Supporting Information

Copper(I)/Ganphos Catalysis: Enantioselective Synthesis of Diversified Spirooxindoles Using Alkyl Substituted Imino Ester and Methyleneindolinones

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1. General Experimental Details

All reactions were performed under nitrogen using solvents dried by standard methods. NMR spectra were obtained using Bruker AV300 spectrometer. Chemical shifts are expressed in parts per million (ppm) downfield from internal TMS. HRMS spectra were obtained on an Agilent 1290-6540 UHPLC Q-Tof HR-MS spectrometer. X-ray crystallographic analyses were performed on an Oxford diffraction Gemini E diffractometer. Melting Point: heating rate: 4 °C/min, the thermometer was not corrected. Enantiomer excesses were determined by chiral HPLC analysis on Chiralcel IA/OD/AD in comparison with the authentic racemates. Chiral HPLC analysis recorded on Shimadzu labtotal LC-20AT. Silica gel (200-300 mesh) was used for the chromatographic separations. All commercially available reagents were used without further purification.

The DFT calculations were performed using the Gaussian16 program[1]. All structures were optimized at the M06-L[2-4]/6-31G(d, p)/SMD_{THF} level, and the corresponding vibrational frequencies were calculated at the same level. Then, frequency calculations at the same level of theory were carried out to identify all of the stationary points as minima (zero imaginary frequency) or transition state (only one frequency), and to provide free energies. The NCI analysis was plotted using Multiwfn[5].

References

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Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, Gaussian16, Gaussian, Inc., Wallingford, CT, 2016.

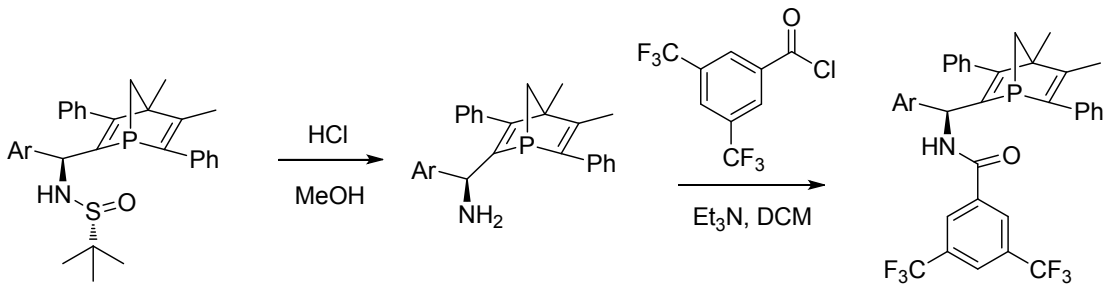
2. Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* 2008, **120**, 215.

3. Y. T. Zhao, D. G. Truhlar, *J. Chem. Theory Comput.* 2008, **4**, 1849.

4. Y. T. Zhao, D. G. Truhlar, *Acc. Chem. Res.* 2008, **41**, 157.

5 T. Lu, F. Chen, *J. Comput. Chem.*, 2011, **33**, 580.

2. General Procedure for the Synthesis of Ligands



Ganphos **A** **Kephos**

Ar = 4-^{t}BuC$_6$H$_4$

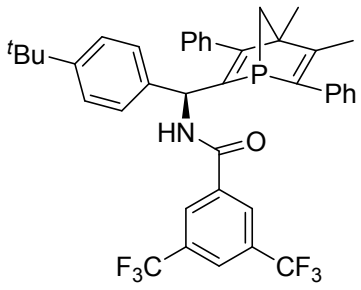
The **Ganphos** was prepared according to the modified procedure of literature.[6]

4 M HCl (4 mmol) was added slowly to the solution of **Ganphos** (0.5 mmol) in MeOH at room temperature and the mixture was stirred for 8 h until completion of the material as indicated by TLC analysis, followed by extracted with aq $NaHCO_3$ and DCM. The combined organic phases were dried over $MgSO_4$ and the solvents were removed in vacuo. Residue was directly purified by chromatography to afford **A**. The isolated yield is 74%.

A stired solution of **A** in DCM was added 3,5-Bis(trifuoromethyl)phenyl isothiocyanate (1.4 eq.) and Et_3N (2.0 eq) under the protection of N_2. The mixture was then stirred at room temperature until completion of **A** as indicated by TLC analysis, after completion of the reaction, the reaction mixture was extracted with aq $NaHCO_3$ and DCM. The organic phases were dried over $MgSO_4$ and the solvents were directly purified by silica gel chromatography using petroleum ether/EtOAc as the eluent to afford the desired **Kephos** in 80% yield.

6. Z.-J. Gan, M.-N. Zhi, R.-P. Han, E.-Q. Li, Z. Duan, F. Mathey. *Org. Lett*. 2019, **21**, 2782.

General Data for Kephos



Kephos

N-((S)-(4-(tert-butyl)phenyl)((1R,4S)-4,5-dimethyl-3,6-diphenyl-1-phosphabicyclo[2.2.1]hepta-2,5-dien-2-yl)methyl)-3,5-bis(trifluoromethyl)benzamide

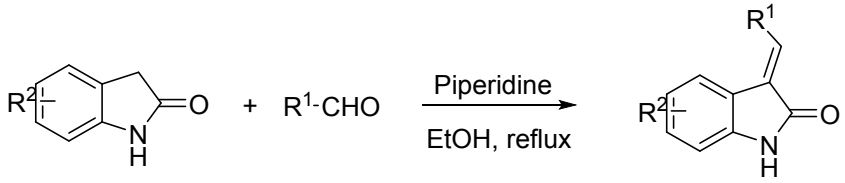
White solid, $\mathbf{R}_f$ = 0.38. (petroleum ether/ ethyl acetate 5/1). **MP:** 76.5-77.5 °C. $[\alpha]_D^{25}$ = 95 (*c* 0.16, CH_2Cl_2).

^{31}P NMR (121 MHz, $CDCl_3$) δ -18.68 (s) ppm. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 1.31 (s, 9H), 1.35 (s, 3H), 2.08 (s, 3H), 2.17 (dd, *J* = 19.6, 9.8 Hz, 2H), 5.86 (t, *J* = 7.9 Hz, 1H), 6.37 (d, *J* = 7.4 Hz, 1H), 6.78 (t, *J* = 7.3 Hz, 1H), 6.91 (t, *J* = 7.6 Hz, 2H), 7.06 (d, *J* = 7.9 Hz, 2H), 7.11 (d, *J* = 6.4 Hz, 2H), 7.29 (d, *J* = 7.3 Hz, 1H), 7.31-7.42 (m, 6H), 7.68 (s, 2H), 7.82 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 15.5, 20.5, 31.4, 34.6, 54.7 (d, $J_{C\text{-}P}$ = 18.8 Hz), 63.5, 71.4 (d, $J_{C\text{-}P}$ = 5.2 Hz), 121.1, 124.6 (d, $J_{C\text{-}F}$ = 10.6 Hz), 126.0, 126.1, 126.9 (d, $J_{C\text{-}P}$ = 2.6 Hz), 127.4, 127.4, 127.5, 127.8, 128.0,

128.1, 128.4, 131.6 (q, $J_{C\text{-}F}$ = 33.7 Hz), 136.1, 137.3, 137.5 (d, $J_{C\text{-}F}$ = 1.8 Hz), 138.2 (d, $J_{C\text{-}P}$ = 20.8 Hz), 147.9 (d, $J_{C\text{-}P}$ = 21.7 Hz), 151.1, 152.8 (d, $J_{C\text{-}P}$ = 26.4 Hz), 157.3, 162.4, 163.4 ppm.

3. Synthesis of starting materials

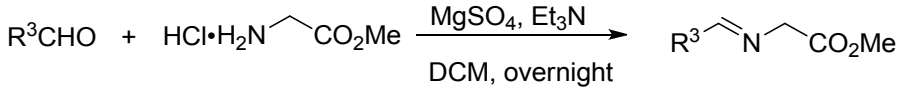
Synthesis of methyleneindolinone derivatives 1.[7]



1

A mixture of oxindole (10 mmol), corresponding aldehyde (11 mmol), and 20 mol% piperidine (2 mmol) were disolved in 15 mL ethanol. After refluxing for 8 hours, the reaction was cooled to room temperature. Crude product was purified by column chromatography on silica gel to give the compound **1**.

Synthesis of glycine imino ester 2.[7]



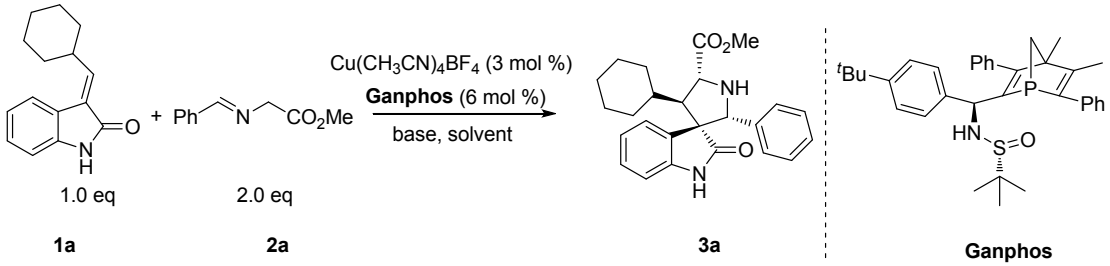
2

To a suspension of glycine methyl ester hydrochloride (1.1 equiv) and $MgSO_4$ (2.0 equiv) in DCM was added Et_3N (1.1 equiv). Then, this solution was stirred at room temperature for 1 h. Subsequently, the aldehyde (1.0 equiv) was added and the reaction was stirred at room temperature overnight. After completion $MgSO_4$ was removed by filtration and the filtrate was washed with water and extracted with DCM. The combined organic phases were dried over anhydrous $MgSO_4$, filtered and dried under reduced pressure.

7. C. Gomez, M. Gicquel, J.-C. Carry, L. Schio, P. Retailleau, A. Voituriez, A. Marinetti, *J. Org. Chem*. **2013**, *78*, 1488.

4. Reaction Conditions

Table S1: Optimization Reaction[a]

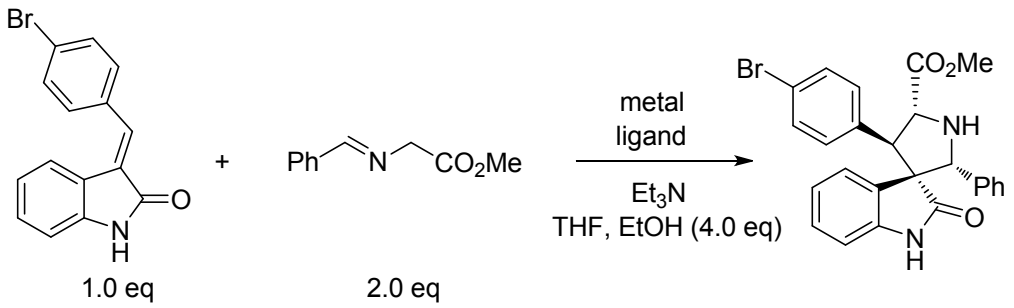


entry	solvent	base	yield (%)[b]	dr[c]	ee (%)[d]
1	THF	Et_3N	86	73:27	92
2	Et_2O	Et_3N	89	80:20	64
3	DCM	Et_3N	trace	-	-
4	CH_3CN	Et_3N	n.r.	-	-
5	EtOAc	Et_3N	96	69:31	79
6	MeOH	Et_3N	94	96:4	78
7	EtOH	Et_3N	94	>20:1	72
8	THF	Cs_2CO_3	59	75:25	91
9	THF	t-BuOK	74	76:24	80
10	THF	K_2CO_3	59	70:30	91
11	THF	DMAP	49.5	76:24	85
12	THF:MeOH/1:1	Et_3N	72	90:10	79
13	THF:MeOH/2:1	Et_3N	77	89:11	76
14[e]	MeOH	Et_3N	54	93:7	62
15[e]	EtOH	Et_3N	trace	-	-
16[e]	THF	Et_3N	74	85:15	95
17[f]	THF	Et_3N	77	86:14	88
18[g]	THF	Et_3N	80	81:19	91
19[h]	THF	Et_3N	89	80:20	89

20[i]	THF	Et_3N	89	83:17	86
21[e, g]	THF	Et_3N	97	89:11	93
22[e, h]	**THF**	**Et_3N**	**80**	**92:8**	**95**
23[e, i]	THF	Et_3N	69	92:8	92

[a] Reaction conditions: **1a** (0.1 mmol), **2a** (0.2 mmol), $Cu(MeCN)_4BF_4$ (3 mol%), **L*** (6 mol%) and base (20 mol%) in solvent (1.0 mL), RT, N_2, 4 h. [b] Yields of isolated product. [c] Determined by ^1H NMR analysis of the crude mixture. [d] Determined by chiral HPLC analysis. [e] The reaction was performed at -20 °C. [f] MeOH (2.0 eq) in THF (1.0 mL). [g] EtOH (3.0 eq) in THF (1.0 mL). [h] EtOH (4.0 eq) in THF (1.0 mL). [i] EtOH (6.0 eq) in THF (1.0 mL).

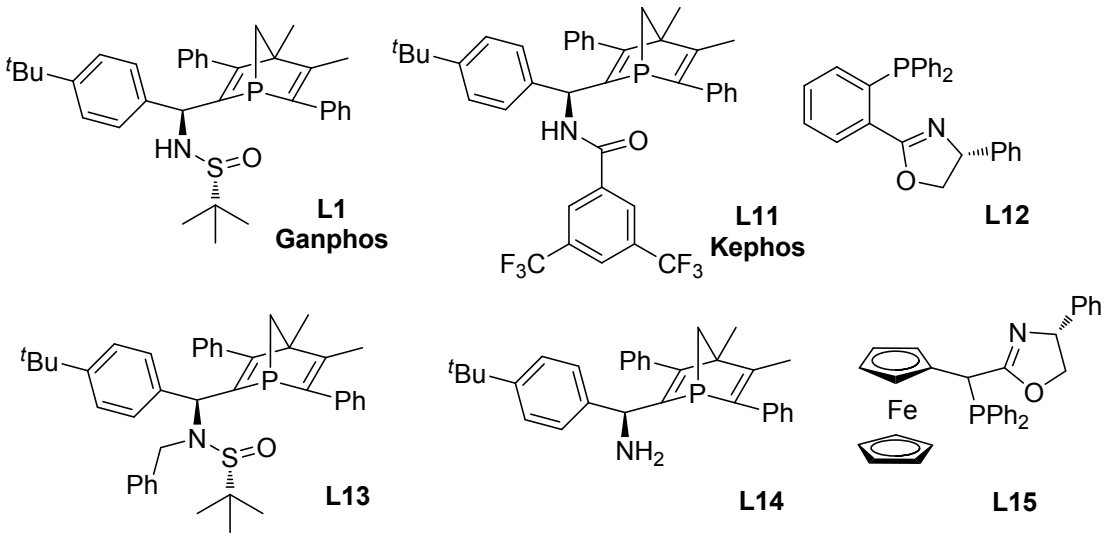
Table S2: Optimization Reaction[a]



1.0 eq **1l** 2.0 eq **2a** **3la**

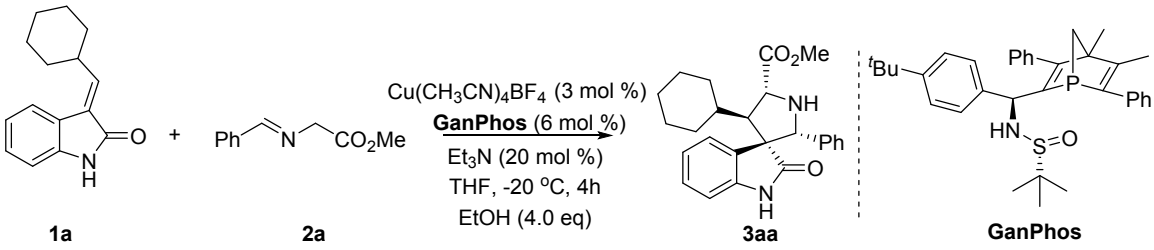
entry	metal	ligand	yield (%)[b]	dr[c]	ee (%)[d]
1	$Cu(MeCN)_4BF_4$	L1	53	20:1	78
2	**$Cu(MeCN)_4BF_4$**	**L11**	**63**	20:1	**90**
3	$Cu(MeCN)_4BF_4$	L12	46	20:1	19
4	$Cu(MeCN)_4BF_4$	L13	63	20:1	84
5	$Cu(MeCN)_4BF_4$	L14	42	20:1	25
6	$Cu(MeCN)_4BF_4$	L15	52	20:1	4.4

[a] Reaction conditions: **1a** (0.1 mmol), **2a** (0.2 mmol), $Cu(MeCN)_4BF_4$ (3 mol%), L (6 mol%) and Et_3N (20 mol%) in THF/EtOH (1.0 mL), -20°C, N_2, 4 h. [b] Yields of isolated product. [c] Determined by ^1H NMR analysis of the crude mixture. [d] Determined by chiral HPLC analysis.



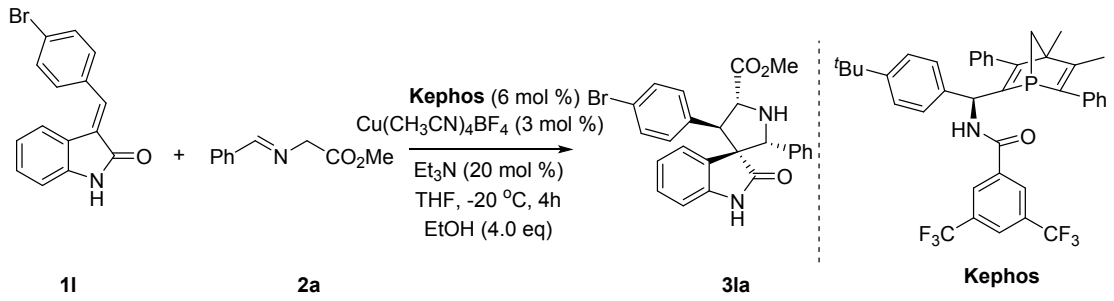
5. General Procedure for Reactions

1) Procedure A: Synthesis of Chiral spiro[pyrrolidin-3,3'-oxindole]s by Ganphos (3aa-3al)



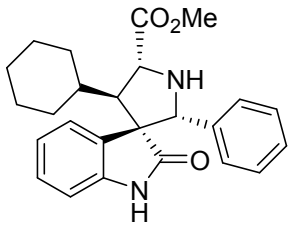
In a Schlenk tube, **Ganphos** (3.3 mg, 0.006 mmol, 6 mol %) and $Cu(CH_3CN)_4BF_4$ (1.1 mg, 0.003 mmol, 3 mol %) were dissolved in THF (1.0 mL) which have EtOH (4.0 eq) as additive. After being stirred for 1h at room temperature, 3-(cyclohexylmethylene)indolin-2-one **1a** (0.1 mmol), glycine imino ester **2a** (0.2 mmol) and Et_3N (2.8 uL, 0.02 mmol) were added subsequently. The reaction mixture was stirred at -20 °C for 4 h. When the reaction was completed as monitored by TLC, the mixture was concentrated and the residue was purified by column chromatography (eluent: ethyl acetate/petroleum ether = 1:2) to afford the cycloadduct 3aa in 80% yield (32.0 mg). Chiral **3ab-3al** were synthesized in the same reaction conditions.

2) Procedure B: Synthesis Chiral of spiro[pyrrolidin-3,3'-oxindole]s by Kephos (3la-3mm)



In a Schlenk tube, **Kephos** (4.7 mg, 0.006 mmol, 6 mol %) and $Cu(CH_3CN)_4BF_4$ (1.1 mg, 0.003 mmol, 3 mol %) were dissolved in THF (1.0 mL) which have EtOH (4.0 eq) as additive. After being stirred for 1h at room temperature, 3-(4-bromobenzylidene)indolin-2-one **1l** (0.1 mmol), glycine imino ester **2a** (0.2 mmol) and Et_3N (2.8 uL, 0.02 mmol) were added subsequently. The reaction mixture was stirred at -20 °C for 4 h. When the reaction was completed as monitored by TLC, the mixture was concentrated and the residue was purified by column chromatography (eluent: ethyl acetate/petroleum ether = 1:2) to afford the cycloadduct. Chiral **3lc-3mm** were synthesized in the same reaction conditions.

6. Characterization of compounds

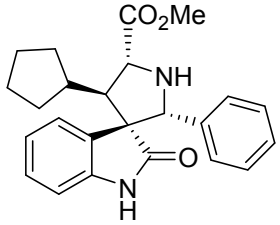


(2'R, 3S, 4'R, 5'R)-Methyl 4'-cyclohexyl-2-oxo-2'-phenylspiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3aa).

White solid (32.0 mg, 80% yield), $\mathbf{R}_f$ = 0.30. (petroleum ether/ ethyl acetate 2/1).

MP: 84.8-85.5 °C. $[\alpha]_D^{25}$ = +37 (*c* 0.23, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.70-1.02 (m, 7H), 1.49-1.78 (m, 4H), 2.88 (t, *J* = 9.6 Hz, 1H), 3.85 (s, 3H), 3.92 (d, *J* = 9.4 Hz, 1H), 4.41 (s, 1H), 6.74 (d, *J* = 7.6 Hz, 1H), 6.84 (d, *J* = 6.7 Hz, 2H), 7.15-7.10 (m, 4H), 7.24 (d, *J* = 7.7 Hz, 1H), 7.36 (d, *J* = 7.1 Hz, 1H), 7.77 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 25.7, 26.0, 26.2, 30.5, 32.1, 38.2, 52.5, 59.0, 63.1, 66.0, 74.7, 109.8, 122.2, 124.5, 126.2, 127.7, 127.8, 128.1, 130.5, 136.1, 140.9, 173.4, 180.4. ppm. **HRMS** (ESI, m/z): Calcd for $C_{25}H_{29}N_2O_3$ $[M+H]^+$: 405.2173, found: 405.2172. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 95% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 20.92. and 29.21 min.



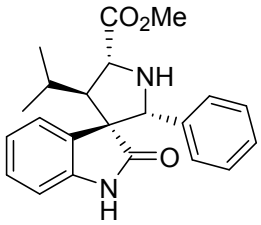
(2'R, 3S, 4'R, 5'R)-Methyl 4'-cyclopentyl-2-oxo-2'-phenylspiro[indoline- 3,3'-pyrrolidine]-5'-carboxylate (3ba).

White solid (38.2 mg, 98% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 142.8-143.3 °C. $[\alpha]_D^{25}$ = +81.3 (*c* 0.30, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.59-0.90 (m, 2H), 1.07 (dd, *J* = 20.1, 9.8 Hz, 1H), 1.16-1.41 (m, 4H), 1.83 (dd, *J* = 11.4, 6.4 Hz, 1H), 1.96 (dd, *J* = 16.8, 7.6 Hz, 1H),

2.89 (dd, *J* = 10.7, 9.7 Hz, 1H), 3.19 (br s, 1H), 3.84 (s, 3H), 3.89 (d, *J* = 9.4 Hz, 1H), 4.48 (s, 1H), 6.74 (d, *J* = 7.6 Hz, 1H), 6.89 (dd, *J* = 7.5, 1.7 Hz, 2H), 7.04-7.15 (m, 4H), 7.23 (dd, *J* = 7.7, 1.1 Hz, 1H), 7.36 (d, *J* = 7.4 Hz, 1H), 8.26 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 24.4, 25.4, 30.5, 31.4, 41.3, 52.4, 60.5, 63.5, 67.3, 74.1, 109.9, 122.3, 124.4, 126.1, 127.7, 127.9, 128.1, 131.0, 136.4, 141.2, 173.4, 180.8 ppm. **HRMS** (ESI, m/z): Calcd for $C_{24}H_{27}N_2O_3$ $[M+H]^+$: 391.2016, found: 391.2015. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 93% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 25.29. and 30.14 min.

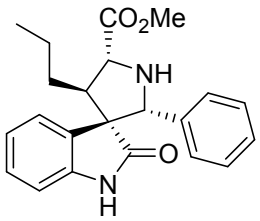


(2'R, 3S, 4'R, 5'R)-Methyl 4'-isopropyl-2-oxo-2'-phenylspiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3ca).

White solid (33.0 mg, 91% yield), $\mathbf{R}_f$ = 0.30. (petroleum ether/ ethyl acetate 2/1).

MP: 71.8-72.4 °C. $[\alpha]_D^{25}$ = +77 (*c* 0.10, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.41 (d, *J* = 6.4 Hz, 3H), 0.93 (d, *J* = 6.7 Hz, 3H), 1.85-1.95 (m, 1H), 2.83 (t, *J* = 9.9 Hz, 1H), 3.84 (s, 3H), 3.90 (d, *J* = 9.5 Hz, 1H), 4.43 (s, 1H), 6.75 (d, *J* = 7.6 Hz, 1H), 6.82-6.88 (m, 2H), 7.14-7.07 (m, 4H), 7.24 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.35 (d, *J* = 7.3 Hz, 1H), 8.09 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 20.6, 21.8, 28.7, 52.4, 60.4, 63.2, 66.4, 74.6, 109.9, 122.3, 124.6, 126.2, 127.7, 127.8, 128.1, 130.6, 136.3, 141.1, 173.4, 180.6 ppm. **HRMS** (ESI, m/z): Calcd for $C_{22}H_{25}N_2O_3$ $[M+H]^+$: 365.1860, found: 365.1857. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 97% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr =24.33 and 34.26 min.

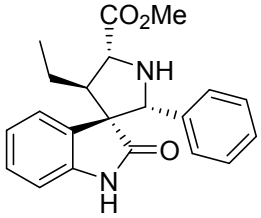


(2'R, 3S, 4'R, 5'R)-Methyl 2-oxo-2'-phenyl-4'-propylspiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3da).

White solid (33.0 mg, 91% yield), $\mathbf{R}_f$ = 0.30. (petroleum ether/ ethyl acetate 2/1).

MP: 65.2-66.0 °C. $[\alpha]_D^{25}$ = +31 (*c* 0.17, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.70 (t, *J* = 7.0 Hz, 3H), 0.77-0.89 (m, 1H), 1.02-1.16 (m, 1H), 1.48-1.75 (m, 2H), 2.78 (dd, *J* = 15.0, 8.5 Hz, 1H), 3.44 (br s, 1H), 3.82 (d, *J* = 5.2 Hz, 1H), 3.86 (s, 3H), 4.47 (s, 1H), 6.72 (d, *J* = 7.7 Hz, 1H), 6.88 (d, *J* = 1.7 Hz, 2H), 7.12 (m, 4H), 7.22 (d, *J* = 1.0 Hz, 1H), 7.36 (d, *J* = 7.4 Hz, 1H), 7.63 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 13.9, 20.7, 33.1, 52.4, 53.3, 62.9, 67.4, 73.2, 109.7, 122.2, 125.0, 126.1, 127.7, 127.9, 128.2, 129.5, 135.8, 141.1, 172.7, 180.3 ppm. **HRMS** (ESI, m/z): Calcd for $C_{22}H_{25}N_2O_3$ $[M+H]^+$: 365.1860, found: 365.1858. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 85% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 21.71 and 27.87 min.



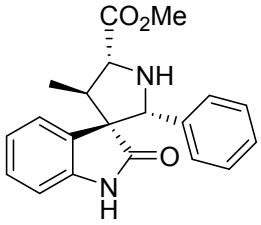
(2'R, 3S, 4'R, 5'R)-Methyl 4'-ethyl-2-oxo-2'-phenylspiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3ea).

White solid (31 mg, 89% yield), $\mathbf{R}_f$ = 0.33. (petroleum ether/ ethyl acetate 2/1).

MP: 69.8-70.2°C. $[\alpha]_D^{25}$ = +24 (*c* 0.20, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.59 (t, *J* = 7.3 Hz, 3H), 1.66 (ddd, *J* = 22.2, 14.4, 6.8 Hz, 2H), 2.68 (dd, *J* = 15.1, 8.3 Hz, 1H), 3.41 (br s, 1H), 3.81 (d, *J* = 2.6 Hz, 1H),

3.85 (s, 3H), 4.46 (s, 1H), 6.73 (d, *J* = 7.6 Hz, 1H), 6.90 (d, *J* = 6.4 Hz, 2H), 7.03-7.15 (m, 4H), 7.22 (d, *J* = 7.6 Hz, 1H), 7.35 (d, *J* = 7.4 Hz, 1H), 8.20 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 12.1, 23.9, 52.4, 55.3, 62.9, 67.2, 73.1, 109.9, 122.2, 124.9, 126.1, 127.7, 127.9, 128.2, 129.5, 136.0, 141.3, 172.7, 180.7 ppm. **HRMS** (ESI, m/z): Calcd for $C_{21}H_{23}N_2O_3$ $[M+H]^+$: 351.1703, found: 351.1705. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 85% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 28.20 and 33.27 min.

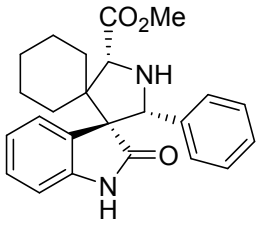


(2'R, 3S, 4'R, 5'R)-Methyl 4'-methyl-2-oxo-2'-phenylspiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3fa).

White solid (24 mg, 72% yield), $\mathbf{R}_f$ = 0.36. (petroleum ether/ ethyl acetate 2/1).

MP: 64.5-65.5 °C. $[\alpha]_D^{25}$ = +27 (*c* 0.10, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 1.17 (d, *J* = 7.1 Hz, 3H) 2.75-2.87 (m, 1H), 3.48 (br s, 1H), 3.78 (d, *J* = 8.1 Hz, 1H), 3.85 (s, 3H), 4.49 (s, 1H), 6.72 (d, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 6.7 Hz, 2H), 7.03-7.16 (m, 4H), 7.22 (d, *J* = 7.5 Hz, 1H), 7.35 (d, *J* = 7.3 Hz, 1H), 8.01 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 16.8. 47.4, 52.3, 63.3, 68.5, 72.3, 109.9, 122.2, 125.2, 126.1, 127.7, 127.9, 128.2, 129.2, 136.1, 141.4, 172.6, 180.3 ppm. **HRMS** (ESI, m/z): Calcd for $C_{20}H_{21}N_2O_3$ $[M+H]^+$: 337.1547, found: 337.1549. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 70% ee (Chiralpak OD-H, hexane/*i*-propanol = 95 : 5, flow rate 1.0 mL/min, λ = 254 nm); tr = 16.27 and 24.09 min.

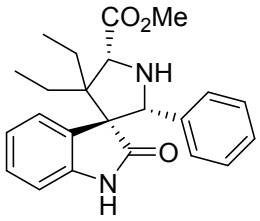


Methyl (2'R, 4'S, 5'R)-2''-oxo-5'-phenyldispiro[cyclohexane-1,3'-pyrrolidine-4', 3''-indoline]-2'-carboxylate (3ga).

White solid (36.3 mg, 92% yield), $\mathbf{R}_f$ = 0.35. (petroleum ether/ ethyl acetate 2/1).

MP: 170.2-171.6 °C. $[\alpha]_D^{25}$ = +40 (*c* 0.10, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 1.15 (dd, *J* = 16.0, 6.3 Hz, 2H), 1.26 (t, *J* = 7.1 Hz, 1H), 1.44 (dt, *J* = 37.2, 11.1 Hz, 5H), 1.70 (t, *J* = 12.5 Hz, 1H), 1.85-1.98 (m, 1H), 3.85 (s, 3H), 3.90 (s, 1H), 4.58 (s, 1H), 6.69 (d, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 6.6 Hz, 2H), 6.96-7.06 (m, 3H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 7.46 (d, *J* = 7.5 Hz, 1H), 8.08 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 22.7, 23.2, 25.3, 30.0, 36.6, 51.9, 55.5, 67.1, 69.6, 69.8, 109.7, 121.7, 126.3, 126.6, 127.5, 127.7, 128.2, 128.5, 135.9, 141.6, 172.5, 178.1 ppm. **HRMS** (ESI, m/z): Calcd for $C_{24}H_{27}N_2O_3$ $[M+H]^+$: 391.2016, found: 391.2018. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 93% ee (Chiralpak OD-H, hexane/*i*-propanol = 95 : 5, flow rate 1.0 mL/min, λ = 254 nm); tr = 16.62 and 24.36min.



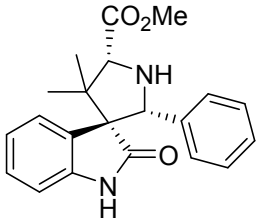
(2'R, 3S, 5'R)-Methyl 4', 4'-diethyl-2-oxo-2'-phenylspiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3ha)

White solid (22.0 mg, 58% yield), $\mathbf{R}_f$ = 0.35. (petroleum ether/ ethyl acetate 2/1).

MP: 89.5-90.2 °C. $[\alpha]_D^{25}$ = -33 (*c* 0.12, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.40 (t, *J* = 7.4 Hz, 3H), 1.12 (t, *J* = 7.2 Hz, 3H), 1.64 (dd, *J* = 14.4, 7.4 Hz, 1H), 1.88 (dd, *J* = 14.4, 7.3 Hz, 1H), 2.05 (dd, *J* = 14.4, 7.1 Hz, 2H), 3.84 (s, 3H), 4.01 (s, 1H), 4.52 (s, 1H), 6.61 (d, *J* = 7.5 Hz, 1H), 6.85 (d, *J* = 7.3 Hz, 2H), 7.10-7.02 (m, 4H), 7.17 (t, *J* = 7.5 Hz, 1H), 7.46 (d, *J* = 7.4 Hz, 1H), 7.61 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 8.3, 8.5, 22.0, 29.7, 52.0, 57.9, 67.2, 69.3, 69.8, 109.6, 121.7, 126.5, 127.7, 127.9, 129.2, 134.4, 141.1, 148.3, 171.6, 177.5 ppm. **HRMS** (ESI, m/z): Calcd for $C_{23}H_{27}N_2O_3$ $[M+H]^+$: 379.2016, found: 379.2013. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 90%

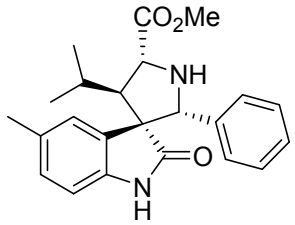
ee (Chiralpak OD-H, hexane/*i*-propanol = 95 : 5, flow rate 1.0 mL/min, λ = 254 nm); tr = 15.03 and 26.41min.



(2'R, 3S, 5'R)-Methyl 4',4'-dimethyl-2-oxo-2'-phenylspiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3ia).

Colorless oil (24.2 mg, 69% yield), $\mathbf{R}_f$ = 0.35. (petroleum ether/ ethyl acetate 2/1). $[\alpha]_D^{25}$ = +16 (*c* 0.10, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 1.01 (s, 3H), 1.47 (s, 3H), 3.83 (s, 3H), 3.88 (s, 1H), 4.59 (s, 1H), 6.69 (d, *J* = 7.6 Hz, 1H), 6.95 (d, *J* = 6.7 Hz, 2H), 7.12-7.03 (m, 4H), 7.21 (t, *J* = 7.7 Hz, 1H), 7.41 (d, *J* = 7.4 Hz, 1H), 7.80 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 21.74, 30.6, 50.7, 51.9, 67.1, 68.6, 71.0, 109.7, 121.8, 126.2, 126.4, 127.5, 127.5, 127.8, 128.3, 135.7, 141.9, 171.6, 178.2 ppm. **HRMS** (ESI, m/z): Calcd for $C_{21}H_{23}N_2O_3$ $[M+H]^+$: 351.1703, found: 351.1702. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 90% ee (Chiralpak OD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 7.48 and 10.53min.

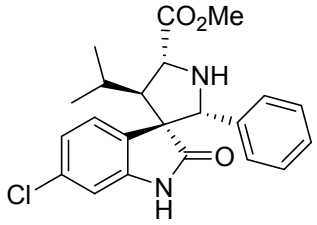


(2'R, 3S, 4'R, 5'R)-Methyl 4'-isopropyl-5-methyl-2-oxo-2'-phenylspiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3ja).

White solid (24.0 mg, 64% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 126.0-126.6°C. $[\alpha]_D^{25}$ = +78 (*c* 0.12, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.42 (d, *J* = 6.4 Hz, 3H), 0.93 (d, *J* = 6.7 Hz, 3H), 1.81-1.95 (m, 1H), 2.42 (s, 3H), 2.82 (t, *J* = 10.0 Hz, 1H), 3.10 (br s, 1H), 3.84 (s, 3H), 3.89 (d, *J* = 9.7 Hz, 1H), 4.42 (s, 1H), 6.64 (d, *J* = 7.9 Hz, 1H), 6.86 (dd, *J* = 7.5, 1.6 Hz, 2H), 7.11-7.04 (m, 4H), 7.15 (s, 1H), 7.87 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 20.8, 21.4, 21.8, 28.7, 52.4, 60.5, 63.3, 66.5, 74.7, 109.6, 125.3, 126.2, 127.6, 127.8, 128.5, 130.8, 131.7, 136.5, 138.6, 173.5, 180.5 ppm. **HRMS** (ESI, m/z): Calcd for $C_{23}H_{27}N_2O_3$ $[M+H]^+$: 379.2016, found: 379.2018. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 83% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 16.56 and 28.54 min.

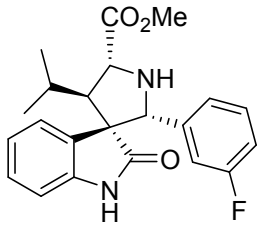


(2'R, 3S, 4'R, 5'R)-Methyl 6-chloro-4'-isopropyl-2-oxo-2'-phenylspiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3ka).

White solid (35.0 mg, 88% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 187.5-188.0 °C. $[\alpha]_D^{25}$ = -95 (*c* 0.12, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.43 (d, *J* = 6.5 Hz, 3H), 0.91 (d, *J* = 6.6 Hz, 3H), 1.98-2.14 (m, 1H), 2.95 (dd, *J* = 10.7, 6.9 Hz, 1H), 3.61 (br s, 1H), 3.80 (s, 3H), 4.10 (d, *J* = 6.9 Hz, 1H), 4.68 (s, 1H), 6.65 (d, *J* = 1.4 Hz, 1H), 6.82 (d, *J* = 7.3 Hz, 2H), 7.03-7.16 (m, 4H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.88 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 21.8, 22.3, 30.1, 52.5, 59.9, 63.8, 64.3, 73.2, 110.3, 122.6, 123.3, 126.1, 127.9, 128.1, 129.2, 133.5, 134.1, 141.6, 175.6, 177.7 ppm. **HRMS** (ESI, m/z): Calcd for $C_{22}H_{24}ClN_2O_3$ $[M+H]^+$: 399.1470, found: 399.1473. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 84% ee (Chiralpak OD-H, hexane/*i*-propanol = 95 : 5, flow rate 1.0 mL/min, λ = 254 nm); tr = 9.98 and 12.07 min.

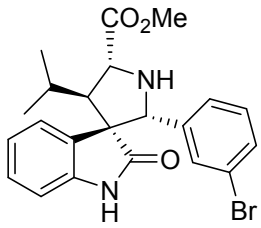


(2'R, 3S, 4'R, 5'R)-Methyl 2'-(3-fluorophenyl)-4'-isopropyl-2-oxospiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3ab)

White solid (24.0 mg, 66% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 52.4-53.2 °C. $[\alpha]_D^{25}$ = +69 (*c* 0.12, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.42 (d, *J* = 6.4 Hz, 3H), 0.93 (d, *J* = 6.7 Hz, 3H), 1.83-1.95 (m, 1H), 2.83 (t, *J* = 9.9 Hz, 1H), 3.04 (br s, 1H), 3.85 (s, 3H), 3.90 (d, *J* = 9.6 Hz, 1H), 4.42 (s, 1H), 6.64 (dd, *J* = 9.6, 1.9 Hz, 2H), 6.76-6.86 (m, 2H), 7.04 (td, *J* = 8.0, 6.1 Hz, 1H), 7.13 (td, *J* = 7.6, 1.0 Hz, 1H), 7.24-7.31 (m, 1H), 7.34 (d, *J* = 7.5 Hz, 1H), 8.04 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 20.6, 21.8, 28.7, 52.5, 60.2, 63.0, 66.3, 73.8, 110.0, 113.4 (d, $J_{C\text{-}F}$ = 22.5 Hz), 114.6 (d, $J_{C\text{-}F}$ = 21.0 Hz), 121.8 (d, $J_{C\text{-}F}$ = 2.8 Hz), 122.5, 124.6, 128.4, 129.3 (d, $J_{C\text{-}F}$ = 8.2 Hz), 130.3, 139.2 (d, $J_{C\text{-}F}$ = 7.3 Hz), 141.0, 162.3 (d, $J_{C\text{-}F}$ = 245.4 Hz), 173.3, 180.3 ppm. **HRMS** (ESI, m/z): Calcd for $C_{22}H_{24}FN_2O_3$ $[M+H]^+$: 383.1765, found: 383.1763. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 90% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 20.94 and 32.37 min.

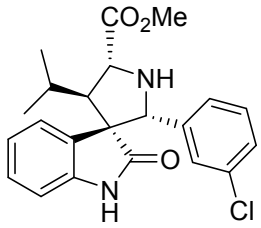


(2'R, 3S, 4'R, 5'R)-Methyl 2'-(3-bromophenyl)-4'-isopropyl-2-oxospiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3ac).

White solid (34.0 mg, 79% yield), $\mathbf{R}_f$ = 0.33. (petroleum ether/ ethyl acetate 2/1).

MP: 106.5-107.2 °C. $[\alpha]_D^{25}$= +86 (*c* 0.10, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.43 (d, *J* = 6.4 Hz, 3H), 0.92 (d, *J* = 6.7 Hz, 3H), 1.83-1.93 (m, 1H), 2.84 (t, *J* = 9.9 Hz, 1H), 3.02 (br s, 1H), 3.85 (s, 3H), 3.90 (d, *J* = 9.6 Hz, 1H), 4.39 (s, 1H), 6.91-6.78 (m, 2H), 6.93 (t, *J* = 7.9 Hz, 1H), 7.06-7.17 (m, 2H), 7.36-7.23 (m, 3H), 8.17 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 20.6, 21.8 28.7, 52.5, 56.0, 63.0, 66.3, 73.6, 110.2, 122.0, 122.5, 124.5, 124.9, 128.4, 129.4, 129.5, 130.3, 130.8, 139.1, 141.0, 173.3, 180.2 ppm. **HRMS** (ESI, m/z): Calcd for $C_{22}H_{24}BrN_2O_3$ $[M+H]^+$: 443.0965, found: 443.0964. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 92% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 21.83 and 33.31 min.

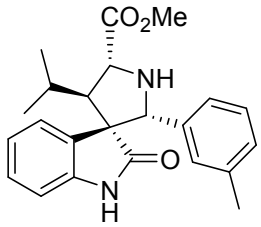


(2'R, 3S, 4'R, 5'R)-Methyl 2'-(3-chlorophenyl)-4'-isopropyl-2-oxospiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3ad).

White solid (36.2 mg, 91% yield), $\mathbf{R}_f$ = 0.31. (petroleum ether/ ethyl acetate 2/1).

MP: 104.2-105.0 °C. $[\alpha]_D^{25}$= +112 (*c* 0.15, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.42 (d, *J* = 6.4 Hz, 3H), 0.92 (d, *J* = 6.7 Hz, 3H), 1.81-1.94 (m, 1H), 2.83 (t, *J* = 9.9 Hz, 1H), 3.02 (br s, 1H), 3.85 (s, 3H), 3.90 (d, *J* = 9.6 Hz, 1H), 4.40 (s, 1H), 6.72 (d, *J* = 7.7 Hz, 1H), 6.81 (d, *J* = 7.6 Hz, 1H), 7.01-6.94 (m, 2H), 7.07-7.17 (m, 2H), 7.24-7.31 (m, 1H), 7.34 (d, *J* = 7.4 Hz, 1H), 8.29 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 20.6, 21.8, 28.7, 52.5, 56.0, 63.0, 66.2, 73.7, 110.2, 122.5, 124.4, 124.5, 126.6, 127.8, 128.4, 129.1, 130.3, 133.7, 138.8, 141.0, 173.3, 180.4 ppm. **HRMS** (ESI, m/z): Calcd for $C_{22}H_{24}ClN_2O_3$ $[M+H]^+$: 399.1470, found: 399.1468. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 89% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 19.96 and 30.63 min.

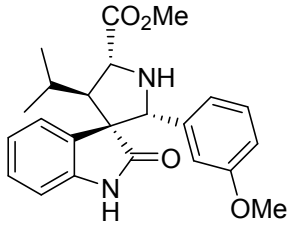


(2'R, 3S, 4'R, 5'R)-Methyl 4'-isopropyl-2-oxo-2'-(m-tolyl)spiro[indoline-3, 3'-pyrrolidine]-5'-carboxylate (3ae).

white solid (32.0 mg, 85% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 62.2-62.8 °C. $[\alpha]_D^{25}$ = +30 (*c* 0.21, CH_2Cl_2)

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.40 (d, *J* = 6.4 Hz, 3H), 0.92 (d, *J* = 6.6 Hz, 3H), 1.89 (qd, *J* = 13.0, 6.5 Hz, 1H), 2.13 (s, 3H), 2.81 (t, *J* = 9.9 Hz, 1H), 3.14 (br s, 1H), 3.83 (s, 3H), 3.88 (d, *J* = 9.5 Hz, 1H), 4.39 (s, 1H), 6.56 (d, *J* = 3.5 Hz, 1H), 6.69-6.82 (m, 2H), 6.91 (d, *J* = 4.8 Hz, 2H), 7.11 (t, *J* = 7.4 Hz, 1H), 7.23 (d, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 7.4 Hz, 1H), 8.41 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 20.6, 21.3, 21.8, 28.6, 52.4, 60.5, 63.2, 66.2, 74.4, 109.9, 122.1, 123.2, 124.5, 126.8, 127.6, 128.0, 128.3, 130.6, 136.1, 137.2, 141.3, 173.4, 180.8 ppm. **HRMS** (ESI, m/z): Calcd for $C_{23}H_{27}N_2O_3$ $[M+H]^+$: 379.2016, found: 379.2019. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 96% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 19.16 and 22.54 min.



(2'R, 3S, 4'R, 5'R)-Methyl 4'-isopropyl-2'-(3-methoxyphenyl)-2-oxospiro-[indoline-3,3'-pyrrolidine]-5'-carboxylate (3af).

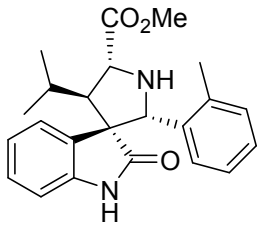
White solid (32.4 mg, 82% yield), $\mathbf{R}_f$ = 0.33. (petroleum ether/ ethyl acetate 2/1).

MP: 59.1-59.8 °C. $[\alpha]_D^{25}$ = +56 (*c* 0.26, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.42 (d, *J* = 6.4 Hz, 3H), 0.93 (d, *J* = 6.6 Hz, 3H), 1.82-1.96 (m, 1H), 2.82 (t, *J* = 9.9 Hz, 1H), 3.12 (br s, 1H), 3.54 (s, 3H), 3.84 (s, 3H),

3.89 (d, *J* = 9.5 Hz, 1H), 4.41 (s, 1H), 6.39 (s, 1H), 6.45 (d, *J* = 7.6 Hz, 1H), 6.65 (dd, *J* = 8.1, 2.2 Hz, 1H), 6.77 (d, *J* = 7.6 Hz, 1H), 6.97 (t, *J* = 7.9 Hz, 1H), 7.11 (t, *J* = 7.4 Hz, 1H), 7.20-7.26 (m, 1H), 7.34 (d, *J* = 7.4 Hz, 1H), 8.22 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 20.6, 21.9, 28.7, 52.4, 54.9, 60.4, 63.2, 66.3, 74.5, 110.0, 111.3, 113.8, 118.4, 122.3, 124.6, 128.1, 128.8, 130.6, 137.9, 141.3, 159.0, 173.4, 180.7 ppm. **HRMS** (ESI, m/z): Calcd for $C_{23}H_{27}N_2O_4$ $[M+H]^+$: 395.1965, found: 399.1964.

HPLC: The product was analyzed by HPLC to determine the enantiomeric excess: 92% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 36.90 and 42.24 min.

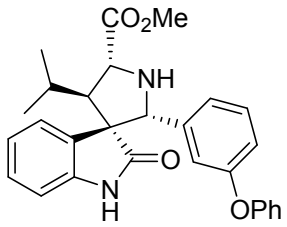


(2'R, 3S, 4'R, 5'R)-Methyl 4'-isopropyl-2-oxo-2'-(o-tolyl)spiro[indoline- 3,3'-pyrrolidine]-5'-carboxylate (3ag).

White solid (20.0 mg, 53% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 177.0-177.6 °C. $[\alpha]_D^{25}$ = -118 (*c* 0.16, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.39 (d, *J* = 6.5 Hz, 3H), 0.91 (d, *J* = 6.5 Hz, 3H), 1.83 (s, 3H), 2.07-2.20 (m, 1H), 3.03 (dd, *J* = 10.6, 7.2 Hz, 1H), 3.43 (br s, 1H), 3.81 (s, 3H), 4.15 (d, *J* = 7.1 Hz, 1H), 5.11 (s, 1H), 6.61 (d, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 4.0 Hz, 1H), 6.94-7.00 (m, 2H), 7.03 (d, *J* = 7.4 Hz, 1H), 7.10 (d, *J* = 7.3 Hz, 1H), 7.47 (t, *J* = 8.5 Hz, 2H), 8.18 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 19.7, 21.7, 22.4, 30.0, 52.4, 59.6, 64.0, 64.4, 68.0, 109.7, 122.1, 123.1, 125.7, 125.8, 127.6, 127.9, 130.2, 130.3, 133.2, 136.9, 140.4, 175.9, 178.4 ppm. **HRMS** (ESI, m/z): Calcd for $C_{23}H_{27}N_2O_3$ $[M+H]^+$: 379.2016, found: 379.2018. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 72% ee (Chiralpak AD-H, hexane/*i*-propanol = 95 : 5, flow rate 1.0 mL/min, λ = 254 nm); tr = 30.08 and 32.47 min.

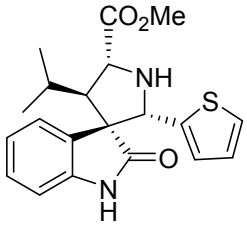


(2'R, 3S, 4'R, 5'R)-Methyl 4'-isopropyl-2-oxo-2'-(3-phenoxyphenyl)spiro-[indoline-3,3'-pyrrolidine]-5'-carboxylate (3ah).

White solid (33.0 mg, 72% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 65.0-66.0 °C. $[\alpha]_D^{25}$ = +98 (*c* 0.17, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.40 (d, *J* = 6.4 Hz, 3H), 0.91 (d, *J* = 6.7 Hz, 3H), 1.82-1.93 (m, 1H), 2.81 (t, *J* = 9.9 Hz, 1H), 3.07 (br s, 1H), 3.81 (s, 3H), 3.88 (d, *J* = 9.5 Hz, 1H), 4.40 (s, 1H), 6.49 (s, 1H), 6.73 (t, *J* = 8.3 Hz, 2H), 6.78 (d, *J* = 7.8 Hz, 3H), 7.06 (t, *J* = 7.7 Hz, 3H), 7.16-7.25 (m, 3H), 7.29 (d, *J* = 7.7 Hz, 1H), 8.28 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 20.6, 21.8, 28.7, 52.4, 60.4, 63.1, 66.3, 74.2, 110.1, 117.3, 118.5, 118.6, 121.1, 122.4, 122.9, 124.5, 128.2, 129.3, 129.6, 130.4, 138.4, 141.1, 156.4, 157.2, 173.3, 180.6 ppm. **HRMS** (ESI, m/z): Calcd for $C_{28}H_{29}N_2O_4$ $[M+H]^+$: 457.2122, found: 457.2124. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 92% ee (Chiralpak AD-H, hexane/*i*-propanol = 90:10, flow rate 1.0 mL/min, λ = 254 nm); tr = 32.42 and 36.80 min.



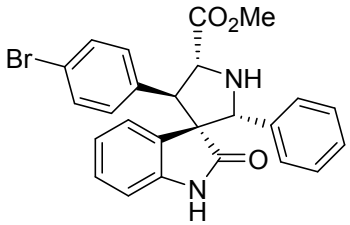
(2'S, 3S, 4'R, 5'R)-Methyl 4'-isopropyl-2-oxo-2'-(thiophen-2-yl)spiro[indoline-3,3'-pyrrolidine]-5'-carboxylate (3ai).

White solid; (25.0 mg, 68% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 65.2-66.0 °C. $[\alpha]_D^{25}$ = +18 (*c* 0.18, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.44 (d, *J* = 6.4 Hz, 3H), 0.94 (d, *J* = 6.6 Hz, 3H), 1.83-1.95 (m, 1H), 2.85 (t, *J* = 9.5 Hz, 1H), 3.22 (br s, 1H), 3.84 (s, 3H), 3.90 (d, *J* =

9.0 Hz, 1H), 4.64 (s, 1H), 6.61 (d, *J* = 3.2 Hz, 1H), 6.69-6.77 (m, 1H), 6.83 (d, *J* = 7.6 Hz, 1H), 6.99 (d, *J* = 4.8 Hz, 1H), 7.10 (t, *J* = 7.4 Hz, 1H), 7.29 (dd, *J* = 11.9, 5.0 Hz, 2H), 8.44 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 20.6, 21.9, 28.8, 52.5, 60.3, 62.9, 66.1, 70.4, 110.2, 122.4, 124.0, 124.2, 124.6, 126.5, 128.4, 129.7, 139.2, 141.6, 173.0, 180.9 ppm. **HRMS** (ESI, m/z): Calcd for $C_{20}H_{23}N_2O_3S$ $[M+H]^+$: 371.1424, found: 371.1426. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 91% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 31.21 and 38.19 min.).

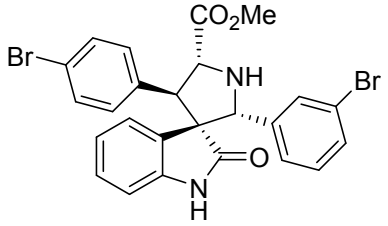


(2'R, 3S, 4'R, 5'R)-Methyl 4'-(4-bromophenyl)-2-oxo-2'-phenylspiro[indoline-3,3'-pyrrolidine]-5'-carboxylate (3la).

White solid; (30.0 mg, 63% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 165.2-166.0 °C. $[\alpha]_D^{25}$ = +165 (*c* 0.13, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.81 (s, 3H), 4.10 (d, *J* = 5.6 Hz, 1H), 4.51 (d, *J* = 5.5 Hz, 1H), 4.68 (s, 1H), 6.25 (d, *J* = 7.5 Hz, 1H), 6.58 (d, *J* = 7.7 Hz, 1H), 6.77 (t, *J* = 7.5 Hz, 1H), 6.94 (d, *J* = 7.3 Hz, 2H), 7.00-7.16 (m, 6H), 7.40 (d, *J* = 8.3 Hz, 2H), 8.10 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 52.6, 56.8, 64.0, 65.9, 72.5, 109.5, 121.4, 122.1, 125.0, 126.3, 127.6, 128.0, 128.1, 128.2, 130.5, 131.6, 135.6, 137.8, 141.0, 172.8, 179.5 ppm. **HRMS** (ESI, m/z): Calcd for $C_{25}H_{22}BrN_2O_3$ $[M+H]^+$: 477.0808, found: 477.0811. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 90% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 24.16 and 28.61 min.).

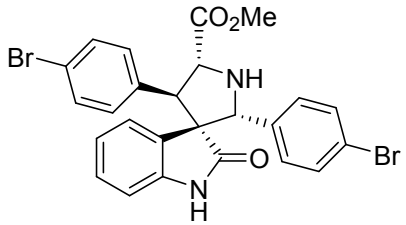


(2'R, 3S, 4'R, 5'R)-Methyl 2'-(3-bromophenyl)-4'-(4-bromophenyl)-2-oxospiro-[indoline-3,3'-pyrrolidine]-5'-carboxylate (3lc).

White solid; (34.0 mg, 61% yield), $\mathbf{R}_f$ = 0.30. (petroleum ether/ ethyl acetate 2/1).

MP: 103.5-104.2 °C. $[\alpha]_D^{25}$ = +61 (*c* 0.10, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.57 (br s, 1H), 3.82 (s, 3H), 4.11 (d, *J* = 6.0 Hz, 1H), 4.52 (d, *J* = 5.7 Hz, 1H), 4.64 (s, 1H), 6.29 (d, *J* = 7.5 Hz, 1H), 6.64 (d, *J* = 7.8 Hz, 1H), 6.81 (t, *J* = 7.5 Hz, 1H), 6.88-7.01 (m, 2H), 7.03-7.15 (m, 4H), 7.29 (d, *J* = 7.7 Hz, 1H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.61 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 52.6, 56.7, 63.8, 65.7, 71.8, 109.6, 120.8, 121.5, 122.2, 122.4, 124.9, 125.0, 127.4, 128.5, 129.6, 130.5, 131.1, 131.6, 137.4, 138.3, 140.7, 172.6, 178.7 ppm. **HRMS** (ESI, m/z): Calcd for $C_{25}H_{21}Br_2N_2O_3$ $[M+H]^+$: 554.9913, found: 554.9915. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 86% ee (Chiralpak IA-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 19.56 and 26.06 min.).



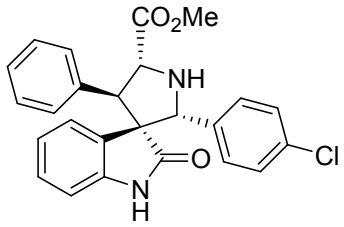
(2'R, 3S, 4'R, 5'R)-Methyl 2',4'-bis(4-bromophenyl)-2-oxospiro[indoline- 3,3'-pyrrolidine]-5'-carboxylate (3lj).

White solid; (50.0 mg, 90% yield), $\mathbf{R}_f$ = 0.30. (petroleum ether/ ethyl acetate 2/1).

MP: 124.3-125.2 °C. $[\alpha]_D^{25}$ = +142 (*c* 0.18, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.80 (s, 3H), 4.09 (d, *J* = 5.8 Hz, 1H), 4.51 (d, *J* = 5.8 Hz, 1H), 4.64 (s, 1H), 6.29 (d, *J* = 7.5 Hz, 1H), 6.61 (d, *J* = 7.7 Hz, 1H), 6.81 (dd, *J* = 12.7, 8.0 Hz, 3H), 7.05 (d, *J* = 8.4 Hz, 2H), 7.10 (t, *J* = 8.0 Hz, 1H), 7.20 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.3 Hz, 2H), 8.11 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 52.6. 56.4, 63.8, 65.7, 71.8, 109.8, 121.5, 122.0, 122.3, 125.0, 127.4, 128.1, 128.5, 130.5, 131.2, 131.6, 135.2, 137.3, 140.8, 172.8, 179.1 ppm. **HRMS** (ESI, m/z): Calcd for $C_{25}H_{21}Br_2N_2O_3$ $[M+H]^+$: 554.9913, found: 554.9914. **HPLC**: The product was

analyzed by HPLC to determine the enantiomeric excess: 88% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 26.09 and 32.46 min.).

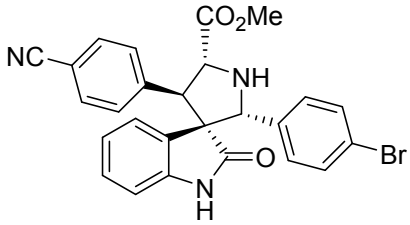


(2'R, 3S, 4'R, 5'R)-Methyl 2'-(4-chlorophenyl)-2-oxo-4'-phenylspiro[indoline-3,3'-pyrrolidine]-5'-carboxylate (3mk).

White solid; (34.0 mg, 79% yield), $\mathbf{R}_f$ = 0.30. (petroleum ether/ ethyl acetate 2/1).

MP: 177.7-178.5 °C. $[\alpha]_D^{25}$ = +180 (*c* 0.10, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.66 (br s, 1H), 3.83 (s, 3H), 4.16 (d, *J* = 5.0 Hz, 1H), 4.60 (d, *J* = 4.1 Hz, 1H), 4.71 (s, 1H), 6.10 (d, *J* = 7.5 Hz, 1H), 6.60 (d, *J* = 7.7 Hz, 1H), 6.71 (t, *J* = 7.5 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 2H), 7.00-7.11 (m, 3H), 7.21 (d, *J* = 7.4 Hz, 2H), 7.28-7.35 (m, 3H), 8.10 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 52.6, 57.0, 64.0, 66.0, 71.8, 109.5, 122.0, 125.1, 127.4, 127.6, 127.8, 128.2, 128.6, 128.9, 133.7, 134.5, 138.7, 140.9, 173.2, 179.5 ppm. **HRMS** (ESI, m/z): Calcd for $C_{25}H_{22}ClN_2O_3$ $[M+H]^+$: 433.1313, found: 433.1311. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 89% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 25.75 and 34.96 min.).

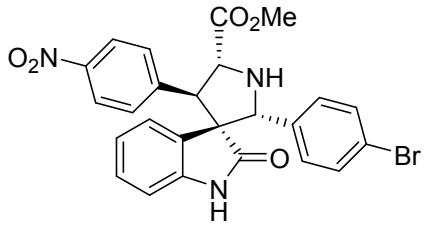


(2'R, 3S, 4'R, 5'R)-Methyl 2'-(4-bromophenyl)-4'-(4-cyanophenyl)-2-oxospiro[indoline-3,3'-pyrrolidine]-5'-carboxylate (3nj).

White solid; (34.0 mg, 68% yield), $\mathbf{R}_f$ = 0.20. (petroleum ether/ ethyl acetate 2/1).

MP: 86.7-87.4 °C. $[\alpha]_D^{25}$ = +166 (*c* 0.17, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.55 (br s, 1H), 3.80 (s, 3H), 4.17 (d, *J* = 5.9 Hz, 1H), 4.55 (s, 1H), 4.63 (s, 1H), 6.27 (d, *J* = 7.5 Hz, 1H), 6.62 (d, *J* = 7.7 Hz, 1H), 6.80 (dd, *J* = 15.4, 7.9 Hz, 3H), 7.11 (t, *J* = 7.7 Hz, 1H), 7.20 (d, *J* = 8.1 Hz, 2H), 7.29 (s, 2H), 7.55 (d, *J* = 8.0 Hz, 2H), 8.19 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 52.7, 56.9, 63.8, 65.2, 71.8, 110.0, 111.5, 118.5, 122.1, 122.4, 124.7, 127.2, 128.1, 128.8, 129.5, 131.2, 132.3, 135.0, 140.8, 143.6, 172.4, 178.9 ppm. **HRMS** (ESI, m/z): Calcd for $C_{26}H_{21}BrN_3O_3$ $[M+H]^+$: 502.0761, found: 502.0760. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 83% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 67.76 and 72.41 min.).

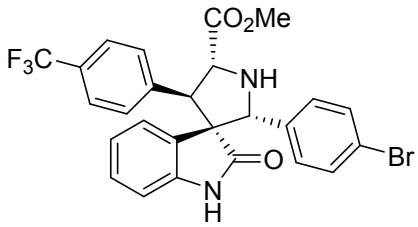


(2'R, 3S, 4'R, 5'R)-Methyl 2'-(4-bromophenyl)-4'-(4-nitrophenyl)-2-oxospiro-[indoline-3,3'-pyrrolidine]-5'-carboxylate (3oj).

White solid; (48.0 mg, 92% yield), $\mathbf{R}_f$ = 0.20. (petroleum ether/ ethyl acetate 2/1).

MP: 88.6-89.4 °C. $[\alpha]_D^{25}$ = +144 (*c* 0.20, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.50 (br s, 1H), 3.80 (s, 3H), 4.23 (d, *J* = 6.4 Hz, 1H), 4.59 (d, *J* = 6.2 Hz, 1H), 4.66 (s, 1H), 6.35 (d, *J* = 7.5 Hz, 1H), 6.63 (d, *J* = 7.7 Hz, 1H), 6.86-6.77 (m, 3H), 7.11 (t, *J* = 7.7 Hz, 1H), 7.21 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.5 Hz, 2H), 8.11 (d, *J* = 8.5 Hz, 2H), 8.15 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 52.8, 56.7, 65.3, 69.2, 72.0, 110.0, 122.1, 122.5, 123.7, 124.7, 127.2, 128.1, 128.9, 129.6, 131.2, 135.0, 140.8, 145.5, 147.2, 172.3, 178.7 ppm. **HRMS** (ESI, m/z): Calcd for $C_{25}H_{21}BrN_3O_5$ $[M+H]^+$: 552.0659, found: 522.0658. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 88% ee (Chiralpak AD-H, hexane/*i*-propanol = 80 : 20, flow rate 1.0 mL/min, λ = 254 nm, tr = 21.03 and 27.59 min.).

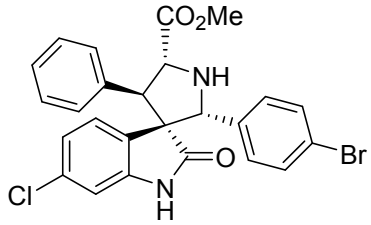


(2'R, 3S, 4'R, 5'R)-Methyl 2'-(4-bromophenyl)-2-oxo-4'-(4-(trifluoromethyl)-phenyl)spiro[indoline-3,3'-pyrrolidine]-5'-carboxylate (3pj).

White solid; (46.0 mg, 85% yield), $\mathbf{R}_f$ = 0.30. (petroleum ether/ ethyl acetate 2/1).

MP: 88.0-89.0 °C. $[\alpha]_D^{25}$ = +119 (*c* 0.27, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.82 (s, 3H), 4.21 (d, *J* = 5.8 Hz, 1H), 4.58 (d, *J* = 5.8 Hz, 1H), 4.66 (s, 1H), 6.21 (d, *J* = 7.5 Hz, 1H), 6.62 (d, *J* = 7.7 Hz, 1H), 6.76 (t, *J* = 7.6 Hz, 1H), 6.85 (d, *J* = 8.3 Hz, 2H), 7.09 (t, *J* = 7.6 Hz, 1H), 7.23 (d, *J* = 8.3 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.77 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 52.7, 56.7, 63.8, 65.6, 72.0, 109.7, 122.1, 122.3, 124.8, 125.5 (d, $J_{C\text{-}F}$ = 3.7 Hz), 127.2, 128.1, 128.6, 129.2, 131.2, 135.0, 140.7, 142.4, 172.6, 178.8 ppm. **HRMS** (ESI, m/z): Calcd for $C_{26}H_{21}BrF_3N_2O_3$ $[M+H]^+$: 545.0682, found: 545.0684. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 81% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 19.00 and 22.67 min.).



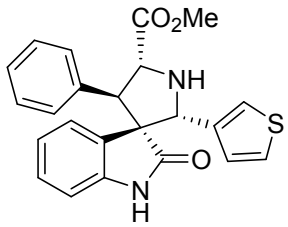
(2'R, 3S, 4'R, 5'R)-Methyl 2'-(4-bromophenyl)-6-chloro-2-oxo-4'-phenylspiro-[indoline-3,3'-pyrrolidine]-5'-carboxylate (3kj).

White solid; (50.0 mg, 98% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 118.0-119.0 °C. $[\alpha]_D^{25}$ = +86 (*c* 0.20, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.63 (br s, 1H), 3.82 (s, 3H), 4.13 (d, *J* = 4.7 Hz, 1H), 4.55 (d, *J* = 3.5 Hz, 1H), 4.64 (s, 1H), 5.90 (d, *J* = 8.2 Hz, 1H), 6.61 (d, *J* = 1.4 Hz,

1H), 6.62-6.70 (m, 1H), 6.84 (d, *J* = 8.4 Hz, 2H), 7.06-7.24 (m, 4H), 7.32 (d, *J* = 6.4 Hz, 3H), 8.10 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 52.6, 56.9, 63.6, 66.0, 71.8, 110.1, 122.0, 122.2, 125.6, 126.0, 127.8, 128.1, 128.7, 128.8, 131.3, 134.0, 134.5, 138.7, 142.0, 173.0, 179.4 ppm. **HRMS** (ESI, m/z): Calcd for $C_{25}H_{21}BrClN_2O_3$ $[M+H]^+$: 511.0419, found: 511.0417. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 86% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 25.72 and 41.60 min.).

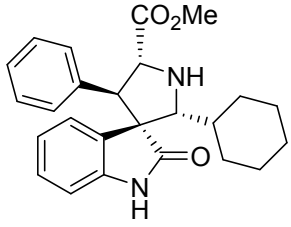


(2'S, 3S, 4'R, 5'R)-Methyl 2-oxo-4'-phenyl-2'-(thiophen-3-yl)spiro[indoline- 3,3'-pyrrolidine]-5'-carboxylate (3mi).

White solid; (40.0 mg, 99% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 162.0-163.0 °C. $[\alpha]_D^{25}$ = +99 (*c* 0.10, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 3.81 (s, 3H), 4.14 (d, *J* = 5.0 Hz, 1H), 4.58 (d, *J* = 4.8 Hz, 1H), 4.80 (s, 1H), 6.03 (d, *J* = 7.5 Hz, 1H), 6.51 (d, *J* = 5.0 Hz, 1H), 6.66 (t, *J* = 7.8 Hz, 2H), 6.91 (s, 1H), 6.96-7.10 (m, 2H), 7.17-7.23 (m, 2H), 7.29 (d, *J* = 7.2 Hz, 3H), 8.16 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 52.5, 57.4, 63.5, 66.3, 68.7, 109.4, 121.4, 121.9, 125.0, 125.3, 125.6, 127.5, 127.5, 128.1, 128.6, 128.9, 136.9, 139.1, 141.3, 173.0, 180.1 ppm. **HRMS** (ESI, m/z): Calcd for $C_{23}H_{21}N_2O_3S$ $[M+H]^+$: 405.1267, found: 405.1268. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 84% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 22.51 and 31.45 min.).

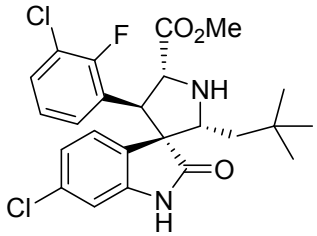


(2'R, 3S, 4'R, 5'R)-Methyl 2'-cyclohexyl-2-oxo-4'-phenylspiro[indoline- 3,3'-pyrrolidine]-5'-carboxylate (3mk).

White solid; (20.0 mg, 50% yield), $\mathbf{R}_f$ = 0.32. (petroleum ether/ ethyl acetate 2/1).

MP: 92.1-93.0 °C. $[\alpha]_D^{25}$ = -14 (*c* 0.12, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.34-0.52 (m, 1H), 0.81-1.11 (m, 5H), 1.51 (s, 1H), 1.76 (dd, *J* = 38.0, 11.0 Hz, 3H), 2.13 (d, *J* = 12.4 Hz, 1H), 2.94 (br s, 1H), 3.41 (d, *J* = 9.3 Hz, 1H), 3.71 (s, 3H), 3.94 (d, *J* = 7.2 Hz, 1H), 4.39 (d, *J* = 7.3 Hz, 1H), 6.33 (d, *J* = 7.5 Hz, 1H), 6.73-6.64 (m, 2H), 7.01 (dd, *J* = 16.5, 7.7 Hz, 3H), 7.14 (d, *J* = 6.3 Hz, 3H), 8.47 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 25.7, 25.9, 26.1, 30.1, 31.9, 39.6, 52.4, 61.2, 62.0, 64.9, 73.8, 109.3, 121.7, 125.1, 127.2, 127.6, 128.1, 128.6, 130.4, 137.8, 140.1, 172.6, 181.3 ppm. **HRMS** (ESI, m/z): Calcd for $C_{25}H_{29}N_2O_3$ $[M+H]^+$: 405.2173, found: 405.2172. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 90% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 22.97 and 66.69 min.).



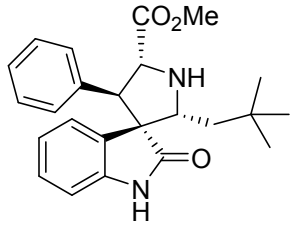
(2'R, 3S, 4'S, 5'R)-Methyl 6-chloro-4'-(3-chloro-2-fluorophenyl)-2'-neopentyl-2-oxospiro[indoline-3,3'-pyrrolidine]-5'-carboxylate (3ql).

White solid; (22.0 mg, 46% yield), $\mathbf{R}_f$ = 0.30. (petroleum ether/ ethyl acetate 2/1).

MP: 167.5-168.5 °C. $[\alpha]_D^{25}$ = -15 (*c* 0.10, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.82 (s, 9H), 1.41 (dd, *J* = 14.1, 9.9 Hz, 2H), 2.99 (br s, 1H), 3.40 (d, *J* = 8.9 Hz, 1H), 3.77 (s, 3H), 4.15 (d, *J* = 6.5 Hz, 1H), 4.44 (d, *J* = 6.3 Hz, 1H), 6.00 (d, *J* = 8.1 Hz, 1H), 6.66 (dd, *J* = 8.1, 1.6 Hz, 1H), 6.87 (d, *J* = 1.5 Hz, 1H), 7.13 (t, *J* = 8.0 Hz, 1H), 7.24-7.33 (m, 1H), 7.39 (t, *J* = 6.8 Hz, 1H), 8.25 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 29.8, 30.2, 43.2, 50.8, 52.6, 62.8, 65.4, 67.1, 110.3, 122.0, 123.8, 124.5, 124.5, 124.8, 125.7, 126.8, 126.8, 129.8, 134.0, 142.4,

172.1, 180.5 ppm. **HRMS** (ESI, m/z): Calcd for $C_{24}H_{26}Cl_2FN_2O_3$ $[M+H]^+$: 479.1299, found: 479.1297. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 94% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 22.21 and 32.85 min.).

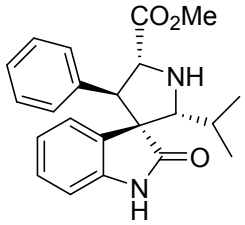


(2'R, 3S, 4'R, 5'R)-Methyl 2'-neopentyl-2-oxo-4'-phenylspiro[indoline-3,3'-pyrrolidine]-5'-carboxylate (3ml).

Yellow solid; (18.0 mg, 46% yield), $\mathbf{R}_f$ = 0.30. (petroleum ether/ ethyl acetate 2/1).

MP: 59.1-60.0 °C. $[\alpha]_D^{25}$ = +43 (*c* 0.13, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.82 (s, 9H), 1.20-1.45 (m, 2H), 3.00 (br s, 1H), 3.58 (d, *J* = 9.4 Hz, 1H), 3.78 (s, 3H), 3.96 (d, *J* = 4.8 Hz, 1H), 4.47 (d, *J* = 4.6 Hz, 1H), 5.86 (d, *J* = 7.6 Hz, 1H), 6.61 (t, *J* = 7.6 Hz, 1H), 6.82 (d, *J* = 7.7 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 1H), 7.15 (d, *J* = 6.7 Hz, 2H), 7.20-7.32 (m, 3H), 8.74 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 29.8, 30.2, 43.6, 52.4, 57.0, 63.4, 66.2, 67.2, 109.3, 121.8, 125.0, 127.3, 127.5, 127.8, 128.4, 128.9, 139.6, 141.2, 173.1, 181.3 ppm. **HRMS** (ESI, m/z): Calcd for $C_{24}H_{29}N_2O_3$ $[M+H]^+$: 393.2173, found: 393.2172. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 84% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 7.68 and 22.61 min.).

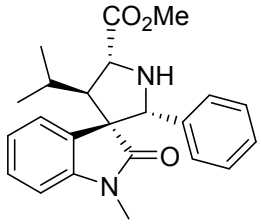


(2'R, 3S, 4'R, 5'R)-Methyl 2'-isopropyl-2-oxo-4'-phenylspiro[indoline- 3,3'-pyrrolidine]-5'-carboxylate (3mm).

Yellow solid; (17.0 mg, 47% yield), $\mathbf{R}_f$ = 0.30. (petroleum ether/ ethyl acetate 2/1).

MP: 46.4-47.3 °C. $[\alpha]_D^{25}$ = -10 (*c* 0.15, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.38 (d, *J* = 6.6 Hz, 3H), 1.09 (d, *J* = 6.6 Hz, 3H), 2.06 (dd, *J* = 14.4, 7.8 Hz, 1H), 3.33 (d, *J* = 9.3 Hz, 1H), 3.72 (s, 3H), 3.97 (d, *J* = 7.1 Hz, 1H), 4.41 (d, *J* = 7.1 Hz, 1H), 6.31 (d, *J* = 7.5 Hz, 1H), 6.61-6.78 (m, 2H), 7.00 (d, *J* = 7.5 Hz, 1H), 7.03-7.09 (m, 2H), 7.15 (t, *J* = 5.9 Hz, 3H), 8.58 (s, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 20.1, 22.0, 30.3, 52.4, 61.1, 62.1, 65.0, 75.3, 109.3, 121.8, 125.2, 127.2, 127.6, 128.1, 128.6, 130.3, 137.9, 140.3, 172.6, 181.3 ppm. **HRMS** (ESI, m/z): Calcd for $C_{22}H_{25}N_2O_3$ $[M+H]^+$: 365.1860, found: 365.1859. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 70% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm, tr = 11.97 and 13.45 min.).

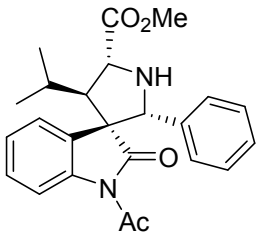


(2'R, 3S, 4'R, 5'R)-Methyl 4'-isopropyl-1-methyl-2-oxo-2'-phenylspiro[indoline-3,3'-pyrrolidine]-5'-carboxylate (3ra).

Colorless oil (17.0 mg, 45% yield), $\mathbf{R}_f$ = 0.42. (petroleum ether/ ethyl acetate 2/1).

$[\alpha]_D^{25}$= +148 (*c* 0.10, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.42 (d, *J* = 6.4 Hz, 3H), 0.98 (d, *J* = 6.7 Hz, 3H), 1.90-2.05 (m, 1H), 2.76 (s, 3H), 2.83 (t, *J* = 9.5 Hz, 1H), 3.86 (s, 3H), 3.91 (d, *J* = 9.1 Hz, 1H), 4.42 (s, 1H), 6.69 (d, *J* = 7.7 Hz, 1H), 6.73-6.81 (m, 2H), 7.05-7.18 (m, 4H), 7.31 (td, *J* = 7.7, 1.0 Hz, 1H), 7.39 (d, *J* = 7.4 Hz, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 20.5, 22.1, 25.8, 28.6, 52.4, 60.2, 63.1, 66.4, 74.8, 108.0, 122.3, 124.4, 125.9, 127.7, 128.2, 129.8, 135.7, 144.1, 173.4, 178.3 ppm. The product was analyzed by HPLC to determine the enantiomeric excess: 75% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 11.30 and 15.89 min.

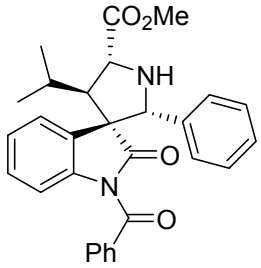


(2'R, 3S, 4'R, 5'R)-Methyl 1-acetyl-4'-isopropyl-2-oxo-2'-phenylspiro[indoline-3,3'-pyrrolidine]-5'-carboxylate (3sa).

White solid (24.0 mg, 59% yield), $\mathbf{R}_f$ = 0.55. (petroleum ether/ ethyl acetate 2/1).

MP: 43.4-44.2 °C. $[\alpha]_D^{25}$= -59 (*c* 0.20, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.41 (d, *J* = 6.6 Hz, 3H), 0.95 (d, *J* = 6.6 Hz, 3H), 2.10 (ddd, *J* = 17.3, 11.9, 5.4 Hz, 1H), 2.30 (s, 3H), 3.02 (dd, *J* = 10.8, 6.7 Hz, 1H), 3.84 (s, 3H), 4.15 (d, *J* = 6.6 Hz, 1H), 4.72 (s, 1H), 6.71 (d, *J* = 7.4 Hz, 2H), 7.06 (t, *J* = 7.4 Hz, 2H), 7.15 (t, *J* = 7.1 Hz, 1H), 7.28-7.34 (m, 2H), 7.52 (dd, *J* = 5.6, 3.0 Hz, 1H), 7.95 (dd, *J* = 6.1, 2.9 Hz, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 22.1, 22.3, 26.1, 30.0, 52.6, 59.9, 64.1, 64.7, 74.5, 116.4, 121.7, 125.4, 125.6, 127.9, 128.5, 128.5, 129.4, 133.6, 139.7, 170.2, 175.5, 176.6 ppm. **HRMS** (ESI, m/z): Calcd for $C_{24}H_{27}N_2O_4$ $[M+H]^+$: 407.1965, found: 407.1964. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 76% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 7.24 and 10.53 min.



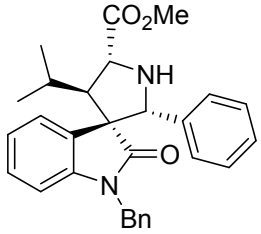
(2'R, 3S, 4'R, 5'R)-Methyl 1-benzoyl-4'-isopropyl-2-oxo-2'-phenylspiro[indoline-3,3'-pyrrolidine]-5'-carboxylate (3ta).

White solid (25.0 mg, 54% yield), $\mathbf{R}_f$ = 0.45. (petroleum ether/ ethyl acetate 2/1).

MP: 44.5-45.2 °C. $[\alpha]_D^{25}$= -100 (*c* 0.10, CH_2Cl_2).

^{1}H NMR (300 MHz, $CDCl_3$) δ 0.47 (d, *J* = 6.6 Hz, 3H), 0.89 (d, *J* = 6.6 Hz, 3H), 2.03 (ddd, *J* = 13.0, 9.1, 4.8 Hz, 1H), 3.05 (dd, *J* = 10.8, 6.7 Hz, 1H), 3.82 (s, 3H), 4.00 (d,

J = 6.7 Hz, 1H), 4.89 (s, 1H), 6.80 (d, *J* = 7.1 Hz, 2H), 6.90-6.97 (m, 2H), 7.22 (d, *J* = 7.6 Hz, 2H), 7.36-7.30 (m, 5H), 7.47-7.56 (m, 2H), 7.60 (dd, *J* = 5.9, 2.9 Hz, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 21.9, 22.3, 30.0, 52.5, 61.6, 64.0, 64.5, 73.2, 115.0, 122.3, 125.2, 125.9, 128.0, 128.2, 128.4, 128.5, 129.2, 130.3, 132.8, 133.9, 134.5, 140.1, 169.0, 175.4, 175.5 ppm. The product was analyzed by HPLC to determine the enantiomeric excess: 70% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 14.65 and 28.80 min.



(2'R, 3S, 4'R, 5'R)-Methyl 1-benzyl-4'-isopropyl-2-oxo-2'-phenylspiro[indoline-3,3'-pyrrolidine]-5'-carboxylate (3ua).

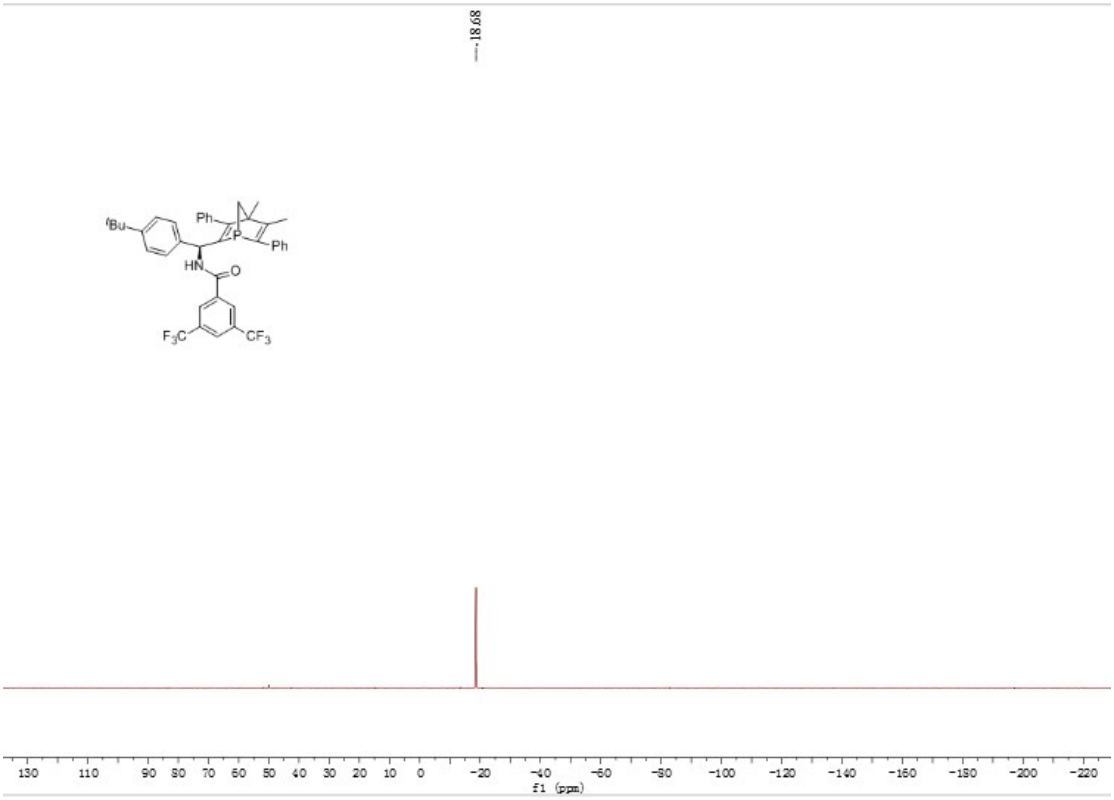
White solid (27.0 mg, 60% yield), $\mathbf{R}_f$ = 0.45. (petroleum ether/ ethyl acetate 2/1).

MP: 47.2-48.0 °C. $[\alpha]_D^{25}$= -88 (*c* 0.10, CH_2Cl_2).

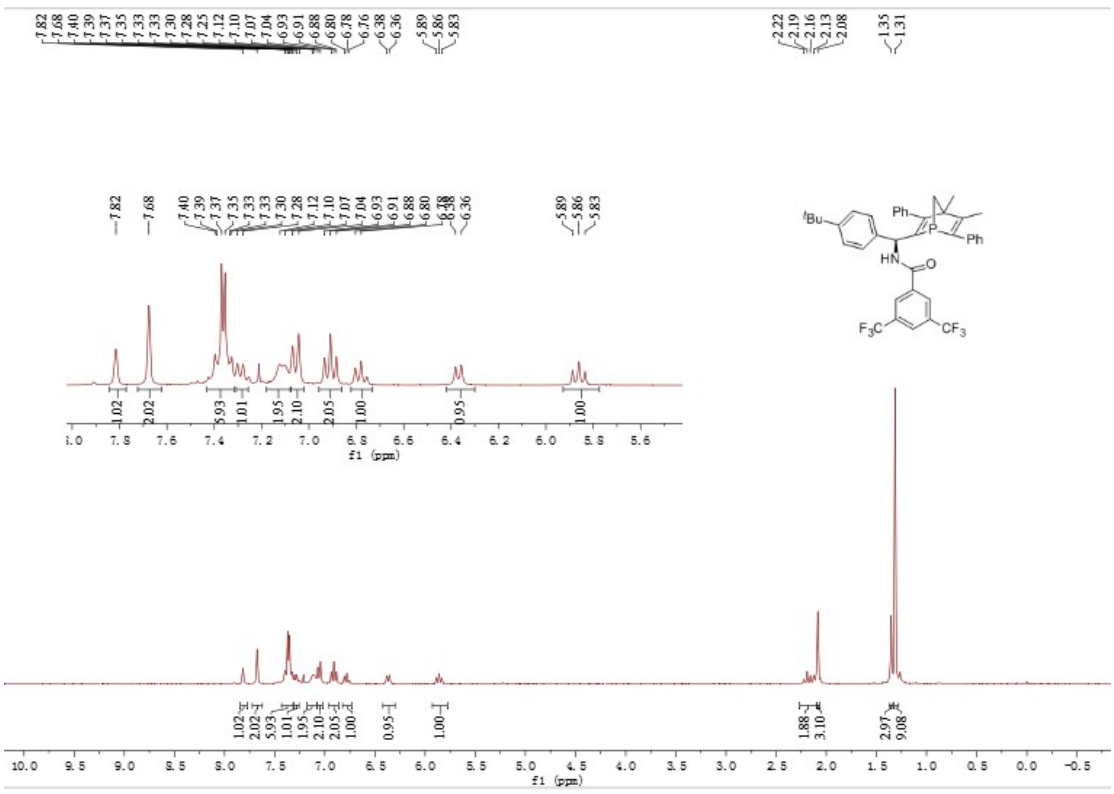
^{1}H NMR (300 MHz, $CDCl_3$) δ 0.37 (d, *J* = 6.4 Hz, 3H), 0.92 (d, *J* = 6.5 Hz, 3H), 2.02-2.19 (m, 1H), 3.00-3.11 (m, 1H), 3.83 (s, 3H), 4.18 (d, *J* = 6.8 Hz, 1H), 4.34 (d, *J* = 15.9 Hz, 1H), 4.73-4.91 (m, 2H), 6.37 (d, *J* = 6.7 Hz, 1H), 6.49 (d, *J* = 7.0 Hz, 2H), 6.84 (d, *J* = 7.4 Hz, 2H), 7.03-7.15 (m, 7H), 7.20 (d, *J* = 7.3 Hz, 1H), 7.50 (d, *J* = 6.2 Hz, 1H) ppm. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 21.7, 22.4, 30.2, 43.3, 52.4, 60.4, 64.1, 64.4, 72.9, 109.3, 122.1, 122.6, 126.4, 126.6, 127.1, 127.9, 127.9, 128.0, 128.5, 130.1, 134.5, 135.2, 142.7, 175.7 ppm. **HRMS** (ESI, m/z): Calcd for $C_{29}H_{31}N_2O_3$ $[M+H]^+$: 455.2329, found: 455.2326. **HPLC**: The product was analyzed by HPLC to determine the enantiomeric excess: 94% ee (Chiralpak AD-H, hexane/*i*-propanol = 90 : 10, flow rate 1.0 mL/min, λ = 254 nm); tr = 24.59 and 28.02 min.

7. Copies of NMR spectra

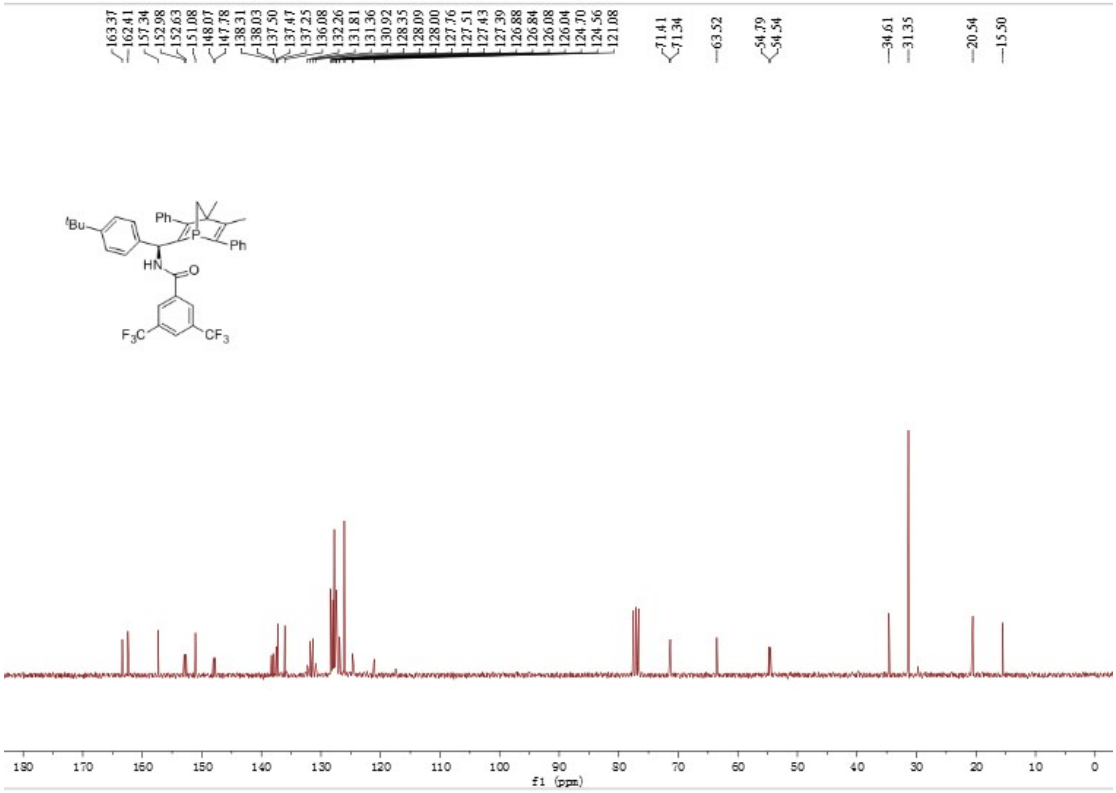
^{31}P NMR of Kephos



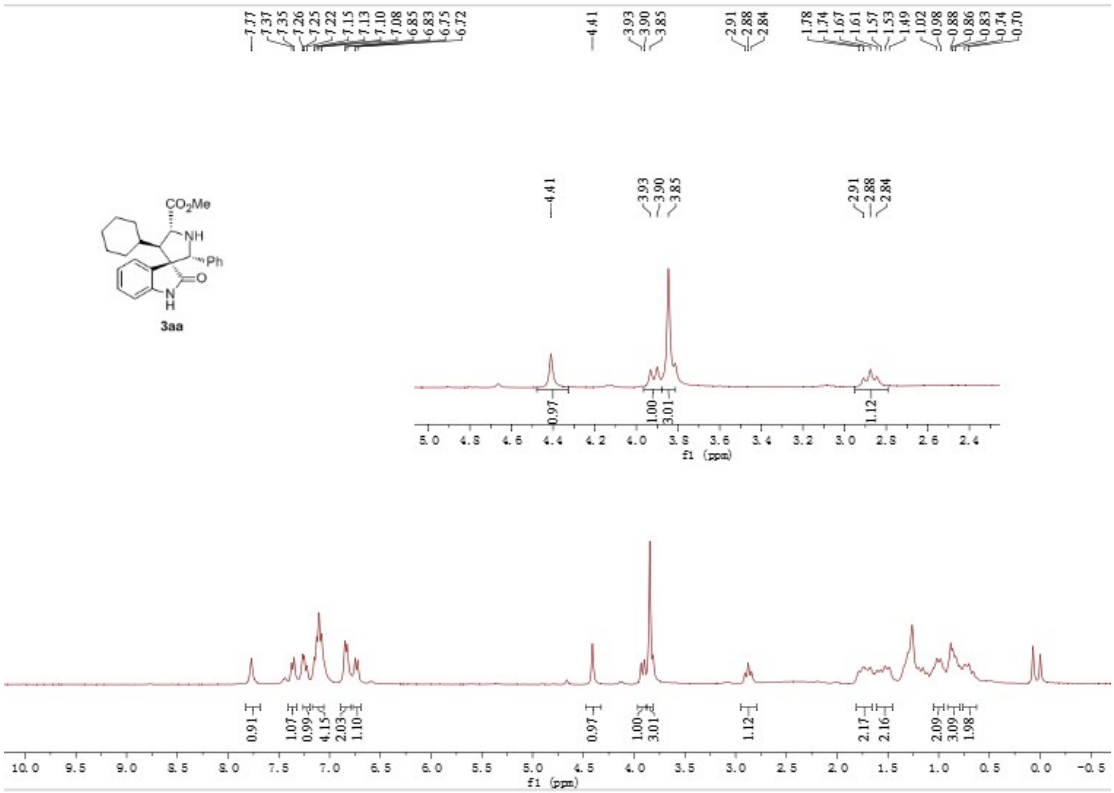
^{1}H NMR of Kephos



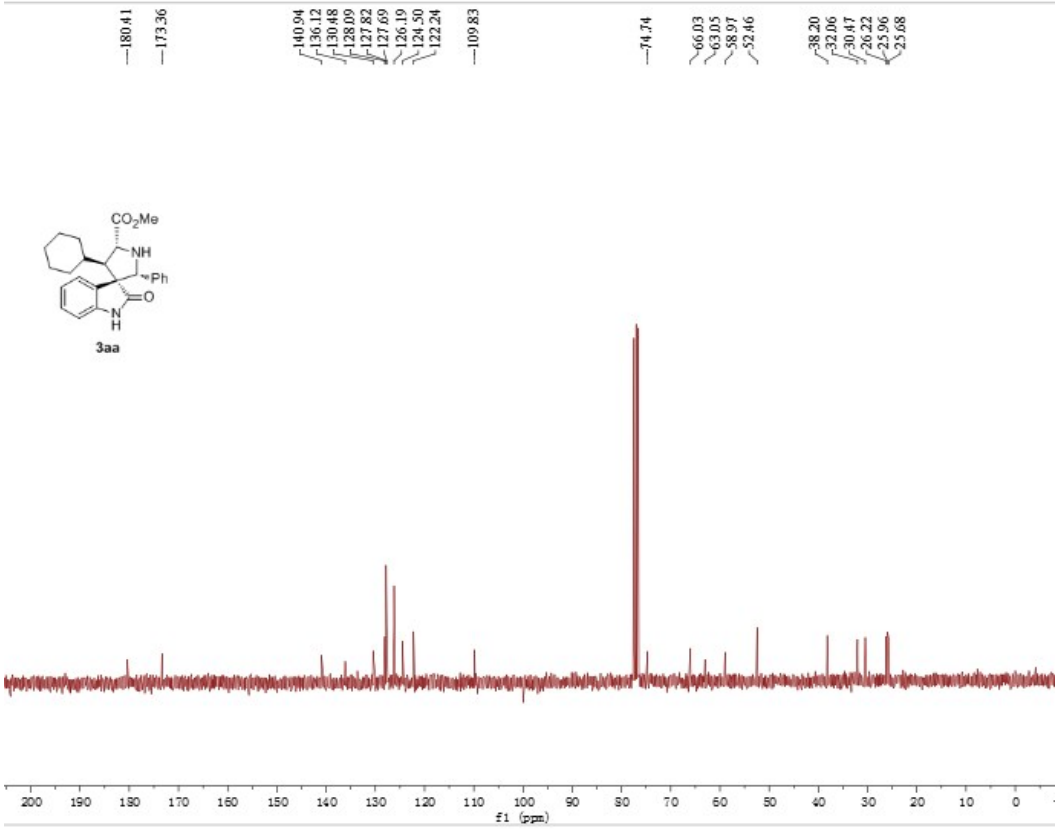
^{13}C NMR of Kephos



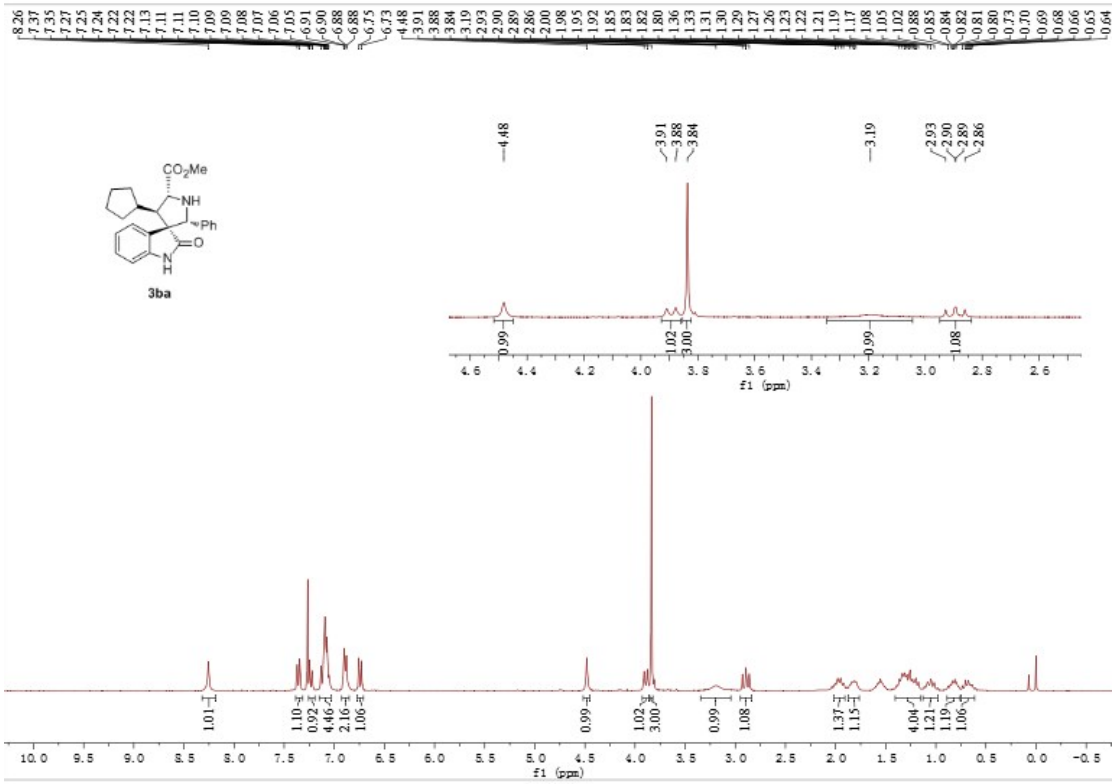
^{1}H NMR of 3aa



^{13}C NMR of 3aa



^{1}H NMR of 3ba



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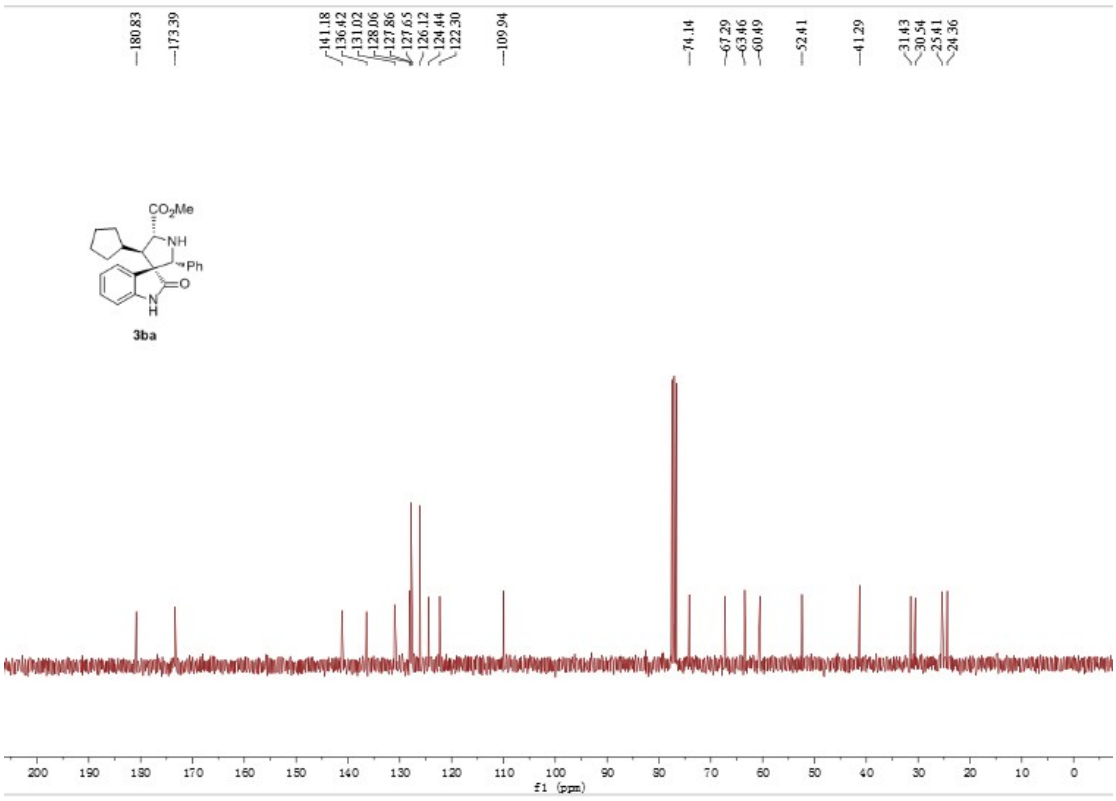
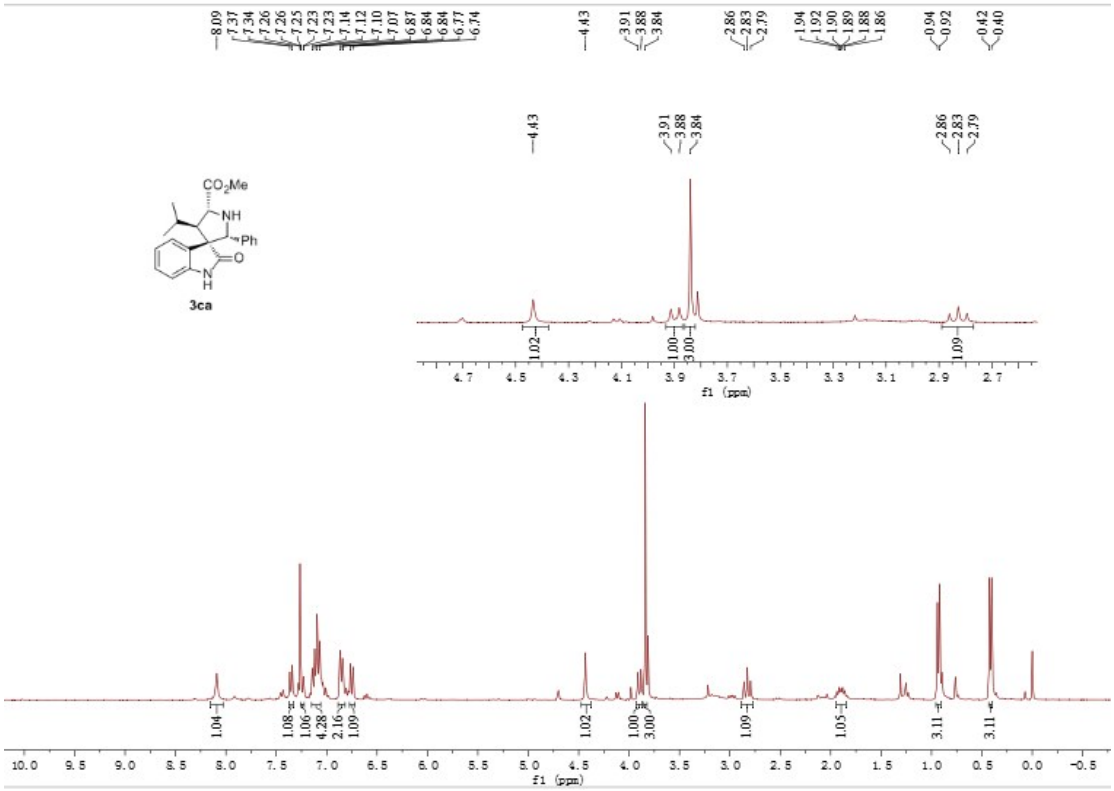
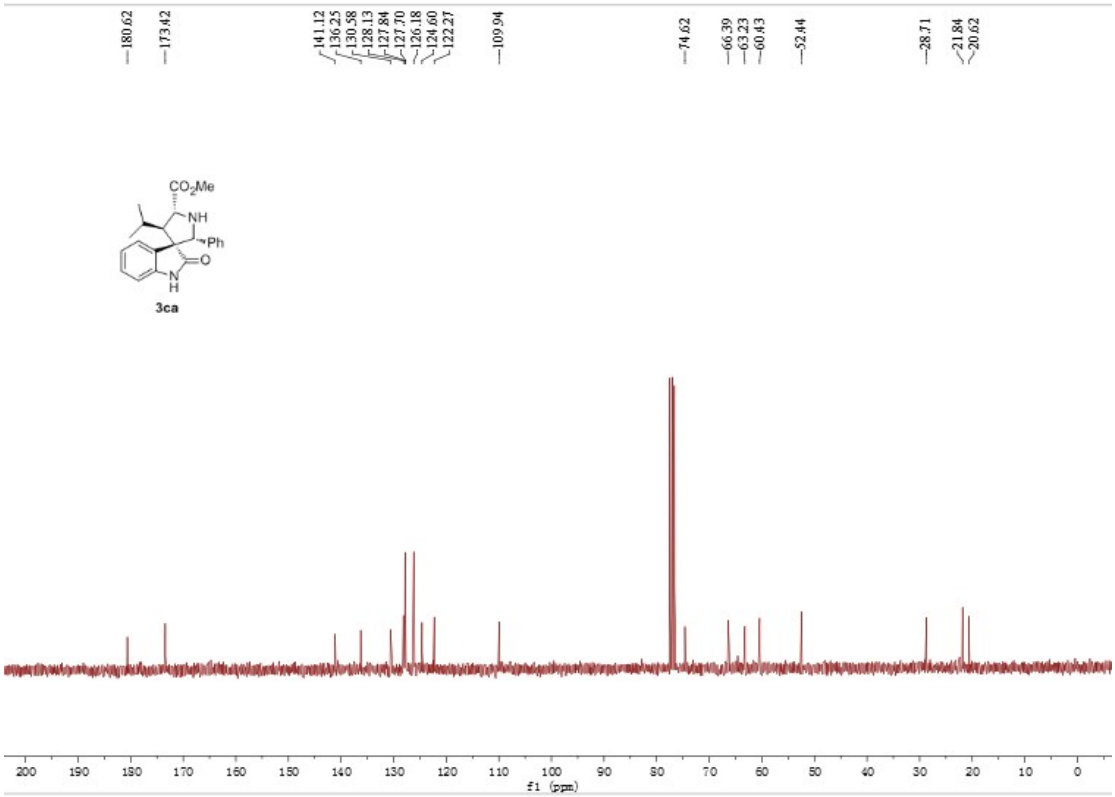


^{1}H NMR of 3ca



^{13}C NMR of 3ca



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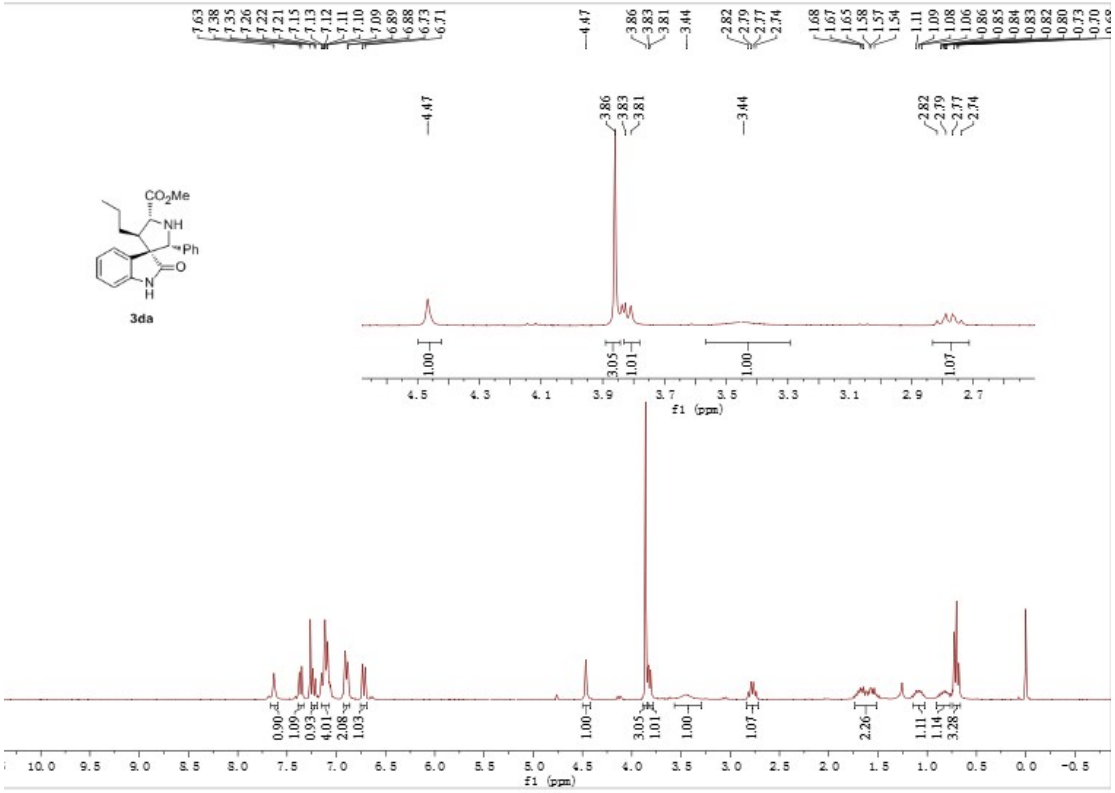
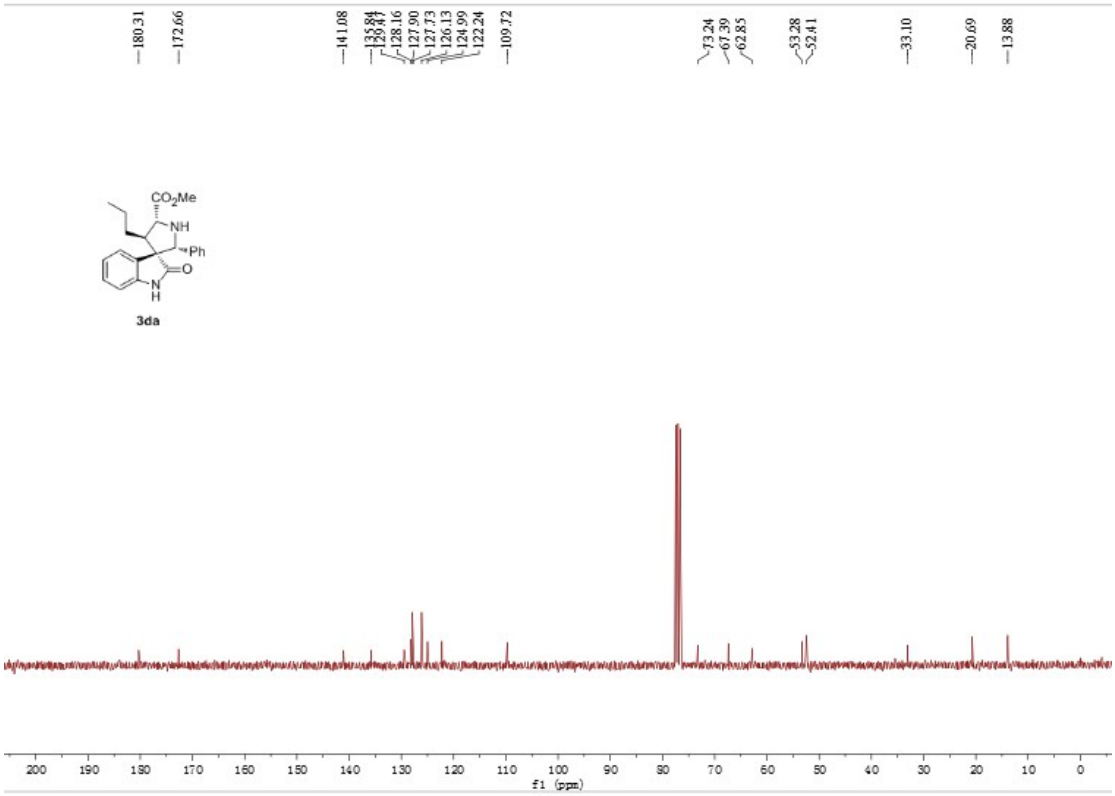


^{13}C NMR of 3da



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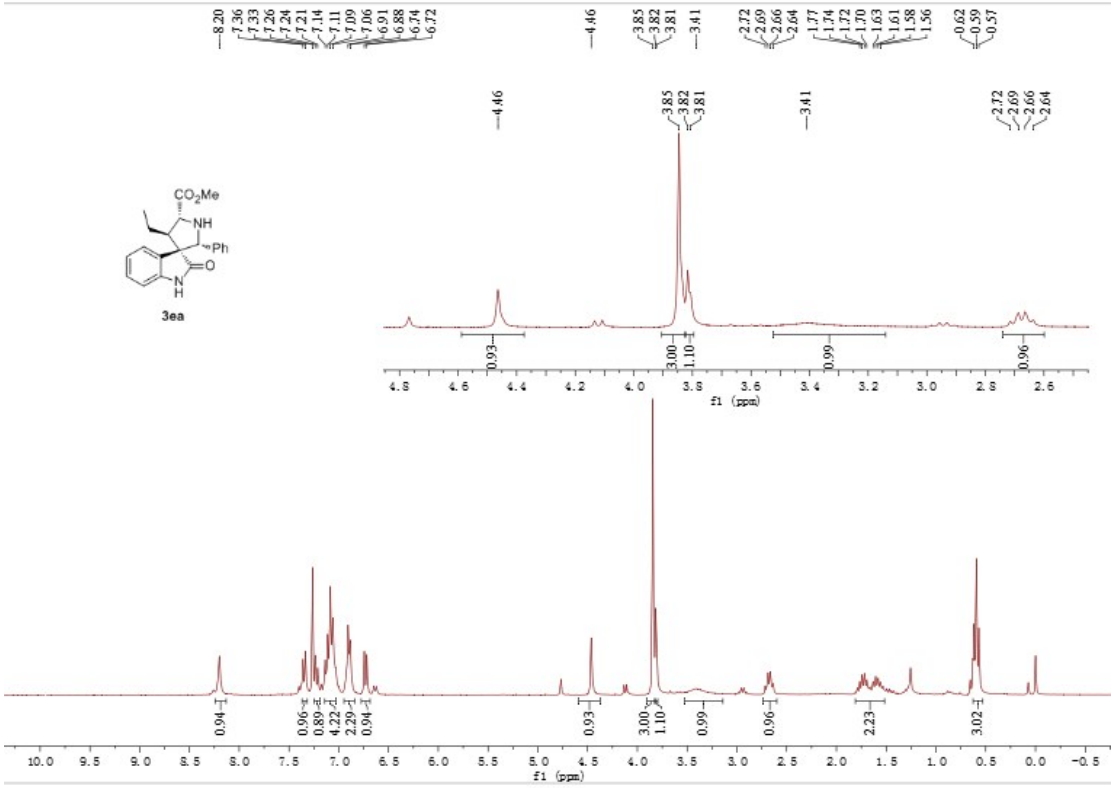
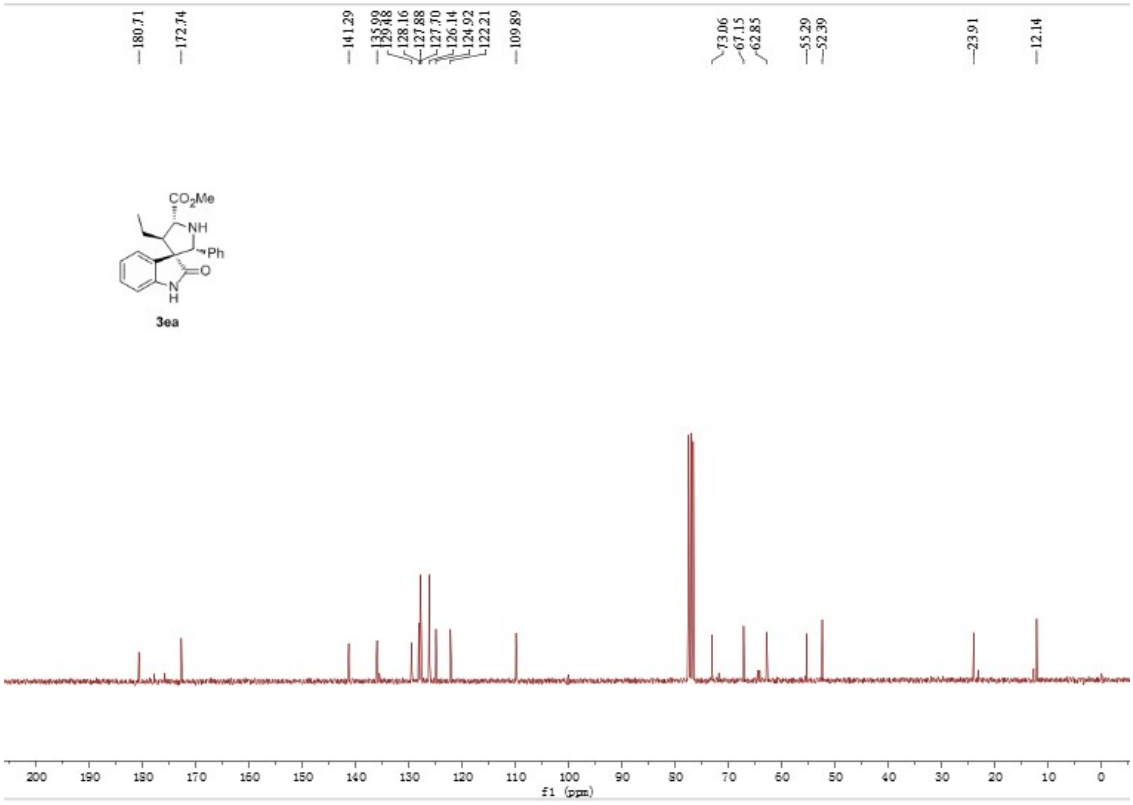
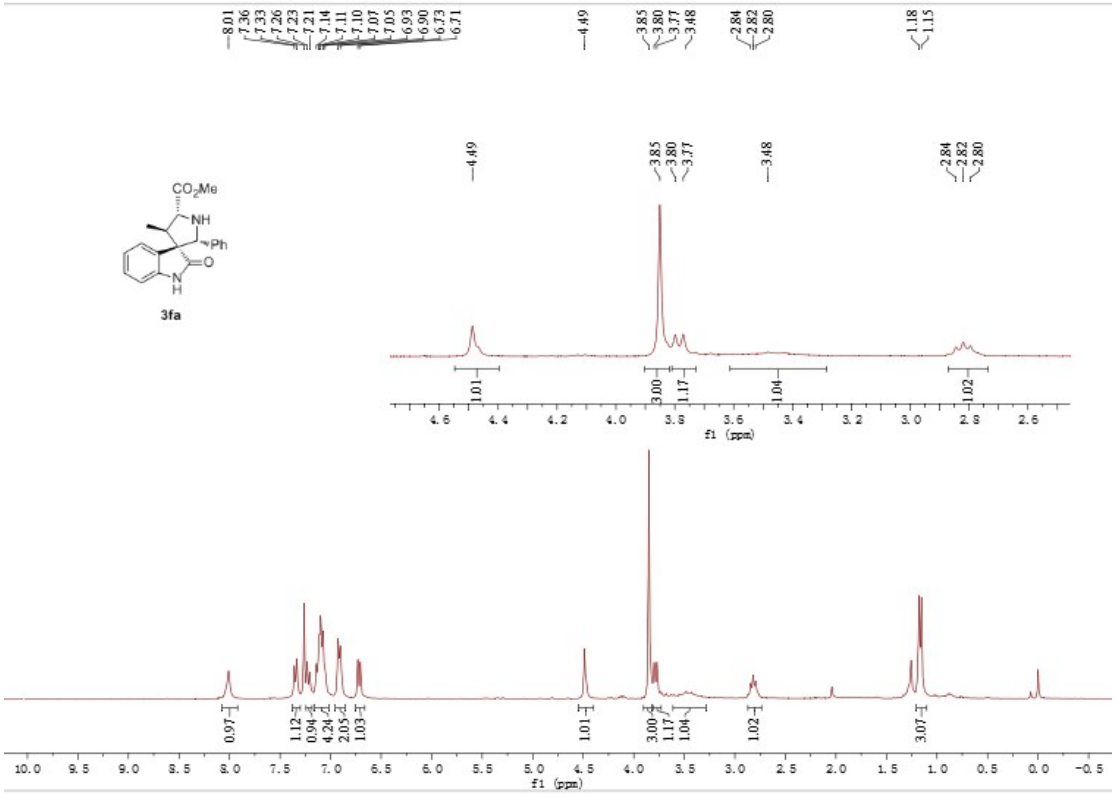


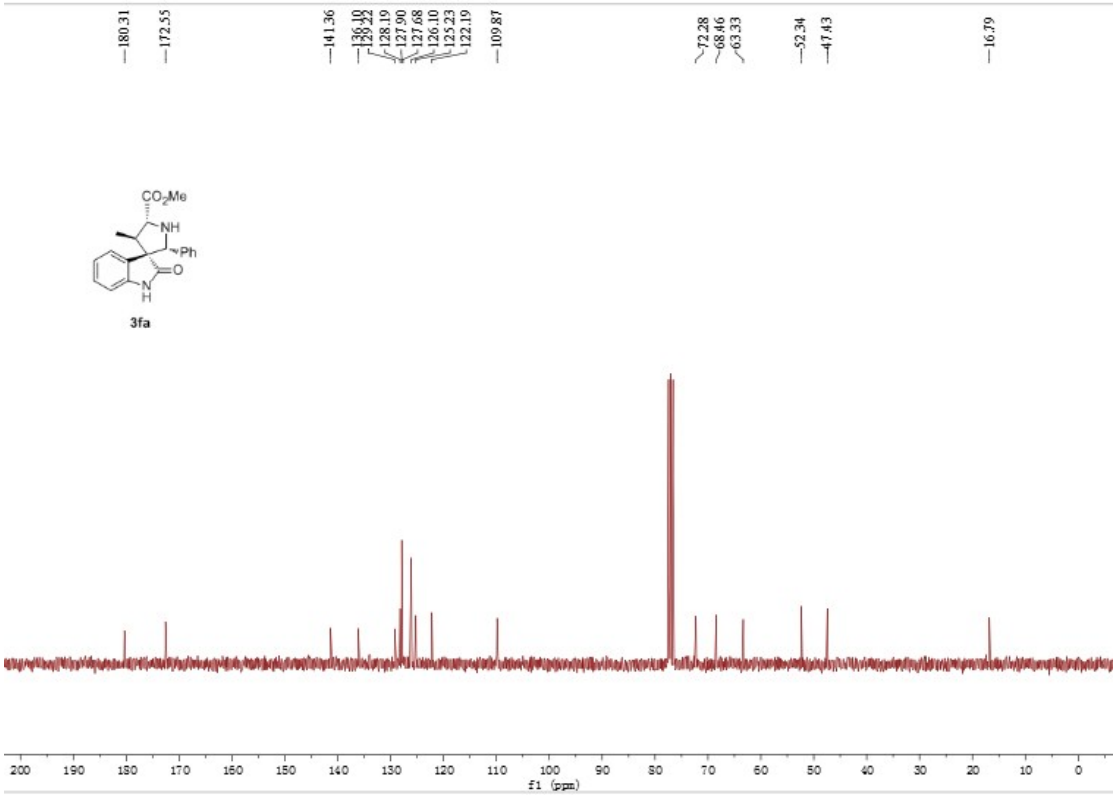
^{13}C NMR of 3ea



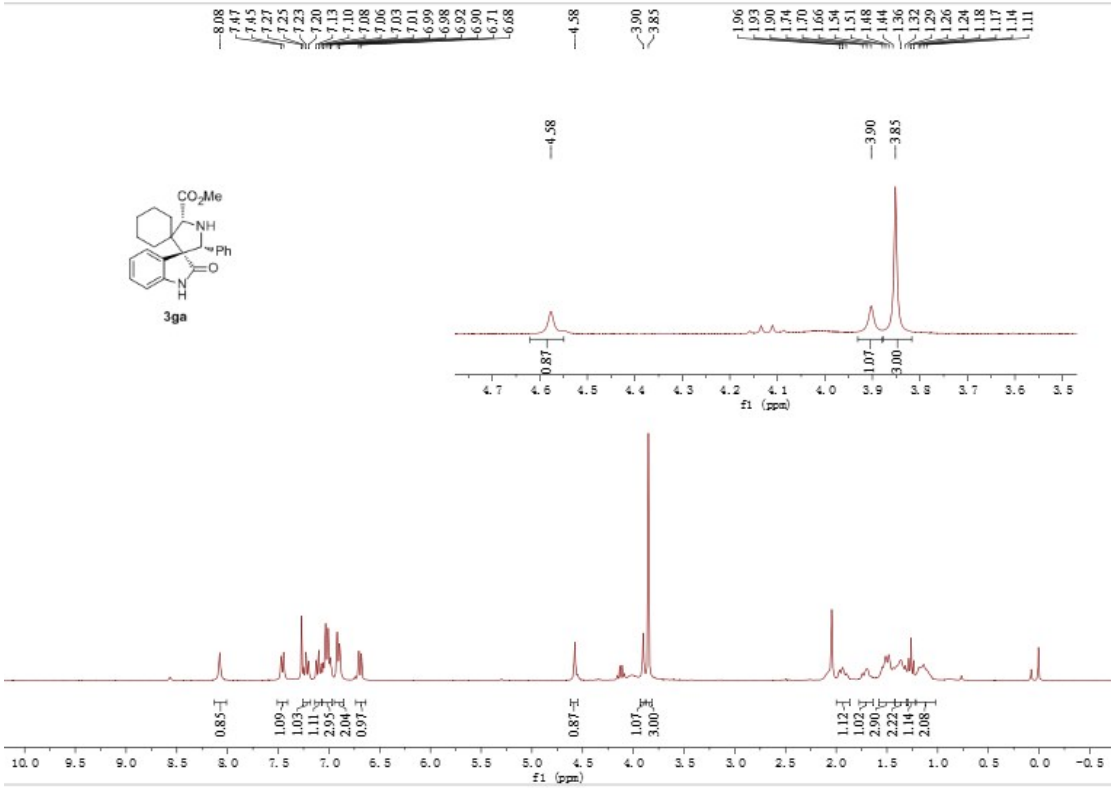
^{1}H NMR of 3fa



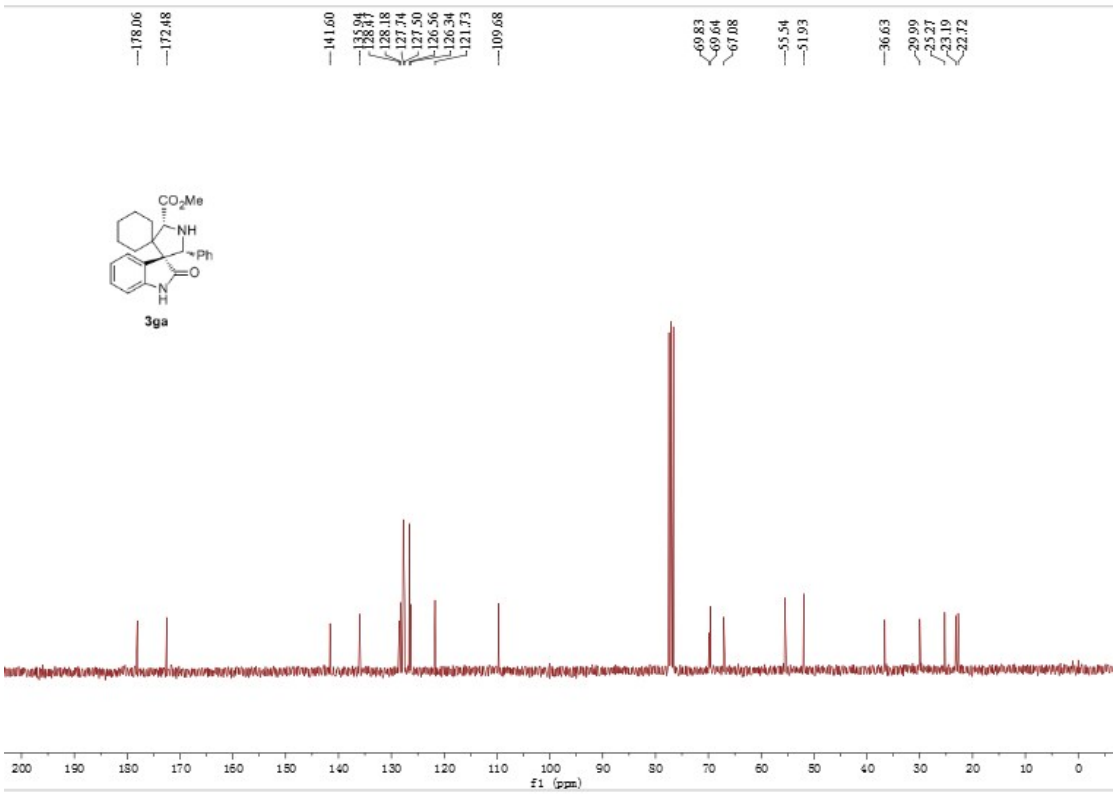
^{13}C NMR of 3fa



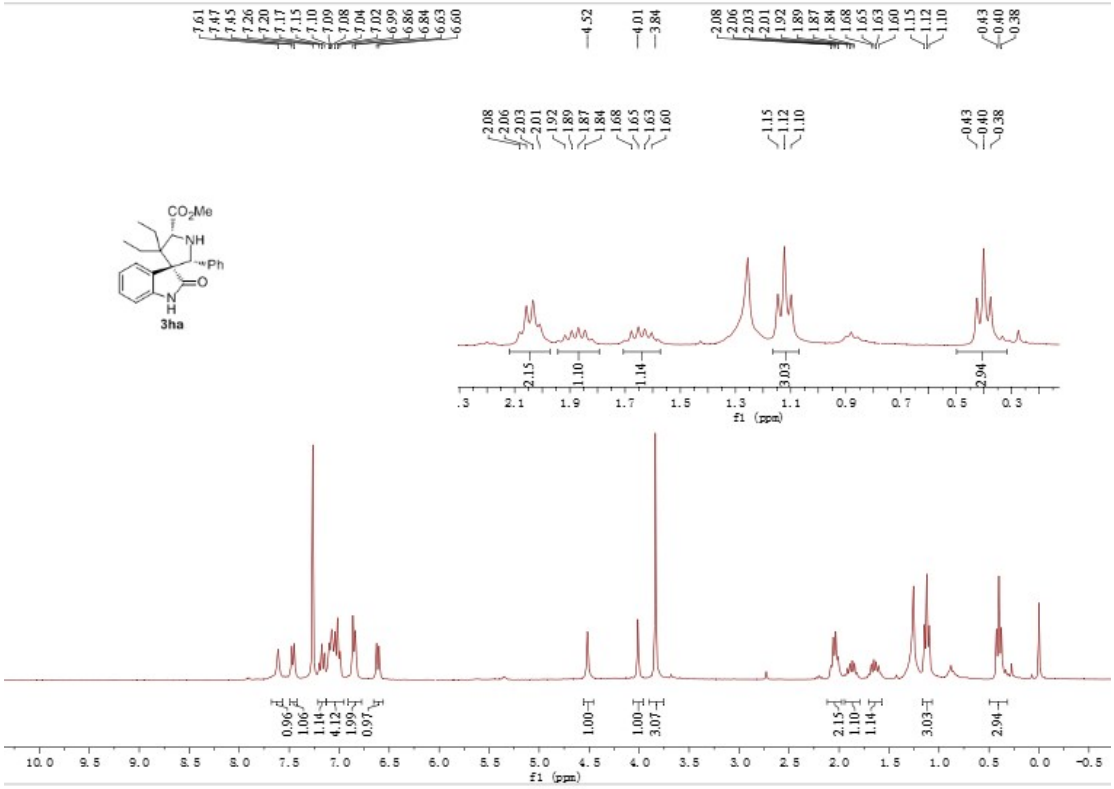
^{1}H NMR of 3ga



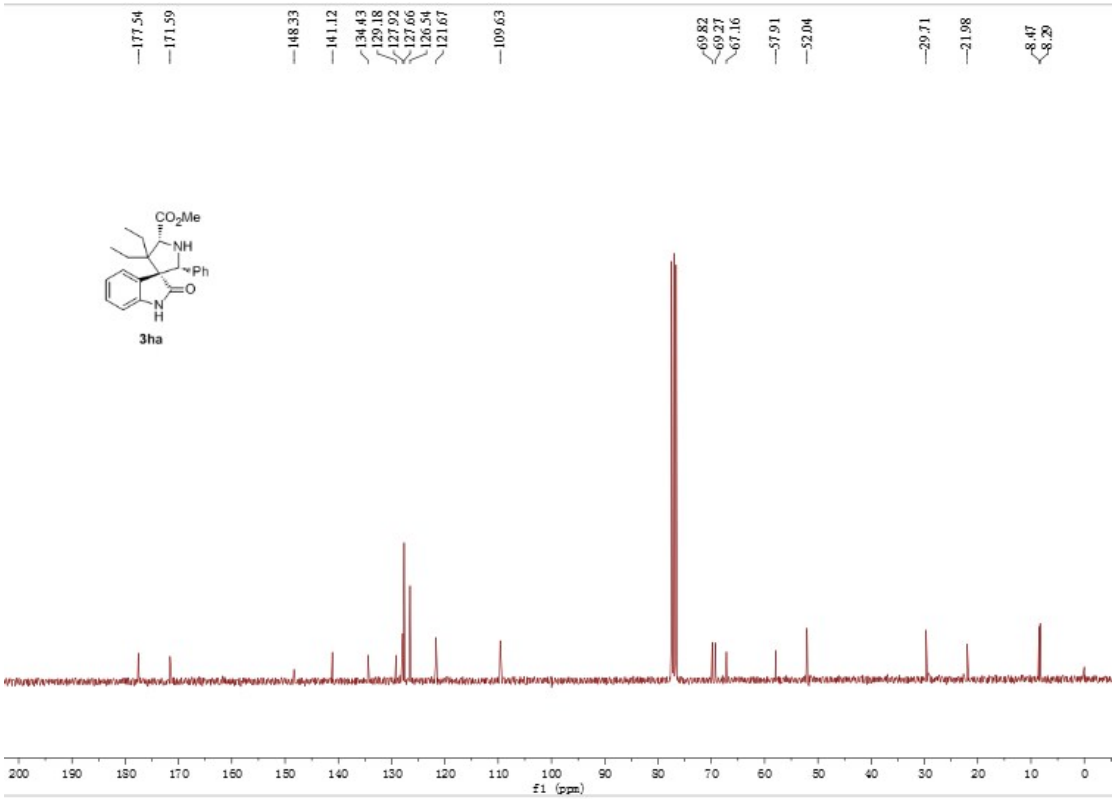
^{13}C NMR of 3ga



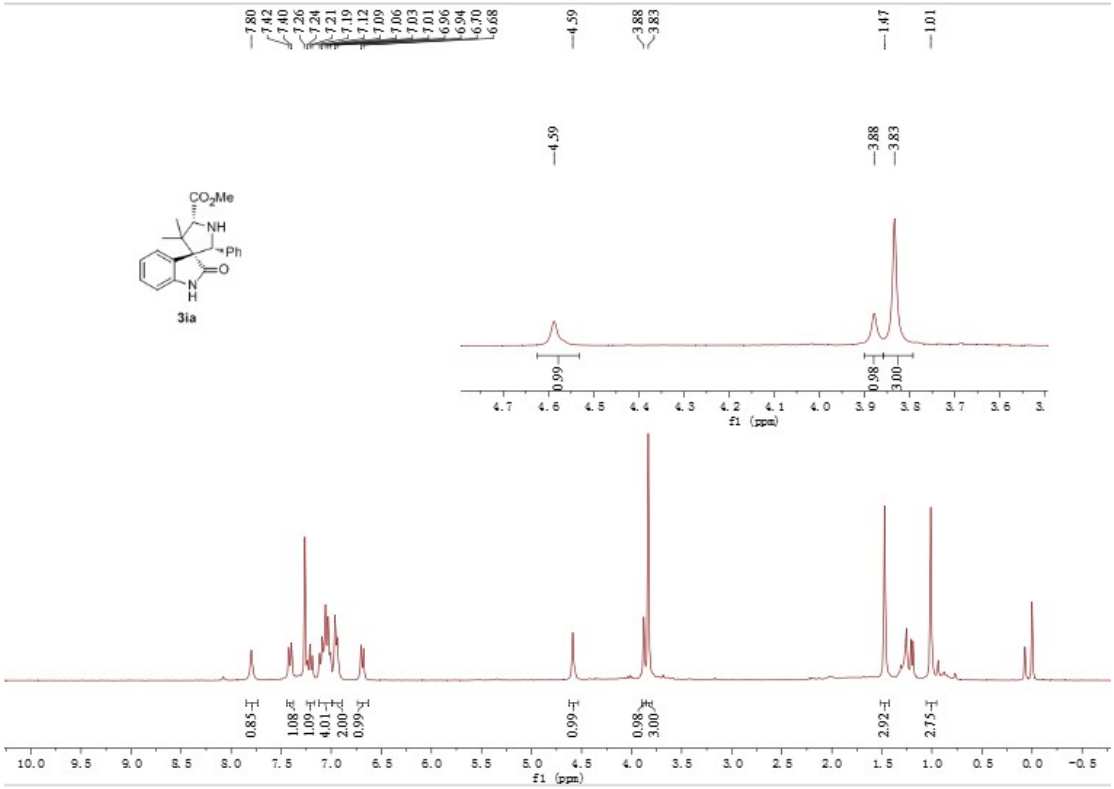
^{1}H NMR of 3ha



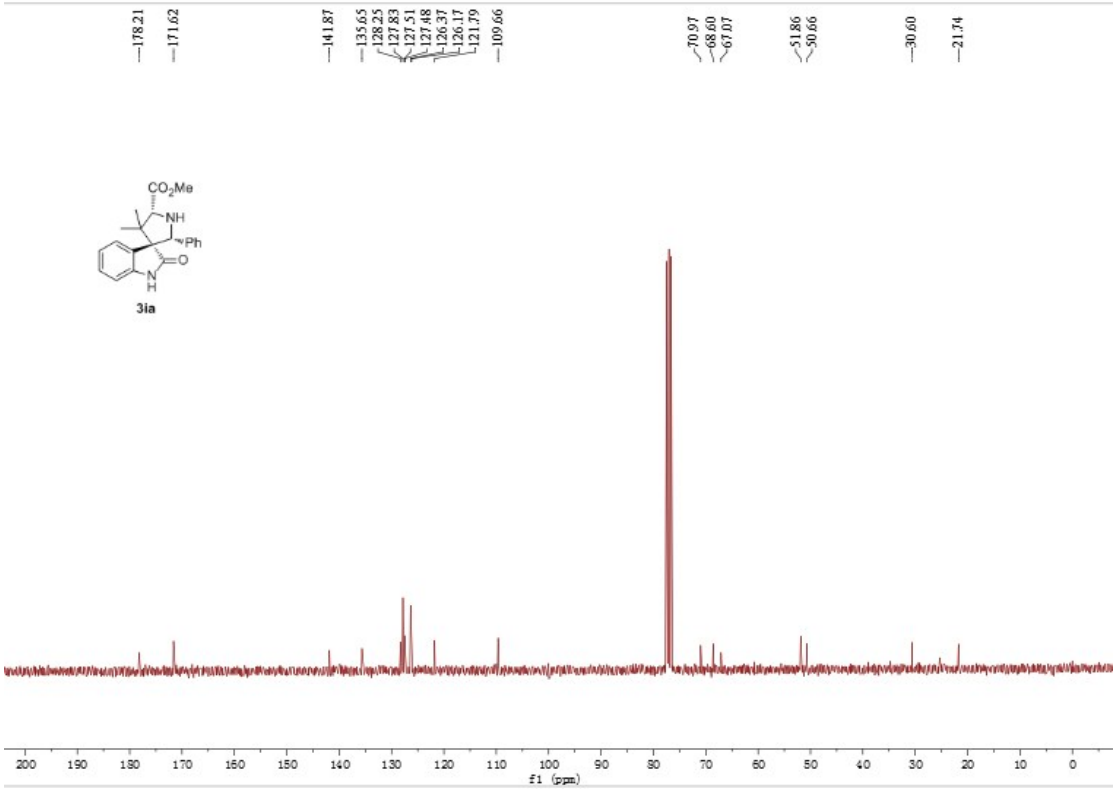
^{13}C NMR of 3ha



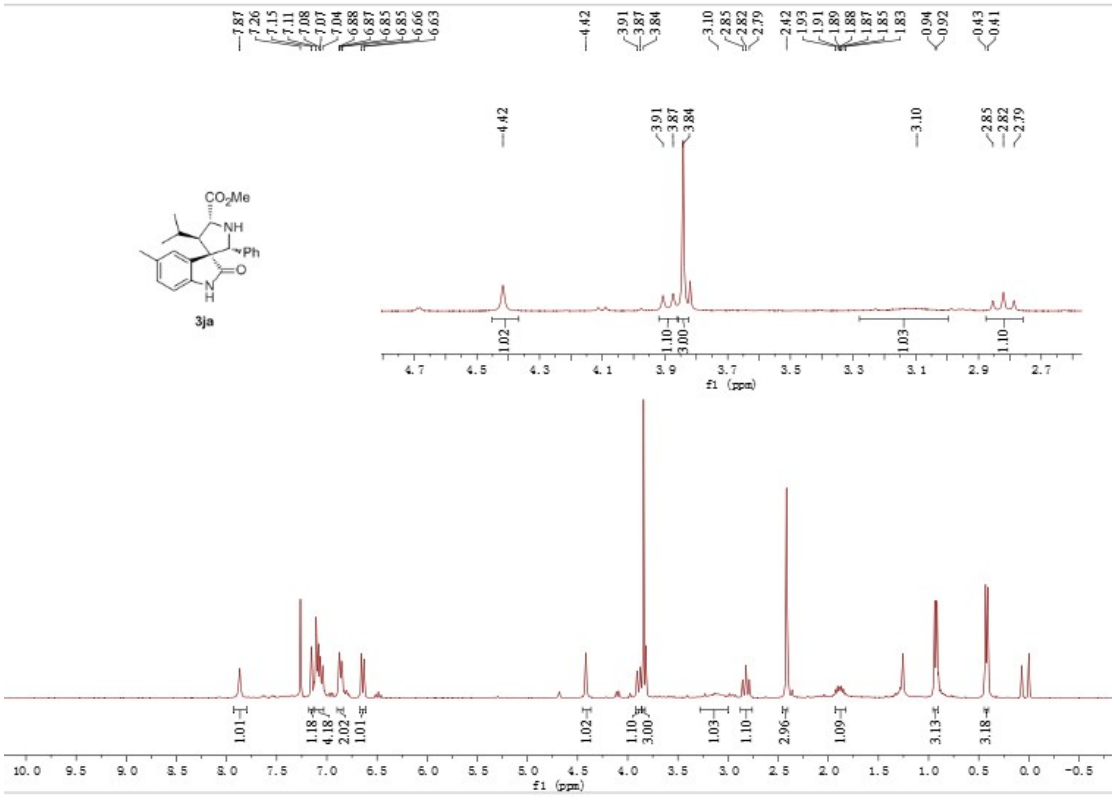
^{1}H NMR of 3ia



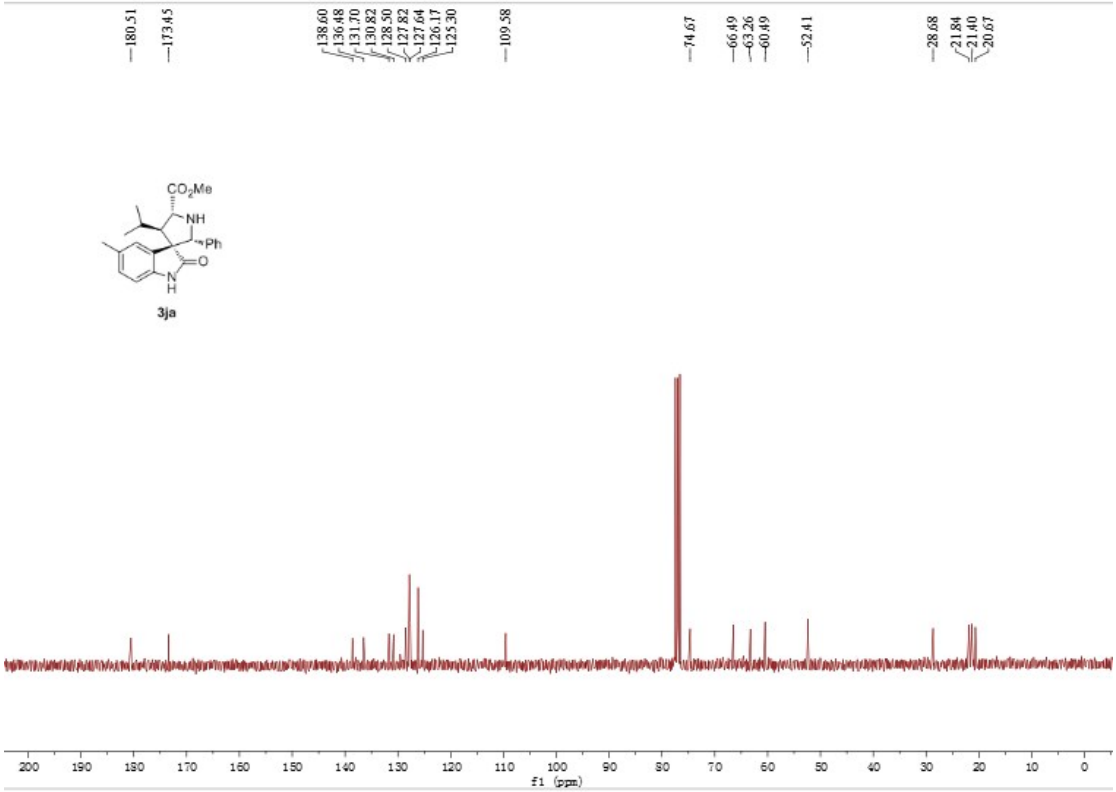
^{13}C NMR of 3ia



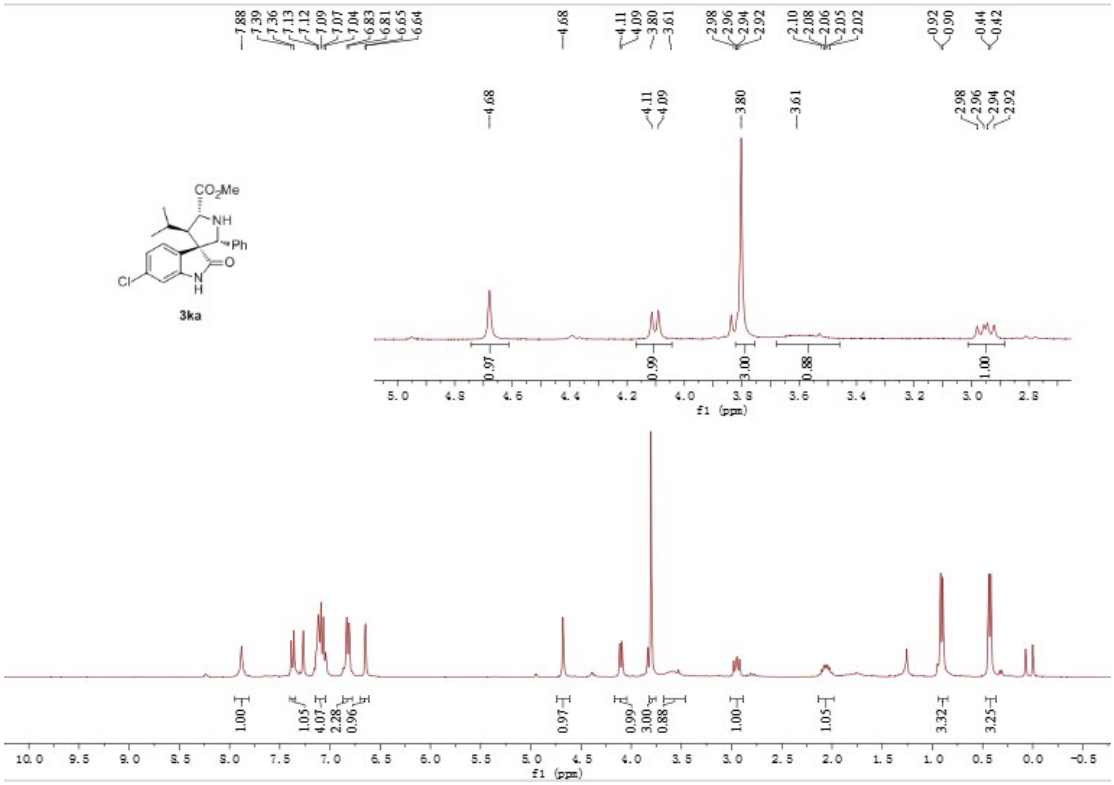
^{1}H NMR of 3ja



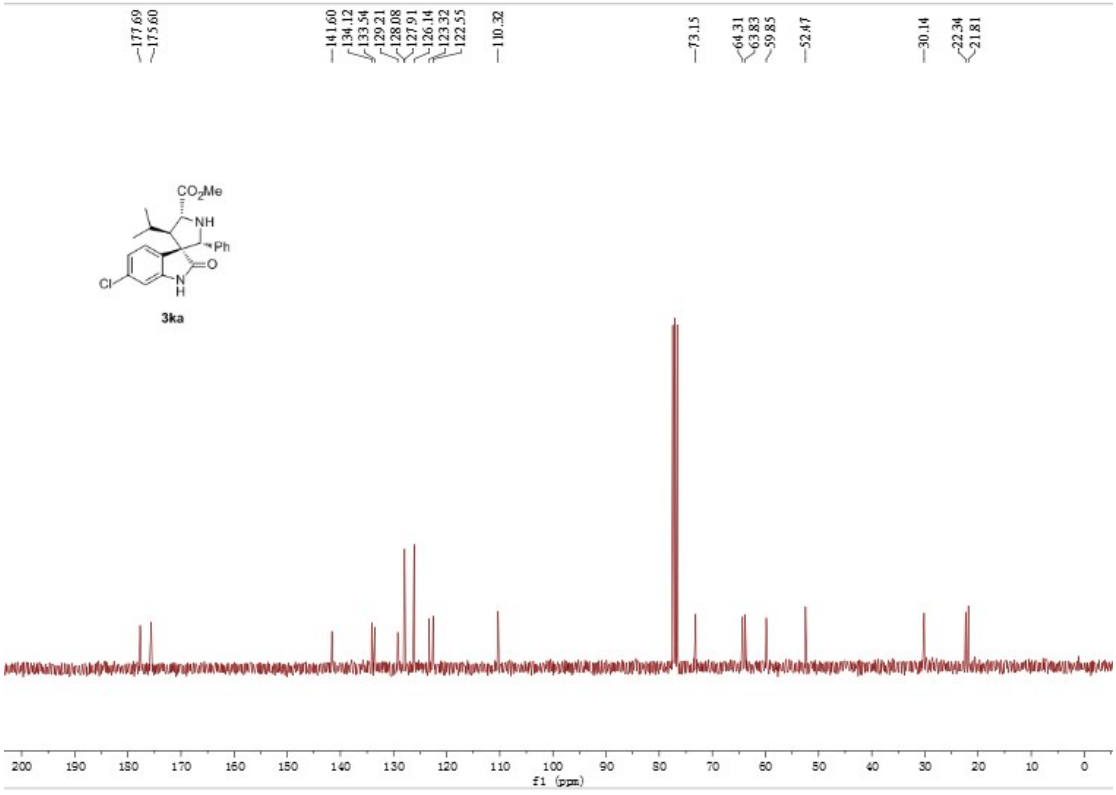
^{13}C NMR of 3ja



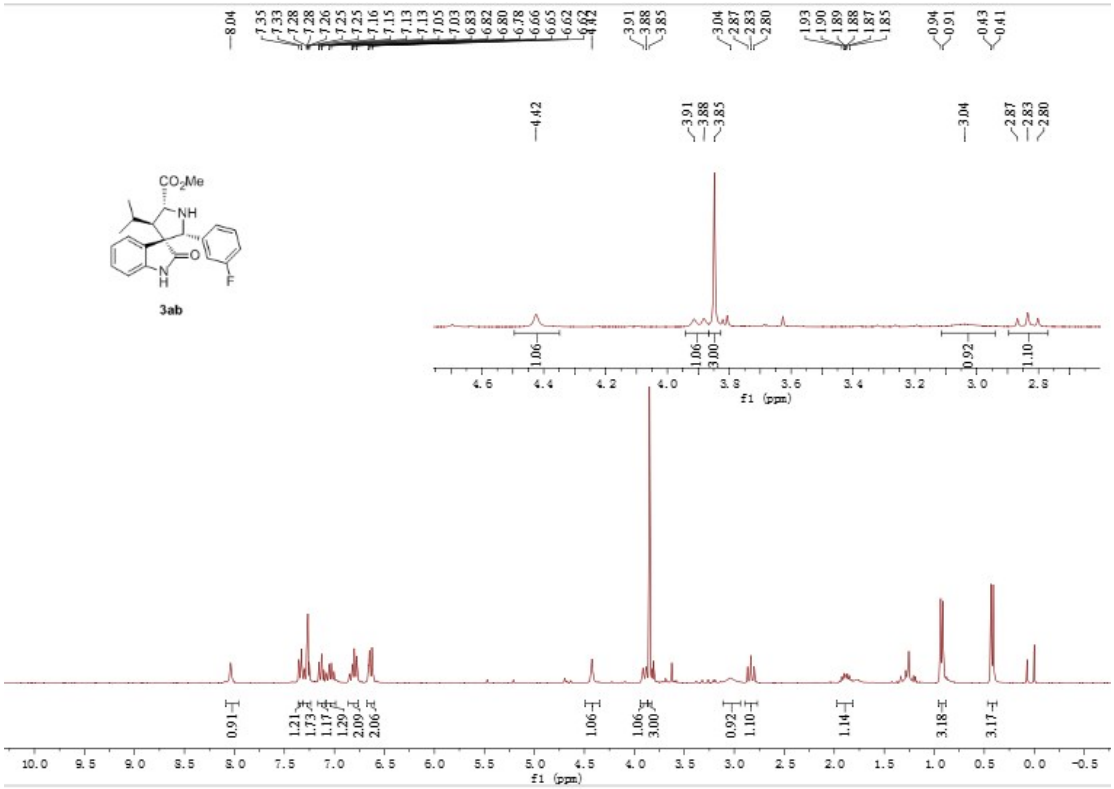
^{1}H NMR of 3ka



^{13}C NMR of 3ka



^{1}H NMR of 3ab



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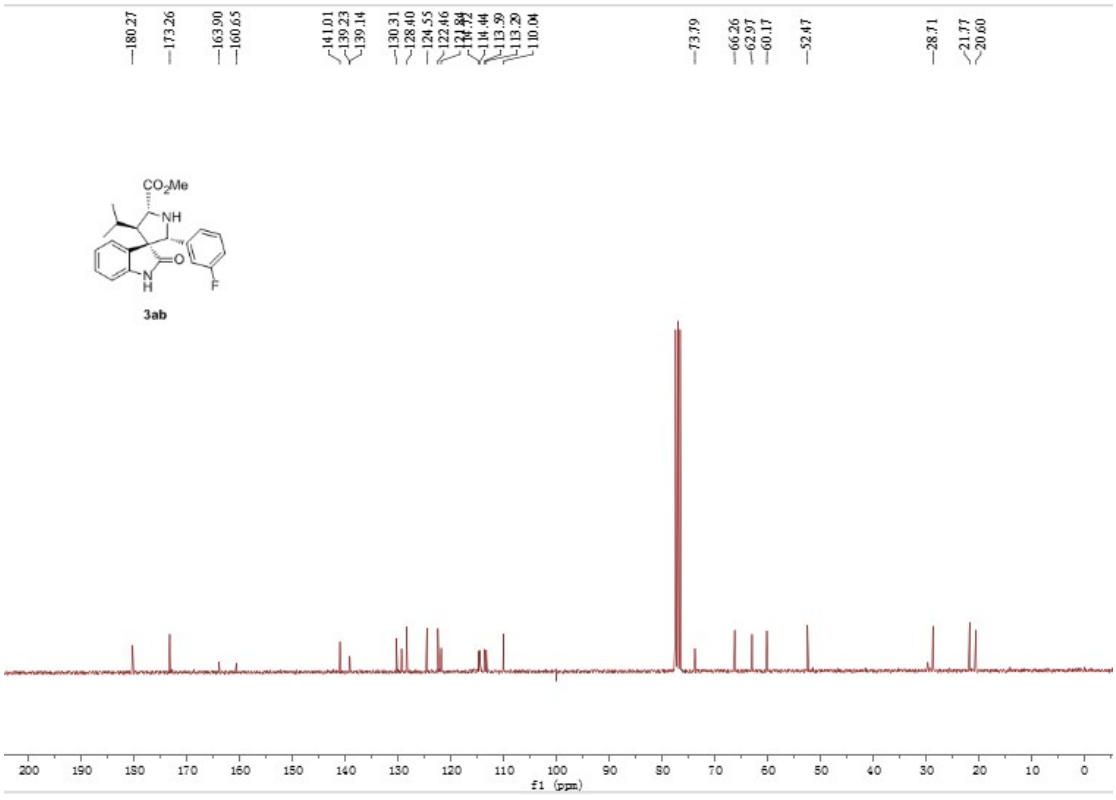
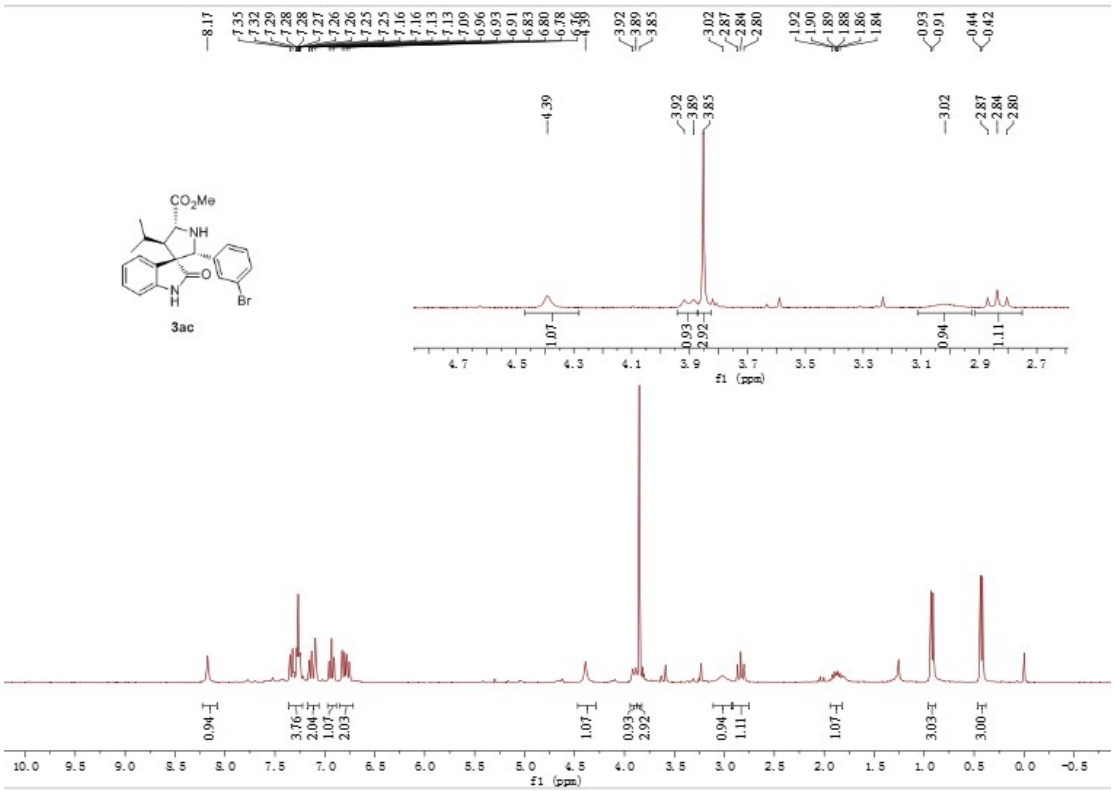
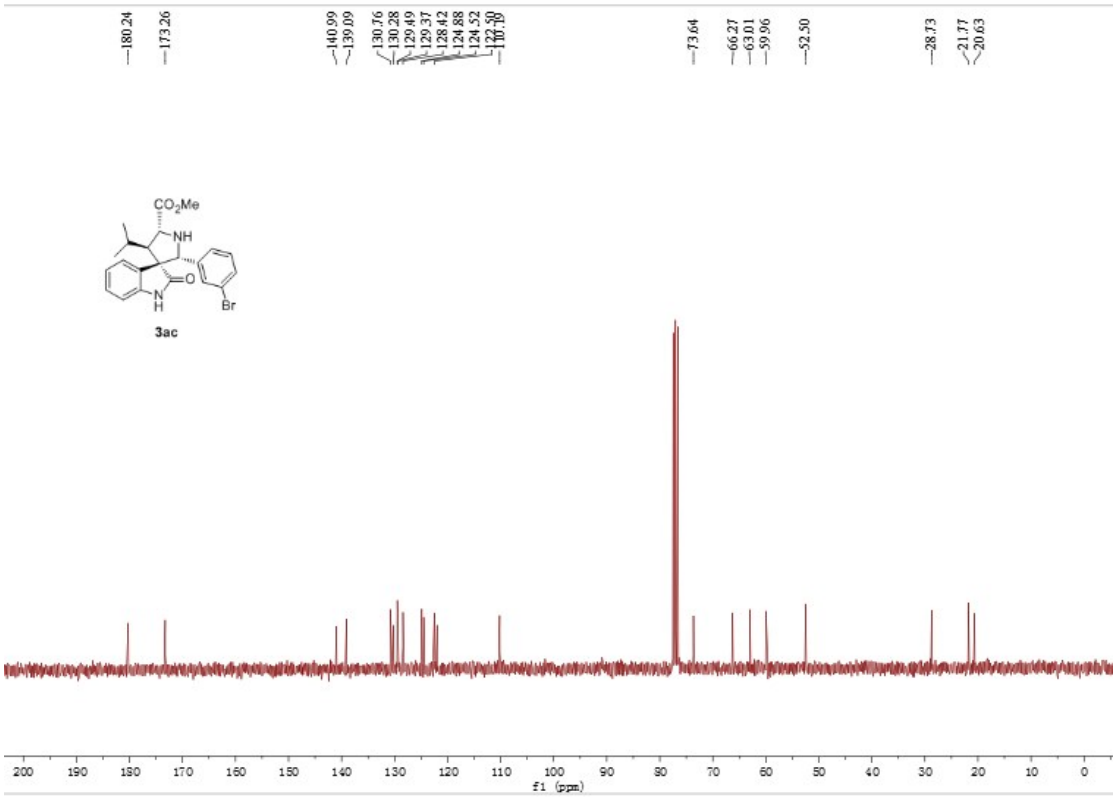


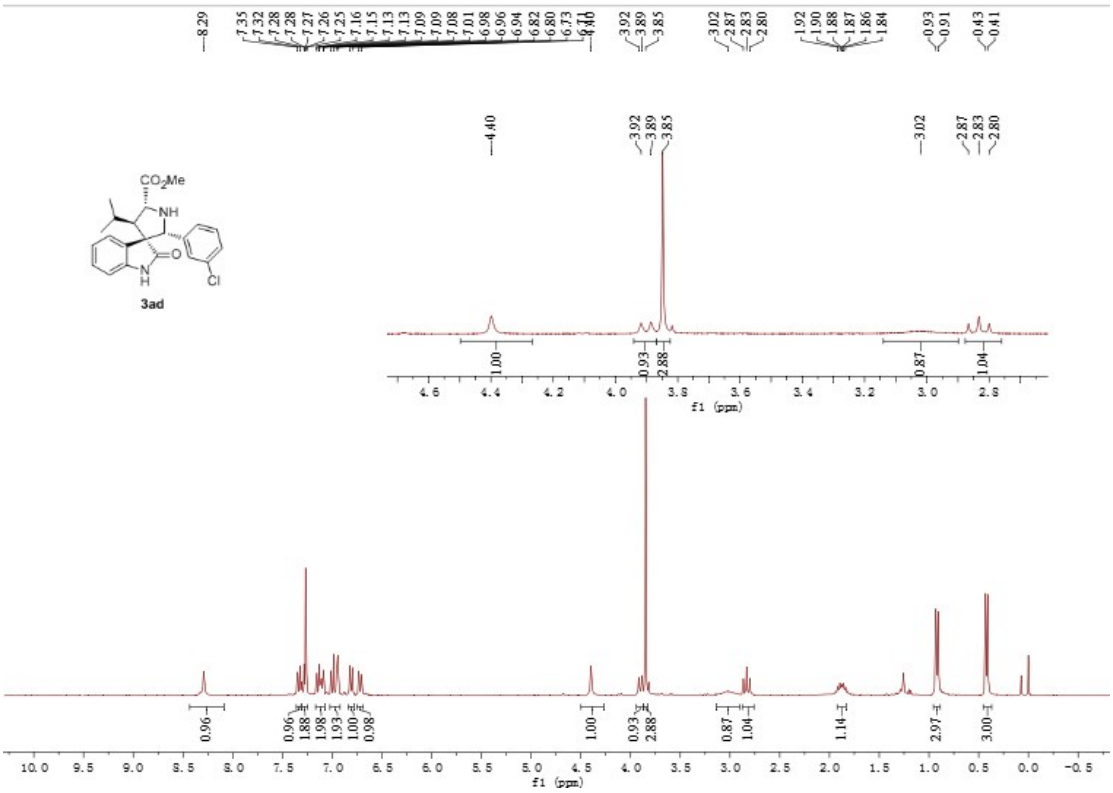
^{1}H NMR of 3ac



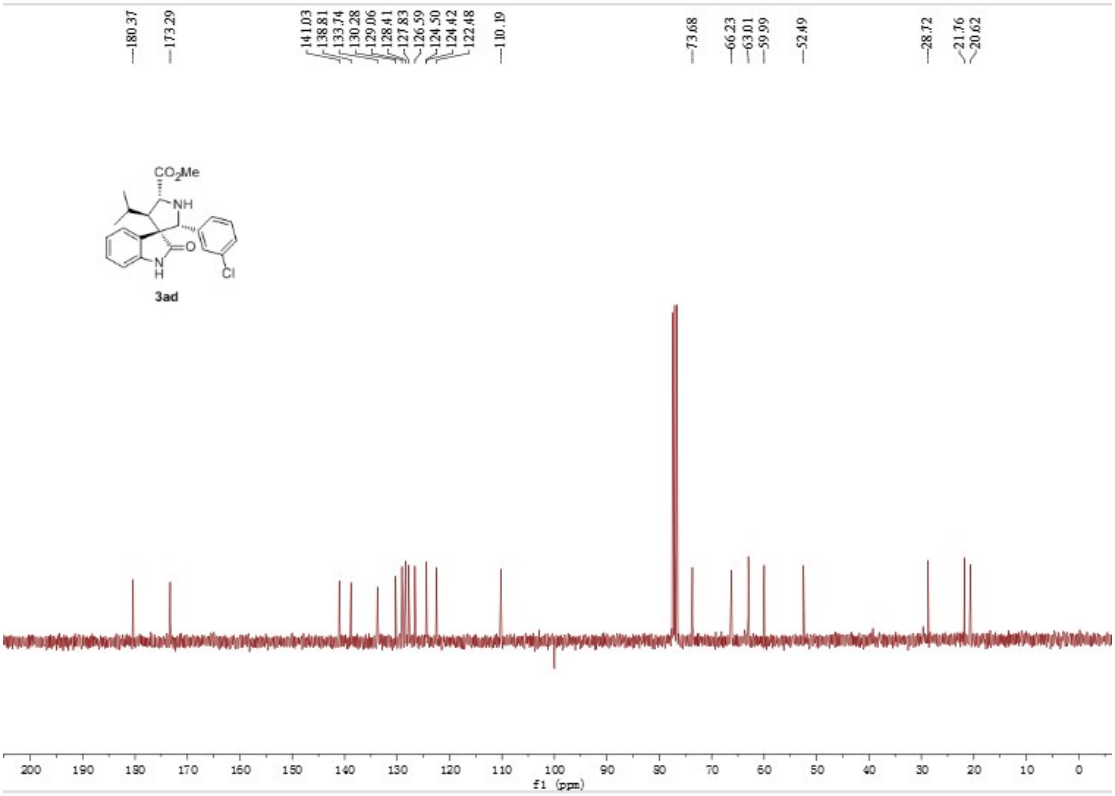
^{13}C NMR of 3ac



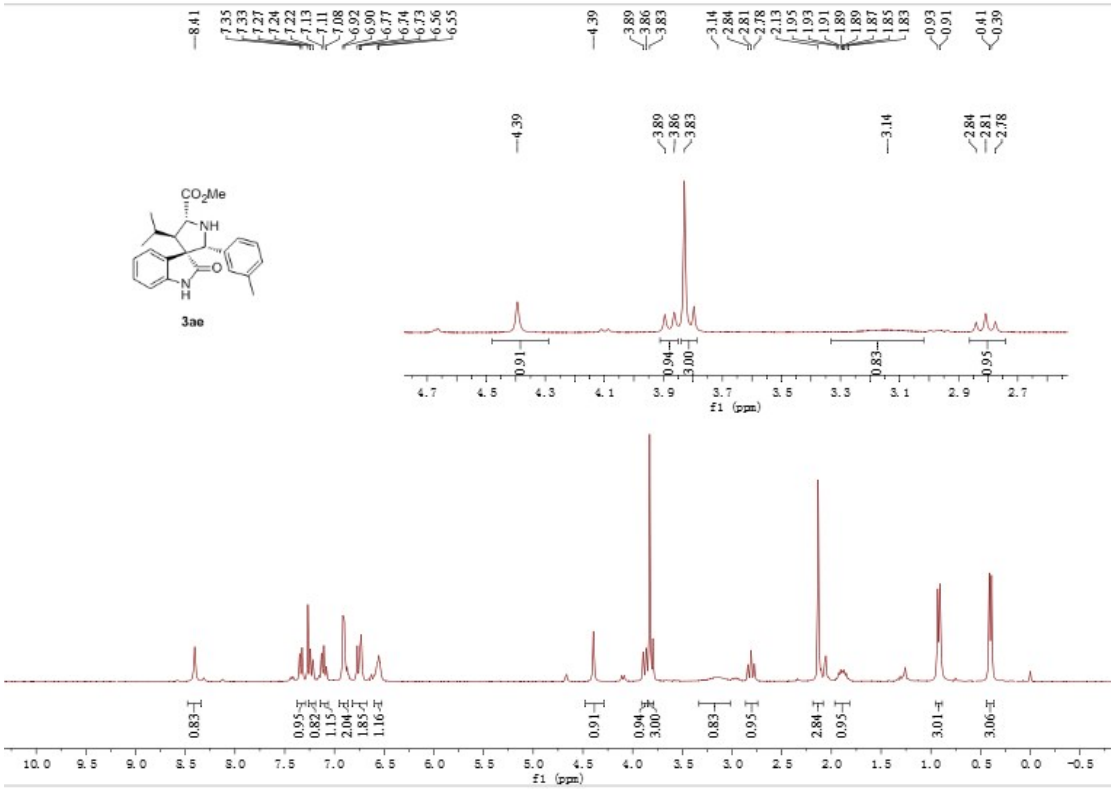
^{1}H NMR of 3ad



^{13}C NMR of 3ad



^{1}H NMR of 3ae



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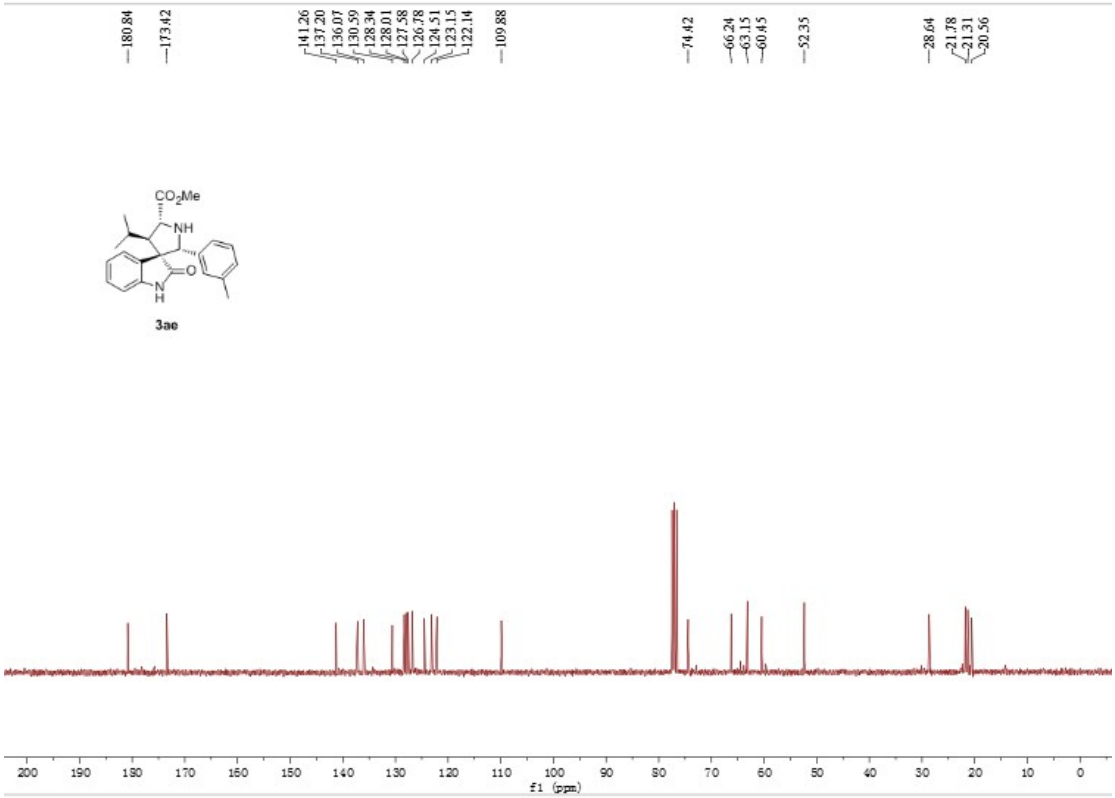

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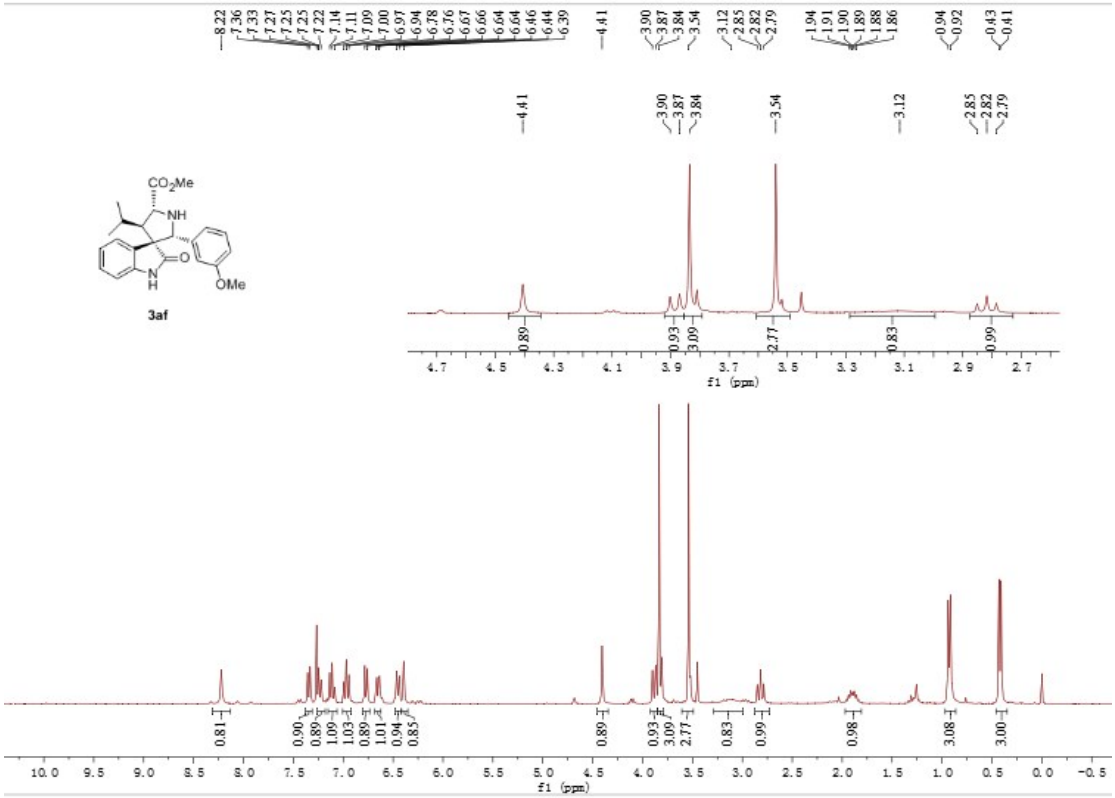

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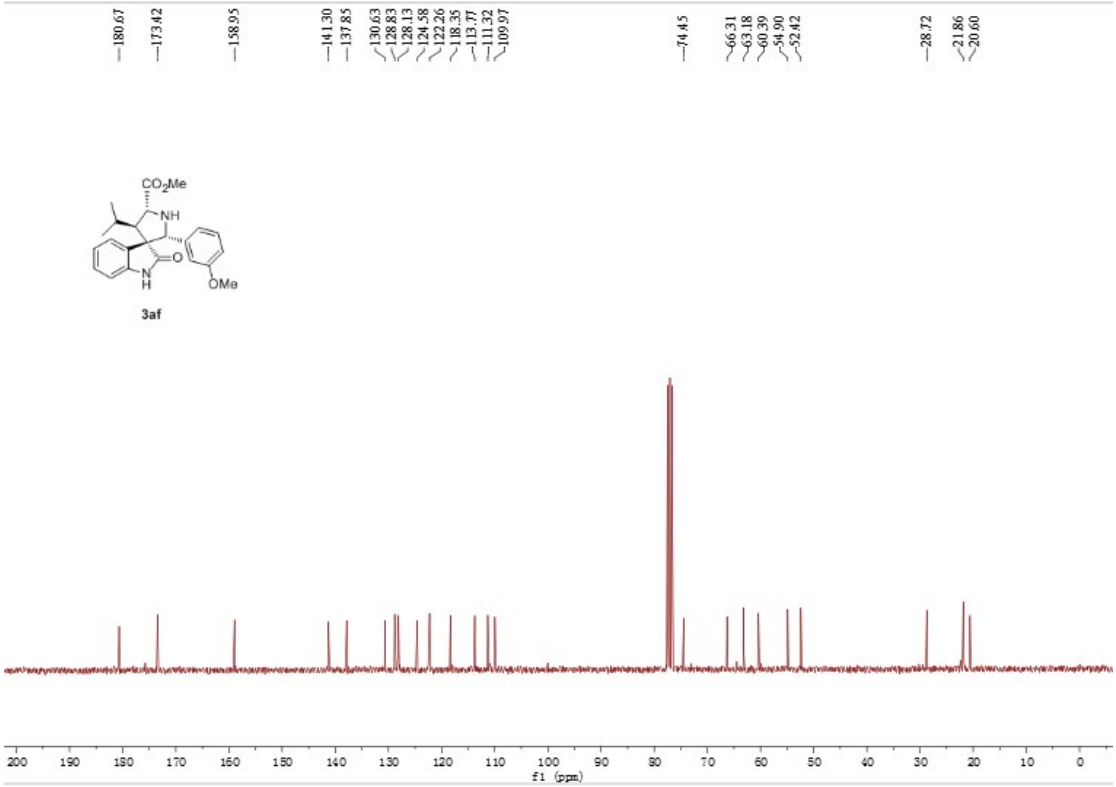
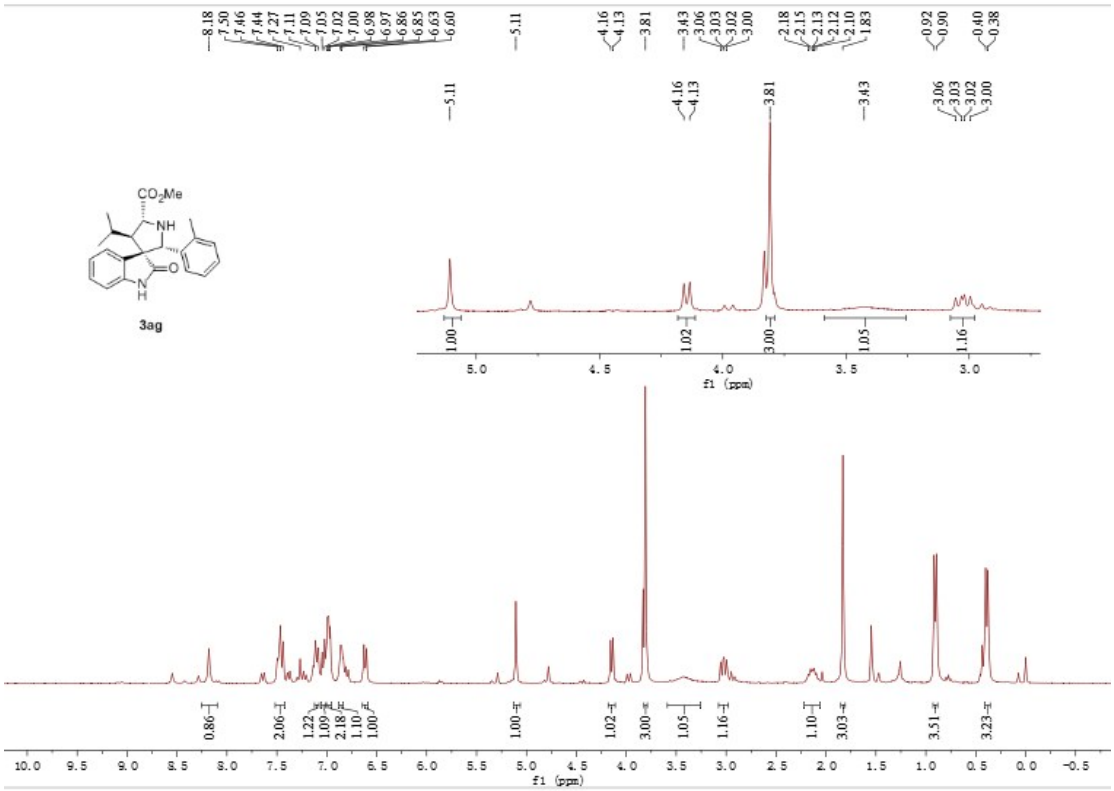
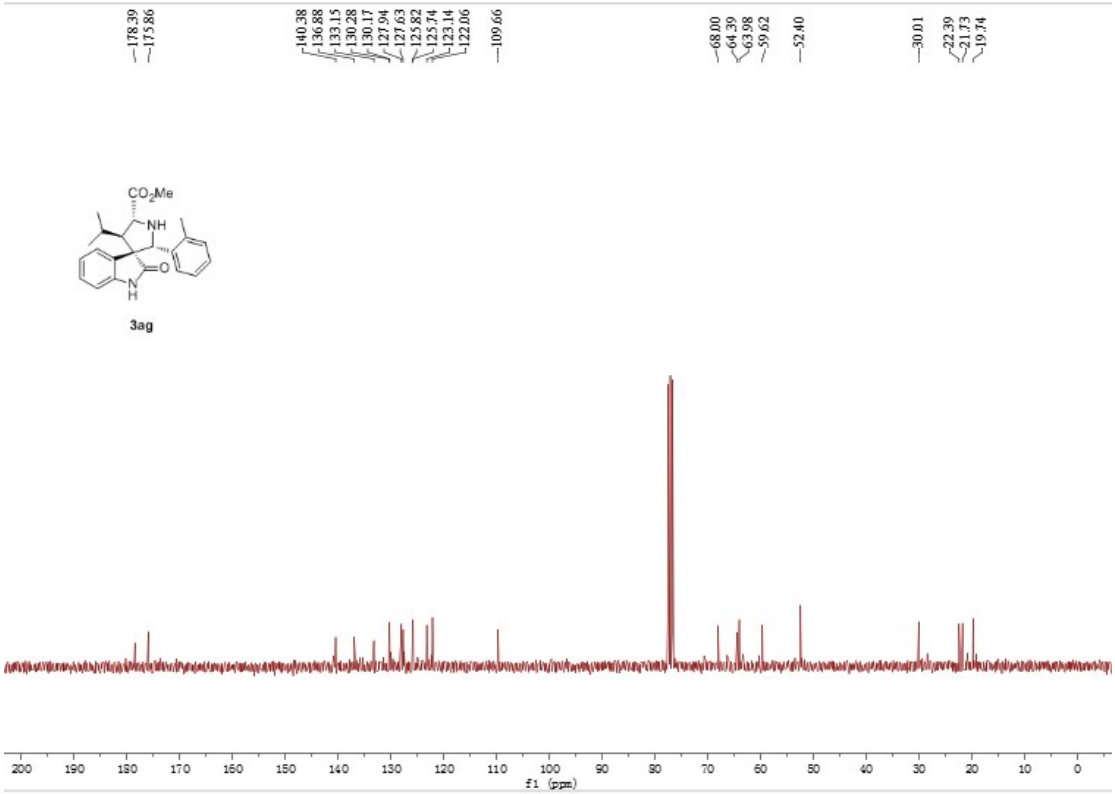


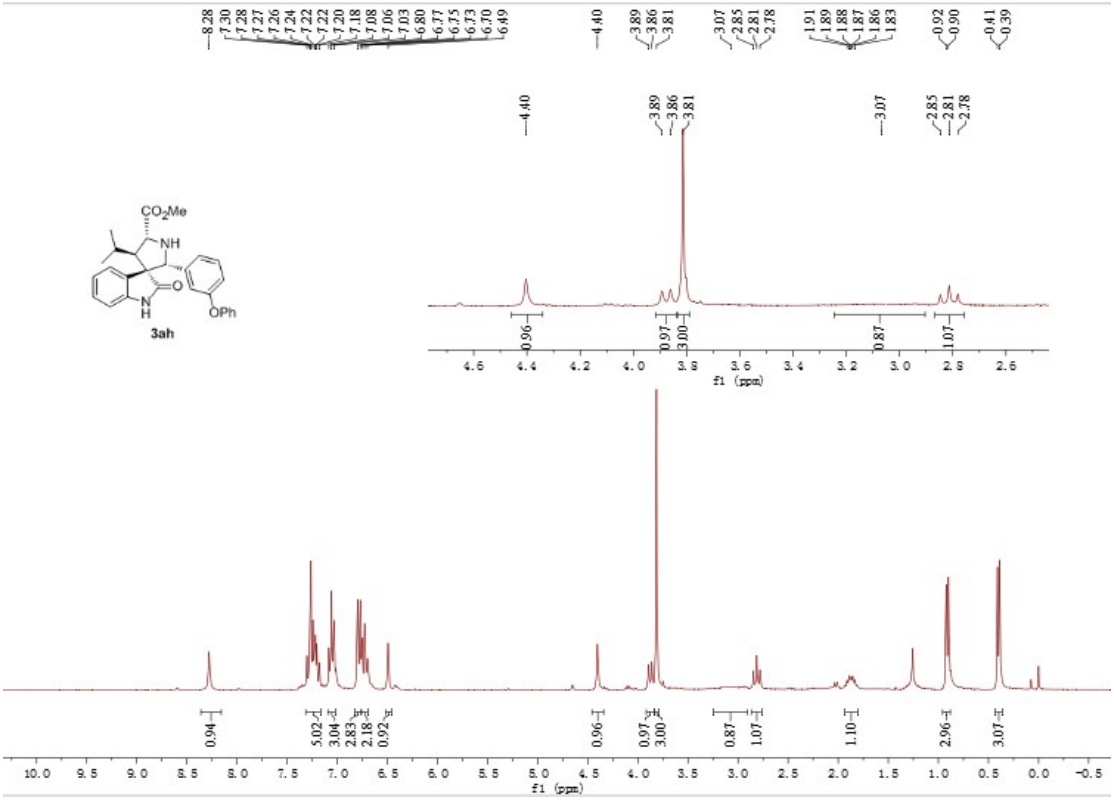
^{1}H NMR of 3ag



^{13}C NMR of 3ag



^{1}H NMR of 3ah



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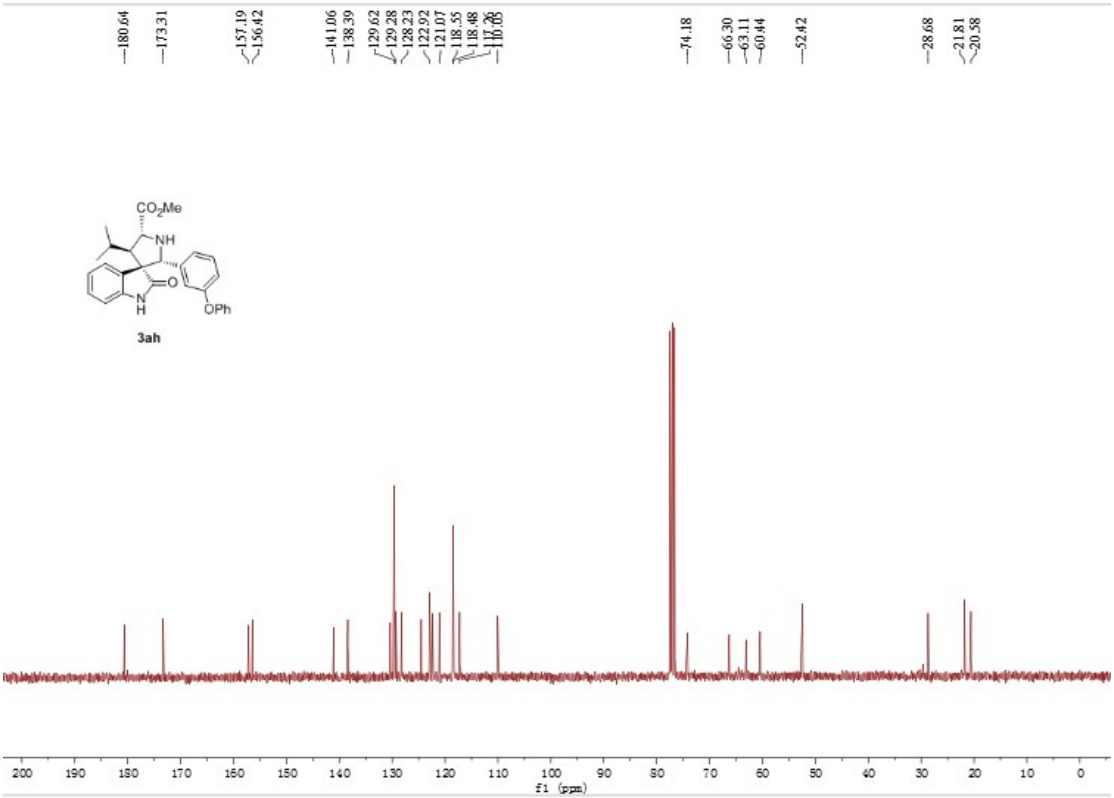

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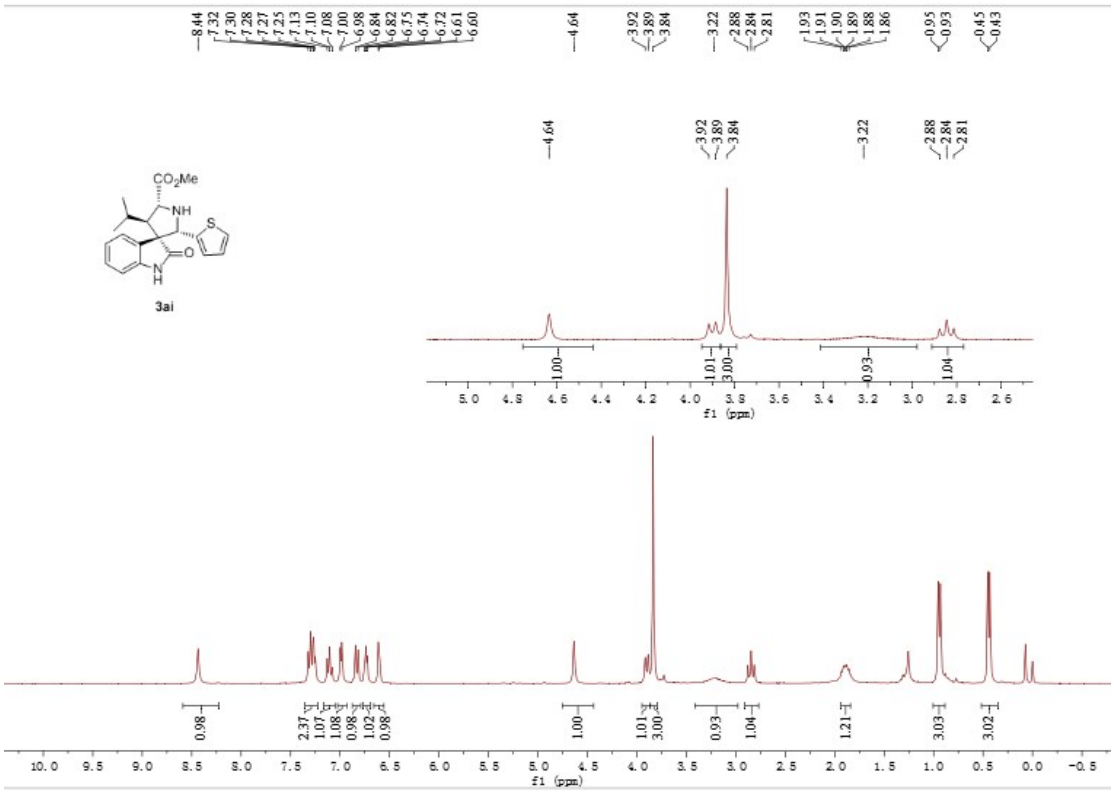

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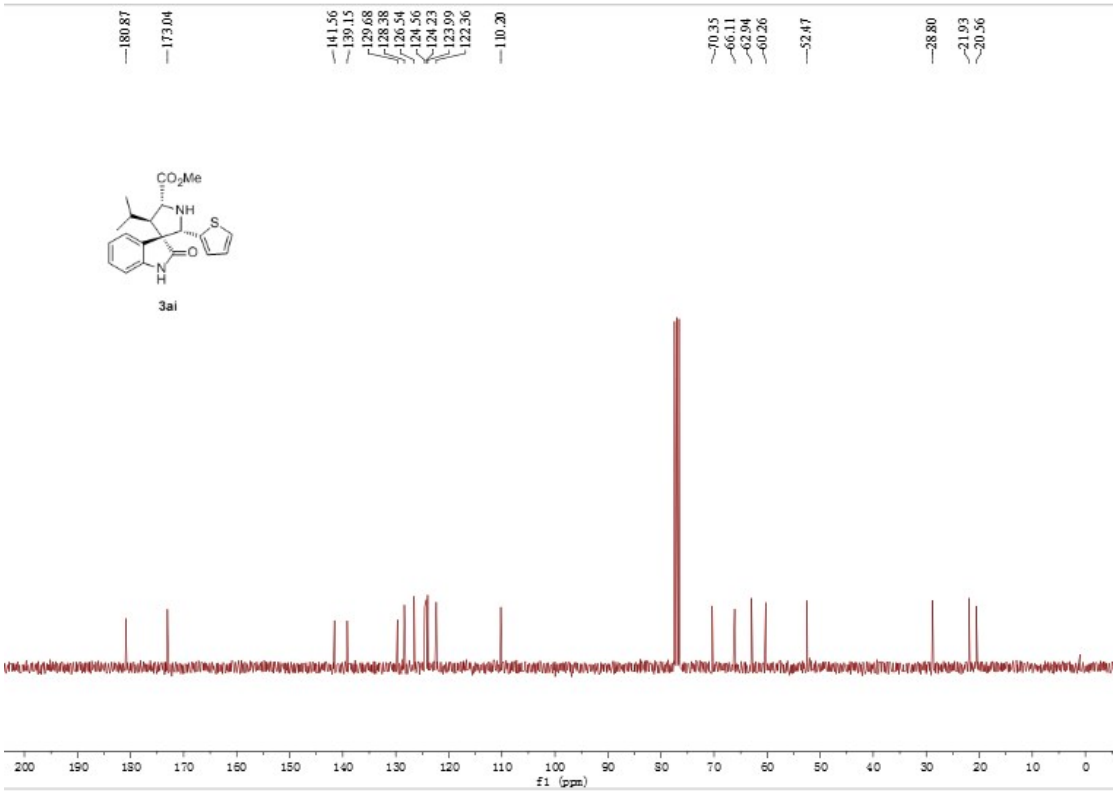

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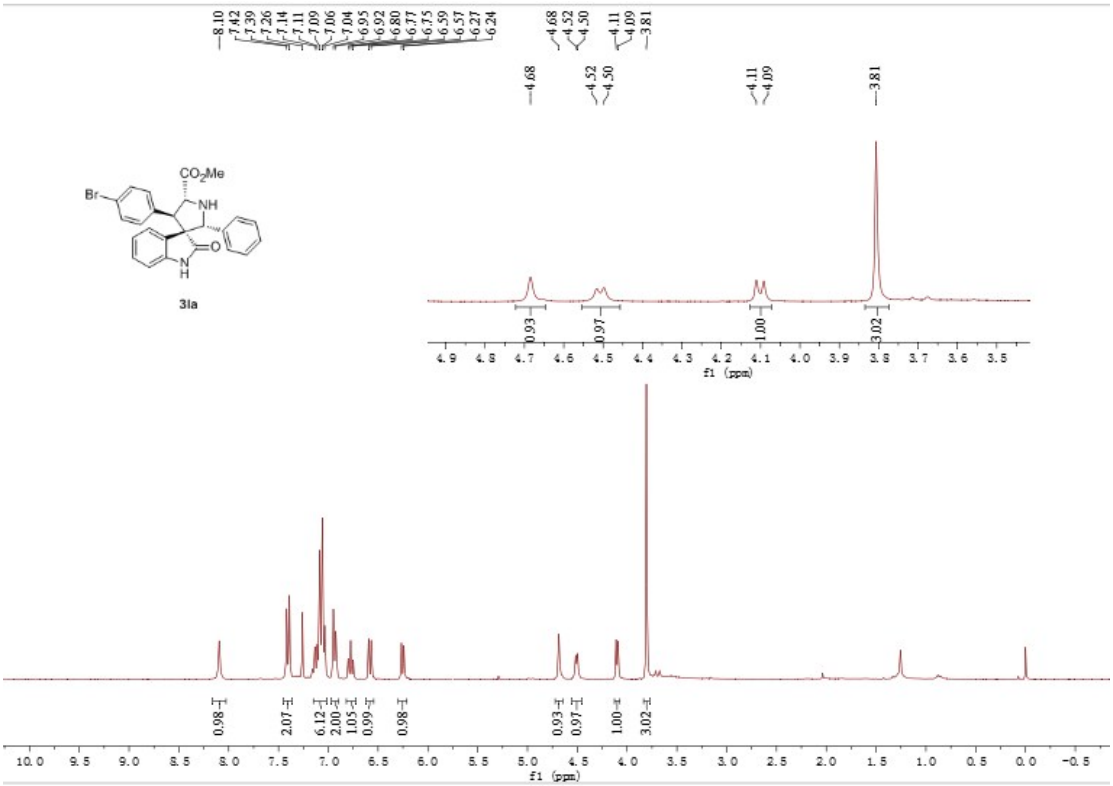

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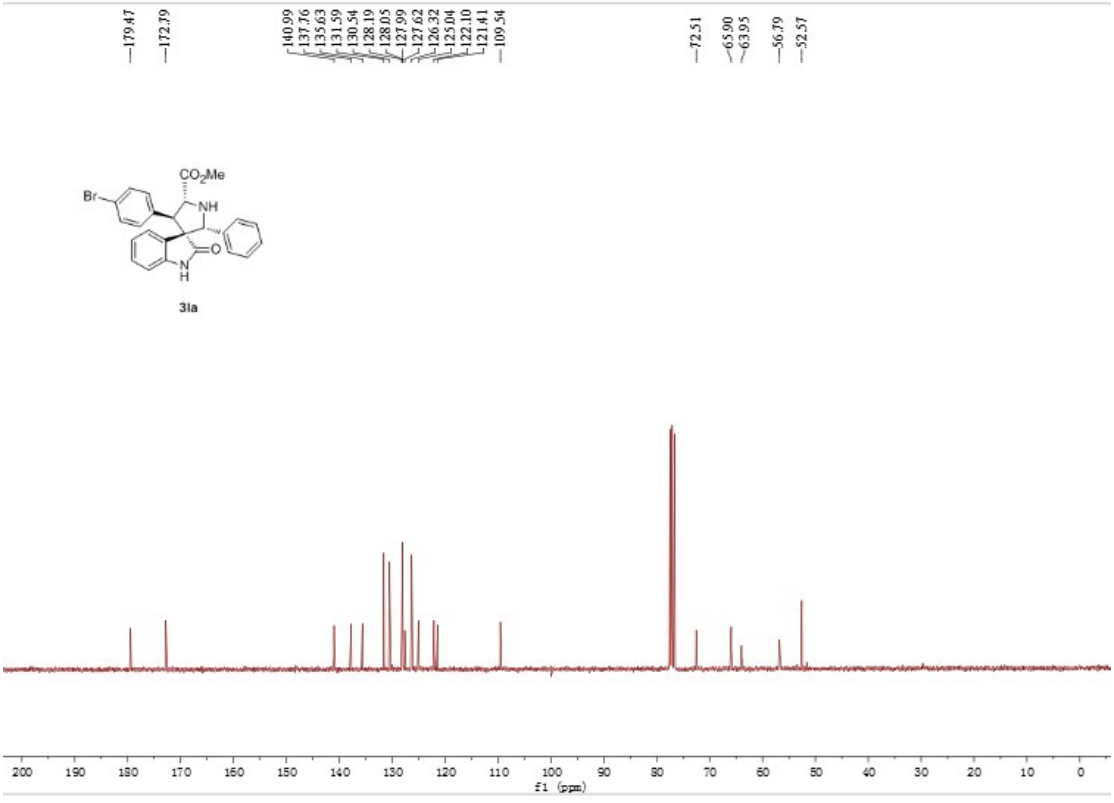

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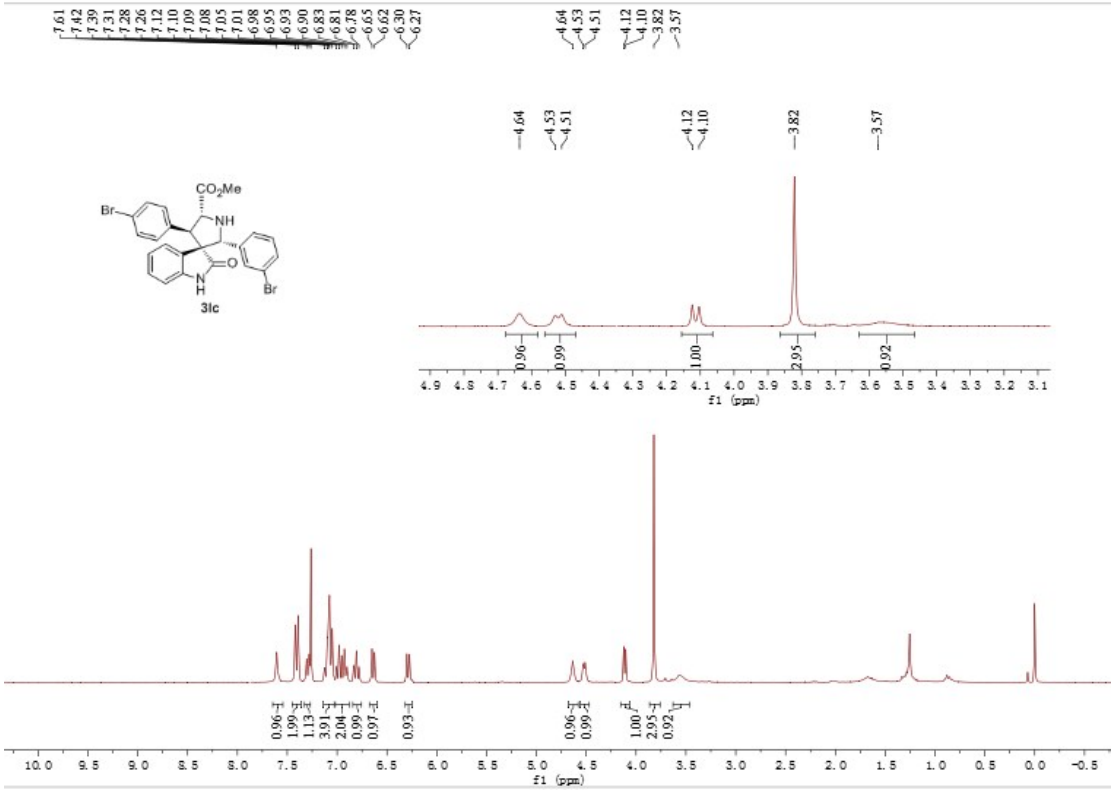

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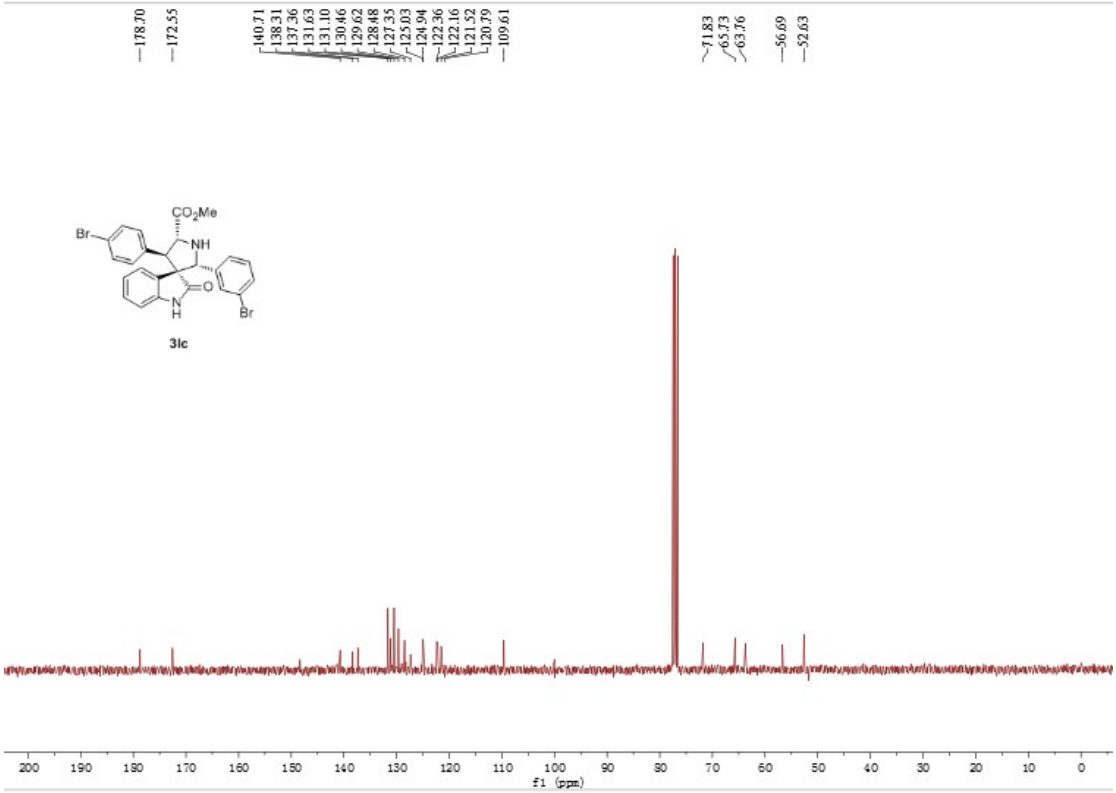

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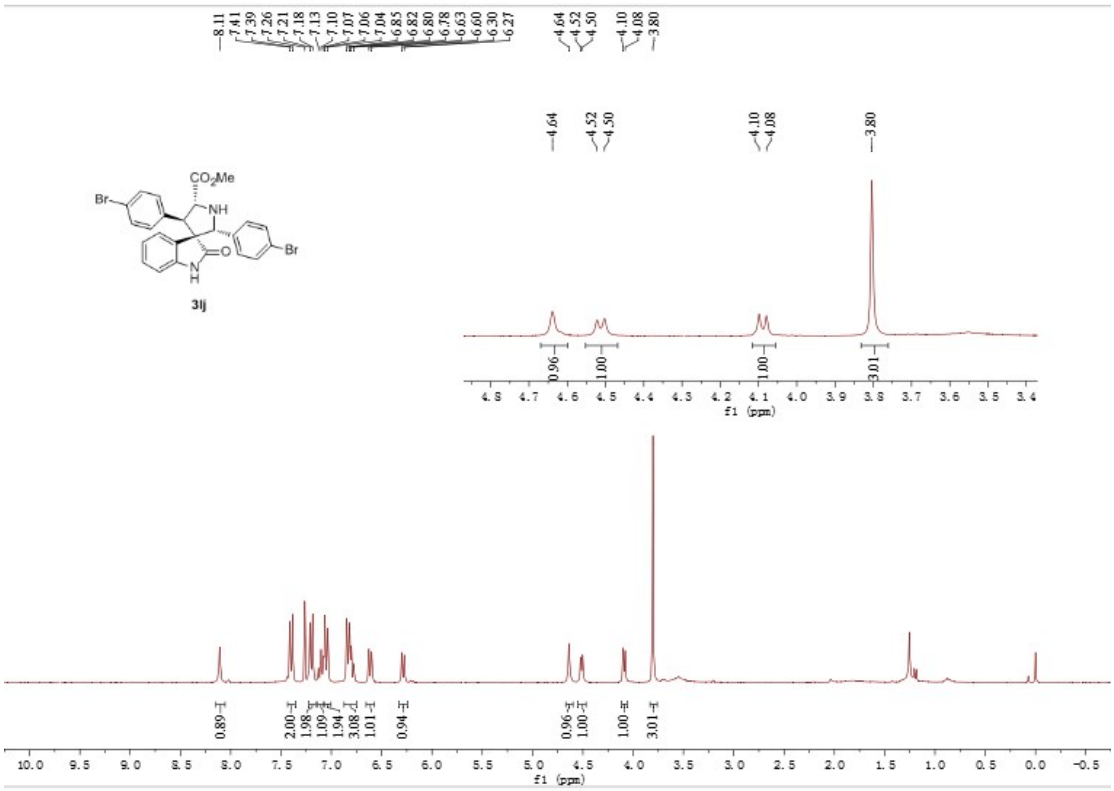

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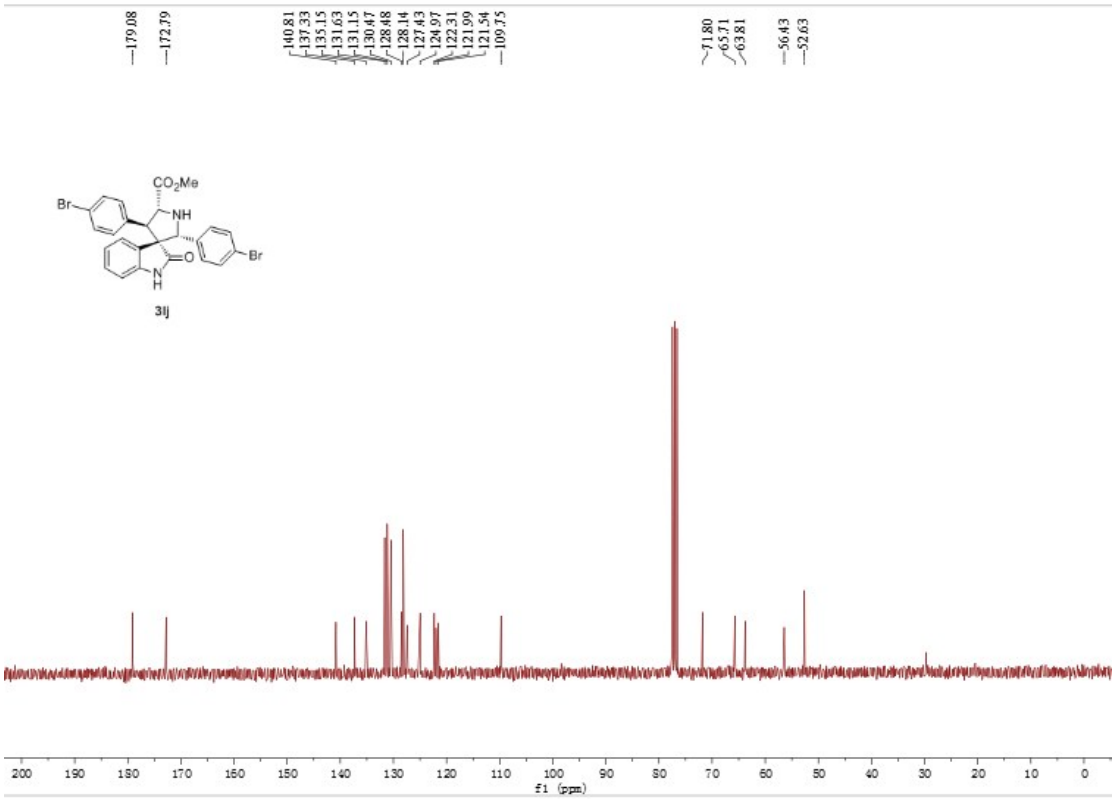
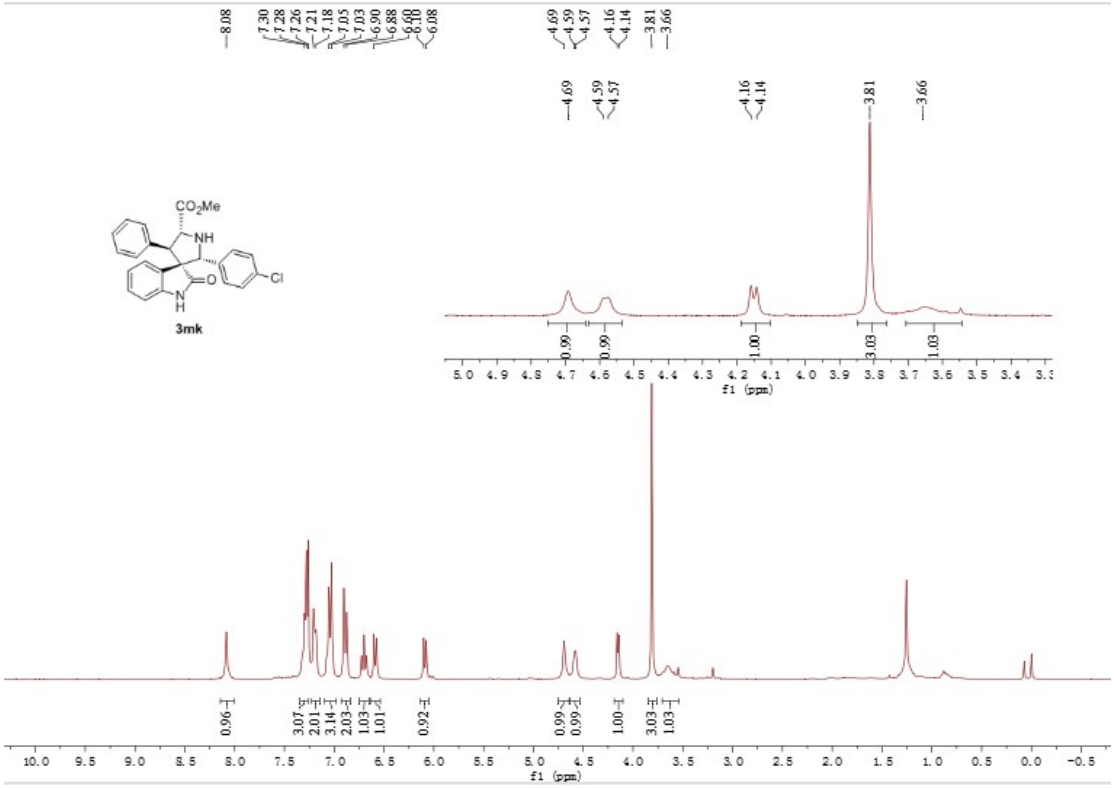


^{1}H NMR of 3mk



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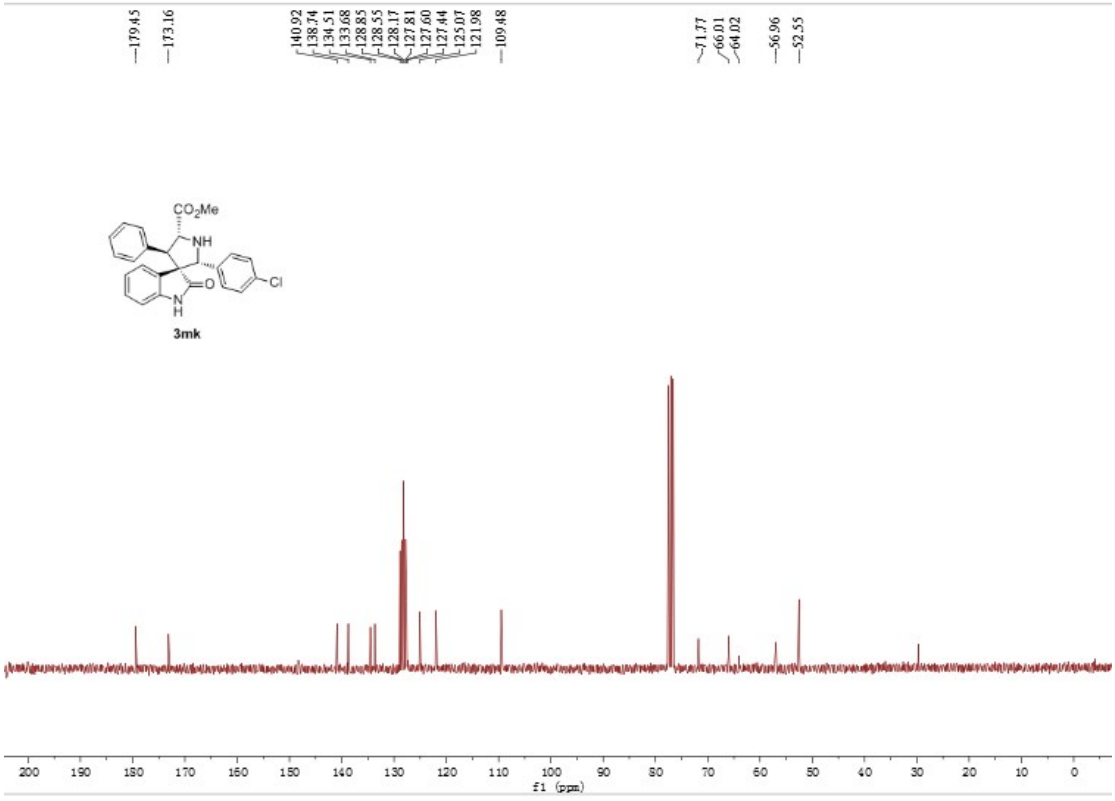

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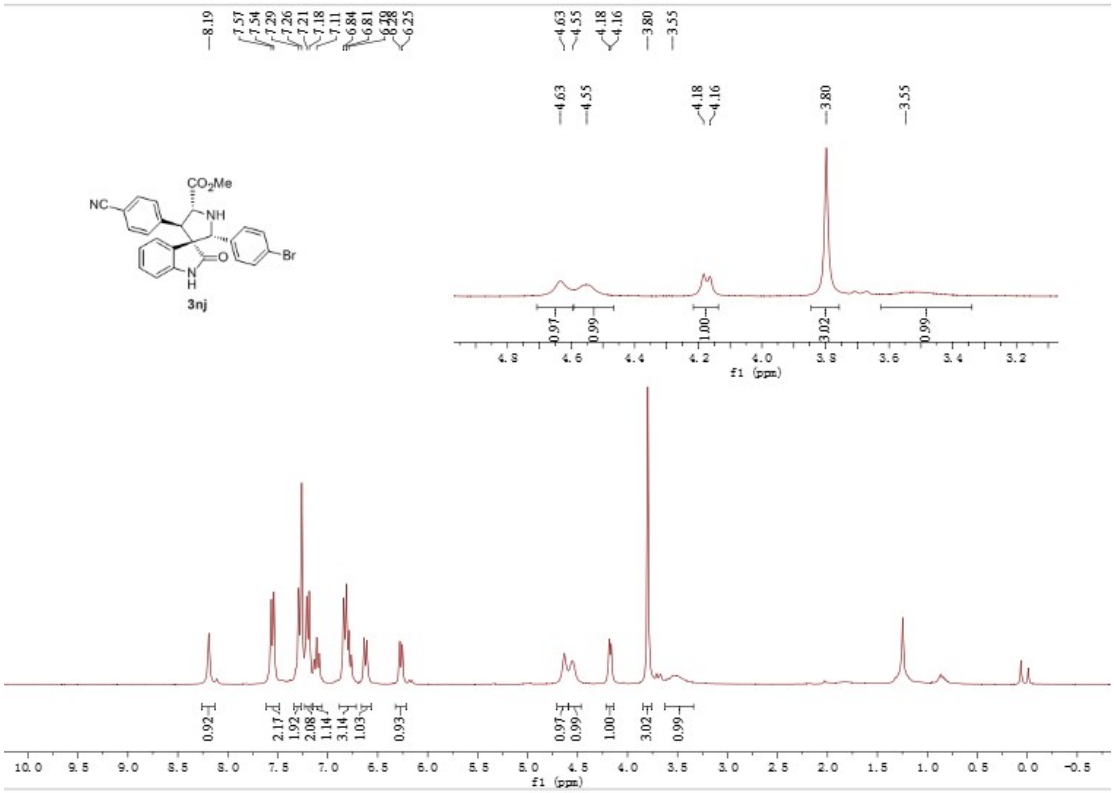

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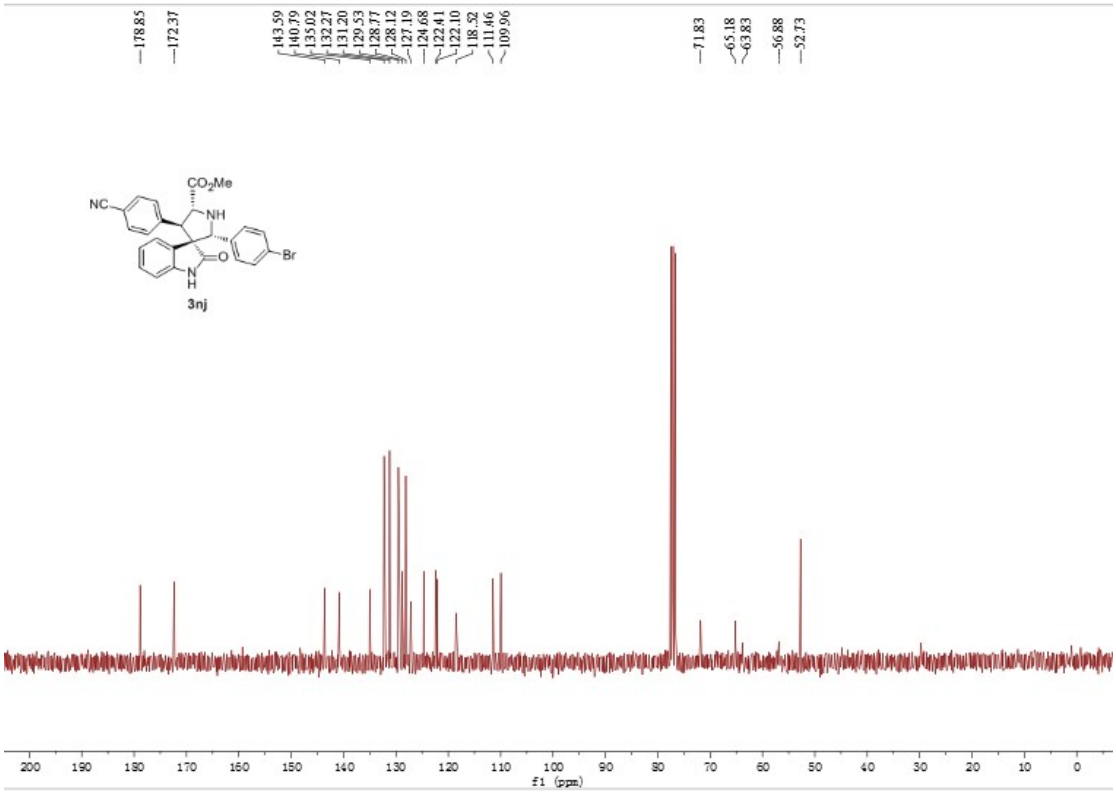
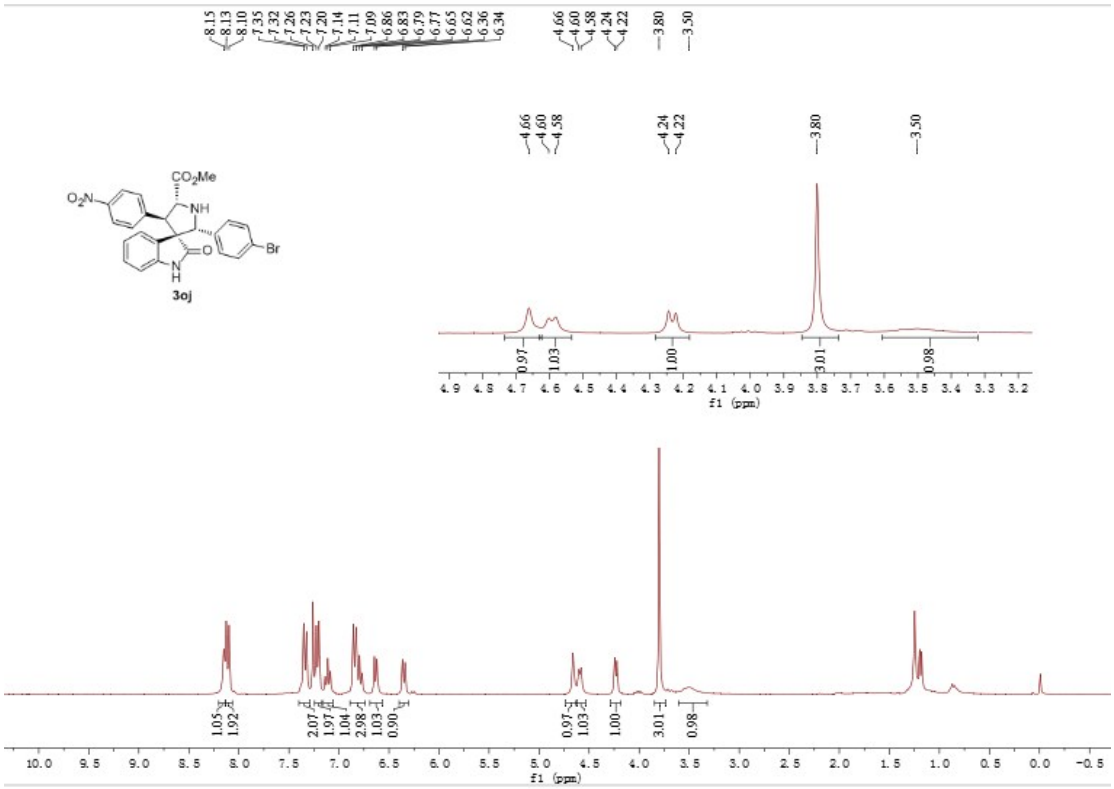


^{1}H NMR of 3oj



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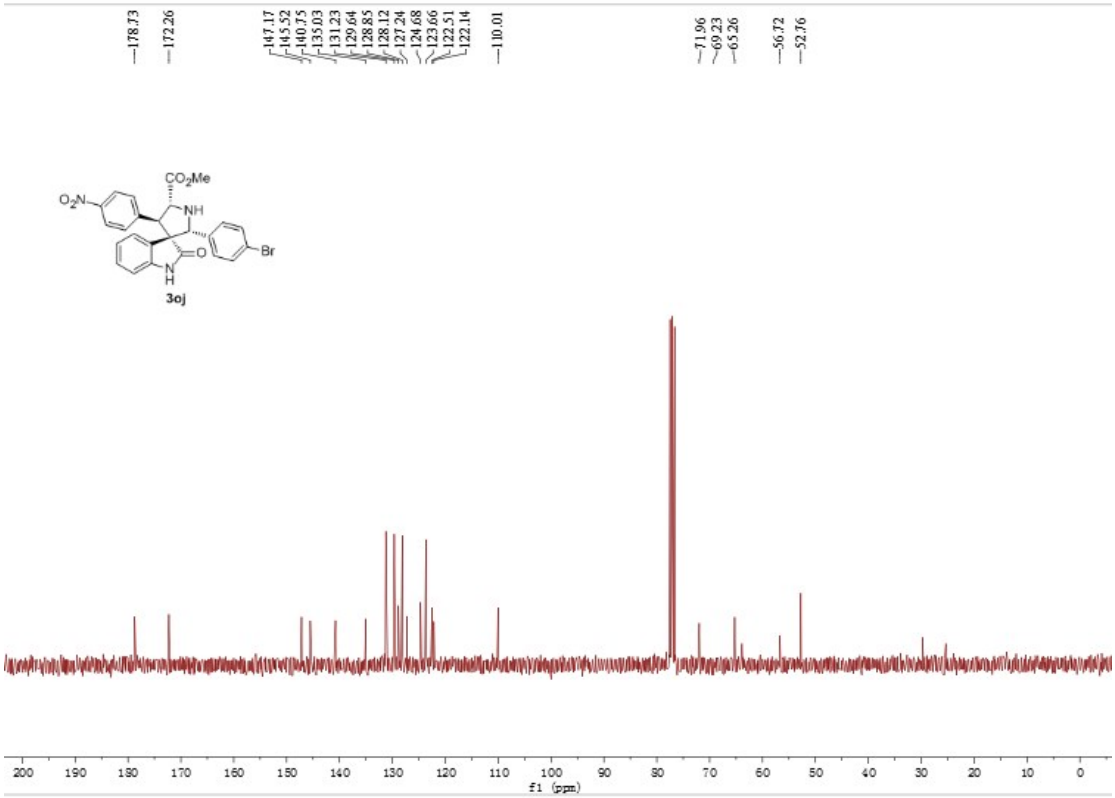

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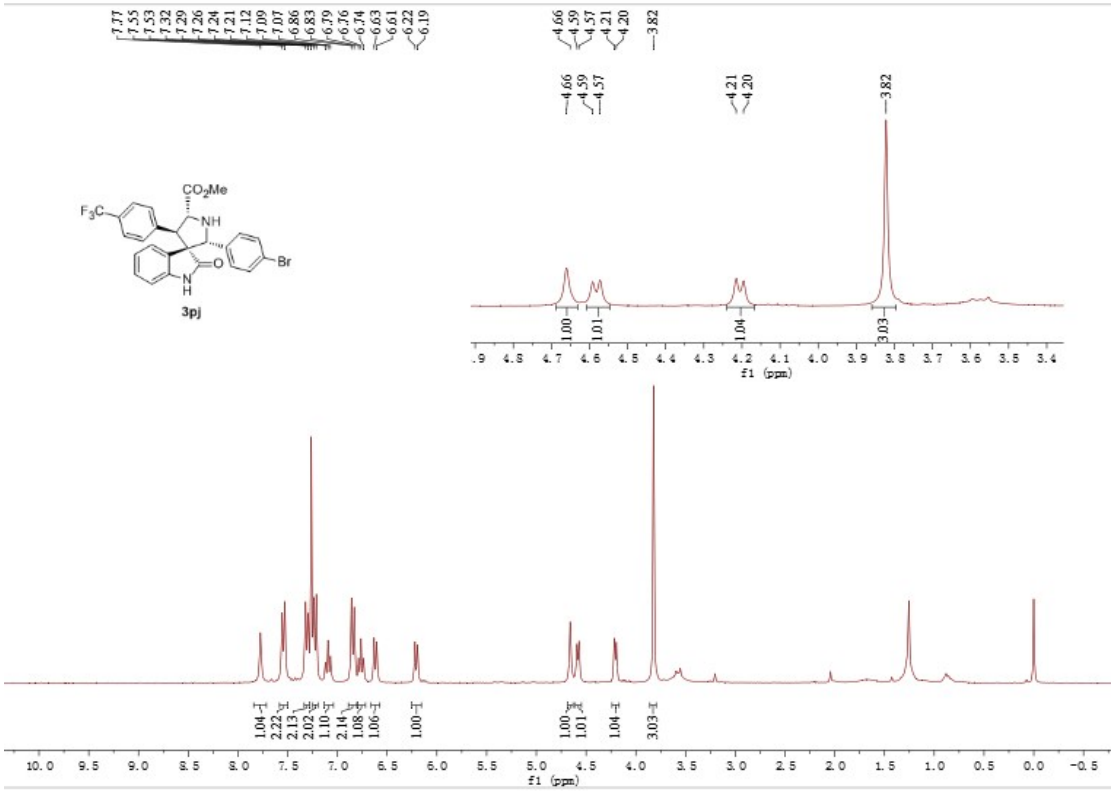
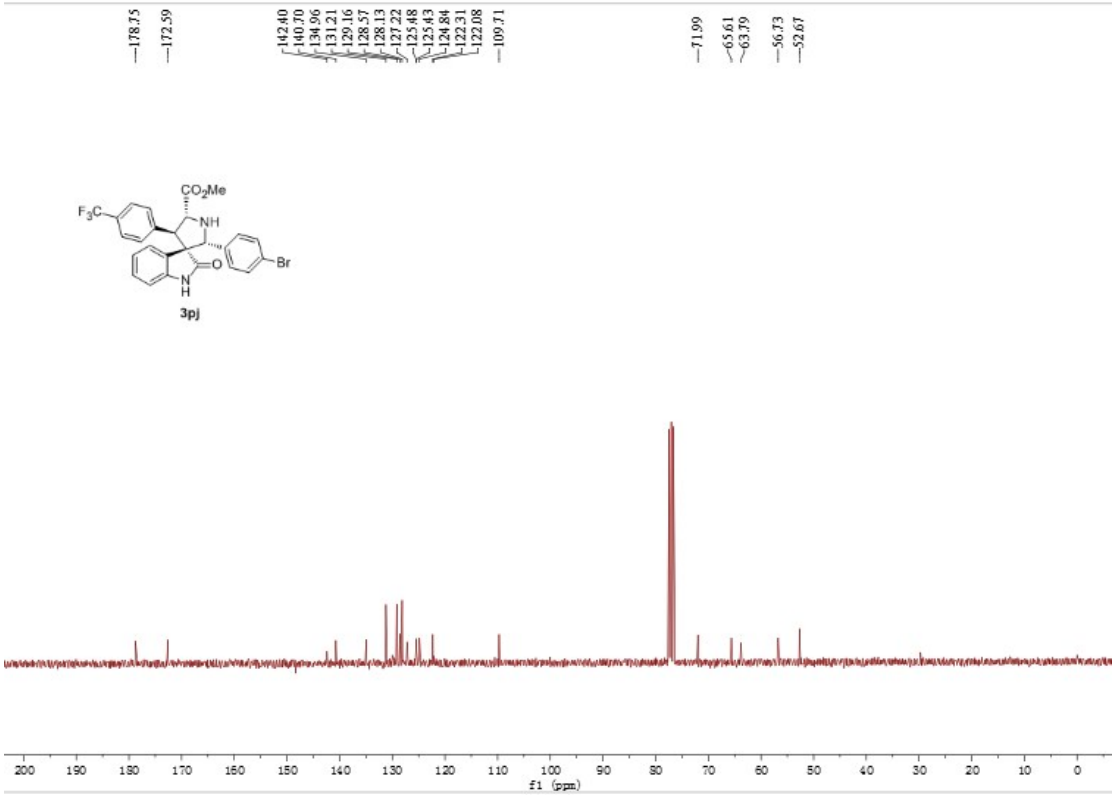


^{13}C NMR of 3pj



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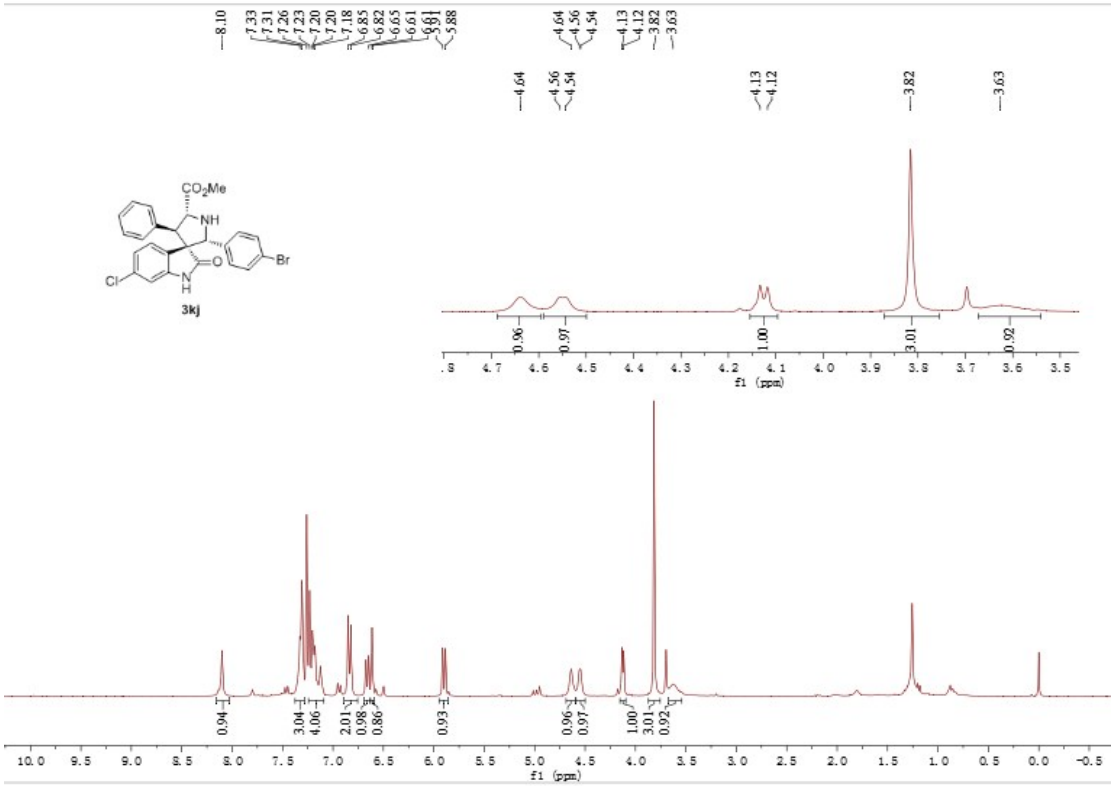

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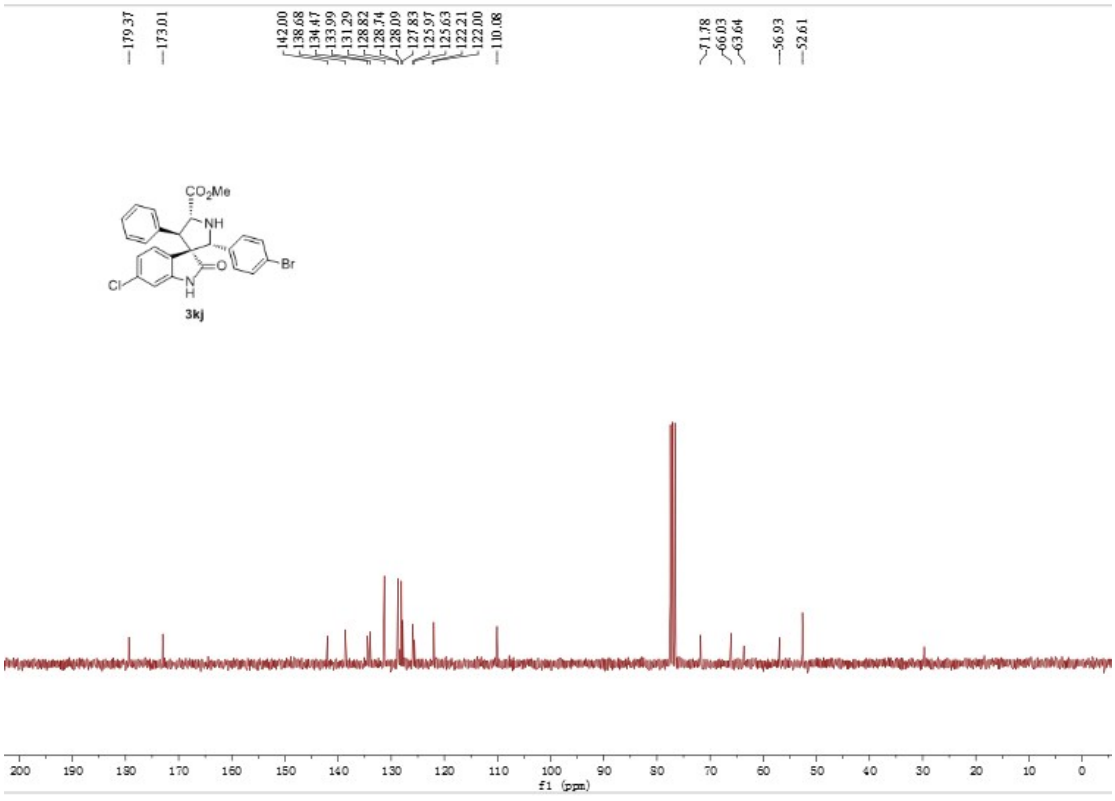

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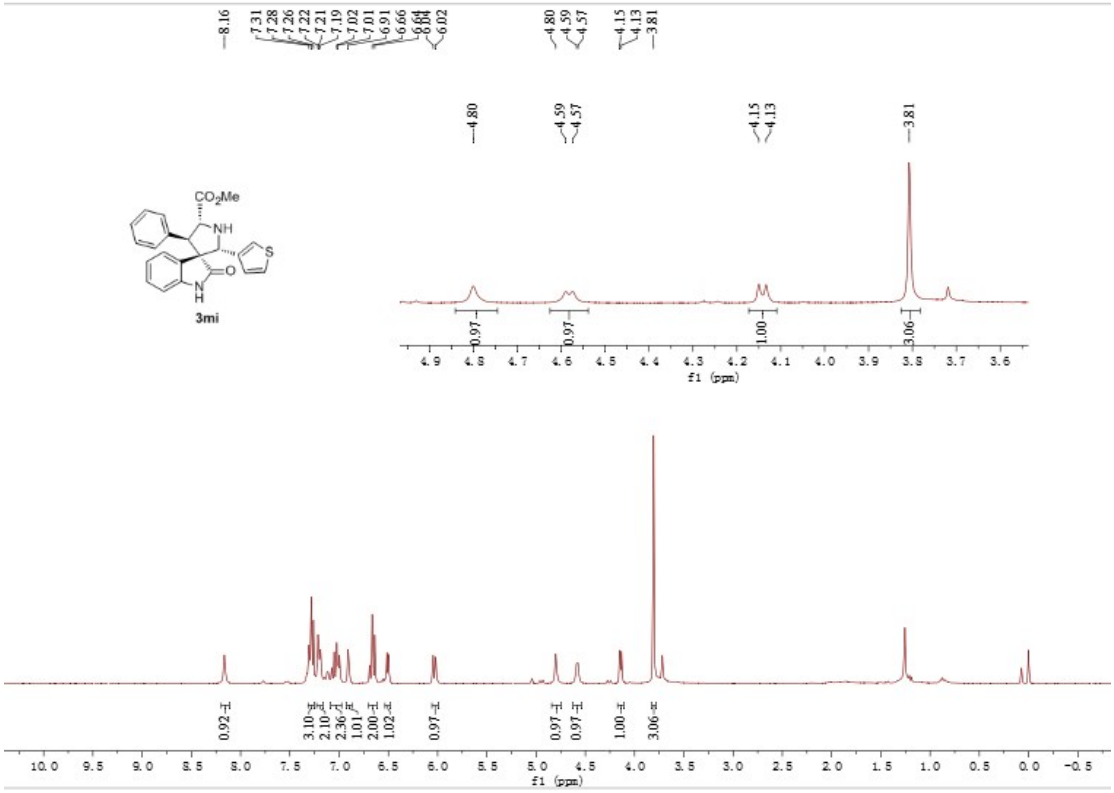

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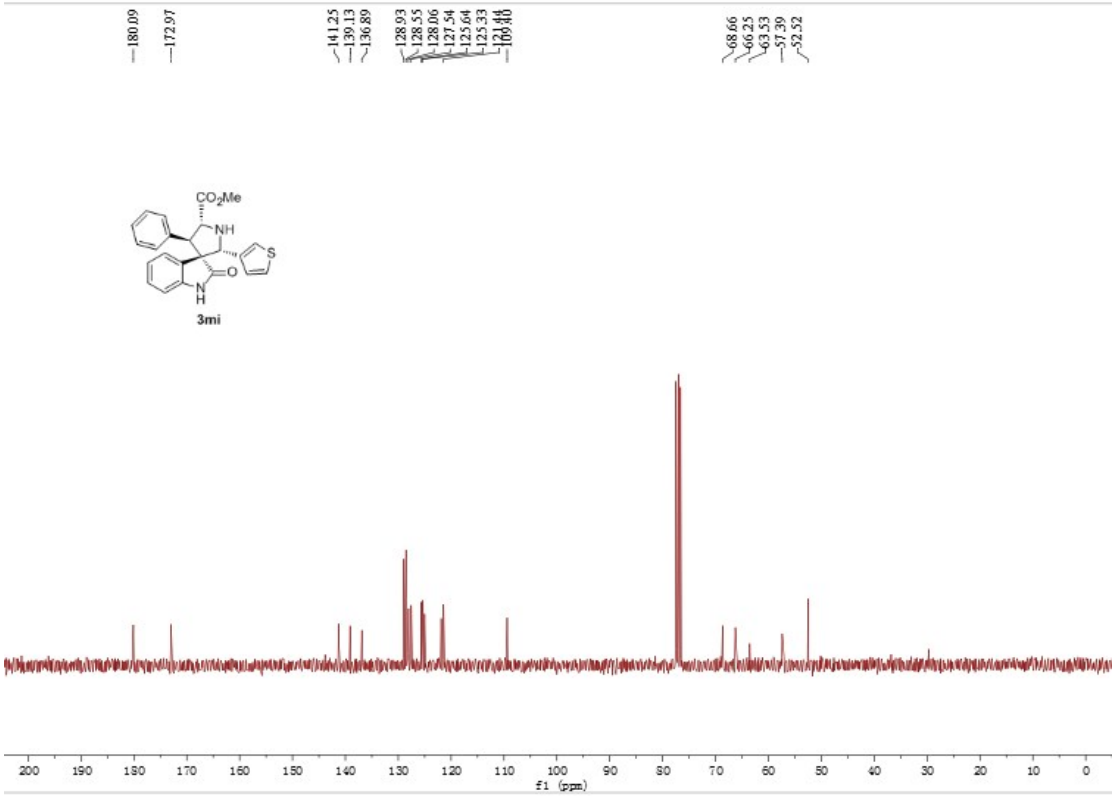
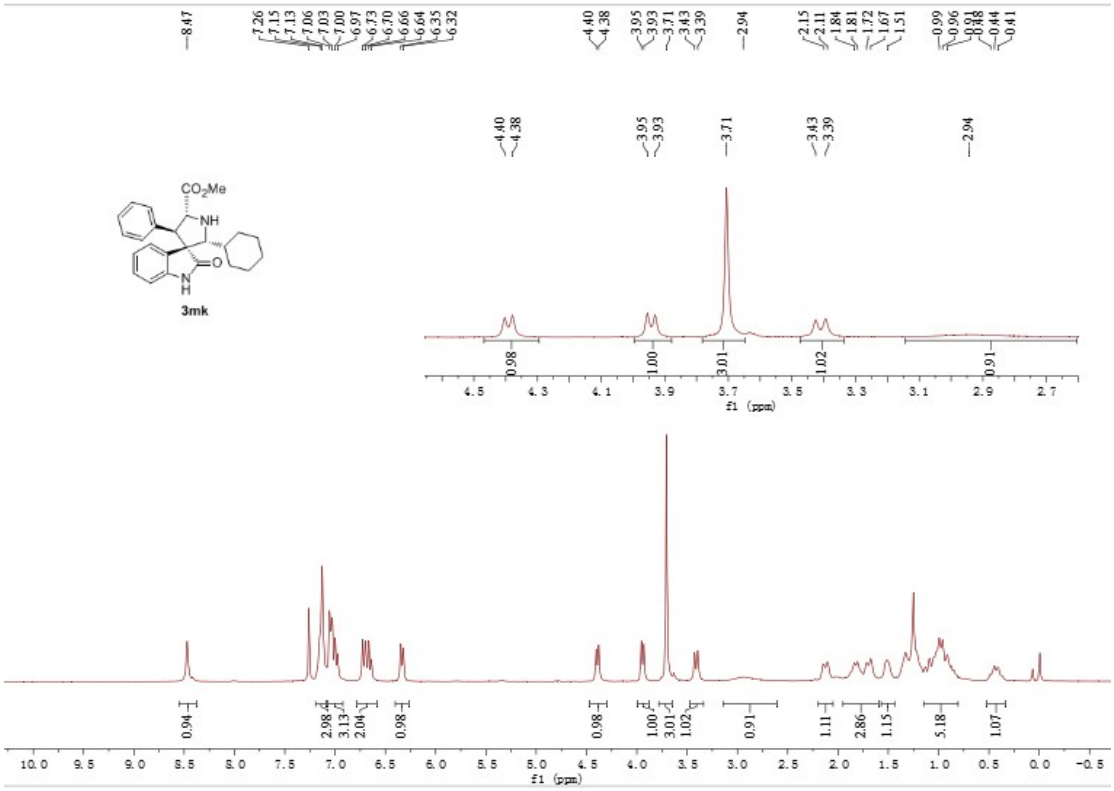
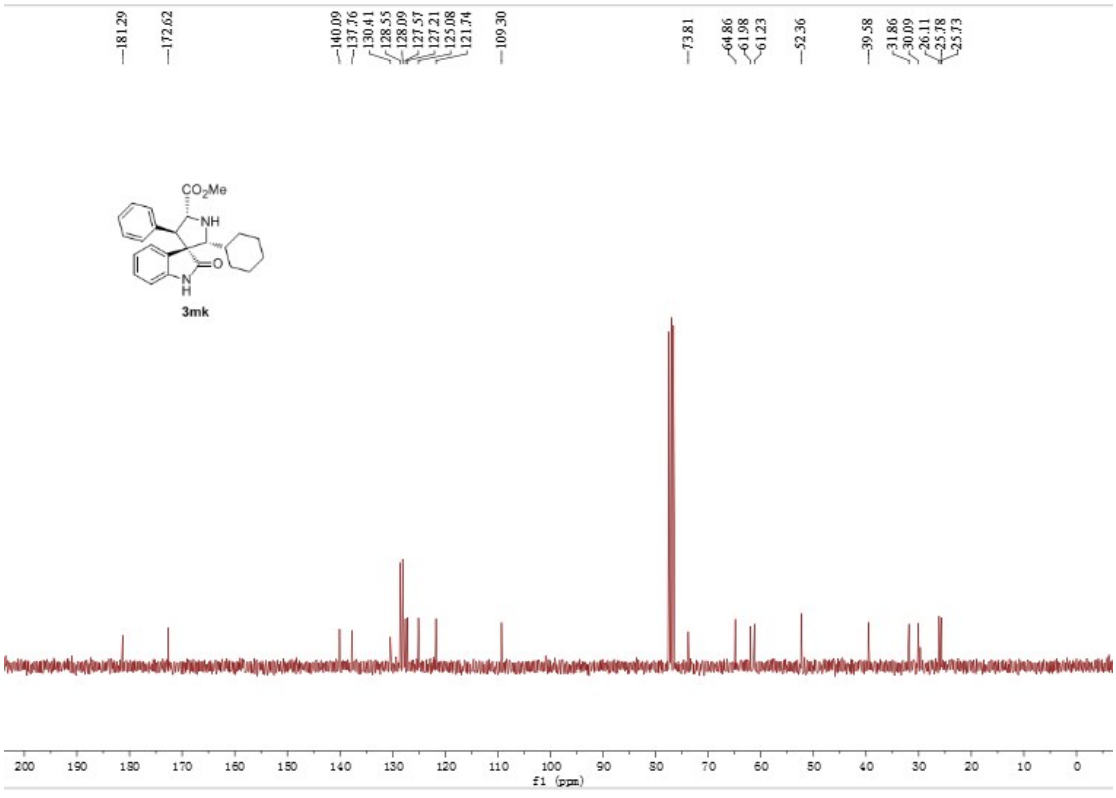


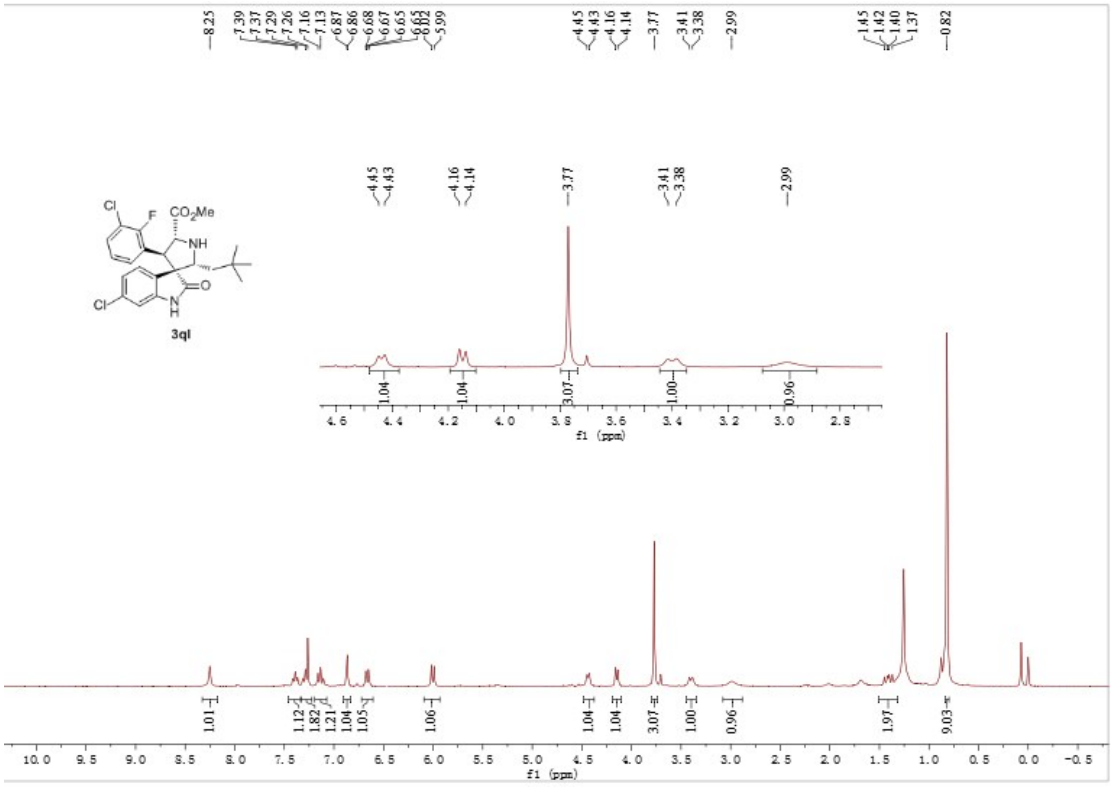
^{1}H NMR of 3mk



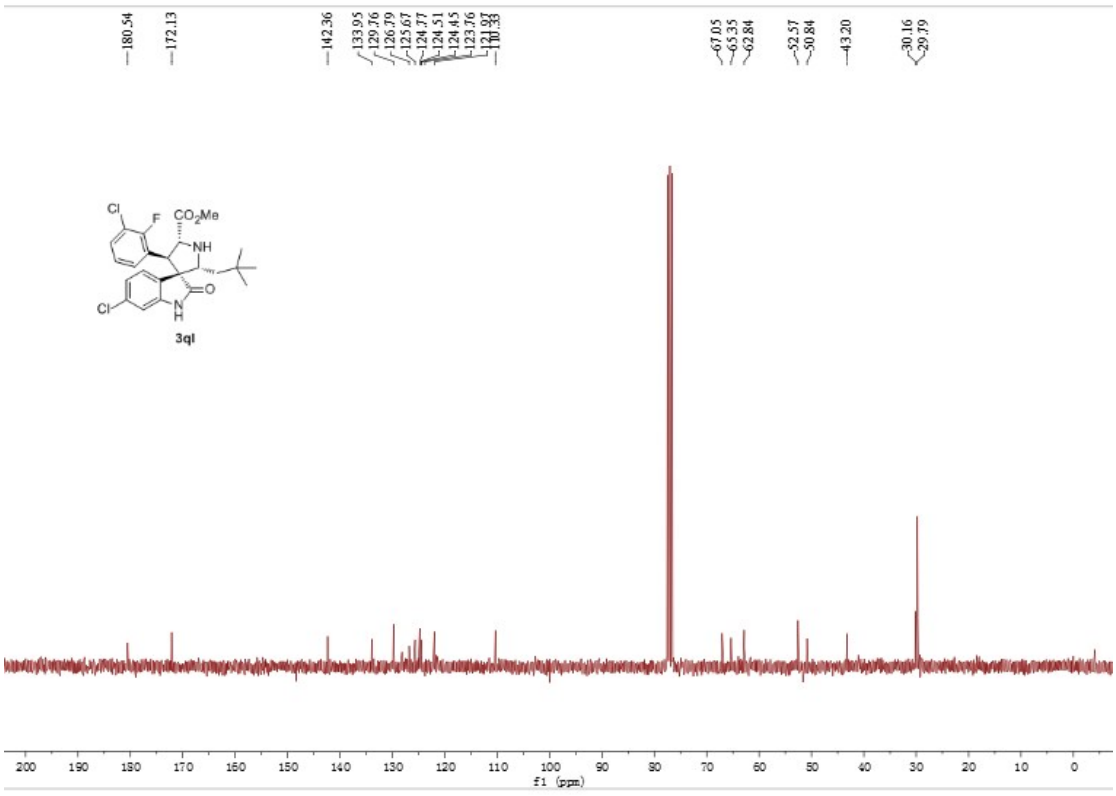
^{13}C NMR of 3mk



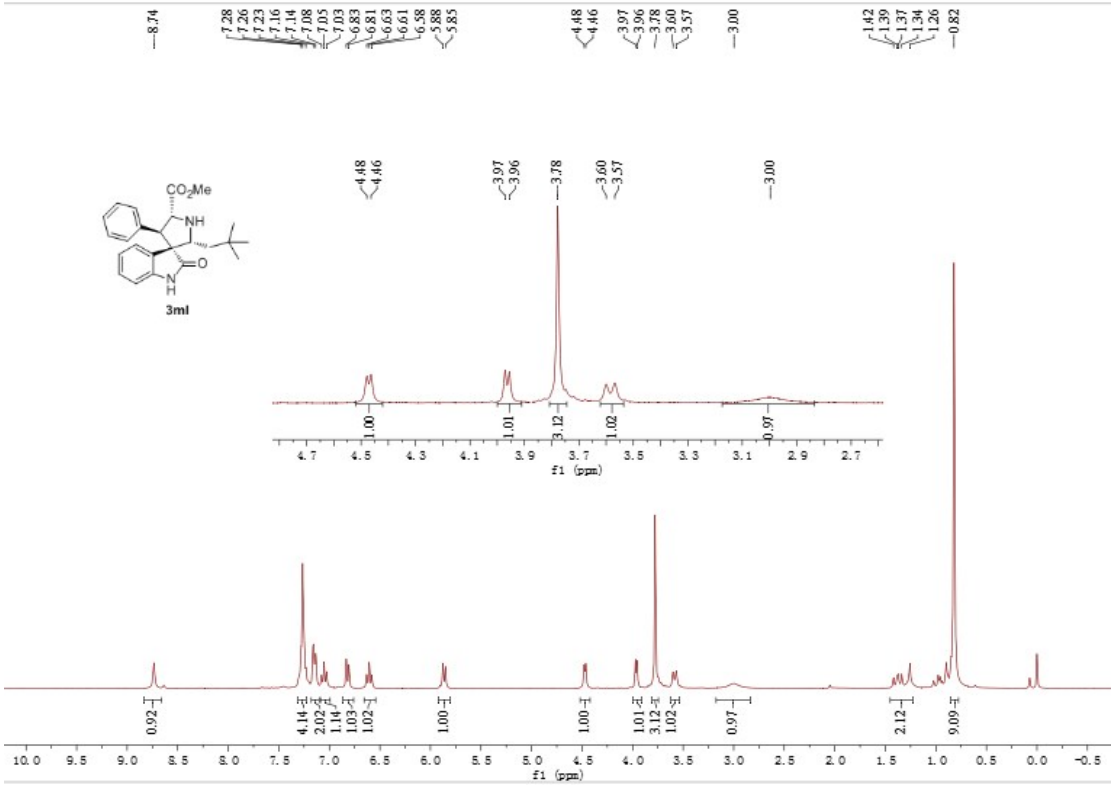
^{1}H NMR of 3ql



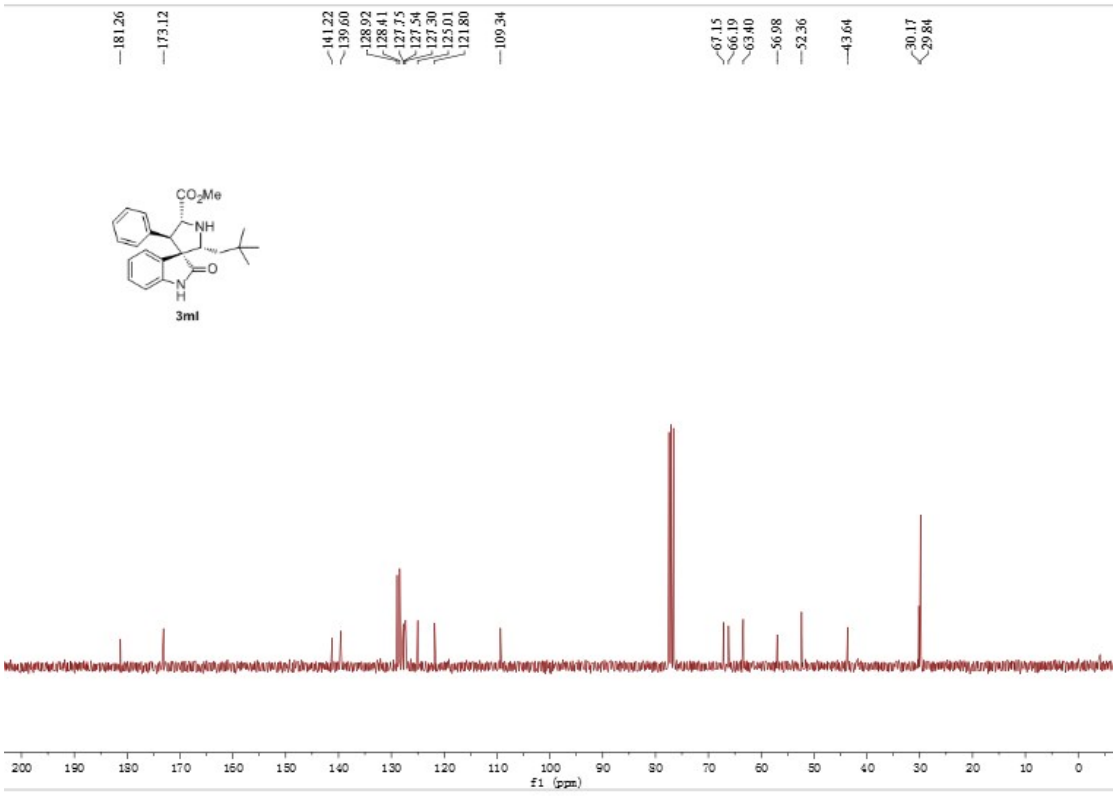
^{13}C NMR of 3ql



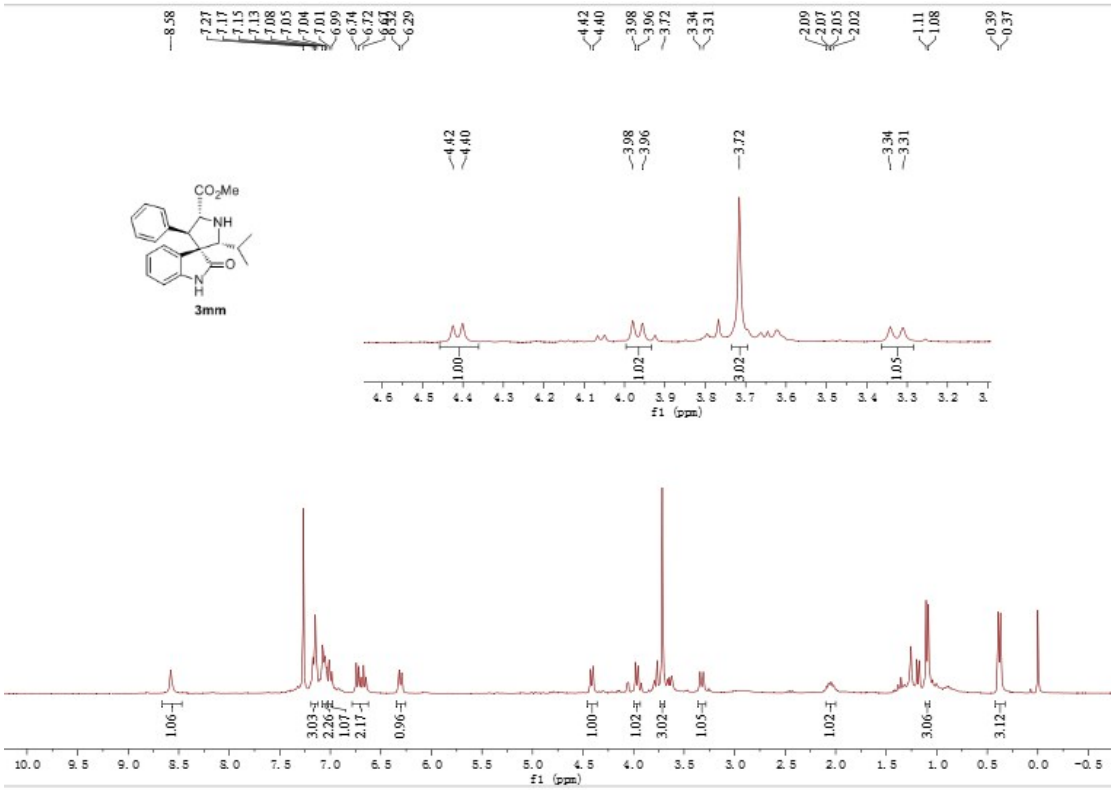
^{1}H NMR of 3ml



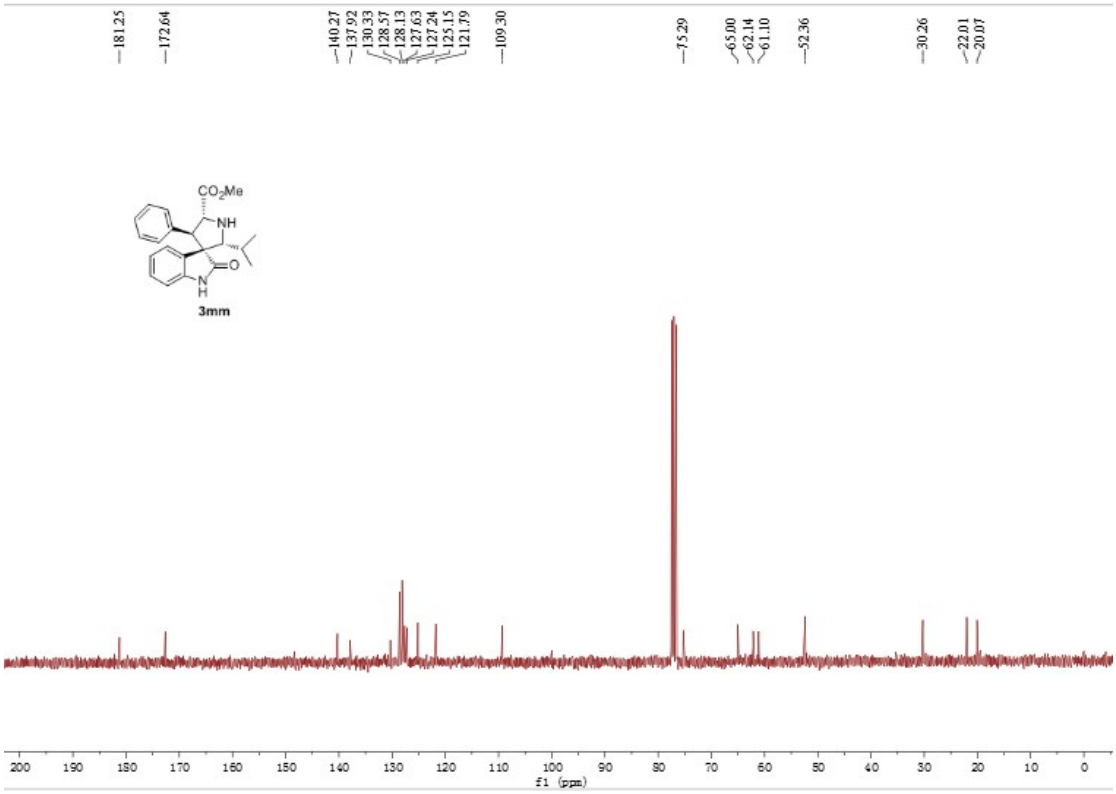
^{13}C NMR of 3ml



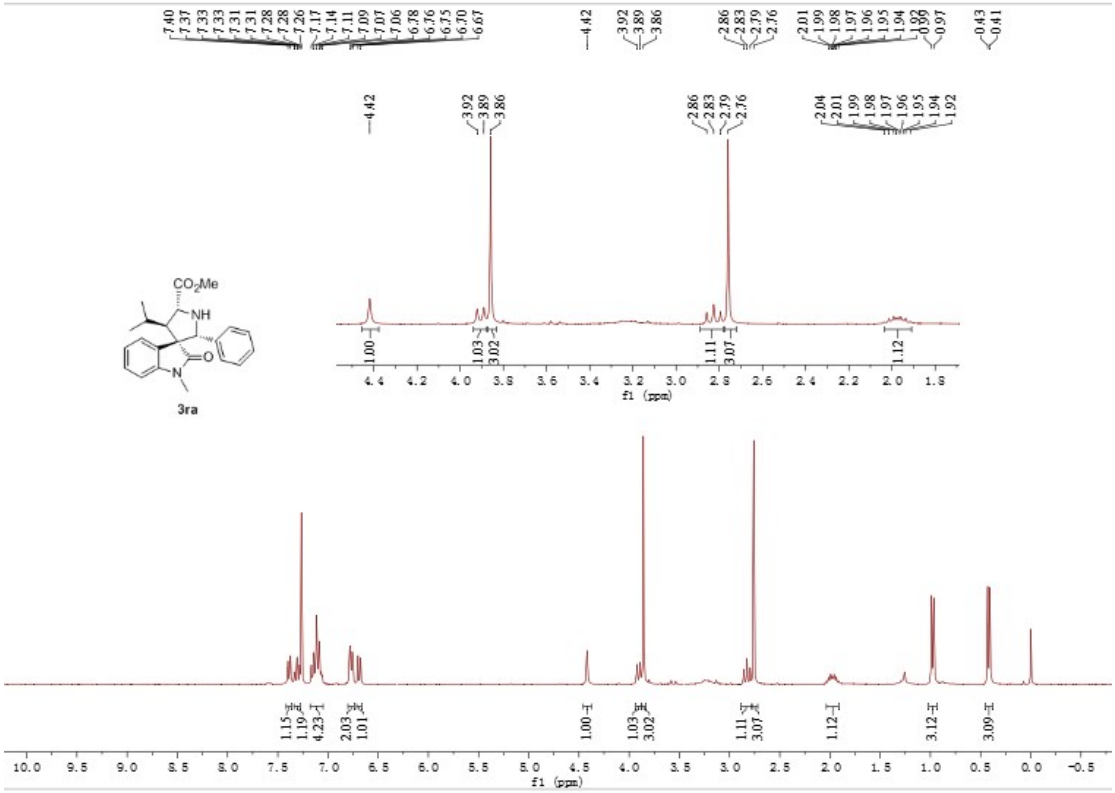
^{1}H NMR of 3mm



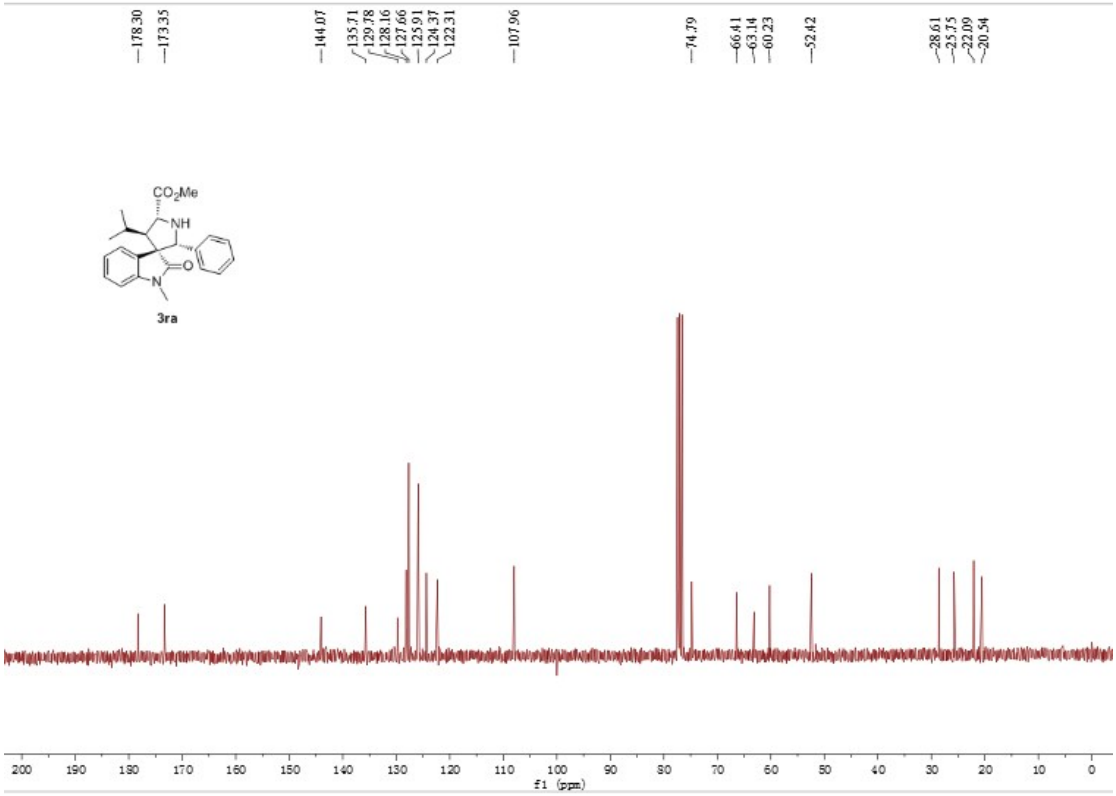
^{13}C NMR of 3mm



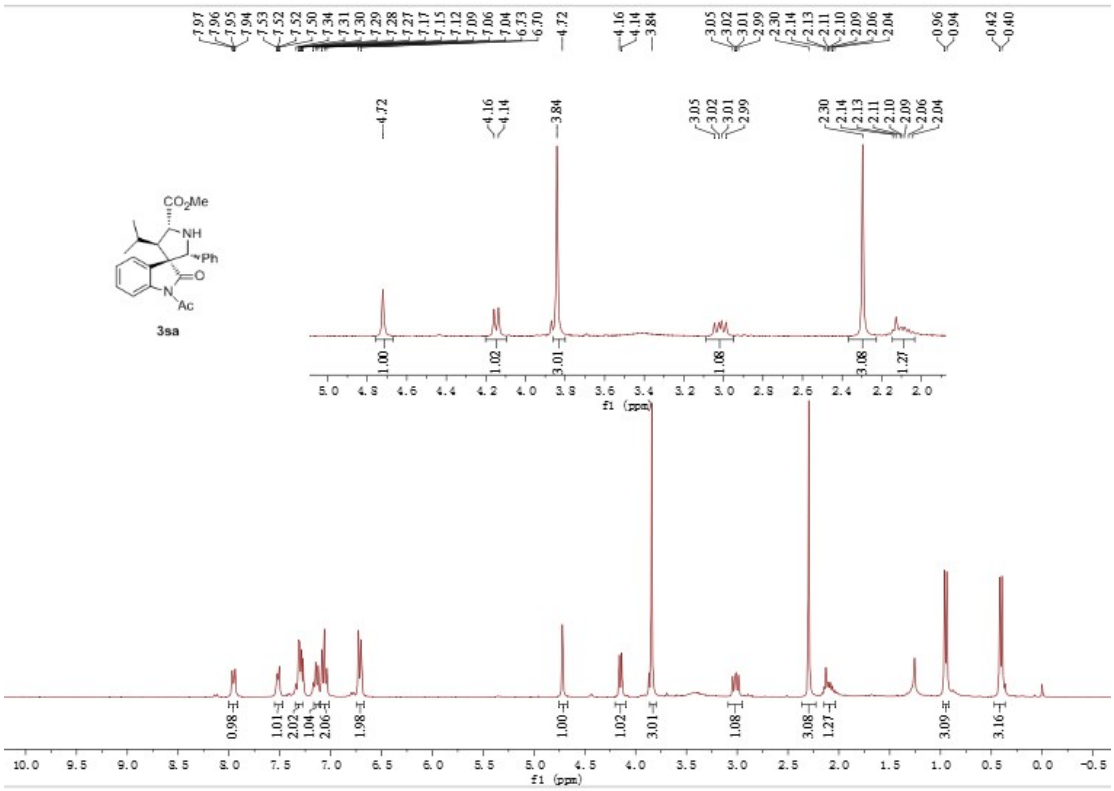
^{1}H NMR of 3ra



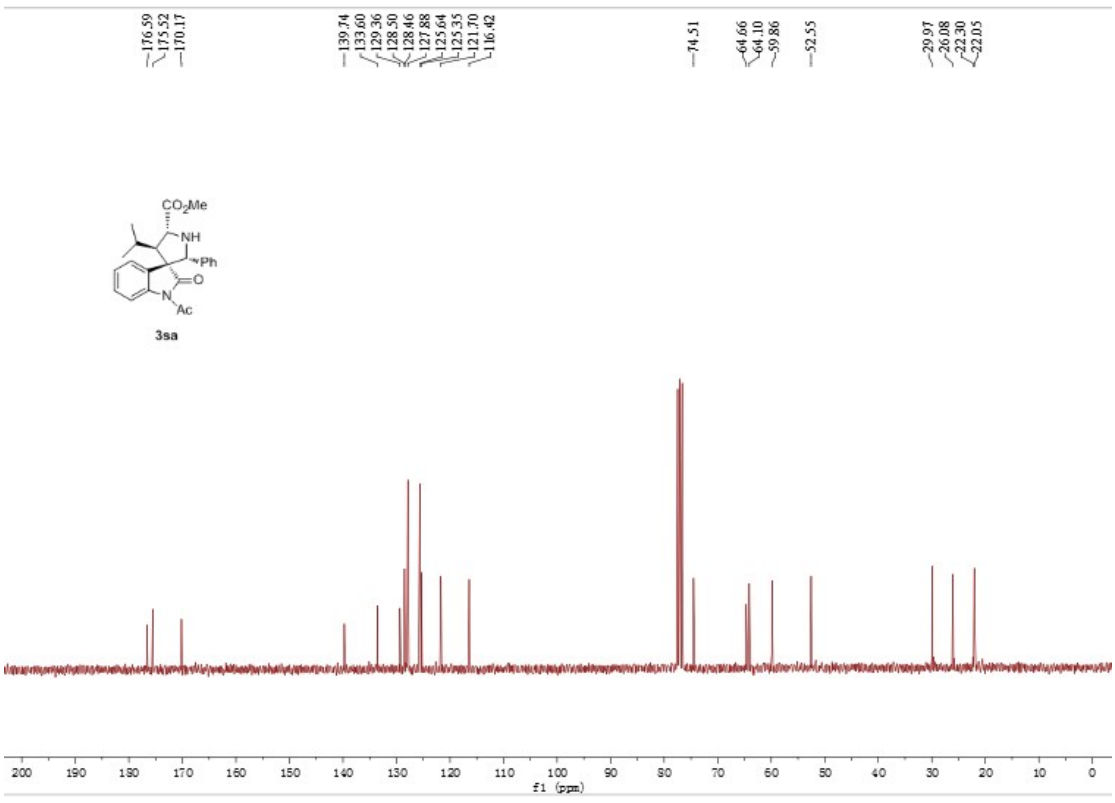
^{13}C NMR of 3ra



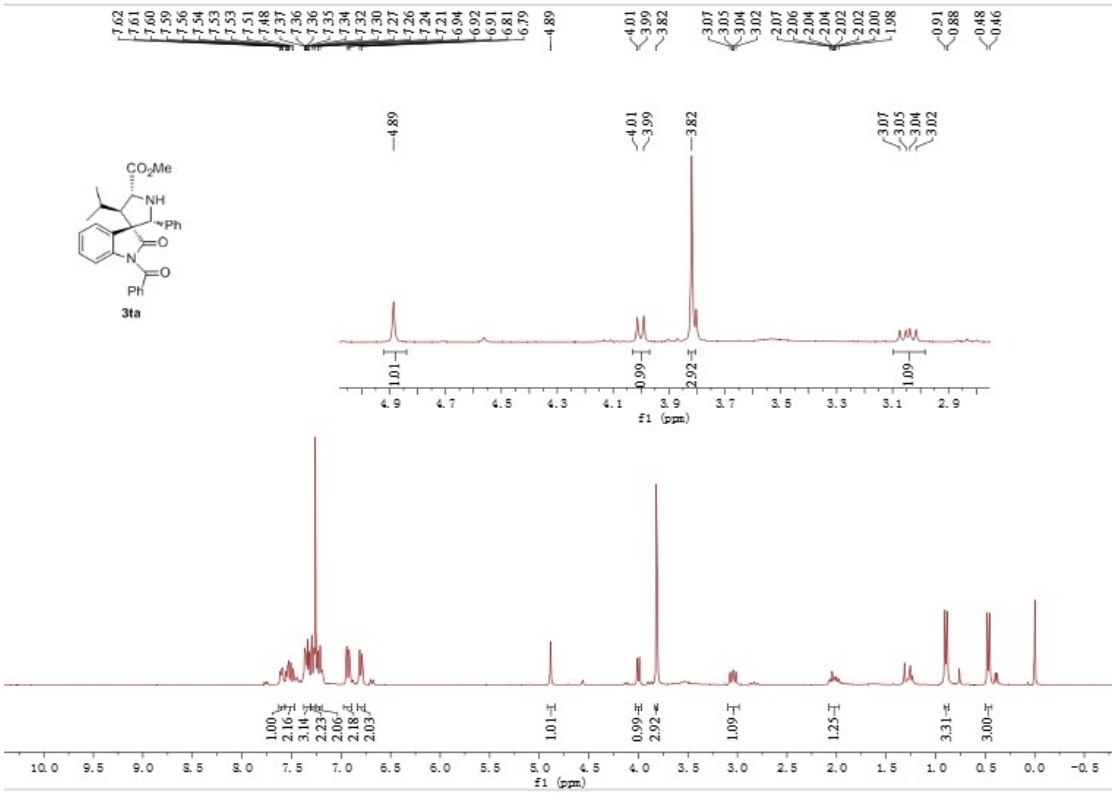
^{1}H NMR of 3sa



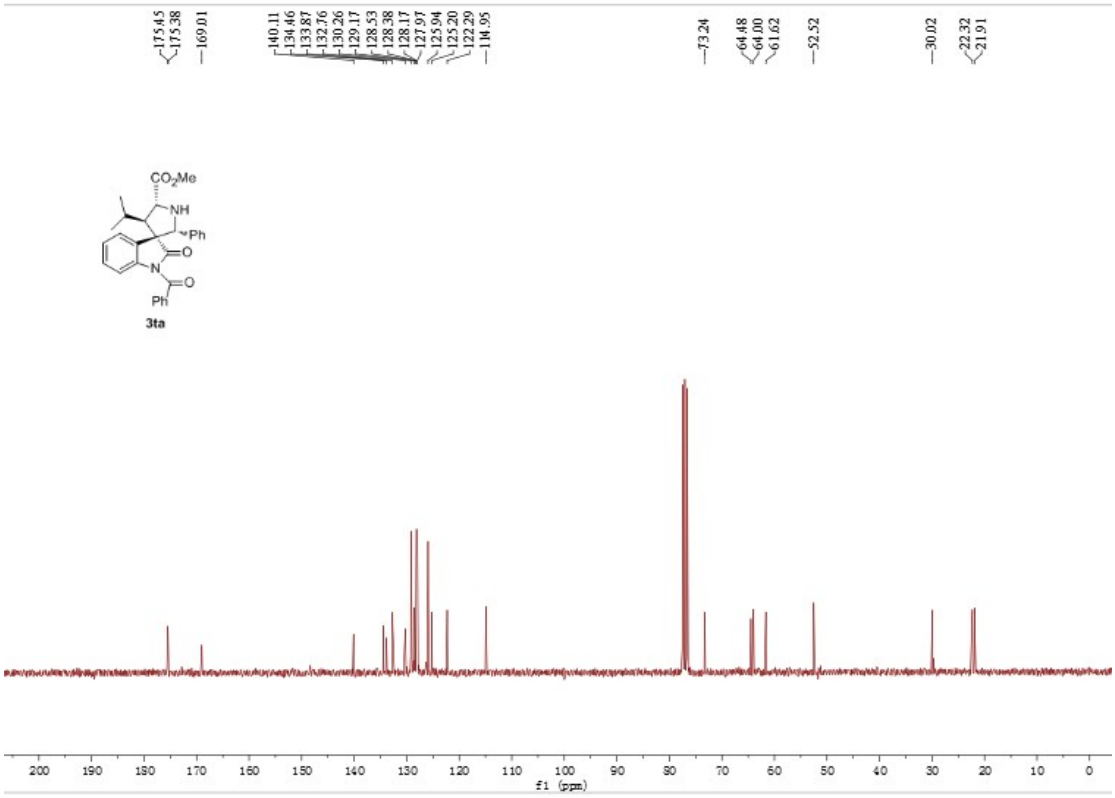
^{13}C NMR of 3sa



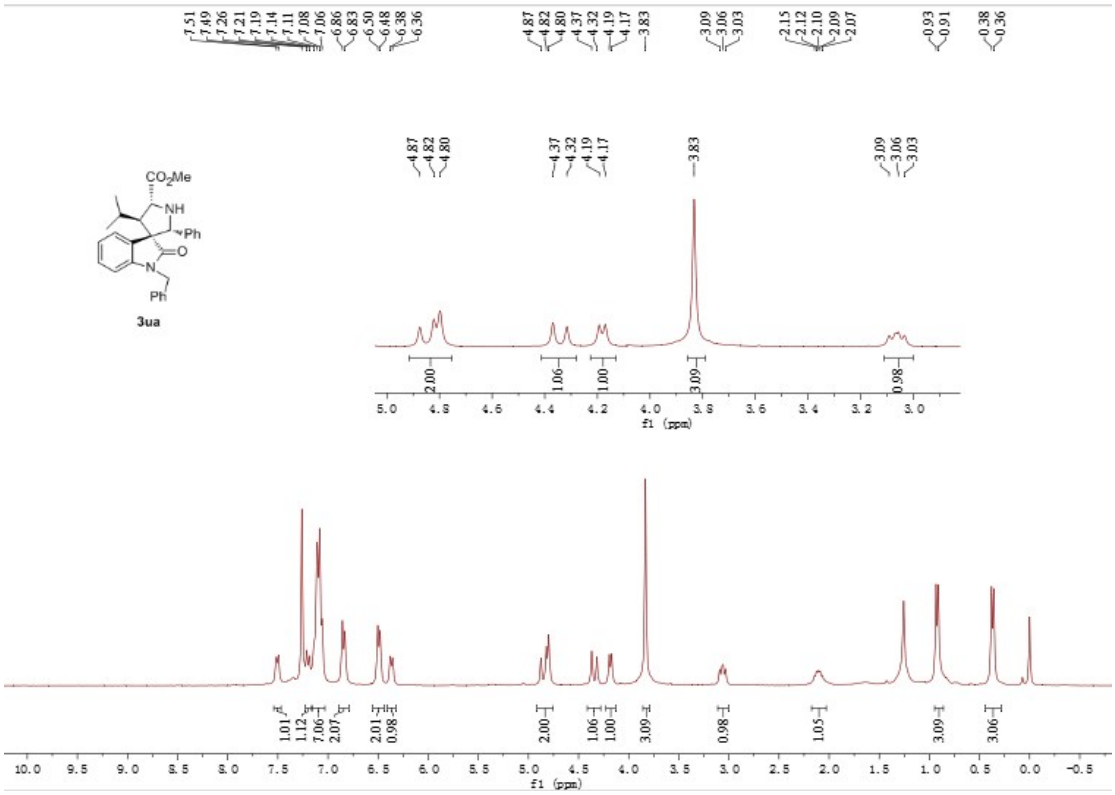
^{1}H NMR of 3ta



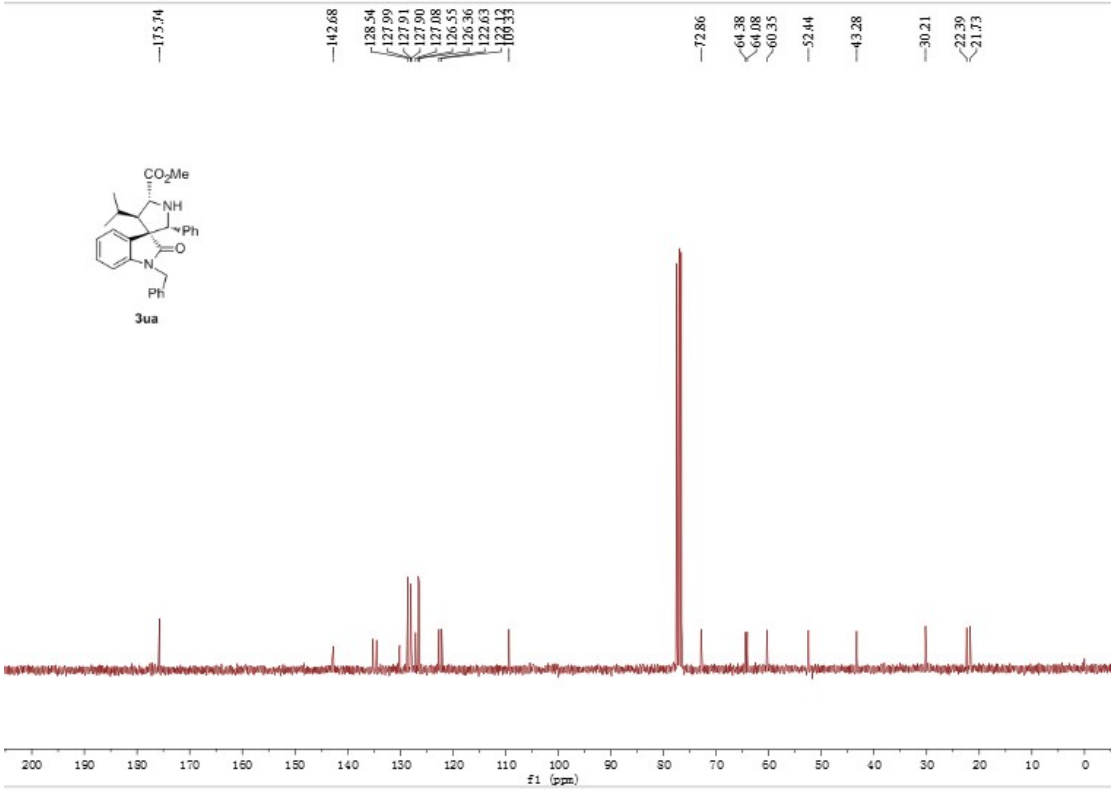
^{13}C NMR of 3ta



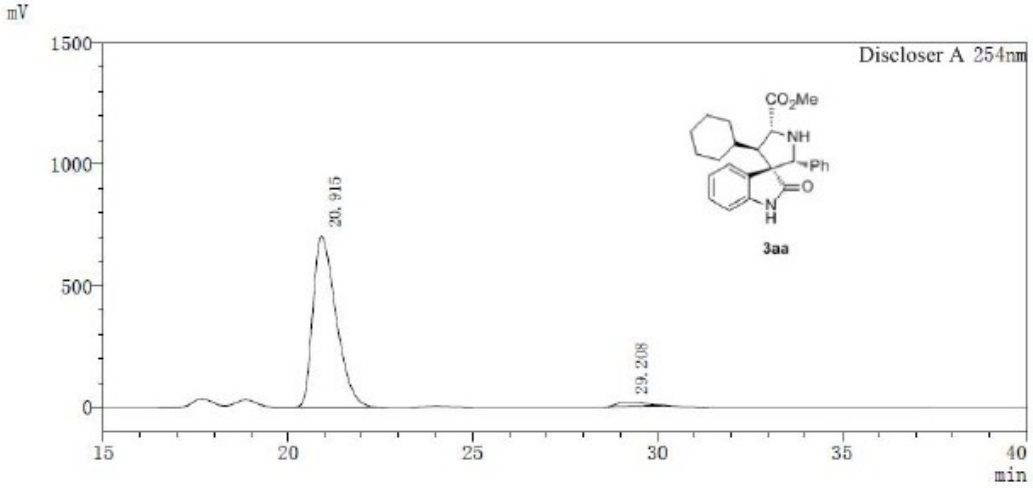
^{1}H NMR of 3ua



^{13}C NMR of 3ua

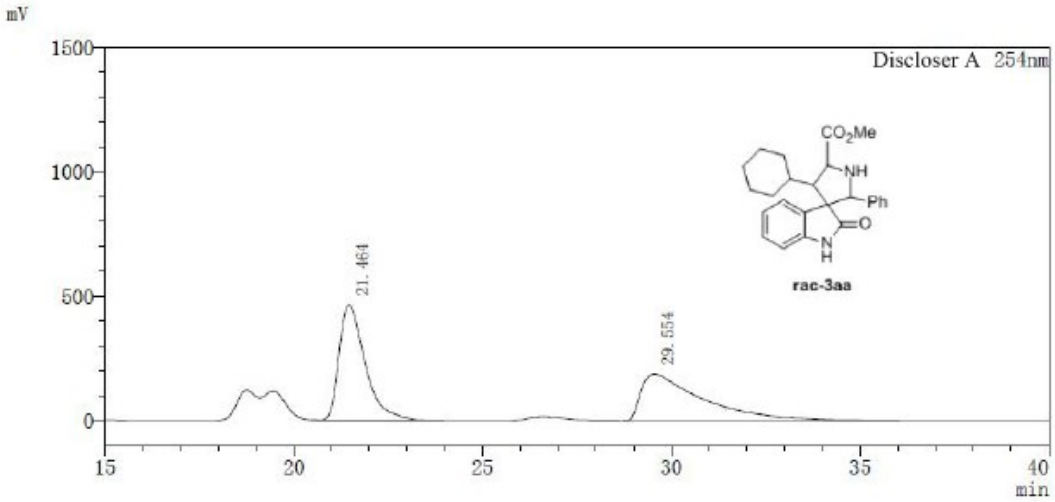


8. Copies of HPLC Chromatograms



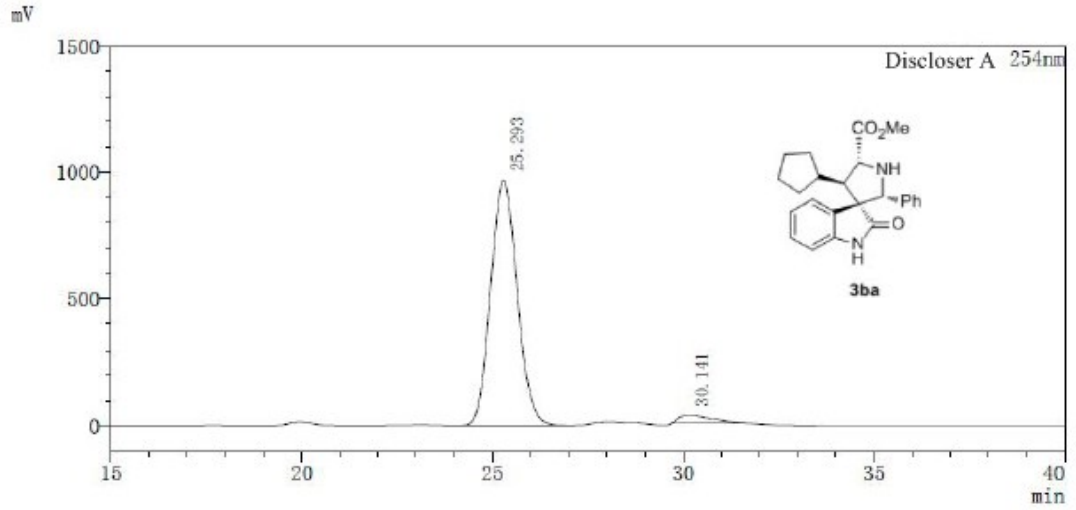
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	20.915	97.526
2	29.208	2.474
Total		100.000



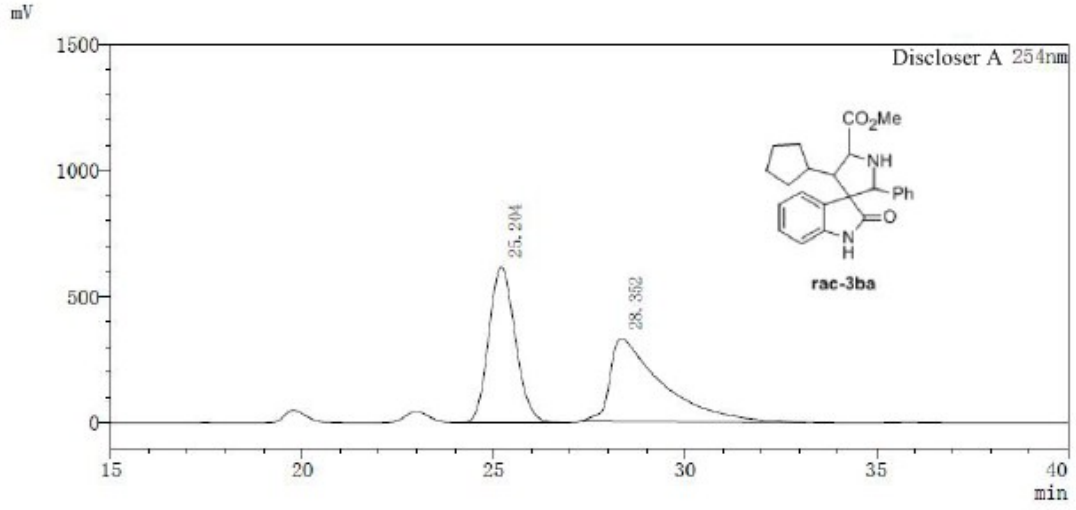
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	21.464	51.439
2	29.554	48.561
Total		100.000



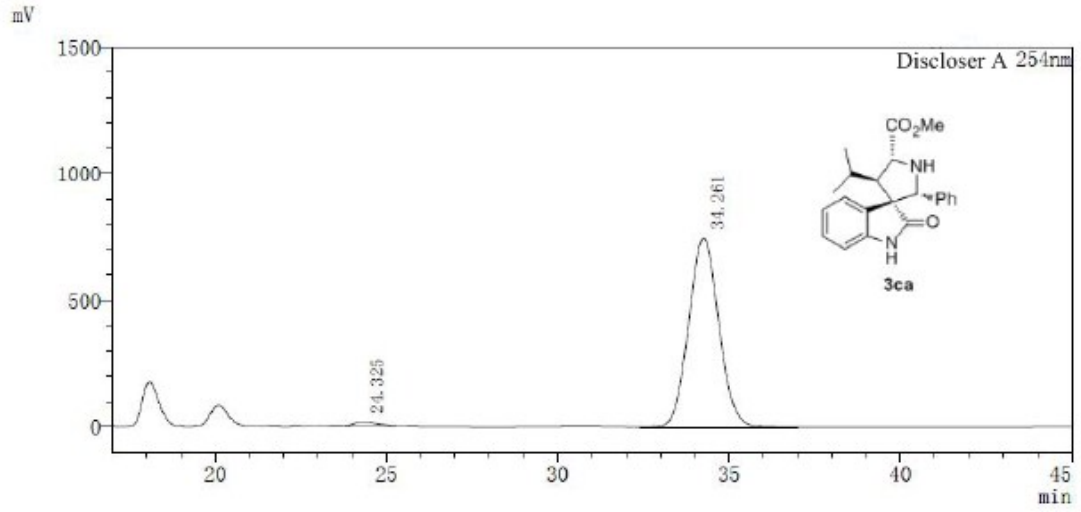
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	25.293	96.319
2	30.141	3.681
Total		100.000



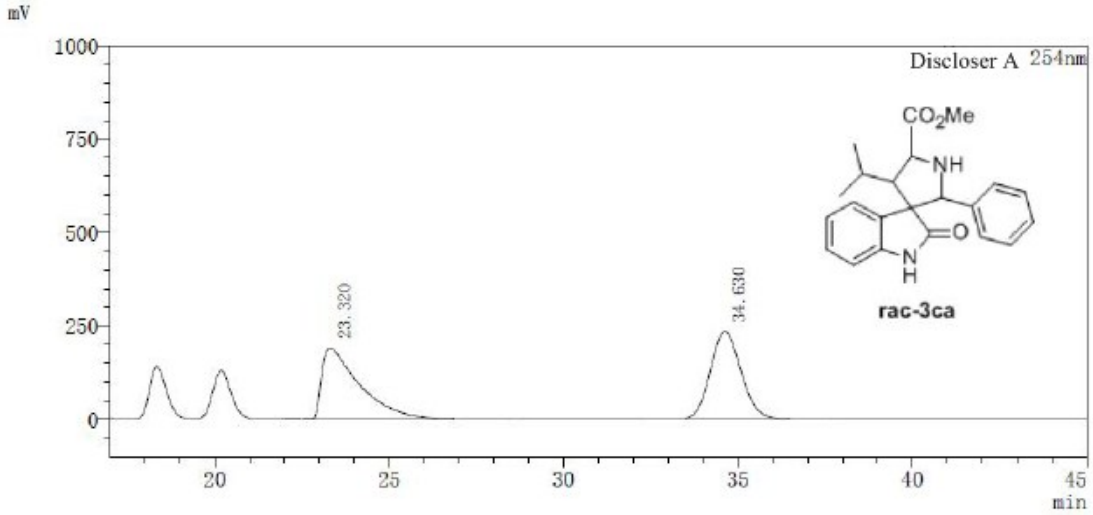
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	25.204	49.163
2	28.352	50.837
Total		100.000



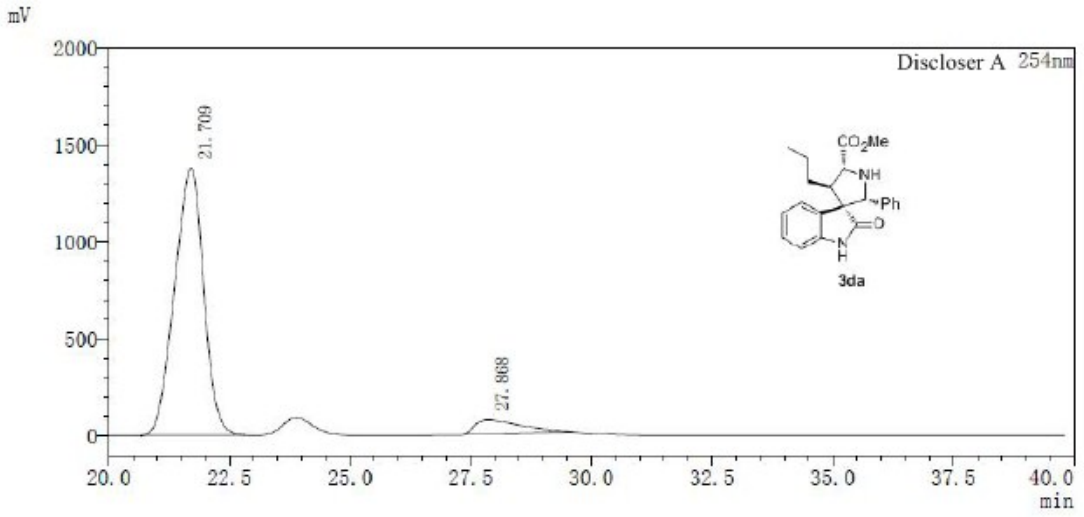
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	24.325	1.481
2	34.261	98.519
Total		100.000



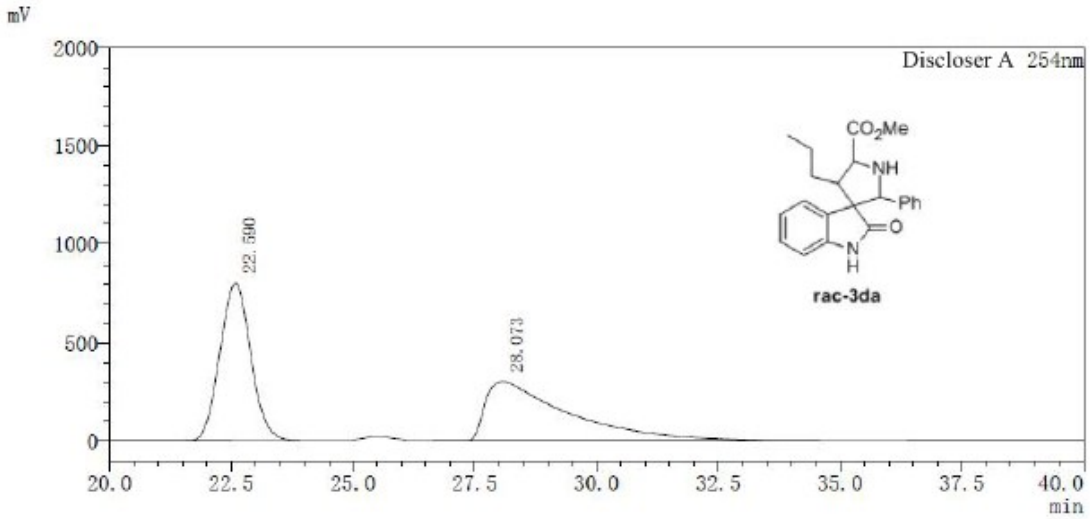
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	23.320	50.326
2	34.630	49.674
Total		100.000



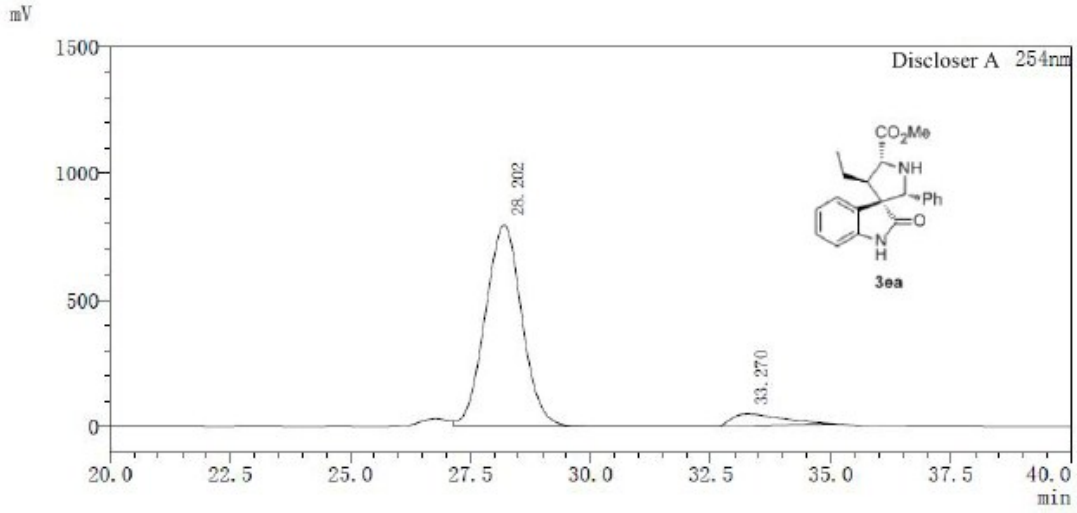
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	21.709	92.410
2	27.868	7.590
Total		100.000



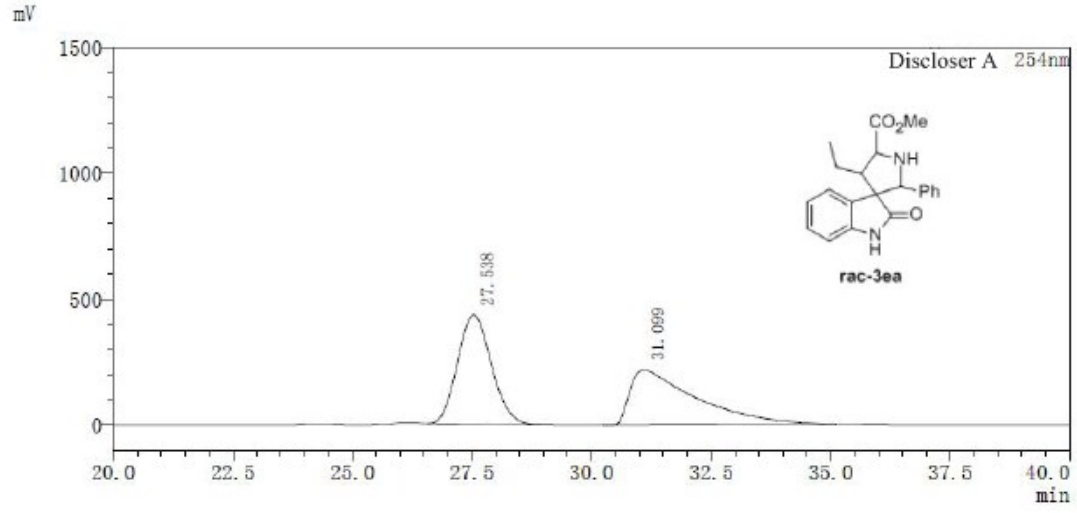
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	22.590	49.550
2	28.073	50.450
Total		100.000



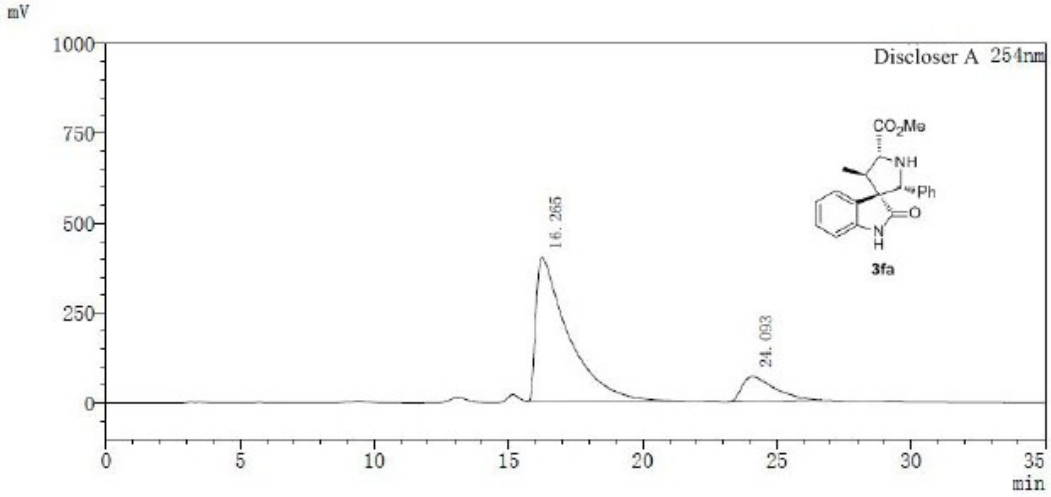
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	28.202	92.677
2	33.270	7.323
Total		100.000



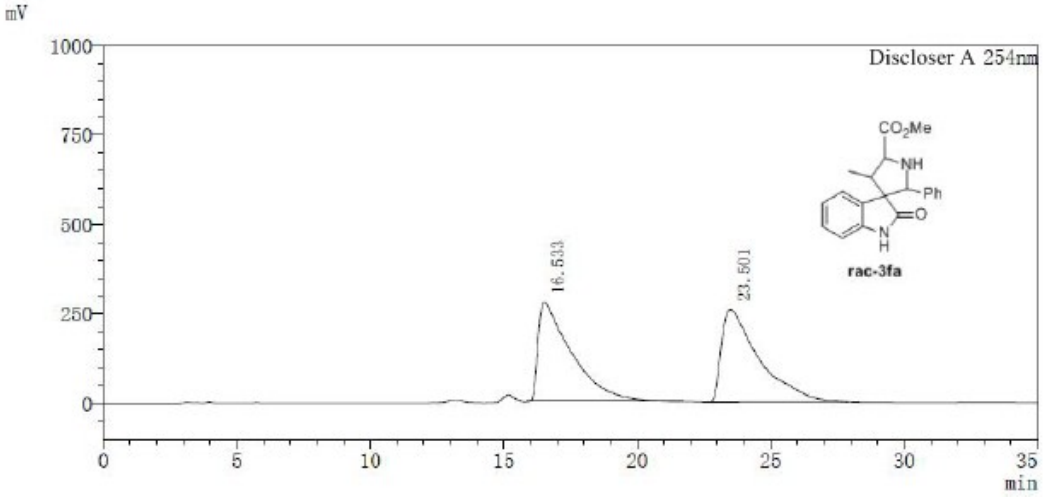
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	27.538	50.313
2	31.099	49.687
Total		100.000



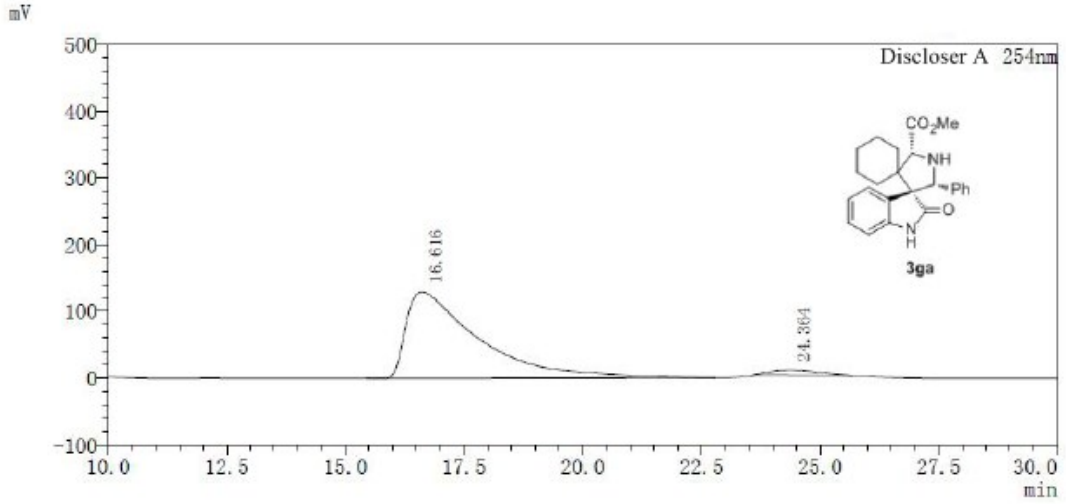
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	16.265	85.113
2	24.093	14.887
Total		100.000



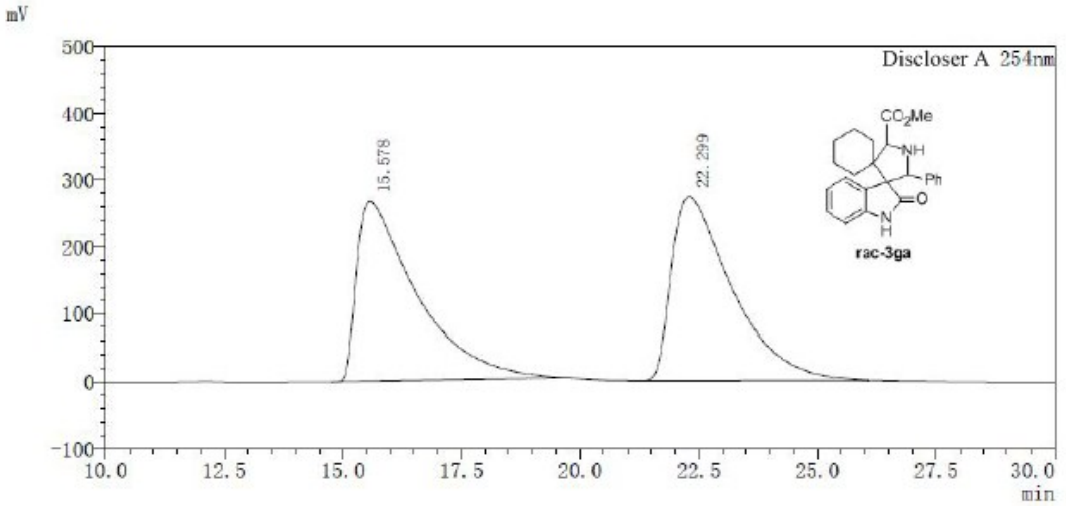
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	16.533	49.059
2	23.501	50.941
Total		100.000



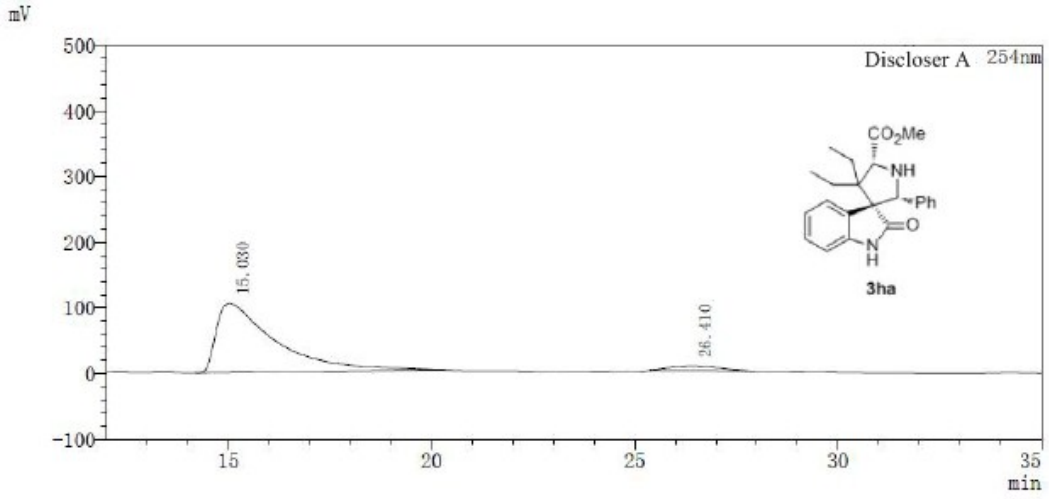
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	16.616	96.277
2	24.364	3.723
Total		100.000



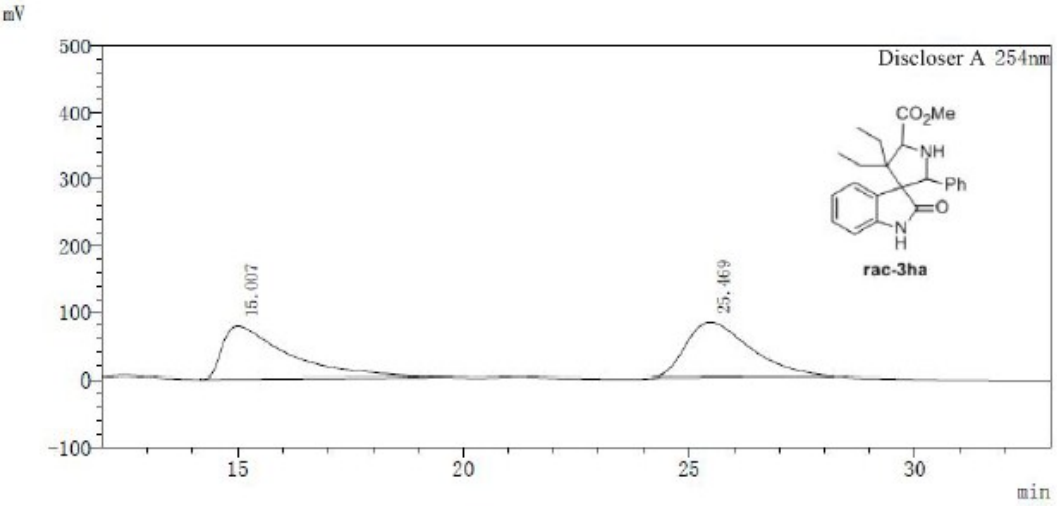
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	15.578	49.302
2	22.299	50.698
Total		100.000



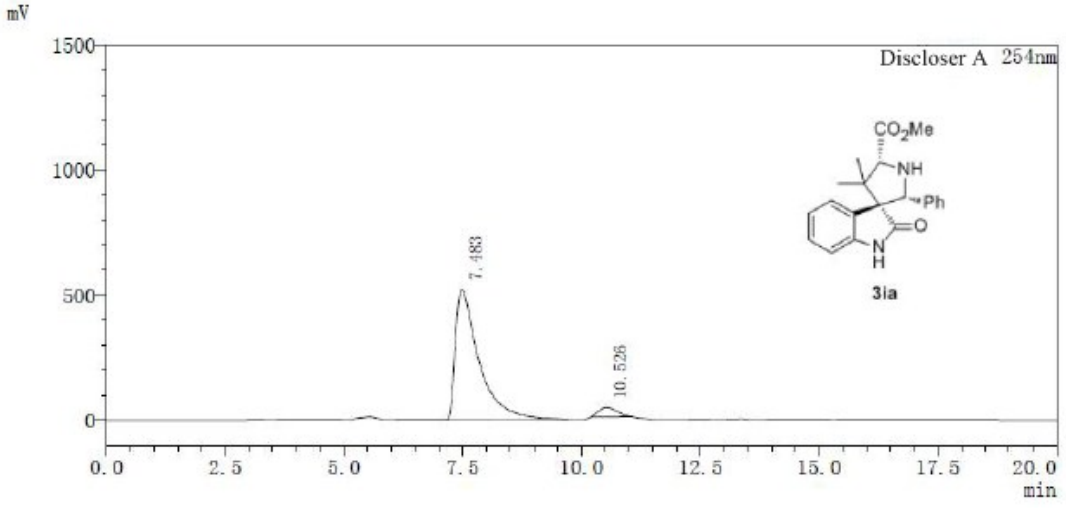
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	15.030	95.062
2	26.410	4.938
Total		100.000



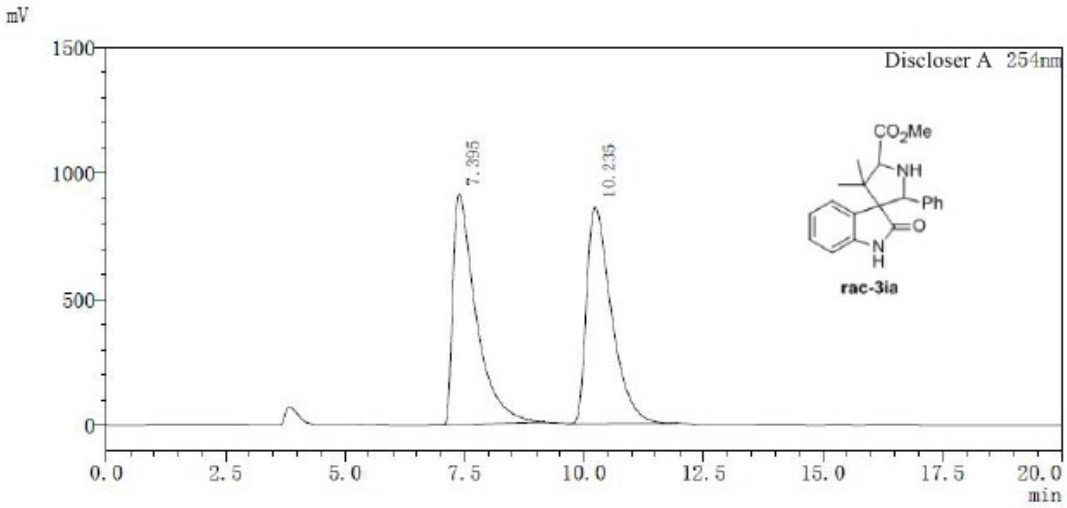
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	15.007	49.505
2	25.469	50.495
Total		100.000



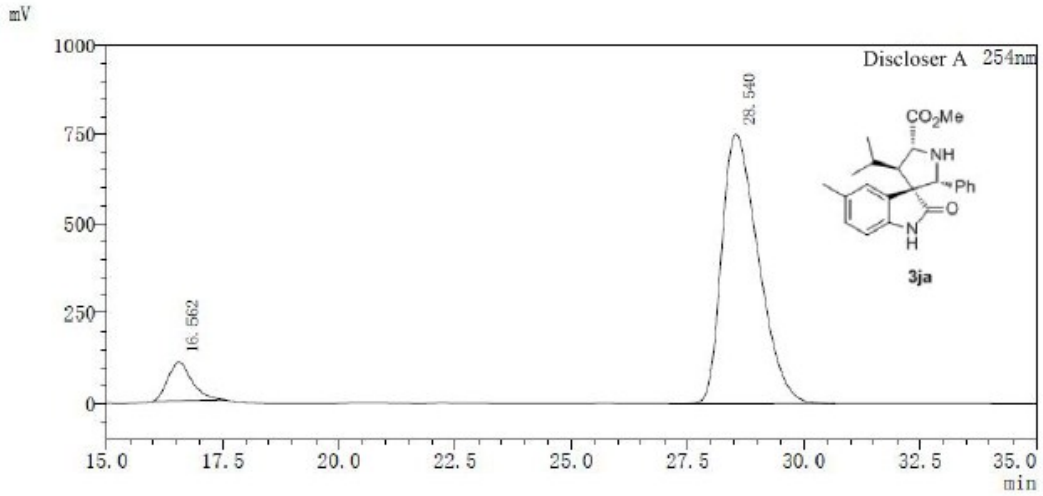
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	7.483	94.704
2	10.526	5.296
Total		100.000



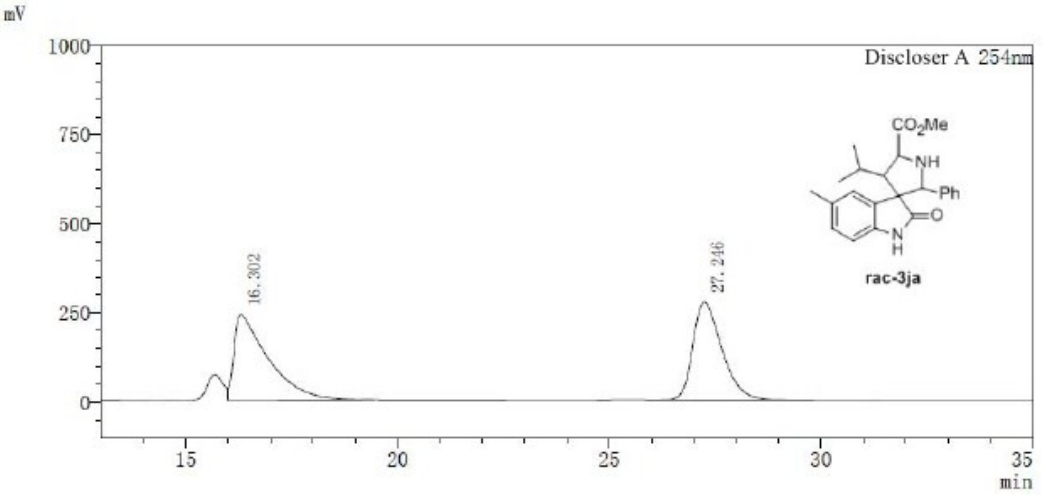
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	7.395	49.649
2	10.235	50.351
Total		100.000



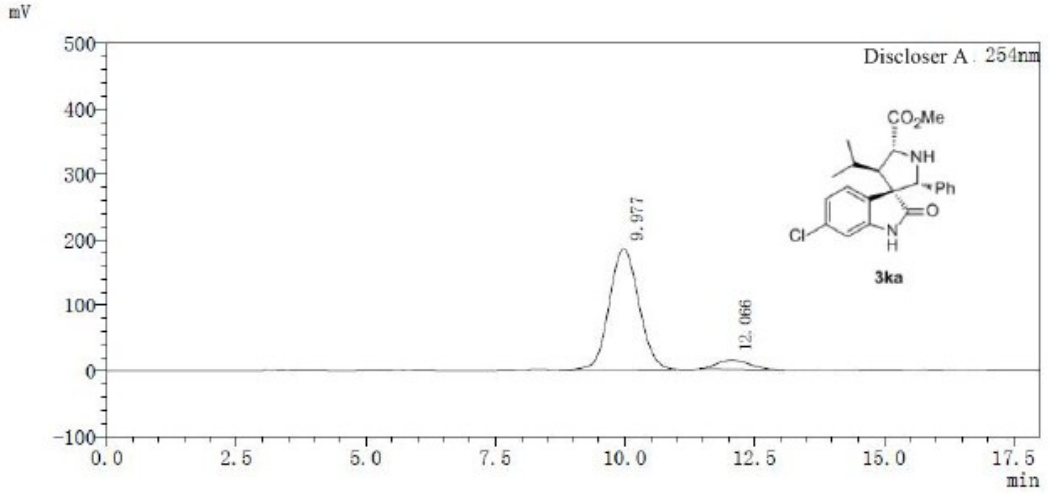
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	16.562	8.721
2	28.540	91.279
Total		100.000



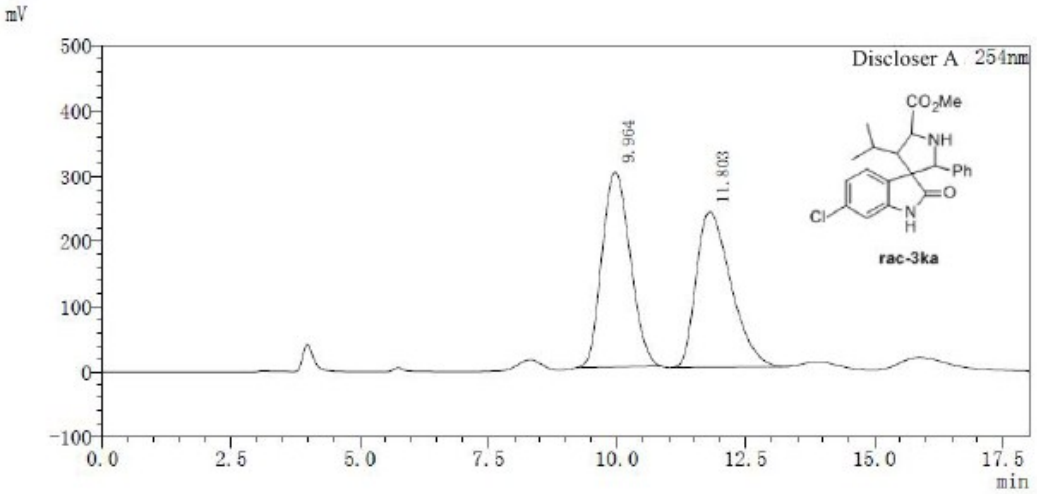
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	16.302	50.824
2	27.246	49.176
Total		100.000



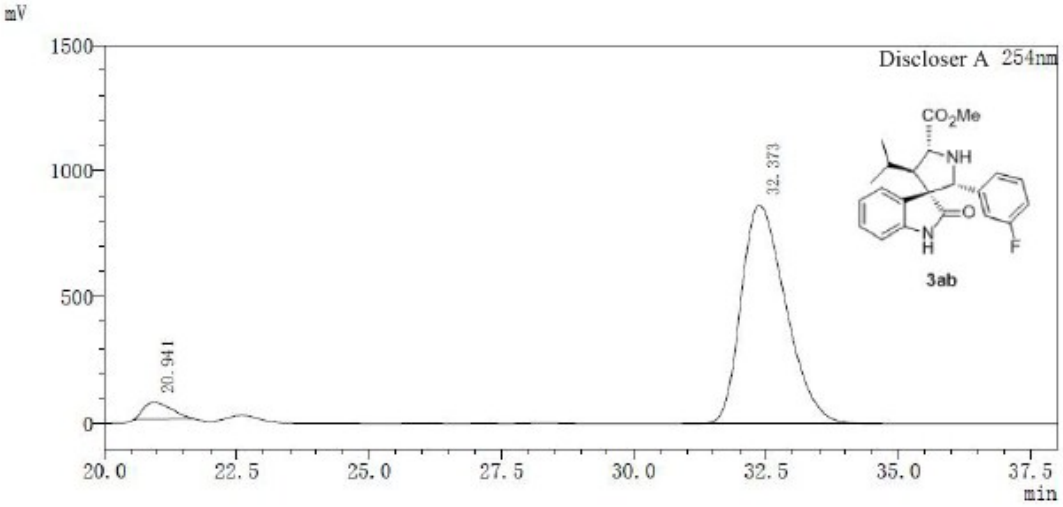
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	9.977	92.206
2	12.066	7.794
Total		100.000



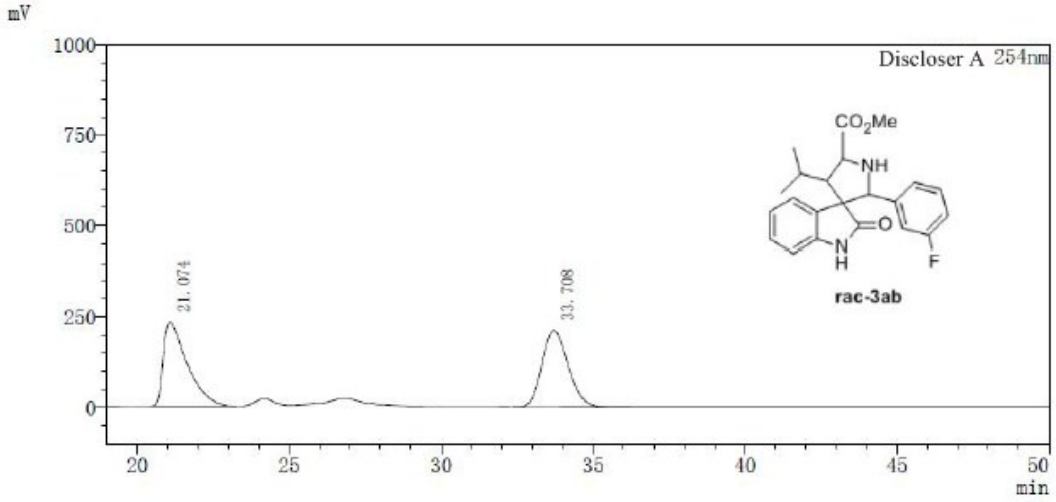
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	9.964	50.456
2	11.803	49.544
Total		100.000



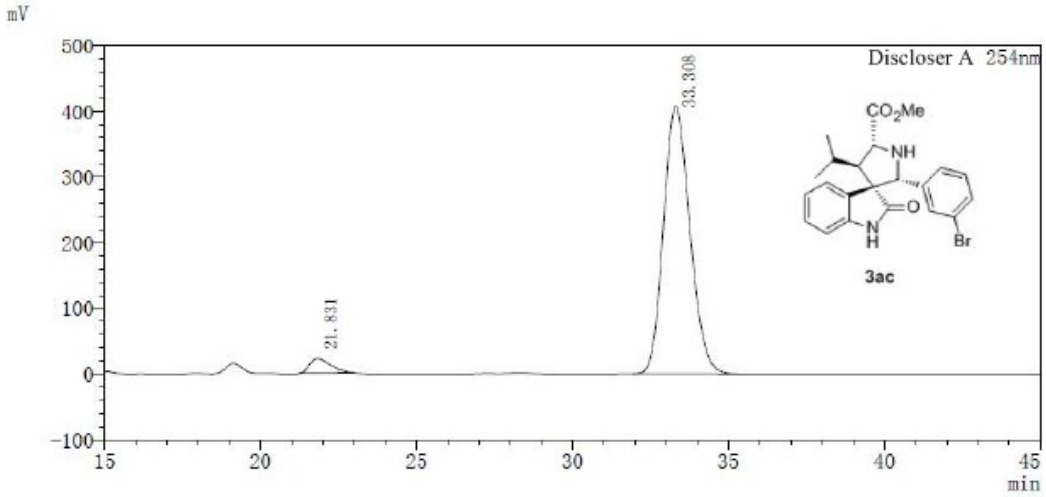
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	20.941	4.591
2	32.373	95.409
Total		100.000



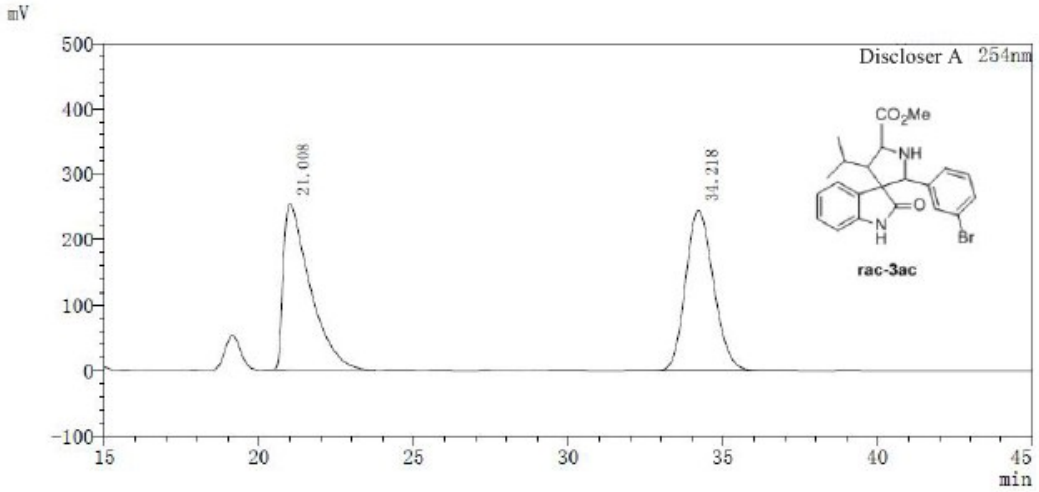
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	21.074	49.824
2	33.708	50.176
Total		100.000



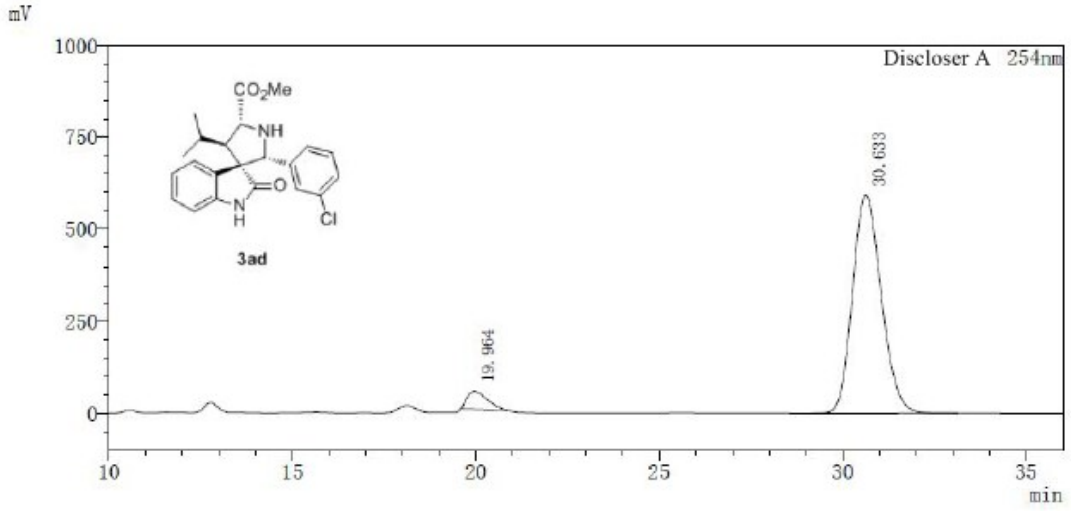
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	21.831	4.183
2	33.308	95.817
Total		100.000



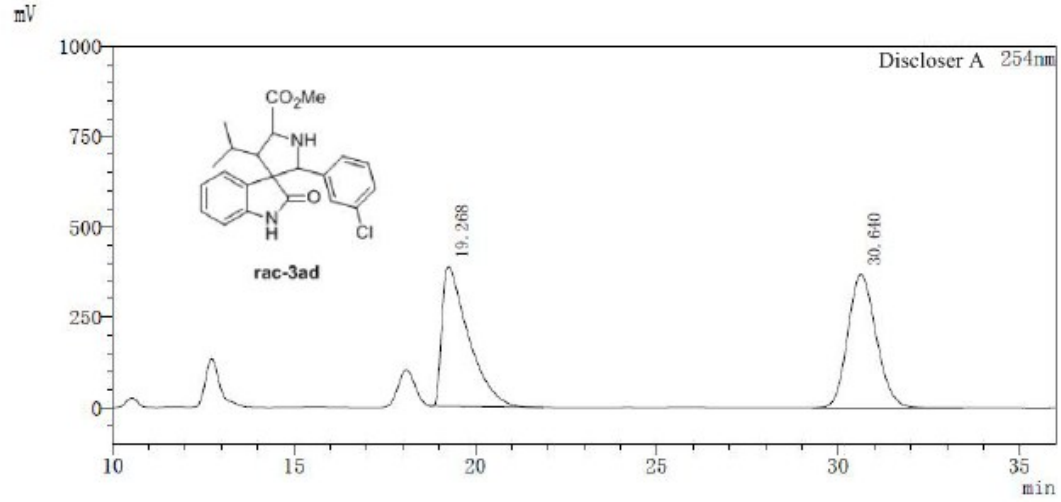
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	21.008	49.650
2	34.218	50.350
Total		100.000



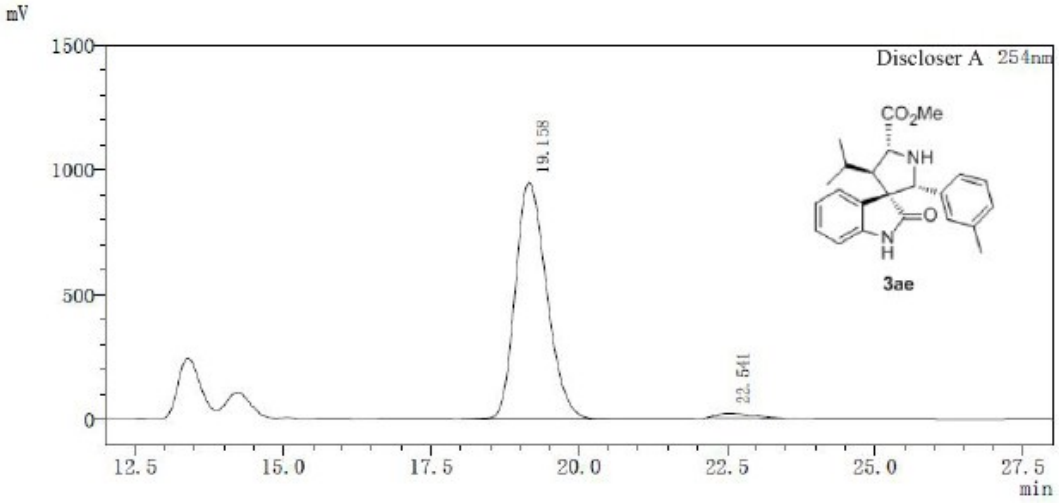
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	19.964	5.485
2	30.633	94.515
Total		100.000



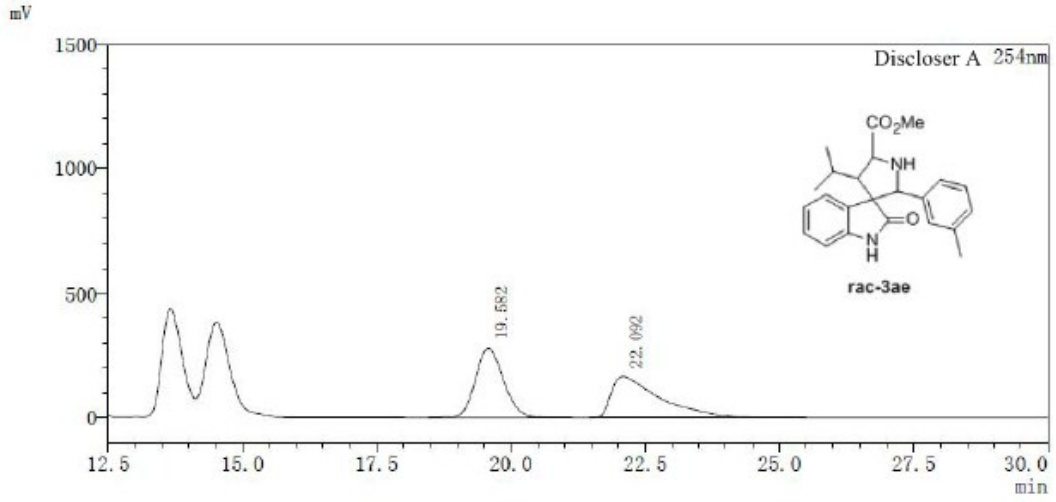
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	19.268	49.498
2	30.640	50.502
Total		100.000



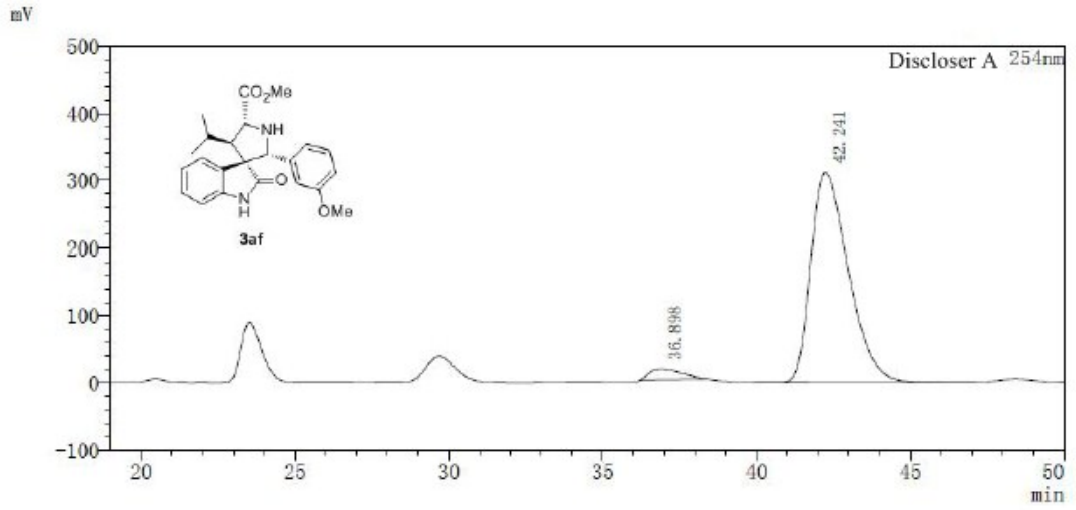
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	19.158	97.843
2	22.541	2.157
Total		100.000



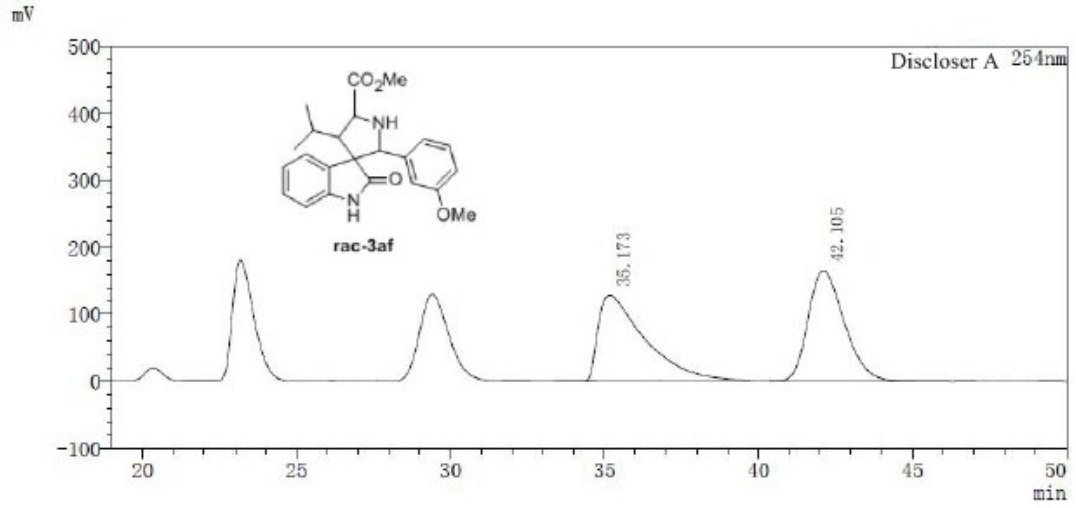
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	19.582	49.430
2	22.092	50.570
Total		100.000



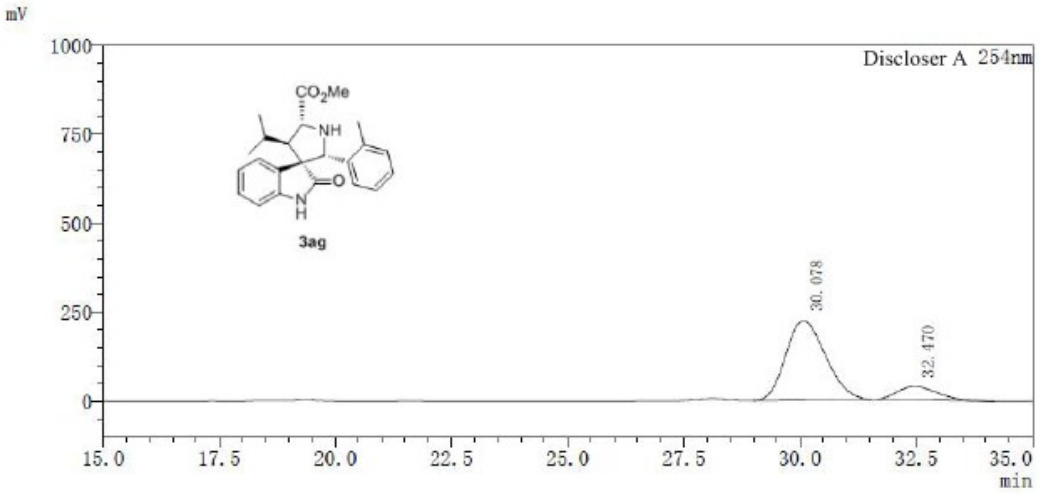
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	36.898	4.251
2	42.241	95.749
Total		100.000



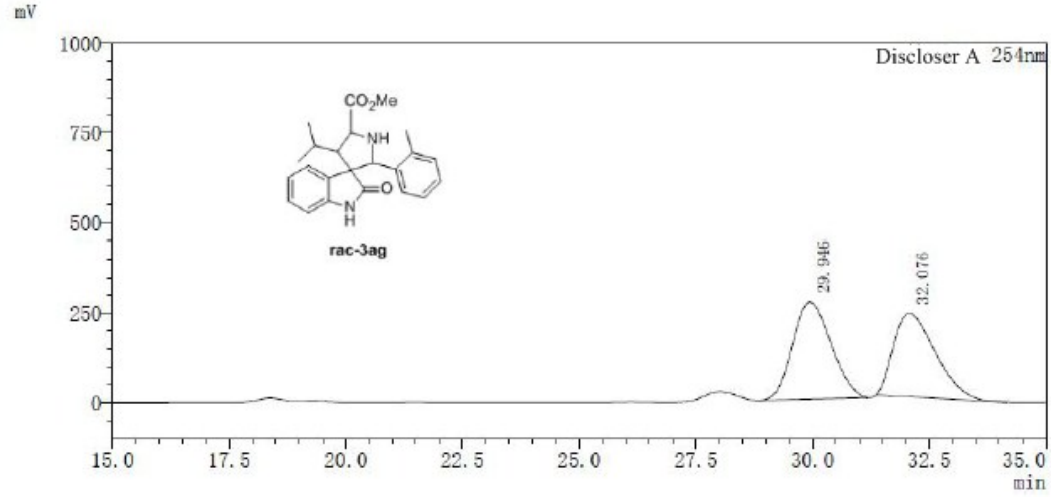
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	35.173	50.102
2	42.105	49.898
Total		100.000



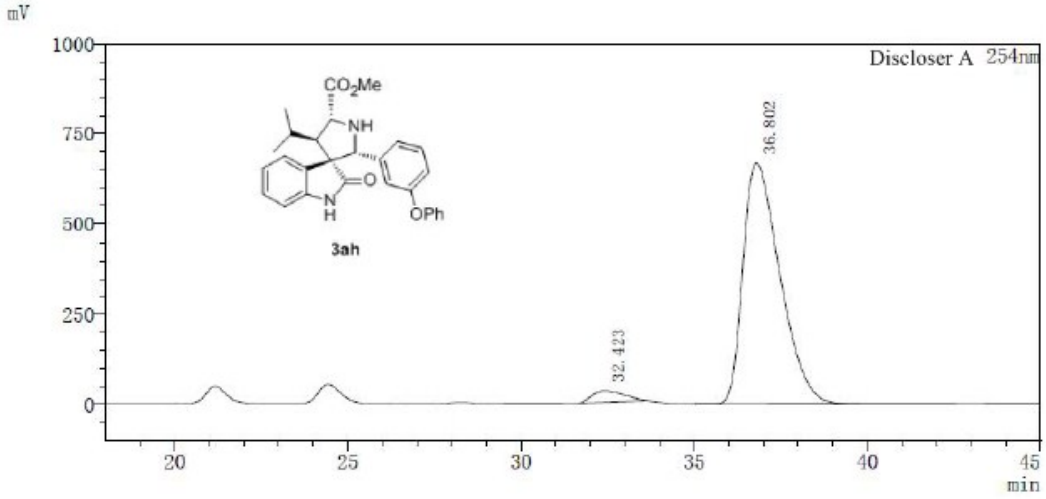
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	30.078	85.953
2	32.470	14.047
Total		100.000



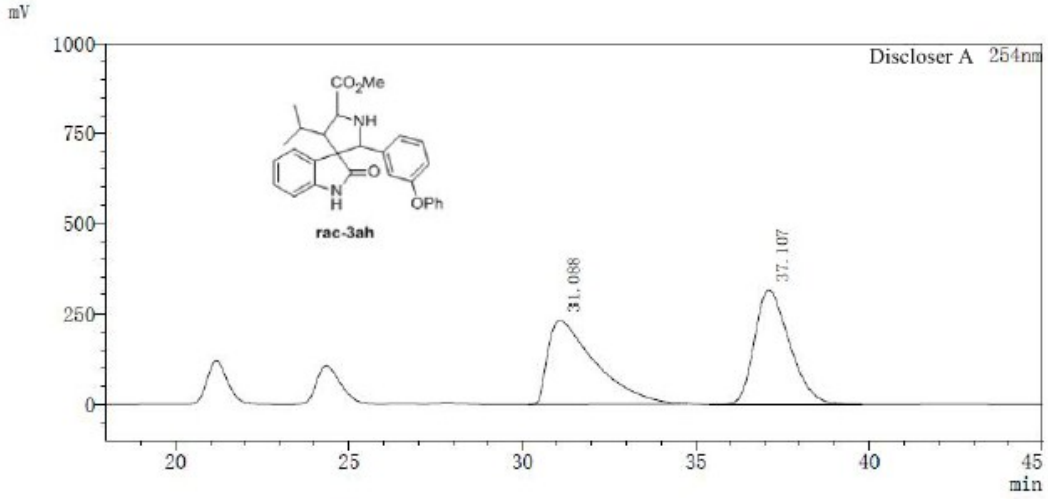
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	29.946	51.716
2	32.076	48.284
Total		100.000



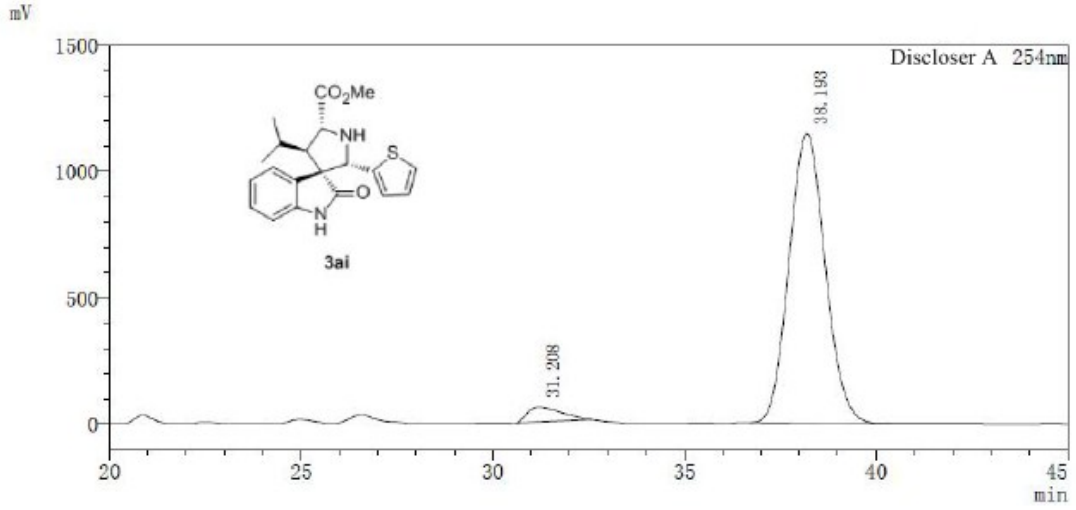
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	32.423	4.110
2	36.802	95.890
Total		100.000



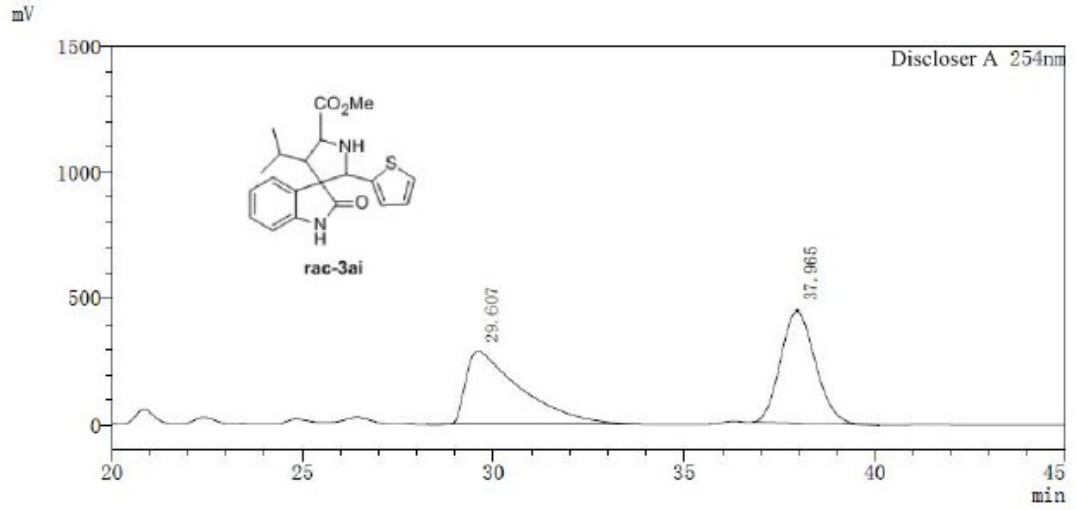
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	31.088	49.808
2	37.107	50.192
Total		100.000



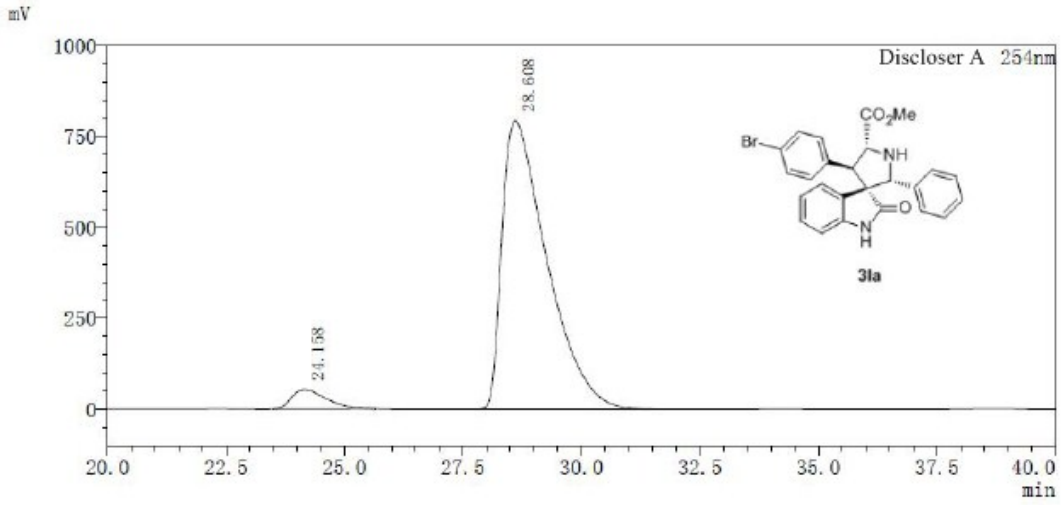
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	31.208	4.549
2	38.193	95.451
Total		100.000



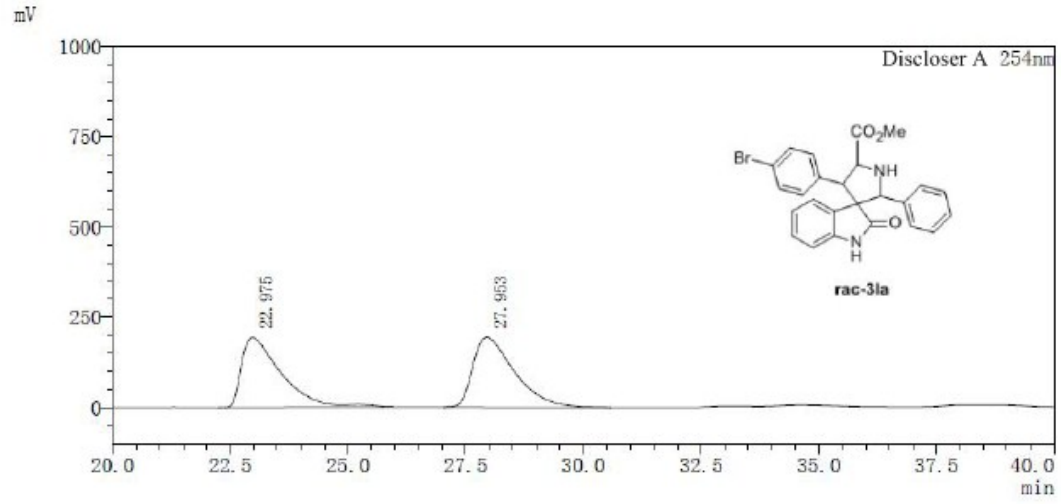
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	29.607	50.751
2	37.965	49.249
Total		100.000



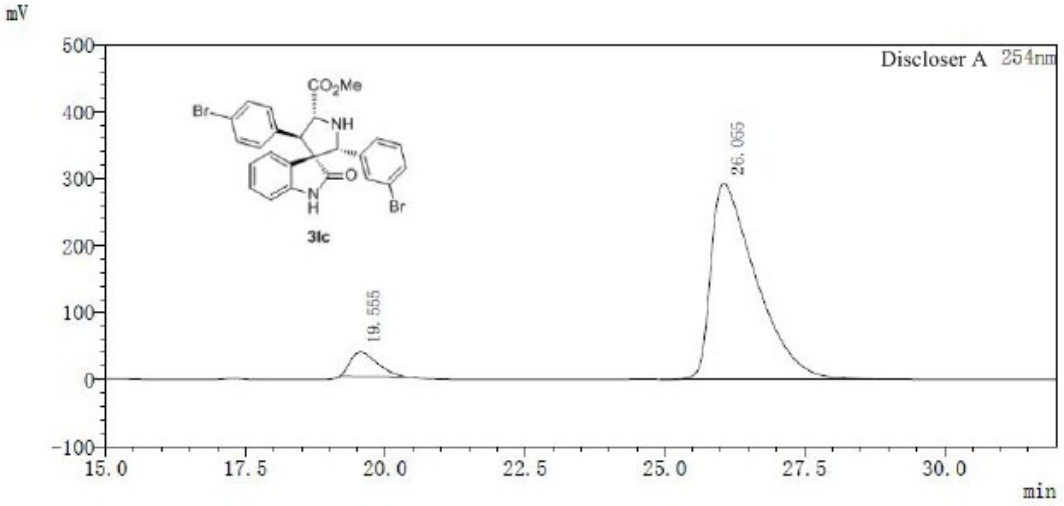
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	24.158	4.946
2	28.608	95.054
Total		100.000



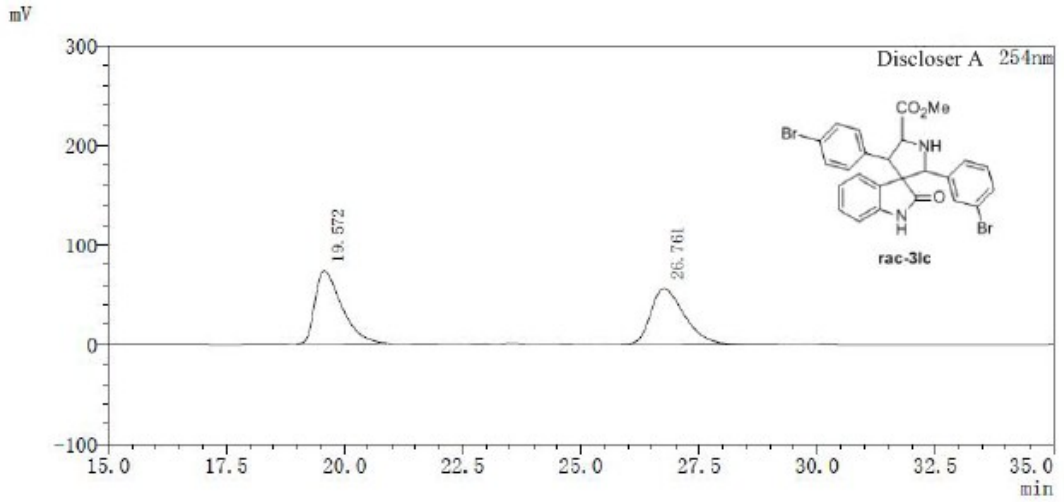
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	22.975	49.001
2	27.953	50.999
Total		100.000



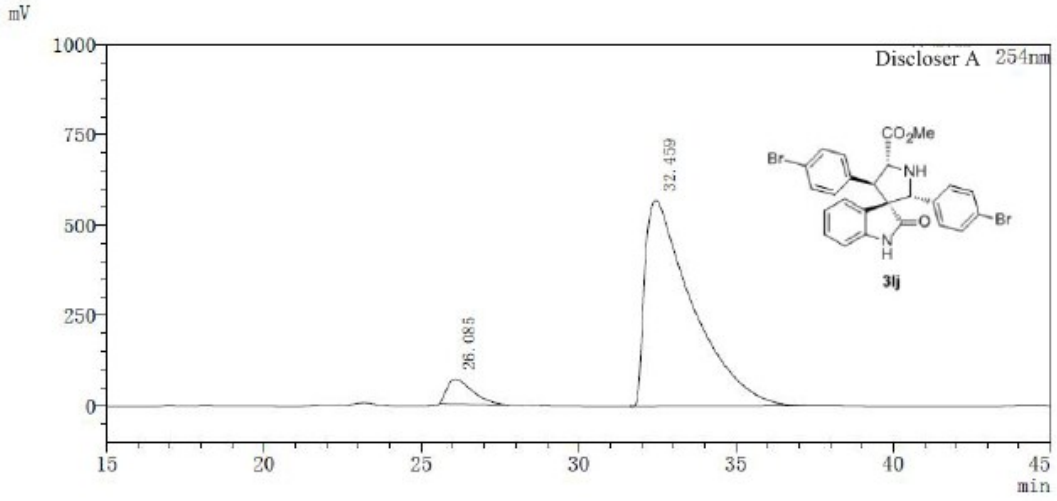
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	19.555	6.962
2	26.055	93.038
Total		100.000



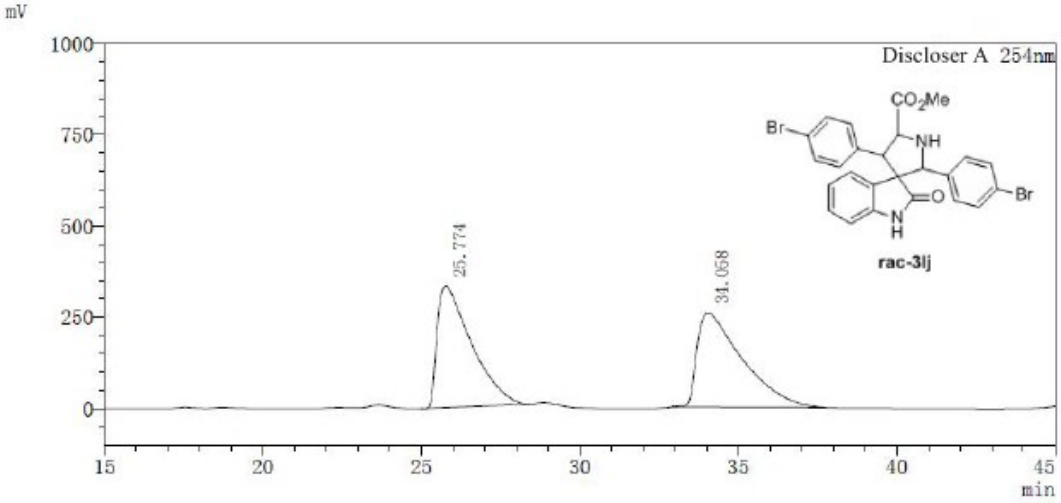
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	19.572	50.822
2	26.761	49.178
Total		100.000



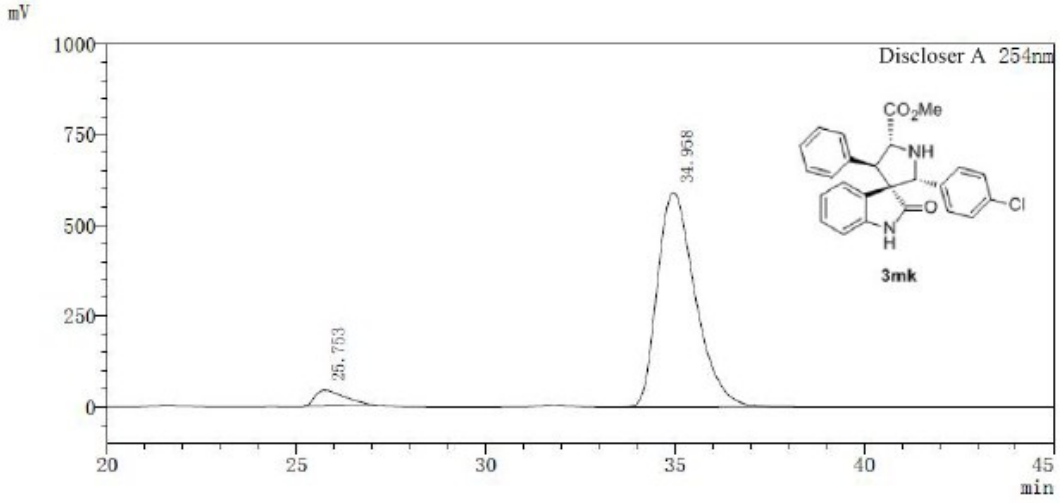
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	26.085	6.085
2	32.459	93.915
Total		100.000



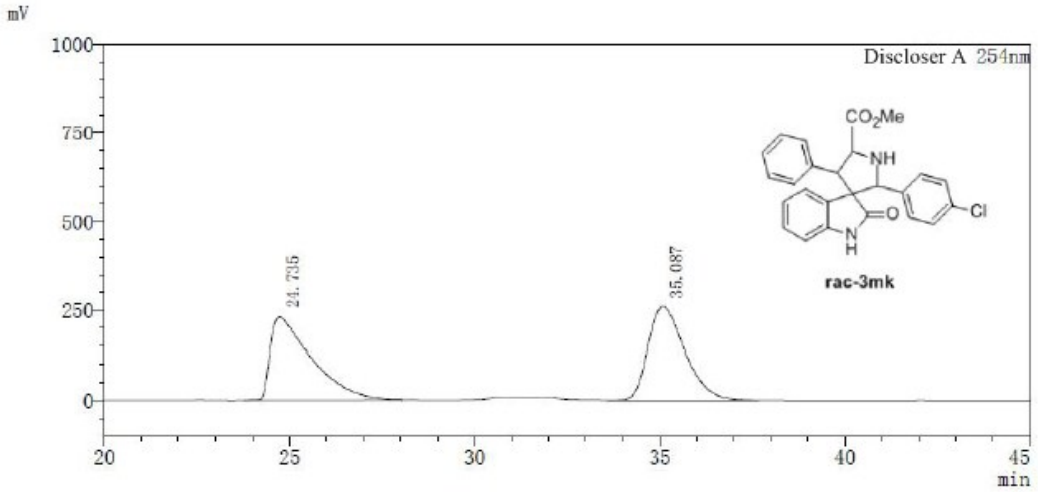
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	25.774	49.449
2	34.058	50.551
Total		100.000



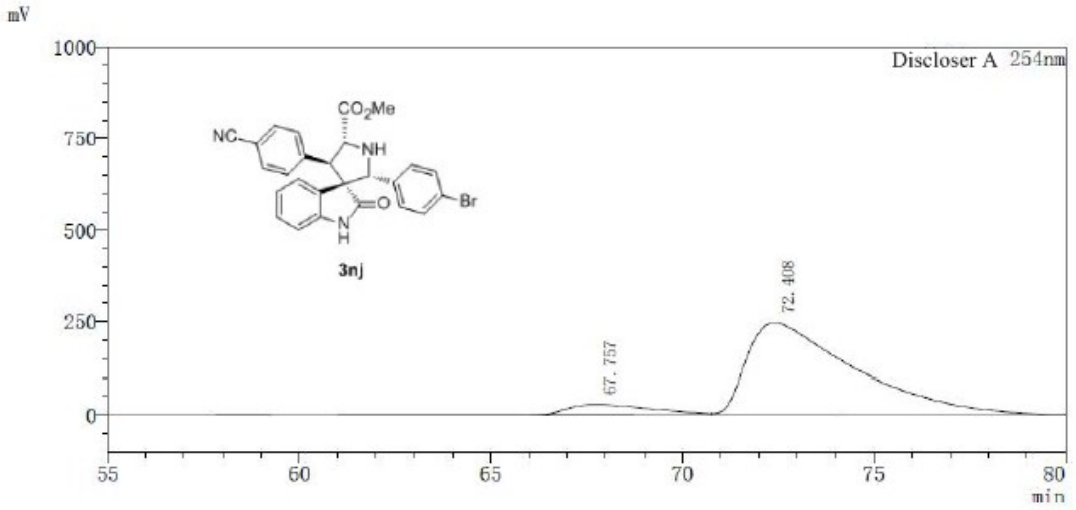
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	25.753	5.444
2	34.958	94.556
Total		100.000



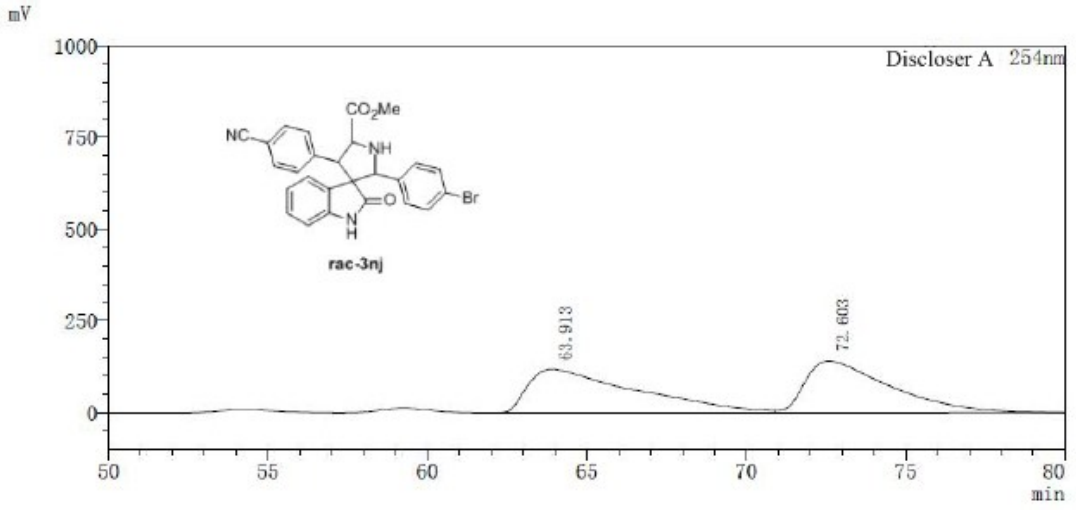
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	24.735	49.879
2	35.087	50.121
Total		100.000



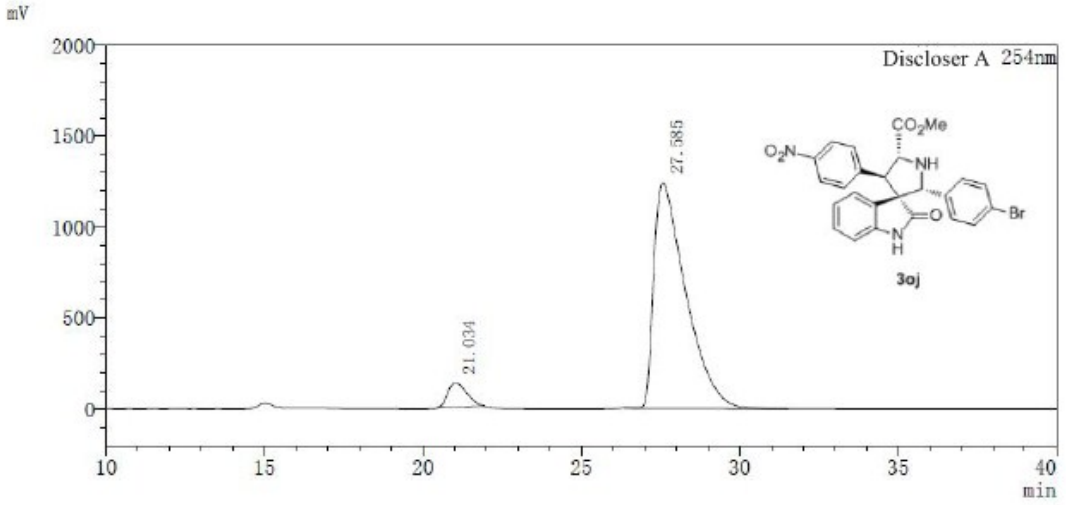
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	67.757	8.472
2	72.408	91.528
Total		100.000



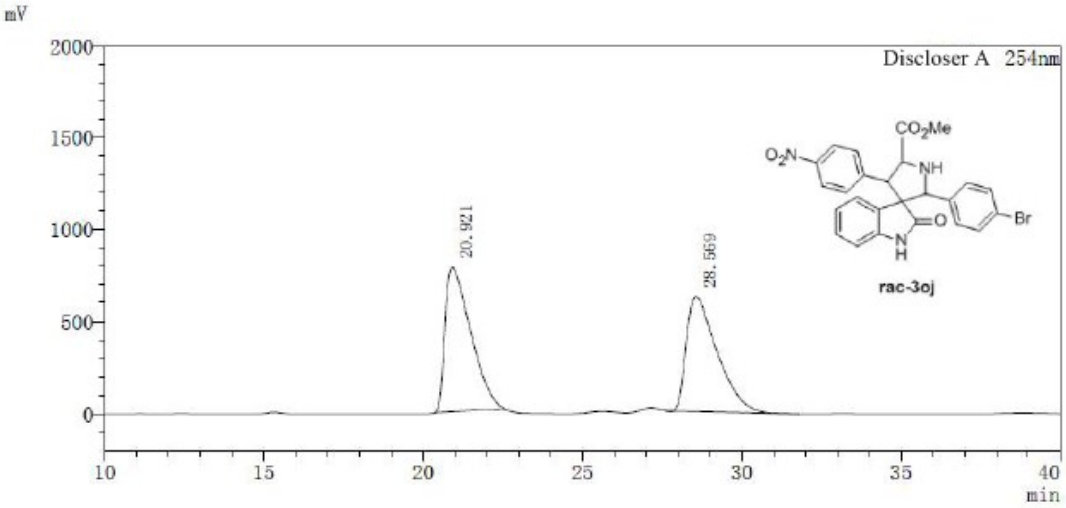
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	63.913	51.713
2	72.603	48.287
Total		100.000



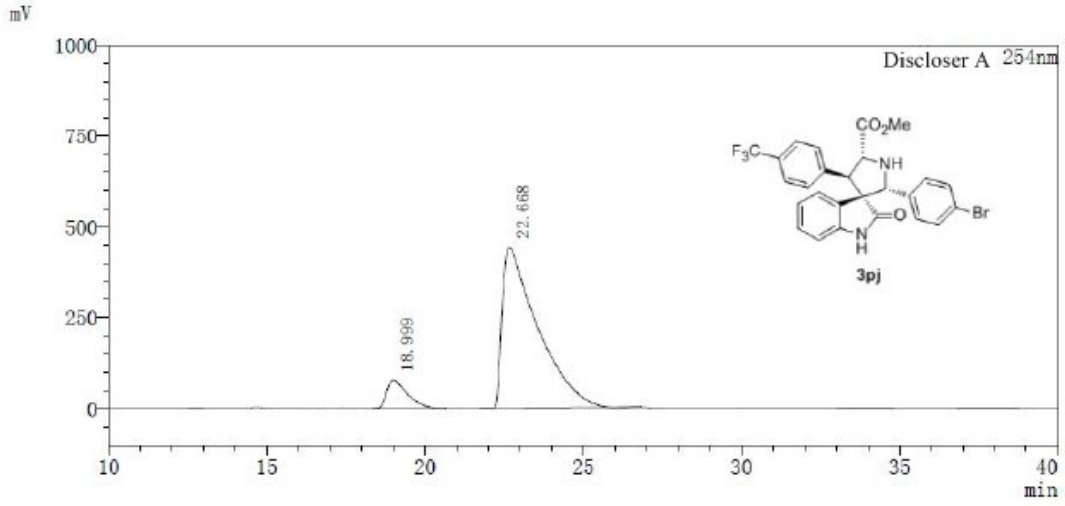
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	21.034	6.138
2	27.585	93.862
Total		100.000



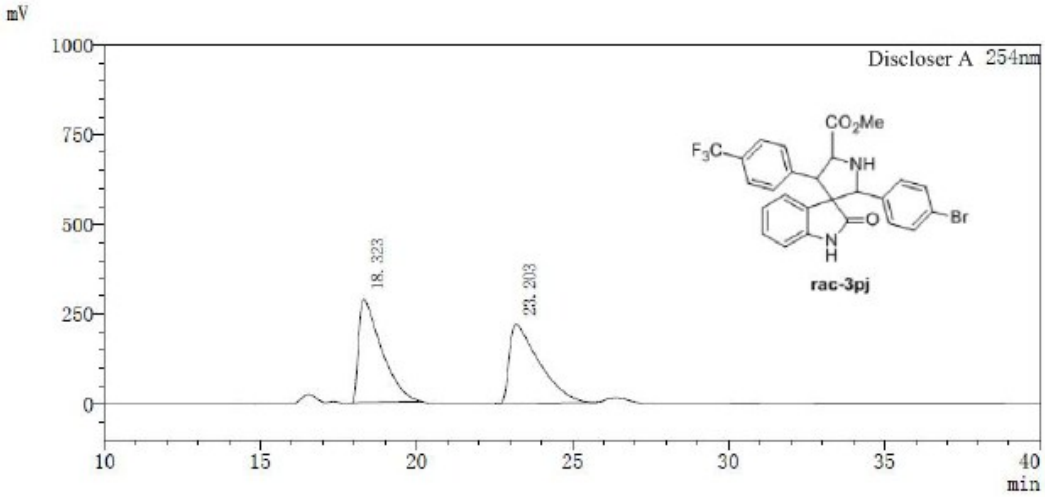
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	20.921	51.077
2	28.569	48.923
Total		100.000



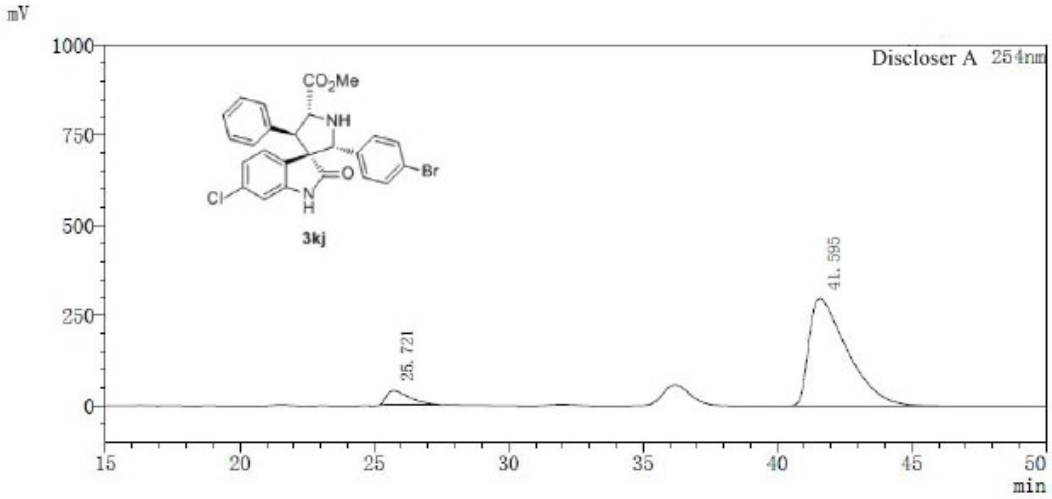
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	18.999	9.470
2	22.668	90.530
Total		100.000



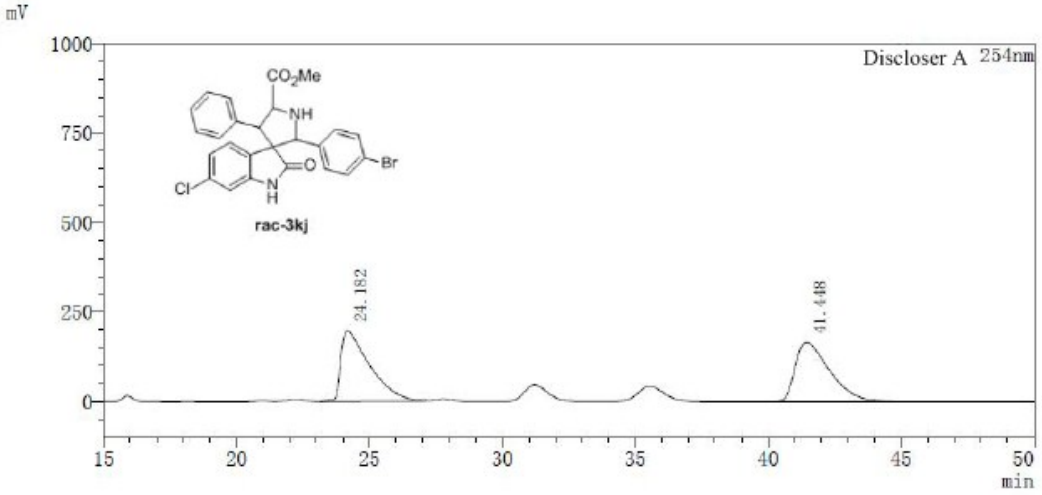
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	18.323	50.238
2	23.203	49.762
Total		100.000



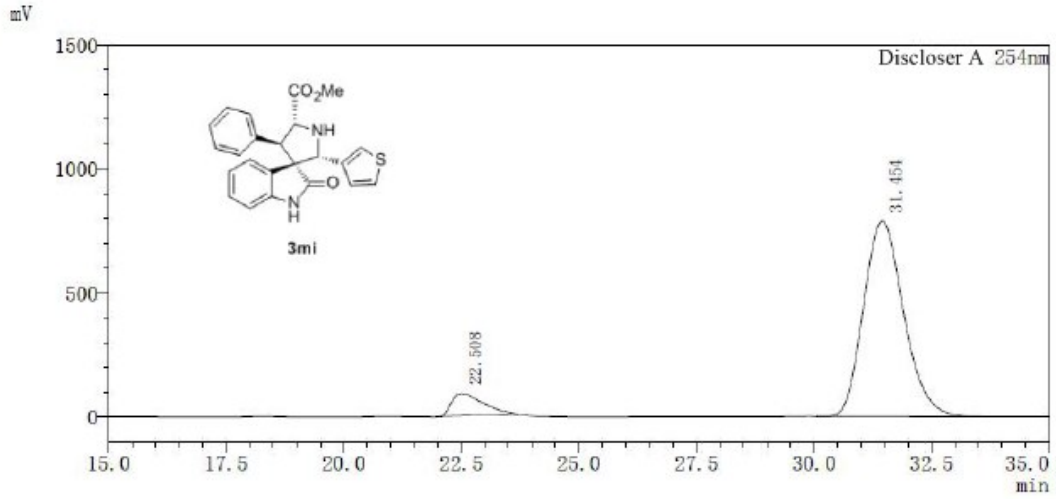
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	25.721	7.181
2	41.595	92.819
Total		100.000



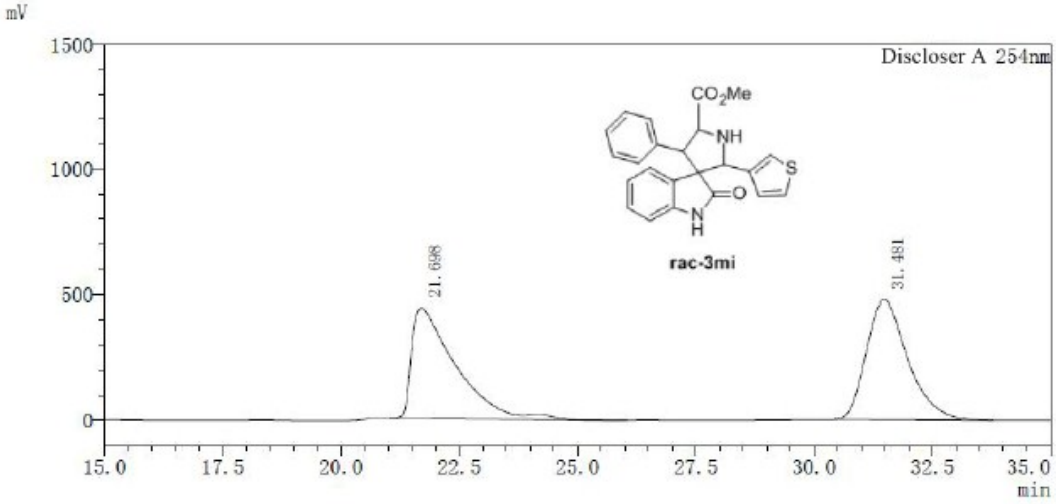
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	24.182	49.733
2	41.448	50.267
Total		100.000



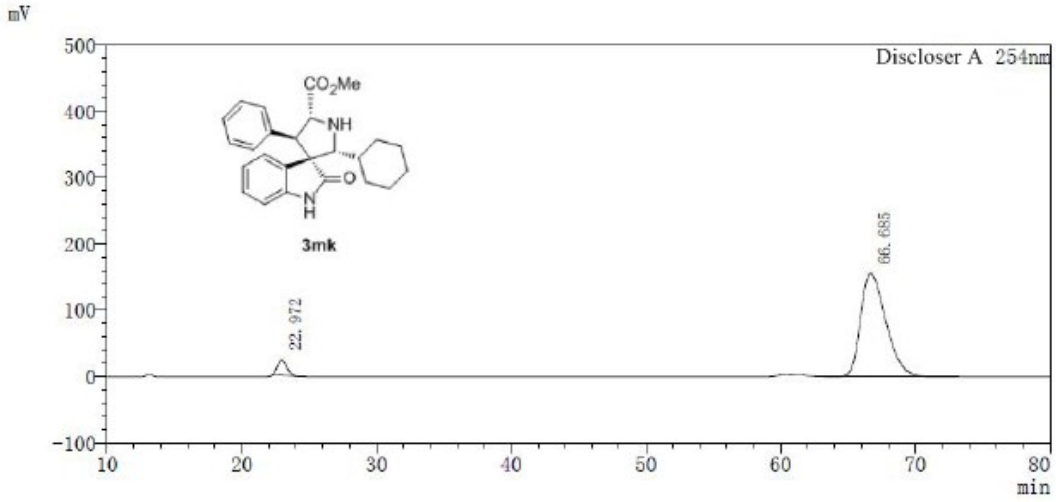
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	22.508	8.047
2	31.454	91.953
Total		100.000



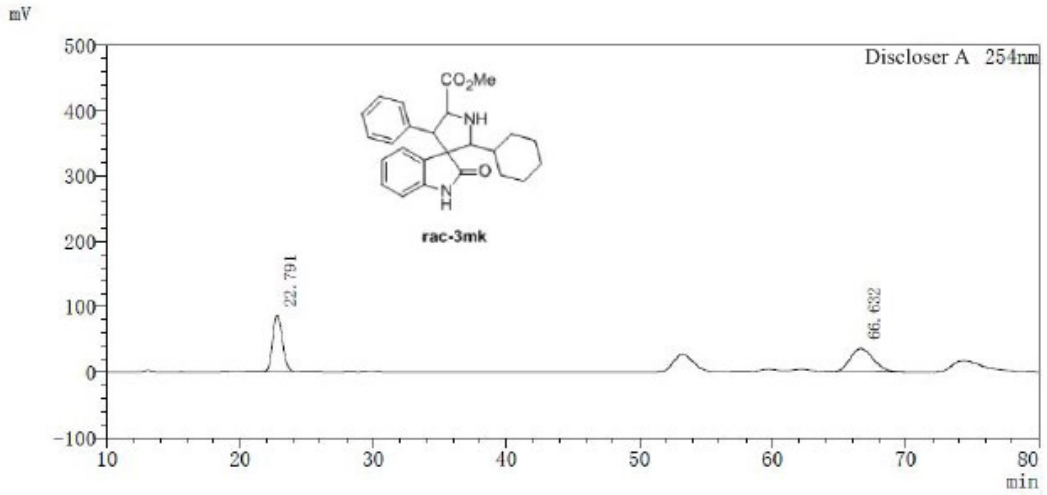
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	21.698	49.544
2	31.481	50.456
Total		100.000



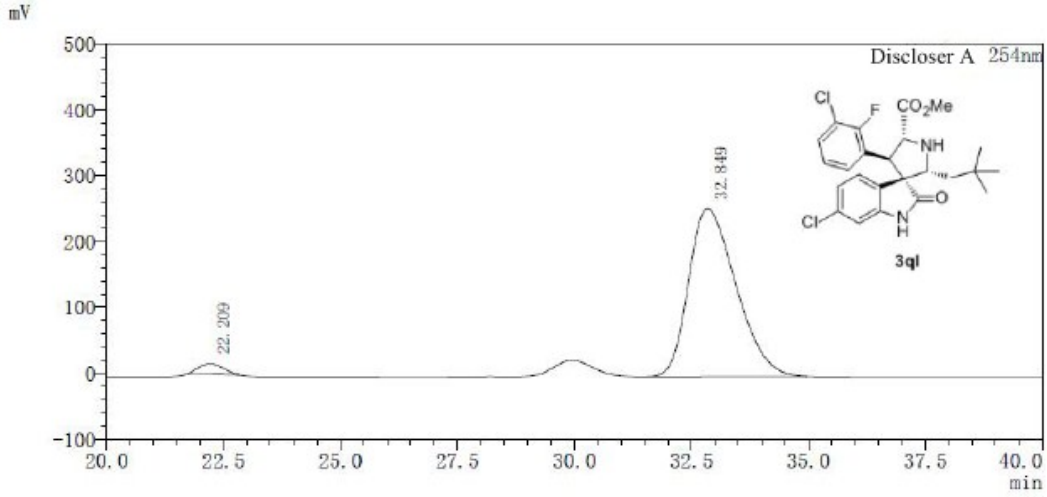
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	22.972	5.203
2	66.685	94.797
Total		100.000



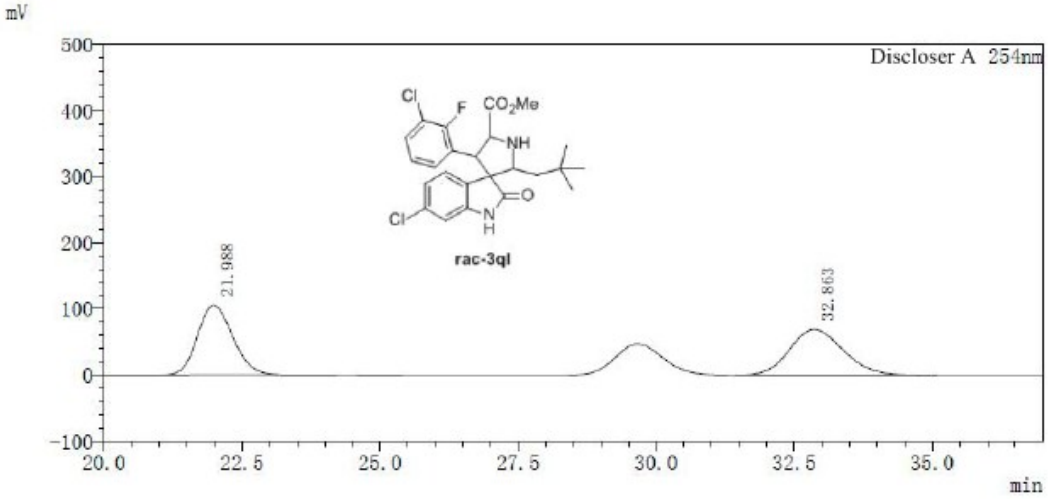
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	22.791	50.699
2	66.632	49.301
Total		100.000



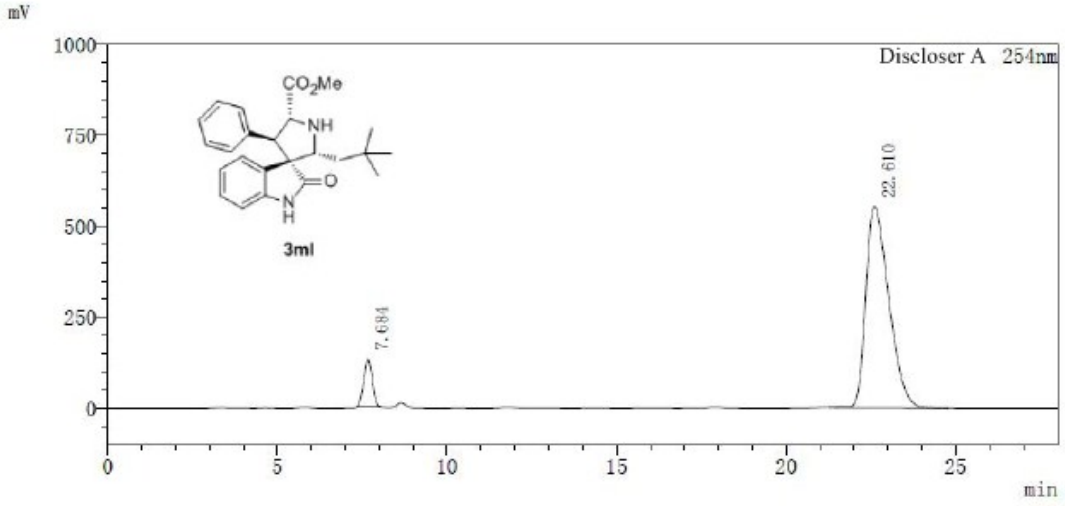
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	22.209	3.121
2	32.849	96.879
Total		100.000



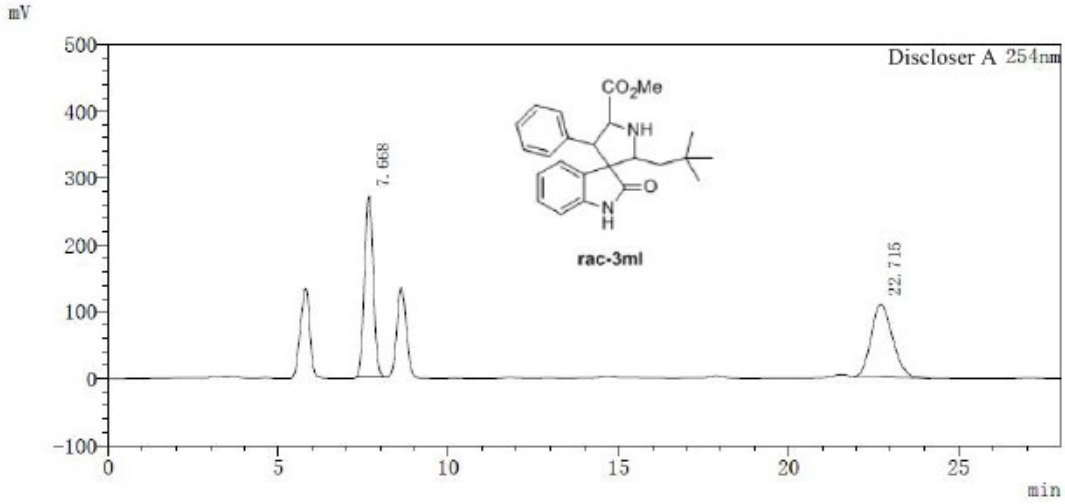
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	21.988	50.040
2	32.863	49.960
Total		100.000



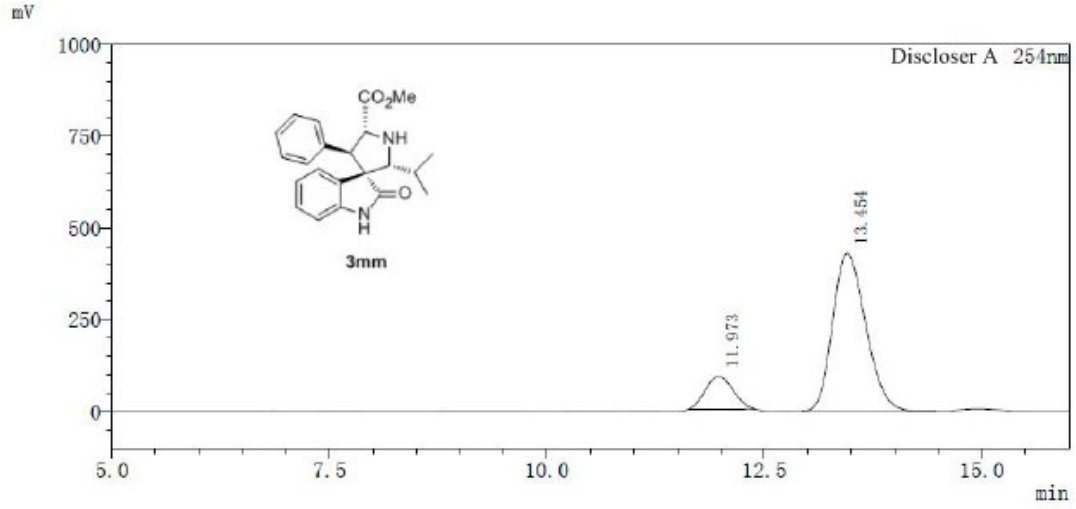
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	7.684	8.224
2	22.610	91.776
Total		100.000



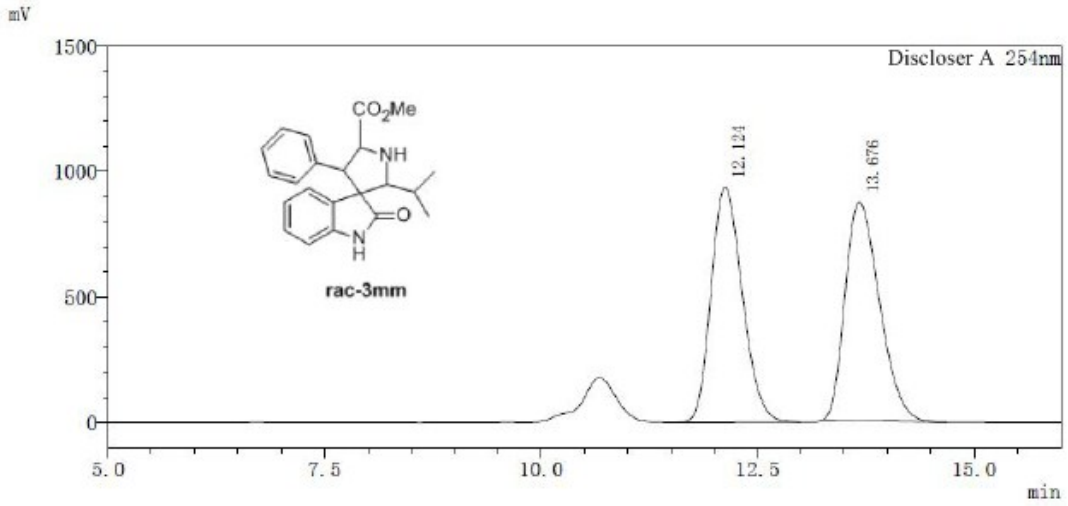
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	7.668	50.611
2	22.715	49.389
Total		100.000



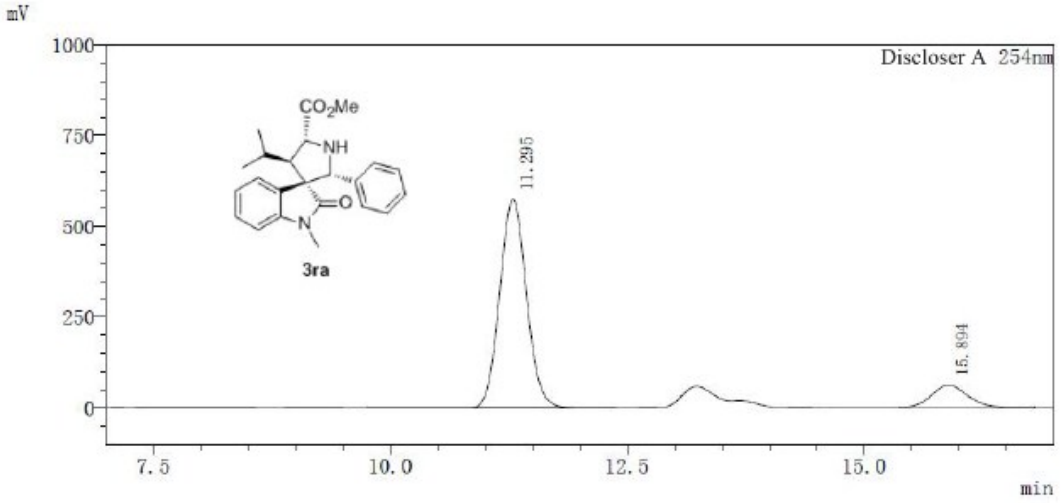
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	11.973	14.891
2	13.454	85.109
Total		100.000



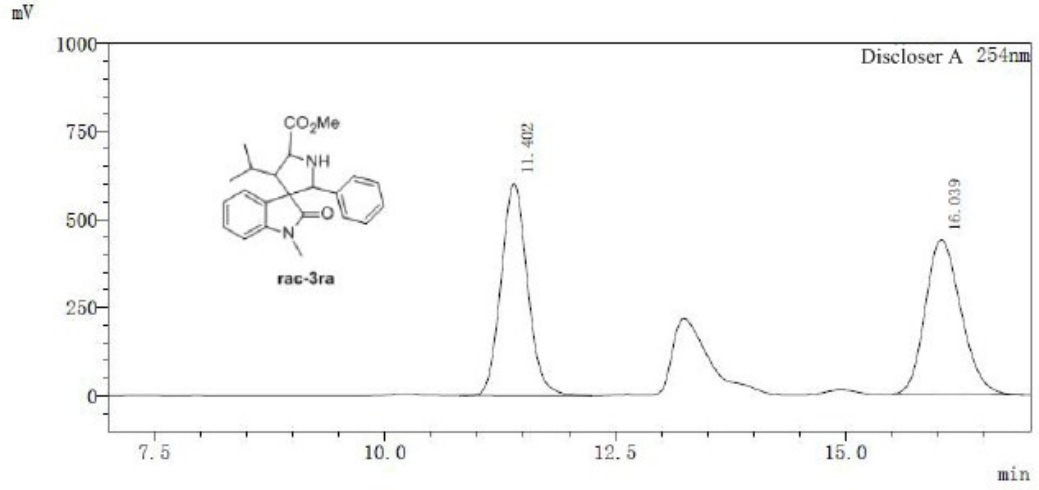
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	12.124	49.438
2	13.676	50.562
Total		100.000



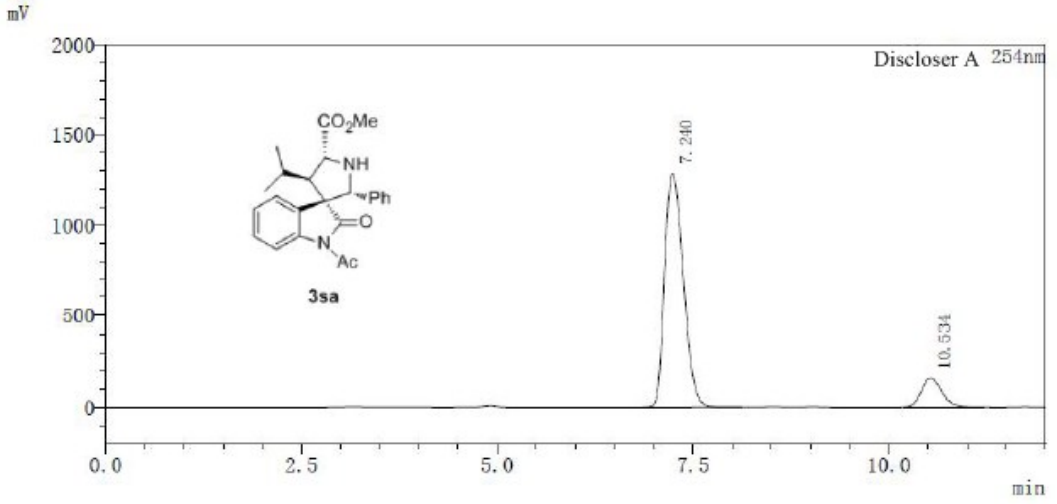
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	11.295	87.434
2	15.894	12.566
Total		100.000



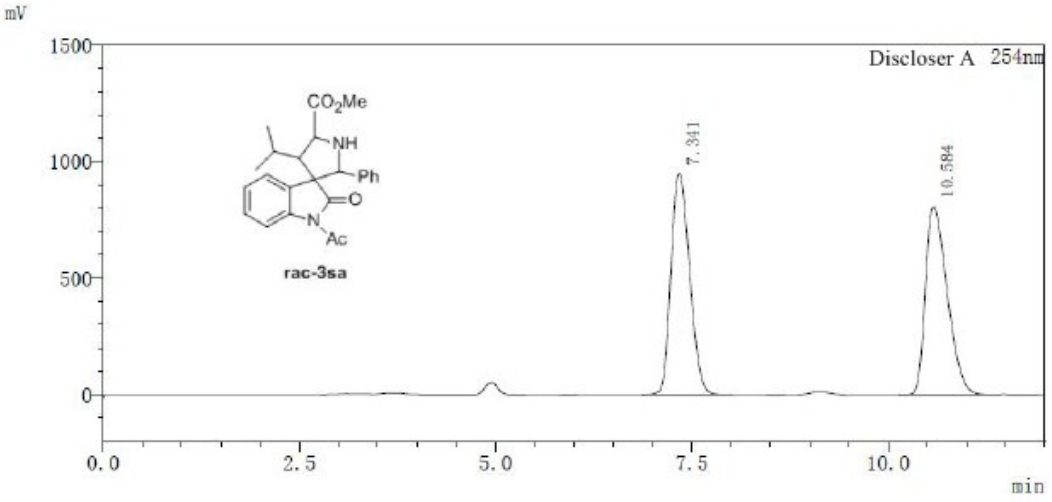
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	11.402	50.442
2	16.039	49.558
Total		100.000



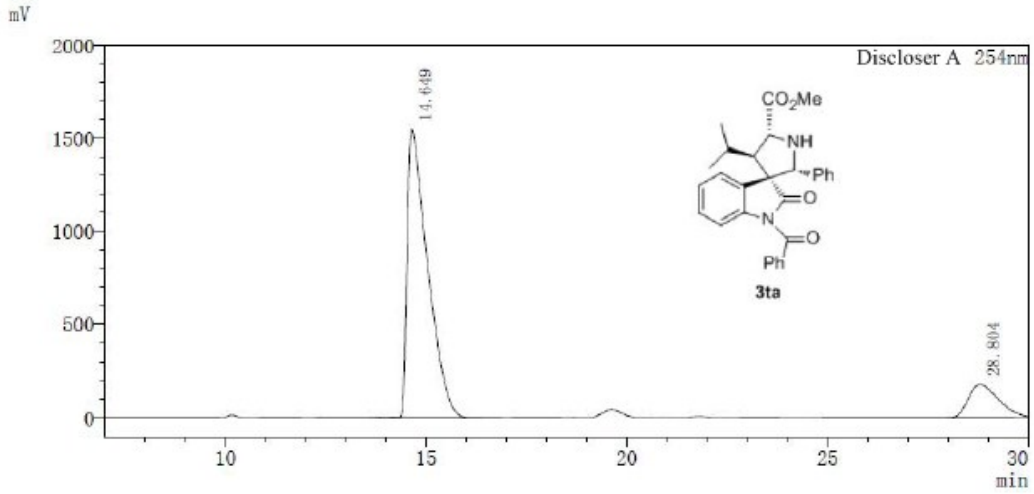
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	7.240	87.835
2	10.534	12.165
Total		100.000



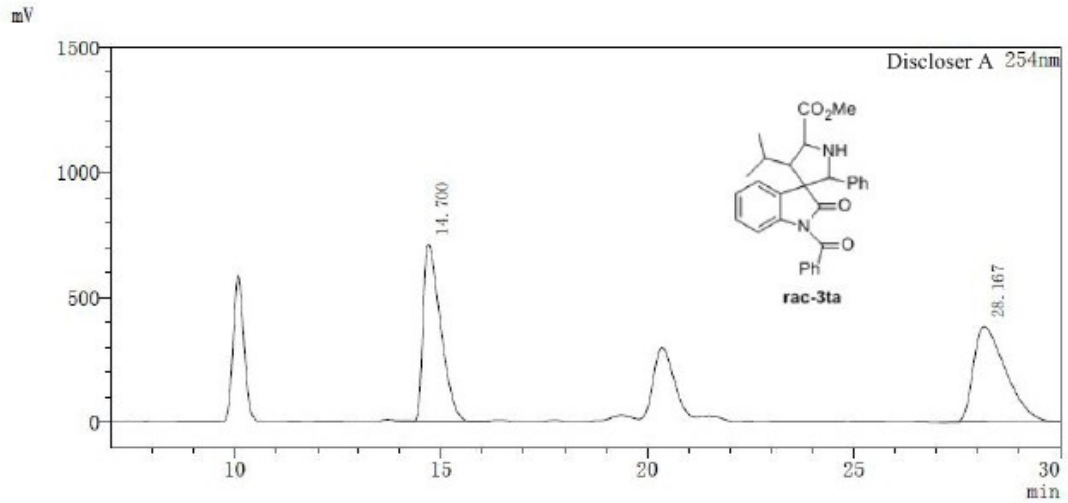
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	7.341	50.063
2	10.584	49.937
Total		100.000



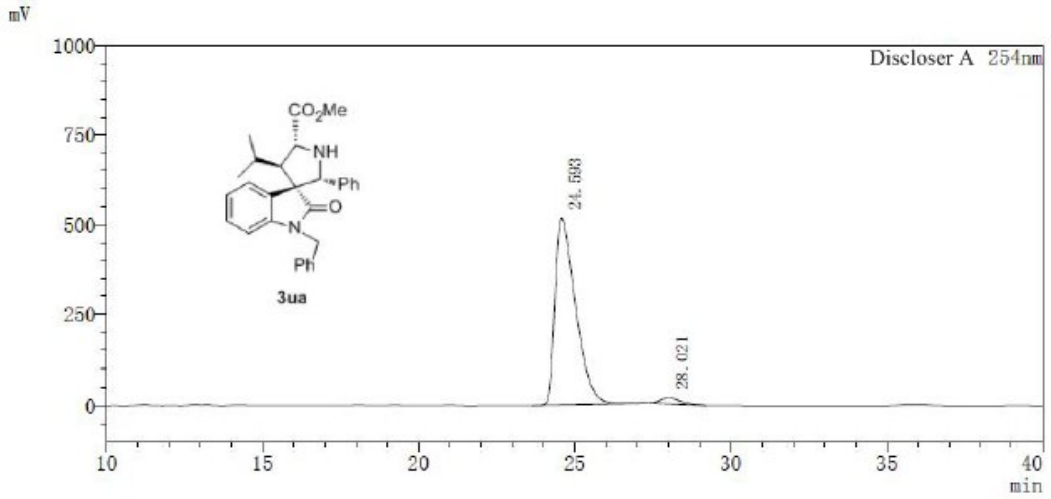
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	14.649	84.980
2	28.804	15.020
Total		100.000



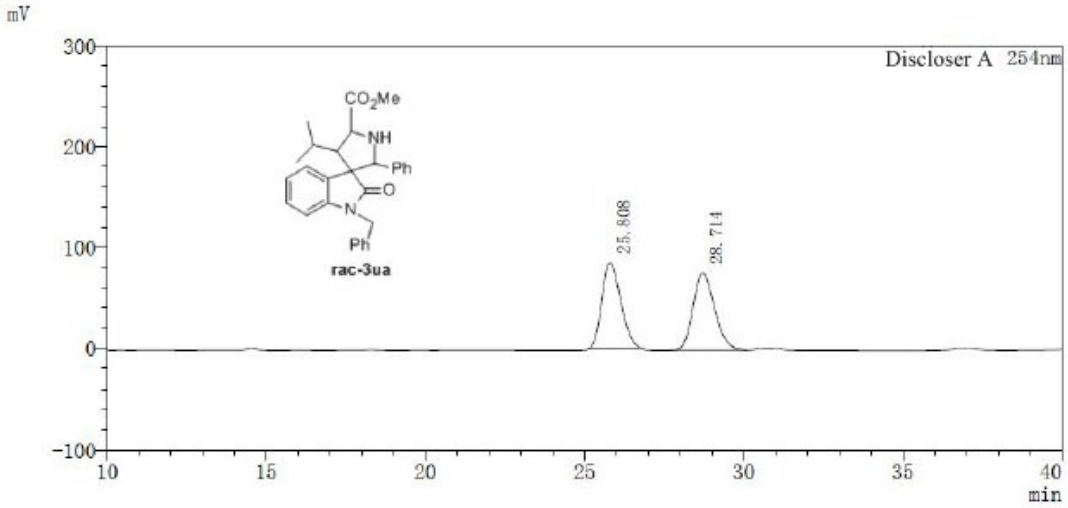
Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	14.700	49.903
2	28.167	50.097
Total		100.000



Discloser A 254 nm

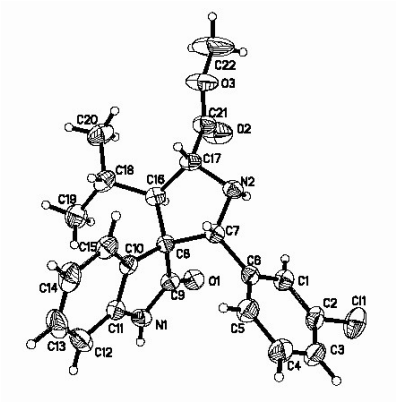
Peak	Reten time (min)	Area (%)
1	24.593	96.998
2	28.021	3.002
Total		100.000

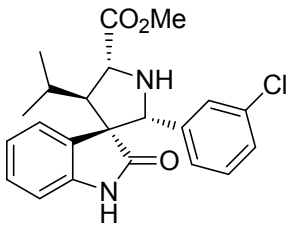


Discloser A 254 nm

Peak	Reten time (min)	Area (%)
1	25.808	49.512
2	28.714	50.488
Total		100.000

9. X-ray crystal structures





3ad

Table S3 Crystal data and structure refinement for 3ad (CCDC 1955469).

Identification code	201909229
Empirical formula	$C_{22}H_{23}ClN_2O_3$
Formula weight	398.87
Temperature/K	293(2)
Crystal system	monoclinic
Space group	C2
a/Å	24.1998(14)
b/Å	12.3700(6)
c/Å	9.5879(6)
α/°	90
β/°	119.944(8)
γ/°	90
Volume/Å^3	2487.0(3)
Z	4

ρ_{calc}g/cm^3	1.065
μ/mm^{-1}	1.526
F(000)	840.0
Crystal size/mm^3	0.17 × 0.12 × 0.09
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.434 to 134.126
Index ranges	-28 ≤ h ≤ 28, -13 ≤ k ≤ 14, -11 ≤ l ≤ 11
Reflections collected	17070
Independent reflections	4120 [R_{int} = 0.0281, R_{sigma} = 0.0257]
Data/restraints/parameters	4120/3/264
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0448, wR_2 = 0.1259
Final R indexes [all data]	R_1 = 0.0472, wR_2 = 0.1292
Largest diff. peak/hole / e Å^{-3}	0.25/-0.20
Flack parameter	0.000(18)

10. Energy, geometrical coordinates and vibrational frequencies of the optimized structures R1

Zero-point correction= 0.871945

Thermal correction to Energy= 0.924878

Thermal correction to Enthalpy= 0.925822

Thermal correction to Gibbs Free Energy= 0.785236

Sum of electronic and zero-point Energies= -4460.003288

Sum of electronic and thermal Energies= -4459.950355

Sum of electronic and thermal Enthalpies= -4459.949410

Sum of electronic and thermal Free Energies= -4460.089997

Cartesian coordinates

C	0.477545	0.182237	0.750986
C	0.357149	-0.486473	3.053787
C	1.175078	0.165783	1.902161
C	-1.057793	0.065939	2.794491
H	-1.809325	-0.373092	3.457892
H	-1.102396	1.158380	2.856650
C	-0.618231	-2.197991	1.665534
C	0.211103	-1.985575	2.713603
C	0.884841	-0.193839	4.445039
H	1.899397	-0.576362	4.596801
H	0.914409	0.885776	4.624429
H	0.238902	-0.642224	5.206222
C	1.033155	-2.986526	3.445962
H	0.615229	-3.212373	4.435510
H	1.116788	-3.930149	2.900906
H	2.043952	-2.601756	3.627613
C	-0.960819	-3.443505	0.984847
C	-1.189555	-3.440266	-0.402922
C	-1.086776	-4.667099	1.667907
C	-1.492895	-4.612090	-1.085083
H	-1.141119	-2.497812	-0.945864
C	-1.392227	-5.838754	0.983189
H	-0.973613	-4.690369	2.748191
C	-1.589561	-5.819936	-0.396511
H	-1.663420	-4.578248	-2.158436
H	-1.488579	-6.771188	1.533585

H	-1.830711	-6.736325	-0.928257
P	-1.200093	-0.535663	1.062766
C	2.554237	0.633675	2.127804
C	2.849254	2.002697	2.143523
C	3.592583	-0.281517	2.347235
C	4.152700	2.446117	2.352288
H	2.046268	2.721130	1.987110
C	4.895572	0.162327	2.545591
H	3.376392	-1.348104	2.326452
C	5.181282	1.527162	2.546470
H	4.365064	3.511971	2.356915
H	5.690959	-0.562058	2.699656
H	6.200667	1.870912	2.701275
C	0.886692	0.549654	-0.650427
H	0.314066	-0.121570	-1.308803
C	2.353910	0.318630	-0.939718
C	2.815172	-0.999685	-1.022923
C	3.277263	1.349229	-1.079540
C	4.162905	-1.270872	-1.209880
H	2.104766	-1.820686	-0.921888
C	4.633049	1.072902	-1.255235
H	2.937530	2.381010	-1.026390
C	5.108723	-0.238942	-1.314281
H	4.488848	-2.307457	-1.269617
H	5.324666	1.906628	-1.334565
N	0.443918	1.928351	-0.978543
H	0.299625	2.484799	-0.140464
S	-0.885536	2.177929	-2.007095
O	-1.854165	0.993474	-1.940040

C	-0.097034	1.975336	-3.697657
C	-1.232471	2.317671	-4.655496
H	-0.861264	2.269992	-5.684000
H	-2.060830	1.610090	-4.561883
H	-1.619601	3.328703	-4.488831
C	0.371271	0.547798	-3.903788
H	-0.408434	-0.169403	-3.626886
H	0.599313	0.397234	-4.964504
H	1.281363	0.326513	-3.338528
C	1.034811	2.981424	-3.791491
H	1.416822	2.995365	-4.817796
H	0.702702	3.997882	-3.551870
H	1.861099	2.719632	-3.124462
C	6.588076	-0.577628	-1.490617
C	7.045783	-1.493441	-0.347930
H	8.104240	-1.751913	-0.467275
H	6.928360	-1.000275	0.623296
H	6.479217	-2.429745	-0.317151
C	7.467260	0.671299	-1.479857
H	8.519267	0.386285	-1.585909
H	7.227408	1.351983	-2.303507
H	7.366945	1.227109	-0.540158
C	6.779726	-1.307778	-2.826192
H	6.200499	-2.236420	-2.864448
H	6.464232	-0.683589	-3.669448
H	7.834131	-1.566899	-2.977237
Cu	-2.692148	-0.054128	-0.324996
C	-4.959396	1.720924	0.713443
H	-6.032756	1.847345	0.898284

N	-4.555314	0.682200	0.012882
C	-5.448682	-0.189047	-0.523539
C	-4.919757	-1.260303	-1.260300
O	-3.691094	-1.456914	-1.463526
O	-5.847486	-2.109637	-1.773882
C	-5.318091	-3.224357	-2.483539
H	-4.728466	-3.872396	-1.826735
H	-6.180353	-3.774777	-2.861723
H	-4.685248	-2.908962	-3.318546
C	-4.089995	2.730873	1.257405
C	-4.633282	3.729182	2.095188
C	-2.706751	2.796438	0.985540
C	-3.836312	4.726893	2.638695
H	-5.699276	3.704961	2.314905
C	-1.914683	3.793240	1.534810
H	-2.279460	2.039015	0.332155
C	-2.467343	4.768292	2.367830
H	-4.284641	5.479805	3.282568
H	-0.849876	3.820740	1.306837
H	-1.843730	5.550392	2.791482
H	-6.520935	-0.061545	-0.385839

Vibrational frequencies

12.8807	15.7056	23.1477
28.4358	33.7473	37.8047
42.2244	51.0325	53.9785
56.0026	60.1946	67.0103
69.4935	73.2860	79.7877
81.8937	86.5359	88.2684
95.4657	104.4766	113.4181

120.2250	128.9712	132.6633
135.1942	143.9172	150.6084
159.8327	168.2484	178.2821
181.5508	189.4131	198.5504
199.8648	204.3080	221.5637
225.8263	228.1745	238.5763
240.6375	246.5607	250.3086
254.9633	261.9192	267.4012
273.0511	274.6641	281.8768
288.6761	291.0226	304.7014
305.9194	317.9791	324.0421
329.3780	335.0063	341.2551
349.1930	353.3309	360.2731
375.3434	378.0237	379.3887
384.7669	391.0467	402.9286
411.6398	414.2785	415.8508
424.8103	427.1935	430.5171
432.5528	434.9952	458.4146
473.5496	479.3620	485.6954
492.2861	507.0678	512.5963
518.6914	535.0228	546.8851
555.1385	560.1063	565.3495
575.1507	582.1852	614.6791
616.0047	625.8350	628.4243
637.3345	637.8273	651.2389
658.1742	666.1526	692.6941
700.2339	706.4636	713.8831
715.5126	718.7400	719.1155
722.5161	739.1402	748.9065

762.2214 764.9010 768.1833

770.6951 806.8805 818.2989

819.7400 832.9454 846.1357

847.9023 848.5568 857.0913

864.5627 865.0380 870.8615

871.4370 898.5095 903.0723

912.8002 916.3421 916.7315

924.1072 934.9190 938.3742

947.7614 952.1586 952.8975

956.2293 962.9608 964.9704

965.6923 968.8833 972.5343

973.1718 987.8590 989.6637

992.9386 996.3814 1009.7469

1013.3587 1014.7227 1016.3936

1022.1159 1022.5753 1030.9484

1031.7880 1033.9350 1040.4127

1043.2318 1046.8731 1053.0225

1055.9394 1056.5578 1061.1064

1061.2420 1080.6362 1098.1716

1102.9217 1110.3726 1111.1280

1121.7700 1134.3717 1136.2128

1161.3161 1166.1279 1166.7789

1166.8189 1167.9045 1184.6081

1186.7069 1195.0499 1196.5761

1197.2656 1197.8639 1203.8791

1207.7997 1214.9145 1231.9480

1234.5368 1242.0336 1242.5044

1253.2532 1268.5699 1271.5217

1296.8759 1297.2844 1298.1558

1313.6664	1319.8848	1326.6498
1332.7859	1336.3785	1342.7438
1345.7595	1372.8702	1377.8648
1379.7592	1382.2478	1385.8848
1388.2460	1391.8824	1396.2138
1398.2871	1399.9888	1402.9488
1407.2050	1418.1299	1439.6862
1440.4666	1443.7320	1457.6848
1458.7907	1460.0555	1463.4429
1464.0587	1464.9185	1467.7056
1469.4844	1469.8996	1470.5381
1472.7792	1474.9052	1475.5298
1476.1543	1476.8212	1481.7872
1483.6638	1487.0346	1492.6995
1492.9780	1493.8212	1500.8631
1506.4846	1525.5693	1526.5140
1531.8112	1546.2038	1562.5874
1614.5098	1623.0467	1625.3199
1628.6407	1646.9519	1654.4809
1656.9929	1665.1544	1668.8797
1669.4177	1693.2941	3038.6336
3045.1207	3049.5583	3051.8135
3051.9737	3056.5754	3057.8274
3059.1210	3059.6435	3061.8207
3084.5959	3087.6499	3124.5042
3139.0610	3139.6806	3141.1433
3146.4921	3148.8655	3149.5317
3150.6644	3152.0083	3152.2007
3152.4047	3152.6874	3158.6258

3162.3913	3167.3740	3167.9094
3168.2104	3169.8496	3171.1655
3175.2670	3175.9528	3177.4235
3177.4509	3180.2550	3184.2681
3189.6641	3191.1912	3193.7792
3194.3831	3197.0115	3198.1221
3198.3790	3198.4608	3202.0996
3207.6261	3216.8805	3217.2372
3217.5414	3217.6224	3564.2444

R2

Zero-point correction= 0.224402

Thermal correction to Energy= 0.236859

Thermal correction to Enthalpy= 0.237803

Thermal correction to Gibbs Free Energy= 0.185826

Sum of electronic and zero-point Energies= -594.840001

Sum of electronic and thermal Energies= -594.827545

Sum of electronic and thermal Enthalpies= -594.826601

Sum of electronic and thermal Free Energies= -594.878578

Cartesian coordinates

C	-1.891257	0.489778	-0.016976
C	-0.695578	-0.263812	-0.058820
C	-0.775898	-1.653915	-0.108429
C	-2.031476	-2.266354	-0.136749
C	-3.196225	-1.500043	-0.106825
C	-3.142836	-0.105434	-0.041353
C	-0.209132	2.053202	0.077451
C	0.407253	0.690386	-0.017387
H	0.121783	-2.265271	-0.115988

H	-2.099067	-3.349361	-0.177255
H	-4.164822	-1.992232	-0.127364
H	-4.048678	0.492693	-0.008906
O	0.345186	3.141035	0.145947
N	-1.576929	1.841943	0.058493
C	1.745327	0.547746	-0.073591
H	2.322691	1.473529	-0.009215
C	2.514827	-0.727598	-0.192557
H	1.938866	-1.420452	-0.822063
C	2.674791	-1.376130	1.186963
H	3.208916	-2.328618	1.105397
H	3.249204	-0.727823	1.857626
H	1.704872	-1.568060	1.656604
C	3.870549	-0.492678	-0.846547
H	4.419159	-1.432687	-0.961587
H	3.769638	-0.040658	-1.838106
H	4.486628	0.178035	-0.236498
H	-2.254244	2.588136	0.109246

Vibrational frequencies

53.8357	86.4030	107.2821
127.9128	149.7500	232.4101
252.8081	260.8507	270.9847
305.5839	349.7837	383.0777
417.2738	422.2194	482.1674
502.0613	529.3505	592.9270
599.8555	632.2863	678.8152
734.2257	757.3911	760.7563
788.5106	862.3648	865.2899
896.4909	906.2556	929.8143

930.4665	967.6863	978.7197
979.9927	999.6872	1057.2688
1118.8672	1132.3731	1157.1160
1171.2440	1196.1151	1206.9183
1229.1559	1267.7348	1299.7262
1319.4821	1345.9577	1370.4913
1380.5564	1395.1481	1407.6604
1445.9610	1464.4009	1469.2434
1480.0891	1486.7194	1506.6475
1522.2724	1648.5952	1675.4839
1730.5435	1824.4846	3048.7498
3052.1702	3059.4344	3138.3592
3148.9180	3149.1689	3153.1326
3155.8466	3194.6069	3198.6179
3210.0443	3224.6195	3662.0621

PreR

Zero-point correction= 1.097339

Thermal correction to Energy= 1.163651

Thermal correction to Enthalpy= 1.164596

Thermal correction to Gibbs Free Energy= 0.997280

Sum of electronic and zero-point Energies= -5054.865591

Sum of electronic and thermal Energies= -5054.799279

Sum of electronic and thermal Enthalpies= -5054.798334

Sum of electronic and thermal Free Energies= -5054.965650

Cartesian coordinates

C	1.551942	-0.232167	-0.639162
C	1.200544	0.572412	-2.871577
C	2.090054	-0.221730	-1.874574

C	-0.214029	0.124456	-2.452731
H	-1.007411	0.644729	-2.996140
H	-0.368073	-0.954770	-2.548344
C	0.574532	2.278919	-1.284192
C	1.240552	2.054902	-2.440481
C	1.508997	0.325602	-4.335730
H	2.522366	0.635731	-4.610214
H	1.419119	-0.739105	-4.573439
H	0.807220	0.870572	-4.974757
C	2.056115	3.024523	-3.219854
H	1.543598	3.346847	-4.135549
H	2.294436	3.921850	-2.643315
H	2.997833	2.568978	-3.547633
C	0.435115	3.505228	-0.504179
C	0.345292	3.434986	0.897472
C	0.327485	4.771868	-1.106485
C	0.182379	4.580515	1.666730
H	0.372060	2.460973	1.382457
C	0.164263	5.917793	-0.334965
H	0.329450	4.850146	-2.190365
C	0.095328	5.830086	1.054553
H	0.110507	4.493319	2.748064
H	0.073549	6.884357	-0.824032
H	-0.039557	6.726739	1.653520
P	-0.078762	0.640965	-0.694441
C	3.353043	-0.854482	-2.288046
C	3.485065	-2.248269	-2.218652
C	4.442541	-0.100471	-2.748321
C	4.673310	-2.872096	-2.587380

H	2.642110	-2.841965	-1.869277
C	5.635220	-0.723851	-3.101171
H	4.361874	0.984089	-2.792998
C	5.755177	-2.110777	-3.022970
H	4.755298	-3.954036	-2.526930
H	6.474755	-0.123059	-3.440666
H	6.686639	-2.594852	-3.304126
C	2.150070	-0.669110	0.673550
H	1.696645	-0.011530	1.431524
C	3.645426	-0.446675	0.738560
C	4.106386	0.874399	0.742711
C	4.584098	-1.472244	0.748405
C	5.464364	1.154478	0.719539
H	3.382917	1.690296	0.745201
C	5.949670	-1.186818	0.710505
H	4.245776	-2.505931	0.750303
C	6.420867	0.127088	0.681555
H	5.789863	2.192930	0.722067
H	6.649807	-2.016995	0.687124
N	1.740318	-2.048915	1.031269
H	1.427033	-2.569145	0.215621
S	0.549337	-2.245445	2.241722
O	-0.283443	-0.968959	2.357606
C	1.601402	-2.205066	3.792882
C	0.594224	-2.425405	4.915597
H	1.126908	-2.473342	5.870739
H	-0.128964	-1.607296	4.971031
H	0.044743	-3.365620	4.795402
C	2.290335	-0.862310	3.937759

H	1.582847	-0.036449	3.807051
H	2.709712	-0.782986	4.946407
H	3.115726	-0.744660	3.229548
C	2.584222	-3.357185	3.693237
H	3.141284	-3.437351	4.632721
H	2.077648	-4.314675	3.529529
H	3.303368	-3.202431	2.883925
C	7.907029	0.475423	0.615379
C	8.164471	1.399065	-0.581972
H	9.226594	1.663494	-0.637977
H	7.889486	0.911644	-1.523602
H	7.596958	2.332199	-0.511319
C	8.780554	-0.766921	0.452426
H	9.833304	-0.474234	0.377665
H	8.692118	-1.451275	1.303109
H	8.525862	-1.324192	-0.456662
C	8.314723	1.203873	1.901878
H	7.736122	2.122848	2.044759
H	8.160760	0.572518	2.783887
H	9.374985	1.480458	1.868688
Cu	-1.336940	0.195731	0.921024
C	-3.614610	-1.867673	0.902395
H	-4.637055	-2.129493	1.203468
N	-3.132714	-0.701317	1.272385
C	-3.884127	0.150962	2.014771
C	-3.263283	1.338690	2.432977
O	-2.052901	1.629457	2.229574
O	-4.068831	2.196937	3.113153
C	-3.435920	3.397808	3.546011

H	-3.022786	3.960714	2.702752
H	-4.212585	3.984029	4.038675
H	-2.625757	3.192769	4.252748
C	-2.921242	-2.842487	0.100212
C	-3.619659	-4.001248	-0.302767
C	-1.587485	-2.706094	-0.338921
C	-3.027248	-4.955755	-1.117703
H	-4.651139	-4.127599	0.025298
C	-1.002786	-3.658147	-1.160999
H	-1.029933	-1.827311	-0.021649
C	-1.713697	-4.790812	-1.562547
H	-3.594116	-5.835261	-1.413899
H	0.024111	-3.514758	-1.496936
H	-1.251339	-5.534814	-2.205352
C	-6.078073	-1.526447	-1.381601
C	-5.842512	-0.213460	-0.908662
C	-6.719193	0.334577	0.024797
C	-7.798399	-0.429755	0.480534
C	-8.003902	-1.724767	0.005296
C	-7.143773	-2.294128	-0.938472
C	-4.153733	-0.856881	-2.437050
C	-4.622569	0.254622	-1.552590
H	-6.572968	1.343484	0.401651
H	-8.483974	-0.008213	1.209630
H	-8.848914	-2.303348	0.369142
H	-7.301882	-3.301908	-1.312286
H	-4.980499	-2.776353	-2.716005
O	-3.171035	-0.901145	-3.165151
N	-5.093517	-1.863427	-2.301235

C	-3.919097	1.401036	-1.462260
H	-3.015239	1.446933	-2.077389
C	-4.269320	2.630306	-0.685254
H	-4.684225	2.321645	0.285217
C	-5.347918	3.426209	-1.427115
H	-5.638679	4.311222	-0.851345
H	-4.980924	3.768598	-2.401255
H	-6.245730	2.824466	-1.601840
C	-3.028136	3.475215	-0.437896
H	-3.267962	4.391550	0.112903
H	-2.279172	2.921731	0.137891
H	-2.571021	3.775016	-1.389895
H	-4.915628	-0.081050	2.275718

Vibrational frequencies

-6.6808	18.3567	21.6328
25.5081	29.0534	31.8122
37.8198	41.0314	44.7743
46.4595	49.8981	53.6084
54.4116	57.9727	65.9278
68.9044	69.3851	73.7518
74.7053	78.2076	81.1806
82.0456	87.7372	91.1835
93.2278	98.9854	101.6001
107.6682	114.6650	119.0910
122.9041	124.6428	132.4805
140.7409	148.6058	151.0931
155.1636	159.5638	165.4972
167.8919	171.3952	177.5719
183.5870	189.8180	199.7815

202.4352	212.2432	214.6719
219.8552	224.4074	237.9655
238.7025	246.0970	252.2181
254.8421	255.8517	256.5088
263.9624	268.0596	272.3267
274.2647	283.3198	285.5341
287.9234	301.0479	307.3947
319.6655	323.2176	326.7400
327.8454	329.7475	332.4102
333.0745	337.8023	341.3761
345.9008	356.1791	360.5412
365.0544	371.7614	373.6330
384.4420	393.1330	408.4734
411.8795	414.2258	422.0198
423.0104	424.4034	425.8503
429.1761	431.1779	436.3711
440.5868	455.8549	472.0130
481.6169	487.9950	493.4688
503.3414	507.6094	507.9042
512.7205	526.0925	531.0663
548.1737	558.3715	559.3849
565.7345	579.7804	582.9247
594.9154	597.7695	608.5670
610.9650	617.8282	628.3283
630.1516	636.0460	637.2353
639.9194	652.8214	660.1129
667.7728	681.8163	701.5868
706.4972	707.2440	711.6339
716.3439	720.5492	721.5212

723.5948	733.2643	735.9235
752.6696	756.1066	761.8257
766.1433	767.2986	768.8595
772.7843	787.6478	811.3730
818.1061	819.8589	838.0254
842.6769	850.3434	855.1981
856.3715	859.3436	862.6356
865.3432	866.2076	871.5816
895.7672	898.4099	900.5824
903.4418	906.4864	909.8326
914.6314	918.0947	919.2787
922.9541	933.4932	939.8750
940.3874	946.5626	952.3368
952.7721	958.9477	961.4005
963.3419	964.4901	968.2342
969.6220	974.5024	976.4720
983.6774	987.6230	990.4577
990.8955	992.9561	996.8610
1002.2521	1012.2341	1014.5102
1015.0490	1017.1289	1021.5699
1031.9889	1033.0129	1034.8404
1038.9698	1039.7242	1042.3643
1044.3851	1051.2916	1052.7481
1055.8728	1056.3794	1059.7872
1063.0316	1077.5354	1096.9958
1103.9380	1112.6405	1113.8896
1116.4012	1117.3146	1128.4843
1134.0547	1140.0201	1157.0805
1157.9897	1164.6448	1167.3983

1167.4806	1169.9873	1173.6446
1178.7394	1190.2164	1192.6244
1192.7968	1192.8144	1195.1701
1197.4486	1199.2458	1202.7243
1207.9506	1218.2330	1232.1757
1232.6015	1234.5119	1239.3167
1240.3144	1254.7046	1269.3043
1269.9032	1270.7645	1292.7410
1296.4848	1298.5325	1300.8096
1310.0450	1316.9588	1318.6217
1324.2383	1328.2446	1341.7603
1345.3197	1347.1639	1350.1880
1373.1306	1375.2622	1376.8455
1380.9312	1380.9847	1383.8084
1384.1887	1387.3167	1390.3021
1392.7551	1393.4941	1395.0663
1395.9556	1401.9348	1405.9114
1411.1495	1411.6767	1433.2089
1435.8501	1443.7533	1449.1798
1450.3834	1453.4686	1454.0707
1457.1938	1458.6527	1461.5179
1464.8765	1464.9784	1466.6037
1467.6591	1468.7559	1470.3505
1470.8648	1471.7015	1471.9641
1474.7644	1478.0078	1478.6984
1479.3613	1481.3511	1481.6772
1481.8756	1490.2336	1491.9066
1495.6037	1497.1142	1502.8721
1504.6521	1521.9055	1524.4796

1528.3158	1528.6374	1543.7937
1562.9674	1616.6029	1623.1675
1627.1921	1627.2329	1643.8222
1645.3295	1653.2042	1654.4943
1661.1237	1669.1630	1669.8675
1675.4132	1692.1977	1721.4134
1815.3889	3032.9247	3044.0025
3044.4756	3045.6395	3046.7690
3049.3692	3054.5030	3054.6222
3055.6822	3058.9664	3061.5087
3061.6112	3062.2698	3079.4650
3096.0865	3120.1826	3125.2521
3134.5599	3137.6698	3138.4841
3141.2777	3144.9773	3145.6019
3146.8249	3148.2650	3151.6816
3153.8061	3154.2179	3154.4107
3154.6713	3155.0246	3155.2880
3159.0143	3161.2294	3161.6103
3163.7313	3168.9593	3169.8155
3171.4202	3171.4999	3171.7785
3174.0560	3179.6279	3184.4089
3186.4521	3187.8357	3188.8170
3189.6006	3191.4827	3191.8718
3193.5399	3194.7493	3198.9448
3200.7089	3203.4150	3207.6536
3208.0188	3211.9531	3213.0336
3218.6900	3220.2466	3220.4645
3224.9295	3567.3463	3678.4951

PreS

Zero-point correction= 1.098629

Thermal correction to Energy= 1.165153

Thermal correction to Enthalpy= 1.166097

Thermal correction to Gibbs Free Energy= 0.998294

Sum of electronic and zero-point Energies= -5054.851475

Sum of electronic and thermal Energies= -5054.784951

Sum of electronic and thermal Enthalpies= -5054.784006

Sum of electronic and thermal Free Energies= -5054.951810

Cartesian coordinates

C	-1.899403	-1.070978	-0.130579
C	-2.553663	-2.072771	-2.226127
C	-2.959992	-1.464407	-0.867656
C	-1.336330	-1.217347	-2.615392
H	-0.826726	-1.581654	-3.513331
H	-1.596288	-0.160286	-2.741535
C	-0.710984	-3.337419	-1.339379
C	-1.931528	-3.443596	-1.914540
C	-3.643969	-2.103327	-3.281474
H	-4.533027	-2.651718	-2.954276
H	-3.961729	-1.089244	-3.542397
H	-3.273475	-2.577247	-4.196170
C	-2.743366	-4.671016	-2.135584
H	-2.793786	-4.952057	-3.195223
H	-2.354421	-5.529812	-1.583974
H	-3.779996	-4.501144	-1.818189
C	0.181707	-4.417465	-0.926743
C	0.232321	-5.641122	-1.622692
C	1.035474	-4.252962	0.175686

C	1.059711	-6.673477	-1.194203
H	-0.358373	-5.771367	-2.525341
C	1.856467	-5.289231	0.605209
H	1.064446	-3.290619	0.680503
C	1.866620	-6.509314	-0.069027
H	1.082786	-7.607326	-1.750292
H	2.502520	-5.134145	1.467058
H	2.511935	-7.317832	0.264965
P	-0.354133	-1.514262	-1.082426
C	-4.368577	-1.443497	-0.424382
C	-5.315625	-0.586021	-1.002080
C	-4.773983	-2.285880	0.620563
C	-6.625178	-0.559613	-0.532892
H	-5.009818	0.089959	-1.798080
C	-6.088042	-2.267396	1.080695
H	-4.045486	-2.960460	1.068150
C	-7.015589	-1.398695	0.509915
H	-7.343538	0.123364	-0.978940
H	-6.385365	-2.928161	1.890855
H	-8.039223	-1.376527	0.873628
C	-2.033415	-0.369318	1.211440
H	-2.427620	-1.075759	1.950585
C	-3.020966	0.779064	1.109016
C	-4.118884	0.875048	1.956875
C	-2.838033	1.771421	0.139803
C	-5.039683	1.913061	1.817118
H	-4.282537	0.105184	2.709402
C	-3.747090	2.811525	0.012846
H	-1.980745	1.711232	-0.532820

C	-4.880913	2.896351	0.836960
H	-5.901764	1.934698	2.477676
H	-3.583210	3.566373	-0.754781
N	-0.824419	0.247217	1.801972
H	-0.489364	1.020862	1.229461
S	0.560093	-0.422982	2.506640
O	1.340796	-1.370185	1.608675
C	-0.200342	-1.543107	3.809700
C	0.970214	-1.819508	4.751595
H	0.646661	-2.504807	5.541819
H	1.804079	-2.291050	4.221849
H	1.335719	-0.904588	5.229636
C	-0.655840	-2.852621	3.185194
H	0.187161	-3.373616	2.724282
H	-1.060926	-3.498228	3.972593
H	-1.429220	-2.738219	2.420368
C	-1.298738	-0.792324	4.542750
H	-0.952624	0.185231	4.893820
H	-2.187112	-0.629516	3.927542
H	-1.601549	-1.369597	5.423731
C	-5.883845	4.027287	0.620936
C	-6.393259	3.982487	-0.825709
H	-7.125863	4.779110	-0.998237
H	-5.583357	4.118354	-1.549398
H	-6.879555	3.025556	-1.046005
C	-5.190007	5.373384	0.864602
H	-5.887096	6.202308	0.697044
H	-4.817223	5.449157	1.891814
H	-4.338639	5.515141	0.190489

C	-7.086493	3.916070	1.555591
H	-7.629978	2.975741	1.406778
H	-6.797172	3.975400	2.610321
H	-7.785936	4.735605	1.359953
Cu	1.550445	-0.648061	-0.694211
C	3.087541	1.418695	-2.440941
H	4.069679	1.804822	-2.742493
N	3.045603	0.256797	-1.812960
C	4.201018	-0.428623	-1.647336
C	4.133081	-1.644844	-0.938480
O	3.102776	-2.086156	-0.386440
O	5.303457	-2.342744	-0.905971
C	5.223789	-3.609059	-0.255811
H	4.567966	-4.292580	-0.804505
H	6.240666	-4.003043	-0.242874
H	4.847826	-3.515523	0.767717
C	1.958184	2.226246	-2.816367
C	0.616551	1.859926	-2.583846
C	2.196903	3.466034	-3.447975
C	-0.426567	2.693520	-2.960108
H	0.438774	0.921860	-2.066629
C	1.149931	4.300113	-3.816088
H	3.225982	3.765857	-3.640757
C	-0.172907	3.922488	-3.575987
H	-1.454005	2.383374	-2.773565
H	1.364015	5.251105	-4.298212
H	-0.993658	4.571554	-3.868968
C	3.119261	4.274637	0.315572
C	4.123590	3.398658	0.790770

C	5.379754	3.918740	1.097329
C	5.612114	5.285364	0.926340
C	4.607944	6.126114	0.444551
C	3.340757	5.629777	0.128413
C	2.153385	2.210891	0.347211
C	3.540325	2.063679	0.822164
H	6.176221	3.274594	1.459762
H	6.588704	5.696419	1.164780
H	4.811541	7.184547	0.308869
H	2.556911	6.279056	-0.250996
O	1.277149	1.332466	0.232792
N	1.956047	3.543053	0.091146
C	4.006962	0.849439	1.199737
H	3.304818	0.018209	1.084514
C	5.325674	0.557715	1.841045
H	5.547859	1.389617	2.527409
C	6.471301	0.488876	0.824946
H	7.435842	0.449027	1.343190
H	6.382168	-0.408299	0.204566
H	6.479106	1.357830	0.159039
C	5.236349	-0.732250	2.647246
H	6.182167	-0.958457	3.149582
H	4.450724	-0.678083	3.408835
H	4.993846	-1.574397	1.987080
H	5.132349	-0.081777	-2.094234
H	1.109196	3.908363	-0.321275

Vibrational frequencies

16.9967	20.0143	25.4807
26.6166	28.2238	35.2312

36.3183	39.9172	44.6020
46.4462	47.7641	55.2420
59.8606	61.0852	68.9272
71.6367	74.3392	78.5123
80.1998	84.7104	87.2583
93.8057	99.5778	100.7724
104.3684	106.7925	113.5537
115.7396	122.7511	128.1959
133.7862	136.2319	140.8191
143.3476	148.4610	154.4204
162.4966	163.9669	165.7735
171.3536	178.1560	186.7060
190.7942	205.6682	207.0673
216.7232	227.5450	229.6853
231.1243	244.3510	249.0804
253.6213	257.4585	261.1483
262.0149	263.7144	270.2030
279.8102	284.5369	288.0681
291.3082	292.2355	293.7328
298.1923	308.9416	317.8085
322.3666	323.7048	328.5966
331.9356	333.7830	338.4267
340.9705	341.8336	346.0400
353.2408	355.6136	365.4488
366.4147	376.9009	377.6828
389.5083	393.5254	396.8207
414.9485	415.3508	418.3621
424.9347	425.9689	427.0315
430.5608	435.6375	442.3128

452.6246	457.0798	467.7617
471.7712	473.1450	485.1354
501.3021	503.7238	512.8427
520.3772	521.8983	529.7167
538.1815	543.0848	558.4706
568.8104	577.1184	579.9232
581.3977	594.1199	600.3816
613.3404	621.2009	628.3784
630.1460	636.1008	638.0230
647.7696	651.5760	665.4128
668.2288	680.2827	690.8181
708.0591	711.1272	715.7592
721.2734	721.6744	726.7396
731.8881	737.6041	755.0664
758.4695	762.0697	764.7149
765.4667	767.4267	773.8799
779.1778	786.1538	800.1815
809.3739	813.8239	829.1189
843.4788	854.0388	859.3976
859.6123	861.7783	864.1274
865.4741	870.7838	870.8450
872.3525	895.5591	898.1097
900.0544	908.2060	911.5901
912.3730	924.0531	925.0676
930.8899	932.9024	936.0968
938.7259	952.2044	952.9789
953.9382	956.6148	962.0753
964.3463	967.9857	972.0240
973.4459	975.3856	976.8969

979.7368	982.1819	987.8304
990.5388	997.3747	1002.5754
1003.3523	1003.4378	1010.4585
1012.9038	1016.0796	1017.9381
1020.0702	1030.6672	1035.5739
1037.3681	1039.2462	1044.4103
1045.4505	1051.3730	1051.7556
1054.0153	1058.6681	1061.0167
1064.6605	1083.7689	1104.8575
1111.5296	1112.0067	1114.2700
1119.7527	1125.3621	1127.6489
1134.5800	1151.2075	1155.4649
1159.9140	1165.3748	1166.3758
1166.8965	1171.9651	1175.2221
1189.9022	1191.8228	1194.9713
1195.1301	1198.0364	1202.9883
1204.4176	1205.6236	1209.1304
1211.3555	1221.8836	1222.4948
1228.5339	1234.4123	1240.0163
1240.0767	1258.6373	1270.4718
1271.4383	1271.9767	1274.9204
1294.7775	1299.5946	1300.4347
1306.1318	1312.6529	1318.5831
1320.6281	1328.4397	1338.7698
1342.0359	1344.0379	1347.8729
1366.5619	1371.1952	1381.1303
1382.1153	1382.4993	1383.3348
1386.6857	1387.5233	1388.5743
1390.5576	1390.9478	1397.9160

1399.4913	1404.9069	1408.2150
1409.2530	1410.7245	1438.9213
1439.2785	1445.3348	1445.8251
1448.0924	1451.9604	1452.2760
1457.8763	1463.5470	1464.3661
1464.6374	1466.7316	1468.2055
1470.1846	1472.4642	1472.6343
1476.0416	1476.0864	1478.8295
1480.1243	1483.2035	1483.2520
1484.2873	1484.6171	1486.0513
1493.3554	1493.6418	1495.8893
1497.3956	1497.9676	1504.8333
1510.8181	1521.5251	1526.3764
1529.4317	1531.6220	1554.3322
1560.3509	1616.2595	1624.3523
1624.8985	1631.0305	1642.3038
1642.7963	1648.5481	1657.6293
1661.2161	1663.9061	1673.3949
1674.2796	1678.9961	1714.9471
1805.9734	3016.4054	3039.5977
3042.0329	3042.6085	3047.6850
3047.9611	3052.3444	3052.5749
3053.1241	3056.3423	3057.1051
3058.5785	3062.9345	3086.9595
3091.0519	3124.7831	3130.6096
3135.3238	3139.5571	3143.9348
3144.4690	3145.9089	3147.0655
3147.2741	3148.1086	3148.9256
3152.7540	3154.2507	3155.4448

3158.5651	3160.7307	3161.0609
3162.4659	3163.1719	3169.2159
3171.8386	3173.3781	3173.8434
3174.4257	3175.5028	3177.1707
3181.6891	3182.7472	3184.6114
3186.9135	3192.7964	3193.6964
3194.7910	3195.4943	3197.3483
3198.0317	3199.0313	3200.1634
3201.1638	3205.3447	3205.3570
3213.1570	3214.1705	3215.9379
3217.5383	3219.6974	3222.1788
3229.2935	3447.0828	3661.8032

TS1R

Zero-point correction= 1.097161

Thermal correction to Energy= 1.163377

Thermal correction to Enthalpy= 1.164321

Thermal correction to Gibbs Free Energy= 0.995675

Sum of electronic and zero-point Energies= -5054.848871

Sum of electronic and thermal Energies= -5054.782655

Sum of electronic and thermal Enthalpies= -5054.781711

Sum of electronic and thermal Free Energies= -5054.950357

Cartesian coordinates

C	1.793500	-0.224014	-0.674746
C	1.230015	0.452763	-2.906483
C	2.281863	-0.141682	-1.925723
C	-0.074632	-0.212976	-2.423089
H	-0.972078	0.158077	-2.922240
H	-0.041673	-1.306053	-2.494549

C	0.378881	2.070488	-1.341278
C	1.025964	1.931965	-2.520226
C	1.532163	0.213609	-4.373467
H	2.466081	0.688765	-4.690952
H	1.625436	-0.858043	-4.577330
H	0.725301	0.604431	-5.001113
C	1.617217	3.003728	-3.364423
H	1.055025	3.141423	-4.297004
H	1.645359	3.966206	-2.847581
H	2.639777	2.743370	-3.665067
C	0.051269	3.276348	-0.585861
C	0.139088	3.262184	0.817166
C	-0.381055	4.461600	-1.207050
C	-0.164305	4.391449	1.568381
H	0.440417	2.344353	1.319302
C	-0.687321	5.590503	-0.453269
H	-0.508694	4.481746	-2.286244
C	-0.577520	5.563627	0.936385
H	-0.083342	4.351591	2.651924
H	-1.027963	6.493009	-0.954509
H	-0.823268	6.445251	1.522040
P	0.039646	0.369039	-0.685553
C	3.624291	-0.526580	-2.400303
C	3.957323	-1.877621	-2.559502
C	4.580612	0.445396	-2.723031
C	5.221231	-2.249635	-3.009893
H	3.213773	-2.637884	-2.324373
C	5.845269	0.072165	-3.166195
H	4.335819	1.498266	-2.595072

C	6.171895	-1.275843	-3.307603
H	5.464935	-3.302859	-3.122478
H	6.579193	0.838947	-3.400177
H	7.161573	-1.564630	-3.651836
C	2.445574	-0.634427	0.616843
H	1.969103	-0.026536	1.402136
C	3.930762	-0.354263	0.661659
C	4.346142	0.980560	0.714704
C	4.903742	-1.346038	0.600365
C	5.693789	1.306907	0.682417
H	3.596903	1.771142	0.764801
C	6.258309	-1.013367	0.556530
H	4.600764	-2.389827	0.559301
C	6.683882	0.316295	0.587529
H	5.984834	2.354840	0.723461
H	6.985651	-1.816885	0.483444
N	2.102583	-2.046021	0.928004
H	1.826590	-2.555092	0.092991
S	0.970062	-2.394770	2.148675
O	0.026609	-1.206809	2.360565
C	2.051100	-2.342711	3.679260
C	1.096425	-2.706484	4.810405
H	1.656026	-2.748973	5.750247
H	0.304753	-1.960920	4.922333
H	0.631063	-3.686246	4.658393
C	2.623985	-0.952900	3.877195
H	1.843068	-0.187547	3.822232
H	3.077644	-0.893368	4.872326
H	3.406066	-0.723963	3.147435

C	3.128787	-3.395192	3.496040
H	3.712372	-3.475725	4.419009
H	2.705196	-4.383876	3.287503
H	3.811415	-3.130694	2.683714
C	8.155509	0.721762	0.525099
C	8.376994	1.649773	-0.675536
H	9.420162	1.983717	-0.713653
H	8.153945	1.134424	-1.616037
H	7.745177	2.542798	-0.626345
C	9.078224	-0.485160	0.369305
H	10.119624	-0.152145	0.307891
H	9.004954	-1.175407	1.216849
H	8.856939	-1.048249	-0.544945
C	8.530199	1.470504	1.810242
H	7.917802	2.368229	1.946128
H	8.395560	0.838291	2.694648
H	9.579376	1.786010	1.779460
Cu	-1.137525	-0.153996	0.974351
C	-3.701265	-1.776557	0.603161
H	-4.792976	-1.806563	0.689612
N	-3.050244	-0.751809	1.087634
C	-3.788393	0.320228	1.558744
C	-3.027306	1.198353	2.408985
O	-1.781816	1.238547	2.427852
O	-3.776872	2.010963	3.174708
C	-3.047841	2.993357	3.917630
H	-2.457464	3.629842	3.250632
H	-3.797937	3.589486	4.436407
H	-2.378764	2.520799	4.641273

C	-3.071353	-2.908460	-0.041119
C	-3.884833	-3.920189	-0.582559
C	-1.677514	-3.028673	-0.184463
C	-3.326300	-5.005803	-1.245564
H	-4.965548	-3.835371	-0.480431
C	-1.123142	-4.114461	-0.845886
H	-1.046822	-2.251866	0.244910
C	-1.941965	-5.108683	-1.384011
H	-3.972656	-5.775926	-1.658523
H	-0.041865	-4.190994	-0.946495
H	-1.504130	-5.957107	-1.902597
C	-6.510529	-1.199680	-1.660284
C	-6.328044	-0.110356	-0.761740
C	-7.365010	0.205592	0.121601
C	-8.553984	-0.529519	0.083350
C	-8.715580	-1.580983	-0.820605
C	-7.686431	-1.934731	-1.701153
C	-4.356145	-0.445889	-1.975017
C	-4.988250	0.385375	-0.952927
H	-7.249204	1.019462	0.835381
H	-9.361809	-0.278306	0.765994
H	-9.647493	-2.140096	-0.838956
H	-7.801546	-2.763924	-2.395225
H	-5.180137	-2.075409	-3.072331
O	-3.229516	-0.390928	-2.478018
N	-5.342069	-1.363606	-2.377108
C	-4.270099	1.353581	-0.241356
H	-3.238233	1.449926	-0.602067
C	-4.857944	2.653288	0.284470

H	-5.377770	2.460536	1.234662
C	-5.872145	3.249980	-0.691746
H	-6.259695	4.201215	-0.309579
H	-5.404323	3.450056	-1.662537
H	-6.722706	2.585858	-0.866234
C	-3.744893	3.669275	0.530716
H	-4.104519	4.537316	1.094505
H	-2.892110	3.245496	1.069917
H	-3.355987	4.035345	-0.427359
H	-4.834772	0.156082	1.828268

Vibrational frequencies

-374.0912	15.0411	17.3105
19.7132	23.5366	28.3978
32.3494	34.3887	36.7743
39.6849	44.5846	47.8592
54.4813	56.4917	58.8901
61.8898	63.2577	70.1273
71.1341	78.0443	79.7078
85.1604	91.2930	92.3069
99.3073	103.2881	105.6335
113.5825	119.8231	124.3717
127.9191	129.8316	140.2513
144.0665	148.6096	151.2277
154.2629	160.8107	168.9023
169.6290	180.8833	187.3901
191.5203	191.8365	208.2367
210.6055	212.3046	222.6334
226.2686	229.2766	238.5712
245.3856	247.7518	249.9949

256.3304 262.1116 270.0400

272.7588 275.6377 276.9126

278.8236 280.7396 289.4635

293.6892 298.7092 300.4455

308.7488 313.4507 318.7599

326.7158 328.8193 335.5181

342.7322 345.3830 351.1513

356.2428 359.4074 362.0158

364.0093 372.3852 375.9892

383.4524 400.7116 408.4156

414.1861 415.2892 421.5245

421.7838 424.5964 424.8093

427.3350 429.7072 431.4459

445.5905 458.8607 472.9047

473.8353 487.4231 488.6124

496.4991 506.1627 508.3383

512.1828 520.8401 527.0651

533.6561 549.5658 555.7537

558.0755 565.4675 575.9351

582.4103 593.2086 596.2171

611.6453 616.2528 627.2741

628.9026 630.3463 631.6939

638.3101 653.6943 661.3683

668.1966 681.5475 702.3607

707.0019 714.8836 715.3651

716.8487 723.8999 725.0418

734.1517 741.6605 745.8611

749.0654 763.4992 765.8704

768.3524 770.6587 773.0577

774.8186	809.1974	817.9593
819.8196	834.8613	840.3503
849.9316	853.1754	853.3507
856.1766	863.4459	866.8484
873.3732	873.7644	889.4734
895.7030	902.3562	905.1814
909.9421	912.5330	918.5393
919.1897	927.3027	932.4617
933.6888	939.1475	940.3090
942.8802	950.0244	951.7303
954.1040	954.4823	962.7500
964.2285	964.9117	967.4398
970.7750	971.4587	977.9995
981.8400	984.1851	988.5432
989.3940	991.6358	992.9905
1008.8654	1014.4570	1014.8631
1015.8328	1016.4825	1017.2915
1026.1907	1033.7121	1037.5302
1037.6553	1038.2131	1041.9661
1046.5756	1047.0794	1047.9973
1051.6429	1054.1483	1057.1906
1060.5973	1065.4897	1095.7883
1102.6181	1110.3105	1111.8022
1113.5976	1122.0148	1124.1838
1134.4470	1139.1889	1148.7313
1158.2654	1160.7241	1161.7550
1167.5234	1167.8539	1169.2992
1183.8319	1186.1835	1189.1945
1192.0979	1194.4523	1198.0141

1198.8573	1206.0136	1206.7817
1210.5252	1211.1772	1212.4367
1231.9229	1234.8050	1240.5466
1241.9395	1253.8969	1262.4925
1269.5379	1274.5181	1279.2244
1294.2010	1297.0541	1299.0052
1309.3291	1319.3296	1320.9916
1324.0120	1333.9790	1335.2427
1343.4685	1347.0389	1351.5249
1364.7628	1374.2226	1376.4074
1381.7941	1383.0263	1384.1270
1386.7136	1390.0053	1391.7873
1391.9265	1392.6398	1394.8941
1401.4072	1404.4357	1409.4266
1409.5968	1409.8450	1435.1951
1440.7597	1446.9123	1448.6940
1449.5783	1451.6427	1452.0880
1455.9702	1457.0308	1460.1905
1464.3191	1464.9640	1465.0638
1467.6900	1470.2427	1470.4104
1470.9677	1472.5418	1476.2741
1476.8309	1477.4842	1479.4262
1481.1426	1481.3994	1483.9518
1484.6046	1484.8928	1485.7612
1493.1616	1494.0068	1495.6033
1502.8644	1513.8260	1522.8024
1523.8928	1533.9327	1548.7614
1550.2918	1596.3402	1623.0153
1624.6859	1627.5681	1627.8969

1630.8345	1653.5198	1657.3732
1659.6106	1664.4667	1673.6293
1675.0569	1678.5754	1698.4237
1761.4374	3033.2538	3043.2808
3043.6455	3045.5208	3046.3440
3047.0124	3048.6207	3053.4209
3054.8199	3057.7705	3058.9540
3061.2844	3063.2482	3088.9034
3101.7472	3103.2025	3118.7077
3128.9565	3131.4135	3131.9223
3136.5541	3138.2010	3145.2191
3145.5257	3146.7289	3146.9125
3151.0357	3152.0411	3156.0424
3156.7060	3160.6410	3162.6034
3163.4122	3163.4469	3163.8583
3165.3855	3167.1699	3169.7258
3171.7422	3174.3196	3176.1982
3182.4431	3182.9298	3183.6055
3184.5666	3187.1082	3189.8584
3191.4322	3195.0021	3195.3478
3196.2717	3197.8428	3198.7461
3199.3520	3202.4716	3206.7321
3207.7482	3208.7599	3210.8284
3217.4828	3217.6941	3218.7793
3221.0653	3563.1464	3676.6358

TS1S

Zero-point correction= 1.098635

Thermal correction to Energy= 1.164219

Thermal correction to Enthalpy= 1.165163

Thermal correction to Gibbs Free Energy= 0.999388

Sum of electronic and zero-point Energies= -5054.841589

Sum of electronic and thermal Energies= -5054.776005

Sum of electronic and thermal Enthalpies= -5054.775061

Sum of electronic and thermal Free Energies= -5054.940836

Cartesian coordinates

C	1.937159	1.033176	-0.151280
C	2.596968	1.970872	-2.274970
C	3.000702	1.388529	-0.903120
C	1.361244	1.128491	-2.635821
H	0.853003	1.479419	-3.539991
H	1.599555	0.063148	-2.735262
C	0.785883	3.289567	-1.400902
C	1.999854	3.358839	-1.993788
C	3.681030	1.956966	-3.336991
H	4.580982	2.498059	-3.027839
H	3.979587	0.931895	-3.576318
H	3.313242	2.415616	-4.260501
C	2.828973	4.566988	-2.252492
H	2.897266	4.804060	-3.321744
H	2.443359	5.451888	-1.740976
H	3.859157	4.396987	-1.914387
C	-0.067270	4.402292	-0.989931
C	-0.138658	5.586772	-1.747656
C	-0.844275	4.316591	0.175815
C	-0.917828	6.658964	-1.326812
H	0.402380	5.653403	-2.687923
C	-1.613269	5.394846	0.599734

H	-0.853189	3.384827	0.737712
C	-1.649611	6.574199	-0.143247
H	-0.959535	7.561995	-1.930423
H	-2.194519	5.308803	1.515590
H	-2.255743	7.413811	0.186770
P	0.396512	1.481674	-1.103967
C	4.409716	1.353144	-0.463311
C	5.344898	0.475827	-1.030118
C	4.826670	2.202422	0.571661
C	6.653665	0.436517	-0.559624
H	5.030037	-0.205332	-1.818165
C	6.140136	2.171807	1.032214
H	4.106874	2.891839	1.010453
C	7.055448	1.282941	0.472841
H	7.362629	-0.261873	-0.996730
H	6.446610	2.838523	1.834051
H	8.078561	1.250744	0.837270
C	2.054309	0.347719	1.201207
H	2.460258	1.055014	1.933230
C	3.021015	-0.819577	1.110783
C	4.118102	-0.924958	1.958539
C	2.823899	-1.816324	0.148738
C	5.024989	-1.976022	1.825264
H	4.292600	-0.152097	2.705809
C	3.720305	-2.867820	0.026631
H	1.966912	-1.749604	-0.522947
C	4.854122	-2.961861	0.849736
H	5.887422	-2.004891	2.485317
H	3.546311	-3.623578	-0.737794

N	0.829446	-0.232945	1.790791
H	0.451499	-0.985728	1.212738
S	-0.522760	0.486352	2.507897
O	-1.260012	1.486795	1.629584
C	0.278106	1.542563	3.840953
C	-0.886419	1.831270	4.787487
H	-0.543136	2.478606	5.601083
H	-1.702113	2.347154	4.270900
H	-1.285813	0.914422	5.233655
C	0.785214	2.852063	3.259328
H	-0.029032	3.402499	2.781239
H	1.178840	3.472452	4.072300
H	1.583344	2.730347	2.521333
C	1.347827	0.735141	4.556215
H	0.968419	-0.240070	4.878858
H	2.232898	0.560656	3.938843
H	1.665748	1.277600	5.453912
C	5.843945	-4.104905	0.636739
C	6.348689	-4.073613	-0.811954
H	7.072700	-4.878508	-0.982573
H	5.534866	-4.205543	-1.532015
H	6.843621	-3.122798	-1.039604
C	5.136694	-5.442239	0.890080
H	5.824694	-6.279402	0.724971
H	4.766414	-5.508154	1.918849
H	4.281667	-5.578754	0.219549
C	7.051152	-4.001562	1.566318
H	7.604141	-3.067888	1.410636
H	6.765230	-4.052316	2.622379

H	7.741025	-4.829541	1.372215
Cu	-1.496171	0.612572	-0.685852
C	-3.216256	-1.463211	-2.172007
H	-4.212619	-1.919306	-2.227753
N	-3.095300	-0.266997	-1.643964
C	-4.233576	0.268829	-1.080960
C	-4.097615	1.661180	-0.727127
O	-3.006251	2.175273	-0.461731
O	-5.255551	2.347066	-0.666863
C	-5.127358	3.702261	-0.218432
H	-4.518652	4.286818	-0.913098
H	-6.141526	4.098517	-0.180520
H	-4.669311	3.745290	0.773792
C	-2.133712	-2.246701	-2.719868
C	-0.786497	-1.846601	-2.649671
C	-2.428484	-3.497752	-3.293745
C	0.220279	-2.662614	-3.143821
H	-0.565275	-0.905564	-2.153055
C	-1.416796	-4.315691	-3.779699
H	-3.466218	-3.824566	-3.336514
C	-0.085776	-3.902164	-3.711087
H	1.257537	-2.338096	-3.079976
H	-1.664739	-5.280826	-4.214004
H	0.706431	-4.541560	-4.091150
C	-3.184212	-4.180600	0.396400
C	-4.211820	-3.235940	0.673544
C	-5.506823	-3.717625	0.894081
C	-5.754063	-5.089069	0.816145
C	-4.729249	-5.991835	0.521173

C	-3.423585	-5.544230	0.308033
C	-2.199089	-2.132305	0.379098
C	-3.593130	-1.928299	0.676154
H	-6.322112	-3.036779	1.122504
H	-6.762056	-5.459110	0.984443
H	-4.946431	-7.054685	0.458126
H	-2.617721	-6.237834	0.082088
O	-1.271726	-1.280473	0.271071
N	-1.993282	-3.490301	0.246093
C	-4.082340	-0.634984	0.911266
H	-3.286100	0.085499	1.118764
C	-5.380158	-0.386509	1.658055
H	-5.494144	-1.239412	2.346149
C	-6.639292	-0.350967	0.793022
H	-7.535221	-0.417717	1.419684
H	-6.702202	0.581512	0.224102
H	-6.671198	-1.178323	0.076756
C	-5.268135	0.875253	2.506153
H	-6.177171	1.043279	3.093347
H	-4.423009	0.818749	3.201505
H	-5.115555	1.759351	1.875966
H	-5.205153	-0.096095	-1.414754
H	-1.112777	-3.896073	-0.034749

Vibrational frequencies

-370.7526	14.3770	18.2954
24.5044	27.4577	29.1152
35.7514	40.4015	47.7429
49.6806	53.8305	54.3227
60.3837	62.9941	64.6255

70.4976	73.2420	77.8666
78.6952	87.1429	88.1797
95.2757	99.4862	102.7409
106.3376	107.8999	117.6985
122.1339	125.0979	130.3687
133.6605	135.6914	148.3518
150.6462	155.6001	158.1501
162.1978	170.2000	172.0052
180.2267	182.2965	193.7860
202.7251	208.3625	213.1037
218.2446	224.4286	228.0813
235.8251	240.9018	242.7358
249.0207	256.4182	260.3008
264.4946	268.7290	269.5629
277.1773	281.7716	284.3357
288.0660	292.3598	296.9520
303.5605	308.5791	312.1154
315.6820	319.0444	325.0140
330.2435	330.7691	340.1460
345.1930	345.7397	348.9823
354.1267	357.4784	360.3424
367.0122	368.8324	370.6590
379.9361	402.4959	407.0822
413.6360	415.4118	420.3779
424.3209	429.9244	430.7634
433.4394	434.9502	452.1824
453.6837	469.4139	471.9386
475.0595	475.4512	489.2395
500.1644	506.6244	518.5968

522.0287	524.3131	529.5706
534.5044	540.9115	544.6736
550.5802	562.9167	570.5556
581.8958	592.7500	604.2409
610.2806	620.2666	628.3853
631.0048	637.1898	639.0184
647.7644	649.9980	666.5634
667.8340	689.6031	689.9630
714.6023	714.7327	717.0755
719.9786	727.1550	728.5361
746.3869	750.7917	751.9042
755.5917	762.5418	764.1587
768.9292	772.5064	773.9275
776.4308	806.9590	811.5649
817.9491	832.4582	842.1156
848.9735	851.3673	856.7398
858.0075	861.5545	863.6558
864.3072	877.6543	891.9056
900.2926	901.7404	905.9369
906.9792	914.2214	921.2881
922.7226	924.0354	931.3668
937.4780	939.7600	940.5396
947.7008	948.2398	954.8226
955.9848	957.5542	960.2040
963.1101	968.7619	968.8964
969.1739	969.8086	974.1072
982.1527	982.9363	988.3059
992.7493	995.4669	1016.1985
1016.8904	1017.6505	1018.2032

1020.5422	1027.3843	1034.3400
1036.0897	1038.3313	1040.7106
1042.0245	1045.1638	1046.7601
1050.4294	1054.8363	1055.5768
1056.7186	1057.2827	1062.3633
1064.9133	1072.7596	1102.5061
1107.8787	1108.7496	1115.7539
1117.0198	1119.6699	1122.9886
1137.5633	1140.3617	1152.3439
1163.1063	1166.4541	1166.8593
1171.3499	1175.7900	1177.7663
1184.4573	1189.7582	1191.5344
1191.9335	1196.9229	1201.7486
1206.5640	1209.6764	1213.8708
1215.0310	1217.4796	1227.7896
1236.0566	1240.1358	1241.3545
1248.1341	1256.4139	1265.8950
1268.6823	1269.5004	1273.0013
1285.0661	1295.7458	1300.8155
1307.7388	1314.7461	1321.2294
1324.9300	1334.9695	1337.1462
1337.7512	1340.0428	1362.4517
1370.2270	1375.1927	1378.3133
1381.4281	1383.0403	1383.8601
1387.4651	1389.4821	1390.1469
1390.3045	1392.5507	1398.5738
1402.5145	1404.0478	1406.1488
1407.5441	1412.7199	1426.6934
1437.6957	1443.0997	1449.8098

1450.8519	1452.6038	1456.8942
1457.4194	1461.6037	1463.0285
1467.8042	1469.3953	1470.6260
1470.8159	1471.7594	1475.0156
1475.2828	1475.5059	1476.2247
1479.8945	1480.6811	1482.1441
1483.2207	1484.9260	1485.5757
1486.1119	1488.9924	1492.5469
1495.5684	1499.9020	1500.7645
1503.2436	1517.3980	1520.5054
1529.1346	1533.1047	1543.6159
1552.2830	1587.9229	1624.6813
1625.9000	1627.2896	1628.6773
1632.0497	1649.6512	1659.7244
1663.0277	1664.1915	1665.4534
1670.5119	1672.8910	1694.1352
1702.7144	3030.1591	3035.3220
3041.5805	3045.0838	3046.0696
3047.5443	3048.8170	3050.8125
3051.7089	3054.7097	3057.6286
3057.8433	3064.4140	3077.7895
3088.2184	3106.0964	3116.9089
3128.9239	3136.7512	3138.3421
3139.2945	3139.5499	3142.1622
3144.1266	3146.5879	3148.0828
3148.2938	3152.8058	3153.7055
3157.2057	3157.8742	3159.7229
3160.9621	3161.5244	3163.7094
3164.1159	3165.4346	3166.5208

3167.4705	3169.3409	3170.8098
3178.0449	3182.4473	3182.9283
3183.8064	3184.8480	3188.6332
3190.2648	3192.7645	3194.9391
3196.0855	3198.5430	3203.1868
3204.4970	3205.5422	3207.0415
3207.3450	3208.0656	3209.6435
3212.7343	3215.9473	3222.2751
3224.2083	3490.9480	3659.9857

M1R

Zero-point correction= 1.099509

Thermal correction to Energy= 1.165946

Thermal correction to Enthalpy= 1.166890

Thermal correction to Gibbs Free Energy= 0.997139

Sum of electronic and zero-point Energies= -5054.857775

Sum of electronic and thermal Energies= -5054.791338

Sum of electronic and thermal Enthalpies= -5054.790394

Sum of electronic and thermal Free Energies= -5054.960145

Cartesian coordinates

C	1.787979	-0.243885	-0.703029
C	1.208237	0.410049	-2.937948
C	2.274762	-0.155108	-1.954042
C	-0.082546	-0.280539	-2.453123
H	-0.991700	0.068794	-2.946574
H	-0.023568	-1.372702	-2.517372
C	0.334095	2.015438	-1.371843
C	0.979782	1.885969	-2.553058
C	1.516210	0.172092	-4.403740

H	2.442759	0.661703	-4.720869
H	1.627686	-0.898358	-4.604687
H	0.703738	0.547944	-5.033135
C	1.565110	2.964087	-3.392919
H	0.999991	3.103669	-4.323333
H	1.590672	3.924694	-2.872491
H	2.587837	2.708119	-3.696837
C	0.034148	3.215641	-0.596698
C	0.155594	3.183257	0.803997
C	-0.384661	4.417131	-1.194769
C	-0.096438	4.312732	1.573657
H	0.454535	2.253734	1.288268
C	-0.641520	5.545604	-0.421949
H	-0.538615	4.451395	-2.270054
C	-0.494120	5.501739	0.963570
H	0.014374	4.261680	2.654019
H	-0.972032	6.461668	-0.904822
H	-0.700421	6.383706	1.563718
P	0.021117	0.309539	-0.720992
C	3.629225	-0.498701	-2.427200
C	3.992050	-1.837221	-2.621951
C	4.567204	0.502005	-2.713423
C	5.267974	-2.169473	-3.068918
H	3.263777	-2.619749	-2.415344
C	5.843985	0.168192	-3.153242
H	4.298646	1.545360	-2.558463
C	6.201006	-1.168077	-3.328262
H	5.534764	-3.213718	-3.209344
H	6.563324	0.956987	-3.357058

H	7.200521	-1.426025	-3.668665
C	2.443622	-0.629512	0.593748
H	1.960670	-0.014337	1.369432
C	3.926542	-0.339931	0.641146
C	4.334952	0.996517	0.706500
C	4.904578	-1.326540	0.573822
C	5.681252	1.329513	0.682325
H	3.581517	1.782930	0.760650
C	6.257618	-0.987013	0.539227
H	4.606847	-2.371505	0.523038
C	6.676768	0.344439	0.585732
H	5.966884	2.378546	0.732434
H	6.989276	-1.786344	0.463552
N	2.109104	-2.040050	0.922213
H	1.824187	-2.558046	0.095205
S	0.988022	-2.377189	2.155051
O	0.031266	-1.194464	2.347099
C	2.072525	-2.287062	3.681729
C	1.128453	-2.661484	4.818143
H	1.691405	-2.684862	5.756578
H	0.321756	-1.931592	4.926811
H	0.683595	-3.651980	4.675004
C	2.615916	-0.883500	3.865138
H	1.819036	-0.135022	3.807421
H	3.073101	-0.806240	4.857371
H	3.389541	-0.644508	3.129641
C	3.171857	-3.317846	3.503571
H	3.756032	-3.382703	4.427379
H	2.768573	-4.315849	3.298903

H	3.849305	-3.042929	2.690293
C	8.147032	0.757012	0.536776
C	8.378224	1.674182	-0.670507
H	9.416320	2.025296	-0.690841
H	8.185216	1.143231	-1.608794
H	7.730125	2.556661	-0.646257
C	9.077705	-0.446412	0.404064
H	10.118300	-0.108860	0.355656
H	8.994471	-1.130614	1.255582
H	8.873086	-1.017228	-0.509123
C	8.503766	1.520035	1.818852
H	7.888799	2.418220	1.938129
H	8.359729	0.896645	2.708008
H	9.552650	1.837028	1.797200
Cu	-1.187408	-0.254032	0.920778
C	-3.739811	-1.798278	0.479907
H	-4.833786	-1.806050	0.508101
N	-3.085004	-0.798339	0.986881
C	-3.883434	0.334411	1.395152
C	-3.107512	1.044776	2.458460
O	-1.875931	1.054847	2.496206
O	-3.870471	1.678218	3.343638
C	-3.167316	2.479398	4.309803
H	-2.564830	3.240835	3.807408
H	-3.938510	2.948525	4.917881
H	-2.521363	1.854252	4.929277
C	-3.099780	-2.954422	-0.121020
C	-3.898659	-3.916866	-0.758510
C	-1.707104	-3.133028	-0.109482

C	-3.319871	-5.020571	-1.372880
H	-4.978818	-3.783543	-0.769618
C	-1.132453	-4.240427	-0.714693
H	-1.098253	-2.385892	0.397220
C	-1.935423	-5.186777	-1.353701
H	-3.948794	-5.755705	-1.867366
H	-0.052992	-4.374093	-0.688027
H	-1.482933	-6.051490	-1.831268
C	-6.513305	-0.909047	-1.843853
C	-6.280022	-0.016187	-0.747081
C	-7.314444	0.173931	0.183996
C	-8.532607	-0.490446	0.012741
C	-8.738906	-1.349059	-1.069899
C	-7.721644	-1.567778	-2.012548
C	-4.344224	-0.139829	-2.008102
C	-4.949546	0.470674	-0.862579
H	-7.169061	0.845488	1.030216
H	-9.331953	-0.336459	0.734542
H	-9.694209	-1.854284	-1.188254
H	-7.875548	-2.242148	-2.852757
H	-5.206371	-1.506393	-3.413927
O	-3.201255	-0.033226	-2.491578
N	-5.350982	-0.959734	-2.579810
C	-4.171539	1.262178	0.107095
H	-3.178057	1.432787	-0.342376
C	-4.758123	2.631478	0.542996
H	-5.374140	2.472961	1.441143
C	-5.646227	3.252785	-0.527356
H	-5.974061	4.252034	-0.217314

H	-5.099137	3.362850	-1.470981
H	-6.537143	2.652984	-0.730549
C	-3.643560	3.618944	0.884671
H	-4.033352	4.509266	1.391784
H	-2.856924	3.199608	1.517358
H	-3.147393	3.953998	-0.034748
H	-4.870316	0.043240	1.784659

Vibrational frequencies

9.0546	18.0624	19.9293
21.6487	28.8891	29.9949
32.8241	38.0489	43.8419
44.7530	47.2740	50.7370
57.5564	59.7508	61.4820
63.4419	68.2823	72.2015
75.2824	78.9209	82.8917
89.9572	95.0691	100.8358
103.9827	106.5359	113.8956
115.6877	118.6708	121.2043
130.5902	135.5777	138.4475
142.0745	149.4835	153.9547
158.9950	167.3689	180.1934
180.4053	183.4862	186.6911
190.5691	207.4226	212.6709
213.9920	218.6815	224.6604
228.1697	229.3221	237.8067
242.4271	247.5026	251.4142
256.7511	260.6334	268.4901
270.8511	272.4043	273.5385
277.4650	289.6095	290.3308

293.2390	299.6292	307.3652
311.8511	317.6491	324.9441
335.6910	336.3113	343.1313
345.4945	348.8009	355.6788
360.5987	361.6681	363.7479
372.4250	375.3932	380.5018
388.4652	407.3501	410.3396
414.3034	414.7296	422.6627
423.4851	424.7611	427.4535
429.0721	434.5786	448.2565
459.0247	473.7425	475.1441
486.1305	494.8532	496.7329
509.1992	510.2353	512.8045
519.9896	531.0184	535.1608
555.8182	557.8620	563.2905
569.6603	574.1711	579.1557
595.0321	599.3856	612.2446
618.1703	618.5618	628.2810
631.1643	633.7300	638.5253
653.9877	658.9936	662.7047
686.0821	700.8256	707.2590
713.3626	714.7110	716.0703
722.1533	726.3774	727.0909
732.3244	740.8393	748.3553
762.3163	767.8005	769.8079
772.7246	778.5843	779.6066
808.4952	817.8158	818.1678
820.3108	833.6498	848.6130
852.2305	855.8471	856.4874

861.1654	865.0211	866.0658
871.2264	879.5059	883.9025
886.5153	901.5099	909.9926
913.8889	913.9987	918.7189
919.7357	922.7462	939.5100
942.5933	947.9406	948.7726
952.6855	953.9902	956.5672
961.9775	962.6852	965.8959
966.6728	969.5372	969.8232
970.3948	974.6201	977.8109
987.5877	988.1754	992.4535
999.0820	1006.0475	1007.0720
1013.0270	1016.7173	1017.3365
1019.1420	1032.1422	1037.0282
1037.1264	1037.5059	1038.6130
1042.1420	1044.8683	1045.8637
1049.1158	1050.4544	1052.5844
1055.2083	1058.6241	1063.2430
1092.2696	1095.1041	1101.0142
1111.3848	1112.6960	1118.8249
1121.5039	1127.3359	1136.0866
1137.7359	1143.4672	1163.6393
1165.7148	1168.2431	1168.6131
1170.8163	1171.5645	1172.5974
1184.2985	1188.6196	1191.2422
1197.2659	1198.2945	1199.3840
1201.6723	1203.3568	1203.8647
1210.4766	1230.8170	1231.7583
1234.5747	1241.3115	1253.6571

1254.1498	1261.0903	1268.3221
1271.4703	1276.3223	1280.7909
1293.6559	1294.3367	1299.0203
1311.7067	1314.1744	1319.5659
1323.6437	1330.7765	1335.8486
1345.7813	1346.2192	1355.9628
1363.3153	1375.3485	1377.6772
1381.4094	1381.7633	1386.2573
1387.8236	1388.7481	1390.7885
1391.5860	1393.5831	1395.9409
1398.9640	1403.8079	1407.5658
1408.9548	1411.5624	1422.6447
1429.0503	1444.4323	1446.6874
1449.6655	1449.8363	1451.8411
1453.6626	1453.9423	1457.6944
1460.6576	1462.8046	1464.3734
1465.3348	1467.4352	1468.6530
1470.1011	1470.7477	1472.6164
1473.1643	1475.0857	1475.1854
1476.5827	1480.1378	1482.0669
1482.1754	1482.9289	1484.4000
1486.8358	1490.3653	1493.5660
1495.4948	1512.3919	1523.7053
1525.6036	1525.8088	1534.4642
1550.4087	1614.1504	1616.6395
1623.2928	1626.6492	1627.7393
1643.9163	1653.5403	1654.7784
1658.3829	1662.5313	1671.7429
1675.5759	1698.3003	1722.3314

1738.1045	3001.6994	3039.0904
3041.0542	3046.9463	3048.8653
3049.1200	3051.7930	3053.7375
3054.3837	3055.6437	3057.2967
3057.4809	3059.9075	3062.1070
3075.0742	3089.3245	3120.0034
3130.4887	3133.3090	3133.3322
3138.4447	3142.7134	3145.3362
3145.8643	3146.0563	3146.5970
3149.1657	3149.9510	3154.9378
3161.5886	3161.8005	3161.8582
3164.4084	3164.4204	3166.0368
3168.6513	3169.1504	3172.9602
3174.5885	3176.2787	3177.2304
3177.5459	3178.8612	3181.5251
3183.2832	3184.3289	3189.2624
3189.6440	3193.4417	3196.3318
3196.4268	3198.3151	3198.9006
3200.5417	3200.9864	3205.0175
3209.3314	3210.3115	3217.0192
3219.6845	3221.3699	3222.1246
3226.5051	3563.3756	3667.0762

M1S

Zero-point correction= 1.101664

Thermal correction to Energy= 1.167157

Thermal correction to Enthalpy= 1.168101

Thermal correction to Gibbs Free Energy= 1.002802

Sum of electronic and zero-point Energies= -5054.853266

Sum of electronic and thermal Energies= -5054.787773

Sum of electronic and thermal Enthalpies= -5054.786829

Sum of electronic and thermal Free Energies= -5054.952129

Cartesian coordinates

C	-1.954845	-1.020177	-0.128887
C	-2.555888	-1.998179	-2.249736
C	-2.997643	-1.406565	-0.894177
C	-1.330721	-1.133974	-2.598553
H	-0.799895	-1.484133	-3.490105
H	-1.590119	-0.075465	-2.714561
C	-0.729649	-3.271018	-1.336469
C	-1.934324	-3.370143	-1.945039
C	-3.621645	-2.017940	-3.329888
H	-4.514358	-2.575554	-3.029391
H	-3.938940	-1.001651	-3.582405
H	-3.229604	-2.476484	-4.243435
C	-2.730428	-4.598658	-2.211858
H	-2.781679	-4.837370	-3.281657
H	-2.328628	-5.473323	-1.695340
H	-3.768043	-4.453569	-1.884882
C	0.155186	-4.363749	-0.936933
C	0.259155	-5.533825	-1.714040
C	0.939587	-4.272099	0.223098
C	1.074196	-6.587532	-1.315884
H	-0.285159	-5.602865	-2.652105
C	1.747536	-5.330983	0.622800
H	0.925064	-3.349986	0.799355
C	1.813944	-6.497613	-0.137492
H	1.138827	-7.479397	-1.933960

H	2.336649	-5.237444	1.532775
H	2.449206	-7.322519	0.174411
P	-0.389085	-1.452621	-1.045199
C	-4.415295	-1.389900	-0.480914
C	-5.354305	-0.532062	-1.070674
C	-4.837152	-2.238159	0.552935
C	-6.671727	-0.510195	-0.623395
H	-5.037006	0.148178	-1.858533
C	-6.158786	-2.224740	0.990536
H	-4.115380	-2.914094	1.008968
C	-7.078151	-1.354957	0.408529
H	-7.383706	0.173694	-1.078299
H	-6.468591	-2.890492	1.791880
H	-8.107805	-1.336375	0.754837
C	-2.107312	-0.313072	1.208496
H	-2.516561	-1.016625	1.942132
C	-3.092675	0.834887	1.087407
C	-4.203011	0.926301	1.919755
C	-2.901037	1.826678	0.119194
C	-5.126210	1.959966	1.768029
H	-4.372830	0.156061	2.670891
C	-3.814088	2.862187	-0.019947
H	-2.033941	1.769792	-0.540910
C	-4.958599	2.943044	0.789419
H	-5.997005	1.978519	2.417226
H	-3.644389	3.617156	-0.785641
N	-0.903077	0.292635	1.815214
H	-0.516639	1.047861	1.243354
S	0.441849	-0.422005	2.546907

O	1.189610	-1.410761	1.661773
C	-0.369237	-1.499684	3.857415
C	0.783780	-1.792199	4.816768
H	0.428185	-2.438824	5.625626
H	1.602686	-2.311650	4.309376
H	1.181493	-0.877338	5.268370
C	-0.860146	-2.808048	3.259280
H	-0.037803	-3.346810	2.781489
H	-1.252158	-3.439904	4.064171
H	-1.654870	-2.688831	2.517821
C	-1.451836	-0.705021	4.568152
H	-1.080727	0.268076	4.906344
H	-2.330381	-0.526830	3.942525
H	-1.777980	-1.258802	5.455893
C	-5.962075	4.071382	0.562393
C	-6.441411	4.038714	-0.894840
H	-7.177690	4.830560	-1.073602
H	-5.618034	4.190882	-1.599860
H	-6.914154	3.080014	-1.136234
C	-5.278829	5.417455	0.834108
H	-5.975013	6.246098	0.660438
H	-4.928444	5.483206	1.869786
H	-4.413456	5.568184	0.180068
C	-7.183282	3.946181	1.470759
H	-7.717854	3.003420	1.305354
H	-6.916663	4.000580	2.531656
H	-7.883389	4.762904	1.265970
Cu	1.450052	-0.487563	-0.578731
C	3.237986	1.398996	-2.118039

H	4.233715	1.858446	-2.142480
N	3.072316	0.265933	-1.499170
C	4.216823	-0.121318	-0.697434
C	4.130558	-1.611381	-0.547461
O	3.065790	-2.157879	-0.306427
O	5.288170	-2.259504	-0.693966
C	5.208962	-3.684865	-0.501628
H	4.483972	-4.124758	-1.189647
H	6.208741	-4.064933	-0.703504
H	4.915849	-3.916787	0.525381
C	2.202800	2.126125	-2.824959
C	0.842409	1.787328	-2.734499
C	2.573512	3.243128	-3.592102
C	-0.110520	2.523340	-3.423665
H	0.568137	0.957438	-2.088332
C	1.616092	3.980711	-4.276519
H	3.623851	3.523207	-3.642135
C	0.270874	3.619622	-4.199641
H	-1.161505	2.252063	-3.349282
H	1.915630	4.840426	-4.869217
H	-0.479664	4.196934	-4.732786
C	3.221387	4.233724	0.526396
C	4.233830	3.233833	0.697183
C	5.554431	3.679547	0.880792
C	5.836159	5.044653	0.874337
C	4.826490	5.996382	0.692441
C	3.500195	5.593363	0.519898
C	2.203097	2.207339	0.458427
C	3.580336	1.961218	0.647764

H	6.361754	2.969394	1.034578
H	6.862969	5.374673	1.015458
H	5.071239	7.055134	0.687935
H	2.704233	6.321992	0.384258
O	1.229993	1.379859	0.353361
N	2.015544	3.582076	0.384511
C	4.061713	0.558511	0.749615
H	3.228308	-0.014528	1.185665
C	5.305239	0.344326	1.651776
H	5.322874	1.203539	2.335781
C	6.643004	0.319821	0.916534
H	7.469705	0.398989	1.630333
H	6.781239	-0.614702	0.362712
H	6.747959	1.141232	0.200305
C	5.155100	-0.905672	2.512613
H	6.001851	-1.016037	3.199091
H	4.238740	-0.871535	3.111911
H	5.116671	-1.819055	1.906565
H	5.163994	0.192305	-1.151409
H	1.118431	4.019979	0.244806

Vibrational frequencies

17.5244	20.8012	23.2039
27.5795	33.5496	40.1276
42.8843	47.6949	53.4318
55.6998	57.4224	60.1244
63.2744	63.4178	69.4892
72.4837	76.4720	77.8531
84.8722	89.1577	91.1266
93.8795	96.5248	108.4123

110.9071	118.6797	121.4025
125.6231	128.7178	130.2645
133.3643	142.0210	145.4377
149.9871	155.5007	158.8462
170.0187	174.0570	183.4068
187.7597	188.4185	194.5097
198.5427	203.2887	213.0926
224.6506	227.3626	228.8520
231.0783	233.8343	242.6633
259.0472	262.6994	264.2713
267.7601	270.4596	272.8845
276.9465	279.7533	282.5248
287.8109	296.3268	299.5079
302.1294	305.1116	312.5264
321.0060	327.8332	330.8643
334.0548	338.5142	341.4654
344.4155	345.7208	347.3709
351.8500	359.2101	361.4571
366.2309	368.7352	378.6919
390.3599	401.0926	405.3086
411.6888	417.5526	418.9939
423.1062	426.5305	427.4710
431.8269	437.1881	443.8533
454.4958	466.2653	469.6392
475.1327	478.8940	487.7386
500.0712	511.5994	521.6744
523.1662	531.7164	533.8788
541.8329	549.4343	560.7757
562.4990	570.2647	580.6066

592.1531	601.7893	611.6602
620.6353	627.3035	628.5260
633.0359	638.6532	647.4597
650.0330	661.8507	667.1948
690.0046	690.3682	710.2031
712.4235	713.6397	716.6896
720.4090	720.6024	733.7932
743.5464	752.7423	754.0523
758.8398	763.0050	774.3032
776.5470	777.2861	793.2176
805.9349	811.1182	816.2157
821.9252	830.9132	849.2324
855.3665	860.2389	860.9628
863.3024	863.7868	870.9072
876.2562	878.3920	883.3588
895.1993	901.2684	903.5256
912.7061	917.3410	924.9305
928.0262	928.1266	934.9057
935.7199	940.5190	950.2956
951.5959	954.3844	956.0478
958.5688	961.2937	961.8613
963.1490	967.3986	971.5956
973.1980	975.6799	979.6459
981.3684	989.0738	992.2308
1001.1021	1001.4798	1015.8516
1016.3705	1017.1945	1020.7196
1022.5777	1027.3129	1028.8265
1036.1985	1037.7018	1039.3156
1043.7478	1045.7523	1049.4782

1050.6681	1052.7170	1057.1647
1058.0677	1061.0871	1069.2869
1076.2137	1103.6469	1110.5104
1111.4662	1113.3680	1119.7139
1122.7225	1128.4916	1137.9831
1141.1227	1149.9990	1156.9081
1157.0166	1165.2695	1171.7682
1172.8050	1173.3236	1174.9825
1187.2872	1187.6194	1193.9118
1194.7433	1201.6478	1204.4887
1205.9533	1207.5309	1209.4433
1213.2708	1217.8475	1232.9846
1234.7294	1239.8424	1252.9420
1256.4373	1257.9909	1266.3538
1266.8738	1270.9122	1272.0786
1287.5727	1288.9242	1300.1567
1303.2330	1312.5373	1315.7751
1327.5070	1335.2977	1338.8931
1346.5132	1348.2107	1351.3756
1365.0412	1371.6861	1376.9161
1377.0182	1383.5429	1385.1918
1385.3382	1388.5934	1390.0377
1390.5023	1392.3458	1398.0902
1402.6785	1406.6788	1407.4283
1411.3637	1412.3002	1412.9983
1424.5085	1429.5923	1438.7563
1448.2625	1449.5823	1451.0772
1452.0753	1455.1936	1459.4716
1463.3318	1465.8896	1465.9357

1467.6366	1468.1948	1470.1314
1472.4977	1472.8456	1475.9110
1477.2055	1479.0541	1480.0471
1482.3841	1482.7159	1482.9007
1484.3617	1486.0191	1488.4891
1488.7009	1497.4949	1499.0277
1502.9600	1511.4535	1523.9723
1526.4732	1532.0742	1534.9624
1552.6148	1608.9463	1615.6841
1624.4419	1627.7049	1628.1126
1628.9914	1649.2429	1651.1307
1658.7458	1663.9527	1664.1432
1672.0838	1675.6844	1686.4481
1788.7812	3029.9470	3033.5544
3038.3897	3041.4960	3045.9814
3048.9881	3049.9324	3052.9427
3054.5576	3055.6838	3058.2477
3058.8623	3064.2341	3074.6522
3078.4435	3079.2249	3088.7441
3116.6721	3128.9729	3136.1768
3141.8675	3143.2316	3145.2672
3146.0157	3147.3100	3148.7862
3149.6437	3150.1730	3152.5168
3152.7537	3156.2923	3157.1889
3158.4917	3158.6071	3164.0053
3170.3336	3170.3793	3170.8163
3171.1824	3171.6393	3174.3453
3175.1991	3175.2505	3177.9495
3179.7511	3183.8966	3186.0877

3187.2362	3188.0065	3189.0117
3189.9386	3197.3018	3198.4682
3199.4999	3200.2491	3202.7300
3207.6634	3210.5697	3212.3843
3214.7594	3215.8962	3217.4841
3230.9497	3488.5645	3669.7235

TS2R

Zero-point correction= 1.101093

Thermal correction to Energy= 1.165779

Thermal correction to Enthalpy= 1.166723

Thermal correction to Gibbs Free Energy= 1.003938

Sum of electronic and zero-point Energies= -5054.839163

Sum of electronic and thermal Energies= -5054.774477

Sum of electronic and thermal Enthalpies= -5054.773533

Sum of electronic and thermal Free Energies= -5054.936319

Cartesian coordinates

C	-1.948509	-1.024092	-0.653303
C	-1.459793	-3.216369	0.194273
C	-2.498259	-2.231634	-0.416798
C	-0.177429	-2.865825	-0.591578
H	0.705140	-3.386223	-0.205450
H	-0.279198	-3.042082	-1.668414
C	-0.425621	-1.555306	1.597383
C	-1.118957	-2.713984	1.616404
C	-1.846761	-4.681012	0.112018
H	-2.746289	-4.910308	0.692578
H	-2.046295	-4.970625	-0.924749
H	-1.037234	-5.314753	0.487837

C	-1.614930	-3.452613	2.808521
H	-1.038960	-4.370944	2.982387
H	-1.553827	-2.849822	3.718298
H	-2.655478	-3.772964	2.676754
C	0.001310	-0.715175	2.711755
C	-0.117791	0.681472	2.614022
C	0.539572	-1.252201	3.892296
C	0.256820	1.507597	3.667514
H	-0.508729	1.116990	1.695918
C	0.919505	-0.424238	4.943591
H	0.689224	-2.326348	3.967461
C	0.773442	0.958346	4.840260
H	0.148439	2.585559	3.572757
H	1.341463	-0.860432	5.845478
H	1.073935	1.603656	5.661516
P	-0.166968	-1.075140	-0.177164
C	-3.905888	-2.610806	-0.608184
C	-4.498484	-2.555974	-1.877043
C	-4.693107	-3.015880	0.479873
C	-5.837951	-2.892938	-2.053012
H	-3.892345	-2.262665	-2.731776
C	-6.033840	-3.338016	0.306836
H	-4.251641	-3.040035	1.474316
C	-6.611381	-3.279961	-0.961317
H	-6.278644	-2.848355	-3.045482
H	-6.631751	-3.631311	1.165619
H	-7.658746	-3.536072	-1.096433
C	-2.574912	0.296693	-1.020627
H	-1.898397	1.053439	-0.594559

C	-3.943868	0.514756	-0.407133
C	-4.076998	0.425095	0.983906
C	-5.077425	0.812749	-1.156369
C	-5.305966	0.623780	1.594533
H	-3.204359	0.180438	1.590531
C	-6.313384	1.011948	-0.538124
H	-4.996503	0.877528	-2.238513
C	-6.457305	0.921624	0.847321
H	-5.375508	0.540862	2.677610
H	-7.174094	1.235483	-1.162023
N	-2.573089	0.547893	-2.484067
H	-2.656628	-0.317419	-3.010043
S	-1.339854	1.472425	-3.205713
O	-0.037804	1.386161	-2.419147
C	-1.948834	3.217593	-2.865541
C	-0.855353	4.094185	-3.464164
H	-1.135718	5.147247	-3.356277
H	0.100339	3.940319	-2.953868
H	-0.708592	3.898433	-4.532129
C	-2.086725	3.478896	-1.376937
H	-1.178177	3.193712	-0.833291
H	-2.246513	4.552145	-1.220677
H	-2.949230	2.958904	-0.947920
C	-3.263871	3.380143	-3.604968
H	-3.599376	4.419938	-3.525292
H	-3.166056	3.147279	-4.671117
H	-4.043803	2.740969	-3.181271
C	-7.794024	1.112932	1.560978
C	-8.173410	-0.193705	2.269828

H	-9.118312	-0.076009	2.812939
H	-8.299163	-1.008862	1.548928
H	-7.409596	-0.501905	2.991922
C	-8.917809	1.478452	0.593322
H	-9.854068	1.612072	1.145604
H	-8.713904	2.413067	0.059197
H	-9.087812	0.694167	-0.152262
C	-7.666187	2.231277	2.602585
H	-6.901217	2.005704	3.352636
H	-7.401388	3.185142	2.133254
H	-8.615735	2.370204	3.132028
Cu	1.111854	0.403566	-0.912007
C	4.125811	0.266372	-1.334986
H	5.035629	0.857660	-1.535226
N	2.977322	0.963783	-1.165917
C	3.334194	2.046523	-0.287160
C	2.117764	2.862205	0.023875
O	0.991462	2.380912	0.084249
O	2.366008	4.153227	0.248164
C	1.229096	4.947687	0.626336
H	0.674471	4.471207	1.437500
H	1.632029	5.905879	0.950359
H	0.564697	5.090037	-0.229764
C	4.169289	-1.049661	-1.985689
C	5.385058	-1.537251	-2.483204
C	3.042509	-1.878324	-2.022246
C	5.467399	-2.820607	-3.014620
H	6.269551	-0.902635	-2.438797
C	3.120181	-3.154639	-2.563764

H	2.128575	-1.475100	-1.589676
C	4.334534	-3.632505	-3.059687
H	6.417033	-3.189087	-3.393996
H	2.236289	-3.787933	-2.590737
H	4.397958	-4.634358	-3.476863
C	6.220833	-1.599997	0.732443
C	6.075048	-0.192360	0.608321
C	7.224329	0.571106	0.397826
C	8.474572	-0.054226	0.333583
C	8.588178	-1.438257	0.462342
C	7.453845	-2.232069	0.661495
C	3.978791	-1.168621	0.916379
C	4.648846	0.104754	0.600517
H	7.158166	1.649999	0.288435
H	9.366456	0.547506	0.178168
H	9.565807	-1.909821	0.404632
H	7.532201	-3.312201	0.755135
H	4.768277	-3.134627	1.017740
O	2.780219	-1.392447	1.097610
N	4.965403	-2.152164	0.903949
C	3.945352	1.371172	1.031757
H	3.060314	1.024719	1.589205
C	4.751484	2.320957	1.956376
H	5.557570	1.716212	2.394124
C	3.882564	2.817713	3.108158
H	4.450663	3.465127	3.785754
H	3.028790	3.402355	2.741360
H	3.481693	1.984338	3.694276
C	5.412301	3.509788	1.261213

H	6.116106	3.999821	1.942502
H	5.970326	3.227905	0.362886
H	4.674289	4.258589	0.957237
H	4.112626	2.698345	-0.714302

Vibrational frequencies

-295.8080	12.9549	21.1326
32.3341	34.3366	37.0280
41.7608	44.5455	46.0302
52.5598	52.8423	55.2256
63.2190	63.2892	69.9551
71.7826	73.6570	77.2454
82.3597	86.2787	92.8176
96.3365	102.0669	104.6061
106.6902	113.2653	116.2691
120.5838	122.9757	124.5220
131.1313	133.4126	137.2009
144.9707	156.1967	159.3943
161.2960	172.5458	175.5850
182.6388	183.8488	192.1500
197.1260	209.0880	212.5386
219.4633	221.3476	228.0006
230.2337	234.2936	242.4258
250.7805	257.0478	258.0041
259.4464	261.7116	265.7497
270.9558	273.6143	278.4490
281.6112	285.4325	290.5913
298.1866	304.4939	317.1809
317.5653	323.5509	328.8766
332.1851	335.0463	341.3161

342.8156	344.9864	349.5507
353.3243	363.9551	366.2117
373.4321	377.3314	386.6837
397.2209	406.6054	412.0395
416.4010	422.4664	424.1037
426.0448	431.5614	432.4323
437.7930	445.2212	450.5638
465.3280	471.1351	473.0844
487.6223	497.5383	507.3939
509.6050	513.4771	522.8615
533.1062	544.6620	553.8674
556.6670	564.8147	567.5755
577.7607	583.4775	588.2439
595.4320	613.1735	616.1386
617.3056	627.8583	628.9872
633.4363	639.5001	641.5090
650.7703	652.8853	659.9806
684.8016	701.9479	706.9543
707.9017	720.1704	723.0481
727.2222	729.3756	739.7901
750.1687	756.4802	764.9999
766.7080	770.3232	772.7962
777.3631	787.3357	800.0261
807.0969	819.1770	820.9569
834.8611	844.6955	846.4731
848.9591	856.7198	865.6249
868.3865	869.4035	881.5832
884.6942	891.0044	901.2163
901.6547	903.4378	910.3942

912.8391 918.7481 929.6740

931.0364 935.8408 942.4024

943.2040 944.1592 945.7202

950.2212 952.1027 952.4120

960.8688 962.2940 964.7700

969.3251 970.2721 975.5517

976.6016 983.1075 987.2749

989.1189 992.8810 1000.2791

1005.5383 1008.8823 1013.5147

1017.1790 1017.8169 1021.5923

1030.4898 1032.9460 1034.1961

1036.3708 1037.7269 1039.0890

1043.5672 1044.8168 1047.4478

1052.8767 1054.0196 1056.6032

1058.1791 1076.5616 1085.8681

1093.3323 1096.7402 1101.4131

1102.1787 1103.7370 1105.8685

1116.9924 1132.5431 1133.6760

1142.0293 1152.5089 1156.9804

1159.7636 1162.9901 1163.8773

1164.9539 1166.5544 1168.9590

1179.5074 1181.6035 1188.4810

1190.3227 1192.1048 1194.2455

1201.3933 1201.7311 1207.5025

1218.2069 1230.9133 1234.4702

1237.3932 1241.5106 1242.3613

1249.2417 1257.3541 1263.2652

1267.4397 1273.9699 1288.9600

1295.2167 1299.1341 1309.5134

1312.5549	1319.6258	1327.2863
1327.6768	1330.0899	1337.5518
1338.2951	1340.1428	1349.1689
1350.0551	1367.1509	1369.8660
1377.6156	1379.0165	1380.0803
1382.8440	1383.4431	1384.4622
1387.3184	1393.1195	1395.3207
1395.7607	1399.6052	1400.2075
1400.4096	1404.9463	1405.3725
1408.5196	1440.1420	1442.7189
1444.8154	1449.4941	1452.4114
1453.8668	1455.5078	1455.9271
1459.4882	1461.1273	1462.8610
1464.6603	1465.1191	1468.4560
1470.3995	1470.6859	1472.7790
1472.9882	1473.4123	1473.8283
1475.5541	1475.8443	1480.1903
1480.3975	1482.5137	1484.3246
1492.5218	1496.9403	1497.9327
1507.1685	1509.6401	1513.1555
1519.5411	1526.4780	1527.7646
1537.8962	1547.6814	1622.5117
1624.6517	1630.3381	1632.7755
1637.3116	1654.3405	1655.6738
1661.1097	1661.9536	1673.3957
1682.8665	1705.6703	1754.5549
1767.0888	2965.8609	2989.2984
2999.4739	3036.5376	3040.7407
3040.8211	3042.2336	3044.8795

3045.7213	3049.1751	3053.3454
3055.5674	3060.6306	3061.1634
3063.3296	3073.8500	3080.3941
3114.1251	3123.4598	3131.2475
3138.9263	3140.8544	3143.9431
3144.6179	3145.1692	3145.7165
3150.6029	3152.6958	3153.2610
3154.3382	3154.7758	3158.4869
3158.7124	3170.5307	3172.1172
3172.9954	3173.5570	3174.0053
3174.0577	3175.1736	3175.5401
3176.1203	3176.1889	3176.6298
3178.7282	3185.5612	3187.9023
3189.4454	3192.1540	3192.6205
3193.9300	3195.2054	3196.3258
3198.5881	3200.3711	3202.7144
3206.2781	3209.2075	3209.2712
3212.1599	3216.0766	3219.4956
3225.5181	3568.5907	3667.0647

TS2S

Zero-point correction= 1.101708

Thermal correction to Energy= 1.166051

Thermal correction to Enthalpy= 1.166995

Thermal correction to Gibbs Free Energy= 1.005928

Sum of electronic and zero-point Energies= -5054.836799

Sum of electronic and thermal Energies= -5054.772456

Sum of electronic and thermal Enthalpies= -5054.771512

Sum of electronic and thermal Free Energies= -5054.932580

Cartesian coordinates

C	-2.054387	-0.709494	-0.319840
C	-2.866773	-1.368618	-2.496103
C	-3.159546	-0.799748	-1.090764
C	-1.471524	-0.795346	-2.803276
H	-1.036374	-1.197696	-3.723584
H	-1.473542	0.299357	-2.839579
C	-1.404420	-3.098112	-1.696601
C	-2.600470	-2.867861	-2.286920
C	-3.906003	-1.049383	-3.554127
H	-4.902144	-1.418788	-3.291260
H	-3.986407	0.031604	-3.704579
H	-3.622980	-1.496285	-4.512608
C	-3.688257	-3.836827	-2.592101
H	-3.775509	-4.042187	-3.666765
H	-3.548572	-4.792745	-2.082063
H	-4.657023	-3.424416	-2.283168
C	-0.791513	-4.374853	-1.345092
C	-1.060044	-5.552168	-2.071833
C	0.112975	-4.459305	-0.272647
C	-0.498899	-6.767491	-1.698537
H	-1.688391	-5.505746	-2.956144
C	0.670404	-5.677774	0.098814
H	0.400679	-3.550613	0.252793
C	0.358174	-6.841002	-0.601294
H	-0.721892	-7.660406	-2.276897
H	1.361511	-5.716794	0.937983
H	0.795614	-7.792320	-0.310220
P	-0.642219	-1.437830	-1.292809

C	-4.548061	-0.577263	-0.636440
C	-5.334787	0.490944	-1.088474
C	-5.099016	-1.471557	0.293206
C	-6.626840	0.670121	-0.602706
H	-4.917346	1.204225	-1.795858
C	-6.396783	-1.299424	0.766249
H	-4.496647	-2.310139	0.639843
C	-7.161652	-0.222239	0.325656
H	-7.220130	1.512276	-0.949529
H	-6.807133	-2.004223	1.484407
H	-8.171164	-0.078774	0.701085
C	-2.049378	-0.139808	1.087656
H	-2.507152	-0.862169	1.772816
C	-2.867069	1.137429	1.150972
C	-3.903489	1.293612	2.065072
C	-2.585428	2.191629	0.275036
C	-4.672182	2.457077	2.080832
H	-4.140633	0.479505	2.748664
C	-3.341483	3.354220	0.305161
H	-1.779036	2.086877	-0.452731
C	-4.415420	3.507752	1.195998
H	-5.493216	2.527251	2.788958
H	-3.103118	4.155783	-0.391532
N	-0.742921	0.241007	1.667544
H	-0.309462	1.031403	1.189583
S	0.524357	-0.646490	2.312190
O	1.155013	-1.658808	1.348679
C	-0.349833	-1.737605	3.567487
C	0.794640	-2.198283	4.468550

H	0.408654	-2.893860	5.220761
H	1.569031	-2.719787	3.896331
H	1.262634	-1.359157	4.993606
C	-0.974873	-2.943607	2.886482
H	-0.210315	-3.540003	2.382095
H	-1.449775	-3.573971	3.646355
H	-1.737499	-2.685657	2.145236
C	-1.336171	-0.899211	4.363198
H	-0.876965	0.025576	4.727668
H	-2.225921	-0.625577	3.790175
H	-1.665194	-1.470429	5.238390
C	-5.248644	4.786987	1.156161
C	-5.806004	4.988015	-0.259281
H	-6.408283	5.902418	-0.306742
H	-5.010073	5.080185	-1.005031
H	-6.445364	4.149777	-0.557113
C	-4.357138	5.983114	1.515157
H	-4.933917	6.914882	1.487505
H	-3.936222	5.879103	2.520987
H	-3.522323	6.090263	0.814582
C	-6.422919	4.738439	2.131055
H	-7.096665	3.902212	1.911664
H	-6.091898	4.643169	3.170746
H	-7.006215	5.661968	2.055633
Cu	1.375800	-1.148900	-0.800242
C	3.603940	0.768943	-1.578374
H	4.691558	0.844482	-1.752225
N	3.144553	-0.450647	-1.203673
C	4.023078	-0.874520	-0.142373

C	3.575010	-2.246833	0.293730
O	2.808518	-2.935018	-0.365795
O	4.117831	-2.663174	1.440771
C	3.604806	-3.913368	1.923827
H	3.918058	-4.736621	1.276880
H	4.023774	-4.041766	2.921691
H	2.512927	-3.870989	1.960331
C	2.840803	1.638070	-2.491700
C	1.453449	1.511084	-2.626886
C	3.496734	2.666253	-3.180908
C	0.739178	2.386358	-3.434627
H	0.978485	0.708012	-2.067729
C	2.780642	3.549228	-3.983979
H	4.575848	2.772677	-3.074216
C	1.399138	3.412230	-4.113231
H	-0.338817	2.275887	-3.534495
H	3.300917	4.344394	-4.511572
H	0.838933	4.099514	-4.742143
C	3.927212	3.880335	-0.116409
C	4.698525	2.702464	0.047973
C	6.083522	2.788715	-0.090583
C	6.673564	4.026359	-0.365411
C	5.891224	5.172024	-0.518368
C	4.499484	5.111915	-0.397859
C	2.447243	2.196011	0.302908
C	3.775568	1.582520	0.199830
H	6.702248	1.900510	0.016995
H	7.753689	4.095866	-0.462724
H	6.366121	6.125283	-0.734993

H	3.884992	5.999835	-0.522517
O	1.360778	1.629098	0.492574
N	2.590563	3.547873	0.042259
C	3.992050	0.277727	0.949674
H	3.051969	0.105830	1.489404
C	5.138852	0.309673	2.000270
H	5.429861	1.362729	2.114069
C	6.404984	-0.443880	1.606013
H	7.195172	-0.264026	2.343204
H	6.238125	-1.524472	1.560720
H	6.795520	-0.130322	0.631396
C	4.635484	-0.152306	3.364985
H	5.428347	-0.104191	4.120337
H	3.807945	0.477004	3.712694
H	4.270211	-1.184369	3.325983
H	5.071618	-0.975460	-0.484179
H	1.811701	4.180912	-0.059232

Vibrational frequencies

-179.8990	16.2580	21.4057
26.5287	31.9192	33.8507
38.6350	42.9902	45.6186
48.1114	51.0921	54.5959
57.1815	60.0938	64.9919
67.2673	72.4960	77.1995
87.3236	89.2557	90.0624
94.8673	95.4051	105.2571
108.7380	119.8193	123.1030
124.4592	129.1757	131.1808
135.6278	138.8082	142.3524

151.5562	155.4898	164.1505
172.1524	177.4144	184.9657
187.2672	197.8708	201.1154
210.3990	215.6404	222.1680
227.3665	229.2379	233.0687
239.4481	240.3599	243.1149
248.2149	251.7930	255.8036
259.7064	262.3583	266.5040
268.7320	270.0707	275.9828
285.4650	294.9586	298.9857
302.3994	304.6578	314.4652
317.5098	332.7226	333.4570
338.2201	340.6735	348.5287
350.0128	350.6501	355.3700
366.5590	367.9841	370.8800
374.2885	376.2261	384.5180
410.6865	411.2553	412.1323
417.2367	422.1676	423.8586
433.0188	433.2526	434.6878
436.9799	455.2376	460.9491
470.0086	474.3428	481.8564
494.3955	502.8123	505.4427
507.7371	518.1584	520.6657
532.2795	546.2068	552.1098
557.1781	562.2593	574.9503
582.7029	584.2939	586.0804
602.0340	612.2682	621.1484
626.6306	629.3561	634.1839
637.3751	647.7317	652.6089

655.3586 658.6646 669.5135

687.8780 695.6422 705.6759

712.2075 715.8502 720.3070

732.6916 737.1132 749.9896

750.1403 756.1820 762.9692

771.5441 773.4746 776.9167

790.2347 792.2182 803.8534

805.3459 810.7652 826.1952

832.5219 856.1100 858.2953

858.9114 862.2942 864.2298

866.5990 873.1005 876.2332

885.6473 891.5657 909.4652

911.6452 915.4642 917.5669

919.7727 920.3574 922.5872

927.9332 939.6938 942.8631

949.3109 949.6126 952.8612

956.5918 958.1464 962.3786

962.8929 965.5405 968.8652

970.2001 971.3837 972.9044

974.5596 986.2242 988.5671

993.0915 995.1791 997.5953

1003.6589 1008.7430 1016.0946

1016.9282 1021.9684 1025.2623

1025.8739 1034.2679 1034.5970

1034.7695 1039.2704 1039.6803

1043.3104 1050.1663 1054.6337

1057.2150 1060.0313 1061.5279

1063.4654 1085.2228 1103.6381

1106.0119 1106.8409 1109.0577

1110.8644	1111.5401	1119.3339
1130.9799	1135.4376	1139.2885
1139.9931	1155.5693	1162.1557
1163.7466	1169.7582	1170.5044
1170.8824	1172.0784	1172.8870
1180.7881	1191.0774	1192.9782
1195.1681	1199.9751	1200.8557
1202.4737	1209.8832	1210.9421
1229.7826	1234.8058	1235.7181
1238.6080	1241.7651	1246.6622
1252.5581	1264.0700	1265.5125
1271.3366	1275.2866	1292.1315
1294.7915	1298.5944	1301.5144
1311.6867	1315.1194	1319.9084
1327.7888	1329.1871	1332.8842
1335.5288	1344.9912	1360.3359
1366.4114	1372.5026	1378.1766
1381.5873	1382.6322	1383.7239
1383.9718	1388.5036	1389.1032
1390.2624	1392.0387	1393.7939
1396.8136	1402.3080	1402.4973
1404.9955	1405.6558	1410.2338
1411.7298	1441.9537	1443.8899
1445.9817	1446.0798	1454.3914
1455.4564	1456.5343	1458.5537
1462.4390	1463.0504	1463.3795
1465.4141	1465.7381	1471.5390
1472.5433	1474.1732	1474.7692
1475.2404	1475.5656	1476.4161

1477.6301	1481.4897	1482.5965
1484.0376	1485.1680	1489.7599
1490.4952	1494.2189	1497.8465
1499.4703	1510.7340	1518.1841
1524.2175	1524.4802	1529.1169
1537.9197	1547.6563	1619.3300
1628.2531	1629.6052	1636.7375
1637.0572	1656.2662	1662.9272
1664.6184	1673.4760	1674.4974
1675.6624	1690.6993	1697.4488
1754.3360	2978.2685	2982.3503
3041.3206	3043.8239	3044.5457
3047.8774	3048.7980	3049.8002
3050.5984	3053.0511	3055.0092
3055.0870	3055.1547	3058.4478
3063.8177	3084.3072	3084.8968
3112.0307	3134.2338	3137.0718
3140.4980	3142.0106	3143.3101
3143.7193	3144.2610	3144.5568
3144.8163	3146.8070	3149.1339
3149.4195	3149.8952	3154.6625
3156.6678	3160.9520	3162.5748
3168.0204	3168.3471	3168.8053
3169.7614	3171.0620	3177.2863
3179.0236	3179.0996	3184.6128
3185.1109	3186.1939	3186.7774
3189.4989	3193.4970	3194.2424
3196.8009	3197.0417	3198.1605
3201.2964	3206.2905	3206.8964

3206.9458	3210.7196	3212.0523
3212.8418	3216.3449	3218.8296
3221.5833	3478.9270	3657.6716

M2R

Zero-point correction= 1.100849

Thermal correction to Energy= 1.166098

Thermal correction to Enthalpy= 1.167042

Thermal correction to Gibbs Free Energy= 1.002697

Sum of electronic and zero-point Energies= -5054.847248

Sum of electronic and thermal Energies= -5054.781999

Sum of electronic and thermal Enthalpies= -5054.781055

Sum of electronic and thermal Free Energies= -5054.945400

Cartesian coordinates

C	-1.913661	-0.744600	-0.426695
C	-1.256470	-3.027948	-0.111240
C	-2.389364	-2.002152	-0.408638
C	-0.070167	-2.443368	-0.907203
H	0.871795	-2.970566	-0.725870
H	-0.278241	-2.391138	-1.982702
C	-0.153282	-1.657479	1.524185
C	-0.812675	-2.822527	1.350412
C	-1.601643	-4.459837	-0.474848
H	-2.449077	-4.842889	0.103734
H	-1.868499	-4.537197	-1.533971
H	-0.747355	-5.120321	-0.296364
C	-1.203472	-3.810337	2.391751
H	-0.642193	-4.748708	2.295510
H	-1.038049	-3.427369	3.402003

H	-2.262448	-4.082312	2.295829
C	0.392710	-1.075177	2.744932
C	0.258616	0.302438	2.981327
C	1.082630	-1.846431	3.695442
C	0.771398	0.883956	4.135185
H	-0.257475	0.918223	2.247330
C	1.594771	-1.263729	4.850277
H	1.242706	-2.904781	3.503907
C	1.440339	0.103612	5.077286
H	0.653549	1.953400	4.295214
H	2.132534	-1.876947	5.569194
H	1.851870	0.559535	5.974144
P	-0.088688	-0.783467	-0.110856
C	-3.781749	-2.456673	-0.593659
C	-4.319128	-2.619529	-1.876374
C	-4.583502	-2.753647	0.515836
C	-5.635628	-3.041534	-2.045730
H	-3.700218	-2.396911	-2.744018
C	-5.899012	-3.173385	0.345520
H	-4.175858	-2.623235	1.516501
C	-6.431410	-3.313881	-0.935389
H	-6.041476	-3.152049	-3.047885
H	-6.511668	-3.385840	1.217862
H	-7.461718	-3.635609	-1.065554
C	-2.583634	0.582095	-0.652018
H	-2.031980	1.301941	-0.026752
C	-4.042244	0.621564	-0.255468
C	-4.380231	0.636410	1.102286
C	-5.074143	0.584995	-1.188647

C	-5.708630	0.596312	1.503541
H	-3.586543	0.663284	1.849711
C	-6.406673	0.536493	-0.782292
H	-4.831801	0.574902	-2.248625
C	-6.755845	0.534973	0.570529
H	-5.937677	0.605593	2.567720
H	-7.178410	0.488243	-1.545573
N	-2.371475	1.001895	-2.064047
H	-2.143961	0.206244	-2.654543
S	-1.284587	2.255421	-2.451255
O	-0.156848	2.345241	-1.427665
C	-2.327073	3.769886	-2.068318
C	-1.450639	4.923602	-2.543608
H	-1.983105	5.868060	-2.392699
H	-0.512815	4.969879	-1.982730
H	-1.210673	4.844421	-3.609490
C	-2.585507	3.873219	-0.576663
H	-1.664396	3.712296	-0.005408
H	-2.951929	4.879591	-0.345768
H	-3.345633	3.162647	-0.238518
C	-3.604315	3.673130	-2.881386
H	-4.158181	4.614075	-2.793723
H	-3.400467	3.510074	-3.945853
H	-4.247999	2.863764	-2.524989
C	-8.202741	0.460384	1.055935
C	-8.396876	-0.820088	1.878704
H	-9.413088	-0.861702	2.287908
H	-8.247636	-1.711732	1.259933
H	-7.696997	-0.878211	2.719332

C	-9.196728	0.437249	-0.102714
H	-10.219419	0.379477	0.284415
H	-9.128813	1.338974	-0.720883
H	-9.041294	-0.431342	-0.752309
C	-8.509806	1.675482	1.940634
H	-7.859491	1.715082	2.820423
H	-8.381175	2.613081	1.388630
H	-9.545139	1.636653	2.298512
Cu	1.135816	0.831094	-0.606508
C	4.073093	0.576705	-1.332291
H	4.968004	1.184256	-1.587561
N	2.972495	1.396385	-1.000027
C	3.488295	2.086769	0.166841
C	2.380257	2.909105	0.756916
O	1.262447	2.455235	0.968272
O	2.707556	4.181888	0.996050
C	1.672955	4.975907	1.595914
H	1.388300	4.562465	2.567264
H	2.095401	5.971880	1.719216
H	0.791844	5.013864	0.950956
C	3.904719	-0.447362	-2.411718
C	4.998332	-0.820613	-3.200533
C	2.688199	-1.105327	-2.595652
C	4.873157	-1.827400	-4.155010
H	5.953538	-0.314464	-3.060132
C	2.555303	-2.103347	-3.554727
H	1.868142	-0.796810	-1.949561
C	3.649939	-2.470933	-4.336755
H	5.730483	-2.106236	-4.762414

H	1.598695	-2.604167	-3.688699
H	3.550254	-3.253221	-5.084926
C	6.267029	-1.720370	-0.088570
C	6.049177	-0.334089	0.019026
C	7.122836	0.532636	-0.140970
C	8.401617	0.009218	-0.367992
C	8.594988	-1.368439	-0.458493
C	7.524645	-2.257796	-0.324966
C	4.010893	-1.482096	0.269018
C	4.583579	-0.085387	0.114823
H	6.971245	1.609379	-0.092031
H	9.247444	0.681927	-0.479158
H	9.591514	-1.762154	-0.640073
H	7.670436	-3.331219	-0.407846
H	4.924171	-3.373823	0.067915
O	2.854940	-1.812324	0.505838
N	5.049626	-2.372631	0.060478
C	3.987180	0.932148	1.107389
H	3.059156	0.473786	1.492591
C	4.871650	1.274288	2.308500
H	5.845404	1.629834	1.938572
C	5.109110	0.025505	3.151700
H	5.722375	0.248773	4.031874
H	4.154202	-0.384268	3.507955
H	5.618881	-0.764208	2.589239
C	4.265935	2.374393	3.172879
H	4.846839	2.509223	4.091810
H	4.238518	3.339002	2.659460
H	3.240177	2.118662	3.472200

H	4.348574	2.748663	-0.062717

Vibrational frequencies

15.3281	21.8822	25.6795
30.8363	35.6390	37.8712
42.6433	43.8741	47.4543
50.4551	54.2110	57.4482
63.3992	68.8128	71.3230
71.9098	75.0692	79.2970
85.4469	86.2547	93.1340
96.1873	101.5343	105.0167
108.1191	110.6283	114.0491
116.9598	123.2982	126.1253
131.7028	132.7038	135.6130
144.8849	156.8979	159.0142
170.8759	175.8821	184.9527
190.6006	195.2948	196.2500
206.6928	218.3836	219.3103
221.2608	226.3409	228.2200
233.1587	240.1606	245.5987
248.0580	254.8168	257.8546
258.7104	263.4197	267.1616
272.6674	277.2290	281.3296
285.1228	289.5640	297.7459
315.5716	315.7798	319.7358
324.4099	326.0337	327.4168
331.9605	339.7029	341.8343
345.8551	346.9355	354.8647
360.0890	365.6855	371.2072
375.4065	384.9255	389.3510

406.6397 411.2276 417.9423

420.2957 423.3124 424.4660

425.3838 428.3829 430.8318

448.6518 451.5635 462.1622

470.8382 472.3341 475.3905

486.5520 497.7358 502.7369

507.1259 513.8077 532.0357

542.5621 550.7130 556.3149

557.3128 566.8540 576.9427

585.4518 589.2559 597.8801

614.6540 616.7285 622.9456

627.5676 628.7621 629.1412

637.3342 642.0916 647.5169

654.0152 660.7927 677.7794

685.1109 701.0172 706.9850

707.2895 720.0911 722.6678

727.2901 730.6136 749.2536

749.5405 762.3924 763.8004

763.9726 771.7528 773.9846

798.4916 806.5894 807.3215

818.4285 820.2481 834.7320

835.2244 843.4943 848.4401

854.5971 857.2813 864.5004

869.3292 872.2054 884.6121

888.8368 898.2245 900.0461

903.8532 906.1546 910.2024

919.5928 922.3524 932.7802

936.2373 941.5574 942.2367

946.2567 950.2854 951.9810

953.0659	953.8475	959.5690
960.3546	960.8999	965.7307
965.7566	972.1575	975.6927
978.0864	980.7424	986.1138
992.0622	992.4522	1001.0677
1010.4068	1014.7854	1017.0817
1019.0202	1023.8558	1029.7731
1030.1719	1031.2975	1033.1271
1037.0297	1037.7387	1040.6969
1041.4359	1043.0658	1047.1395
1049.5708	1054.6615	1055.3979
1057.3002	1062.7073	1080.8692
1088.5157	1094.9220	1100.1755
1101.3742	1102.2768	1115.9884
1126.5131	1134.9104	1140.8961
1154.0467	1157.2411	1161.1540
1163.2894	1164.4810	1165.2365
1168.8338	1169.2016	1173.7635
1175.6012	1186.0617	1186.7060
1188.1082	1194.4462	1195.1617
1200.4241	1204.9602	1206.7706
1208.5818	1231.3083	1232.9858
1234.1287	1241.9836	1247.8747
1258.1414	1259.8700	1265.1982
1266.5160	1273.7860	1278.7942
1295.1349	1298.9436	1304.5937
1308.9880	1313.4078	1320.6092
1321.1486	1329.3612	1331.3838
1333.2956	1337.9903	1346.9354

1347.5745	1355.7605	1369.9209
1378.1523	1378.8706	1379.4226
1380.8229	1383.4554	1384.8364
1386.0224	1388.1970	1388.4377
1393.6049	1394.7430	1399.5572
1400.2966	1401.7607	1406.7163
1407.3277	1418.3505	1435.1557
1442.8692	1445.5007	1451.1255
1451.9155	1453.7882	1455.9401
1457.0706	1461.2002	1462.0540
1464.3994	1464.8804	1469.7209
1470.2150	1471.8646	1472.2329
1472.3850	1473.4330	1474.5513
1477.4253	1480.1848	1480.4214
1481.0826	1482.9927	1483.7765
1488.4896	1493.9710	1494.2565
1495.4021	1508.4302	1508.8209
1515.5662	1523.2522	1527.2616
1533.6687	1551.5578	1622.0891
1624.2749	1632.2571	1642.5435
1645.0867	1653.9060	1655.2608
1669.0984	1671.7794	1675.9744
1684.3068	1707.7145	1772.8346
1794.1464	2867.1100	2914.3228
3007.1455	3029.5373	3037.8984
3039.1297	3043.0941	3045.4581
3046.9096	3048.5224	3053.5818
3054.4395	3060.0153	3062.6725
3063.1601	3073.1792	3074.3140

3114.3243	3118.1697	3131.6916
3134.9274	3138.8986	3140.6147
3144.2307	3144.7739	3147.1980
3150.5962	3153.2564	3154.0083
3154.4287	3155.5539	3157.0296
3157.8740	3160.4129	3161.5531
3166.2381	3169.0621	3169.7609
3171.1295	3174.2893	3174.6484
3175.4447	3176.8091	3177.1099
3179.2977	3183.8412	3185.4668
3187.8668	3192.2791	3192.3138
3193.2110	3194.6710	3196.2964
3200.4420	3201.5629	3201.8482
3202.8015	3208.5433	3208.8762
3216.4483	3217.9042	3218.6016
3225.2573	3557.8027	3650.3348

M2S

Zero-point correction= 1.102230

Thermal correction to Energy= 1.167208

Thermal correction to Enthalpy= 1.168152

Thermal correction to Gibbs Free Energy= 1.005614

Sum of electronic and zero-point Energies= -5054.839535

Sum of electronic and thermal Energies= -5054.774557

Sum of electronic and thermal Enthalpies= -5054.773612

Sum of electronic and thermal Free Energies= -5054.936151

Cartesian coordinates

C	2.084249	0.699143	-0.331617
C	2.950353	1.487220	-2.444294

C	3.200608	0.786459	-1.086944
C	1.532959	1.012287	-2.805640
H	1.129021	1.511930	-3.691806
H	1.479990	-0.074214	-2.933661
C	1.563718	3.217519	-1.519943
C	2.754183	2.977283	-2.116586
C	3.980009	1.214336	-3.524833
H	4.991951	1.508022	-3.229463
H	4.006523	0.150480	-3.778254
H	3.724615	1.764010	-4.436517
C	3.885426	3.919089	-2.337601
H	3.987573	4.211012	-3.390707
H	3.783164	4.834281	-1.749662
H	4.833917	3.440330	-2.063605
C	1.003846	4.488877	-1.074363
C	1.317539	5.704076	-1.715001
C	0.097442	4.528054	-0.000640
C	0.798058	6.909274	-1.256797
H	1.948659	5.697152	-2.598769
C	-0.418099	5.736335	0.455098
H	-0.227556	3.594115	0.454499
C	-0.061378	6.934785	-0.159218
H	1.053902	7.832694	-1.770401
H	-1.111374	5.740078	1.293278
H	-0.466769	7.877706	0.197520
P	0.718393	1.570172	-1.254382
C	4.572653	0.422053	-0.677164
C	5.258759	-0.648168	-1.268352
C	5.217486	1.161831	0.323882

C	6.544130	-0.980270	-0.853664
H	4.765915	-1.241421	-2.035463
C	6.508744	0.834980	0.730130
H	4.693652	1.999323	0.782838
C	7.173536	-0.241245	0.146629
H	7.058147	-1.818741	-1.316282
H	6.993245	1.418641	1.508492
H	8.178461	-0.502441	0.467250
C	2.012425	0.052985	1.040304
H	2.440725	0.738940	1.780355
C	2.814496	-1.233430	1.090925
C	3.825630	-1.418803	2.028244
C	2.550139	-2.265617	0.184819
C	4.587022	-2.586644	2.037817
H	4.048928	-0.622062	2.736666
C	3.297792	-3.434258	0.208487
H	1.762161	-2.140455	-0.559063
C	4.346805	-3.615379	1.123293
H	5.387808	-2.678662	2.766195
H	3.072325	-4.218538	-0.511609
N	0.669584	-0.323015	1.536459
H	0.223757	-1.072705	1.008473
S	-0.565834	0.557796	2.243247
O	-1.107563	1.699681	1.377964
C	0.298045	1.456156	3.646064
C	-0.871196	1.850384	4.549234
H	-0.497045	2.435259	5.395608
H	-1.604207	2.463989	4.013999
H	-1.388291	0.971858	4.949868

C	0.993346	2.707678	3.136358
H	0.278474	3.379784	2.655022
H	1.437700	3.238702	3.985462
H	1.792690	2.502838	2.417652
C	1.219327	0.491856	4.371949
H	0.701768	-0.435228	4.639457
H	2.103246	0.223287	3.787458
H	1.561803	0.956977	5.303141
C	5.167239	-4.903045	1.086233
C	5.752581	-5.098059	-0.318215
H	6.333930	-6.026038	-0.364147
H	4.973579	-5.159840	-1.084668
H	6.419744	-4.271845	-0.586595
C	4.254799	-6.091711	1.416496
H	4.822238	-7.029470	1.396540
H	3.811709	-5.988934	2.412932
H	3.435135	-6.185355	0.696282
C	6.322071	-4.876929	2.084884
H	7.005493	-4.042166	1.890997
H	5.971749	-4.794612	3.119340
H	6.900718	-5.803242	2.007371
Cu	-1.314547	1.305980	-0.843111
C	-3.550986	-0.669411	-1.548712
H	-4.596602	-0.632743	-1.921560
N	-3.063607	0.619254	-1.265848
C	-3.928150	1.038742	-0.188115
C	-3.487604	2.399617	0.282474
O	-2.660459	3.077608	-0.313061
O	-4.115546	2.823286	1.384458

C	-3.630983	4.071267	1.902586
H	-3.862358	4.892689	1.219834
H	-4.141514	4.217222	2.854063
H	-2.548911	4.016667	2.048247
C	-2.765263	-1.536042	-2.484681
C	-1.386178	-1.381549	-2.638176
C	-3.410660	-2.555606	-3.194645
C	-0.666207	-2.221288	-3.481915
H	-0.918836	-0.572739	-2.078331
C	-2.691366	-3.405189	-4.031056
H	-4.489027	-2.675377	-3.091911
C	-1.314752	-3.240244	-4.178131
H	0.406964	-2.083053	-3.598389
H	-3.207147	-4.191639	-4.576184
H	-0.752307	-3.897467	-4.836561
C	-4.459681	-3.658594	-0.089865
C	-4.959346	-2.346979	-0.190727
C	-6.281451	-2.165762	-0.581509
C	-7.096604	-3.281552	-0.799701
C	-6.585022	-4.571356	-0.658704
C	-5.248132	-4.779038	-0.310058
C	-2.658847	-2.296021	0.285183
C	-3.823906	-1.390623	-0.053989
H	-6.680391	-1.163042	-0.718681
H	-8.134566	-3.141235	-1.088480
H	-7.227644	-5.429566	-0.835620
H	-4.835347	-5.780424	-0.226428
O	-1.503711	-1.970737	0.554579
N	-3.102271	-3.597042	0.207032

C	-3.837032	-0.130570	0.842392
H	-2.800257	-0.070813	1.188645
C	-4.693372	-0.095904	2.114524
H	-4.310886	0.769500	2.675500
C	-4.437322	-1.330898	2.971950
H	-4.937636	-1.250745	3.943749
H	-4.813843	-2.239971	2.486577
H	-3.366533	-1.475207	3.160959
C	-6.187198	0.132879	1.919352
H	-6.661017	0.372357	2.878006
H	-6.394840	0.965697	1.238820
H	-6.692669	-0.755166	1.528582
H	-4.991829	1.142009	-0.502243
H	-2.498469	-4.396102	0.333662

Vibrational frequencies

22.2684	23.5999	26.5019
32.3648	38.4251	41.4108
45.8837	51.1769	55.7206
57.8733	60.6068	62.9745
68.3880	72.5052	76.3312
80.6874	84.4871	84.6742
92.0366	94.0432	97.4277
99.8325	103.7694	109.2644
111.8902	116.2997	121.8698
125.3609	129.2932	131.7751
137.3901	141.5886	146.5599
149.8888	168.7728	171.3268
177.3940	185.7516	194.1160
200.5072	206.2337	215.0874

222.3536	224.5590	228.6242
229.6502	231.6117	239.8216
242.1496	244.6712	246.8057
249.4874	259.0991	263.7960
267.5576	269.0954	271.1965
275.8222	279.1561	279.9574
286.0185	287.1589	291.4928
303.8977	310.2162	314.4427
323.5883	329.8569	331.3382
334.8119	344.6491	346.9818
352.0765	357.3731	363.3956
368.8147	369.6878	375.2272
381.4574	385.4145	390.3601
399.9035	411.0144	415.9058
418.4024	426.9940	428.2640
439.8140	445.1847	446.5827
452.8820	455.4258	462.0980
467.0628	468.7000	472.5152
482.7657	490.8165	505.9658
508.2875	514.6302	537.3946
537.8652	547.7373	555.2784
566.8695	572.3697	576.5281
579.6200	586.5334	590.7196
613.7072	620.0474	624.8723
629.3837	629.9876	635.5821
638.0861	639.4186	648.7435
653.5156	657.8868	676.0277
684.1898	693.2997	694.8566
714.0251	721.2074	726.1447

729.0331	731.2116	735.2120
751.0770	752.5359	765.0774
770.0713	772.0707	776.4015
796.0114	803.9454	806.9740
814.0158	822.4677	833.1002
834.7601	846.8854	854.6696
858.1100	860.1921	864.8669
872.8363	875.3510	880.1108
888.6007	896.2273	898.6707
904.0167	912.3022	917.2923
918.5627	924.0330	928.4218
938.9206	941.3019	944.0641
944.5782	948.0984	950.1560
950.7225	950.9129	959.8259
961.9804	965.4269	969.4589
969.8402	970.5036	975.9114
986.2094	987.9985	989.5717
991.2371	993.3826	1001.6794
1014.7221	1016.1394	1018.1679
1020.9636	1024.0665	1028.5053
1032.4767	1035.0133	1036.9933
1041.6819	1043.1866	1045.3199
1047.8774	1051.8694	1052.4804
1056.3564	1058.7598	1062.3879
1065.5474	1069.0053	1086.3197
1102.3664	1103.7047	1111.1586
1119.2758	1120.0754	1122.5133
1129.7769	1134.9948	1137.1125
1149.2591	1156.6130	1165.4541

1168.0030	1168.6585	1169.2962
1175.6523	1175.7645	1184.3458
1187.3052	1190.7711	1193.3058
1197.9078	1202.9937	1206.4390
1208.9152	1212.6539	1213.0169
1215.6136	1216.2299	1234.5257
1236.0199	1236.2250	1240.8552
1253.6843	1258.2008	1262.5583
1267.7320	1269.7402	1273.3683
1289.2189	1299.6202	1300.3280
1311.0687	1311.3698	1319.5998
1324.5168	1328.9909	1330.2704
1332.4963	1335.9026	1347.5800
1354.9317	1365.7881	1367.9036
1376.5004	1378.3482	1379.7881
1384.5088	1385.4925	1388.0344
1390.0962	1390.7060	1391.0358
1391.6045	1394.2754	1394.7148
1402.6834	1406.5704	1413.4033
1413.7696	1415.8247	1436.8473
1444.4851	1452.6077	1453.5159
1455.6478	1458.0274	1460.9498
1461.0709	1462.3651	1465.7704
1465.9020	1467.1831	1468.3112
1469.5281	1471.6789	1473.7088
1475.4430	1478.1979	1479.3471
1482.8180	1482.9377	1484.6308
1485.5610	1486.2639	1486.7022
1487.6708	1490.0424	1494.9329

1495.5282	1507.4783	1511.1272
1518.7263	1524.6782	1532.7532
1534.0481	1546.1564	1623.6285
1625.3848	1628.1644	1640.7385
1642.1280	1647.1120	1656.4580
1660.2169	1666.0313	1671.0232
1673.4557	1674.2856	1768.7630
1780.9809	2875.4321	2892.1850
3037.9745	3043.4995	3045.8320
3047.1642	3052.3582	3055.4954
3056.5813	3060.5298	3060.6301
3063.4049	3063.9725	3067.9120
3082.1151	3086.4166	3095.8476
3119.9890	3126.3656	3136.6635
3137.2736	3141.8131	3142.8533
3144.2599	3147.0763	3148.5533
3149.7226	3152.6207	3153.0124
3156.5766	3158.0160	3161.1720
3162.1445	3162.7962	3165.1618
3165.7387	3166.1186	3167.1533
3169.8290	3172.8174	3174.9403
3177.2578	3180.5086	3182.9947
3183.6558	3184.9253	3185.3513
3187.8500	3189.8504	3192.1875
3192.3679	3193.4780	3196.4053
3201.5941	3202.2774	3209.0277
3209.0848	3212.6752	3212.8647
3215.0154	3216.0151	3218.6780
3225.0281	3544.2947	3648.3698

$NEt_3•H^+$

Zero-point correction= 0.222507

Thermal correction to Energy= 0.231637

Thermal correction to Enthalpy= 0.232581

Thermal correction to Gibbs Free Energy= 0.189262

Sum of electronic and zero-point Energies= -292.630801

Sum of electronic and thermal Energies= -292.621671

Sum of electronic and thermal Enthalpies= -292.620727

Sum of electronic and thermal Free Energies= -292.664046

Cartesian coordinates

N	0.060166	-0.186572	0.677381
C	-1.414547	-0.559884	0.699515
H	-1.475672	-1.456943	1.319334
H	-1.915282	0.250328	1.233376
C	0.312138	1.305172	0.633036
H	-0.222959	1.710682	1.494890
H	1.380185	1.433646	0.819717
C	0.839890	-0.982344	-0.339216
H	0.567798	-2.025350	-0.157697
H	0.461248	-0.703586	-1.324154
C	-2.033956	-0.811259	-0.652319
H	-3.102417	-0.981184	-0.500458
H	-1.930833	0.029528	-1.340658
H	-1.630417	-1.705433	-1.132209
C	-0.112518	1.972455	-0.647597
H	-1.196989	1.979044	-0.775678
H	0.215741	3.013588	-0.614305
H	0.344514	1.517302	-1.530611

C	2.326921	-0.770492	-0.225949
H	2.830950	-1.495772	-0.868108
H	2.637222	0.224475	-0.554167
H	2.686121	-0.930965	0.795274
H	0.422060	-0.475240	1.588971

Vibrational frequencies

70.6953	108.6034	140.9538
234.3508	246.4202	270.8266
294.7613	317.7945	387.3084
406.5656	466.8093	596.7278
721.5898	786.8123	804.8426
827.1906	889.1158	898.5910
1024.8115	1040.7649	1058.4452
1075.1619	1083.3735	1114.1247
1169.6652	1194.4967	1202.7150
1294.9524	1322.0651	1333.2344
1354.8583	1377.9330	1396.6555
1399.4524	1412.8404	1419.6810
1439.4908	1450.9268	1460.3531
1462.7944	1467.0919	1471.8625
1475.5269	1481.9872	1490.9222
1496.3781	1513.6432	3075.5939
3081.5818	3090.4426	3096.3452
3116.5954	3125.7995	3159.9168
3165.5503	3174.6729	3179.1002
3182.7810	3188.0374	3194.9191
3197.5417	3201.1989	3483.0150

Cat+NEt_3

Zero-point correction= 0.898993

Thermal correction to Energy= 0.949075

Thermal correction to Enthalpy= 0.950019

Thermal correction to Gibbs Free Energy= 0.818031

Sum of electronic and zero-point Energies= -4159.991771

Sum of electronic and thermal Energies= -4159.941689

Sum of electronic and thermal Enthalpies= -4159.940744

Sum of electronic and thermal Free Energies= -4160.072733

Cartesian coordinates

C	-0.461368	-0.646679	-0.770124
C	-0.247351	-2.890640	-1.602790
C	-1.176375	-1.696530	-1.212298
C	0.953139	-2.185334	-2.267475
H	1.768063	-2.874736	-2.506727
H	0.666231	-1.621318	-3.160748
C	1.243056	-2.576791	0.260516
C	0.338981	-3.426436	-0.279313
C	-0.893316	-3.943285	-2.482669
H	-1.768954	-4.401313	-2.012163
H	-1.222062	-3.508701	-3.431597
H	-0.178100	-4.739695	-2.710222
C	-0.212726	-4.674122	0.310057
H	0.151166	-5.567833	-0.212490
H	0.041314	-4.780966	1.367036
H	-1.304900	-4.692388	0.213386
C	1.962443	-2.631648	1.528487
C	2.244387	-1.439626	2.221003
C	2.411864	-3.840333	2.088925
C	2.904123	-1.457747	3.444438

H	1.928635	-0.488248	1.790410
C	3.077240	-3.855455	3.310018
H	2.259238	-4.769818	1.547545
C	3.319914	-2.667467	3.997484
H	3.100980	-0.523265	3.964185
H	3.419701	-4.801117	3.721183
H	3.841404	-2.682900	4.950275
P	1.338186	-1.101340	-0.843682
C	-2.641879	-1.871737	-1.292157
C	-3.311711	-1.688089	-2.508368
C	-3.374162	-2.281777	-0.171784
C	-4.687596	-1.879387	-2.594467
H	-2.747748	-1.377398	-3.385626
C	-4.749732	-2.475215	-0.260519
H	-2.860976	-2.430215	0.776108
C	-5.411646	-2.269141	-1.469578
H	-5.195131	-1.720608	-3.542210
H	-5.305881	-2.782621	0.621283
H	-6.486858	-2.414400	-1.534195
C	-0.833642	0.705269	-0.227365
H	-0.244257	0.837351	0.693956
C	-2.287689	0.893999	0.125407
C	-2.716131	0.634538	1.429919
C	-3.235533	1.287213	-0.816168
C	-4.056697	0.749735	1.773552
H	-1.985212	0.336173	2.181201
C	-4.581214	1.389483	-0.471849
H	-2.922708	1.506016	-1.835384
C	-5.023574	1.120840	0.827755

H	-4.358250	0.549137	2.799966
H	-5.291042	1.679970	-1.241036
N	-0.353938	1.743056	-1.185433
H	-0.194707	1.368023	-2.116917
S	0.917161	2.786630	-0.810104
O	1.911444	2.113492	0.159010
C	0.102184	4.077435	0.273803
C	1.201385	5.120970	0.448746
H	0.804420	5.963879	1.022425
H	2.057908	4.715633	0.995249
H	1.554906	5.511334	-0.511769
C	-0.303196	3.485217	1.609154
H	0.517338	2.921608	2.063107
H	-0.564004	4.301176	2.291484
H	-1.180596	2.838263	1.523960
C	-1.077211	4.629876	-0.505210
H	-1.494585	5.482848	0.039498
H	-0.783614	4.986092	-1.498807
H	-1.866030	3.881412	-0.624209
C	-6.489443	1.225341	1.245449
C	-6.958187	-0.123920	1.805288
H	-7.995504	-0.054566	2.152222
H	-6.912247	-0.905475	1.039469
H	-6.347465	-0.449725	2.653751
C	-7.397329	1.600727	0.076358
H	-8.437113	1.652390	0.415251
H	-7.141174	2.577946	-0.346847
H	-7.350068	0.858506	-0.729041
C	-6.624063	2.293116	2.339069

H	-6.026589	2.043243	3.222063
H	-6.295823	3.274770	1.980349
H	-7.668049	2.383709	2.660000
Cu	2.772235	0.377669	-0.493489
N	4.735204	0.788570	-0.352408
C	5.037898	0.549393	1.084110
H	4.344744	1.191661	1.643732
H	4.745664	-0.485760	1.294870
C	5.428193	-0.155069	-1.277604
H	5.371298	-1.140389	-0.801810
H	4.814112	-0.219788	-2.183427
C	4.935519	2.208105	-0.723188
H	4.417574	2.803058	0.036651
H	5.998831	2.481569	-0.679311
C	6.453109	0.794500	1.567835
H	6.469950	0.740570	2.660402
H	7.155509	0.043776	1.198677
H	6.824572	1.783944	1.285570
C	6.856085	0.168011	-1.677131
H	7.546592	0.208019	-0.832456
H	7.215151	-0.610845	-2.356104
H	6.929410	1.118097	-2.215217
C	4.361969	2.508351	-2.089095
H	4.337532	3.585744	-2.272630
H	4.934653	2.044082	-2.897731
H	3.331840	2.132270	-2.155035

Vibrational frequencies

22.7264	27.5672	30.2866
36.3649	38.3759	41.2391

43.5868	56.4900	62.4552
68.9548	78.6090	80.2884
81.1001	90.3458	95.5107
97.1525	103.4495	106.9435
109.9208	115.4176	120.1457
131.9641	133.2485	146.1682
153.8126	159.3758	171.5571
177.9996	182.8489	188.6429
192.1881	199.2799	215.9160
223.1833	227.9829	237.0144
240.9978	249.3235	255.1472
262.9303	265.9793	269.7371
271.3924	275.8536	278.5021
279.4691	285.1300	296.9465
302.5316	310.2326	320.7931
323.6463	333.0219	335.3453
335.9392	352.9261	361.1406
363.7928	363.9293	366.1828
373.6734	376.2686	382.9576
391.1060	402.3614	411.7747
412.6135	420.9896	424.6237
429.5335	436.3880	441.1749
470.4206	473.6240	476.7933
491.9640	494.0637	510.1614
514.1924	533.7171	551.5008
554.6925	560.7571	571.7010
581.4092	603.3911	614.4426
623.2711	629.6425	636.9857
641.2065	654.5891	656.1693

698.8596	707.0049	716.6915
722.9315	730.3634	735.4922
748.6831	768.3271	773.3276
775.5720	782.7091	797.0849
807.5044	813.8237	816.4089
832.2728	841.6140	851.7823
860.6917	861.6532	867.1918
876.0448	894.1486	906.9792
911.0269	911.5557	918.6493
928.3854	931.2875	942.7352
943.8010	945.0949	946.3162
953.5859	954.9101	957.9510
966.2772	967.4524	971.4696
974.1489	985.4998	989.9903
992.8348	1005.0739	1016.4158
1017.6989	1019.1986	1020.6915
1028.3762	1033.1010	1034.2345
1035.7109	1039.6484	1044.6811
1047.3615	1054.9922	1058.4175
1063.1183	1074.0984	1076.8518
1086.0723	1093.1989	1103.3754
1110.8575	1113.7575	1117.9060
1119.9591	1136.9178	1137.7546
1160.7308	1165.3130	1171.2986
1171.9763	1178.8703	1183.1216
1197.2668	1199.7999	1203.3643
1205.8232	1216.8298	1217.9751
1231.8970	1235.2764	1240.7431
1250.2420	1269.5122	1273.1917

1276.6378	1292.4752	1300.0452
1311.9359	1316.6338	1320.4477
1328.8253	1340.5096	1342.0773
1342.2558	1350.3688	1367.9115
1378.1017	1378.5963	1383.0606
1385.4516	1385.5663	1388.0030
1390.7250	1394.5461	1397.8489
1397.9974	1398.7125	1398.8587
1403.9464	1414.0422	1417.0896
1422.4163	1432.6621	1443.1612
1448.5090	1450.8142	1453.1363
1455.0985	1457.2916	1458.3289
1461.0575	1465.3433	1466.6236
1467.2554	1468.1822	1470.8427
1473.0822	1473.6822	1474.5862
1475.1513	1476.2422	1477.7891
1481.1311	1483.3316	1483.6684
1486.9335	1490.0349	1490.4186
1492.1522	1494.2553	1502.1594
1517.3996	1528.1247	1531.9992
1549.1655	1622.7703	1626.3317
1631.1491	1655.8893	1657.3000
1666.3971	1670.3101	1702.1478
3041.4116	3045.5372	3045.6931
3048.8789	3050.4213	3053.6088
3055.6732	3056.6136	3056.7047
3060.1451	3060.2124	3064.6689
3070.6398	3071.3979	3075.1738
3086.6233	3117.7069	3121.4586

3125.1292	3126.1126	3139.8179
3141.9082	3142.5874	3144.9447
3145.4868	3150.3616	3153.3593
3153.4251	3155.7168	3157.3400
3159.9862	3160.5185	3161.3247
3162.1184	3162.8980	3168.2655
3168.8815	3174.7200	3175.2543
3178.8313	3179.7248	3180.9497
3183.1138	3183.5338	3188.9142
3189.7786	3195.7337	3195.8752
3197.3998	3202.4993	3203.9782
3204.5374	3214.9444	3217.1798
3223.6683	3227.5233	3554.1996

PR

Zero-point correction= 0.426235

Thermal correction to Energy= 0.449985

Thermal correction to Enthalpy= 0.450929

Thermal correction to Gibbs Free Energy= 0.373681

Sum of electronic and zero-point Energies= -1187.506863

Sum of electronic and thermal Energies= -1187.483113

Sum of electronic and thermal Enthalpies= -1187.482169

Sum of electronic and thermal Free Energies= -1187.559417

Cartesian coordinates

C	0.259927	-0.906368	-0.746327
H	0.301182	-0.484839	-1.761139
N	-1.013458	-1.593880	-0.629258
C	-1.973395	-0.483762	-0.632931
C	-3.312616	-1.017339	-0.182223

O	-3.496599	-1.541323	0.898185
O	-4.259004	-0.870371	-1.121004
C	-5.566691	-1.318538	-0.732467
H	-5.920605	-0.757906	0.136567
H	-6.212154	-1.131649	-1.588994
H	-5.554460	-2.383350	-0.490775
C	1.479398	-1.759847	-0.542150
C	2.711088	-1.308759	-1.033536
C	1.437702	-2.971869	0.152731
C	3.874783	-2.039376	-0.817976
H	2.752301	-0.377925	-1.597029
C	2.601318	-3.709238	0.359399
H	0.493786	-3.353398	0.532258
C	3.823447	-3.243793	-0.118678
H	4.821283	-1.672581	-1.205668
H	2.550293	-4.651408	0.898715
H	4.729998	-3.819763	0.046590
C	2.094507	1.649591	0.632365
C	1.049926	1.469194	-0.288903
C	1.052506	2.190836	-1.472900
C	2.082231	3.108709	-1.711924
C	3.102734	3.281203	-0.778246
C	3.127911	2.548229	0.411111
C	0.760522	0.034786	1.571903
C	0.159379	0.370180	0.204521
H	0.266432	2.041554	-2.210624
H	2.087667	3.685912	-2.631720
H	3.898775	3.993461	-0.977067
H	3.928834	2.673279	1.133737

H	2.501678	0.740085	2.524683
O	0.322978	-0.771732	2.378440
N	1.897170	0.796795	1.717541
C	-1.380252	0.576533	0.331689
H	-1.645688	0.216808	1.337879
C	-1.891740	2.012475	0.195016
H	-1.503666	2.433555	-0.744537
C	-1.388781	2.869507	1.350707
H	-1.739507	3.902570	1.257764
H	-1.758267	2.480368	2.307761
H	-0.295875	2.898770	1.406484
C	-3.414551	2.059187	0.136854
H	-3.768433	3.095015	0.137854
H	-3.813295	1.581139	-0.762611
H	-3.860677	1.562672	1.008832
H	-2.049441	-0.087539	-1.654205
H	-1.071256	-2.007072	0.304077

Vibrational frequencies

32.1638	44.1040	59.2409
65.4445	68.4032	79.9003
91.5201	101.6008	120.2798
131.3917	155.8992	163.6671
175.9403	198.9176	218.7214
225.3258	243.9271	246.4086
252.8624	269.0290	277.1846
316.5138	319.3493	351.0949
364.6988	384.4239	404.9130
413.3129	427.7900	463.5931
477.0502	496.2847	511.3148

527.9750	559.4593	572.8777
592.5374	614.4274	631.9868
640.3106	655.7480	682.8024
714.6216	719.0280	732.7210
757.5447	766.0195	771.9385
796.0247	806.5438	856.1438
858.5299	872.0940	886.4759
898.1074	915.7021	923.0467
928.0009	932.9571	947.8076
965.6857	969.3438	973.4529
979.9097	980.0414	992.3799
996.0445	1019.5052	1042.8345
1053.1936	1061.2648	1069.3200
1078.6373	1103.1438	1112.1942
1132.1497	1146.1312	1154.6468
1169.5701	1171.2246	1177.8380
1187.4318	1196.7942	1200.4444
1205.3389	1213.8723	1224.9826
1246.7240	1262.1376	1264.5058
1281.2202	1301.9001	1315.2066
1327.7192	1345.4713	1348.3557
1361.3266	1371.4042	1378.9180
1387.8469	1397.0840	1399.2827
1411.3613	1419.1080	1448.7926
1455.9333	1462.4869	1470.8978
1474.0149	1484.4790	1485.4829
1491.5680	1510.8292	1514.1469
1518.7051	1524.2456	1546.4633
1644.7955	1657.0247	1667.0912

1679.4487	1820.9308	1830.1473
3034.5608	3045.9697	3050.1807
3053.5611	3058.4955	3076.3905
3077.3427	3133.6974	3137.6343
3158.6393	3167.1487	3174.2078
3176.5702	3177.1125	3190.9785
3193.8711	3196.9513	3204.7945
3206.9117	3216.3349	3220.3989
3221.0783	3475.8010	3648.7262

PS

Zero-point correction= 0.426235

Thermal correction to Energy= 0.449985

Thermal correction to Enthalpy= 0.450929

Thermal correction to Gibbs Free Energy= 0.373681

Sum of electronic and zero-point Energies= -1187.506863

Sum of electronic and thermal Energies= -1187.483113

Sum of electronic and thermal Enthalpies= -1187.482169

Sum of electronic and thermal Free Energies= -1187.559417

Cartesian coordinates

C	-0.259927	-0.906368	-0.746327
H	-0.301182	-0.484839	-1.761139
N	1.013458	-1.593880	-0.629258
C	1.973395	-0.483762	-0.632931
C	3.312616	-1.017339	-0.182223
O	3.496599	-1.541323	0.898185
O	4.259004	-0.870371	-1.121004
C	5.566691	-1.318538	-0.732467
H	5.920605	-0.757906	0.136567

H	6.212154	-1.131649	-1.588994
H	5.554460	-2.383350	-0.490775
C	-1.479398	-1.759847	-0.542150
C	-2.711088	-1.308759	-1.033536
C	-1.437702	-2.971869	0.152731
C	-3.874783	-2.039376	-0.817976
H	-2.752301	-0.377925	-1.597029
C	-2.601318	-3.709238	0.359399
H	-0.493786	-3.353398	0.532258
C	-3.823447	-3.243793	-0.118678
H	-4.821283	-1.672581	-1.205668
H	-2.550293	-4.651408	0.898715
H	-4.729998	-3.819763	0.046590
C	-2.094507	1.649591	0.632365
C	-1.049926	1.469194	-0.288903
C	-1.052506	2.190836	-1.472900
C	-2.082231	3.108709	-1.711924
C	-3.102734	3.281203	-0.778246
C	-3.127911	2.548229	0.411111
C	-0.760522	0.034786	1.571903
C	-0.159379	0.370180	0.204521
H	-0.266432	2.041554	-2.210624
H	-2.087667	3.685912	-2.631720
H	-3.898775	3.993461	-0.977067
H	-3.928834	2.673279	1.133737
H	-2.501678	0.740085	2.524683
O	-0.322978	-0.771732	2.378440
N	-1.897170	0.796795	1.717541
C	1.380252	0.576533	0.331689

H	1.645688	0.216808	1.337879
C	1.891740	2.012475	0.195016
H	1.503666	2.433555	-0.744536
C	1.388781	2.869507	1.350707
H	1.739507	3.902570	1.257764
H	1.758267	2.480368	2.307761
H	0.295875	2.898770	1.406484
C	3.414551	2.059187	0.136854
H	3.768433	3.095015	0.137854
H	3.813295	1.581139	-0.762611
H	3.860677	1.562672	1.008832
H	2.049441	-0.087539	-1.654205
H	1.071256	-2.007072	0.304077

Vibrational frequencies

32.1638	44.1040	59.2409
65.4446	68.4032	79.9004
91.5201	101.6008	120.2798
131.3917	155.8992	163.6671
175.9403	198.9176	218.7214
225.3258	243.9271	246.4086
252.8624	269.0290	277.1846
316.5138	319.3493	351.0949
364.6988	384.4239	404.9130
413.3129	427.7900	463.5931
477.0502	496.2847	511.3149
527.9750	559.4593	572.8777
592.5374	614.4274	631.9868
640.3106	655.7480	682.8024
714.6216	719.0280	732.7210

757.5447	766.0195	771.9385
796.0247	806.5438	856.1438
858.5299	872.0940	886.4759
898.1074	915.7021	923.0467
928.0009	932.9571	947.8076
965.6857	969.3438	973.4529
979.9097	980.0414	992.3799
996.0445	1019.5053	1042.8345
1053.1936	1061.2648	1069.3200
1078.6373	1103.1438	1112.1942
1132.1496	1146.1312	1154.6468
1169.5700	1171.2246	1177.8380
1187.4318	1196.7942	1200.4444
1205.3388	1213.8723	1224.9826
1246.7240	1262.1376	1264.5058
1281.2202	1301.9001	1315.2066
1327.7192	1345.4713	1348.3557
1361.3266	1371.4042	1378.9180
1387.8469	1397.0840	1399.2827
1411.3613	1419.1080	1448.7926
1455.9333	1462.4869	1470.8978
1474.0149	1484.4790	1485.4829
1491.5680	1510.8292	1514.1469
1518.7051	1524.2456	1546.4633
1644.7955	1657.0247	1667.0912
1679.4487	1820.9308	1830.1473
3034.5608	3045.9697	3050.1807
3053.5611	3058.4955	3076.3905
3077.3427	3133.6974	3137.6343

3158.6393	3167.1487	3174.2078
3176.5702	3177.1125	3190.9786
3193.8711	3196.9513	3204.7945
3206.9116	3216.3349	3220.3989
3221.0783	3475.8010	3648.7262