Axially chiral styrene-based organocatalysts and their application in asymmetric cascade Michael/cyclization reaction

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Content

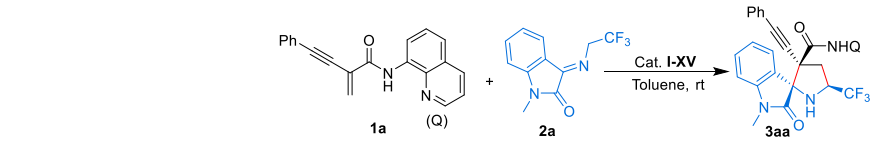
1. General information

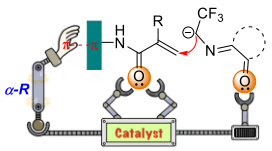
Reagents: All commercial materials were used as received unless otherwise noted. All other solvents (DCM, DCE, THF, et al) used in this manuscript were purchased from Energy in anhydrous form. Toluene and Et_2O were purified by standard procedures prior to use.

Enynamide **1a-1y** were prepared according to the literature procedure.[1]
Isatinimine **2a-2g** were prepared according to the literature procedure.[2]

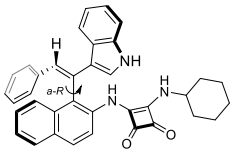
Instruments: Flash chromatography was carried out on 200-300 mesh silica gel, eluting with a mixture of petroleum ether (b.p. 60-90 °C) and ethyl acetate. ^{1}H NMR and ^{13}C NMR spectra were acquired on a Bruker AVANCE III HD spectrometer (400M or 500M) and calibrated using residual solvent peaks as internal reference. Enantiomeric excesses were measured on an Agilent HPLC. Optical rotations were measured on a Rudolph Research Analytical (Autopol VI). High resolution mass spectra (HRMS) were operated on a Bruker Daltonics SolariX 7.0 Tesla Fourier Transform Ion Cyclotron Resonance (FT-ICR) Mass Spectrometer using the electrospray ionization (ESI) technique.

Table S1. Optimization of the Catalyst [a]

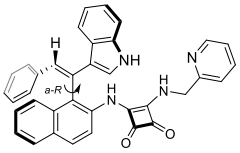




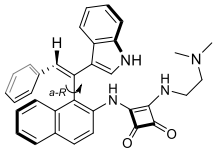
type A
Racemic amine



Cat. **I**
n.d



Cat. **II**
45%[b], 15% ee[c], 1:1 dr[d]

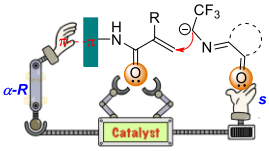


Cat. **III**
49%, 30% ee, 9:1 dr

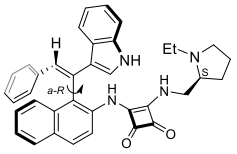
Et_3N
~ 10% yield

DABCO
Complex

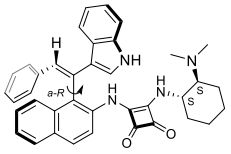
Et_3N + Cat.**I**
21% yield, 3% ee



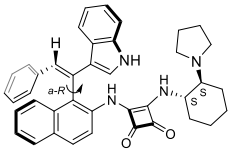
type B
Chiral matched amine



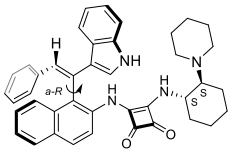
Cat. **IV**
52%, 73% ee, 8:1 dr



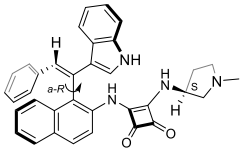
Cat. **V**
57%, 81% ee, 12:1 dr



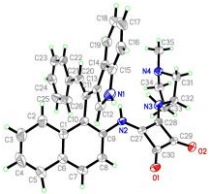
Cat. **VI**
60%, 81% ee, 14:1 dr



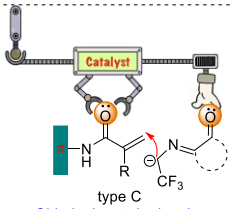
Cat. **VII**
58%, 49% ee, 7:1 dr



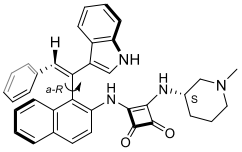
Cat. **VIII**
78%, 90% ee, 12:1 dr



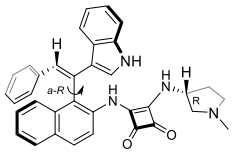
X-ray structure of Cat. **VIII**



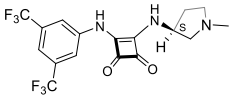
type C
Chiral mismatched amine



Cat. **IX**
35%, -29% ee, 9:1 dr

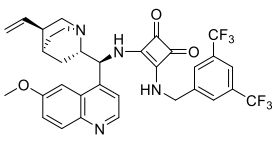


Cat. **X**
75%, -37% ee, 10:1 dr

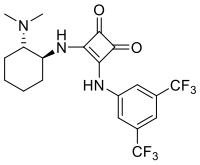


Cat. **XI**
72%, 59% ee, 4:1 dr

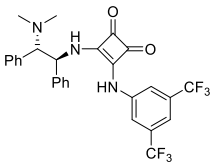
Commercially available catalysts



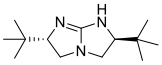
Cat. **XII**
75%, 68% ee, 15:1 dr



Cat. **XIII**
58%, 53% ee, 12:1 dr



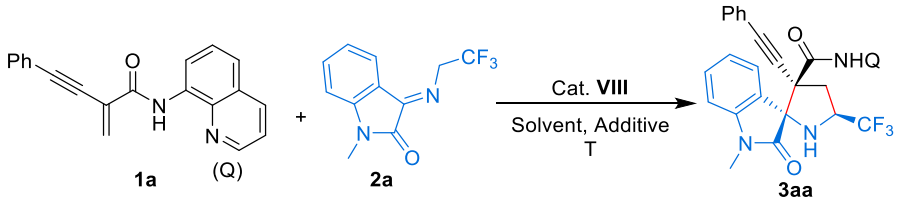
Cat. **XIV**
37%, 28% ee, 8:1 dr



Cat. **XV**
<10% yield

[a] Reaction conditions: **1a** (0.1 mmol), **2a** (0.15 mmol) and organocatalyst (10 mol%) in Toluene (1.0 mL) stirred at the indicated temperature for 12 h. [b] Isolated yield. [c] The ee value was determined by HPLC analysis. [d] The dr value was determined by ^{1}H NMR analysis.

Table S2. Asymmetric Cascade Michael/Cyclization Reaction [a]



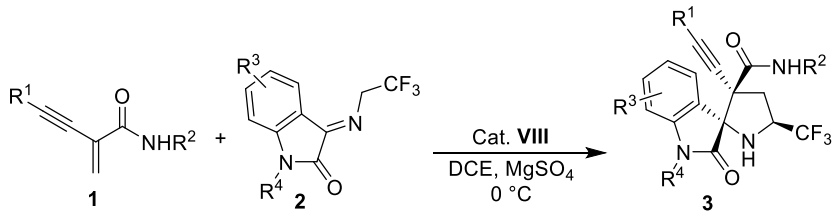
entry	solvent	additive	T (°C)	yield (%)[b]	ee (%)[c]	dr[d]
1	Toluene	----	rt	78	90	12:1
2	DCM	----	rt	81	89	13:1
3	Et_2O	----	rt	46	69	8:1
4	DCE	----	rt	83	91	13:1
5	DCE	----	0	81	92	14:1
6	DCE	3Å MS	0	80	92	14:1
7	DCE	4Å MS	0	81	94	14:1
8	DCE	5Å MS	0	78	93	14:1
9	DCE	$MgSO_4$	0	82	94	14:1

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (0.3 mmol), additive (60 mg) and Cat. **VIII** (10 mol%) in solvent (2.0 mL) stirred at the indicated temperature for 24 h. [b] Isolated yield. [c] The ee value was determined by HPLC analysis. [d] The dr value was determined by ^{1}H NMR analysis.

The results of 4Å MS as additive and $MgSO_4$ as additive in the template reaction were comparable, but the overall results in the substrate expansion were better with $MgSO_4$, so $MgSO_4$ was selected as an additive.

2. General procedure for synthesis of the products

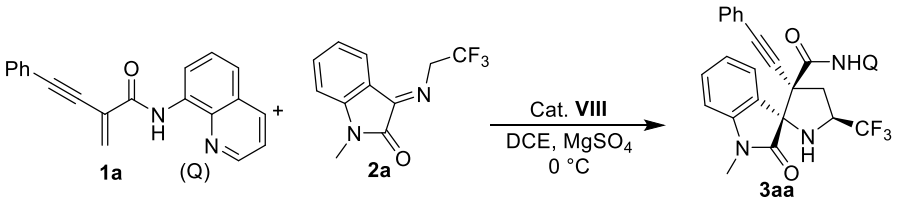
2.1 General procedure for the synthesis of spiro[pyrrolidin-3,20-oxindole] 3



1 2 3

To a mixture of enynamide **1** (0.2 mmol), *N*-2,2,2-trifluoroethylisatin **2** (0.3 mmol), $MgSO_4$ (60 mg) and Cat. **VIII** (0.02 mmol, 10 mol%, 10.7 mg) was added DCE (2.0 mL). Then reaction mixture was stirred at 0 ℃ for 24 hours. Next, the reaction mixture was concentrated under reduced pressure. The resulting residue was purified by flash column chromatography to give the corresponding spiro[pyrrolidin-3,2′-oxindole] **3**.

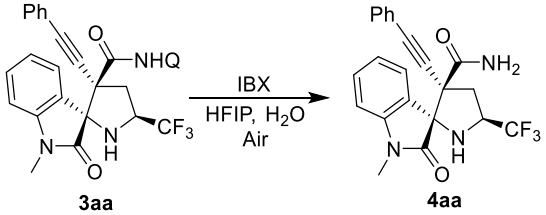
2.2 Gram scale synthesis



1a (Q) 2a 3aa

To a mixture of enynamide **1a** (596 mg, 2 mmol), *N*-2,2,2-trifluoroethylisatin **2a** (726 mg, 3 mmol), $MgSO_4$ (600 mg) and Cat. **VIII** (108 mg, 0.2 mmol, 10 mol%) was added DCE (20 mL). Then reaction mixture was stirred at 0 ℃ for 24 hours. Next, the reaction mixture was concentrated under reduced pressure. The resulting residue was purified by flash column chromatography to give the corresponding spiro[pyrrolidin-3,2′-oxindole] **3aa** (886 mg, 82% yield, 93% ee, 13:1 dr).

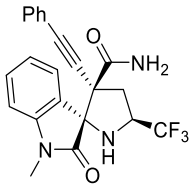
2.3 Synthetic applicability experiments



3aa 4aa

To a dried sealing tube were added (3*R*,3'*R*,5'*S*)-1-methyl-2-oxo-3'-(phenylethynyl)-*N*-(quinolin-8-yl)-5'-(trifluoromethyl)spiro[indoline-3,2'-pyrrolidine]-3'-carboxamide **3aa** (84 mg, 0.1 mmol, 1.0 eq) and IBX (56 mg, 0.2 mmol, 2.0 eq). The mixture in 2.0 mL of mixed solvent (V_{HFIP}/V_{H2O} = 1:1) was stirred at 60 °C in oil bath under air atmosphere for 5 h. The reaction was quenched by the addition of $NaHCO_3$ (aq. 3.0 mL), extracted with dichloromethane, dried over

anhydrous Na_2SO_4. Then the organic solvent was concentrated under reduced pressure and resulting residue was purified by silica gel flash column (petroleum ether/ethyl acetate = 1/1) to give primary amide product **4aa** as a yellow solid (60 mg, 72% yield).[3]

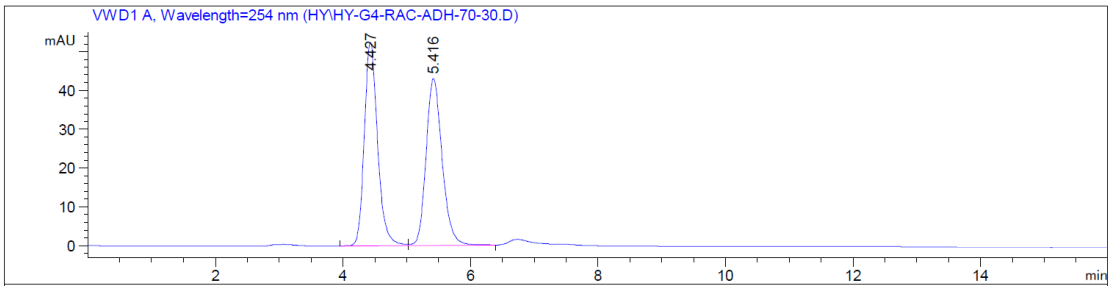


4aa

60 mg, 72% yield, white soild. $[\alpha]^{20}_D$ -202.80 (c 0.5, $CHCl_3$, 99% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 80:20, 1.0 mL/min, 254 nm): tR (minor) = 4.4 min, tR (major) = 5.4 min.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.77 (d, J = 7.4 Hz, 1H), 7.51 – 7.45 (m, 2H), 7.43 – 7.36 (m, 4H), 7.10 (t, J = 7.6 Hz, 1H), 6.83 (d, J = 7.8 Hz, 1H), 5.62 (s, 1H), 5.43 (s, 1H), 4.45 – 4.36 (m, 1H), 3.77 (t, J = 11.6 Hz, 1H), 3.14 (s, 3H), 2.56 (dd, J = 12.2, 6.0 Hz, 2H), 1.87 (s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 175.6, 168.3, 145.2, 131.7, 130.9, 129.3, 128.6, 125.8, 125.7 (q, J_{CF} = 279.3 Hz), 125.0, 122.2, 121.4, 108.4, 88.7, 86.5, 70.8, 58.2 (q, J_{CF} = 32.3 Hz), 57.6, 35.2, 26.3. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.1. **HRMS**: calculated for $C_{22}H_{19}F_3N_3O_2$ [M+H$^+$] 414.1424, found 414.1432.



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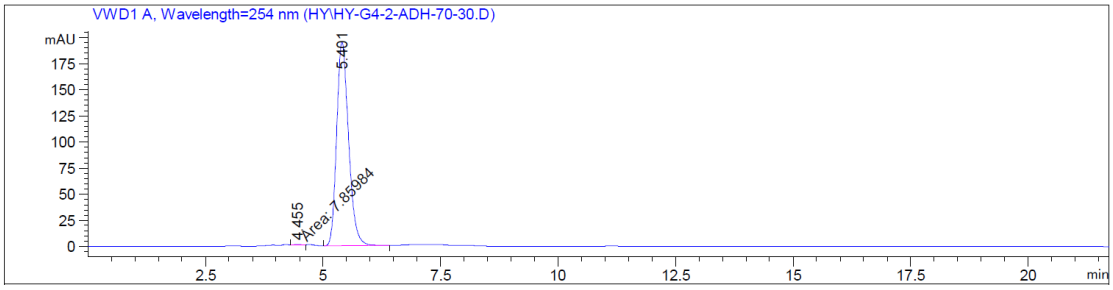
2	5.416	VB	0.2681	752.19098	42.98846	49.8300



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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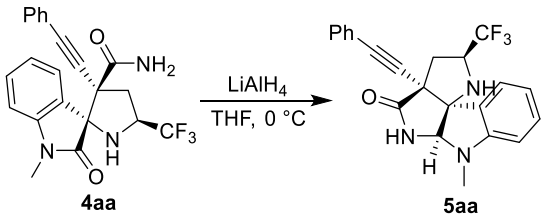
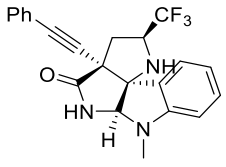
2	5.401	BB	0.2716	3444.35840	195.49182	99.7723



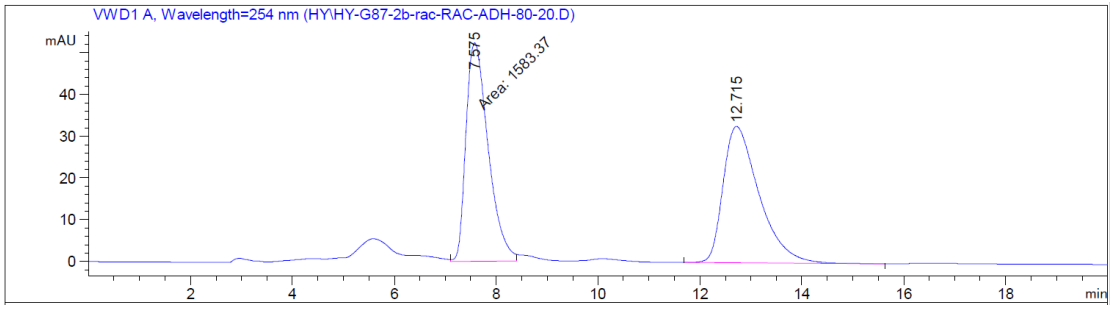
To primary amide **11a** (65 mg, 0.15 mmol, 1.0 eq) in THF (10 mL) at 0 °C, $LiAlH_4$ (74 mg, 1.9 mmol, 13 eq) was added under nitrogen atmosphere. The resulting mixture was stirred for 2 hours at 0 °C, and then quenched with several drops of saturated brine. The reaction mixture was subsequently washed with ethyl acetate. The combined organic layers were dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by silica gel chromatography (PE/EA = 4/1), affording product **11b** (24 mg) as a yellow oil in 41% yield with 99% ee.[4]



24 mg, 41% yield, yellow oil. $[\alpha]^{20}_D$ -102.60 (c 0.5, $CHCl_3$, 99% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 80:20, 1.0 mL/min, 254 nm): tR (minor) = 7.6 min, tR (major) = 12.6 min.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, J = 7.5 Hz, 1H), 7.30 – 7.13 (m, 6H), 6.82 (t, J = 7.5 Hz, 1H), 6.62 (s, 1H), 6.51 (d, J = 7.9 Hz, 1H), 4.93 (s, 1H), 4.46 – 4.34 (m, 1H), 2.89 (s, 3H), 2.85 (dd, J = 13.8, 8.1 Hz, 1H), 2.72 (dd, J = 13.8, 7.5 Hz, 1H), 2.65 – 2.53 (s, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 174.8, 150.8, 131.7, 130.8, 128.4, 128.1, 127.4, 125.4 (q, J_{CF} = 279.5 Hz), 124.7, 122.3, 118.2, 107.4, 87.5, 85.7, 85.4, 81.0, 60.2 (q, J_{CF} = 31.5 Hz), 55.1, 38.3, 32.6. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -77.1. **HRMS**: calculated for $C_{22}H_{19}F_3N_3O$ [M+H$^+$] 398.1475, found 398.1472.



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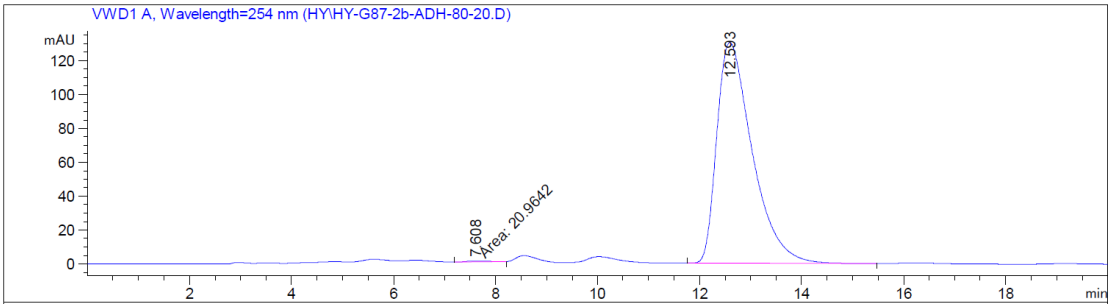

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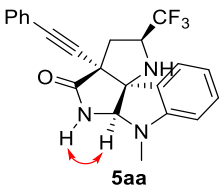
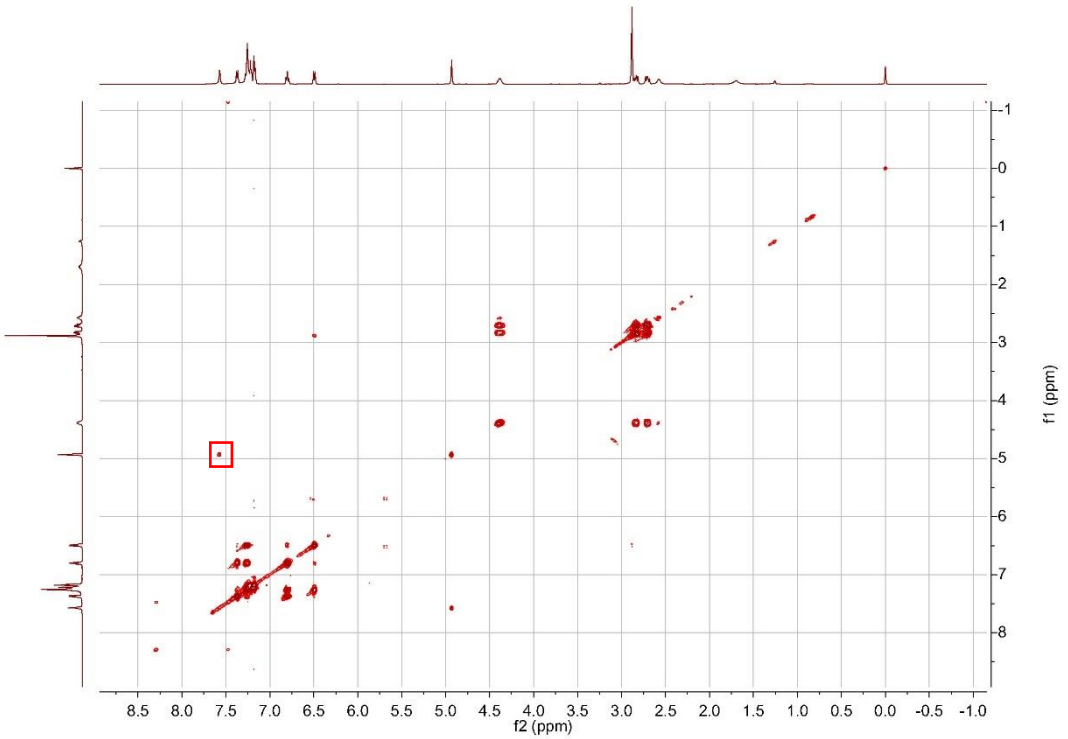
2	12.593	BB	0.7313	6294.61377	130.38011	99.6681

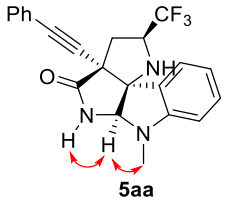
Cosy spectra



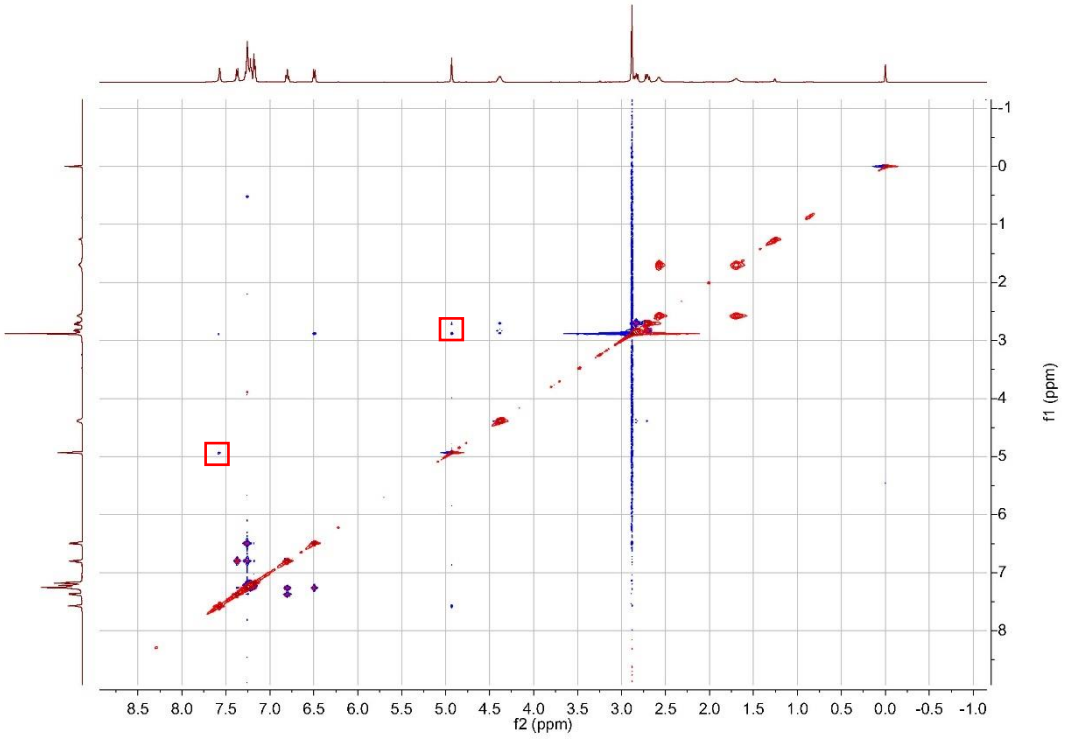
5aa



Noesy spectra

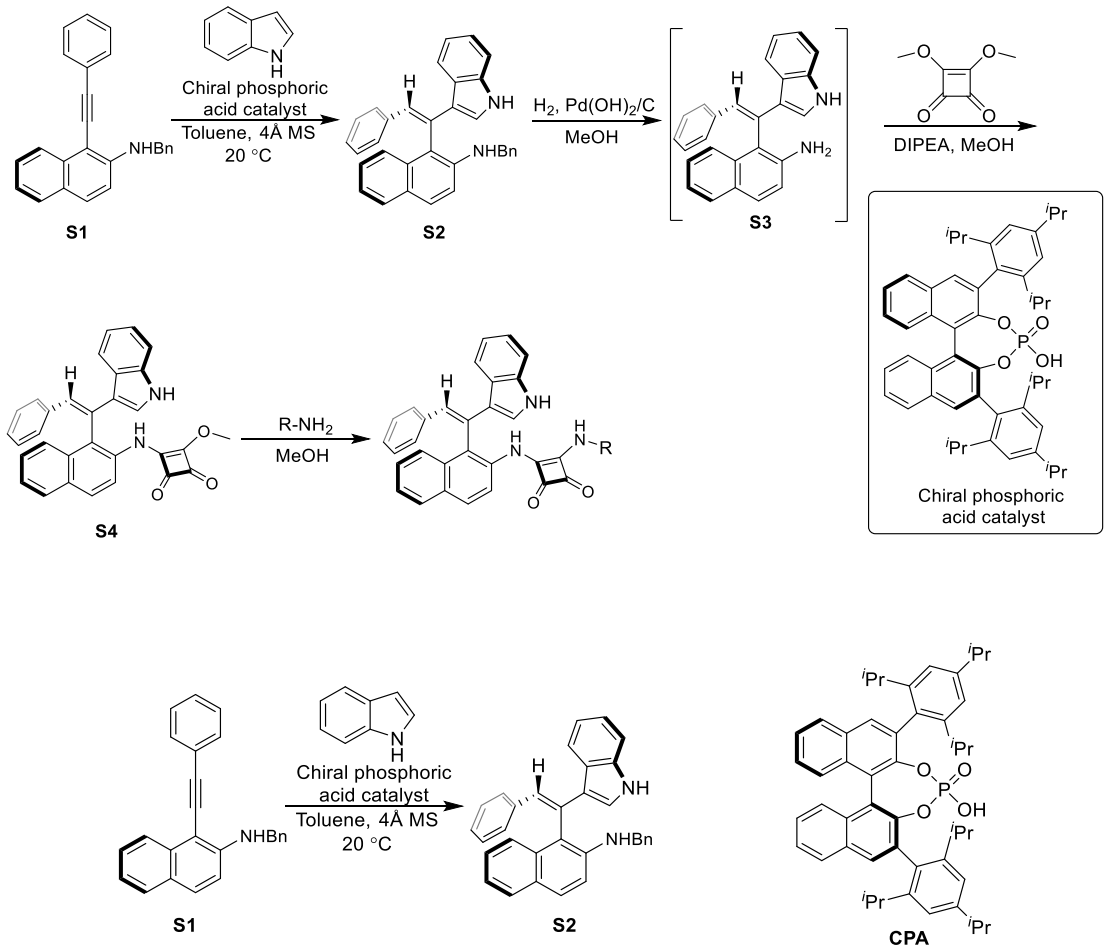


5aa

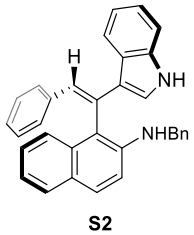


3. The synthesis of catalysts

Figure S1: Synthesis route of catalysts



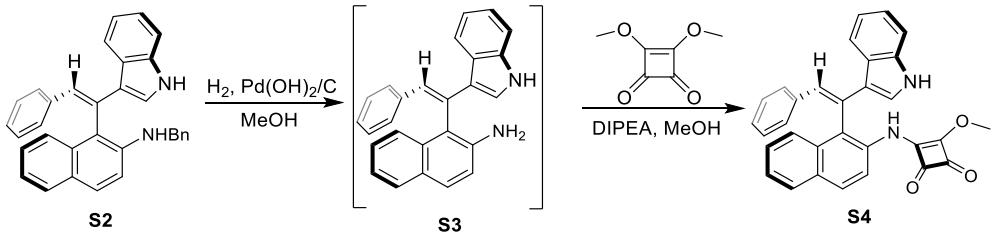
To a solution of **S1** (3.2 g, 9.6 mmol, 1.0 eq), **CPA** (242.8 mg, 0.96 mmol, 0.1 eq) and 4Å MS (4.8 g) in toluene (96 mL), indole (1.7 g, 14.4 mmol, 1.5 eq) was added in one portion at 20 ºC and monitored by TLC. After stirring for 48 h, the mixture was directly purified through flash column chromatography on silica gel to give the pure product **S2**.[5]



S2

3.8 g, 89% yield, yellow foam. $[\alpha]^{20}_{D}$ -152.40 (c 0.5, $CHCl_3$)

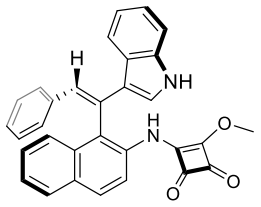
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (m, 8.20 – 8.11, 1H), 7.93 (s, 1H), 7.75 – 7.69 (m, 1H), 7.72 – 7.67 (m, 1H), 7.67 (dd, J = 8.4, 1.2 Hz, 1H), 7.65 (s, 1H), 7.38 – 7.31 (m, 1H), 7.25 (m, 7.28 – 7.24, 2H), 7.24 – 7.12 (m, 2H), 7.13 – 7.06 (m, 2H), 7.09 – 6.98 (m, 7H), 6.88 – 6.83 (m, 2H), 6.59 (d, J = 2.7 Hz, 1H), 4.81 (t, J = 6.3 Hz, 1H), 4.37 – 4.22 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 141.9, 139.7, 137.5, 137.3, 133.1, 131.4, 128.9, 128.4, 128.3, 128.2, 127.9, 127.9, 127.4, 126.9, 126.8, 126.6, 126.6, 125.6, 125.3, 124.5, 122.5, 121.9, 120.9, 120.7, 118.5, 118.1, 114.1, 111.7, 47.8. **HRMS**: calculated for $C_{33}H_{27}N_2^+$ [M+H$^+$] 451.2169, found 451.2175.



S2 **S3** **S4**

S2 (900 mg, 2.0 mmol, 93% ee), $Pd(OH)_2/C$ (90 mg) and MeOH (20 mL) was placed in a hydrogenation tube equipped with a stirring bar. The hydrogenation tube was then put into an autoclave. The system was filled and evacuated with hydrogen for 3 times. The autoclave was pressurized with hydrogen to 7.5 bar hydrogen pressure, and the reaction mixture was stirred at 50 °C for 24 h. After the completion of the reaction, the mixture was filtered and the solvent was evaporated to afford the crude product **S3**.

To a flame-dried round bottom flask equipped with a stir bar, **S3** (235 mg, 0.5 mmol, 99% ee), *N′,N′*-dimethylethane-1,2-diamine (183 mg, 0.62 mmol), DIPEA (26 μL, 0.25 mmol) and $MeOH/CH_2Cl_2$ (4:1, 5.0 mL) was added and the mixture was stirred at 50 ºC for 4 h. After the completion of the reaction, the mixture was filtered and the solid was purified through flash chromatography on silica gel eluted with PE/EA to afford Cat. **II** 250 mg (95% yield) as a white solid. [5]

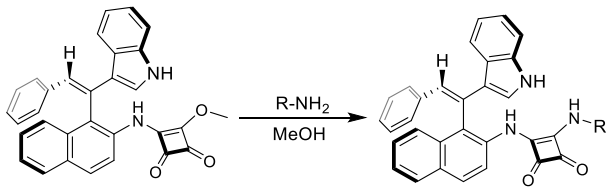


S4

250 mg, 95% yield, white soild. $[\alpha]^{20}_D$ -204.00 (c 0.5, DMSO)

^{1}H NMR (400 MHz, DMSO) δ 11.19 (d, J = 1.6, 1H), 10.42 (s, 1H), 7.99 (dd, J = 13.8, 8.5 Hz, 2H), 7.77 (dd, J = 16.1, 8.2 Hz, 2H), 7.54 (s, 1H), 7.50 – 7.38 (m, 3H), 7.34 (t, J = 7.4 Hz, 1H), 7.14 (t, J = 7.5 Hz, 1H), 7.05 (t, J = 7.5 Hz, 1H), 7.02 – 6.92 (m, 3H), 6.85 – 6.78 (m, 2H), 6.74 (d, J = 2.5 Hz, 1H), 4.10 (s, 3H). **^{13}C NMR** (101 MHz, DMSO) δ 188.0, 183.9, 177.7, 170.4, 137.5, 137.1, 132.5, 131.8, 131.6, 130.5, 130.1, 128.3, 128.2, 127.9, 127.8, 126.9, 126.4, 126.1, 126.1, 125.7, 124.7, 123.9, 121.6, 120.1, 119.8, 117.4, 112.0, 59.9.

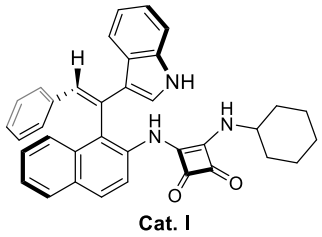
HRMS: calculated for $C_{31}H_{22}N_2NaO_3^+$ [M+Na$^+$] 493.1523, found 493.1520.



S4 **Catalyst**

To a flame-dried round bottom flask equipped with a stir bar, **S4** (47 mg, 0.1 mmol, 99% ee), R-NH_2 (0.12 mmol) and MeOH (1.0 mL) was added and the mixture was stirred at 60 ºC for 4 h. After the completion of the reaction, the mixture was filtered and the solid was purified through

flash chromatography on silica gel eluted with DCM/MeOH to afford catalyst. [5]



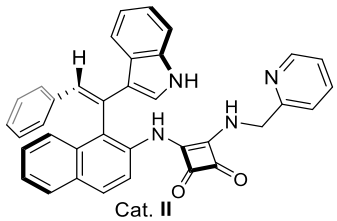
Cat. I

51 mg, 92% yield, yellow soild. $[\alpha]^{20}_{D}$ 29.60 (c 0.5, DMSO)

^{1}H NMR (400 MHz, DMSO) δ 11.24 (s, 1H), 8.86 (s, 1H), 8.06 – 7.95 (d, J = 8.8 Hz, 2H), 7.92 (d, J = 8.1 Hz, 1H), 7.82 – 7.68 (m, 3H), 7.61 (s, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.36 (t, J = 7.3 Hz, 1H), 7.28 (t, J = 7.5 Hz, 1H), 7.15 (t, J = 7.5 Hz, 1H), 7.07 (t, J = 7.5 Hz, 1H), 7.02 – 6.95 (m, 3H), 6.94 – 6.89 (m, 2H), 6.86 (s, 1H), 3.76 (s, 1H), 1.96 – 1.77 (m, 2H), 1.65 (d, J = 15.1 Hz, 2H), 1.54 (d, J = 11.2 Hz, 1H), 1.36 – 1.03 (m, 5H).

^{13}C NMR (101 MHz, DMSO) δ 184.3, 179.9, 168.2, 164.1, 137.2, 133.6, 131.5, 130.6, 130.3, 128.2, 128.0, 127.7, 126.8, 126.7, 126.4, 126.0, 125.7, 125.0, 124.8, 124.8, 122.4, 121.7, 120.1, 119.9, 117.2, 112.2, 54.9, 52.5, 34.0, 33.6, 24.7, 24.3.

HRMS: calculated for $C_{36}H_{31}N_3NaO_2^+$ [M+Na$^+$] 560.2308, found 560.2305.

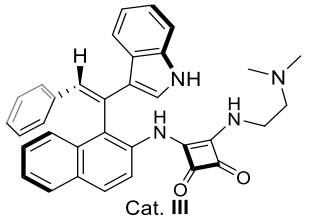


Cat. II

38 mg, 67% yield, yellow soild. $[\alpha]^{20}_{D}$ 46.40 (c 0.5, DMSO)

^{1}H NMR (400 MHz, DMSO) δ 11.23 (s, 1H), 9.12 (s, 1H), 8.64 (t, J = 5.6 Hz, 1H), 8.53 (d, J = 3.8 Hz, 1H), 8.00 (d, J = 8.9 Hz, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.87 – 7.74 (m, 3H), 7.71 (d, J = 8.4 Hz, 1H), 7.61 (s, 1H), 7.41 (d, J = 8.0 Hz, 1H), 7.37 (t, J = 7.4 Hz, 1H), 7.32 – 7.26 (m, 3H), 7.15 (t, J = 7.2 Hz, 1H), 7.07 (t, J = 7.4 Hz, 1H), 6.98 – 6.93 (m, 3H), 6.93 – 6.86 (m, 2H), 6.83 (d, J = 1.8 Hz, 1H), 4.93 – 4.69 (m, 2H). **^{13}C NMR** (101 MHz, DMSO) δ 184.6, 180.3, 168.9, 164.3, 157.2, 149.2, 137.3, 133.5, 131.5, 130.6, 128.0, 127.7, 126.8, 126.4, 125.7, 124.9, 122.7, 121.7, 120.1, 119.9, 117.1, 112.2, 64.9, 48.2, 15.2.

HRMS: calculated for $C_{36}H_{26}N_4NaO_2^+$ [M+Na$^+$] 569.1948, found 569.1942.

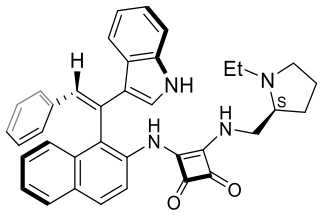


Cat. III

46 mg, 87% yield, yellow soild. $[\alpha]^{20}_{D}$ 120.00 (c 0.5, DMSO)

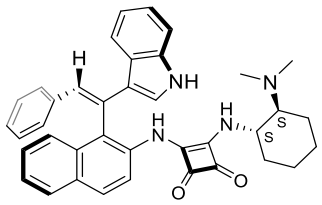
^{1}H NMR (400 MHz, DMSO) δ 11.24 (s, 1H), 9.14 (s, 1H), 8.16 – 8.05 (m, 1H), 8.00 (d, J = 9.0 Hz, 1H), 7.93 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.75 (dd, J = 15.2, 8.7 Hz, 2H), 7.64 (s, 1H), 7.42 (d, J = 8.0 Hz, 1H), 7.37 (t, J = 7.1 Hz, 1H), 7.29 (t, J = 7.2 Hz, 1H), 7.16 (t, J = 7.3 Hz, 1H),

7.09 (t, *J* = 7.2 Hz, 1H), 7.04 – 6.97 (m, 3H), 6.96 – 6.91 (m, 2H), 6.83 (s, 1H), 3.70 – 3.53 (m, 2H), 2.35 (t, *J* = 5.7 Hz, 2H), 2.11 (s, 6H). **^{13}C NMR** (101 MHz, DMSO) *δ* 185.3, 180.6, 169.4, 164.6, 137.8, 137.7, 134.1, 131.9, 131.0, 130.8, 128.6, 128.5, 128.5, 128.2, 127.2, 127.1, 126.8, 126.6, 126.2, 125.4, 125.3, 125.2, 122.9, 122.2, 120.7, 120.4, 117.5, 112.6, 59.8, 45.5, 41.6.
HRMS: calculated for $C_{34}H_{31}N_4O_2^+$ [M+H$^+$] 527.2442, found 527.2436.



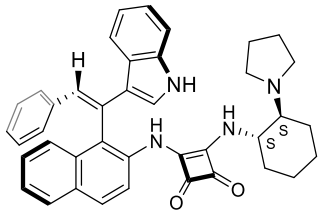
Cat. **IV**

54 mg, 95% yield, yellow soild. $[\alpha]^{20}_D$ 28.80 (c 0.5, DMSO)
^{1}H NMR (400 MHz, DMSO) *δ* 11.25 (s, 1H), 9.08 (s, 1H), 8.01 (d, *J* = 8.9 Hz, 2H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.81 (d, *J* = 8.9 Hz, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.65 (s, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.33 – 7.27 (m, 1H), 7.17 (t, *J* = 7.2 Hz, 1H), 7.10 (t, *J* = 7.3 Hz, 1H), 7.02 – 6.98 (m, 3H), 6.97 – 6.93 (m, 2H), 6.84 (s, 1H), 3.69 – 3.57 (m, 1H), 3.48-3.40 (m, 1H), 2.91 (t, *J* = 6.8 Hz, 1H), 2.80 – 2.68 (m, 1H), 2.51 – 2.44 (m, 1H), 2.25 – 2.14 (m, 1H), 2.07 (q, *J* = 8.9 Hz, 1H), 1.79 – 1.66 (m, 1H), 1.58 – 1.35 (m, 3H), 0.95 (t, *J* = 7.1 Hz, 3H).
^{13}C NMR (101 MHz, DMSO) *δ* 184.7, 180.1, 169.4, 164.1, 137.3, 137.2, 133.7, 131.4, 130.6, 130.3, 128.2, 128.0, 127.8, 126.7, 126.4, 126.1, 125.7, 125.0, 124.8, 124.7, 122.4, 121.7, 120.1, 119.9, 117.1, 112.1, 63.3, 53.1, 48.1, 46.4, 27.7, 22.6, 13.6.
HRMS: calculated for $C_{37}H_{35}N_4O_2^+$ [M+H$^+$] 567.2755, found 567.2748.



Cat. **V**

49 mg, 85% yield, yellow soild. $[\alpha]^{20}_D$ 63.60 (c 0.5, DMSO)
^{1}H NMR (400 MHz, DMSO) *δ* 11.24 (s, 1H), 9.14 (s, 1H), 8.16 – 8.05 (m, 1H), 8.00 (d, *J* = 9.0 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.75 (dd, *J* = 15.2, 8.7 Hz, 2H), 7.64 (s, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 7.1 Hz, 1H), 7.29 (t, *J* = 7.2 Hz, 1H), 7.16 (t, *J* = 7.3 Hz, 1H), 7.09 (t, *J* = 7.2 Hz, 1H), 7.04 – 6.97 (m, 3H), 6.96 – 6.91 (m, 2H), 6.83 (s, 1H), 3.70 – 3.53 (m, 2H), 2.35 (t, *J* = 5.7 Hz, 2H), 2.11 (s, 6H). **^{13}C NMR** (101 MHz, DMSO) *δ* 185.3, 180.6, 169.4, 164.6, 137.8, 137.7, 134.1, 131.9, 131.0, 130.8, 128.6, 128.5, 128.5, 128.2, 127.2, 127.1, 126.8, 126.6, 126.2, 125.4, 125.3, 125.2, 122.9, 122.2, 120.7, 120.4, 117.5, 112.6, 59.8, 45.5, 41.6.
HRMS: calculated for $C_{38}H_{37}N_4O_2^+$ [M+H$^+$] 581.2911, found 581.2918.

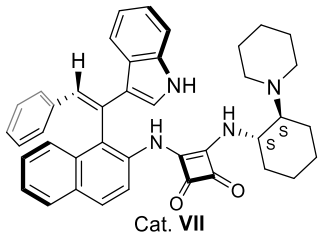


Cat. **VI**

52 mg, 86% yield, yellow soild. $[\alpha]^{20}_{D}$ 43.60 (c 0.5, DMSO)

^{1}H NMR (400 MHz, DMSO) δ 11.25 (s, 1H), 8.91 (s, 1H), 7.95 (dd, J = 24.3, 8.4 Hz, 3H), 7.84 – 7.68 (m, 3H), 7.60 (s, 1H), 7.40 (d, J = 8.0 Hz, 1H), 7.36 (t, J = 7.2, 1H), 7.28 (t, J = 7.6, 1H), 7.14 (t, J = 7.2, 1H), 7.06 (t, J = 7.2, 1H), 6.96 (s, 3H), 6.93 – 6.88 (m, 2H), 6.86 (s, 1H), 3.92 (s, 1H), 2.40 – 2.21 (m, 3H), 1.91 (s, 1H), 1.76 – 1.54 (m, 4H), 1.44 (s, 4H), 1.34 – 1.02 (m, 6H). **^{13}C NMR** (101 MHz, DMSO) δ 184.3, 179.7, 168.8, 163.8, 137.2, 133.6, 131.6, 130.5, 130.2, 128.2, 128.0, 127.7, 127.0, 126.6, 126.4, 125.9, 125.6, 125.0, 124.8, 122.4, 121.7, 120.1, 119.8, 117.3, 112.1, 62.3, 54.9, 47.5, 33.0, 23.7, 23.2.

HRMS: calculated for $C_{40}H_{39}N_4O_2^+$ [M+H$^+$] 607.3068, found 607.3060.

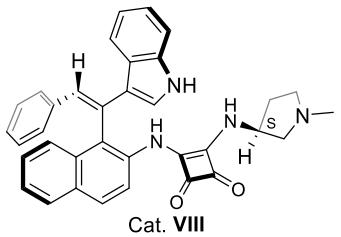


Cat. **VII**

48 mg, 77% yield, yellow soild. $[\alpha]^{20}_{D}$ 138.80 (c 0.5, DMSO)

^{1}H NMR (400 MHz, DMSO) δ 11.21 (s, 1H), 8.80 (s, 1H), 7.99 (d, J = 9.0 Hz, 1H), 7.92 (d, J = 8.1 Hz, 1H), 7.89 – 7.75 (m, 3H), 7.71 (d, J = 8.4 Hz, 1H), 7.62 (s, 1H), 7.41 – 7.32 (m, 2H), 7.28 (t, J = 7.5 Hz, 1H), 7.13 (t, J = 7.4 Hz, 1H), 7.07 (t, J = 7.4 Hz, 1H), 7.02 – 6.95 (m, 3H), 6.94 – 6.89 (m, 2H), 6.81 (d, J = 2.2 Hz, 1H), 3.96 – 3.77 (m, 1H), 2.45 (s, 2H), 2.06 (s, 3H), 1.99 – 1.89 (m, 1H), 1.83 – 1.52 (m, 4H), 1.32 – 0.92 (m, 11H). **^{13}C NMR** (101 MHz, DMSO) δ 184.6, 179.8, 169.5, 163.5, 137.3, 133.7, 131.4, 130.5, 130.3, 128.2, 128.0, 127.8, 126.7, 126.3, 125.8, 124.9, 124.8, 124.7, 121.6, 120.1, 119.8, 116.9, 112.1, 68.4, 54.9, 54.1, 49.3, 34.1, 26.1, 24.8, 24.6, 24.4, 23.6.

HRMS: calculated for $C_{41}H_{41}N_4O_2^+$ [M+H$^+$] 621.3224, found 621.3212.



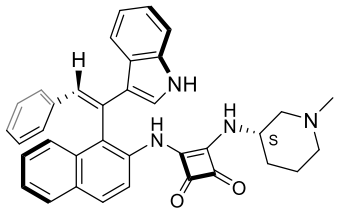
Cat. **VIII**

48 mg, 89% yield, yellow soild. $[\alpha]^{20}_{D}$ 114.40 (c 0.5, DMSO)

^{1}H NMR (400 MHz, DMSO) δ 11.25 (s, 1H), 9.05 (s, 1H), 8.37 (d, J = 8.7 Hz, 1H), 7.99 (d, J = 9.0 Hz, 1H), 7.92 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.78 (d, J = 8.9 Hz, 1H), 7.73 (d, J = 8.4 Hz, 1H), 7.64 (s, 1H), 7.42 (d, J = 8.1 Hz, 1H), 7.36 (t, J = 7.3 Hz, 1H), 7.28 (t, J = 7.4 Hz, 1H), 7.16 (t, J = 7.4 Hz, 1H), 7.09 (t, J = 7.4 Hz, 1H), 7.02 – 6.96 (m, 3H), 6.95 – 6.91 (m, 2H), 6.84 (s, 1H), 4.64 – 4.45 (m, 1H), 2.82 – 2.71 (m, 1H), 2.52 – 2.48 (m, 1H), 2.32 (dd, J = 9.6, 6.0 Hz, 1H),

2.27 – 2.21 (m, 1H), 2.18 (s, 3H), 2.08 (q, *J* = 8.4 Hz, 1H), 1.64 – 1.54 (m, 1H). **^{13}C NMR** (101 MHz, DMSO) *δ* 184.6, 180.0, 167.8, 163.9, 137.3, 133.6, 131.5, 130.6, 130.3, 128.2, 128.1, 127.7, 126.7, 126.4, 126.0, 125.7, 125.0, 124.9, 124.7, 122.3, 121.7, 120.2, 120.0, 117.1, 112.2, 62.8, 54.3, 53.4, 41.2, 33.5.

HRMS: calculated for $C_{35}H_{31}N_4O_2^+$ [M+H$^+$] 539.2442, found 539.2433.

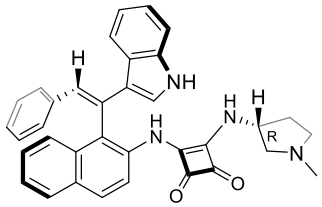


Cat. **IX**

43 mg, 78% yield, yellow soild. $[\alpha]^{20}_D$ 64.00 (c 0.5, DMSO)

^{1}H NMR (400 MHz, DMSO) *δ* 11.25 (d, *J* = 2.0 Hz, 1H), 9.18 (s, 1H), 8.19 (d, *J* = 8.4 Hz, 1H), 7.98 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.72 (dd, *J* = 15.4, 8.7 Hz, 2H), 7.62 (s, 1H), 7.42 (d, *J* = 8.0 Hz, 1H), 7.37 (t, *J* = 7.3 Hz, 1H), 7.28 (t, *J* = 7.4 Hz, 1H), 7.15 (t, *J* = 7.4 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 7.01 – 6.95 (m, 3H), 6.94 – 6.89 (m, 2H), 6.87 (d, *J* = 2.5 Hz, 1H), 4.15 (s, 1H), 2.46 – 2.35 (m, 1H), 2.34 – 2.13 (m, 3H), 2.09 (s, 3H), 1.72 – 1.57 (m, 2H), 1.53 – 1.33 (m, 2H). **^{13}C NMR** (101 MHz, DMSO) *δ* 184.4, 180.2, 168.1, 164.3, 137.3, 137.2, 133.6, 131.5, 130.7, 130.3, 128.1, 128.0, 127.7, 126.8, 126.6, 126.4, 126.3, 125.7, 125.1, 124.9, 124.8, 122.8, 121.7, 120.1, 119.9, 117.3, 112.2, 60.1, 54.9, 49.4, 46.0, 30.2, 21.5.

HRMS: calculated for $C_{36}H_{33}N_4O_2^+$ [M+H$^+$] 553.2598, found 553.2595.

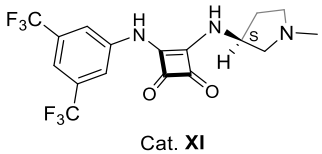


Cat. **X**

46 mg, 85% yield, yellow soild. $[\alpha]^{20}_D$ 35.60 (c 0.5, DMSO)

^{1}H NMR (400 MHz, DMSO) *δ* 11.22 (s, 1H), 9.02 (s, 1H), 8.33 (d, *J* = 8.6 Hz, 1H), 7.99 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.73 (dd, *J* = 16.3, 8.7 Hz, 3H), 7.62 (s, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.38 – 7.34 (m, 1H), 7.28 (t, *J* = 7.4 Hz, 1H), 7.15 (t, *J* = 7.5 Hz, 2H), 7.07 (t, *J* = 7.4 Hz, 1H), 6.99 (d, *J* = 7.0 Hz, 4H), 7.01 – 6.96 (m, 2H), 6.82 (s, 1H), 4.62 – 4.46 (m, qH), 2.76 – 2.68 (m, 1H), 2.57 (d, *J* = 9.3 Hz, 1H), 2.42 – 2.35 (m, 1H), 2.22 (s, 3H), 2.18 (s, 1H), 2.08 (q, *J* = 8.0 Hz, 1H). **^{13}C NMR** (101 MHz, DMSO) *δ* 184.5, 179.9, 167.8, 163.9, 137.2, 133.6, 131.4, 130.6, 130.3, 128.1, 127.7, 126.7, 126.4, 125.7, 124.9, 124.7, 122.3, 121.7, 120.1, 119.9, 117.1, 112.2, 63.0, 54.3, 53.4, 41.3, 33.3.

HRMS: calculated for $C_{35}H_{31}N_4O_2^+$ [M+H$^+$] 539.2442, found 539.2440.



Cat. **XI**

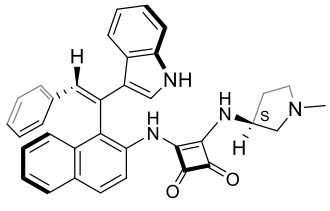
39 mg, 95% yield, white soild. $[\alpha]^{20}_{D}$ 11.60 (c 0.5, DMSO)

^{1}H NMR (400 MHz, $CDCl_3$) δ 13.36 (s, 1H), 8.37 (s, 1H), 8.11 – 7.81 (m, 2H), 7.49 (s, 1H), 4.63 – 4.27 (m, 1H), 3.33 – 3.17 (m, 1H), 3.14 (d, J = 11.1 Hz, 1H), 2.72 – 2.63 (m, 1H), 2.56 (s, 3H), 2.49 – 2.20 (m, 2H), 1.99 – 1.89 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 186.8, 180.6, 167.5, 164.6, 140.9, 132.7 (q, J_{CF} = 33.5 Hz), 127.2, 124.5, 121.8, 119.0, 115.9, 62.0, 55.2, 52.8, 40.9, 34.7.

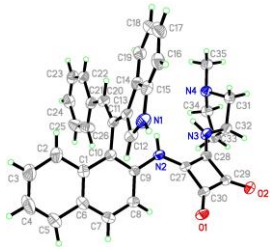
HRMS: calculated for $C_{17}H_{16}F_6N_3O_2^+$ [M+H$^+$] 408.1141, found 408.1138.

4. X-ray structure

Crystal data and structure refinement for Cat. VIII.



Cat. **VIII**

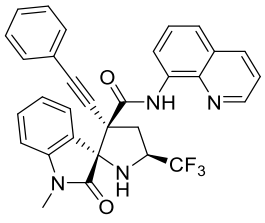


X-ray structure of cat. **VIII** (CCDC 2251865)

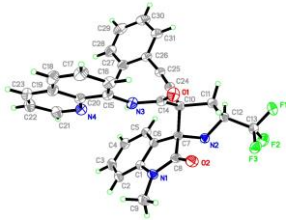
Identification code	a_a
Empirical formula	C36 H34 N4 O3
Formula weight	570.67
Temperature	173(2) K
Wavelength	1.54178 Å
Crystal system	Tetragonal
Space group	$P4_3$
Unit cell dimensions	a = 11.977(5) Å
	b = 11.977 Å
	c = 42.045(13) Å
Volume	6031(5) $Å^3$
Z	8
Density (calculated)	1.257 Mg/m^3
Absorption coefficient	0.645 mm^{-1}
F(000)	2416
Crystal size	0.160 x 0.150 x 0.140 mm^3
Theta range for data collection	3.690 to 67.142°.
Index ranges	-13<=h<=14, -14<=k<=13, -50<=l<=48
Reflections collected	61410
Independent reflections	10685 [R(int) = 0.0898]
Completeness to theta = 67.142°	99.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7528 and 0.6348
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10685 / 3 / 794
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0488, wR2 = 0.1268
R indices (all data)	R1 = 0.0656, wR2 = 0.1399
Absolute structure parameter	-0.14(13)

Extinction coefficient	n/a
Largest diff. peak and hole	0.599 and -0.344 e.Å^{-3}

Crystal data and structure refinement for 3aa.



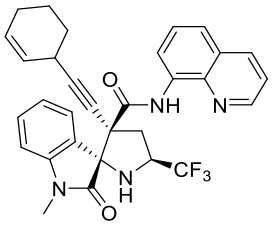
3aa



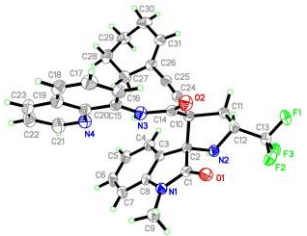
X-ray structure of **3aa** (CCDC 2025863)

Empirical formula	C31 H23 F3 N4 O2
Formula weight	540.53
Temperature	297(2) K
Wavelength	1.54178 A
Crystal system, space group	Orthorhombic, P2(1)2(1)2(1)
Unit cell dimensions	a = 10.5810(3) A alpha = 90 deg. b = 12.0311(3) A beta = 90 deg. c = 20.7727(5) A gamma = 90 deg.
Volume	2644.39(12) A^3
Z, Calculated density	4, 1.358 Mg/m^3
Absorption coefficient	0.846 mm^-1
F(000)	1120
Crystal size	0.200 x 0.180 x 0.150 mm
Theta range for data collection	4.246 to 72.395 deg
Limiting indices	-13<=h<=12, -14<=k<=14, -25<=l<=25
Reflections collected / unique	31504 / 5208 [R(int) = 0.0341]
Completeness to theta = 67.679	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5208 / 0 / 370
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0834
R indices (all data)	R1 = 0.0379, wR2 = 0.0889
Absolute structure parameter	0.05(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.105 and -0.126 e.A^-3

Crystal data and structure refinement for 3ta.



3ta



X-ray structure of **3ta** (CCDC 2251573)

Identification code	t_a
Empirical formula	C31 H27 F3 N4 O2
Formula weight	544.56
Temperature	173(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 10.5678(2) Å
	b = 11.8802(3) Å
	c = 21.0636(4) Å
Volume	2644.48(10) $Å^3$
Z	4
Density (calculated)	1.368 Mg/m^3
Absorption coefficient	0.847 mm^{-1}
F(000)	1136
Crystal size	0.180 x 0.160 x 0.140 mm^3
Theta range for data collection	4.272 to 68.443°.
Index ranges	-12<=h<=12, -14<=k<=14, -25<=l<=25
Reflections collected	31549
Independent reflections	4856 [R(int) = 0.0426]
Completeness to theta = 67.679°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7531 and 0.6409
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4856 / 0 / 368
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0293, wR2 = 0.0738
R indices (all data)	R1 = 0.0320, wR2 = 0.0759
Absolute structure parameter	-0.01(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.177 and -0.166 $e.Å^{-3}$

5. Theoretical calculations on the role of chiral organocatalysts

Figure S2: Proposed catalytic cycle.

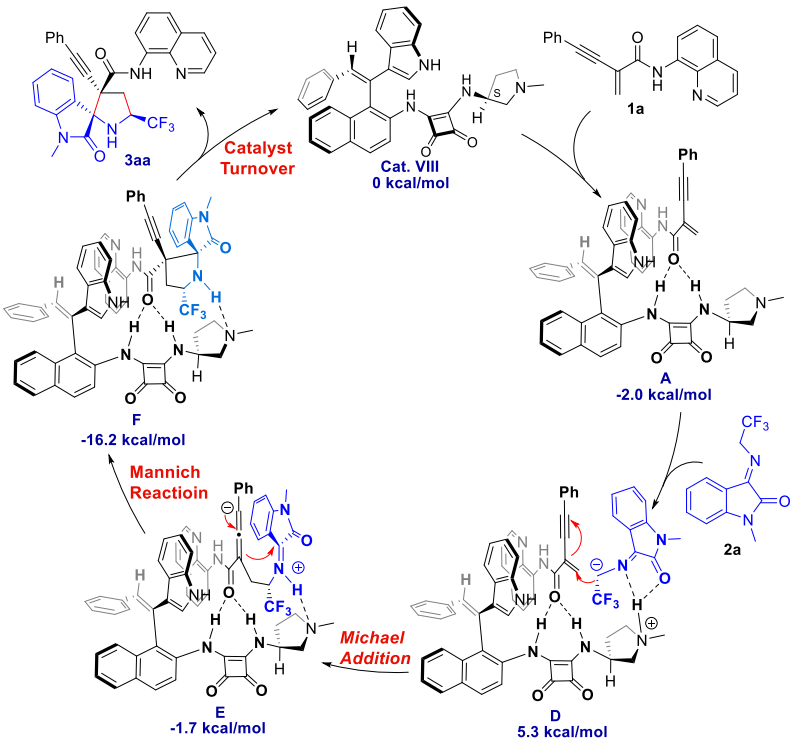


Figure S3: Visualization of noncovalent interactions in TS1 and TS2

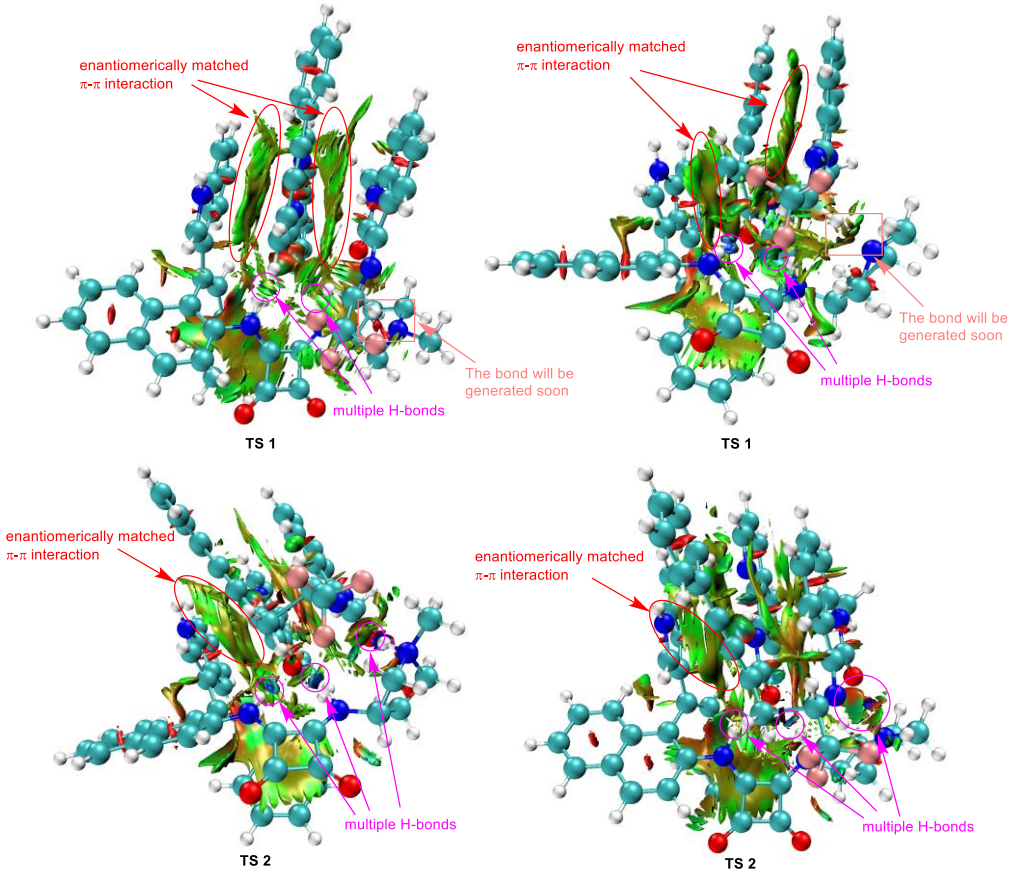
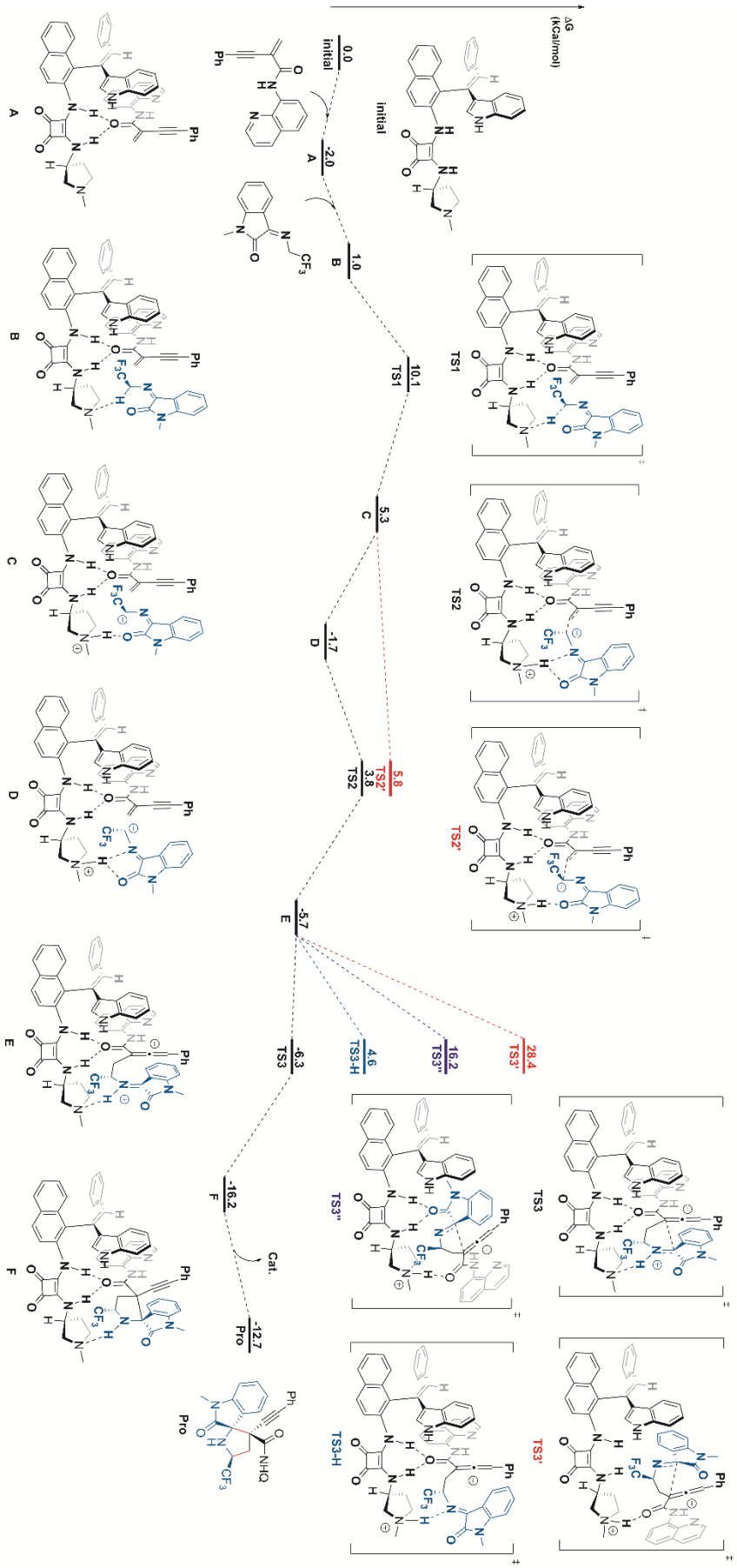


Figure S4: Proposed mechanistic DFT calculation of the reaction



Details of Computational Studies for Determination of the Mechanism

The M06-2X density functional[6] with 6-31G(d,p) basis set[7] was employed for the computational study. Vibrational frequency analyses were carried out at the same level to confirm all the optimized structures as minima (no imaginary frequency) or transition states (only one imaginary frequency), and provided the thermal relative Gibbs free energy correction. To verify that each transition state connects to its appropriate reactant and product, the intrinsic reaction coordinate (IRC) calculations[8] were employed. The solvent effect of dichloroethane in the reaction was evaluated using the SMD solvation model[9]. This model was used for single point energy calculations based on the gas phase optimized geometries at 6-311++G(d,p) basis set[10, 11]. For the purpose of discussion, the solvation Gibbs free energy was used and it was obtained from the addition of solvation single point energy and gas-phase thermal correction to Gibbs free energy. All calculations were carried out by Gaussian 16 program package[7].

Coordinates and Energies:

1a

Zero-point correction= 0.291102 (Hartree/Particle)
Thermal correction to Energy= 0.306604
Thermal correction to Enthalpy= 0.307469
Thermal correction to Gibbs Free Energy= 0.248103
Sum of electronic and zero-point Energies= -954.582546
Sum of electronic and thermal Energies= -954.567045
Sum of electronic and thermal Enthalpies= -954.566180
Sum of electronic and thermal Free Energies= -954.625546
SCF Done: E(RM062X) = -955.128819916

C	-0.46645700	3.15097700	-0.03793600
C	-1.52591200	2.18999400	-0.02812900
C	-2.32926900	1.28208800	-0.00845600
C	-3.24520000	0.18284800	0.03925800
C	-4.58840200	0.34206600	-0.32522800
C	-2.78276000	-1.07357600	0.45955500
C	-5.45468800	-0.74323100	-0.27085000
H	-4.93893800	1.31604700	-0.64909700
C	-3.65750600	-2.15123700	0.51170900
H	-1.73812900	-1.17976400	0.73752000
C	-4.99299500	-1.98970400	0.14630000
H	-6.49419200	-0.61587000	-0.55445100
H	-3.29827000	-3.12065000	0.84289600
H	-5.67353400	-2.83381300	0.18818500
C	0.96287200	2.64361400	0.02477300

O	1.90663100	3.41187400	0.07852000
N	1.06382900	1.28374200	0.00823200
H	0.20982400	0.73763800	-0.06115300
C	2.22274400	0.51375800	0.03394900
C	2.00905900	-0.90371000	-0.04821800
C	3.50797200	1.00514300	0.12531600
C	3.12374900	-1.77930500	-0.04358800
C	4.60453000	0.11110100	0.13589400
H	3.66551100	2.07235400	0.18466900
C	0.51888800	-2.63888300	-0.23342800
C	2.85236800	-3.16638100	-0.14302000
C	4.43380600	-1.24591300	0.05314000
H	5.60468300	0.52568700	0.20908400
C	1.55684000	-3.60032800	-0.24220600
H	-0.51951500	-2.95800800	-0.31252600
H	3.68179100	-3.86838700	-0.14235000
H	5.28274900	-1.92243200	0.05786000
H	1.31560700	-4.65383600	-0.32470600
N	0.72589300	-1.34643400	-0.13595900
C	-0.65606300	4.47362000	-0.09488500
H	0.21006200	5.12593200	-0.09330700
H	-1.65019200	4.90130900	-0.14037700

2a

Zero-point correction= 0.191753 (Hartree/Particle)
Thermal correction to Energy= 0.204106
Thermal correction to Enthalpy= 0.204971
Thermal correction to Gibbs Free Energy= 0.153558
Sum of electronic and zero-point Energies= -908.333044
Sum of electronic and thermal Energies= -908.320691
Sum of electronic and thermal Enthalpies= -908.319826
Sum of electronic and thermal Free Energies= -908.371239
SCF Done: E(RM062X) = -908.802647265

C	1.34851800	-0.74782600	-0.00000500
C	2.41780000	0.16018300	0.00000200
C	3.73407300	-0.27007600	0.00000800
C	3.95419900	-1.65161300	0.00000600
C	2.89922600	-2.56341600	-0.00000200
C	1.57746400	-2.11273900	-0.00000700
C	0.11090700	0.04010200	-0.00000800
C	0.55955800	1.50459600	-0.00000500
H	4.56188200	0.43064200	0.00001400

H	4.97522800	-2.01930500	0.00001000
H	3.10865600	-3.62709500	-0.00000300
H	0.73799100	-2.80024700	-0.00001200
N	1.93515700	1.47844500	0.00000200
O	-0.14410500	2.49331100	-0.00000800
N	-1.07222300	-0.41223200	-0.00001100
C	-2.18705000	0.51429600	-0.00001300
H	-2.18304400	1.16678700	0.87906200
H	-2.18305500	1.16676800	-0.87910200
C	-3.47071600	-0.28059100	0.00000400
F	-4.52545000	0.55000300	0.00000200
F	-3.56950700	-1.06342000	1.07995000
F	-3.56952200	-1.06344300	-1.07992500
C	2.75739100	2.66518800	0.00000500
H	3.39024700	2.69561300	0.89190100
H	3.39025200	2.69561500	-0.89188600
H	2.08623500	3.52436400	0.00000500

Initial/Cat. VIII

Zero-point correction= 0.581945 (Hartree/Particle)
Thermal correction to Energy= 0.610631
Thermal correction to Enthalpy= 0.611496
Thermal correction to Gibbs Free Energy= 0.522116
Sum of electronic and zero-point Energies= -1719.974845
Sum of electronic and thermal Energies= -1719.946159
Sum of electronic and thermal Enthalpies= -1719.945294
Sum of electronic and thermal Free Energies= -1720.034674
SCF Done: E(RM062X) = -1721.02325728

O	-1.92950000	-3.95049300	-2.06946800
N	-4.82911900	2.34514100	0.47293700
O	-4.72818400	-2.24114500	-2.32879600
N	-0.47763200	-1.09956300	-0.87300800
H	-0.43877400	-0.10082300	-0.70891200
N	4.15938500	1.36575900	-2.39440500
H	4.69849500	1.18226300	-3.22410100
C	4.86142800	4.68032600	-0.89585300
H	5.44440500	5.58833500	-1.00830300
C	4.98207300	3.67322900	-1.83702700
H	5.65490300	3.76760500	-2.68342600
C	4.21116100	2.52336100	-1.64993700
C	3.31932600	2.36871200	-0.56191800
C	2.72045300	1.05771400	-0.69562000

C	1.71427600	0.40615800	0.15045500
C	1.71656600	-1.08976500	0.10919400
C	-1.68411600	-1.57565000	-1.27070200
C	-4.70648600	0.68732600	-1.14136200
H	-5.06491000	0.31123500	-2.10001800
C	-4.87272900	2.19498300	-0.97727500
H	-4.07669100	2.76518400	-1.46467500
H	-5.84641900	2.51778900	-1.39197800
C	-5.12947200	3.68478200	0.93445600
H	-5.08236600	3.71864500	2.02692900
H	-6.13496100	4.01933500	0.62174400
H	-4.39217000	4.38875900	0.53941100
N	-3.28133700	0.36379300	-1.04900900
H	-2.80002500	0.82890700	-0.28143800
C	-5.77933300	1.33954600	0.95150400
H	-6.81714700	1.69922200	0.82605800
H	-5.62477600	1.13682700	2.01625100
C	-5.52226200	0.11765700	0.04947800
H	-6.45216200	-0.34008000	-0.29235600
H	-4.94123900	-0.65443400	0.56039400
C	-3.60405000	-2.03928000	-1.93859200
C	-2.28661600	-2.82355900	-1.83159600
C	0.70308500	-3.21270200	-0.55844300
H	-0.12231000	-3.74229400	-1.02232600
C	1.79622400	-3.89436700	-0.10633400
H	1.83119500	-4.97614500	-0.19981400
C	4.01494600	-3.93356700	0.99334900
H	4.02717600	-5.01579200	0.89613100
C	5.05593200	-3.27195000	1.59179000
H	5.90933800	-3.82231900	1.97369900
C	5.01028100	-1.86423400	1.71971700
H	5.82904100	-1.34357800	2.20600400
C	3.94205100	-1.14913400	1.23979900
H	3.91867000	-0.06991100	1.35001900
C	2.85322700	-1.80640100	0.60146600
C	0.81704900	1.14296900	0.84549700
H	0.83111900	2.21915300	0.68555300
C	-0.26685100	0.65599800	1.71439800
C	-0.17234100	-0.51319800	2.48455600
H	0.75713100	-1.07237900	2.49628000
C	-1.25581700	-0.95159300	3.23629800
H	-1.16468100	-1.85953900	3.82378000
C	-2.45129100	-0.23357500	3.24523200
H	-3.29416500	-0.58402800	3.83233700

C	-2.54999100	0.94397200	2.50945000
H	-3.46493400	1.52629600	2.50244700
C	-1.46427300	1.38638400	1.75853400
H	-1.54947300	2.31161700	1.19069000
C	4.00610000	4.53958600	0.21272800
H	3.95138500	5.33884700	0.94423900
C	3.24107100	3.39975400	0.38958700
H	2.60673900	3.29923200	1.26370700
C	3.28158500	0.49039400	-1.81464800
H	3.10467100	-0.48858000	-2.23717300
C	-2.88894000	-0.88698600	-1.35188000
C	0.65482500	-1.79669600	-0.44258400
C	2.89379400	-3.22388700	0.49450700

A

Zero-point correction= 0.874441 (Hartree/Particle)
Thermal correction to Energy= 0.919717
Thermal correction to Enthalpy= 0.920582
Thermal correction to Gibbs Free Energy= 0.795486
Sum of electronic and zero-point Energies= -2674.595287
Sum of electronic and thermal Energies= -2674.550012
Sum of electronic and thermal Enthalpies= -2674.549147
Sum of electronic and thermal Free Energies= -2674.674242
SCF Done: E(RM062X) = -2676.18052241

C	-1.47180600	0.63090900	-2.19206700
C	-2.82979800	1.07101800	-2.28293900
C	-4.00376500	1.37327400	-2.24510800
C	-5.38909200	1.71694100	-2.13219200
C	-6.06427500	2.37568100	-3.16770300
C	-6.07436100	1.38455100	-0.95246000
C	-7.40841500	2.69802300	-3.02207500
H	-5.52961200	2.62602700	-4.07767900
C	-7.41708500	1.71365100	-0.81770900
H	-5.53032500	0.87586500	-0.16088300
C	-8.08635900	2.36926600	-1.85016200
H	-7.92896300	3.20766900	-3.82599300
H	-7.94427000	1.46123200	0.09713600
H	-9.13524300	2.62467300	-1.74129100
C	-1.10944800	-0.31862100	-1.07358300
O	0.05933400	-0.64828100	-0.87757600
N	-2.15590900	-0.77979000	-0.35586800
H	-3.08461400	-0.42380400	-0.57257900

C	-2.11994900	-1.60519100	0.76767100
C	-3.39498600	-1.84706000	1.37563800
C	-0.98259400	-2.15683800	1.31679500
C	-3.46620500	-2.62560000	2.55777800
C	-1.07548000	-2.92153000	2.50413900
H	-0.03016400	-2.00962100	0.82867700
C	-5.66213400	-1.50414100	1.34469400
C	-4.74988400	-2.81797800	3.12645200
C	-2.27738700	-3.15604500	3.12052000
H	-0.16226100	-3.32544600	2.93155300
C	-5.84804400	-2.26182700	2.52557300
H	-6.52055900	-1.05647300	0.84539200
H	-4.84339100	-3.40605700	4.03529800
H	-2.33738100	-3.74208100	4.03229500
H	-6.84418900	-2.39069700	2.93281600
N	-4.49117200	-1.29735400	0.78951400
C	-0.50181100	1.01430500	-3.03147600
H	0.50900900	0.64334800	-2.89400200
H	-0.70615000	1.69215000	-3.85183800
O	6.02017600	-0.41661100	-1.59854500
N	-0.11689000	-4.28978700	-0.92795500
O	5.04990800	-3.55293700	-2.07288900
N	2.78336000	0.42150400	-1.30907200
H	1.83079300	0.22382000	-1.00576800
N	-1.37397500	3.32813300	-0.34856800
H	-1.84112600	3.88324500	-1.04614700
C	-3.73238300	1.72960700	2.01209300
H	-4.78211900	1.63562400	2.27463900
C	-3.36657400	2.52630100	0.94138800
H	-4.10514500	3.06733500	0.35718400
C	-2.00546100	2.60585000	0.63641900
C	-1.01068500	1.89704500	1.35439500
C	0.25698500	2.19712500	0.71713600
C	1.58948900	1.62677800	0.93670200
C	2.71353200	2.29224800	0.20793700
C	3.53206700	-0.68410500	-1.56943100
C	1.89908600	-4.07271300	-2.03062900
H	2.57749700	-4.38934500	-2.82453600
C	0.44465200	-4.46603900	-2.26187000
H	-0.06240300	-3.82658300	-2.99127800
H	0.38456500	-5.51569900	-2.60698400
C	-1.47934200	-4.75622500	-0.78773300
H	-1.81403200	-4.60959600	0.24368800
H	-1.58292200	-5.82799300	-1.03867100

H	-2.13909300	-4.17921200	-1.44287400
N	1.95613000	-2.61871000	-1.92265500
H	1.12707000	-2.16345300	-1.54708800
C	0.82807800	-4.95771500	-0.02806500
H	0.58810500	-6.03195300	0.06441500
H	0.76041000	-4.51991100	0.97462500
C	2.21157300	-4.77417700	-0.69180400
H	2.69219000	-5.73815100	-0.87372500
H	2.90167700	-4.16638900	-0.10459600
C	4.53309600	-2.47142000	-1.91410600
C	4.97490400	-1.01767400	-1.67425500
C	4.44703600	2.19758200	-1.50705100
H	4.91822900	1.64161100	-2.30897900
C	4.94733000	3.39993200	-1.09384700
H	5.82081100	3.82155700	-1.58280400
C	4.84174000	5.38141200	0.39224000
H	5.70295200	5.79714400	-0.12386200
C	4.26000200	6.05357600	1.43595300
H	4.65241000	7.01330400	1.75585200
C	3.14898100	5.48903700	2.10589100
H	2.69958500	6.01985100	2.93914000
C	2.63753300	4.27770600	1.71513900
H	1.78782800	3.84820200	2.23558600
C	3.20952300	3.56481500	0.62514200
C	1.76384100	0.46689000	1.60750900
H	0.86941400	-0.03071800	1.97295300
C	2.99404900	-0.33056100	1.73342900
C	4.29369100	0.20217200	1.71690500
H	4.43797000	1.27637800	1.71016200
C	5.40297600	-0.63503900	1.69897500
H	6.39590300	-0.20200200	1.64421100
C	5.24790100	-2.01955300	1.73352000
H	6.11654800	-2.66847200	1.70410500
C	3.96824600	-2.56112600	1.81763900
H	3.83632600	-3.63698400	1.88312100
C	2.85656400	-1.72500200	1.81656200
H	1.85861000	-2.15531500	1.86493000
C	-2.76315900	1.05295900	2.77651200
H	-3.07972500	0.45032700	3.62235000
C	-1.41689800	1.13150300	2.46312500
H	-0.69232500	0.61287800	3.08035800
C	-0.02838700	3.07985300	-0.29962700
H	0.65095100	3.53422800	-1.00681800
C	3.13547300	-1.99357600	-1.81272400

C	3.31269800	1.64360800	-0.85909500
C	4.33989500	4.12516200	-0.03412700

B

Zero-point correction= 1.067842 (Hartree/Particle)
Thermal correction to Energy= 1.126312
Thermal correction to Enthalpy= 1.127177
Thermal correction to Gibbs Free Energy= 0.974619
Sum of electronic and zero-point Energies= -3582.959994
Sum of electronic and thermal Energies= -3582.901524
Sum of electronic and thermal Enthalpies= -3582.900659
Sum of electronic and thermal Free Energies= -3583.053217
SCF Done: E(RM062X) = -3585.00398603

C	-3.26180258	-0.24678111	0.00000000
C	-1.87324658	-0.52118911	-0.19993700
C	-0.68083258	-0.74057611	-0.22830000
C	0.72219042	-1.01922111	-0.20078700
C	1.53972542	-0.74410811	-1.30544800
C	1.28087742	-1.56959411	0.96344000
C	2.90106442	-1.01661511	-1.24118400
H	1.09616042	-0.31298711	-2.19683500
C	2.64310842	-1.83968311	1.01444000
H	0.62567442	-1.77594711	1.80607500
C	3.45478942	-1.56316311	-0.08463200
H	3.53315142	-0.80432711	-2.09722600
H	3.07443742	-2.27197211	1.91207400
H	4.51786942	-1.77577411	-0.04115800
C	-3.75203258	-0.08688511	1.41956300
O	-4.91497758	0.22108489	1.66027700
N	-2.79965158	-0.24134611	2.36775300
H	-1.88547358	-0.58540711	2.08172400
C	-2.94316258	-0.08055411	3.74313800
C	-1.74965058	-0.31098011	4.50546000
C	-4.10690558	0.28067689	4.39027800
C	-1.79315158	-0.20144311	5.91820300
C	-4.12190858	0.40085589	5.80072100
H	-5.00652658	0.46932789	3.82028900
C	0.47962942	-0.85602011	4.51798800
C	-0.59115158	-0.46161011	6.62216500
C	-3.00610658	0.16007189	6.55813800
H	-5.05221258	0.68963289	6.28052500
C	0.54419542	-0.79071511	5.92974800

H	1.37314542	-1.09877411	3.94407500
H	-0.58827458	-0.39354311	7.70651500
H	-3.02955658	0.24673989	7.63984200
H	1.48006042	-0.99385911	6.43726300
N	-0.61429658	-0.63128411	3.82776300
C	-4.13913158	-0.08436511	-0.99949400
H	-5.18404358	0.11827489	-0.78109100
H	-3.82488358	-0.14683411	-2.03513900
C	-2.09177958	2.93723189	-1.37239100
C	-1.08313358	2.65763189	-0.44160300
C	0.23415242	2.47506589	-0.82672800
C	0.51863442	2.58421089	-2.19201800
C	-0.47686058	2.85857589	-3.12995900
C	-1.80113458	3.03659189	-2.72193900
C	-3.35625758	3.04159089	-0.63011700
C	-2.97984358	2.81349089	0.84020300
H	1.01183442	2.24015389	-0.10757800
H	1.54332042	2.44795389	-2.52469000
H	-0.21911358	2.93701489	-4.18029600
H	-2.59540258	3.25020989	-3.42991000
N	-1.62518458	2.58637889	0.85128800
O	-3.70912258	2.81628889	1.81528900
N	-4.49889958	3.23574389	-1.13902400
C	-5.67161958	3.23586089	-0.28803700
H	-5.91032458	2.20843189	0.02293600
H	-5.56321158	3.84752289	0.62099200
C	-6.83873958	3.75608389	-1.08820200
F	-7.95796858	3.75797689	-0.34210400
F	-7.08231658	3.01885189	-2.17692700
F	-6.62925358	5.01827789	-1.49417000
C	-0.86015458	2.29794089	2.04249700
H	-0.38418458	1.31396989	1.96353600
H	-0.09361058	3.06345389	2.19736400
H	-1.55239858	2.29491489	2.88626400
O	-10.71902858	0.98351489	0.65156800
N	-5.80532658	5.22252689	2.29393400
O	-9.88517158	3.25104289	2.90833900
N	-7.53750258	-0.01124911	0.58530100
H	-6.63533558	-0.17065511	1.02947500
N	-3.65088258	-3.43766411	-0.36592200
H	-3.14560858	-3.53769211	-1.23050500
C	-1.45232458	-3.65769211	2.60169000
H	-0.42584158	-3.80327011	2.92481800
C	-1.75171158	-3.66669711	1.25148400

H	-0.98105158	-3.81153211	0.49992900
C	-3.08706458	-3.46665411	0.88717700
C	-4.11981058	-3.22918011	1.82909600
C	-5.33328558	-2.99256411	1.06774600
C	-6.66072258	-2.54445111	1.50685200
C	-7.69800958	-2.42283011	0.43307800
C	-8.27741658	0.96163889	1.19360200
C	-6.85892558	3.56540789	3.55443500
H	-7.64514458	3.40214189	4.29479000
C	-7.13378858	4.84200289	2.75152500
H	-7.81674658	4.68145289	1.91368300
H	-7.57612358	5.60804789	3.41733600
C	-5.74840858	6.51423389	1.64453600
H	-4.71923458	6.72887589	1.34134600
H	-6.09423458	7.33217389	2.30229300
H	-6.37156858	6.50041389	0.74588800
N	-6.79884458	2.37233289	2.70581800
H	-5.89099058	2.08366489	2.34853900
C	-4.96013258	5.10684489	3.47594900
H	-5.08173758	5.99068189	4.13042300
H	-3.90757958	5.03171189	3.18811100
C	-5.47504358	3.84010589	4.18664900
H	-5.55881358	3.99518689	5.26422500
H	-4.80245758	2.99556589	4.01983900
C	-9.32527358	2.41930189	2.23204700
C	-9.70829458	1.35034089	1.20180300
C	-9.14368158	-1.02109311	-0.94845300
H	-9.46801258	-0.02252211	-1.21646300
C	-9.71315858	-2.12679211	-1.51309000
H	-10.49739658	-2.01573411	-2.25622000
C	-9.87504758	-4.58969311	-1.73238200
H	-10.64737758	-4.45675311	-2.48513700
C	-9.48033958	-5.84540711	-1.34937200
H	-9.93363158	-6.72285011	-1.79891000
C	-8.48569058	-5.99835011	-0.35492600
H	-8.18698058	-6.99449311	-0.04426200
C	-7.89963958	-4.90072911	0.22278600
H	-7.14179058	-5.02475911	0.98934000
C	-8.27634158	-3.58496311	-0.16584600
C	-6.87881458	-2.10413111	2.76531500
H	-6.02257958	-2.06708011	3.43178700
C	-8.08771058	-1.47647011	3.31791300
C	-9.39361858	-1.72796311	2.86735500
H	-9.57147158	-2.49806411	2.12520800

C	-10.46352958	-0.98732411	3.35667700
H	-11.45999358	-1.17010411	2.96909600
C	-10.25982358	0.00644489	4.31288200
H	-11.09213058	0.60769089	4.66276700
C	-8.97797258	0.22600689	4.81159700
H	-8.81125758	0.98833489	5.56663700
C	-7.90875958	-0.51836811	4.32755200
H	-6.90664658	-0.34010811	4.70958100
C	-2.46436958	-3.48312711	3.56498000
H	-2.20267958	-3.50328111	4.61854500
C	-3.78191058	-3.27792411	3.19614400
H	-4.53464858	-3.16982111	3.96719300
C	-4.98429458	-3.14822611	-0.25532900
H	-5.60993958	-3.05472411	-1.13160300
C	-7.92081458	1.96155289	2.09089600
C	-8.12542958	-1.16786311	0.02805400
C	-9.29382458	-3.43418711	-1.14997400

TS1

Zero-point correction= 1.063516 (Hartree/Particle)
Thermal correction to Energy= 1.121311
Thermal correction to Enthalpy= 1.122176
Thermal correction to Gibbs Free Energy= 0.972103
Sum of electronic and zero-point Energies= -3582.946537
Sum of electronic and thermal Energies= -3582.888742
Sum of electronic and thermal Enthalpies= -3582.887877
Sum of electronic and thermal Free Energies= -3583.037950
SCF Done: E(RM062X) = -3584.98694055

C	-1.80257511	-0.61158797	0.00000000
C	-0.43403911	-0.95520497	-0.23531900
C	0.73823989	-1.26157197	-0.29087700
C	2.11313289	-1.65862197	-0.29599500
C	2.96980389	-1.30340397	-1.34648000
C	2.60464389	-2.40650197	0.78534400
C	4.30344189	-1.69187597	-1.31010000
H	2.58244089	-0.71094697	-2.16866700
C	3.94011789	-2.79101497	0.80914900
H	1.91926689	-2.67060997	1.58709600
C	4.79097489	-2.43445497	-0.23555500
H	4.96620889	-1.41471697	-2.12340100
H	4.31968889	-3.37436597	1.64244500
H	5.83300989	-2.73617097	-0.21378500

C	-2.27705711	-0.57565997	1.43234500
O	-3.40875611	-0.19241397	1.71814500
N	-1.34860411	-0.93393597	2.35005800
H	-0.47996311	-1.34923897	2.01961100
C	-1.48434611	-0.91436397	3.73552700
C	-0.36112111	-1.42796997	4.46670700
C	-2.57868111	-0.43064097	4.42351500
C	-0.41819811	-1.48603997	5.88249500
C	-2.60516911	-0.48140597	5.83753500
H	-3.41902011	-0.02099197	3.88084100
C	1.74922989	-2.32883897	4.41949300
C	0.70574889	-2.03083597	6.55208300
C	-1.56607511	-1.00414397	6.56102600
H	-3.48331511	-0.09778497	6.34798400
C	1.78765089	-2.45673897	5.82797900
H	2.60650989	-2.63992897	3.82347000
H	0.69254389	-2.09973697	7.63631300
H	-1.60006511	-1.05024597	7.64493800
H	2.66371289	-2.87646597	6.30868100
N	0.72468689	-1.84172697	3.75957800
C	-2.66595911	-0.28911997	-0.97329800
H	-3.69692111	-0.04210997	-0.73949100
H	-2.35153911	-0.25833097	-2.01031400
C	0.30663489	2.63849103	-0.80483400
C	1.18307689	2.08472303	0.14014000
C	2.51358289	1.83965903	-0.15226100
C	2.95735289	2.17800803	-1.43570600
C	2.09740889	2.72941903	-2.38470500
C	0.75363289	2.95879103	-2.07457300
C	-1.02144711	2.69018203	-0.18229200
C	-0.82608011	2.17974503	1.23623200
H	3.18308189	1.38757803	0.57218300
H	3.99572589	1.99573003	-1.69535200
H	2.47449189	2.98001403	-3.37021800
H	0.06295789	3.37628303	-2.79999100
N	0.49853689	1.83478703	1.33947400
O	-1.65480411	2.11001203	2.13251900
N	-2.10327911	3.05206403	-0.74291800
C	-3.34838411	2.92237703	-0.06372400
H	-3.49404111	1.93654903	0.39380000
H	-3.46798311	3.76283003	0.96763300
C	-4.46632211	3.19058303	-1.02504400
F	-5.65651911	3.15006703	-0.39310200
F	-4.52711811	2.28982503	-2.02477400

F	-4.36390711	4.40136103	-1.59592700
C	1.09703089	1.24532703	2.51304400
H	1.44655189	0.22925003	2.29632000
H	1.93775989	1.85440903	2.85911300
H	0.33050789	1.20377403	3.28894100
O	-9.11979611	1.11508703	0.82372200
N	-3.72920211	4.83225503	2.15347900
O	-7.99394211	3.30454103	3.03222700
N	-6.03925411	-0.13622897	0.60799700
H	-5.13415511	-0.38965797	1.00033500
N	-2.46252111	-3.70916197	-0.74002700
H	-1.97506511	-3.74205697	-1.61988600
C	-0.27644611	-4.50293297	2.13746500
H	0.73419989	-4.78024097	2.42236000
C	-0.57937011	-4.30627497	0.80266500
H	0.17229189	-4.42035297	0.02700800
C	-1.89301311	-3.94221097	0.48891900
C	-2.89322211	-3.73627497	1.47172700
C	-4.08674211	-3.30452497	0.76959200
C	-5.36222411	-2.79592697	1.28820400
C	-6.40873111	-2.50108397	0.25950400
C	-6.66959511	0.86713403	1.27254900
C	-4.95206111	3.37089103	3.52267800
H	-5.75046811	3.35621703	4.26685800
C	-5.09695811	4.60530503	2.62329800
H	-5.77670811	4.44441103	1.78234100
H	-5.46132911	5.46346203	3.21269700
C	-3.53457111	6.07894903	1.43174700
H	-2.48601811	6.16328803	1.13287500
H	-3.80401211	6.95289903	2.04378600
H	-4.14660311	6.06952003	0.52582800
N	-5.02965511	2.12083503	2.76562000
H	-4.16624511	1.71146303	2.41751700
C	-2.88109711	4.67182703	3.33838500
H	-2.86765011	5.61016703	3.91707300
H	-1.85875811	4.42941003	3.03782800
C	-3.54747911	3.54020203	4.14308100
H	-3.61803011	3.80169903	5.20034100
H	-2.97612511	2.61298903	4.06087900
C	-7.54432111	2.40557103	2.35615300
C	-8.06145311	1.38282203	1.33976900
C	-7.74988711	-0.87193897	-0.96816200
H	-7.98824111	0.16908803	-1.15039500
C	-8.42095811	-1.87482097	-1.60821600

H	-9.20338311	-1.63626997	-2.32269100
C	-8.79484411	-4.28866397	-2.02705700
H	-9.56634111	-4.02910397	-2.74694100
C	-8.49920611	-5.60058897	-1.76094600
H	-9.03181911	-6.39628597	-2.27149600
C	-7.50251211	-5.91915397	-0.80863000
H	-7.28138811	-6.95937997	-0.59162800
C	-6.81700411	-4.92667197	-0.15518800
H	-6.05744911	-5.17723897	0.57810300
C	-7.09095511	-3.55636497	-0.42136900
C	-5.50992711	-2.44117297	2.58338200
H	-4.63538611	-2.52312297	3.22265300
C	-6.64703011	-1.75096197	3.20994000
C	-7.98011811	-1.86343197	2.78334700
H	-8.24161011	-2.57333197	2.00660500
C	-8.96858211	-1.05983497	3.33955700
H	-9.98584411	-1.13325997	2.97030900
C	-8.65605911	-0.14050097	4.34024400
H	-9.42516311	0.50876803	4.74500300
C	-7.34891111	-0.06051997	4.81361600
H	-7.09668411	0.64351603	5.60092000
C	-6.36099311	-0.86792397	4.26194500
H	-5.33879111	-0.79985797	4.62410100
C	-1.26310111	-4.36329597	3.13276500
H	-0.99796211	-4.54333197	4.17034100
C	-2.55666511	-3.98968097	2.81599800
H	-3.29590811	-3.91054997	3.60401400
C	-3.76516511	-3.32439897	-0.56937200
H	-4.38767111	-3.06905997	-1.41516700
C	-6.20159211	1.81160403	2.17797200
C	-6.73350411	-1.18550597	-0.02964300
C	-8.10896311	-3.23873297	-1.36422800

C

Zero-point correction=	1.067276 (Hartree/Particle)
Thermal correction to Energy=	1.125326
Thermal correction to Enthalpy=	1.126191
Thermal correction to Gibbs Free Energy=	0.974638
Sum of electronic and zero-point Energies=	-3582.954388
Sum of electronic and thermal Energies=	-3582.896339
Sum of electronic and thermal Enthalpies=	-3582.895474
Sum of electronic and thermal Free Energies=	-3583.047027

SCF Done: E(RM062X) = -3584.99706436

C	-1.60944206	-0.38626609	0.00000000
C	-0.28758806	-0.73584109	-0.41773500
C	0.85861394	-1.07567609	-0.62310400
C	2.20441594	-1.51682209	-0.82624000
C	2.96961594	-1.03099409	-1.89429800
C	2.76216494	-2.44045309	0.07227900
C	4.27884294	-1.46777009	-2.05792900
H	2.53667294	-0.29699809	-2.56595200
C	4.07214694	-2.87051309	-0.10295300
H	2.14866994	-2.80240209	0.89399200
C	4.83192594	-2.38559209	-1.16674800
H	4.87168294	-1.08571209	-2.88267400
H	4.50141194	-3.59033809	0.58738500
H	5.85434294	-2.72344009	-1.30120100
C	-1.92311706	-0.49936309	1.46806400
O	-3.01015806	-0.13853909	1.92266300
N	-0.91817006	-0.99167009	2.22858300
H	-0.07815206	-1.31910209	1.75568600
C	-0.90278906	-1.16881109	3.60756100
C	0.32040694	-1.70159109	4.13947200
C	-1.94835306	-0.89249609	4.46489900
C	0.43047894	-1.94450509	5.53170500
C	-1.81461206	-1.13632009	5.85248900
H	-2.87507906	-0.50697609	4.06622100
C	2.44959994	-2.46087909	3.73921500
C	1.65533094	-2.48471509	5.99715400
C	-0.66276006	-1.65058509	6.38622200
H	-2.65919606	-0.91332809	6.49670900
C	2.66520894	-2.74402709	5.10870600
H	3.23892194	-2.64843009	3.01212300
H	1.77450094	-2.68652209	7.05807900
H	-0.57024906	-1.84048609	7.45089200
H	3.61416094	-3.15587009	5.43219000
N	1.32907694	-1.96591609	3.26731300
C	-2.57035006	0.03284091	-0.83571800
H	-3.56408006	0.26449591	-0.46782100
H	-2.37138006	0.15457391	-1.89484200
C	0.85779294	2.70988691	-0.97332600
C	1.80862094	2.12174391	-0.11217900
C	3.13375294	1.91711391	-0.48500800
C	3.50422094	2.32358691	-1.76166700
C	2.57123994	2.90305891	-2.63728500
C	1.24877794	3.09614391	-2.25773900

C	-0.39434406	2.73949791	-0.25998700
C	-0.13544006	2.19565591	1.00288500
H	3.84481494	1.44435891	0.18566500
H	4.52927194	2.18023791	-2.08842400
H	2.89270794	3.20730291	-3.62827600
H	0.52485694	3.54107091	-2.93245100
N	1.17923194	1.83305791	1.09058400
O	-0.93416806	2.04602591	2.05102700
N	-1.57798506	3.15861391	-0.81892900
C	-2.72059306	2.96111991	-0.28575900
H	-2.92009706	2.45154091	0.66302000
H	-1.44204006	2.95560791	2.23125200
C	-3.94958506	3.39348391	-1.03493900
F	-4.69494506	4.24295491	-0.29403200
F	-4.74400206	2.33298091	-1.29610600
F	-3.67853306	3.99289791	-2.18708300
C	1.78516694	1.13357591	2.19995200
H	2.09664994	0.13010791	1.89008400
H	2.65382594	1.68698891	2.56888300
H	1.04294194	1.04388191	2.99452100
O	-7.96763506	2.72078891	0.26199300
N	-1.88826606	4.30077591	2.77195100
O	-6.46940706	4.51393091	2.58012600
N	-5.65557506	0.30381591	0.81476600
H	-4.87204506	-0.12709909	1.30111300
N	-2.42742806	-3.35625609	-1.03573000
H	-1.95818506	-3.32219209	-1.92568400
C	-0.20180406	-4.45959209	1.70583400
H	0.80373294	-4.79684209	1.93871700
C	-0.53269806	-4.14809709	0.39913900
H	0.19185694	-4.22956409	-0.40587900
C	-1.83733606	-3.70956409	0.15445800
C	-2.80274706	-3.54127209	1.17901400
C	-3.99041606	-2.99867609	0.54792400
C	-5.21491006	-2.44974209	1.14248600
C	-6.23365906	-1.93761209	0.17027000
C	-5.98131506	1.53870991	1.25793500
C	-3.84568006	3.41838791	3.74385300
H	-4.70563406	3.77941291	4.31049900
C	-3.33852406	4.53478791	2.81524200
H	-3.78120906	4.50247591	1.81771200
H	-3.54765606	5.52237991	3.25494600
C	-1.13229206	5.36088491	2.11107300
H	-0.06703306	5.11590991	2.13041500

H	-1.29002006	6.32985891	2.60579100
H	-1.45348006	5.43055891	1.06873000
N	-4.26718606	2.22622091	3.01227900
H	-3.57638606	1.50993291	2.79683100
C	-1.53896606	4.08162391	4.18449800
H	-1.59004606	5.03218591	4.73751500
H	-0.52558606	3.67906191	4.26393100
C	-2.62552106	3.10078891	4.64537700
H	-2.85333106	3.20372091	5.70685800
H	-2.29305006	2.07148091	4.47210300
C	-6.32562706	3.42740591	2.06605700
C	-7.02218406	2.58166291	0.99641400
C	-7.35808706	-0.05232809	-0.90565400
H	-7.48684106	1.02033191	-0.99145200
C	-8.09410506	-0.91006409	-1.67302800
H	-8.81176906	-0.51451509	-2.38614800
C	-8.70593506	-3.21381409	-2.35441600
H	-9.41860206	-2.80039209	-3.06300800
C	-8.55756706	-4.57049409	-2.22198500
H	-9.14984606	-5.24833009	-2.82782400
C	-7.63377506	-5.08883309	-1.28408300
H	-7.52776706	-6.16341909	-1.17398400
C	-6.87392006	-4.24748909	-0.51126500
H	-6.16976906	-4.65189009	0.20879800
C	-6.99735706	-2.83531909	-0.63503400
C	-5.33651206	-2.22230909	2.46780700
H	-4.48405506	-2.43313409	3.10671900
C	-6.44986106	-1.50258709	3.11095900
C	-7.79234806	-1.71634509	2.77363800
H	-8.04520406	-2.50353309	2.07009300
C	-8.79183806	-0.92335409	3.32639300
H	-9.82694506	-1.09594209	3.05008700
C	-8.47102506	0.09457391	4.22266000
H	-9.25311106	0.72194091	4.63737300
C	-7.14204806	0.30127891	4.58351100
H	-6.88023706	1.09443391	5.27729100
C	-6.14392006	-0.50115109	4.04190400
H	-5.10438806	-0.32231509	4.30720000
C	-1.15666006	-4.36334309	2.73635900
H	-0.87421206	-4.63662709	3.74857800
C	-2.44226306	-3.91566909	2.48762900
H	-3.15587206	-3.87231709	3.30159900
C	-3.70312706	-2.92542809	-0.79746800
H	-4.33052006	-2.56809409	-1.60166500

C	-5.34735806	2.33493891	2.20768300
C	-6.42212506	-0.56803409	0.02951000
C	-7.94057606	-2.31744009	-1.56615100

D

Zero-point correction= 1.066860 (Hartree/Particle)
Thermal correction to Energy= 1.124779
Thermal correction to Enthalpy= 1.125644
Thermal correction to Gibbs Free Energy= 0.976104
Sum of electronic and zero-point Energies= -3582.963983
Sum of electronic and thermal Energies= -3582.906064
Sum of electronic and thermal Enthalpies= -3582.905199
Sum of electronic and thermal Free Energies= -3583.054738
SCF Done: E(RM062X) = -3585.00968370

H	-1.79184550	-0.57939913	0.00000000
O	-6.09870550	5.47717387	2.32191700
N	-2.76287450	-1.15626513	0.18010900
O	-6.70758050	2.54053287	0.94613500
N	-2.82740050	4.89961087	1.88491800
H	-2.03870450	4.51373987	1.36732500
N	2.42669450	6.38744287	1.89321900
H	3.06921650	6.25864287	2.65965500
C	4.10237150	6.83309787	-1.38051500
H	5.06841250	6.91160787	-1.86907000
C	4.04522150	6.65171787	-0.01047700
H	4.94597550	6.58952987	0.59404500
C	2.77935450	6.54200287	0.57296300
C	1.58392050	6.62431987	-0.18095200
C	0.48932350	6.52120187	0.75773200
C	-0.95675050	6.54251287	0.49997600
C	-1.81084750	7.07210387	1.60662500
C	-4.00331350	4.25857087	1.68244600
C	-4.16098350	0.78360987	0.18030500
H	-5.23848150	0.91799387	0.29192200
C	-3.68243150	-0.39360813	1.05768800
H	-3.15237350	-0.06661613	1.94920300
H	-4.51108750	-1.05465913	1.33641500
C	-2.40850850	-2.49540913	0.67014700
H	-1.68473350	-2.93619313	-0.01780000
H	-3.30437650	-3.12108013	0.72412600
H	-1.96310650	-2.38698513	1.65854100
N	-3.54457250	2.03938287	0.55877500

H	-2.53069650	2.13317487	0.51106400
C	-3.40337850	-1.11020913	-1.15898800
H	-4.27087850	-1.78048913	-1.15878400
H	-2.68014250	-1.43578313	-1.90874700
C	-3.79427750	0.36168987	-1.26862900
H	-4.61184350	0.53013087	-1.97030400
H	-2.92408250	0.93864287	-1.59514400
C	-5.73605350	3.19581387	1.25555500
C	-5.44637950	4.55972487	1.88624100
C	-3.54989750	6.75152487	3.29152300
H	-4.26219550	6.08484787	3.76184100
C	-3.45535950	8.05877687	3.67176700
H	-4.09080750	8.44156687	4.46508200
C	-2.43462250	10.30103687	3.43251000
H	-3.07422350	10.65886887	4.23485100
C	-1.56322350	11.14966887	2.80041200
H	-1.49803950	12.19096387	3.09858400
C	-0.75446850	10.66673987	1.74566400
H	-0.07666150	11.34435987	1.23631400
C	-0.81957350	9.35253187	1.35683900
H	-0.19820250	8.99741587	0.54157200
C	-1.70027650	8.44314687	2.00593400
C	-1.45499150	6.01871887	-0.64093800
H	-0.74169050	5.54559987	-1.31335600
C	-2.87059150	5.83973487	-1.00093000
C	-3.88524850	6.74406987	-0.65252400
H	-3.62581150	7.68046087	-0.16956600
C	-5.21787150	6.43955587	-0.90434900
H	-5.99262750	7.13475687	-0.59894600
C	-5.56470450	5.23831587	-1.52340300
H	-6.60800850	4.99370087	-1.69349600
C	-4.56351250	4.35340487	-1.91431400
H	-4.82295750	3.41674587	-2.39929800
C	-3.22965450	4.65614387	-1.66063200
H	-2.44964950	3.95120987	-1.93942800
C	2.92642250	6.92024287	-2.15263500
H	3.00646050	7.06750887	-3.22499700
C	1.67562550	6.82206687	-1.56979700
H	0.77864550	6.90921987	-2.17409400
C	1.06093250	6.38850587	2.00107300
H	0.57765150	6.28793187	2.96299300
C	-4.27611350	3.01711587	1.11830000
C	-2.72358950	6.25282887	2.25037900
C	-2.53166250	8.93941387	3.04854700

C	0.31532350	3.09979887	2.67911200
C	1.57107050	3.38480587	3.29829700
C	2.68923650	3.63584687	3.69387400
C	4.03047550	3.97546987	4.05753000
C	4.45819750	3.98027787	5.39154900
C	4.92992150	4.32447787	3.03526900
C	5.76787950	4.33242487	5.69656500
H	3.75972150	3.70851587	6.17557600
C	6.23462550	4.68113087	3.35422200
H	4.57847550	4.30115587	2.00587500
C	6.65674350	4.68507787	4.68291700
H	6.09593650	4.33484487	6.73072100
H	6.92655250	4.95594487	2.56350400
H	7.67642950	4.96265387	4.92858800
C	0.24667650	3.15476487	1.17446100
O	-0.83729450	3.12718287	0.58306600
N	1.44171350	3.25567187	0.55044900
H	2.28426050	3.25169187	1.12259800
C	1.68637550	3.36408187	-0.81653300
C	3.06756350	3.51311187	-1.17780500
C	0.72660750	3.31082687	-1.80599500
C	3.42253550	3.61931987	-2.54709700
C	1.09968550	3.45834887	-3.16238900
H	-0.30466750	3.14113087	-1.53357800
C	5.25701450	3.58710287	-0.50258800
C	4.80363750	3.71163487	-2.84923300
C	2.40882050	3.61252287	-3.53856200
H	0.31880850	3.43415387	-3.91608600
C	5.72374250	3.68498687	-1.83431600
H	5.96762450	3.56439387	0.32362700
H	5.11314650	3.79573387	-3.88754100
H	2.68716750	3.71438987	-4.58299800
H	6.78825750	3.74199287	-2.03153900
N	3.98818950	3.51502787	-0.18060300
C	-0.79076050	2.77241687	3.36261000
H	-1.70935650	2.53976687	2.83654600
H	-0.79472850	2.72724287	4.44538500
C	1.94327850	0.19845287	1.70933400
C	2.56688250	0.27976687	0.43686900
C	3.93235750	0.44104787	0.27259700
C	4.71457250	0.55654787	1.42212200
C	4.12852550	0.50242887	2.68690400
C	2.75391050	0.31783887	2.84164700
C	0.52410050	0.03848987	1.44839100

C	0.35431450	0.05721387	0.03147900
H	4.37265450	0.50702287	-0.71857500
H	5.78649750	0.69891587	1.32874000
H	4.75011150	0.61210287	3.57002200
H	2.33603150	0.30132587	3.84116000
N	1.58921650	0.19468387	-0.54995000
O	-0.70855950	-0.03562913	-0.66275900
N	-0.55705550	-0.17558413	2.23341300
C	-0.51139950	-0.25160513	3.51638400
H	0.37841950	-0.16855413	4.13669200
C	-1.78997950	-0.49598413	4.24728200
F	-1.56590750	-0.69512413	5.55126300
F	-2.46455550	-1.57400413	3.78416200
F	-2.66501850	0.53286387	4.14967300
C	1.83542150	0.16472487	-1.97099400
H	2.43646650	1.02682487	-2.27502500
H	2.35683950	-0.75587213	-2.25421500
H	0.86933950	0.20920487	-2.47366600

TS2

Zero-point correction= 1.069621 (Hartree/Particle)
Thermal correction to Energy= 1.126522
Thermal correction to Enthalpy= 1.127387
Thermal correction to Gibbs Free Energy= 0.979358
Sum of electronic and zero-point Energies= -3582.954283
Sum of electronic and thermal Energies= -3582.897382
Sum of electronic and thermal Enthalpies= -3582.896517
Sum of electronic and thermal Free Energies= -3583.044546
SCF Done: E(RM062X) = -3585.00419549

H	-0.35407725	-1.52347457	-0.01994337
O	-4.51928325	4.32701143	1.85696763
N	-1.21278025	-2.13073557	-0.02930237
O	-5.12167125	1.45103943	0.35687063
N	-1.25088425	3.80583143	1.33884163
H	-0.45806725	3.42942243	0.81536163
N	3.97793175	5.37855443	1.36995263
H	4.62330275	5.20921943	2.12671463
C	5.63206775	5.87985443	-1.90706537
H	6.59522375	5.96105143	-2.40098037
C	5.58304375	5.67912843	-0.53913237
H	6.48709875	5.60059543	0.05846463
C	4.32132175	5.56326643	0.05096763

C	3.12049375	5.66171443	-0.69304137
C	2.03353775	5.53502243	0.25108163
C	0.58611575	5.53188643	0.00520663
C	-0.26746125	6.00342943	1.13828663
C	-2.41849925	3.16081143	1.13164663
C	-2.60811325	-0.25462757	-0.46588037
H	-3.68093825	-0.06101957	-0.52350737
C	-2.34163025	-1.36719457	0.56841763
H	-2.04136725	-0.97432857	1.53664363
H	-3.18605625	-2.05623657	0.67000463
C	-0.87027125	-3.39096857	0.65546363
H	-0.00792925	-3.83229557	0.15390263
H	-1.72501425	-4.06876557	0.60841563
H	-0.61916925	-3.15576657	1.68970263
N	-1.96899425	0.99224743	-0.10274637
H	-0.94842525	1.05994643	-0.07977837
C	-1.57343025	-2.24045857	-1.47360437
H	-2.37153625	-2.98494157	-1.55584237
H	-0.69239325	-2.55659757	-2.03097737
C	-2.04239425	-0.82204757	-1.79861737
H	-2.78261625	-0.81061257	-2.59898737
H	-1.18388725	-0.21909957	-2.10458537
C	-4.14997825	2.10058543	0.68486363
C	-3.86521425	3.43734943	1.37114463
C	-1.97196825	5.58543443	2.83689563
H	-2.66180125	4.88681643	3.29408463
C	-1.89505625	6.87812543	3.26779463
H	-2.52234025	7.21681243	4.08723063
C	-0.92287725	9.14792843	3.09700963
H	-1.55547825	9.46238443	3.92275663
C	-0.07901425	10.03684843	2.48345563
H	-0.02887225	11.06728043	2.81996763
C	0.72165575	9.61007143	1.39857863
H	1.37821275	10.31952743	0.90500863
C	0.67594075	8.31035143	0.96169863
H	1.29199775	7.99733943	0.12555463
C	-0.17668125	7.35988143	1.58944863
C	0.08507975	5.03775743	-1.14788237
H	0.79823675	4.60048443	-1.84410937
C	-1.33190725	4.85244243	-1.49897337
C	-2.35254625	5.73501143	-1.11352337
H	-2.09735325	6.65850743	-0.60407637
C	-3.68458425	5.42551043	-1.36253337
H	-4.46301225	6.10363943	-1.02908737

C	-4.02589025	4.24100643	-2.01614937
H	-5.06836425	3.99155243	-2.18462837
C	-3.01952025	3.37879543	-2.44266737
H	-3.27425325	2.45335743	-2.95153537
C	-1.68629625	3.68650443	-2.19164937
H	-0.90231025	2.99749343	-2.49703937
C	4.45135275	5.98150443	-2.66963137
H	4.52425775	6.14276343	-3.74050937
C	3.20405075	5.87962343	-2.07922837
H	2.30372975	5.97753843	-2.67681437
C	2.61410775	5.37437043	1.48669563
H	2.13906375	5.23173643	2.44702063
C	-2.69451525	1.93920443	0.52494663
C	-1.15652225	5.14393643	1.76218663
C	-1.00006925	7.79993543	2.66314763
C	1.82966575	2.06197843	2.14576563
C	3.05175075	2.37102343	2.77481563
C	4.15878575	2.63162843	3.21368663
C	5.49103875	2.96210443	3.59866963
C	5.89875675	2.98709343	4.94158063
C	6.42634475	3.27019943	2.59141163
C	7.20958475	3.31462743	5.26627063
H	5.17952275	2.74963543	5.71820163
C	7.73173575	3.60471443	2.93111263
H	6.09904475	3.23396843	1.55427763
C	8.12993175	3.62686543	4.26689963
H	7.51455675	3.33130143	6.30772963
H	8.44448975	3.84872243	2.14835063
H	9.15016775	3.88716043	4.52837163
C	1.75269275	2.13249643	0.69149763
O	0.67777475	2.02203643	0.06094863
N	2.94763275	2.34045043	0.04524163
H	3.78340275	2.39735343	0.62164663
C	3.19418675	2.42122943	-1.31278837
C	4.58032475	2.55763943	-1.67975237
C	2.24277275	2.34073643	-2.31351037
C	4.93985175	2.64911443	-3.04985937
C	2.62390075	2.45610343	-3.66958737
H	1.20965875	2.18627443	-2.03938437
C	6.77256775	2.62089943	-1.00225737
C	6.32172075	2.74254743	-3.34821437
C	3.93270975	2.61463243	-4.04704737
H	1.84605275	2.41178743	-4.42611437
C	7.24125575	2.72166243	-2.33239637

H	7.48122675	2.59407743	-0.17412837
H	6.63271375	2.82181243	-4.38658337
H	4.21461075	2.69973643	-5.09186837
H	8.30591375	2.78120143	-2.52879437
N	5.50223275	2.55172643	-0.68335637
C	0.72157075	1.58013843	2.88056663
H	-0.23935225	1.59807943	2.37631863
H	0.67926175	1.81939543	3.94066263
C	3.48041075	-0.59831257	1.43241063
C	4.16153375	-0.61109757	0.19274463
C	5.53297775	-0.49536557	0.08270463
C	6.26724675	-0.35821257	1.26437063
C	5.62934575	-0.35942257	2.50043863
C	4.24022175	-0.47787057	2.59503763
C	2.05373775	-0.74165657	1.11104963
C	1.98020775	-0.86597057	-0.37079937
H	6.01826575	-0.48596357	-0.88829337
H	7.34524375	-0.24473557	1.21386163
H	6.21239875	-0.23708957	3.40714063
H	3.77890975	-0.44352957	3.57377263
N	3.24226175	-0.75903157	-0.85855037
O	0.96084775	-1.02070557	-1.05746337
N	0.92886275	-0.80796457	1.77099563
C	0.88868675	-0.39505657	3.06485363
H	1.77955475	-0.45868357	3.68915963
C	-0.32790925	-0.79988657	3.83971263
F	-0.19149725	-0.46551057	5.12800763
F	-0.56385825	-2.13299557	3.79622263
F	-1.46331125	-0.21793557	3.40072763
C	3.58208875	-0.82442057	-2.26120937
H	4.16069975	0.05579343	-2.55484337
H	4.16035575	-1.72937357	-2.47341537
H	2.64836375	-0.84000857	-2.82301537

TS2’

Zero-point correction=	1.069351 (Hartree/Particle)
Thermal correction to Energy=	1.126006
Thermal correction to Enthalpy=	1.126871
Thermal correction to Gibbs Free Energy=	0.980004
Sum of electronic and zero-point Energies=	-3582.948592
Sum of electronic and thermal Energies=	-3582.891937
Sum of electronic and thermal Enthalpies=	-3582.891072
Sum of electronic and thermal Free Energies=	-3583.037939

SCF Done: E(RM062X) = -3585.00170730

C	-0.42278892	0.88880408	0.08306188
C	0.83283408	0.49074408	-0.41967412
C	1.94374408	0.10003708	-0.74268112
C	3.28990208	-0.27992792	-1.02115812
C	3.90769108	0.03664708	-2.24038112
C	4.03306408	-0.94550192	-0.03057112
C	5.23777608	-0.30106192	-2.45750112
H	3.33884208	0.56367008	-2.99907112
C	5.36211008	-1.27830892	-0.25829712
H	3.54409208	-1.17299492	0.91387888
C	5.97139208	-0.95796892	-1.47084212
H	5.70667708	-0.04774592	-3.40319912
H	5.92945808	-1.78921992	0.51440788
H	7.00973108	-1.21953392	-1.64637912
C	-0.82152292	0.43632208	1.40015788
O	-1.92560992	0.73750708	1.90244888
N	0.10232208	-0.29651992	2.10324788
H	0.96410008	-0.53682192	1.62105588
C	-0.04629792	-0.90132992	3.34192388
C	1.06408808	-1.70595792	3.77677288
C	-1.15035692	-0.78714492	4.16651388
C	0.97610208	-2.41976892	5.00032188
C	-1.21459592	-1.50730192	5.38055788
H	-1.97747592	-0.16912692	3.85140688
C	3.18514908	-2.48704992	3.36831188
C	2.08947408	-3.21550192	5.36490588
C	-0.19137492	-2.31858392	5.79618488
H	-2.11185792	-1.41358792	5.98549988
C	3.19277608	-3.25668592	4.55397988
H	4.05477608	-2.49621692	2.71200688
H	2.05031608	-3.78433092	6.29008888
H	-0.25278092	-2.87811392	6.72431388
H	4.06123708	-3.85530892	4.80444188
N	2.17216208	-1.74335592	2.98859888
C	-1.37303092	1.65000908	-0.68157912
H	-2.42154192	1.41322008	-0.50225312
H	-1.12926492	1.77854708	-1.73325712
C	2.26030708	3.33922108	0.16052088
C	2.89381208	2.61023708	1.17830688
C	4.22364308	2.23202308	1.10086488
C	4.92136508	2.59401608	-0.05388012
C	4.30157408	3.30393108	-1.08415912

C	2.95888408	3.67114208	-0.99124612
C	0.84913108	3.43717408	0.51848888
C	0.74741508	2.85410508	1.88935788
H	4.69751708	1.65087108	1.88486688
H	5.95772308	2.29028608	-0.16080312
H	4.86808908	3.55326708	-1.97505412
H	2.45524608	4.19857108	-1.79476212
N	1.96992708	2.34427508	2.20358788
O	-0.20248892	2.93042308	2.70284988
N	-0.09568692	3.86678608	-0.26036212
C	-1.38385992	3.43489908	-0.05774212
H	-1.77654892	3.23056008	0.94314388
C	-2.38622092	4.18176208	-0.88690712
F	-3.61259892	3.64993408	-0.74478512
F	-2.08733792	4.19717008	-2.18366712
F	-2.49480592	5.48027908	-0.49244312
C	2.28542508	1.67707408	3.44600788
H	2.68764008	0.68066308	3.23980088
H	3.01469308	2.25788408	4.02012388
H	1.35977808	1.57574708	4.01404588
H	-1.10522092	4.24934108	2.55147388
O	-7.14262892	2.51125508	0.03431888
N	-1.53118392	5.16471708	2.89826988
O	-6.03828992	4.64422508	2.29869788
N	-4.43833692	0.60056608	0.70920188
H	-3.58828192	0.34089208	1.21484888
N	-0.31576492	-2.57420292	-0.30306012
H	0.42869008	-2.25584792	-0.90594612
C	0.81702908	-4.83340192	2.40755588
H	1.65983208	-5.41096692	2.77405788
C	0.95312608	-4.09080292	1.24719388
H	1.88658408	-4.06723092	0.69266388
C	-0.15576392	-3.35694192	0.81867088
C	-1.38384792	-3.34990892	1.52481988
C	-2.29060192	-2.50832692	0.77643288
C	-3.65130692	-2.07423592	1.11204188
C	-4.53164892	-1.67555892	-0.03097112
C	-5.00877092	1.74064708	1.12416188
C	-3.43939692	3.99682508	3.68911388
H	-4.40715292	4.25298608	4.12174488
C	-3.01579592	5.13538808	2.74247688
H	-3.29153392	4.97376008	1.69980388
H	-3.40199692	6.10587808	3.06943588
C	-0.84280892	6.28746608	2.22980688

H	0.23046208	6.19187508	2.40114888
H	-1.21063792	7.22933208	2.64209988
H	-1.05218992	6.22922508	1.16116188
N	-3.57834792	2.72607408	2.99768688
H	-2.74536492	2.15919308	2.81878288
C	-1.33374592	5.05103608	4.37425788
H	-1.59517592	6.01596408	4.81921688
H	-0.28846592	4.81237908	4.57239888
C	-2.31102992	3.93270208	4.75121288
H	-2.69087392	4.05671308	5.76516888
H	-1.80268692	2.96714108	4.68631588
C	-5.71441792	3.55817108	1.85790188
C	-6.21459392	2.57246008	0.80006088
C	-5.80864092	0.02649808	-1.23701312
H	-6.12131692	1.06085108	-1.31753012
C	-6.26195392	-0.91378992	-2.11793712
H	-6.93417792	-0.62358492	-2.92035212
C	-6.33497192	-3.25330192	-2.92704212
H	-6.99861992	-2.93921392	-3.72817312
C	-5.96675092	-4.56739792	-2.79750512
H	-6.33158192	-5.31066092	-3.49884612
C	-5.11351892	-4.95732692	-1.73878612
H	-4.83263092	-6.00039192	-1.63338812
C	-4.63868892	-4.03231992	-0.84375712
H	-3.98631192	-4.34271592	-0.03425812
C	-4.99082592	-2.65896292	-0.96167312
C	-4.03154792	-1.92056792	2.39845488
H	-3.28437592	-2.10994092	3.16661788
C	-5.29507892	-1.31805692	2.85799588
C	-6.53767192	-1.60103092	2.27631688
H	-6.60537792	-2.37026192	1.51322388
C	-7.67191592	-0.89309392	2.65799888
H	-8.62487692	-1.11436792	2.18845388
C	-7.58980892	0.10252408	3.63035288
H	-8.47495192	0.66321308	3.91219588
C	-6.36615992	0.37070308	4.23839988
H	-6.29076892	1.14398208	4.99703988
C	-5.23263892	-0.34199892	3.86184288
H	-4.27247192	-0.11284192	4.31910288
C	-0.39576692	-4.84900492	3.12278588
H	-0.46909592	-5.44241792	4.02886788
C	-1.49197992	-4.11927492	2.69529488
H	-2.42401892	-4.15086792	3.25023388
C	-1.59072392	-2.07606992	-0.32518312

H	-1.91715592	-1.41935592	-1.11935512
C	-4.59953492	2.64088608	2.10687888
C	-4.93489692	-0.35741592	-0.18667812
C	-5.86624692	-2.27362292	-2.01525612

E

Zero-point correction= 1.072997 (Hartree/Particle)
Thermal correction to Energy= 1.129740
Thermal correction to Enthalpy= 1.130605
Thermal correction to Gibbs Free Energy= 0.983271
Sum of electronic and zero-point Energies= -3582.968460
Sum of electronic and thermal Energies= -3582.911717
Sum of electronic and thermal Enthalpies= -3582.910852
Sum of electronic and thermal Free Energies= -3583.058186
SCF Done: E(RM062X) = -3585.02335127

H	-0.79399142	0.30042918	0.00000000
O	-3.85488342	6.15059318	1.66509400
N	-1.68787642	-0.20697582	-0.20357400
O	-4.73610042	3.30768418	0.24856400
N	-0.67872542	5.49576018	0.74129300
H	0.04170858	5.04909518	0.16932900
N	4.70957658	6.48489718	0.93976100
H	5.31099658	6.25094918	1.71566200
C	6.48868958	6.71191518	-2.30206800
H	7.46587058	6.66224318	-2.77204100
C	6.38332058	6.55586518	-0.93149700
H	7.25640058	6.38172318	-0.30878900
C	5.10361458	6.60633018	-0.37274400
C	3.94090058	6.83160318	-1.14924800
C	2.82558558	6.84964018	-0.23035400
C	1.39316658	7.00627318	-0.50509100
C	0.57988458	7.55207418	0.62467400
C	-1.90156842	4.94713818	0.62809700
C	-2.59980742	1.72853718	-1.19330500
H	-3.55931942	2.14170218	-1.50573600
C	-2.83538742	0.74192718	-0.04102200
H	-2.82098542	1.20932018	0.93986100
H	-3.75430342	0.16163618	-0.16818900
C	-1.71009042	-1.39202982	0.67858500
H	-0.82860542	-1.99688582	0.46318000
H	-2.62039442	-1.96112882	0.48218800
H	-1.68077142	-1.05762182	1.71408800

N	-1.74787542	2.82247318	-0.77099700
H	-0.72529642	2.76398818	-0.80431900
C	-1.73620842	-0.50955682	-1.67098400
H	-2.60678942	-1.15663082	-1.81647700
H	-0.82312842	-1.01574382	-1.97098000
C	-1.92690642	0.87407618	-2.29720600
H	-2.53936742	0.81964018	-3.19758300
H	-0.95498742	1.29743218	-2.55843100
C	-3.71873242	3.95832818	0.39276500
C	-3.30010842	5.26664318	1.06116100
C	-1.14790442	7.28344618	2.33031600
H	-1.91077242	6.66009218	2.77868900
C	-0.90998942	8.54088518	2.80447200
H	-1.47973442	8.91961918	3.64809600
C	0.31457358	10.68840618	2.68770800
H	-0.26836242	11.04734618	3.53168600
C	1.24915458	11.49263518	2.08919300
H	1.42225558	12.49928718	2.45559500
C	1.98323358	11.00997618	0.98079000
H	2.71215458	11.65381918	0.49898300
C	1.78298758	9.73832418	0.50643100
H	2.35023958	9.38212418	-0.34667600
C	0.83175658	8.87362718	1.11671000
C	0.85686958	6.58522218	-1.67139200
H	1.51960358	6.06908918	-2.36326600
C	-0.56923142	6.59030118	-2.03544100
C	-1.45297742	7.61995618	-1.67937900
H	-1.06737842	8.50790818	-1.18877600
C	-2.81372342	7.50225018	-1.93624000
H	-3.48658042	8.29862318	-1.63539000
C	-3.31836242	6.36662318	-2.57052100
H	-4.38341342	6.27441718	-2.75691300
C	-2.44542142	5.35695018	-2.96501400
H	-2.82599742	4.46863518	-3.46163300
C	-1.08374942	5.47115918	-2.70274900
H	-0.40712642	4.66475318	-2.97533300
C	5.34717658	6.93492118	-3.09751900
H	5.46345558	7.05573118	-4.16984900
C	4.08354658	7.00247318	-2.53734700
H	3.21700158	7.19265318	-3.16189800
C	3.35341258	6.64079518	1.02140800
H	2.84208458	6.56058318	1.97001300
C	-2.31894842	3.78043718	-0.01217200
C	-0.40819142	6.78746418	1.22452900

C	0.07690158	9.37294918	2.21420700
C	1.93713258	3.45218818	1.59772100
C	3.11053358	3.65522718	2.32791300
C	4.19441158	3.81513518	2.87473300
C	5.51591458	3.98028818	3.37148100
C	5.80669758	4.01782118	4.74651800
C	6.57892158	4.09692018	2.44978000
C	7.11698458	4.17018218	5.18227700
H	4.99489658	3.92893518	5.46072400
C	7.88293758	4.26023318	2.90111600
H	6.34711358	4.04822218	1.38743700
C	8.16123958	4.29563318	4.26688700
H	7.32525258	4.19777918	6.24733000
H	8.69075458	4.35756718	2.18082000
H	9.18086058	4.42144618	4.61522700
C	1.98323858	3.50323418	0.17071000
O	0.96175358	3.43429218	-0.56851700
N	3.24469958	3.61653418	-0.39580100
H	4.03386958	3.62158818	0.24455600
C	3.60179558	3.60456918	-1.72497000
C	5.02061458	3.54357718	-1.98519300
C	2.73130458	3.61039818	-2.80408900
C	5.49393358	3.52085418	-3.32403800
C	3.22967458	3.60824918	-4.12520100
H	1.66862858	3.61596418	-2.61269500
C	7.14671758	3.37305618	-1.13334600
C	6.89529058	3.42399418	-3.51036500
C	4.57318958	3.56881218	-4.40057600
H	2.51414358	3.63497418	-4.94187500
C	7.72506858	3.34399418	-2.42289100
H	7.78130258	3.30607018	-0.24906800
H	7.29204958	3.41000218	-4.52217800
H	4.94417558	3.56538318	-5.42065100
H	8.80062858	3.26225018	-2.53374300
N	5.85697458	3.47552218	-0.91818200
C	0.70849358	2.95802618	2.27683100
H	-0.17496242	3.11592418	1.65517800
H	0.54835258	3.44698318	3.24225700
C	3.37475358	0.65957418	1.04452900
C	4.07514158	0.49887318	-0.17176900
C	5.45211358	0.47170718	-0.24555800
C	6.16473358	0.61205118	0.95026000
C	5.50505158	0.75052918	2.16536000
C	4.10879458	0.77634118	2.22216300

C	1.94278458	0.61837618	0.69586600
C	1.89722458	0.37753718	-0.80389100
H	5.96235058	0.37649018	-1.19870100
H	7.24975858	0.61873618	0.92444000
H	6.07515158	0.87481418	3.07955600
H	3.62836658	0.90879818	3.18248200
N	3.17821958	0.36313518	-1.24709800
O	0.88620358	0.26453018	-1.48169800
N	0.81172658	0.74921718	1.28605200
C	0.79150058	1.40492918	2.55831700
H	1.66461858	1.20916618	3.18892200
C	-0.41241042	0.94419218	3.34353700
F	-0.47495342	1.53856118	4.53648600
F	-0.39521042	-0.38631982	3.55504200
F	-1.56675642	1.20870318	2.69794800
C	3.56089258	0.24044118	-2.63575500
H	4.20973758	1.07273918	-2.92291800
H	4.07787458	-0.70851382	-2.80938500
H	2.64780258	0.27853518	-3.22955800

TS3

Zero-point correction= 1.071420 (Hartree/Particle)
Thermal correction to Energy= 1.127881
Thermal correction to Enthalpy= 1.128746
Thermal correction to Gibbs Free Energy= 0.981252
Sum of electronic and zero-point Energies= -3582.977380
Sum of electronic and thermal Energies= -3582.920919
Sum of electronic and thermal Enthalpies= -3582.920054
Sum of electronic and thermal Free Energies= -3583.067548
SCF Done: E(RM062X) = -3585.02220337

C	-3.48489172	-1.20686437	-0.17051016
C	-2.33269772	-1.61610937	-0.90637016
C	-1.25715272	-1.89185737	-1.39828616
C	0.03146928	-2.28482037	-1.87626616
C	0.47829428	-1.94141637	-3.15925016
C	0.86810628	-3.02416037	-1.02241616
C	1.73945328	-2.34239237	-3.58320016
H	-0.16879972	-1.36143137	-3.80866016
C	2.12615328	-3.42211437	-1.45926816
H	0.51293628	-3.26378337	-0.02206216
C	2.56403528	-3.08397837	-2.73867816
H	2.08103328	-2.07701837	-4.57823816

H	2.76779828	-3.99779137	-0.79875916
H	3.54608528	-3.39679637	-3.07748116
C	-3.64715872	-1.88283837	1.16493684
O	-4.74212272	-1.97640837	1.72042884
N	-2.48026972	-2.27245937	1.73881684
H	-1.63126772	-2.20838837	1.18230284
C	-2.26492372	-2.72914137	3.03542184
C	-0.89680872	-3.02978337	3.34415184
C	-3.22871672	-2.86837937	4.01118284
C	-0.56218372	-3.51779437	4.63199184
C	-2.87454372	-3.36716437	5.28659484
H	-4.25069872	-2.59897537	3.78792384
C	1.29384128	-3.03848337	2.65960384
C	0.80548728	-3.78911437	4.88006384
C	-1.58199572	-3.69928637	5.59952684
H	-3.65848172	-3.48490037	6.02788384
C	1.73525028	-3.55254337	3.90092684
H	2.01323728	-2.82745037	1.86878084
H	1.09983928	-4.17657537	5.85170884
H	-1.32124972	-4.08588437	6.57978084
H	2.79012828	-3.74327337	4.06216984
N	0.03463428	-2.78791737	2.38352784
C	-4.75429472	-0.91701037	-0.92999316
H	-5.61550172	-1.10372437	-0.28571216
H	-4.84764572	-1.53954037	-1.82304616
C	-1.81791872	1.07694863	-0.19710216
C	-0.90092972	0.89493563	0.85421484
C	0.46826028	0.94836363	0.65808884
C	0.92315828	1.21773863	-0.63612416
C	0.03201928	1.43842763	-1.68242016
C	-1.34753972	1.35878463	-1.47000116
C	-3.15605972	0.79402563	0.35651084
C	-2.94412872	0.70044163	1.85028784
H	1.16058428	0.79233063	1.47835584
H	1.99090128	1.26243763	-0.82334716
H	0.41054628	1.66040963	-2.67409216
H	-2.03176972	1.51785363	-2.29688416
N	-1.58718772	0.67855163	2.05478684
O	-3.80526172	0.59000863	2.70197684
N	-4.34883972	1.31599463	-0.11492016
C	-4.75387372	0.58725463	-1.29886116
H	-4.04331372	0.77185963	-2.11106116
C	-6.10367572	1.04503563	-1.80155816
F	-6.45297072	0.34312363	-2.88653516

F	-6.10091772	2.34064663	-2.13415016
F	-7.05443572	0.86502363	-0.87340216
C	-0.97460472	0.47512863	3.34703284
H	-0.23635572	-0.32933237	3.28445384
H	-0.48943372	1.39126163	3.69819784
H	-1.76543072	0.18877263	4.04207784
H	-5.09123472	1.35564163	0.60868984
O	-10.26250372	-2.90067537	-0.50834016
N	-6.55451472	2.37020763	1.70407884
O	-10.40329672	-0.26995037	1.47238584
N	-6.97746172	-3.12634937	0.20208784
H	-6.17965272	-3.00877937	0.82306684
N	-1.89810472	-4.95556437	-0.36612616
H	-1.26201372	-4.69830037	-1.10479416
C	-0.20624972	-6.33040237	2.63010584
H	0.75884428	-6.59773337	3.04869084
C	-0.27150772	-5.80090537	1.35384884
H	0.62165728	-5.65486637	0.75256084
C	-1.53594472	-5.46329037	0.85948784
C	-2.72275072	-5.65693937	1.60771484
C	-3.82282772	-5.24529637	0.76473884
C	-5.26279872	-5.22271637	1.05849284
C	-6.17816172	-5.37414937	-0.11451416
C	-8.03545772	-2.32369037	0.48966484
C	-7.73689972	0.68223163	2.78741784
H	-8.67947772	0.43232763	3.27837984
C	-7.91780172	1.85700463	1.82432284
H	-8.33755972	1.56217463	0.86193684
H	-8.58640672	2.61049063	2.28126284
C	-6.46790172	3.62188863	0.97400384
H	-5.42436572	3.94608763	0.92266784
H	-7.06334472	4.41982563	1.45076084
H	-6.82807472	3.47616063	-0.04700116
N	-7.26132372	-0.51185637	2.08940084
H	-6.26611472	-0.71613937	2.06941184
C	-6.12087672	2.48372163	3.09949784
H	-6.58076772	3.37494563	3.56458884
H	-5.03503072	2.57593663	3.16336884
C	-6.65530272	1.20039563	3.76214984
H	-7.08105572	1.40892963	4.74530084
H	-5.86053272	0.46195163	3.88532884
C	-9.55716972	-1.03868737	1.07569184
C	-9.48396072	-2.26798637	0.16571684
C	-7.91352472	-4.48846137	-1.59030116

H	-8.58017872	-3.67348937	-1.84388216
C	-7.94420172	-5.66012637	-2.28949616
H	-8.62938772	-5.77419737	-3.12465516
C	-7.12755372	-7.96627337	-2.66887816
H	-7.81264172	-8.05268737	-3.50804116
C	-6.32493172	-9.01799737	-2.30914616
H	-6.36061272	-9.95035237	-2.86306016
C	-5.45563972	-8.88870937	-1.20135316
H	-4.83232872	-9.72761937	-0.90830516
C	-5.39432272	-7.71691437	-0.48984816
H	-4.72781972	-7.63516237	0.36232384
C	-6.20116172	-6.60166237	-0.85022016
C	-5.70446772	-4.96970737	2.30935284
H	-4.95221172	-4.74609437	3.06350684
C	-7.10330972	-4.75642537	2.71883884
C	-8.17821372	-5.50032037	2.21257684
H	-7.98251072	-6.34826537	1.56394984
C	-9.48637972	-5.14345037	2.51844584
H	-10.30919572	-5.71363037	2.10014584
C	-9.74637272	-4.05075437	3.34554084
H	-10.76978572	-3.76376337	3.56340884
C	-8.68581972	-3.32887437	3.88591284
H	-8.87735872	-2.47537437	4.52938084
C	-7.37612872	-3.68501737	3.57981884
H	-6.54995872	-3.09715237	3.97322284
C	-1.37318272	-6.53366037	3.39394284
H	-1.28746072	-6.95501337	4.39045984
C	-2.62264672	-6.20804437	2.89709184
H	-3.51390772	-6.38735137	3.48945084
C	-3.26301672	-4.83927937	-0.42345616
H	-3.75426972	-4.47390137	-1.31480616
C	-8.10400872	-1.19876537	1.31037184
C	-7.02373472	-4.34040437	-0.49235916
C	-7.09276472	-6.74499737	-1.94988016

TS3’

Zero-point correction=	1.070077 (Hartree/Particle)
Thermal correction to Energy=	1.126667
Thermal correction to Enthalpy=	1.127532
Thermal correction to Gibbs Free Energy=	0.978251
Sum of electronic and zero-point Energies=	-3582.900138
Sum of electronic and thermal Energies=	-3582.843548
Sum of electronic and thermal Enthalpies=	-3582.842683

Sum of electronic and thermal Free Energies= -3582.991965
SCF Done: E(RM062X) = -3584.96397884

C	-2.11373391	0.07510730	0.00000000
C	-0.96103191	-0.55316870	-0.59157800
C	0.03501209	-1.18391470	-0.88012400
C	1.15877609	-2.02344070	-1.16779000
C	0.94909509	-3.30179070	-1.70690200
C	2.46234509	-1.60315770	-0.86623700
C	2.03478609	-4.13463070	-1.95267900
H	-0.06956491	-3.62211170	-1.90146900
C	3.53993209	-2.44717970	-1.10982100
H	2.61189309	-0.61786470	-0.43584700
C	3.32951409	-3.71181270	-1.65708200
H	1.86890609	-5.12197270	-2.37156400
H	4.54763009	-2.11531870	-0.87880500
H	4.17285609	-4.36701670	-1.85032600
C	-1.80136791	0.76696930	1.25393700
O	-2.56103491	1.64515930	1.75408400
N	-0.70963491	0.33028530	1.92219000
H	-0.10591991	-0.32279970	1.42370100
C	-0.29792991	0.58906830	3.22323700
C	0.97893209	0.02469730	3.56072300
C	-1.01538791	1.26950430	4.18435400
C	1.50025609	0.20114130	4.86571100
C	-0.47597591	1.43460730	5.48183100
H	-2.00408291	1.63673030	3.94682400
C	2.78723409	-1.21790170	2.88664600
C	2.76253809	-0.38544970	5.13513300
C	0.75070209	0.92820130	5.82560800
H	-1.06309791	1.97107430	6.22043700
C	3.40691109	-1.09199970	4.15386400
H	3.26909009	-1.78277670	2.09038100
H	3.19949809	-0.27039670	6.12332100
H	1.15408509	1.06102130	6.82459700
H	4.37036009	-1.55622470	4.33050500
N	1.62561809	-0.68070570	2.59517000
C	-3.08001691	0.79786330	-0.91864700
H	-2.82324191	0.59532130	-1.95955200
H	-3.07236491	1.88123930	-0.76256700
C	-3.58365791	-1.16766970	1.91631900
C	-2.61133391	-1.90642270	2.61023600
C	-2.55003291	-1.92837370	3.99473500
C	-3.51965391	-1.20523370	4.69853700

C	-4.53594191	-0.52719670	4.03111100
C	-4.57604191	-0.52702270	2.63129600
C	-3.34370591	-1.36664870	0.43809100
C	-2.41652391	-2.59057570	0.44344000
H	-1.79270791	-2.50478970	4.51584600
H	-3.49164691	-1.20199870	5.78358500
H	-5.31124791	-0.01245470	4.59137800
H	-5.40874291	-0.08176170	2.09535500
N	-1.83295891	-2.62908570	1.70032400
O	-2.18161991	-3.36351570	-0.46135600
N	-4.22503891	-1.21839270	-0.55225500
C	-4.49384491	0.16639930	-0.64205600
H	-4.90024091	0.67221430	0.25835800
C	-5.47947291	0.49186830	-1.73602700
F	-5.64687091	1.84089530	-1.82197300
F	-6.69501591	-0.02599970	-1.49143500
F	-5.09274491	0.07181230	-2.93913200
C	-0.77546091	-3.54105470	2.06047200
H	0.07865509	-2.98477770	2.46200100
H	-1.12503391	-4.27066970	2.79875000
H	-0.47111891	-4.05889970	1.14906700
H	-2.83857091	2.91146130	1.08671600
O	-9.22157091	2.29905530	-1.29212600
N	-3.01064891	3.97936530	0.92580800
O	-7.16040691	4.61335130	-0.26896100
N	-8.01625091	0.29605630	1.19748800
H	-7.50411291	0.07422230	2.04607300
N	-5.16348391	-3.82327570	0.51772900
H	-4.57407791	-3.80001870	-0.30651200
C	-3.58793391	-5.51172770	3.41429100
H	-2.76899891	-6.15989270	3.71245500
C	-3.72096091	-5.15053970	2.08263100
H	-3.02106691	-5.48250370	1.32092600
C	-4.79008691	-4.31759270	1.74819000
C	-5.71414591	-3.83435270	2.70833600
C	-6.65628691	-3.00600070	1.98719600
C	-7.78177391	-2.21342570	2.47908100
C	-8.82999391	-1.94472270	1.44681500
C	-7.82794991	1.52130130	0.67927400
C	-5.20925491	3.94060730	1.88730400
H	-5.94763491	4.73793630	1.98429900
C	-4.44429391	4.16312030	0.56083300
H	-4.72212991	3.45369730	-0.22306000
H	-4.58677391	5.18025230	0.18620400

C	-2.04364291	4.50177030	-0.05533300
H	-1.03419991	4.25364630	0.27596800
H	-2.15826691	5.58513430	-0.13630500
H	-2.23426791	4.03837630	-1.02405600
N	-5.93172891	2.67751330	1.95974800
H	-5.35715591	1.86750530	2.18041600
C	-2.88399591	4.54549230	2.29900600
H	-2.87853691	5.63739730	2.21714900
H	-1.94822691	4.19638530	2.74019800
C	-4.13476391	4.01511330	2.99544300
H	-4.43955291	4.64588430	3.83026900
H	-3.93806691	3.00803830	3.37619500
C	-7.42854491	3.47121330	0.04114100
C	-8.39872391	2.39030330	-0.42174700
C	-9.81599391	-0.52113770	-0.27061900
H	-9.83992991	0.42673630	-0.79315400
C	-10.66779891	-1.52547570	-0.63411100
H	-11.37315191	-1.36295370	-1.44401900
C	-11.54383091	-3.82717570	-0.34350200
H	-12.25240591	-3.64796370	-1.14753200
C	-11.50922391	-5.03477470	0.30445500
H	-12.19193291	-5.82862470	0.01972600
C	-10.57948291	-5.24835070	1.34939800
H	-10.55699291	-6.20631370	1.85880900
C	-9.70604991	-4.25888370	1.72315600
H	-8.99377091	-4.42941970	2.52418800
C	-9.71790591	-2.99756570	1.06693100
C	-7.82132491	-1.73553970	3.74470600
H	-6.94123691	-1.92534670	4.35586700
C	-8.85890391	-0.92681970	4.40346100
C	-10.20225791	-0.87076170	3.99694200
H	-10.54160791	-1.47439070	3.16342900
C	-11.11247191	-0.06619070	4.67250800
H	-12.14619091	-0.04103570	4.34253300
C	-10.71402391	0.69405530	5.76988100
H	-11.43096491	1.31945130	6.29176400
C	-9.39142491	0.63106830	6.19992900
H	-9.06986991	1.20502630	7.06342100
C	-8.48085991	-0.17418570	5.52705300
H	-7.45236891	-0.23339170	5.87548300
C	-4.50867091	-5.07078670	4.38256400
H	-4.38840491	-5.38944370	5.41304800
C	-5.56686891	-4.24311170	4.04319600
H	-6.27725691	-3.92853770	4.80082800

C	-6.26015591	-3.03127870	0.66711900
H	-6.65835491	-2.48577770	-0.17628800
C	-6.92569391	2.52156930	1.03528000
C	-8.89156791	-0.73016570	0.78617100
C	-10.65556991	-2.78394070	0.02105300

TS3”

Zero-point correction= 1.071371 (Hartree/Particle)
Thermal correction to Energy= 1.127701
Thermal correction to Enthalpy= 1.128566
Thermal correction to Gibbs Free Energy= 0.980618
Sum of electronic and zero-point Energies= -3582.920273
Sum of electronic and thermal Energies= -3582.863943
Sum of electronic and thermal Enthalpies= -3582.863078
Sum of electronic and thermal Free Energies= -3583.011026
SCF Done: E(RM062X) = -3584.98569766

C	-2.62875537	-0.03218884	0.00000000
C	-1.47336337	0.27612216	0.80678400
C	-0.47512537	0.61994016	1.40357200
C	0.70589763	1.09961216	2.05332300
C	0.76914263	1.22361216	3.44784700
C	1.81017963	1.48218616	1.27545500
C	1.91920063	1.71963116	4.05079000
H	-0.08819537	0.93141916	4.04493700
C	2.95555863	1.97386716	1.88815000
H	1.74465263	1.38548616	0.19521400
C	3.01429563	2.09485116	3.27574800
H	1.96062963	1.81356816	5.13113300
H	3.80801463	2.26407416	1.28155700
H	3.91031863	2.48023516	3.75120300
C	-2.24543637	-0.44459684	-1.37311100
O	-2.94352237	-1.19574284	-2.08887700
N	-1.14591437	0.18155916	-1.86586900
H	-0.62007937	0.75521916	-1.20654500
C	-0.82909137	0.45470416	-3.19365100
C	0.20668063	1.43728216	-3.36131400
C	-1.45072737	-0.07283584	-4.30518200
C	0.54199163	1.88466116	-4.66268600
C	-1.08466337	0.37286316	-5.59798400
H	-2.23379937	-0.80637484	-4.18015700
C	1.71900363	2.84719916	-2.36905400
C	1.53801763	2.88924516	-4.75851900

C	-0.12290537	1.33053716	-5.78726700
H	-1.59542537	-0.05421484	-6.45496000
C	2.12307063	3.37538316	-3.61916100
H	2.16492763	3.21782016	-1.44753000
H	1.82106363	3.26207316	-5.73899800
H	0.14081663	1.67399616	-6.78256700
H	2.88352763	4.14679916	-3.65819300
N	0.80516963	1.91566016	-2.23954100
C	-3.67472737	-0.87804284	0.70605500
H	-3.37507437	-1.04362584	1.74161300
H	-3.81194937	-1.85479784	0.23625400
C	-2.68343037	2.66752116	-0.07462500
C	-2.41231137	3.12875116	-1.36576600
C	-1.49388937	4.13612116	-1.61517400
C	-0.85387737	4.70127616	-0.50727200
C	-1.13471737	4.27336516	0.79170500
C	-2.05535637	3.24096416	1.01496500
C	-3.63007837	1.51073216	-0.14540000
C	-4.05323637	1.57121516	-1.65219600
H	-1.29881437	4.49205016	-2.62222000
H	-0.12938837	5.49495516	-0.66514800
H	-0.62252237	4.73081016	1.63193400
H	-2.28526337	2.88082216	2.01237100
N	-3.23321137	2.46181816	-2.28879300
O	-4.98593937	0.99517116	-2.21447500
N	-4.56313637	1.33071316	0.81839900
C	-4.99105637	-0.01761284	0.69674500
H	-5.53529237	-0.28147184	-0.22557200
C	-5.89430037	-0.45221484	1.82606300
F	-6.25176937	-1.75392684	1.63839200
F	-7.02889937	0.24963016	1.90090400
F	-5.30309237	-0.38697084	3.02431900
C	-3.35593437	2.84501216	-3.67856000
H	-3.66841937	3.89215416	-3.75832300
H	-2.40062037	2.70281316	-4.19570400
H	-4.11003237	2.19843516	-4.12901700
H	-3.77650537	-2.45345684	-1.64408800
O	-10.05076237	-0.87074384	0.66950500
N	-4.15775937	-3.44857884	-1.74493800
O	-8.63895237	-3.35662384	-0.96571200
N	-7.70259937	1.17044316	-0.72794500
H	-6.88051137	1.38581516	-1.29126100
N	-4.19910537	5.44963716	-0.30038000
H	-3.43971237	5.48004816	0.36548800

C	-3.51420237	7.40276216	-3.37592600
H	-2.84244137	8.12743016	-3.82474300
C	-3.28350637	6.97200816	-2.08036200
H	-2.44395437	7.34151316	-1.49955900
C	-4.17113237	6.03519516	-1.54269100
C	-5.25838337	5.51405116	-2.28417100
C	-5.92208137	4.55725616	-1.43148900
C	-7.11271437	3.75427816	-1.74009200
C	-8.07606837	3.54016516	-0.61837900
C	-8.11776737	-0.10259984	-0.76836900
C	-6.23372037	-2.71858984	-2.67855700
H	-7.13684737	-3.25436584	-2.97542300
C	-5.62513137	-3.45374284	-1.46266600
H	-5.82773437	-2.95501684	-0.51084300
H	-5.95708837	-4.49446584	-1.40655700
C	-3.35122937	-4.35619484	-0.90713000
H	-2.29673737	-4.20987684	-1.14505400
H	-3.64705437	-5.38760584	-1.10898700
H	-3.52779537	-4.12026284	0.14280800
N	-6.60155937	-1.34815284	-2.38965800
H	-5.87065237	-0.63486984	-2.41333600
C	-4.06159737	-3.69345884	-3.21474000
H	-4.28317037	-4.75082584	-3.39086300
H	-3.04794237	-3.46060484	-3.54446100
C	-5.13730437	-2.76381184	-3.77026900
H	-5.51757137	-3.10650584	-4.73243400
H	-4.71926537	-1.76038984	-3.89824700
C	-8.51528037	-2.14826584	-0.89296800
C	-9.14999437	-0.99138284	-0.11884400
C	-9.22301037	2.07119816	0.96209800
H	-9.39796637	1.06981916	1.33330900
C	-9.85045437	3.14168116	1.53014500
H	-10.52926637	2.98856616	2.36423600
C	-10.30478637	5.57271916	1.62869800
H	-10.97969737	5.39569416	2.46185700
C	-10.11360137	6.83868616	1.13861300
H	-10.63182237	7.68304116	1.58140700
C	-9.24354337	7.04127016	0.04265000
H	-9.10400337	8.04200016	-0.35382900
C	-8.57459237	5.98704316	-0.52681200
H	-7.91493237	6.15963116	-1.37064300
C	-8.73809437	4.66441916	-0.02851900
C	-7.26473437	3.20684516	-2.96398100
H	-6.44118137	3.31868116	-3.66819600

C	-8.37523137	2.33759116	-3.38974400
C	-9.71323937	2.62182216	-3.08975500
H	-9.95910437	3.55342516	-2.58901800
C	-10.71436637	1.71491816	-3.41816900
H	-11.74681237	1.94331416	-3.17391700
C	-10.39763037	0.51323016	-4.05031600
H	-11.18118937	-0.19763984	-4.29185300
C	-9.07204037	0.23019916	-4.36866600
H	-8.81388537	-0.70719784	-4.85238300
C	-8.07041437	1.14141816	-4.05039400
H	-7.02961437	0.91016116	-4.26556500
C	-4.61429137	6.92839416	-4.11770200
H	-4.77826337	7.30447516	-5.12230200
C	-5.48835637	5.99618316	-3.58379800
H	-6.33889137	5.63868916	-4.15665300
C	-5.23263537	4.54903616	-0.24260600
H	-5.38239237	3.91523316	0.62371900
C	-7.60190137	-1.17752984	-1.48810700
C	-8.33256837	2.26964316	-0.12575200
C	-9.63552437	4.46208316	1.05580200

TS3-H

Zero-point correction= 1.067869 (Hartree/Particle)
Thermal correction to Energy= 1.124030
Thermal correction to Enthalpy= 1.124895
Thermal correction to Gibbs Free Energy= 0.980131
Sum of electronic and zero-point Energies= -3582.960494
Sum of electronic and thermal Energies= -3582.904334
Sum of electronic and thermal Enthalpies= -3582.903469
Sum of electronic and thermal Free Energies= -3583.048232
SCF Done: E(RM062X) = -3585.00381951

C	-2.01716739	-2.11373387	0.00000000
C	-3.17081339	-1.95280187	-0.76862700
C	-4.23994939	-1.83860787	-1.35335300
C	-5.54384439	-1.69719487	-1.90173000
C	-5.79441239	-1.79813187	-3.28090900
C	-6.62626439	-1.46945887	-1.02634700
C	-7.08936339	-1.67166787	-3.76743600
H	-4.96493539	-1.97358287	-3.95785100
C	-7.91479339	-1.33489487	-1.52905400
H	-6.42225339	-1.40910487	0.04097400
C	-8.15460639	-1.43720987	-2.89861100

H	-7.26915039	-1.75100887	-4.83495600
H	-8.74008239	-1.15073987	-0.84677700
H	-9.16223539	-1.33321687	-3.28677600
C	-2.08956039	-1.94392487	1.42432500
O	-1.08180439	-1.95692787	2.17743200
N	-3.36173739	-1.77971487	1.94441700
H	-4.13344539	-1.80092987	1.28343400
C	-3.75677739	-1.68901787	3.26188400
C	-5.18278639	-1.69342287	3.48012100
C	-2.91685339	-1.64133387	4.36192400
C	-5.69476839	-1.60208187	4.80137100
C	-3.45213839	-1.53472287	5.66482700
H	-1.84965439	-1.69261487	4.20490800
C	-7.28638639	-1.88916887	2.57955800
C	-7.10286439	-1.64733387	4.95125700
C	-4.80325939	-1.50512887	5.89913500
H	-2.75966739	-1.47860387	6.49938500
C	-7.90245739	-1.79618487	3.84832000
H	-7.89655039	-2.01920687	1.68521200
H	-7.52904139	-1.57085887	5.94812600
H	-5.20292239	-1.42324087	6.90497900
H	-8.98247639	-1.84365387	3.93183700
N	-5.98861339	-1.83193987	2.39609000
C	-0.77812839	-2.63469387	-0.62787500
H	0.09669861	-2.45748087	-0.00116800
H	-0.60108239	-2.19321387	-1.61279200
C	-3.50251839	-4.82899387	0.59051800
C	-4.28083739	-4.86997787	1.77240200
C	-5.66035539	-4.88893587	1.76218400
C	-6.29974339	-4.86973487	0.51870300
C	-5.56559839	-4.86098387	-0.66152400
C	-4.16962839	-4.83652487	-0.63622800
C	-2.10097639	-4.82240687	1.02936500
C	-2.14728239	-4.89151087	2.54670100
H	-6.22572539	-4.89365287	2.68822700
H	-7.38412739	-4.86059687	0.47709800
H	-6.07795039	-4.83385787	-1.61698000
H	-3.63798839	-4.81510787	-1.57831400
N	-3.45840739	-4.89817587	2.90671600
O	-1.18701839	-4.88844387	3.29463100
N	-0.93545239	-4.79696387	0.46026800
C	-0.88152439	-4.20012687	-0.84223800
H	-1.76996139	-4.39915487	-1.44536300
C	0.28321661	-4.71582687	-1.64841300

F	0.31821261	-4.14647387	-2.85481700
F	0.21549961	-6.04657987	-1.83138200
F	1.46109061	-4.46556287	-1.04647000
C	-3.91874839	-4.93352487	4.27698700
H	-4.60816339	-4.10708987	4.46917500
H	-4.41559539	-5.88543087	4.48938400
H	-3.04294939	-4.82088987	4.91583000
H	0.38081961	-5.14250787	1.26656600
O	3.87268361	0.43244313	-0.16399800
N	1.43343161	-5.75441587	1.69077900
O	4.62238161	-2.41753487	1.29639200
N	0.66529461	-0.06177787	0.75030900
H	-0.07135439	-0.44958487	1.34322200
N	-4.68637139	1.01866013	0.36213600
H	-5.27108839	0.75854913	-0.41772800
C	-6.55488439	1.51987513	3.52248800
H	-7.54687339	1.53238313	3.96299400
C	-6.41374439	1.26245713	2.17049100
H	-7.27340239	1.06990513	1.53461700
C	-5.11691139	1.23873013	1.65015800
C	-3.97238339	1.48578813	2.44647300
C	-2.82913539	1.41409313	1.56597100
C	-1.40123039	1.54866113	1.88040700
C	-0.53970039	2.02938813	0.75742300
C	1.86296361	-0.66800887	0.87717800
C	2.41376961	-3.89349787	2.75717000
H	3.37192861	-3.50363787	3.10302100
C	2.65280161	-4.89875887	1.62983600
H	2.77834061	-4.43517587	0.65554200
H	3.51834261	-5.53812087	1.84435000
C	1.51816761	-6.97184787	0.86496700
H	0.57119761	-7.51108887	0.92870700
H	2.33093061	-7.60550387	1.23160500
H	1.70491161	-6.69306487	-0.16998800
N	1.60730861	-2.77792387	2.28902600
H	0.58903361	-2.76255487	2.38536800
C	1.33404461	-6.05048387	3.15185700
H	2.09103361	-6.81517087	3.36379600
H	0.34445661	-6.42856287	3.39293800
C	1.68002861	-4.72099487	3.83577200
H	2.32052061	-4.88947787	4.70268500
H	0.77677461	-4.20804687	4.16510700
C	3.63253961	-1.73136887	1.13675000
C	3.27392161	-0.41677587	0.44955500

C	1.22520761	1.65529813	-0.88839000
H	1.98626461	1.00011913	-1.29182900
C	1.02819961	2.89782213	-1.41735100
H	1.62851861	3.22950413	-2.25963600
C	-0.15005739	5.07510513	-1.41841400
H	0.46224861	5.38760413	-2.26008900
C	-1.08172339	5.92238913	-0.87709200
H	-1.22297639	6.91706713	-1.28721200
C	-1.85407039	5.50001213	0.22979000
H	-2.58028539	6.17793813	0.66689500
C	-1.69403439	4.24438013	0.75899200
H	-2.29000739	3.93552213	1.61104600
C	-0.74722239	3.33586913	0.20841300
C	-0.91306239	1.15694913	3.07699600
H	-1.60935439	0.68481313	3.76756100
C	0.50507161	1.13099813	3.47294400
C	1.41562761	2.14031413	3.13007100
H	1.05671061	3.03377413	2.62890900
C	2.76912161	1.99357713	3.41077000
H	3.46455261	2.77450213	3.12095500
C	3.23750261	0.84766213	4.05352900
H	4.29699861	0.73219513	4.25771300
C	2.33694461	-0.14423987	4.43167600
H	2.69017961	-1.04162887	4.93190900
C	0.98260561	-0.00060087	4.14707200
H	0.28513661	-0.79471387	4.40222500
C	-5.43144739	1.76637313	4.33688900
H	-5.57641639	1.96710613	5.39359400
C	-4.15018939	1.75699813	3.81424200
H	-3.29547939	1.96387513	4.44996900
C	-3.32348539	1.13803813	0.31407100
H	-2.78543939	0.98816613	-0.61108800
C	2.22050261	-1.84666687	1.53536200
C	0.44616361	1.21817213	0.21607900
C	0.04599561	3.77499313	-0.88737700

F

Zero-point correction=	1.073434 (Hartree/Particle)
Thermal correction to Energy=	1.130180
Thermal correction to Enthalpy=	1.131045
Thermal correction to Gibbs Free Energy=	0.982892
Sum of electronic and zero-point Energies=	-3582.990252
Sum of electronic and thermal Energies=	-3582.933506

Sum of electronic and thermal Enthalpies= -3582.932641
Sum of electronic and thermal Free Energies= -3583.080794
SCF Done: E(RM062X) = -3585.03963857

C	-3.35836911	0.18240343	0.00000000
C	-4.52731311	0.96364243	-0.39038100
C	-5.52316211	1.60630943	-0.63428900
C	-6.66989511	2.43841543	-0.85322100
C	-7.42343311	2.35142043	-2.03038300
C	-7.02724511	3.36519543	0.13878100
C	-8.51798111	3.18847043	-2.21253600
H	-7.14530211	1.62509443	-2.78658200
C	-8.12225911	4.19912743	-0.05592300
H	-6.43542211	3.40655143	1.05075800
C	-8.86784111	4.11351743	-1.23043100
H	-9.10049311	3.12018443	-3.12524100
H	-8.39564711	4.91645943	0.71229300
H	-9.72171311	4.76581543	-1.38043600
C	-2.68614411	0.78256043	1.25657900
O	-1.50683411	0.53548743	1.48511700
N	-3.49177511	1.50710843	2.05535300
H	-4.44193811	1.69519643	1.74541400
C	-3.19555211	2.05388143	3.30511600
C	-4.28475411	2.75557943	3.92068200
C	-1.98555611	1.95830643	3.95544500
C	-4.09322111	3.36626343	5.18476500
C	-1.81362911	2.58787743	5.21231600
H	-1.16658811	1.41809943	3.49961900
C	-6.48185111	3.40627943	3.82870900
C	-5.20514111	4.03324343	5.75308500
C	-2.82755111	3.28219643	5.81778700
H	-0.84605511	2.51134643	5.69899400
C	-6.40076611	4.05173543	5.08375700
H	-7.42080611	3.40952143	3.27585900
H	-5.09343811	4.51900443	6.71869300
H	-2.68340211	3.76196143	6.78087400
H	-7.27334411	4.54763743	5.49339300
N	-5.47323311	2.78552543	3.26211800
C	-2.29841911	0.01985243	-1.12259900
H	-1.40647311	0.60489643	-0.88328300
H	-2.69322411	0.35935343	-2.08148800
C	-4.94399511	-1.81414057	-0.45175000
C	-5.91687911	-2.22727157	0.46484500
C	-7.15834511	-2.69621857	0.06852700

C	-7.42077611	-2.73981457	-1.30336000
C	-6.47336611	-2.31822457	-2.23046600
C	-5.22731611	-1.84381757	-1.80529700
C	-3.72885211	-1.34860257	0.32414900
C	-4.15511711	-1.60643157	1.78587800
H	-7.89994311	-3.01481257	0.79312500
H	-8.38346911	-3.10387857	-1.64667800
H	-6.70137911	-2.35406657	-3.28995600
H	-4.50740811	-1.48852857	-2.53647600
N	-5.43860411	-2.08135057	1.77449800
O	-3.45823611	-1.44300557	2.76588200
N	-2.52495111	-2.10069857	0.05032800
C	-1.96798911	-1.49747657	-1.14983200
H	-2.41733511	-1.96509057	-2.03313000
C	-0.48720011	-1.77533057	-1.25499900
F	0.05480289	-1.08094657	-2.26301500
F	-0.24174411	-3.07435257	-1.47554700
F	0.15217089	-1.43526357	-0.12904100
C	-6.15748311	-2.46037057	2.96801200
H	-7.08407411	-1.88571957	3.05461500
H	-6.39525611	-3.52825757	2.95040900
H	-5.51174111	-2.24324357	3.81886900
H	-1.87568411	-2.02817357	0.84749800
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Pro

Zero-point correction= 0.489293 (Hartree/Particle)
Thermal correction to Energy= 0.516878
Thermal correction to Enthalpy= 0.517743
Thermal correction to Gibbs Free Energy= 0.430056
Sum of electronic and zero-point Energies= -1862.965003
Sum of electronic and thermal Energies= -1862.937417
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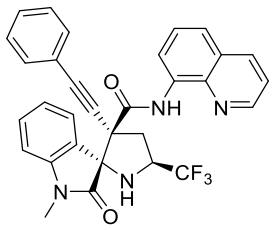
7. NMR data

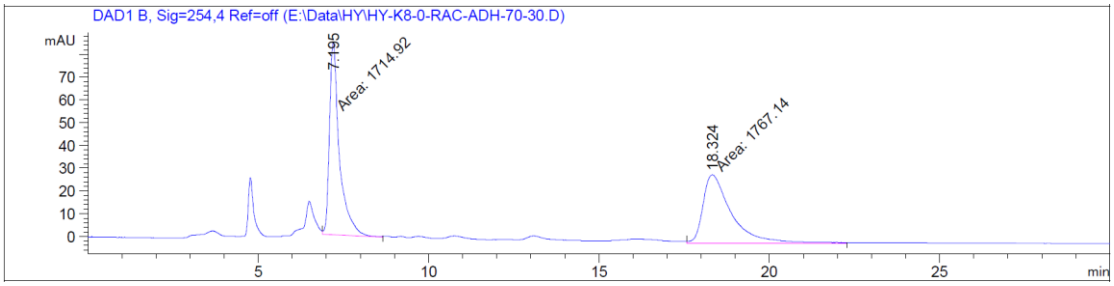


3aa

85 mg, 89% yield, white soild. $[\alpha]^{20}_{D}$ -130.40 (c 0.5, $CHCl_3$, 94% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 7.2 min, tR (major) = 18.3 min.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.58 (p, J = 4.4 Hz, 1H), 8.47 (dd, J = 4.3, 1.8 Hz, 1H), 8.04 (dd, J = 8.3, 1.8 Hz, 1H), 7.87 (d, J = 7.5 Hz, 2H), 7.59 – 7.50 (m, 3H), 7.42 (d, J = 4.8 Hz, 2H), 7.39 – 7.30 (m, 6H), 7.16 (t, J = 7.6 Hz, 2H), 6.61 (d, J = 7.7 Hz, 1H), 4.61 – 4.45 (m, 1H), 3.98 (t, J = 11.6 Hz, 1H), 2.92 (s, 3H), 2.76 (dd, J = 12.1, 6.0 Hz, 1H), 2.69 (d, J = 8.6 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.6, 164.2, 147.8, 145.1, 138.1, 135.9, 133.7, 131.7, 130.6, 129.1, 128.5, 127.5, 127.1, 125.8 (q, J_{CF} = 279.8 Hz), 125.5, 125.1, 122.1, 121.7, 121.6, 121.4, 116.2, 108.4, 89.5, 86.6, 77.3, 77.2, 77.0, 76.7, 71.1, 59.2, 58.3 (q, J_{CF} = 32.0 Hz), 35.0, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8. **HRMS**: calculated for $C_{31}H_{24}F_3N_4O_2^+$ [M+H$^+$] 541.1846, found 541.1850.



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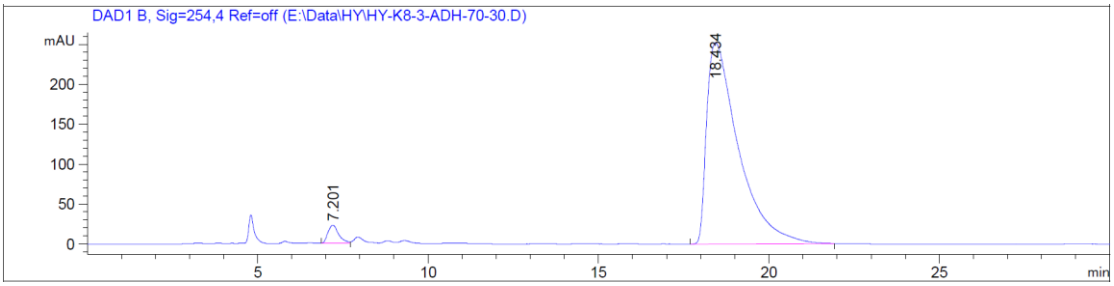

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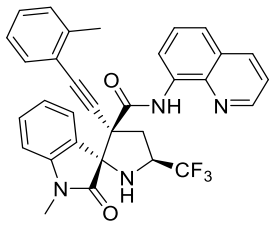
1	7.201	BV	0.3460	494.57498	22.54270	2.9457
2	18.434	BB	0.9199	1.62950e4	252.17310	97.0543



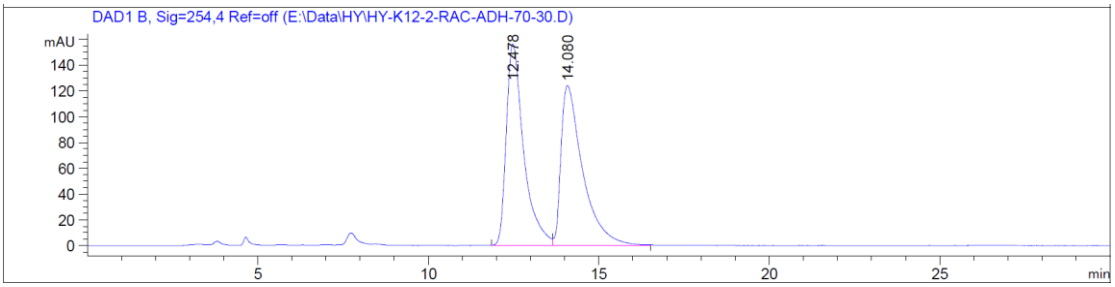
3ba

90 mg, 81% yield, white soild. $[\alpha]^{20}_{D}$ -73.60 (c 0.5, $CHCl_3$, 91% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 12.5 min, tR (major) = 14.1 min.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.00 (s, 1H), 8.59 (q, *J* = 4.2 Hz, 1H), 8.44 (d, *J* = 4.1 Hz, 1H), 8.07 (d, *J* = 8.2 Hz, 1H), 7.87 (d, *J* = 7.5 Hz, 1H), 7.53 (d, *J* = 7.5 Hz, 1H), 7.48 – 7.42 (m, 2H), 7.38 – 7.32 (m, 2H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.23 – 7.12 (m, 3H), 6.60 (d, *J* = 7.8 Hz, 1H), 4.60 – 4.48 (m, 1H), 3.99 (t, *J* = 11.6 Hz, 1H), 2.92 (s, 3H), 2.77 (dd, *J* = 12.2, 6.0 Hz, 1H), 2.39 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.7, 164.4, 147.8, 145.2, 140.6, 138.1, 136.0, 133.8, 132.3, 130.6, 129.7, 129.1, 127.6, 127.2, 125.8 (q, J_{CF} = 279.5 Hz), 125.7, 125.7, 125.3, 122.2, 121.8, 121.5, 121.4, 116.3, 108.4, 90.2, 88.6, 71.1, 59.5, 58.3 (q, J_{CF} = 32.3 Hz), 35.4, 26.2, 20.8. **^{19}F NMR** (376 MHz, $CDCl_3$) *δ* -74.9. **HRMS**: calculated for $C_{32}H_{25}F_3N_4NaO_2^+$ [M+H$^+$] 577.1822, found 577.1817.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
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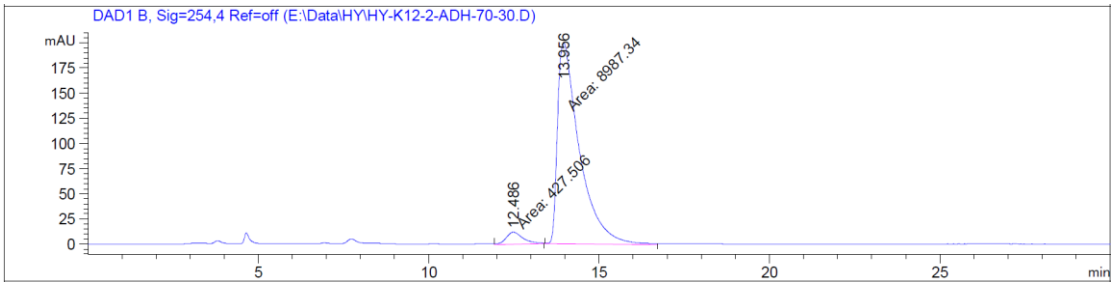
2	14.080	VB	0.6383	5435.80713	123.79910	49.5817



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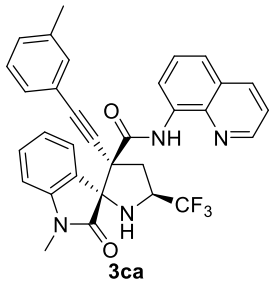


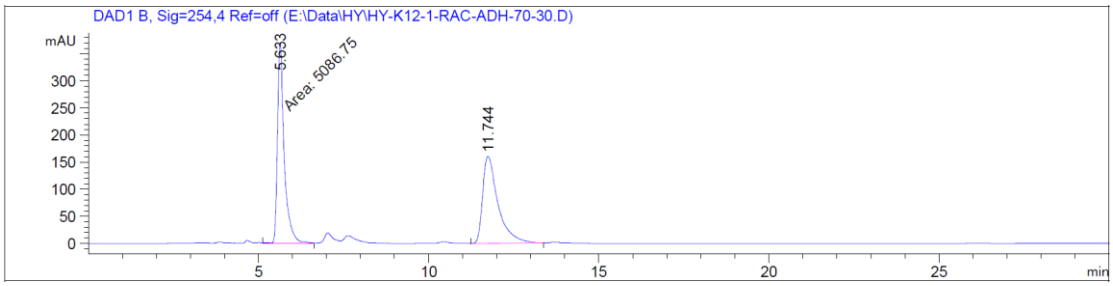
3ca

92 mg, 83% yield, white soild. $[\alpha]^{20}_{D}$ -165.60 (c 0.5, $CHCl_3$, 93% ee)

HPLC (Daicel Chiralpak AD-H, hexane/i-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 5.6 min, tR (major) = 11.7 min.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.62 – 8.54 (m, 1H), 8.48 (dd, J = 4.2, 1.6 Hz, 1H), 8.04 (dd, J = 8.3, 1.6 Hz, 1H), 7.88 (d, J = 7.4 Hz, 1H), 7.44 – 7.39 (d, J = 4.2 Hz, 2H), 7.39 – 7.31 (m, 4H), 7.28 – 7.22 (m, 1H), 7.21 – 7.13 (m, 2H), 6.60 (d, J = 7.8 Hz, 1H), 4.65 – 4.43 (m, 1H), 3.97 (t, J = 11.6 Hz, 1H), 2.92 (s, 3H), 2.81 – 2.62 (m, 2H), 2.34 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.6, 164.3, 147.8, 145.1, 138.2, 138.2, 135.9, 133.7, 132.2, 130.6, 130.0, 128.7, 128.3, 127.5, 127.0, 125.7 (q, J_{CF} = 279.6 Hz), 125.5, 125.1, 122.1, 121.7, 121.4, 121.4, 116.2, 108.3, 89.8, 86.2, 71.1, 59.2, 58.3 (q, J_{CF} = 32.3 Hz), 35.1, 26.1, 21.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8.

HRMS: calculated for $C_{32}H_{26}F_3N_4O_2^+$ [M+H$^+$] 555.2002, found 555.1999.



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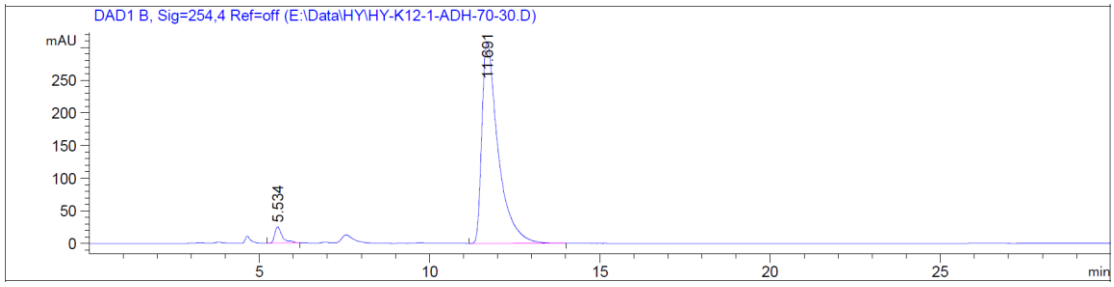

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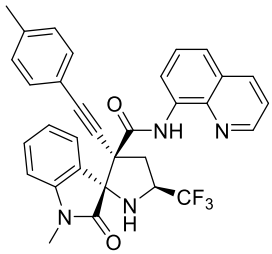
2	11.691	BB	0.4866	1.01945e4	307.63757	96.4250

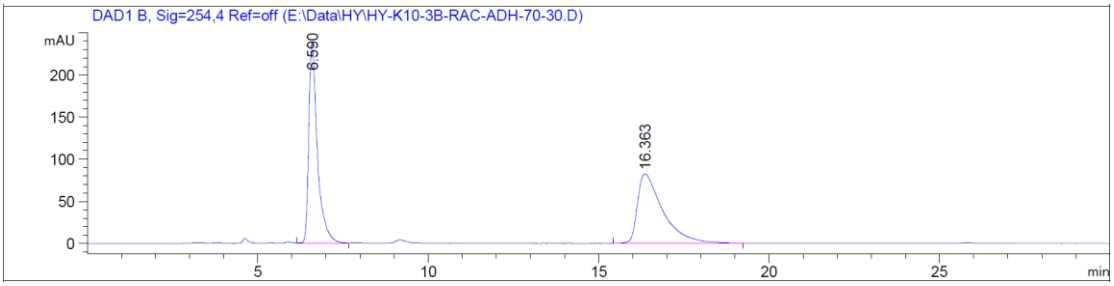


3da

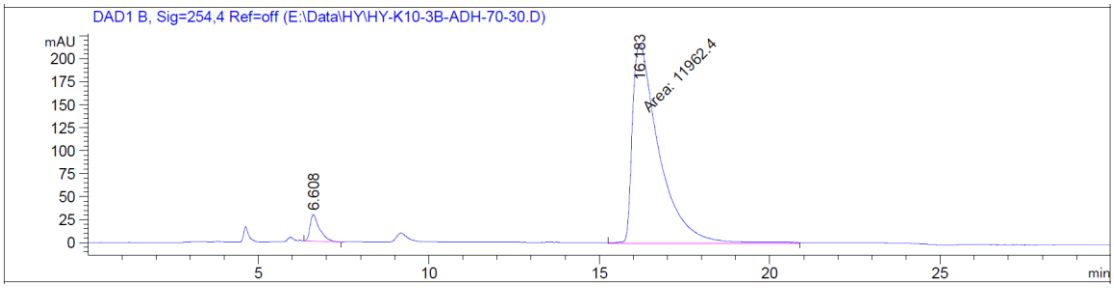
83 mg, 75% yield, white soild. $[\alpha]^{20}_{D}$ -125.20 (c 0.5, $CHCl_3$, 91% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 6.5 min, tR (major) = 16.3 min.

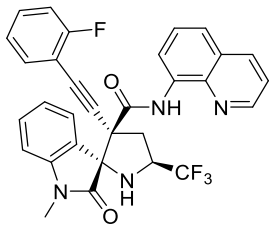
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.57 (dd, J = 5.1, 4.0 Hz, 1H), 8.46 (dd, J = 4.3, 1.7 Hz, 1H), 8.03 (dd, J = 8.3, 1.7 Hz, 1H), 7.87 (d, J = 7.5 Hz, 1H), 7.44 (d, J = 8.2 Hz, 2H), 7.42 – 7.38 (m, 2H), 7.37 – 7.31 (m, 2H), 7.19 – 7.12 (m, 3H), 6.59 (d, J = 7.7 Hz, 1H), 4.62 – 4.15 (m, 1H), 3.97 (t, J = 11.6 Hz, 1H), 2.91 (s, 3H), 2.81 – 2.64 (m, 2H), 2.35 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.6, 164.3, 147.8, 145.0, 139.3, 138.1, 135.9, 133.7, 131.5, 130.5, 129.2, 127.5, 127.0, 125.8 (q, J_{CF} = 279.5 Hz), 125.5, 125.1, 122.1, 121.7, 121.4, 118.5, 116.2, 108.3, 89.8, 85.9, 71.1, 59.3, 58.3 (q, J_{CF} = 32.2 Hz), 35.0, 26.0, 21.4. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8. **HRMS**: calculated for $C_{32}H_{26}F_3N_4O_2^+$ [M+H$^+$] 555.2002, found 555.2009.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.590	BB	0.2580	4158.33545	237.85574	49.5255
2	16.363	BB	0.7342	4238.02490	82.38226	50.4745



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.608	BB	0.2729	553.19788	28.96019	4.4201
2	16.183	MM	0.9157	1.19624e4	217.72339	95.5799



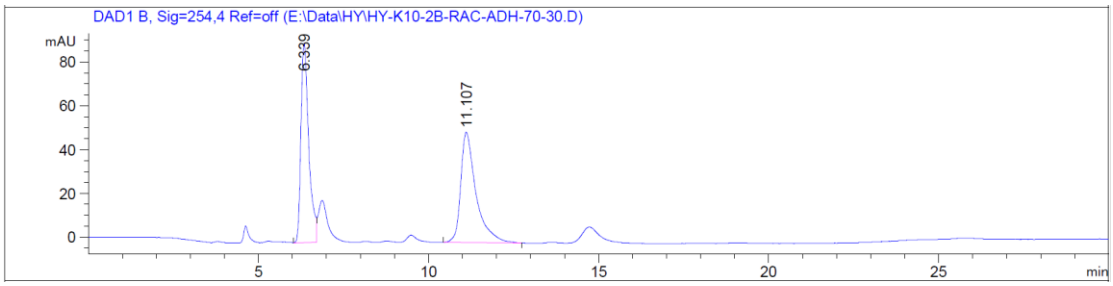
3ea

83 mg, 74% yield, brown soild. $[\alpha]^{20}_{D}$ -130.00 (c 0.5, $CHCl_3$, 91% ee)

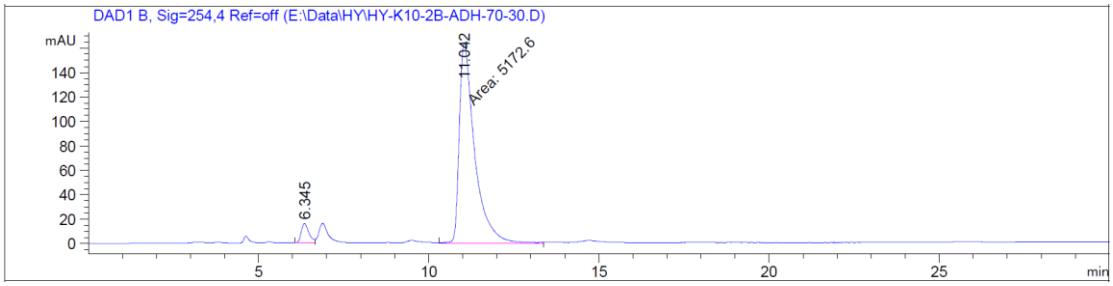
HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 6.3 min, tR (major) = 11.1 min.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.00 (s, 1H), 8.58 (p, J = 4.4 Hz, 1H), 8.46 (dd, J = 4.2, 1.6 Hz, 1H), 8.04 (dd, J = 8.3, 1.6 Hz, 1H), 7.96 (d, J = 7.4 Hz, 1H), 7.50 (td, J = 7.5, 1.6 Hz, 2H), 7.42 (d, J = 4.5 Hz, 2H), 7.40 – 7.32 (m, 4H), 7.20 – 7.09 (m, 4H), 6.63 (d, J = 7.8 Hz, 1H), 4.61 – 4.49 (m, 2H), 4.01 (t, J = 11.6 Hz, 1H), 2.93 (s, 3H), 2.80 (dd, J = 12.2, 6.0 Hz, 1H), 2.32 – 2.75 (m, 1H).

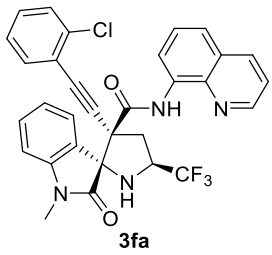
^{13}C NMR (101 MHz, $CDCl_3$) δ 175.6, 164.1, 164.0, 161.6, 147.9, 145.1, 138.1, 135.9, 133.7, 133.6, 130.9, 130.9, 130.6, 127.5, 127.0, 125.8 (q, J_{CF} = 279.6 Hz), 125.3, 125.2, 125.2, 124.1, 124.1, 122.4, 121.8, 121.7, 121.5, 116.3, 115.7, 115.5, 110.3, 110.2, 108.3, 91.6, 91.6, 83.0, 59.4, 58.1 (q, J_{CF} = 32.3 Hz), 35.4, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.9, -109.3. **HRMS**: calculated for $C_{31}H_{23}F_4N_4O_2^+$ [M+H$^+$] 559.1752, found 559.1756.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.339	BV	0.2384	1455.15784	91.06264	48.0023
2	11.107	BB	0.4531	1576.27332	50.36798	51.9977



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.345	BV	0.2349	246.29396	15.88579	4.5451
2	11.042	MM	0.5242	5172.60498	164.45439	95.4549

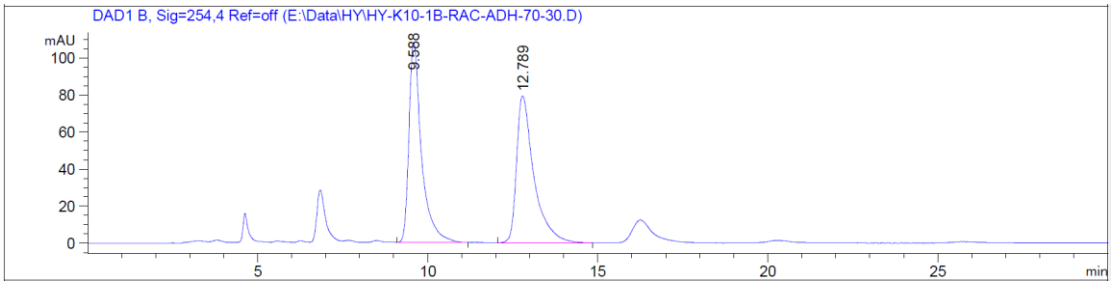


3fa

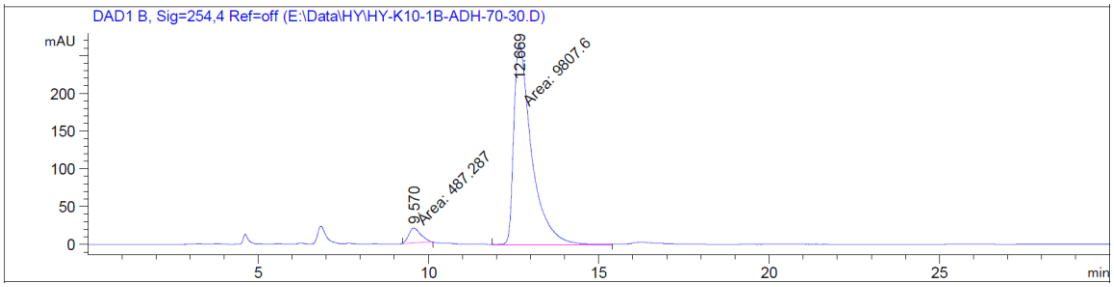
88 mg, 77% yield, yellow soild. $[\alpha]^{20}_{D}$ -101.60 (c 0.5, $CHCl_3$, 90% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 9.5 min, tR (major) = 12.7 min.

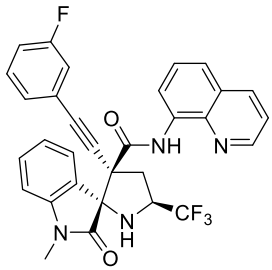
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.60 (p, J = 4.4 Hz, 1H), 8.48 (dd, J = 4.3, 1.7 Hz, 1H), 8.07 (dd, J = 8.3, 1.7 Hz, 1H), 7.94 (dd, J = 7.6, 1.3 Hz, 1H), 7.55 (dd, J = 7.6, 1.8 Hz, 1H), 7.49 – 7.41 (m, 3H), 7.39 – 7.29 (m, 3H), 7.27 – 7.22 (m, 1H), 7.14 (t, J = 7.5 Hz, 1H), 6.63 (d, J = 7.6 Hz, 1H), 4.71 – 4.51 (m, 1H), 4.02 (t, J = 11.6 Hz, 1H), 2.95 (s, 3H), 2.81 (dd, J = 12.1, 6.1 Hz, 1H), 2.71 (d, J = 7.8 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.7, 164.1, 148.0, 145.2, 138.3, 136.3, 136.1, 133.8, 133.6, 130.7, 130.2, 129.5, 127.7, 127.2, 126.7, 125.9 (q, J_{CF} = 279.8 Hz), 125.5, 125.4, 122.4, 121.9, 121.7, 121.6, 116.5, 108.4, 91.7, 86.4, 70.9, 59.6, 58.3 (q, J_{CF} = 32.8 Hz), 35.5, 26.2. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.9. **HRMS**: calculated for $C_{31}H_{23}ClF_3N_4O_2^+$ [M+H$^+$] 575.1456, found 575.1465.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.588	BB	0.3778	2773.75000	107.93480	49.6533
2	12.789	BB	0.5190	2812.48853	79.45441	50.3467



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.570	MM	0.4102	487.28708	19.80113	4.7333
2	12.669	MM	0.6111	9807.60352	267.46814	95.2667

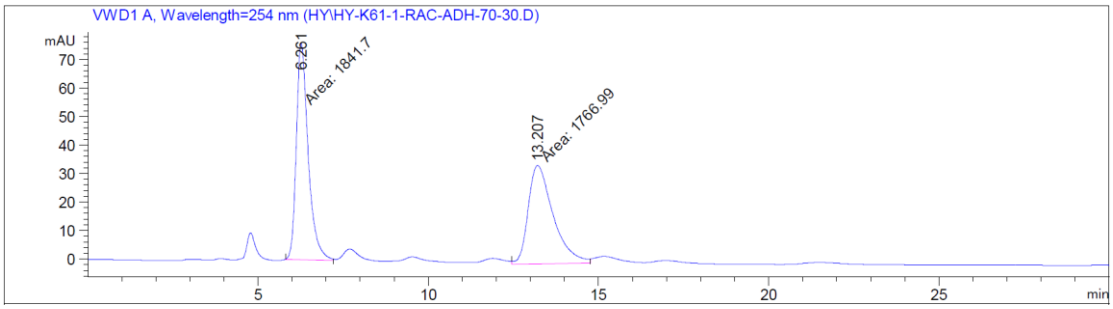


3ga

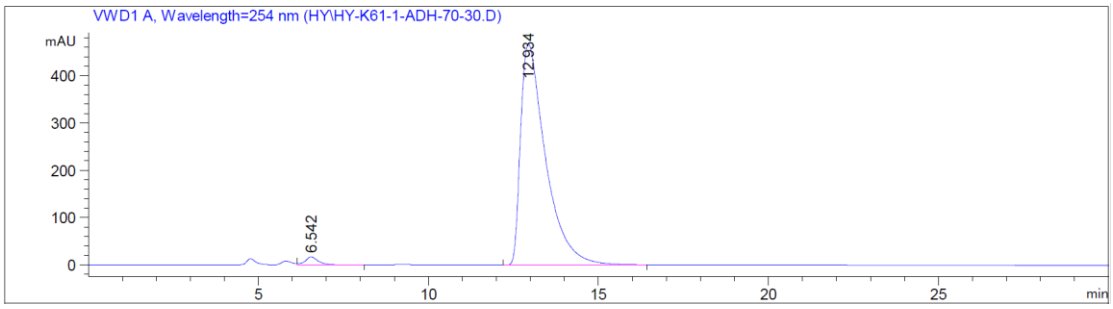
82 mg, 73% yield, yellow soild. $[\alpha]^{20}_{D}$ -107.20 (c 0.5, $CHCl_3$, 96% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 6.2 min, tR (major) = 13.2 min.

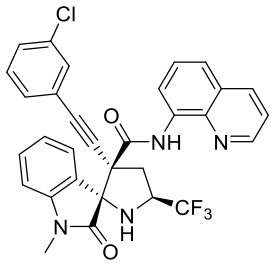
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.01 (s, 1H), 8.58 (p, J = 4.5 Hz, 1H), 8.50 (dd, J = 4.2, 1.6 Hz, 1H), 8.06 (dd, J = 8.3, 1.5 Hz, 1H), 7.83 (d, J = 7.5 Hz, 1H), 7.46 – 7.41 (m, 2H), 7.39 – 7.31 (m, 4H), 7.30 – 7.26 (m, 1H), 7.17 (t, J = 7.6 Hz, 1H), 7.12 – 7.06 (m, 1H), 6.62 (d, J = 7.8 Hz, 1H), 4.59 – 4.46 (m, 1H), 3.97 (t, J = 11.6 Hz, 1H), 2.92 (s, 3H), 2.82 – 2.58 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.5, 163.9, 163.5, 161.0, 147.9, 145.1, 138.1, 136.0, 133.6, 130.7, 130.2, 130.1, 127.6, 127.5, 127.5, 127.1, 125.7 (q, J_{CF} = 279.7 Hz), 125.5, 125.0, 123.4, 123.3, 122.1, 121.9, 121.5, 118.7, 118.5, 116.6, 116.4, 116.3, 108.4, 88.4, 88.3, 87.7, 71.2, 59.2, 58.3 (q, J_{CF} = 32.4 Hz), 34.9, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.9, -112.2. **HRMS**: calculated for $C_{31}H_{22}F_4N_4NaO_2^+$ [M+Na$^+$] 581.1571, found 581.1564.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.261	MM	0.4035	1841.69800	76.07048	51.0351
2	13.207	MM	0.8522	1766.99231	34.55627	48.9649



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.542	VB	0.3930	450.35464	16.68103	1.8535
2	12.934	BB	0.7584	2.38478e4	468.09219	98.1465

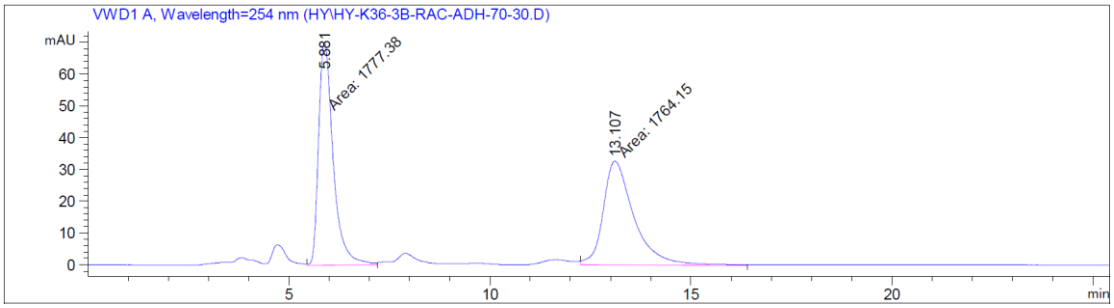


3ha

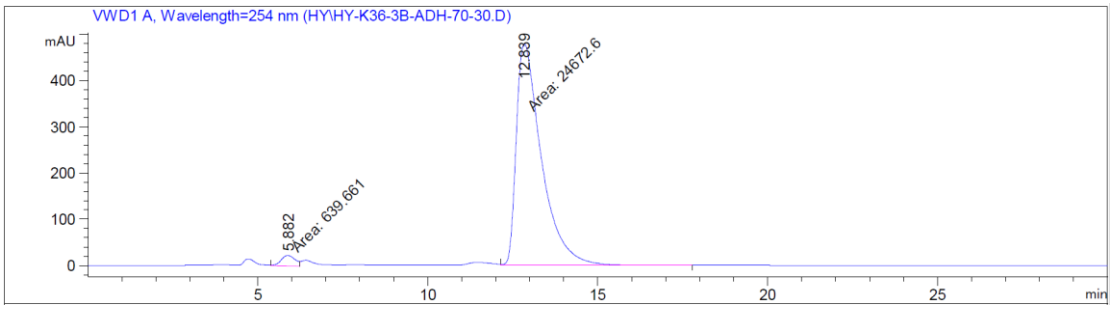
90 mg, 78% yield, white soild. $[\alpha]^{20}_{D}$ -108.40 (c 0.5, $CHCl_3$, 95% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 5.8 min, tR (major) = 13.1 min.

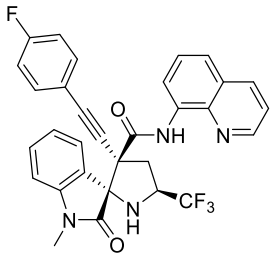
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.02 (s, 1H), 8.61 – 8.54 (m, 1H), 8.52 (dd, J = 4.2, 1.6 Hz, 1H), 8.06 (dd, J = 8.3, 1.6 Hz, 1H), 7.81 (d, J = 7.3 Hz, 1H), 7.59 – 7.55 (m, 1H), 7.45 – 7.39 (m, 3H), 7.38 – 7.27 (m, 4H), 7.17 (t, J = 7.6 Hz, 1H), 6.61 (d, J = 7.8 Hz, 1H), 4.62 – 4.44 (m, 1H), 3.97 (t, J = 11.6 Hz, 1H), 2.92 (s, 3H), 2.80 – 2.64 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.5, 163.8, 147.9, 145.0, 138.1, 136.0, 134.2, 133.6, 131.6, 130.7, 129.8, 129.7, 129.4, 127.6, 127.0, 125.7 (q, J_{CF} = 279.5 Hz), 125.4, 124.9, 123.2, 122.1, 121.8, 121.5, 116.2, 108.4, 88.2, 88.0, 71.2, 59.2, 58.3 (q, J_{CF} = 32.4 Hz), 34.8, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8. **HRMS**: calculated for $C_{31}H_{23}ClF_3N_4O_2^+$ [M+H$^+$] 575.1456, found 575.1459.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.881	MM	0.4214	1777.38330	70.29691	50.1869
2	13.107	MM	0.8982	1764.14795	32.73529	49.8131



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.882	MM	0.4743	639.66138	22.47787	2.5271
2	12.839	FM	0.8582	2.46726e4	479.16650	97.4729

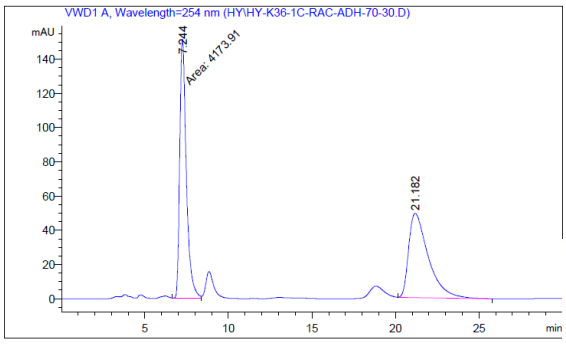


3ia

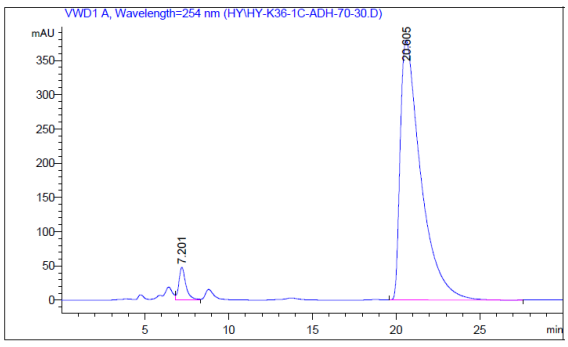
102 mg, 91% yield, white soild. $[\alpha]^{20}_{D}$ -113.60 (c 0.5, $CHCl_3$, 92% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 7.2 min, tR (major) = 21.2 min.

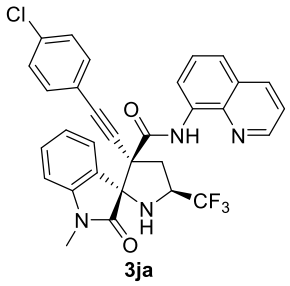
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.01 (s, 1H), 8.62 – 8.54 (m, 1H), 8.47 (dd, J = 4.2, 1.5 Hz, 1H), 8.06 (dd, J = 8.3, 1.5 Hz, 1H), 7.85 (d, J = 7.4 Hz, 1H), 7.57 – 7.50 (m, 2H), 7.42 (d, J = 4.3 Hz, 2H), 7.39 – 7.32 (m, 2H), 7.17 (t, J = 7.6 Hz, 1H), 7.10 – 7.02 (m, J = 8.6 Hz, 2H), 6.62 (d, J = 7.8 Hz, 1H), 4.62 – 4.44 (m, 1H), 3.97 (t, J = 11.6 Hz, 1H), 2.92 (s, 3H), 2.81 – 2.62 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.6, 164.2, 164.1, 161.6, 147.8, 145.1, 138.1, 136.0, 133.7, 133.6, 133.6, 130.6, 127.6, 127.1, 125.8 (q, J_{CF} = 279.6 Hz), 125.5, 125.0, 122.1, 121.8, 121.5, 117.7, 117.7, 116.2, 115.9, 115.7, 108.4, 88.5, 86.4, 86.4, 71.1, 59.2, 58.2 (q, J_{CF} = 32.3 Hz), 35.0, 26.0. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8, -109.2. **HRMS**: calculated for $C_{31}H_{23}F_4N_4O_2^+$ [M+H$^+$] 559.1752, found 559.1754.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.244	FM	0.4585	4173.90674	151.73819	51.0229
2	21.182	BB	1.2176	4006.55078	49.22283	48.9771



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.201	VB	0.4213	1313.07190	46.80666	3.8950
2	20.605	BB	1.2565	3.23985e4	379.32565	96.1050

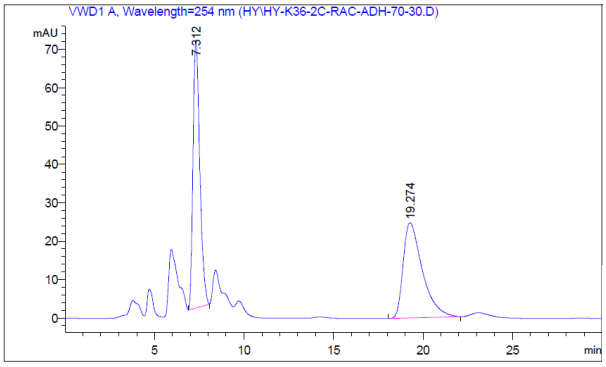


3ja

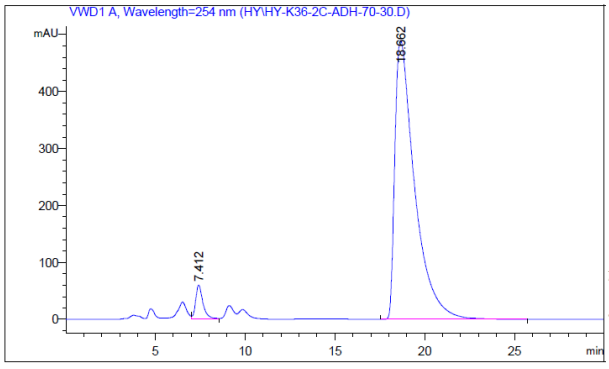
79 mg, 69% yield, yellow soild. $[\alpha]^{20}_{D}$ -153.60 (c 0.5, $CHCl_3$, 92% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 7.3 min, tR (major) = 19.3 min.

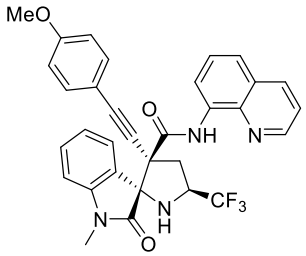
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.01 (s, 1H), 8.58 (p, *J* = 4.4 Hz, 1H), 8.48 (dd, *J* = 4.2, 1.5 Hz, 1H), 8.07 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.82 (d, *J* = 7.5 Hz, 1H), 7.50 – 7.43 (m, 4H), 7.40 – 7.32 (m, 4H), 7.15 (t, *J* = 7.6 Hz, 1H), 6.63 (d, *J* = 7.8 Hz, 1H), 4.59 – 4.44 (m, 1H), 3.96 (t, *J* = 11.6 Hz, 1H), 2.93 (s, 3H), 2.80 – 2.61 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.6, 164.1, 147.9, 145.2, 138.2, 136.1, 135.2, 133.7, 132.9, 130.7, 128.9, 127.6, 127.2, 125.7 (q, J_{CF} = 279.6 Hz), 125.6, 125.0, 122.1, 121.8, 121.5, 120.1, 116.3, 108.5, 88.4, 87.7, 71.1, 59.2, 58.3 (q, J_{CF} = 32.3 Hz), 35.0, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) *δ* -74.9. **HRMS**: calculated for $C_{31}H_{23}ClF_3N_4O_2^+$ [M+H$^+$] 575.1456, found 575.1462.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.312	VB	0.4062	1844.61658	69.83212	49.9050
2	19.274	BB	1.1139	1851.63806	24.83438	50.0950



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.412	VB	0.4150	1608.45276	58.45368	4.1161
2	18.662	BB	1.1270	3.74691e4	489.52780	95.8839

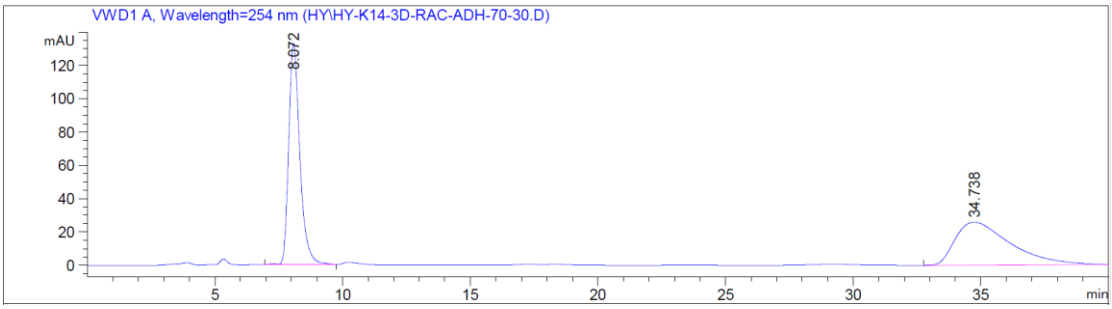


3ka

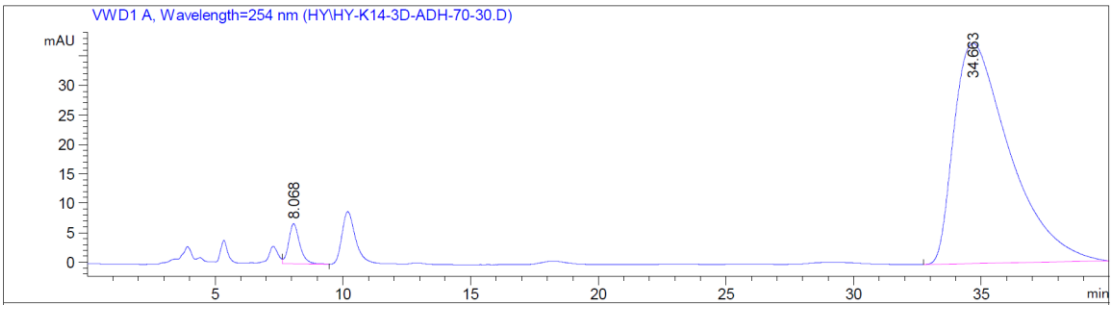
97 mg, 85% yield, white soild. $[\alpha]^{20}_{D}$ -182.40 (c 0.5, $CHCl_3$, 93% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 8.1 min, tR (major) = 34.7 min.

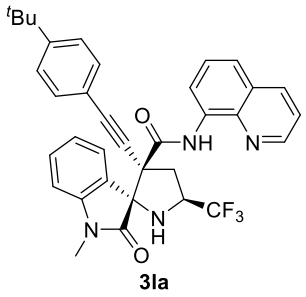
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.62 – 8.53 (m, 1H), 8.46 (dd, J = 4.2, 1.6 Hz, 1H), 8.03 (dd, J = 8.3, 1.6 Hz, 1H), 7.89 – 7.84 (m, 2H), 7.52 – 7.44 (m, 2H), 7.43 – 7.38 (m, 2H), 7.36 – 7.30 (m, 2H), 7.19 – 7.12 (m, 1H), 6.92 – 6.84 (m, 2H), 6.59 (d, J = 7.7 Hz, 1H), 4.62 – 4.44 (m, 1H), 3.96 (t, J = 11.6 Hz, 1H), 3.80 (s, 3H), 2.90 (s, 3H), 2.80 – 2.65 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.7, 164.4, 160.1, 147.8, 145.0, 138.1, 135.9, 133.7, 133.1, 130.5, 127.5, 127.0, 125.8 (q, J_{CF} = 279.6 Hz), 125.5, 125.1, 122.1, 121.7, 121.4, 116.1, 114.0, 113.5, 108.3, 89.6, 85.1, 71.1, 59.2, 58.2 (q, J_{CF} = 32.3 Hz), 55.2, 35.0, 26.0. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.7. **HRMS**: calculated for $C_{31}H_{23}F_4N_4O_2^+$ [M+H$^+$] 571.1952, found 571.1961.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.072	VB R	0.4556	4006.42407	132.95314	50.8633
2	34.738	BBA	2.2654	3870.41797	25.81208	49.1367



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.068	VB	0.4463	200.76123	6.76389	3.4145
2	34.663	BBA	2.2805	5678.88232	37.42001	96.5855

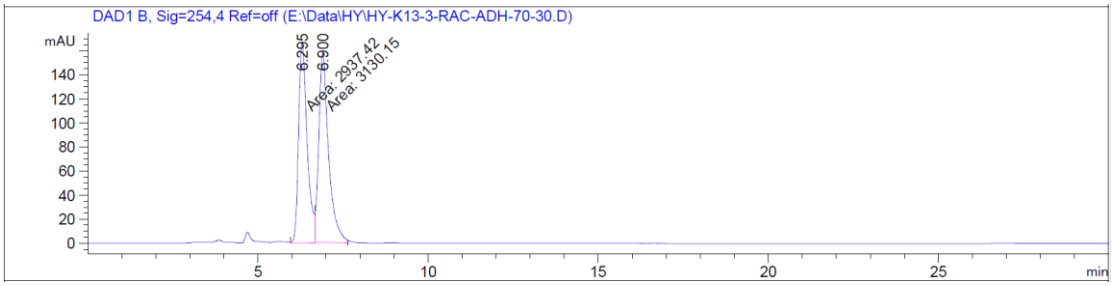


3la

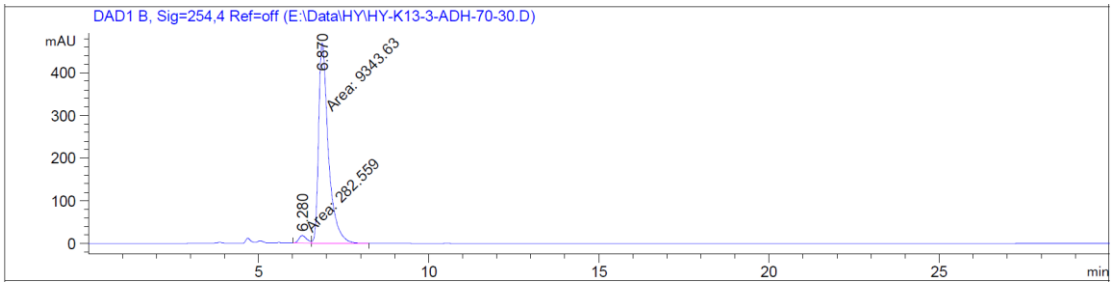
87 mg, 73% yield, yellow soild. $[\alpha]^{20}_{D}$ -118.00 (c 0.5, $CHCl_3$, 94% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90:10, 1.0 mL/min, 254 nm): tR (minor) = 29.6 min, tR (major) = 36.0 min.

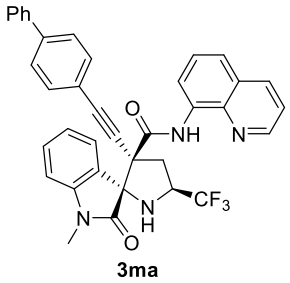
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.62 – 8.54 m, 1H), 8.48 (dd, J = 4.2, 1.6 Hz, 1H), 8.04 (dd, J = 8.3, 1.6 Hz, 1H), 7.90 (d, J = 7.5 Hz, 1H), 7.52 – 7.47 (m, 2H), 7.41 (dd, J = 5.9, 1.9 Hz, 3H), 7.39 – 7.31 (m, 3H), 7.18 (t, J = 7.6 Hz, 1H), 6.60 (d, J = 7.8 Hz, 1H), 4.61 – 4.44 (m, 1H), 3.97 (t, J = 11.6 Hz, 1H), 2.92 (s, 3H), 2.81 – 2.61 (m, 2H), 1.32 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.7, 164.4, 152.5, 147.8, 145.1, 138.2, 135.9, 133.7, 131.4, 130.5, 127.5, 127.0, 125.8 (q, J_{CF} = 279.6 Hz), 125.6, 125.5, 125.2, 122.2, 121.7, 121.4, 118.6, 116.2, 108.3, 89.7, 85.9, 71.1, 59.3, 58.3 (q, J_{CF} = 32.3 Hz), 35.1, 34.8, 31.0, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8. **HRMS**: calculated for $C_{32}H_{26}F_3N_4O_2^+$ [M+H$^+$] 597.2472, found 597.2479.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.295	MM	0.2945	2937.42163	166.22252	48.4118
2	6.900	FM	0.3315	3130.15161	157.37370	51.5882



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.280	MF	0.2682	282.55850	17.55734	2.9353
2	6.870	FM	0.3320	9343.62891	469.01605	97.0647

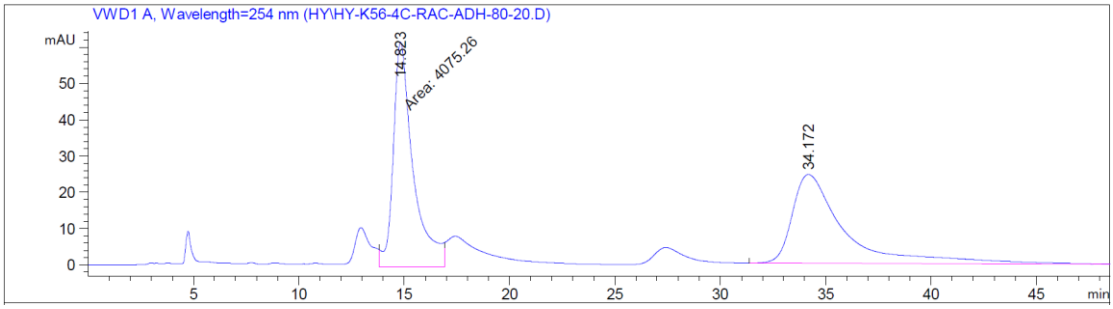


3ma

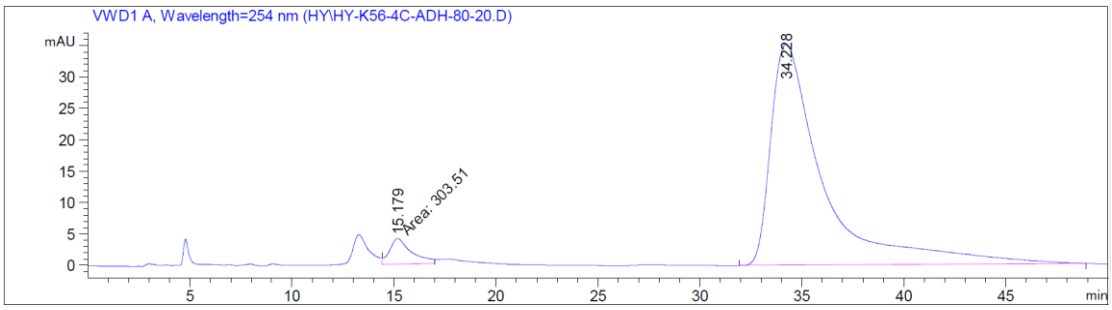
113 mg, 92% yield, yellow soild. $[\alpha]_{20}^{D}$ -196.40 (c 0.5, $CHCl_3$, 91% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 80:20, 1.0 mL/min, 254 nm): tR (minor) = 14.8 min, tR (major) = 34.2 min.

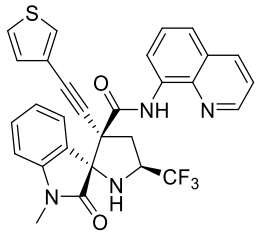
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.06 (s, 1H), 8.64 – 8.55 (m, 1H), 8.50 (dd, J = 4.2, 1.6 Hz, 1H), 8.05 (dd, J = 8.3, 1.6 Hz, 1H), 7.90 (d, J = 7.4 Hz, 1H), 7.64 – 7.55 (m, 6H), 7.47 – 7.40 (m, 4H), 7.39 – 7.32 (m, 3H), 7.18 (t, J = 7.6 Hz, 1H), 6.61 (d, J = 7.8 Hz, 1H), 4.65 – 4.47 (m, 1H), 3.99 (t, J = 11.6 Hz, 1H), 2.93 (s, 3H), 2.85 – 2.50 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.7, 164.3, 147.9, 145.1, 141.8, 139.9, 138.2, 136.0, 133.7, 132.1, 130.6, 128.8, 127.8, 127.6, 127.1, 126.9, 125.8 (q, J_{CF} = 279.5 Hz), 125.6, 125.1, 122.2, 121.8, 121.5, 120.4, 116.3, 108.4, 89.5, 87.3, 71.2, 59.3, 58.3 (q, J_{CF} = 32.4 Hz), 35.1, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8. **HRMS**: calculated for $C_{37}H_{28}F_3N_4O_2^+$ [M+H$^+$] 617.2159, found 617.2160.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.823	MM	1.0962	4075.25781	61.95957	49.1343
2	34.172	BBA	2.4273	4218.85645	24.49642	50.8657



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.179	MM	1.2427	303.51022	4.07064	4.5882
2	34.228	BB	2.5420	6311.46387	35.26560	95.4118



3na

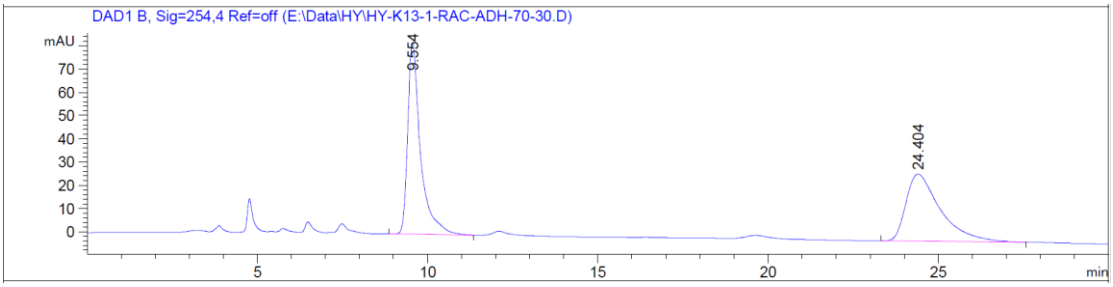
82 mg, 75% yield, brown soild. $[\alpha]^{20}_{D}$ -142.40 (c 0.5, $CHCl_3$, 94% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 9.5 min, tR (major) = 24.4 min.

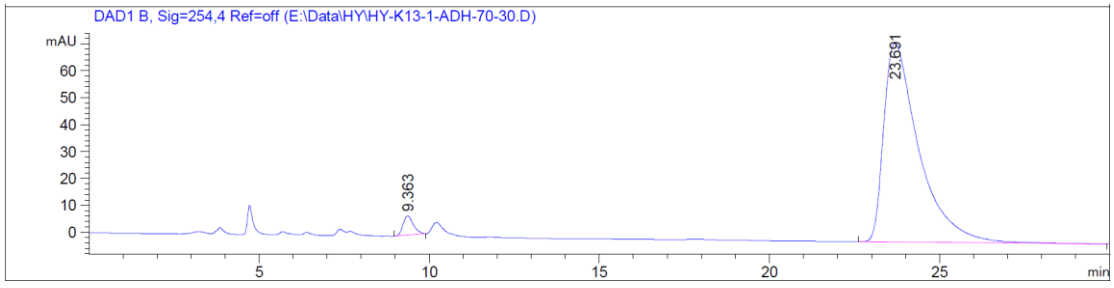
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.97 (s, 1H), 8.60 – 8.53 (p, J = 4.4 Hz, 1H), 8.50 (dd, J = 4.2, 1.7 Hz, 1H), 8.06 (dd, J = 8.3, 1.7 Hz, 1H), 7.88 – 7.83 (m, 1H), 7.45 – 7.41 (m, 2H), 7.40 – 7.29 (m, 4H), 7.23 – 7.16 (m, 1H), 7.02 (dd, J = 5.1, 3.7 Hz, 1H), 6.63 (d, J = 7.7 Hz, 1H), 4.60 – 4.42 (m, 1H), 3.96 (t, J = 12.0 Hz, 1H), 2.93 (s, 3H), 2.77 (dd, J = 12.2, 6.0 Hz, 1H), 2.67 (d, J = 7.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.6, 164.0, 147.9, 145.2, 138.2, 135.9, 133.7, 132.9, 130.6, 128.1, 127.6, 127.2, 127.1, 125.8 (q, J_{CF} = 279.5 Hz), 125.6, 125.1, 122.3, 121.8, 121.5, 121.5, 116.3, 108.4, 90.4, 83.0, 71.1, 59.5, 58.2 (q, J_{CF} = 32.3 Hz), 34.9, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.9.

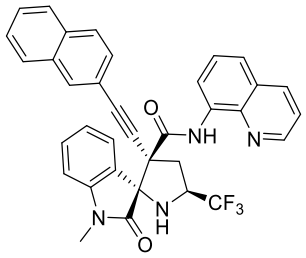
HRMS: calculated for $C_{29}H_{22}F_3N_4O_2S^+$ [M+H$^+$] 547.1410, found 547.1418.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.554	BB	0.3811	2151.06250	82.26332	51.4805
2	24.404	BB	1.0030	2027.33923	28.87894	48.5195



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.363	BB	0.3208	151.43472	7.15719	2.7710
2	23.691	BBA	1.0601	5313.59229	73.96822	97.2290

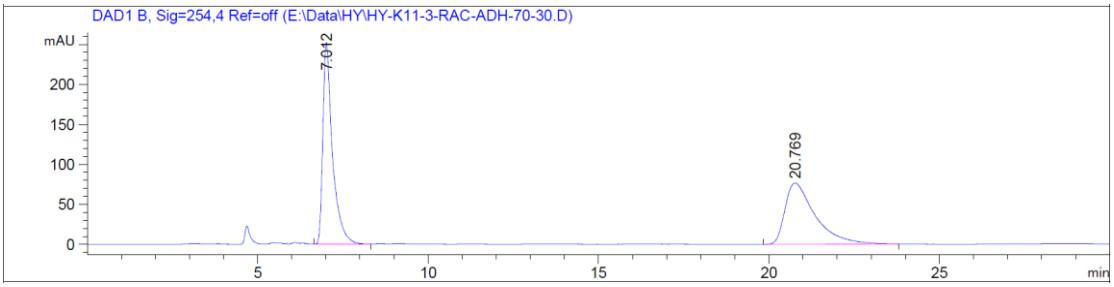


3oa

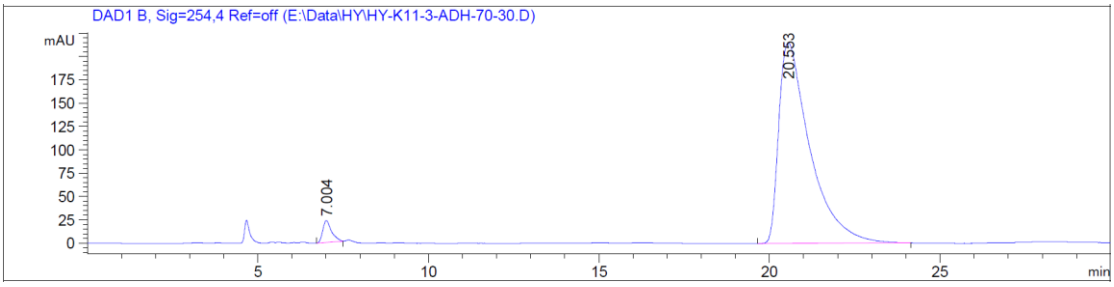
90 mg, 76% yield, yellow soild. $[\alpha]_{20}^{D}$ -174.40 (c 0.5, $CHCl_3$, 94% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 7.0 min, tR (major) = 20.8 min.

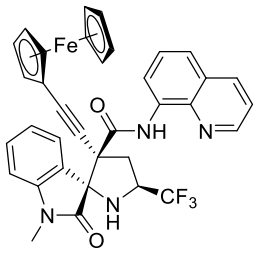
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.11 (s, 1H), 8.64 – 8.57 (m, 1H), 8.49 (dd, J = 4.2, 1.5 Hz, 1H), 8.06 (s, 1H), 8.03 (dd, J = 8.3, 1.5 Hz, 1H), 7.91 (d, J = 7.4 Hz, 1H), 7.84 – 7.76 (m, 3H), 7.56 (dd, J = 8.5, 1.3 Hz, 1H), 7.52 – 7.46 (m, 2H), 7.45 – 7.39 (m, 2H), 7.38 – 7.31 (m, 2H), 7.16 (t, J = 7.5 Hz, 1H), 6.60 (d, J = 7.8 Hz, 1H), 4.69 – 4.50 (m, 1H), 4.02 (t, J = 11.6 Hz, 1H), 2.92 (s, 3H), 2.86 – 2.66 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.6, 164.2, 147.8, 145.1, 138.2, 136.0, 133.7, 133.0, 132.7, 131.9, 130.6, 128.2, 127.9, 127.7, 127.6, 127.5, 127.1, 127.1, 126.8, 125.8 (q, J_{CF} = 279.6 Hz), 125.6, 125.1, 122.1, 121.8, 121.5, 118.8, 116.2, 108.3, 90.0, 86.9, 71.2, 59.4, 58.3 (q, J_{CF} = 32.2 Hz), 35.0, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.7. **HRMS**: calculated for $C_{35}H_{26}F_3N_4O_2^+$ [M+H$^+$] 591.2002, found 591.2000.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.012	BB	0.2842	4924.34668	251.76924	51.1120
2	20.769	BB	0.8716	4710.07813	76.57426	48.8880



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.004	BB	0.2672	417.84659	23.52635	2.9679
2	20.553	BB	0.9157	1.36611e4	215.47522	97.0321

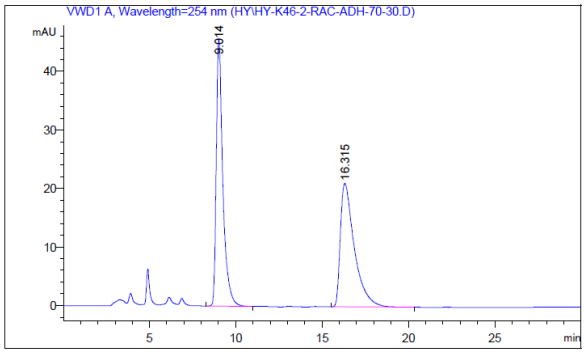


3pa

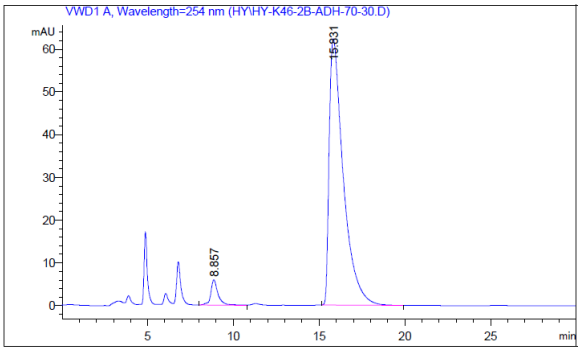
114 mg, 85% yield, yellow soild. $[\alpha]^{20}_{D}$ 97.60 (c 0.5, $CHCl_3$, 91% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 9.0 min, tR (major) = 16.3 min.

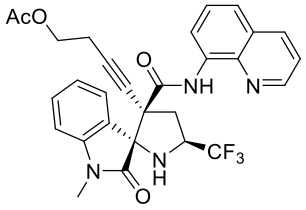
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 8.63 (dd, J = 6.7, 1.8 Hz, 1H), 8.51 (d, J = 3.7 Hz, 1H), 8.07 (d, J = 8.1 Hz, 1H), 7.96 (d, J = 7.4 Hz, 1H), 7.50 – 7.43 (m, 2H), 7.39 (t, J = 7.7 Hz, 1H), 7.35 (dd, J = 8.2, 4.2 Hz, 1H), 7.29 (d, J = 7.5 Hz, 1H), 6.58 (d, J = 7.7 Hz, 1H), 4.55 (s, 1H), 4.52 – 4.41 (m, 2H), 4.25 (d, J = 10.8 Hz, 2H), 4.08 (s, 5H), 3.91 (t, J = 11.6 Hz, 1H), 2.89 (s, 3H), 2.81 – 2.46 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.7, 164.7, 147.9, 145.3, 138.1, 136.0, 133.9, 130.6, 127.6, 127.3, 125.9, 125.8 (q, J_{CF} = 279.6 Hz), 125.4, 122.0, 121.7, 121.5, 116.3, 108.4, 88.6, 82.7, 71.5, 71.4, 70.9, 69.8, 69.1, 69.0, 67.1, 63.5, 59.4, 58.2 (q, J_{CF} = 32.2 Hz), 35.1, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.0. **HRMS**: calculated for $C_{35}H_{27}F_3FeN_4NaO_2^+$ [M+Na$^+$] 671.1328, found 671.1322.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.014	BB	0.3923	1206.85974	45.67237	50.3790
2	16.315	BB	0.8331	1188.70007	21.10540	49.6210



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.857	BB	0.4268	172.51584	5.90663	4.6220
2	15.831	BB	0.8470	3560.00439	62.26898	95.3780

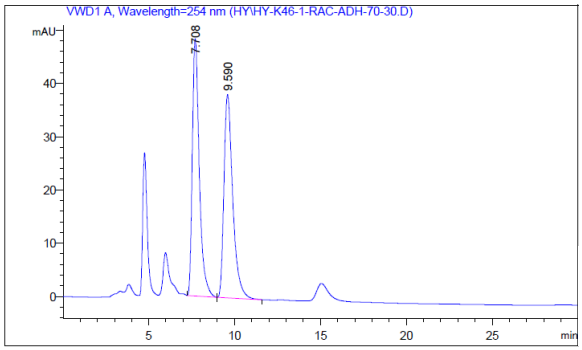


3qa

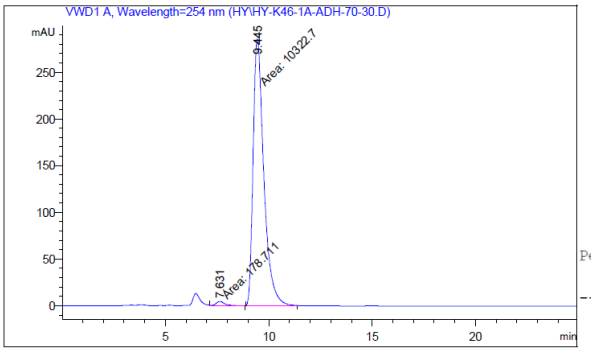
90 mg, 79% yield, yellow soild. $[\alpha]^{20}_{D}$ -174.40 (c 0.5, $CHCl_3$, 96% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 7.7 min, tR (major) = 9.5 min.

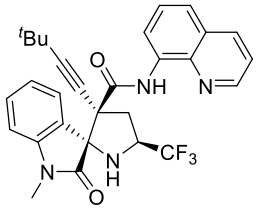
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 8.63 (dd, J = 6.7, 1.8 Hz, 1H), 8.51 (d, J = 3.7 Hz, 1H), 8.07 (d, J = 8.1 Hz, 1H), 7.96 (d, J = 7.4 Hz, 1H), 7.50 – 7.43 (m, 2H), 7.39 (t, J = 7.7 Hz, 1H), 7.35 (dd, J = 8.2, 4.2 Hz, 1H), 7.29 (d, J = 7.5 Hz, 1H), 6.58 (d, J = 7.7 Hz, 1H), 4.55 (s, 1H), 4.52 – 4.41 (m, 2H), 4.25 (d, J = 10.8 Hz, 2H), 4.08 (s, 5H), 3.91 (t, J = 11.6 Hz, 1H), 2.89 (s, 3H), 2.81 – 2.46 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.7, 164.7, 147.9, 145.3, 138.1, 136.0, 133.9, 130.6, 127.6, 127.3, 125.9, 125.8 (q, J_{CF} = 279.6 Hz), 125.4, 122.0, 121.7, 121.5, 116.3, 108.4, 88.6, 82.7, 71.5, 71.4, 70.9, 69.8, 69.1, 69.0, 67.1, 63.5, 59.4, 58.2 (q, J_{CF} = 32.2 Hz), 35.1, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.0. **HRMS**: calculated for $C_{29}H_{25}F_3N_4NaO_4^+$ [M+Na$^+$] 573.1720, found 573.1718.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.708	BB	0.4285	1359.96313	48.30423	50.0182
2	9.590	BB	0.5370	1358.97327	38.20714	49.9818



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.631	MM	0.5821	178.71089	5.11684	1.7018
2	9.445	MM	0.6019	1.03227e4	285.82288	98.2982

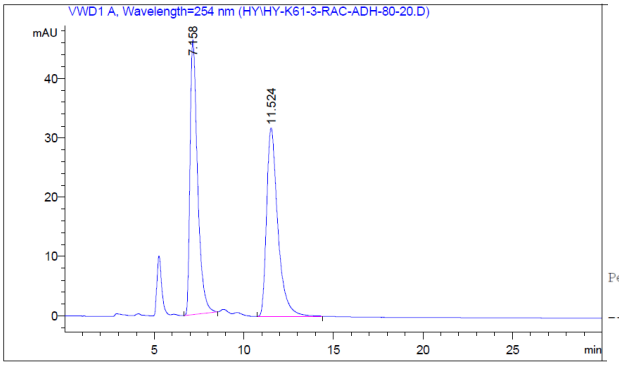


3ra

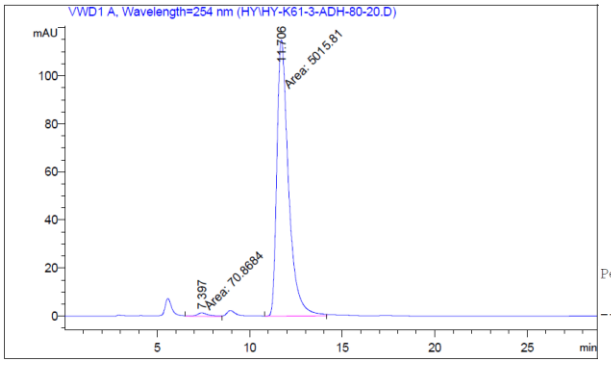
28 mg, 27% yield, yellow soild. $[\alpha]^{20}_{D}$ -67.40 (c 0.5, $CHCl_3$, 97% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 80:20, 1.0 mL/min, 254 nm): tR (minor) = 7.1 min, tR (major) = 11.5 min.

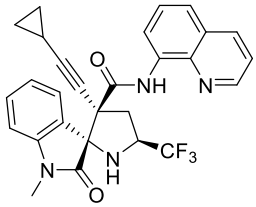
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.04 (s, 1H), 8.56 (p, J = 4.5 Hz, 1H), 8.49 (dd, J = 4.2, 1.5 Hz, 1H), 8.06 (dd, J = 8.3, 1.5 Hz, 1H), 7.83 (d, J = 7.3 Hz, 1H), 7.45 – 7.40 (m, 2H), 7.35 (dd, J = 8.3, 4.2 Hz, 1H), 7.29 (d, J = 7.7 Hz, 1H), 7.14 (t, J = 7.5 Hz, 1H), 6.51 (d, J = 7.8 Hz, 1H), 4.51 – 4.33 (m, 1H), 3.84 (t, J = 11.5 Hz, 1H), 2.90 (s, 3H), 2.71 – 2.47 (m, 2H), 1.33 (s, 9H).**^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.8, 164.9, 147.7, 144.8, 138.2, 135.9, 133.8, 130.4, 127.5, 127.0, 125.7 (q, J_{CF} = 279.5 Hz), 125.6, 125.2, 121.6, 121.4, 116.0, 107.9, 98.7, 76.3, 71.2, 58.8, 58.2 (q, J_{CF} = 32.3 Hz), 35.0, 30.6, 27.8, 26.0. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.7. **HRMS**: calculated for $C_{29}H_{28}F_3N_4O_2^+$ [M+H$^+$] 521.2159, found 521.1961.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.158	BB	0.4430	1354.39819	46.33311	49.4745
2	11.524	BB	0.6538	1383.16821	31.77761	50.5255



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.397	MM	0.7867	70.86840	1.50129	1.3932
2	11.706	MF	0.7273	5015.81152	114.93947	98.6068

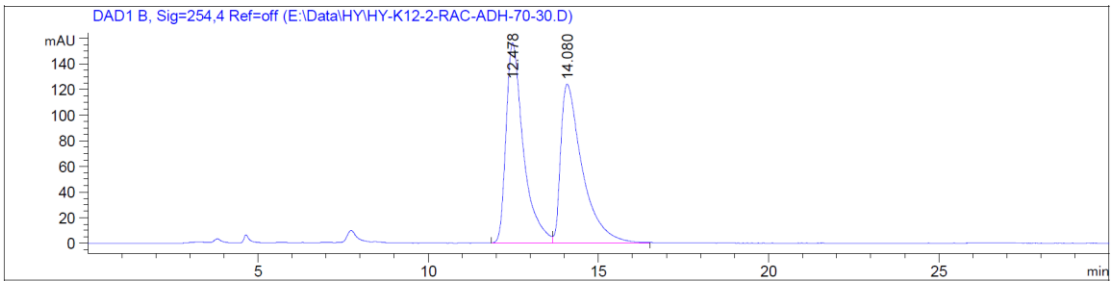


3sa

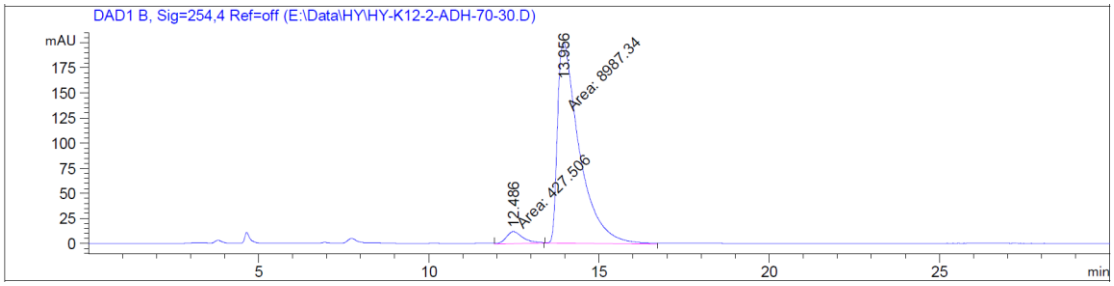
91 mg, 90% yield, yellow soild. $[\alpha]^{20}_{D}$ -86.80 (c 0.5, $CHCl_3$, 91% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 12.5 min, tR (major) = 14.1 min.

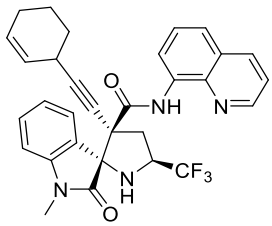
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 8.63 – 8.46 (m, 2H), 8.08 (dd, J = 8.3, 1.8 Hz, 1H), 7.79 (d, J = 7.2 Hz, 1H), 7.47 – 7.41 (m, 2H), 7.37 (dd, J = 8.3, 4.2 Hz, 1H), 7.31 (t, J = 7.6 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 6.57 (d, J = 7.6 Hz, 1H), 4.54 – 4.35 (m, 1H), 3.83 (t, J = 11.6 Hz, 1H), 2.67 – 2.51 (m, 2H), 2.58 (dd, J = 12.0, 6.2 Hz, 2H), 1.48 – 1.34 (m, 1H), 0.95 – 0.78 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.2, 165.2, 148.1, 145.4, 138.6, 136.3, 134.2, 130.7, 128.0, 127.5, 126.2, 126.1 (q, J_{CF} = 279.5 Hz), 125.4, 122.1, 122.0, 121.8, 116.6, 108.5, 93.9, 73.1, 71.4, 59.2, 58.6 (q, J_{CF} = 32.2 Hz), 35.5, 26.4, 8.6, 8.5. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.9. **HRMS**: calculated for $C_{28}H_{24}F_3N_4O_2^+$ [M+H$^+$] 505.1846, found 505.1846.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.478	BV	0.5270	5527.52930	156.15616	50.4183
2	14.080	VB	0.6383	5435.80713	123.79910	49.5817



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.486	MM	0.5865	427.50595	12.14859	4.5408
2	13.956	MM	0.7483	8987.34473	200.18144	95.4592

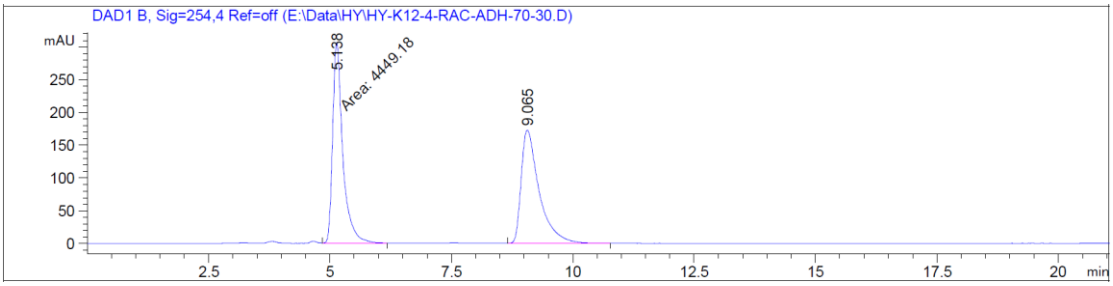


3ta

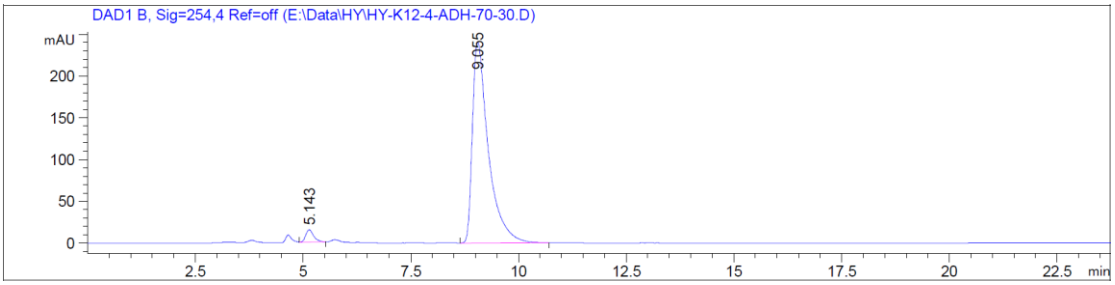
89 mg, 82% yield, yellow soild. $[\alpha]^{20}_{D}$ -131.60 (c 0.5, $CHCl_3$, 94% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90:10, 1.0 mL/min, 254 nm): tR (minor) = 5.1 min, tR (major) = 9.1 min.

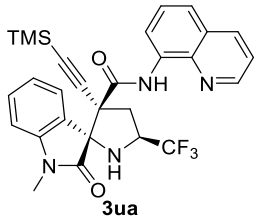
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.92 (s, 1H), 8.60 – 8.52 (m, 1H), 8.47 (dd, *J* = 4.1, 1.3 Hz, 1H), 8.05 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.84 (d, *J* = 7.5 Hz, 1H), 7.42 (d, *J* = 4.4 Hz, 2H), 7.38 – 7.31 (m, 2H), 7.17 (t, *J* = 7.6 Hz, 1H), 6.58 (d, *J* = 7.8 Hz, 1H), 6.35 – 6.20 (m, 1H), 4.54 – 4.37 (m, 1H), 3.90 (t, *J* = 11.5 Hz, 1H), 2.91 (s, 3H), 2.77 – 2.38 (m, 2H), 2.26 – 2.18 (m, 2H), 2.16 – 2.10 (m, 2H), 1.70 – 1.56 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.8, 164.6, 147.8, 145.1, 138.2, 136.6, 135.9, 133.8, 130.4, 127.5, 127.1, 125.8 (q, J_{CF} = 279.5 Hz), 125.6, 125.2, 122.0, 121.6, 121.4, 119.6, 116.2, 108.2, 91.3, 83.7, 70.9, 59.2, 58.2 (q, J_{CF} = 32.2 Hz), 35.2, 28.8, 26.0, 25.6, 22.1, 21.3. **^{19}F NMR** (376 MHz, $CDCl_3$) *δ* -74.8. **HRMS**: calculated for $C_{31}H_{28}F_3N_4O_2^+$ [M+H$^+$] 545.2159, found 545.2155.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.138	FM	0.2420	4449.18066	306.47208	50.1090
2	9.065	BB	0.3814	4429.81885	172.60815	49.8910



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.143	VB	0.1947	191.55075	14.82431	3.0065
2	9.055	BB	0.3797	6179.61279	240.56281	96.9935

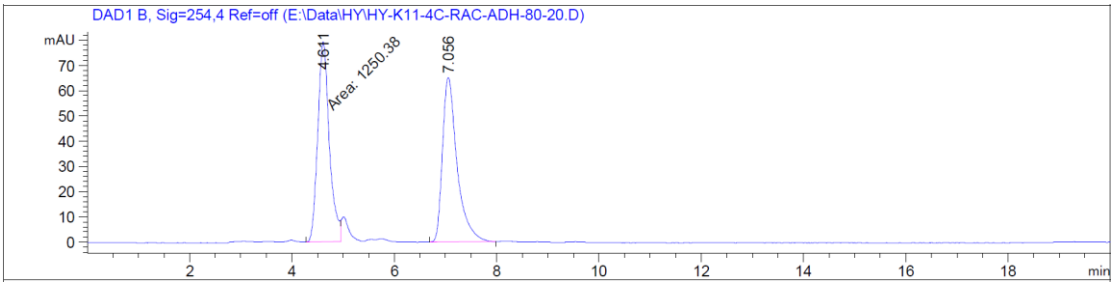


3ua

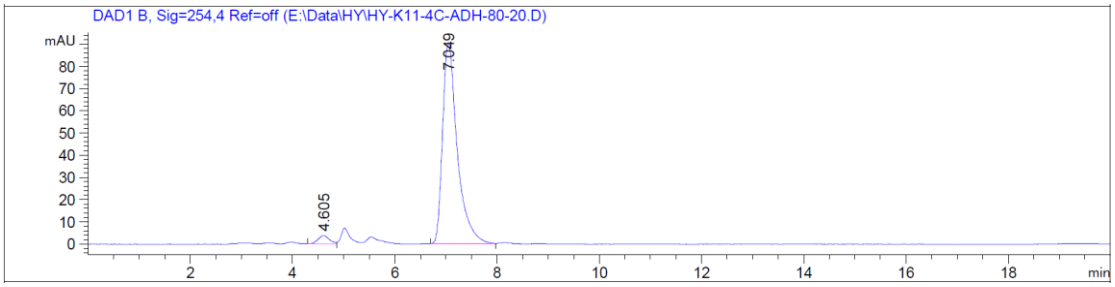
69 mg, 62% yield, white soild. $[\alpha]^{20}_{D}$ -76.80 (c 0.5, $CHCl_3$, 92% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90:10, 1.0 mL/min, 254 nm): tR (minor) = 4.6 min, tR (major) = 7.0 min.

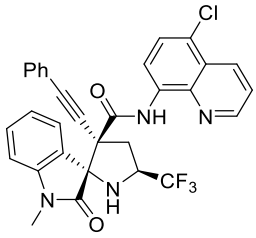
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.97 (s, 1H), 8.60 – 8.53 (m, 1H), 8.49 (dd, J = 4.2, 1.7 Hz, 1H), 8.07 (dd, J = 8.3, 1.8 Hz, 1H), 7.85 (d, J = 7.5 Hz, 1H), 7.44 (d, J = 4.6 Hz, 2H), 7.36 (dd, J = 8.3, 4.2 Hz, 1H), 7.31 (t, J = 7.7 Hz, 1H), 7.14 (t, J = 7.6 Hz, 1H), 6.54 (d, J = 7.3 Hz, 1H), 4.52-4.34 (m, 1H), 3.86 (t, J = 11.6 Hz, 1H), 2.90 (s, 3H), 2.63 (dd, J = 12.3, 6.1 Hz, 2H), 0.26 (s, 9H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.0, 164.5, 148.2, 145.4, 138.6, 136.3, 134.2, 130.9, 128.0, 127.5, 126.1 (q, J_{CF} = 279.8 Hz), 125.7, 125.6, 122.1, 122.1, 121.8, 116.6, 108.5, 103.0, 95.7, 71.1, 59.9, 58.7 (q, J_{CF} = 32.4 Hz), 35.1, 26.5, 0.0. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.9. **HRMS**: calculated for $C_{28}H_{27}F_3N_4NaO_2Si^+$ [M+Na^+] 559.1748, found 559.1758.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.611	MF	0.2630	1250.37512	79.24776	49.1787
2	7.056	BB	0.2975	1292.13721	65.11919	50.8213



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.605	BV	0.2198	56.26894	3.69165	3.0477
2	7.049	BB	0.2971	1790.03320	90.36163	96.9523



3va

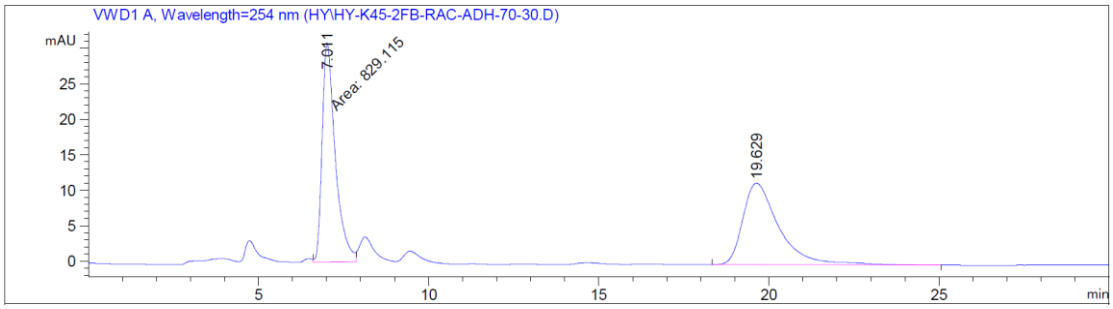
94 mg, 79% yield, white soild. $[\alpha]^{20}_{D}$ -128.80 (c 0.5, $CHCl_3$, 94% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90:10, 1.0 mL/min, 254 nm): tR (minor) = 7.0 min, tR (major) = 19.6 min.

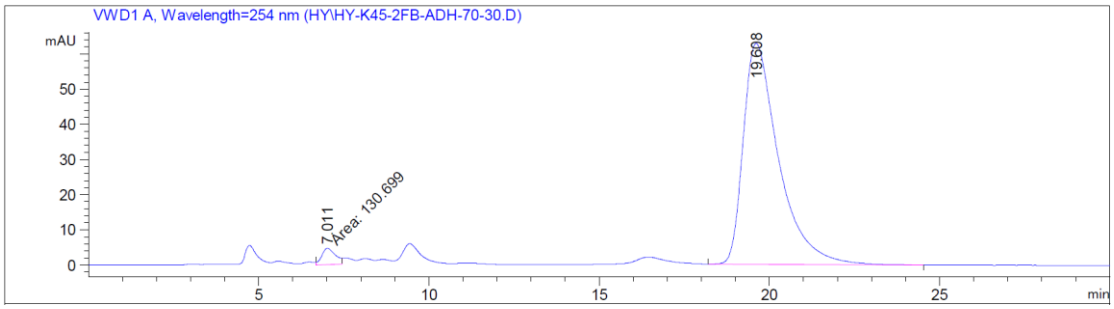
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.96 (s, 1H), 8.56 – 8.48 (m, 2H), 8.43 (dd, J = 8.5, 1.6 Hz, 1H), 7.88 (dd, J = 7.6, 0.8 Hz, 1H), 7.57 – 7.52 (m, 2H), 7.50 – 7.43 (m, 2H), 7.40 – 7.33 (m, 4H), 7.18 (td, J = 7.6, 0.9 Hz, 1H), 6.61 (d, J = 7.7 Hz, 1H), 4.62 – 4.44 (m, 1H), 3.96 (t, J = 11.2, 1H), 2.93 (s, 3H), 2.80 – 2.62 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.8, 163.8, 150.4, 148.3, 145.2, 139.0, 131.7, 130.9, 130.5, 129.1, 128.5, 127.3, 125.8, 125.8 (q, J_{CF} = 279.5 Hz), 125.1, 122.1, 121.8, 120.5, 120.1, 116.5, 108.4, 104.1, 89.4, 86.9, 71.2, 59.2, 58.4 (q, J_{CF} = 32.3 Hz), 55.7, 35.1, 26.2.

^{19}F NMR (376 MHz, $CDCl_3$) δ -74.8.

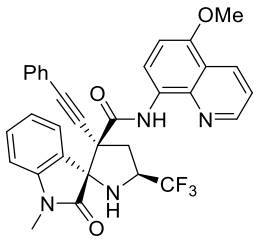
HRMS: calculated for $C_{31}H_{22}ClF_3N_4NaO_2^+$ [M+Na^+] 597.1276, found 597.1277.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.011	MF	0.4469	829.11536	30.92293	49.3639
2	19.629	BB	1.0991	850.48352	11.49601	50.6361



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.011	MM	0.4654	130.69930	4.68016	2.7975
2	19.608	BB	1.0833	4541.34375	62.83101	97.2025



3wa

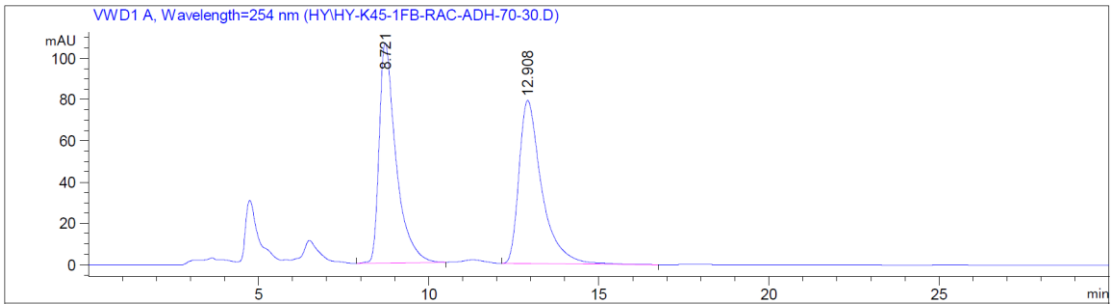
98 mg, 91% yield, yellow soild. $[\alpha]^{20}_{D}$ -122.40 (c 0.5, $CHCl_3$, 94% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 8.7 min, tR (major) = 12.9 min.

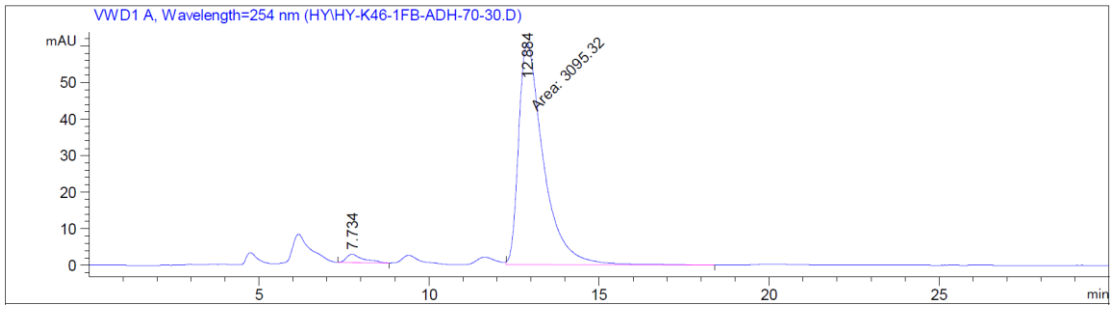
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.55 – 8.41 (m, 2H), 7.87 (dd, J = 7.6, 0.8 Hz,), 7.59 – 7.51 (m, 2H), 7.41 – 7.31 (m, 5H), 7.15 (td, J = 7.6, 0.9 Hz, 1H), 6.74 (d, J = 8.6 Hz, 1H), 6.62 (d, J = 7.7 Hz, 1H), 4.60 – 4.44 (m, 1H), 4.00 – 3.88 (m, 4H), 2.94 (s, 3H), 2.85 – 2.45 (m, 2H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.8, 163.8, 150.4, 148.3, 145.2, 139.0, 131.7, 130.9, 130.5, 129.1, 128.5, 127.3, 125.8, 125.8 (q, J_{CF} = 279.5 Hz), 125.1, 122.1, 121.8, 120.5, 120.1, 116.5, 108.4, 104.1, 89.4, 86.9, 71.2, 59.2, 58.4 (q, J_{CF} = 32.3 Hz), 55.7, 35.1, 26.2. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.9.

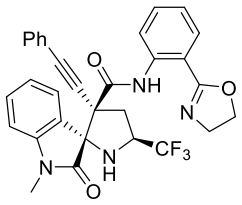
HRMS: calculated for $C_{32}H25F_3N_4NaO_3^+$ [M+Na^+] 593.1771, found 593.1763.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.721	BB	0.5076	3666.19189	106.50940	49.9526
2	12.908	BB	0.6912	3673.15186	79.18708	50.0474



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.734	BB	0.4928	79.65002	2.30710	2.5087
2	12.884	FM	0.8507	3095.32422	60.64151	97.4913

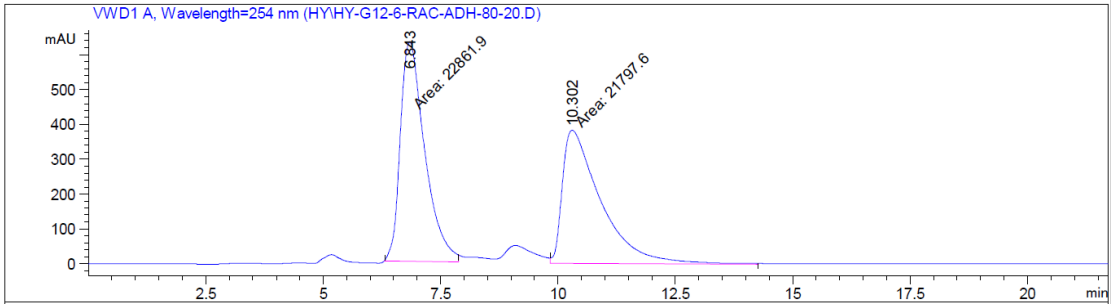


3xa

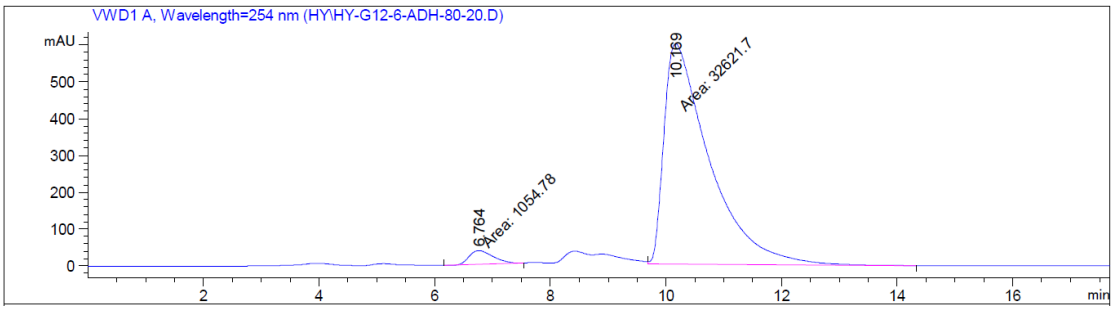
87 mg, 78% yield, yellow soild. $[\alpha]^{20}_{D}$ -139.20 (c 0.5, $CHCl_3$, 94% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 80:20, 1.0 mL/min, 254 nm): tR (minor) = 6.8 min, tR (major) = 10.3 min.

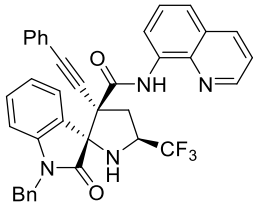
^{1}H NMR (400 MHz, $CDCl_3$) δ 12.41 (s, 1H), 8.53 (dd, J = 8.4, 0.8 Hz, 1H), 7.84 – 7.78 (m, 1H), 7.75 (dd, J = 7.9, 1.5 Hz, 1H), 7.52 – 7.47 (m, 2H), 7.39 – 7.29 (m, 5H), 7.07 (td, J = 7.6, 0.8 Hz, 1H), 7.02 (td, J = 7.9, 1.1 Hz, 1H), 6.71 (d, J = 7.7 Hz, 1H), 4.58 – 4.43 (m, 1H), 4.28 – 4.14 (m, 2H), 3.88 (t, J = 11.5 Hz, 1H), 3.77 (t, J = 9.5 Hz, 2H), 3.03 (s, 3H), 2.76 (dd, J = 12.0, 6.0 Hz, 1H), 2.66 – 2.45 (m, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.2, 165.7, 164.0, 145.1, 139.1, 132.2, 131.6, 130.1, 129.0, 128.8, 128.4, 126.7, 125.8 (q, J_{CF} = 279.5 Hz), 124.7, 122.6, 122.0, 121.9, 119.8, 113.4, 108.1, 88.7, 86.7, 70.8, 66.0, 59.6, 58.3 (q, J_{CF} = 32.2 Hz), 54.3, 35.7, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -75.1. **HRMS**: calculated for $C_{31}H_{26}F_3N_4O_3^+$ [M+H$^+$] 559.1952, found 559.1956.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.843	MM	0.6044	2.28619e4	630.42719	51.1916
2	10.302	MM	0.9510	2.17976e4	382.02557	48.8084



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.764	MM	0.4745	1054.77625	37.04625	3.1321
2	10.169	FM	0.9088	3.26217e4	598.23950	96.8679



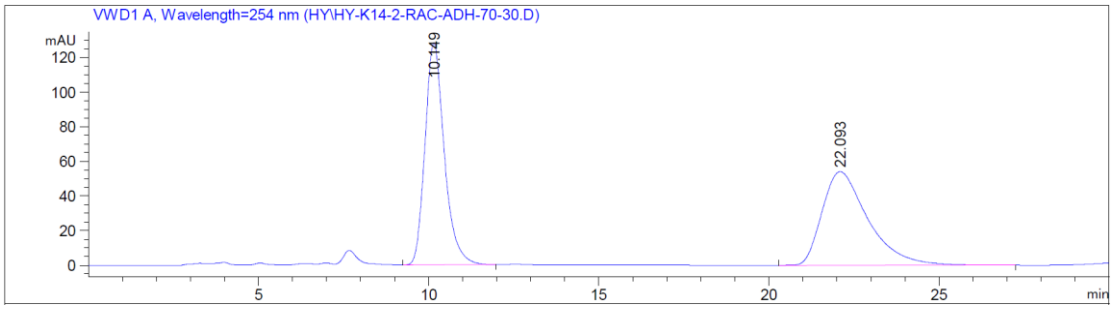
3ab

101 mg, 82% yield, white soak. $[\alpha]^{20}_{D}$ -108.00 (c 0.5, $CHCl_3$, 91% ee)

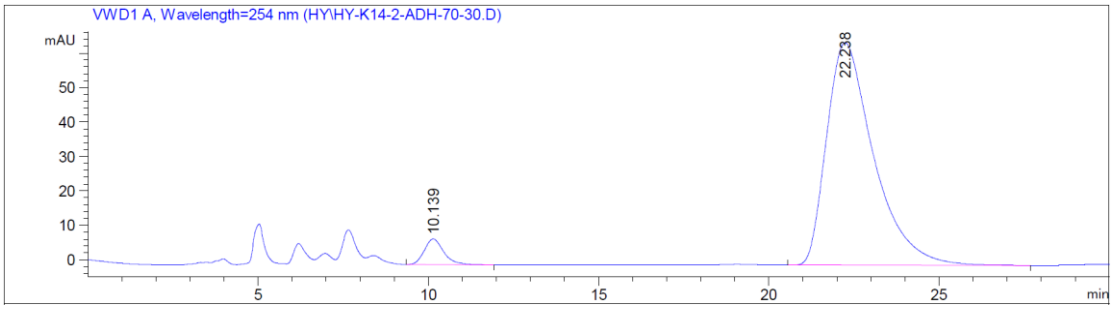
HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 10.1 min, tR (major) = 22.1 min.

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.07 (s, 1H), 8.62 (dd, J = 6.7, 2.3 Hz, 1H), 8.30 (dd, J = 4.2, 1.7 Hz, 1H), 7.99 (dd, J = 8.3, 1.6 Hz, 1H), 7.96 – 7.91 (m, 1H), 7.55 – 7.49 (m, 2H), 7.48 – 7.41 (m, 2H), 7.37 – 7.31 (m, 3H), 7.30 – 7.22 (m, 3H), 7.16 (td, J = 7.6, 0.9 Hz, 1H), 7.01 (d, J = 7.3 Hz, 2H), 6.85 (t, J = 7.4 Hz, 1H), 6.70 (t, J = 7.7 Hz, 2H), 6.54 (d, J = 7.7 Hz, 1H), 5.09 (d, J = 15.7 Hz, 1H), 4.62 – 4.48 (m, 1H), 4.29 (d, J = 15.7 Hz, 1H), 4.07 (t, J = 11.6 Hz, 1H), 2.86 – 2.67 (m, 2H).

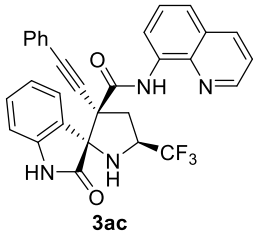
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.7, 144.5, 138.1, 135.8, 135.1, 133.8, 131.7, 130.5, 129.1, 128.5, 128.0, 127.6, 127.1, 127.0, 126.9, 125.8 (q, J_{CF} = 279.5 Hz), 125.4, 125.3, 122.3, 121.8, 121.6, 121.4, 116.3, 109.6, 89.5, 86.7, 70.9, 59.0, 58.2 (q, J_{CF} = 32.3 Hz), 44.1, 35.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.7. **HRMS**: calculated for $C_{37}H_{28}F_3N_4O_2^+$ [M+H$^+$] 617.2159, found 617.2164.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.149	BB	0.6000	5051.51416	128.12273	49.9324
2	22.093	BB	1.4162	5065.19531	54.00531	50.0676



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.139	BB	0.6018	295.43027	7.43158	4.5518
2	22.238	BB	1.4490	6194.92822	64.58998	95.4482

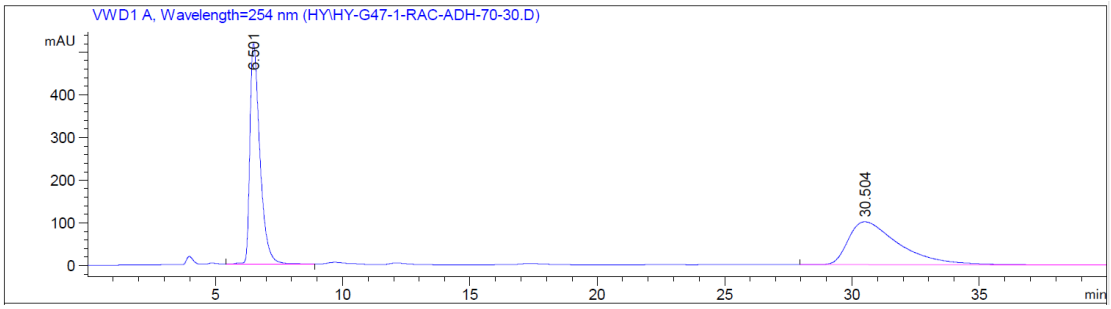


3ac

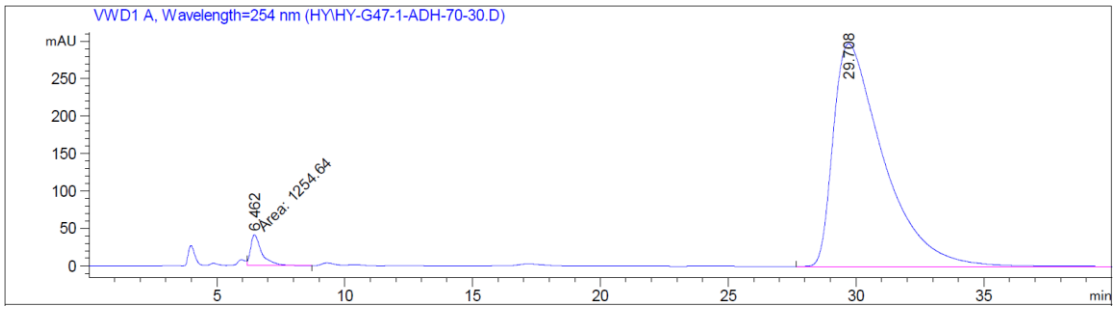
63 mg, 60% yield, white soild. $[\alpha]^{20}_{D}$ -41.60 (c 0.5, $CHCl_3$, 94% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 6.5 min, tR (major) = 29.7 min.

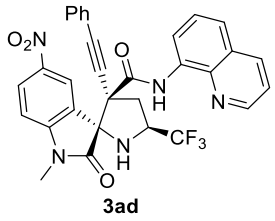
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.14 (s, 1H), 8.58 – 8.47 (m, 2H), 8.00 (dd, J = 8.3, 1.6 Hz, 1H), 7.87 (d, J = 7.5 Hz, 1H), 7.58 – 7.51 (m, 2H), 7.39 – 7.26 (m, 7H), 7.13 (td, J = 7.6, 0.9 Hz, 1H), 6.72 (d, J = 7.7 Hz, 1H), 4.58 – 4.42 (m, 1H), 3.92 (t, J = 11.6 Hz, 1H), 2.77 – 2.60 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 178.0, 164.2, 147.8, 142.6, 138.3, 135.9, 133.7, 131.7, 130.6, 129.1, 128.5, 127.6, 127.1, 125.9, 125.8 (q, J_{CF} = 279.5 Hz), 125.4, 122.1, 121.8, 121.7, 121.4, 116.5, 110.6, 89.6, 86.6, 71.3, 59.1, 58.2 (q, J_{CF} = 32.3 Hz), 35.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8. **HRMS**: calculated for $C_{30}H_{22}F_3N_4O_2^+$ [M+H$^+$] 527.1689, found 527.1690.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.501	VV R	0.4144	1.41515e4	517.00842	50.2868
2	30.504	BBA	2.0550	1.39901e4	100.68818	49.7132



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.462	FM	0.5090	1254.63513	41.08524	3.0112
2	29.708	BBA	1.9728	4.04107e4	297.11548	96.9888

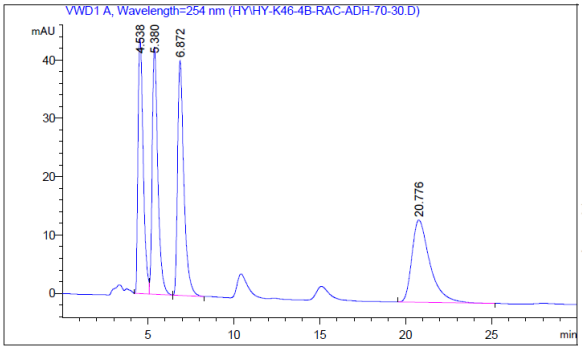


3ad

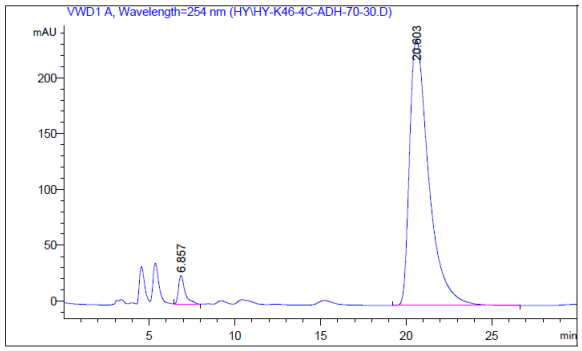
67 mg, 69% yield, brown soild. $[\alpha]^{20}_{D}$ -110.00 (c 0.5, $CHCl_3$, 93% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 6.8 min, tR (major) = 20.8 min.

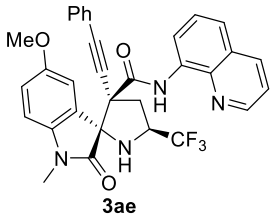
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.25 (s, 1H), 8.91 (d, J = 2.3 Hz, 1H), 8.57 (dd, J = 4.2, 1.6 Hz, 1H), 8.50 (dd, J = 7.1, 1.9 Hz, 1H), 8.32 (dd, J = 8.7, 2.3 Hz, 1H), 8.10 (dd, J = 8.3, 1.6 Hz, 1H), 7.69 – 7.62 (m, 2H), 7.50 – 7.43 (m, 2H), 7.43 – 7.36 (m, 5H), 6.77 (d, J = 8.7 Hz, 1H), 4.69 – 4.52 (m, 1H), 3.93 (t, J = 11.5 Hz, 1H), 3.13 (s, 2H), 2.88 (dd, J = 12.0, 6.0 Hz, 1H), 2.77 (d, J = 8.1 Hz, 1H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.2, 164.1, 151.0, 148.2, 142.8, 138.2, 136.2, 133.4, 131.9, 129.5, 128.6, 127.7, 127.5, 127.1, 126.8, 125.8 (q, J_{CF} = 279.6 Hz), 122.2, 121.7, 121.1, 120.9, 116.5, 107.8, 90.9, 85.2, 69.8, 60.2, 58.6 (q, J_{CF} = 32.7 Hz), 35.6, 26.7. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.9. **HRMS**: calculated for $C_{31}H_{23}F_3N_5O_4^+$ [M+H$^+$] 586.1697, found 586.1702.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.538	BV	0.3339	922.74243	43.77431	23.4471
2	5.380	VB	0.3482	958.76483	42.33028	24.3625
3	6.872	BB	0.3854	1025.00696	40.20594	26.0457
4	20.776	BB	1.0983	1028.90308	14.11658	26.1447



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.857	VB	0.3944	670.95911	25.38545	3.5062
2	20.603	BB	1.1693	1.84657e4	238.48943	96.4938

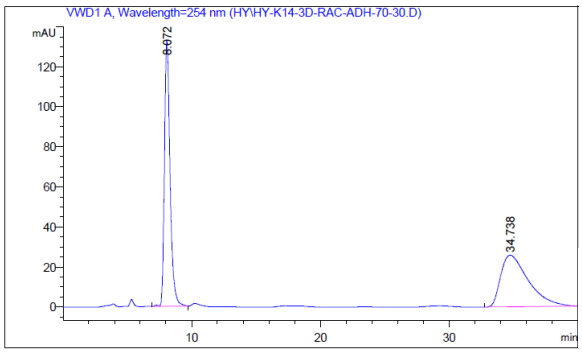


3ae

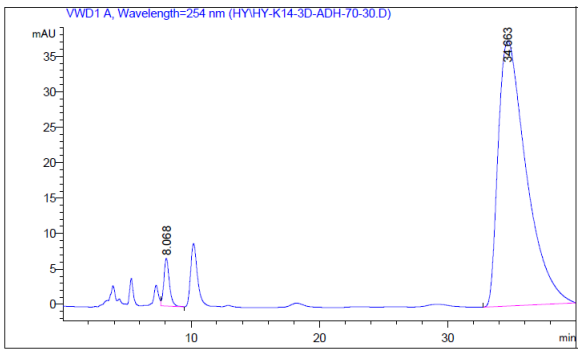
92 mg, 81% yield, yellow soak. $[\alpha]^{20}_{D}$ -75.60 (c 0.5, $CHCl_3$, 93% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH =70:30, 1.0 mL/min, 254 nm): tR (minor) = 8.0 min, tR (major) = 34.7 min.

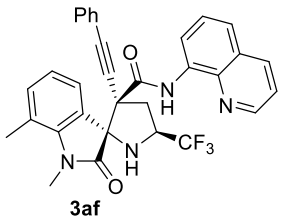
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.03 (s, 1H), 8.62 – 8.53 (m, 1H), 8.50 (dd, J = 4.2, 1.6 Hz, 1H), 8.06 (dd, J = 8.3, 1.6 Hz, 1H), 7.61 – 7.52 (m, 3H), 7.42 (d, J = 4.2 Hz, 2H), 7.39 – 7.31 (m, 4H), 6.87 (dd, J = 8.5, 2.6 Hz, 1H), 6.50 (d, J = 8.5 Hz, 1H), 4.64 – 4.44 (m, 1H), 3.98 (t, J = 11.6 Hz, 1H), 3.69 (s, 3H), 2.89 (s, 3H), 2.80 – 2.59 (m, 2H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 175.5, 164.2, 155.7, 147.8, 138.4, 138.1, 136.0, 133.7, 131.7, 129.1, 128.4, 127.5, 127.1, 126.6, 125.8 (q, J_{CF} = 279.6 Hz), 121.7, 121.5, 116.2, 115.5, 112.2, 108.7, 89.7, 86.6, 71.3, 59.3, 58.3 (q, J_{CF} = 32.3 Hz), 55.8, 34.9, 26.1. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.8. **HRMS**: calculated for $C_{32}H_{26}F_3N_4O_3^+$ [M+H$^+$] 571.1952, found 571.1961.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.072	VB R	0.4556	4006.42407	132.95314	50.8633
2	34.738	BBA	2.2654	3870.41797	25.81208	49.1367



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.068	VB	0.4463	200.76123	6.76389	3.4145
2	34.663	BBA	2.2805	5678.88232	37.42001	96.5855

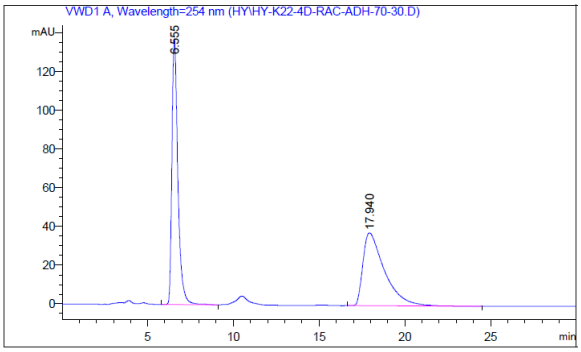


3af

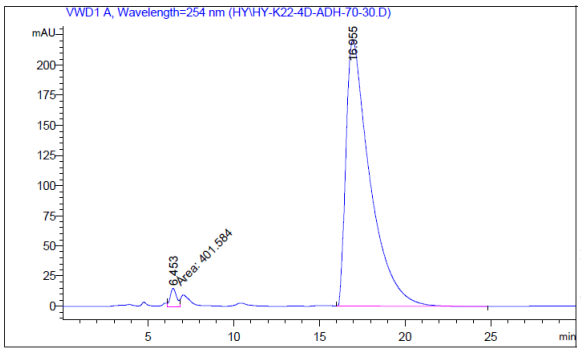
65 mg, 59% yield, white soak. $[\alpha]^{20}_{D}$ -213.60 (c 0.5, $CHCl_3$, 96% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 6.6 min, tR (major) = 17.9 min.

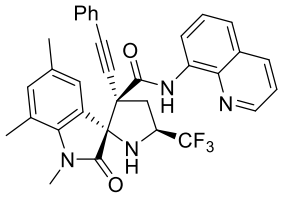
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.95 (s, 1H), 8.65 – 8.58 (m, 1H), 8.44 (dd, J = 4.2, 1.7 Hz, 1H), 8.06 (dd, J = 8.3, 1.6 Hz, 1H), 7.73 – 7.67 (m, 1H), 7.56 – 7.50 (m, 2H), 7.46 – 7.41 (m, 2H), 7.39 – 7.32 (m, 4H), 7.09 – 7.03 (m, 2H), 4.62 – 4.42 (m, 1H), 3.95 (t, J = 11.7 Hz, 1H), 3.10 (s, 3H), 2.73 (dd, J = 12.2, 6.0 Hz, 1H), 2.66 – 2.52 (m, 1H), 2.08 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.5, 164.3, 147.8, 142.7, 138.1, 135.9, 134.3, 133.8, 131.6, 129.0, 128.4, 127.5, 127.1, 126.1, 125.8 (q, J_{CF} = 279.6 Hz), 123.0, 122.0, 121.7, 121.7, 121.4, 120.0, 116.0, 89.8, 86.5, 70.9, 59.5, 58.3 (q, J_{CF} = 32.2 Hz), 34.7, 29.4, 18.6. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.9. **HRMS**: calculated for $C_{32}H_{26}F_3N_4O_2^+$ [M+H$^+$] 555.2002, found 555.2011.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.555	BB	0.3659	3313.88843	137.14241	50.2397
2	17.940	BB	1.2810	3282.26147	37.65121	49.7603



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.453	MM	0.4406	401.58411	15.18926	1.8382
2	16.955	BB	1.3882	2.14449e4	220.96831	98.1618

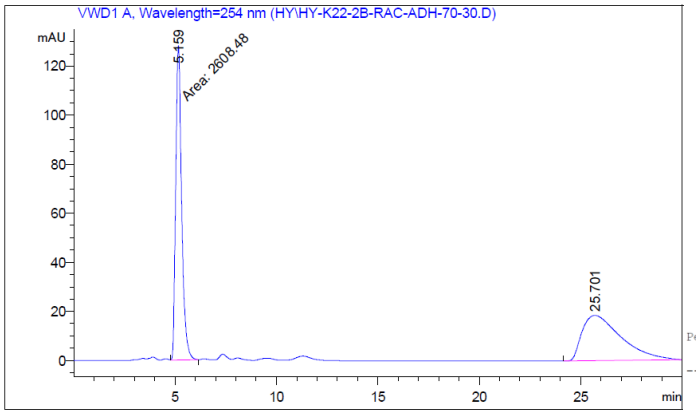


3ag

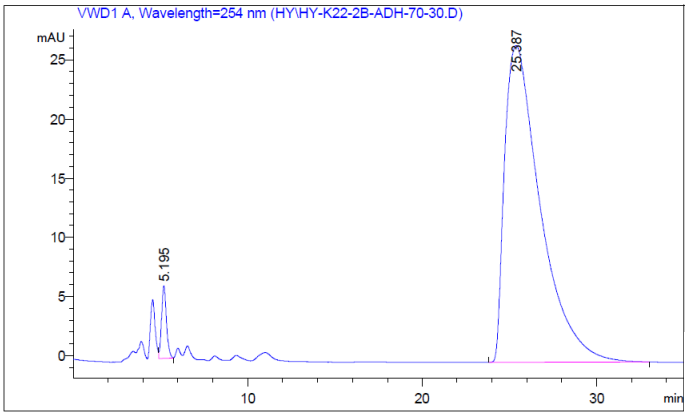
90 mg, 79% yield, yellow soild. $[\alpha]^{20}_{D}$ -140.80 (c 0.5, $CHCl_3$, 94% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 70:30, 1.0 mL/min, 254 nm): tR (minor) = 5.1 min, tR (major) = 25.7 min.

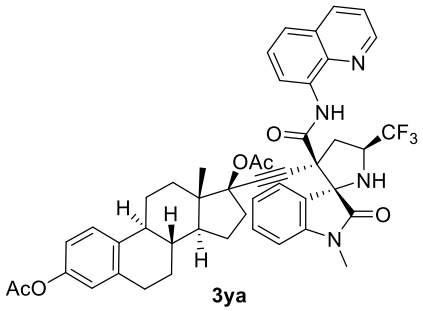
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.94 (s, 1H), 8.61 (dd, J = 5.5, 3.5 Hz, 1H), 8.45 (dd, J = 4.2, 1.6 Hz, 1H), 8.06 (dd, J = 8.3, 1.5 Hz, 1H), 7.58 – 7.50 (m, 4H), 7.45 – 7.41 (m, 2H), 7.40 – 7.32 (m, 5H), 4.62 – 4.42 (m, 2H), 3.95 (t, J = 11.7 Hz, 1H), 3.07 (s, 2H), 2.72 (dd, J = 12.2, 5.9 Hz, 1H), 2.61 (s, 1H), 2.32 (s, 3H), 2.03 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 176.5, 164.3, 147.7, 140.2, 138.0, 135.9, 134.7, 133.8, 131.6, 131.3, 129.0, 128.4, 127.5, 127.1, 126.1, 125.8 (q, J_{CF} = 279.6 Hz), 123.8, 121.7, 121.6, 121.4, 119.6, 116.0, 89.9, 86.7, 71.1, 59.5, 58.3 (q, J_{CF} = 32.1 Hz), 34.6, 29.4, 20.8, 18.4. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -74.9. **HRMS**: calculated for $C_{33}H_{28}F_3N_4O_2^+$ [M+H$^+$] 569.2159, found 569.2169.



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.159	FM	0.3390	2608.47949	128.24103	51.2173
2	25.701	BBA	2.0275	2484.48242	18.46800	48.7827



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.195	VB	0.2970	119.45296	6.13933	3.0408
2	25.387	BB	2.1238	3808.94067	26.77308	96.9592

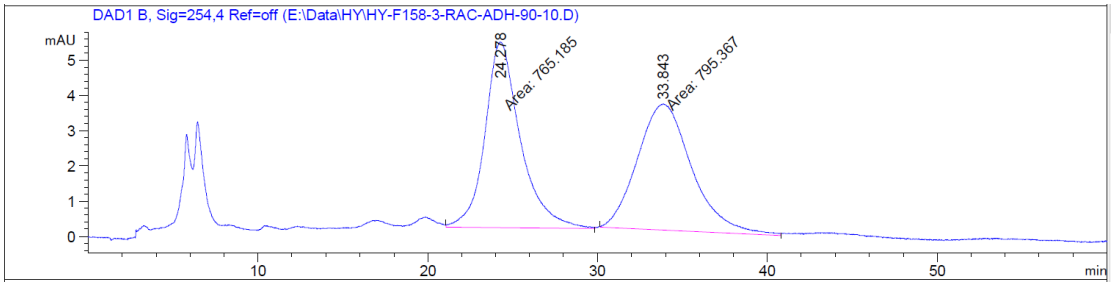


3ya

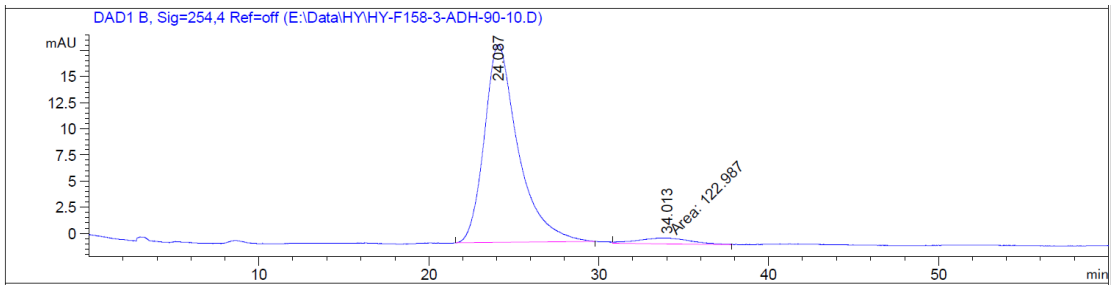
124 mg, 76% yield, white soild. $[\alpha]^{20}_{D}$ -89.20 (c 0.5, $CHCl_3$, 91% ee)

HPLC (Daicel Chiralpak AD-H, hexane/*i*-PrOH = 90:10, 1.0 mL/min, 254 nm): tR (major) = 24.3 min, tR (minor) = 33.8min.

^{1}H NMR (400 MHz, $CDCl_3$) δ 11.16 (s, 1H), 8.95 – 8.82 (m, 2H), 8.18 (dd, J = 8.3, 1.6 Hz, 1H), 7.70 (d, J = 7.3 Hz, 1H), 7.59 – 7.52 (m, 2H), 7.48 (dd, J = 8.3, 4.2 Hz, 1H), 7.37 (td, J = 7.8, 0.9 Hz, 1H), 7.23 (d, J = 8.5 Hz, 1H), 7.20 – 7.14 (m, 1H), 6.90 (d, J = 7.7 Hz, 1H), 6.82 (dd, J = 8.5, 2.5 Hz, 1H), 6.78 – 6.74 (m, 1H), 4.61 – 4.47 (m, 1H), 3.63 (d, J = 14.3 Hz, 1H), 3.53 (d, J = 13.4 Hz, 1H), 3.31 – 3.16 (m, 4H), 2.89 – 2.75 (m, 3H), 2.58 (d, J = 13.4 Hz, 1H), 2.38 – 2.29 (m, 2H), 2.26 (s, 3H), 2.23 – 2.07 (m, 3H), 2.05 (s, 3H), 2.01 – 1.93 (m, 1H), 1.93 – 1.77 (m, 3H), 1.62 – 1.48 (m, 3H), 1.37 – 1.20 (m, 2H), 1.01 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 174.9, 169.8, 169.4, 167.1, 148.4, 148.0, 143.3, 138.9, 138.0, 137.4, 136.3, 134.0, 132.7, 129.4, 127.9, 127.3, 126.3, 123.9, 123.9 (q, J_{CF} = 282.2 Hz), 123.0, 122.3, 121.6, 121.4, 118.6, 117.2, 108.7, 88.5, 86.1, 84.7, 73.8 (q, J_{CF} = 29.9 Hz), 67.9, 51.6, 49.9, 48.7, 48.3, 43.6, 38.7, 37.3, 34.0, 29.3, 27.0, 26.6, 26.2, 23.3, 21.3, 21.0, 13.5. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -67.9. **HRMS**: calculated for $C_{47}H_{46}F_3N_4O_6$ [M+H$^+$] 819.3364, found 819.3367.



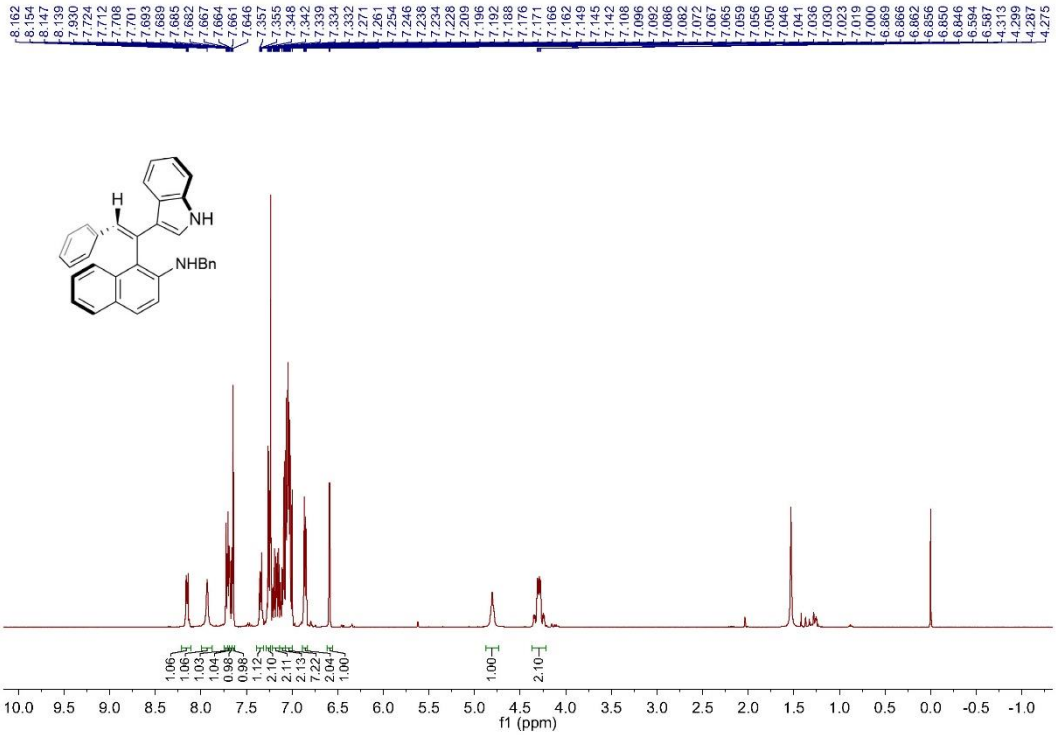
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.278	MM	2.4178	765.18481	5.27462	49.0330
2	33.843	MM	3.7004	795.36707	3.58239	50.9670



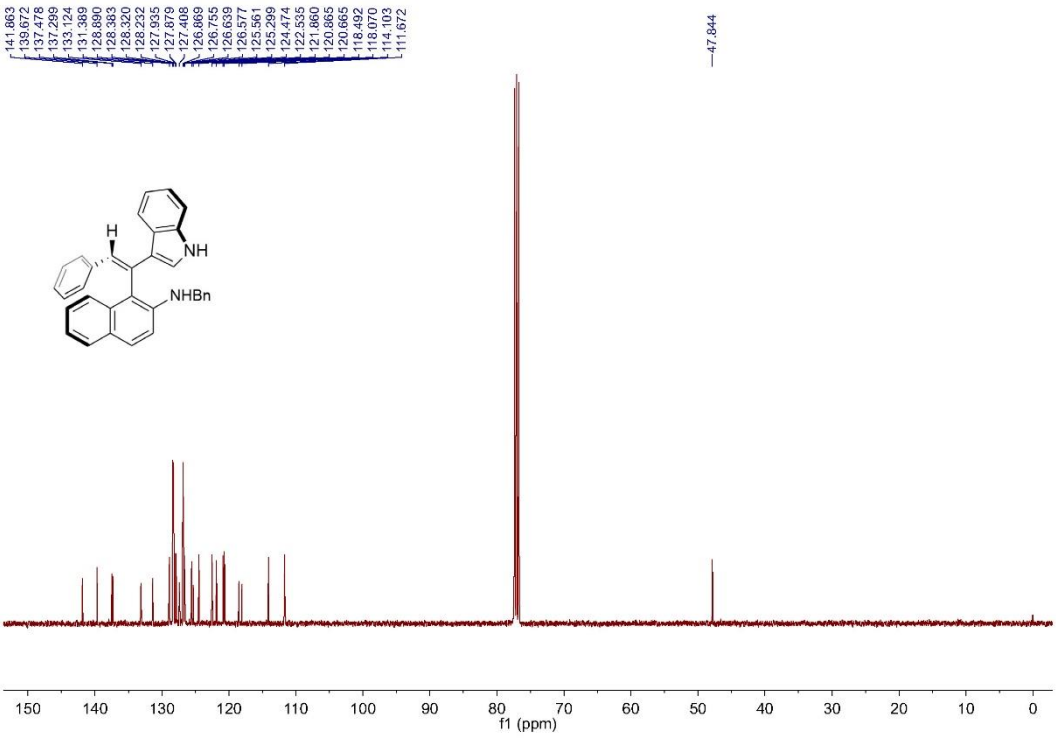
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	24.087	BB	1.6870	2623.06738	18.92596	95.5213
2	34.013	MM	3.6121	122.98669	5.67471e-1	4.4787

8. NMR spectras

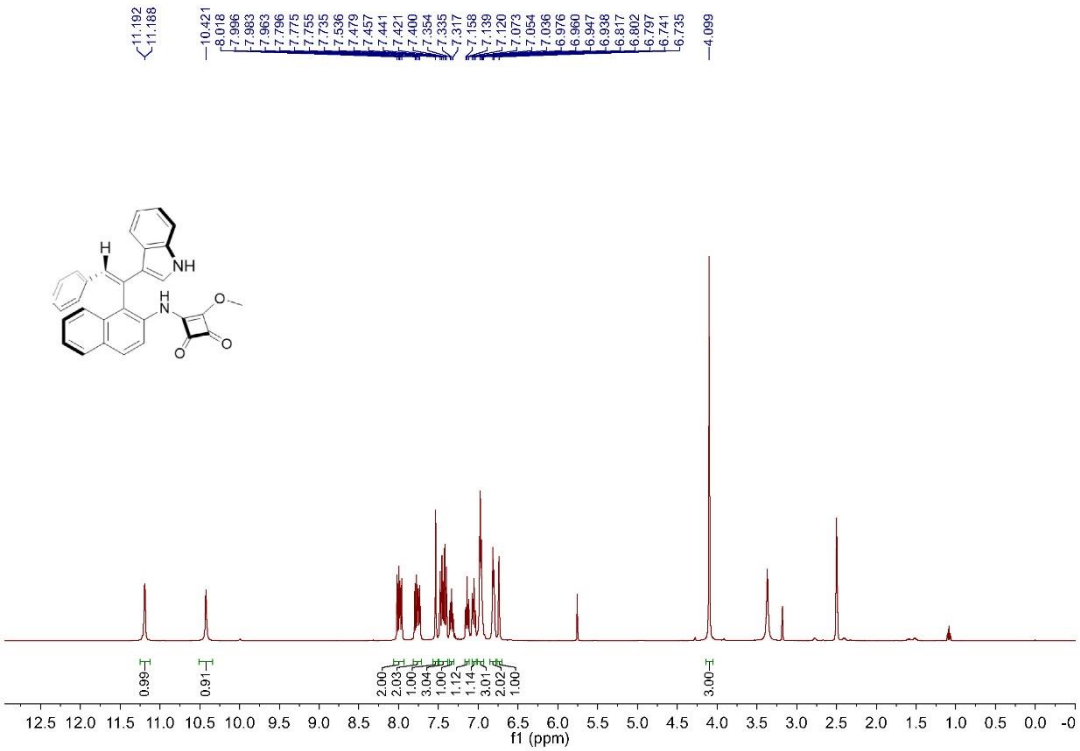
^{1}H NMR spectrum of **S2** in $CDCl_3$, 400 MHz



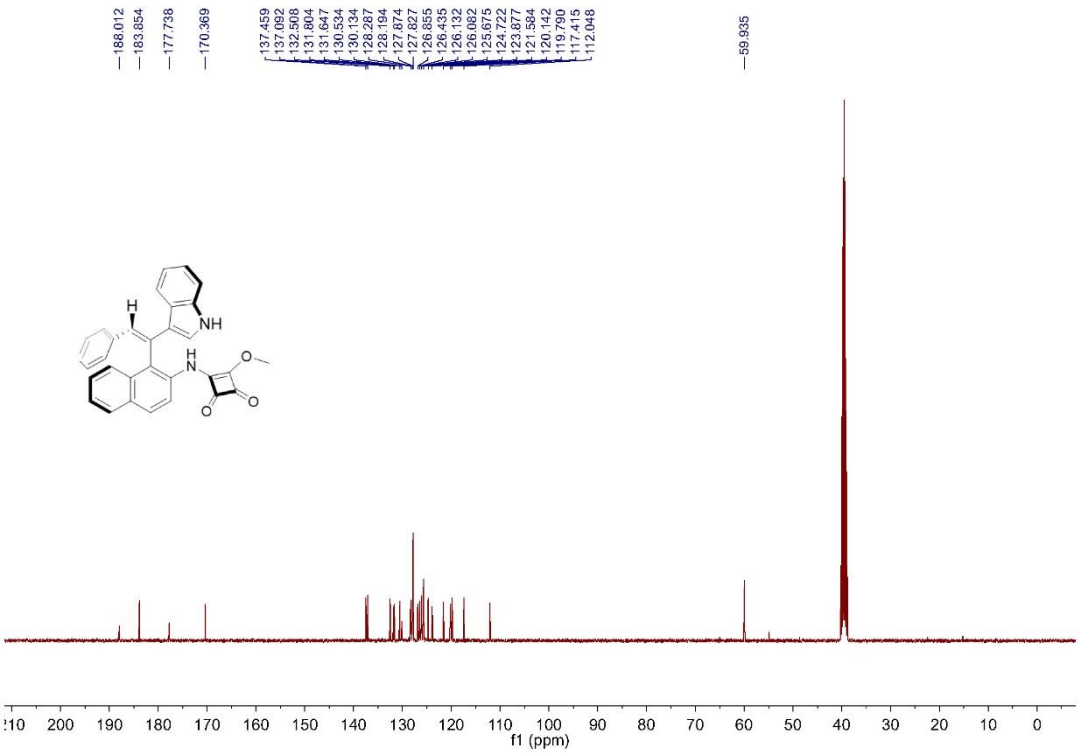
^{13}C NMR spectrum of **S2** in $CDCl_3$, 101 MHz



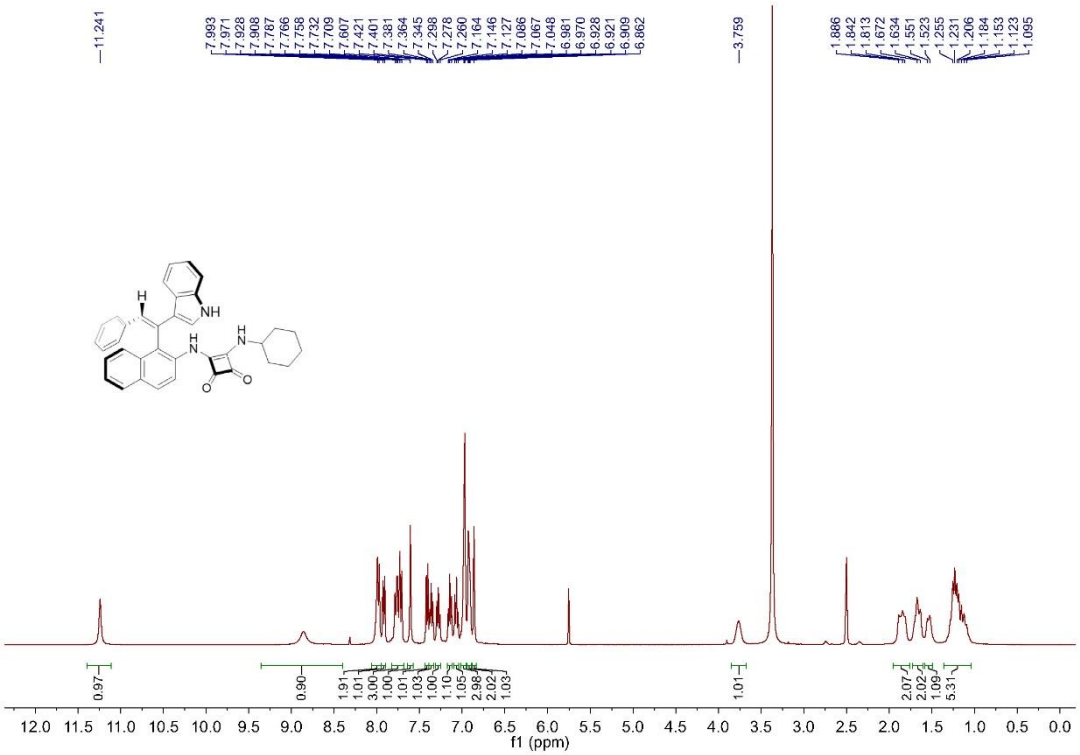
^{1}H NMR spectrum of **S3** in DMSO, 400 MHz



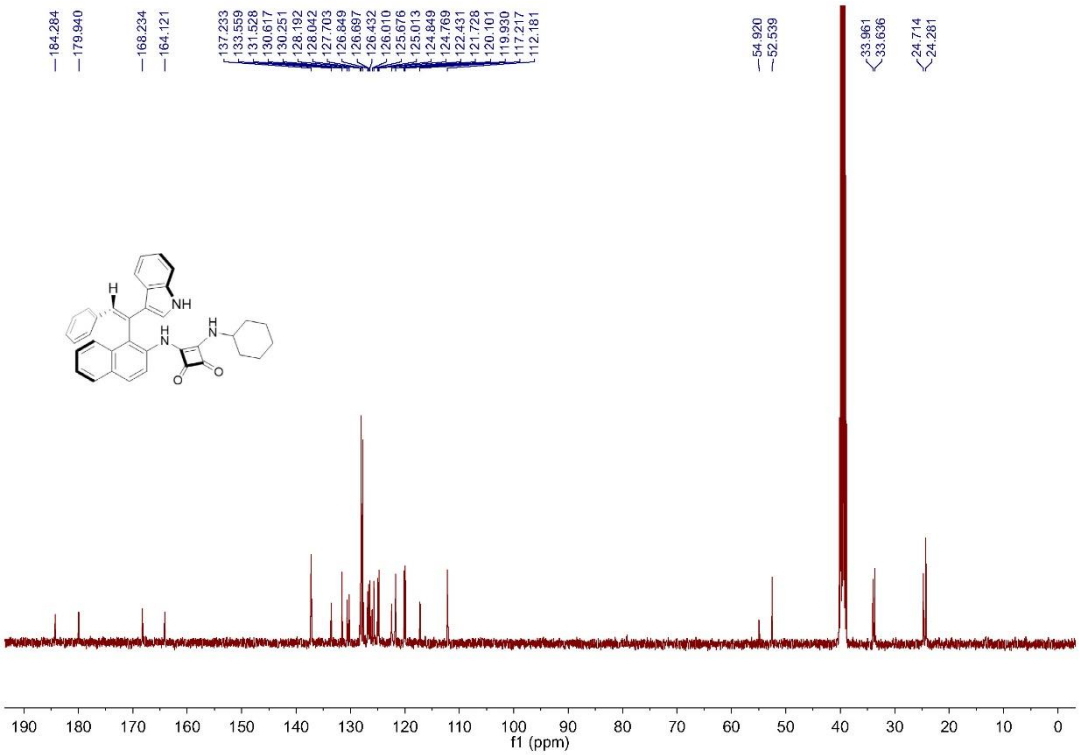
^{13}C NMR spectrum of **S3** in DMSO, 101 MHz



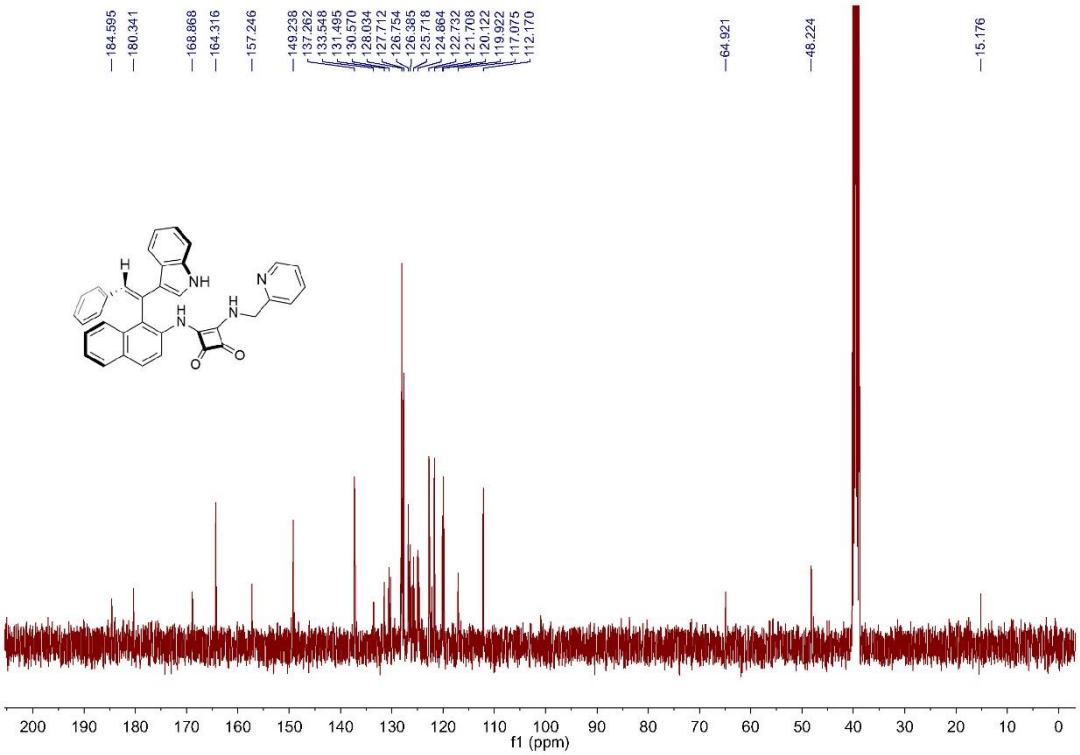
^{1}H NMR spectrum of **Cat. I** in DMSO, 400 MHz



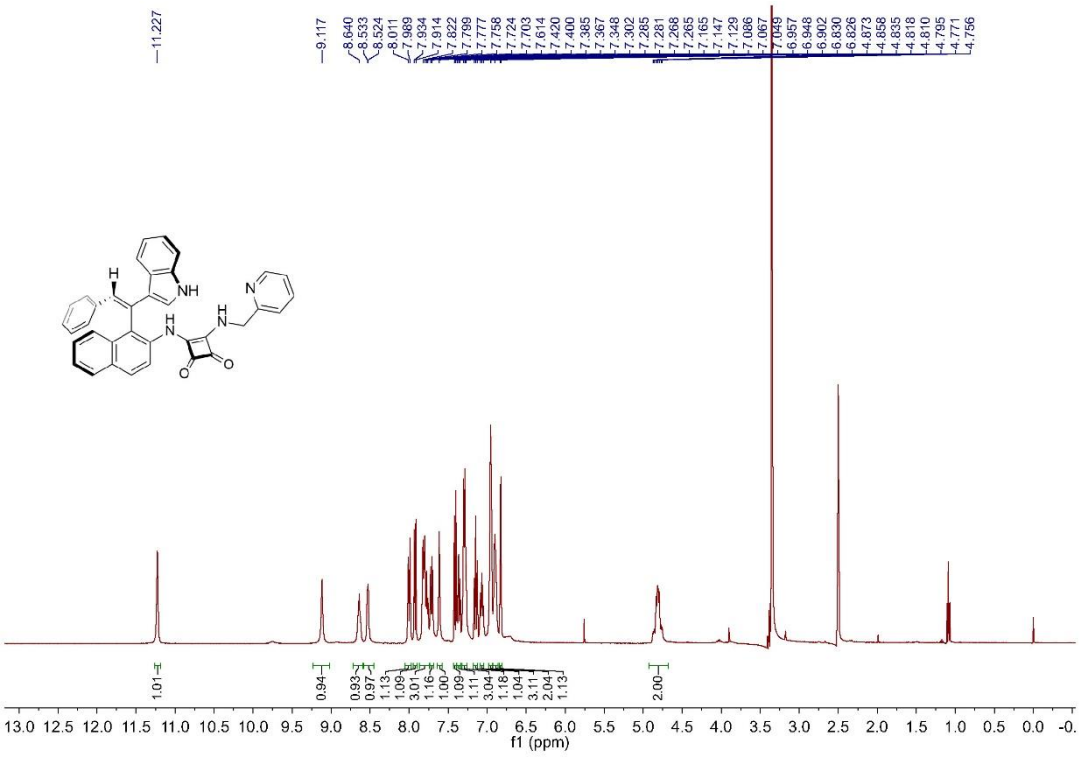
^{13}C NMR spectrum of **Cat. I** in DMSO, 101 MHz



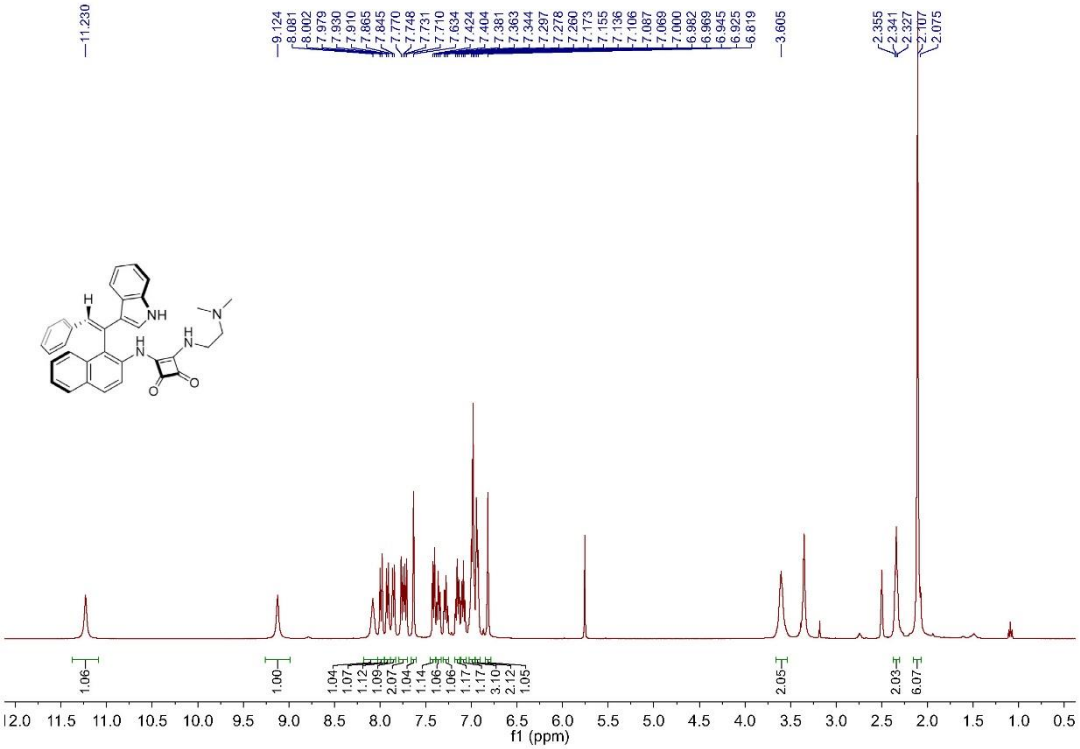
^{1}H NMR spectrum of **Cat. II** in DMSO, 400 MHz



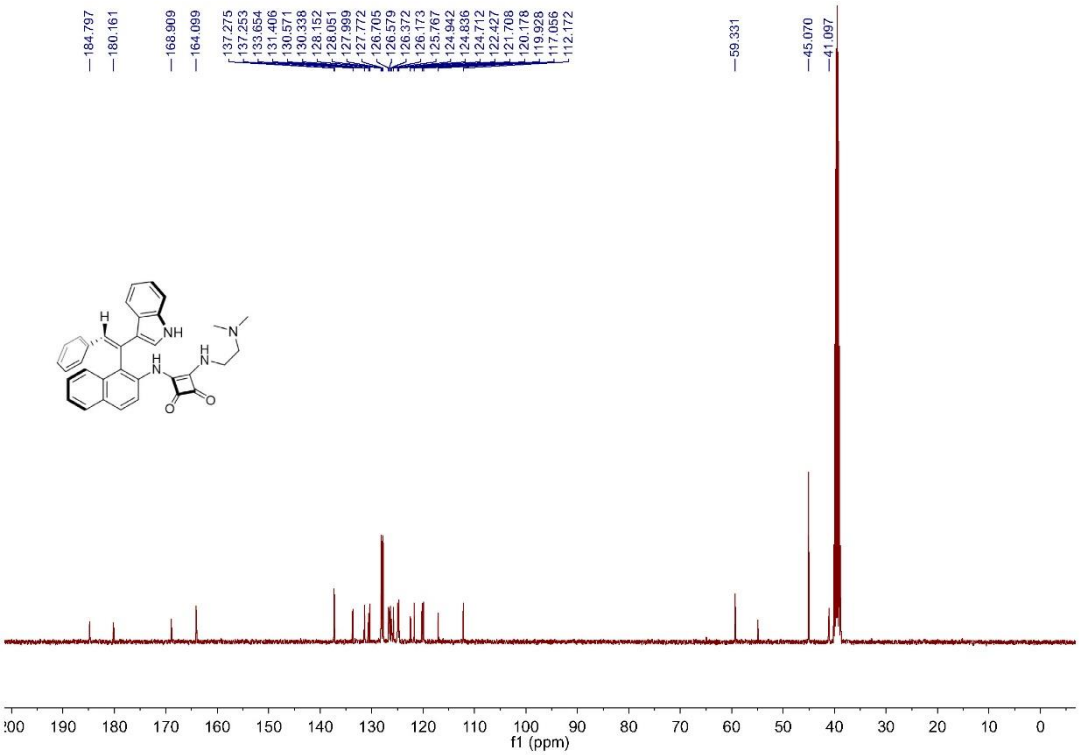
^{13}C NMR spectrum of **Cat. II** in DMSO, 101 MHz



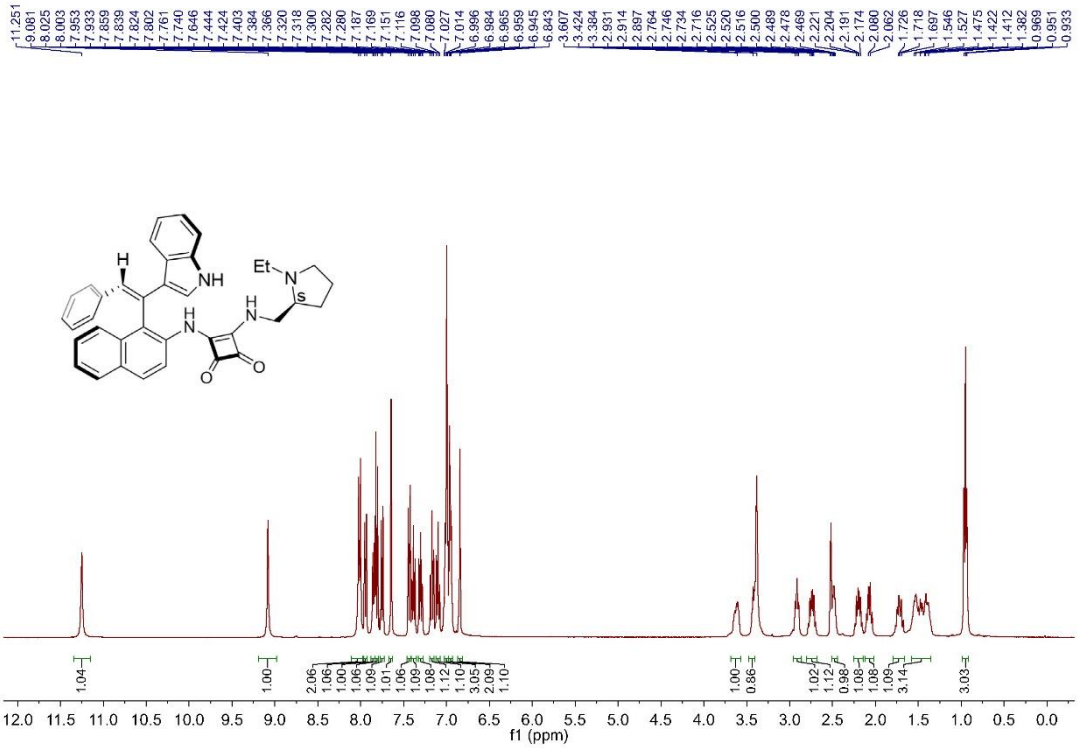
^{1}H NMR spectrum of **Cat. III** in DMSO, 400 MHz



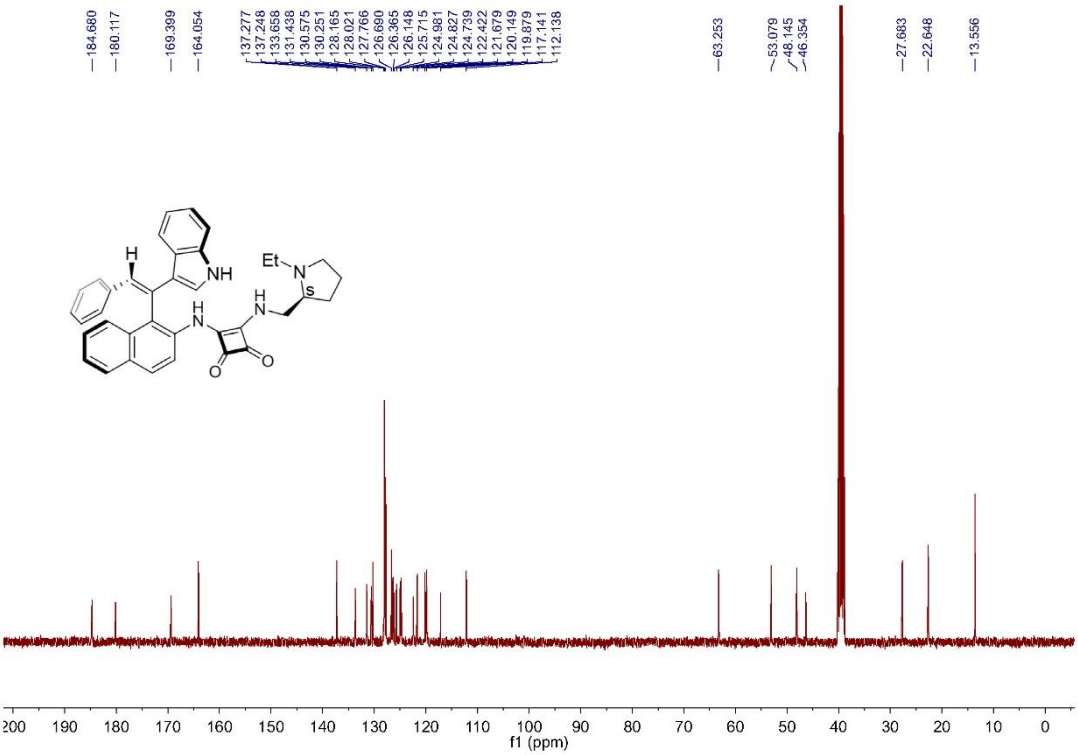
^{13}C NMR spectrum of **Cat. III** in DMSO, 101 MHz



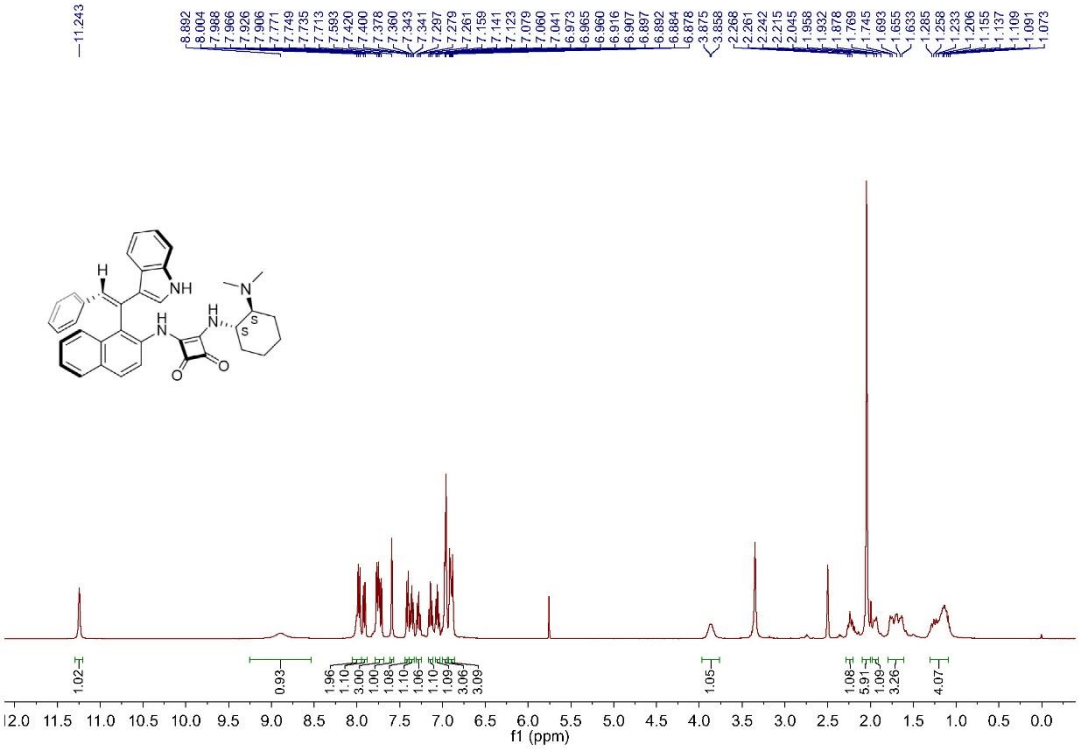
^{1}H NMR spectrum of **Cat. IV** in DMSO, 400 MHz



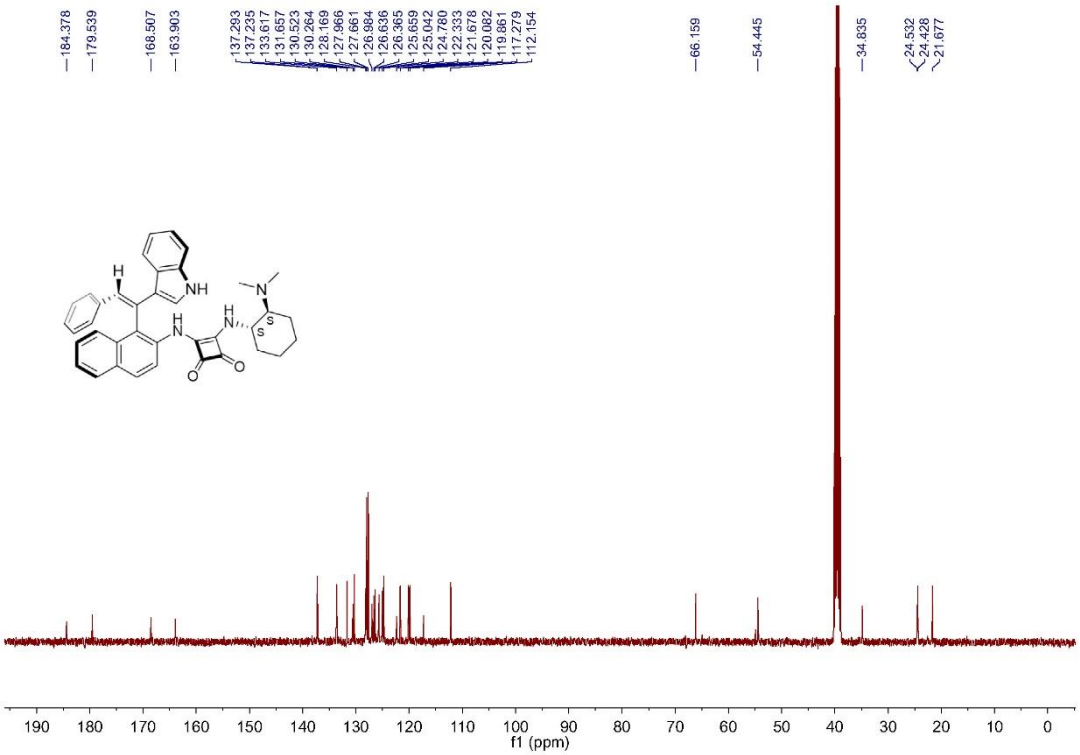
^{13}C NMR spectrum of **Cat. IV** in DMSO, 101 MHz



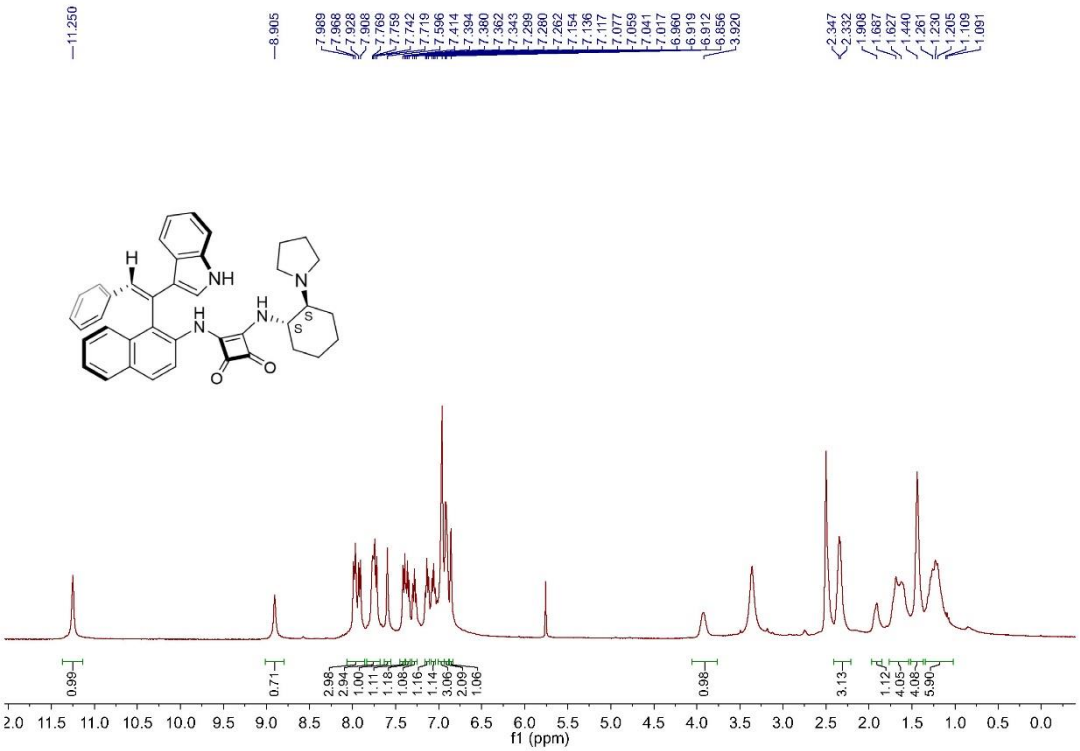
^{1}H NMR spectrum of **Cat. V** in DMSO, 400 MHz



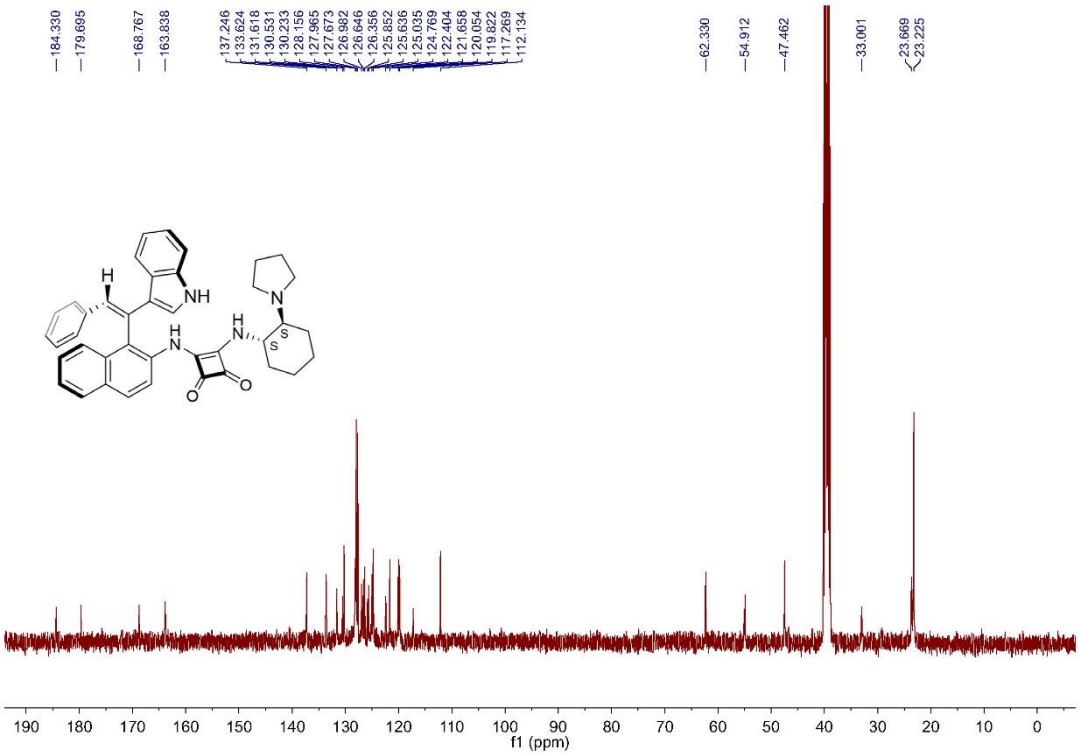
^{13}C NMR spectrum of **Cat. V** in DMSO, 101 MHz



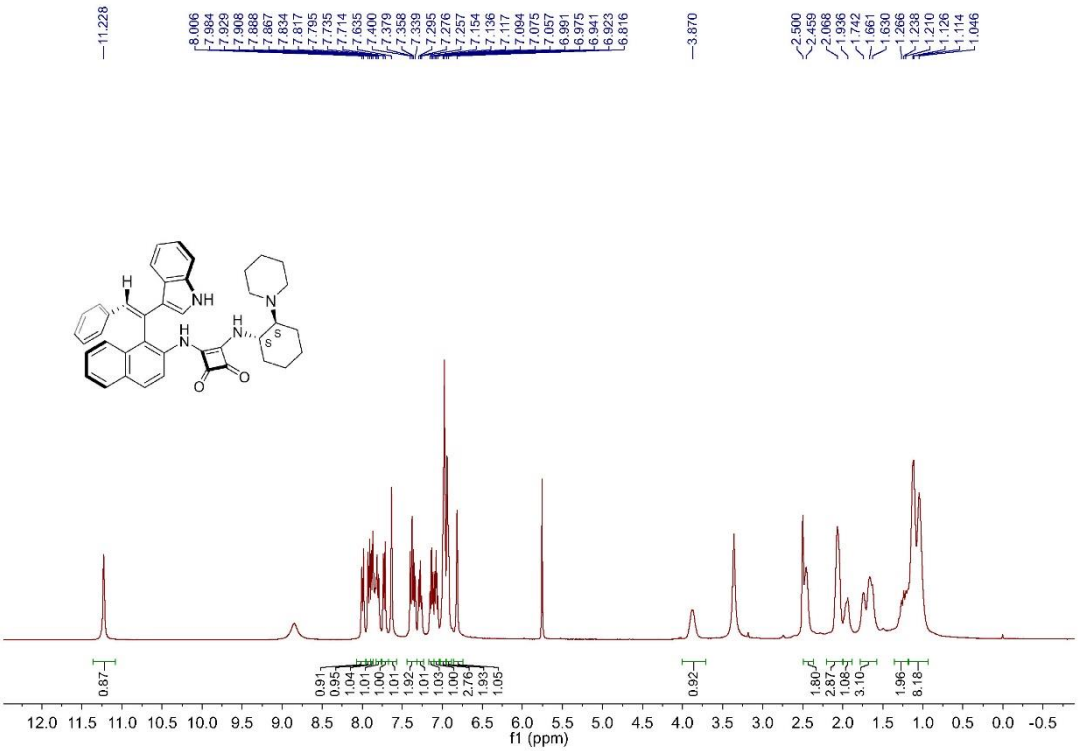
[1]H NMR spectrum of **Cat. VI** in DMSO, 400 MHz



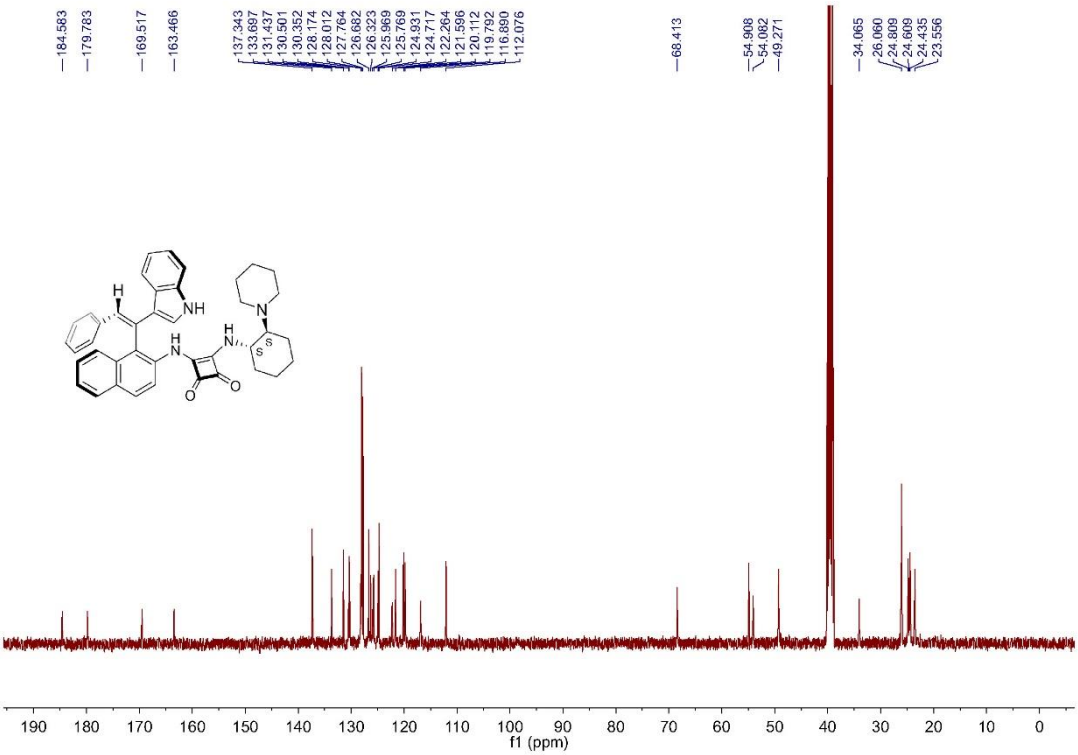
[13]C NMR spectrum of **Cat. VI** in DMSO, 101 MHz



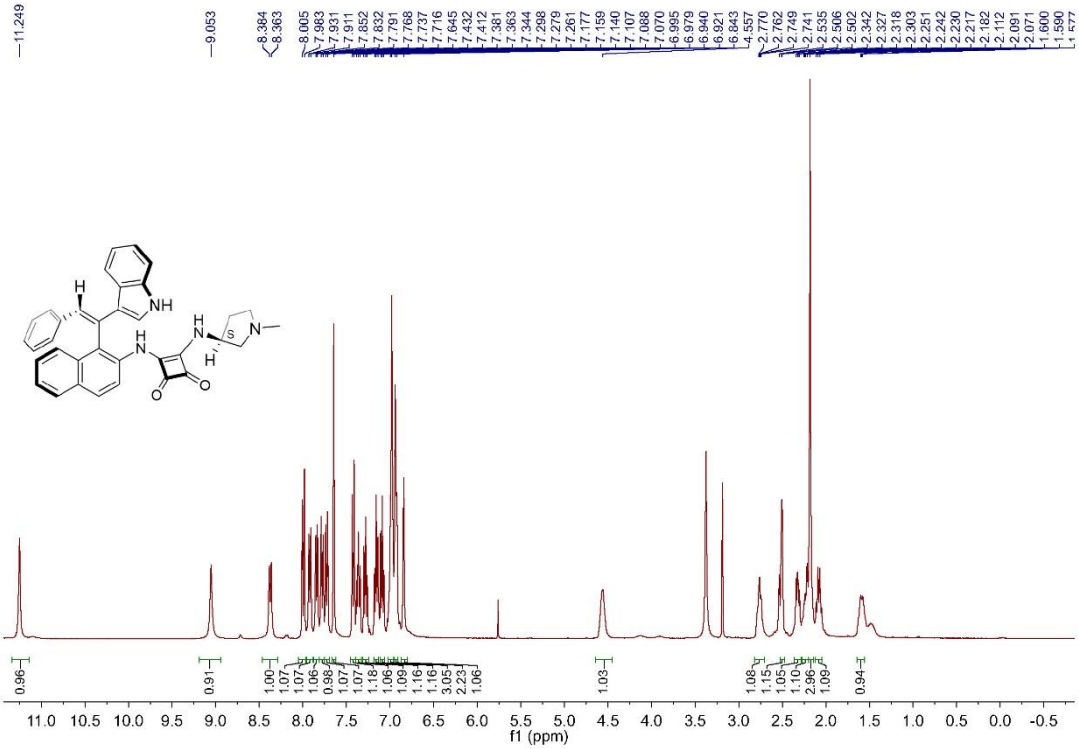
[1]H NMR spectrum of **Cat. VII** in DMSO, 400 MHz



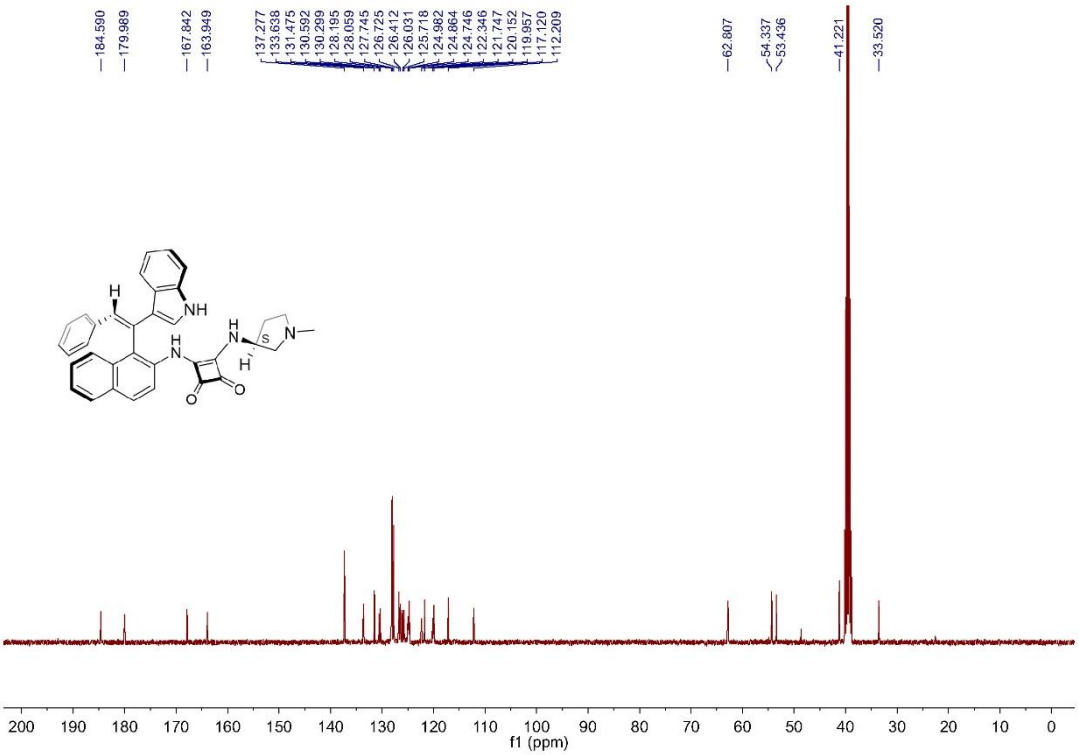
[13]C NMR spectrum of **Cat. VII** in DMSO, 101 MHz



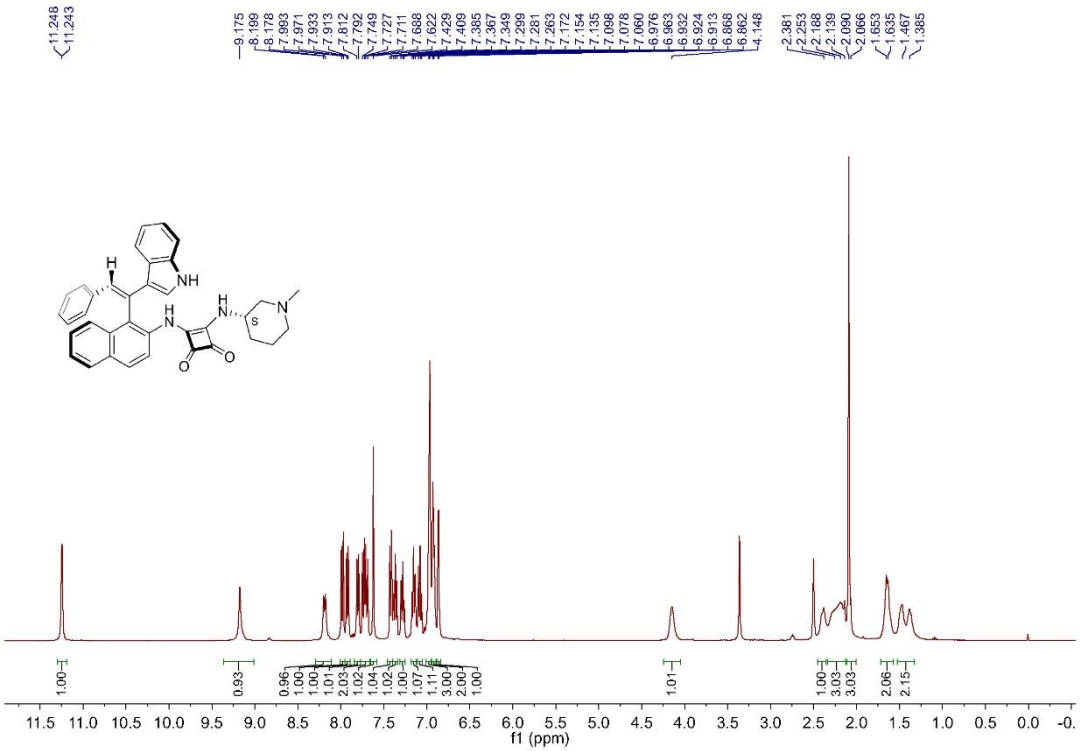
^{1}H NMR spectrum of **Cat. VIII** in DMSO, 400 MHz



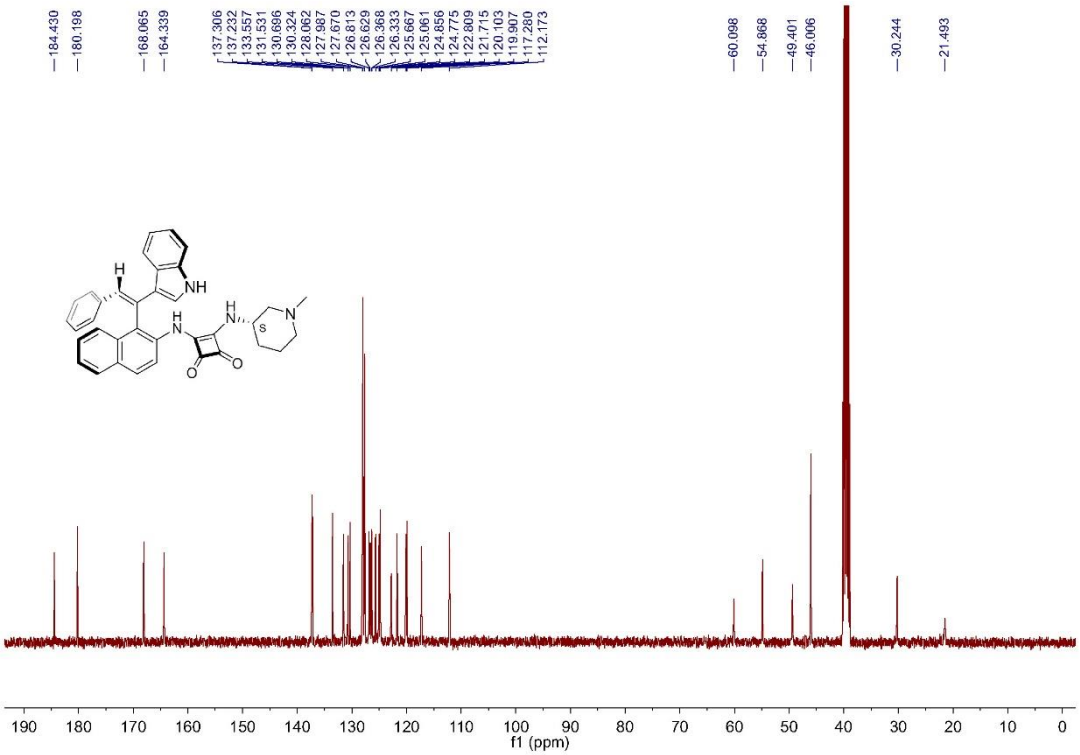
^{13}C NMR spectrum of **Cat. VIII** in DMSO, 101 MHz



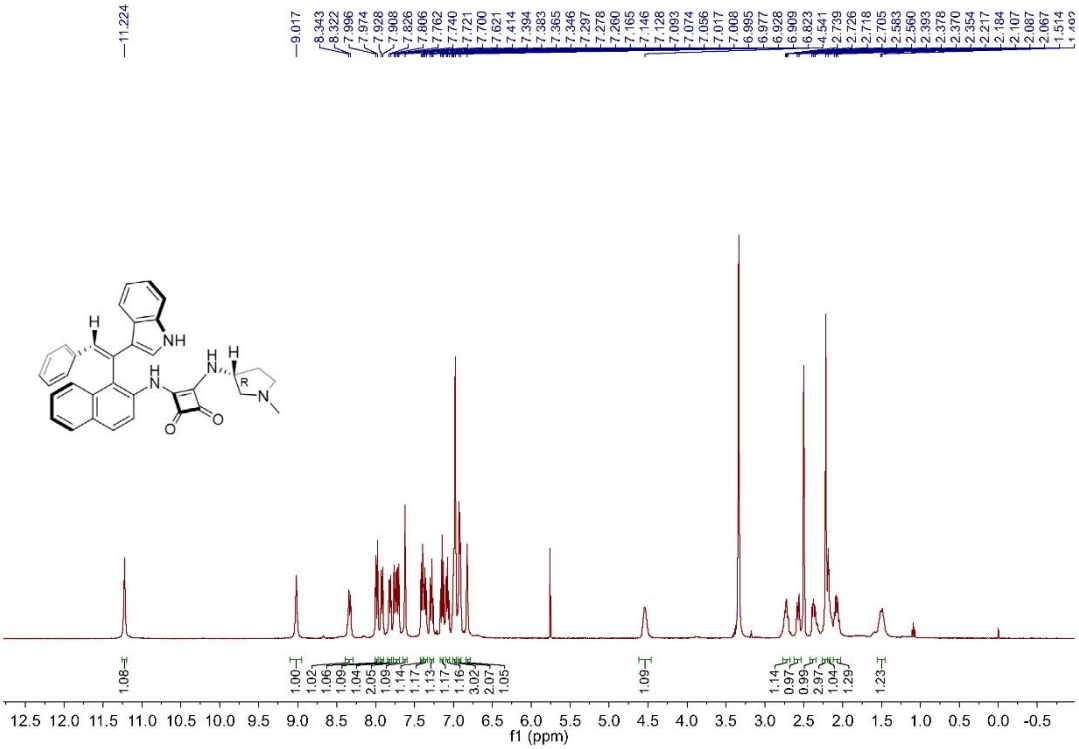
^{1}H NMR spectrum of **Cat. IX** in DMSO, 400 MHz



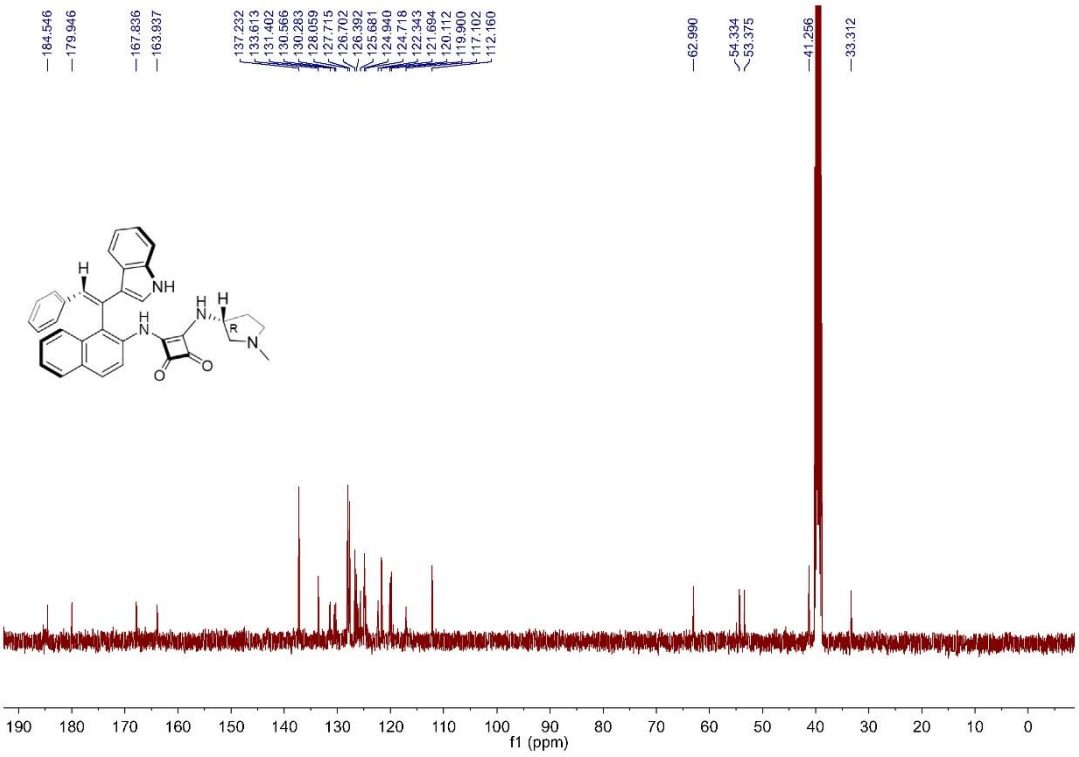
^{13}C NMR spectrum of **Cat. IX** in DMSO, 101 MHz



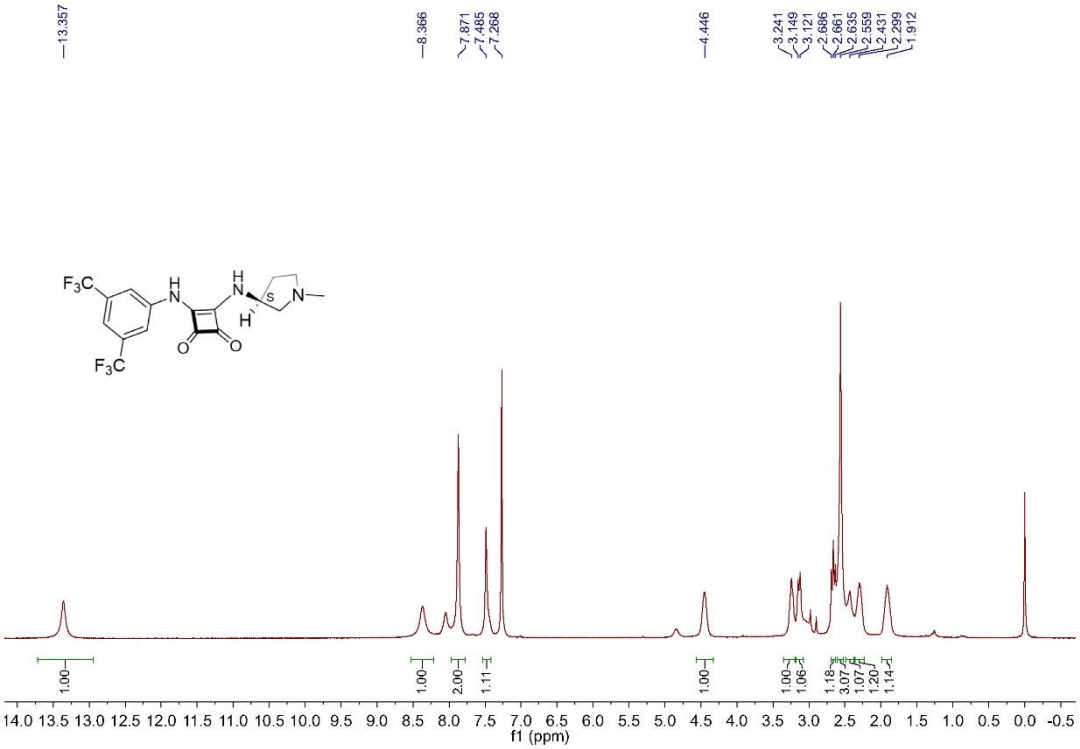
^{1}H NMR spectrum of **Cat. X** in DMSO, 400 MHz



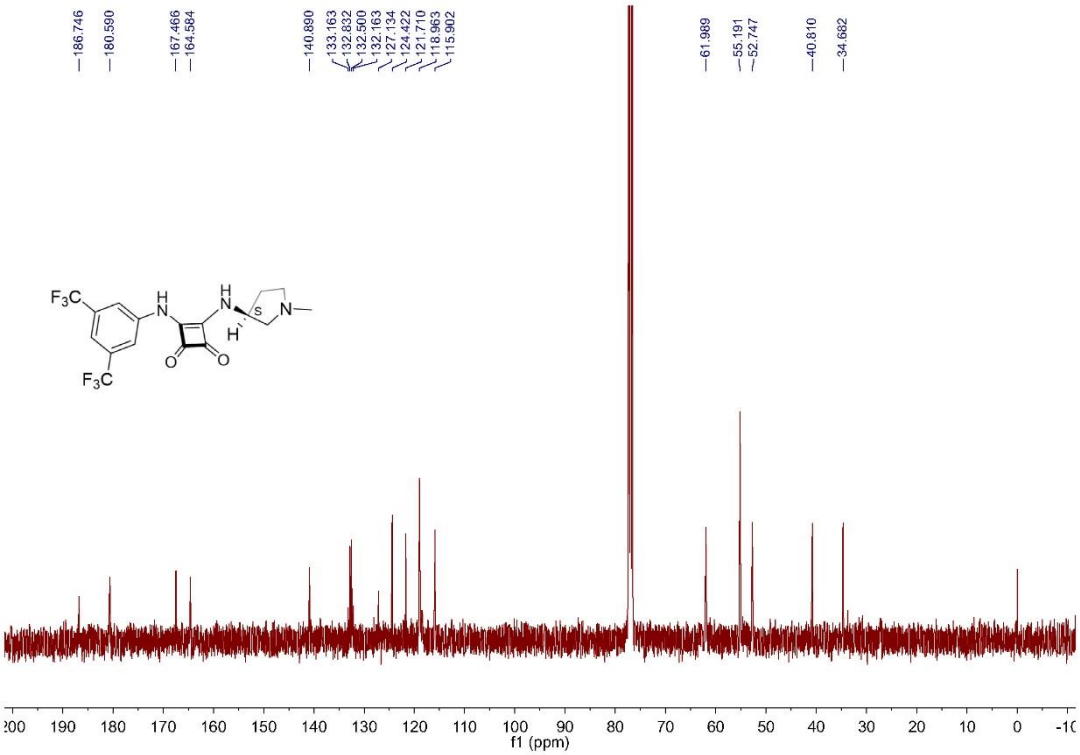
^{13}C NMR spectrum of **Cat. X** in DMSO, 101 MHz



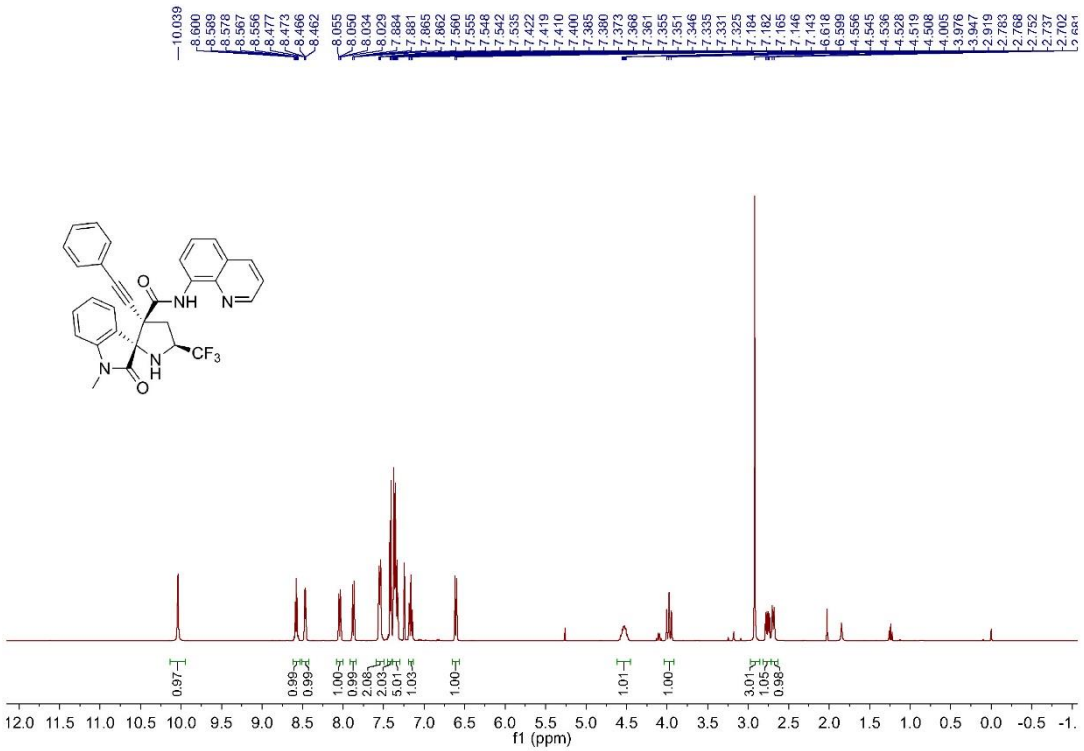
^{1}H NMR spectrum of **Cat. XI** in $CDCl_3$, 400 MHz



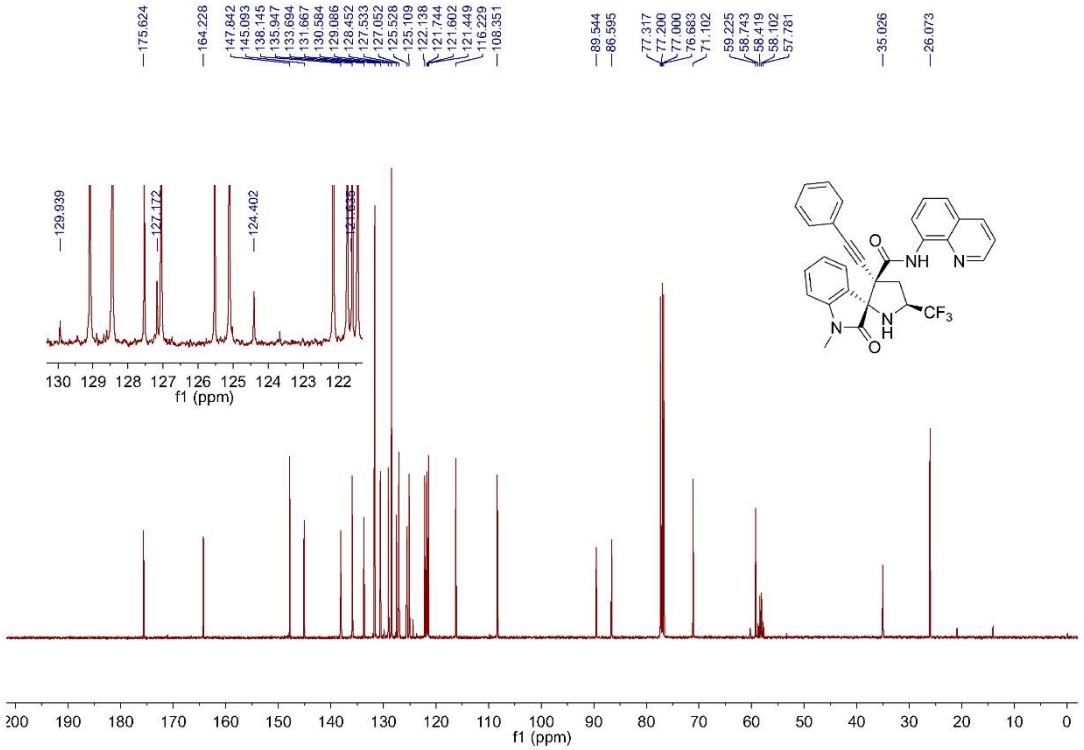
^{13}C NMR spectrum of **Cat. XI** in $CDCl_3$, 101 MHz



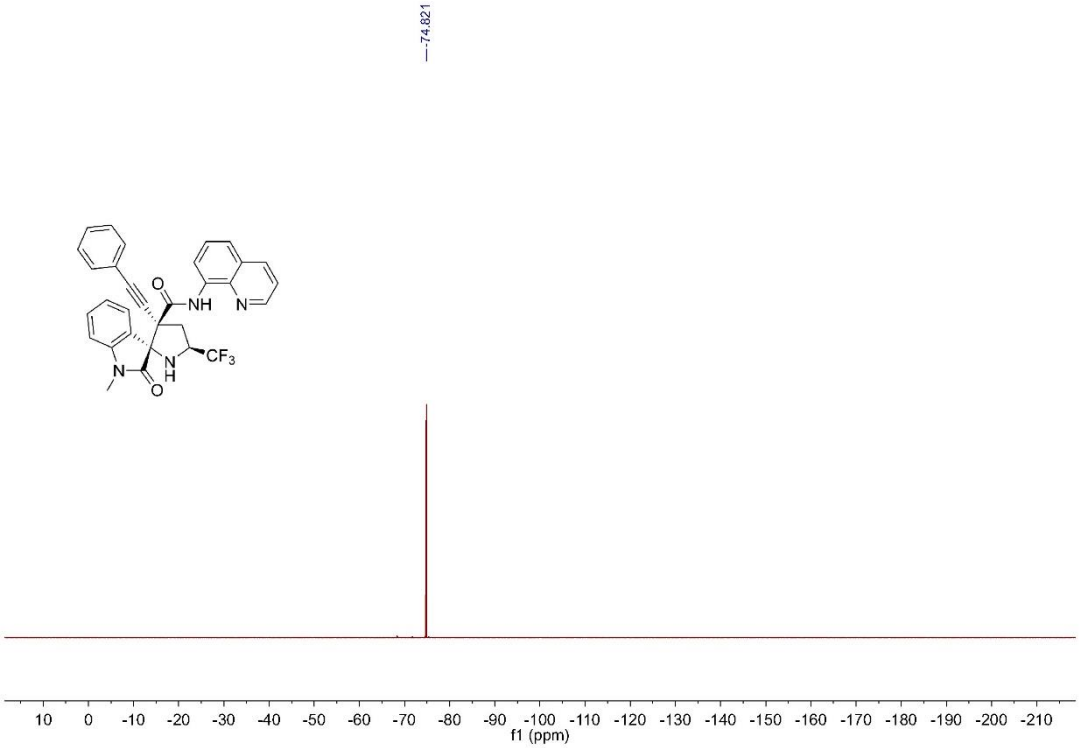
^{1}H NMR spectrum of **3aa** in $CDCl_3$, 400 MHz



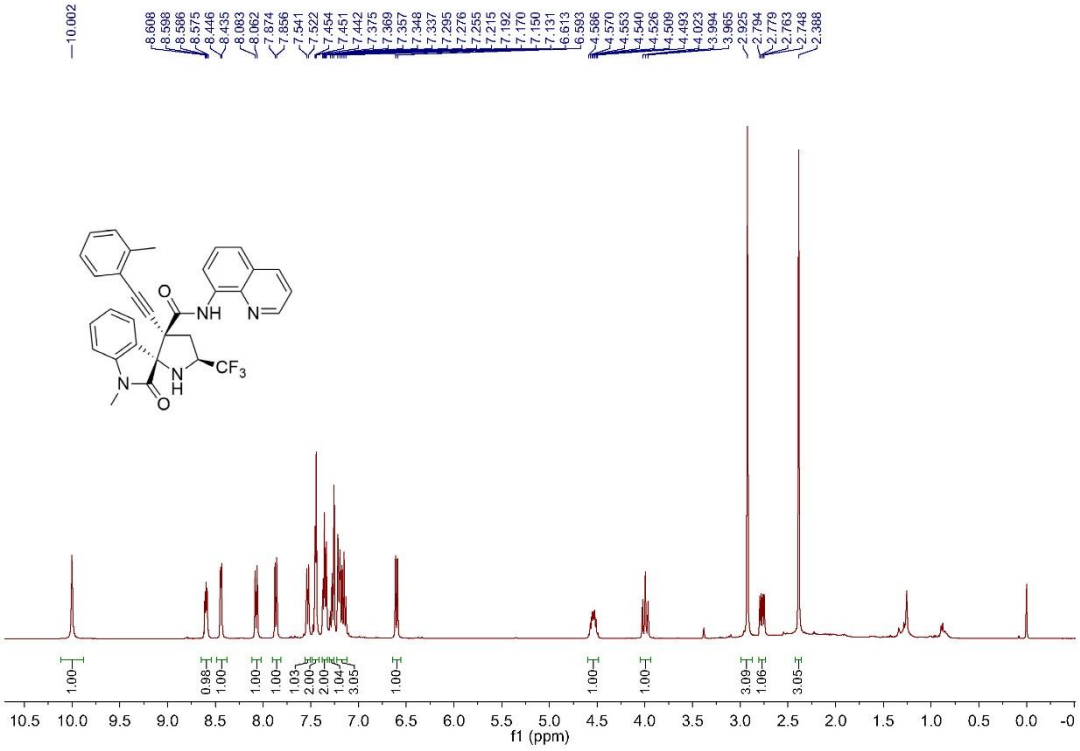
^{13}C NMR spectrum of **3aa** in $CDCl_3$, 101 MHz



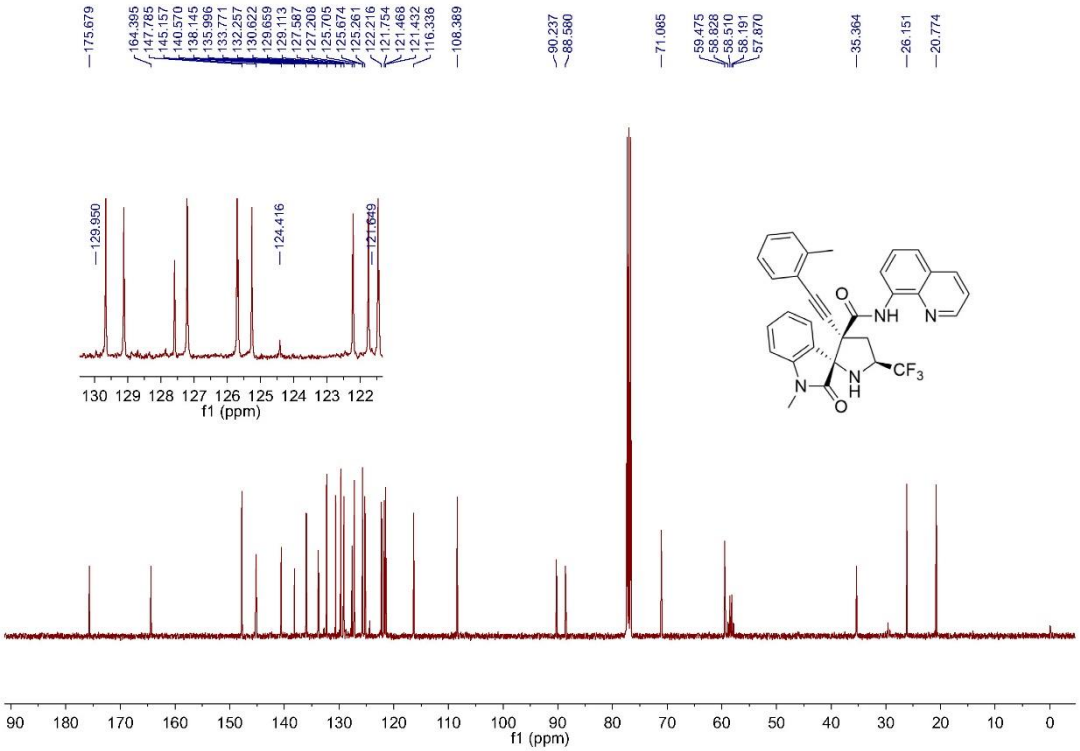
^{19}F NMR spectrum of **3aa** in $CDCl_3$, 376 MHz



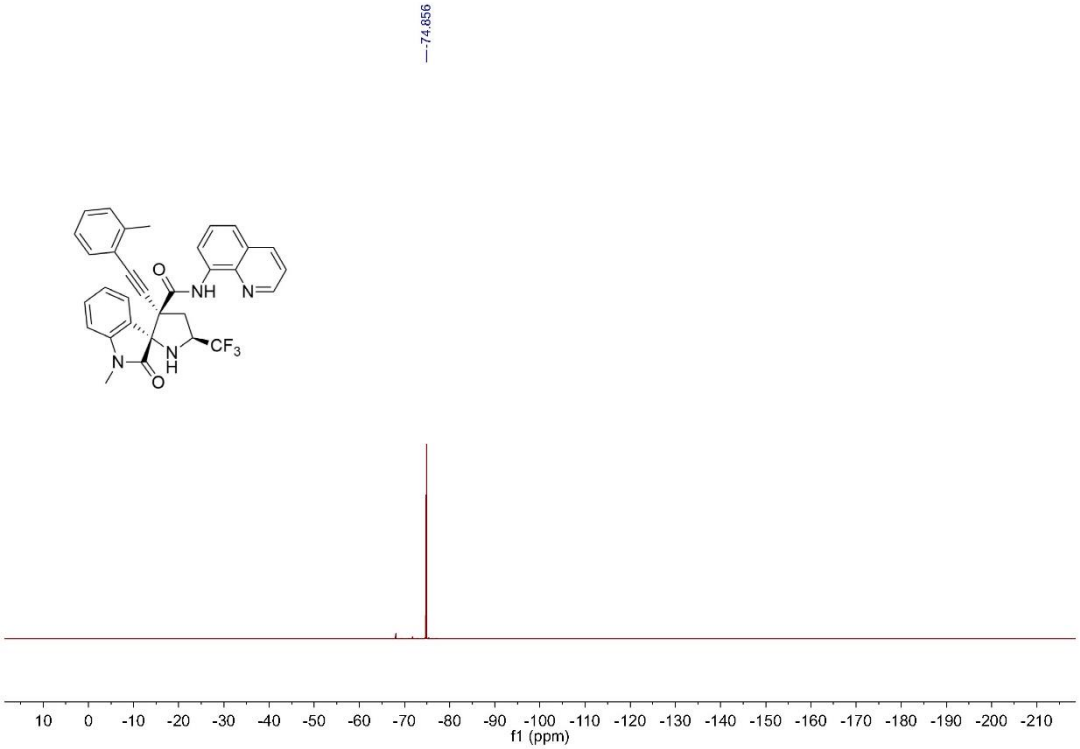
^{1}H NMR spectrum of **3ba** in $CDCl_3$, 400 MHz



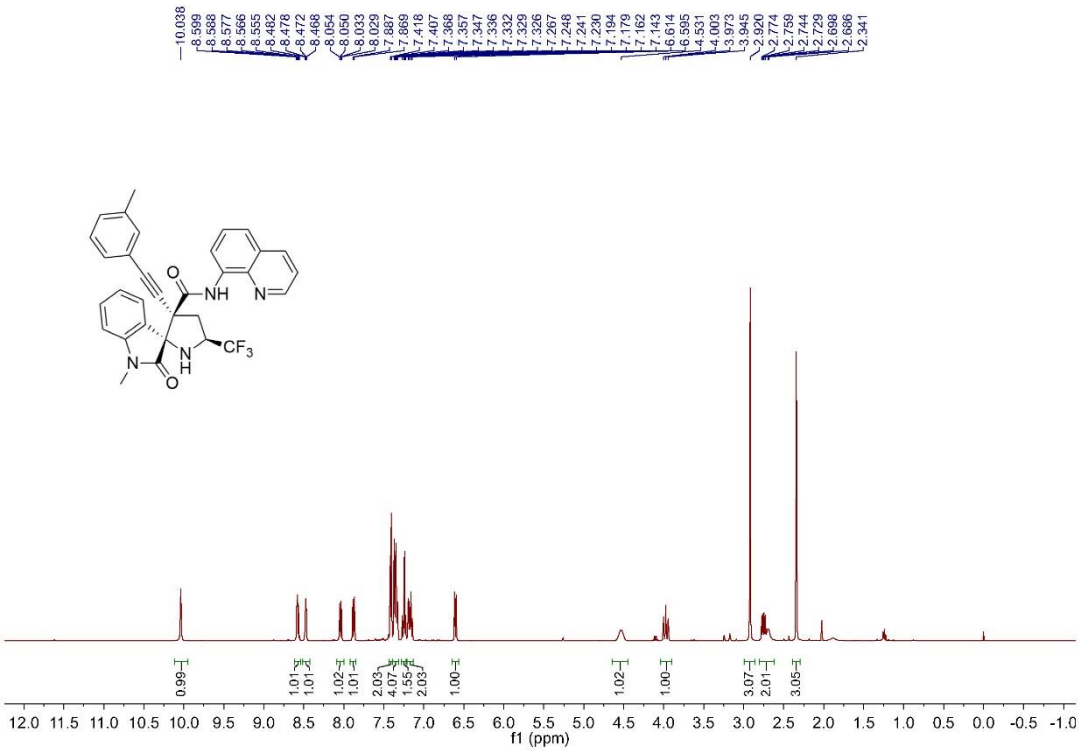
^{13}C NMR spectrum of **3ba** in $CDCl_3$, 101 MHz



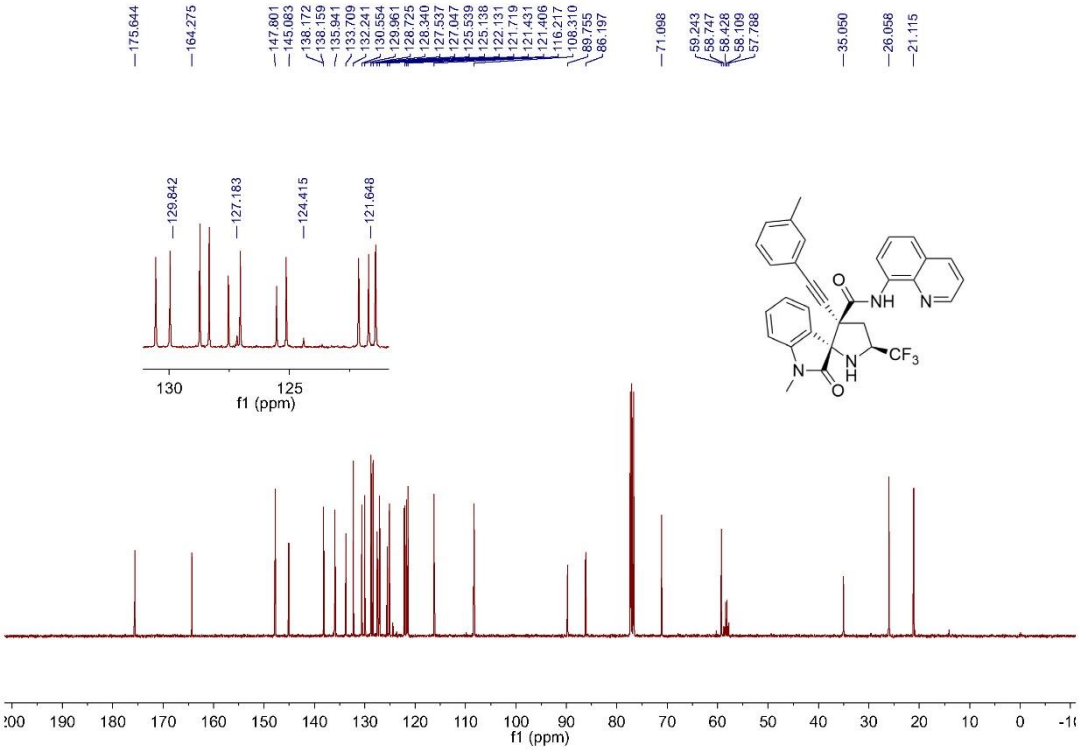
^{19}F NMR spectrum of **3ba** in $CDCl_3$, 376 MHz



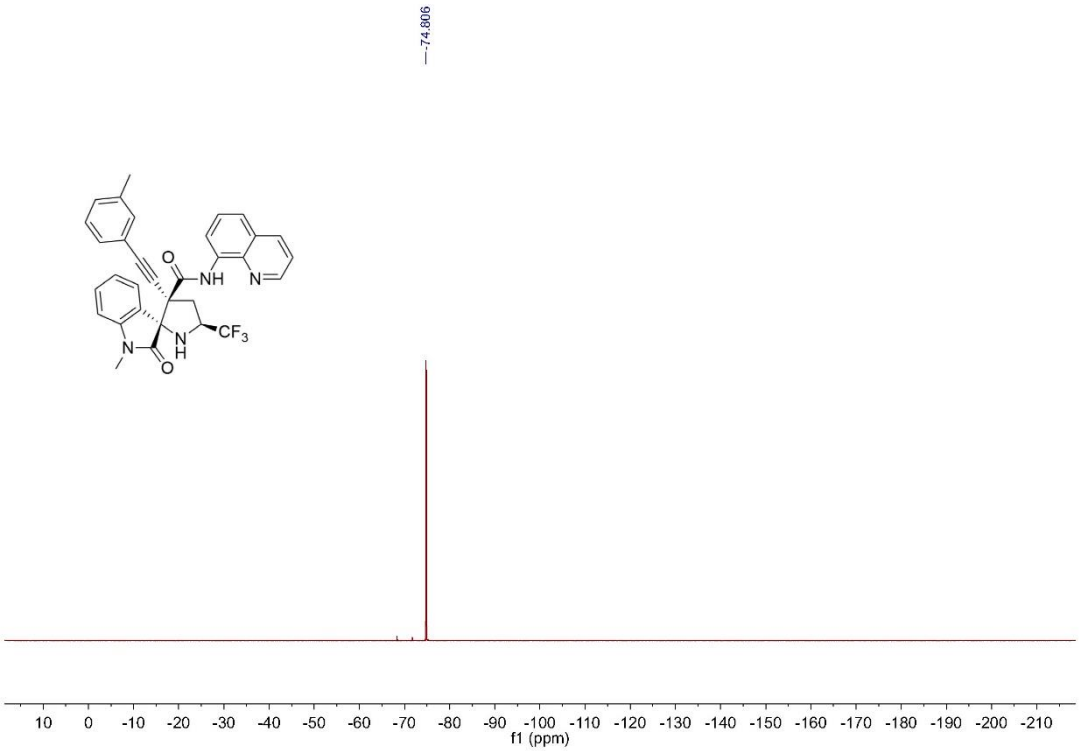
^{1}H NMR spectrum of **3ca** in $CDCl_3$, 400 MHz



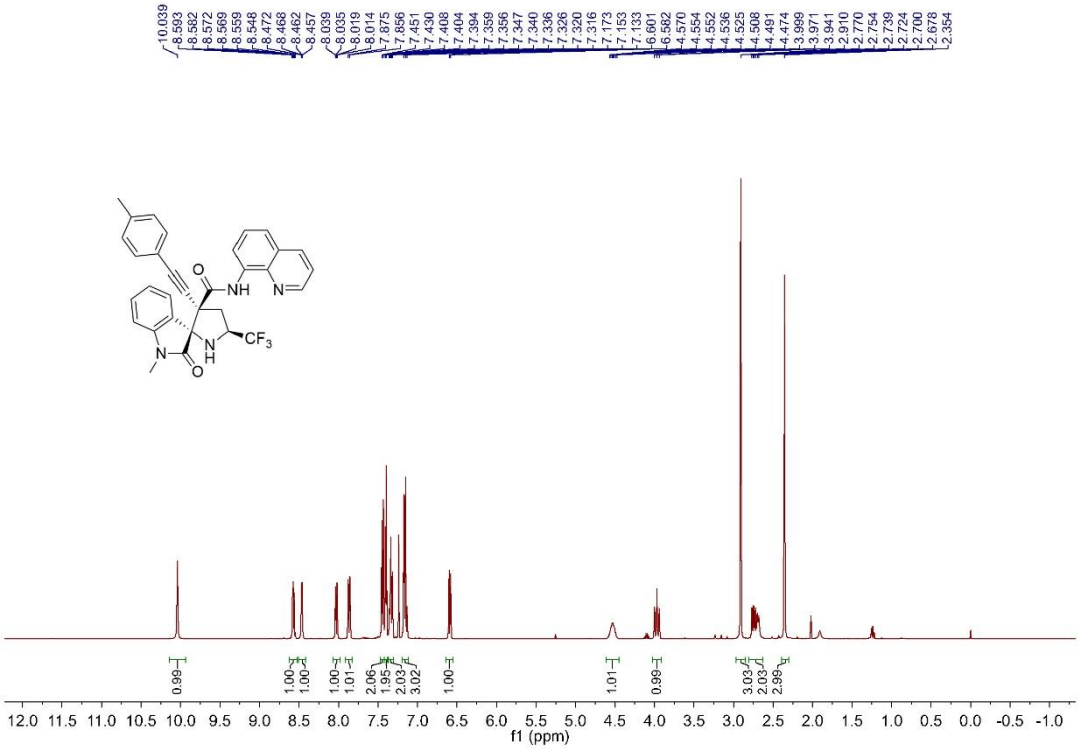
^{13}C NMR spectrum of **3ca** in $CDCl_3$, 101 MHz



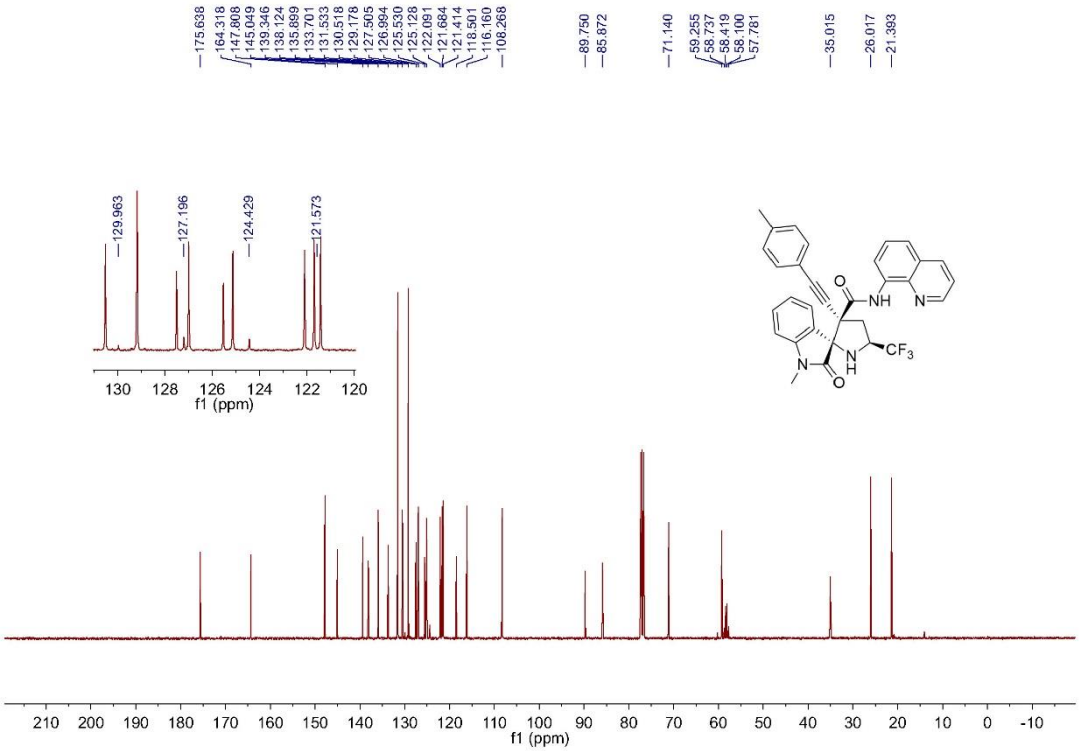
^{19}F NMR spectrum of **3ca** in $CDCl_3$, 376 MHz



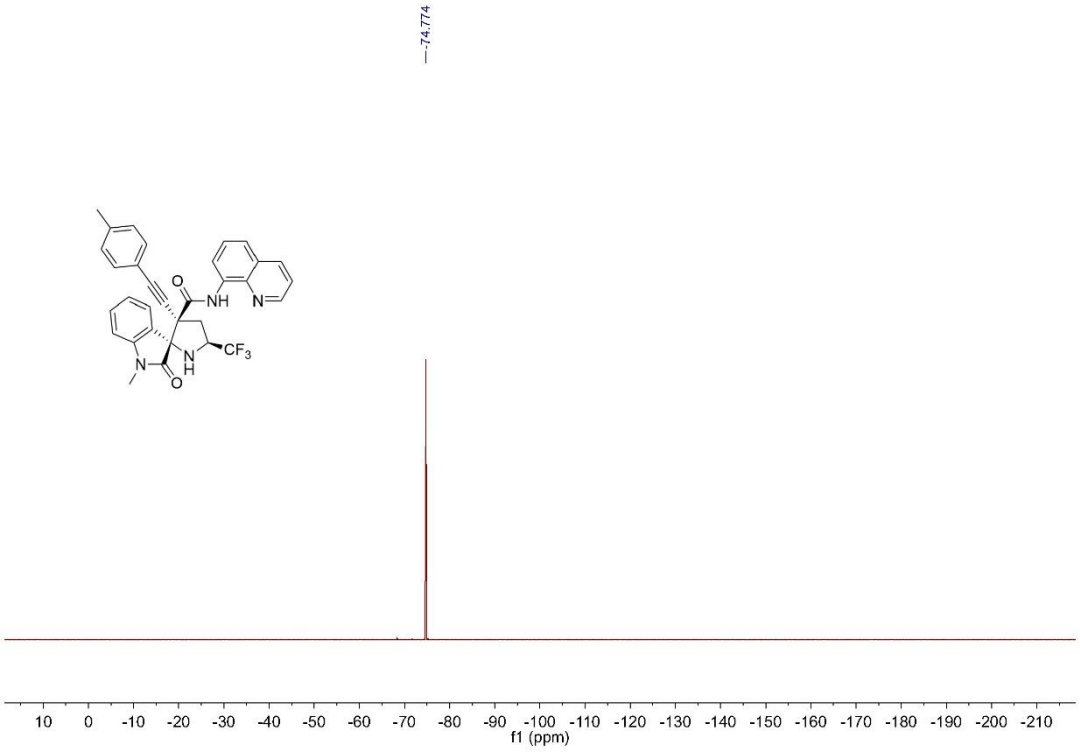
^{1}H NMR spectrum of **3da** in $CDCl_3$, 400 MHz



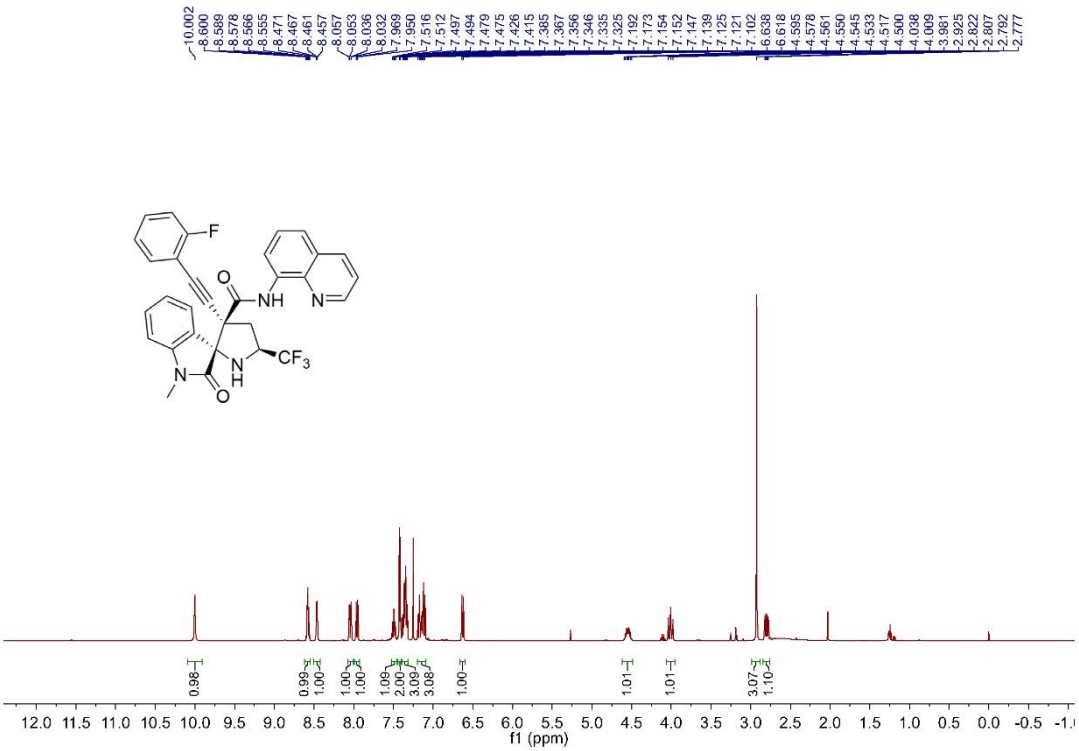
^{13}C NMR spectrum of **3da** in $CDCl_3$, 101 MHz



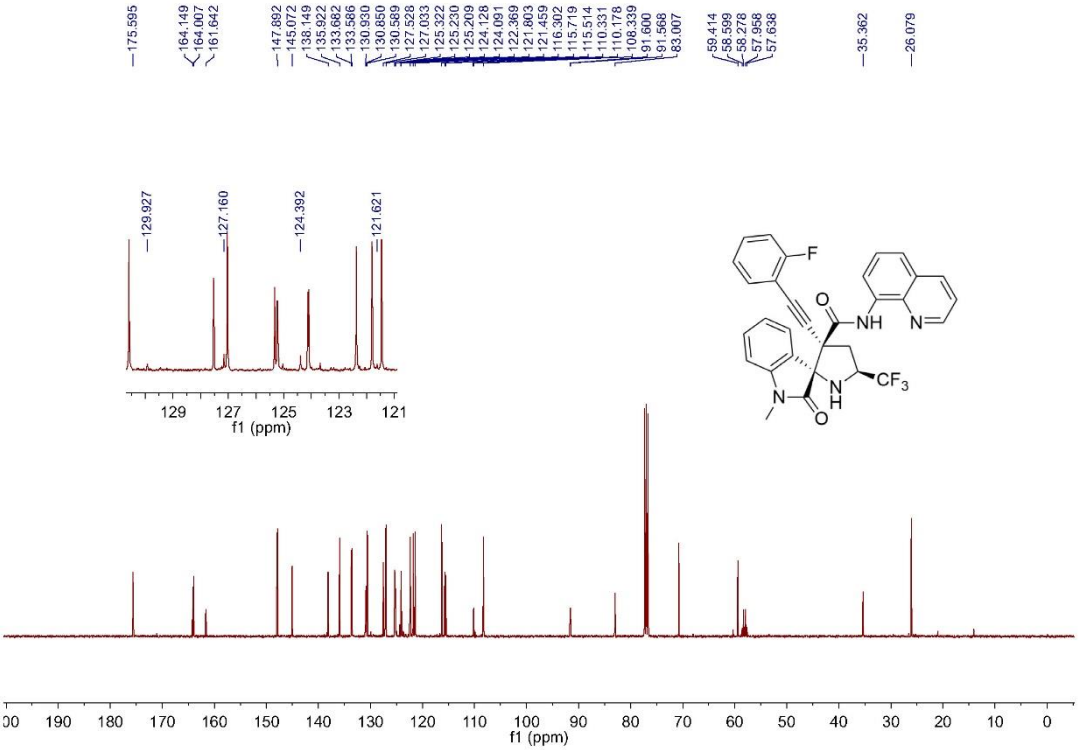
^{19}F NMR spectrum of **3da** in $CDCl_3$, 376 MHz



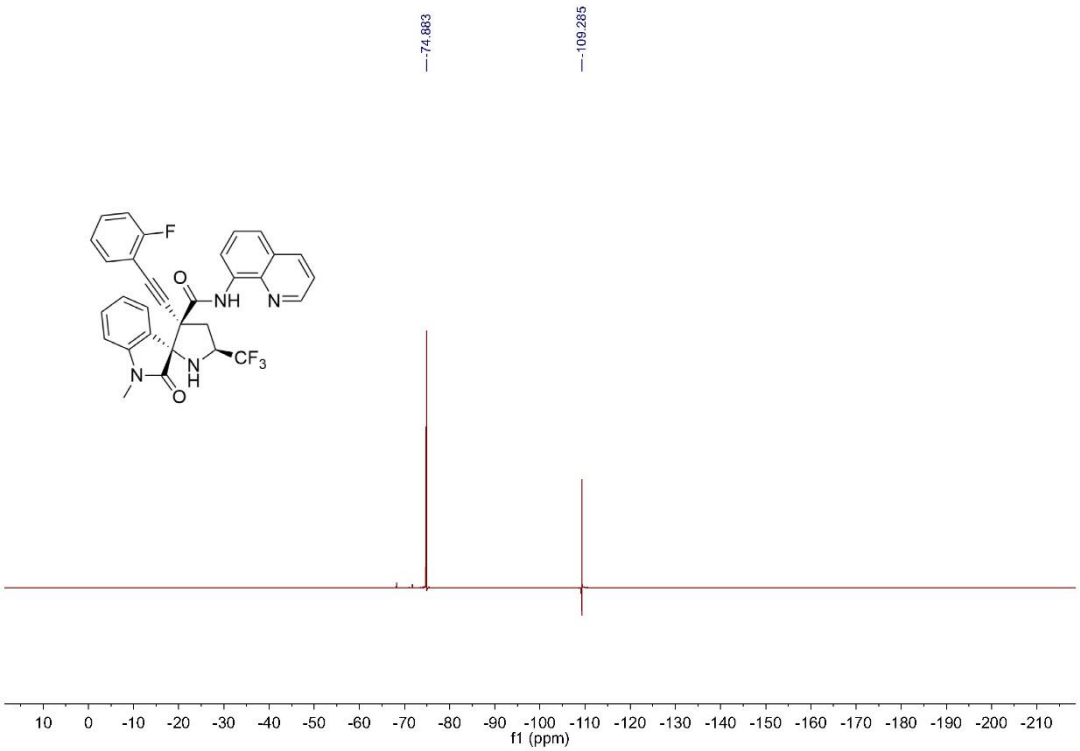
^{1}H NMR spectrum of **3ea** in $CDCl_3$, 400 MHz



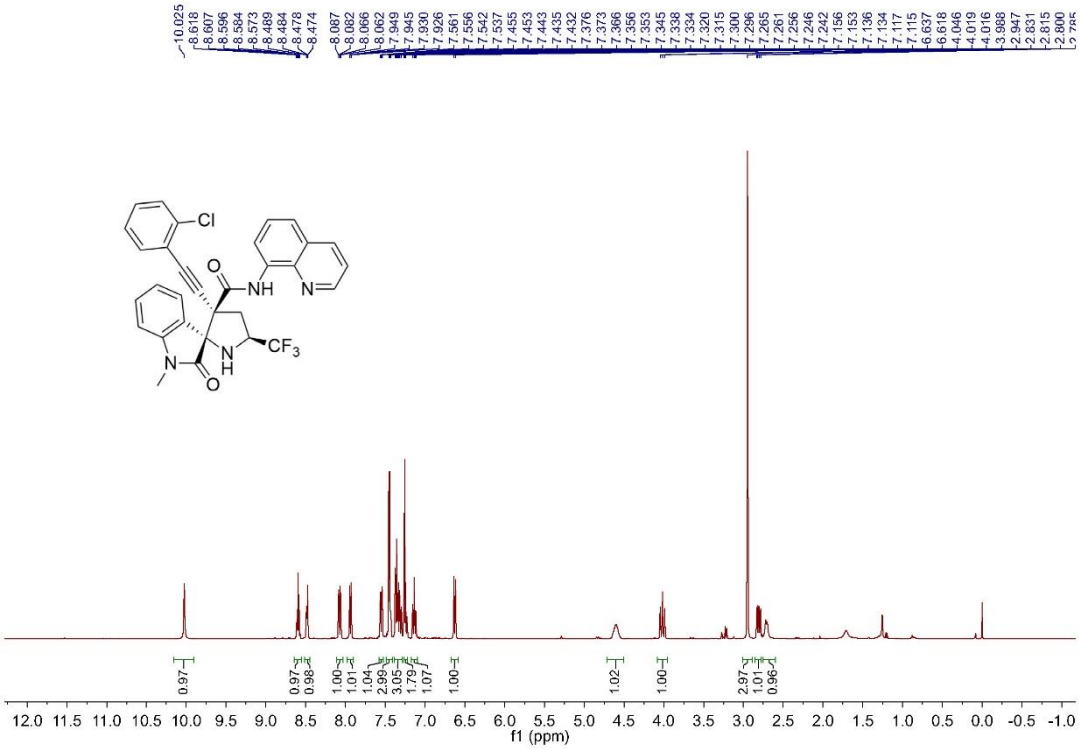
^{13}C NMR spectrum of **3ea** in $CDCl_3$, 101 MHz



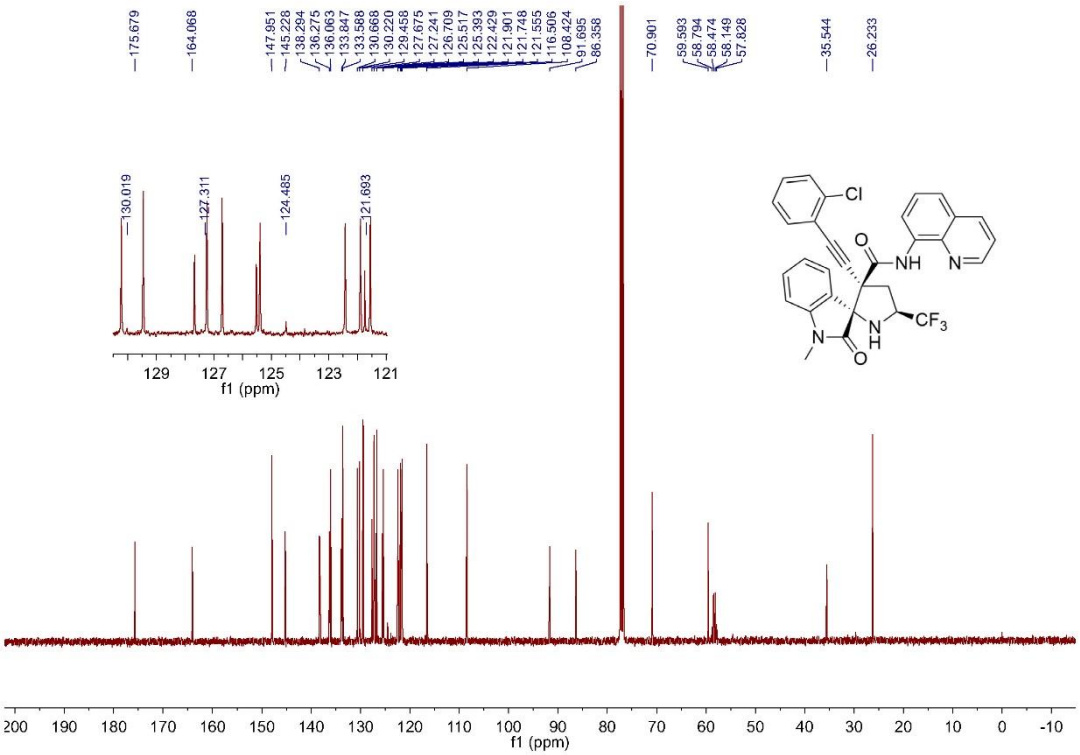
^{19}F NMR spectrum of **3ea** in $CDCl_3$, 376 MHz



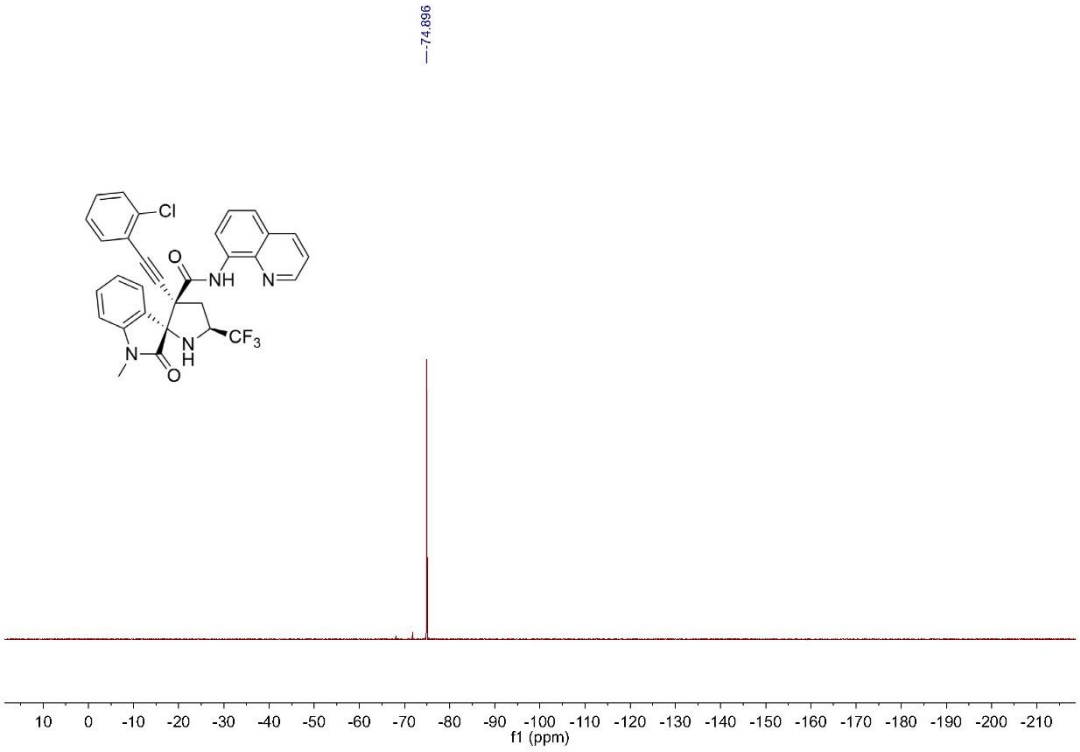
^{1}H NMR spectrum of **3fa** in $CDCl_3$, 400 MHz



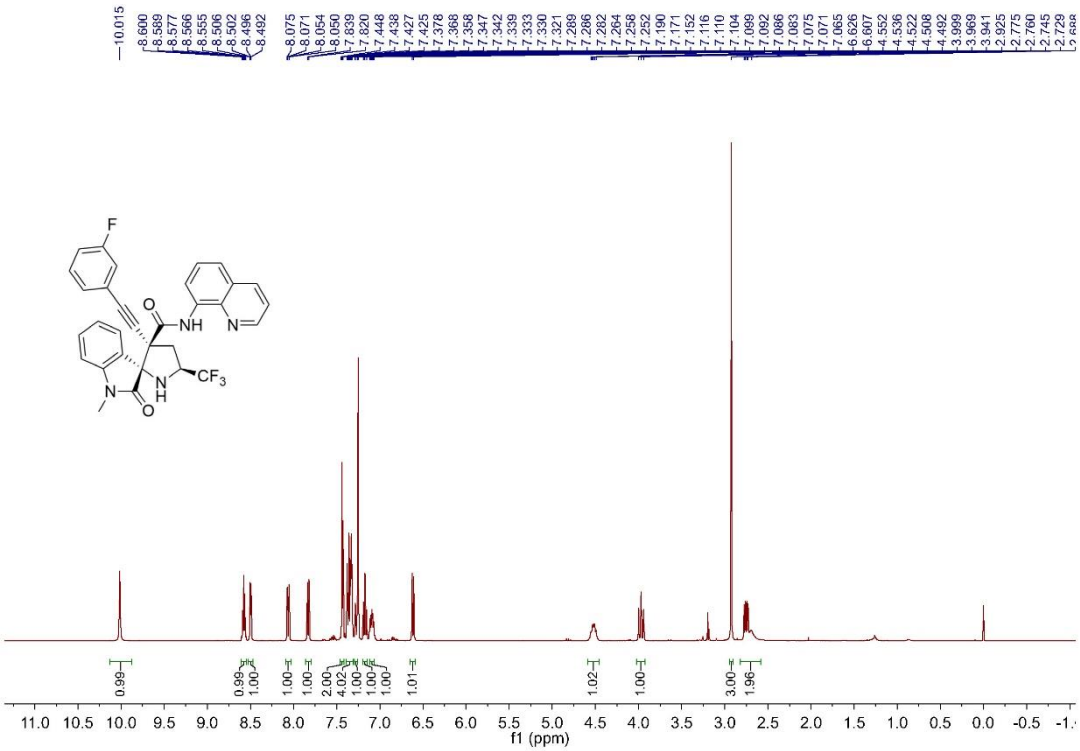
^{13}C NMR spectrum of **3fa** in $CDCl_3$, 101 MHz



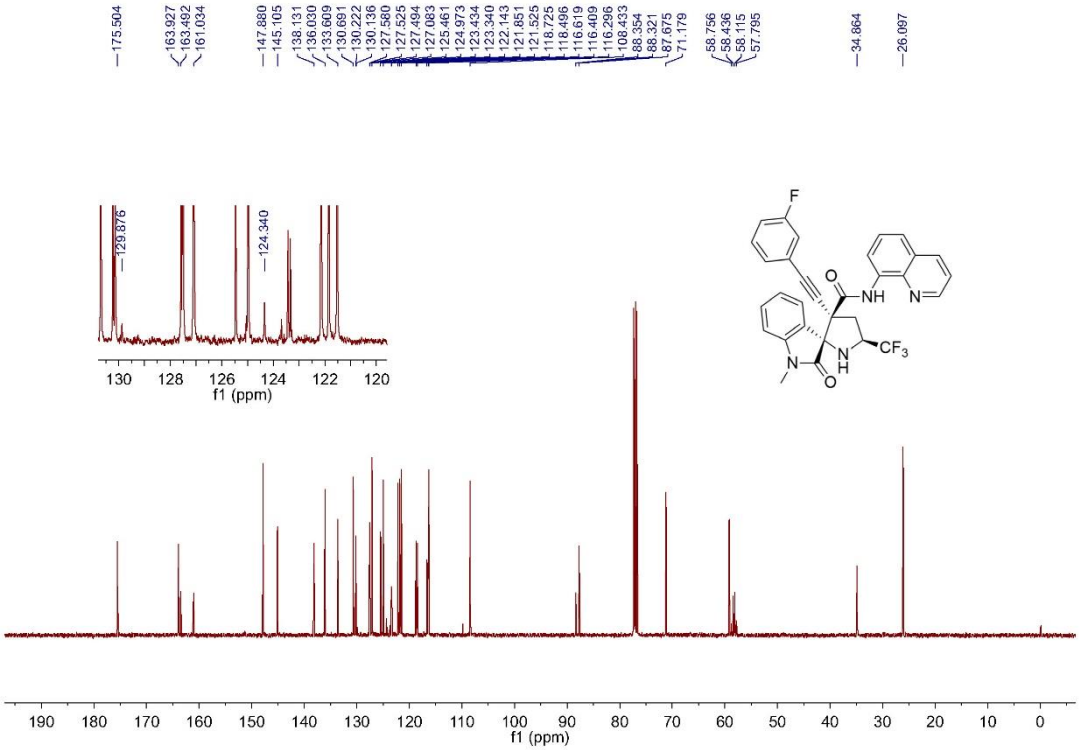
^{19}F NMR spectrum of **3fa** in $CDCl_3$, 376 MHz



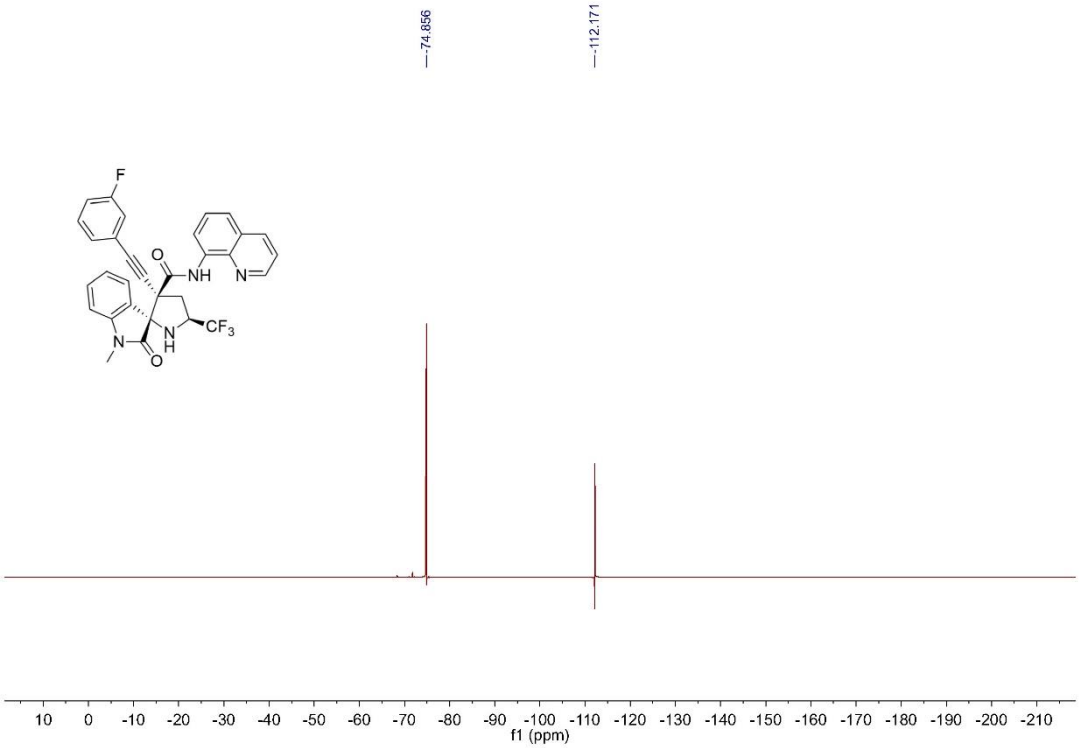
^{1}H NMR spectrum of **3ga** in $CDCl_3$, 400 MHz



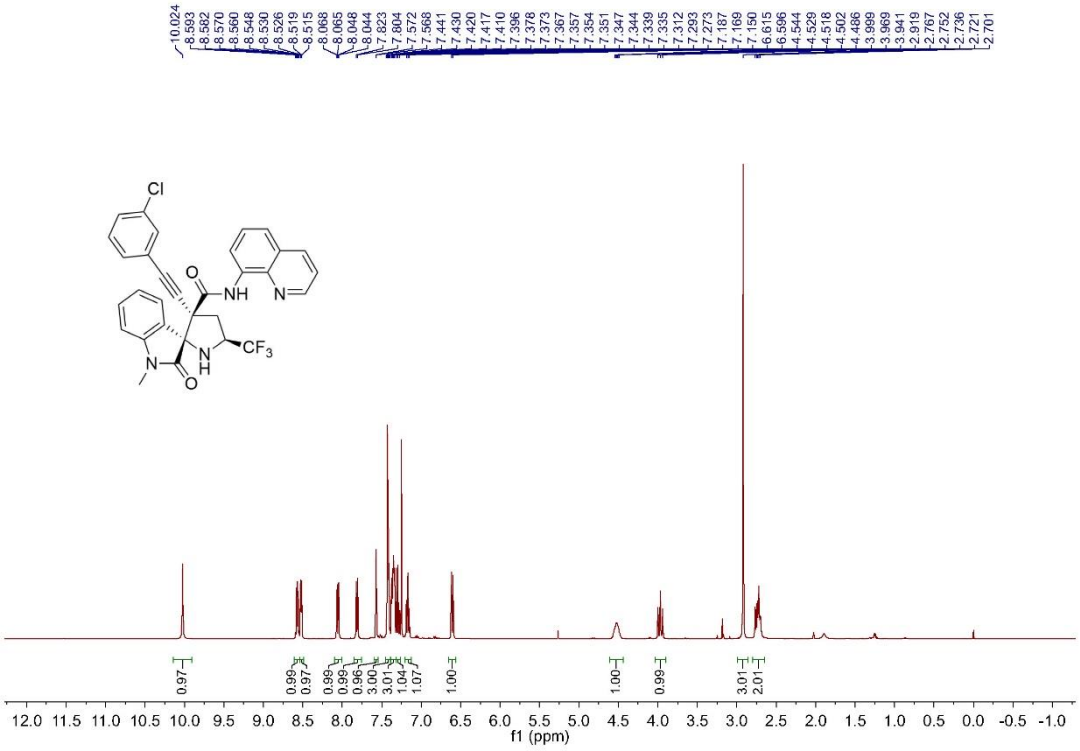
^{13}C NMR spectrum of **3ga** in $CDCl_3$, 101 MHz



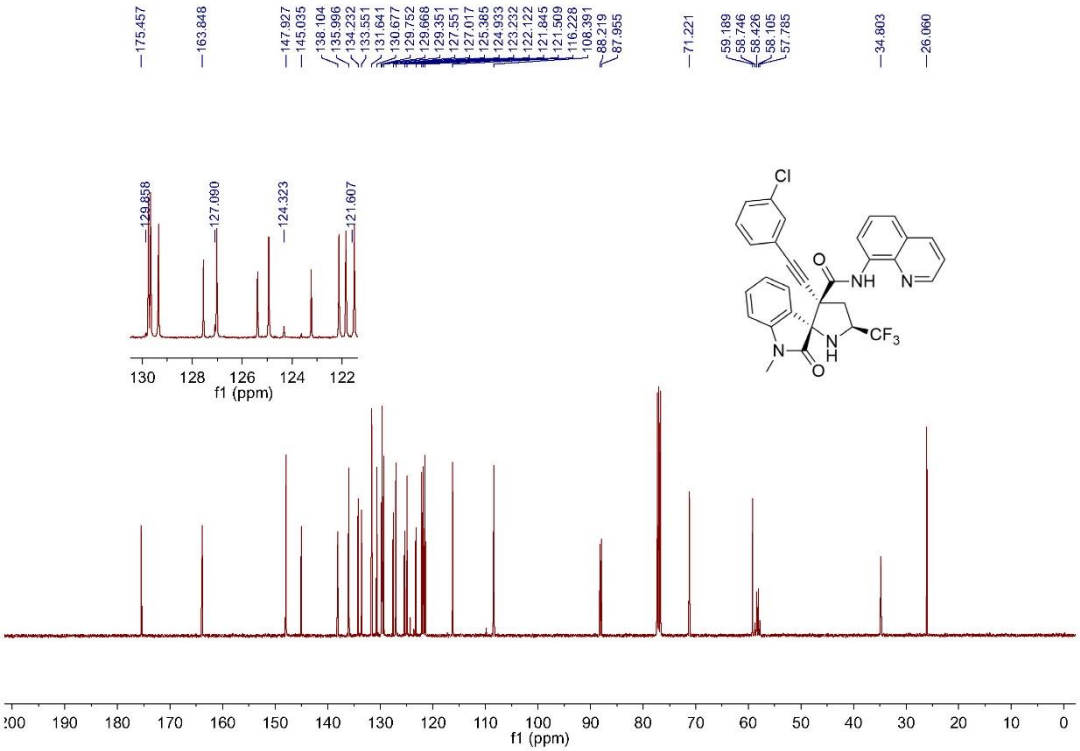
^{19}F NMR spectrum of **3ga** in $CDCl_3$, 376 MHz



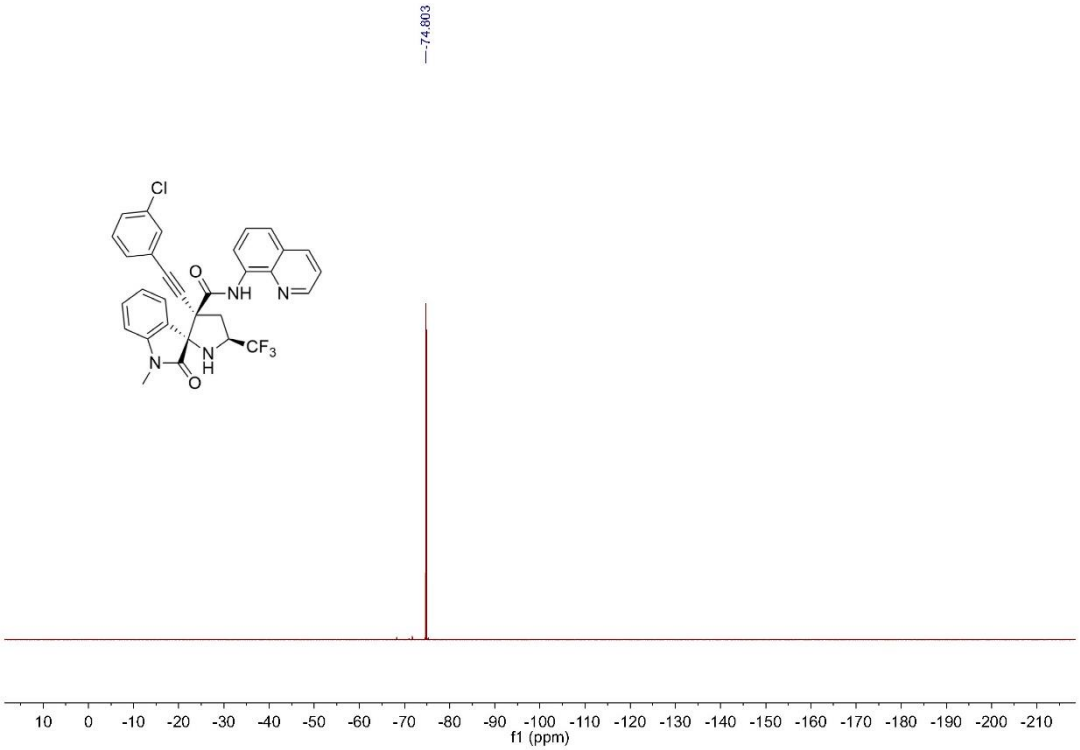
^{1}H NMR spectrum of **3ha** in $CDCl_3$, 400 MHz



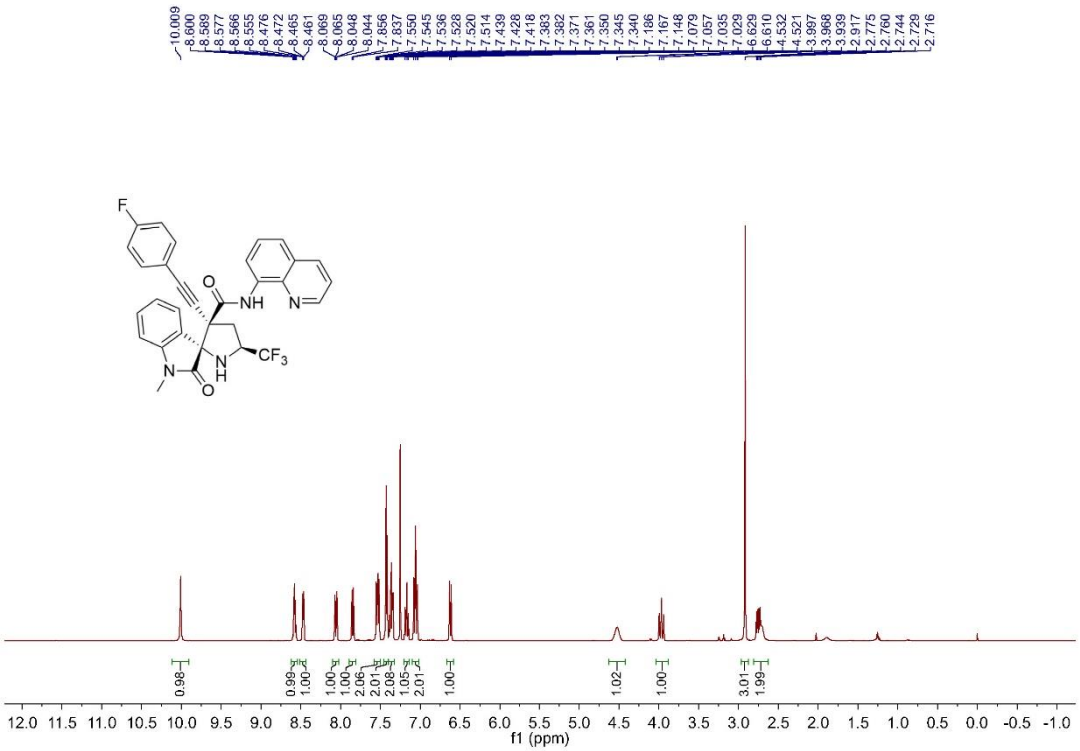
^{13}C NMR spectrum of **3ha** in $CDCl_3$, 101 MHz



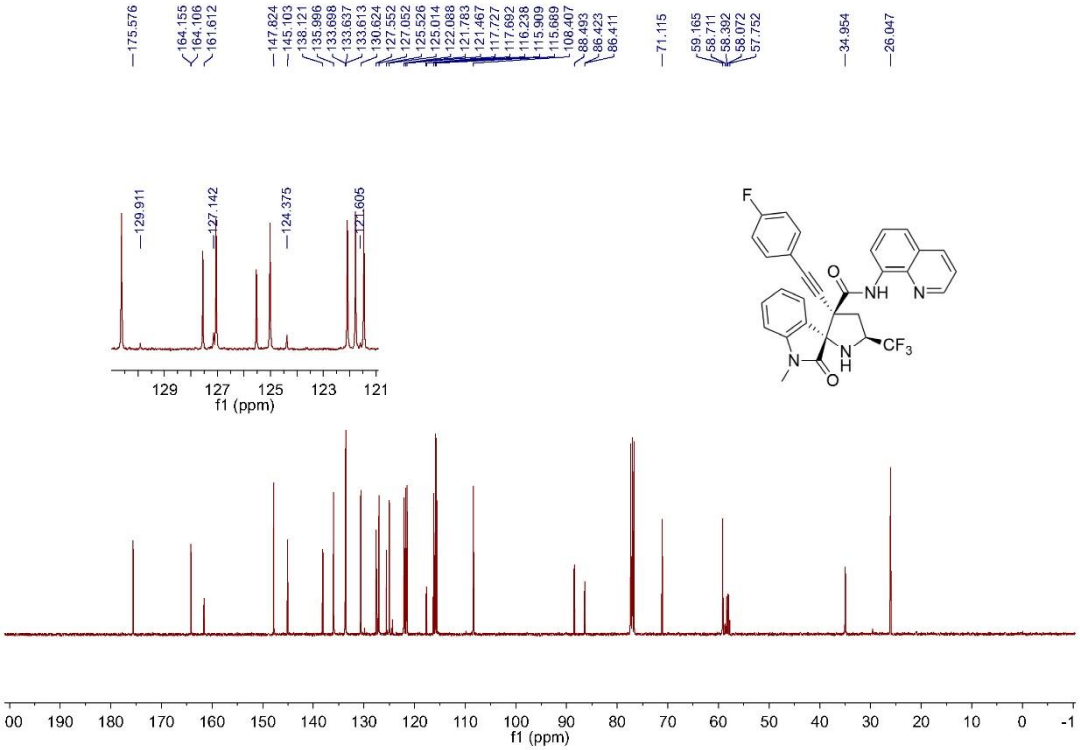
^{19}F NMR spectrum of **3ha** in $CDCl_3$, 376 MHz



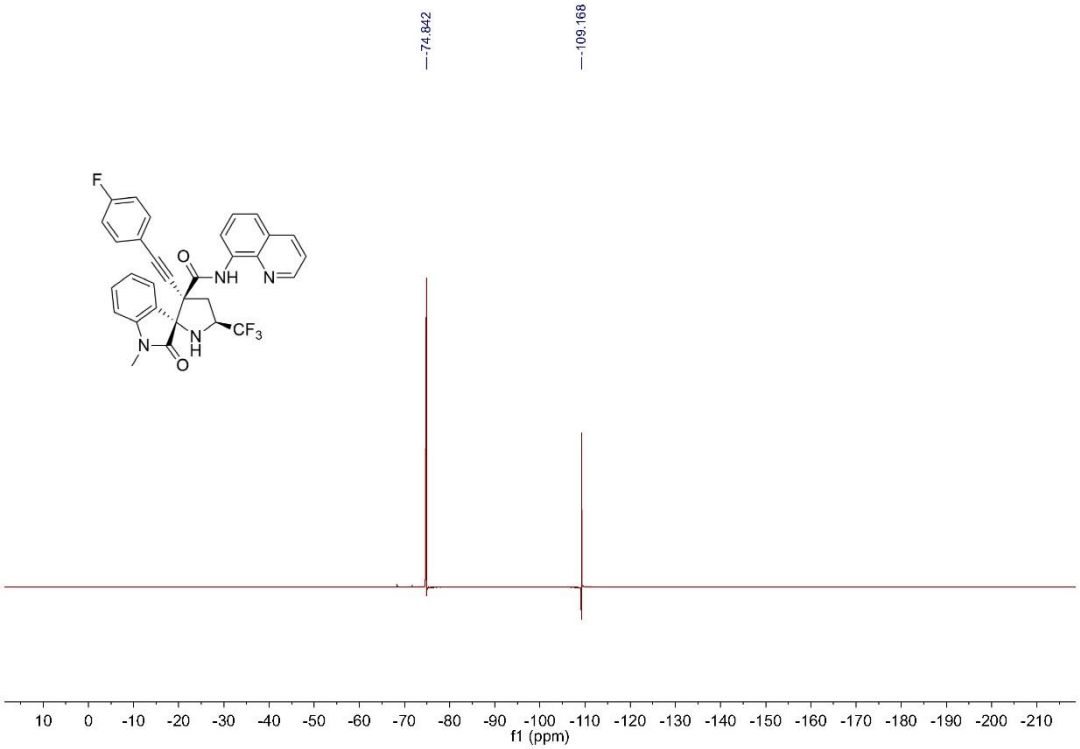
^{1}H NMR spectrum of **3ia** in $CDCl_3$, 400 MHz



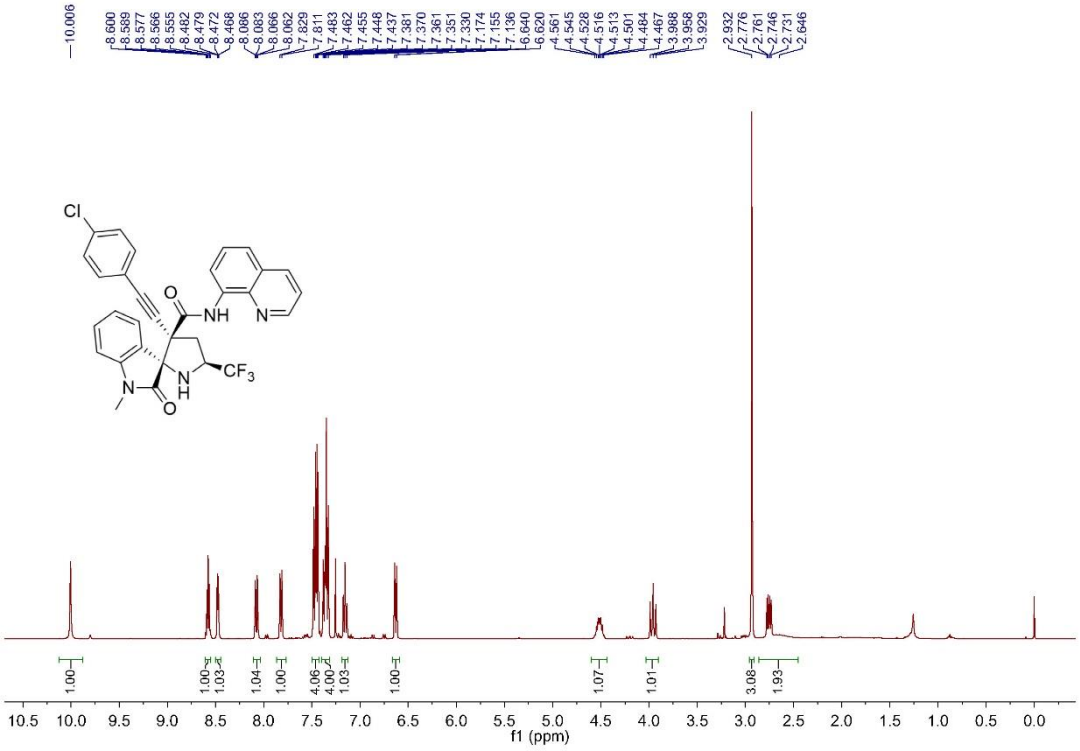
^{13}C NMR spectrum of **3ia** in $CDCl_3$, 101 MHz



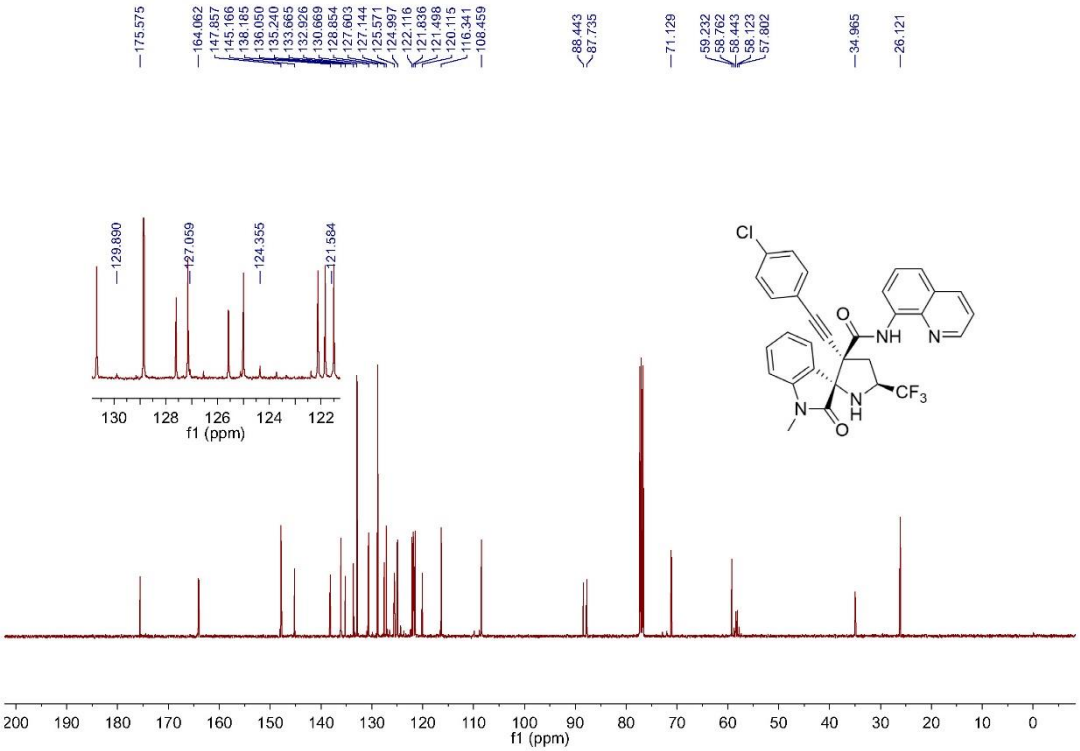
^{19}F NMR spectrum of **3ia** in $CDCl_3$, 376 MHz



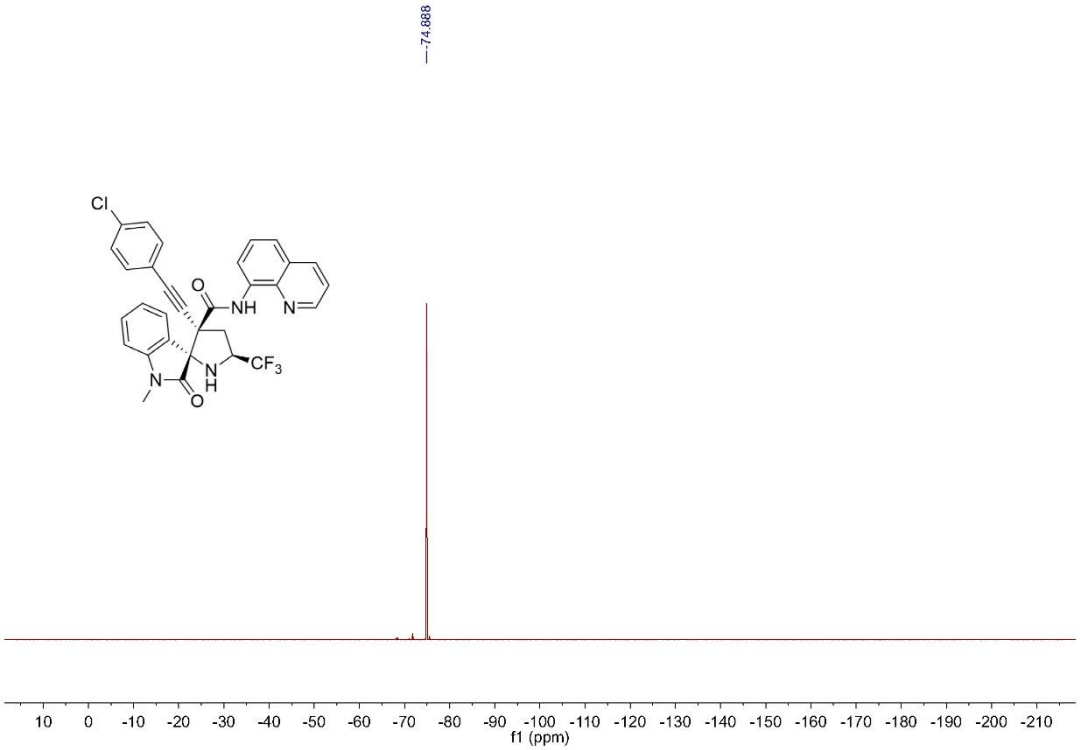
^{1}H NMR spectrum of **3ja** in $CDCl_3$, 400 MHz



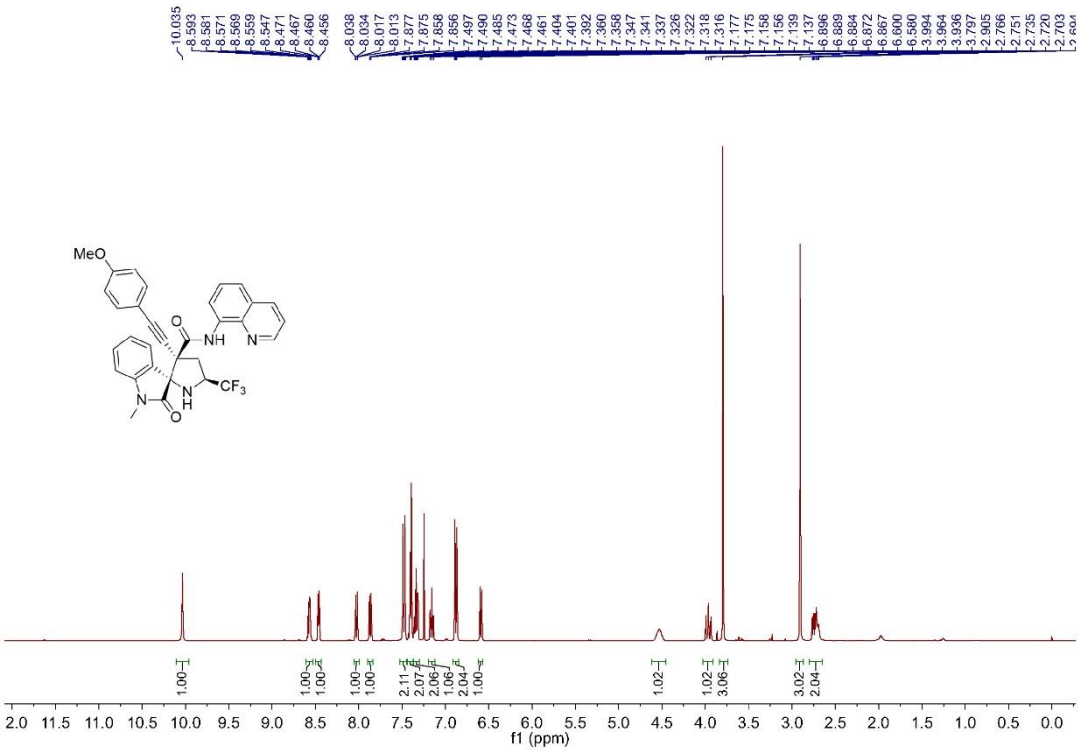
^{13}C NMR spectrum of **3ja** in $CDCl_3$, 101 MHz



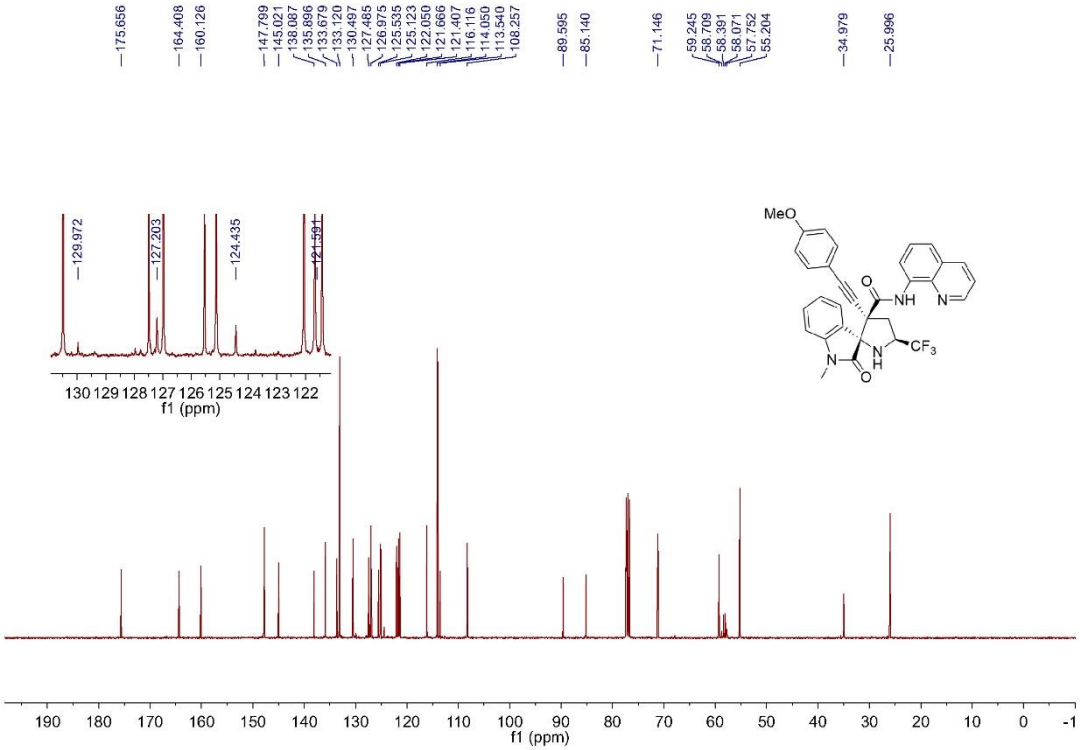
^{19}F NMR spectrum of **3ja** in $CDCl_3$, 376 MHz



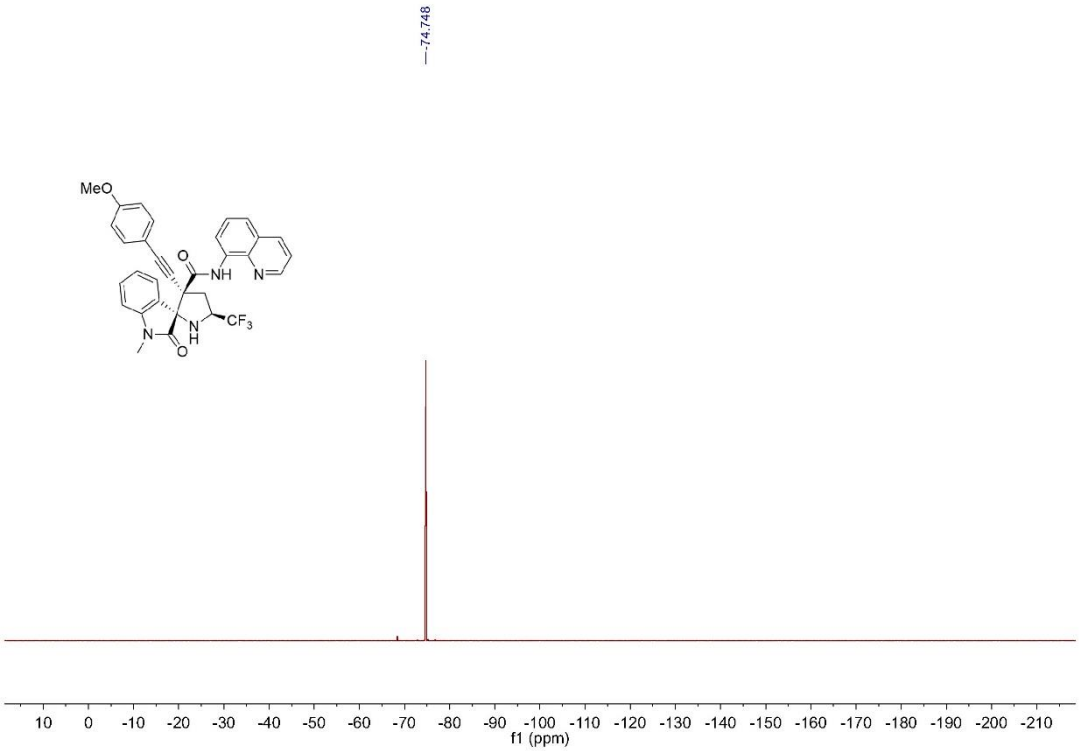
^{1}H NMR spectrum of **3ka** in $CDCl_3$, 400 MHz



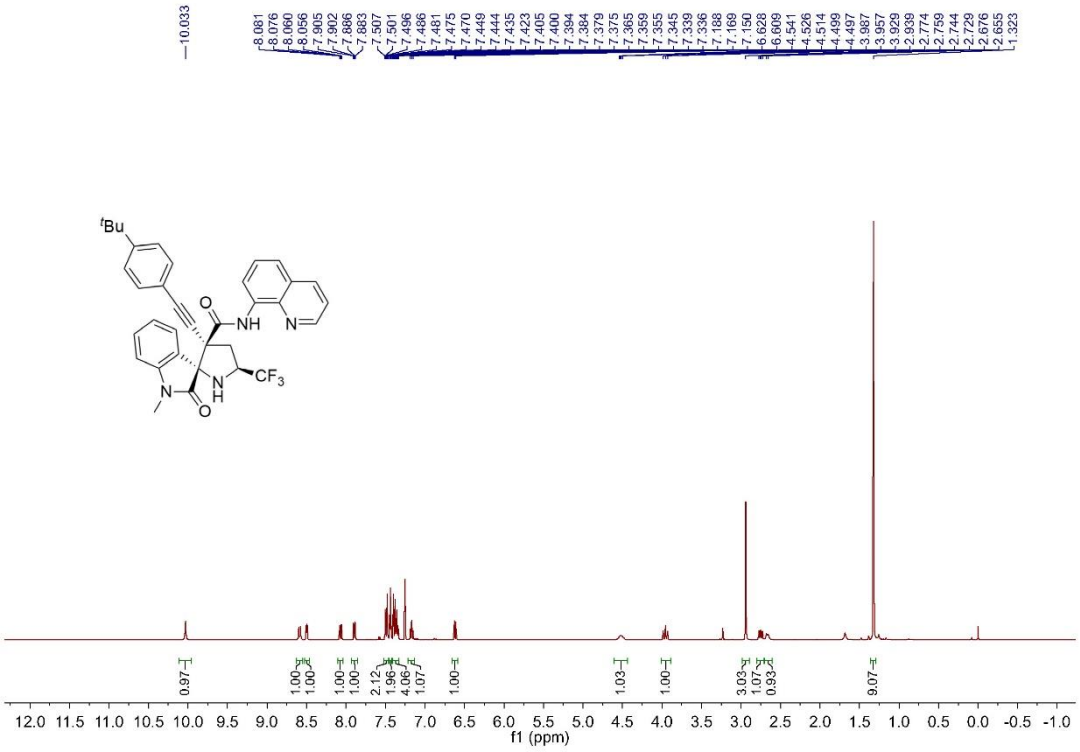
^{13}C NMR spectrum of **3ka** in $CDCl_3$, 101 MHz



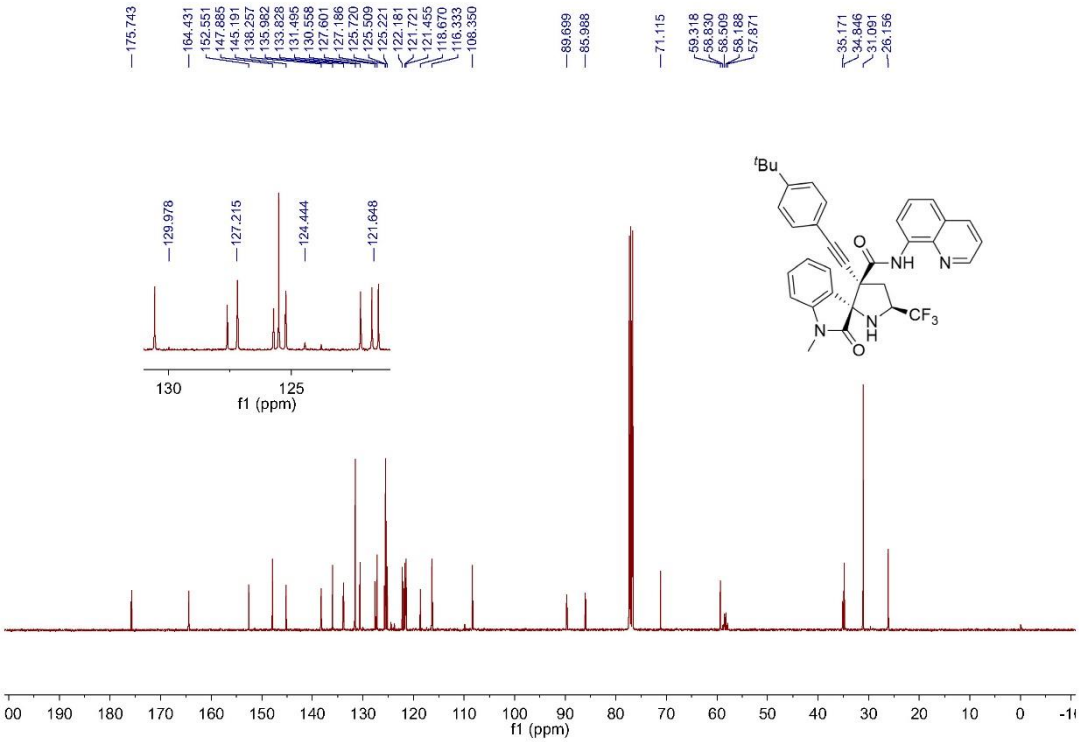
^{19}F NMR spectrum of **3ka** in $CDCl_3$, 376 MHz



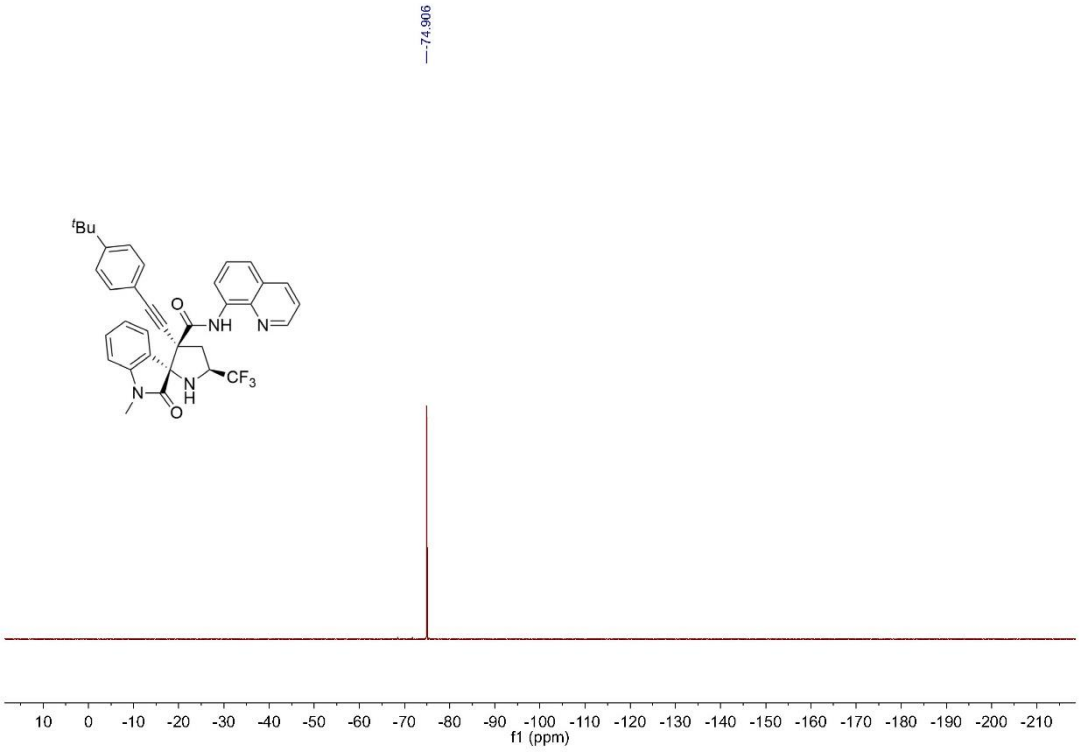
^{1}H NMR spectrum of **3la** in $CDCl_3$, 400 MHz



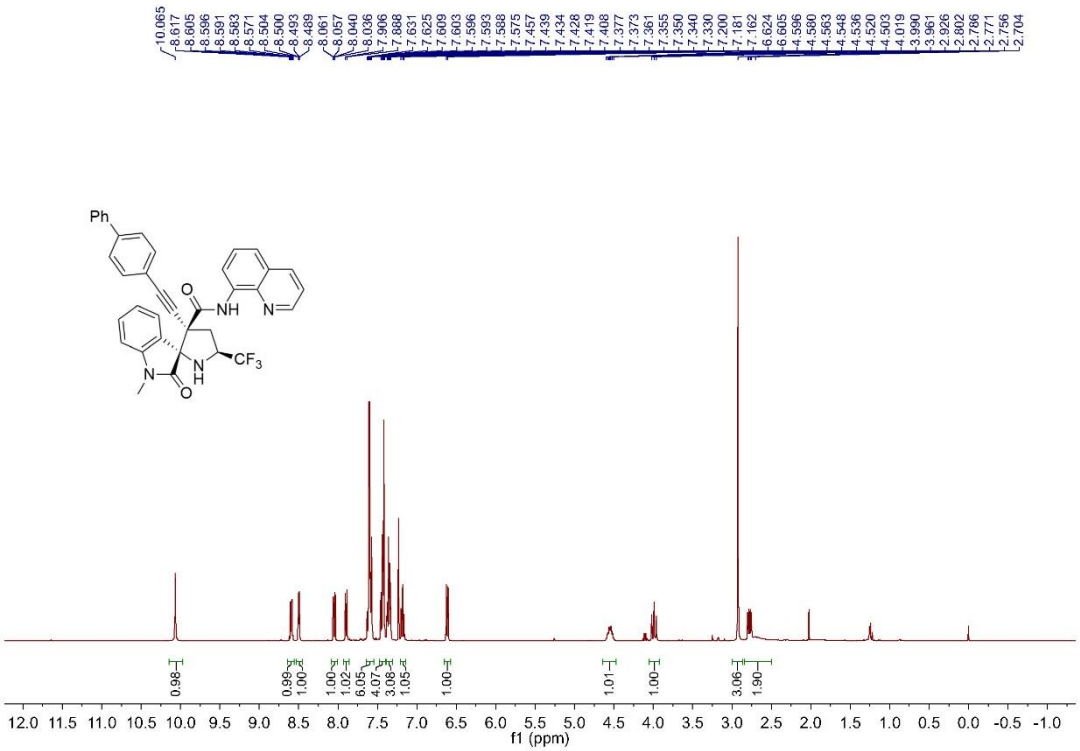
^{13}C NMR spectrum of **3la** in $CDCl_3$, 101 MHz



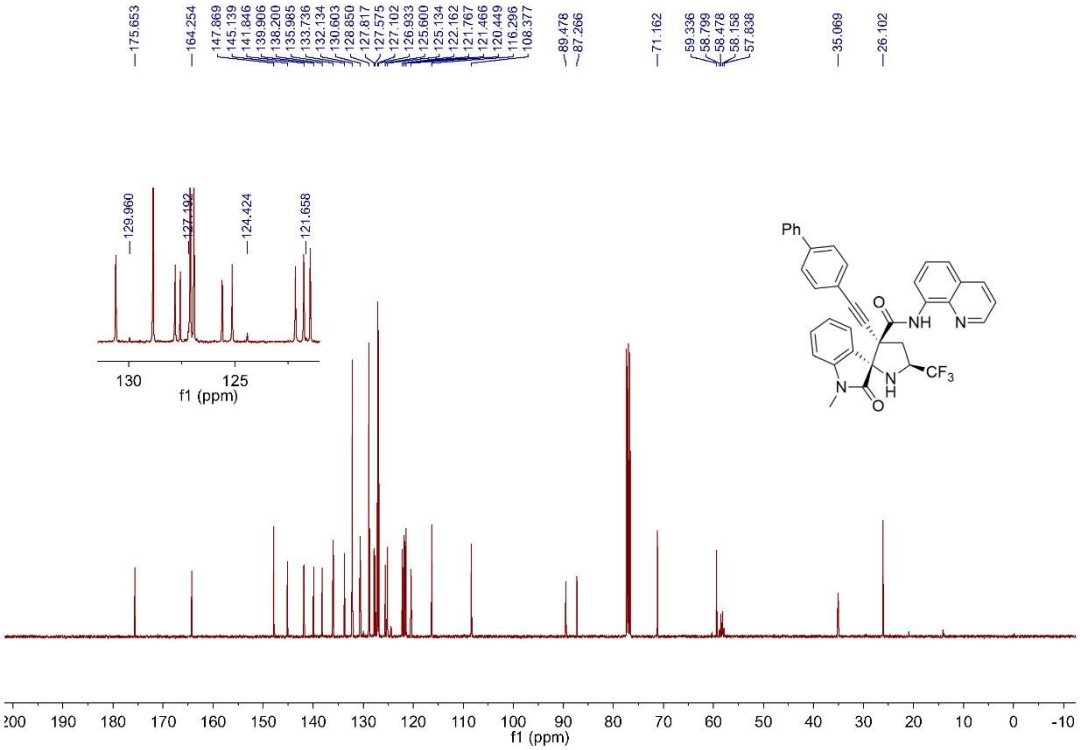
^{19}F NMR spectrum of **3la** in $CDCl_3$, 376 MHz



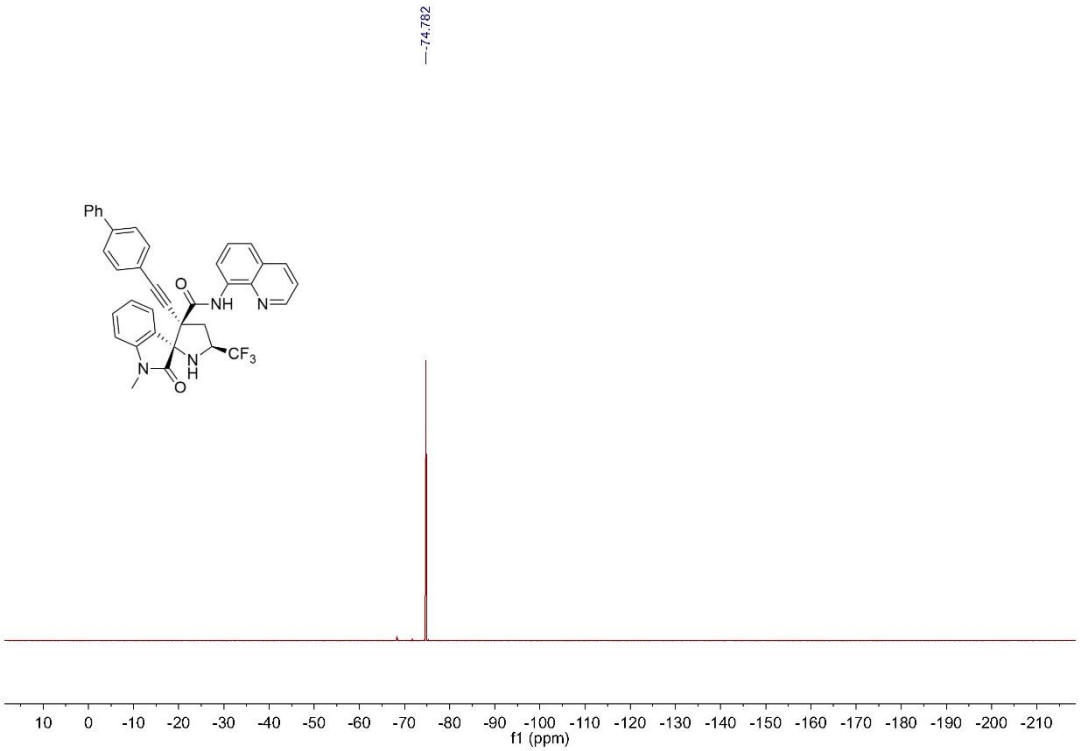
^{1}H NMR spectrum of **3ma** in $CDCl_3$, 400 MHz



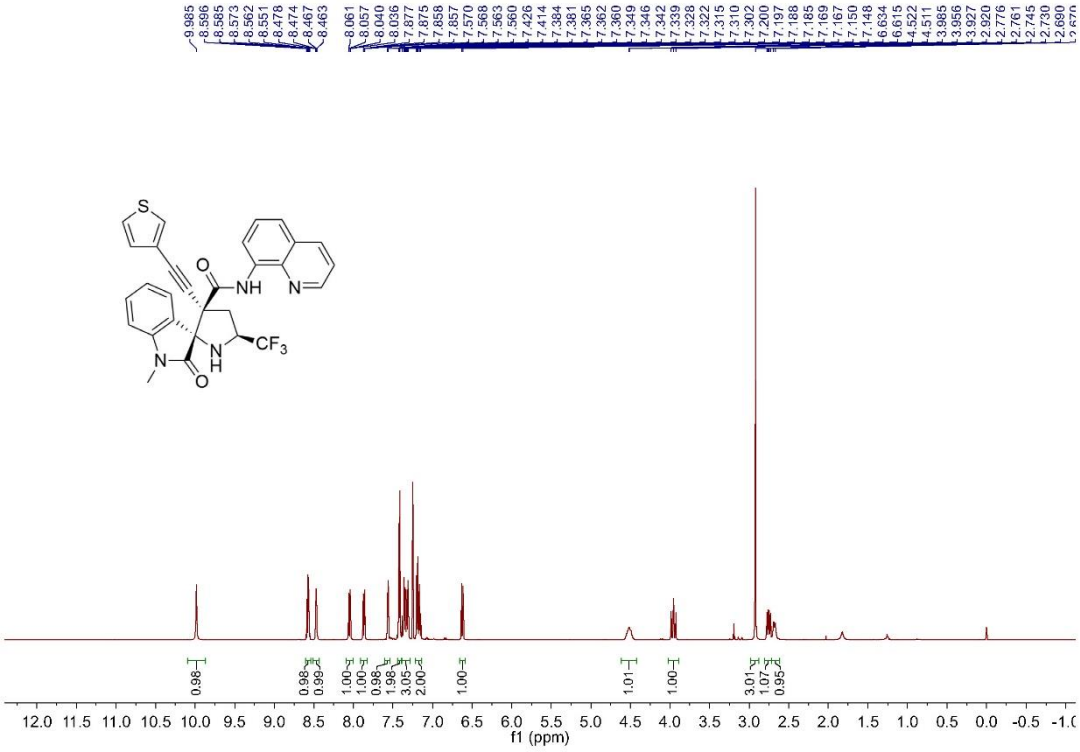
^{13}C NMR spectrum of **3ma** in $CDCl_3$, 101 MHz



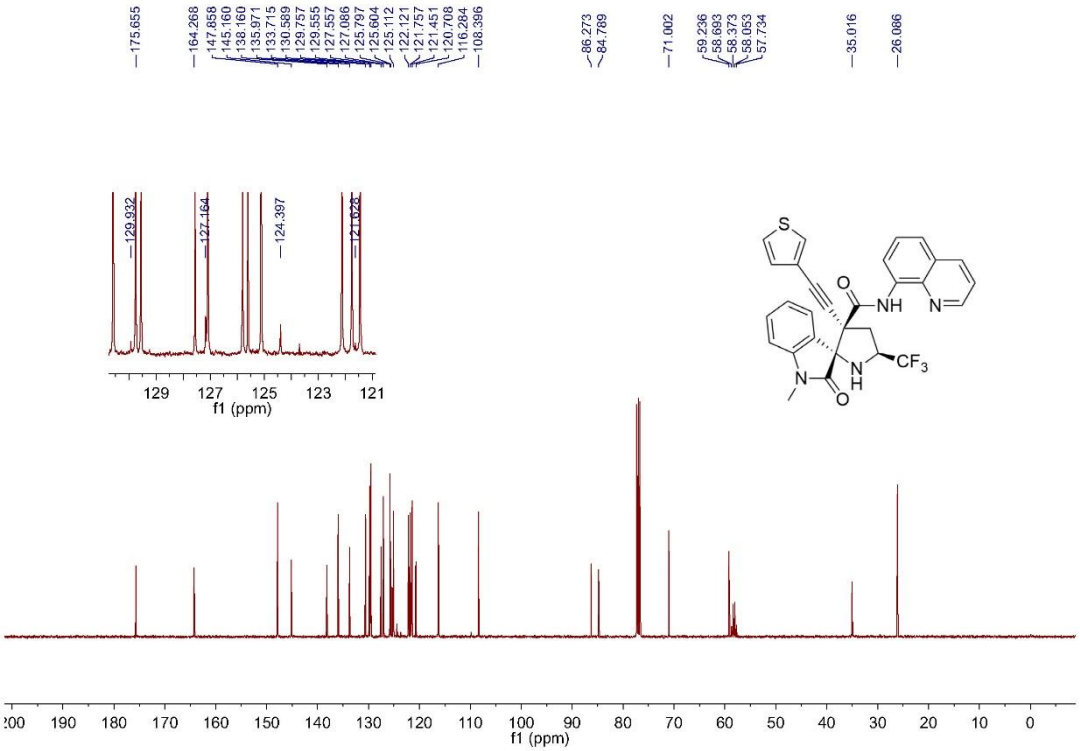
^{19}F NMR spectrum of **3ma** in $CDCl_3$, 376 MHz



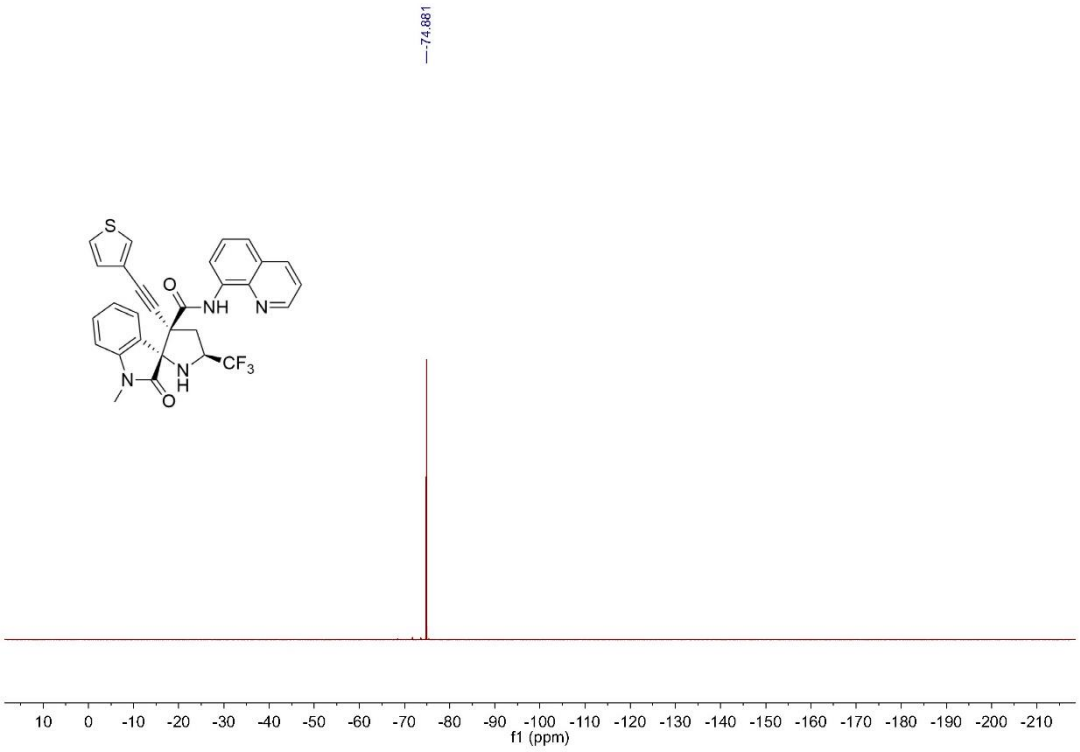
^{1}H NMR spectrum of **3na** in $CDCl_3$, 400 MHz



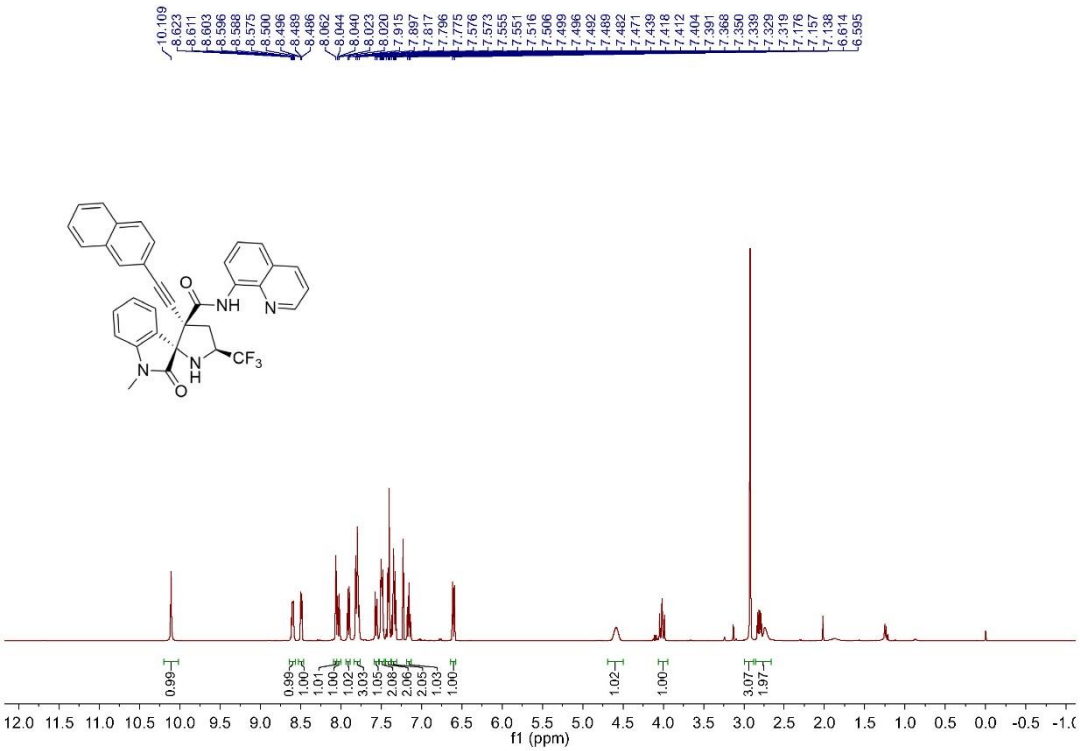
^{13}C NMR spectrum of **3na** in $CDCl_3$, 101 MHz



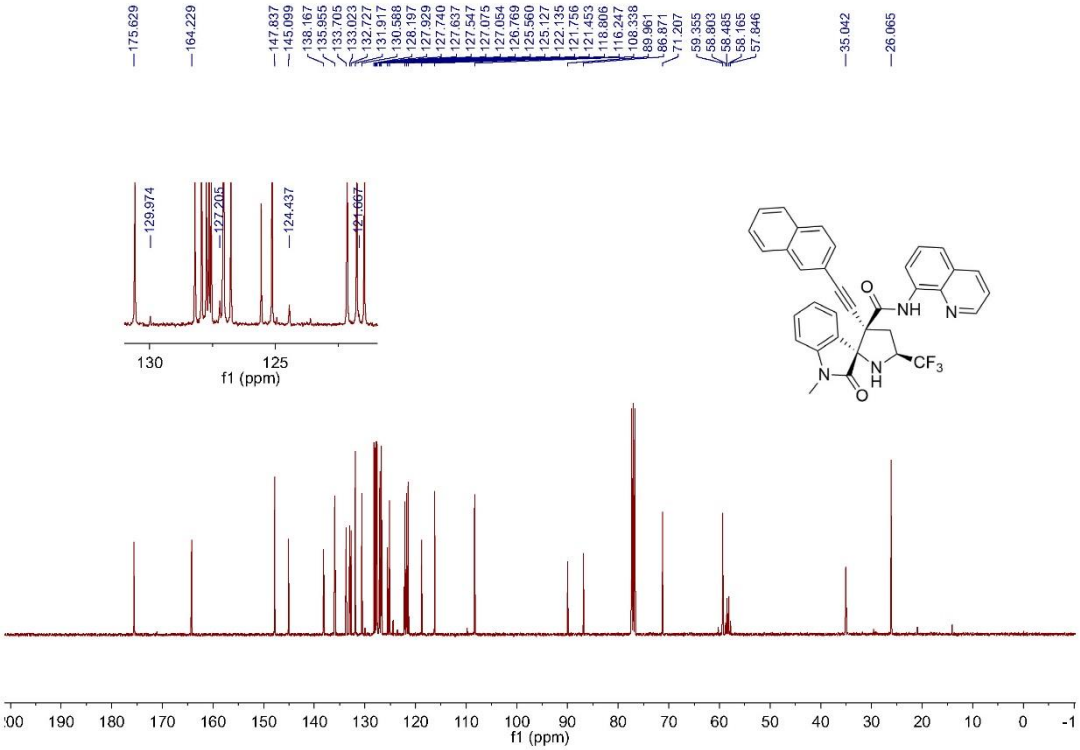
^{19}F NMR spectrum of **3na** in $CDCl_3$, 376 MHz



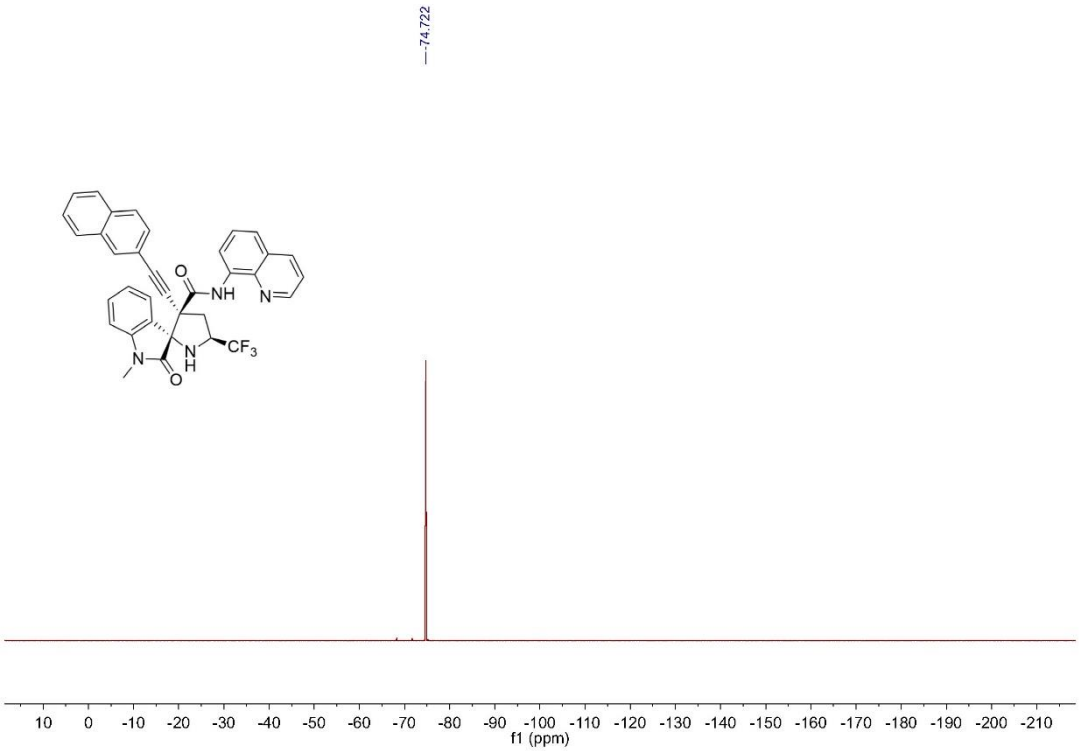
^{1}H NMR spectrum of **3oa** in $CDCl_3$, 400 MHz



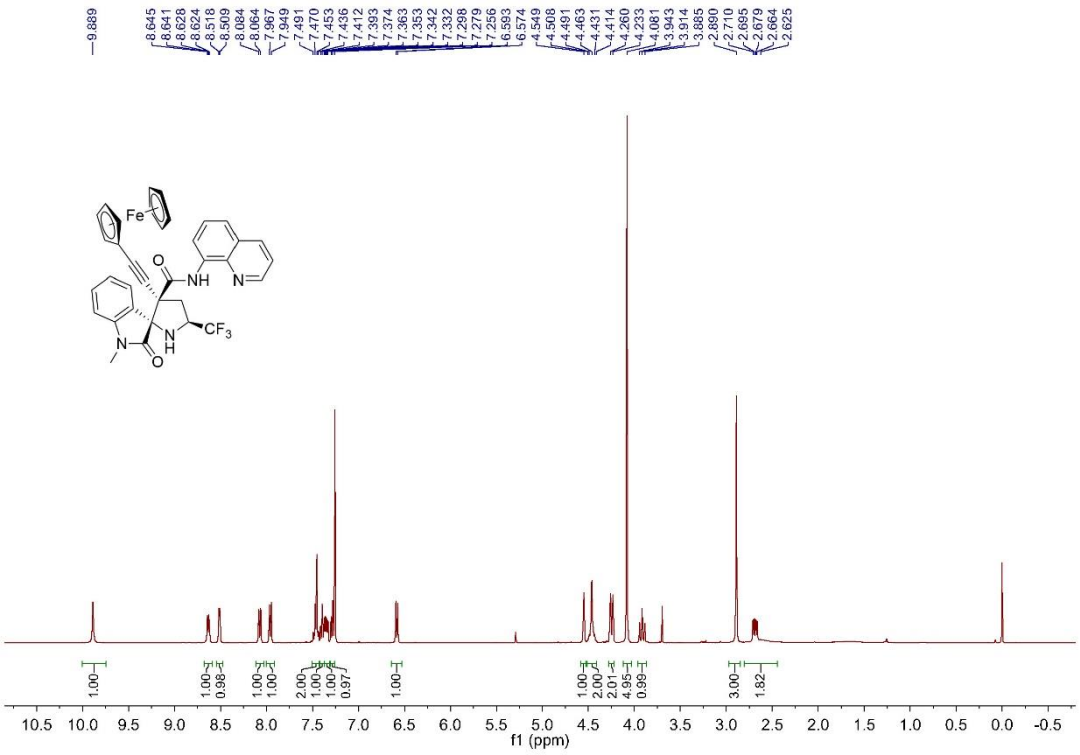
^{13}C NMR spectrum of **3oa** in $CDCl_3$, 101 MHz



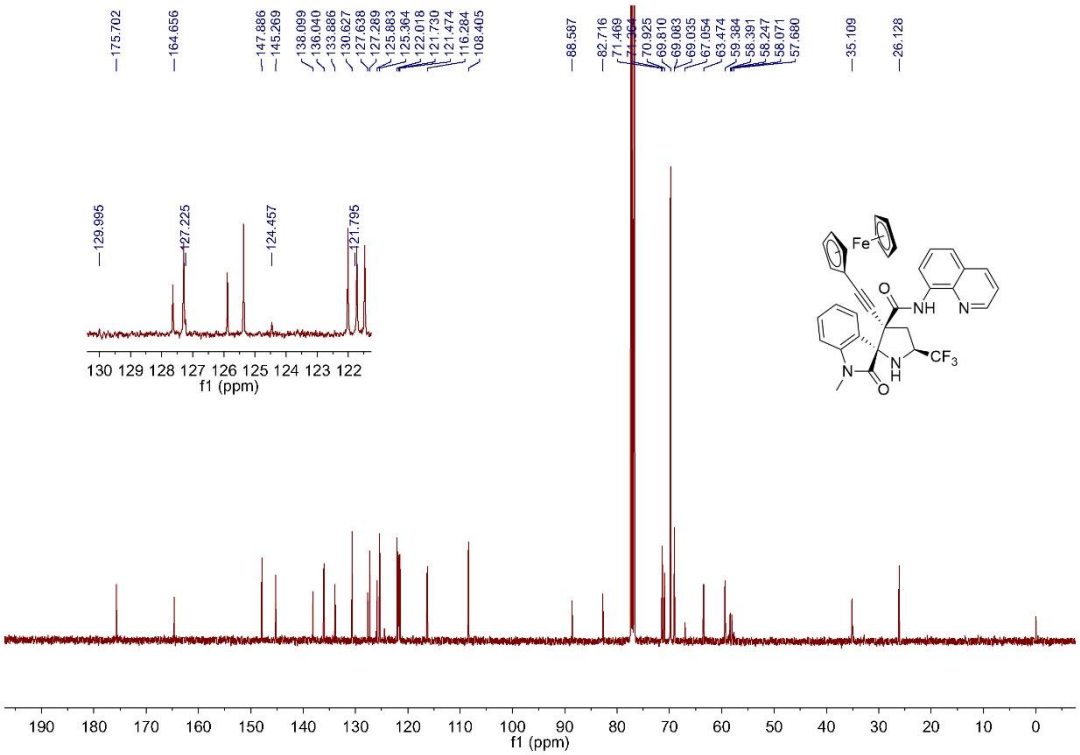
^{19}F NMR spectrum of **3oa** in $CDCl_3$, 376 MHz



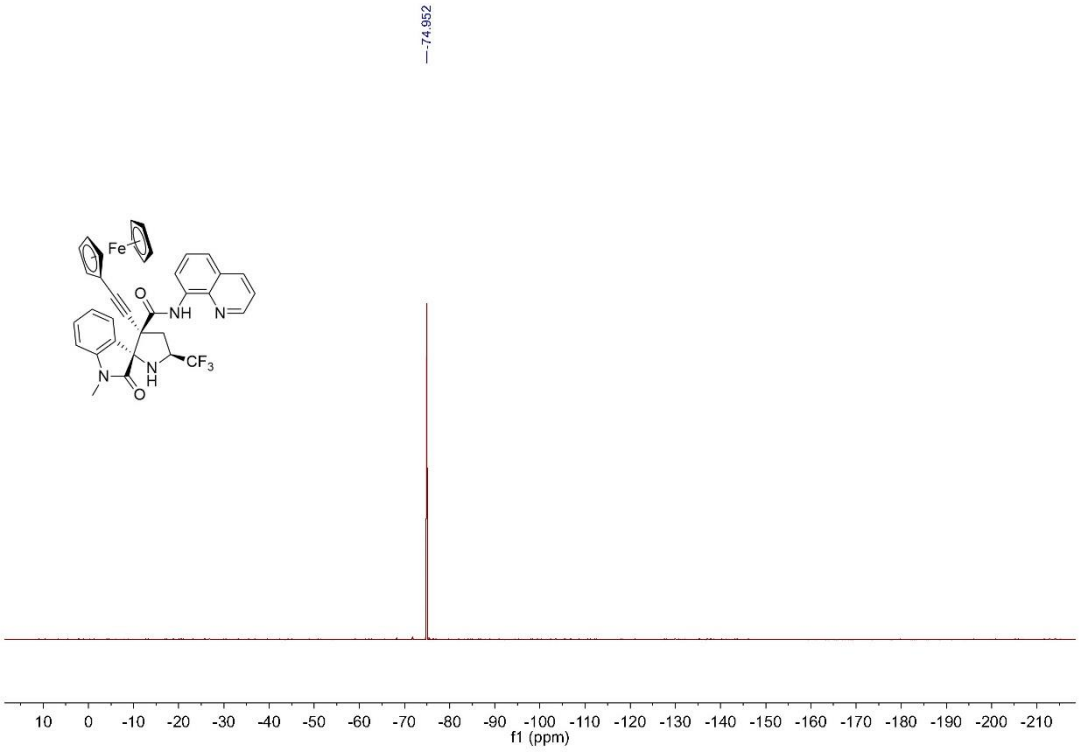
^{1}H NMR spectrum of **3pa** in $CDCl_3$, 400 MHz



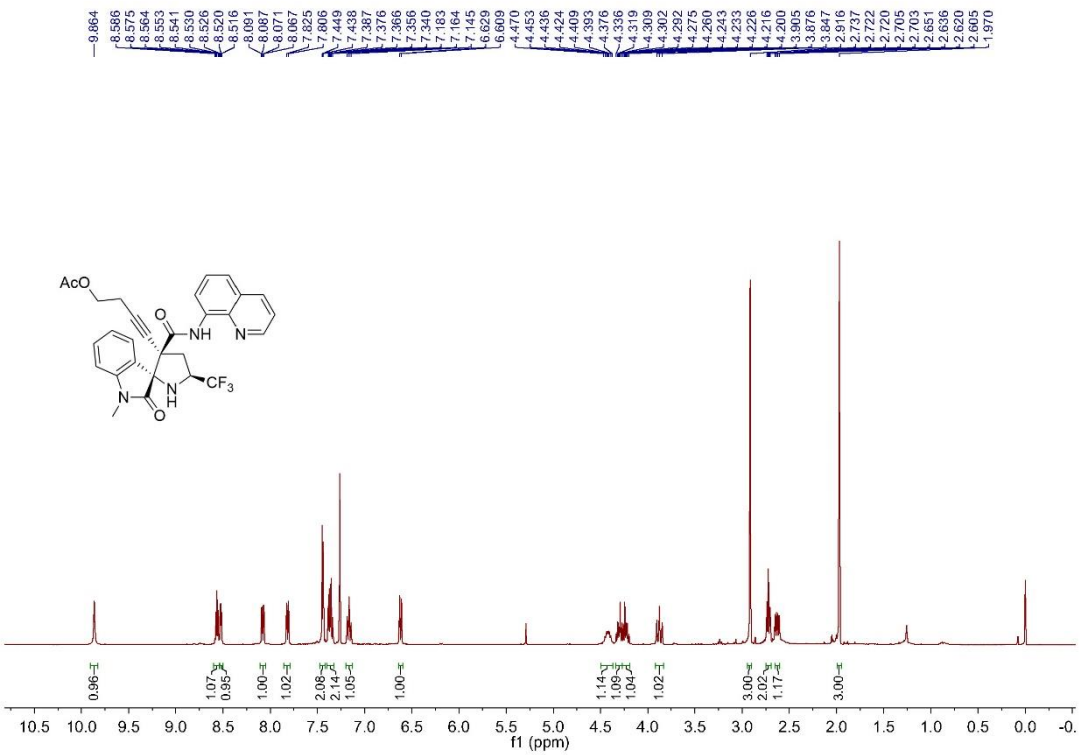
^{13}C NMR spectrum of **3pa** in $CDCl_3$, 101 MHz



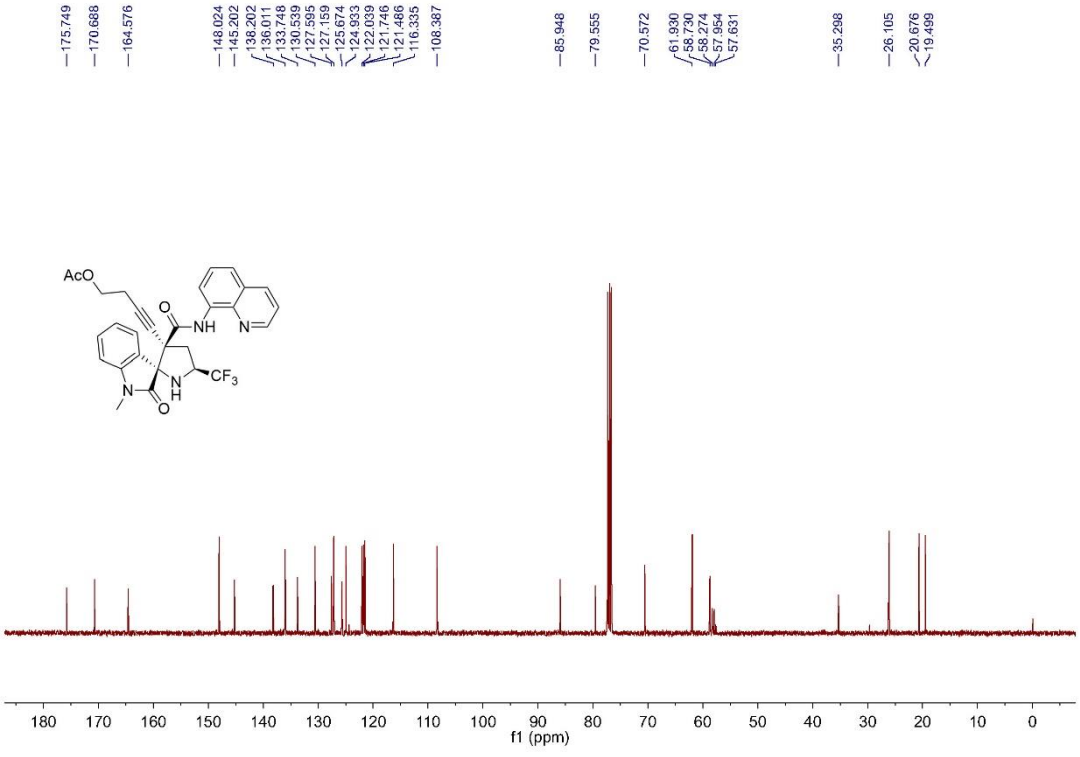
^{19}F NMR spectrum of **3pa** in $CDCl_3$, 376 MHz



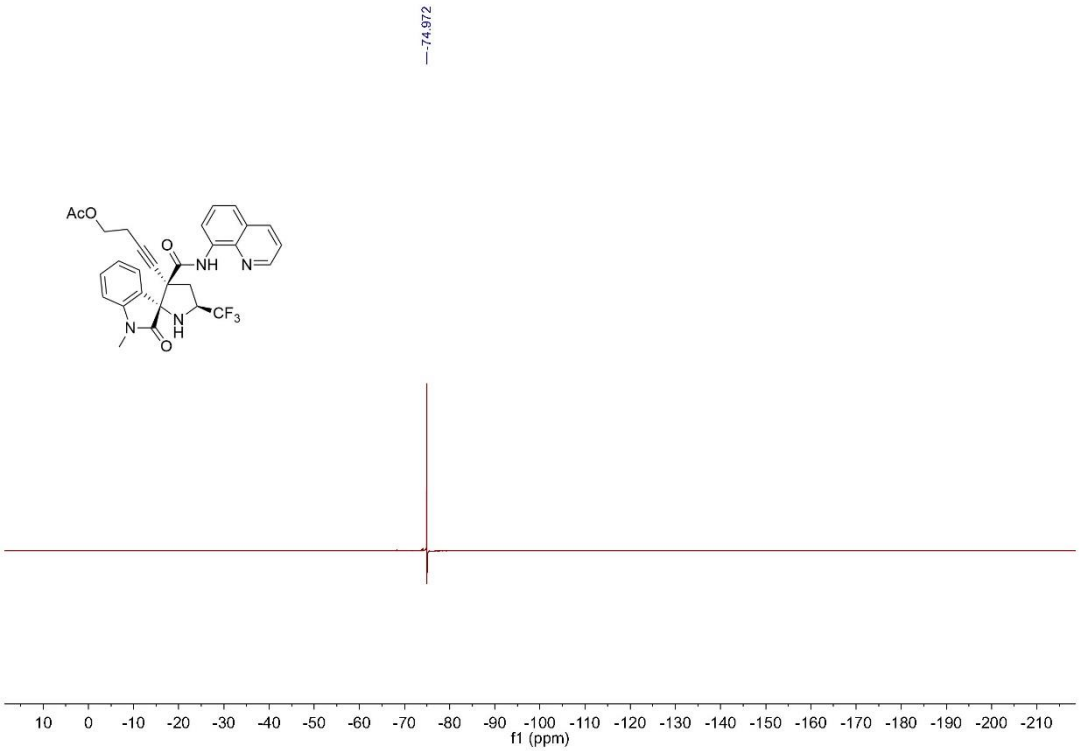
^{1}H NMR spectrum of **3qa** in $CDCl_3$, 400 MHz



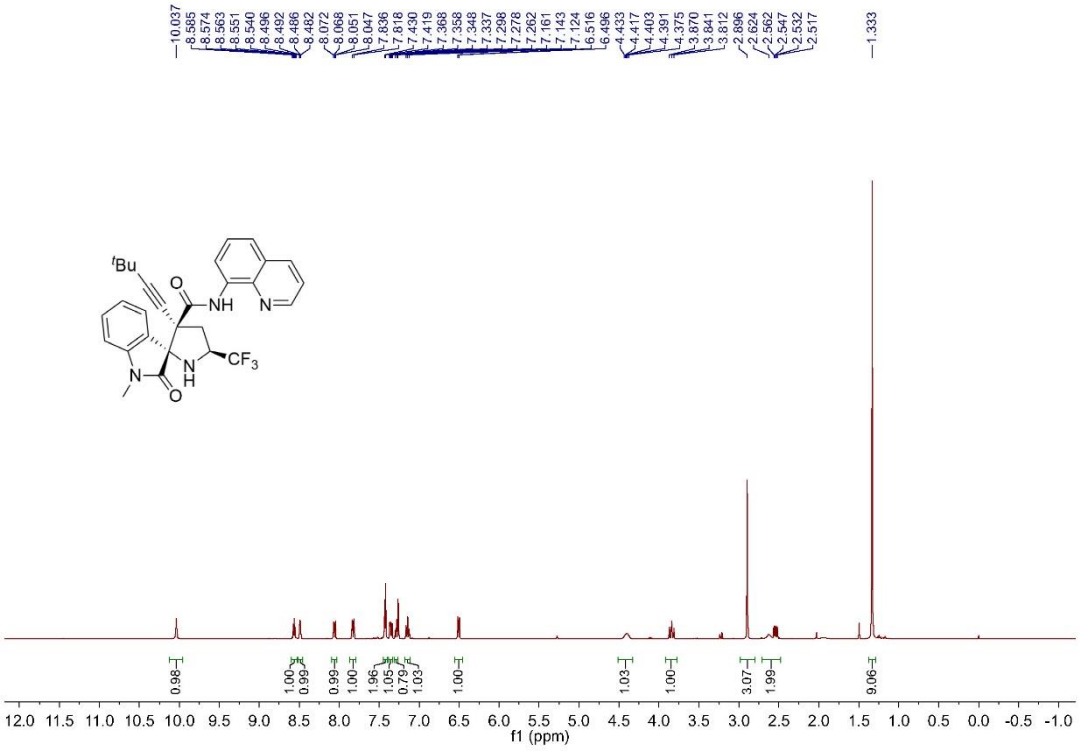
^{13}C NMR spectrum of **3qa** in $CDCl_3$, 101 MHz



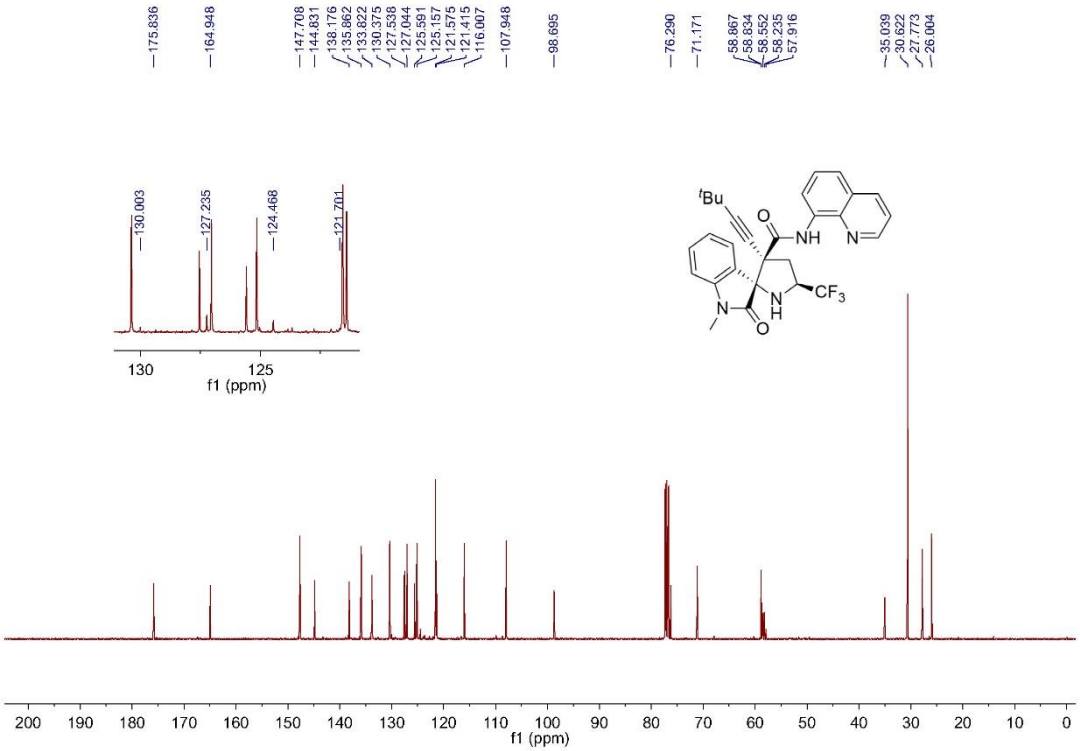
^{19}F NMR spectrum of **3qa** in $CDCl_3$, 376 MHz



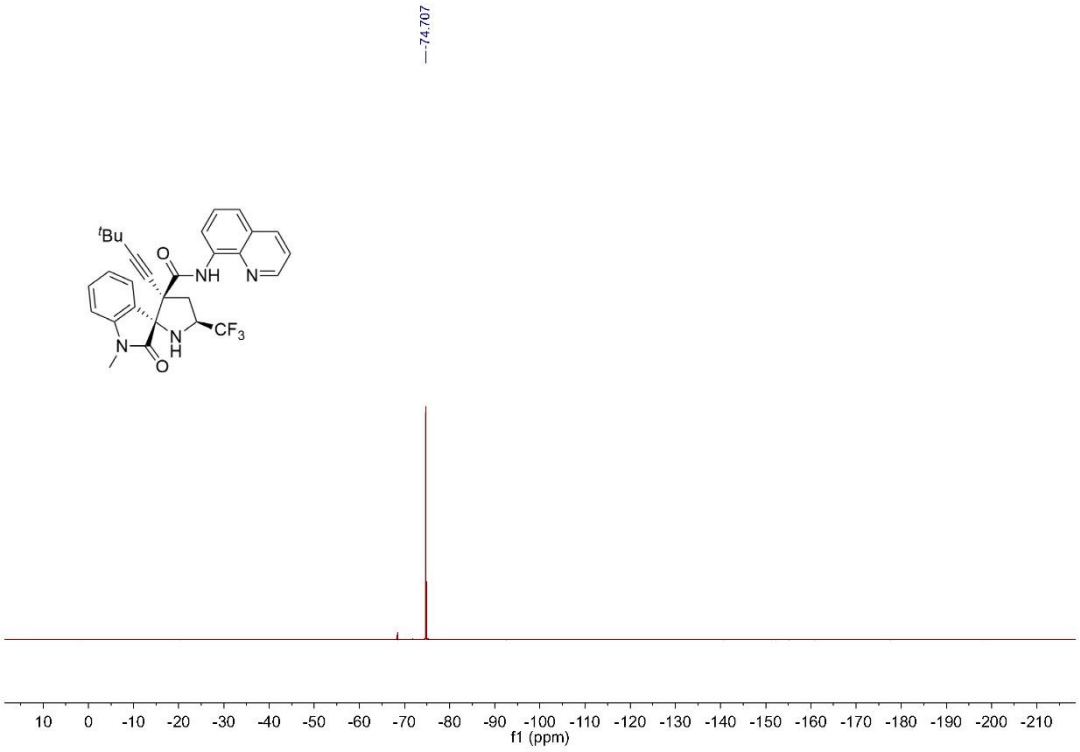
^{1}H NMR spectrum of **3ra** in $CDCl_3$, 400 MHz



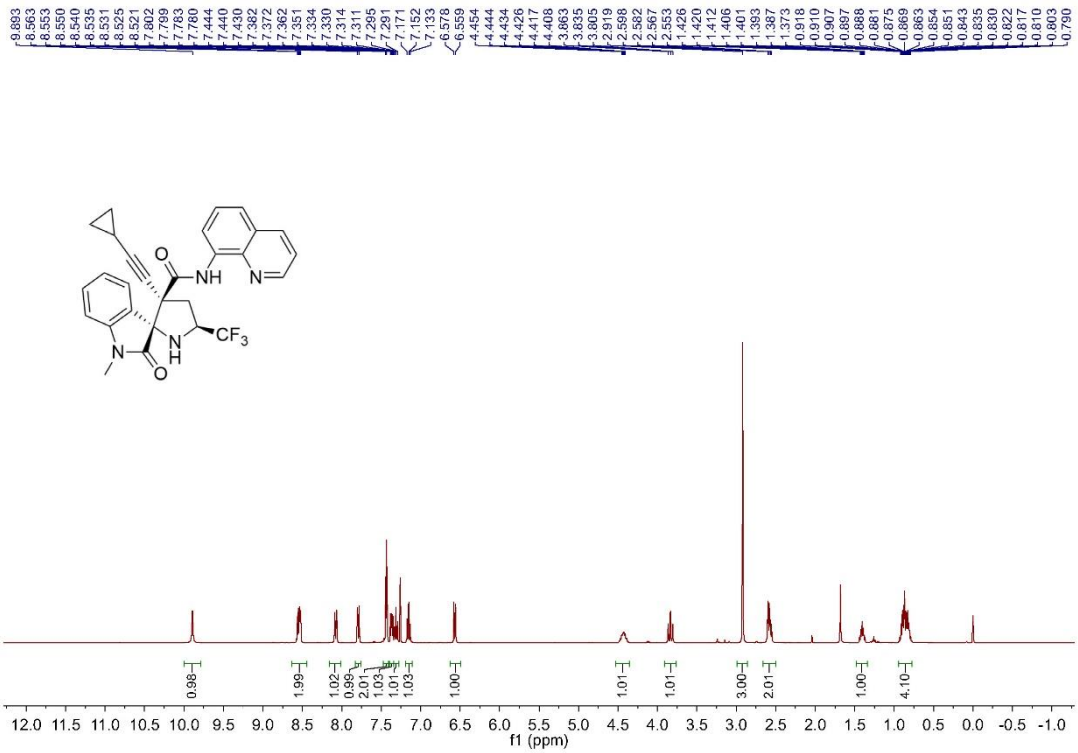
^{13}C NMR spectrum of **3ra** in $CDCl_3$, 101 MHz



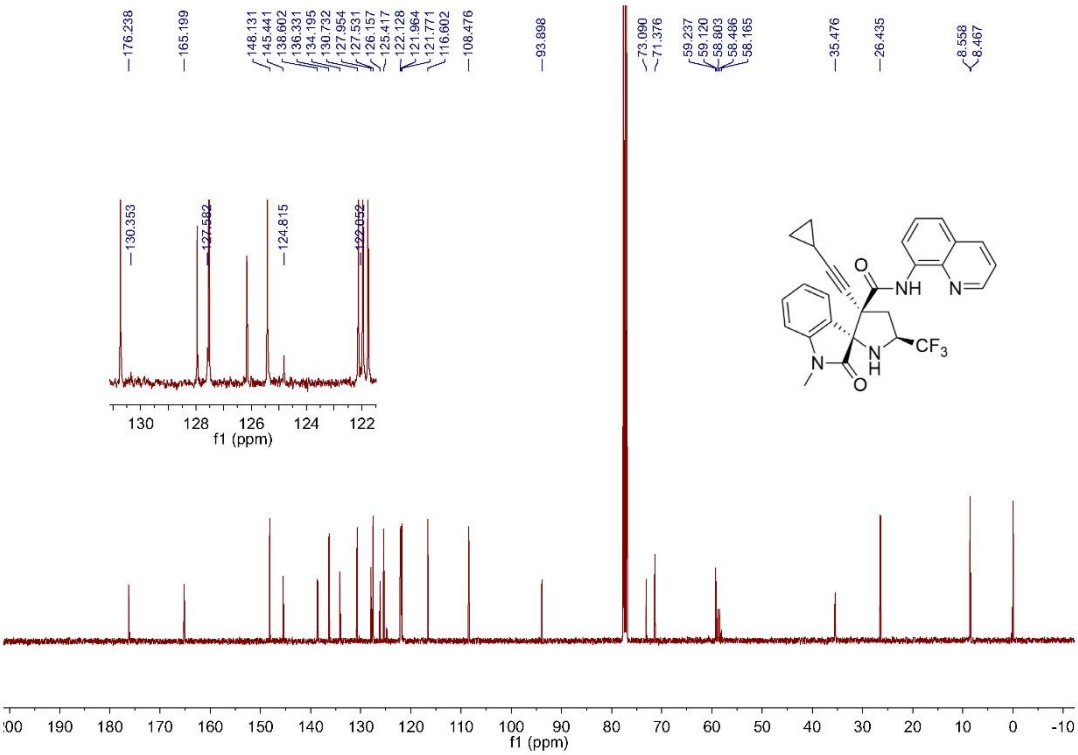
^{19}F NMR spectrum of **3ra** in $CDCl_3$, 376 MHz



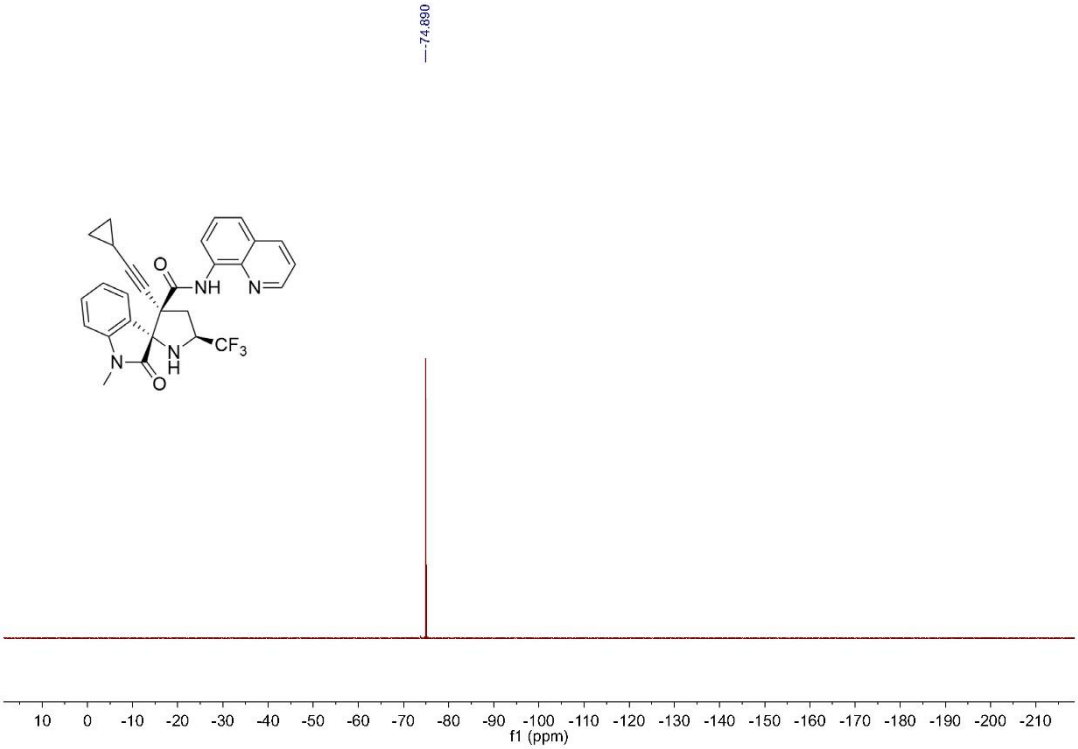
^{1}H NMR spectrum of **3sa** in $CDCl_3$, 400 MHz



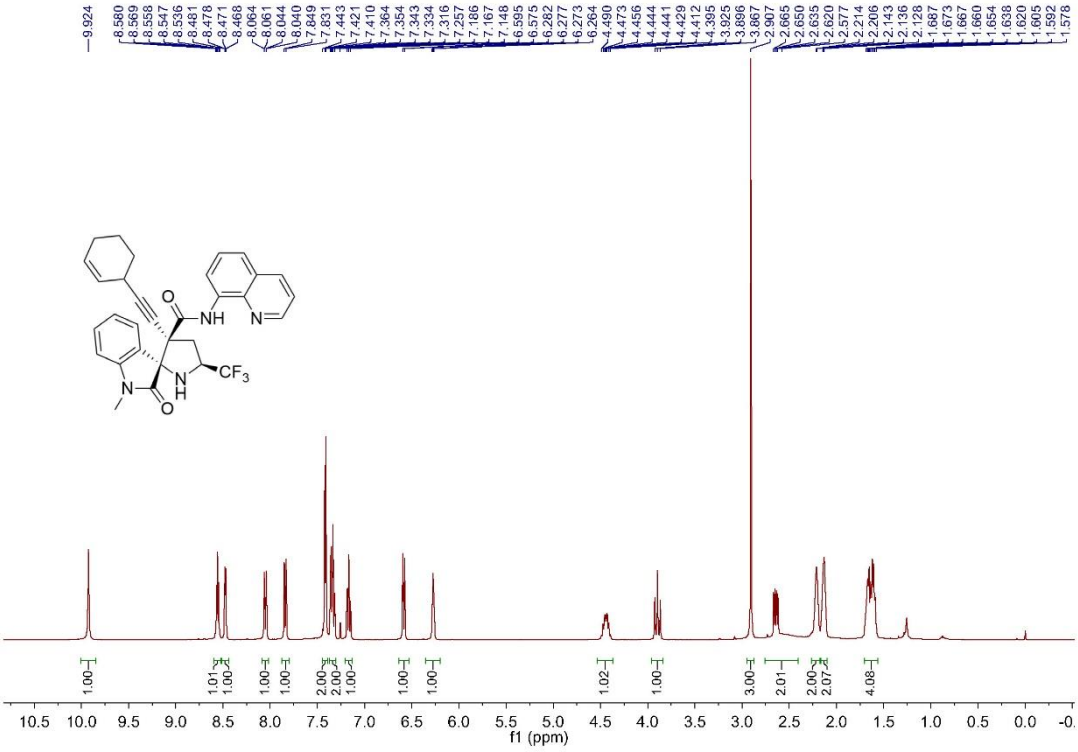
^{13}C NMR spectrum of **3sa** in $CDCl_3$, 101 MHz



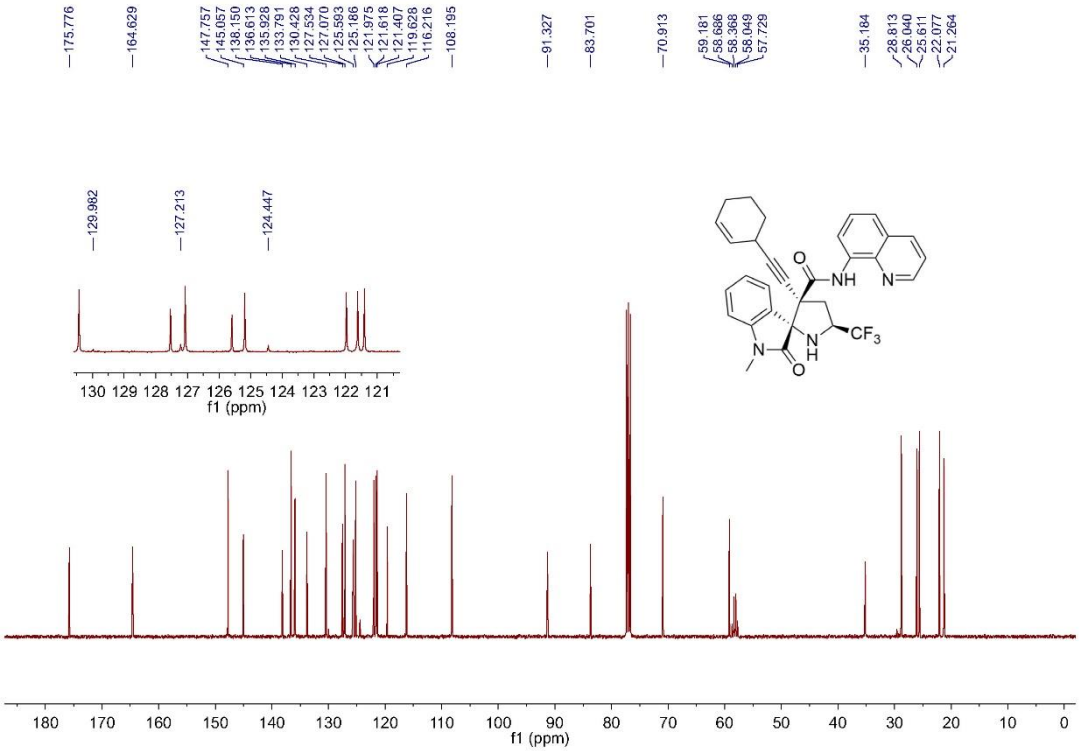
^{19}F NMR spectrum of **3sa** in $CDCl_3$, 376 MHz



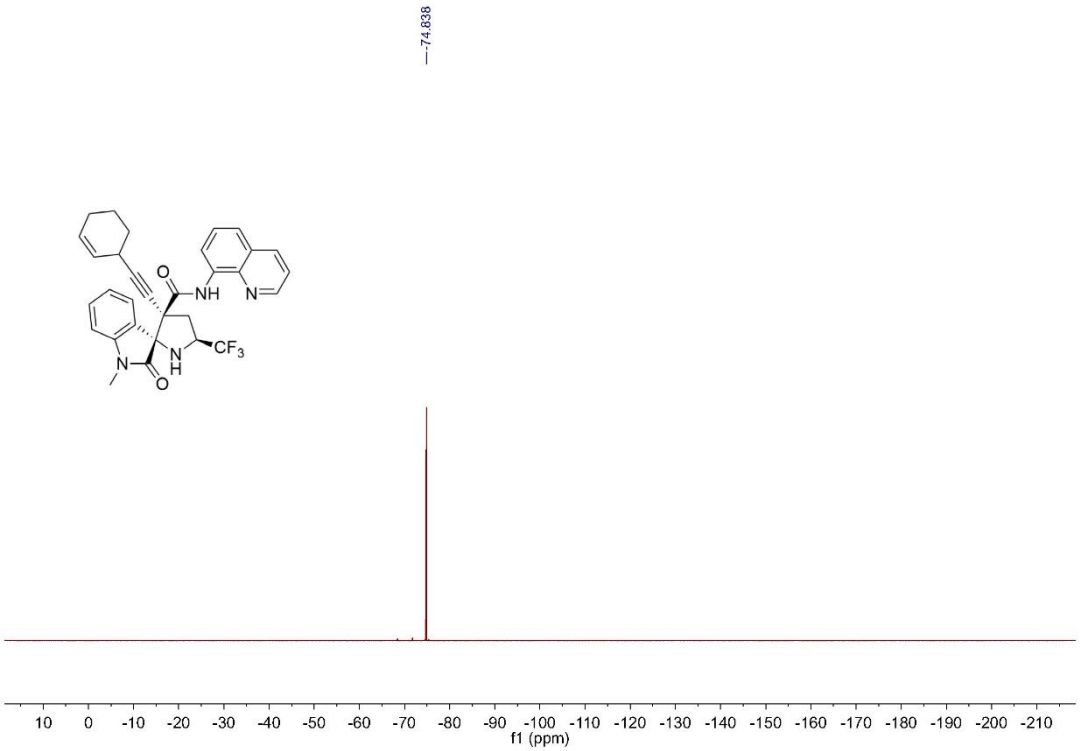
^{1}H NMR spectrum of **3ta** in $CDCl_3$, 400 MHz



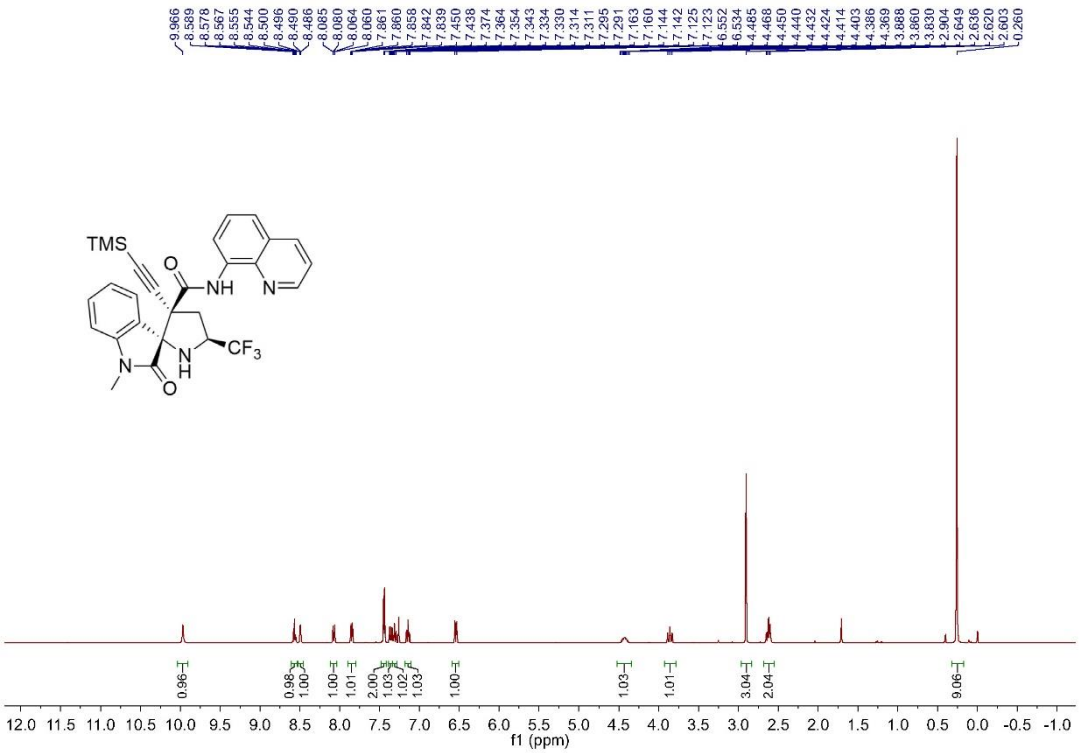
^{13}C NMR spectrum of **3ta** in $CDCl_3$, 101 MHz



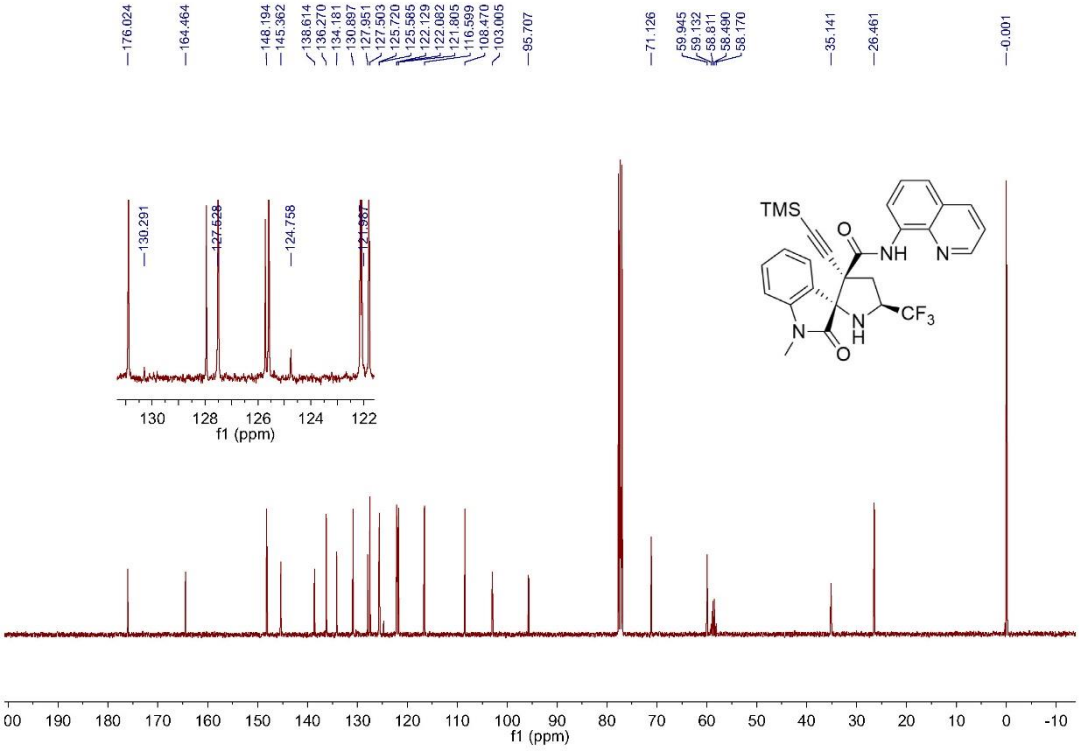
^{19}F NMR spectrum of **3ta** in $CDCl_3$, 376 MHz



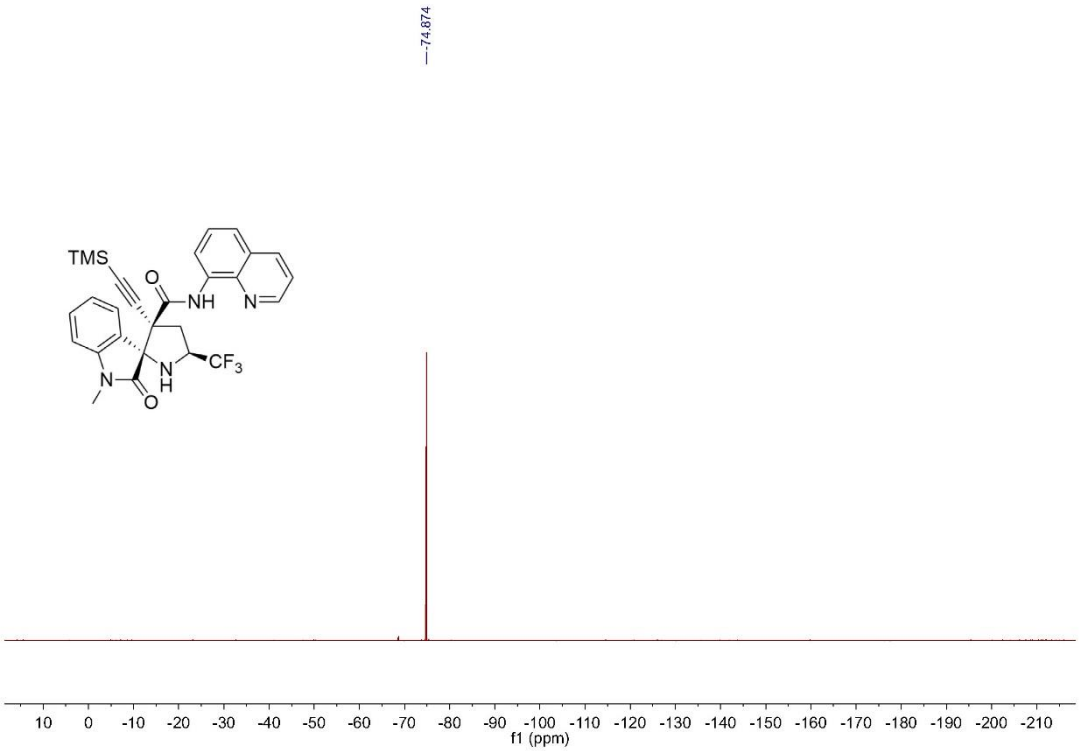
^{1}H NMR spectrum of **3ua** in $CDCl_3$, 400 MHz



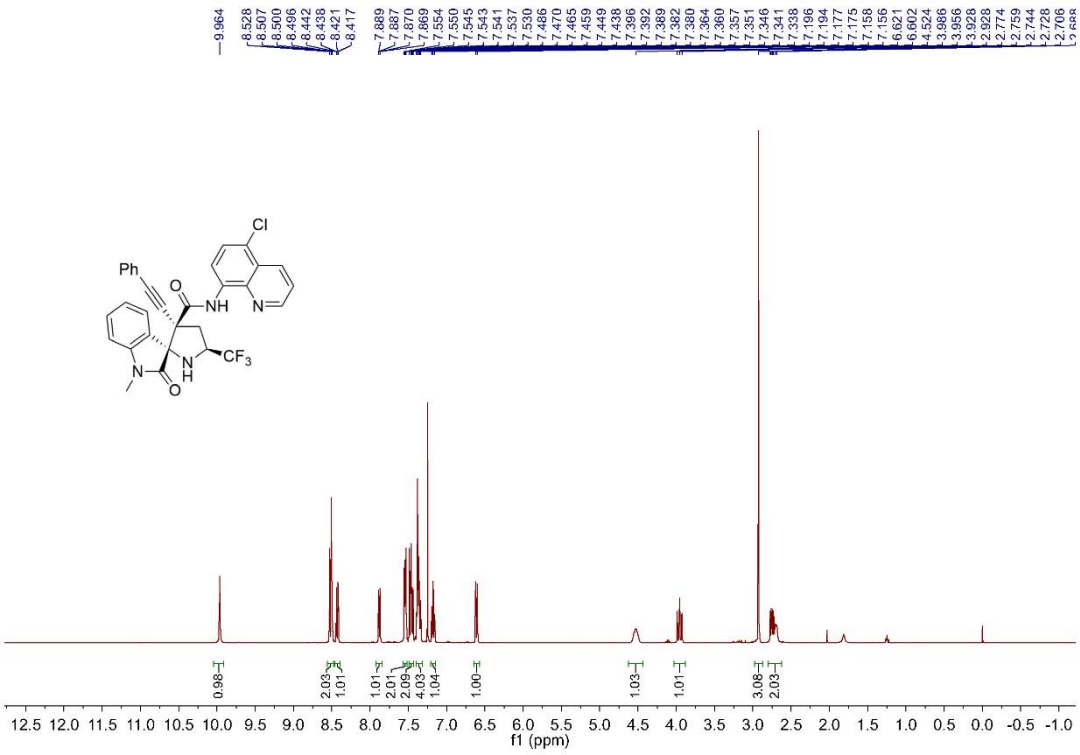
^{13}C NMR spectrum of **3ua** in $CDCl_3$, 101 MHz



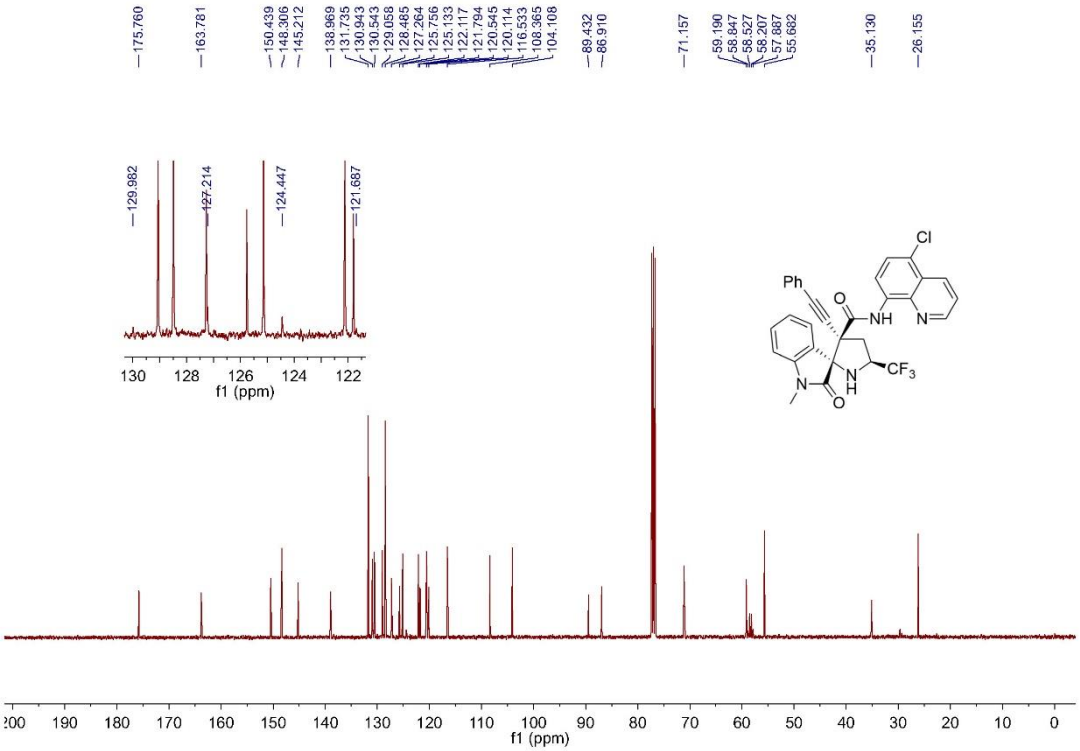
^{19}F NMR spectrum of **3ua** in $CDCl_3$, 376 MHz



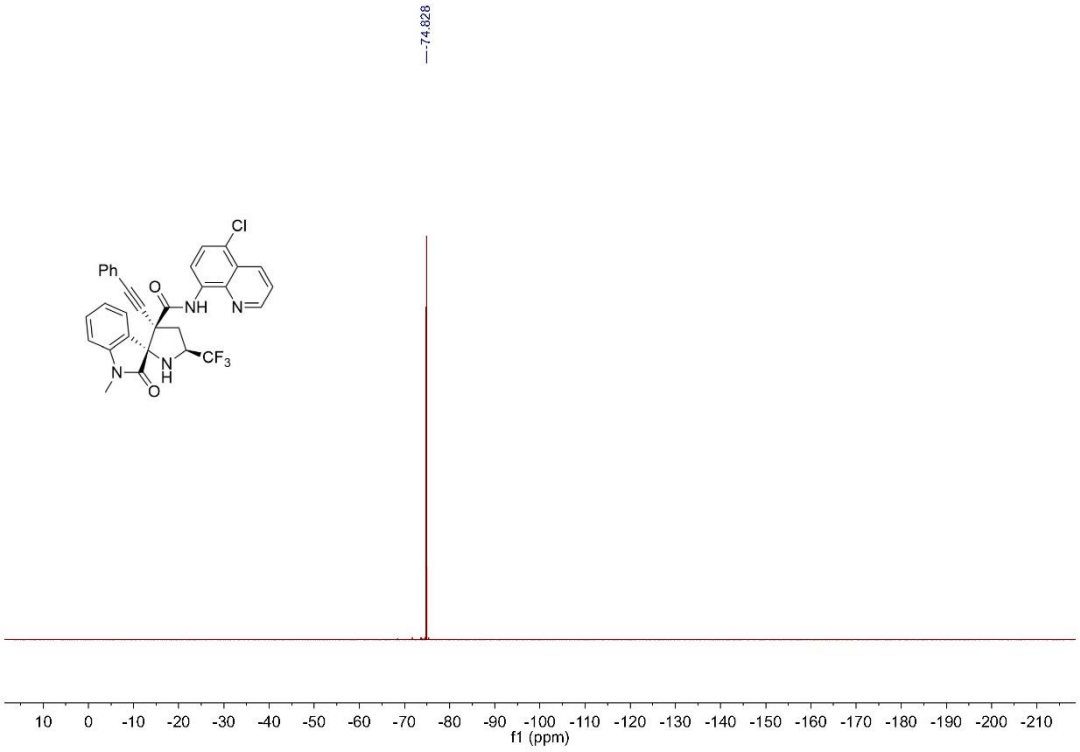
^{1}H NMR spectrum of **3va** in $CDCl_3$, 400 MHz



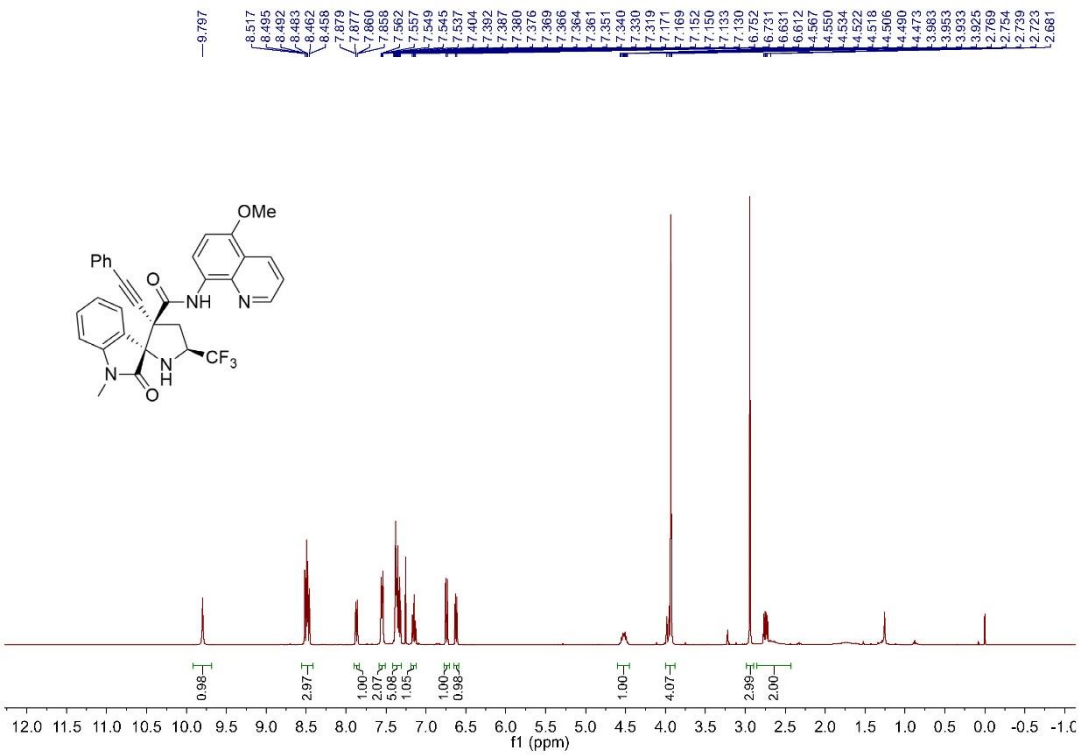
^{13}C NMR spectrum of **3va** in $CDCl_3$, 101 MHz



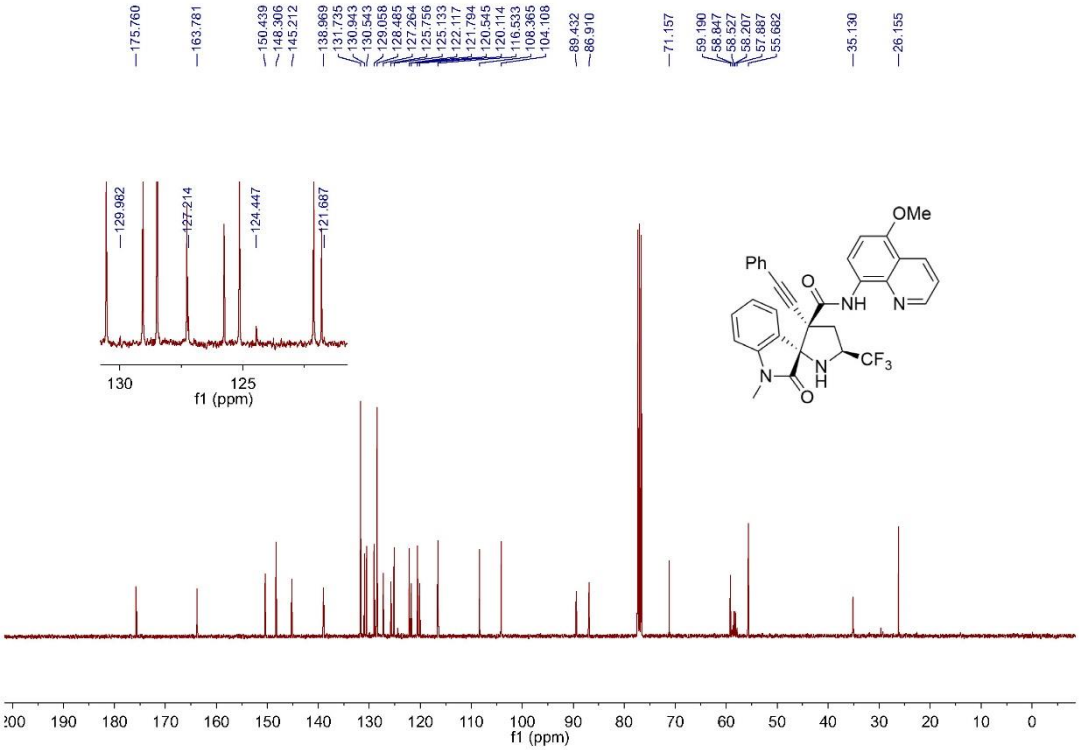
^{19}F NMR spectrum of **3va** in $CDCl_3$, 376 MHz



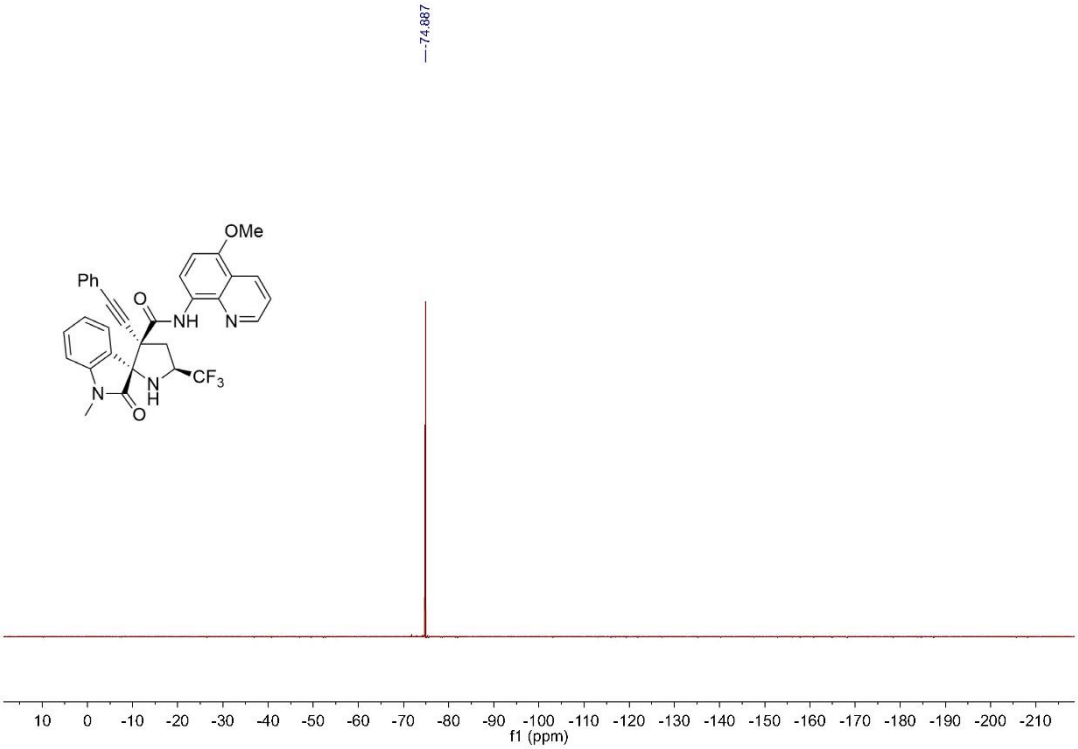
^{1}H NMR spectrum of **3wa** in $CDCl_3$, 400 MHz



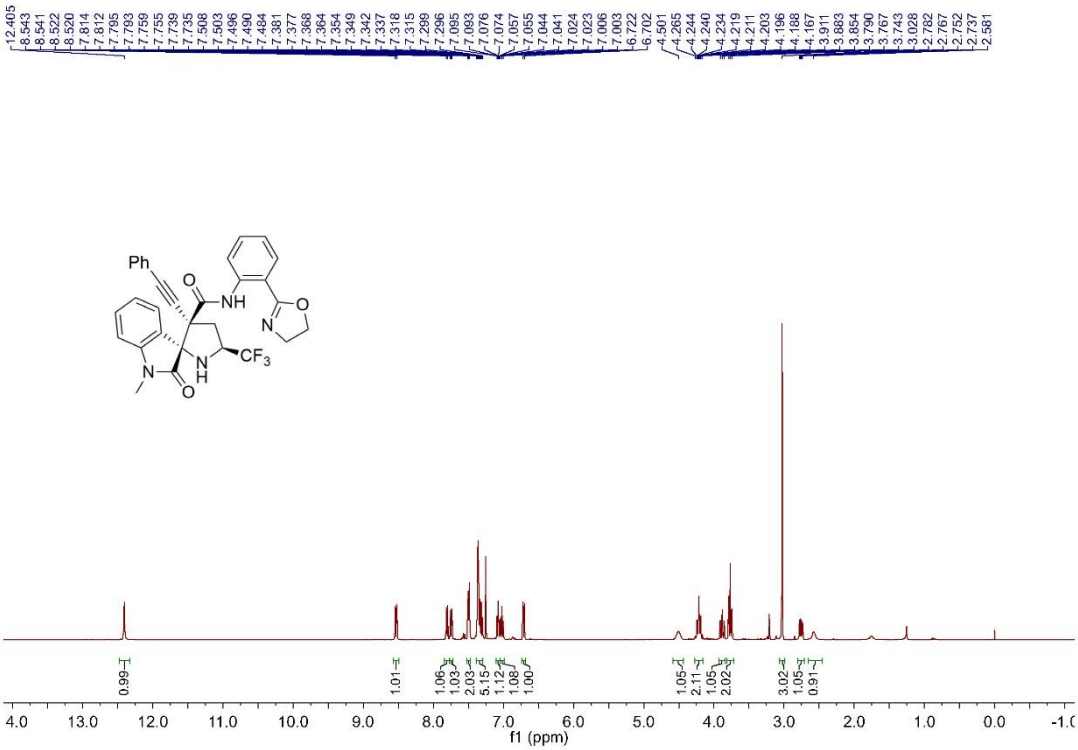
^{13}C NMR spectrum of **3wa** in $CDCl_3$, 101 MHz



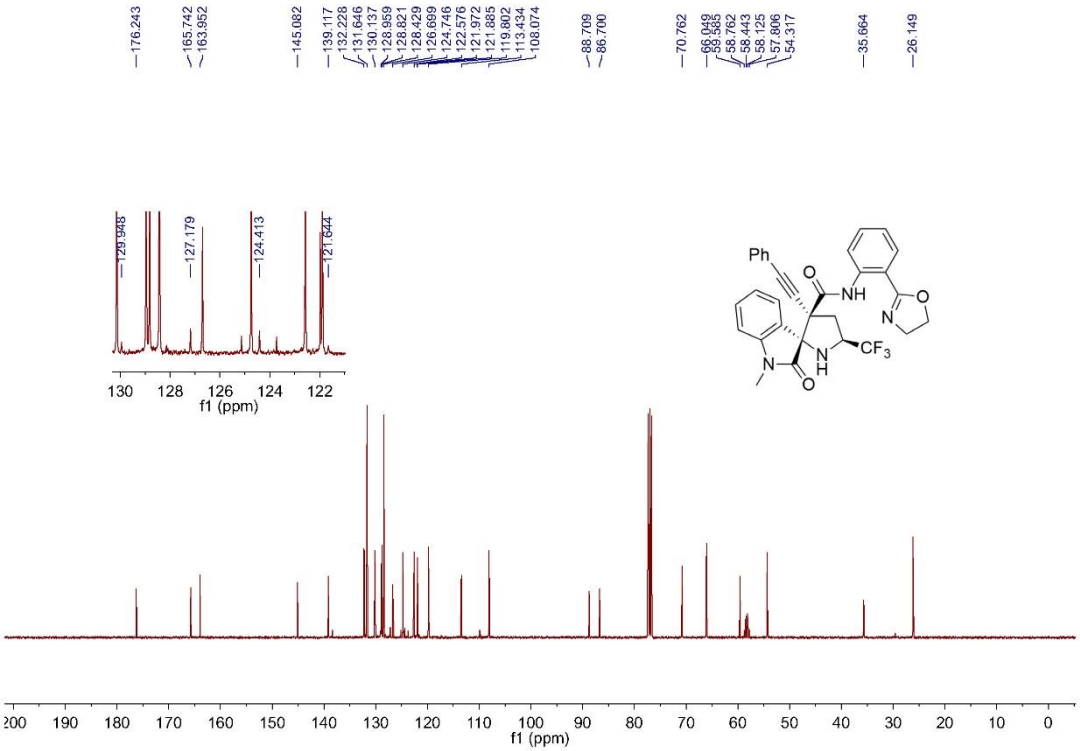
^{19}F NMR spectrum of **3wa** in $CDCl_3$, 376 MHz



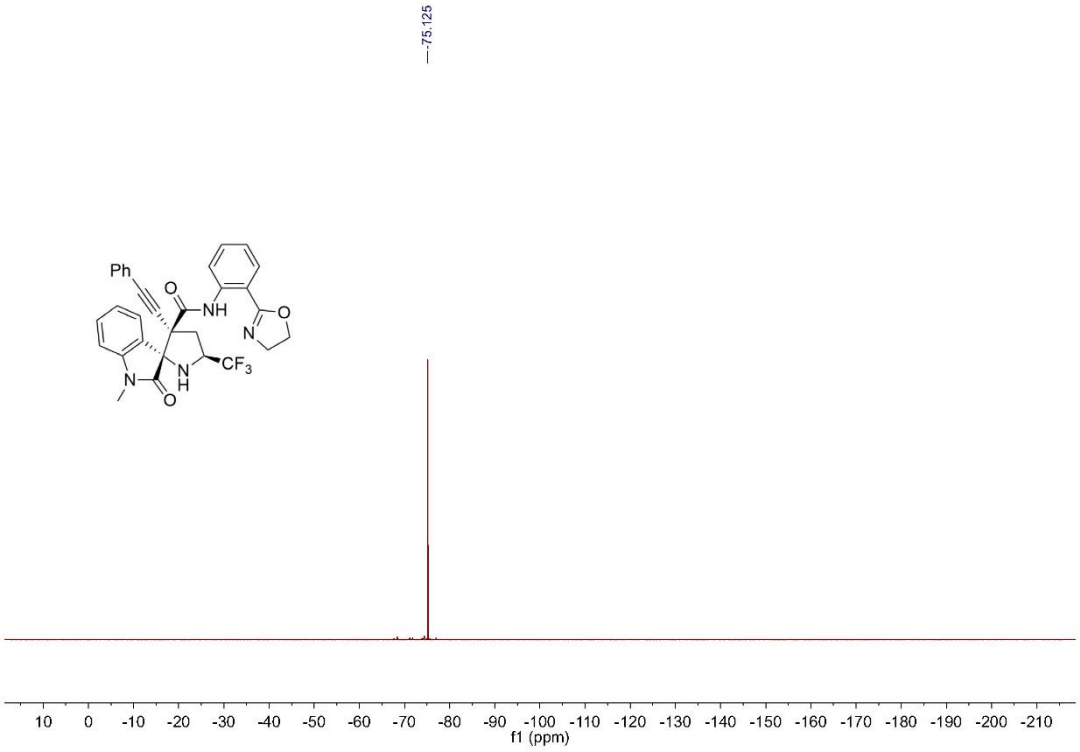
^{1}H NMR spectrum of **3xa** in $CDCl_3$, 400 MHz



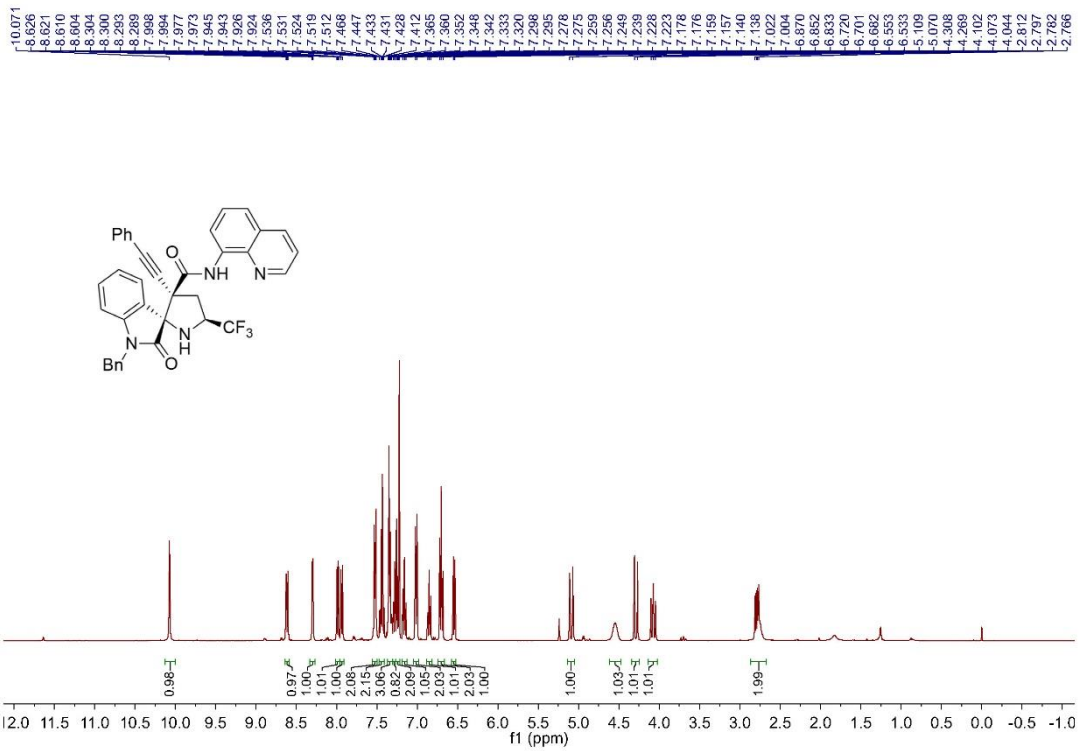
^{13}C NMR spectrum of **3xa** in $CDCl_3$, 101 MHz



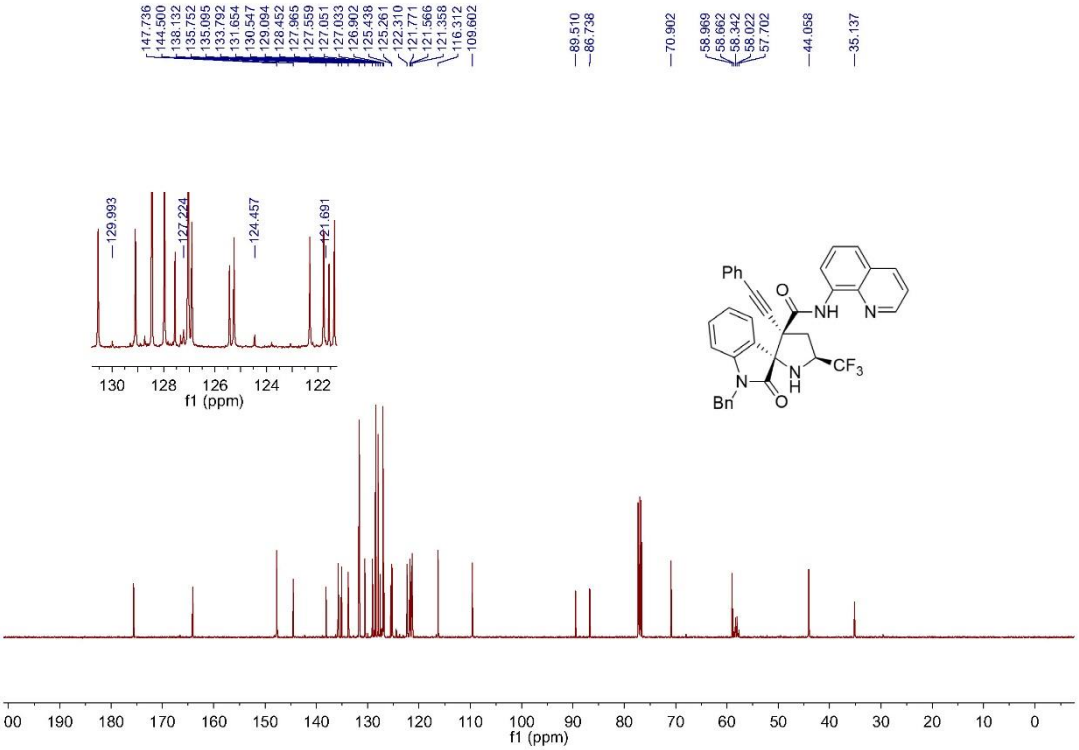
^{19}F NMR spectrum of **3xa** in $CDCl_3$, 376 MHz



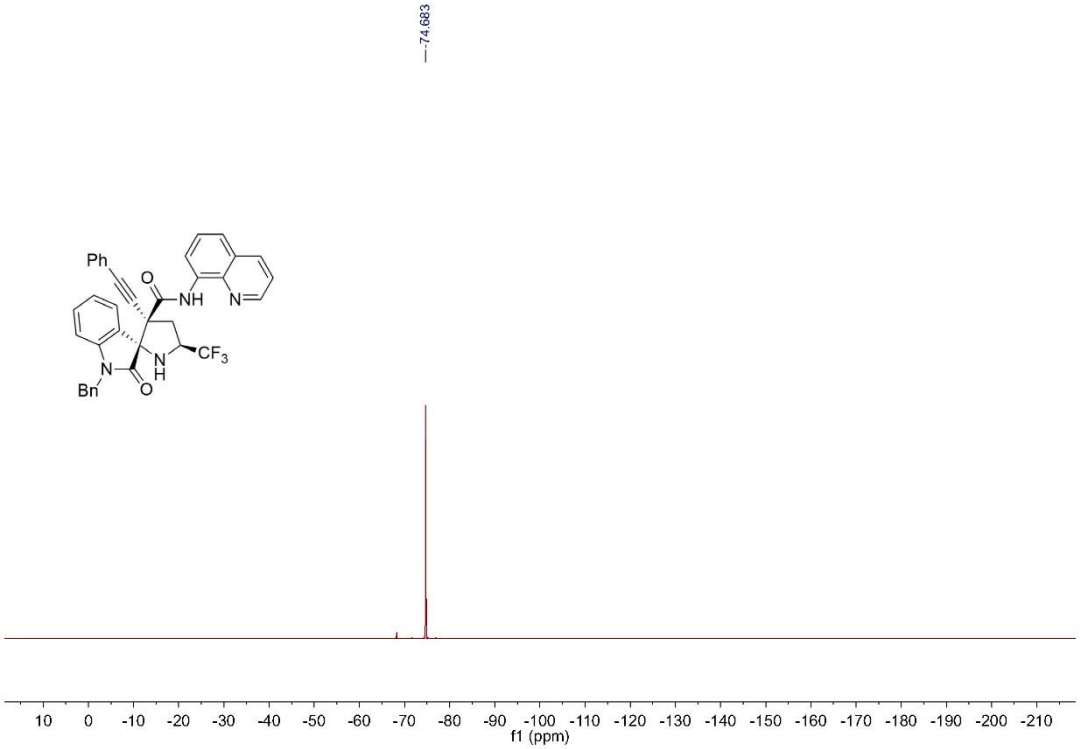
^{1}H NMR spectrum of **3ab** in $CDCl_3$, 400 MHz



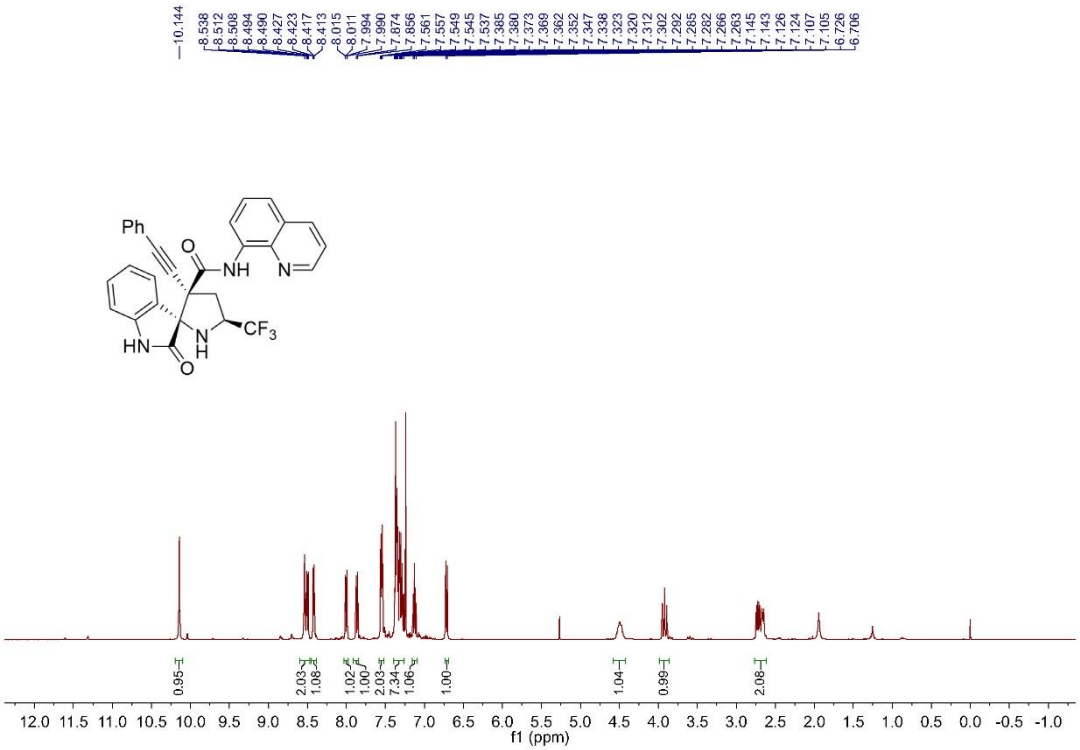
^{13}C NMR spectrum of **3ab** in $CDCl_3$, 101 MHz



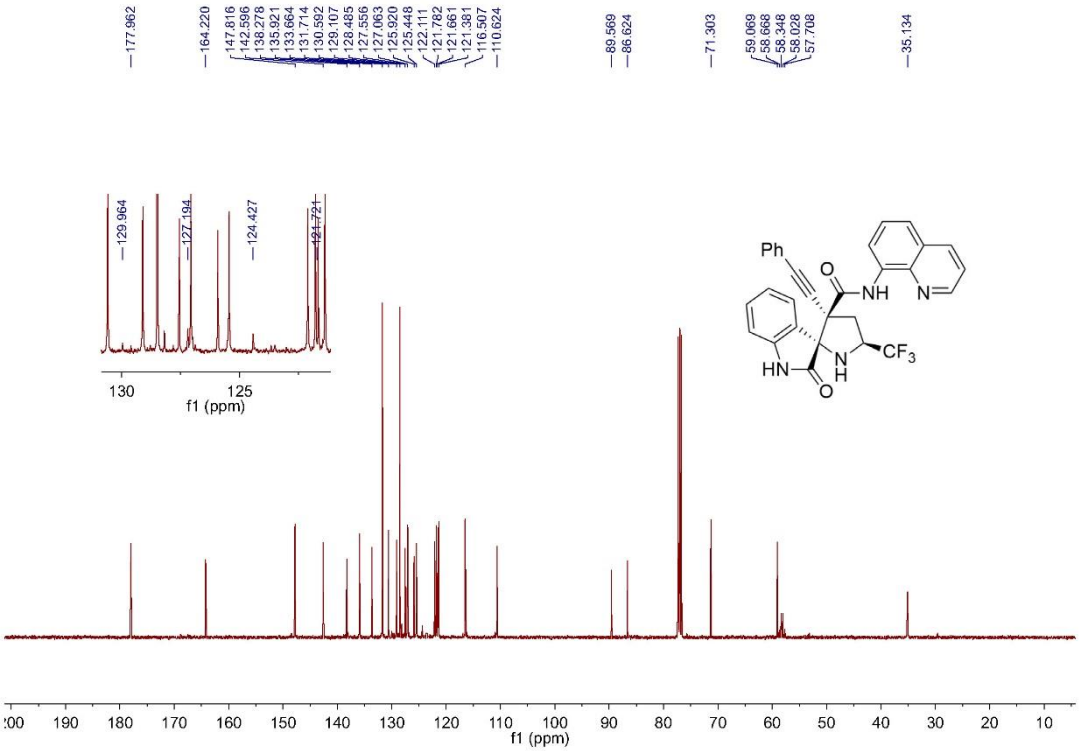
^{19}F NMR spectrum of **3ab** in $CDCl_3$, 376 MHz



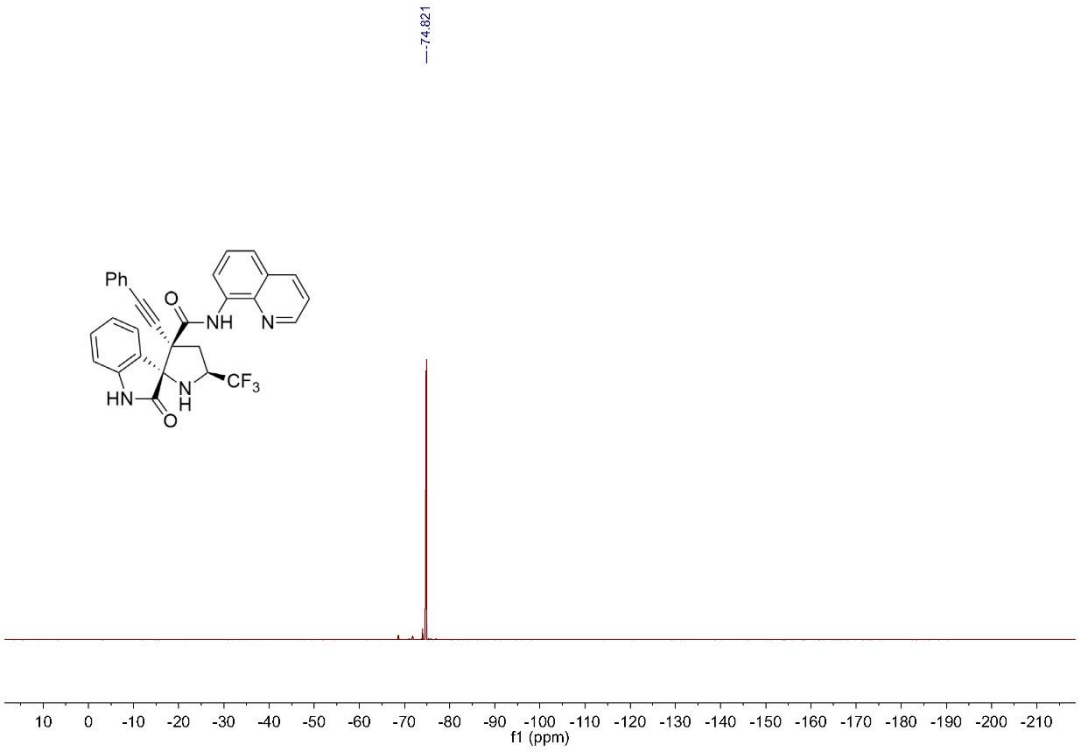
^{1}H NMR spectrum of **3ac** in $CDCl_3$, 400 MHz



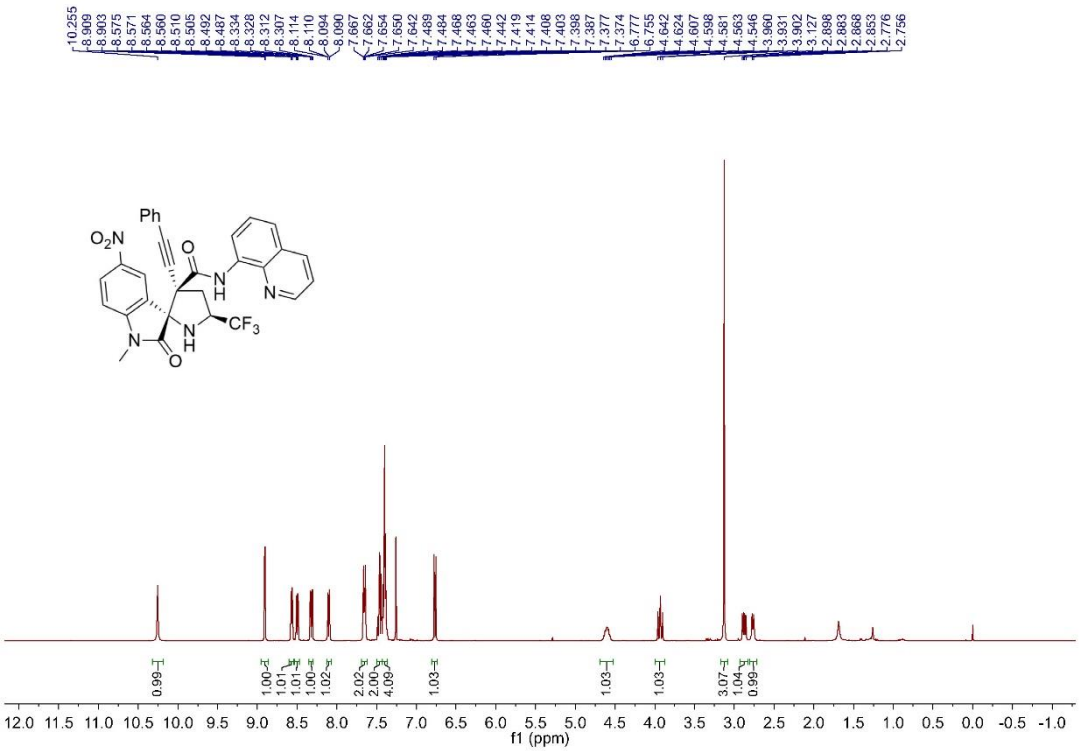
^{13}C NMR spectrum of **3ac** in $CDCl_3$, 101 MHz



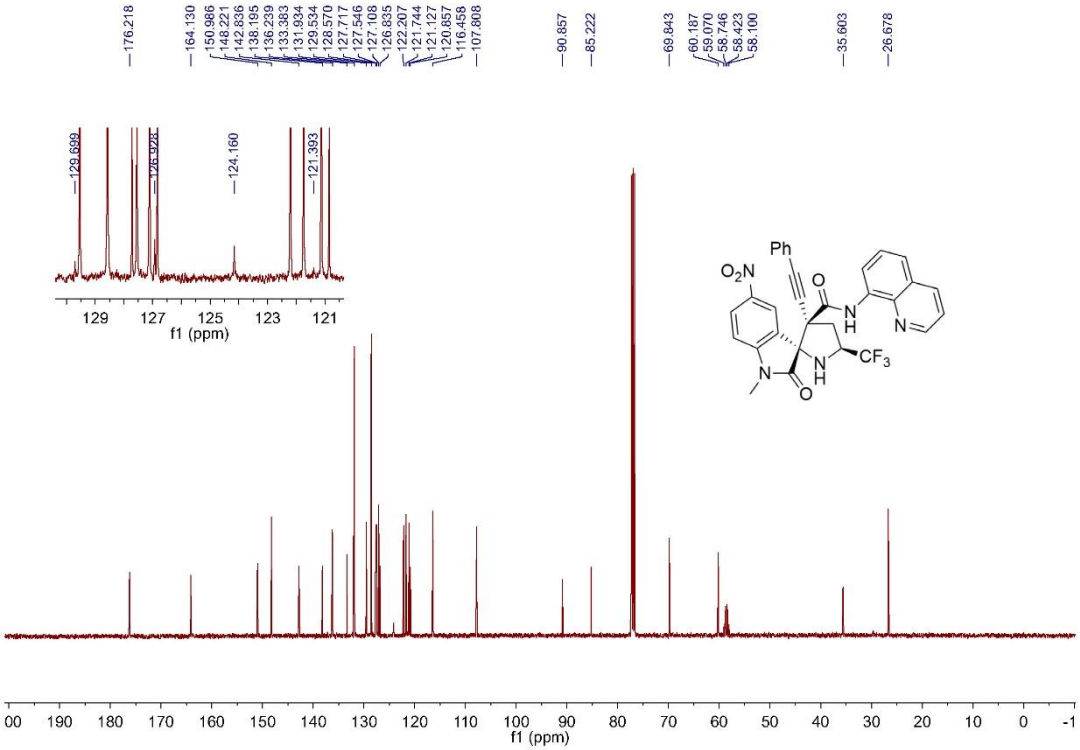
^{19}F NMR spectrum of **3ac** in $CDCl_3$, 376 MHz



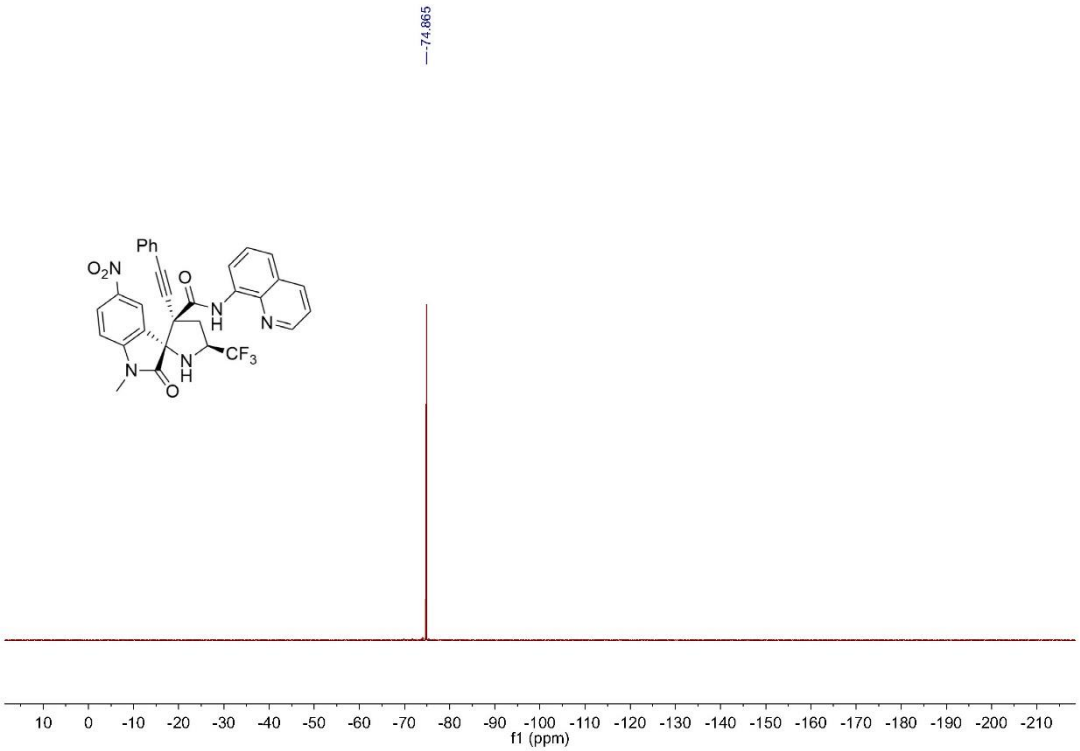
^{1}H NMR spectrum of **3ad** in $CDCl_3$, 400 MHz



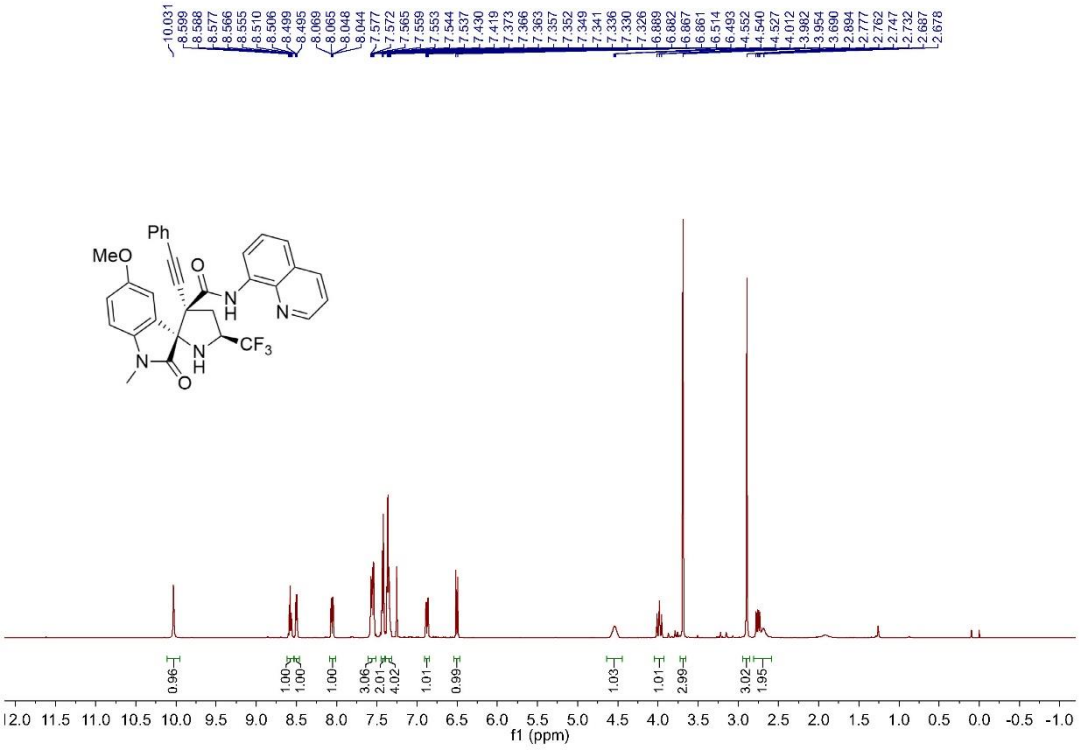
^{13}C NMR spectrum of **3ad** in $CDCl_3$, 101 MHz



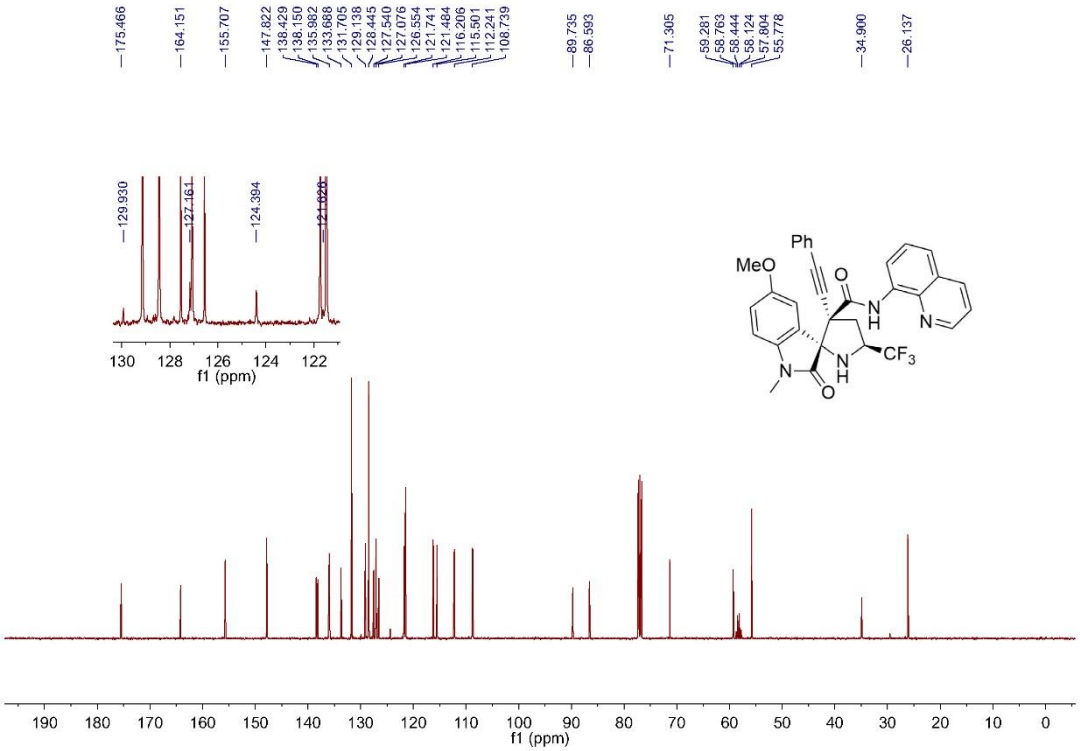
^{19}F NMR spectrum of **3ad** in $CDCl_3$, 400 MHz



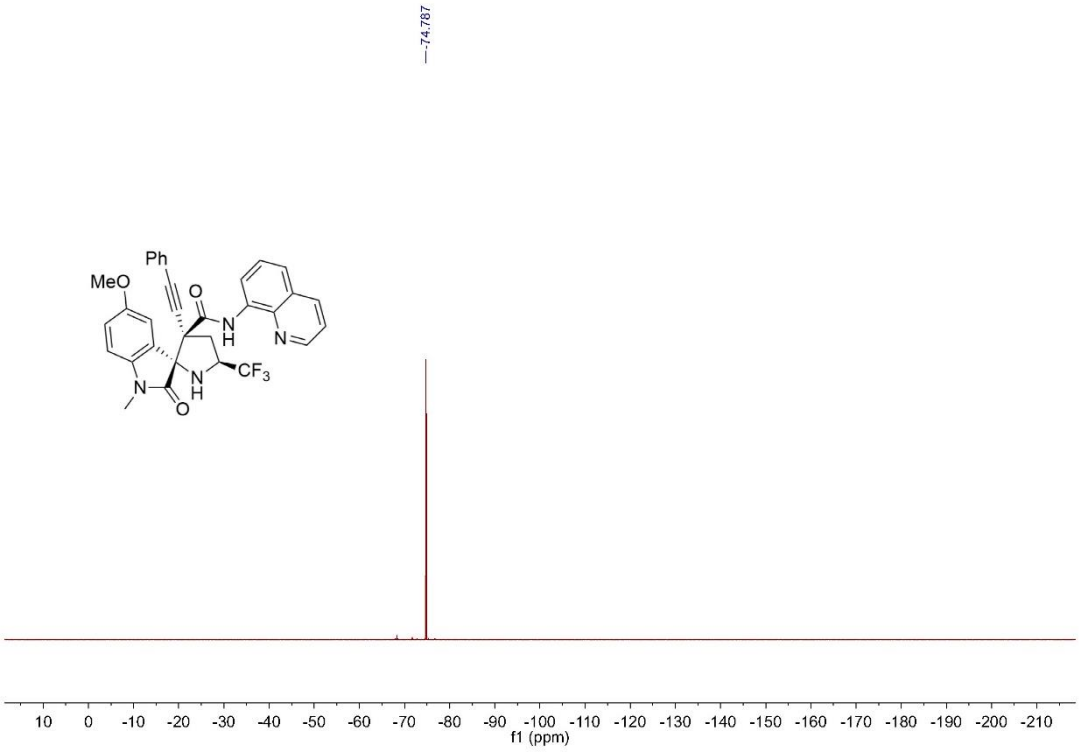
^{1}H NMR spectrum of **3ae** in $CDCl_3$, 400 MHz



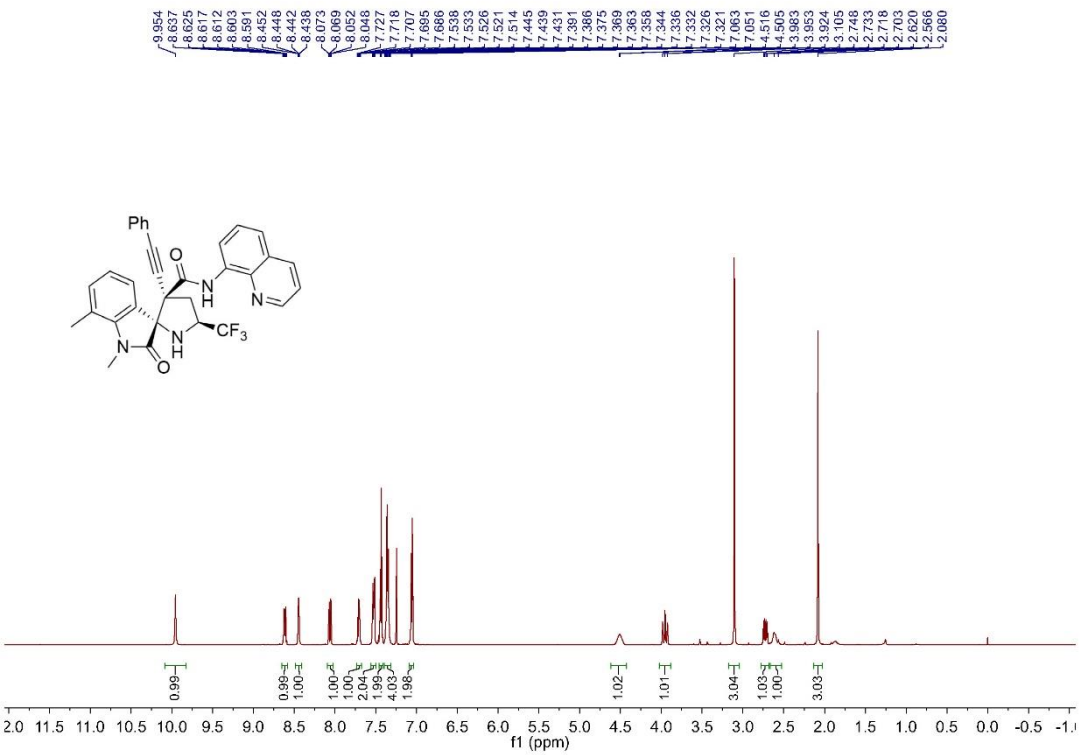
^{13}C NMR spectrum of **3ae** in $CDCl_3$, 101 MHz



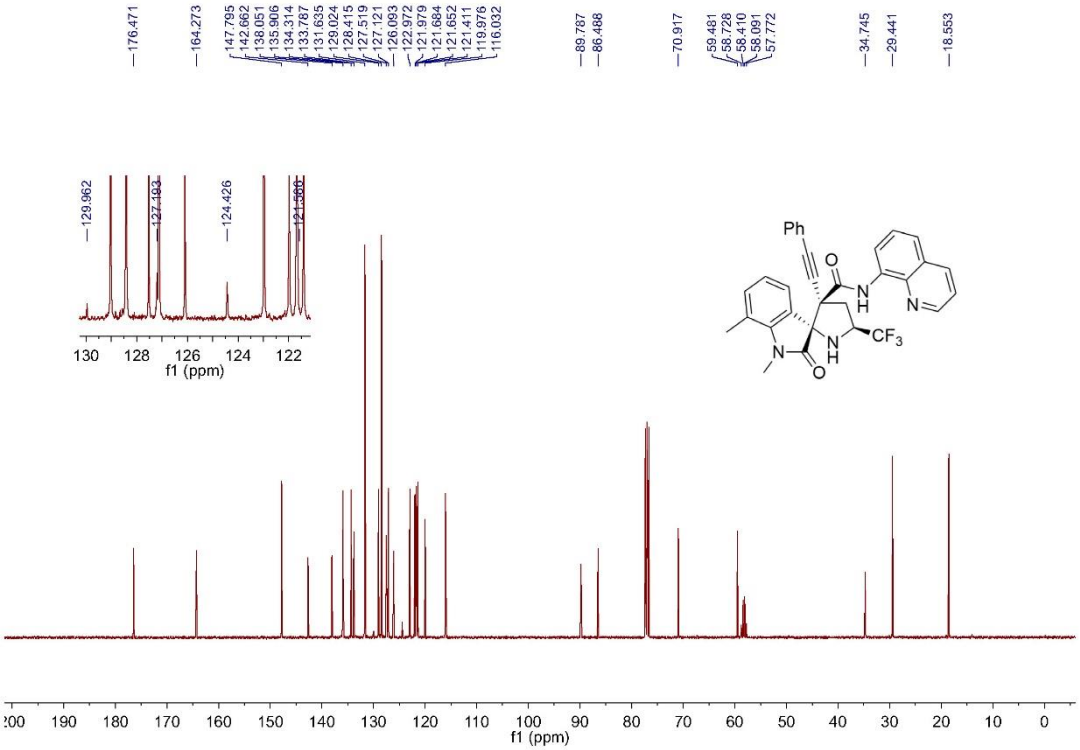
^{19}F NMR spectrum of **3ae** in $CDCl_3$, 376 MHz



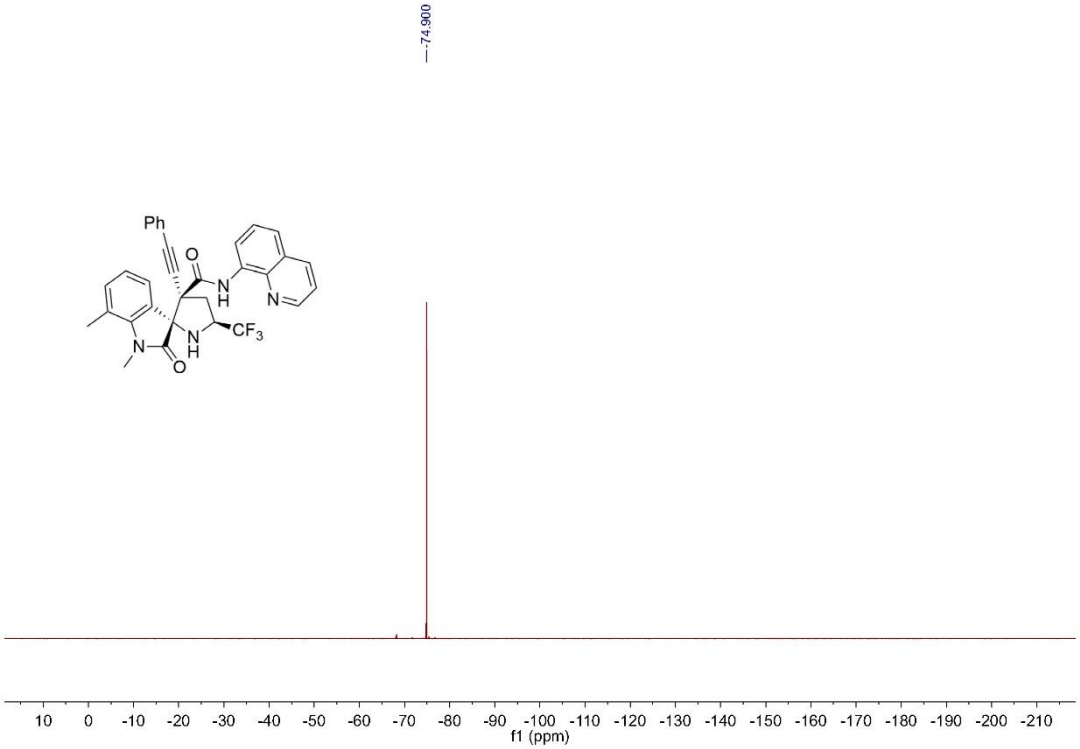
^{1}H NMR spectrum of **3af** in $CDCl_3$, 400 MHz



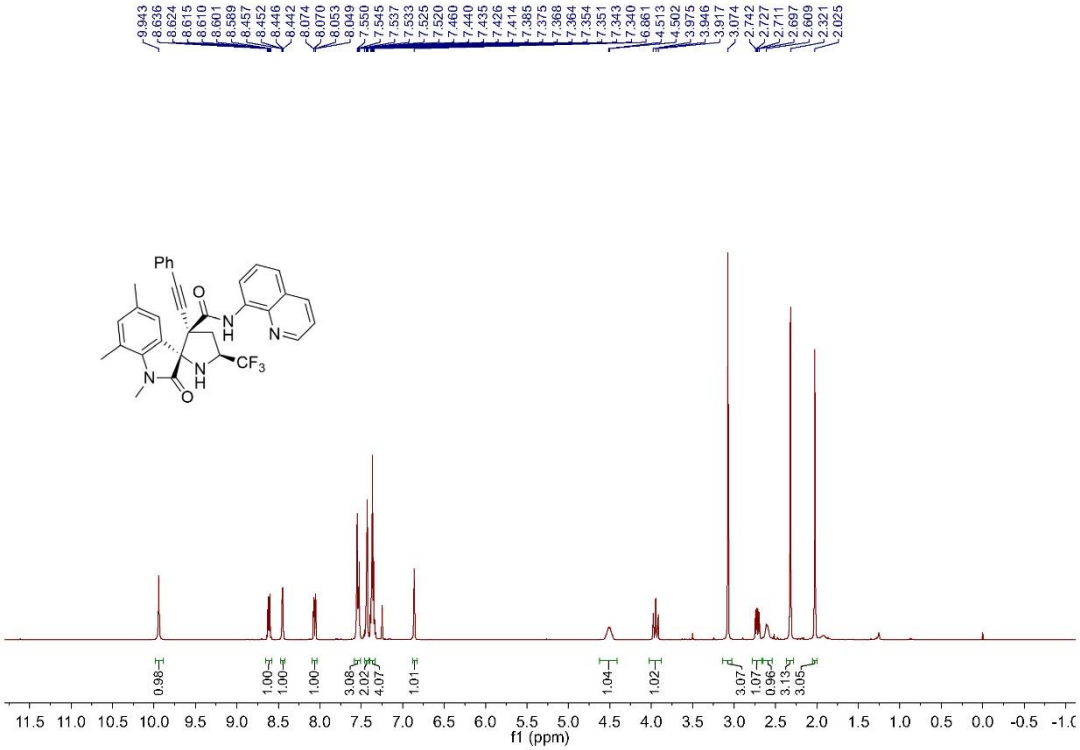
^{13}C NMR spectrum of **3af** in $CDCl_3$, 101 MHz



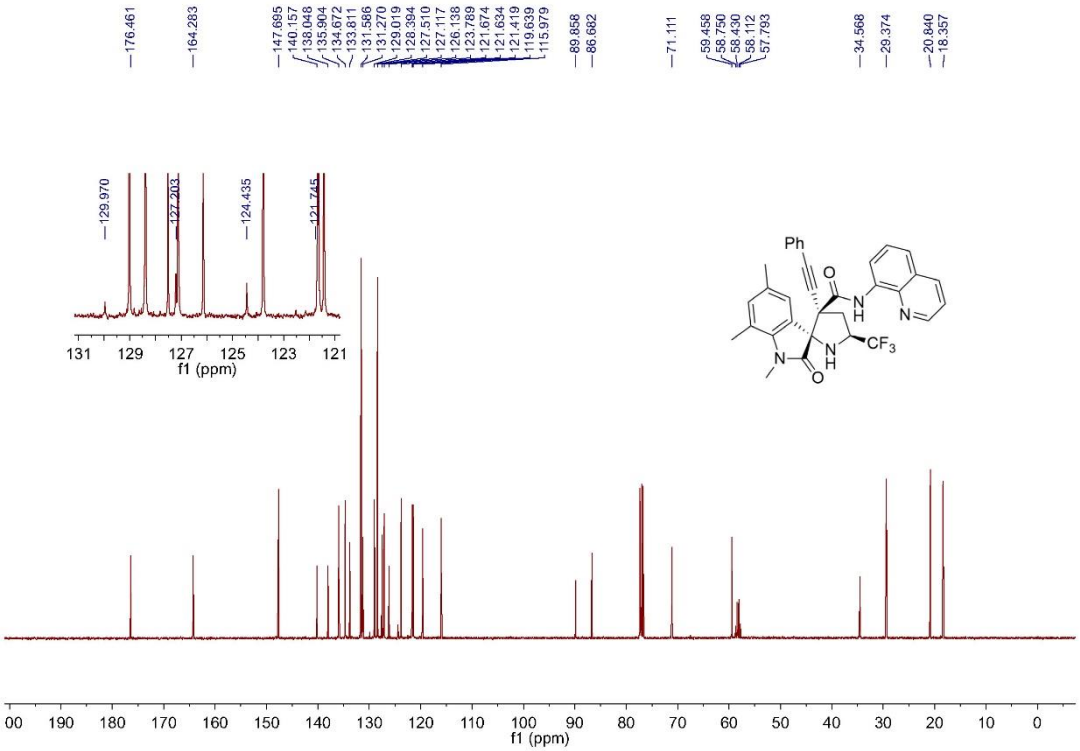
^{19}F NMR spectrum of **3af** in $CDCl_3$, 376 MHz



^{1}H NMR spectrum of **3ag** in $CDCl_3$, 400 MHz

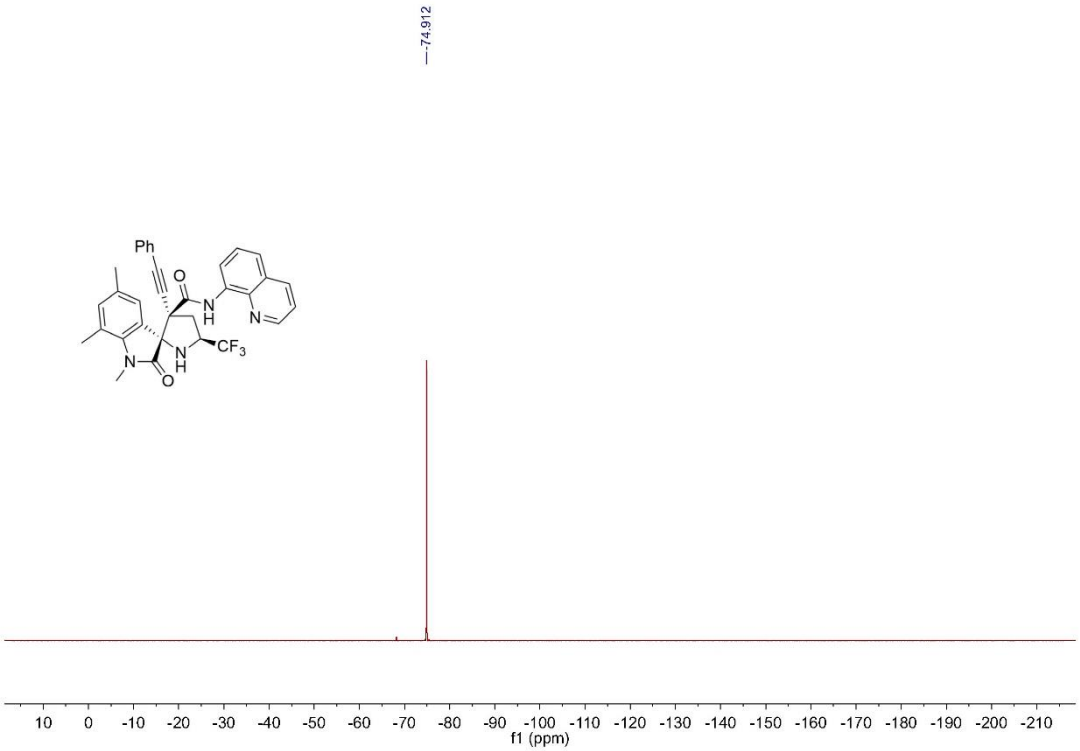


^{13}C NMR spectrum of **3ag** in $CDCl_3$, 400 MHz

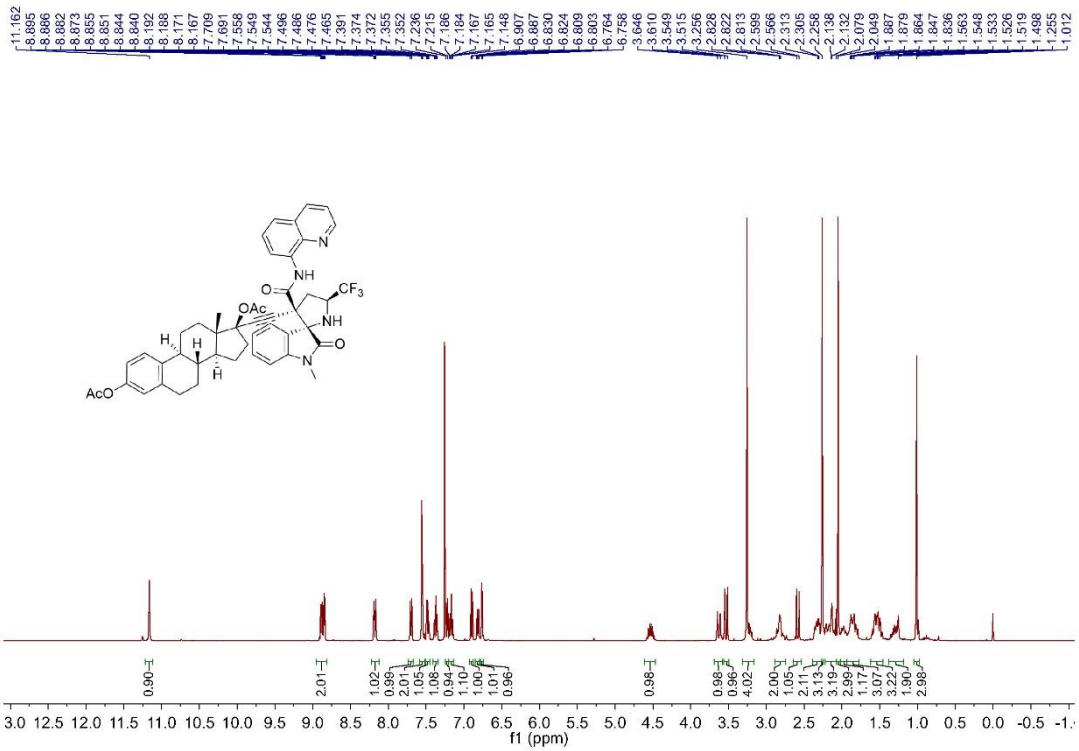


^{19}F NMR spectrum of **3ag** in $CDCl_3$, 376 MHz

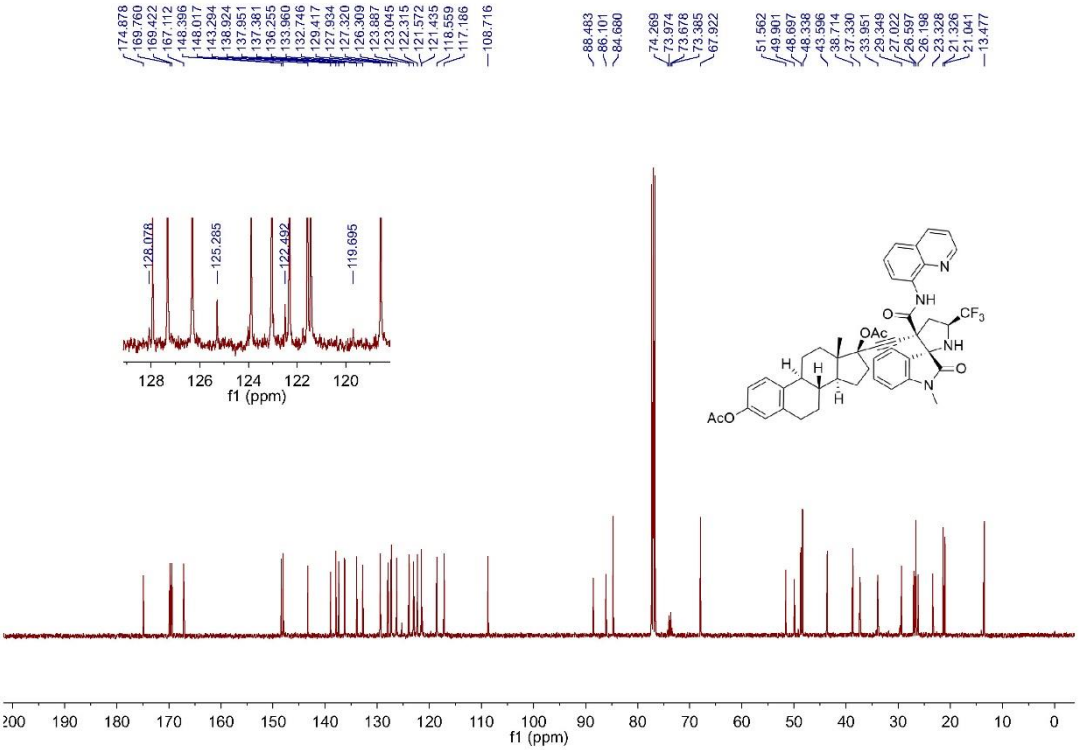
f



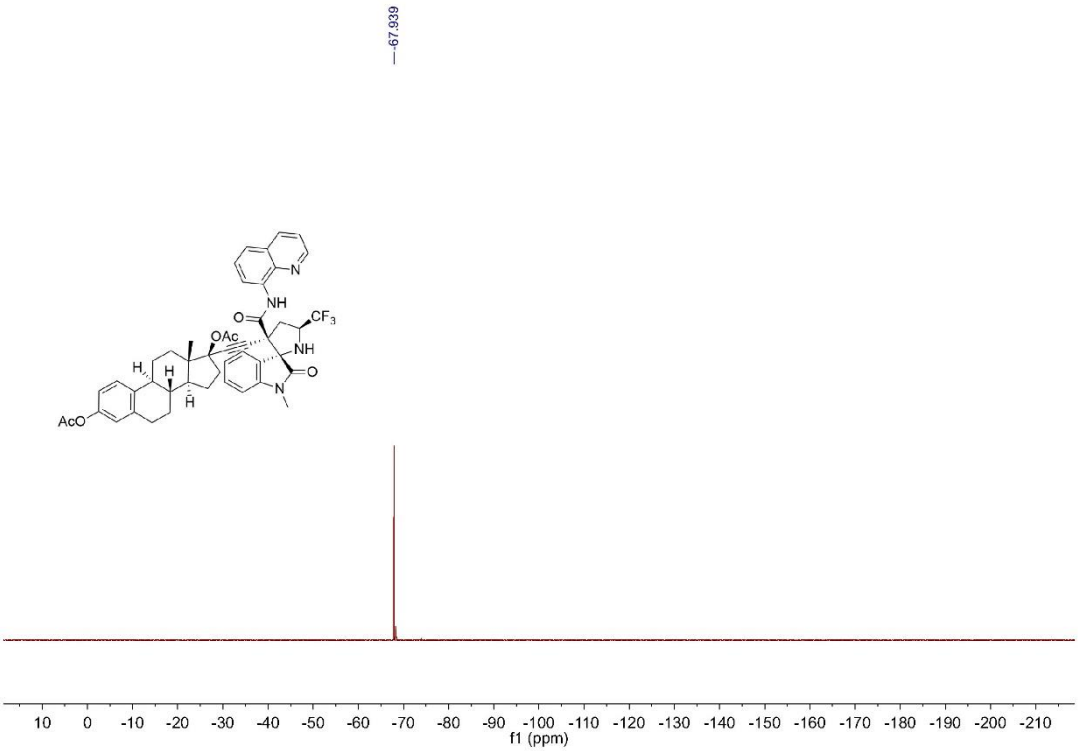
^{1}H NMR spectrum of **3ya** in $CDCl_3$, 400 MHz



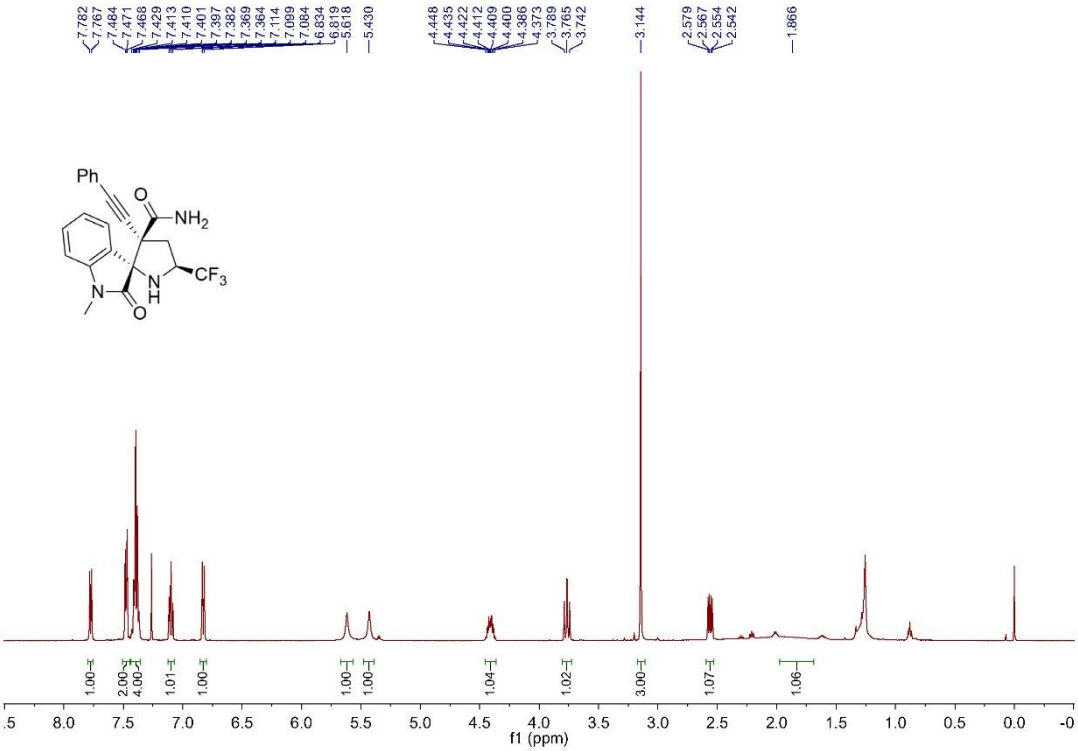
^{13}C NMR spectrum of **3ya** in $CDCl_3$, 101 MHz



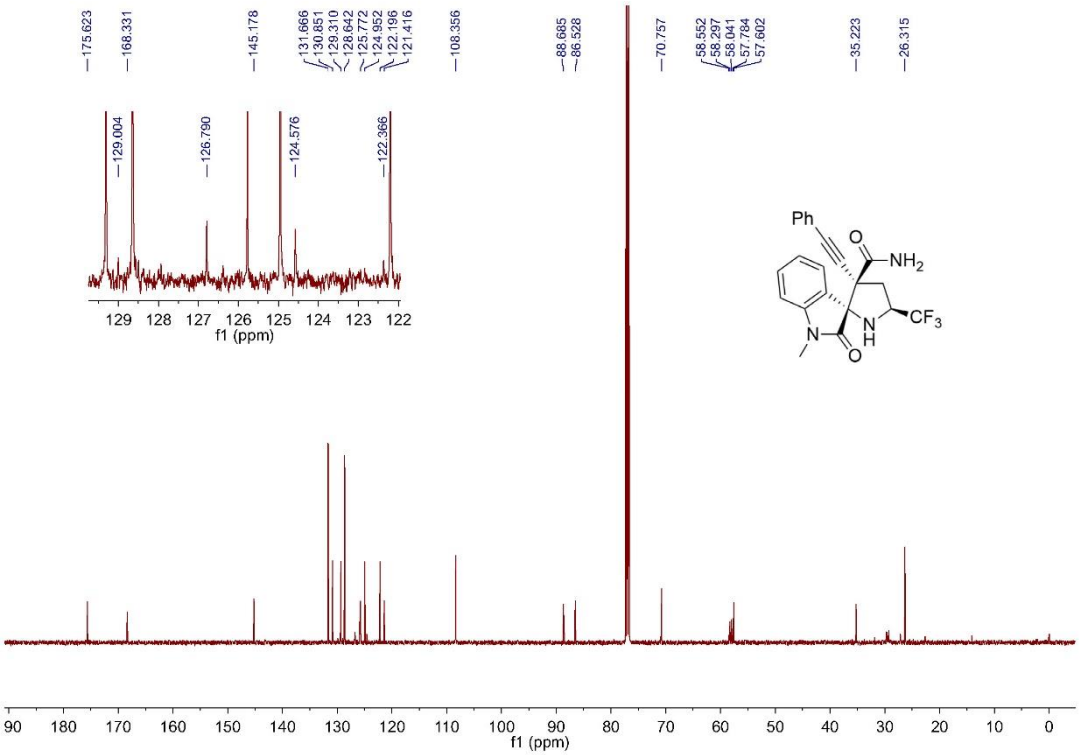
^{19}F NMR spectrum of **3ya** in $CDCl_3$, 376 MHz



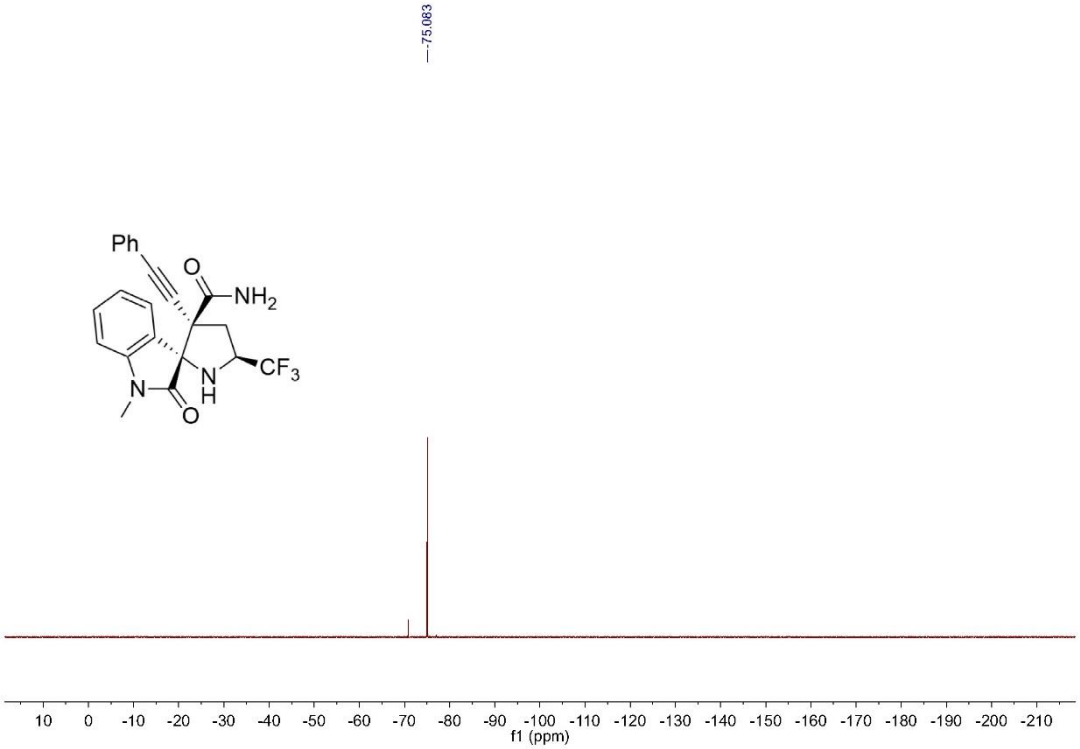
^{1}H NMR spectrum of **4aa** in $CDCl_3$, 500 MHz



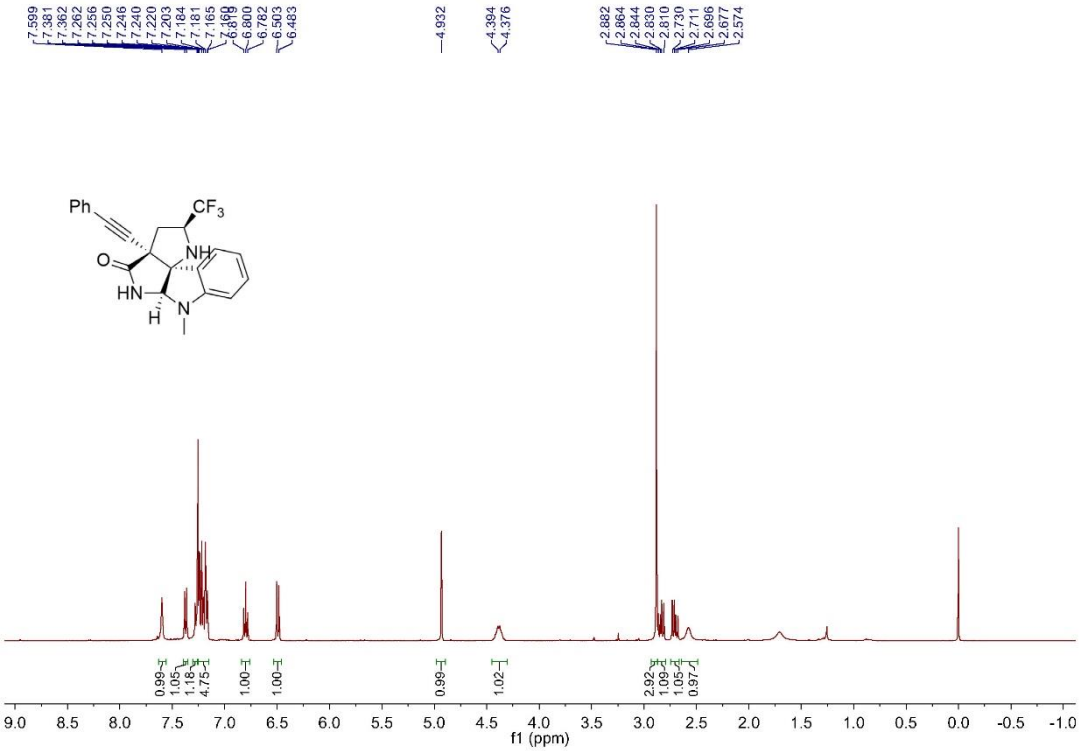
^{13}C NMR spectrum of **4aa** in $CDCl_3$, 126 MHz



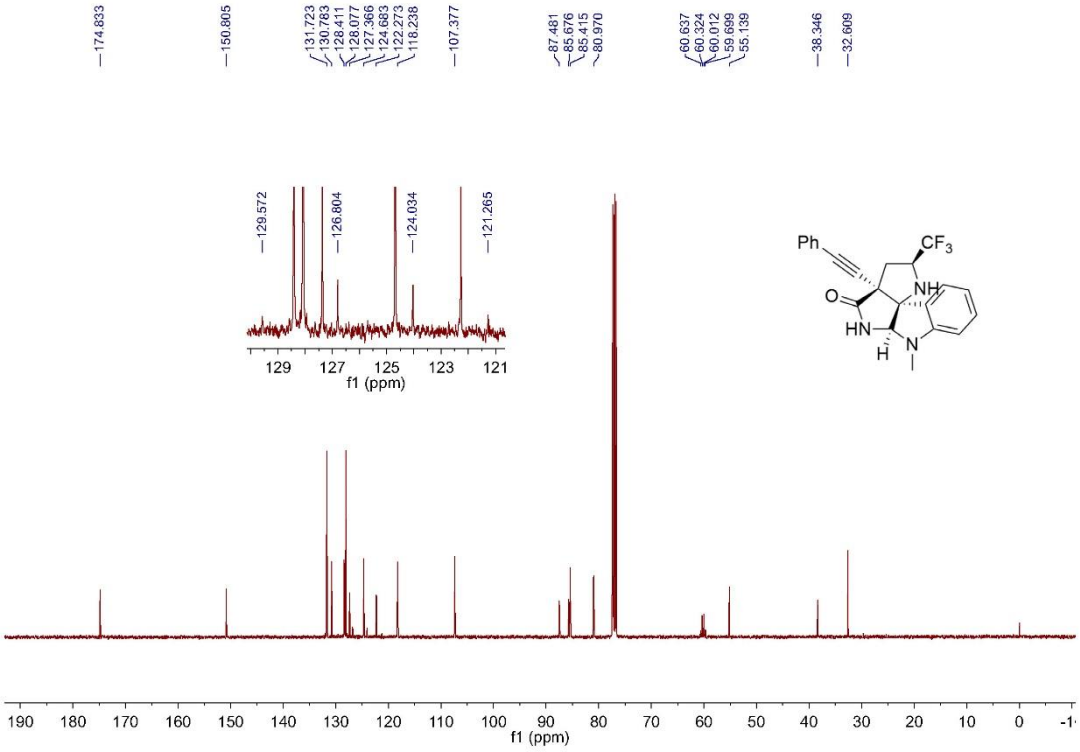
^{19}F NMR spectrum of **4aa** in $CDCl_3$, 376 MHz



^{1}H NMR spectrum of **5aa** in $CDCl_3$, 400 MHz



^{13}C NMR spectrum of **5aa** in $CDCl_3$, 101 MHz



^{19}F NMR spectrum of **5aa** in $CDCl_3$, 376 MHz