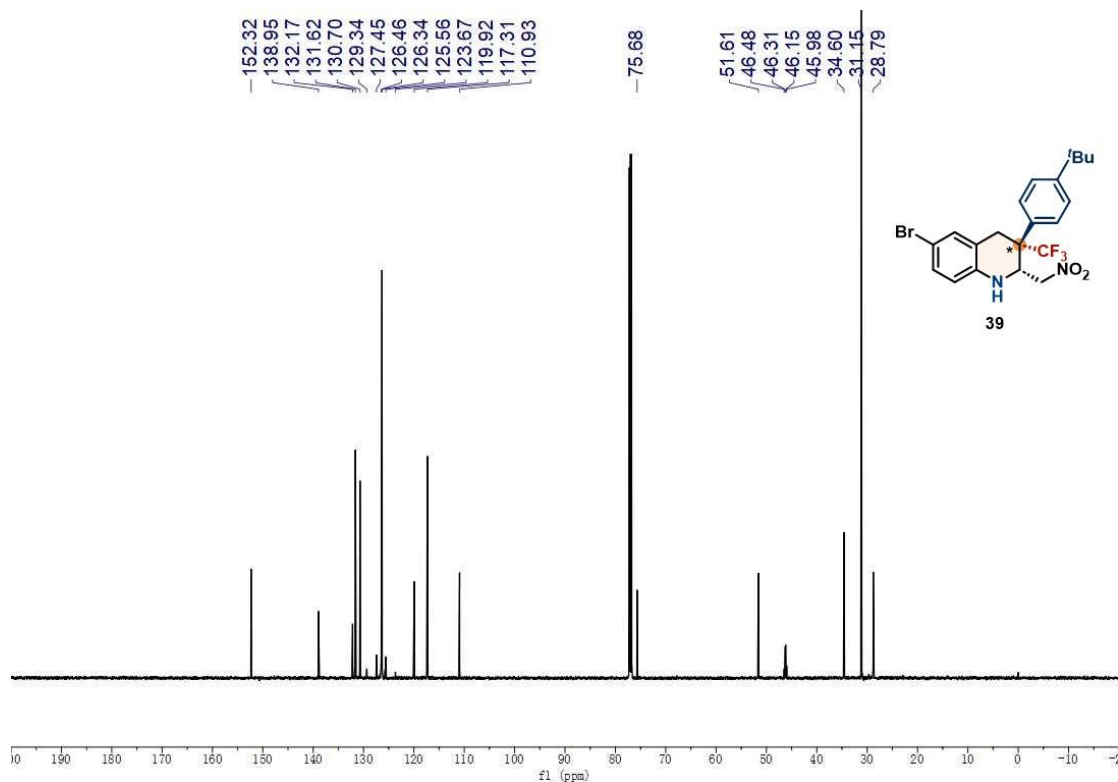
Supplementary Fig. S121. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 38



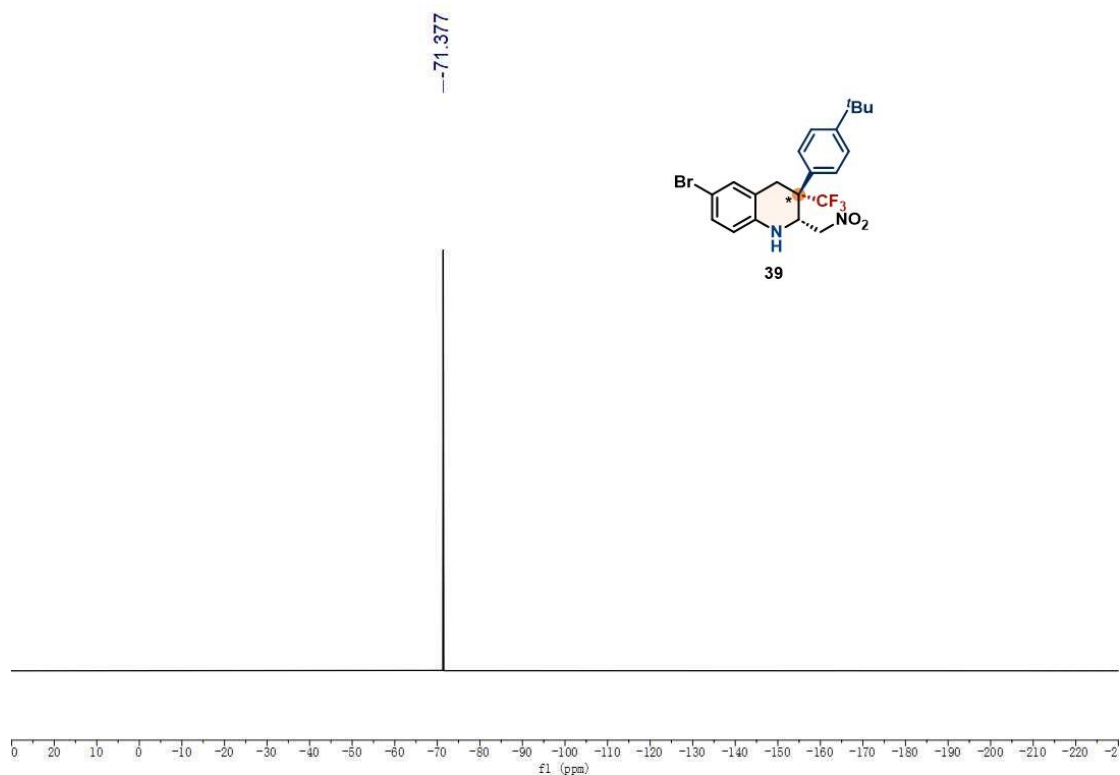
Supplementary Fig. S122. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 38



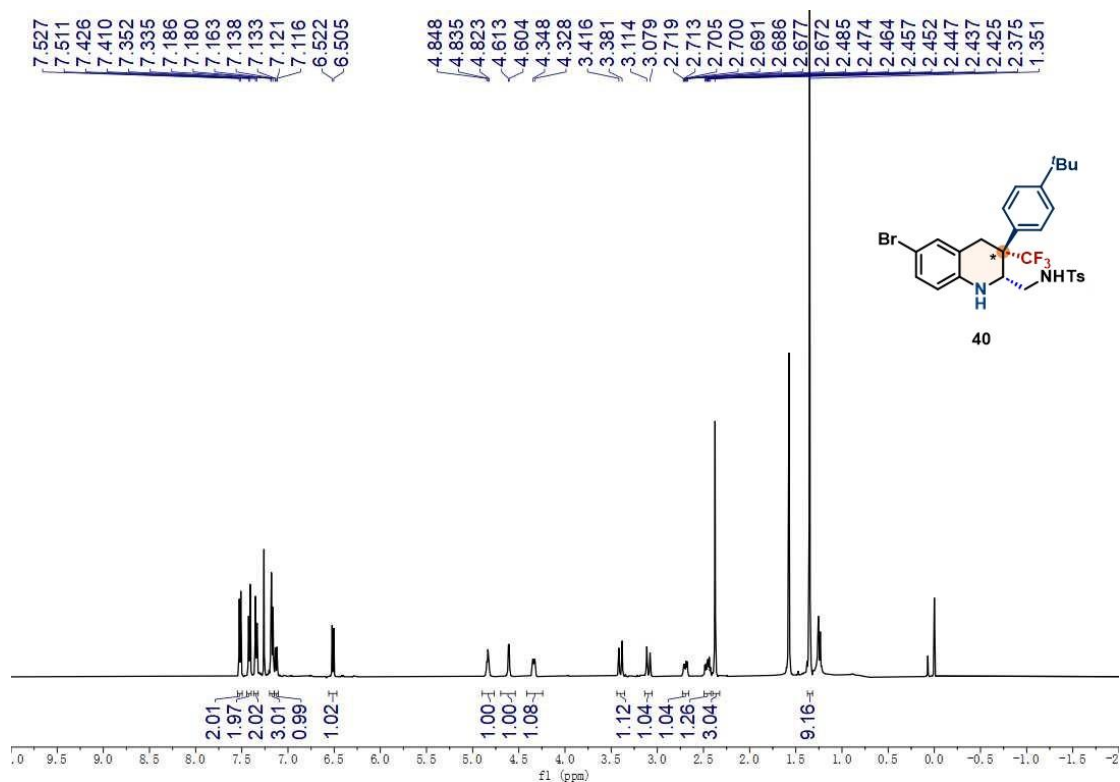
Supplementary Fig. S123. ¹H NMR (600 MHz, CDCl₃) Spectrum of (2S,3R)-39



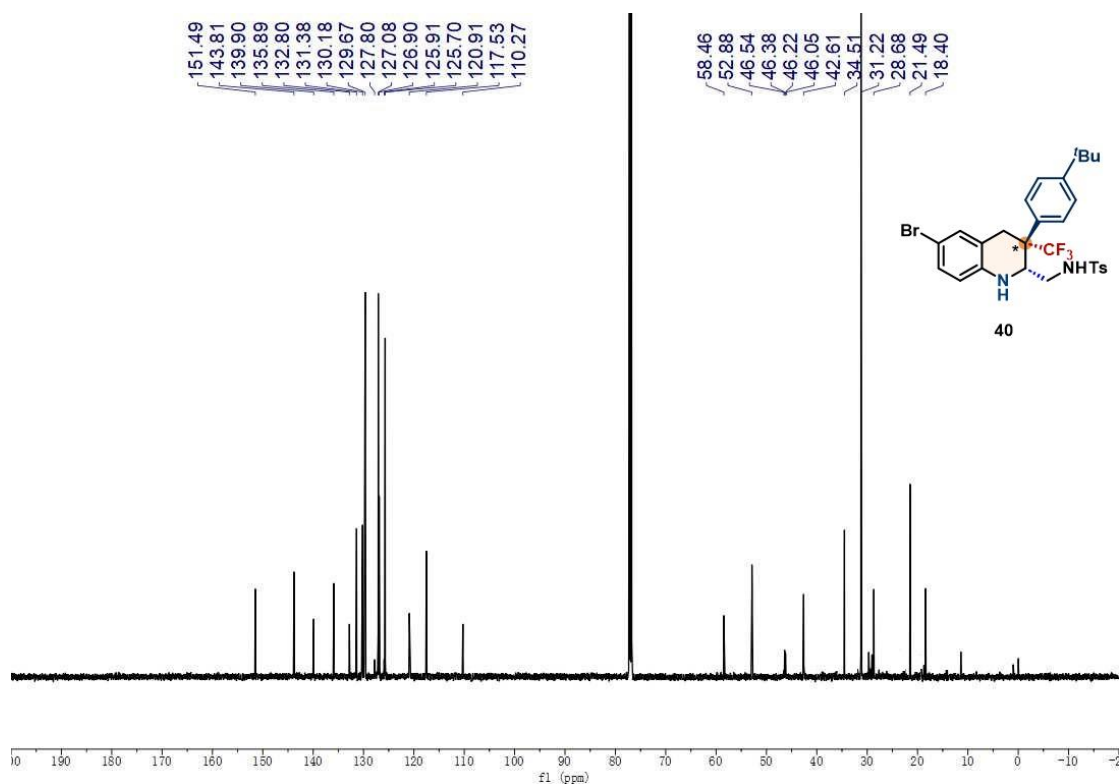
Supplementary Fig. S124. ¹³C NMR (150 MHz, CDCl₃) Spectrum of (2S,3R)-39



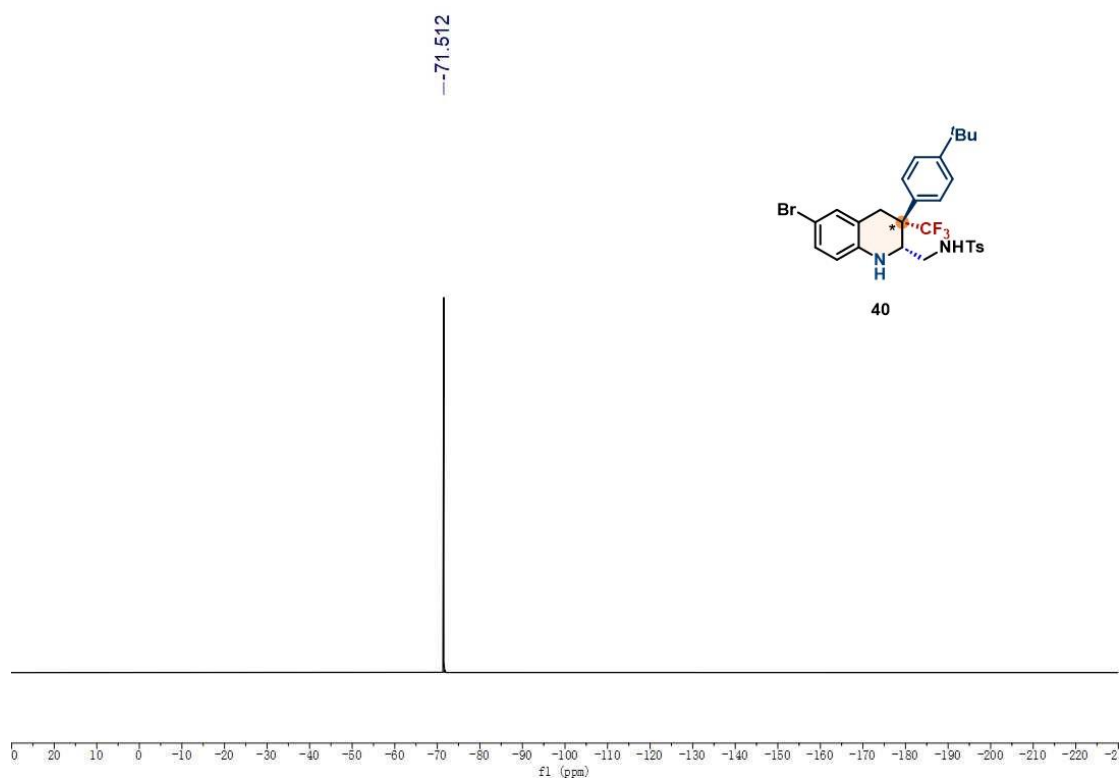
Supplementary Fig. S125. ^{19}F NMR (564 MHz, CDCl_3) Spectrum of (2*S*,3*R*)-39



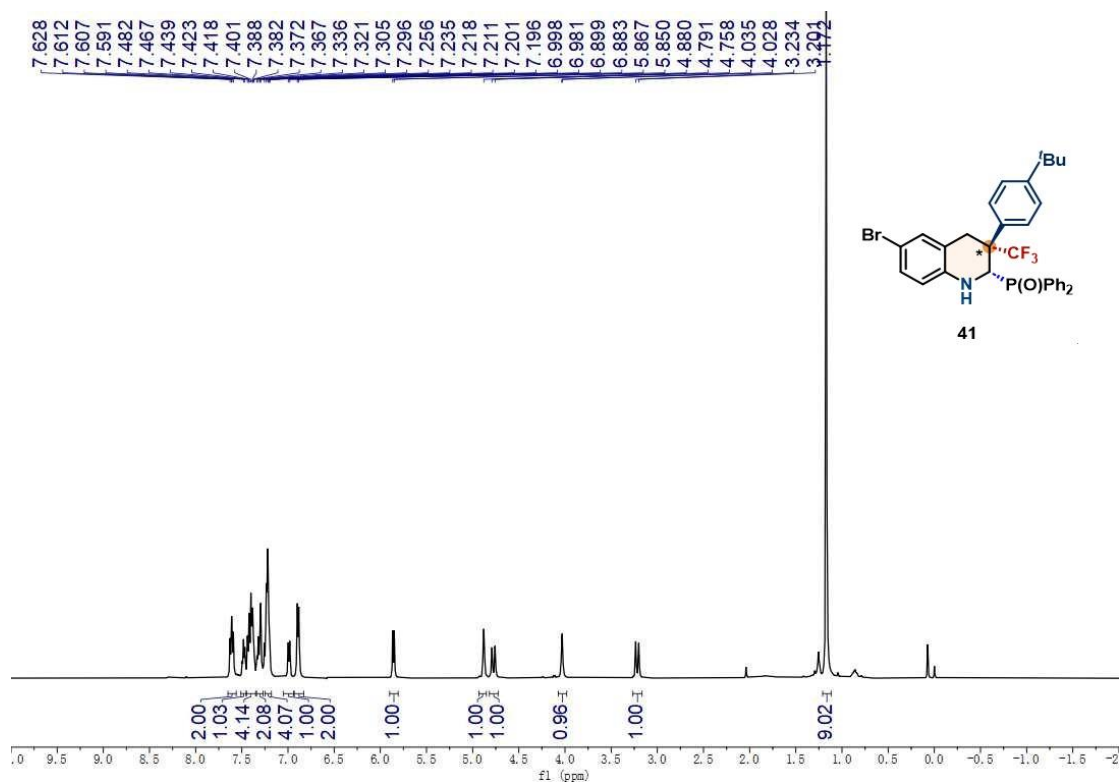
Supplementary Fig. S126. ^{19}F NMR (500 MHz, CDCl_3) Spectrum of (2*S*,3*R*)-40



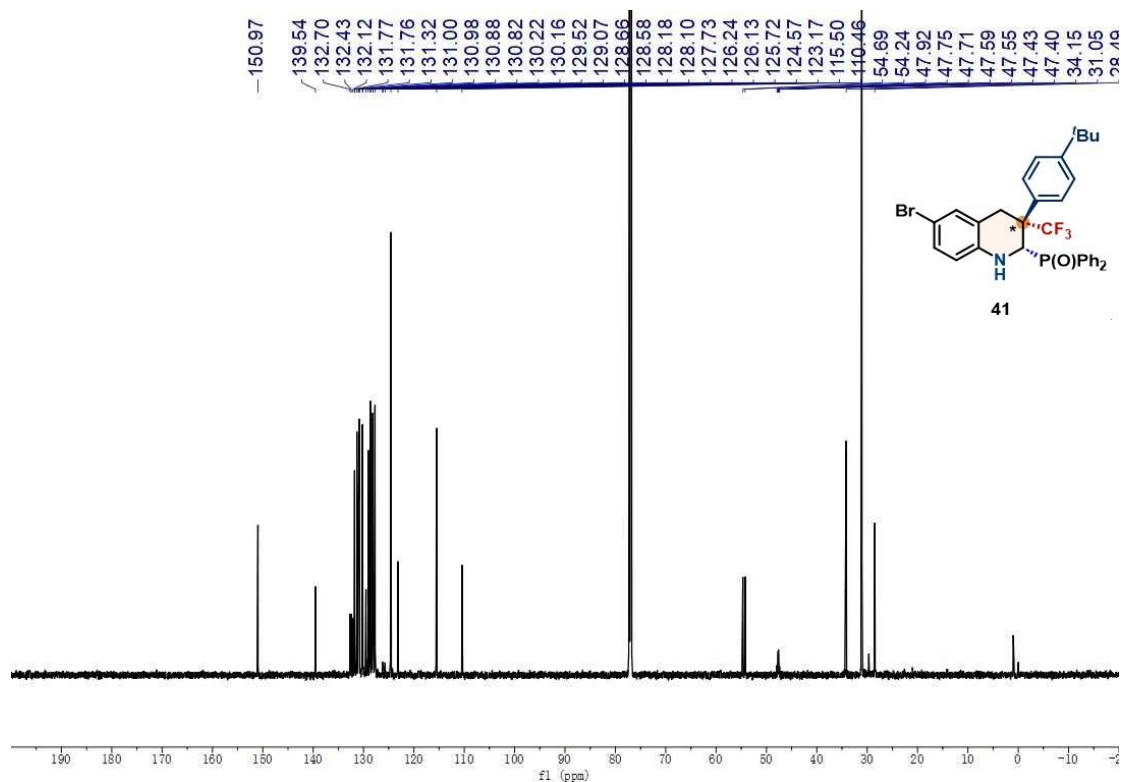
Supplementary Fig. S127. ¹³C NMR (150 MHz, CDCl₃) Spectrum of (2S,3R)-40



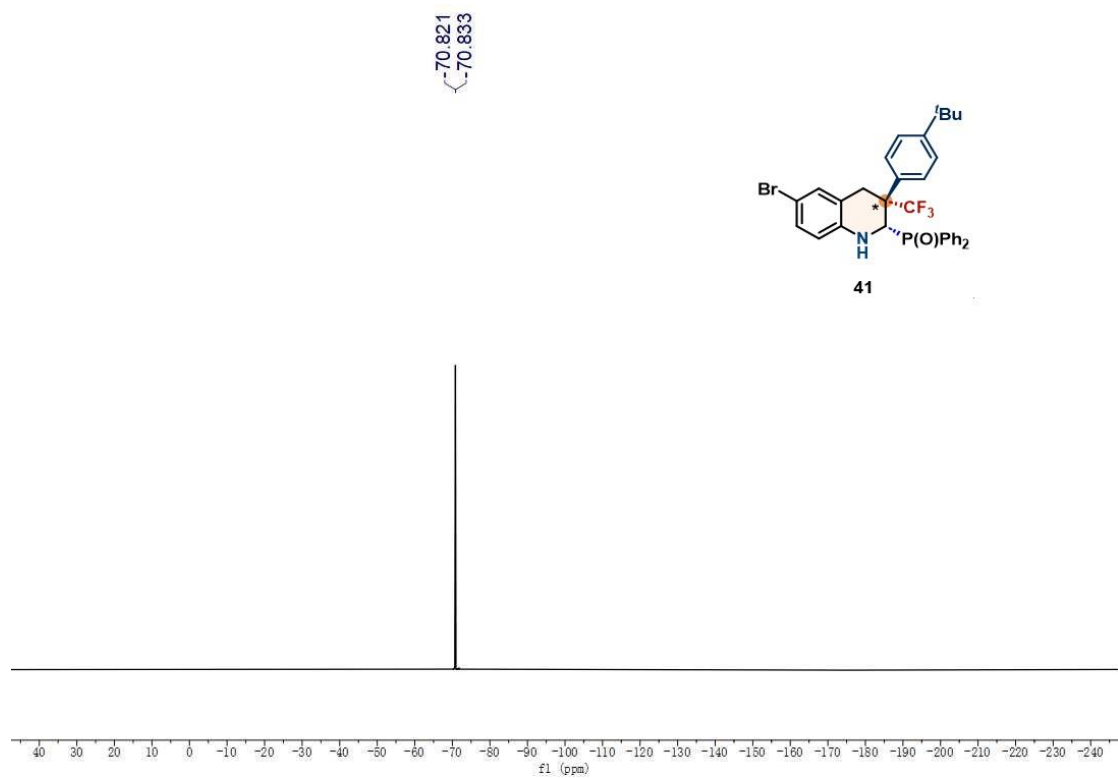
Supplementary Fig. S128. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of (2S,3R)-40



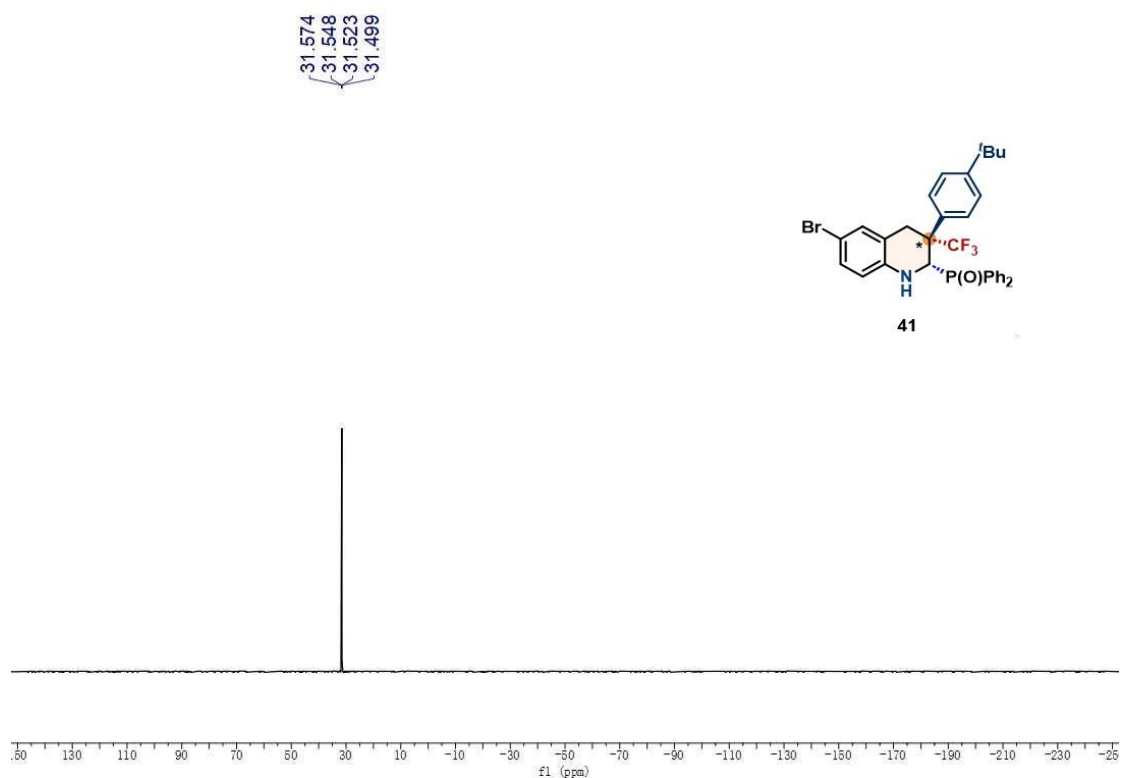
Supplementary Fig. S129. ¹H NMR (500 MHz, CDCl₃) Spectrum of (2*R*,3*S*)-41



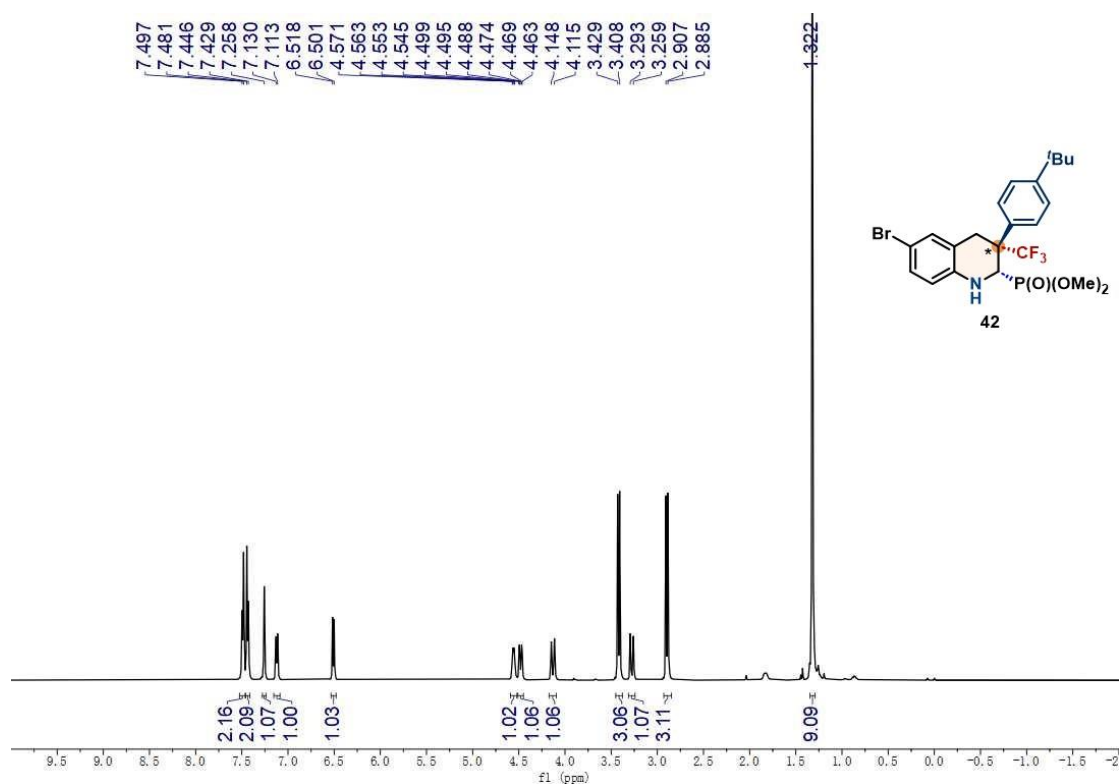
Supplementary Fig. S130. ¹³C NMR (150 MHz, CDCl₃) Spectrum of (2*R*,3*S*)-41



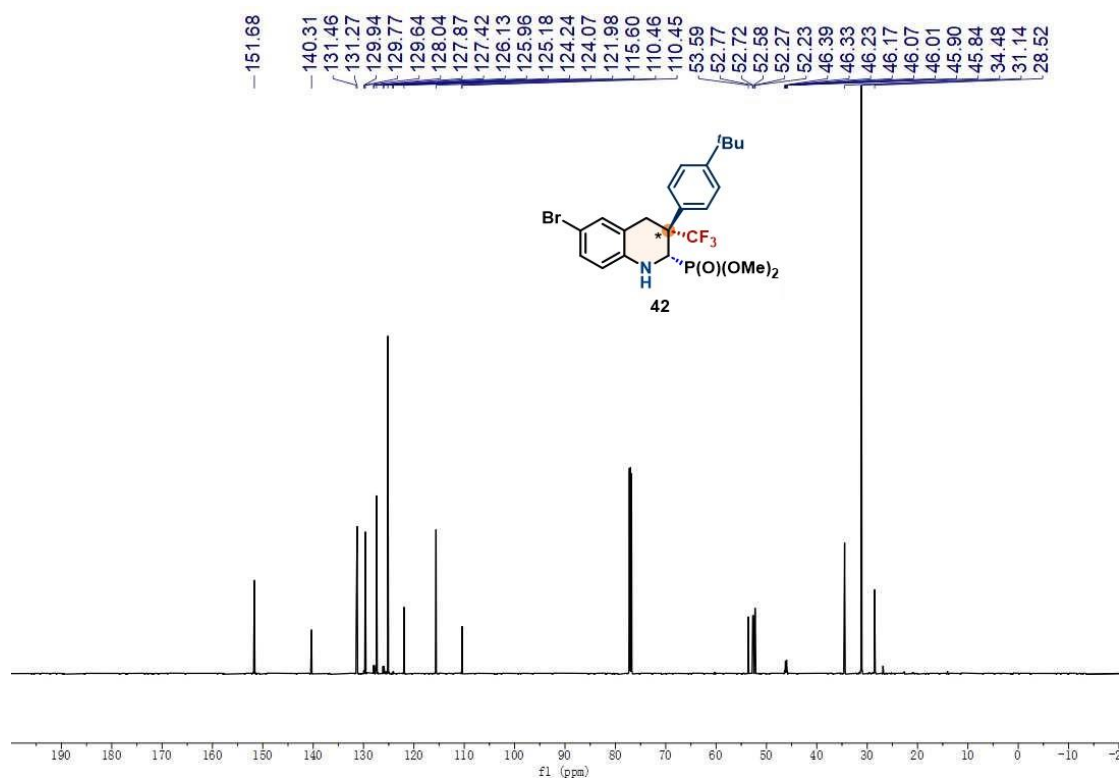
Supplementary Fig. S131. ¹⁹F NMR (470 MHz, CDCl₃) Spectrum of (2*R*,3*S*)-41



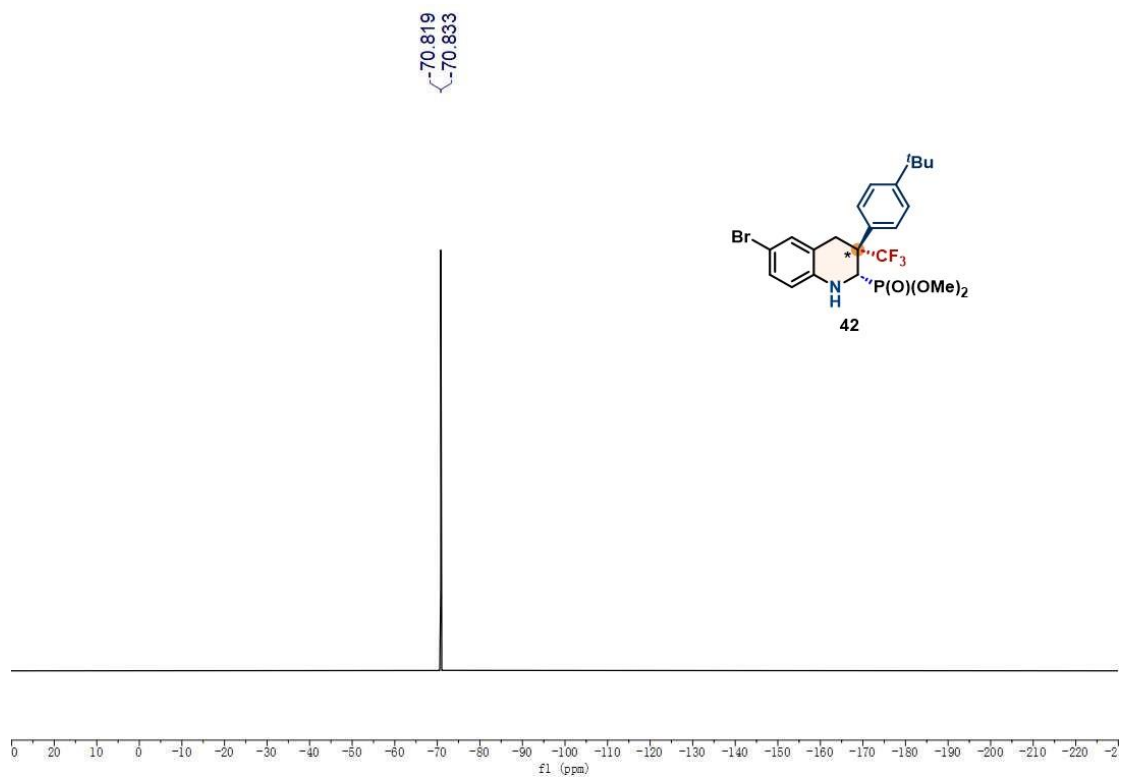
Supplementary Fig. S132. ³¹P NMR (202 MHz, CDCl₃) Spectrum of (2*R*,3*S*)-41



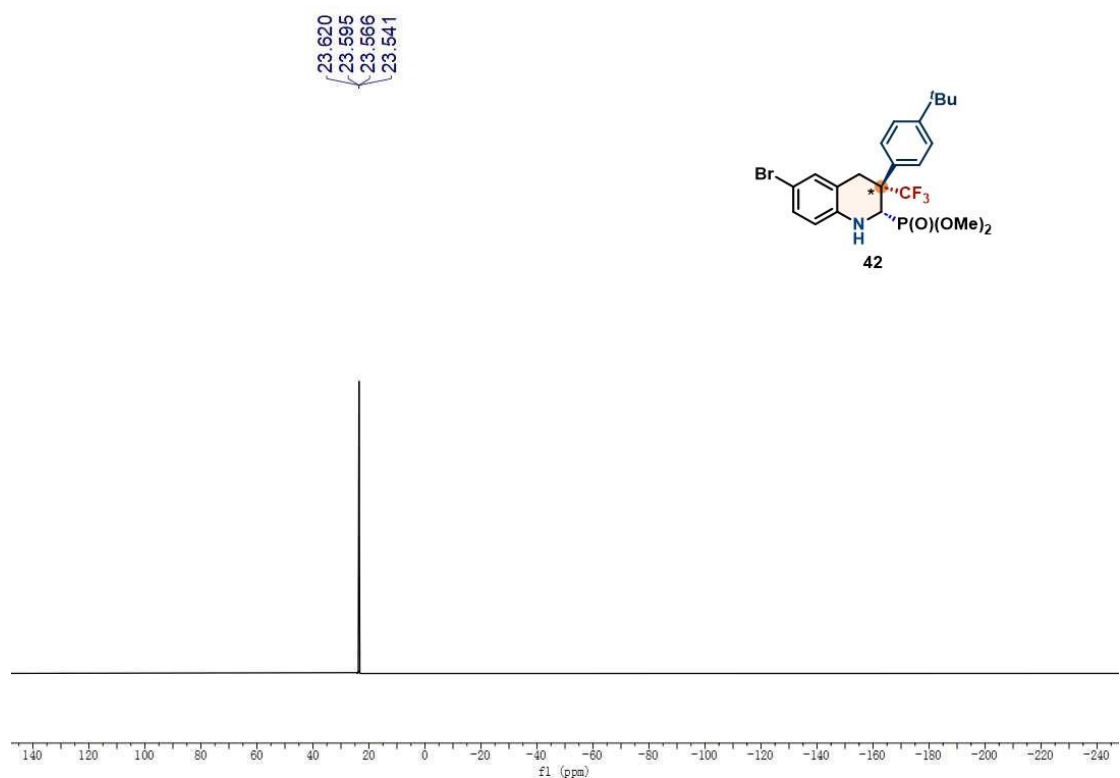
Supplementary Fig. S133. ¹H NMR (500 MHz, CDCl₃) Spectrum of (2R,3S)-42



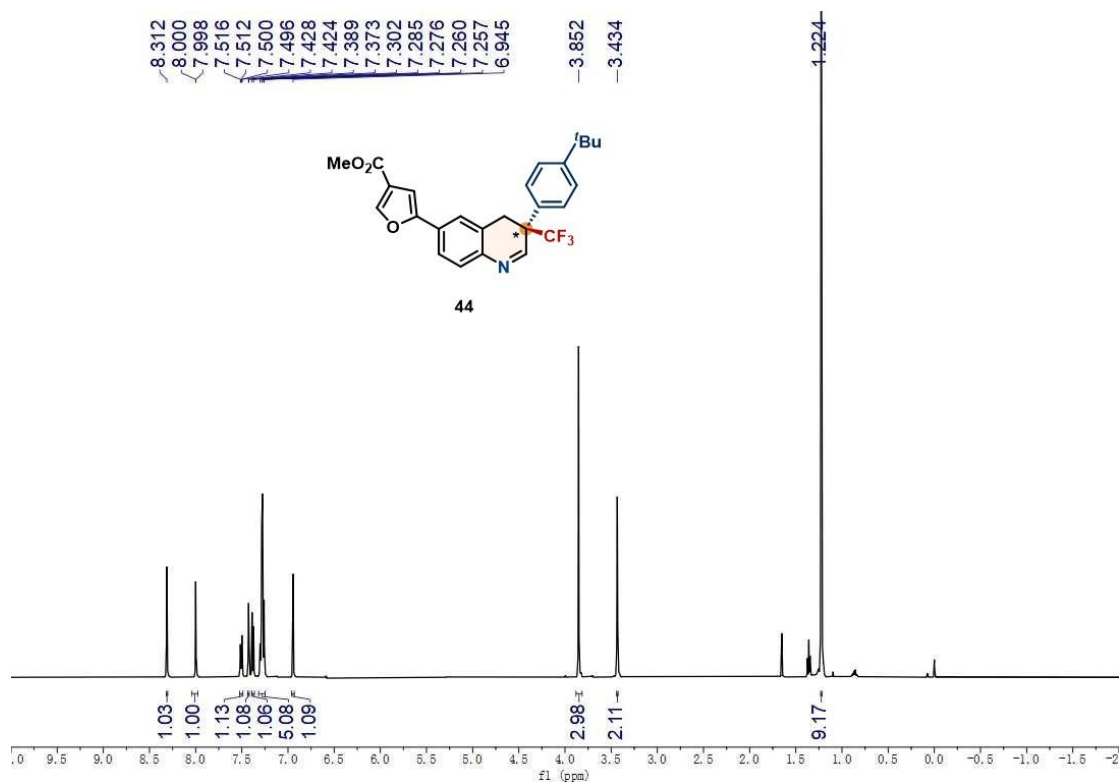
Supplementary Fig. S134. ¹³C NMR (150 MHz, CDCl₃) Spectrum of (2R,3S)-42



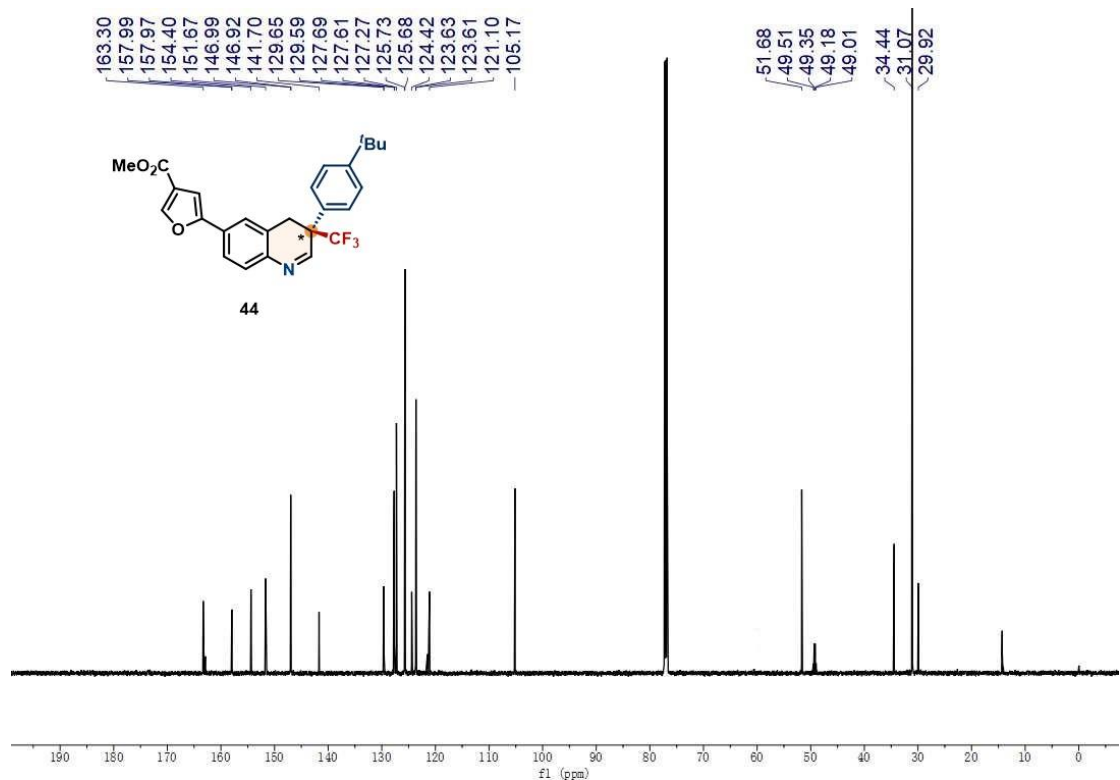
Supplementary Fig. S135. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of (2*R*,3*S*)-42



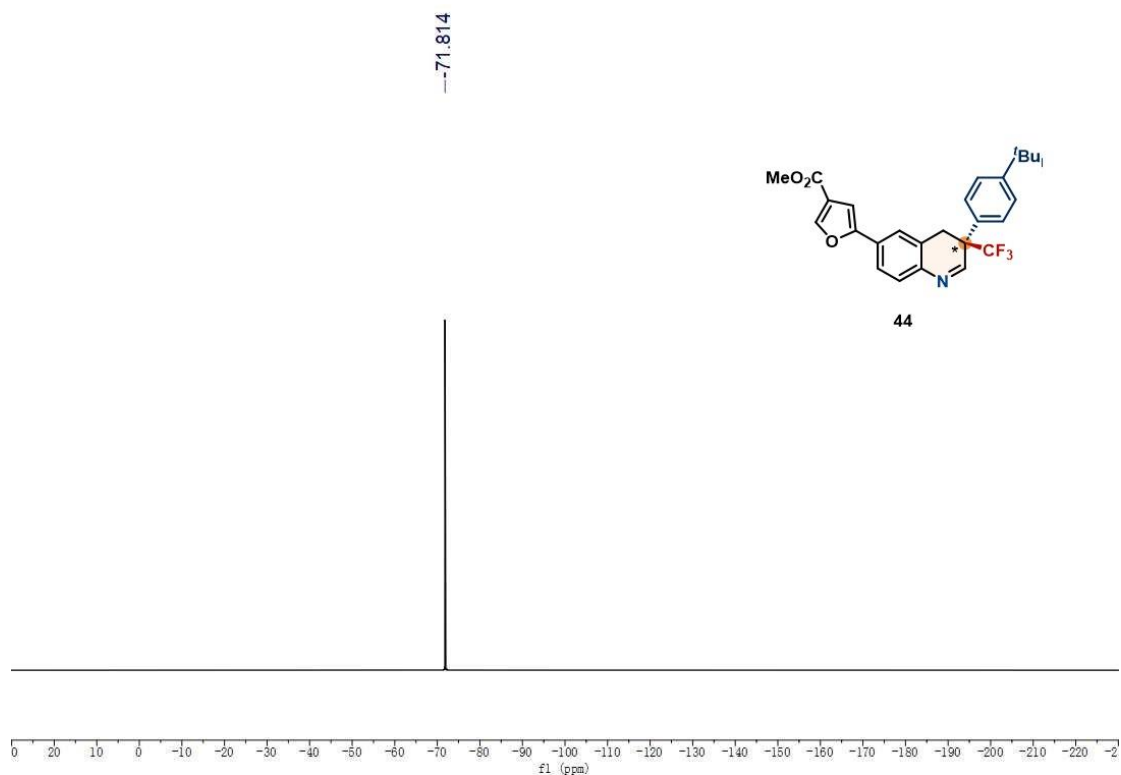
Supplementary Fig. S136. ³¹P NMR (243 MHz, CDCl₃) Spectrum of (2*R*,3*S*)-42



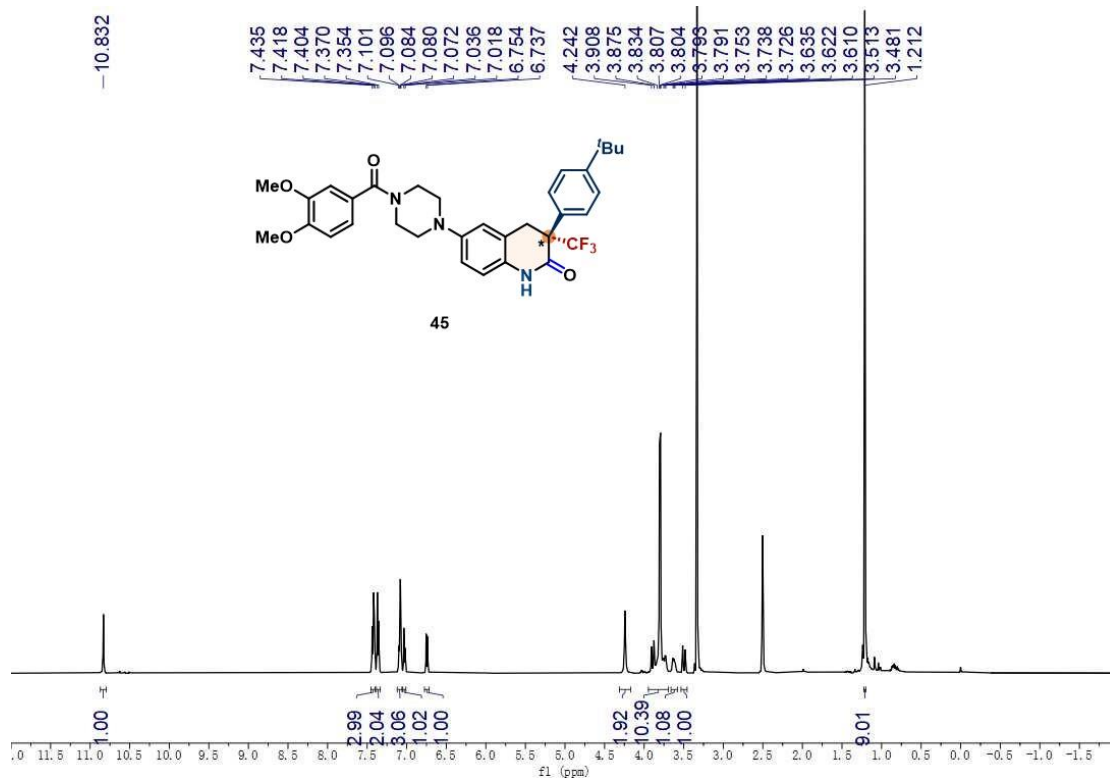
Supplementary Fig. S137. ¹³C NMR (500 MHz, CDCl₃) Spectrum of 44



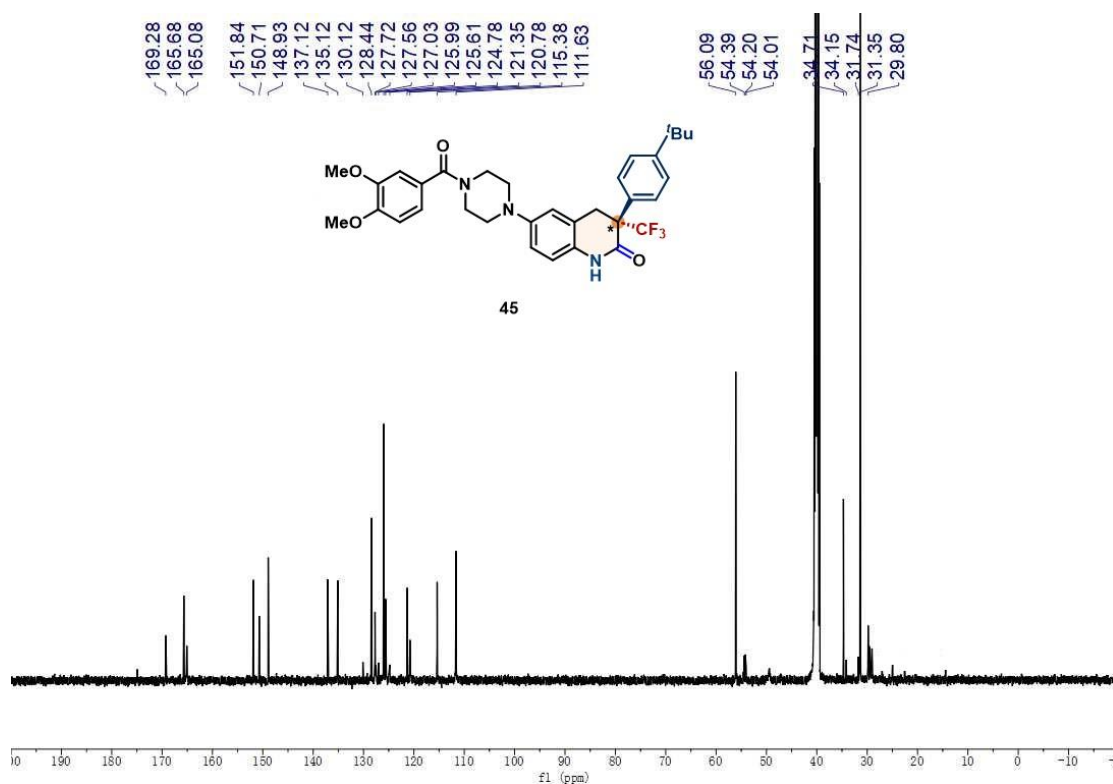
Supplementary Fig. S138. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 44



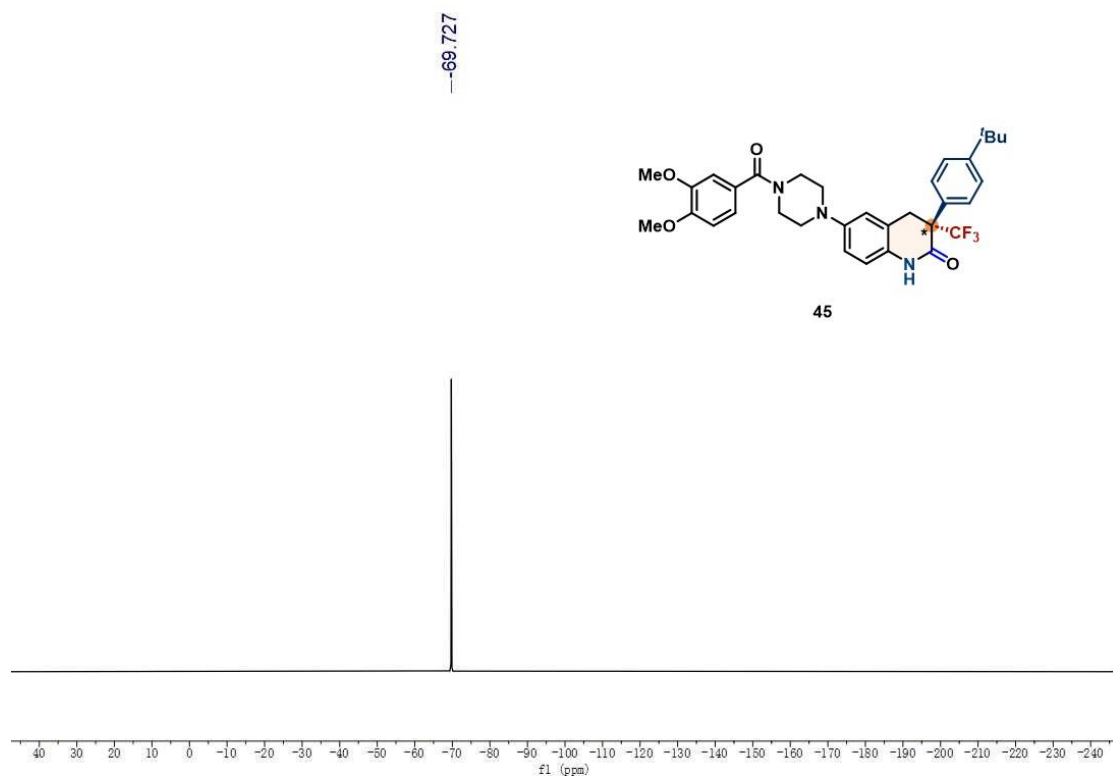
Supplementary Fig. S139. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 44



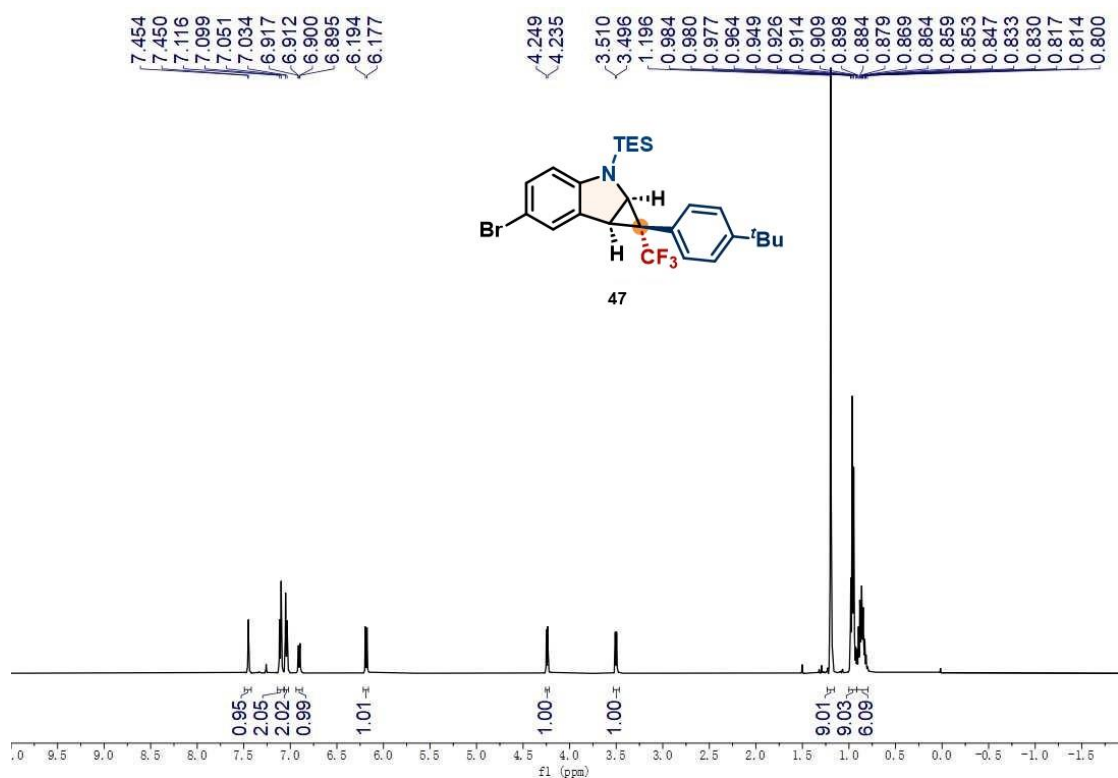
Supplementary Fig. S140. ¹H NMR (500 MHz, DMSO) Spectrum of 45



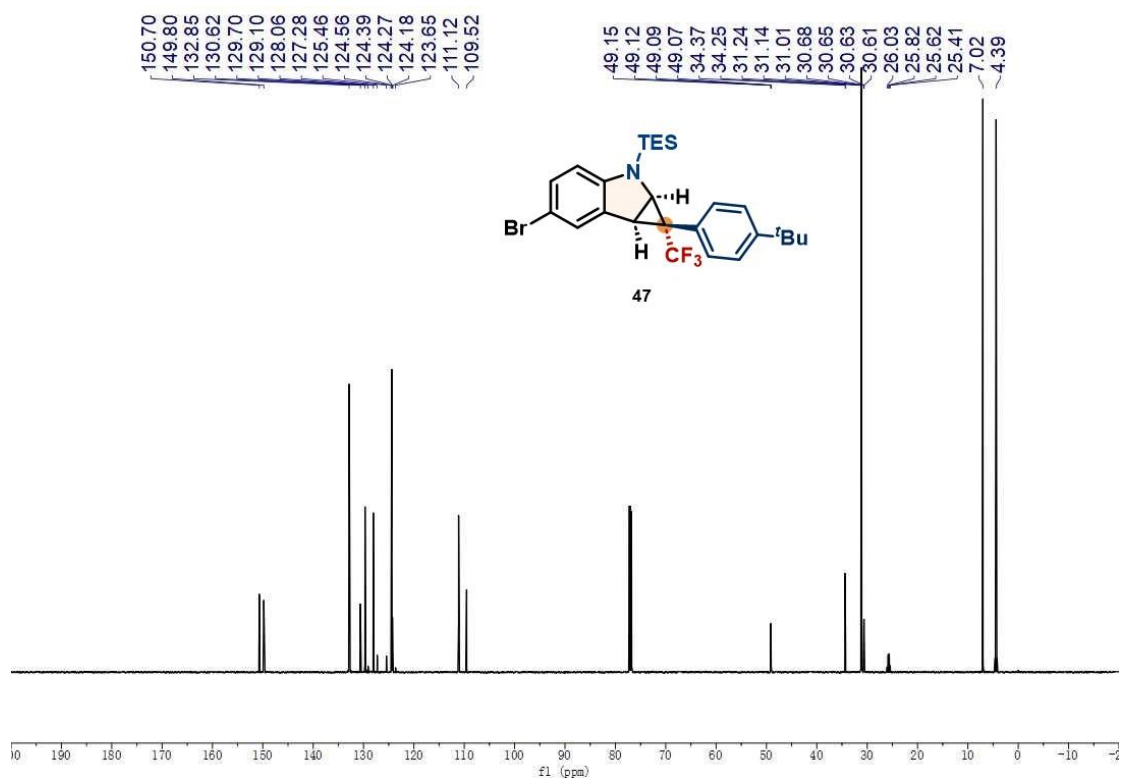
Supplementary Fig. S141. ¹³C NMR (125 MHz, DMSO) Spectrum of 45



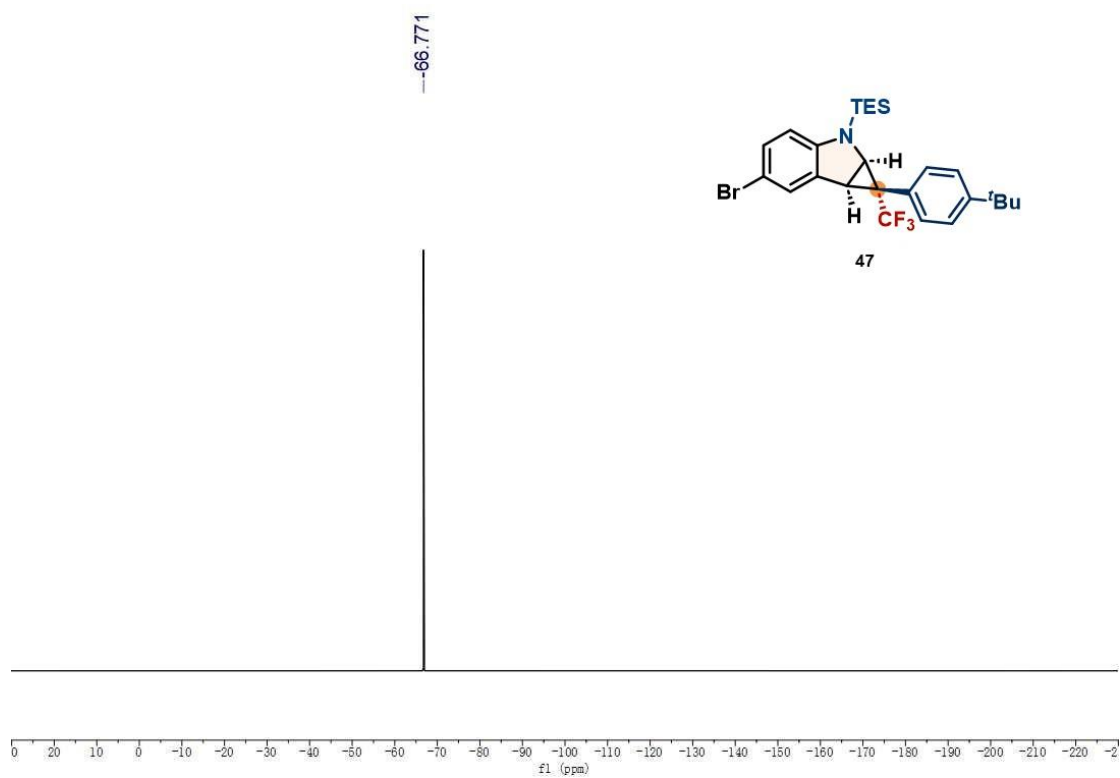
Supplementary Fig. S142. ¹⁹F NMR (470 MHz, DMSO) Spectrum of 45



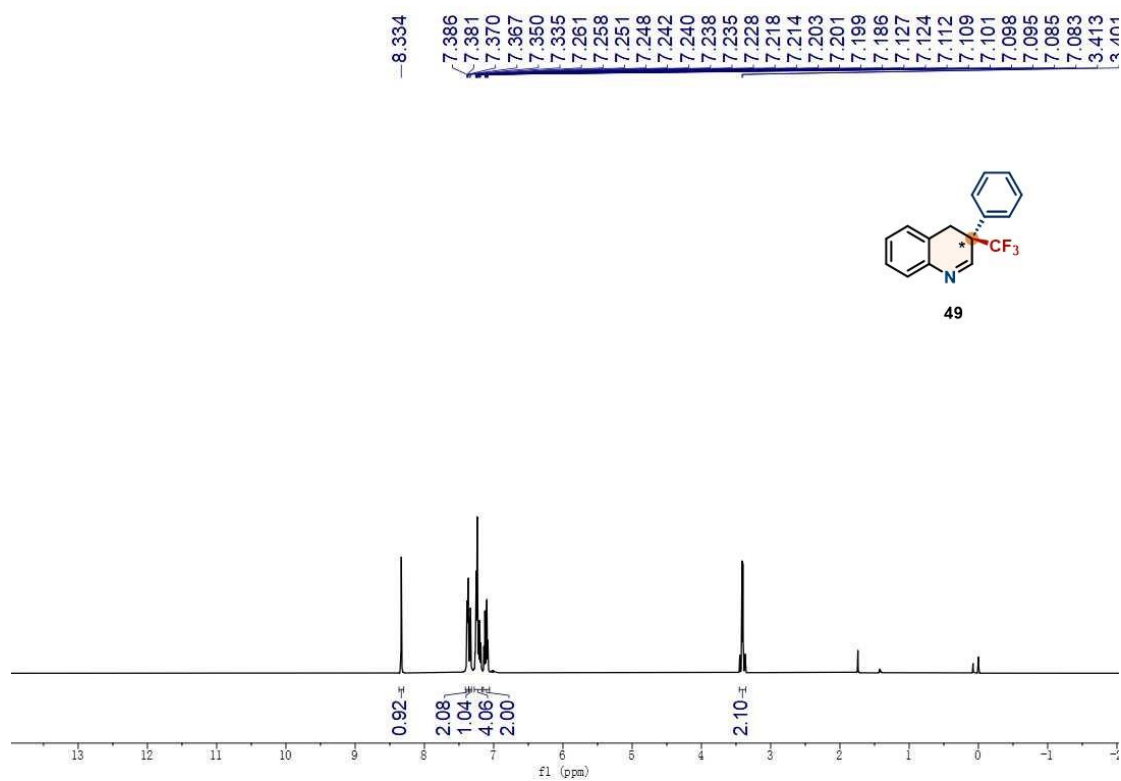
Supplementary Fig. S143. ¹H NMR (500 MHz, CDCl₃) Spectrum of 47



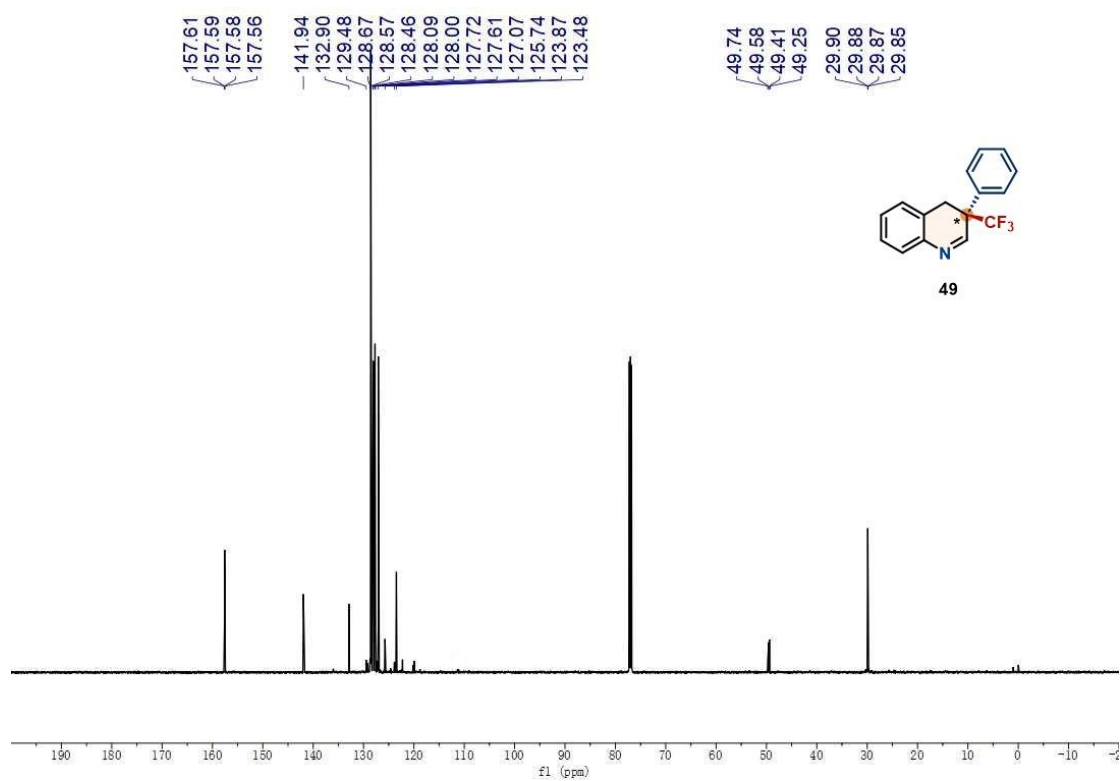
Supplementary Fig. S144. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 47



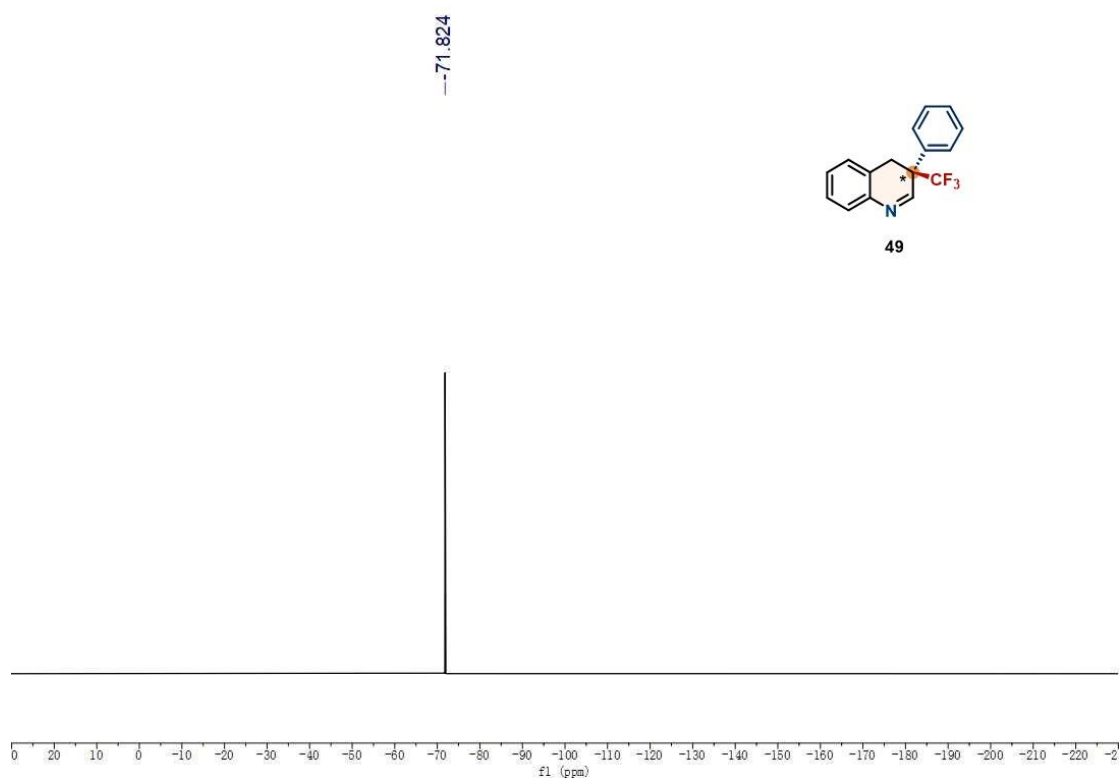
Supplementary Fig. S145. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 47



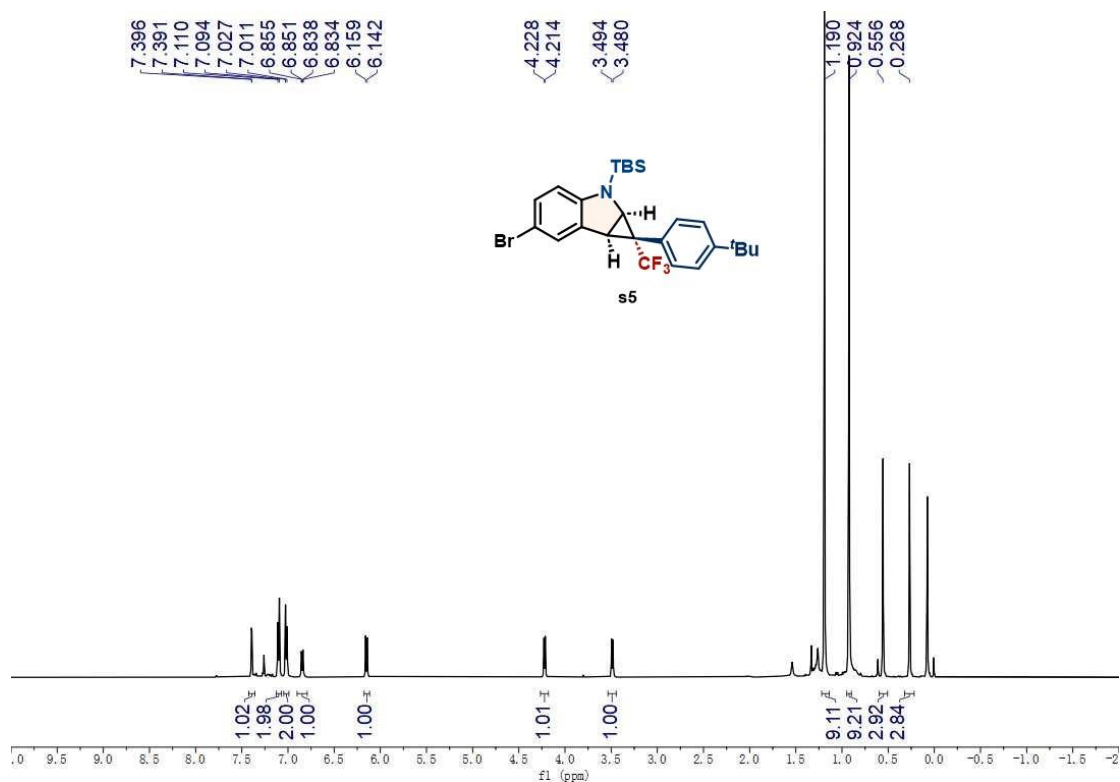
Supplementary Fig. S146. ¹H NMR (500 MHz, CDCl₃) Spectrum of 49



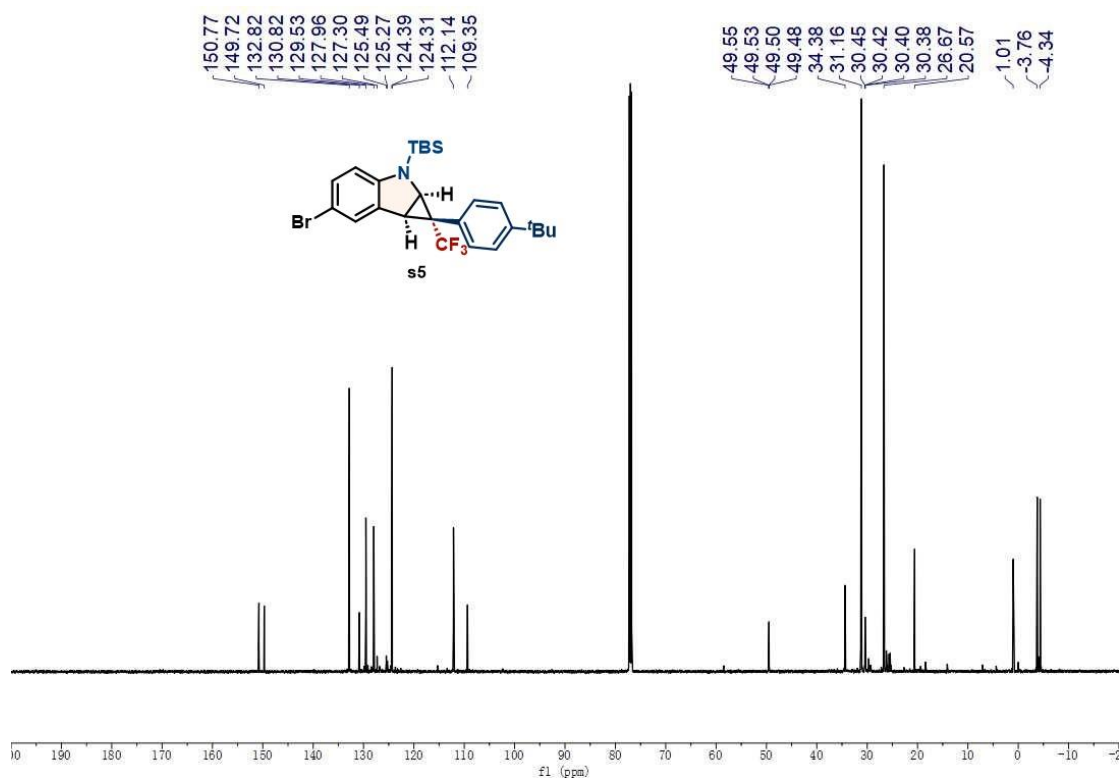
Supplementary Fig. S1457. ¹³C NMR (150 MHz, CDCl₃) Spectrum of 49



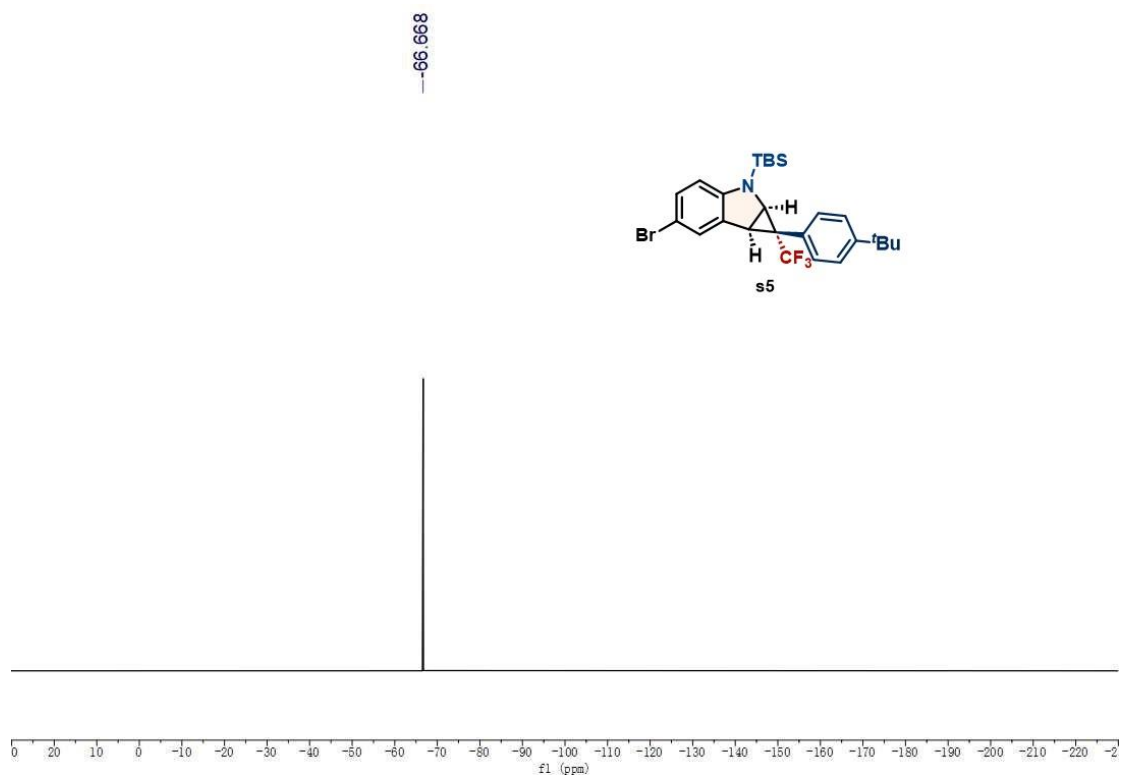
Supplementary Fig. S148. ¹⁹F NMR (564 MHz, CDCl₃) Spectrum of 49



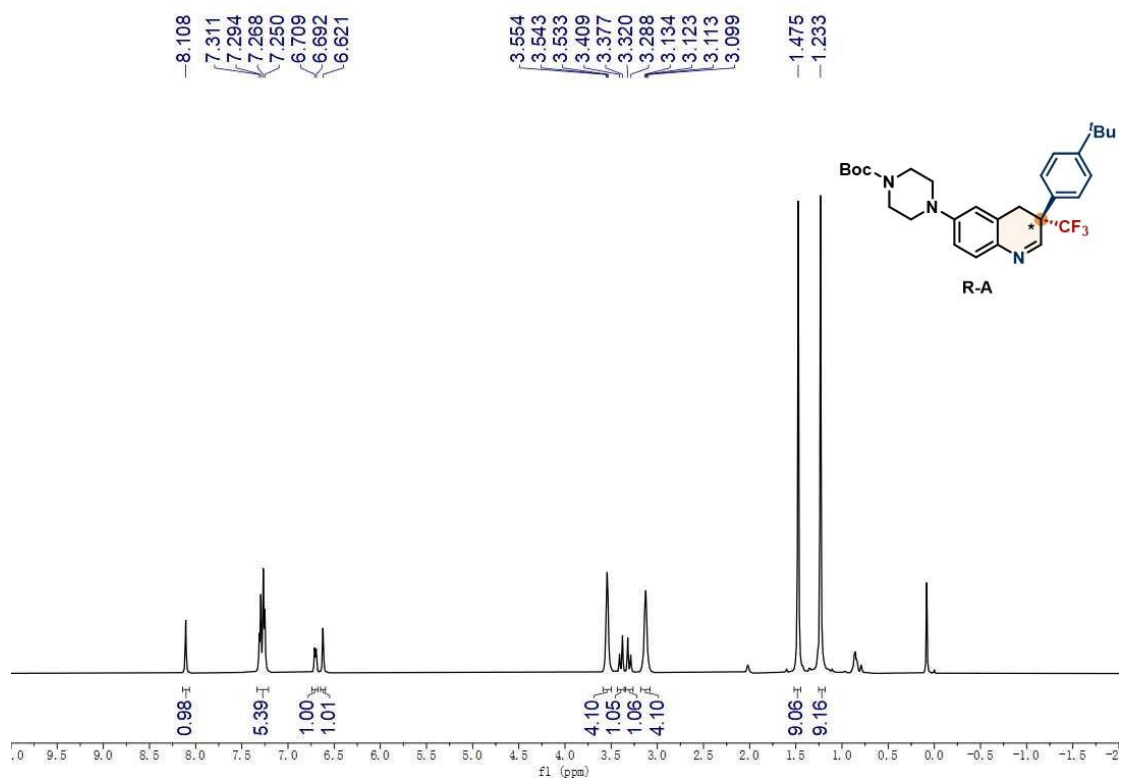
Supplementary Fig. S149. ¹H NMR (500 MHz, CDCl₃) Spectrum of s5



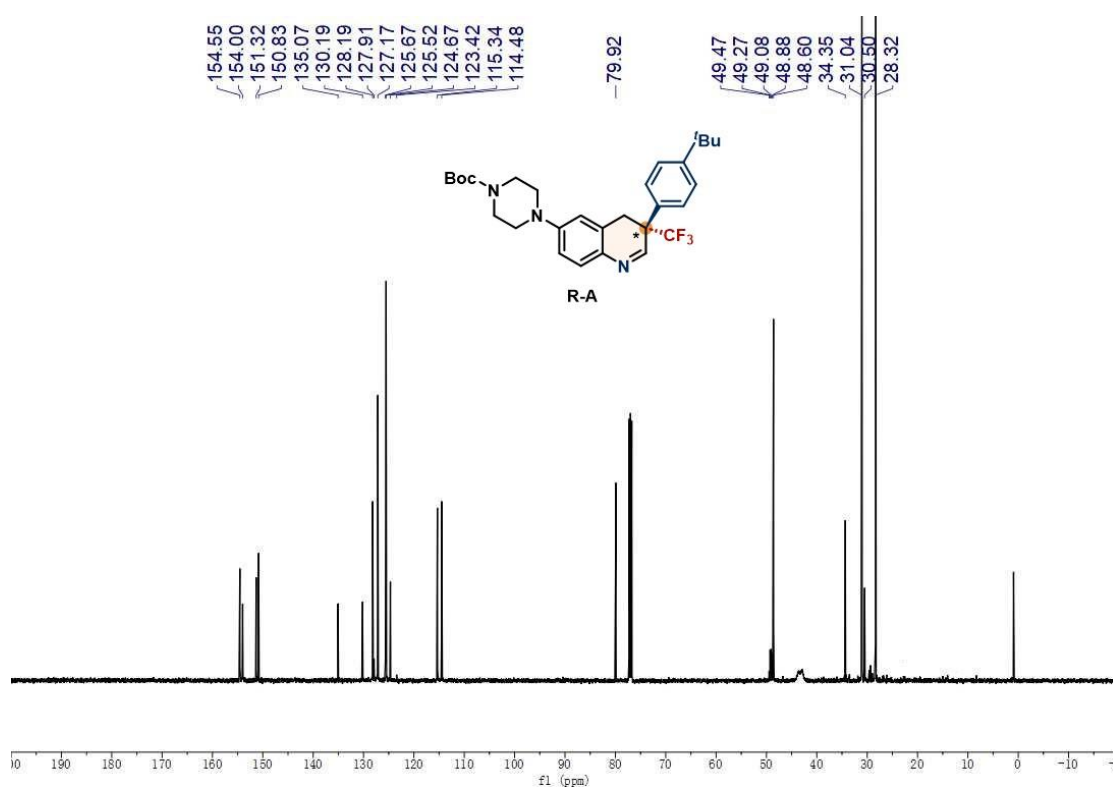
Supplementary Fig. S150. ¹³C NMR (150 MHz, CDCl₃) Spectrum of s5



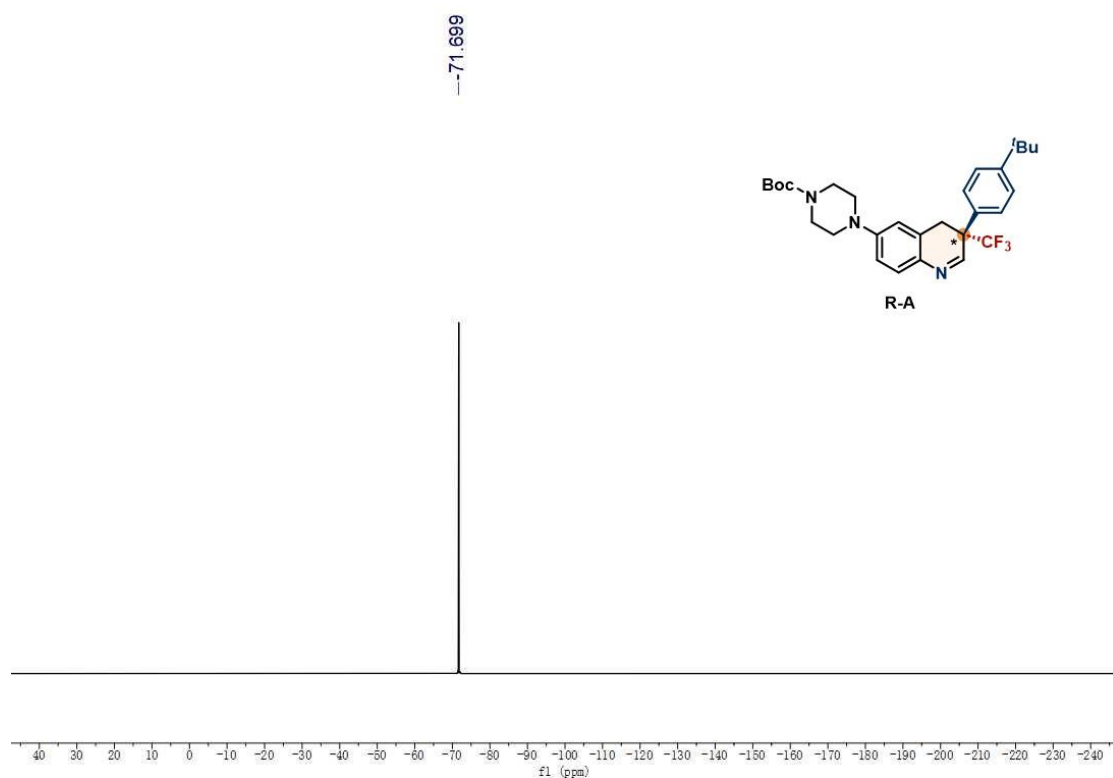
Supplementary Fig. S151. ^{19}F NMR (564 MHz, CDCl_3) Spectrum of s5



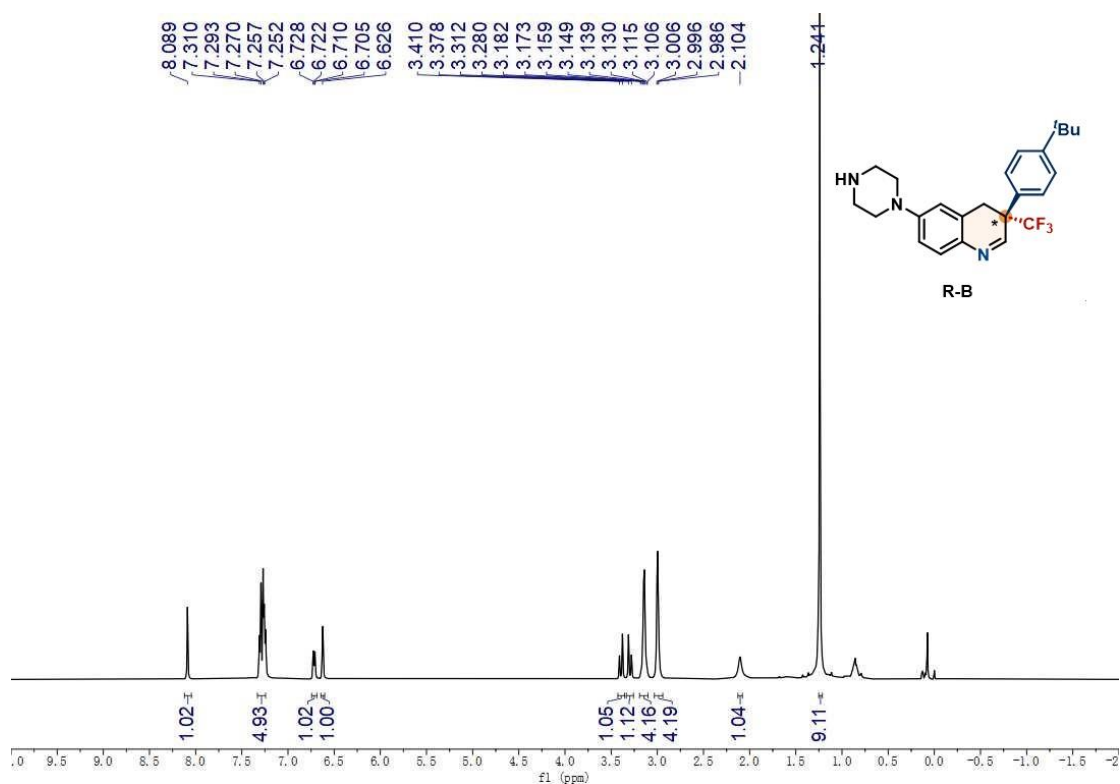
Supplementary Fig. S152. ^1H NMR (500 MHz, CDCl_3) Spectrum of R-A



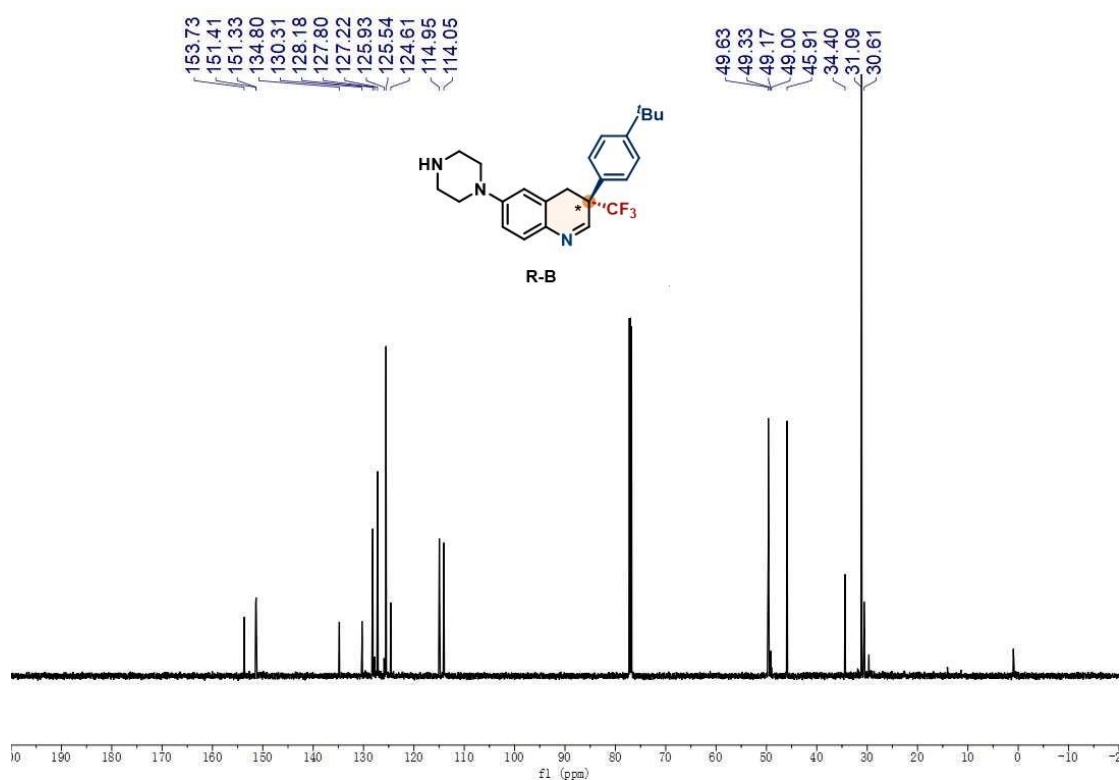
Supplementary Fig. S153. ¹³C NMR (125 MHz, CDCl₃) Spectrum of R-A



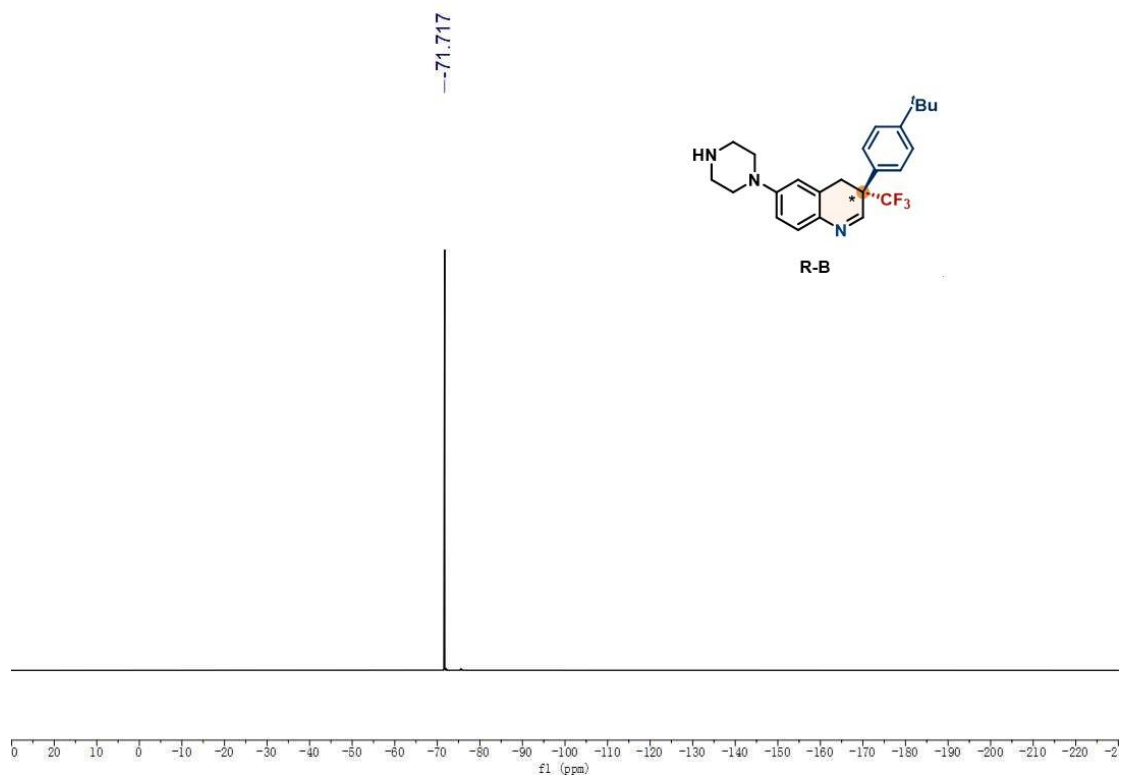
Supplementary Fig. S154. ¹⁹F NMR (470 MHz, CDCl₃) Spectrum of R-A



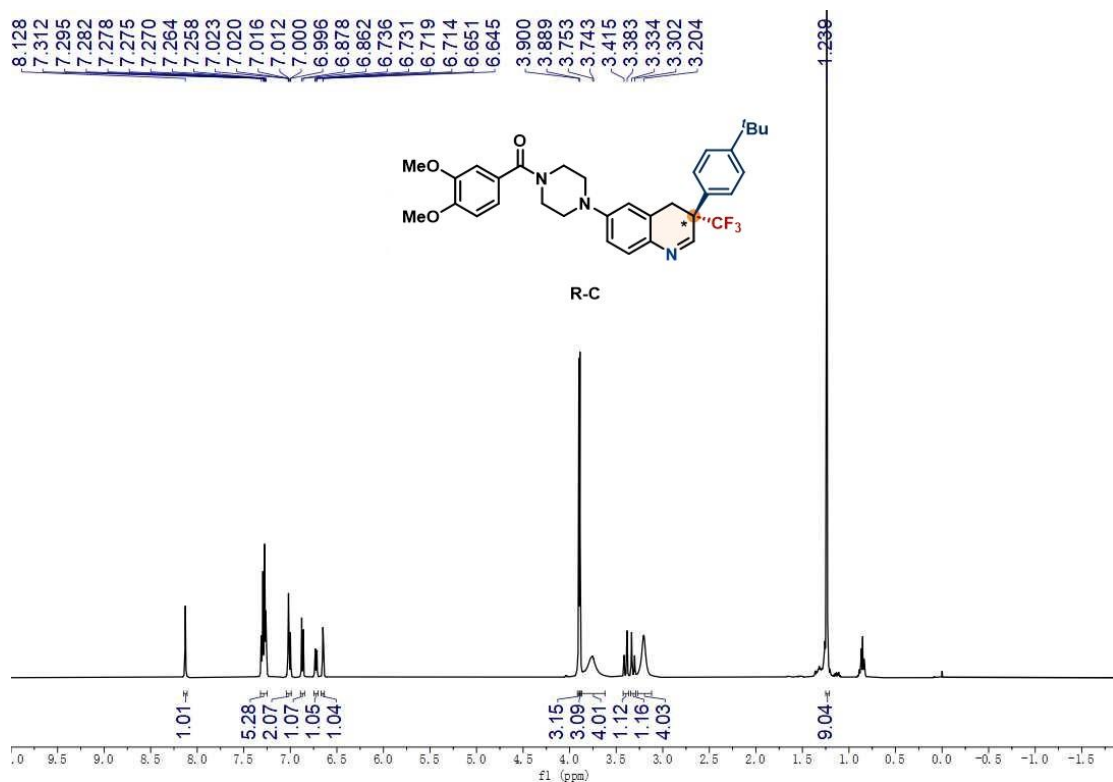
Supplementary Fig. S155. ¹H NMR (500 MHz, CDCl₃) Spectrum of R-B



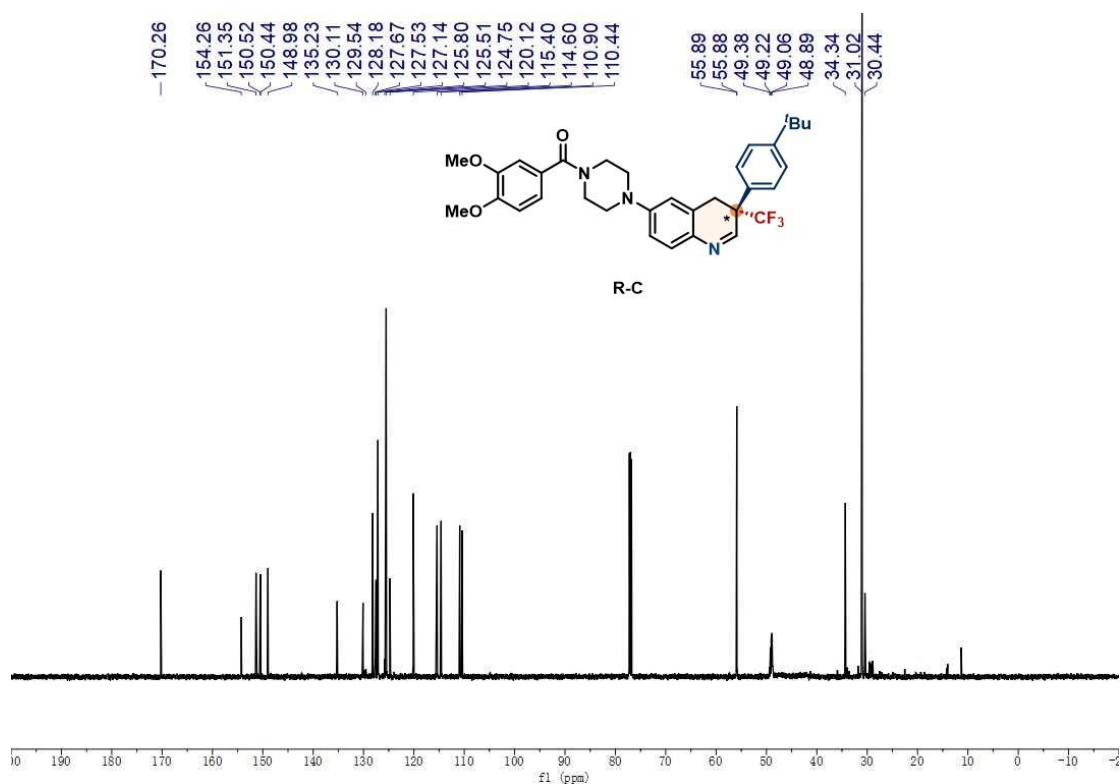
Supplementary Fig. S156. ¹³C NMR (150 MHz, CDCl₃) Spectrum of R-B



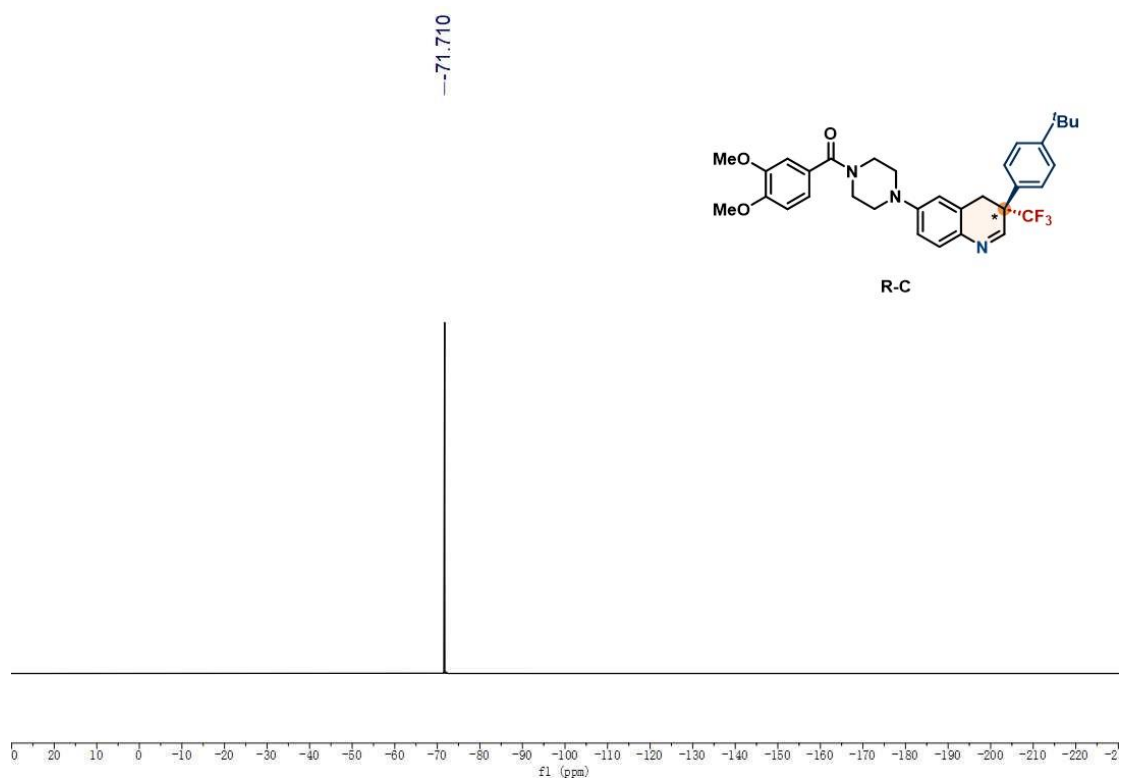
Supplementary Fig. S157. ^{19}F NMR (564 MHz, CDCl_3) Spectrum of R-B



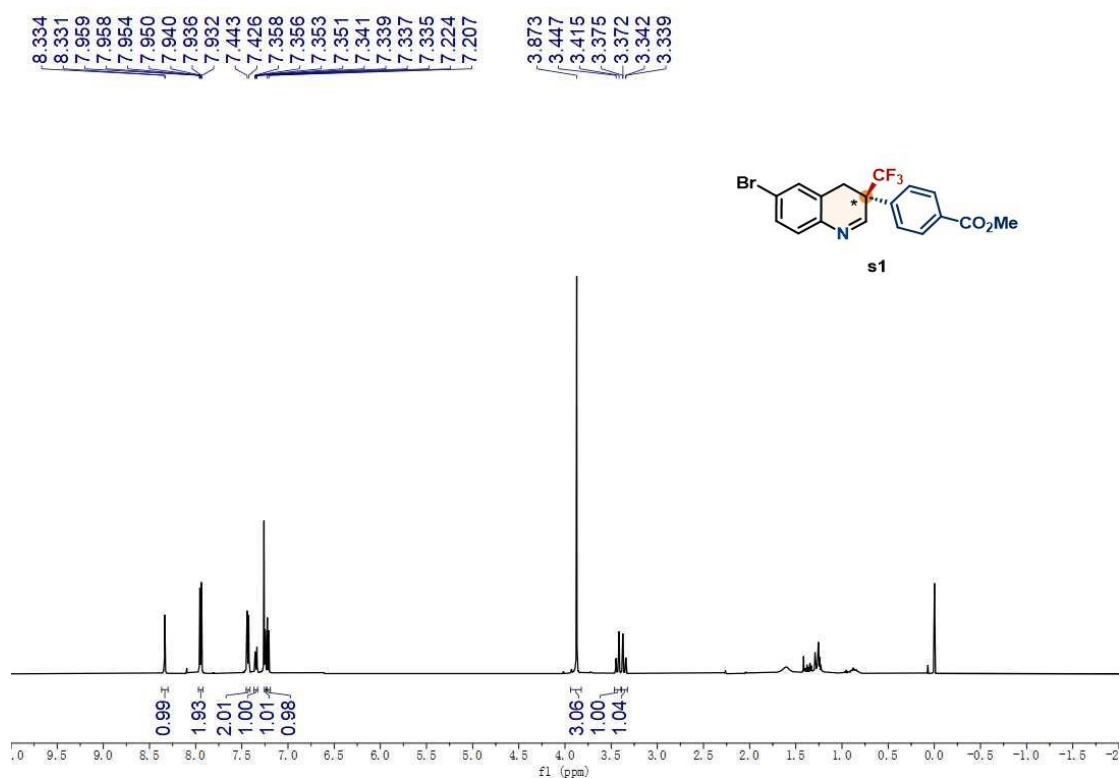
Supplementary Fig. S158. ^1H NMR (500 MHz, CDCl_3) Spectrum of R-C



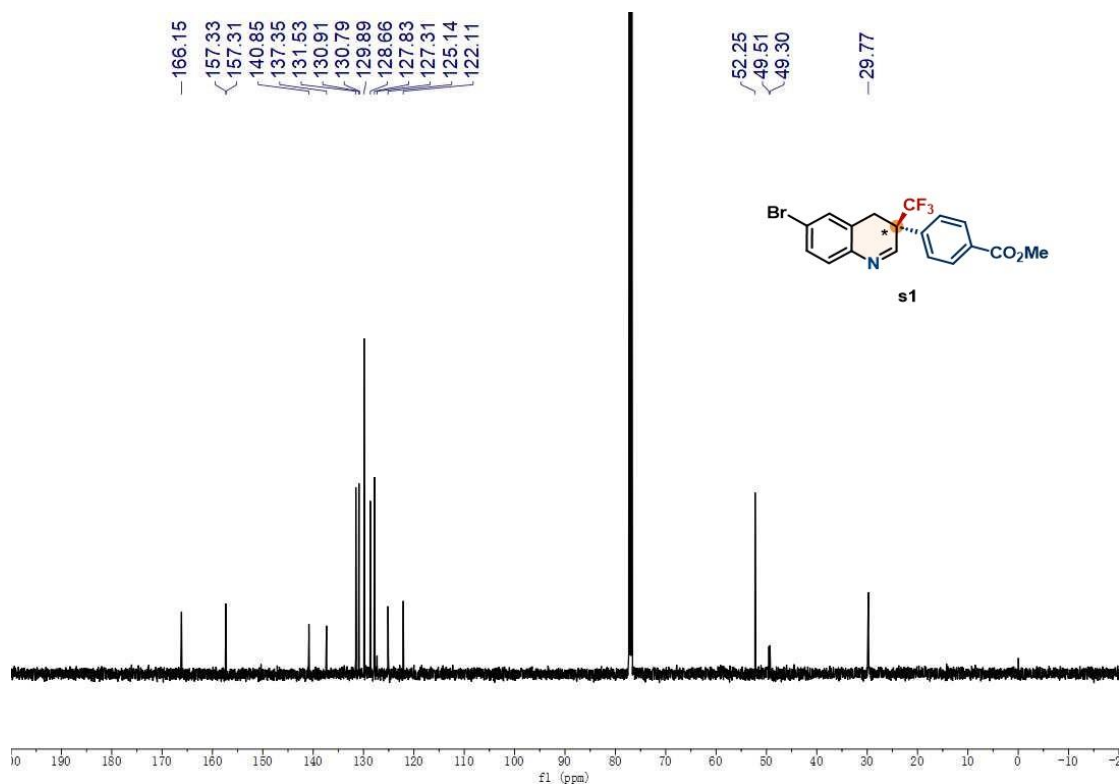
Supplementary Fig. S159. ^{13}C NMR S (150 MHz, CDCl_3) spectrum of R-C



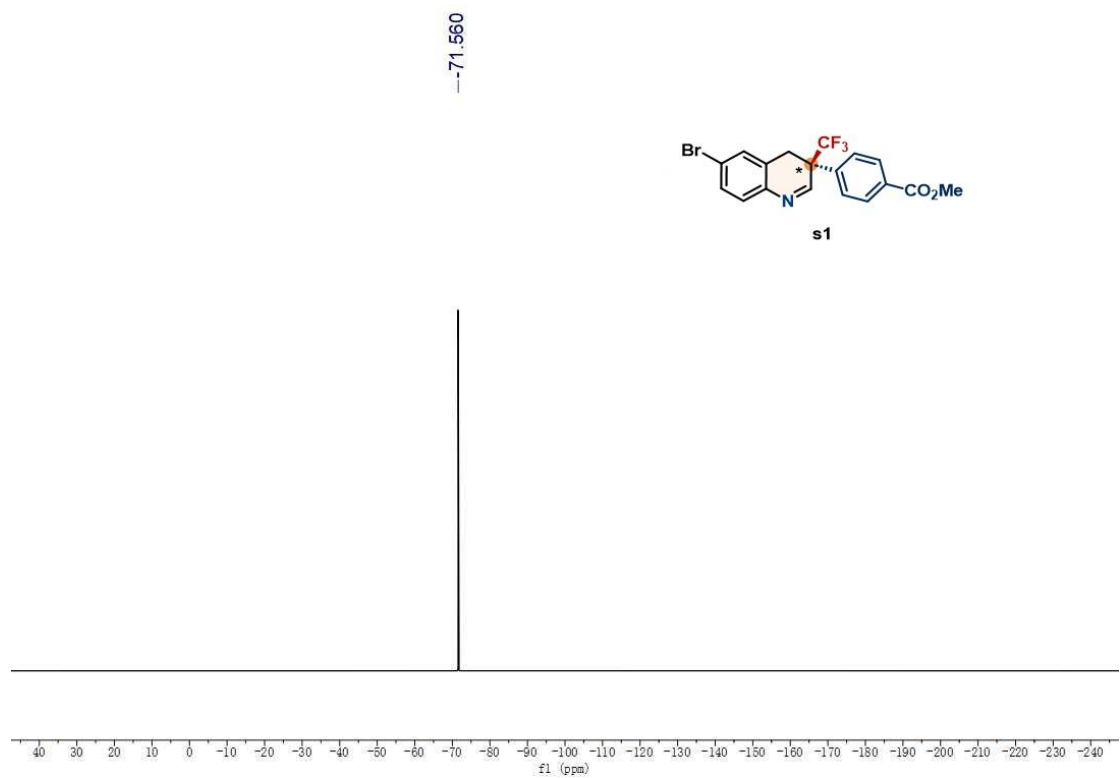
Supplementary Fig. S160. ^{19}F NMR (564 MHz, CDCl_3) Spectrum of R-C



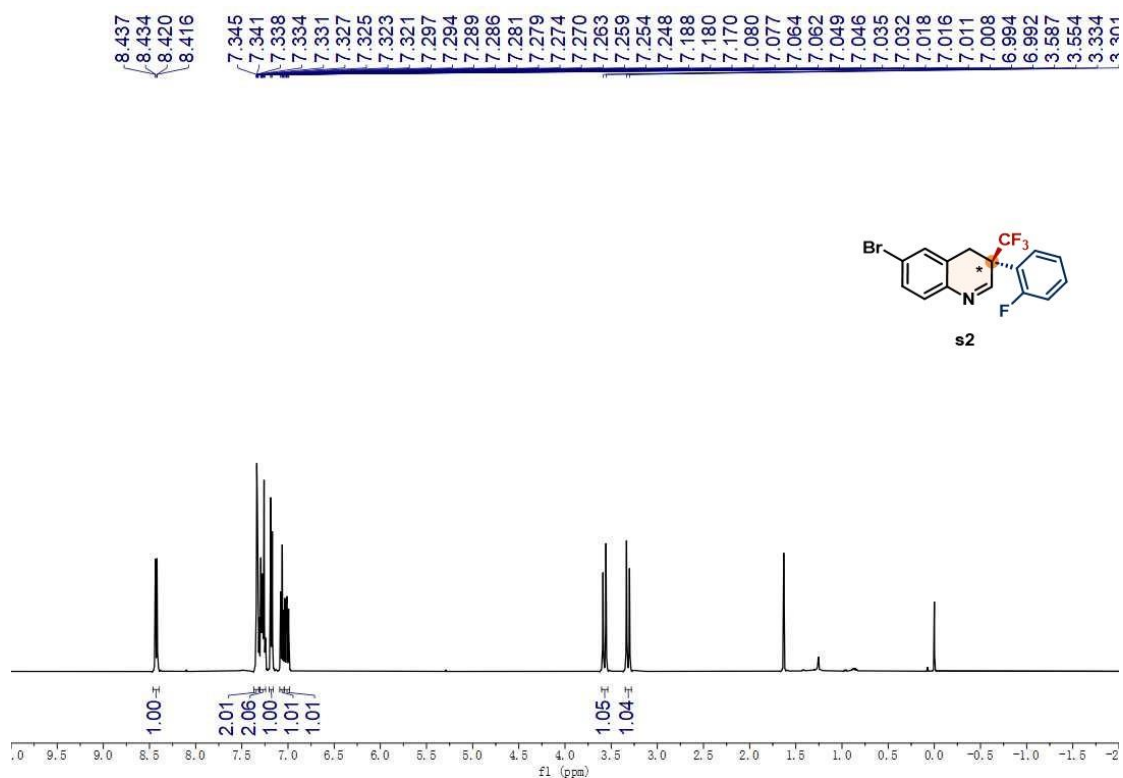
Supplementary Fig. S161. ¹H NMR (500 MHz, CDCl₃) Spectrum of s1



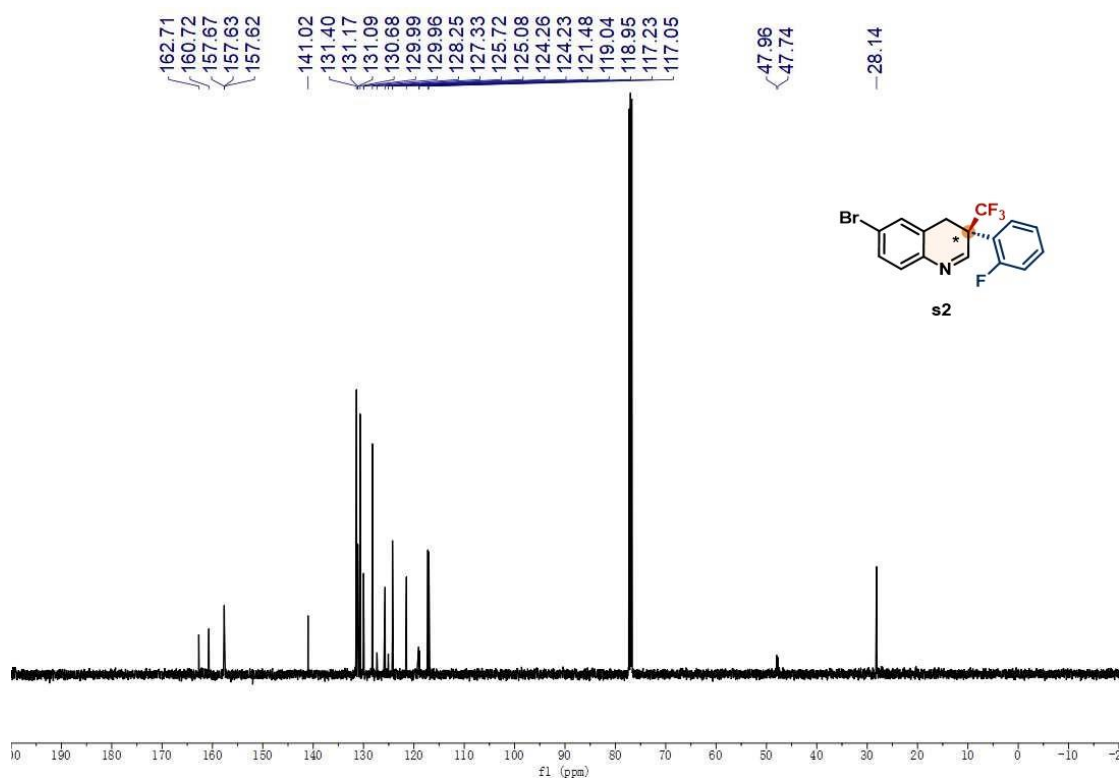
Supplementary Fig. S162. ¹³C NMR (125 MHz, CDCl₃) Spectrum of s1



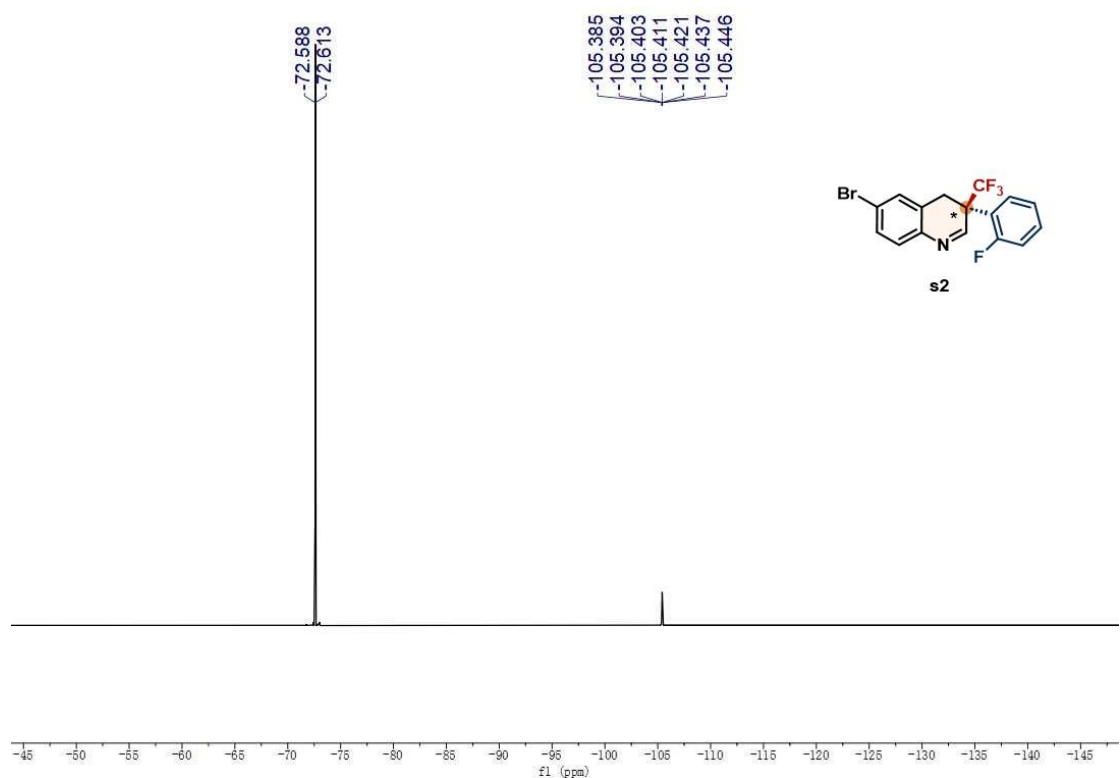
Supplementary Fig. S163. ¹⁹F NMR (470 MHz, CDCl₃) Spectrum of **s1**



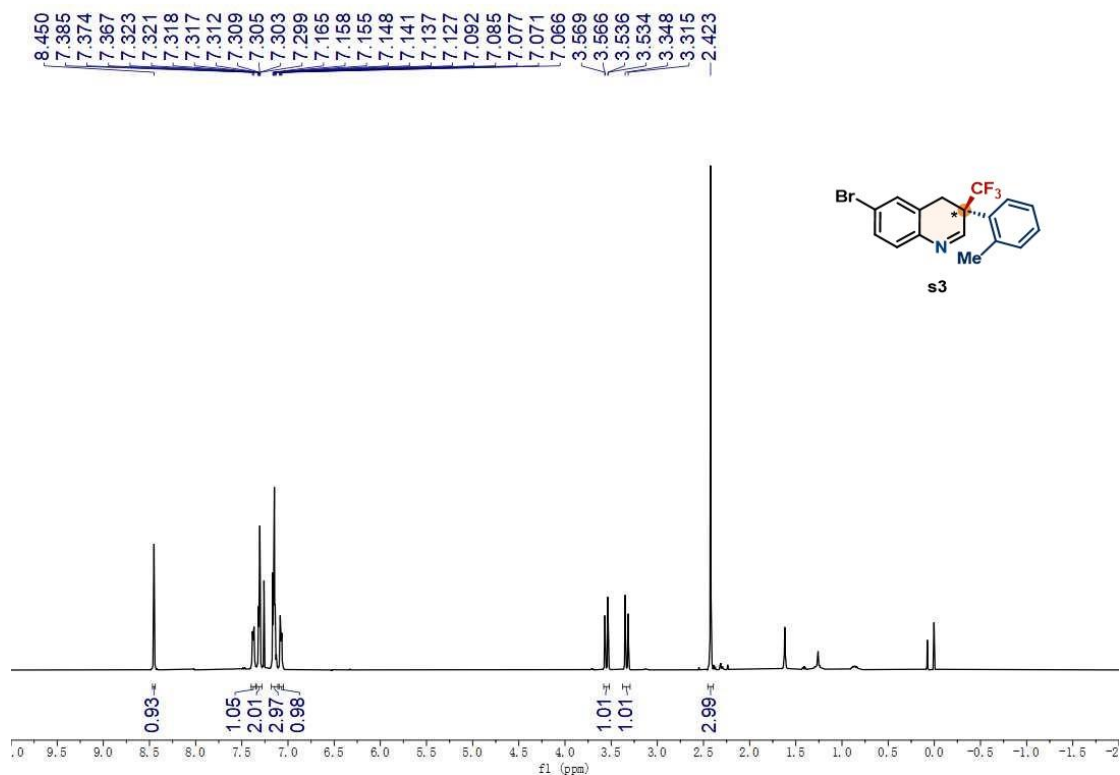
Supplementary Fig. S164. ¹H NMR (500 MHz, CDCl₃) Spectrum of **s2**



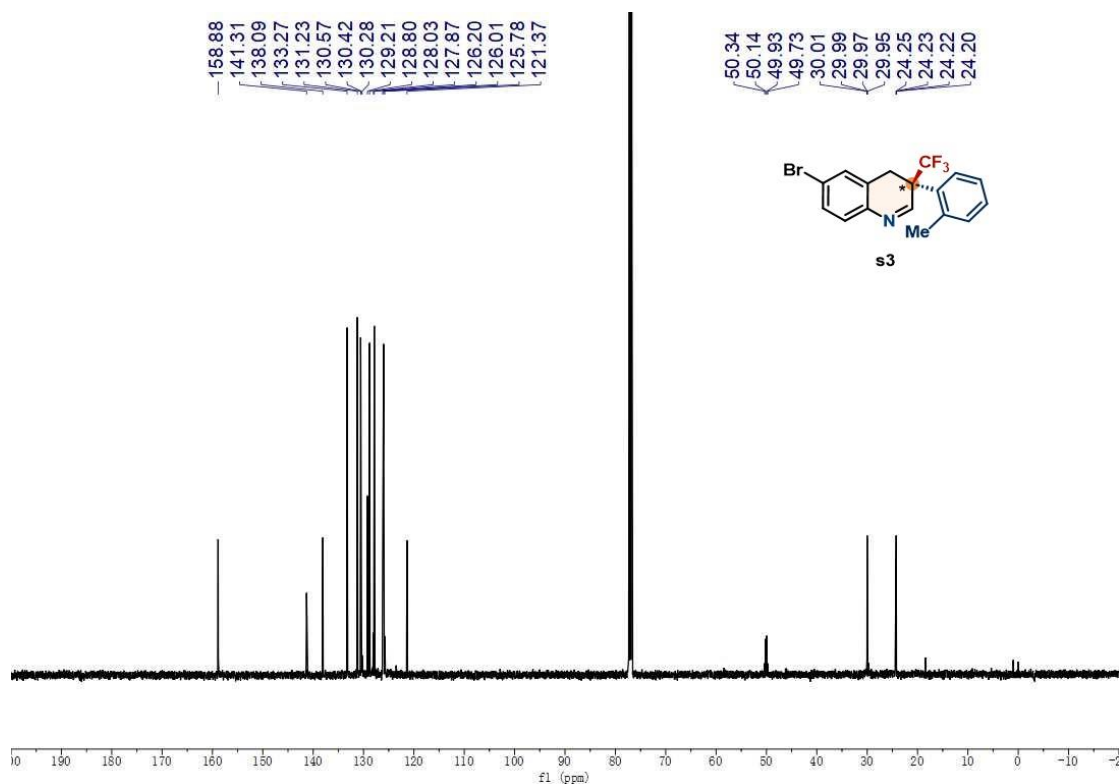
Supplementary Fig. S165. ¹³C NMR (125 MHz, CDCl₃) Spectrum of s2



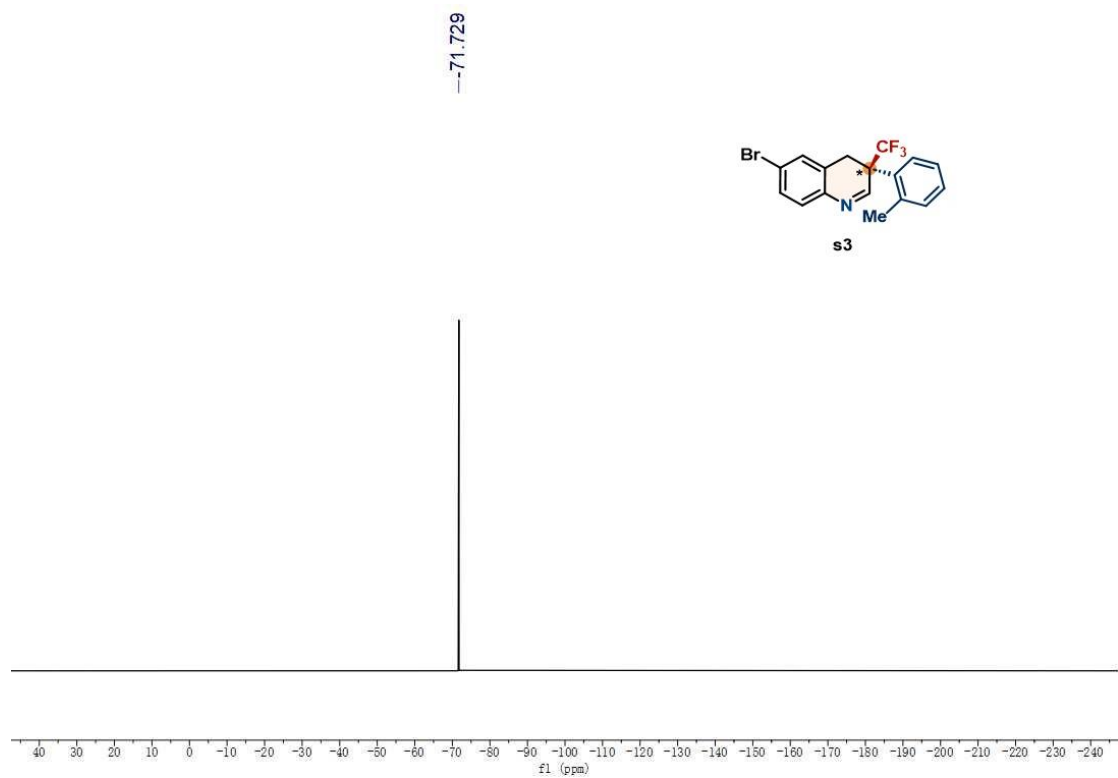
Supplementary Fig. S166. ¹⁹F NMR (470 MHz, CDCl₃) Spectrum of s2



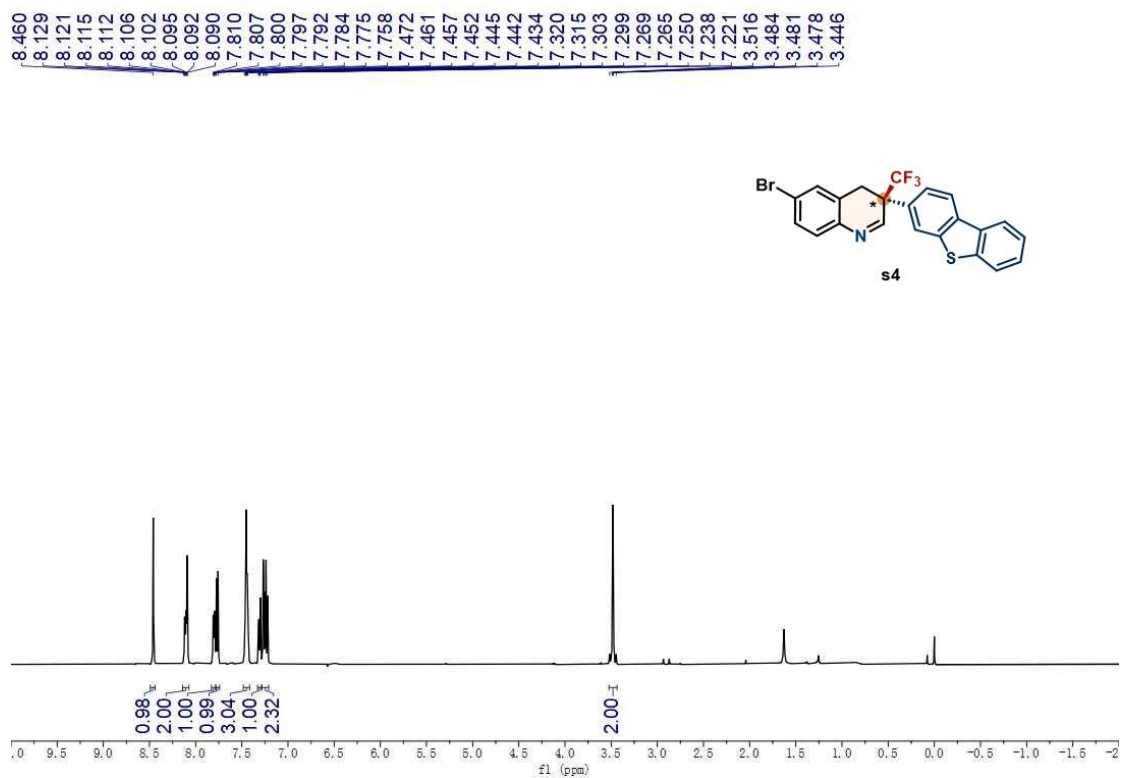
Supplementary Fig. S167. ¹H NMR (500 MHz, CDCl₃) Spectrum of s3



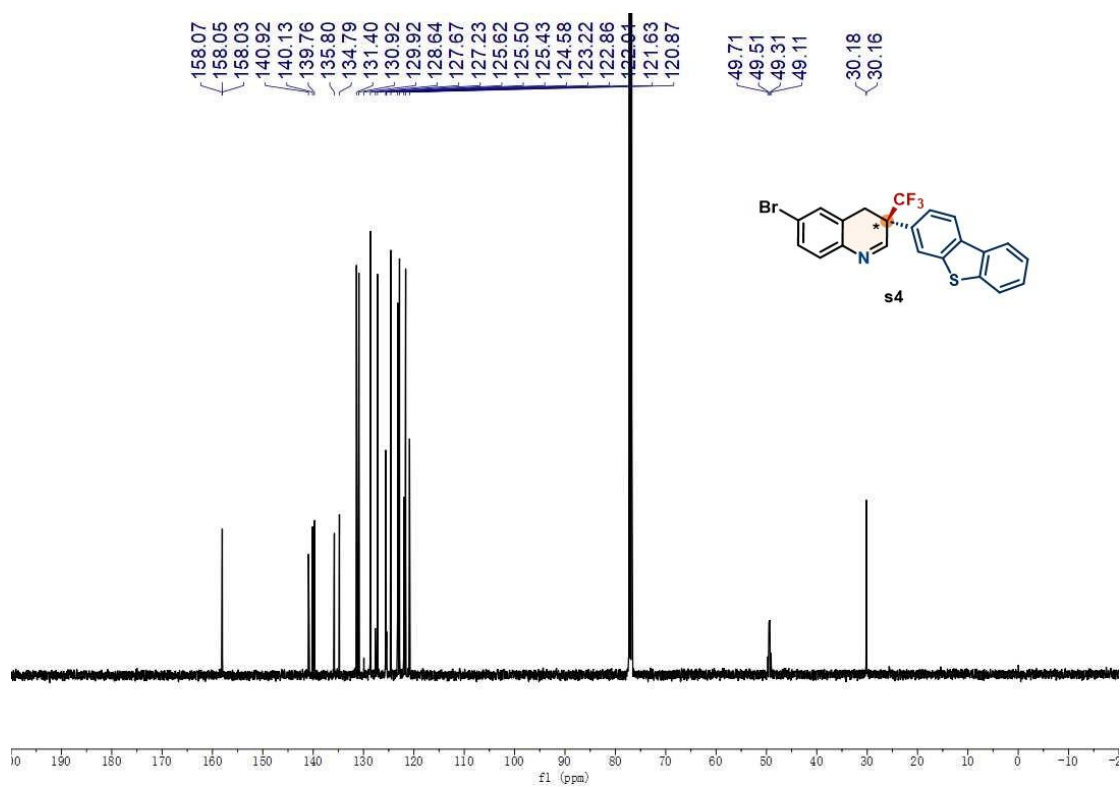
Supplementary Fig. S168. ¹³C NMR (125 MHz, CDCl₃) Spectrum of s3



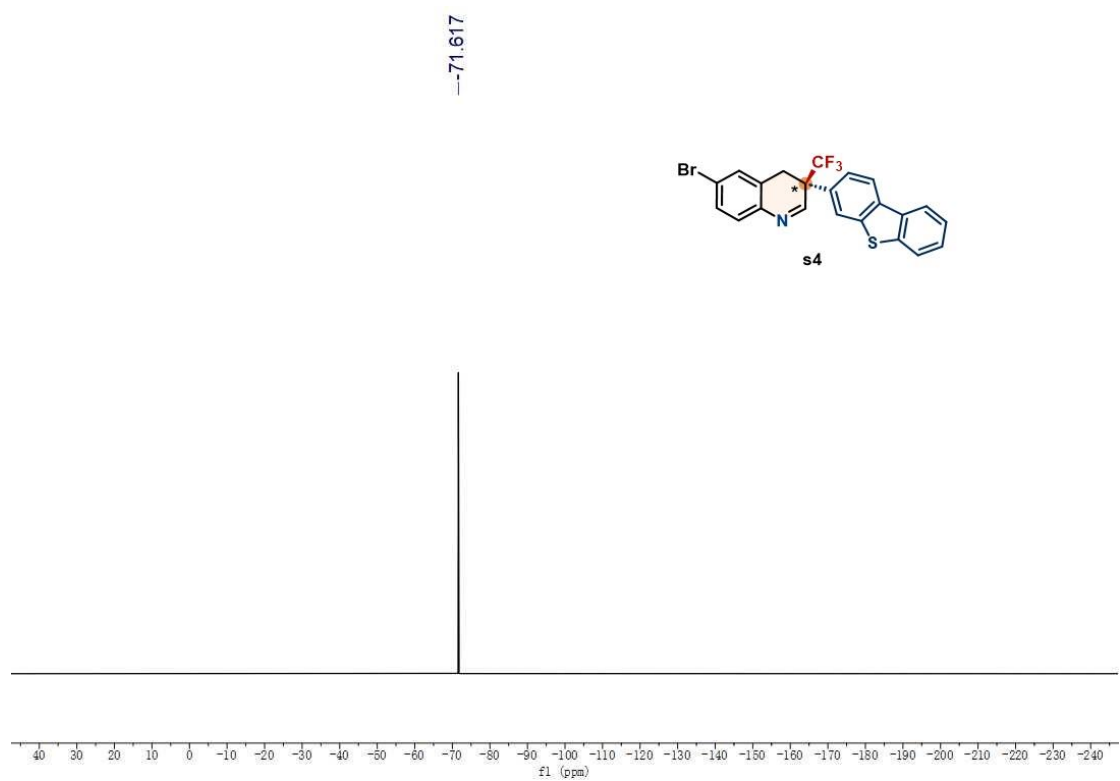
Supplementary Fig. S169. ^{19}F NMR (470 MHz, CDCl_3) Spectrum of **s3**



Supplementary Fig. S170. ^1H NMR (500 MHz, CDCl_3) Spectrum of **s4**



Supplementary Fig. S171. ¹³C NMR (125 MHz, CDCl₃) Spectrum of **s4**



Supplementary Fig. S172. ¹⁹F NMR (470 MHz, CDCl₃) Spectrum of **s4**

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