

Enantioselective [4+1] Annulation Reactions of α -Substituted Ammonium Ylides to Construct Spirocyclic Oxindoles

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Supporting Information

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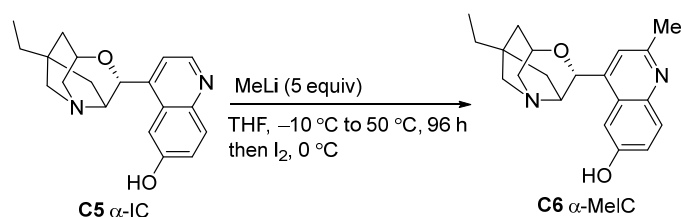
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1. General methods

^1H NMR and ^{13}C NMR data were obtained on an Agilent 600 MHz operating at 600 MHz and 150 MHz, respectively. Chemical shifts are given in parts per million (δ) from tetramethylsilane with the solvent resonance as the internal standard in CDCl_3 solution. Data are presented as follows: chemical shift, integration, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet) and coupling constant in Hertz (Hz). The ee value determination was carried out using chiral high performance liquid chromatography (HPLC) with Daicel Chiracel chiral columns IA Column (250×4.6 mm), Chiralpak IE Column (250×4.6 mm), Chiralpak IF Column (250×4.6 mm) or Chiralpak OD-H Column (250×4.6 mm). UV detection was monitored at 254 nm by Waters with a 2996 UV-detector. ESI-HRMS was recorded on a Bruker Apex-2. Optical rotation data were examined in CHCl_3 solution at 20 °C on Autopol-IV Automatic Polarimeter. Melting point was detected on Buchi M-560. Column chromatography was performed on silica gel (300-400 mesh) eluting with ethyl acetate (EA) and petroleum ether (PE) and dichloromethane (CH_2Cl_2). TLC was performed on glass-backed silica plates. UV light and I_2 were used to visualize products. All chemicals were used without purification as commercially available unless otherwise noted. THF, EA, PE, CH_2Cl_2 , MeCN and toluene were freshly distilled before use. Catalysts **C2** was commercially available. Catalysts **C1**,^{1a} **C3**,^{1b} **C4**,^{1b} **C5**^{1b} were prepared according to the literature procedures. 1-Azadienes were prepared according to the literature procedure.² 3-Bromooxindoles were prepared according to the literature.³

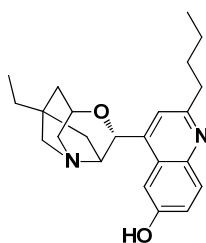
- (1) (a) Jaric, M.; Haag, B. A.; Manolikakes, S. M.; Knochel, P. *Org. Lett.* **2011**, *13*, 2306. (b) Nakamoto, Y.; Urabe, F.; Takahashi, K.; Ishihara, J.; Hatakeyama, S. *Chem. –Eur. J.* **2013**, *19*, 1265.
- (2) (a) Liu, H.; Zhang, Q.; Wang, L.; Tong, X. *Chem. –Eur. J.* **2010**, *16*, 1968. (b) Morales, S.; Guijarro, F. G.; Ruano, J. L. G.; Cid, M. B. *J. Am. Chem. Soc.* **2014**, *136*, 1082.
- (3) Li, J.; Du, T.; Zhang, G.; Peng, Y. *Chem. Commun.* **2013**, *49*, 1330.

2. Preparation of 2'-substituted catalysts⁴

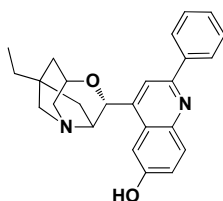


Under an argon atmosphere condition, $\alpha\text{-IC}$ **C5** (1.24 g, 4 mmol) was dissolved in dry THF (48

mL) and cooled to $-10\text{ }^{\circ}\text{C}$ in an ice/EtOH bath. Methyllithium (1.6 M, 12.5 mL, 20 mmol) was added and the reaction mixture was stirred for 30 min. Then it was warmed to $50\text{ }^{\circ}\text{C}$ and stirred until **C5** was consumed (96 h). It was cooled to $0\text{ }^{\circ}\text{C}$ before iodine (3 g, 12 mmol) was added. After 15 min, the mixture was quenched with saturated aqueous sodium thiosulfate (40 mL). The aqueous phase was extracted with CH_2Cl_2 (20 mL $\times$ 3). The collected organic phases were dried over anhydrous MgSO_4 , followed by filtration, evaporation and purification by column chromatography ($\text{CH}_2\text{Cl}_2/\text{MeOH} = 60/1$) to give α -MeIC **C6** as a white solid (300 mg, 23% yield; *the synthetic procedure has not been further optimized*); mp $164\text{--}165\text{ }^{\circ}\text{C}$; $[\alpha]_{\text{D}}^{20} = -39.0$ ($c = 0.8$ in CHCl_3); ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.87 (d, $J = 7.8$ Hz, 1H), 7.78 (s, 1H), 7.43 (s, 1H), 7.19 (d, $J = 7.8$ Hz, 1H), 5.86 (s, 1H), 4.43 (s, 1H), 4.04 (dd, $J = 22.7, 12.2$ Hz, 2H), 2.95–2.88 (m, 2H), 2.84 (d, $J = 10.8$ Hz, 1H), 2.71 (s, 3H), 2.02 (d, $J = 13.9$ Hz, 1H), 1.88 (d, $J = 12.6$ Hz, 2H), 1.44 (d, $J = 5.9$ Hz, 2H), 1.19 (t, $J = 11.0$ Hz, 1H), 0.90 (t, $J = 7.5$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 155.61, 155.32, 142.85, 142.68, 130.43, 124.88, 121.58, 119.02, 105.94, 69.71, 68.13, 66.67, 64.12, 53.10, 42.83, 41.67, 37.00, 29.08, 25.24, 9.36; ESI-HRMS: calcd. for $\text{C}_{20}\text{H}_{24}\text{N}_2\text{O}_2 + \text{H}^+$ 325.1911, found 325.1912.

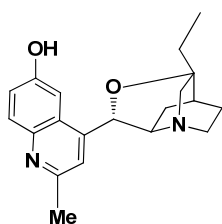


Catalyst **C7** was prepared according to the same procedure using *n*-butyllithium as the alkylation reagent for 48 h in 35% yield. A yellow solid; mp $217\text{--}219\text{ }^{\circ}\text{C}$; $[\alpha]_{\text{D}}^{20} = -13.7$ ($c = 1.0$ in CHCl_3); ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.96 (d, $J = 9.0$ Hz, 1H), 7.44 (s, 1H), 7.39–7.29 (m, 2H), 5.94 (s, 1H), 4.92 (d, $J = 10.5$ Hz, 1H), 4.80 (d, $J = 11.0$ Hz, 2H), 3.80 (d, $J = 10.7$ Hz, 1H), 3.60 (d, $J = 13.3$ Hz, 1H), 3.28 (d, $J = 10.9$ Hz, 1H), 2.96 (t, $J = 7.8$ Hz, 2H), 2.36 (br, 1H), 2.17 (d, $J = 14.3$ Hz, 1H), 2.09 (d, $J = 12.5$ Hz, 1H), 1.93 (d, $J = 14.5$ Hz, 1H), 1.77 (dd, $J = 15.5, 7.0$ Hz, 3H), 1.65–1.52 (m, 2H), 1.43 (dd, $J = 14.8, 7.3$ Hz, 2H), 0.95 (t, $J = 7.4$ Hz, 6H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 159.58, 155.17, 143.28, 139.58, 131.29, 124.19, 122.03, 118.84, 103.59, 70.13, 68.83, 68.31, 67.81, 56.67, 43.12, 40.03, 38.71, 36.21, 32.26, 28.60, 22.62, 13.99, 8.86; ESI-HRMS: calcd. for $\text{C}_{23}\text{H}_{30}\text{N}_2\text{O}_2 + \text{H}^+$ 367.2381, found 367.2386.



Catalyst **C8** was prepared according to the same procedure using phenyllithium as phenylation reagent for 48 h in 40% yield. Brown oil; $[\alpha]_{\text{D}}^{20} = +36.0$ ($c = 0.5$ in CHCl_3); ^1H NMR (600 MHz, CDCl_3): δ (ppm) 8.00 (s, 1H), 7.93 (t, $J = 8.3$

Hz, 3H), 7.76 (s, 2H), 7.36 (d, $J = 6.7$ Hz, 3H), 5.70 (s, 1H), 4.73 (d, $J = 9.9$ Hz, 1H), 4.52 (s, 2H), 3.60 (d, $J = 13.5$ Hz, 1H), 3.32 (s, 2H), 2.70 (br, 1H), 1.89 (s, 2H), 1.79 (d, $J = 12.0$ Hz, 1H), 1.53 (t, $J = 10.9$ Hz, 1H), 1.35 (d, $J = 6.9$ Hz, 2H), 0.73 (t, $J = 7.0$ Hz, 3H); ^{13}C NMR (150 MHz, DMSO): δ (ppm) 154.90, 152.69, 144.92, 143.17, 139.07, 131.23, 129.94, 129.32, 127.55, 125.21, 124.38, 116.38, 112.22, 67.84, 67.16, 65.41, 63.63, 51.73, 42.43, 34.93, 27.85, 25.91, 9.17; ESI-HRMS: calcd. for $\text{C}_{25}\text{H}_{26}\text{N}_2\text{O}_2 + \text{H}^+$ 387.2068, found 387.2072.

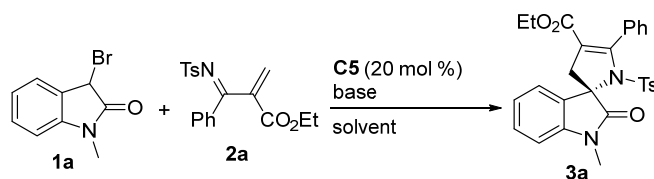


Catalyst **C9** was prepared from β -ICD according to the same procedure using methyllithium as alkylation reagent for 96 h in 15% yield. A brown solid; mp 185–187 °C; $[\alpha]_{\text{D}}^{20} = -52.2$ ($c = 1.0$ in CHCl_3); ^1H NMR (600 MHz, CDCl_3): δ (ppm) 8.04 (s, 1H), 7.87 (d, $J = 9.0$ Hz, 1H), 7.50 (s, 1H), 7.19 (dd, $J = 9.0, 1.7$

Hz, 1H), 5.99 (s, 1H), 3.73 (d, $J = 13.5$ Hz, 1H), 3.53 (d, $J = 6.0$ Hz, 1H), 3.28–3.18 (m, 1H), 3.10 (d, $J = 11.8$ Hz, 1H), 2.80 (d, $J = 13.6$ Hz, 1H), 2.71 (s, 3H), 2.22 (s, 1H), 1.88 (dd, $J = 12.3, 6.3$ Hz, 1H), 1.76 (t, $J = 10.0$ Hz, 1H), 1.70 (dd, $J = 15.2, 7.8$ Hz, 2H), 1.67–1.58 (m, 1H), 1.26 (dd, $J = 12.7, 6.2$ Hz, 1H), 1.03 (t, $J = 7.4$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 155.73, 155.04, 142.74, 141.91, 130.17, 125.30, 121.92, 119.69, 106.53, 76.98, 72.48, 56.40, 53.79, 46.45, 32.94, 27.43, 25.20, 23.16, 23.07, 7.37; ESI-HRMS: calcd. for $\text{C}_{20}\text{H}_{24}\text{N}_2\text{O}_2 + \text{H}^+$ 325.1911, found 325.1923.

(4) Johansson, C. C. C.; Bremeyer, N.; Ley, S. V.; Owen, D. R.; Smith, S. C.; Gaunt, M. J. *Angew. Chem., Int. Ed.* **2006**, *45*, 6024.

3. More screening conditions for enantioselective [4+1] annulation reaction^a

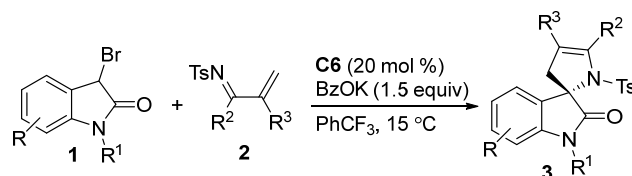


entry	catalyst	base	solvent	t (h)	T (°C)	yield ^b (%)	ee ^c (%)
1	C5	AcOK	PhCF_3	80	0	60	51
2	C5	AcOK	PhCF_3	14	25	75	79
3	C5	AcOK	PhCF_3	5	55	78	59
4	C5	BzOK	CH_3CN	48	15	65	73
5	C5	BzOK	toluene	48	15	60	84

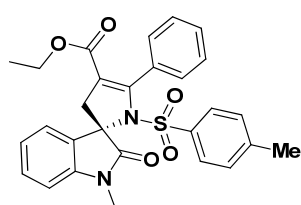
6	C5	BzOK	1,4-dioxane	48	15	30	30
7	C5	BzOK	THF	48	15	<20	/
8	C5	BzOK	CHCl ₃	36	15	64	86
9	C5	AcOLi	PhCF ₃	72	35	40	71
10	C5	4-NO ₂ BzOK	PhCF ₃	24	35	64	73
11	C5	4-MeOBzOK	PhCF ₃	12	35	65	86
12 ^d	C5	BzOK	PhCF ₃	48	15	73	89
13 ^e	C5	BzOK	PhCF ₃	40	15	71	86
14 ^f	C5	BzOK	PhCF ₃	48	15	68	89

^a Unless noted otherwise, reactions were performed with **1a** (0.05 mmol), **2a** (0.05 mmol), catalyst (20 mol %), base (0.05 mmol) in solvent (0.5 mL). ^b Yield of isolated product. ^c Determined by chiral HPLC analysis. ^d With 0.075 mmol of **2a** and base. ^e With 0.25 mL solvent. ^f With **1a** (0.75 mmol.), **2a** (0.05 mmol), catalyst (10 mol %), base (0.075) in 0.5 mL solvent.

4. General procedure for enantioselective [4+1] annulation reaction



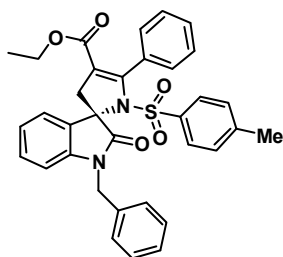
To a mixture of 3-bromooxindole **1** (0.15 mmol), tertiary amine **C6** (20 mol %) and BzOK (0.15 mmol) in PhCF₃ (2 mL) was added 1-azadiene **2** (0.1 mmol) in three portions (generally at 0 h, 12 h, 24 h, respectively). The mixture was stirred at 15 °C. After completion, the mixture was directly subjected to column chromatography using (EtOAc/petroleum ether/DCM = 3:20:3) as eluent to give the product **3**. The corresponding racemic product (for HPLC analysis) was prepared using DABCO (30 mol %) as the catalyst.



(S)-Ethyl-1-methyl-2-oxo-5'-phenyl-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3a). White solid; 75% yield; $[\alpha]_{\text{D}}^{20} = -4.3$ ($c = 1.75$ in CHCl₃); 98% ee, determined by HPLC analysis on Daicel chiralpak IA, *n*-hexane/*i*-PrOH = 80/20, 1 mL/min, $\lambda = 254$ nm, T = 25

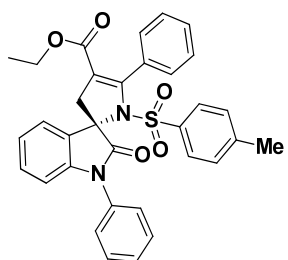
°C, $t_{\text{minor}} = 8.438$ min, $t_{\text{major}} = 11.304$ min; ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.58 (d, $J = 7.3$ Hz, 1H), 7.38 (t, $J = 7.8$ Hz, 2H), 7.31 (t, $J = 7.5$ Hz, 1H), 7.28-7.24 (m, 1H), 7.15 (dd, $J = 16.3, 7.9$ Hz, 3H), 6.96 (d, $J = 8.1$ Hz, 2H), 6.91 (d, $J = 7.7$ Hz, 2H), 6.59 (d, $J = 7.5$ Hz, 1H), 3.87 (q, $J = 7.1$ Hz,

2H), 3.50 (d, $J = 15.8$ Hz, 1H), 3.31 (s, 3H), 3.04 (d, $J = 15.8$ Hz, 1H), 2.32 (s, 3H), 0.87 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 176.22, 163.99, 152.01, 143.83, 142.41, 136.62, 131.59, 130.54, 129.92, 129.07, 128.98, 128.75, 128.36, 126.96, 123.27, 122.46, 108.86, 108.77, 70.97, 59.77, 41.36, 26.86, 21.55, 13.72; ESI-HRMS: calcd. for $\text{C}_{28}\text{H}_{26}\text{N}_2\text{O}_5\text{S}+\text{Na}^+$ 525.1455, found 525.1470.



(S)-Ethyl-1-benzyl-2-oxo-5'-phenyl-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3b). Red solid; 54% yield; $[\alpha]_{\text{D}}^{20} = -7.5$ ($c = 0.4$ in CHCl_3); 90% ee, determined by HPLC analysis on Daicel chiralpak IF, n -hexane/ i -PrOH = 80/20, 1 mL/min, $\lambda = 254$ nm, $T = 25$ °C, $t_{\text{minor}} = 19.595$ min, $t_{\text{major}} = 23.472$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.60

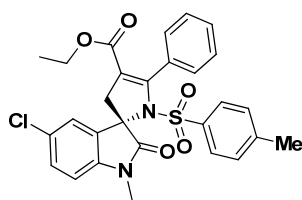
(d, $J = 7.3$ Hz, 1H), 7.45 (d, $J = 7.4$ Hz, 1H), 7.41 (d, $J = 7.6$ Hz, 2H), 7.33-7.28 (m, 5H), 7.24 (d, $J = 7.9$ Hz, 3H), 7.12 (t, $J = 7.5$ Hz, 1H), 7.00 (d, $J = 8.1$ Hz, 2H), 6.93 (t, $J = 7.4$ Hz, 1H), 6.74 (d, $J = 7.8$ Hz, 1H), 6.61 (d, $J = 7.5$ Hz, 1H), 5.05 (s, 2H), 3.94-3.82 (m, 2H), 3.58 (d, $J = 15.7$ Hz, 1H), 3.10 (d, $J = 15.7$ Hz, 1H), 2.35 (s, 3H), 0.90 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 176.41, 163.99, 152.15, 143.86, 141.32, 136.66, 135.42, 131.74, 130.56, 129.88, 129.69, 129.08, 129.01, 128.78, 128.44, 127.56, 127.22, 126.97, 123.34, 122.39, 110.03, 108.64, 71.11, 59.80, 44.48, 41.94, 21.54, 13.73; ESI-HRMS: calcd. for $\text{C}_{34}\text{H}_{30}\text{N}_2\text{O}_5\text{S}+\text{Na}^+$ 601.1768, found 601.1781.



(S)-Ethyl-2-oxo-1,5'-diphenyl-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3c). Colourless oil; 60% yield; $[\alpha]_{\text{D}}^{20} = +2.5$ ($c = 0.20$ in CHCl_3); 90% ee, determined by HPLC analysis on Daicel chiralpak IE, n -hexane/ i -PrOH = 80/20, 0.8 mL/min, $\lambda = 254$ nm, $T = 25$ °C, $t_{\text{major}} = 39.208$ min, $t_{\text{minor}} = 43.261$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.67

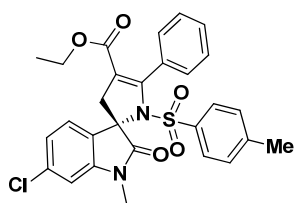
(d, $J = 7.2$ Hz, 1H), 7.57-7.51 (m, 3H), 7.50-7.41 (m, 3H), 7.37 (dd, $J = 14.7, 7.3$ Hz, 1H), 7.33-7.27 (m, 2H), 7.21 (t, $J = 8.5$ Hz, 2H), 7.18 (dd, $J = 7.7, 3.7$ Hz, 1H), 6.97 (d, $J = 8.4$ Hz, 2H), 6.92 (t, $J = 7.6$ Hz, 1H), 6.83 (d, $J = 7.9$ Hz, 1H), 6.58 (d, $J = 7.5$ Hz, 1H), 3.90 (q, $J = 7.1$ Hz, 2H), 3.65 (d, $J = 15.8$ Hz, 1H), 3.20 (d, $J = 15.8$ Hz, 1H), 2.34 (s, 3H), 0.91 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 175.91, 164.02, 151.99, 143.89, 142.73, 136.55, 134.56, 131.29, 130.55, 129.85, 129.72, 129.09, 129.01, 128.80, 128.43, 127.16, 126.98, 126.01, 123.73, 122.79,

110.09, 108.68, 71.11, 59.83, 41.57, 21.55, 13.75; ESI-HRMS: calcd. for $C_{33}H_{28}N_2O_5S+Na^+$ 587.1612, found 587.1622.



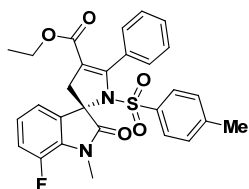
(S)-Ethyl-5-chloro-1-methyl-2-oxo-5'-phenyl-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3d). Brown oil; 71% yield; $[\alpha]_D^{20} = -13.0$ ($c = 0.3$ in $CHCl_3$); 89% ee, determined by HPLC analysis on Daicel chiralpak IA, n -hexane/ i -PrOH = 90/10, 0.5 mL/min, $\lambda = 254$ nm,

$T = 25$ °C, $t_{minor} = 24.474$ min, $t_{major} = 38.007$ min; 1H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.50 (s, 1H), 7.40 (s, 1H), 7.38-7.32 (m, 2H), 7.28 (s, 1H), 7.15 (d, $J = 8.1$ Hz, 2H), 6.98 (d, $J = 8.2$ Hz, 2H), 6.93 (s, 1H), 6.84 (d, $J = 8.3$ Hz, 1H), 6.61 (d, $J = 7.5$ Hz, 1H), 3.87 (d, $J = 7.1$ Hz, 2H), 3.49 (d, $J = 16.0$ Hz, 1H), 3.30 (s, 3H), 3.02 (d, $J = 15.9$ Hz, 1H), 2.34 (s, 3H), 0.88 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 175.82, 163.81, 151.92, 144.06, 141.04, 136.35, 132.91, 130.59, 129.88, 129.04, 128.89, 128.52, 128.34, 127.18, 126.98, 123.05, 109.88, 108.71, 70.64, 59.88, 41.31, 26.97, 21.54, 13.69; ESI-HRMS: calcd. for $C_{28}H_{25}N_2ClO_5S+Na^+$ 559.1065, found 559.1072.



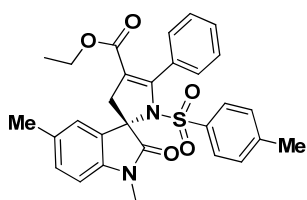
(S)-Ethyl-6-chloro-1-methyl-2-oxo-5'-phenyl-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3e). Yellow solid; 61% yield; $[\alpha]_D^{20} = +1.4$ ($c = 0.25$ in $CHCl_3$); 89% ee, determined by HPLC analysis on Daicel chiralpak IE, n -hexane/ i -PrOH = 60/40, 0.5 mL/min, $\lambda = 254$

nm, $T = 25$ °C, $t_{major} = 26.661$ min, $t_{minor} = 29.791$ min; 1H NMR (600 MHz, $CDCl_3$): δ (ppm) 7.51 (d, $J = 7.9$ Hz, 1H), 7.40 (d, $J = 7.5$ Hz, 1H), 7.33 (t, $J = 7.5$ Hz, 1H), 7.28 (d, $J = 7.4$ Hz, 1H), 7.19 (d, $J = 8.1$ Hz, 2H), 7.15-7.12 (m, 1H), 6.99 (d, $J = 8.2$ Hz, 2H), 6.93-6.88 (m, 2H), 6.56 (d, $J = 7.5$ Hz, 1H), 3.92-3.82 (m, 2H), 3.49 (d, $J = 15.9$ Hz, 1H), 3.31 (s, 3H), 3.02 (d, $J = 15.9$ Hz, 1H), 2.34 (s, 3H), 0.88 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ (ppm) 176.24, 163.86, 151.89, 144.01, 143.70, 136.37, 135.69, 130.50, 129.96, 129.78, 129.04, 128.82, 128.33, 127.16, 123.40, 123.11, 109.72, 108.69, 70.46, 59.85, 41.28, 26.98, 21.54, 13.69; ESI-HRMS: calcd. for $C_{28}H_{25}N_2ClO_5S+Na^+$ 559.1065, found 559.1083.



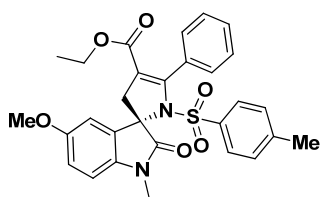
(S)-Ethyl-7-fluoro-1-methyl-2-oxo-5'-phenyl-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3f). Yellow solid; 62% yield; $[\alpha]_D^{20} =$

-6.5 (c = 0.2 in CHCl₃); 82% ee, determined by HPLC analysis on Daicel chiralpak IA, *n*-hexane/*i*-PrOH = 80/20, 0.8 mL/min, λ = 254 nm, T = 25 °C, t_{major} = 7.799 min, t_{minor} = 9.907 min; ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.41 (t, J = 7.2 Hz, 2H), 7.34 (t, J = 7.2 Hz, 1H), 7.29 (d, J = 7.2 Hz, 1H), 7.20 (d, J = 8.0 Hz, 2H), 7.14-7.08 (m, 2H), 6.99 (d, J = 8.0 Hz, 2H), 6.91 (t, J = 7.4 Hz, 1H), 6.56 (d, J = 7.7 Hz, 1H), 3.88 (q, J = 7.1 Hz, 2H), 3.53 (s, 3H), 3.50 (d, J = 15.9 Hz, 1H), 3.04 (d, J = 15.9 Hz, 1H), 2.35 (s, 3H), 0.88 (t, J = 7.1 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 176.06, 163.87, 151.90, 148.74, 147.12 (d, $^1J_{\text{C,F}}$ = 244.7 Hz) 143.99, 136.41, 134.42, 130.52, 129.80, 129.03, 128.87, 128.81, 128.38, 127.15, 126.97 (d, $^2J_{\text{C,F}}$ = 26.5 Hz), 124.04, 124.00 (d, $^3J_{\text{C,F}}$ = 6.3 Hz), 118.28, 118.26 (d, $^3J_{\text{C,F}}$ = 3.2 Hz), 117.94, 117.81 (d, $^2J_{\text{C,F}}$ = 19.3 Hz), 108.66, 70.82, 59.84, 41.54, 29.44, 21.54, 13.69; ESI-HRMS: calcd. for C₂₈H₂₅FN₂O₅S+Na⁺ 543.1361, found 543.1373.



(S)-Ethyl-1,5-dimethyl-2-oxo-5'-phenyl-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate(3g). Orange solid; 70% yield; $[\alpha]_{\text{D}}^{20}$ = -26.0 (c = 0.6 in CHCl₃); 99% ee, determined by HPLC analysis on Daicel chiralpak IA, *n*-hexane/*i*-PrOH = 90/10, 1 mL/min, λ = 254 nm, T = 25 °C,

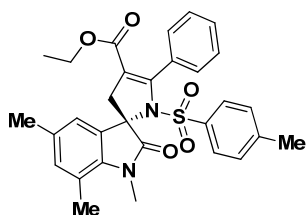
t_{minor} = 12.188 min, t_{major} = 16.455 min; ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.43 (d, J = 7.5 Hz, 1H), 7.37-7.32 (m, 2H), 7.28 (t, J = 7.4 Hz, 1H), 7.18 (d, J = 8.2 Hz, 3H), 6.97 (d, J = 8.3 Hz, 2H), 6.94 (t, J = 7.5 Hz, 1H), 6.81 (d, J = 7.9 Hz, 1H), 6.62 (d, J = 7.6 Hz, 1H), 3.88 (q, J = 7.1 Hz, 2H), 3.50 (d, J = 15.8 Hz, 1H), 3.30 (s, 3H), 3.03 (d, J = 15.8 Hz, 1H), 2.39 (s, 3H), 2.34 (s, 3H), 0.89 (t, J = 7.1 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 176.15, 164.07, 152.03, 143.79, 140.03, 136.68, 132.85, 131.56, 130.54, 130.17, 129.93, 129.13, 128.93, 128.38, 127.07, 123.22, 108.74, 108.61, 71.07, 59.76, 41.43, 26.86, 21.52, 21.18, 13.71; ESI-HRMS: calcd. for C₂₉H₂₈N₂O₅S+Na⁺ 539.1612, found 539.1617.



(S)-Ethyl-5-methoxy-1-methyl-2-oxo-5'-phenyl-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3h). Brown solid; 66% yield; $[\alpha]_{\text{D}}^{20}$ = -11.8 (c = 0.45 in CHCl₃); 96% ee, determined by HPLC analysis on Daicel chiralpak IA, *n*-hexane/*i*-PrOH = 80/20, 1 mL/min, λ

= 254 nm, T = 25 °C, t_{minor} = 8.236 min, t_{major} = 19.312 min; ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.41 (d, J = 7.5 Hz, 1H), 7.34 (t, J = 7.5 Hz, 1H), 7.28 (t, J = 7.5 Hz, 1H), 7.21 (d, J = 8.2 Hz, 2H),

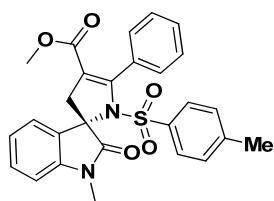
7.18 (d, $J = 2.4$ Hz, 1H), 6.98 (d, $J = 8.2$ Hz, 2H), 6.95-6.88 (m, 2H), 6.82 (d, $J = 8.5$ Hz, 1H), 6.60 (d, $J = 7.6$ Hz, 1H), 3.88 (q, $J = 7.1$ Hz, 2H), 3.84 (s, 3H), 3.51 (d, $J = 15.9$ Hz, 1H), 3.30 (s, 3H), 3.04 (d, $J = 15.9$ Hz, 1H), 2.34 (s, 3H), 0.89 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 175.91, 163.97, 156.39, 152.02, 143.82, 136.66, 135.82, 132.70, 130.56, 129.87, 128.96, 128.77, 128.39, 127.10, 113.86, 110.11, 109.23, 108.73, 71.24, 59.77, 55.86, 41.41, 26.92, 21.52, 13.72; ESI-HRMS: calcd. for $\text{C}_{29}\text{H}_{28}\text{N}_2\text{O}_6\text{S}+\text{Na}^+$ 555.1561, found 555.1569.



(S)-Ethyl-1,5,7-trimethyl-2-oxo-5'-phenyl-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3i). Yellow solid; 74% yield;

$[\alpha]_{\text{D}}^{20} = -19.3$ ($c = 0.8$ in CHCl_3); 99% ee, determined by HPLC analysis on Daicel chiralpak IA, n -hexane/ i -PrOH = 60/40, 1 mL/min, $\lambda = 254$ nm,

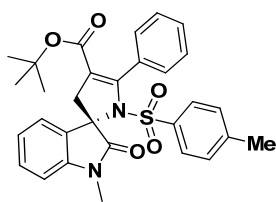
$T = 25$ °C, $t_{\text{major}} = 15.381$ min, $t_{\text{minor}} = 24.681$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.42 (d, $J = 7.5$ Hz, 1H), 7.33 (t, $J = 7.5$ Hz, 1H), 7.28 (t, $J = 7.4$ Hz, 1H), 7.19 (d, $J = 8.1$ Hz, 3H), 6.98 (d, $J = 8.2$ Hz, 2H), 6.96-6.90 (m, 2H), 6.62 (d, $J = 7.6$ Hz, 1H), 3.88 (q, $J = 7.1$ Hz, 2H), 3.57 (s, 3H), 3.48 (d, $J = 15.8$ Hz, 1H), 3.00 (d, $J = 15.8$ Hz, 1H), 2.56 (s, 3H), 2.34 (d, $J = 3.3$ Hz, 6H), 0.89 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 177.02, 164.09, 152.00, 143.72, 137.63, 136.77, 134.09, 132.74, 130.49, 129.97, 129.16, 128.91, 128.73, 128.40, 127.06, 121.03, 120.18, 108.58, 70.73, 59.72, 41.85, 30.26, 21.52, 20.86, 18.93, 13.71; ESI-HRMS: calcd. for $\text{C}_{30}\text{H}_{30}\text{N}_2\text{O}_5\text{S}+\text{Na}^+$ 553.1768, found 553.1779.



(S)-Methyl-1-methyl-2-oxo-5'-phenyl-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3j). White solid; 74% yield; $[\alpha]_{\text{D}}^{20} = -5.3$ ($c = 0.4$ in CHCl_3); 99% ee, determined by HPLC analysis on Daicel chiralpak

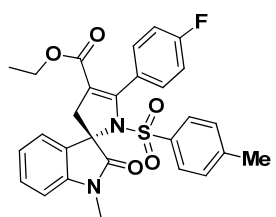
IE, n -hexane/ i -PrOH = 60/40, 1 mL/min, $\lambda = 254$ nm, $T = 25$ °C, $t_{\text{major}} = 18.248$ min, $t_{\text{minor}} = 19.914$ min;

^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.57 (d, $J = 7.3$ Hz, 1H), 7.39 (dd, $J = 14.1, 6.9$ Hz, 2H), 7.33 (t, $J = 7.5$ Hz, 1H), 7.28 (t, $J = 7.4$ Hz, 1H), 7.15 (dd, $J = 14.5, 7.8$ Hz, 3H), 6.97 (d, $J = 8.1$ Hz, 2H), 6.95-6.89 (m, 2H), 6.59 (d, $J = 7.5$ Hz, 1H), 3.50 (d, $J = 15.8$ Hz, 1H), 3.44 (s, 3H), 3.32 (s, 3H), 3.03 (d, $J = 15.8$ Hz, 1H), 2.33 (s, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 176.17, 164.31, 152.54, 143.86, 142.41, 136.56, 131.53, 130.46, 129.95, 129.76, 128.99, 128.87, 128.35, 127.06, 123.29, 122.43, 108.87, 108.26, 71.05, 51.10, 41.30, 26.87, 21.54; ESI-HRMS: calcd. for $\text{C}_{27}\text{H}_{24}\text{N}_2\text{O}_5\text{S}+\text{Na}^+$ 511.1299, found 511.1301.



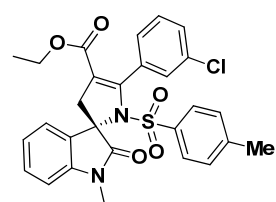
(S)-tert-Butyl-1-methyl-2-oxo-5'-phenyl-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3k). White solid; 67% yield; $[\alpha]_{\text{D}}^{20} = +26.3$ ($c = 0.3$ in CHCl_3); 93% ee, determined by HPLC analysis on Daicel chiralpak IE, n -hexane/ i -PrOH = 60/40, 0.5 mL/min, $\lambda = 254$ nm, $T = 25$ °C,

$t_{\text{minor}} = 24.216$ min, $t_{\text{major}} = 28.299$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.59 (d, $J = 7.3$ Hz, 1H), 7.41-7.35 (m, 2H), 7.32-7.26 (m, 1H), 7.23 (d, $J = 7.4$ Hz, 1H), 7.14 (dd, $J = 7.5, 4.9$ Hz, 3H), 6.95 (d, $J = 8.1$ Hz, 2H), 6.90 (t, $J = 8.0$ Hz, 2H), 6.59 (d, $J = 7.5$ Hz, 1H), 3.46 (d, $J = 15.9$ Hz, 1H), 3.31 (s, 3H), 2.99 (d, $J = 15.9$ Hz, 1H), 2.32 (s, 3H), 1.06 (s, 9H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 176.38, 163.51, 150.40, 143.66, 142.43, 136.78, 131.71, 130.78, 130.04, 129.83, 129.56, 128.93, 128.32, 126.91, 123.21, 122.52, 110.62, 108.82, 80.10, 70.68, 41.57, 27.69, 26.85, 21.51; ESI-HRMS: calcd. for $\text{C}_{30}\text{H}_{30}\text{N}_2\text{O}_5\text{S}+\text{Na}^+$ 553.1768, found 553.1769.



(S)-Ethyl-5'-(4-fluorophenyl)-1-methyl-2-oxo-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3l). White solid; 73% yield; $[\alpha]_{\text{D}}^{20} = -6.0$ ($c = 0.1$ in CHCl_3); 96% ee, determined by HPLC analysis on Daicel chiralpak IA, n -hexane/ i -PrOH = 80/20, 1mL/min, $\lambda = 254$ nm, $T = 25$ °C,

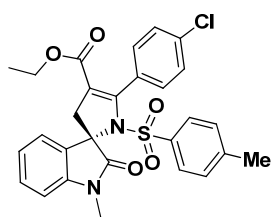
$t_{\text{minor}} = 8.661$ min, $t_{\text{major}} = 13.223$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.57 (d, $J = 7.2$ Hz, 1H), 7.40 (t, $J = 6.6$ Hz, 2H), 7.25 (d, $J = 11.8$ Hz, 2H), 7.20-7.14 (m, 2H), 7.04 (d, $J = 7.4$ Hz, 2H), 6.93 (d, $J = 7.5$ Hz, 1H), 6.65-6.56 (m, 2H), 3.89 (q, $J = 7.1$ Hz, 2H), 3.50 (d, $J = 15.9$ Hz, 1H), 3.33 (s, 3H), 3.05 (d, $J = 15.9$ Hz, 1H), 2.36 (s, 3H), 0.94 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 176.16, 163.88, 162.17, 150.93, 144.15, 142.39 (d, $^1J_{\text{C,F}} = 264.8$ Hz), 136.61, 132.58, 132.52 (d, $^3J_{\text{C,F}} = 8.5$ Hz), 132.00, 131.95 (d, $^3J_{\text{C,F}} = 8.5$ Hz), 131.49, 130.10, 130.01, 129.07, 128.27, 124.97, 124.95 (d, $^4J_{\text{C,F}} = 3.5$ Hz), 123.34, 122.42, 114.42, 114.28, 114.21, 114.06 (dd, $^2J_{\text{C,F}} = 32.4, 21.9$ Hz), 109.23, 108.93, 70.90, 59.93, 41.31, 26.88, 21.57, 13.80; ESI-HRMS: calcd. for $\text{C}_{28}\text{H}_{25}\text{FN}_2\text{O}_5\text{S}+\text{Na}^+$ 543.1361, found 543.1365.



(S)-Ethyl-5'-(3-chlorophenyl)-1-methyl-2-oxo-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3m). Yellow solid; 63% yield; $[\alpha]_{\text{D}}^{20} = -5.2$ ($c = 0.25$ in CHCl_3); 97% ee, determined by HPLC analysis on Daicel chiralpak IA, n -hexane/ i -PrOH = 70/30, 0.3 mL/min, $\lambda = 254$ nm, $T = 25$ °C,

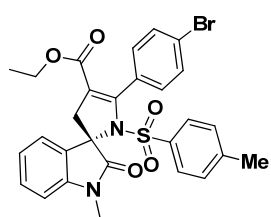
$t_{\text{minor}} = 23.707$ min, $t_{\text{major}} = 33.419$ min; due to the *meta*-Cl substitution, conformational

isomers were observed (ratio = 1.5:1), ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.61 (d, $J = 7.3$ Hz, 1H), 7.53 (d, $J = 6.9$ Hz, 1H), 7.43-7.35 (m, 3H), 7.36-7.27 (m, 4H), 7.24 (d, $J = 8.0$ Hz, 2H), 7.17 (d, $J = 8.0$ Hz, 2H), 7.12 (d, $J = 7.6$ Hz, 1H), 7.08 (d, $J = 7.6$ Hz, 2H), 7.01 (d, $J = 7.8$ Hz, 1H), 6.97 (d, $J = 7.7$ Hz, 1H), 6.93 (t, $J = 8.3$ Hz, 2H), 6.72 (d, $J = 7.6$ Hz, 1H), 6.35 (s, 1H), 3.96-3.83 (m, 3H), 3.50 (t, $J = 14.6$ Hz, 2H), 3.33 (s, 5H), 3.06 (d, $J = 15.9$ Hz, 2H), 2.39 (s, 3H), 2.36 (s, 2H), 0.96-0.84 (m, 5H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 176.15, 163.71, 150.08, 144.70, 144.21, 142.64, 142.29, 136.45, 136.13, 133.11, 131.58, 131.15, 130.77, 130.33, 130.11, 130.00, 129.70, 129.33, 129.11, 128.86, 128.53, 128.37, 128.27, 123.41, 123.25, 122.57, 122.39, 109.60, 109.23, 108.98, 108.90, 70.96, 59.96, 41.33, 26.88, 21.60, 21.55, 13.73, 13.69; ESI-HRMS: calcd. for $\text{C}_{28}\text{H}_{25}\text{ClN}_2\text{O}_5\text{S}+\text{Na}^+$ 559.1065, found 559.1074.



(S)-Ethyl-5'-(4-chlorophenyl)-1-methyl-2-oxo-1'-tosyl-1',3'-dihydrospiro [indoline-3,2'-pyrrole]-4'-carboxylate (3n). Orange solid; 70% yield; $[\alpha]_{\text{D}}^{20} = +6.0$ ($c = 0.2$ in CHCl_3); 93% ee, determined by HPLC analysis on Daicel chiralpak IA, n -hexane/ i -PrOH = 80/20, 1 mL/min, $\lambda = 254$ nm, $T =$

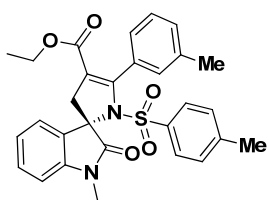
25°C , $t_{\text{minor}} = 8.973$ min, $t_{\text{major}} = 13.444$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.55 (d, $J = 7.3$ Hz, 1H), 7.39 (t, $J = 7.7$ Hz, 1H), 7.32 (d, $J = 13.8$ Hz, 2H) 7.23 (d, $J = 8.2$ Hz, 2H), 7.15 (t, $J = 7.5$ Hz, 1H), 7.03 (d, $J = 8.1$ Hz, 2H), 6.90 (dd, $J = 15.6, 7.8$ Hz, 2H), 6.52 (d, $J = 8.2$ Hz, 1H), 3.89 (q, $J = 7.1$ Hz, 2H), 3.49 (d, $J = 16.0$ Hz, 1H), 3.31 (s, 3H), 3.04 (d, $J = 16.0$ Hz, 1H), 2.35 (s, 3H), 0.93 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 176.09, 163.78, 150.73, 144.24, 142.41, 136.51, 135.15, 131.87, 131.43, 130.03, 129.07, 128.33, 127.52, 127.25, 123.34, 122.43, 109.21, 108.93, 70.96, 59.98, 41.34, 26.87, 21.60, 13.80; ESI-HRMS: calcd. for $\text{C}_{28}\text{H}_{25}\text{ClN}_2\text{O}_5\text{S}+\text{Na}^+$ 559.1065, found 559.1077.



(S)-Ethyl-5'-(4-bromophenyl)-1-methyl-2-oxo-1'-tosyl-1',3'-dihydrospiro [indoline-3,2'-pyrrole]-4'-carboxylate (3o). Yellow solid; 67% yield; $[\alpha]_{\text{D}}^{20} = +18.0$ ($c = 0.4$ in CHCl_3); 96% ee, determined by HPLC analysis on Daicel chiralpak IA, n -hexane/ i -PrOH = 70/30, 0.3 mL/min, $\lambda = 254$ nm, $T =$

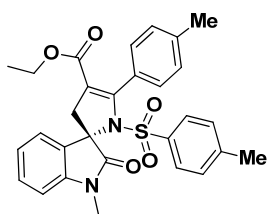
25°C , $t_{\text{minor}} = 9.057$ min, $t_{\text{major}} = 13.282$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.55 (d, $J = 7.3$ Hz, 1H), 7.46 (d, $J = 8.0$ Hz, 1H), 7.39 (t, $J = 7.7$ Hz, 1H), 7.28 (d, $J = 8.2$ Hz, 1H), 7.23 (d, $J = 8.2$ Hz, 2H), 7.15 (t, $J = 7.5$ Hz, 1H), 7.04 (t, $J = 8.1$ Hz, 3H), 6.92 (d, $J = 7.8$ Hz, 1H), 6.47 (d, $J = 8.0$

Hz, 1H), 3.90 (q, $J = 7.1$ Hz, 2H), 3.49 (d, $J = 16.0$ Hz, 1H), 3.32 (s, 3H), 3.04 (d, $J = 15.9$ Hz, 1H), 2.37 (s, 3H), 0.94 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 176.08, 163.76, 150.71, 144.25, 142.43, 136.52, 132.09, 131.5, 130.39, 130.21, 130.02, 129.07, 128.33, 128.04, 123.32, 122.44, 109.20, 108.92, 70.97, 59.98, 41.36, 26.86, 21.58, 13.79; ESI-HRMS: calcd. for $\text{C}_{28}\text{H}_{25}\text{BrN}_2\text{O}_5\text{S}+\text{Na}^+$ 603.0563, found 603.0565.



(S)-Ethyl-1-methyl-2-oxo-5'-(m-tolyl)-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3p). White solid; 66% yield; $[\alpha]_{\text{D}}^{20} = -8.5$ ($c = 0.2$ in CHCl_3); 95% ee, determined by HPLC analysis on Daicel chiralpak IA, n -hexane/ i -PrOH = 80/20, 1 mL/min, $\lambda = 254$ nm, $T = 25^\circ\text{C}$,

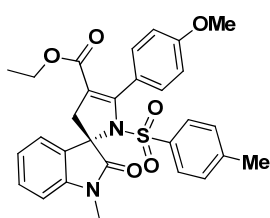
$t_{\text{minor}} = 9.326$ min, $t_{\text{major}} = 12.969$ min; due to the *meta*-Me substitution, conformational isomers were observed (ratio = 1.5:1), ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.60 (d, $J = 7.2$ Hz, 1H), 7.57 (d, $J = 7.3$ Hz, 1H), 7.38 (t, $J = 7.8$ Hz, 2H), 7.26 (s, 1H), 7.23 (d, $J = 7.1$ Hz, 3H), 7.15 (t, $J = 7.0$ Hz, 2H), 7.11 (d, $J = 8.1$ Hz, 1H), 7.09-7.03 (m, 2H), 7.00 (d, $J = 8.0$ Hz, 2H), 6.96 (d, $J = 8.0$ Hz, 1H), 6.91 (t, $J = 7.2$ Hz, 2H), 6.85 (s, 1H), 6.49 (d, $J = 7.5$ Hz, 1H), 6.24 (s, 1H), 3.87 (dd, $J = 14.0$, 6.9 Hz, 3H), 3.49 (dd, $J = 15.8$, 9.8 Hz, 2H), 3.31 (s, 5H), 3.03 (d, $J = 15.7$ Hz, 2H), 2.34 (s, 3H), 2.32 (s, 2H), 2.31 (s, 2H), 1.97 (s, 3H), 0.89 (q, $J = 7.2$ Hz, 5H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 175.79, 163.30, 144.18, 143.91, 143.28, 143.22, 142.42, 141.06, 139.50, 138.32, 136.21, 132.87, 131.10, 130.02, 129.15, 129.04, 128.35, 128.22, 126.04, 123.28, 122.68, 115.73, 115.39, 115.14, 113.08, 111.00, 110.87, 110.34, 108.82, 70.72, 60.31, 60.19, 41.48, 41.44, 26.95, 26.85, 21.55, 13.97; ESI-HRMS: calcd. for $\text{C}_{29}\text{H}_{28}\text{N}_2\text{O}_5\text{S}+\text{H}^+$ 517.1792, found 517.1799.



(S)-Ethyl-1-methyl-2-oxo-5'-(p-tolyl)-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3q). Yellow solid; 73% yield; $[\alpha]_{\text{D}}^{20} = -4.0$ ($c = 0.25$ in CHCl_3); 97% ee, determined by HPLC analysis on Daicel chiralpak IA, n -hexane/ i -PrOH = 80/20, 1.0 mL/min, $\lambda = 254$ nm, $T = 25^\circ\text{C}$,

$t_{\text{minor}} = 8.173$ min, $t_{\text{major}} = 14.822$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.57 (d, $J = 7.3$ Hz, 1H), 7.39 (t, $J = 7.7$ Hz, 1H), 7.29 (d, $J = 7.6$ Hz, 1H), 7.19 (d, $J = 8.2$ Hz, 2H), 7.17-7.12 (m, 2H), 6.98 (d, $J = 8.2$ Hz, 2H), 6.92 (d, $J = 7.7$ Hz, 1H), 6.74 (d, $J = 7.7$ Hz, 1H), 6.49 (d, $J = 7.8$ Hz, 1H), 3.90 (q, $J = 7.1$ Hz, 2H), 3.50 (d, $J = 15.8$ Hz, 1H), 3.33 (s, 3H), 3.03 (d, $J = 15.8$ Hz, 1H), 2.34 (d, $J = 5.7$ Hz, 6H), 0.94 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 176.26, 164.01,

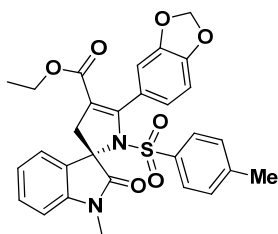
152.47, 143.77, 142.41, 138.72, 136.70, 131.63, 130.32, 129.87, 128.81, 128.40, 127.79, 125.99, 123.25, 122.48, 108.81, 108.50, 70.89, 59.74, 41.35, 29.67, 26.84, 21.55, 13.81; ESI-HRMS: calcd. for C₂₉H₂₈N₂O₅S+Na⁺ 539.1612, found 539.1625.



(S)-Ethyl-5'-(4-methoxyphenyl)-1-methyl-2-oxo-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3r). Yellow solid; 64% yield;

[α]_D²⁰ = +55.5 (c = 0.6 in CHCl₃); 97% ee, determined by HPLC analysis on Daicel chiralpak IA, *n*-hexane/*i*-PrOH = 80/20, 0.8 mL/min, λ = 254 nm, T

= 25 °C, *t*_{minor} = 12.539 min, *t*_{major} = 22.839 min; ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.57 (d, *J* = 7.3 Hz, 1H), 7.39 (t, *J* = 7.7 Hz, 1H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.22 (d, *J* = 8.2 Hz, 2H), 7.16 (t, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 8.1 Hz, 2H), 6.92 (d, *J* = 7.8 Hz, 1H), 6.86 (d, *J* = 6.9 Hz, 1H), 6.53 (d, *J* = 8.0 Hz, 1H), 6.46 (d, *J* = 6.5 Hz, 1H), 3.91 (q, *J* = 7.1 Hz, 2H), 3.81 (s, 3H), 3.49 (d, *J* = 15.8 Hz, 1H), 3.33 (s, 3H), 3.03 (d, *J* = 15.8 Hz, 1H), 2.34 (s, 3H), 0.95 (t, *J* = 7.1 Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 176.32, 164.08, 160.01, 152.18, 143.74, 142.40, 136.75, 133.69, 131.67, 130.16, 128.91, 128.45, 123.27, 122.47, 121.03, 112.60, 108.83, 108.59, 70.77, 59.75, 55.23, 41.33, 26.84, 21.53, 13.87; ESI-HRMS: calcd. for C₂₉H₂₈N₂O₆S+Na⁺ 555.1561, found 555.1566.

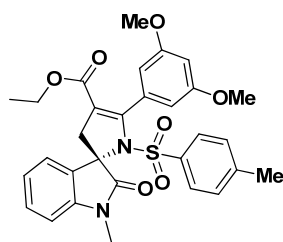


(S)-Ethyl-5'-(benzo[d][1,3]dioxol-5-yl)-1-methyl-2-oxo-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3s). White solid; 73% yield;

[α]_D²⁰ = -6.0 (c = 0.2 in CHCl₃); 97% ee, determined by HPLC analysis on Daicel chiralpak IA, *n*-hexane/*i*-PrOH = 80/20, 1 mL/min, λ =

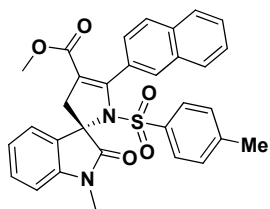
254 nm, T = 25 °C, *t*_{minor} = 12.028 min, *t*_{major} = 14.346 min; conformational isomers were observed (ratio=1.25:1), ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.56 (d, *J* = 7.3 Hz, 2H), 7.39 (t, *J* = 7.7 Hz, 2H), 7.31 (dd, *J* = 14.7, 8.0 Hz, 4H), 7.16 (dd, *J* = 12.9, 7.2 Hz, 2H), 7.06 (d, *J* = 7.9 Hz, 4H), 6.92 (d, *J* = 7.8 Hz, 2H), 6.90 (d, *J* = 8.1 Hz, 1H), 6.84 (s, 1H), 6.78 (d, *J* = 8.0 Hz, 1H), 6.38 (d, *J* = 8.0 Hz, 1H), 6.09 (d, *J* = 8.0 Hz, 1H), 6.02 (s, 1H), 5.97 (d, *J* = 15.9 Hz, 2H), 5.88 (d, *J* = 11.9 Hz, 2H), 3.94 (dt, *J* = 6.9, 5.3 Hz, 4H), 3.48 (dd, *J* = 15.9, 8.9 Hz, 2H), 3.02 (dd, *J* = 15.7, 13.2 Hz, 2H), 2.36 (s, 6H), 0.99 (dd, *J* = 12.0, 6.9 Hz, 6H); ¹³C NMR (150 MHz, CDCl₃): 163.89, 159.42, 151.69, 146.57, 144.07, 136.40, 134.39, 129.92, 128.96, 128.90, 128.56, 128.52, 128.33, 124.62, 124.19, 123.31, 122.59, 122.34, 117.11, 111.15, 110.29, 108.85, 107.34, 107.19, 106.27, 101.18, 101.01,

70.61, 59.84, 41.28, 29.32, 26.86, 21.52, 13.92; ESI-HRMS: calcd. for C₂₉H₂₆N₂O₇S+Na⁺ 569.1353, found 569.1359.



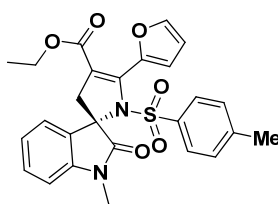
(S)-Ethyl-5'-(3,5-dimethoxyphenyl)-1-methyl-2-oxo-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3t). White solid; 74% yield; $[\alpha]_D^{20} = -13.0$ ($c = 0.4$ in CHCl₃); 99% ee, determined by HPLC analysis on Daicel chiralpak IA, *n*-hexane/*i*-PrOH = 90/10, 1 mL/min, $\lambda = 254$ nm, $T = 25$ °C, $t_{\text{minor}} = 17.305$ min, $t_{\text{major}} = 26.368$ min; ¹H NMR (600 MHz, CDCl₃):

δ (ppm) 7.59 (d, $J = 7.3$ Hz, 1H), 7.39 (t, $J = 7.7$ Hz, 1H), 7.28 (d, $J = 8.0$ Hz, 2H), 7.17 (t, $J = 7.5$ Hz, 1H), 7.02 (d, $J = 8.0$ Hz, 2H), 6.92 (d, $J = 7.8$ Hz, 1H), 6.53 (s, 1H), 6.37 (s, 1H), 5.70 (s, 1H), 3.91 (dd, $J = 9.6, 7.4$ Hz, 2H), 3.80 (s, 3H), 3.49 (d, $J = 15.6$ Hz, 1H), 3.46 (s, 3H), 3.33 (s, 3H), 3.04 (d, $J = 15.9$ Hz, 1H), 2.34 (s, 3H), 0.94 (t, $J = 7.0$ Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 176.35, 163.86, 159.50, 151.66, 143.79, 142.40, 136.53, 131.62, 130.42, 129.90, 128.95, 128.56, 123.33, 122.49, 108.87, 108.40, 107.09, 101.91, 70.89, 59.79, 55.45, 54.79, 41.31, 26.87, 21.44, 13.82; ESI-HRMS: calcd. for C₃₀H₃₀N₂O₇S+Na⁺ 585.1666, found 585.1672.



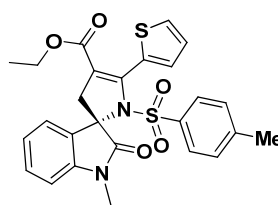
(S)-Methyl-1-methyl-5'-(naphthalen-2-yl)-2-oxo-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3u). Orange solid; 71% yield; $[\alpha]_D^{20} = +14.2$ ($c = 0.5$ in CHCl₃); 92% ee, determined by HPLC analysis on Daicel chiralpak IA, *n*-hexane/*i*-PrOH = 90/10, 1 mL/min, $\lambda = 254$ nm, $T =$

25 °C, $t_{\text{minor}} = 24.808$ min, $t_{\text{major}} = 34.858$ min; conformational isomers were observed (ratio = 1.6:1), ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.83 (d, $J = 8.4$ Hz, 2H), 7.81-7.76 (m, 2H), 7.69-7.64 (m, 2H), 7.56-7.52 (m, 2H), 7.49 (dd, $J = 15.5, 8.1$ Hz, 2H), 7.41 (dt, $J = 15.5, 8.0$ Hz, 4H), 7.30 (d, $J = 8.2$ Hz, 1H), 7.20 (dd, $J = 13.7, 6.6$ Hz, 2H), 7.12 (d, $J = 8.0$ Hz, 2H), 6.95 (dd, $J = 16.6, 7.6$ Hz, 4H), 6.75 (d, $J = 7.9$ Hz, 2H), 6.68 (d, $J = 7.9$ Hz, 2H), 3.56 (d, $J = 15.1$ Hz, 2H), 3.42 (d, $J = 3.8$ Hz, 5H), 3.35 (s, 5H), 3.10 (t, $J = 15.1$ Hz, 1H), 2.28 (s, 2H), 2.18 (s, 3H); ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 176.19, 164.38, 152.53, 143.89, 143.83, 142.65, 142.28, 136.71, 136.32, 133.00, 132.17, 132.05, 131.69, 131.45, 130.09, 130.02, 129.93, 129.55, 128.83, 128.80, 128.45, 128.29, 128.20, 127.60, 127.56, 127.41, 126.91, 126.77, 126.74, 126.52, 126.29, 126.03, 125.63, 123.38, 123.28, 122.68, 122.38, 108.92, 108.88, 108.64, 108.40, 71.21, 70.89, 51.13, 41.41, 41.36, 26.88, 21.45, 21.34; ESI-HRMS: calcd. for C₃₂H₂₈N₂O₅S+Na⁺ 561.1455, found 561.1462.



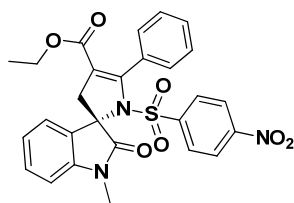
(S)-Ethyl-5'-(furan-2-yl)-1-methyl-2-oxo-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3v). Orange solid; 55% yield; $[\alpha]_{\text{D}}^{20} = -14.0$ ($c = 0.2$ in CHCl_3); 93% ee, determined by HPLC analysis on Daicel chiralpak IA, n -hexane/ i -PrOH = 60/40, 0.5 mL/min, $\lambda = 254$ nm, $T = 25$ °C,

$t_{\text{minor}} = 11.156$ min, $t_{\text{major}} = 13.328$ min; ^1H NMR (600 MHz, CDCl_3): δ 7.48 (d, $J = 7.3$ Hz, 1H), 7.38-7.36 (m, 3H), 7.30 (d, $J = 0.9$ Hz, 1H), 7.11-7.08 (m, 3H), 6.89 (d, $J = 7.8$ Hz, 1H), 6.52 (d, $J = 3.2$ Hz, 1H), 6.38 (dd, $J = 3.3, 1.7$ Hz, 1H), 3.97 (dd, $J = 7.1$ Hz, 2H), 3.49 (d, $J = 16.4$ Hz, 1H), 3.30 (s, 3H), 3.02 (d, $J = 16.4$ Hz, 1H), 2.35 (s, 3H), 1.02 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 175.78, 163.29, 143.88, 143.20, 142.45, 141.05, 139.54, 136.27, 131.11, 130.00, 129.03, 128.35, 123.25, 122.68, 115.13, 113.08, 110.84, 108.81, 70.72, 60.16, 41.50, 26.83, 21.51, 13.96; ESI-HRMS: calcd. for $\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_6\text{S}+\text{Na}^+$ 515.1248, found 515.1249.



(S)-Ethyl-1-methyl-2-oxo-5'-(thiophen-2-yl)-1'-tosyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3w). Yellow solid; 60% yield; $[\alpha]_{\text{D}}^{20} = -8.6$ ($c = 0.28$ in CHCl_3); 93% ee, determined by HPLC analysis on Daicel chiralpak IE, n -hexane/ i -PrOH = 60/40, 0.5 mL/min, $\lambda = 254$ nm, $T = 25$ °C,

$t_{\text{major}} = 34.040$ min, $t_{\text{minor}} = 37.610$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.56 (d, $J = 7.3$ Hz, 1H), 7.38 (t, $J = 7.8$ Hz, 1H), 7.32-7.28 (m, 3H), 7.15 (t, $J = 7.5$ Hz, 1H), 7.03 (d, $J = 8.2$ Hz, 2H), 6.91 (d, $J = 7.8$ Hz, 2H), 3.94 (q, $J = 7.0$ Hz, 2H), 3.49 (d, $J = 16.2$ Hz, 1H), 3.31 (s, 3H), 3.02 (d, $J = 16.2$ Hz, 1H), 2.33 (s, 3H), 0.97 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 176.12, 163.57, 144.46, 143.83, 142.35, 136.45, 131.70, 131.47, 129.96, 129.07, 128.83, 128.26, 127.61, 126.03, 123.31, 122.51, 111.84, 108.85, 70.67, 60.02, 41.43, 26.86, 21.58, 13.79; ESI-HRMS: calcd. for $\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_5\text{S}_2+\text{Na}^+$ 531.1019, found 531.1027.



(S)-Ethyl-1-methyl-1'-((4-nitrophenyl)sulfonyl)-2-oxo-5'-phenyl-1',3'-dihydrospiro[indoline-3,2'-pyrrole]-4'-carboxylate (3x). Yellow solid; 65% yield; $[\alpha]_{\text{D}}^{20} = -32.5$ ($c = 0.4$ in CHCl_3); 90% ee, determined by HPLC analysis on Daicel chiralpak IA, n -hexane/ i -PrOH = 60/40, 0.5

mL/min, $\lambda = 254$ nm, $T = 25$ °C, $t_{\text{minor}} = 14.658$ min, $t_{\text{major}} = 15.888$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 8.03 (d, $J = 8.7$ Hz, 2H), 7.59 (d, $J = 7.4$ Hz, 1H), 7.53 (d, $J = 8.6$ Hz, 2H), 7.44 (dd, $J = 16.5, 8.1$ Hz, 2H), 7.38 (d, $J = 7.3$ Hz, 1H), 7.35 (d, $J = 7.4$ Hz, 1H), 7.19 (t, $J = 7.5$ Hz,

1H), 6.97 - 6.91 (m, 2H), 6.60 (d, $J = 7.3$ Hz, 1H), 3.89 (dt, $J = 6.9, 4.2$ Hz, 2H), 3.54 (d, $J = 16.1$ Hz, 1H), 3.34 (s, 3H), 3.09 (d, $J = 16.1$ Hz, 1H), 0.89 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 175.94, 163.56, 150.48, 149.90, 144.92, 142.36, 131.29, 131.00, 130.29, 129.72, 129.38, 128.57, 127.50, 127.17, 123.45, 122.35, 110.28, 109.12, 71.17, 60.08, 41.42, 26.92, 13.66; ESI-HRMS: calcd. for $\text{C}_{27}\text{H}_{23}\text{N}_3\text{O}_7\text{S}+\text{Na}^+$ 556.1149, found 556.1160.

5. Mechanistic studies by ^1H NMR, ESI-MS and computational calculations

(1) General information for ^1H NMR analysis

^1H NMR data were obtained on an Agilent 600 MHz. Chemical shifts were given in parts per million (δ) from tetramethylsilane with the solvent resonance as the internal standard in CD_3OD solution.

(2) General information for ESI-MS analysis

ESI-MS data were obtained using a Waters SQ Detector mass spectrometer equipped with an ESI source and controlled by Mass Lynx software. The spray voltage was set to 3500 V for positive mode. The heated capillary temperature was at 350 $^\circ\text{C}$. The Mass range was adjusted between 100 to 1000 Da. The analysis was introduced as a solution in acetonitrile/water 1: 1 (v/v) dilution and injected in the infusion mode with a flow rate of 5 $\mu\text{L}/\text{min}$ at an electrospray voltage of 3500 V.

(3) General information for DFT calculations

All calculations were carried out with the GAUSSIAN 09 packages.⁵ The recently developed M05-2x functional,⁶ together with the standard 6-31G(d) basis set, were used for optimizing the geometry of all the minima and transition states. Houk's group and Cheng's group reported very good agreement between the M05-2x functional predictions and experimental observation for the cinchona alkaloid derivatives catalyzed reactions.⁷ In addition, all the optimized structures were confirmed by frequency calculations to be either minima or transition states using the same level of theory. Frequency calculations were carried out at the same level of theory for thermochemical analysis and to confirm that the number of imaginary frequencies of intermediate and transition states was 0 and 1, respectively. For transition states, intrinsic reaction coordinate analysis (IRC) was done to verify that they connect the right reactants.⁸

To take solvent effects into account, solution-phase single-point calculations were performed on the gas-phase geometries.⁹ The solution-phase single point energy calculations were done using M05-2x method at a larger basis set 6-311+G(2d,p). Solvent effect was accounted for using

self-consistent reaction field (SCRF) method, using SMD model and UAKS radii.¹⁰ Toluene was used as the solvent, because α -IC **C5** catalyzed reaction also can be carried out in toluene with 93% ee value and 65% yield. Solution-phase single-point energies corrected by the gas-phase Gibbs free energy corrections were used to describe all the reaction energetics. All of these energies correspond to the reference state of 1 mol/L, 298 K. All energetics reported throughout the text are in kcal/mol, and the bond lengths are in angstroms (Å). Structures were generated using GaussView 5.0.8 and CYLview.

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(10) (a) Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, 113, 6378. (b) Ribeiro, R. F.; Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2011**, 115, 14556.

(4) ^1H NMR studies on the formation of ammonium ylide

^1H NMR analysis has been applied to clarify the formation of ammonium ylide. Equimolar of **1a** (Figure S1) and DABCO (Figure S2) were reacted and the proton signal at C3 of **1a** shifted from 5.50 to 5.18 ppm with the formation of the ammonium salt (**I**) (Figure S3). After the addition of BzOK, the absence of the signal at 5.18 ppm represents the completion of the deprotonation and the formation of ammonium ylide (**II**) (Figure S4). These results strongly supported that the DABCO-catalyzed [4+1] annulation reaction would proceed via ammonium ylide pathway.

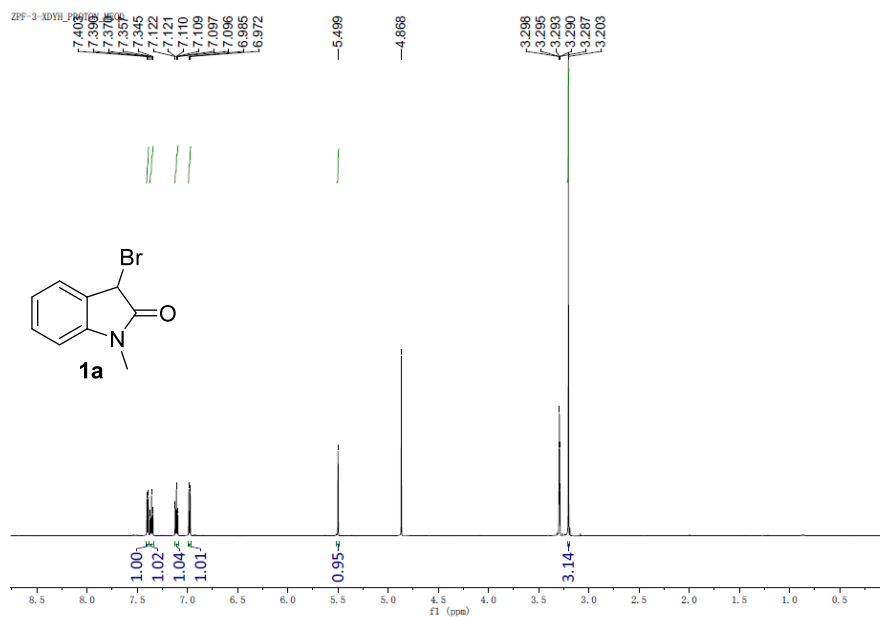


Figure S1. ^1H NMR of **1a**

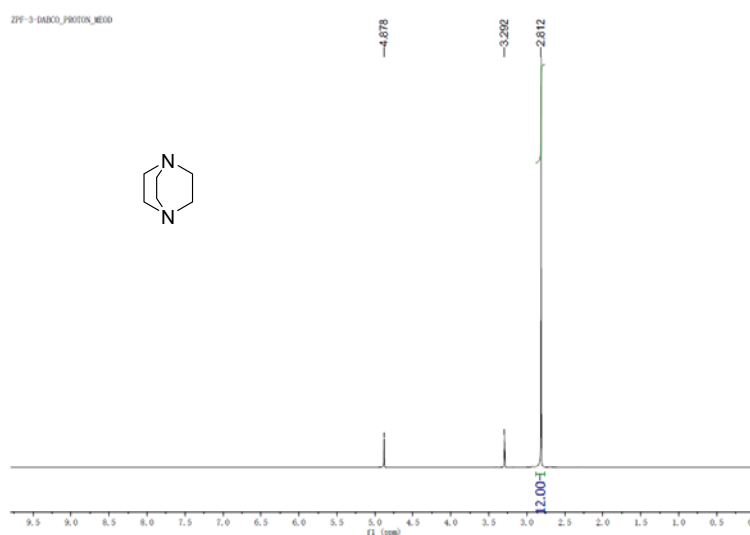


Figure S2. ^1H NMR of DABCO

Preparation of ammonium salt

DABCO (11.2 mg, 0.1 mmol) was added to a stirred solution of **1a** (22.6mg, 0.1 mmol) in CHCl₃ (1.0 mL). The reaction was stirred at room temperature for 2 h. Then CHCl₃ was removed under

reduced pressure to afford ammonium salt as a pink solid (32 mg, 95%). ^1H NMR (600 MHz, CD_3OD): δ (ppm) 7.67 (d, $J = 7.6$ Hz, 1H), 7.58 (t, $J = 7.8$ Hz, 1H), 7.25 (t, $J = 7.7$ Hz, 1H), 7.16 (d, $J = 7.9$ Hz, 1H), 5.18 (s, 1H), 3.93 (td, $J = 8.9, 4.6$ Hz, 3H), 3.62 (d, $J = 8.6$ Hz, 3H), 3.26 (s, 3H), 3.25-3.18 (m, 6H).

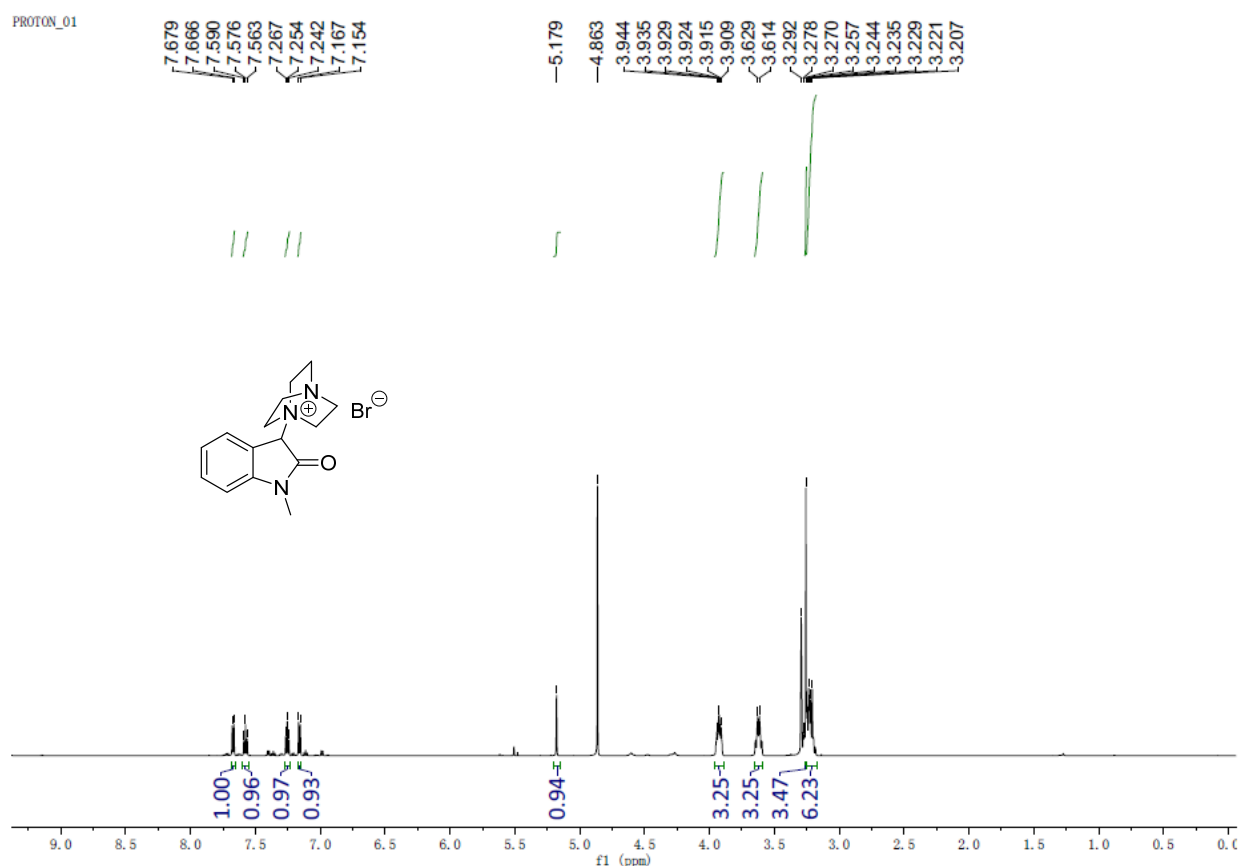


Figure S3. ^1H NMR of ammonium salt

Preparation of ammonium ylide

BzOK (8 mg, 0.05 mmol) was added to a stirred solution of ammonium salt (11.9 mg, 0.05 mmol) in CD_3OD (0.5 mL). The reaction was stirred at room temperature for 30 min. ^1H NMR (600 MHz, CD_3OD): δ (ppm) 7.92 (d, $J = 7.1$ Hz, 2H), 7.66 (d, $J = 7.6$ Hz, 1H), 7.56 (t, $J = 7.7$ Hz, 1H), 7.39 (t, $J = 7.2$ Hz, 1H), 7.33 (t, $J = 7.5$ Hz, 2H), 7.24 (t, $J = 7.6$ Hz, 1H), 7.14 (d, $J = 8.0$ Hz, 1H), 3.91 (dd, $J = 12.8, 7.5$ Hz, 3H), 3.61 (dd, $J = 17.4, 8.7$ Hz, 3H), 3.24 (s, 3H), 3.24-3.15 (m, 6H), 3.01 (s, 1H).

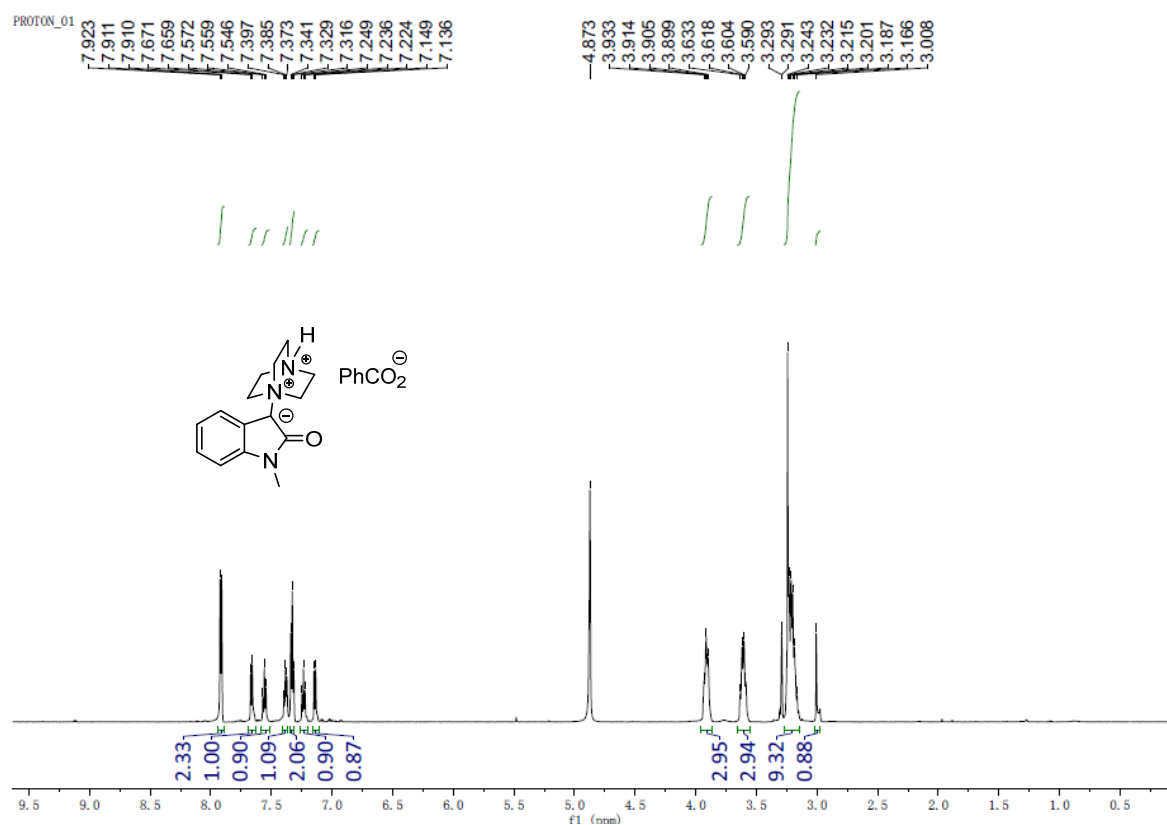


Figure S4. ^1H NMR of ammonium ylide

(5) Mass spectroscopy study on the catalytic reaction mixture¹¹

The formation of the quaternary ammonium salt **I** was supported by ESI-MS. After blending the catalyst **C5** and 3-bromooxindole **1a** for 30 minutes, a typical spectrum obtained was shown in Figure S5. A characteristic signal $[\text{I}-\text{Br}]^+$ consistent with quaternary ammonium salt **I** was observed at m/z 456. BzOK (1.5 equiv relative to 1-azadiene **2a**) was added to the reaction mixture and stirring for 1 hour. The Figure S6 showed similar signals as Figure S1 with a distinguished peak at m/z 456, which may belong to the ammonium cation of **I** ($[\text{I}-\text{Br}]^+$ m/z 456) or the protonated **II** ($[\text{II}+\text{H}]^+$ m/z 456).^{11a}

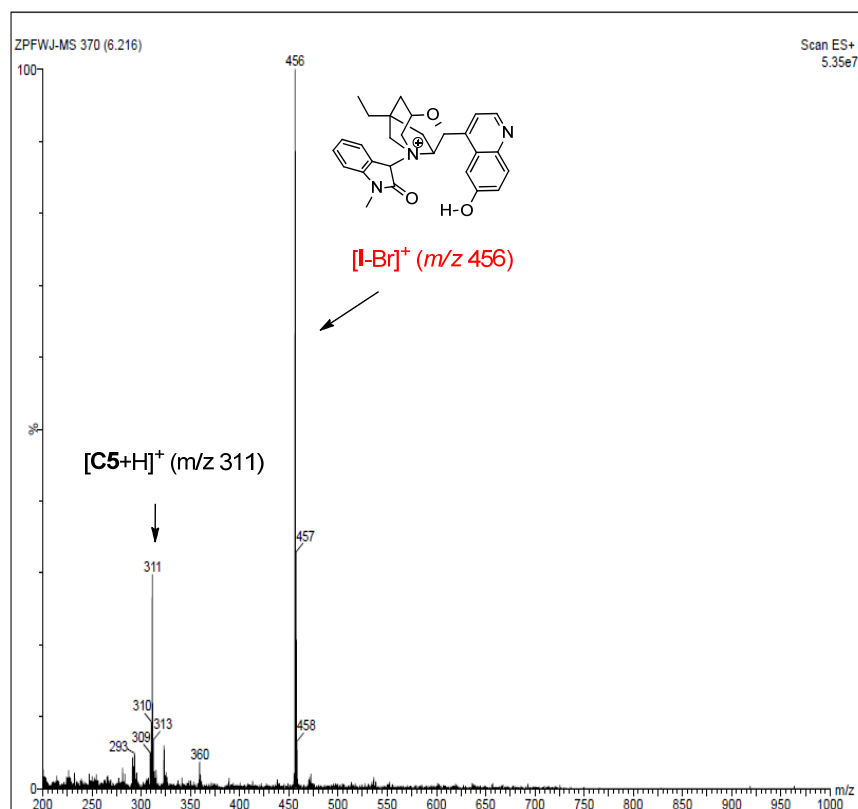


Figure S5. MS study on the mixture of catalyst **C5** and 3-bromooxindole **1a**

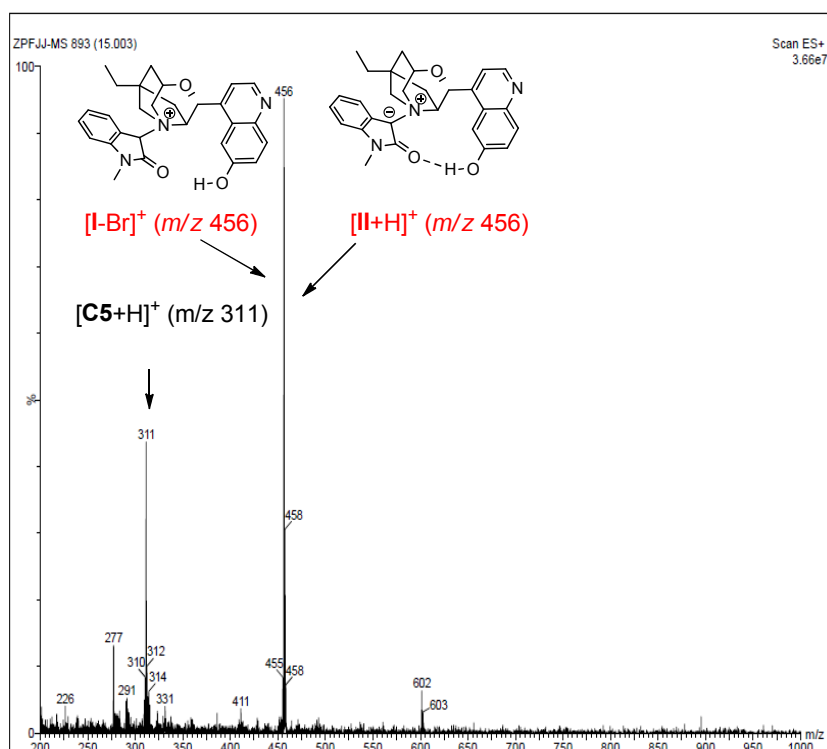


Figure S6. MS study on the mixture of catalyst **C5**, 3-bromooxindole **1a**, and BzOK

After 1-azadiene **2a** was added to the mixture and stirred for 10 minutes, a characteristic peak at m/z 813 belonging to the product of Michael-type addition was detected, apart from those of

catalyst $[\mathbf{C5}+\text{H}]^+$ (m/z 311), 1-azadiene $[\mathbf{2a}+\text{Na}]^+$ (m/z 380), product $[\mathbf{3a}+\text{H}]^+$ (m/z 503), intermediate of $[\mathbf{I}-\text{Br}]^+$ or $[\mathbf{II}+\text{H}]$ at m/z 456 (Figure S7). Mechanistically speaking, the [4+1] annulation reaction should proceed via ammonium ylide or enolate pathway.

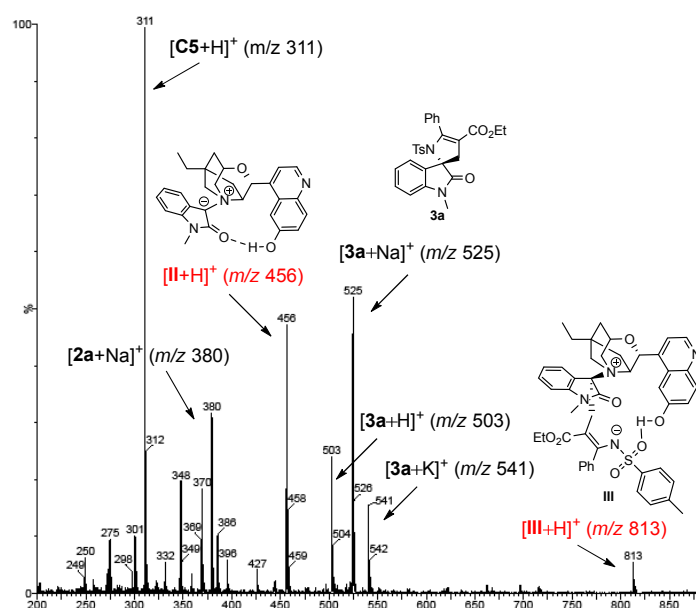


Figure S7. MS study on the mixture of catalyst **C5**, 3-bromooxindole **1a**, BzOK, and 1-azadiene **2a**

In the above work, excess **1a** was used, which would form the ammonium ylide intermediate under the catalysis of **C5** continuously regardless of the completion of the annulation reaction. Subsequently, we used excess 1-azadiene **2a** and monitored the reaction by MS. As outlined in the following figures, the intensity of the intermediate signal ($[\mathbf{I}-\text{Br}]^+$ or $[\mathbf{II}+\text{H}]^+$ m/z 456) at 6 h (**Figure S9**) grows significantly than that at 1 h (**Figure S8**). While at 18 h (**Figure S10**) the intensity started to drop in comparison with that of **3a** and it continues to present the least intensity on the sample taken after 28 h (**Figure S11**). Therefore, these experiments proved that the intensity of the m/z 456 changed with the progress of the annulation reaction. In addition, the intensity of the key zwitterionic intermediate **III** ($[\mathbf{III}+\text{H}]^+$ m/z 813) also changed with the progress of the reaction.

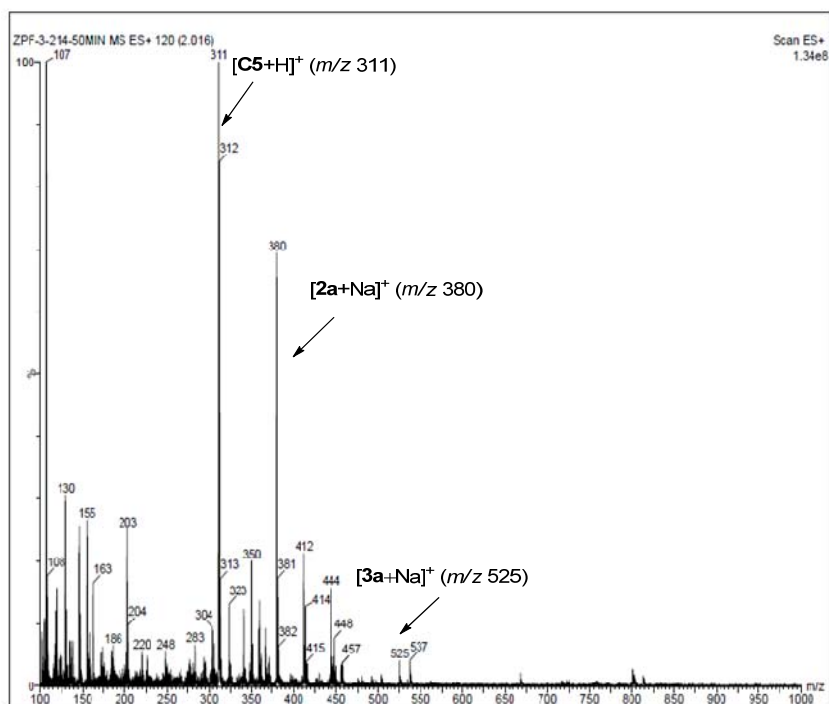


Figure S8. MS study on the mixture of **C5**, 3-bromooxindole **1a**, BzOK, and 1-azadiene **2a** at 1 h

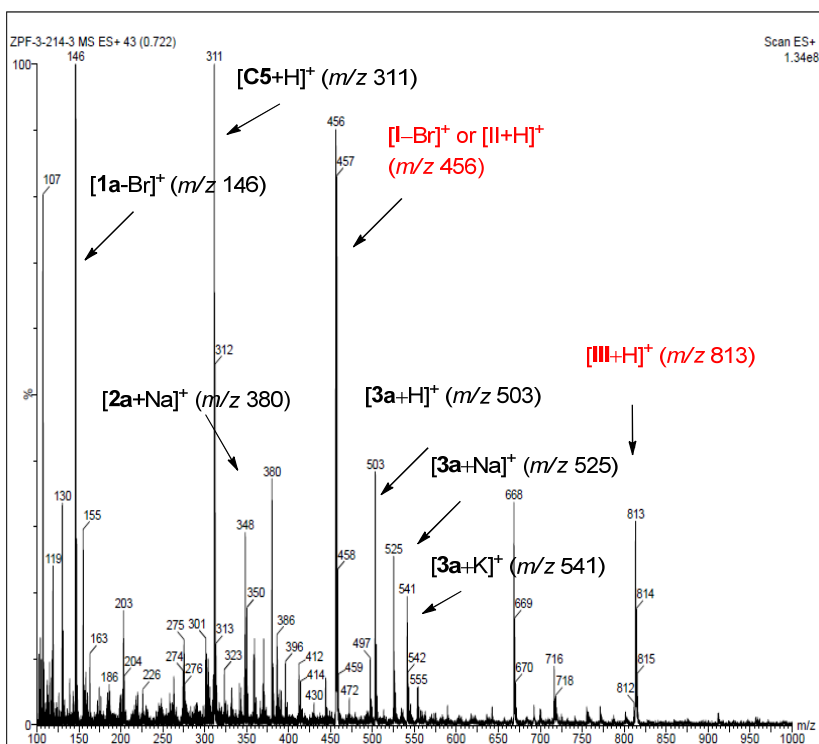


Figure S9. MS study on the mixture of **C5**, 3-bromooxindole **1a**, BzOK, and 1-azadiene **2a** at 6 h

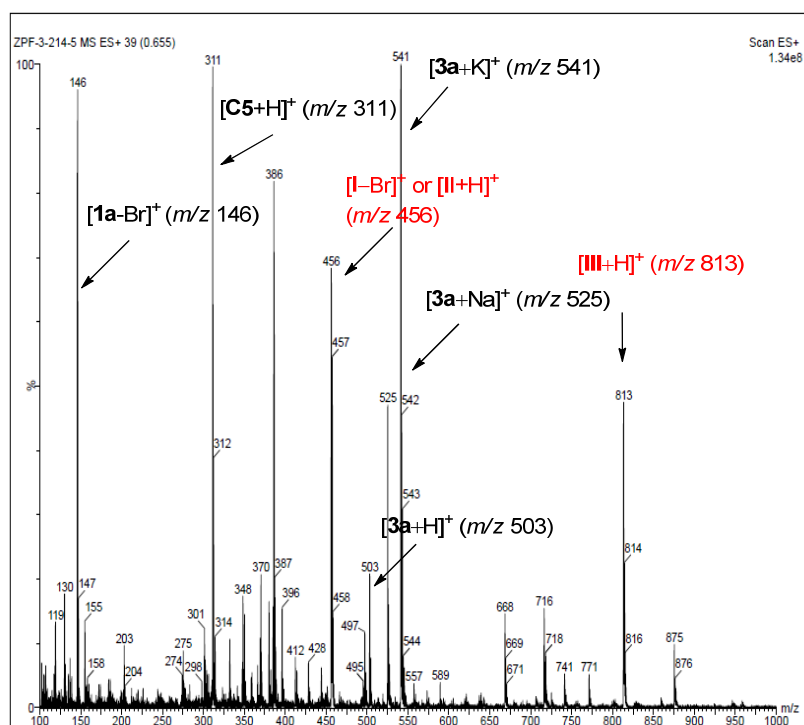


Figure S10. MS study on the mixture of **C5**, 3-bromooxindole **1a**, BzOK, and 1-azadiene **2a** at 18 h

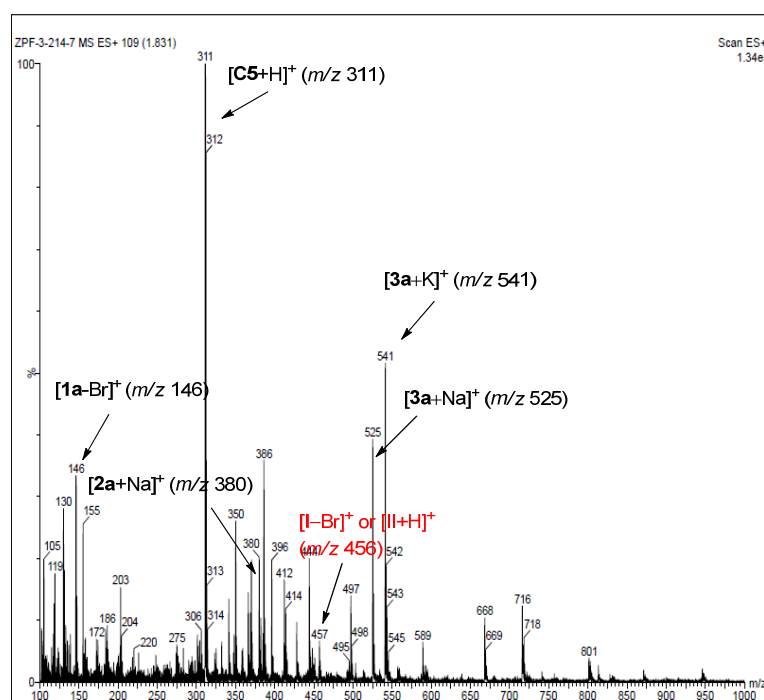


Figure S11. MS study on the mixture of **C5**, 3-bromooxindole **1a**, BzOK, and 1-azadiene **2a** at 28 h

(11) (a) Liu, Y.-L.; Wang, X.; Zhao, Y.-L.; Zhu, F.; Zeng, X.-P.; Chen, L.; Wang, C.-H.; Zhao, X.-L.; Zhou, J. *Angew. Chem., Int. Ed.* **2013**, 52, 13735. (b) Peng, J.; Huang, X.; Zheng, P.-F.; Chen, Y.-C. *Org. Lett.* **2013**, 15, 5534.

(6) Mechanistic studies by computational calculations

To better understand the asymmetric selectivity of this reaction, we conducted a computational investigation of the novel asymmetric ammonium ylide reaction catalyzed by **C5**. First, the formation of the ammonium ylide intermediate **II** from reaction of **C5** and 3-bromooxindole **1a** was calculated in toluene, as shown in Figures S12 and S13. The intermediate **R-I** was formed through a Walden inversion S_N2 reaction of **S-1a** and **C5** with a Gibbs free energy barriers of 26.0 kcal/mol (**S-TS1**). Then, the proton at C3 of **R-I** was deprotonated by BzOK via the transition state **R-TS2** (13.7 kcal/mol) to produce a conformation of ammonium ylide **II-1**. The reaction started from the other enantiomer **R-1a** was also calculated, which showed similar process with producing another conformation **II-2**.

That computational study on the potential energy for the formation of the ylide from **1a** reveals that both transition state energies of the ammonium bromide and ammonium salt are quite high (see Figure S13, around 25.0 kcal/mol and 22.0 kcal/mol, respectively), theoretically suggesting that the equilibrium lies much to the side of the starting materials. However, when the reaction of an equimolar mixture of **1a** and **C5** were conducted in toluene, nearly quantitative precipitation was obtained, suggesting that the poor solubility of the ammonium salt in toluene might drive the equilibrium forward. We also obtained the ^1H NMR spectrum of ammonium salt in CD_3OD . The signal of C3 proton of **1a** at 5.50 ppm disappeared, which shows the clean formation of the diastereomeric ammonium salts (**R-I** and **S-I**) from **1a** and **C5** (Figure S14).

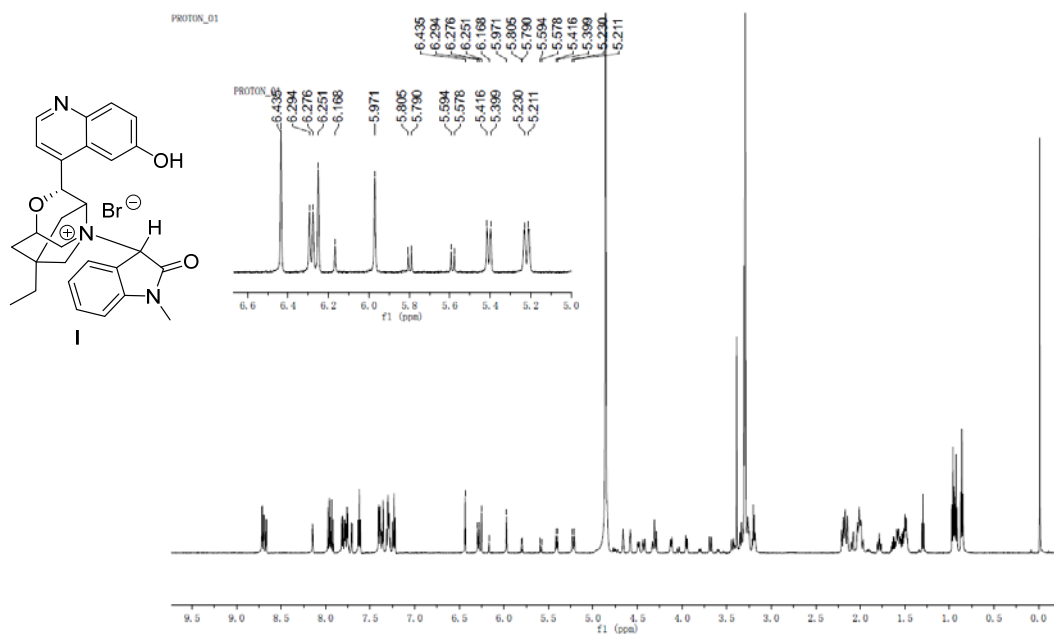


Figure S14. The ^1H NMR spectrum of **R-I** and **S-I** in CD_3OD .

Meanwhile, computational study on the potential energy for the formation of the ylide from **1a** and **C5** in methanol reveals that the free-Gibbs energies of **R-I** (-15.5 kcal/mol) is much lower than that of **S-1a** and **C5** (0.0 kcal/mol) in methanol (Figure S13), which shows the ammonium bromide could be quite stable in methanol, as illustrated in the above ^1H NMR spectrum. On the other hand, although the energies of ammonium salt is quite high in toluene, the formation of the ammonium salt would be promoted by the generation of energetically stable *S* or *R-I-A* before moving toward the second transition state for the ylide formation, which means that the formation of the ammonium salt is theoretically viable.

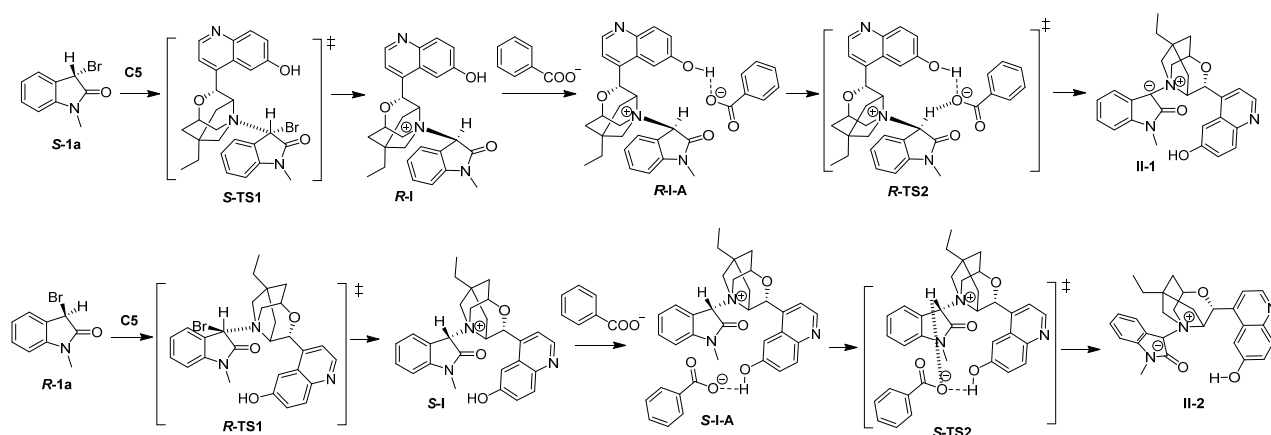


Figure S12. Different approaches for the formation of ammonium ylide **II** from **1a** and **C5**.

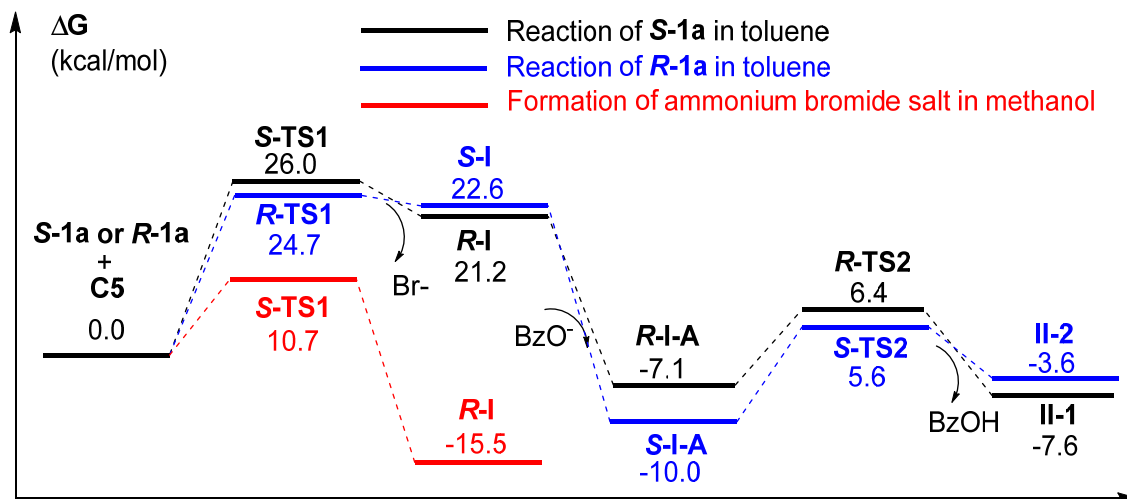


Figure S13. Computed potential energy surface for the formation of ammonium ylide **II** from **1a** and **C5**. Energies are obtained at the M05-2x/ 6-311+G (2d,p) (in toluene or methanol) level and are given in kcal/mol relative to reactants.

In order to rationalize the conversion of each conformations, a full scan (360°) of dihedral angle α (marked by red in Figure S15) was implemented. The conformation **II**, with a hydrogen bond between the phenolic hydroxyl (OH) and carbonyl (C=O, O1 atom), was considered as the most stable conformation, which could be converted from **II-1** and **II-2** via **II-TS1** and **II-TS2**,

respectively. These convertible conformations would further conduct the addition reaction to **2a**.

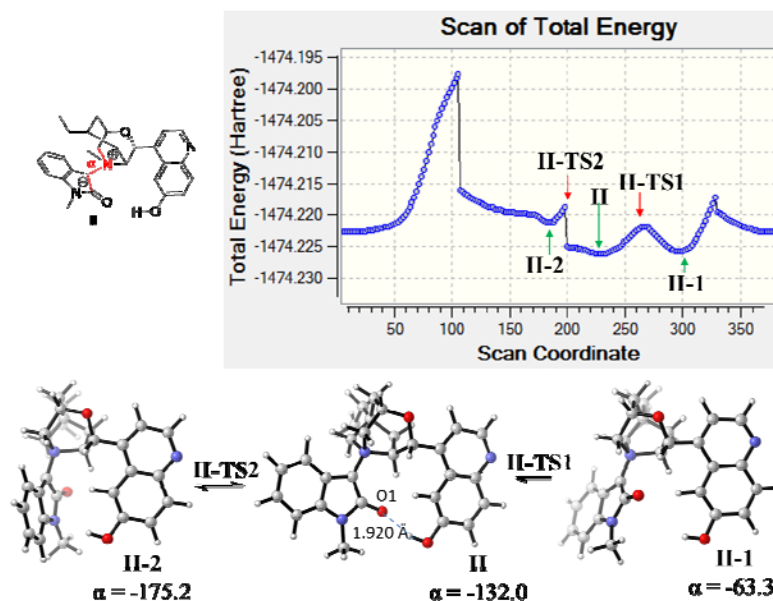


Figure S15. Scan of the dihedral angle α in ammonium ylide using the M05-2x/ 6-31G (d) method.

The preferable conformation of another start material **2a** [ethyl (Z)-2-(phenyl (tosylimino) methyl) acrylate] was rationalized. The three single bond rotations, C2-C5, C2-C3, or N1-S, will lead to 8 reactive conformations, **D1** to **D8** (Figure S16). Among these conformations, **D5** have the lowest energy. And, in **D5**, the oxygens of sulfimide (O2 atom) and carboxyl (O3 atom) are at the same side around the terminal C of olefin (C1) (Figure S16). It will be easy for them to form hydrogen bonds with the OH of **C5** in the corresponding transition states and intermediates. It is rationalized that the conformation **D5** is favored (Figure S17), and thereby leading to the formation of different transition states.

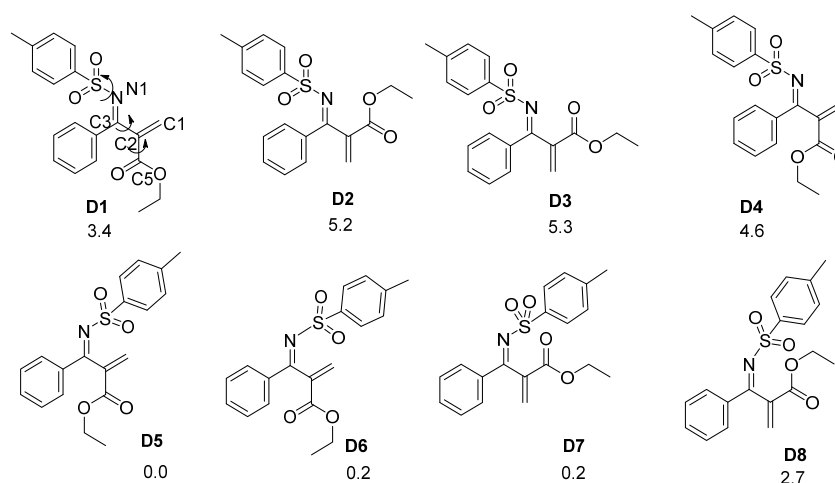


Figure S16. The structures and relative Gibbs free energies [in kcal/mol; at the M05-2X/ 6-311+G(2d,p) //6-31G(d) level] for **2** (**D1-D8**) (toluene as solvent).

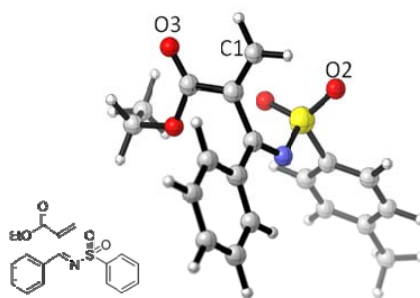


Figure S17. Optimized structure of **D5**

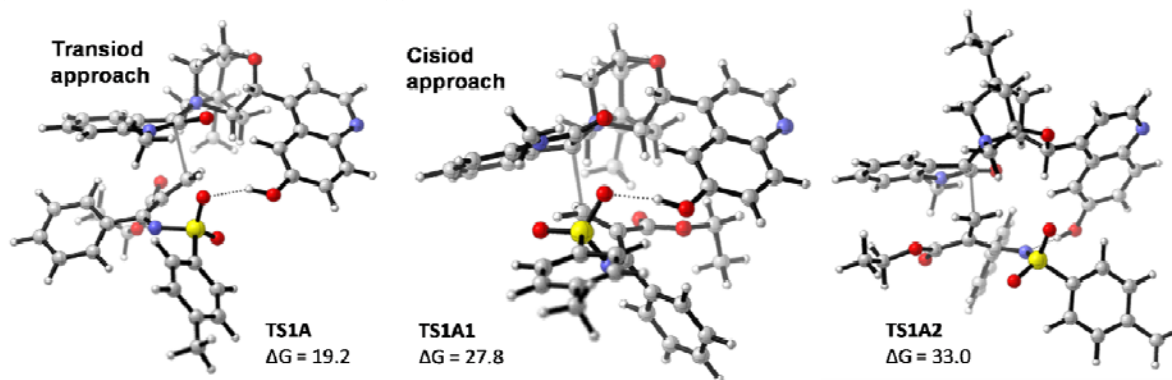


Figure S18. The structure and relative Gibbs free energies [in kcal/mol; at the M05-2X/6-311+G(2d,p)//6-31G(d) level] for **TS1A**, **TS1A1**, and **TS1A2**

The addition step of the ammonium ylide to the olefin compound was assumed to be rate-limiting,¹⁴ and was assumed to occur via a transition state with an end-on arrangement of **D5** and ylide groups. First, the transition states (TSs), in which the ammonium and tosylimino groups are in an anti-like relation with respect to the new C-C bond (*transoid* approach, defined by Aggarwal¹²), are considered as more favorable states due to the steric hindrance from **C5**. The calculations showed that the Gibbs free energies of the **TS1A** is 8.6 kcal/mol lower than that of **TS1A1** via *cisoid* approach, where the ammonium and tosylimino are gauche or even eclipsed with respect to each other (see Figure S18). Second, because the OH group of catalyst is crucial for enantiocontrol, the formation of hydrogen bonds with different atoms was also calculated. The results showed that **TS1A2** with a hydrogen bond between OH of **C5** and N atom of N-Ts imine had 13.8 kcal/mol higher Gibbs free energies than that of **TS1A** (see Figure S18). Therefore, the **path A** and **B** involving hydrogen bonding interaction between OH of **C5** and oxygen atom of N-Ts imine or ester group and *transoid* approach was considered as more rational pathway. Interestingly, in these TSs of step 1, the conformation of **II** would be converted to **II-1** and **II-2** by breaking the hydrogen bond between the phenolic hydroxyl (OH) and carbonyl (C=O, O1 atom). The conformations of ammonium ylide in **TS1A** and **TS1B** were similar as **II-1** with similar dihedral

angles α (-66.9 and -56.0 degree, respectively). Meanwhile, the conformations of ammonium ylide in **TS1C** and **TS1D** were similar with **II-2**. Since the energy of **II-2** is 4.0 kcal/mol higher than **II-1**, the conformations of ammonium ylide in **TS1C** and **TS1D** may be another result leading to the higher energies.

Although α -IC (**C5**) was developed as an enantiocomplementary catalyst of β -ICD **C4**, an interesting result showed that **C4**-catalyzed reactions have the same chiral selectivity as that of **C5**. The calculated pathways of β -ICD (**path A–D**) leading to the enantiomers (*R* and *S*) was shown in Figure S19, S20 and S21. The paths **β A** and **β B** via *Re*-face attacks leading to final products with *S* configuration also have obvious lower Gibbs free energy barriers. The reason for selectivity of ammonium ylide **β II** via *Re*-face attack was similar with the reaction of intermediate **II** of α -IC. The steric repulsion of atoms with short distances was shown in Figure S20. The steric hindrances in **β -TS1C** and **β -TS1D** were the main factor for the higher energy barriers. These results indicate that the Path **β A** and **β B** are the favorable pathways to form product with *S*-configuration, which were consistent with the experimental results.

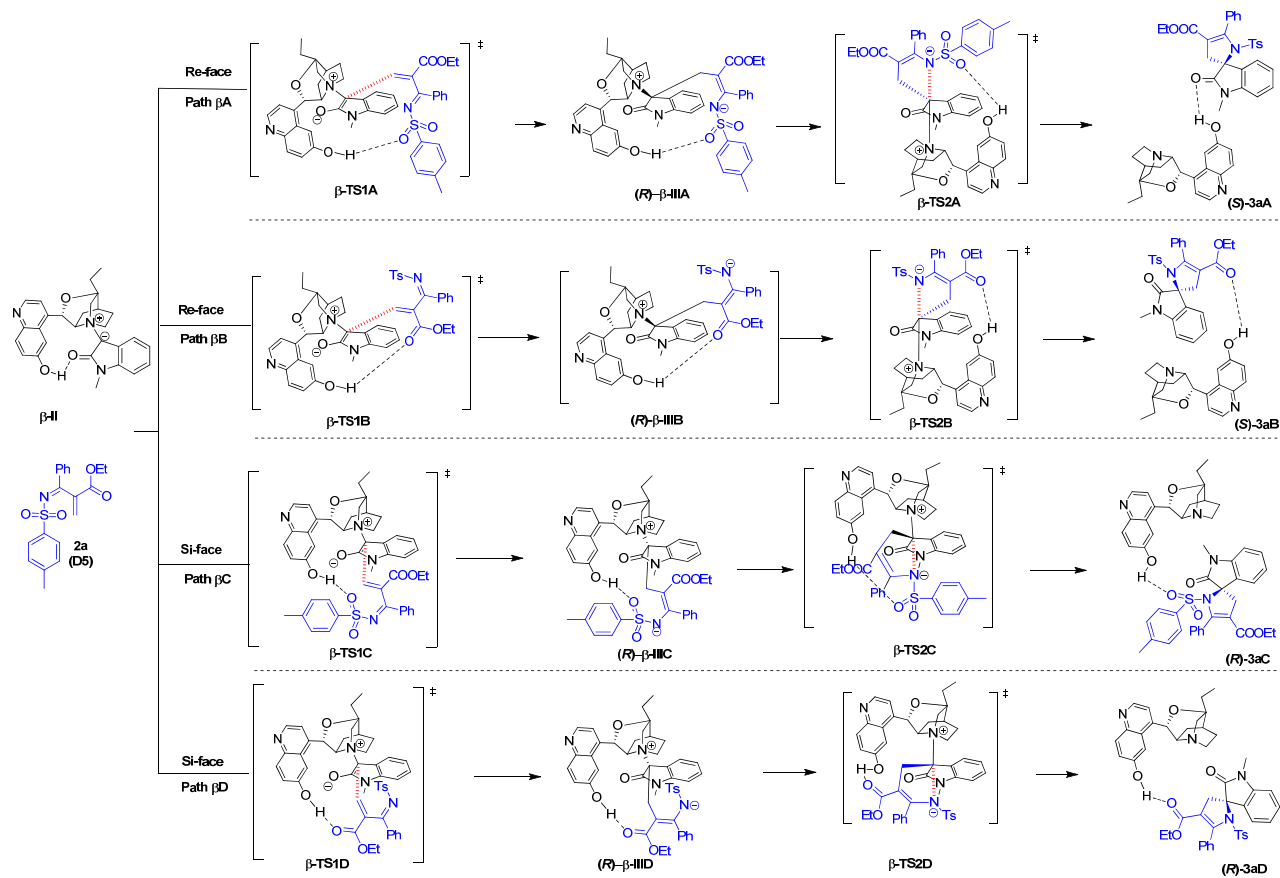


Figure S19. Different approaches of [4+1] annulation reaction from **β -II** to produce the corresponding stereochemical outcomes

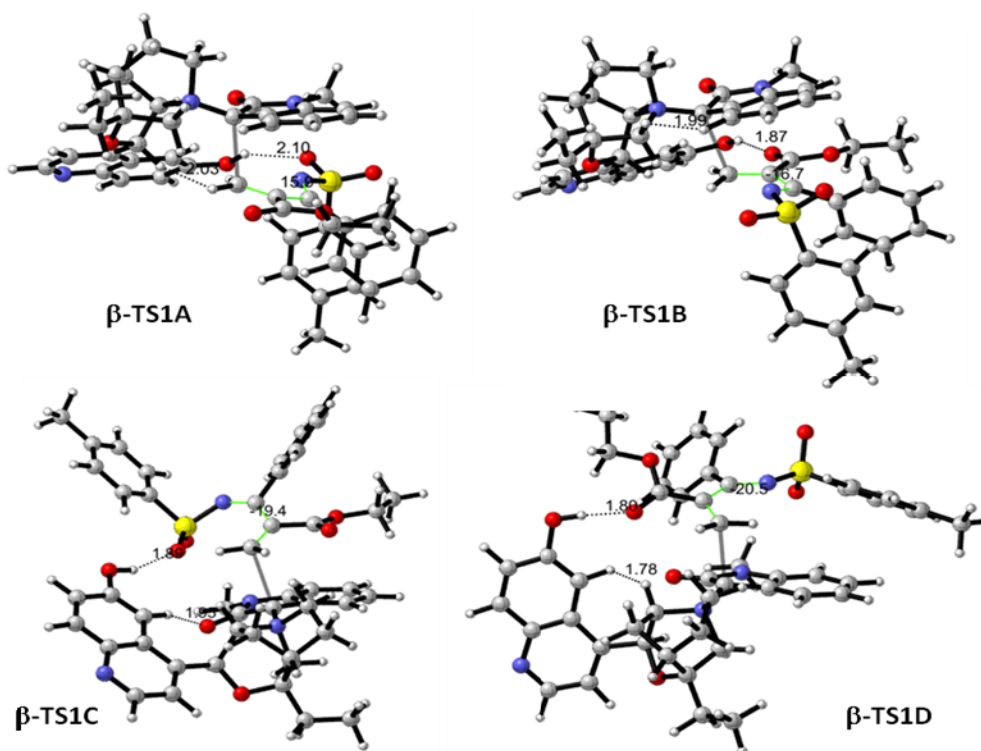


Figure S20. Optimized structure of β -TS1A-D. The bond distances of the optimized structures are in angstroms. The dihedral angle between double bonds, C1-C2 and C3-N, were marked by green and labeled.

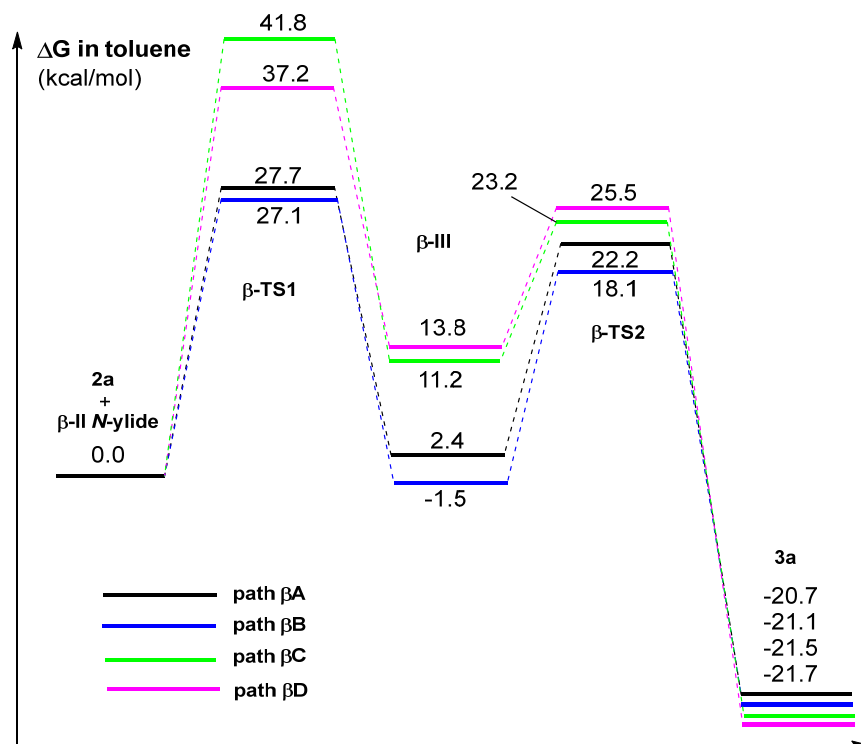
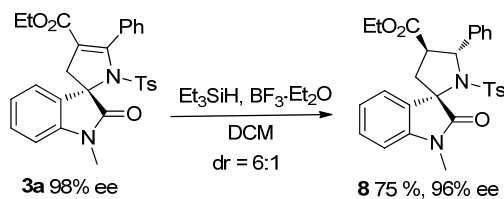


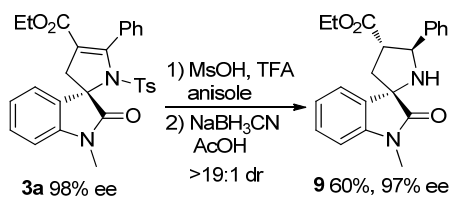
Figure S21. Computed potential energy surface for the [4+1] annulation reaction between ammonium ylide β -II and D5. Energies are obtained at the M05-2x/ 6-311+G(2d,p) (toluene) level and are given in kcal/mol relative to reactants.

(12) Aggarwal, V. K.; Harvey, J. N.; Richardson, J., *J. Am. Chem. Soc.* **2002**, *124*, 5747

6. Transformations of spirocyclic product **3a**



Under an argon atmosphere condition, to a solution of **3a** (0.1 mmol) in CH_2Cl_2 (2 mL), triethyl silicane (4 mmol) was added boron trifluoride diethyl ether (4 mmol). The mixture was stirred at room temperature for 24 h. After completion, the solvent was evaporated under reduced pressure and the crude residue was subjected to column chromatography with PE/EtOAc = 5/1 as eluent to give separable diastereomer **8** as a white solid ($\text{dr} = 6:1$). 75% yield; $[\alpha]_{\text{D}}^{20} = -37.3$ ($c = 0.4$ in CHCl_3); 96% ee, determined by HPLC analysis on Daicel chiralpakIA, n -hexane/ i -PrOH = 80/20, 1 mL/min, $\lambda = 254$ nm, $T = 25$ °C, $t_{\text{minor}} = 15.716$ min, $t_{\text{major}} = 16.897$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.40 (dd, $J = 7.7, 7.2$ Hz, 1H), 7.29 (d, $J = 7.1$ Hz, 1H), 7.26 (d, $J = 6.6$ Hz, 2H), 7.22 (t, $J = 7.3$ Hz, 1H), 7.17 (t, $J = 7.3$ Hz, 2H), 7.10 (t, $J = 7.4$ Hz, 1H), 6.92 (d, $J = 7.8$ Hz, 1H), 6.84 (d, $J = 8.0$ Hz, 2H), 6.72 (d, $J = 8.2$ Hz, 2H), 5.61 (d, $J = 7.3$ Hz, 1H), 4.13 (q, $J = 7.1$ Hz, 2H), 3.30-3.23 (m, 4H), 2.87 (dd, $J = 13.2, 8.0$ Hz, 1H), 2.46 (dd, $J = 13.2, 8.2$ Hz, 1H), 2.29 (s, 3H), 1.19 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 177.08, 170.27, 143.90, 142.65, 138.41, 137.57, 129.73, 129.61, 128.44, 128.24, 128.17, 127.96, 127.46, 123.07, 122.39, 108.84, 69.67, 67.07, 61.36, 51.78, 39.88, 26.77, 21.37, 14.02; ESI-HRMS: calcd. for $\text{C}_{28}\text{H}_{28}\text{N}_2\text{O}_5\text{S} + \text{Na}^+$ 527.1612, found 527.1614.



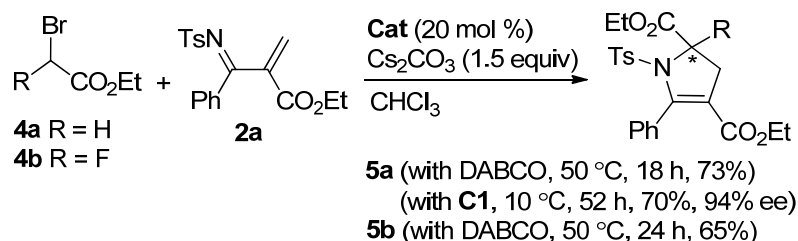
The cycloadduct **3a** (0.1 mmol) was treated with MsOH (1 mL) and anisole-trifluoroacetic acid (3: 1, 1 mL) in an ice-bath for 30 min.¹³ Then it was stirred at room temperature for 1 h. The mixture was diluted with CH_2Cl_2 (10 mL), neutralized by saturated NaHCO_3 and extracted with CH_2Cl_2 (3×5 mL). The combined organic phases were dried over MgSO_4 and concentrated under reduced pressure. Under an argon atmosphere condition, the residue was dissolved in AcOH (1mL) and NaBH_3CN was added. After stirred for 2 hours, the reaction was diluted with CH_2Cl_2 (5 mL), neutralized by saturated NaHCO_3 and extracted with CH_2Cl_2 (3×5 mL). The combined organic

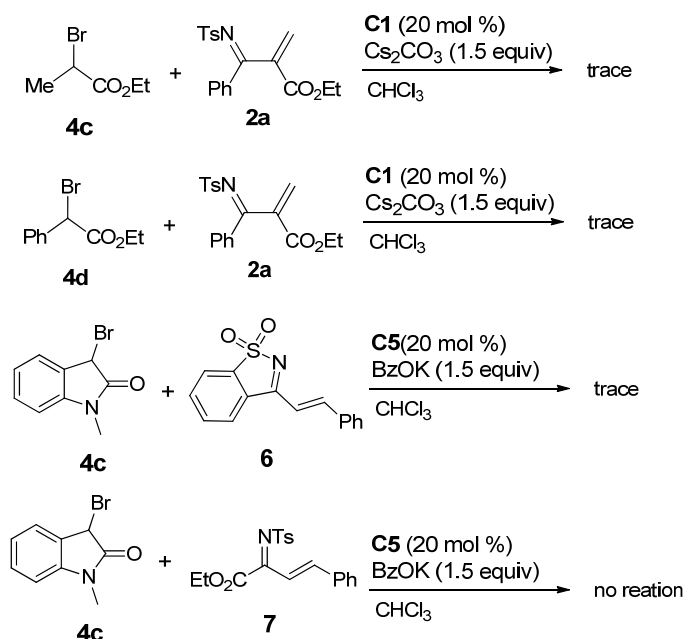
phases were dried (MgSO₄) and concentrated under reduced pressure. The residue was purified by flash chromatography (PE/EA = 5: 1) to afford **9** as colourless oil. 60% yield; $[\alpha]_D^{20} = +27.3$ ($c = 0.3$ in CHCl₃); >19:1 dr, 97% ee, determined by HPLC analysis on Daicel chiralpak IA, *n*-hexane/*i*-PrOH = 80/20, 1 mL/min, $\lambda = 254$ nm, $T = 25$ °C, $t_{\text{minor}} = 8.180$ min, $t_{\text{major}} = 10.053$ min; ¹H NMR (600 MHz, CDCl₃): δ (ppm) 7.61 (d, $J = 7.2$ Hz, 2H), 7.52 (d, $J = 7.3$ Hz, 1H), 7.34 (t, $J = 7.6$ Hz, 2H), 7.30 (ddd, $J = 10.8, 8.7, 4.2$ Hz, 2H), 7.12 (t, $J = 7.3$ Hz, 1H), 6.83 (d, $J = 7.8$ Hz, 1H), 4.87 (d, $J = 9.9$ Hz, 1H), 4.09 (qd, $J = 7.1, 3.7$ Hz, 2H), 3.61 (ddd, $J = 10.9, 10.0, 7.7$ Hz, 1H), 3.22 (s, 3H), 2.61 (dd, $J = 13.1, 7.7$ Hz, 1H), 2.50 (dd, $J = 13.0, 11.1$ Hz, 1H), 2.35 (br, 1H), 1.14 (t, $J = 7.1$ Hz, 3H); ¹³C NMR (150 MHz, CDCl₃): δ (ppm) 179.41, 172.95, 143.14, 141.15, 133.28, 129.01, 128.47, 127.79, 127.40, 123.29, 123.13, 108.20, 67.23, 66.95, 60.71, 52.33, 41.89, 26.33, 14.09; ESI-HRMS: calcd. for C₂₁H₂₂N₂O₃+H⁺ 351.1704, found 351.1711.

(13) Lu, L.-Q.; Zhang, J.-J.; Li, F.; Cheng, Y.; An, J.; Chen, J.-R.; Xiao, W.-J. *Angew. Chem., Int. Ed.* **2010**, *49*, 4495.

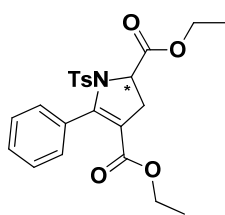
7. Exploration of more ammonium ylide precursors and other 1-azadienes

Some acyclic α -bromo substituted esters with different substitutions at α -position were tested in the reactions with 1-azadienes **2a**. Only **4a** and **4b** exhibited the same [4+1] annulation reaction pattern catalyzed by DABCO in the presence of a stronger base. Unfortunately, the enantioselective attempts were not successful with **4b** and no reaction was observed with **4c** and **4d**. Furthermore, β -substituted 1-azadienes **6** and **7** also failed to give the [4+1] annulation reactions product, probably due to the steric hindrance and the relatively lower reactivity.



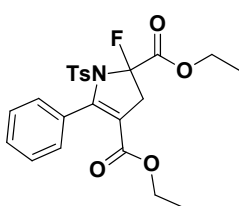


1-Azadienes **2a** (0.12 mmol) was treated with ylide precursor **4** (0.1 mmol) in the presence of tertiary amine catalyst (20 mol %) and Cs_2CO_3 (0.15 mmol) in CHCl_3 (2 mL). The mixture was stirred at 50 °C or 10 °C. After completion, the mixture was directly subjected to column chromatography using (petroleum ether/ethyl acetate = 5: 1) as eluent to yield the desired product **5**.



Diethyl-5-phenyl-1-tosyl-2,3-dihydro-1H-pyrrole-2,4-dicarboxylate (5a).

White solid; 70% yield; $[\alpha]_{\text{D}}^{20} = +108.5$ ($c = 0.6$ in CHCl_3); 94% ee, determined by HPLC analysis on Daicel chiralpak OD-H, n -hexane/ i -PrOH = 80/20, 1 mL/min, $\lambda = 254$ nm, $T = 25$ °C, $t_{\text{major}} = 9.344$ min, $t_{\text{minor}} = 11.179$ min; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.36 (d, $J = 8.1$ Hz, 1H), 7.31 (t, $J = 7.2$ Hz, 1H), 7.19 (t, $J = 7.4$ Hz, 2H), 7.14 (dd, $J = 15.3, 7.8$ Hz, 4H), 5.13 (dd, $J = 11.7, 4.4$ Hz, 1H), 4.32 (q, $J = 7.1$ Hz, 2H), 4.00-3.83 (m, 2H), 3.25 (dd, $J = 16.4, 11.7$ Hz, 1H), 2.94 (dd, $J = 16.5, 4.4$ Hz, 1H), 2.39 (s, 3H), 1.37 (t, $J = 7.1$ Hz, 3H), 0.95 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 171.10, 164.09, 151.36, 144.13, 136.08, 130.04, 129.64, 129.30, 129.20, 127.88, 127.01, 112.75, 61.96, 60.83, 60.05, 33.42, 21.58, 14.15, 13.74; ESI-HRMS: calcd. for $\text{C}_{23}\text{H}_{25}\text{NO}_6\text{S} + \text{Na}^+$ 466.1295, found 466.1301.

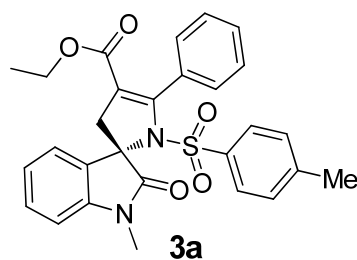
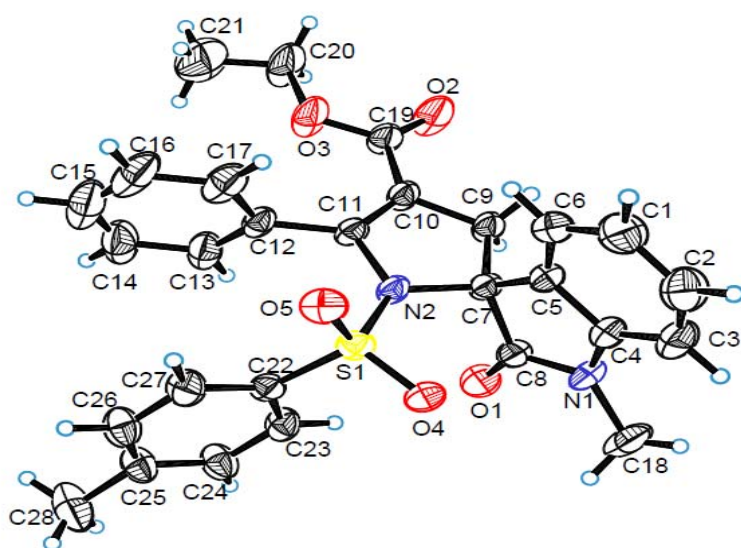


Diethyl-2-fluoro-5-phenyl-1-tosyl-2,3-dihydro-1H-pyrrole-2,4-dicarboxylate (5b).

White solid; 65% yield; ^1H NMR (600 MHz, CDCl_3): δ (ppm) 7.32 (t, $J = 7.5$ Hz, 1H), 7.22 (d, $J = 8.3$ Hz, 3H), 7.10 (dd, $J = 15.5, 7.5$ Hz, 2H), 7.04 (d, $J = 8.2$ Hz, 2H), 6.79 (d, $J = 7.1$ Hz, 1H), 4.55-4.41 (m, 2H), 3.89 (q, $J = 7.1$ Hz,

2H), 3.34 (ddd, $J = 51.2, 35.4, 18.0$ Hz, 2H), 2.37 (s, 3H), 1.45 (t, $J = 7.1$ Hz, 3H), 0.90 (t, $J = 7.1$ Hz, 3H); ^{13}C NMR (150 MHz, CDCl_3): δ (ppm) 166.77, 166.52 (d, $^2J_{\text{C,F}} = 37.8$ Hz), 163.27, 149.96, 149.93, 144.54, 135.88, 130.23, 129.15, 129.14, 128.42, 128.41, 128.01, 127.17, 126.95 (d, $^3J_{\text{C,F}} = 33.7$ Hz), 108.08, 104.34, 102.79 (d, $^1J_{\text{C,F}} = 234.65$ Hz), 63.31, 60.09, 41.15, 40.98 (d, $^2J_{\text{C,F}} = 25.5$ Hz), 21.59, 14.00, 13.69; ESI-HRMS: calcd. for $\text{C}_{23}\text{H}_{24}\text{FNO}_6\text{S} + \text{Na}^+$ 484.1201, found 484.1207.

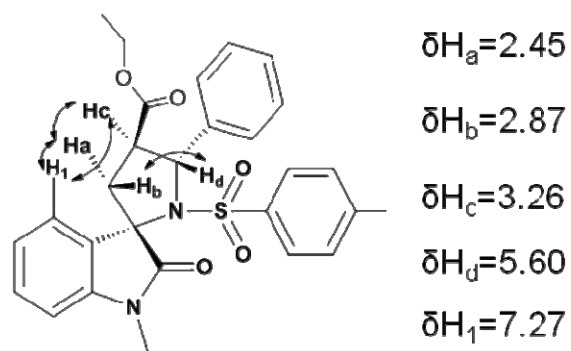
8. Crystal data and structural refinement for enantiopure 3a



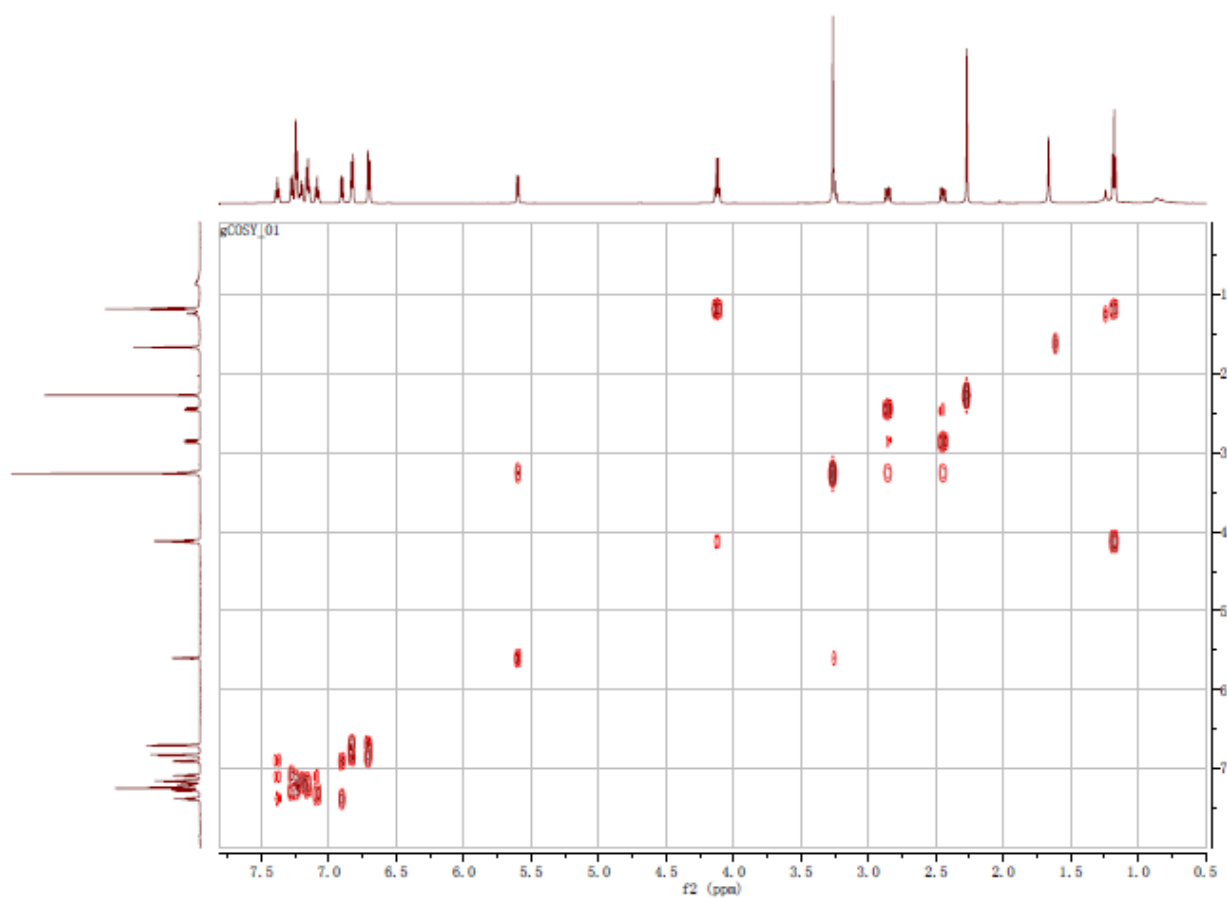
Identification code	3a
Empirical formula	$\text{C}_{28}\text{H}_{26}\text{N}_2\text{O}_5\text{S}$
Formula weight	502.57
Temperature/K	290(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
$a/\text{\AA}$	8.6152(6)
$b/\text{\AA}$	9.5235(5)
$c/\text{\AA}$	32.448(2)
$\alpha/^\circ$	90
$\beta/^\circ$	90
$\gamma/^\circ$	90
Volume/ $\text{\AA}^3$	2662.2(3)

Z	4
$\rho_{\text{calc}}/\text{mg}/\text{mm}^3$	1.254
m/mm^{-1}	0.161
F(000)	1056.0
Crystal size/ mm^3	$0.39 \times 0.38 \times 0.3$
Radiation	MoK α ($\lambda = 0.71073$)
2 Θ range for data collection	6.5 to 58.324°
Index ranges	$-10 \leq h \leq 11, -7 \leq k \leq 12, -27 \leq l \leq 41$
Reflections collected	12749
Independent reflections	6125 [$R_{\text{int}} = 0.0448, R_{\text{sigma}} = 0.0654$]
Data/restraints/parameters	6125/0/325
Goodness-of-fit on F^2	1.035
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0665, wR_2 = 0.1592$
Final R indexes [all data]	$R_1 = 0.1008, wR_2 = 0.1806$
Largest diff. peak/hole / $\text{e } \text{\AA}^{-3}$	0.20/-0.26

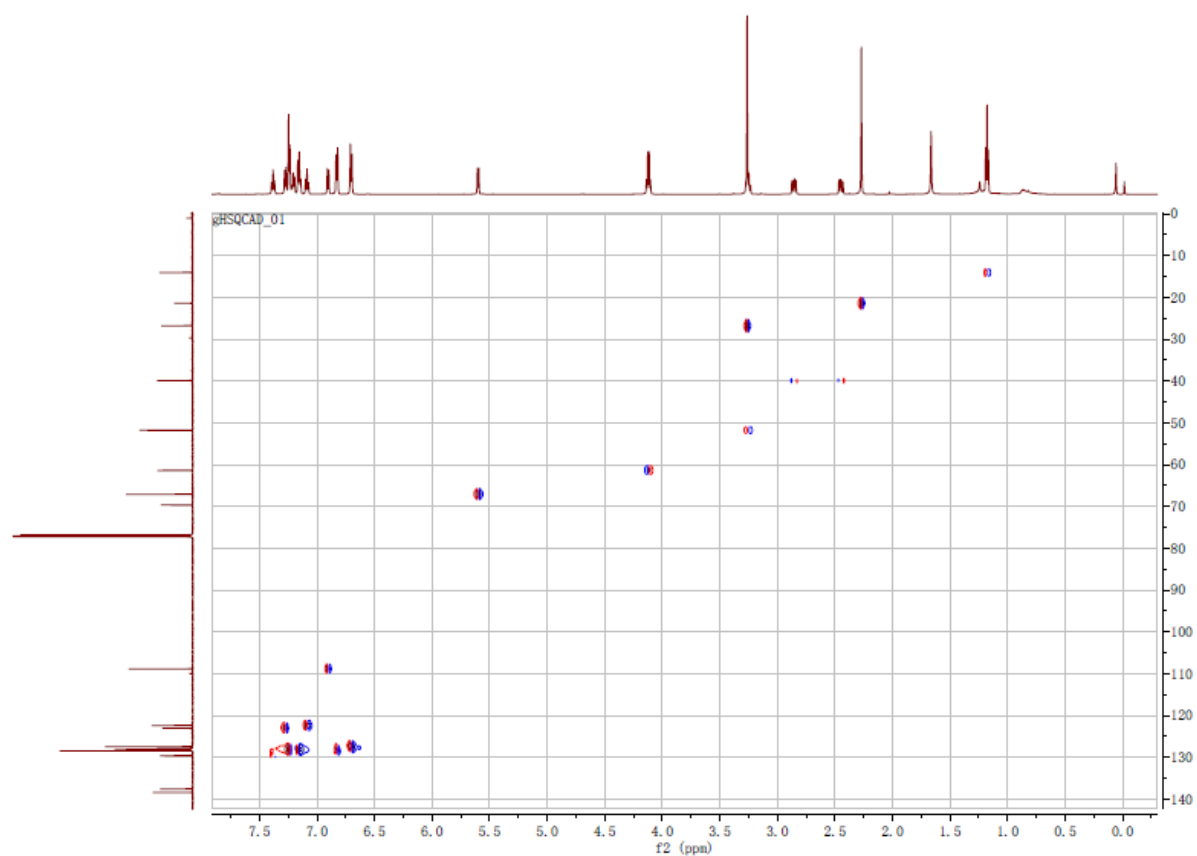
9. Structural analysis of chiral 8 and 9



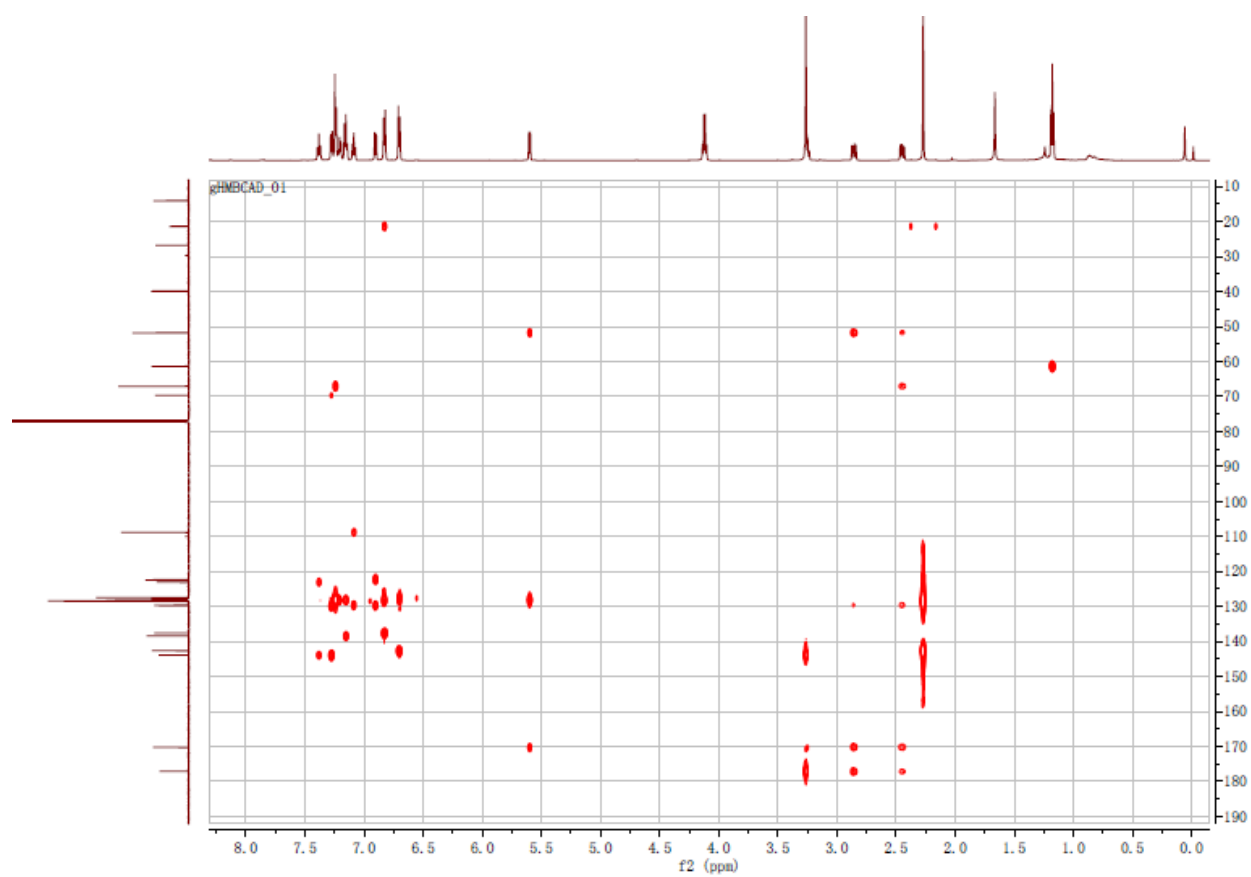
Structure of 8



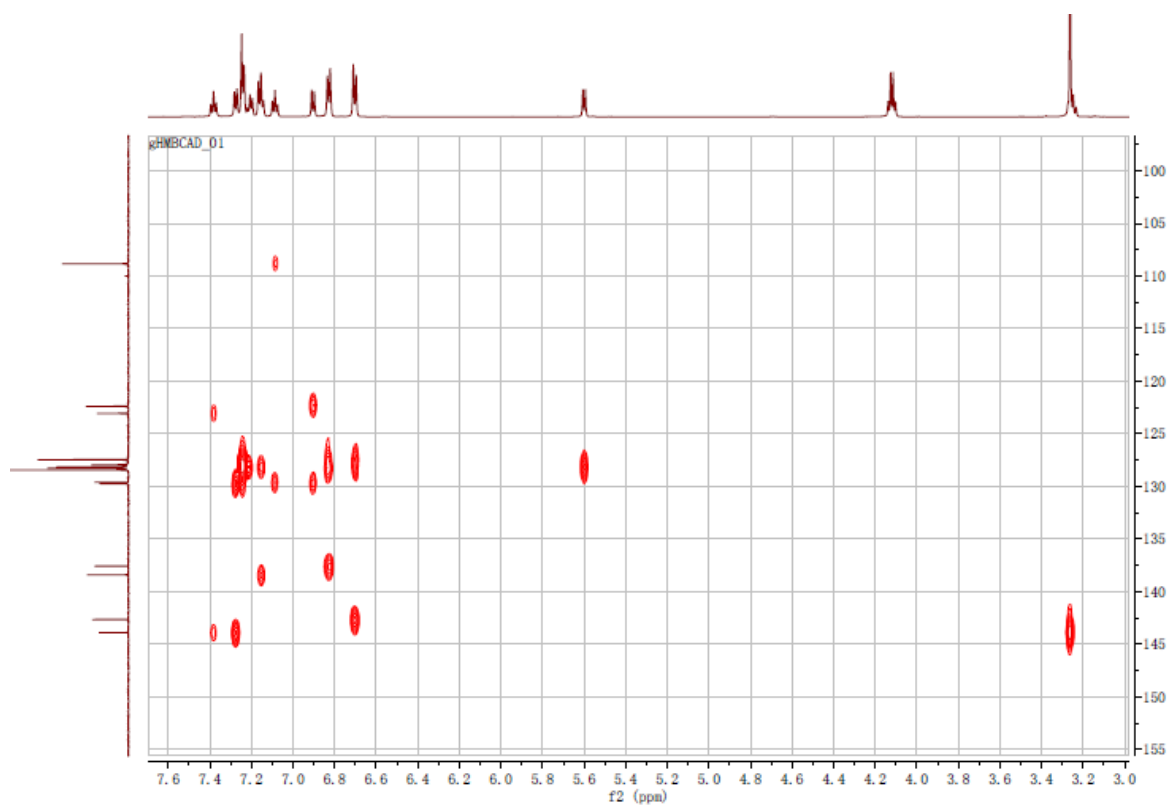
COSY of 8



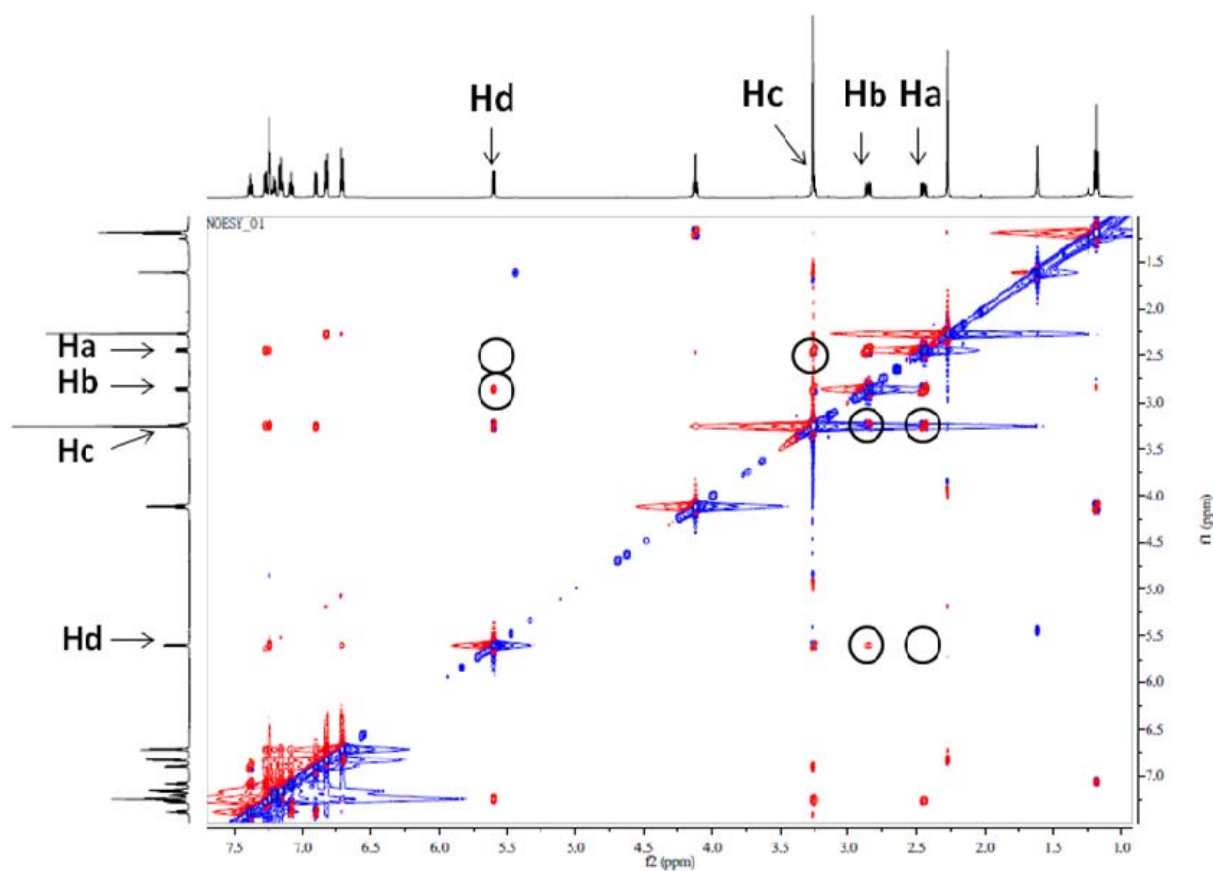
HSQC of 8



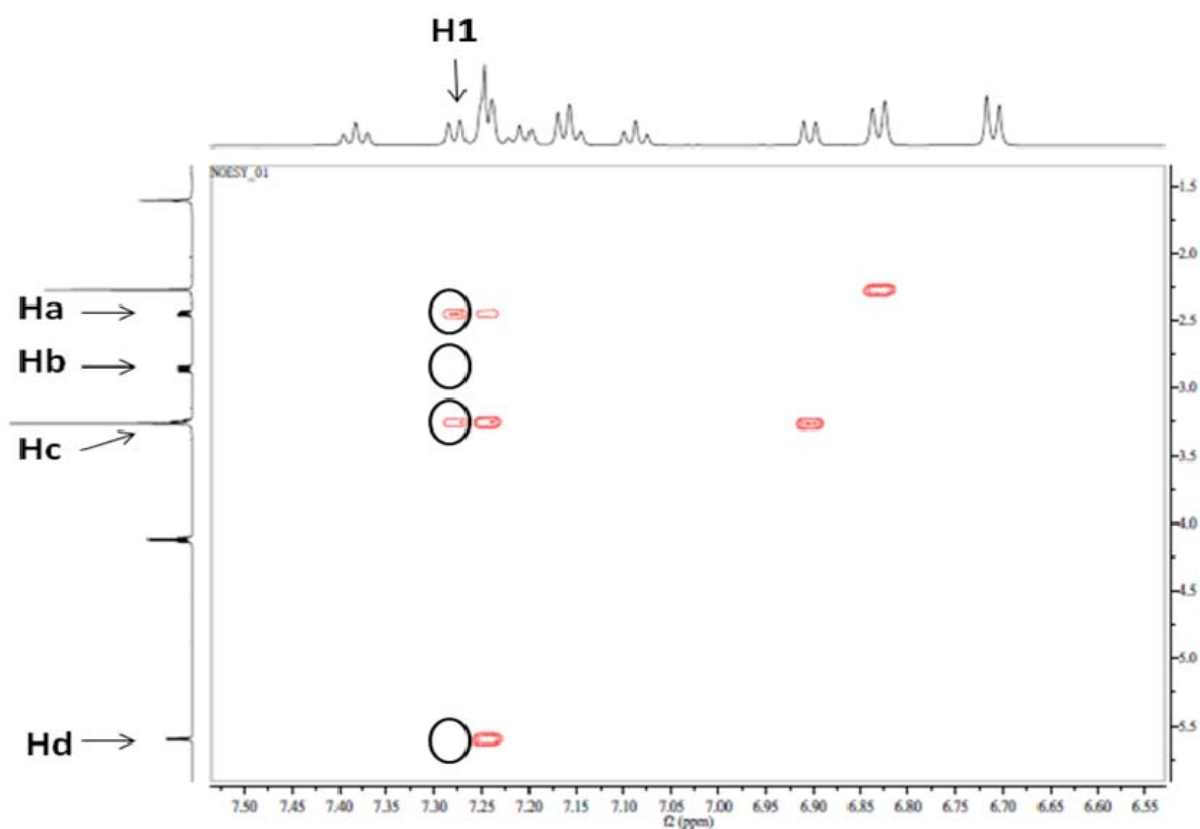
HMBC of 8



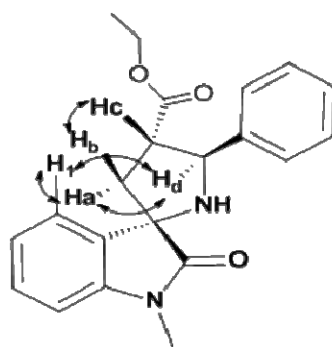
HMBC of 8



NOESY of 8



NOSEY of 8



$\delta H_a = 2.50$

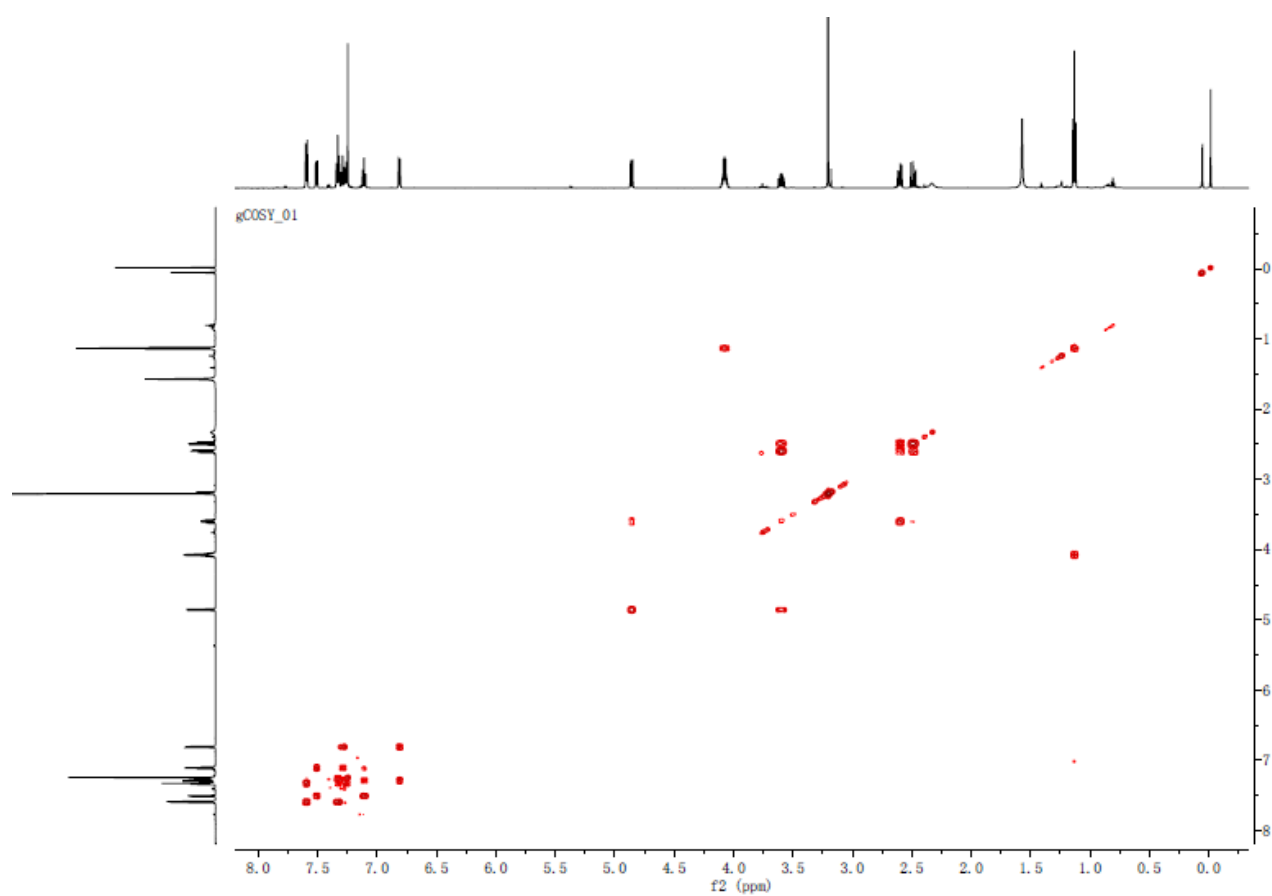
$\delta H_b = 2.61$

$\delta H_c = 3.61$

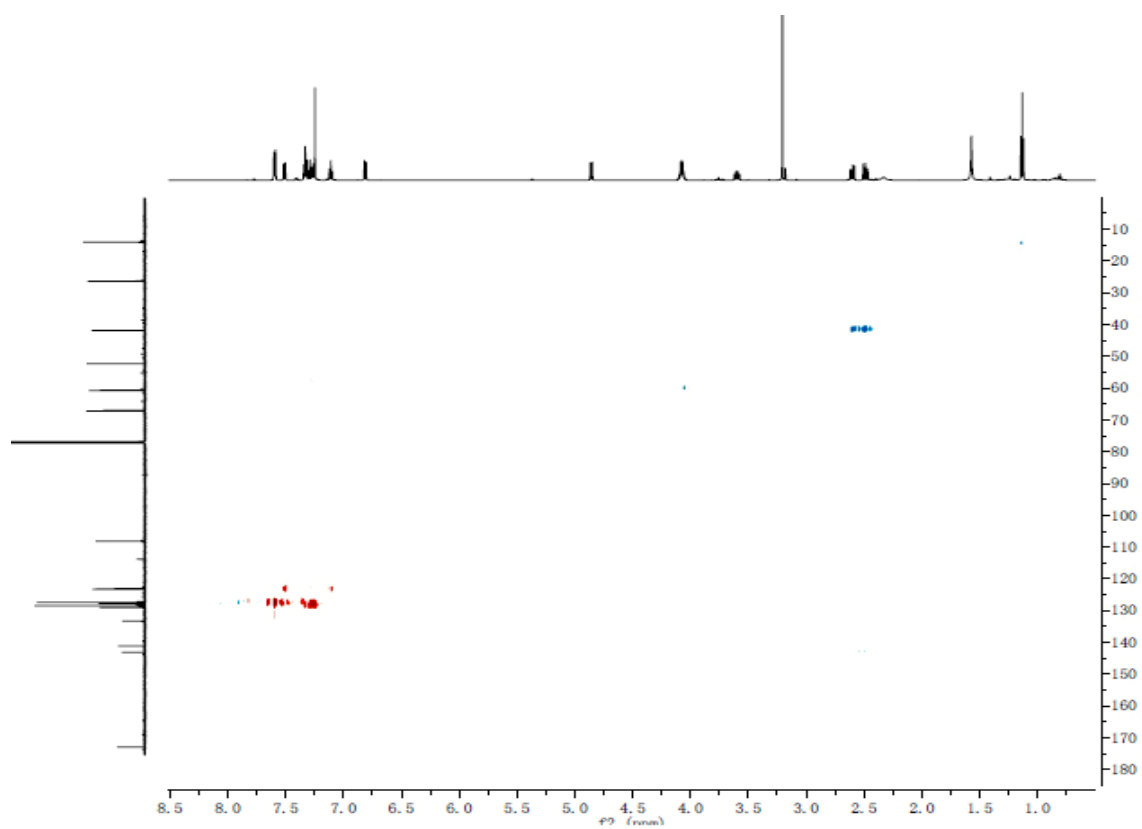
$\delta H_d = 4.86$

$\delta H_1 = 7.52$

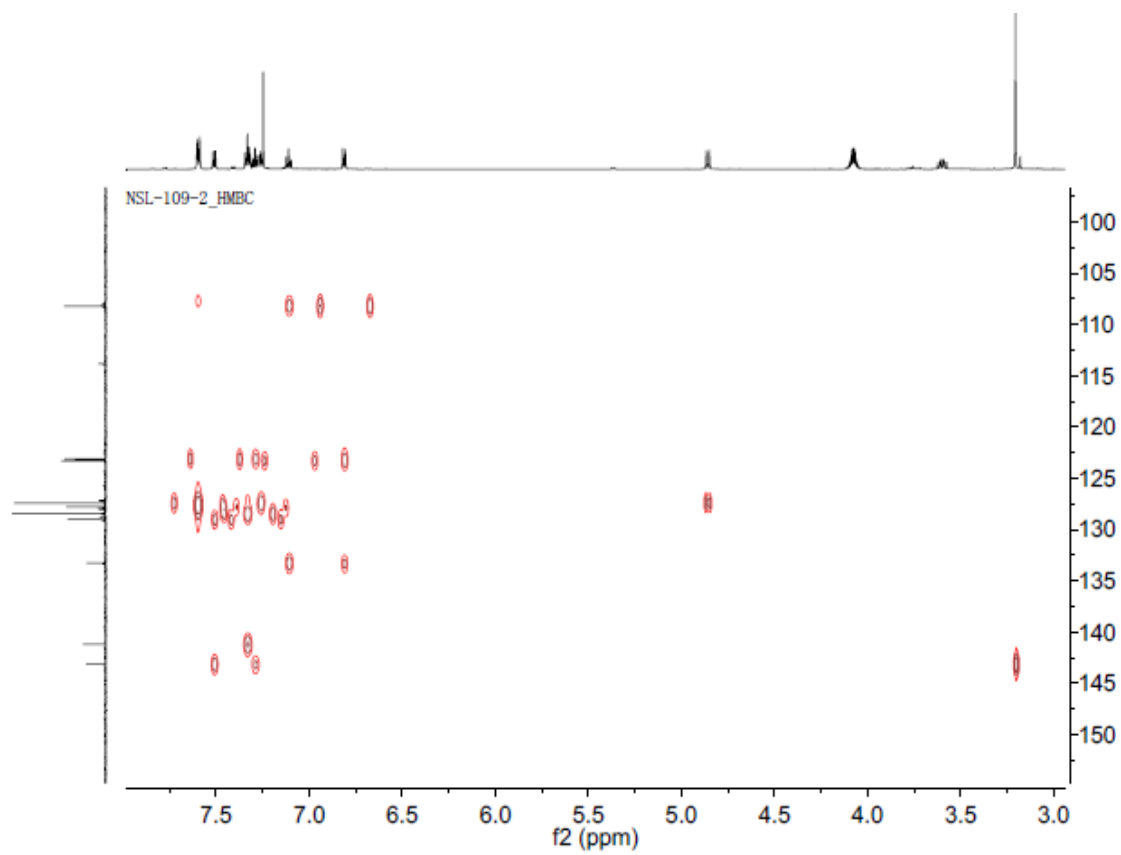
Structure of 9



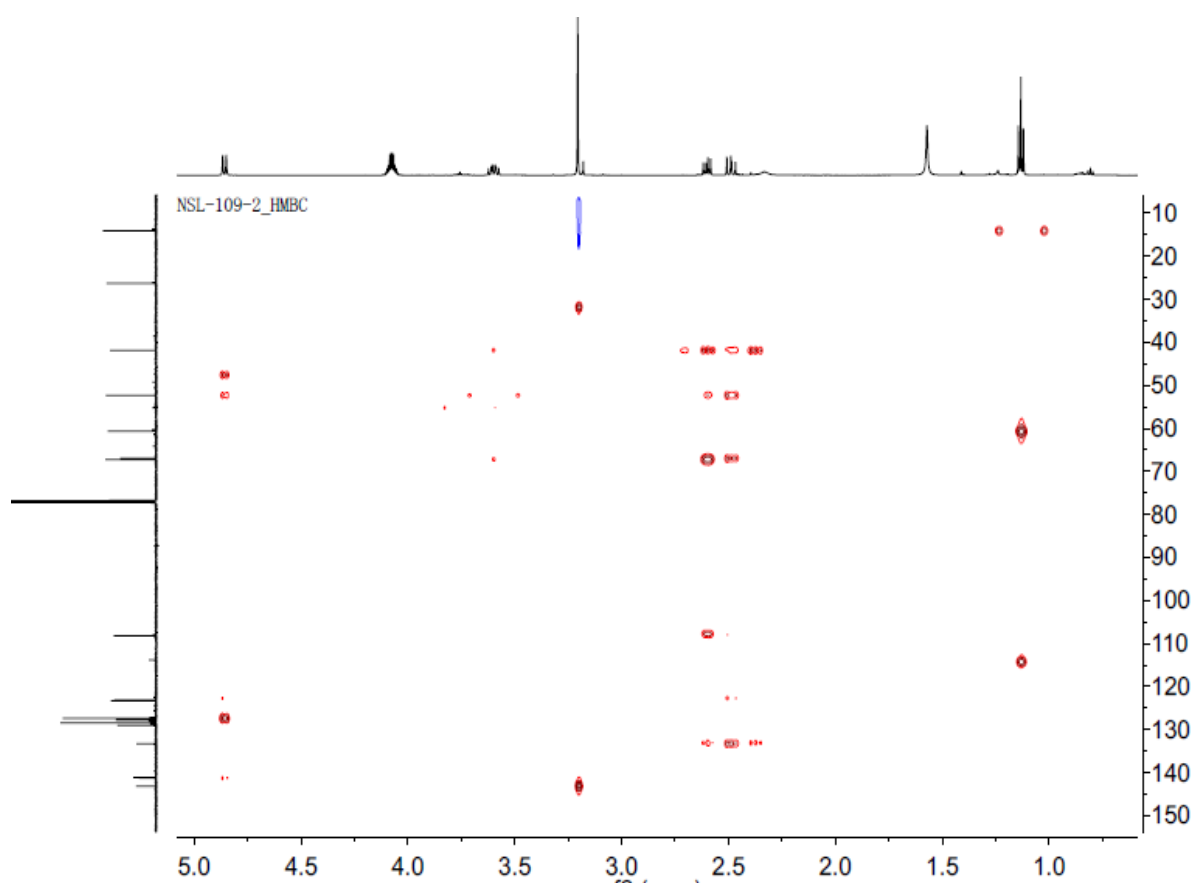
COSY of 9



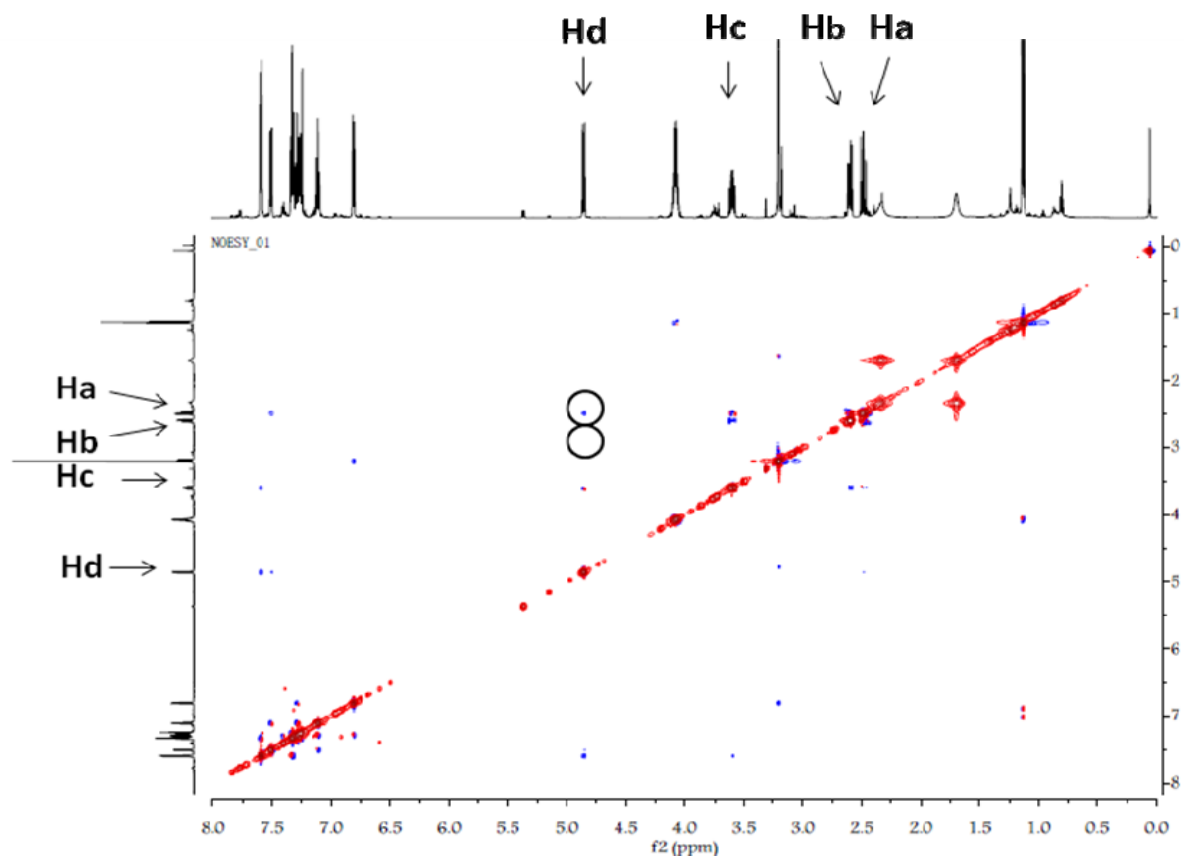
HSQC of 9



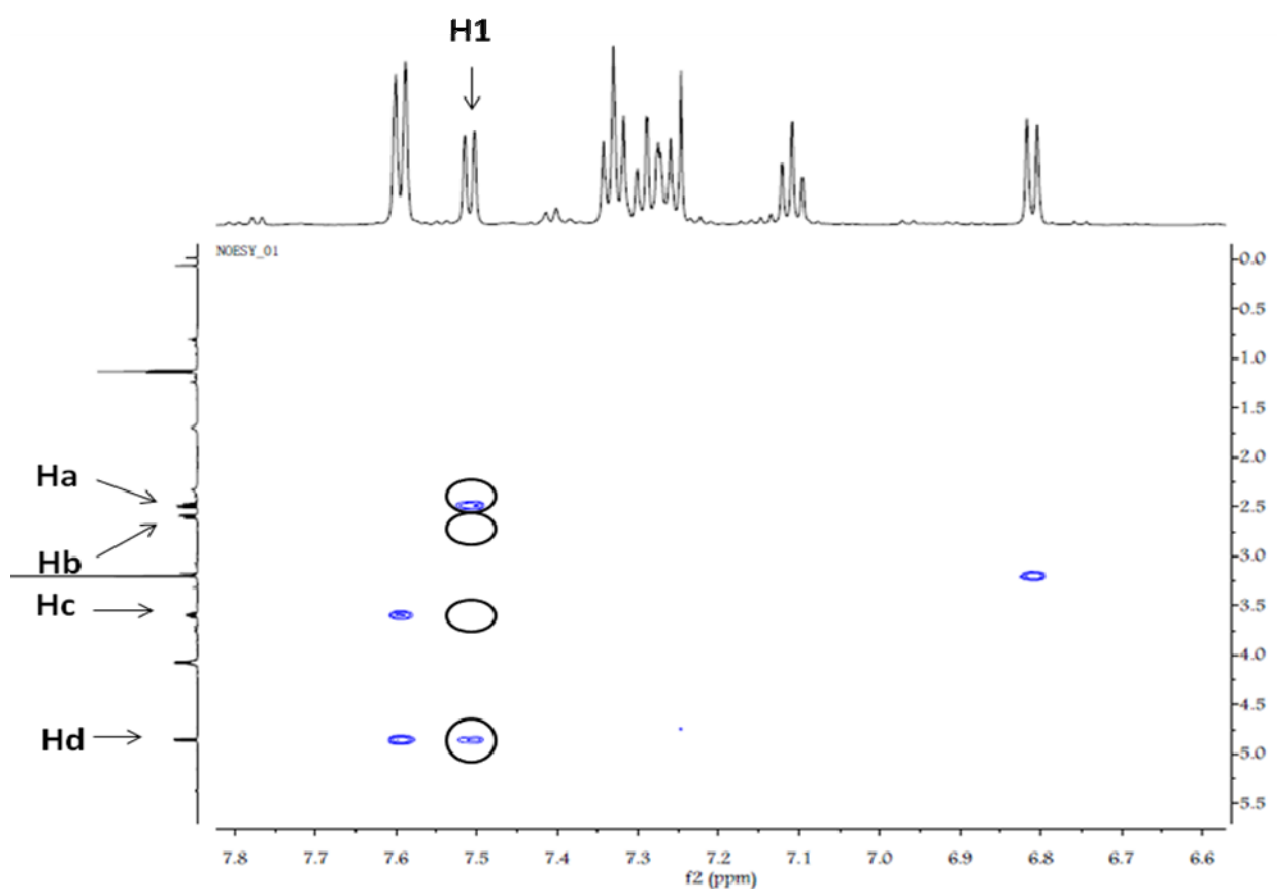
HMBC of 9



HMBC of 9

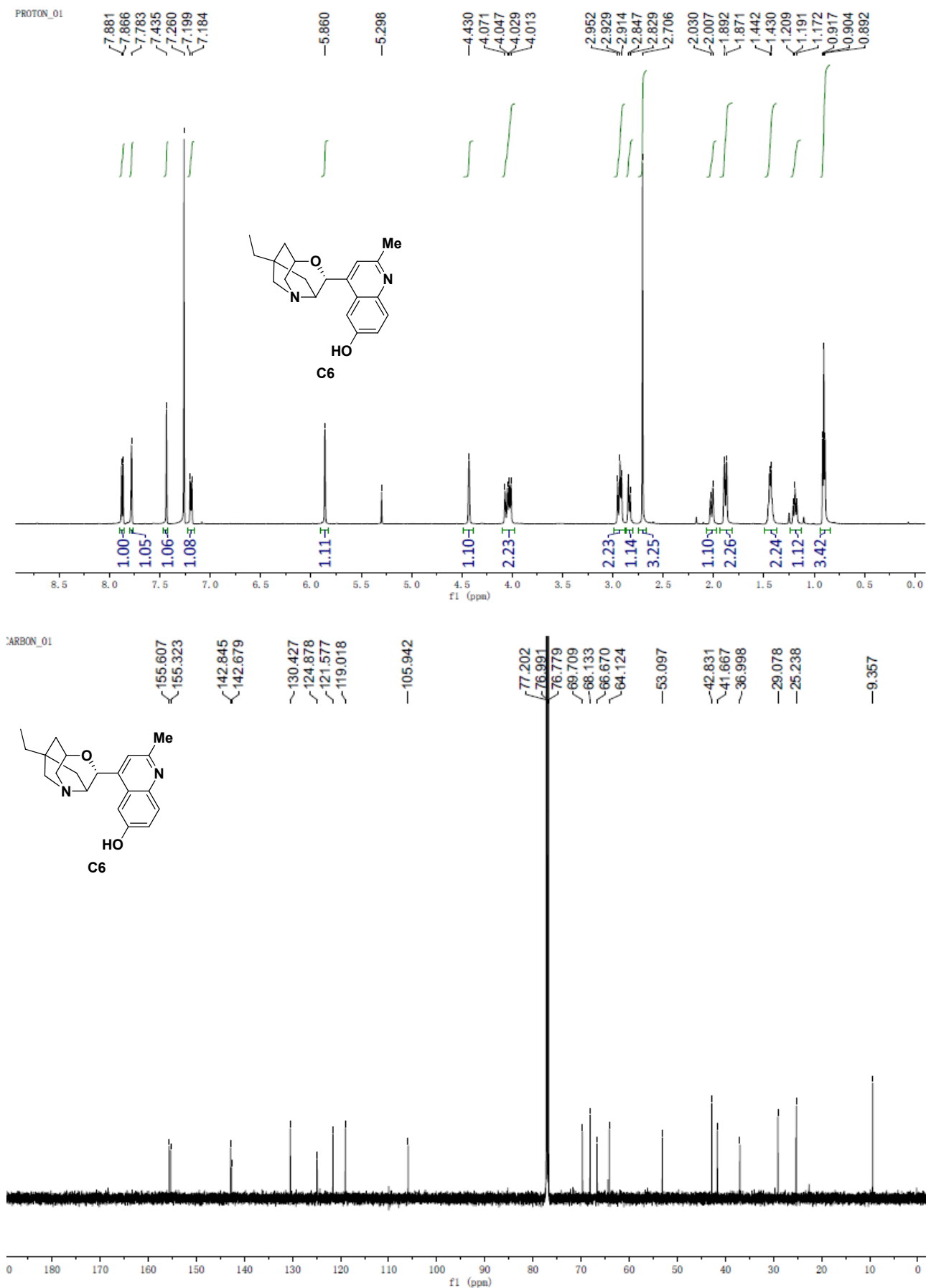


NOESY of 9

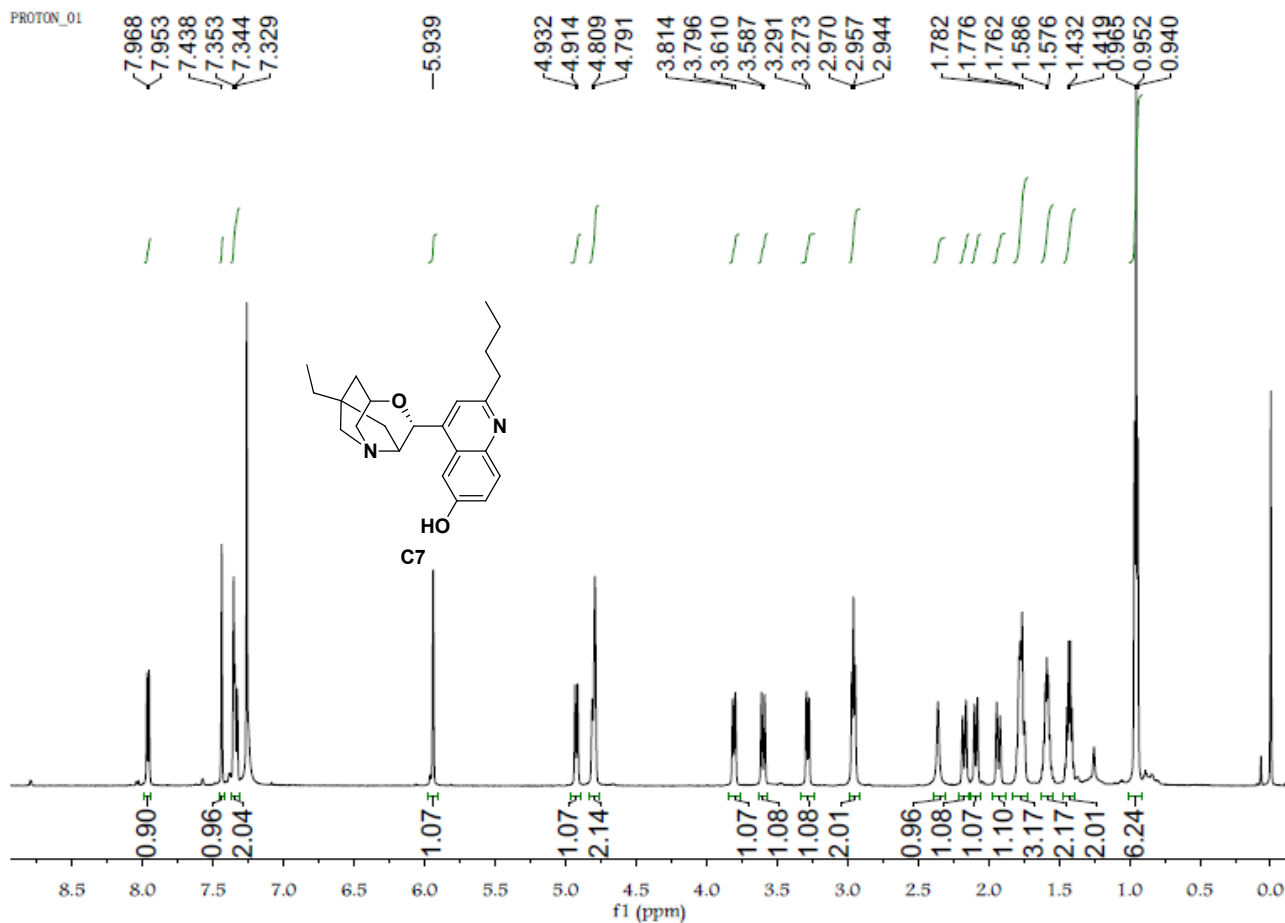


NOSEY of 9

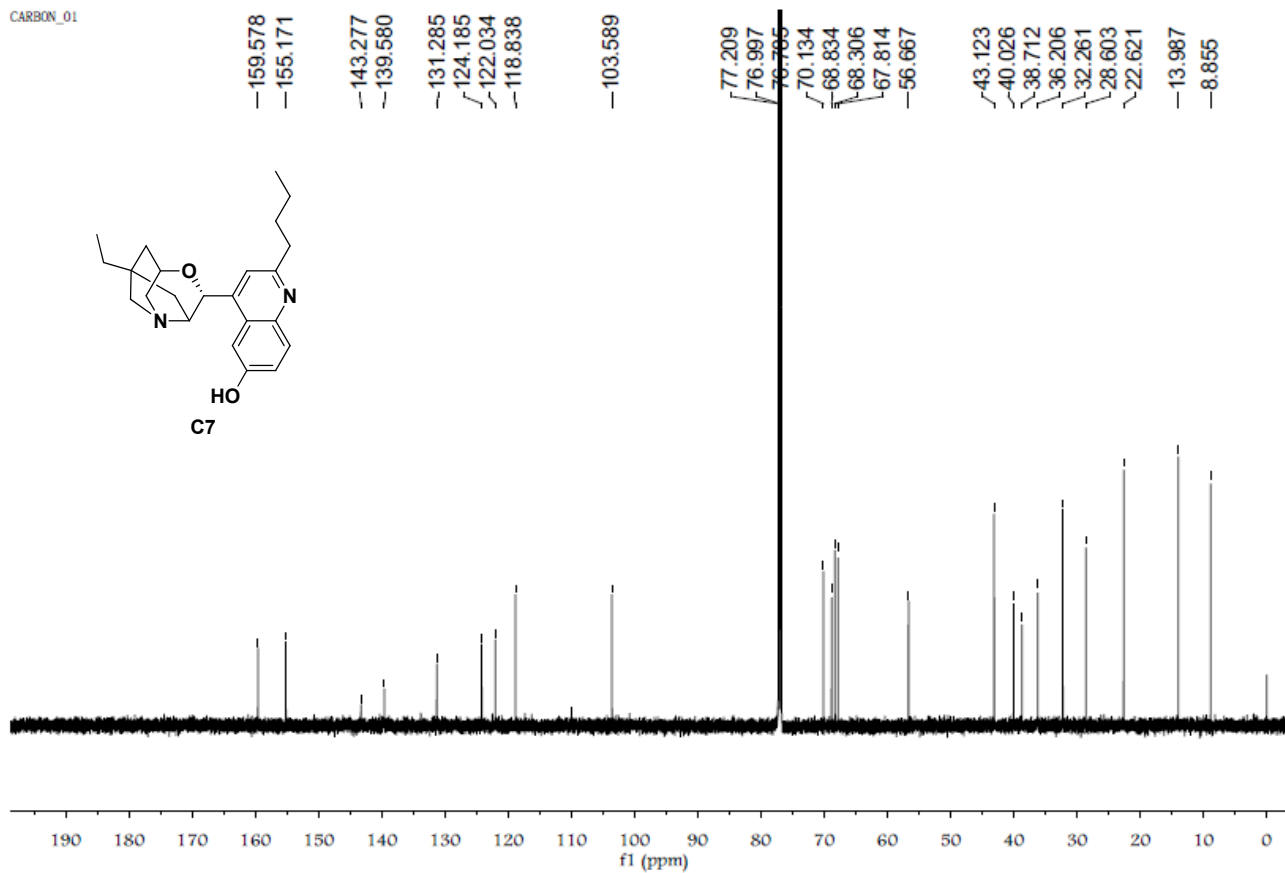
10. NMR spectra and HPLC chromatograms



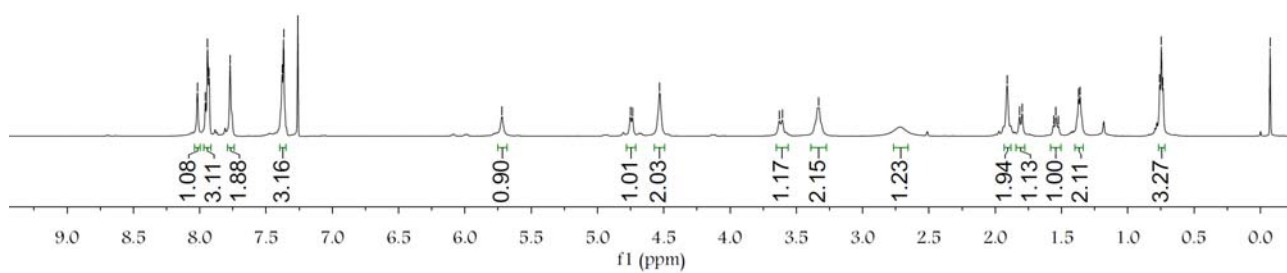
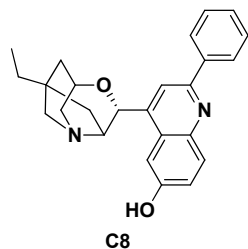
PROTON_01



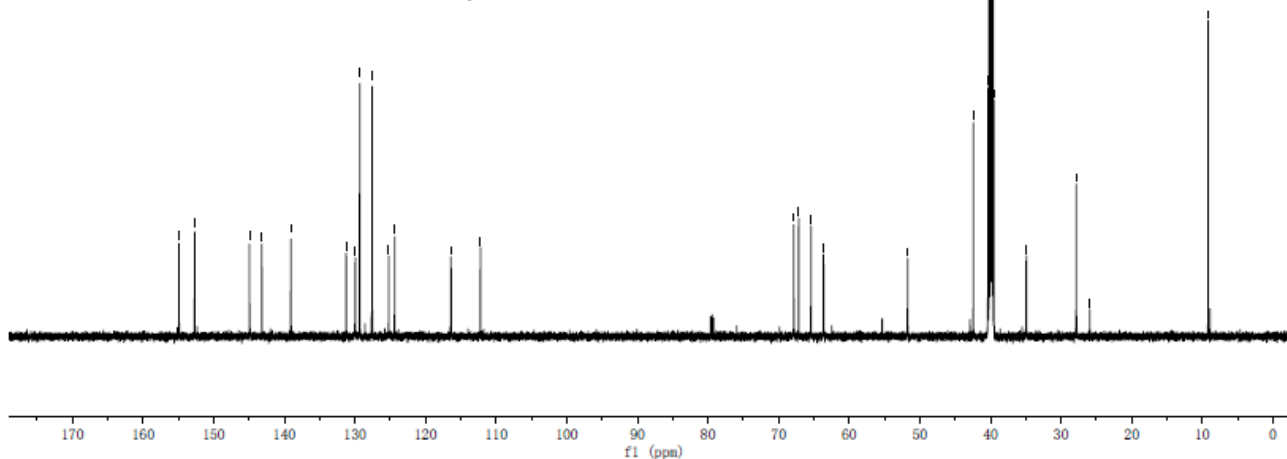
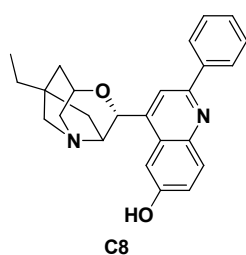
CARBON_01

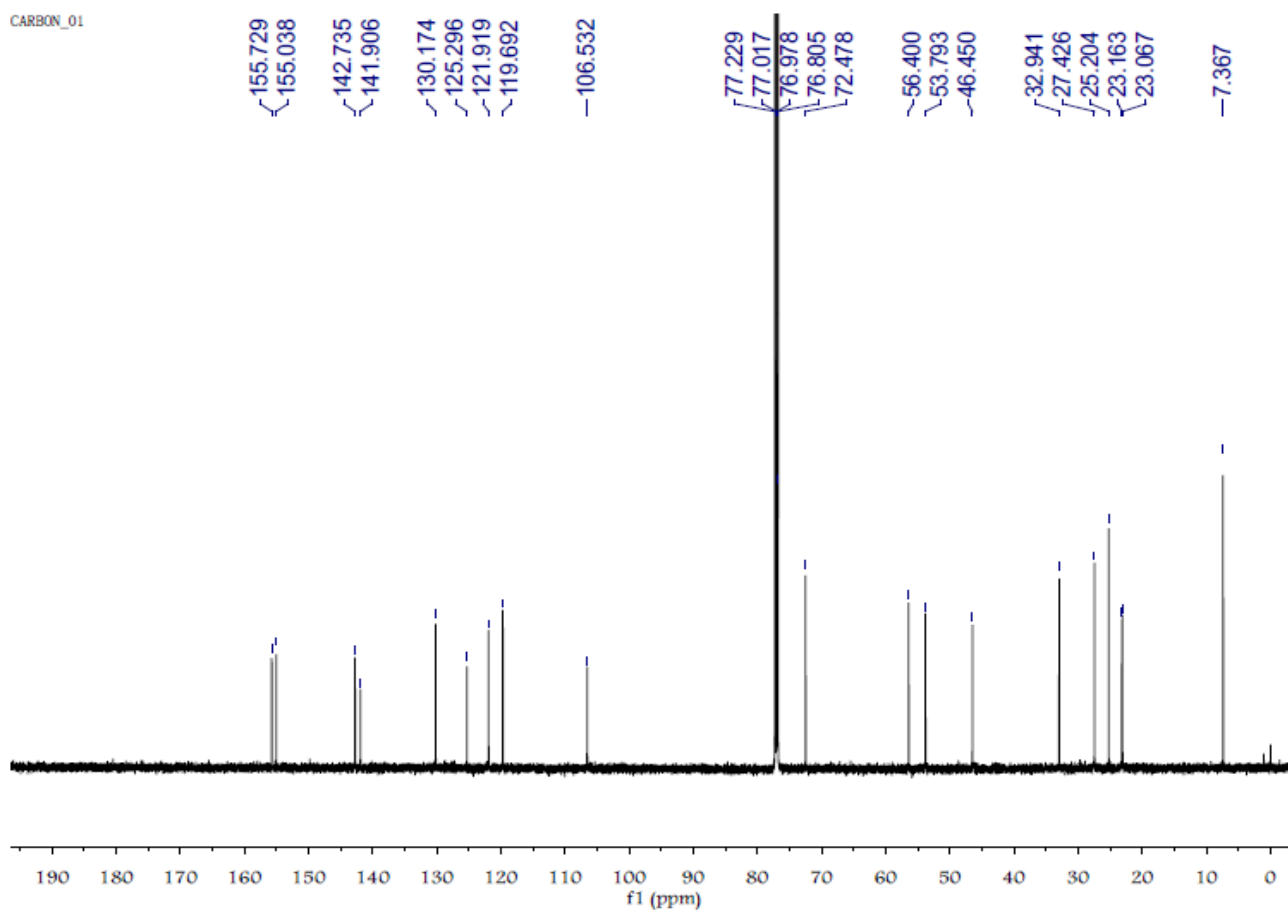
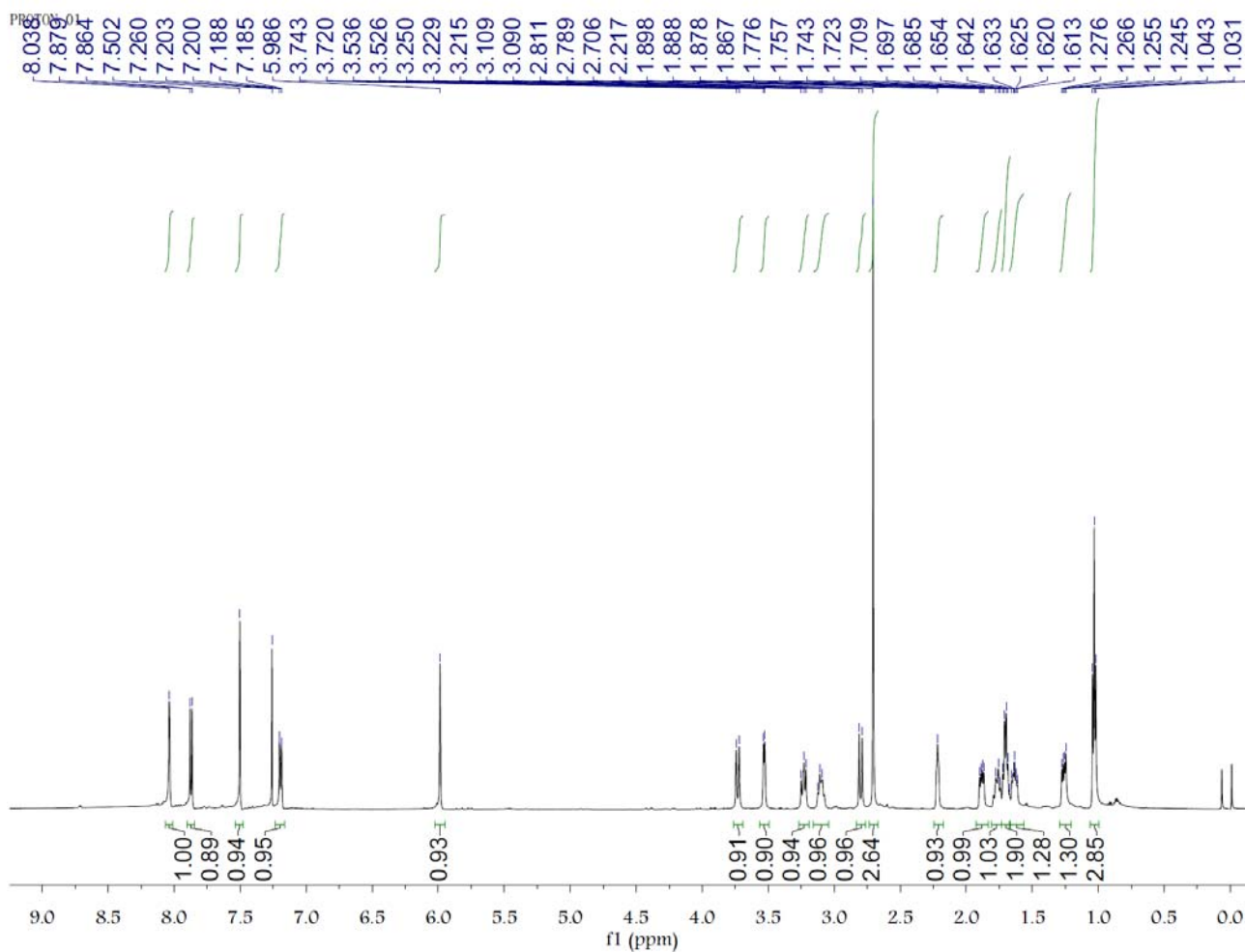


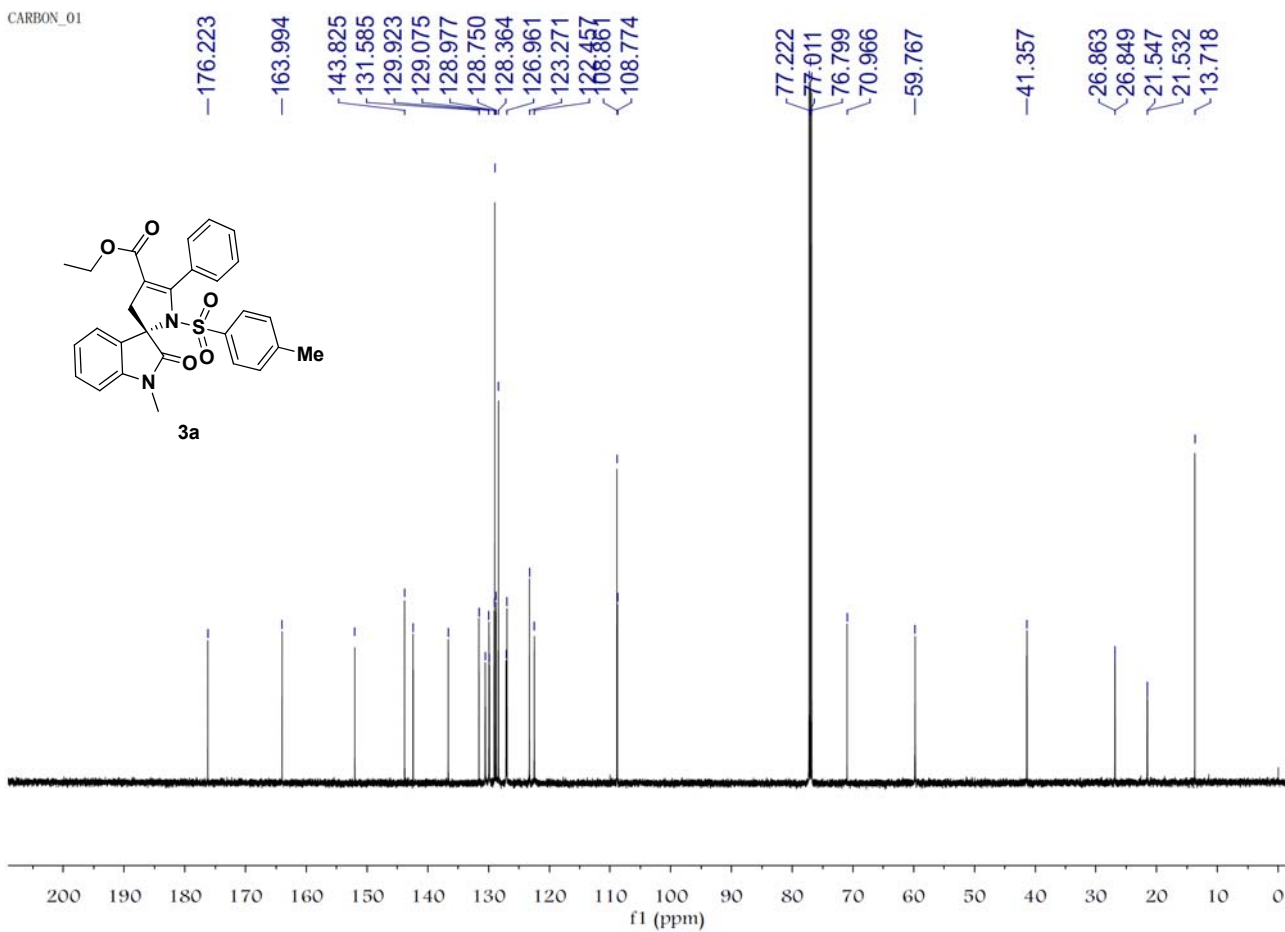
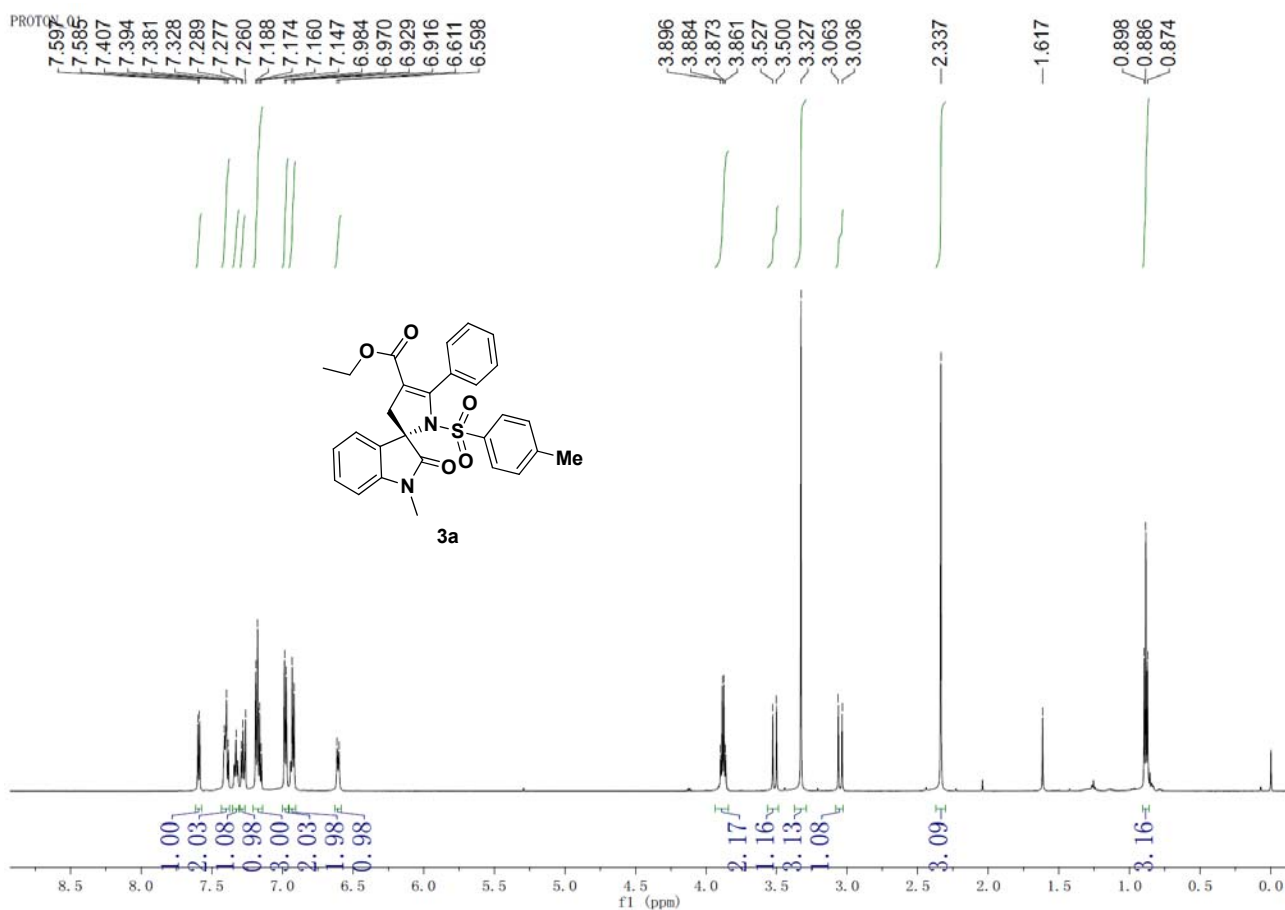
PROTON_01

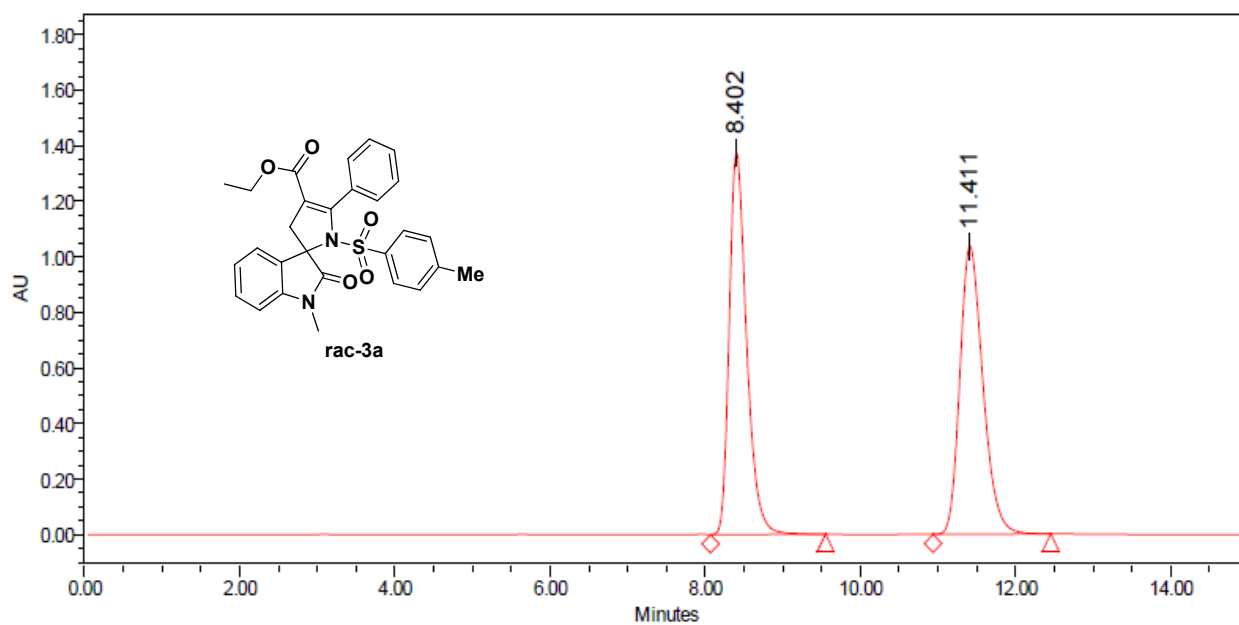


CARBON_01



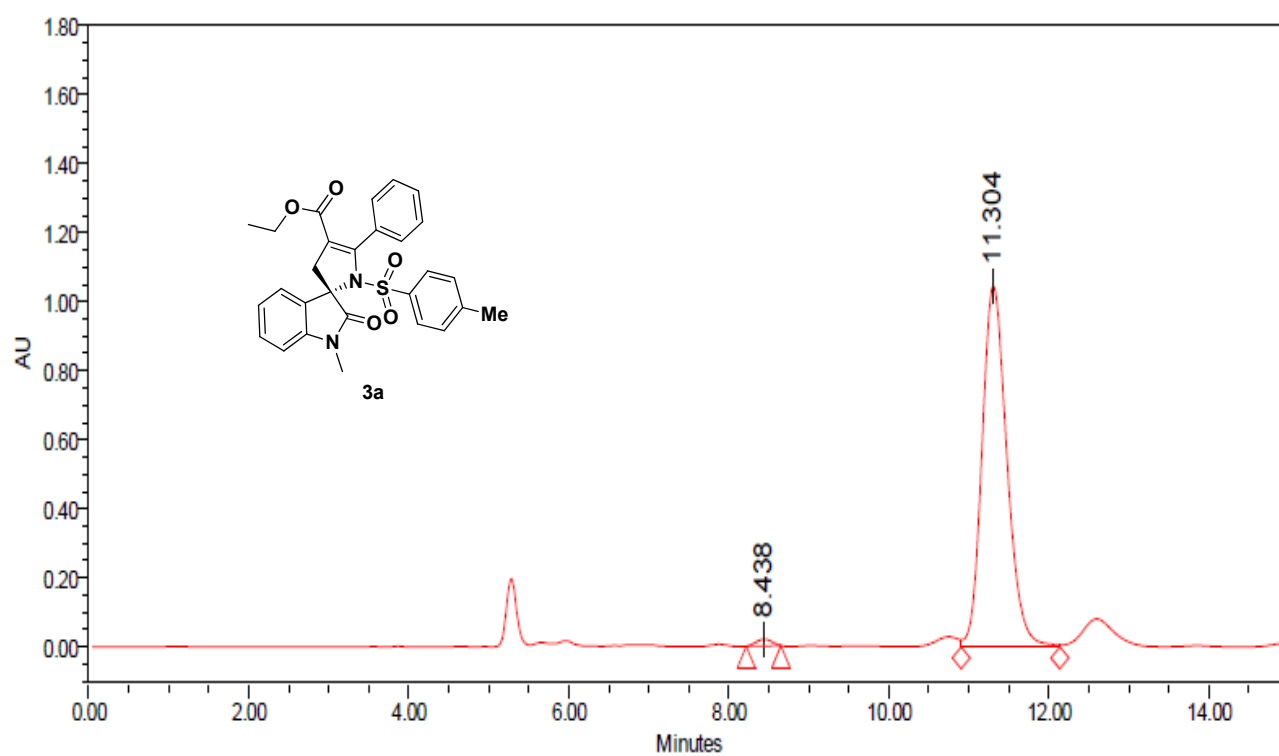






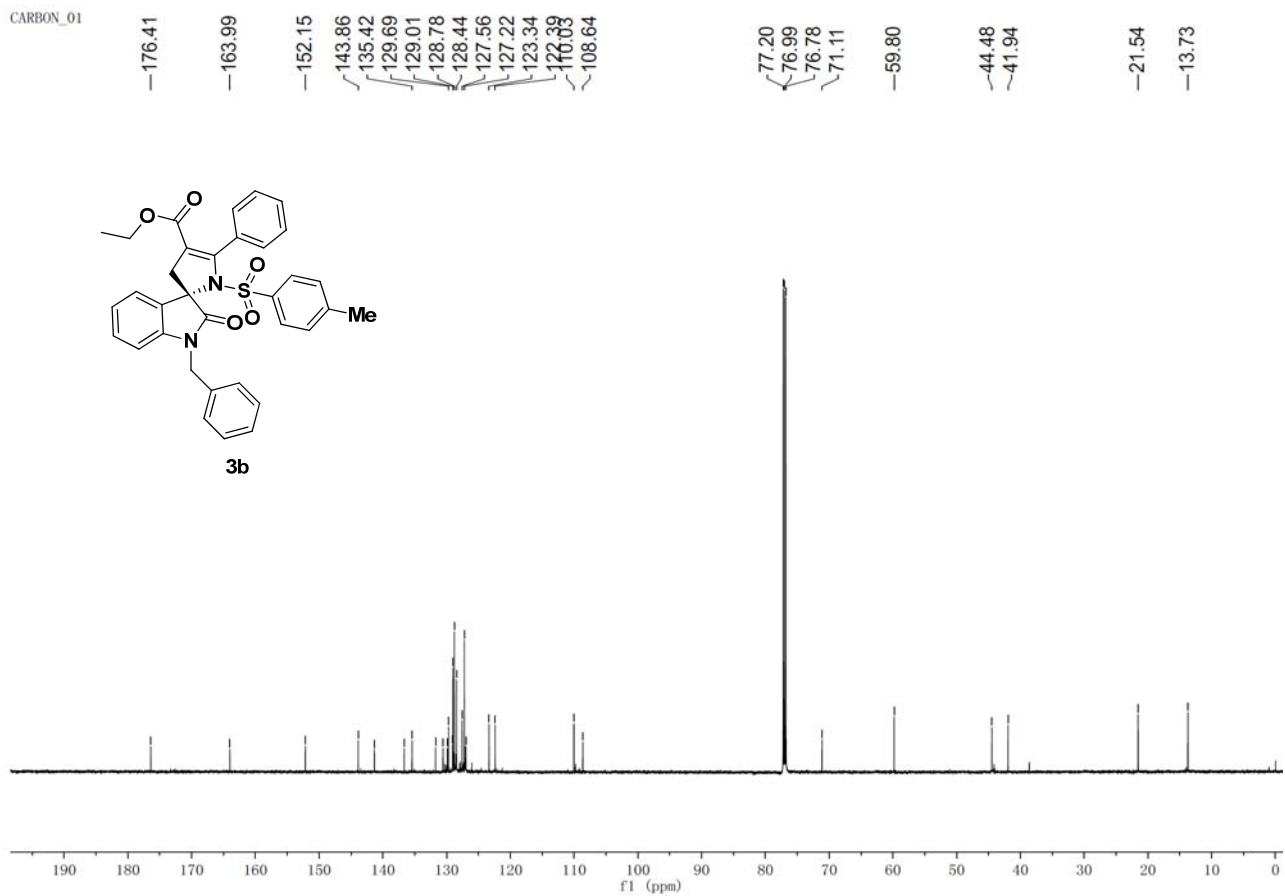
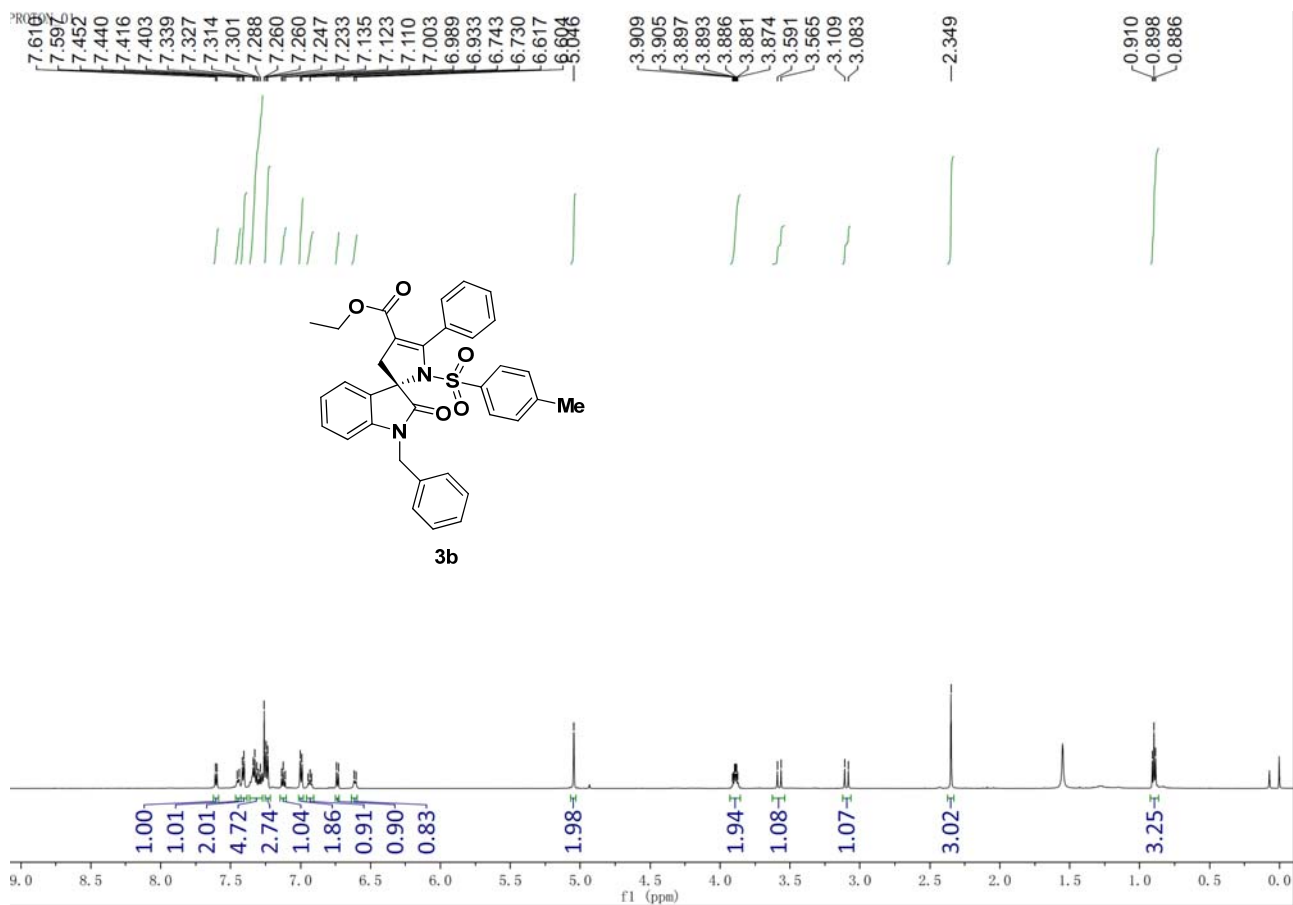
Peak Results

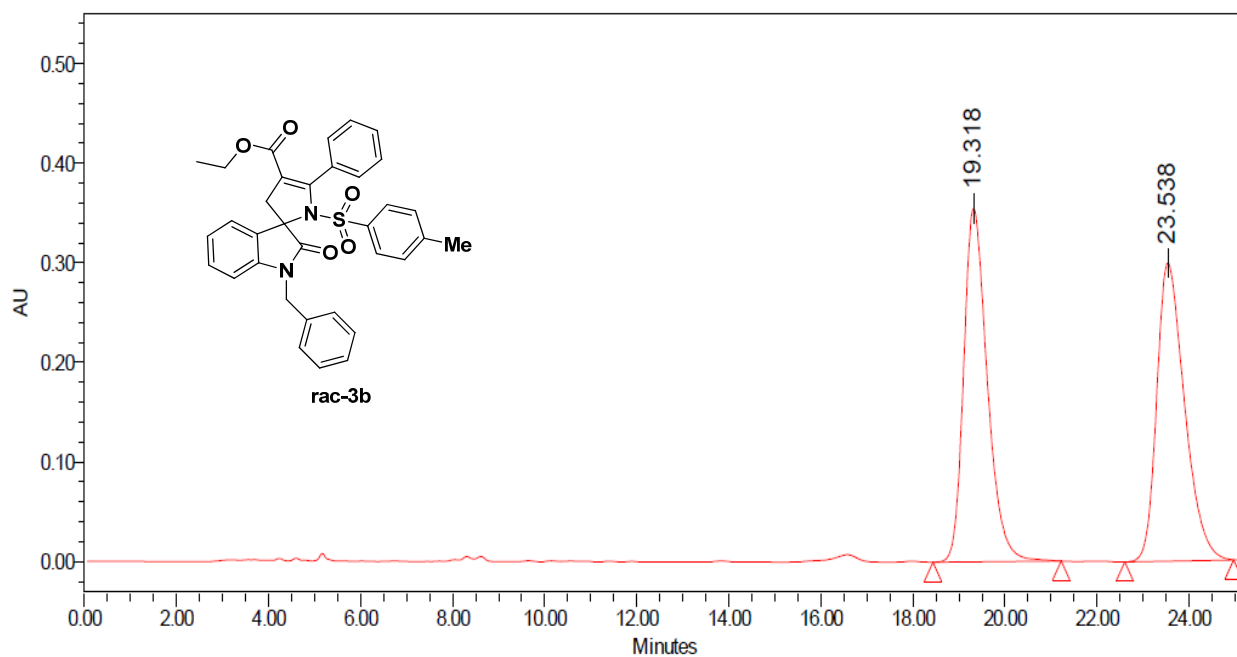
	Name	RT	Area	Height	% Area
1		8.402	21421444	1376230	50.08
2		11.411	21357114	1036842	49.92



Peak Results

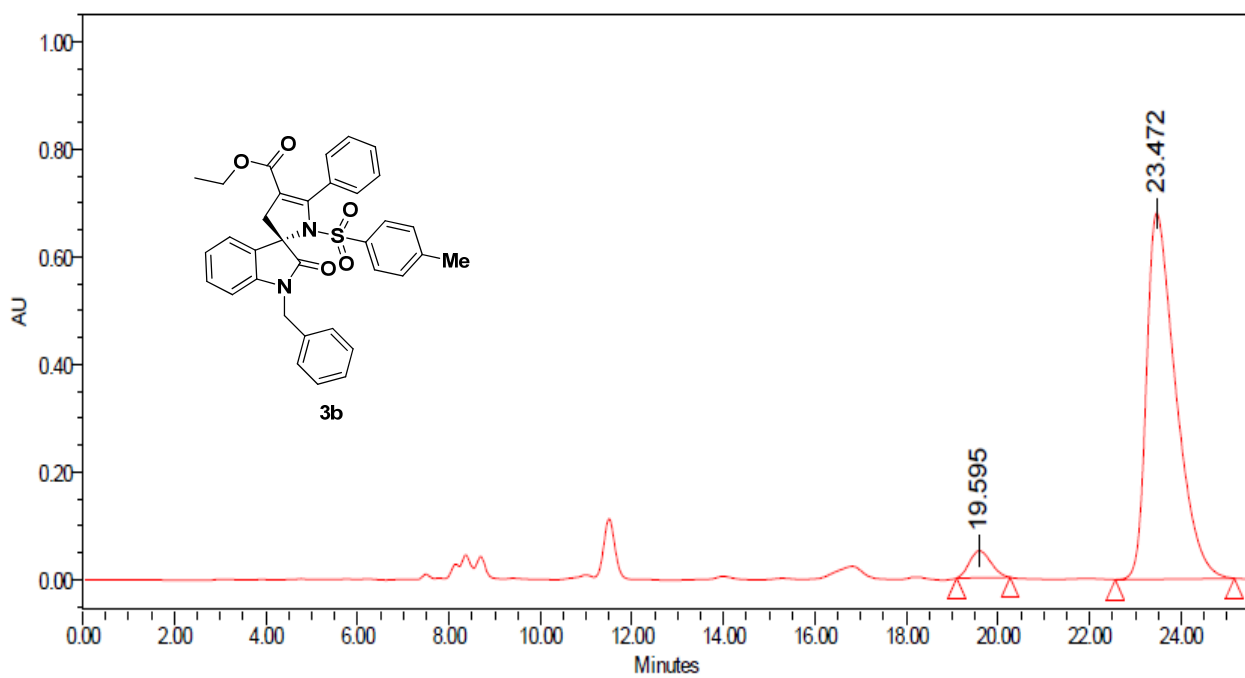
	Name	RT	Area	Height	% Area
1		8.438	260205	19200	1.14
2		11.304	22543038	1046438	98.86





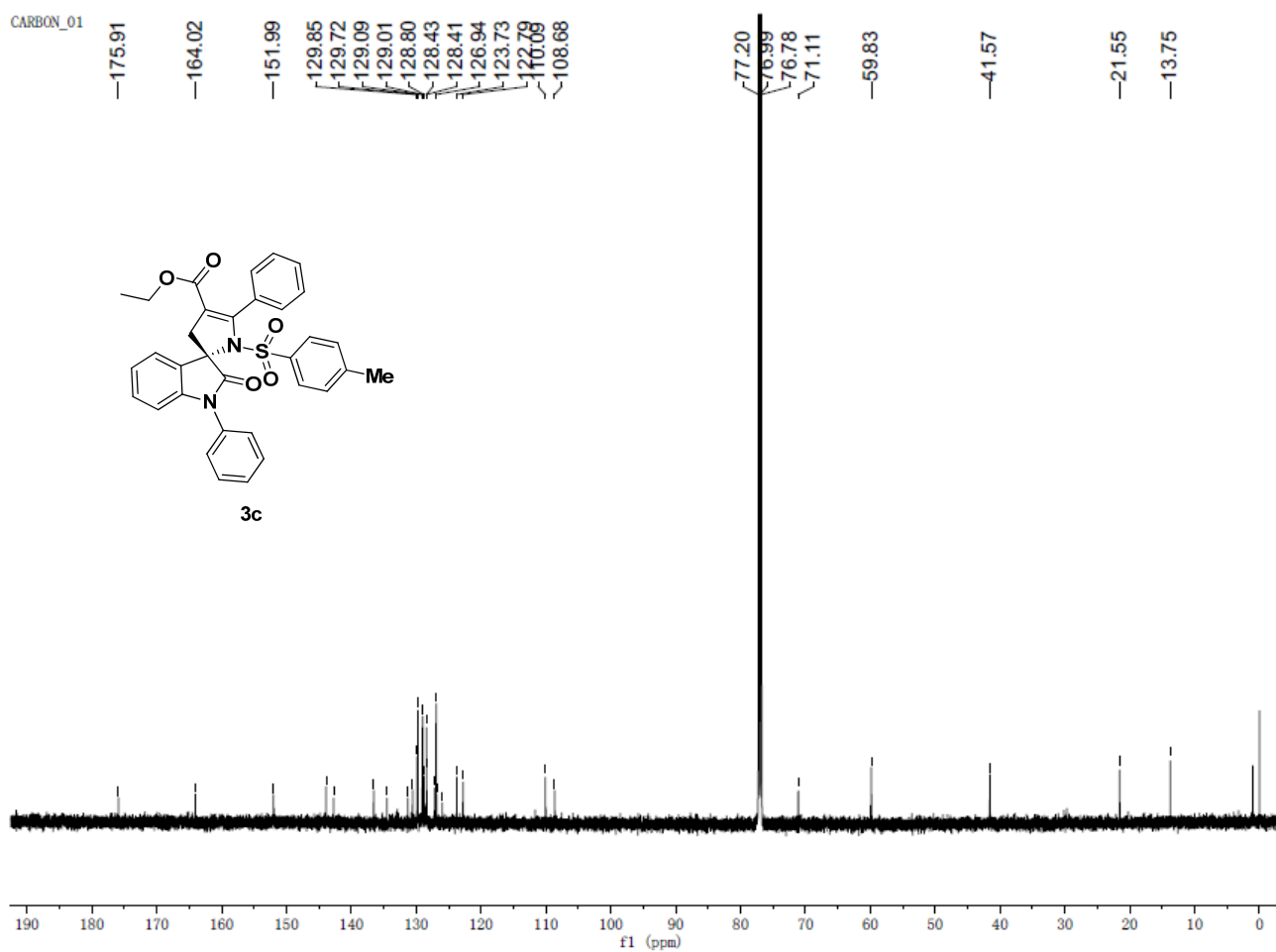
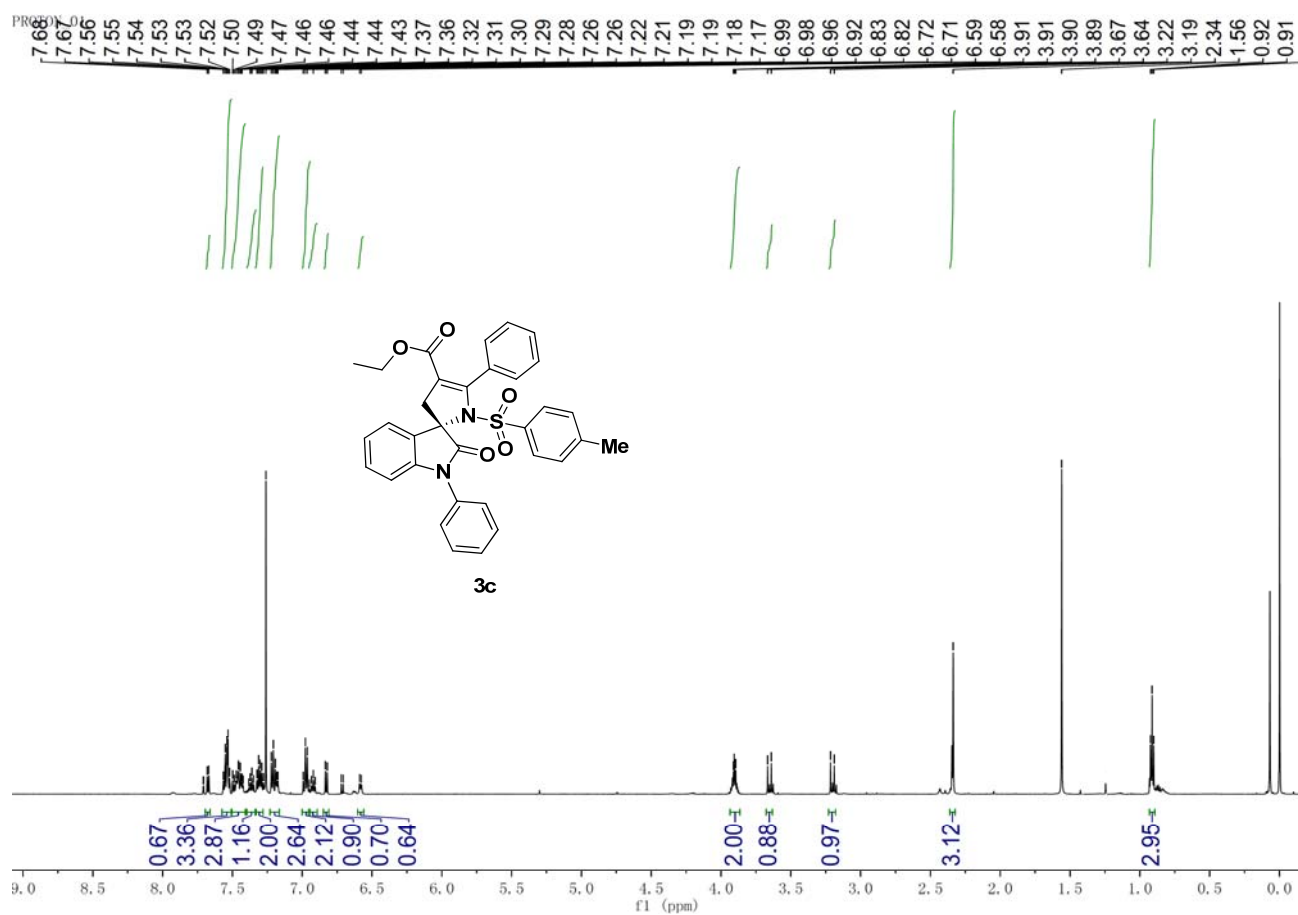
Peak Results

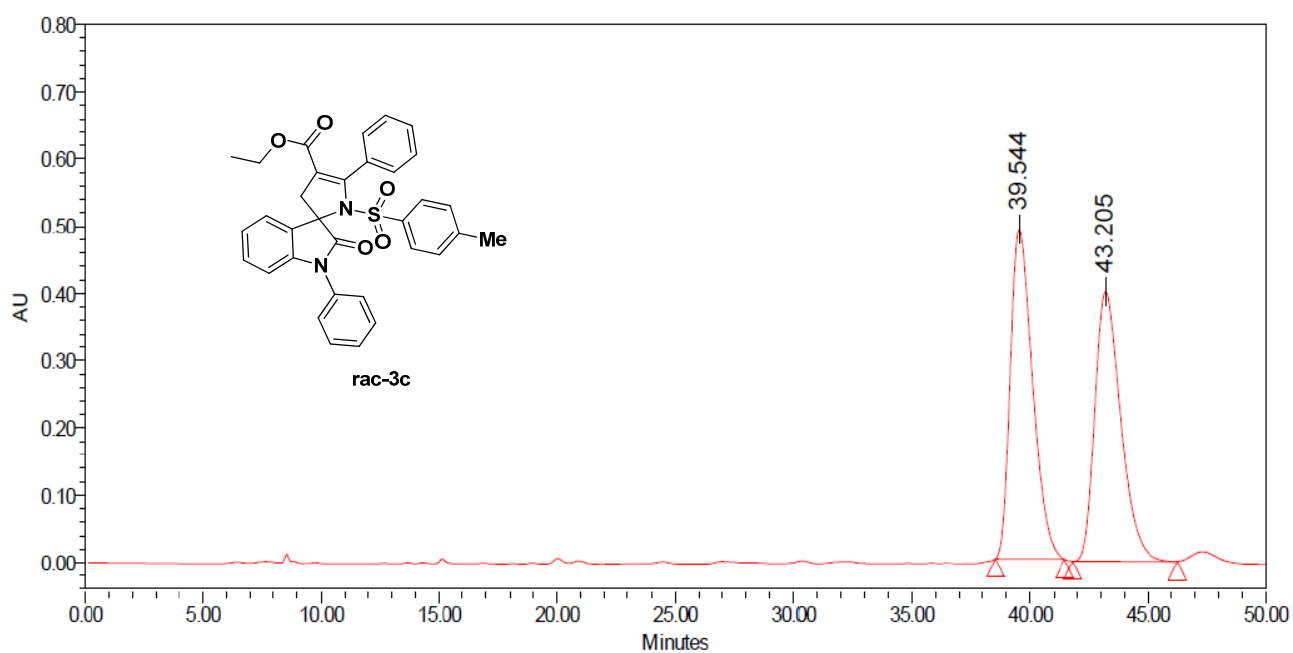
	Name	RT	Area	Height	% Area
1		19.318	12677627	355077	50.21
2		23.538	12571134	299570	49.79



Peak Results

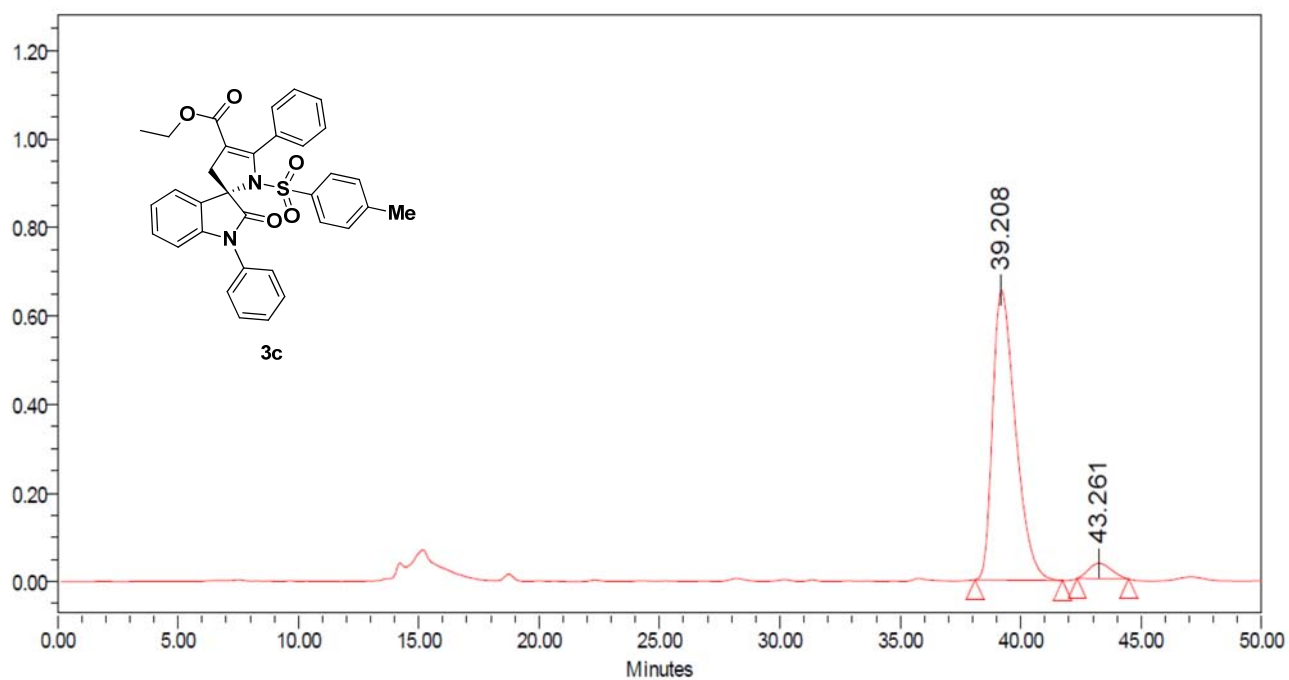
	Name	RT	Area	Height	% Area
1		19.595	1625372	50065	5.11
2		23.472	30195666	680685	94.89





Peak Results

	Name	RT	Area	Height	%Area
1		39.544	31671673	489776	51.10
2		43.205	30311639	400744	48.90



Peak Results

Name	RT	Area	Height	%Area
	39.208	43145238	653764	94.92
	43.261	2306742	34973	5.08

PROTON_01

7.497
7.399
7.366
7.363
7.353
7.349
7.341
7.284
7.248
7.159
7.146
6.990
6.976
6.931
6.847
6.833

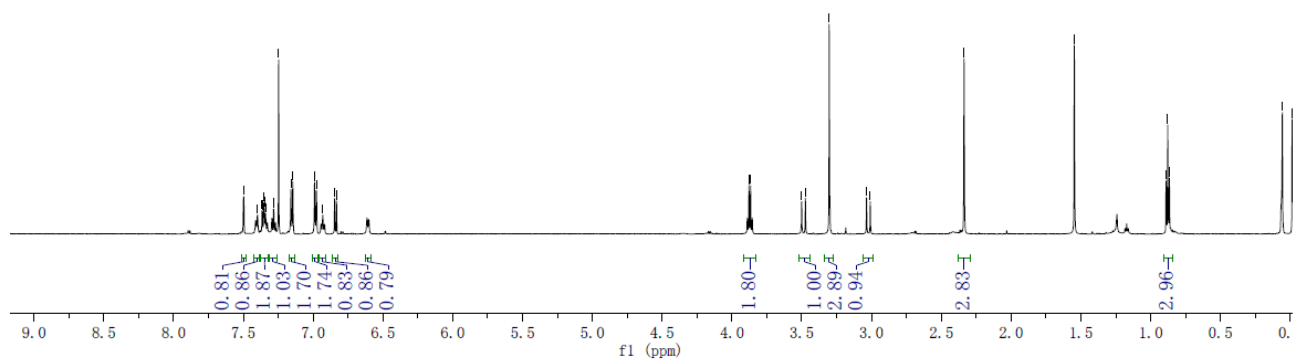
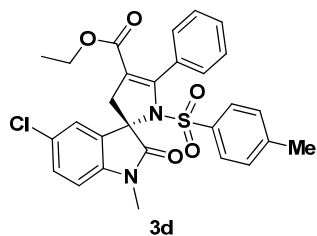
3.878
3.866
3.501
3.474
3.303
3.036
3.009

2.337

1.547

0.890
0.878
0.866

0.057
0.013



CARBON_01

175.82
163.81
151.92
144.06
129.88
129.84
129.04
128.89
128.82
128.34
126.98
123.88
108.71

77.19
76.98
76.77
70.64

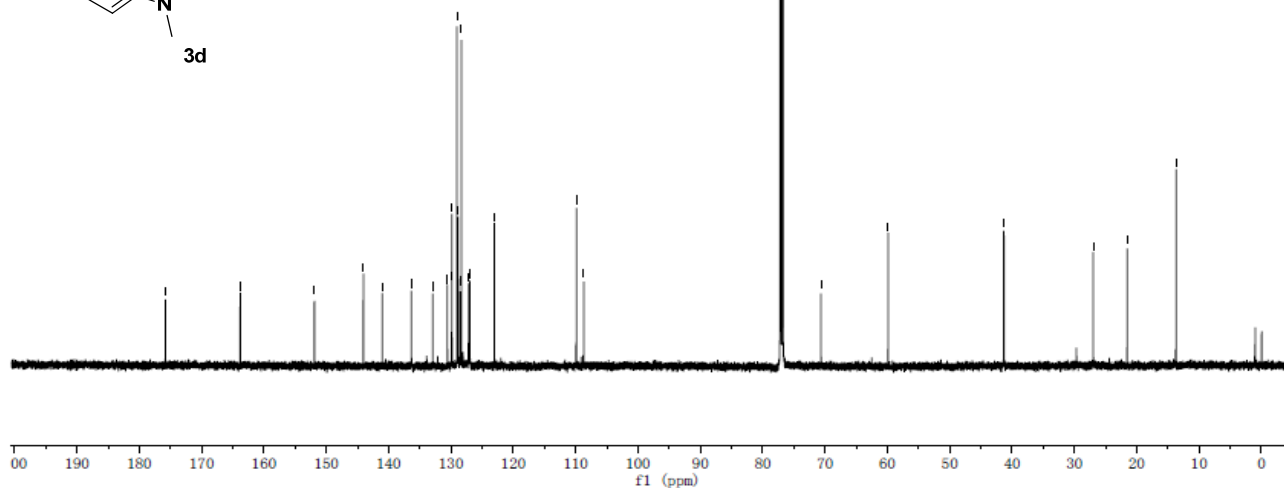
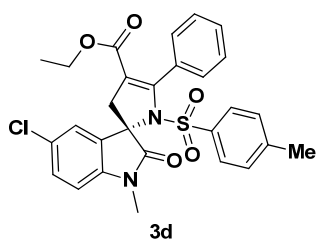
59.88

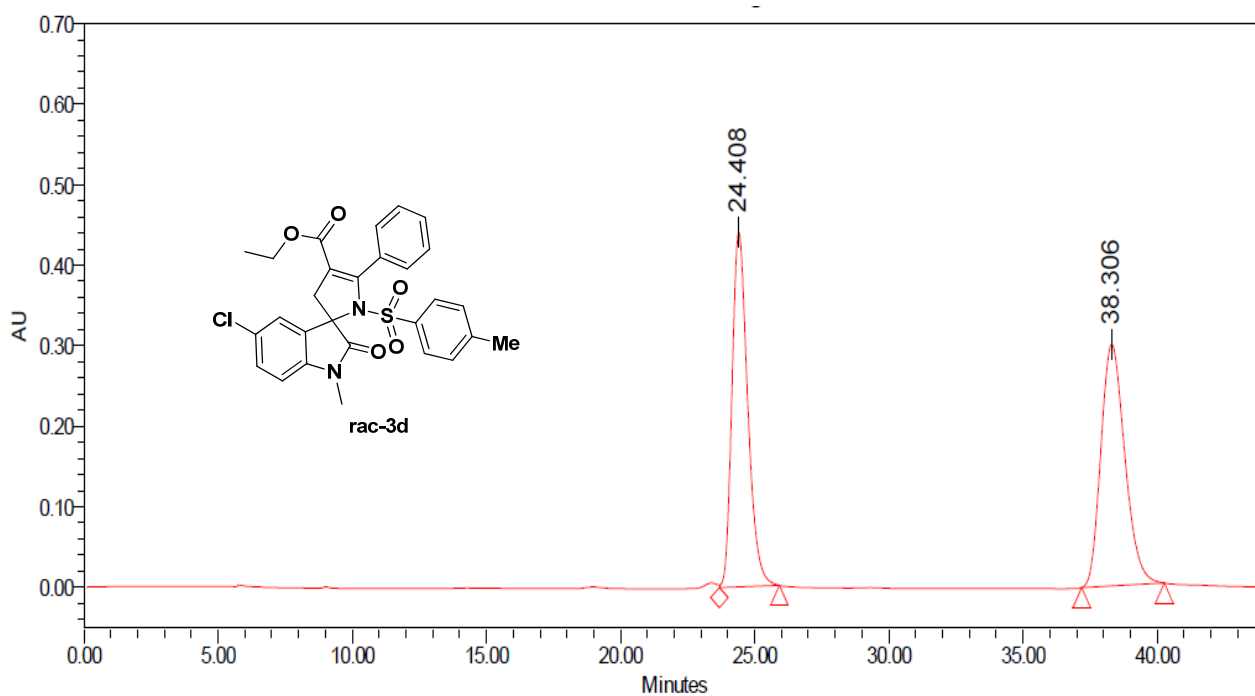
41.31

26.97

21.54

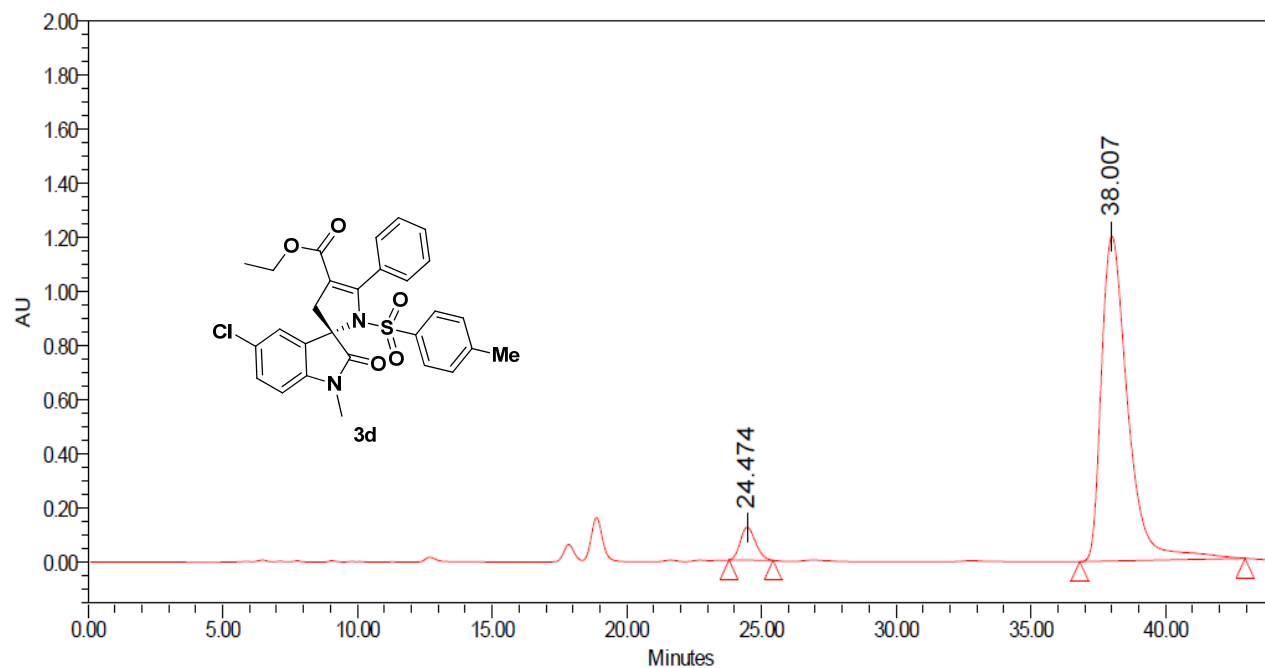
13.69





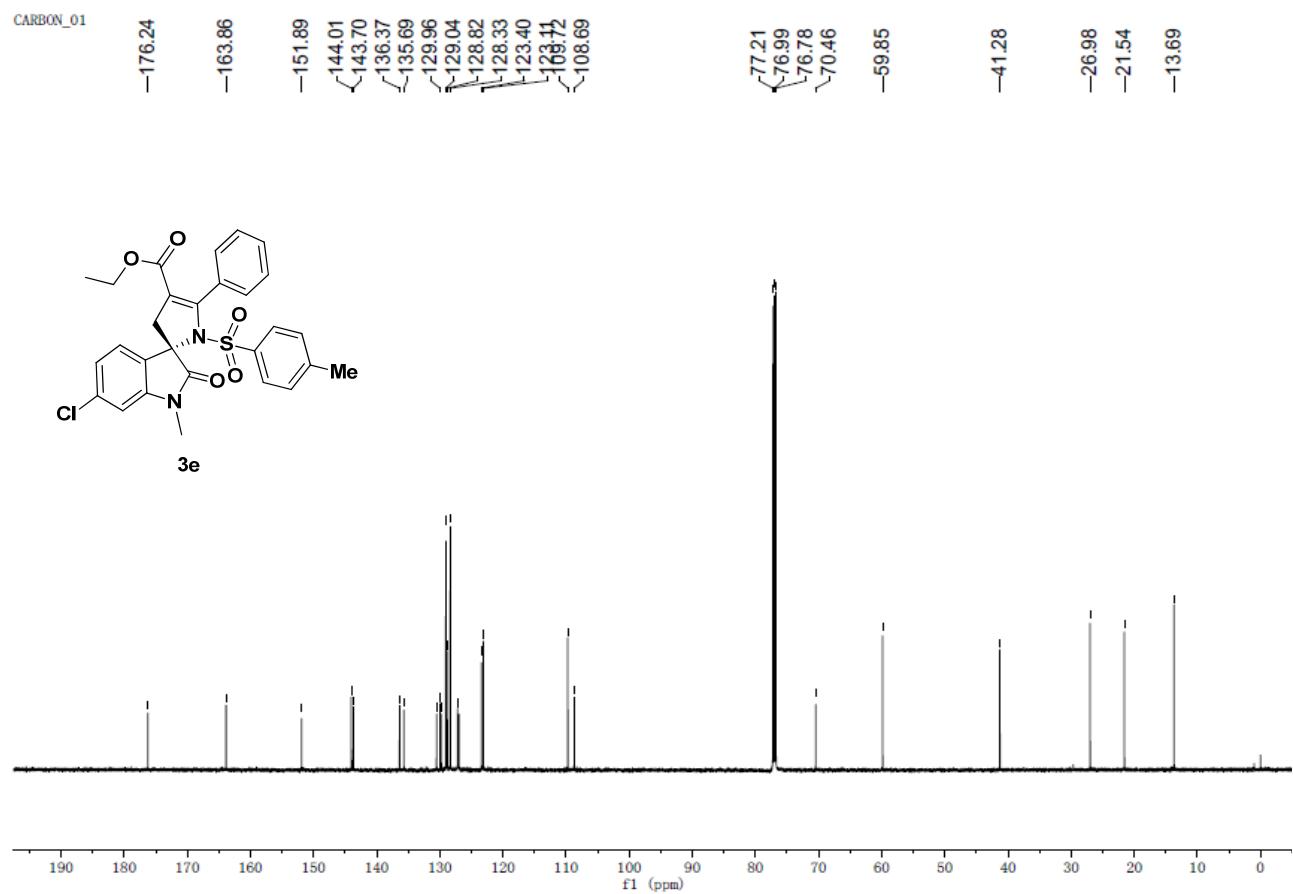
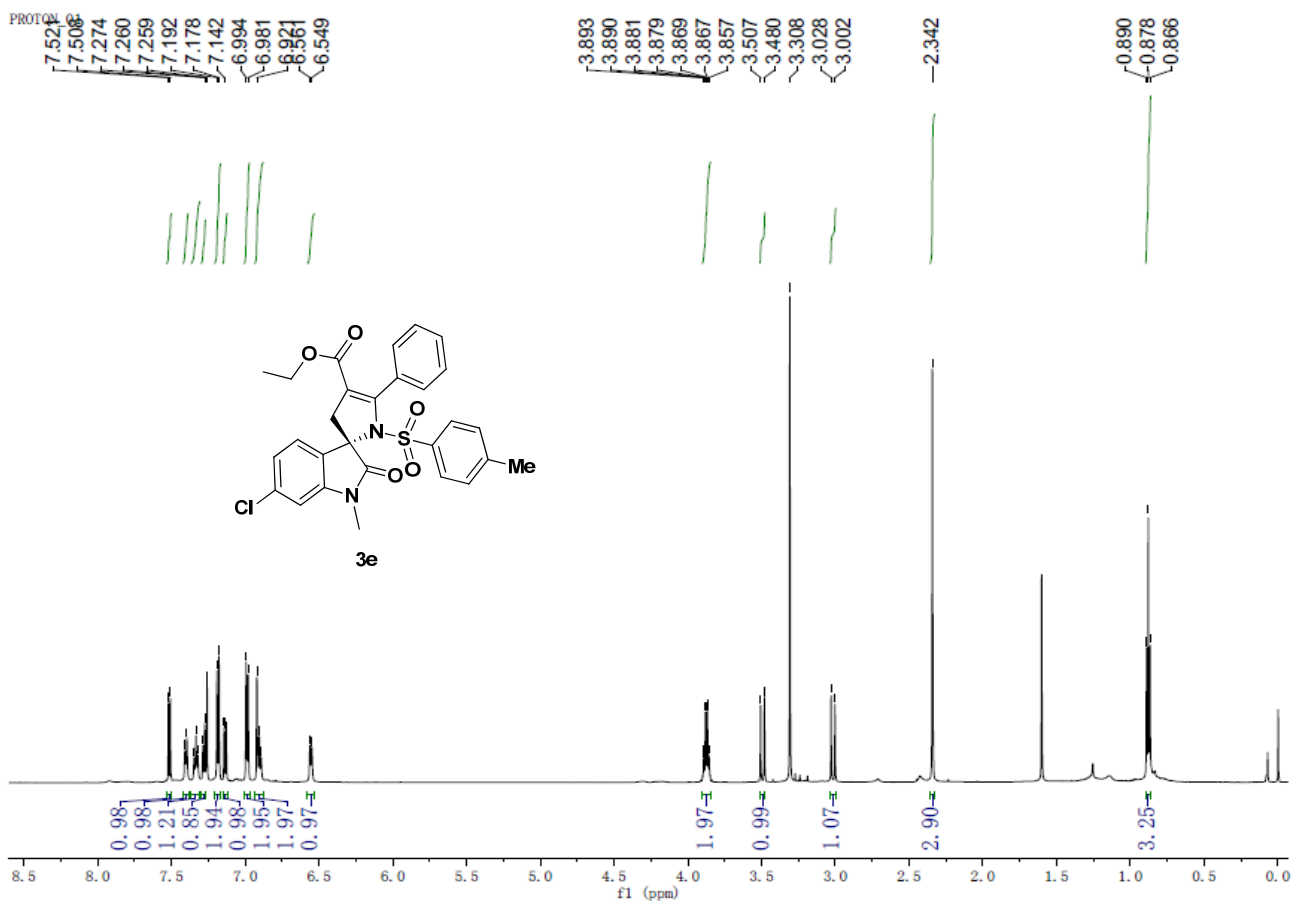
Peak Results

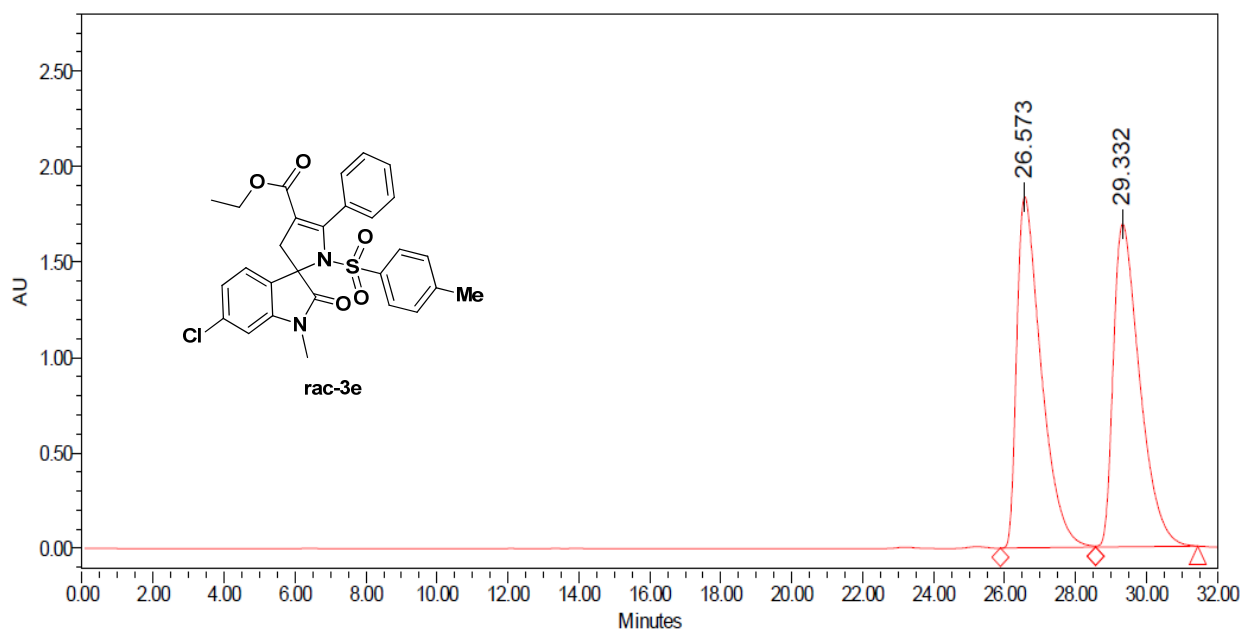
	Name	RT	Area	Height	% Area
1		24.408	17988017	440717	49.06
2		38.306	18678565	300201	50.94



Peak Results

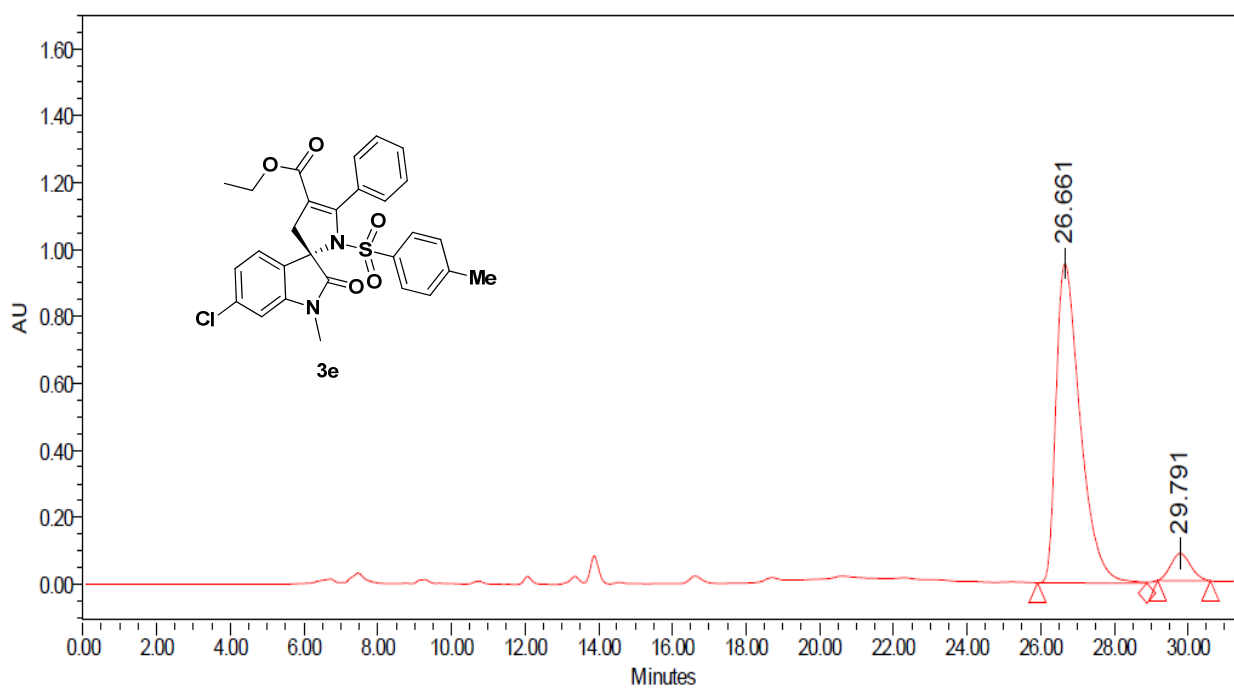
	Name	RT	Area	Height	% Area
1		24.474	4831496	122040	5.59
2		38.007	81654519	1200673	94.41





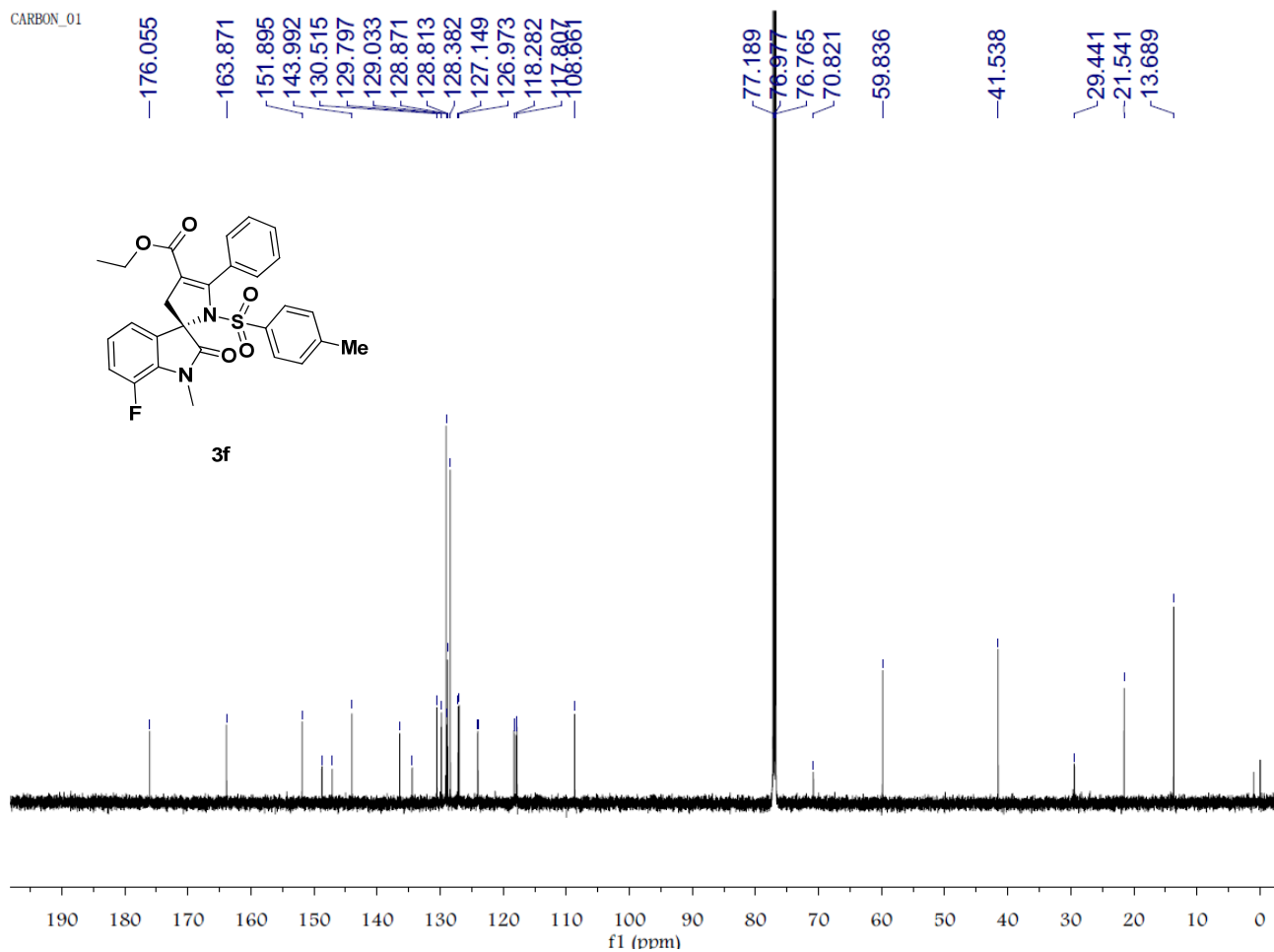
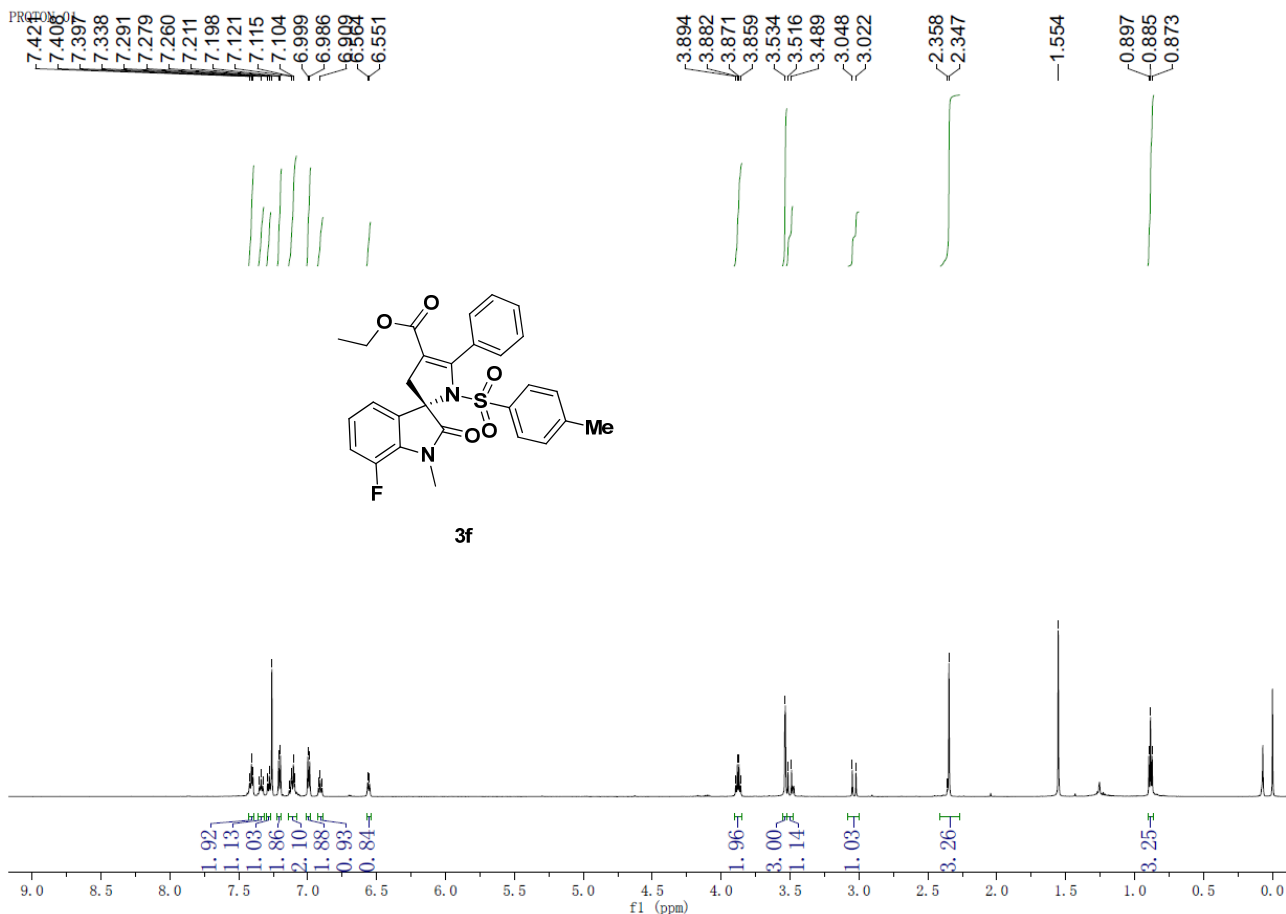
Peak Results

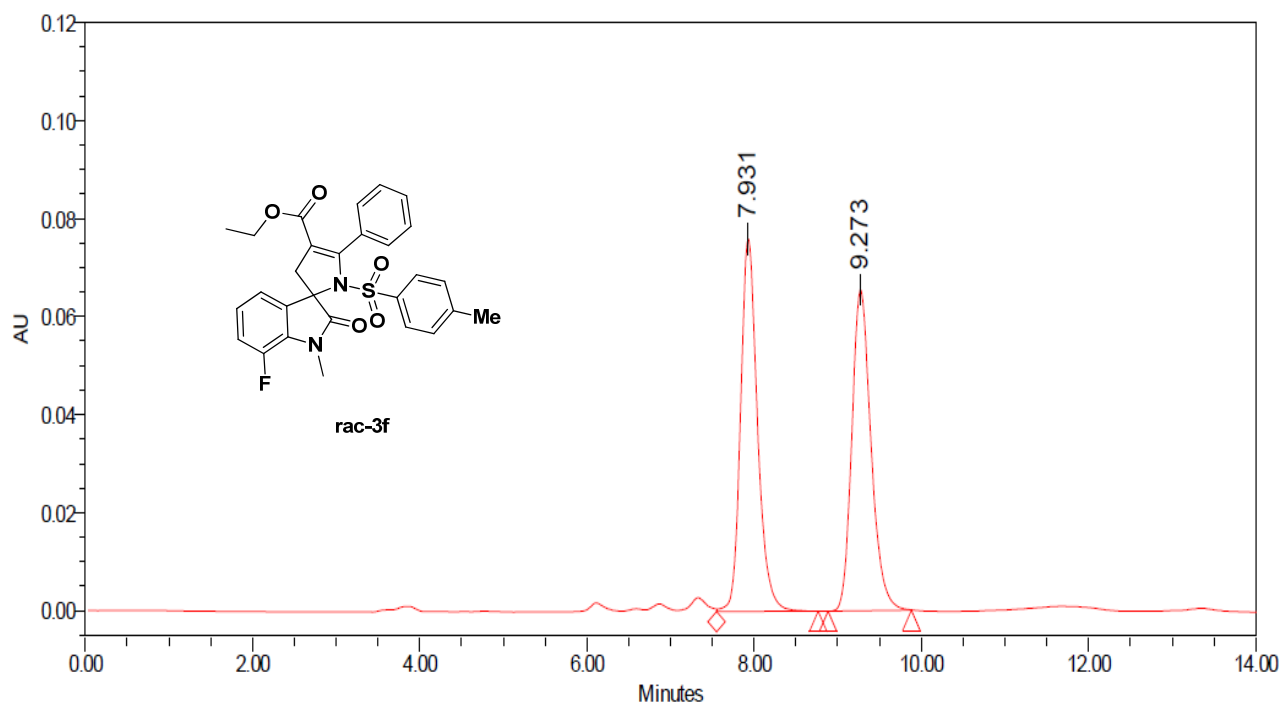
	Name	RT	Area	Height	%Area
1		26.573	87962695	1838483	50.20
2		29.332	87259103	1691023	49.80



Peak Results

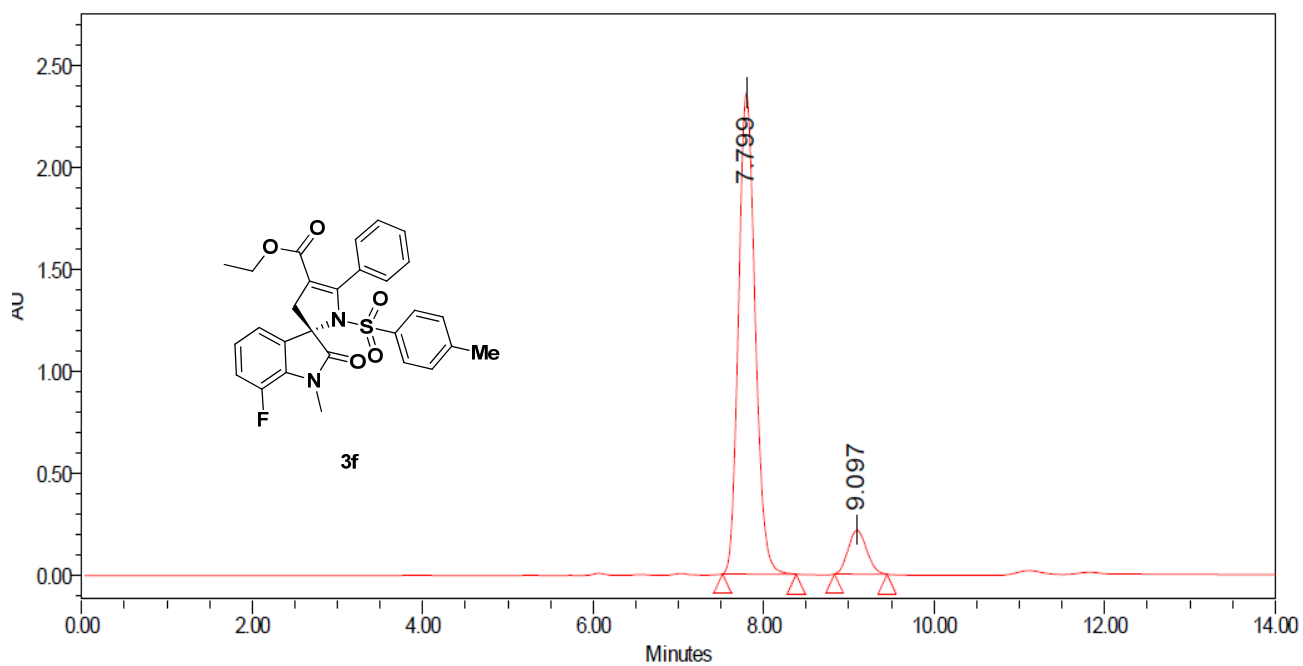
	Name	RT	Area	Height	%Area
1		26.661	43454240	954202	93.42
2		29.791	3061194	81006	6.58





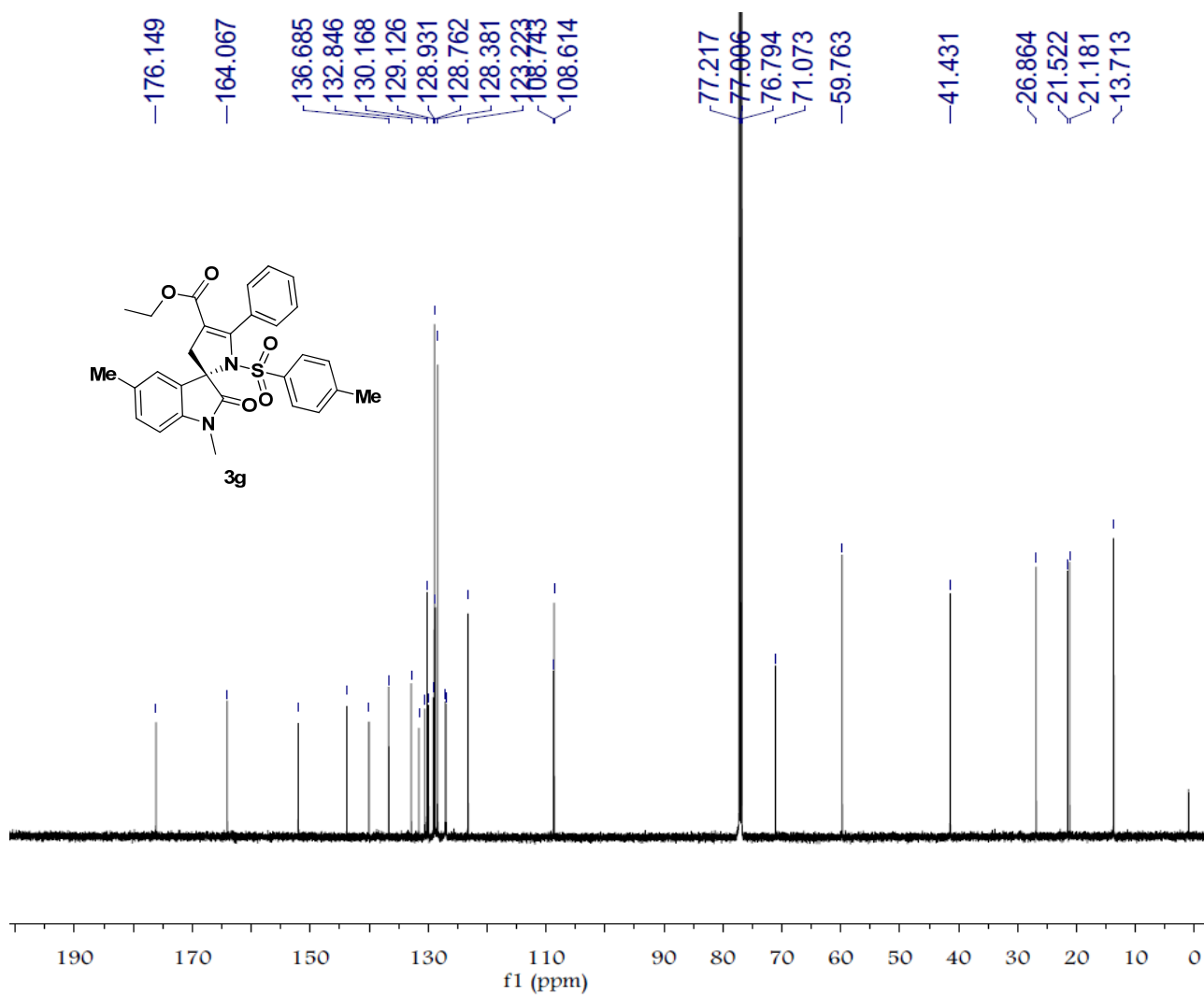
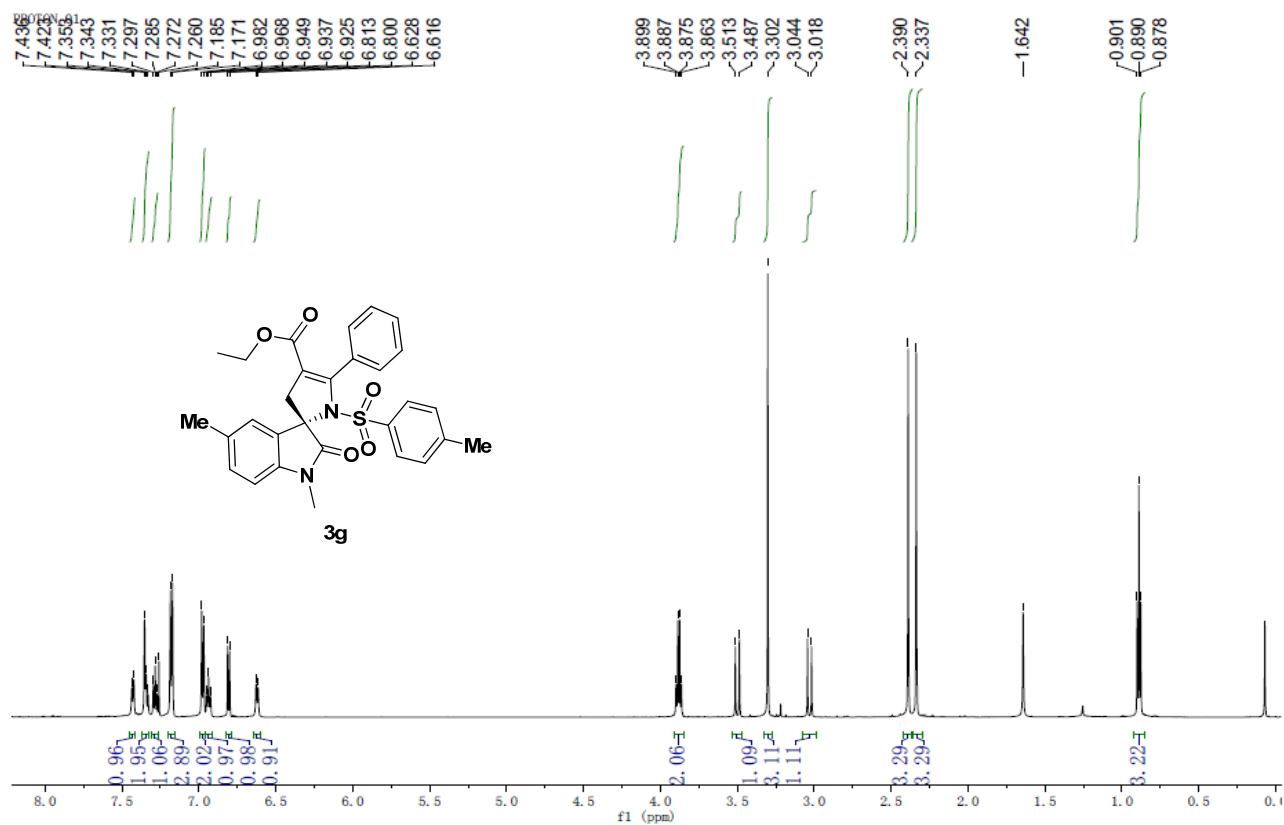
Peak Results

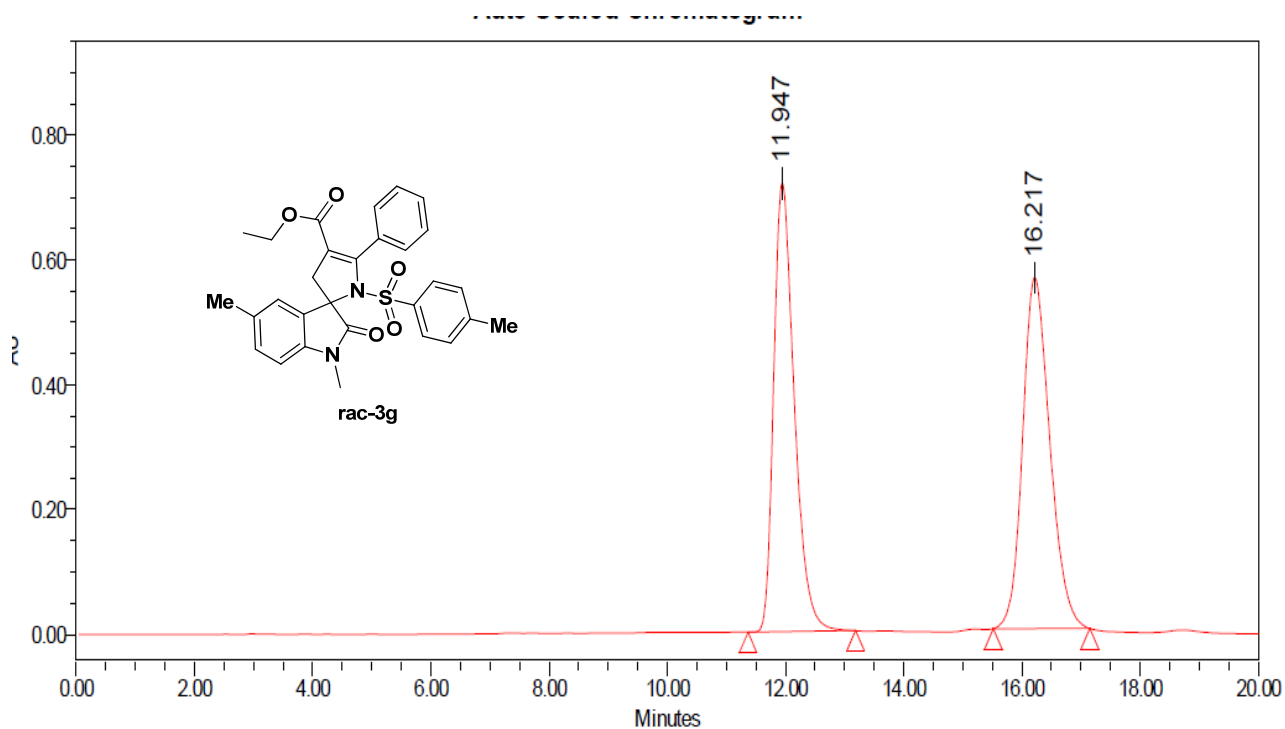
	Name	RT	Area	Height	% Area
1		7.931	1067623	76082	50.54
2		9.273	1044768	65624	49.46



Peak Results

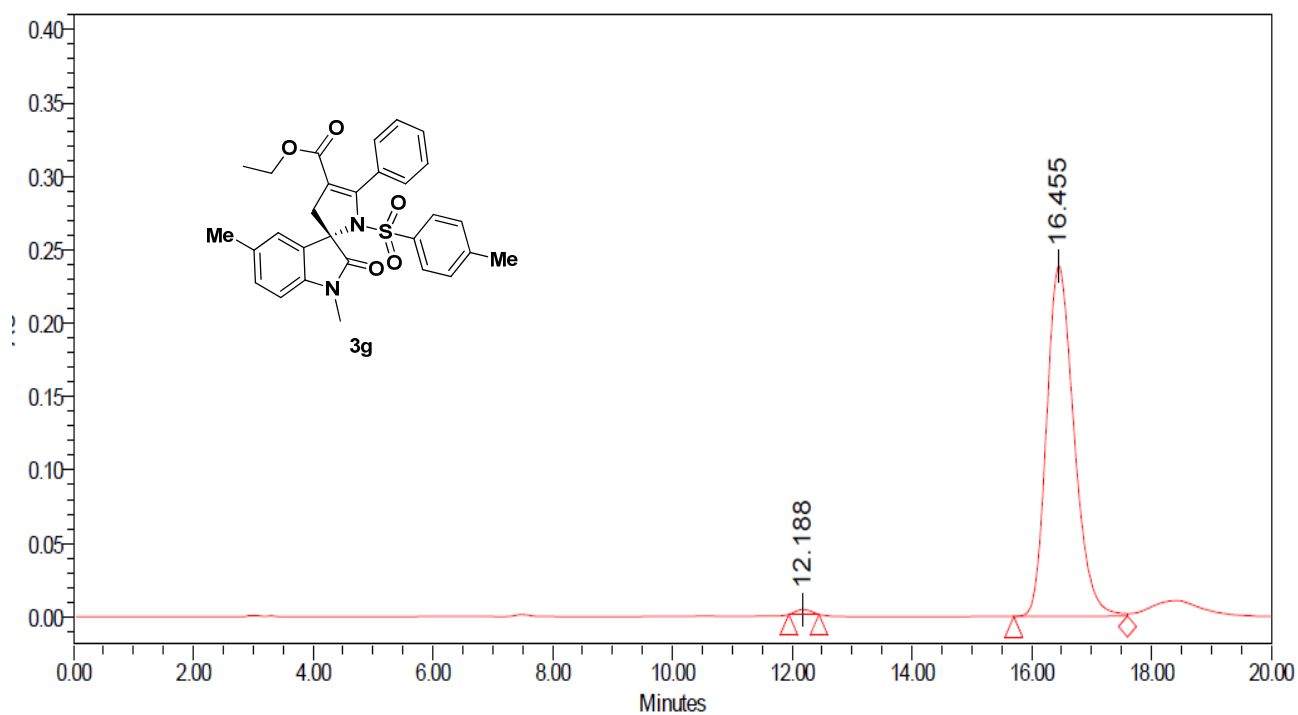
	Name	RT	Area	Height	% Area
1		7.799	31865811	2359679	90.74
2		9.097	3251098	215639	9.26





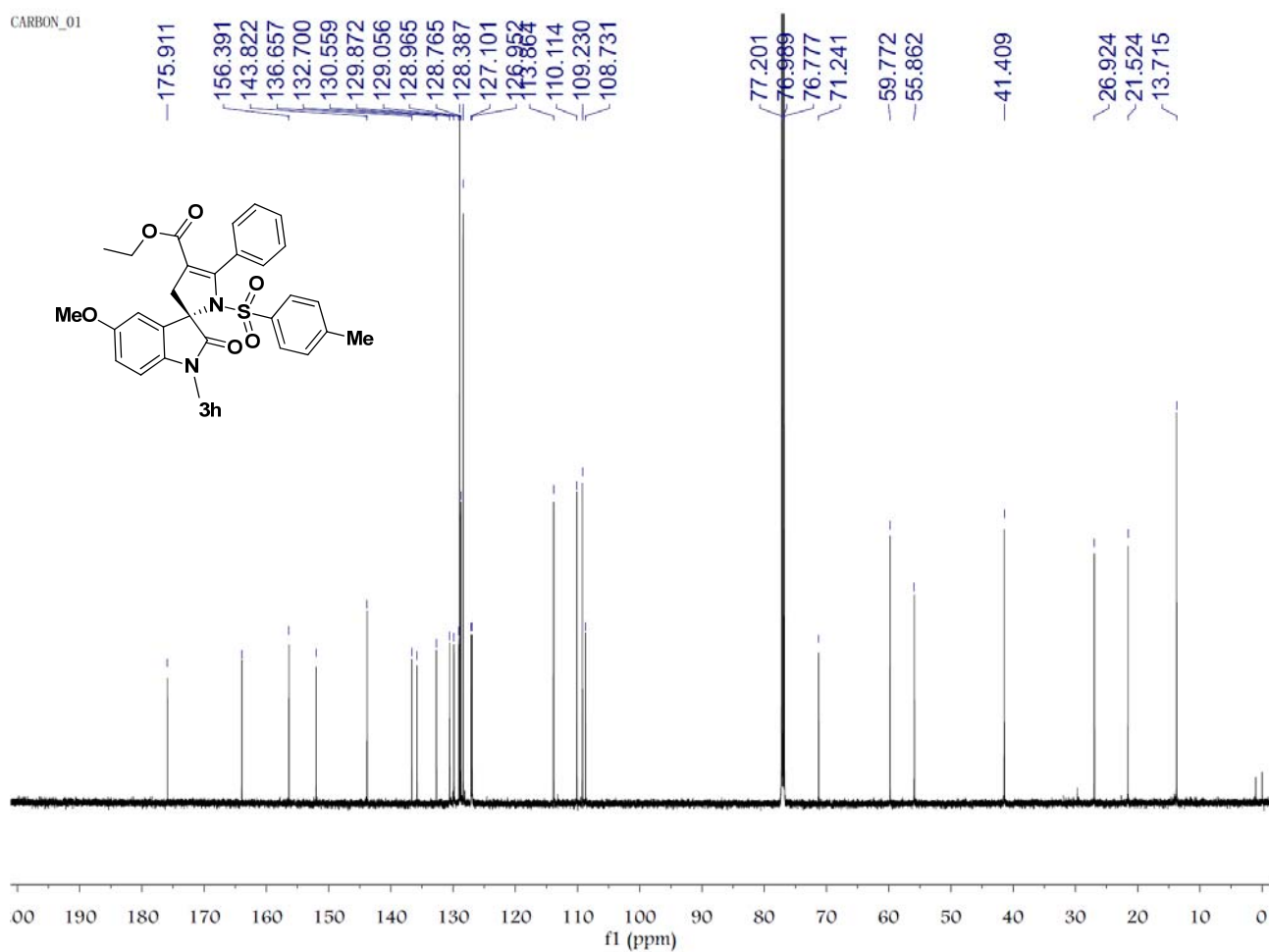
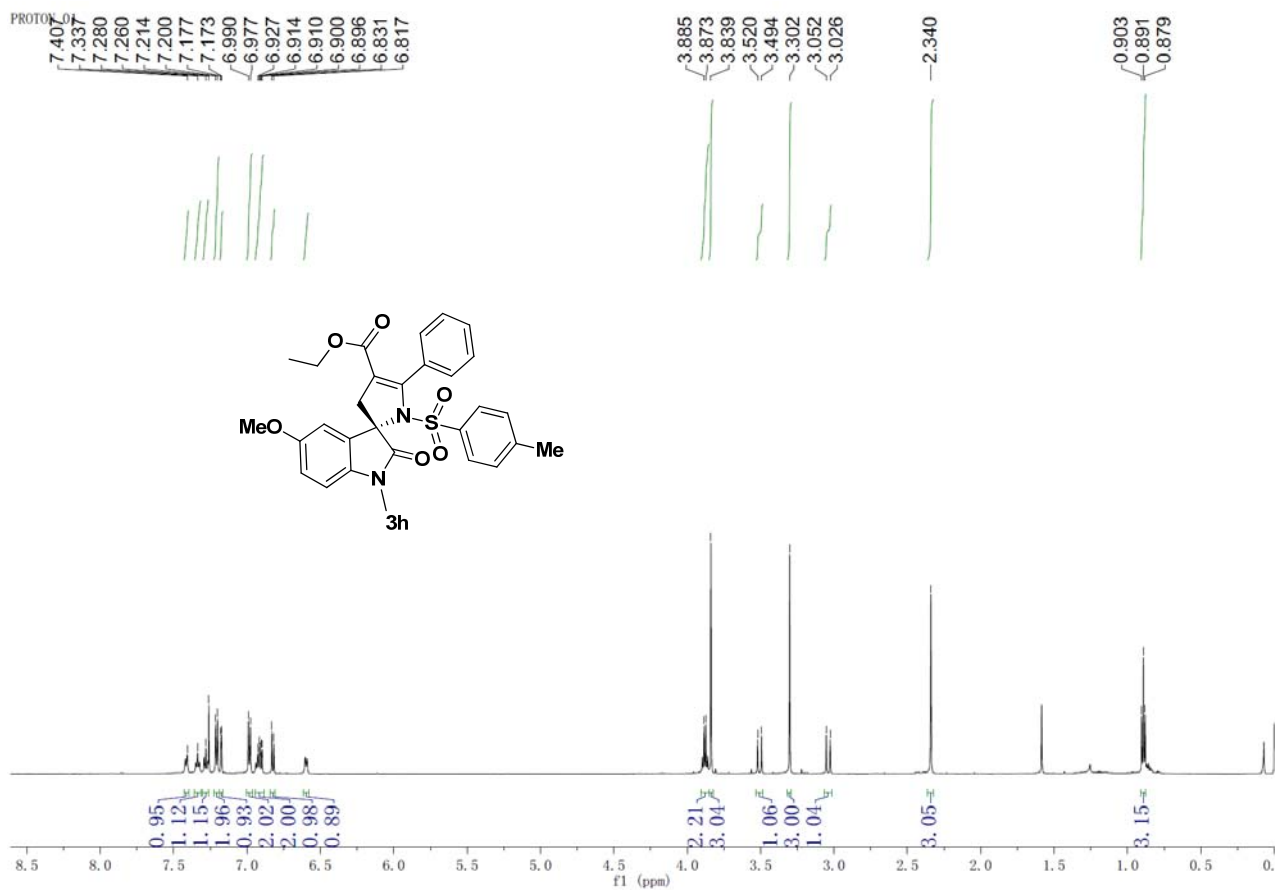
Peak Results

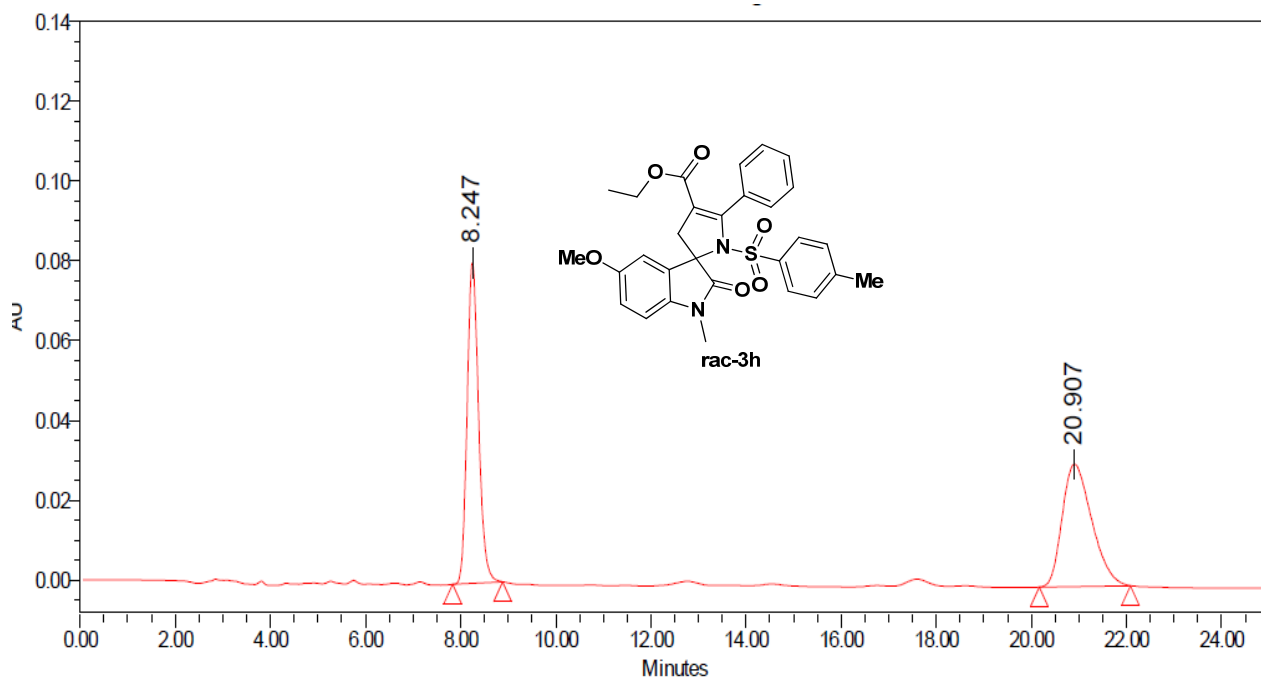
	Name	RT	Area	Height	% Area
1		11.947	17333974	718966	49.06
2		16.217	17994665	562350	50.94



Peak Results

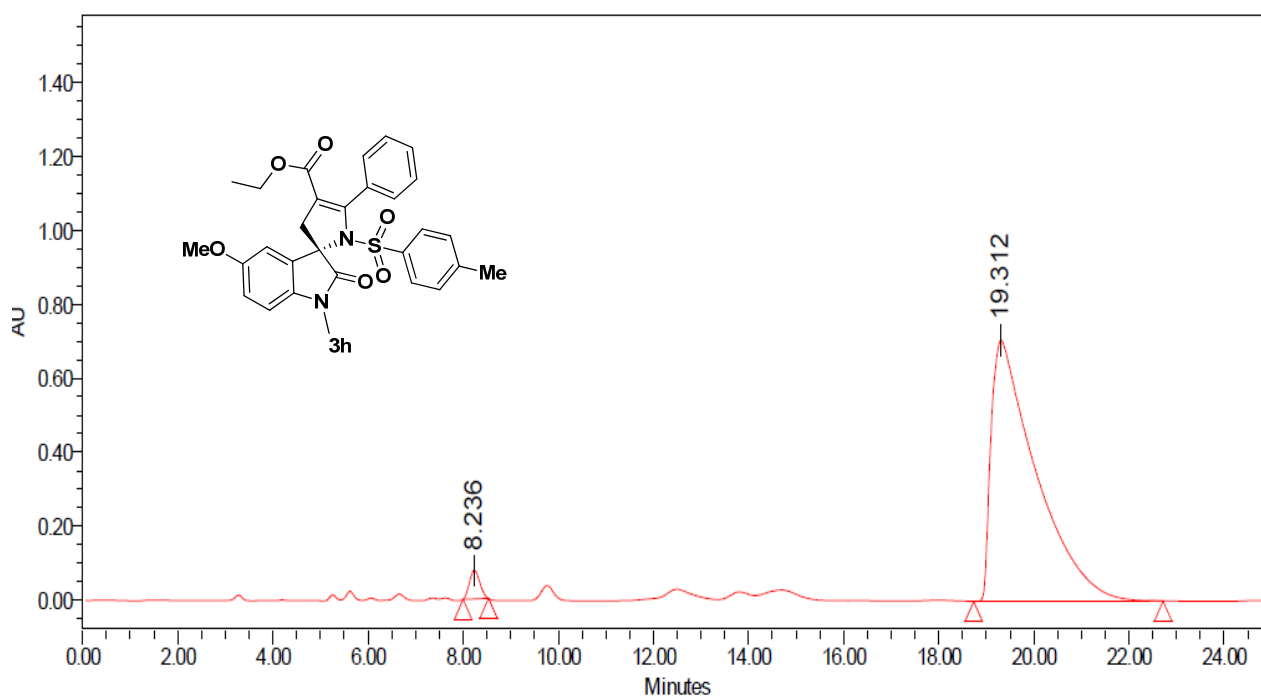
	Name	RT	Area	Height	% Area
1		12.188	56707	3265	0.74
2		16.455	7587890	238463	99.26





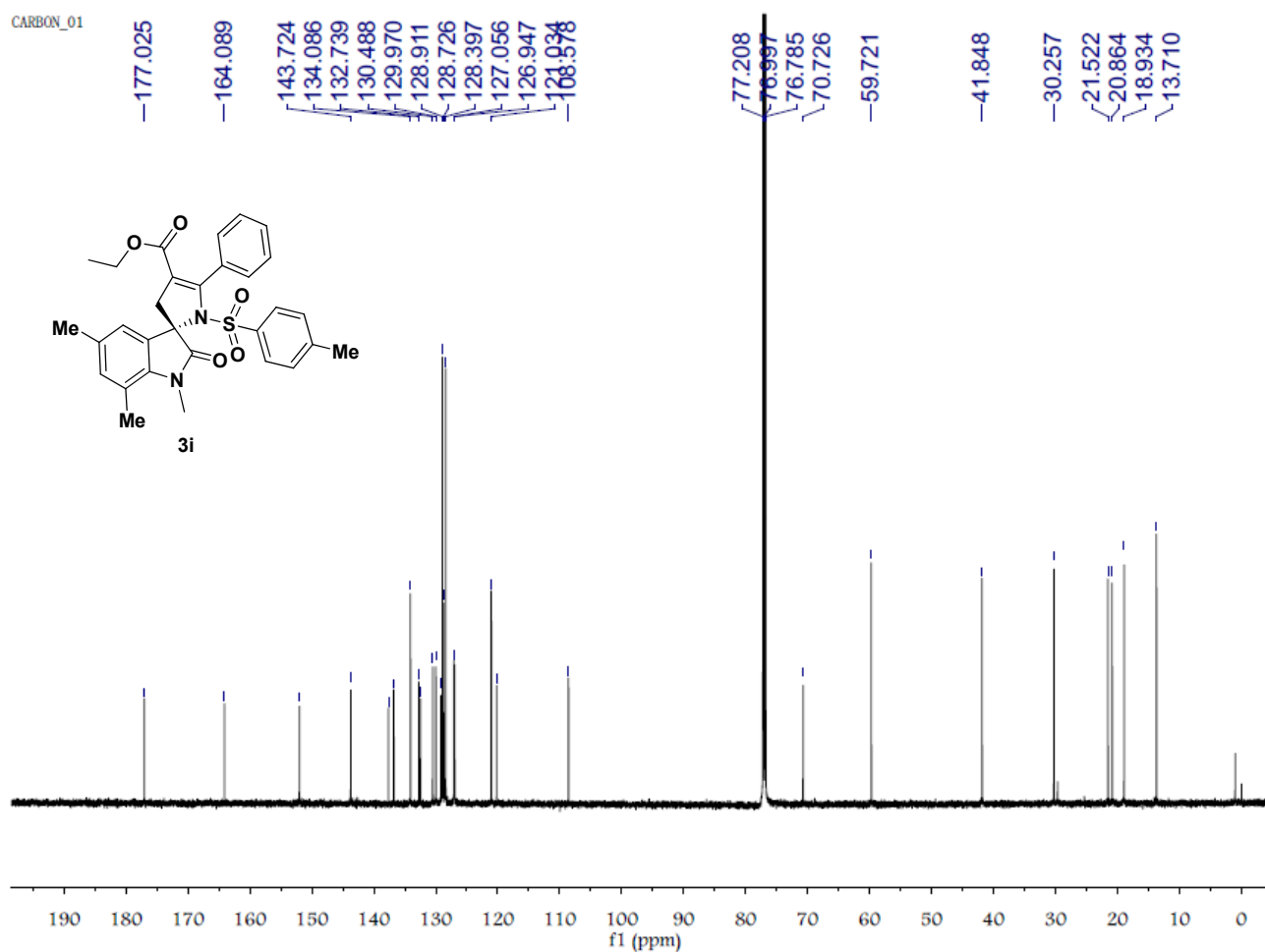
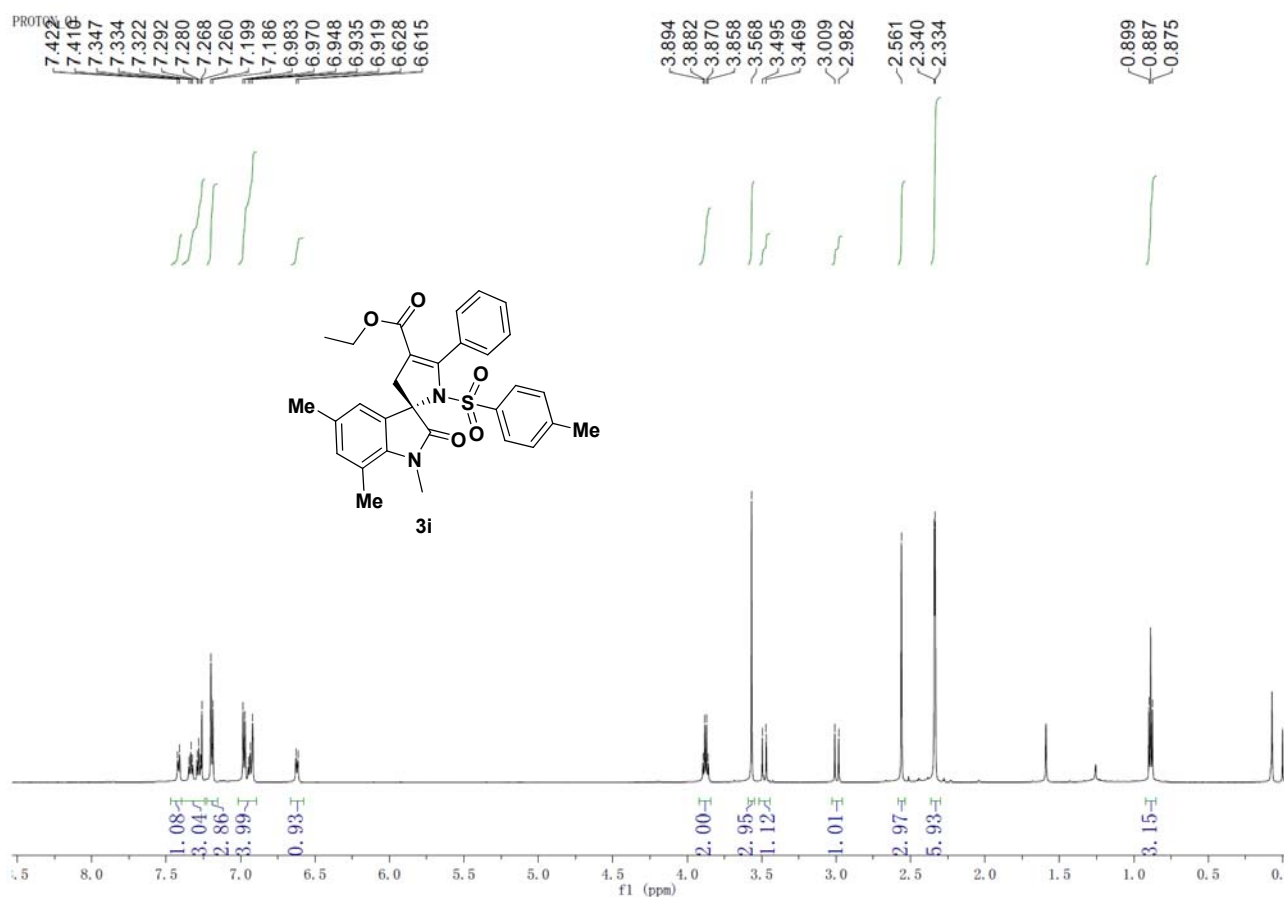
Peak Results

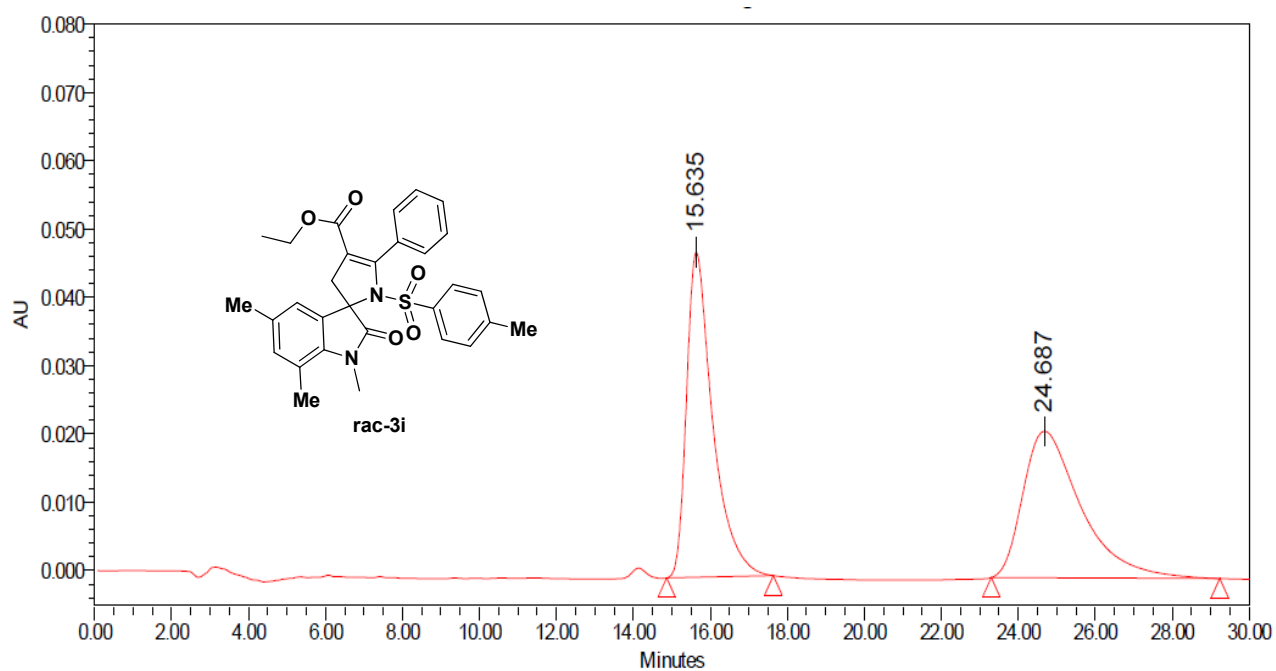
	Name	RT	Area	Height	% Area
1		8.247	1342002	80414	50.28
2		20.907	1326865	30711	49.72



Peak Results

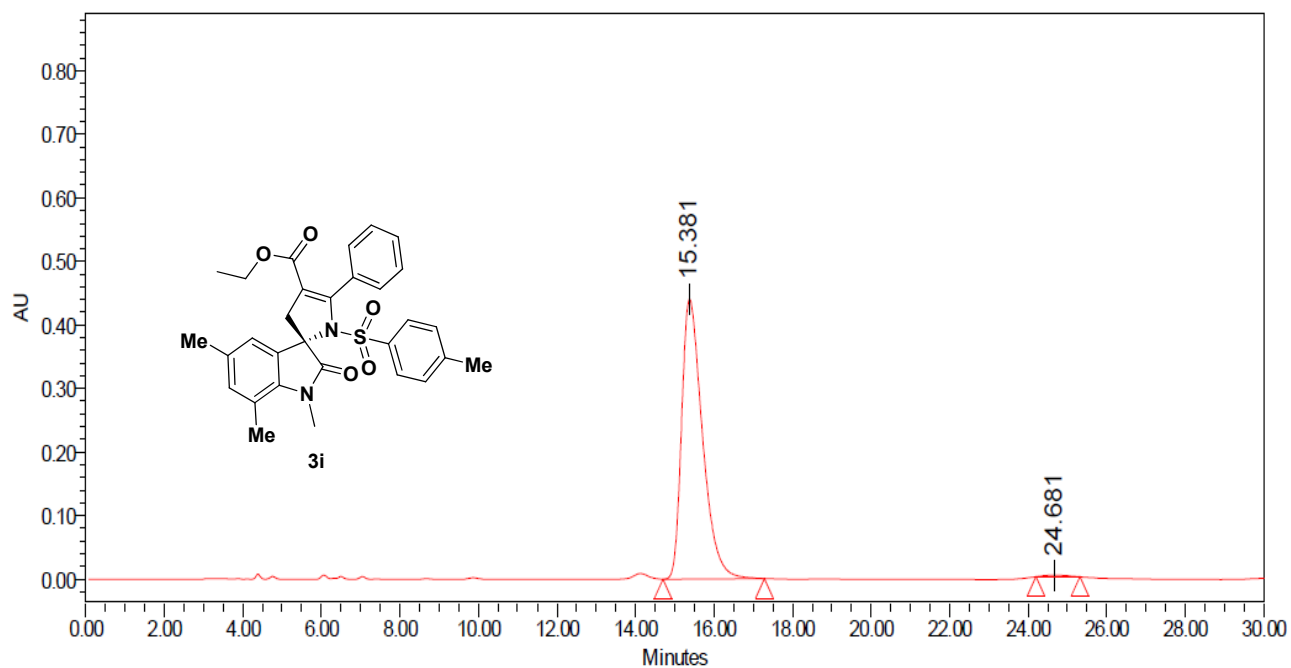
	Name	RT	Area	Height	% Area
1		8.236	1166191	77512	2.46
2		19.312	46171052	705073	97.54





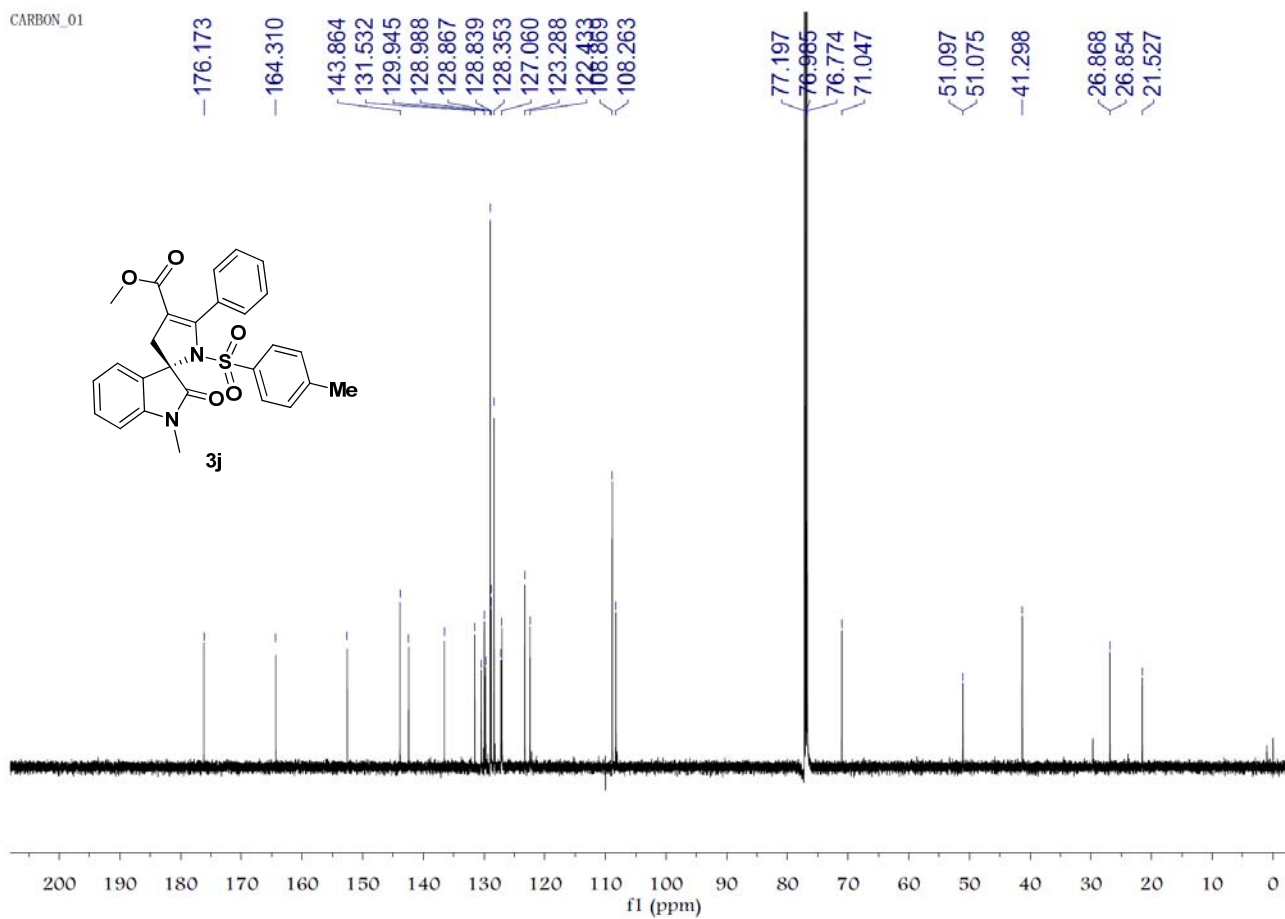
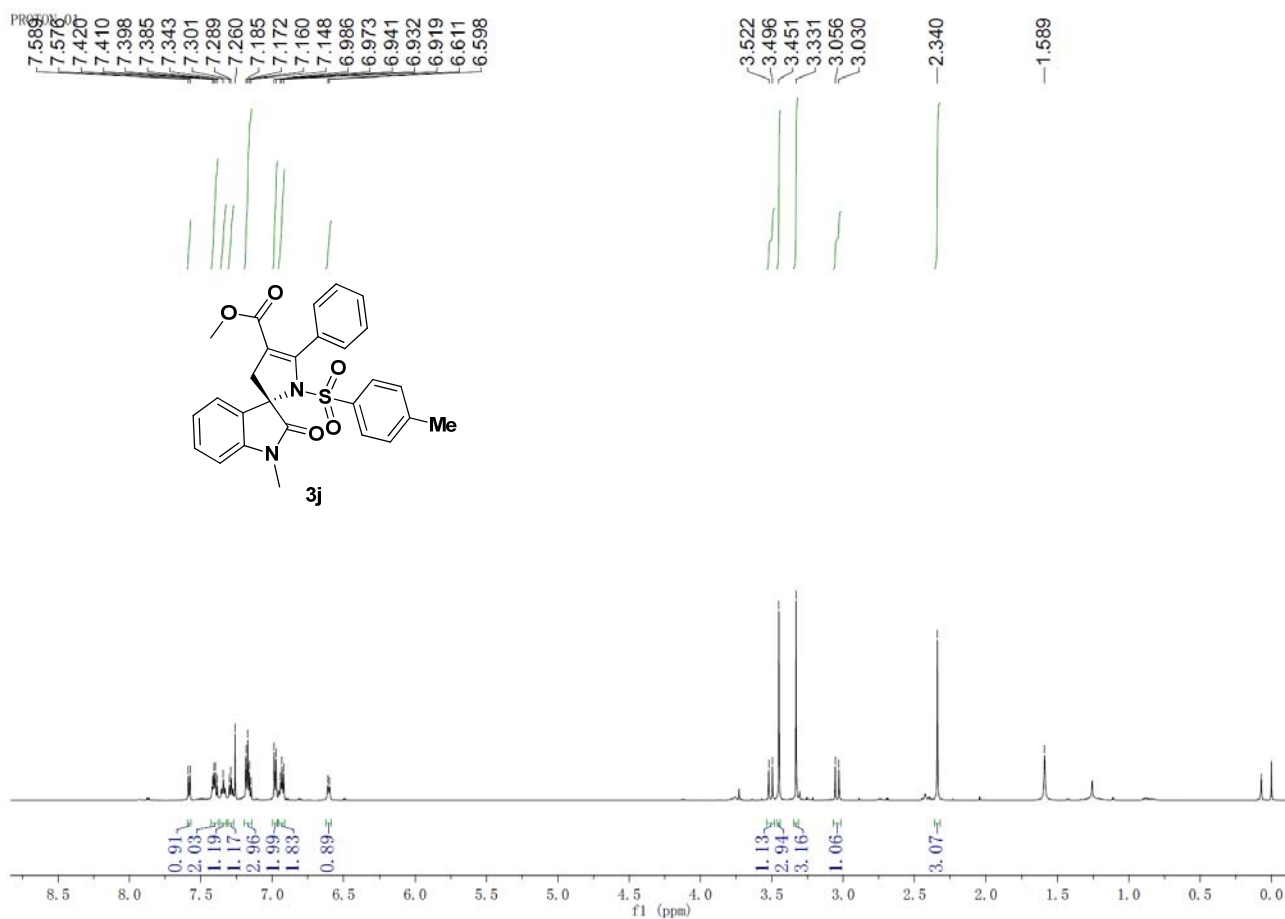
Peak Results

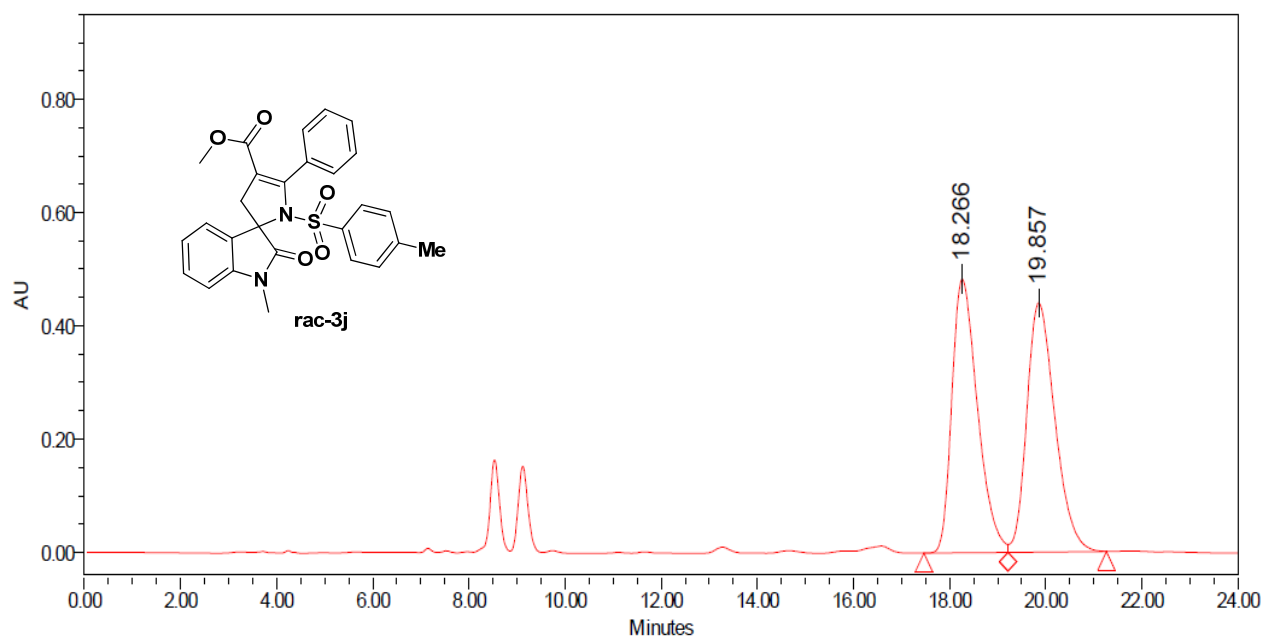
	Name	RT	Area	Height	% Area
1		15.635	2246598	47574	49.99
2		24.687	2247934	21438	50.01



Peak Results

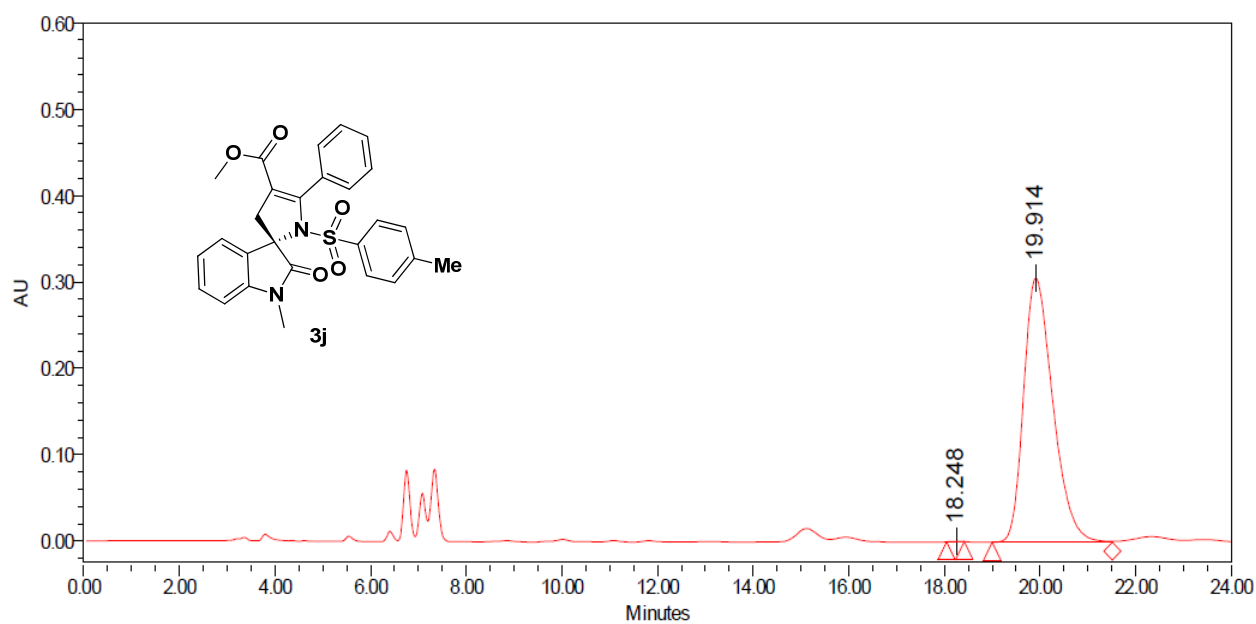
	Name	RT	Area	Height	% Area
1		15.381	16216595	440258	99.40
2		24.681	98117	2346	0.60





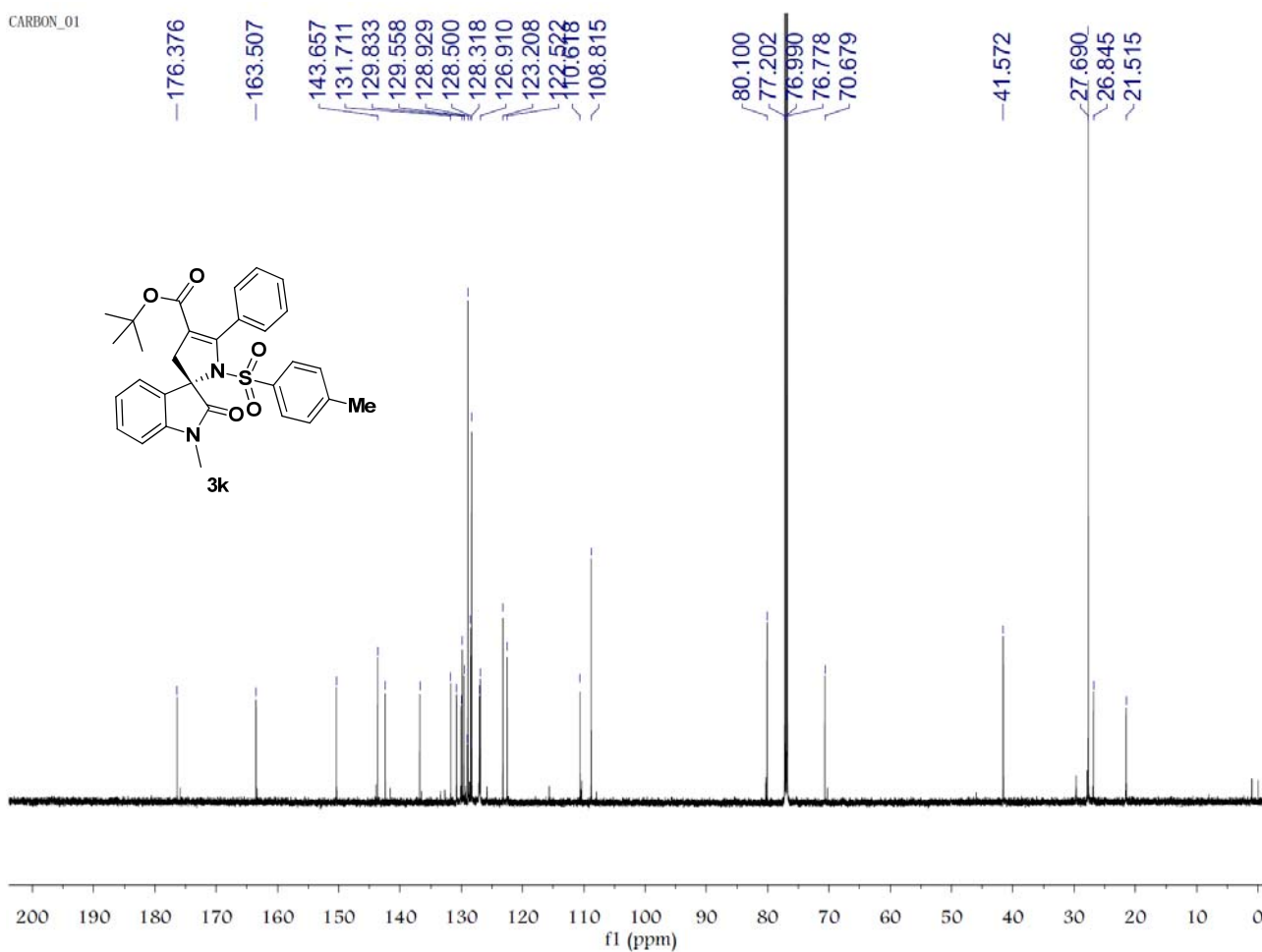
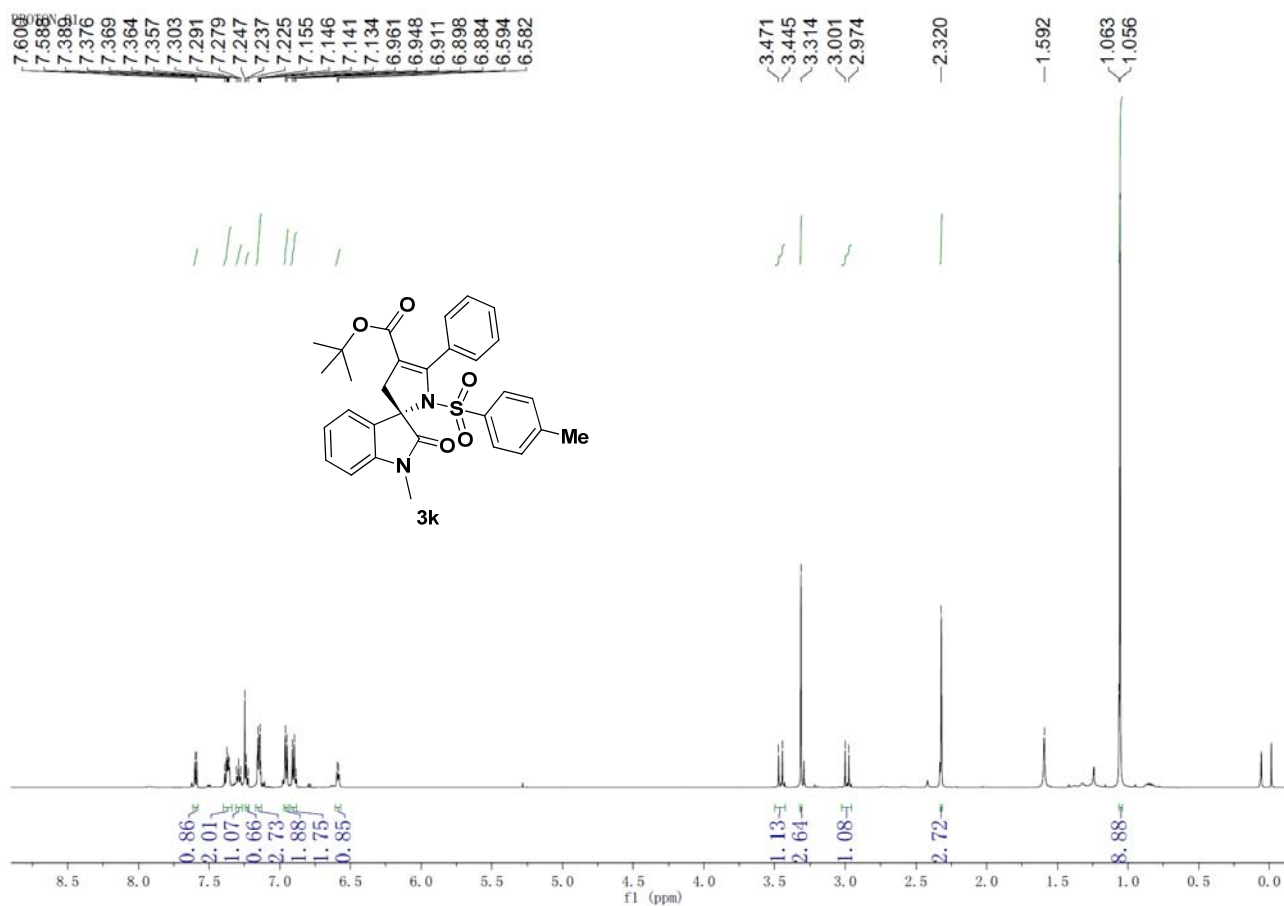
Peak Results

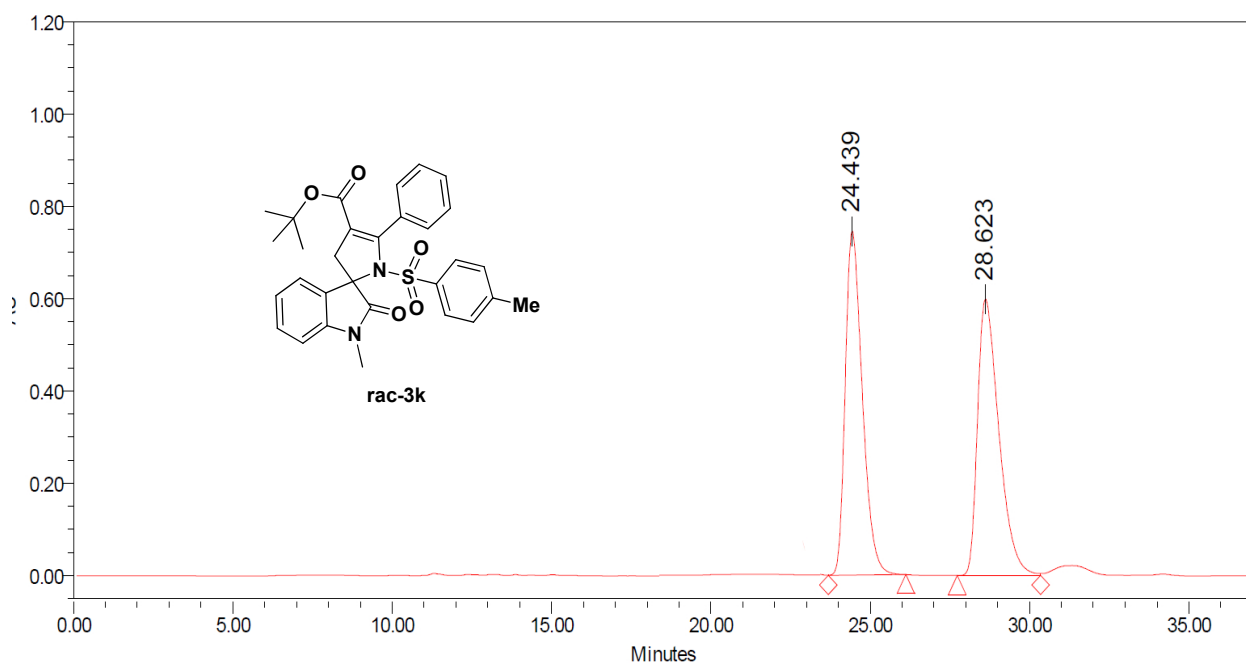
	Name	RT	Area	Height	%Area
1		18.266	17884536	483288	49.91
2		19.857	17947343	440207	50.09



Peak Results

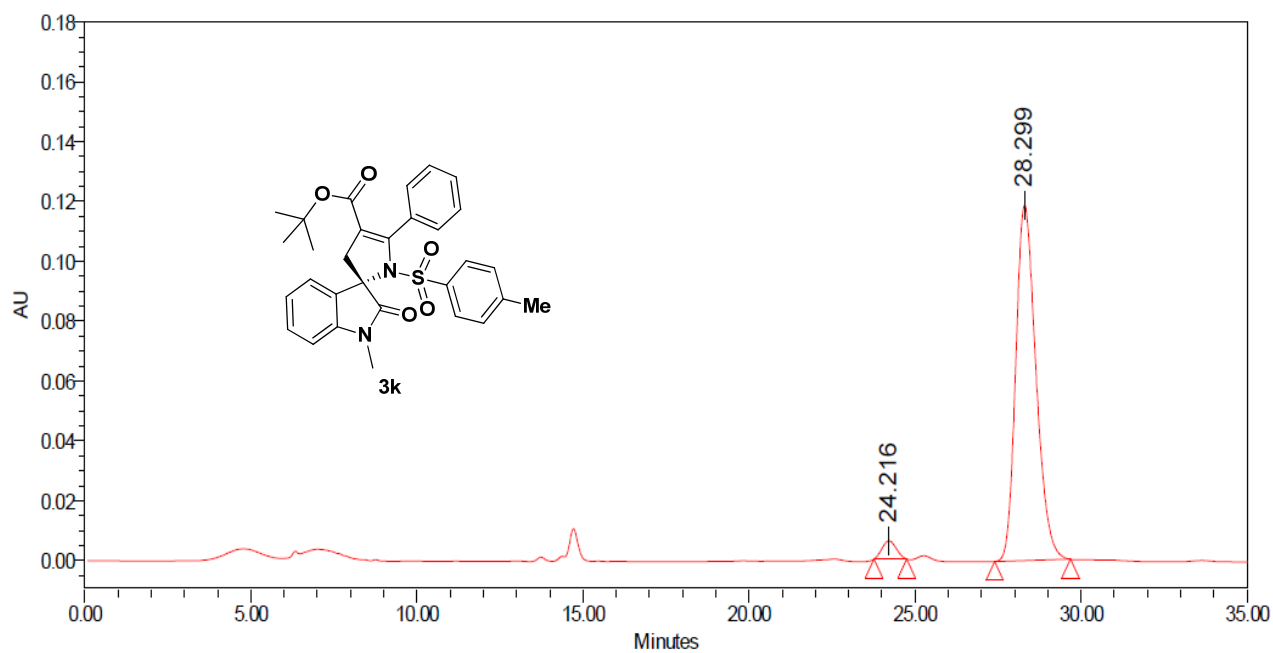
	Name	RT	Area	Height	%Area
1		18.248	4296	304	0.03
2		19.914	13012050	305905	99.97





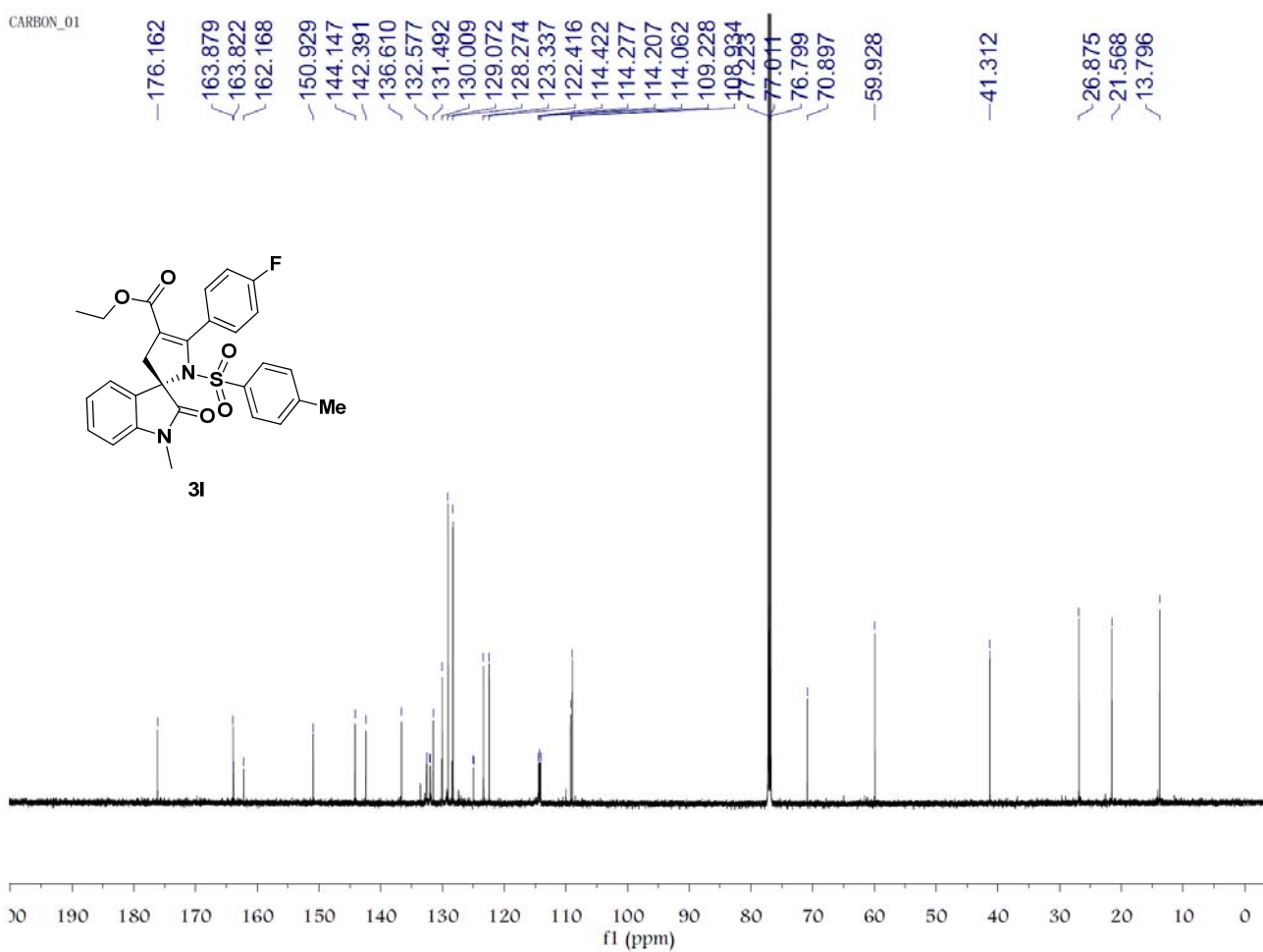
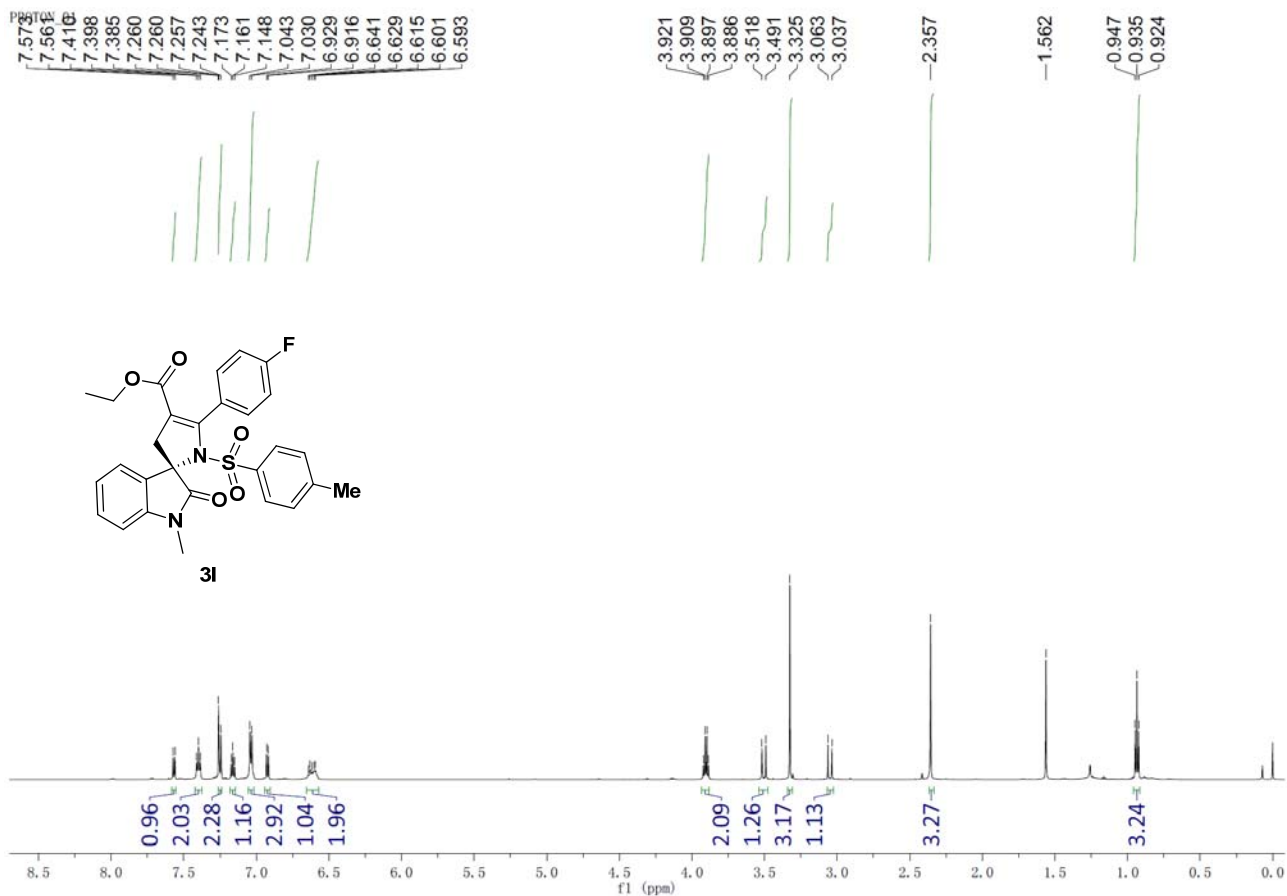
Peak Results

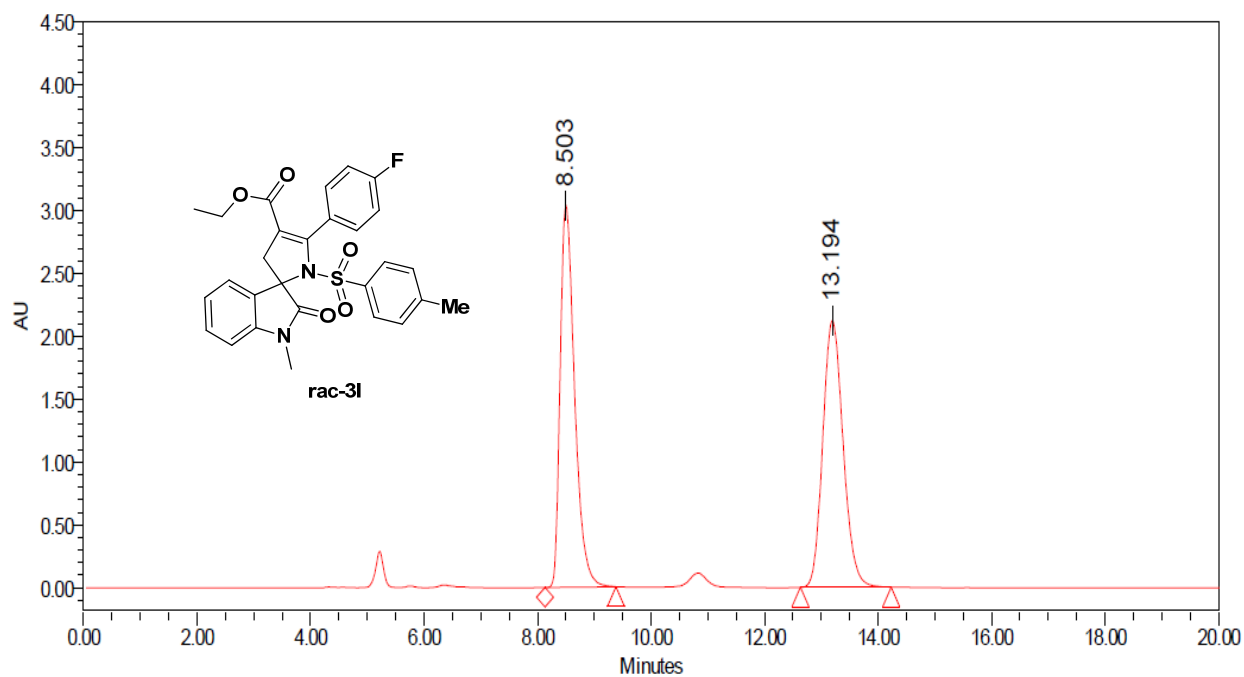
	Name	RT	Area	Height	% Area
1		24.439	27698112	744820	49.92
2		28.623	27791373	598650	50.08



Peak Results

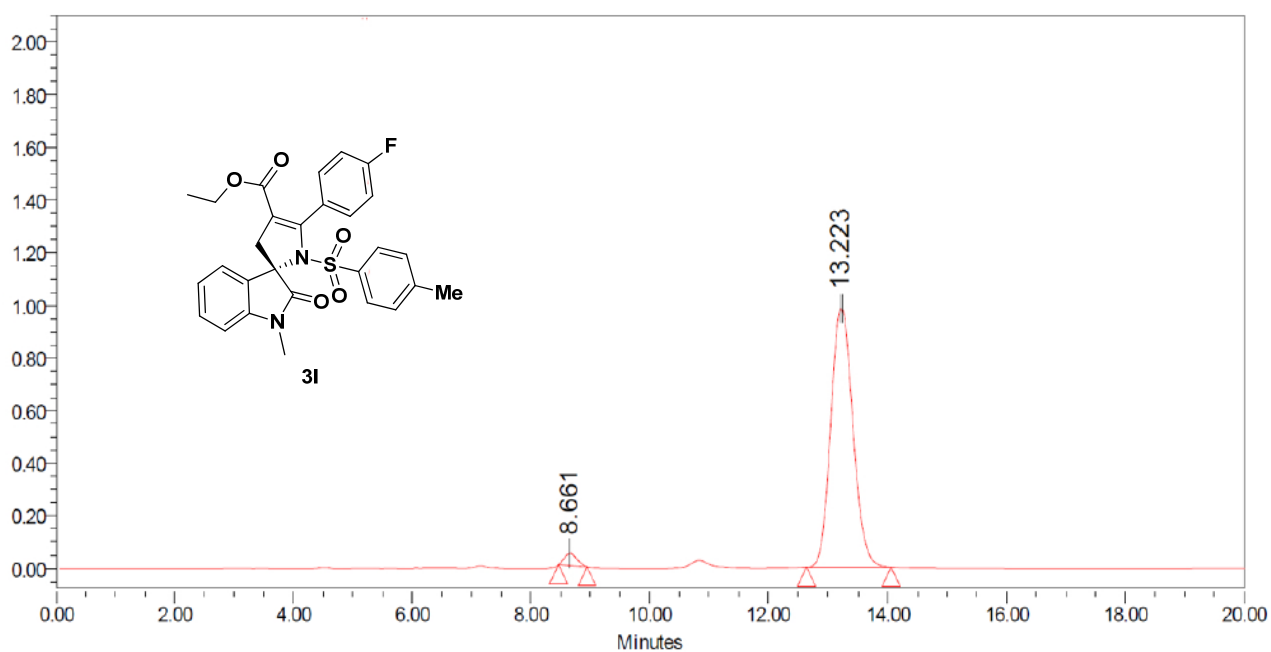
	Name	RT	Area	Height	% Area
1		24.216	181085	6097	3.49
2		28.299	5013882	118781	96.51





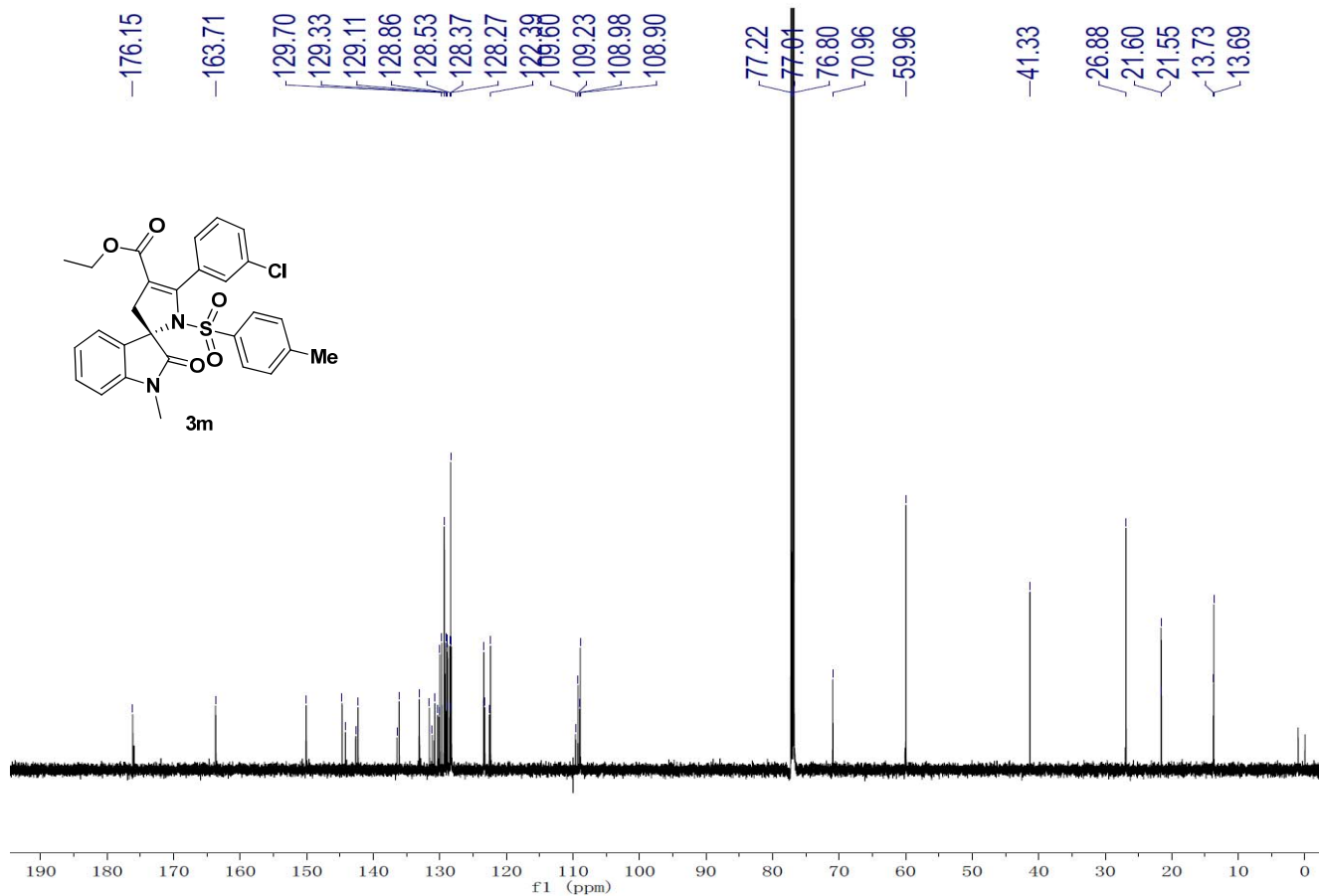
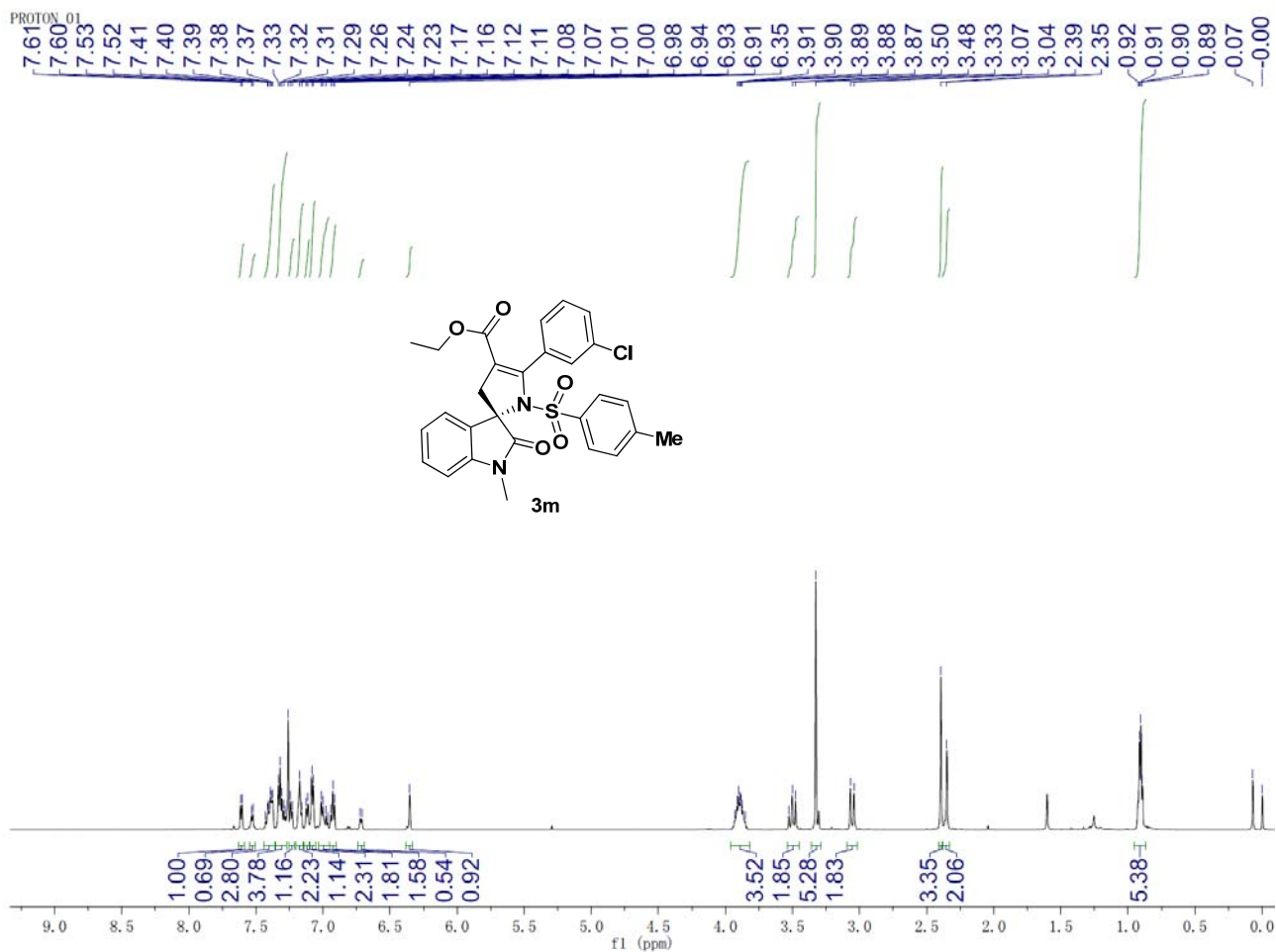
Peak Results

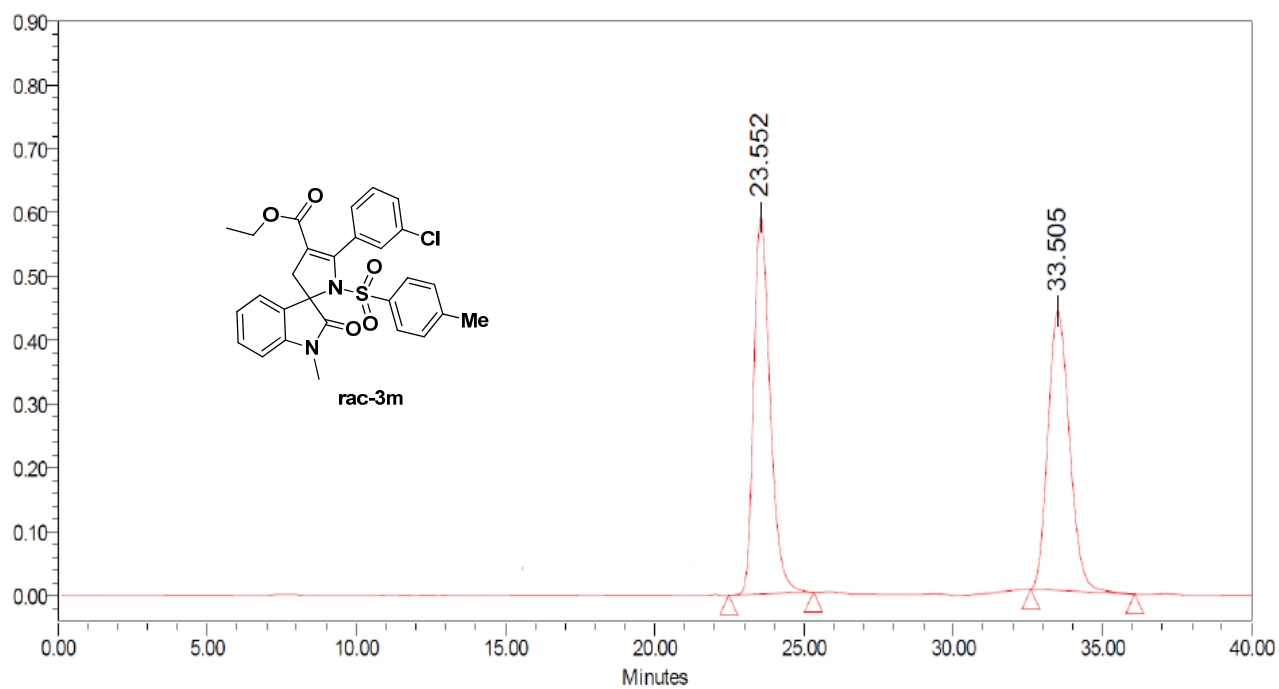
	Name	RT	Area	Height	% Area
1		8.503	53625142	3038625	50.37
2		13.194	52847572	2122666	49.63



Peak Results

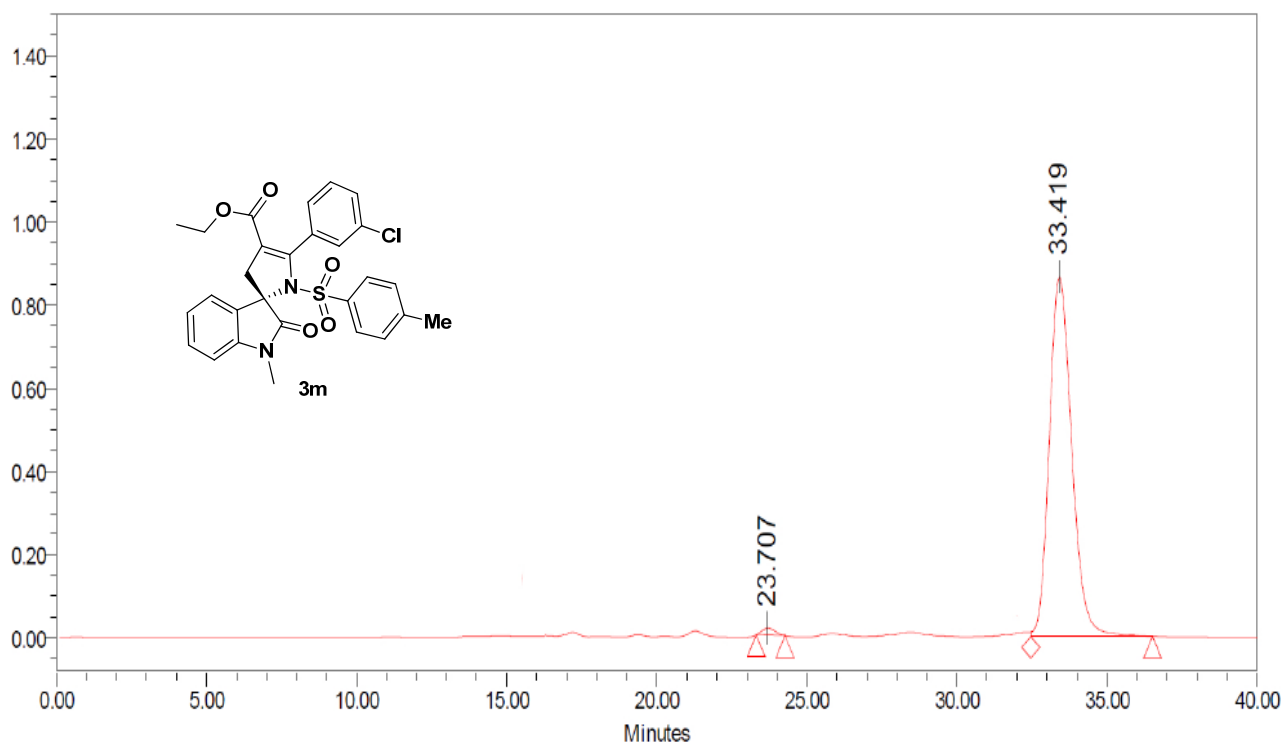
	Name	RT	Area	Height	% Area
1		8.661	653993	43715	2.61
2		13.223	24384075	985042	97.39





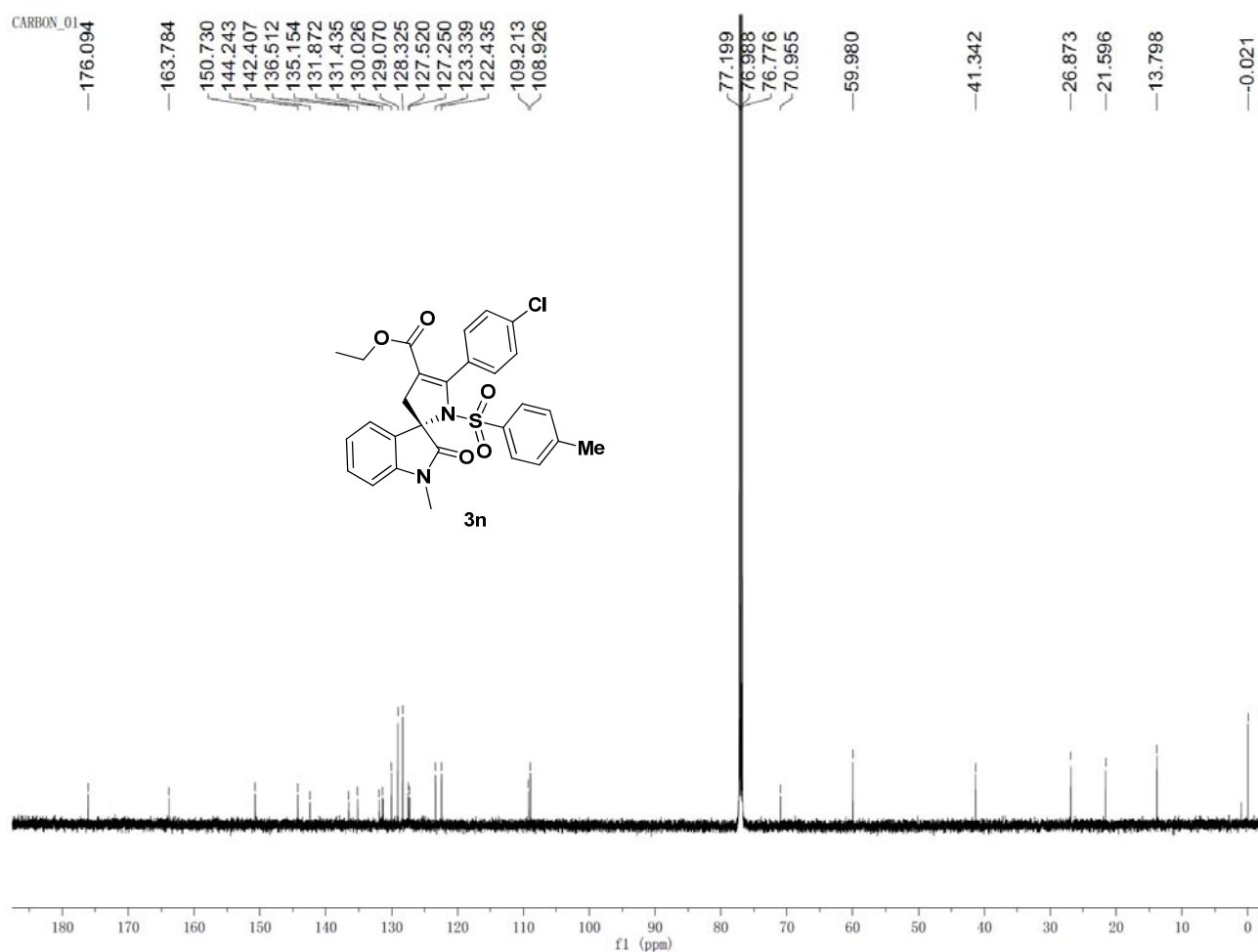
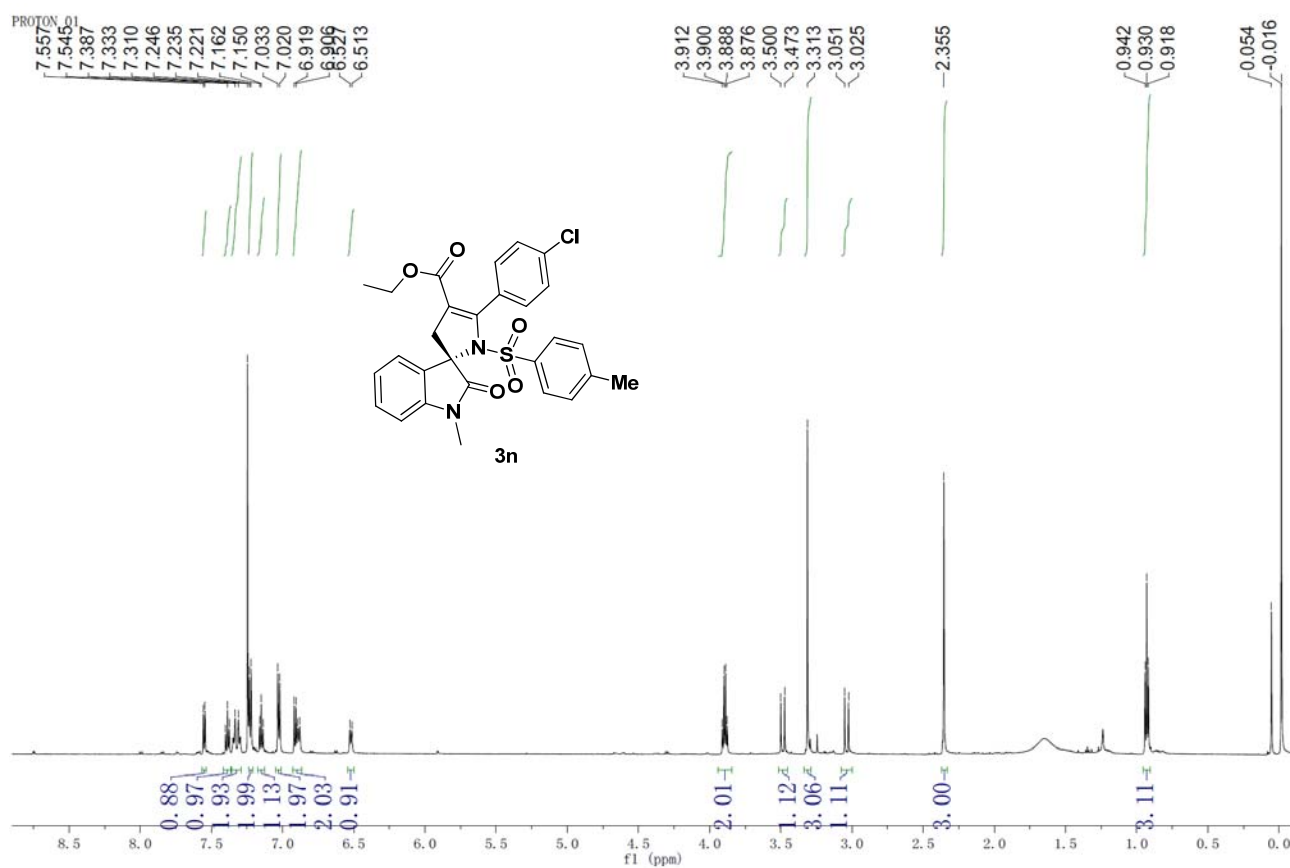
Peak Results

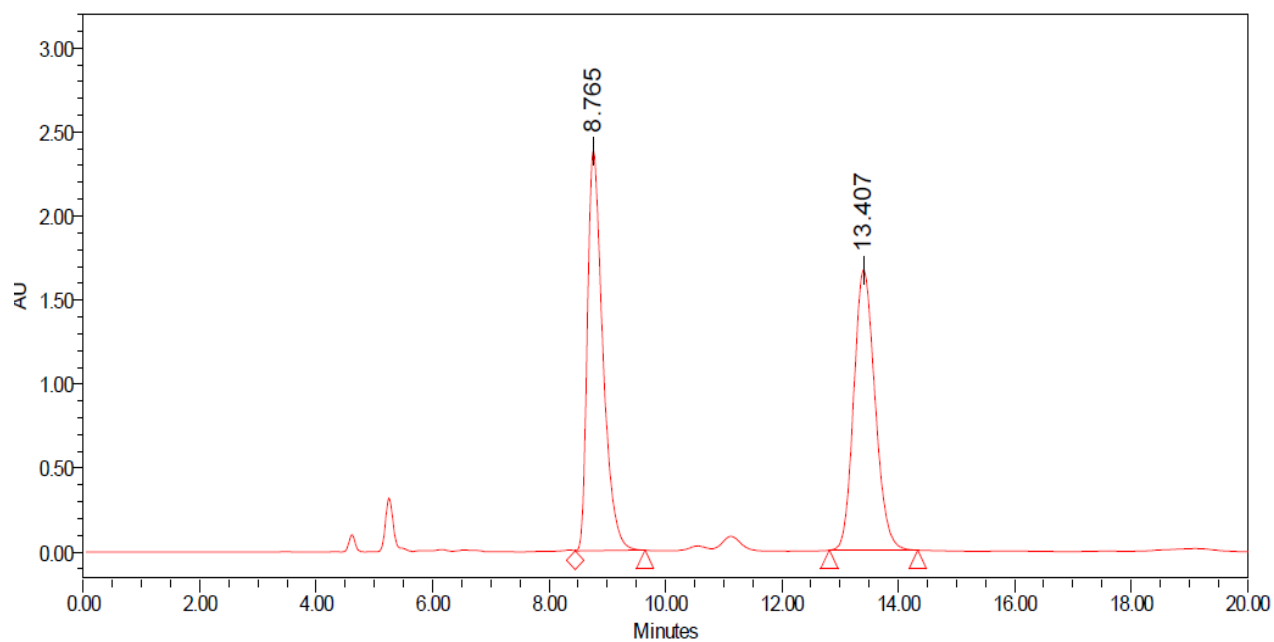
	Name	RT	Area	Height	% Area
1		23.552	22443644	590698	50.24
2		33.505	22225044	437698	49.76



Peak Results

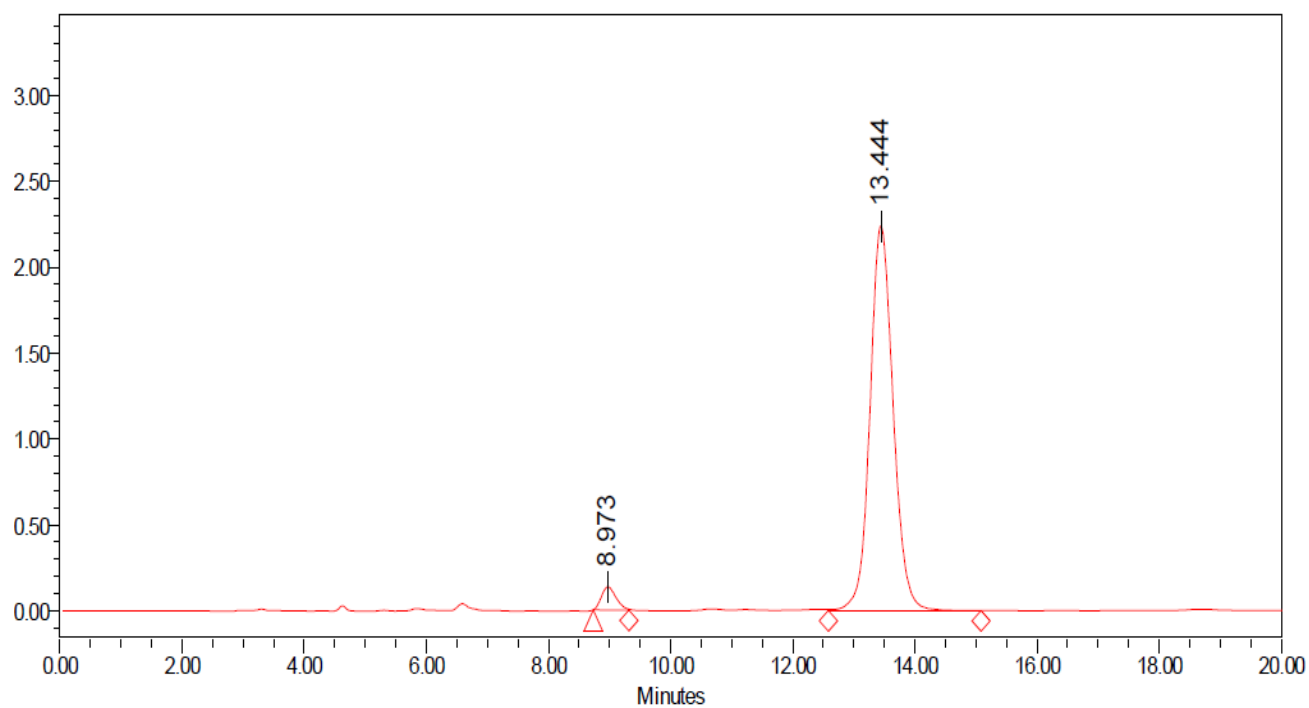
	Name	RT	Area	Height	% Area
1		23.707	536540	17535	1.17
2		33.419	45168017	866711	98.83





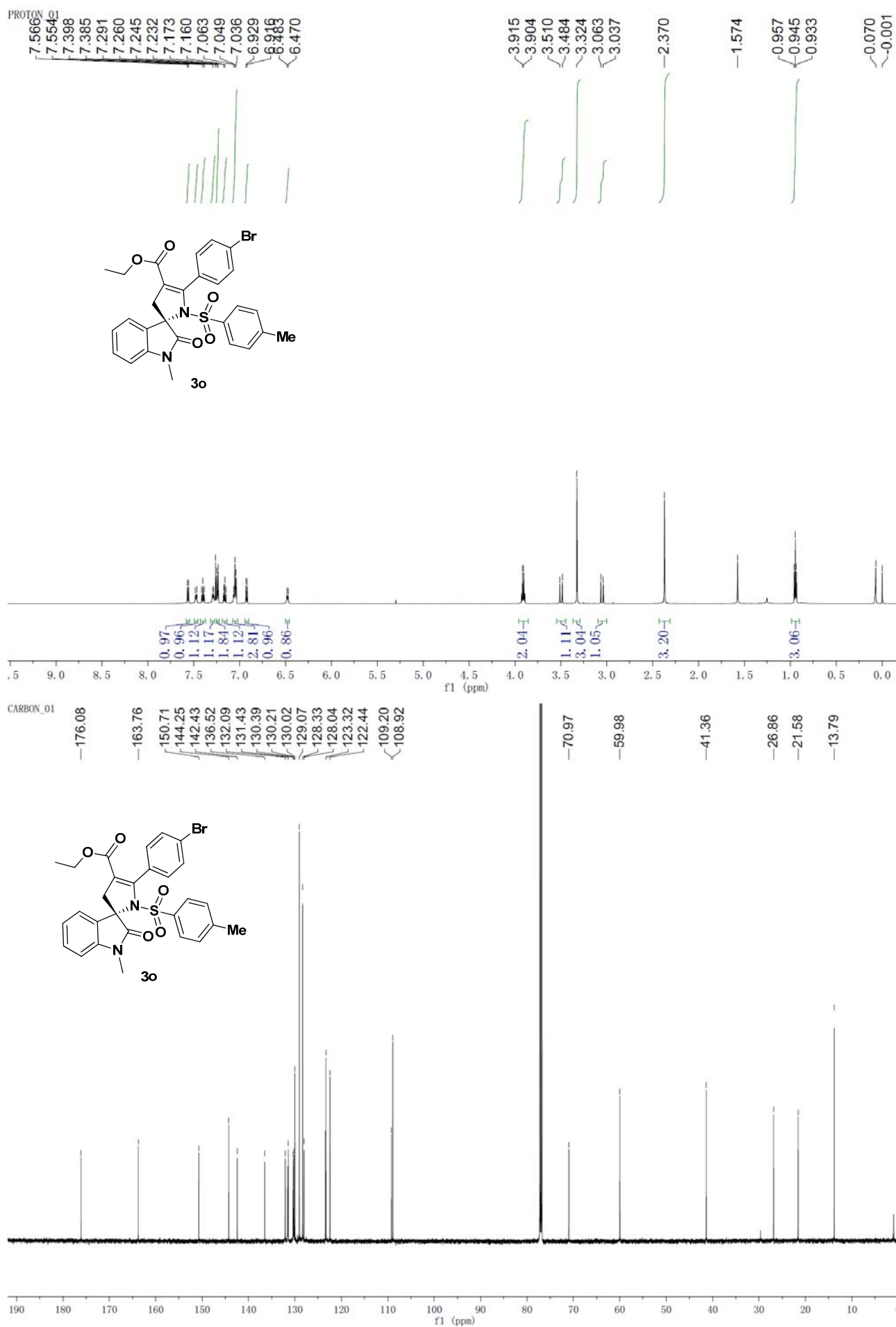
Peak Results

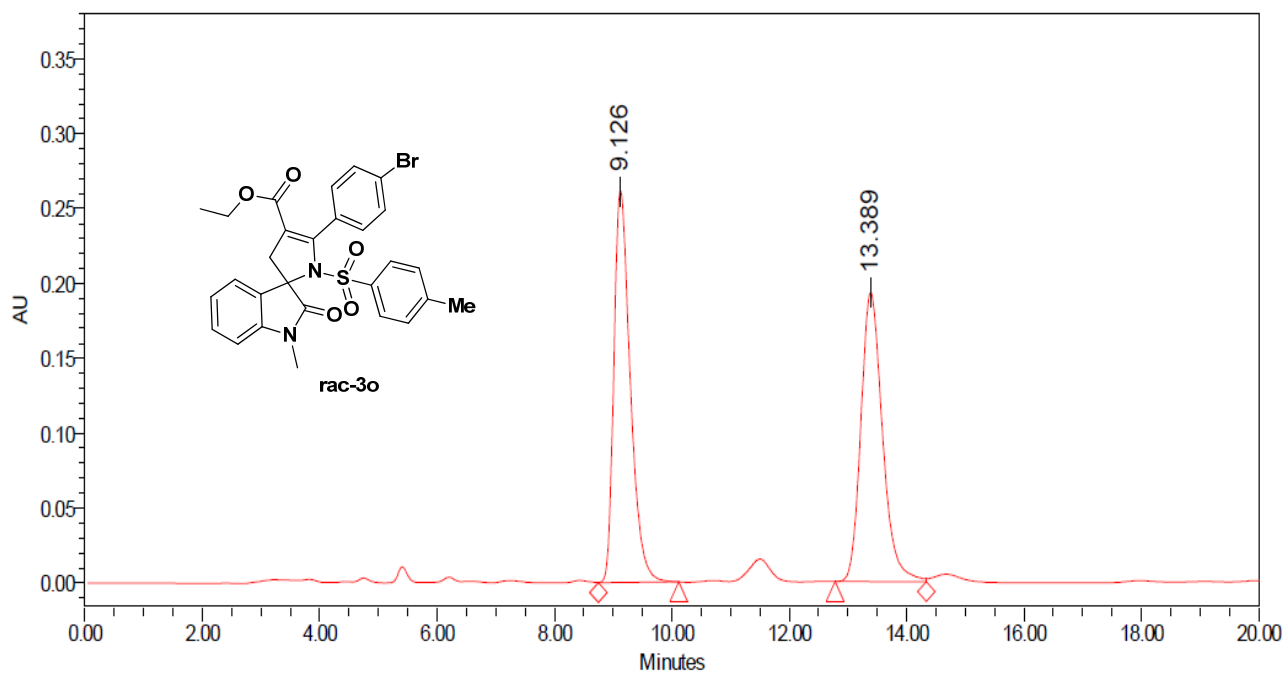
	Name	RT	Area	Height	% Area
1		8.765	43746031	2383218	50.76
2		13.407	42441320	1669505	49.24



Peak Results

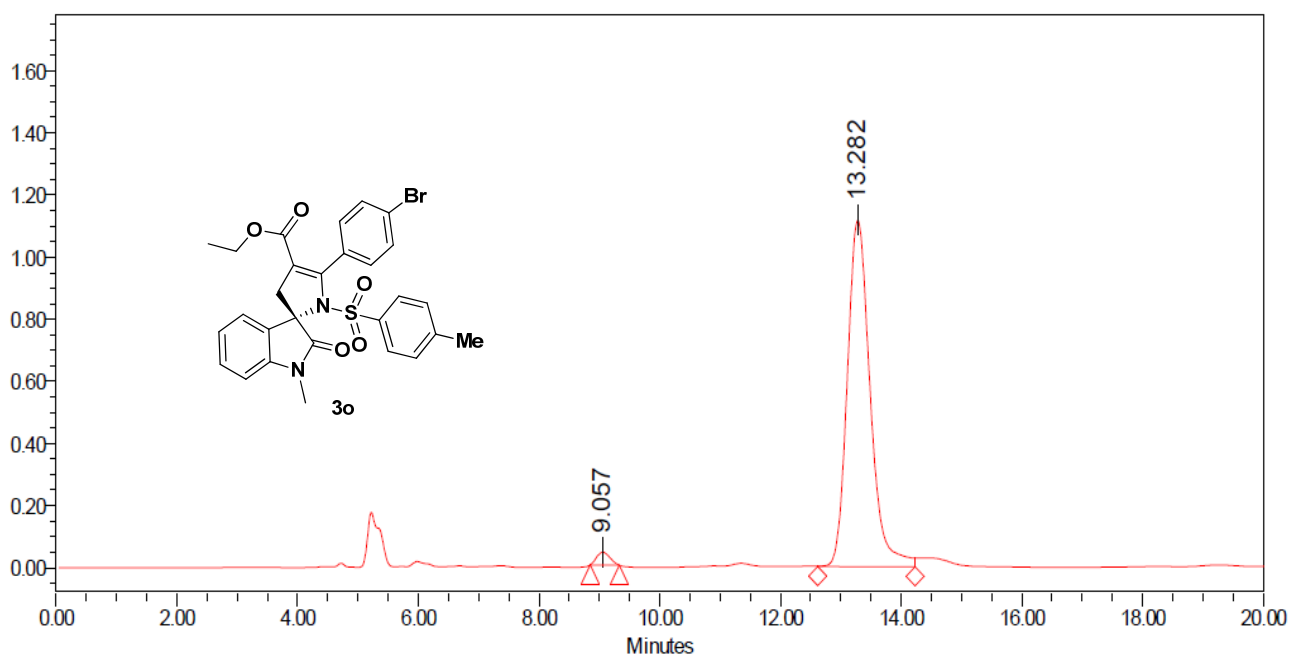
	Name	RT	Area	Height	% Area
1		8.973	2229071	134620	3.64
2		13.444	59065996	2239292	96.36





Peak Results

	Name	RT	Area	Height	% Area
1		9.126	5078274	261389	50.64
2		13.389	4950380	193106	49.36

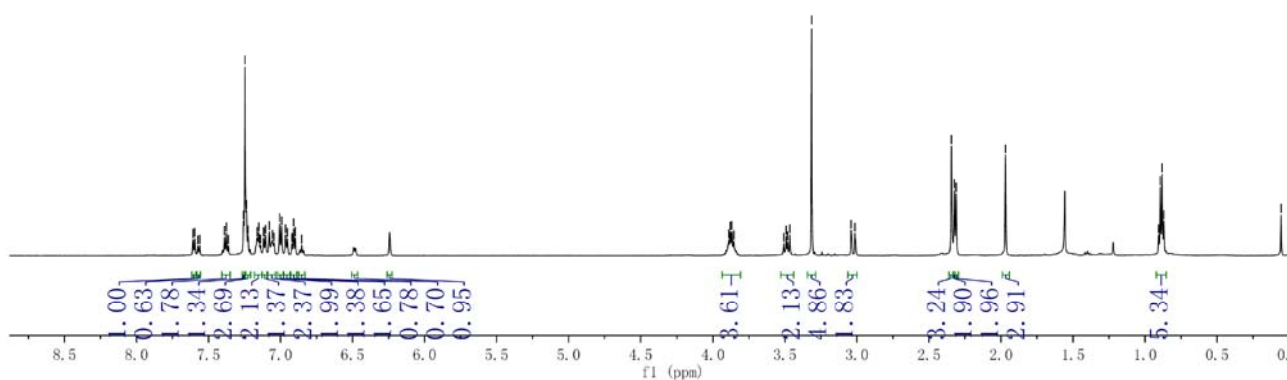
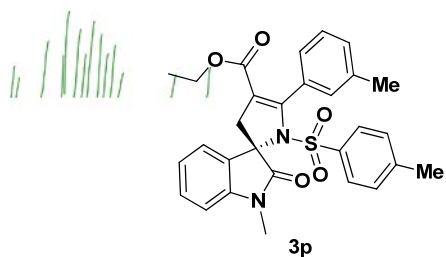


Peak Results

	Name	RT	Area	Height	% Area
1		9.057	625627	41131	2.09
2		13.282	29348250	1116501	97.91

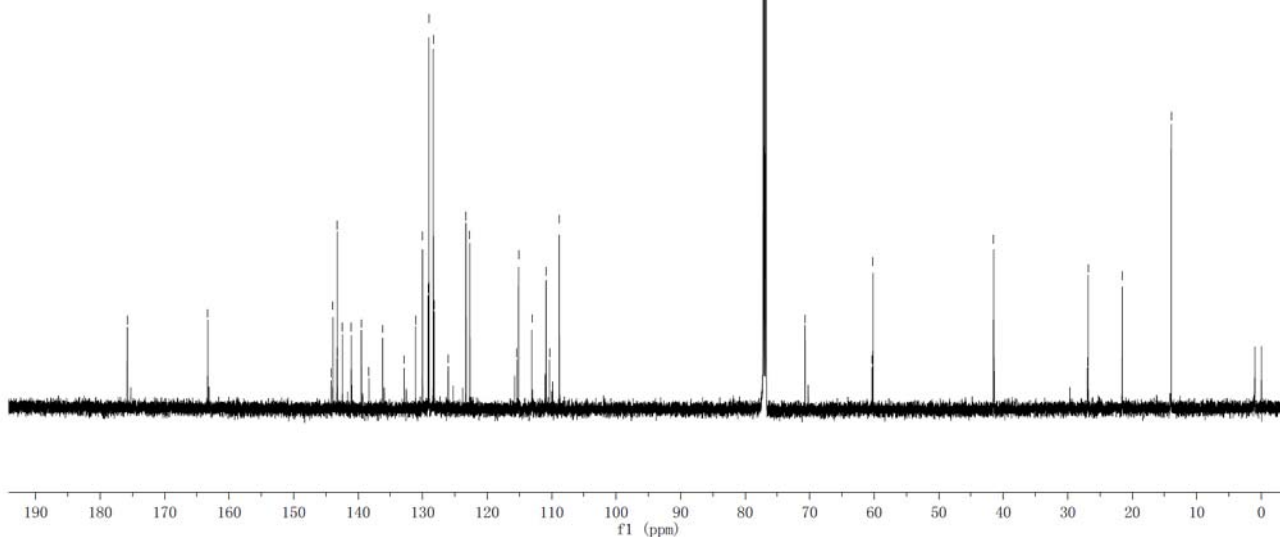
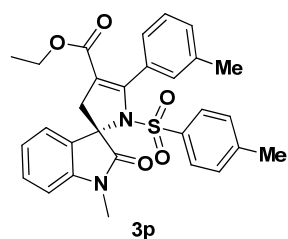
PROTON_01

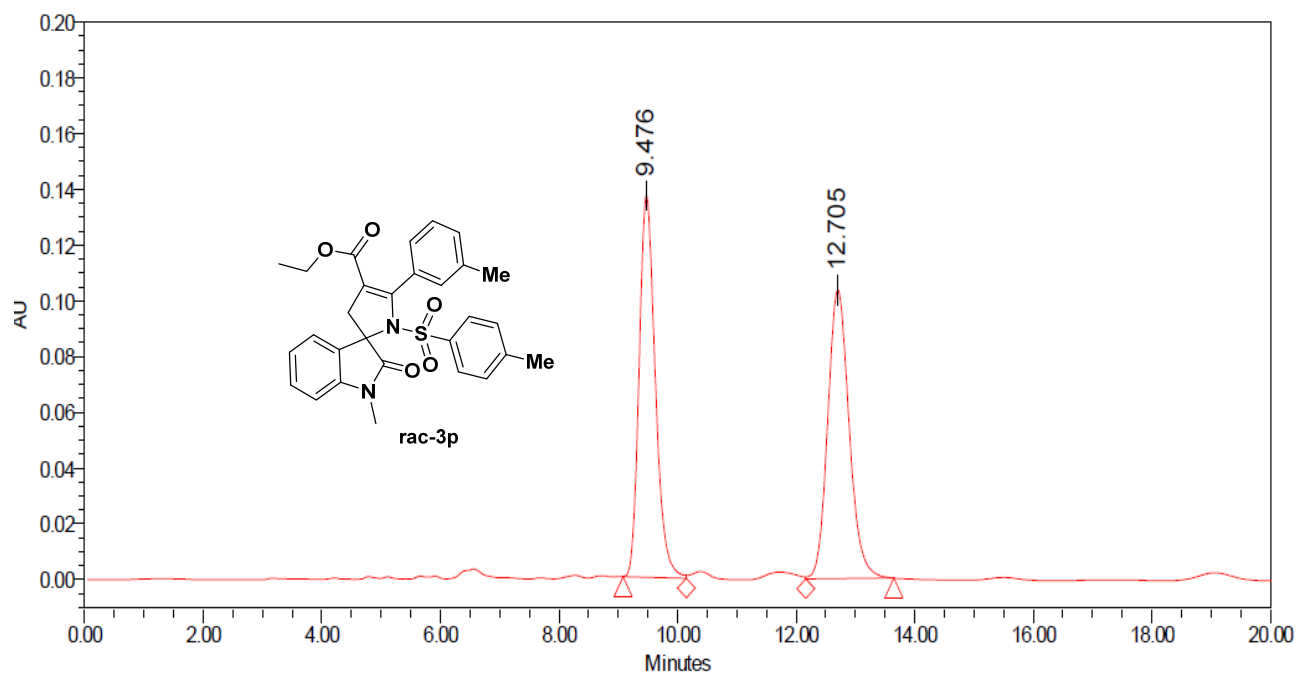
7.608, 7.596, 7.573, 7.561, 7.389, 7.376, 7.363, 7.256, 7.247, 7.236, 7.225, 7.162, 7.151, 7.139, 7.117, 7.103, 7.077, 7.056, 7.045, 7.006, 6.993, 6.965, 6.952, 6.921, 6.909, 6.897, 6.853, 3.890, 3.881, 3.869, 3.855, 3.508, 3.492, 3.482, 3.465, 3.315, 3.040, 3.014, 2.344, 2.324, 2.312, 1.969, 1.564, 0.905, 0.893, 0.881, 0.869, 0.056



CARBON_01

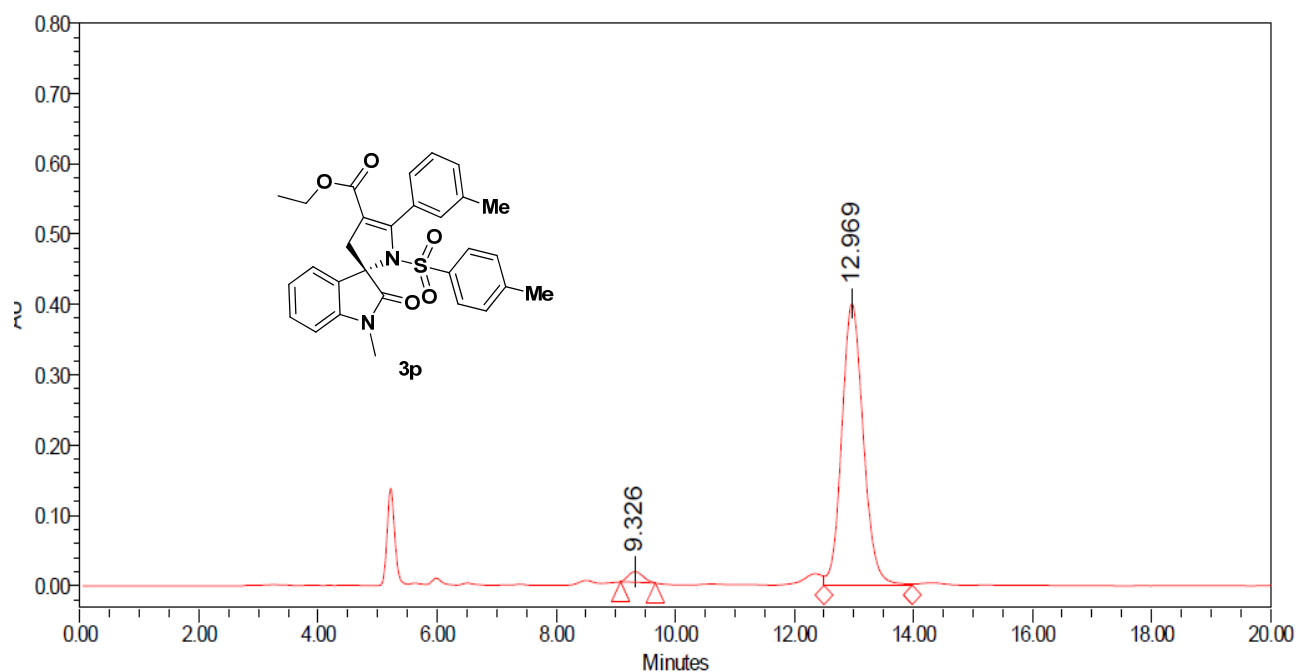
175.79, 163.30, 143.91, 143.22, 139.50, 131.10, 130.02, 129.15, 129.04, 128.35, 128.22, 123.28, 122.68, 122.39, 115.14, 113.08, 110.87, 110.34, 108.82, 77.19, 76.98, 76.76, 70.72, 60.31, 60.19, 41.48, 26.95, 26.85, 21.55, 13.97





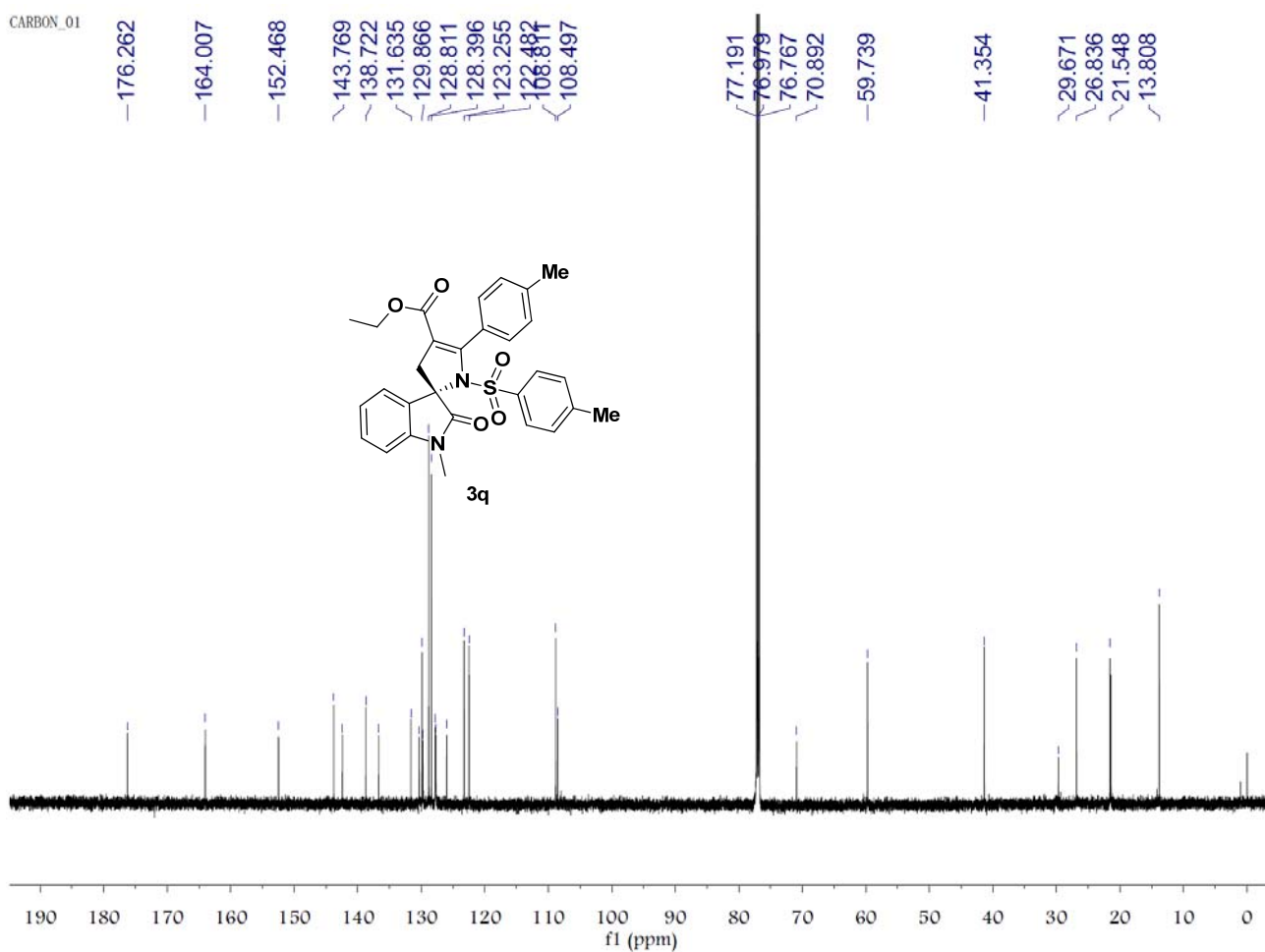
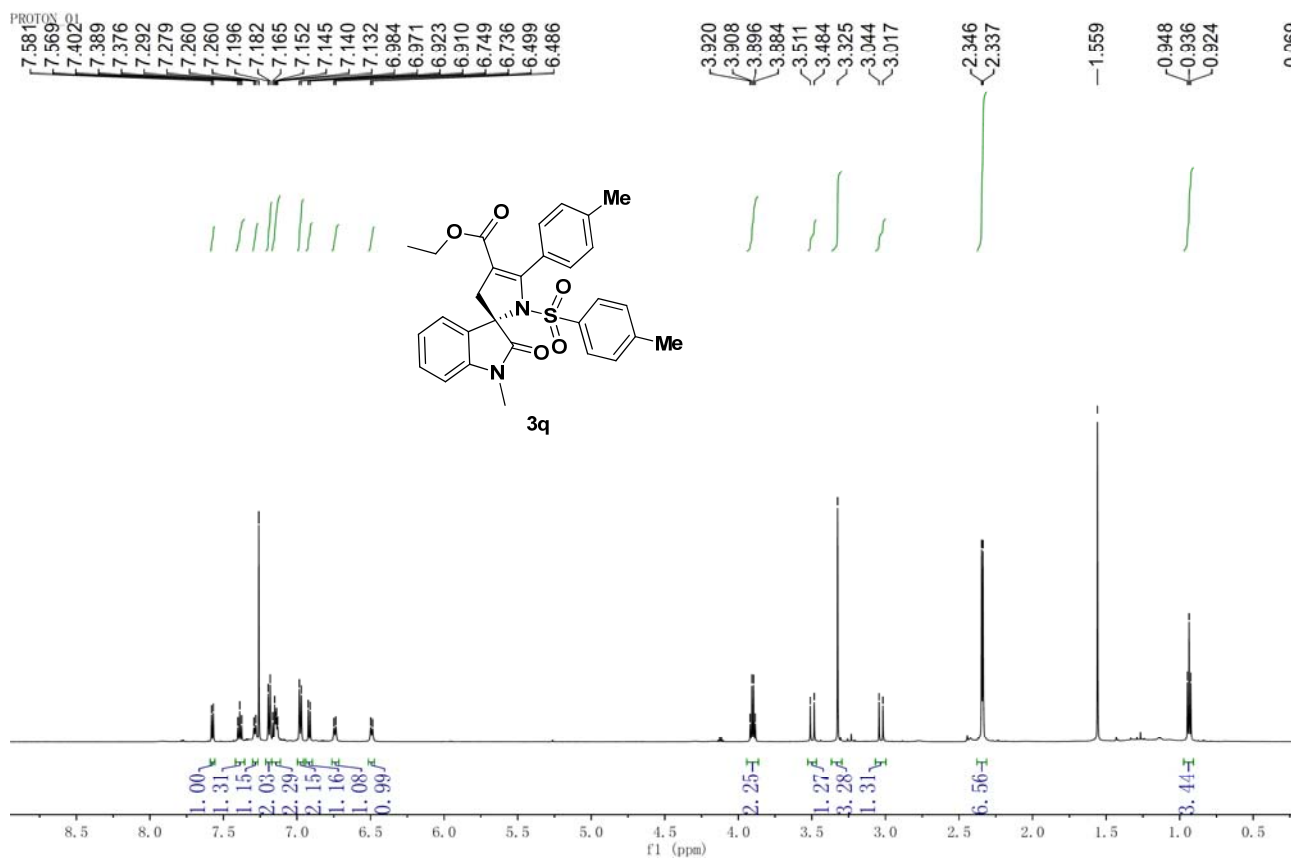
Peak Results

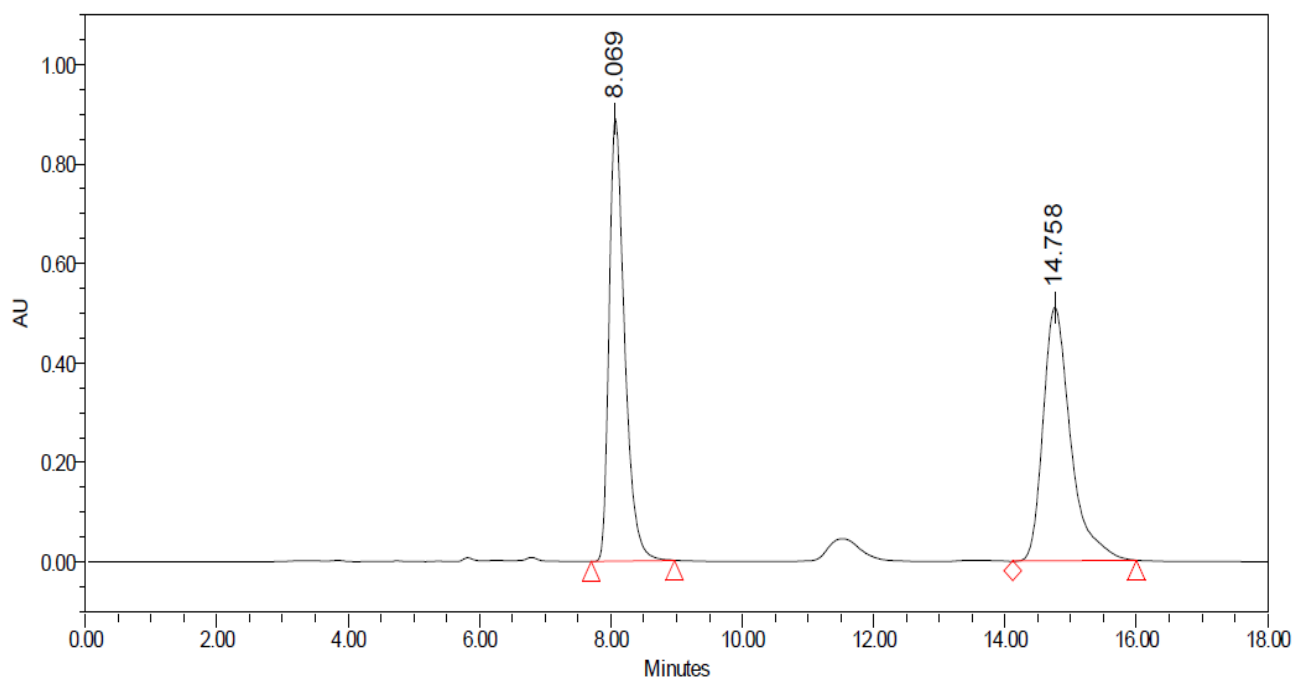
	Name	RT	Area	Height	% Area
1		9.476	2595633	137110	49.91
2		12.705	2604610	103650	50.09



Peak Results

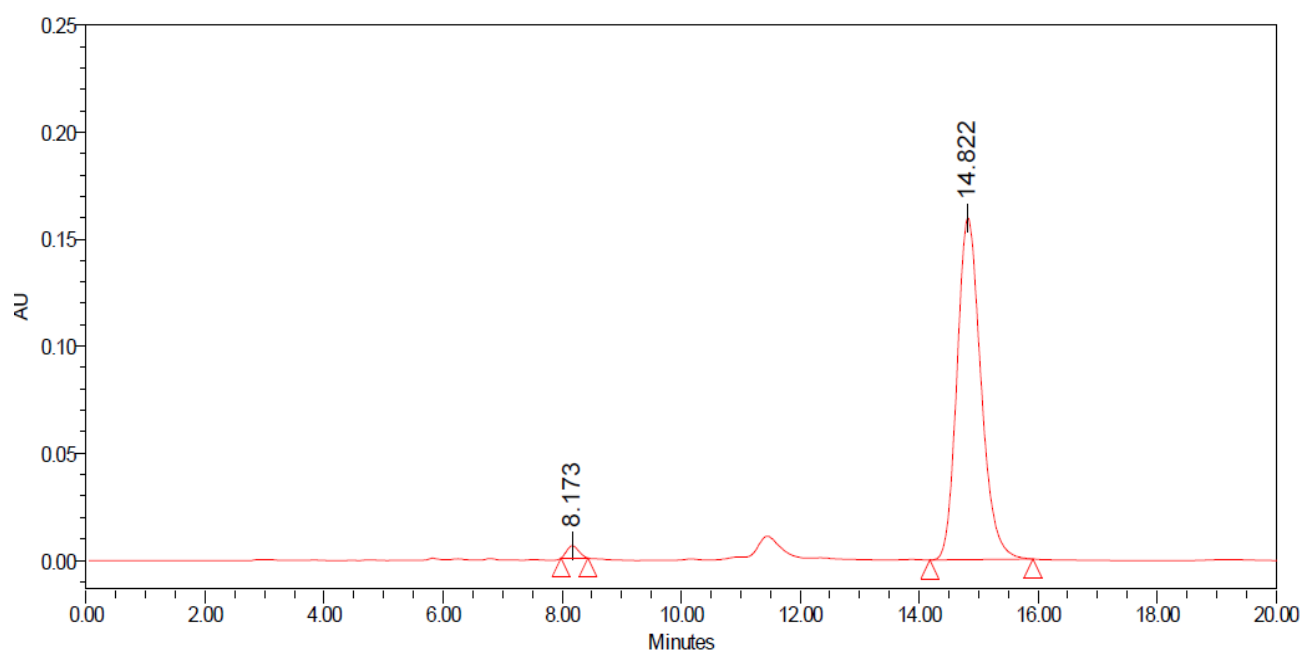
	Name	RT	Area	Height	% Area
1		9.326	257820	14837	2.51
2		12.969	10033790	400314	97.49





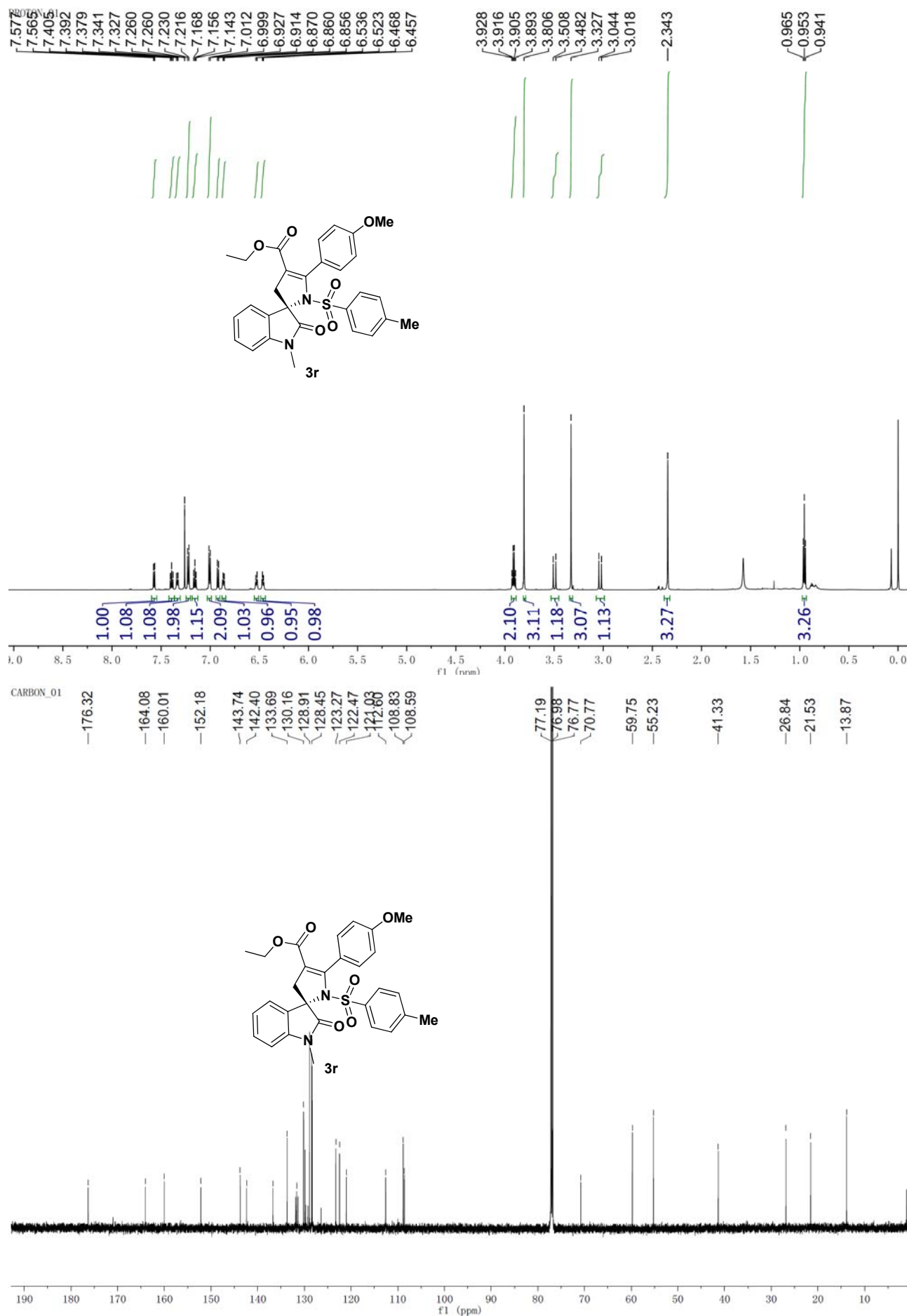
Peak Results

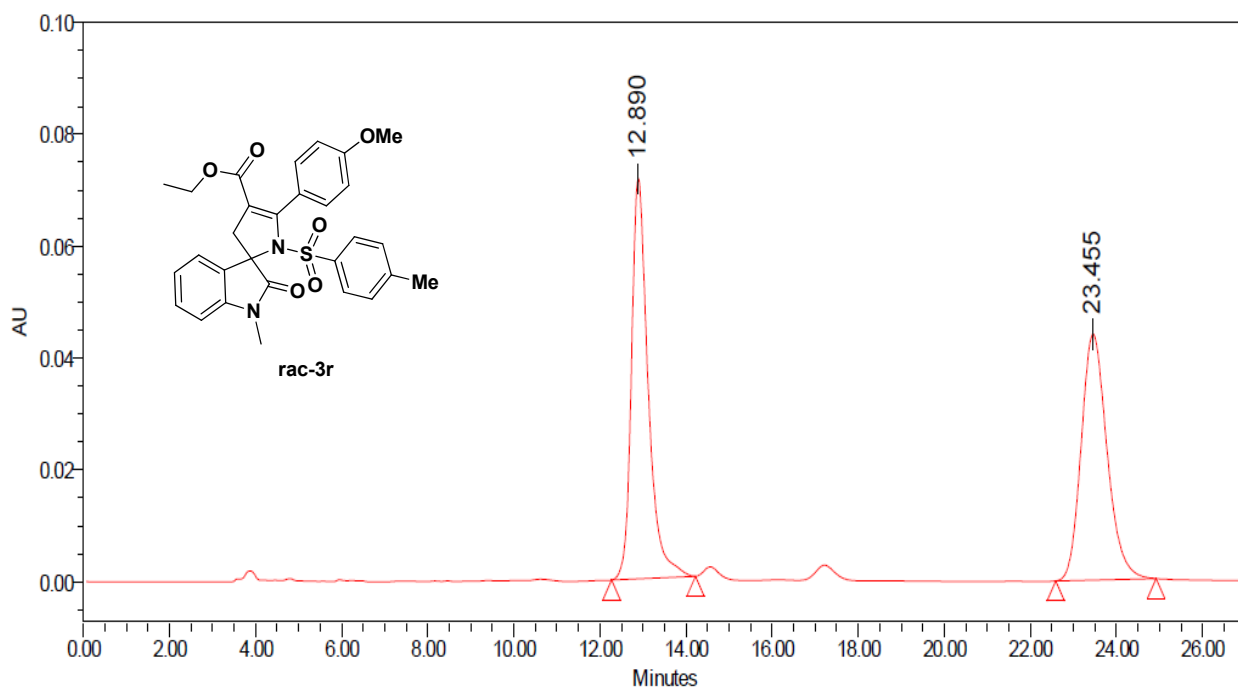
	Name	RT	Area	Height	% Area
1		8.069	14601029	891099	49.59
2		14.758	14839636	509259	50.41



Peak Results

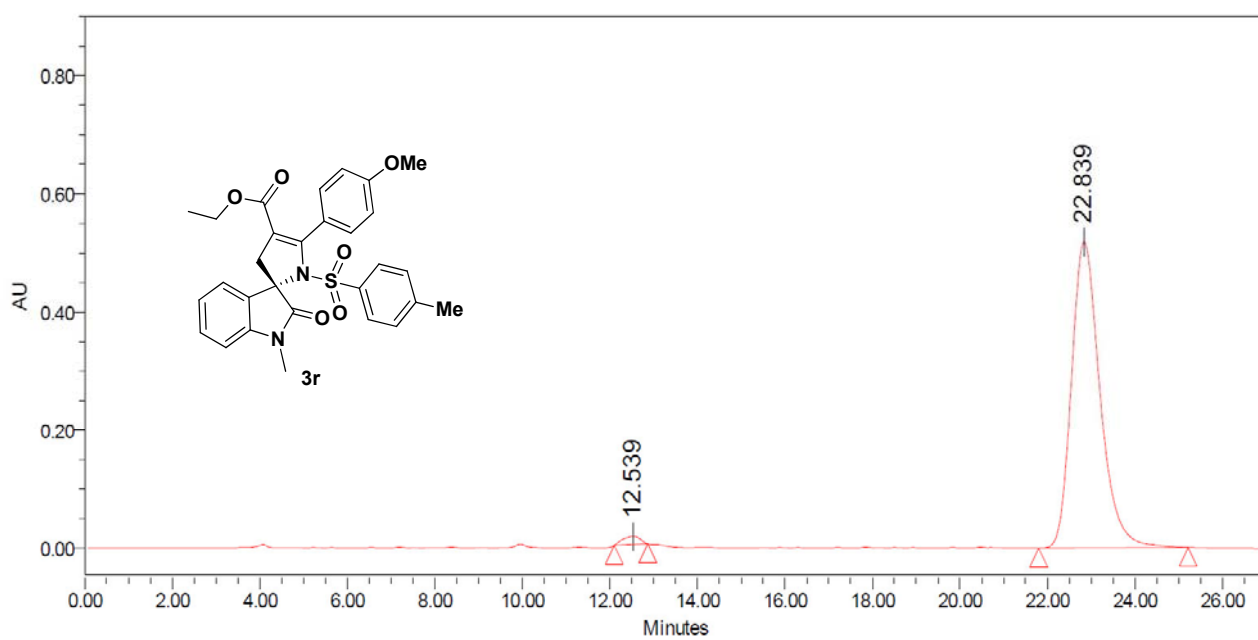
	Name	RT	Area	Height	% Area
1		8.173	79227	5748	1.75
2		14.822	4454918	159639	98.25





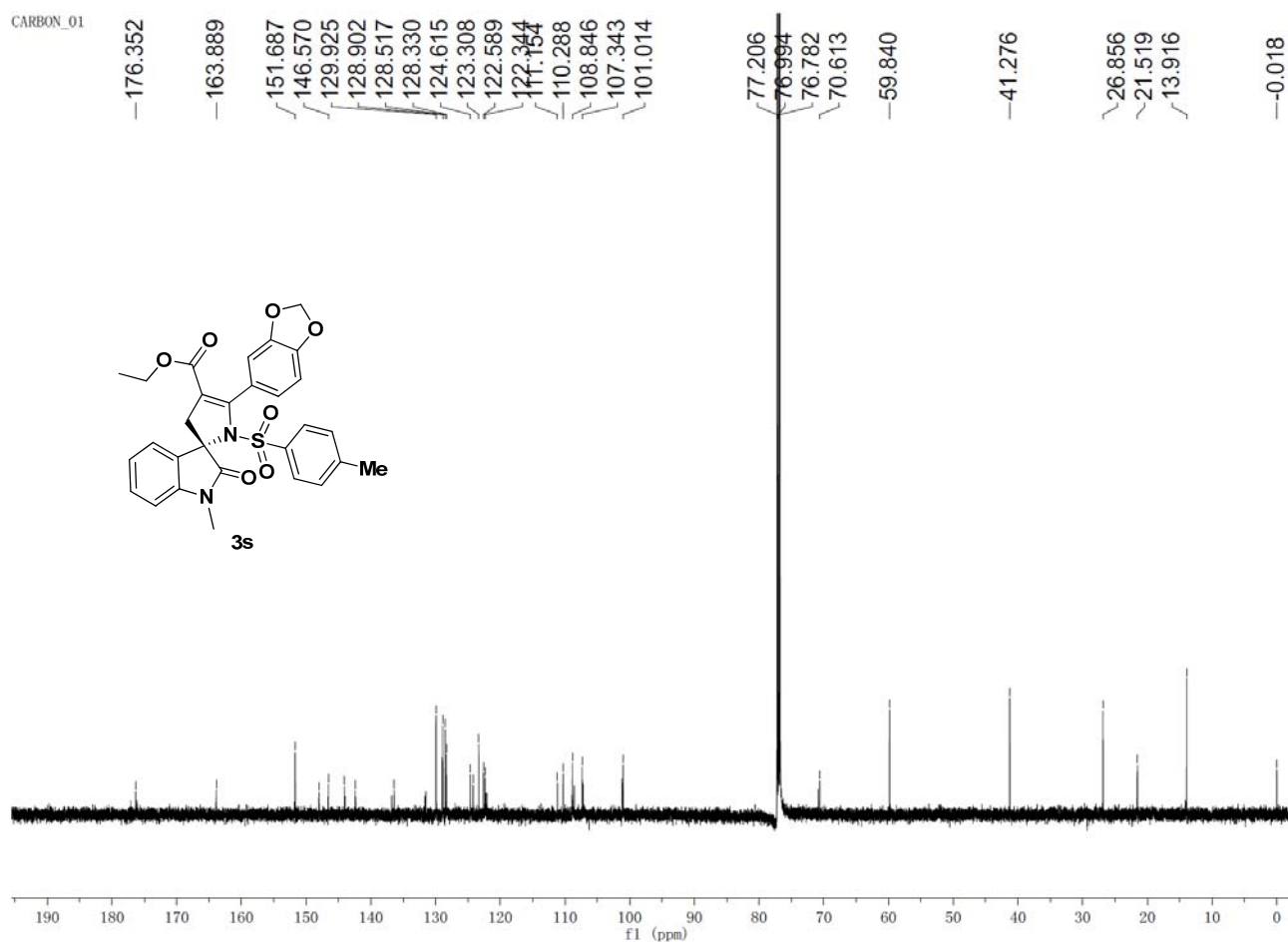
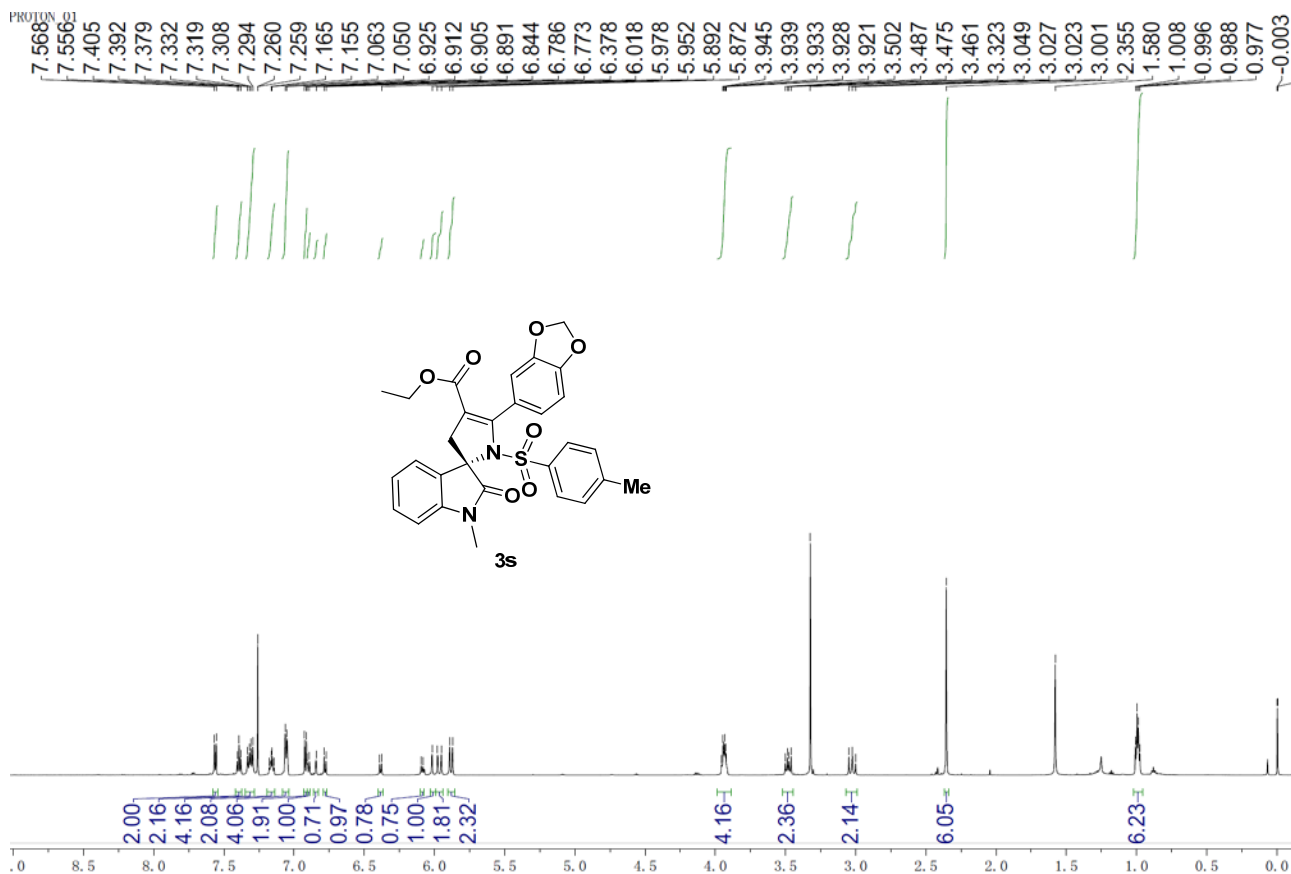
Peak Results

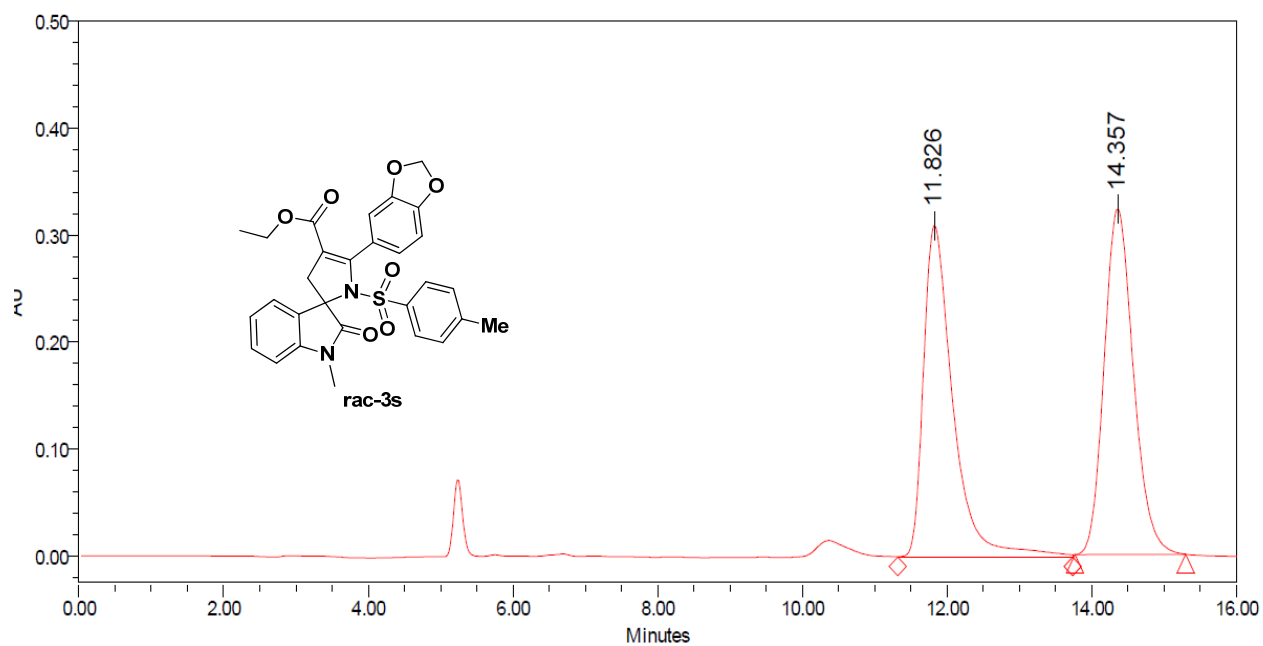
	Name	RT	Area	Height	% Area
1		12.890	1931592	71654	51.25
2		23.455	1837565	43988	48.75



Peak Results

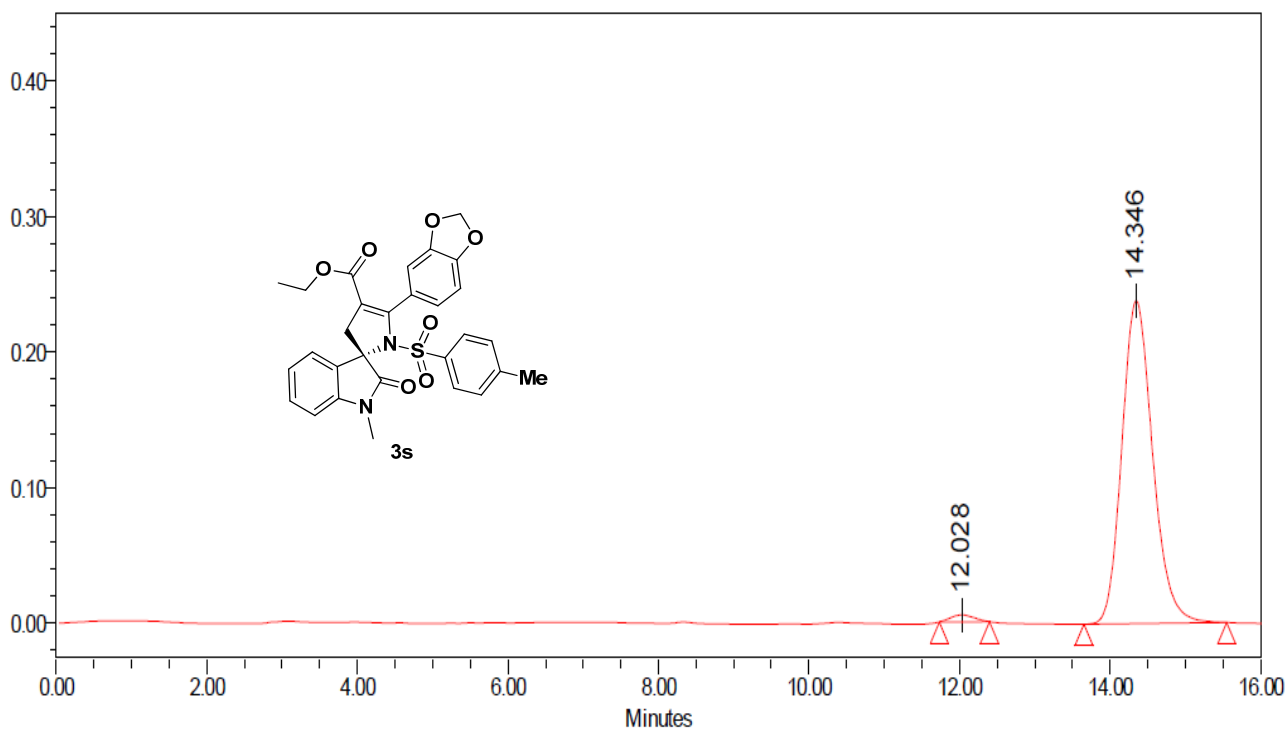
	Name	RT	Area	Height	% Area
1		12.539	393110	13983	1.64
2		22.839	23568568	519658	98.36





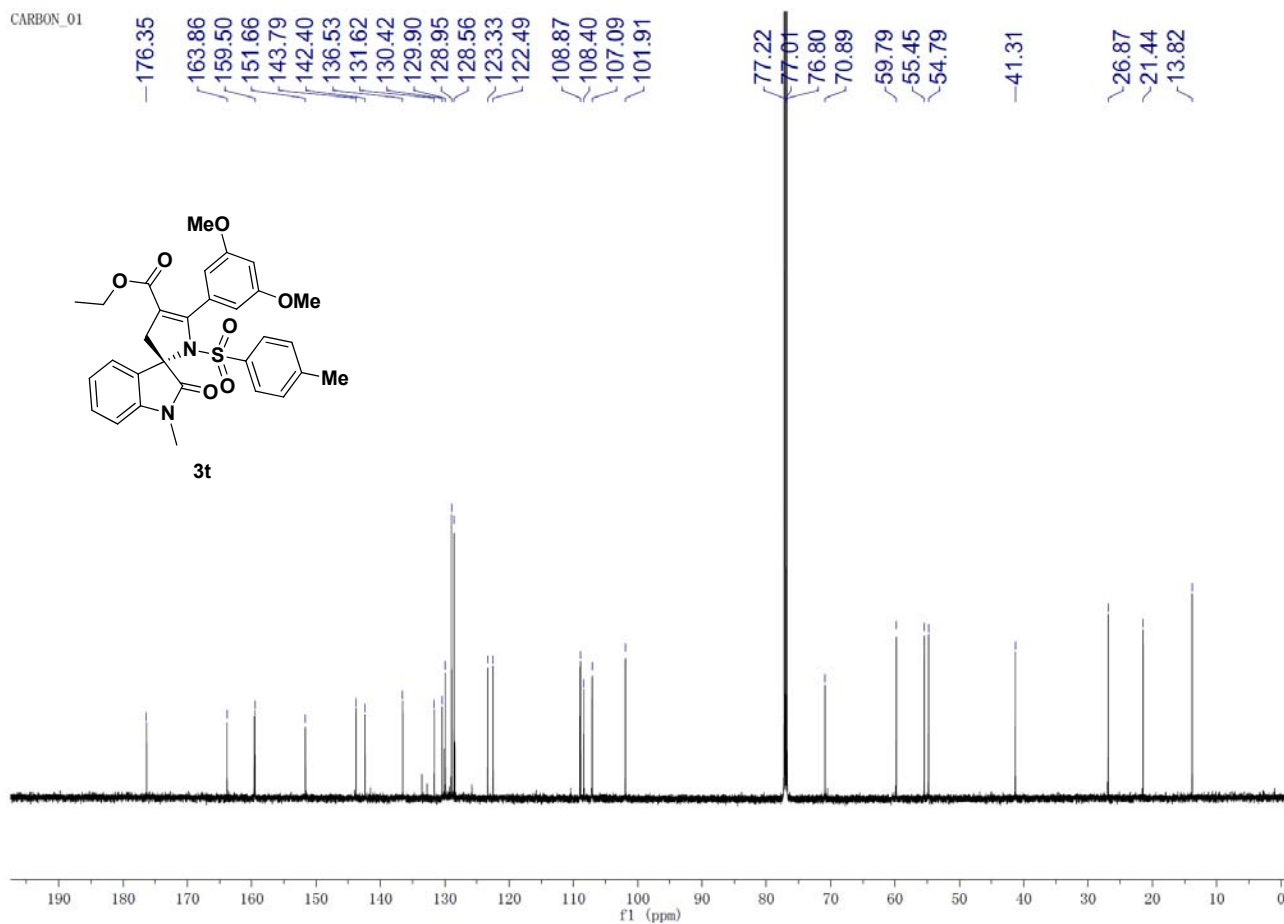
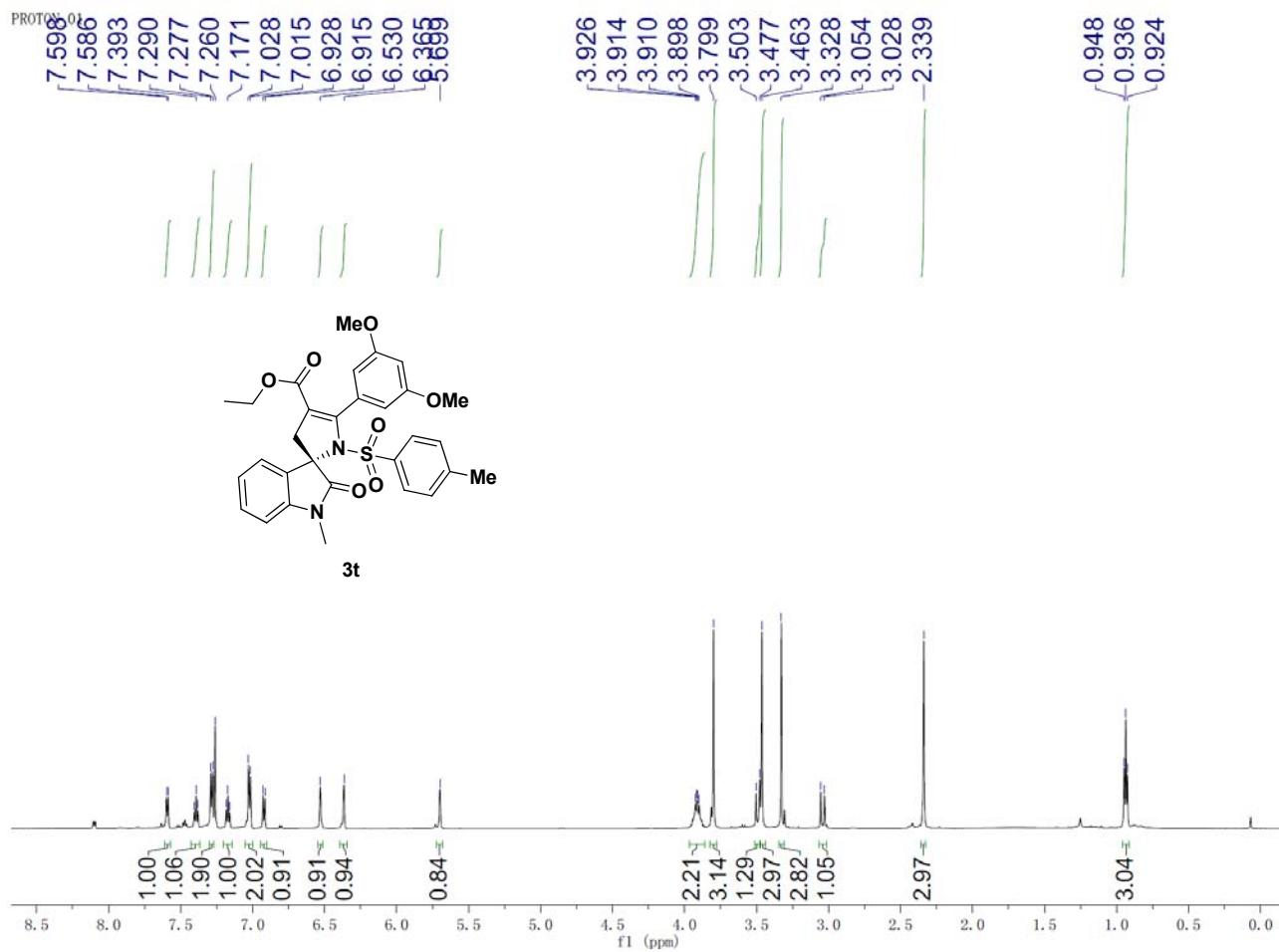
Peak Results

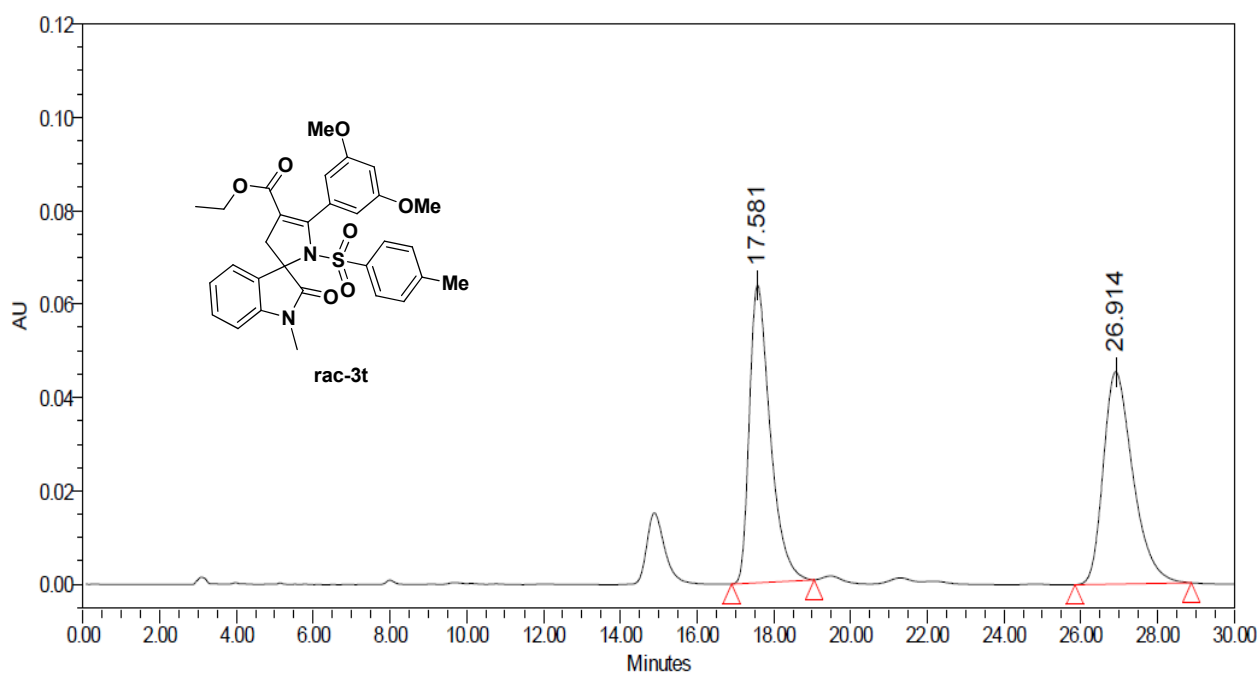
	Name	RT	Area	Height	% Area
1		11.826	8798525	310453	49.20
2		14.357	9083561	323529	50.80



Peak Results

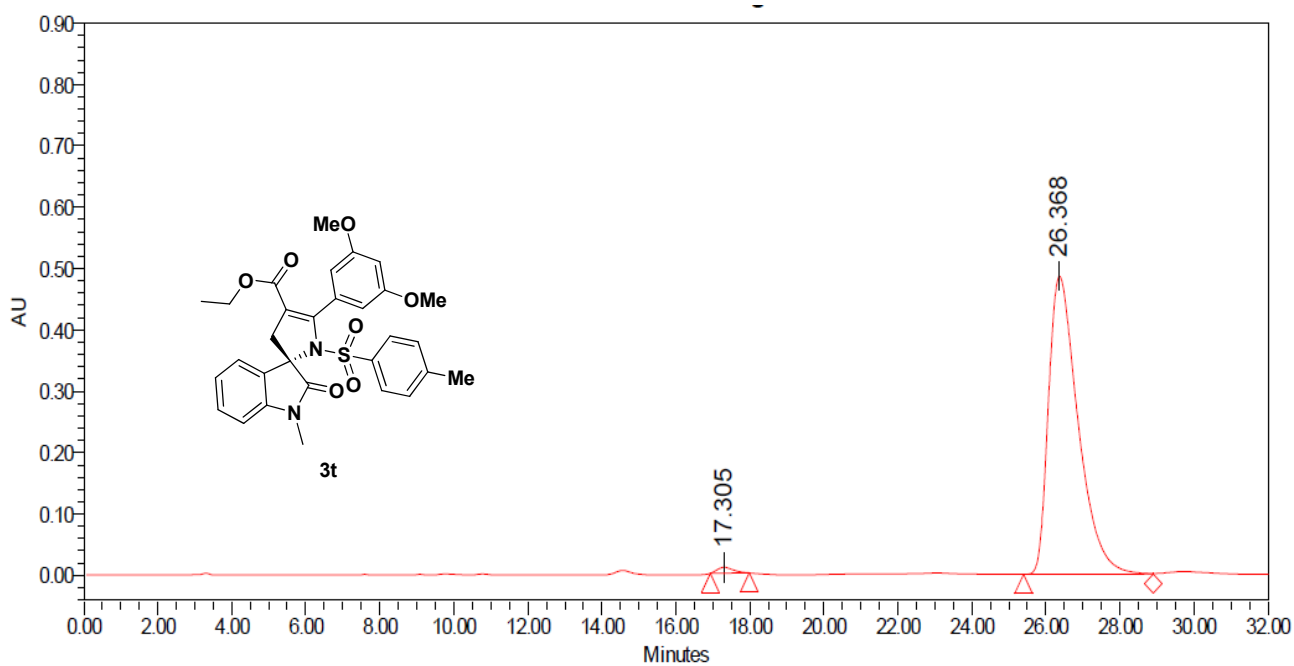
	Name	RT	Area	Height	% Area
1		12.028	111825	5084	1.63
2		14.346	6766915	238358	98.37





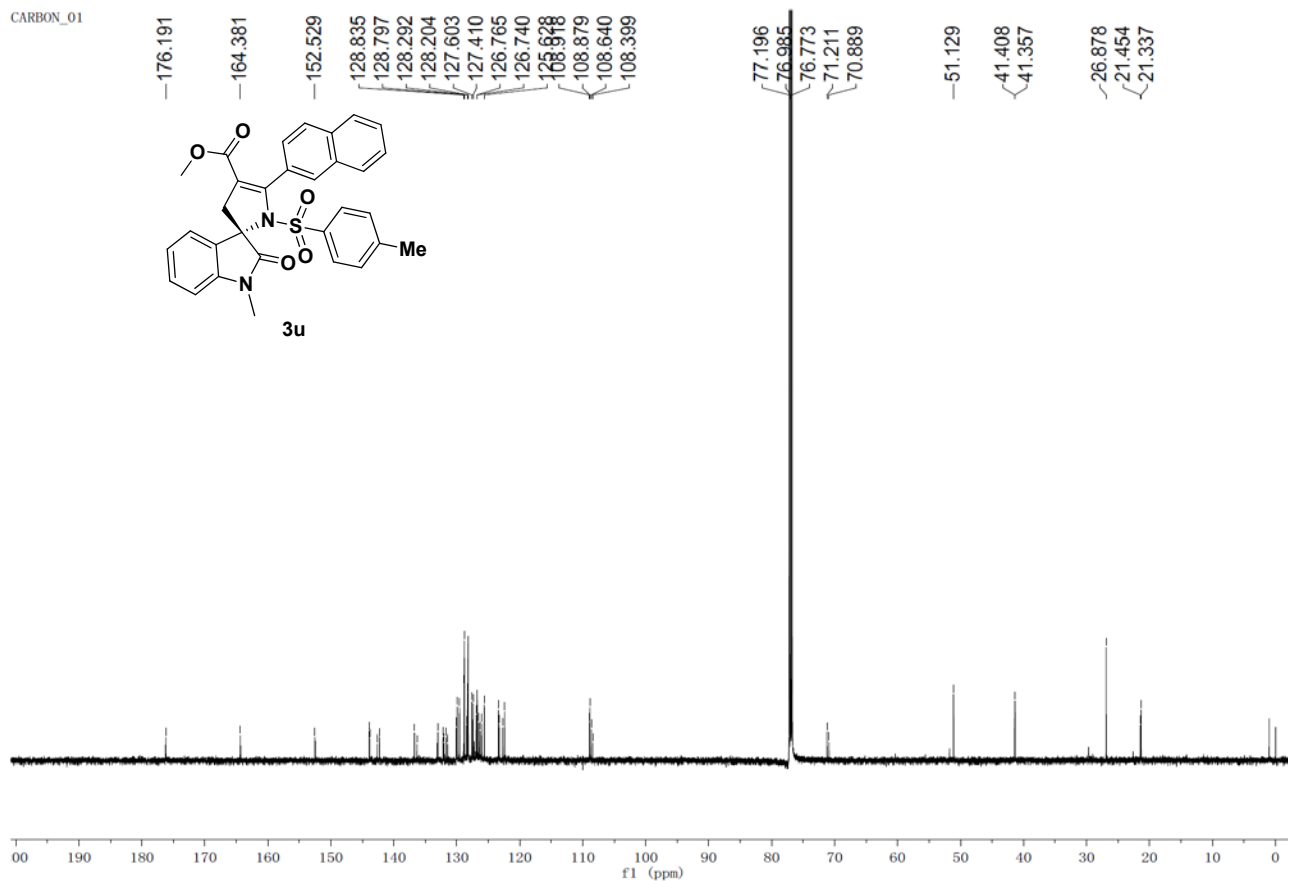
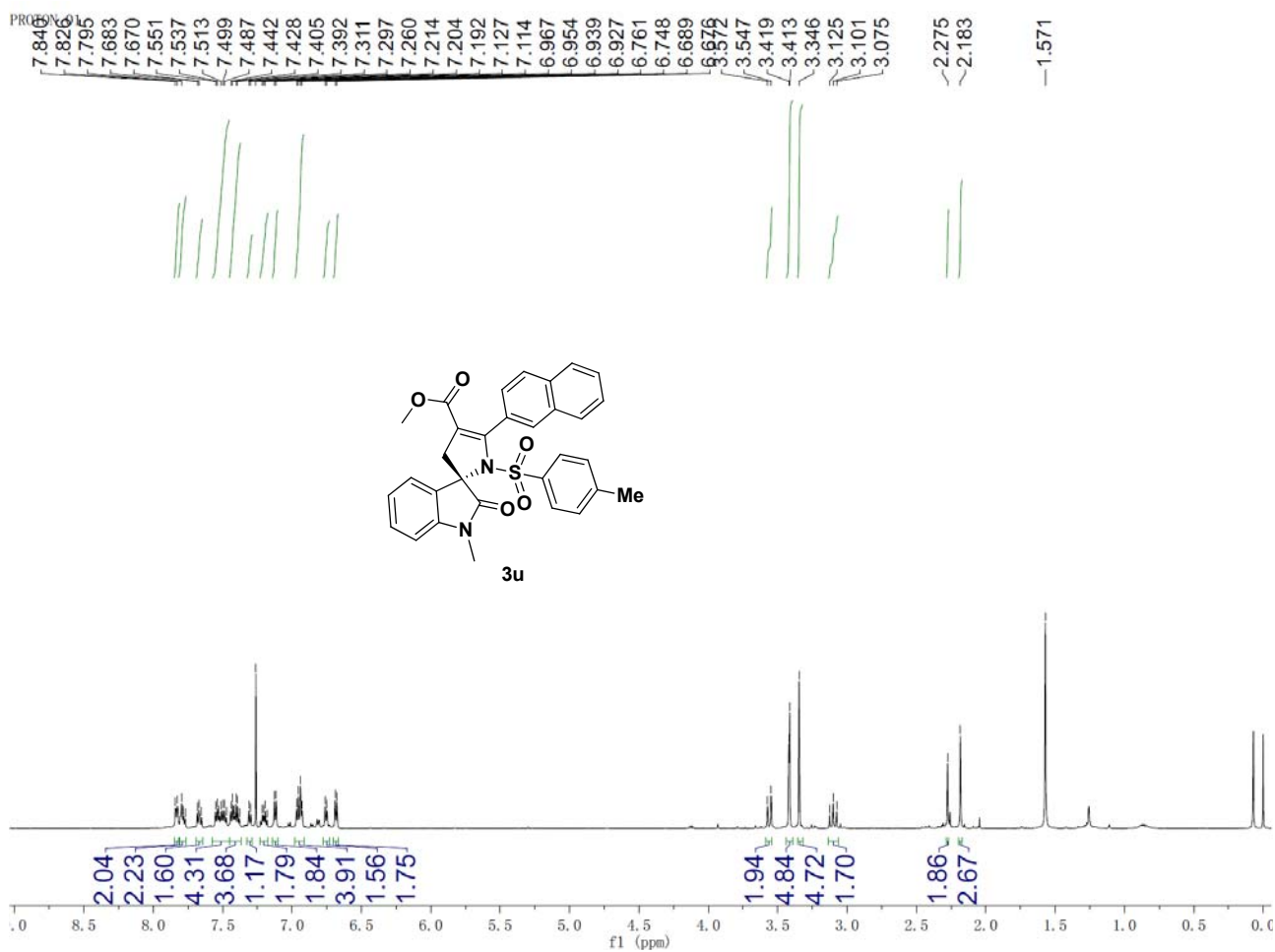
Peak Results

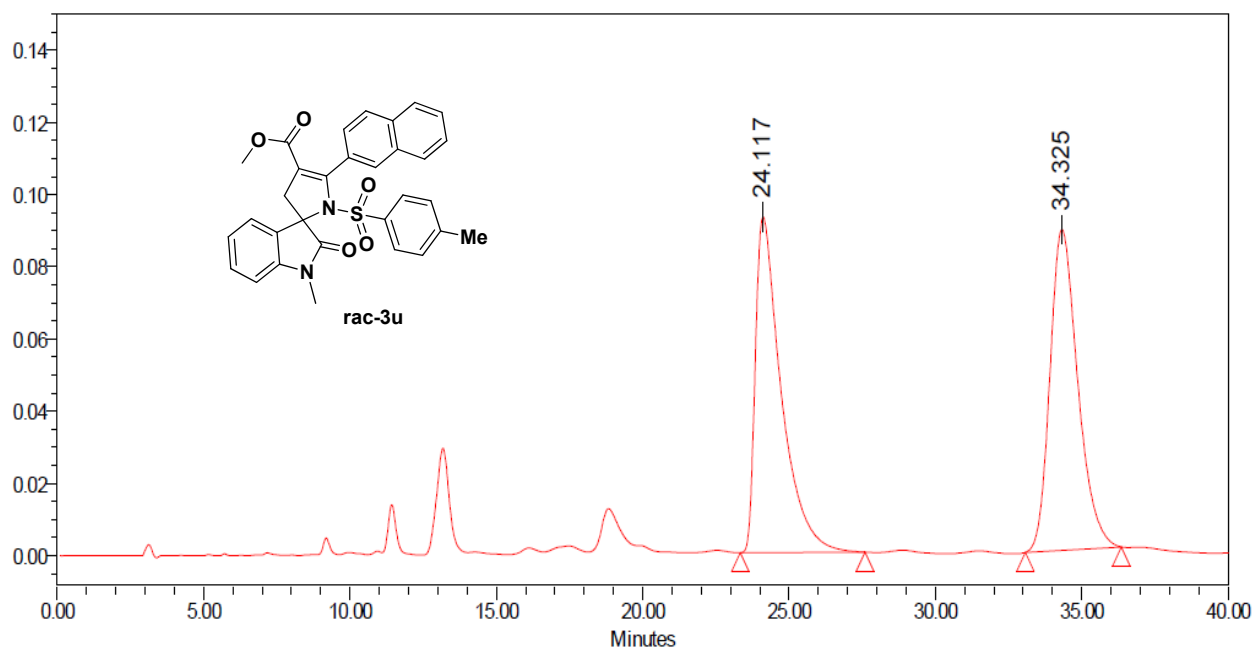
	Name	RT	Area	Height	% Area
1		17.581	2405704	63783	49.62
2		26.914	2442777	45465	50.38



Peak Results

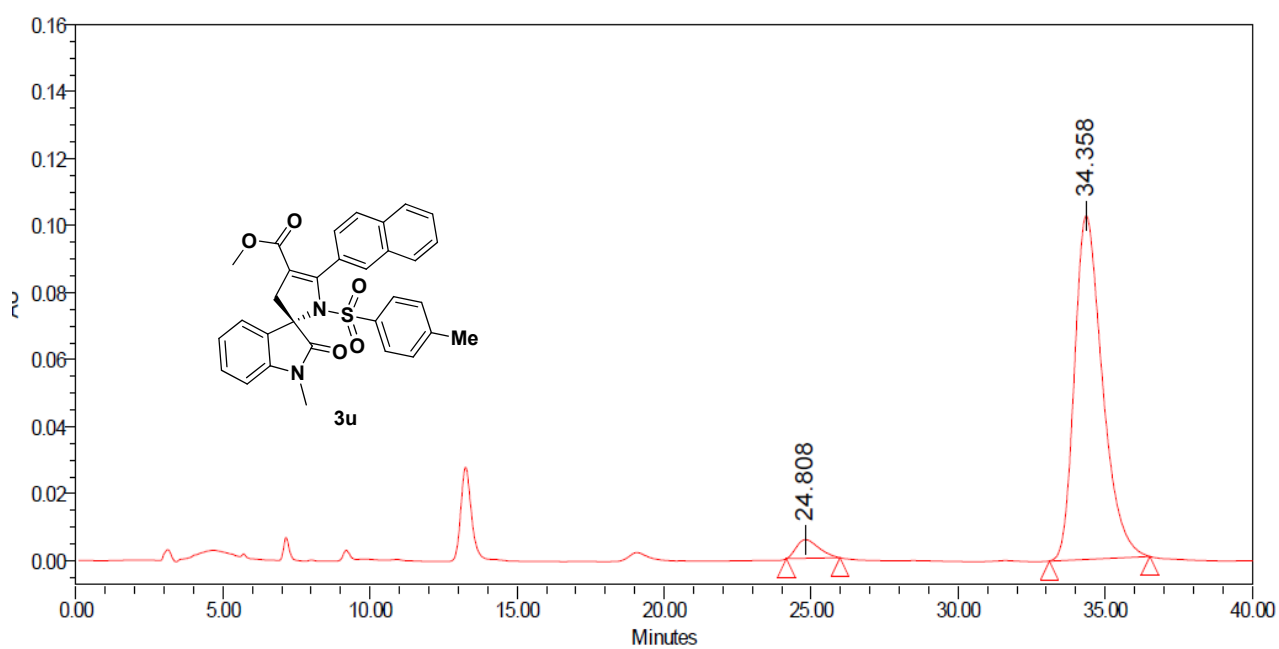
	Name	RT	Area	Height	% Area
1		17.305	284147	9377	1.04
2		26.368	27043009	486356	98.96





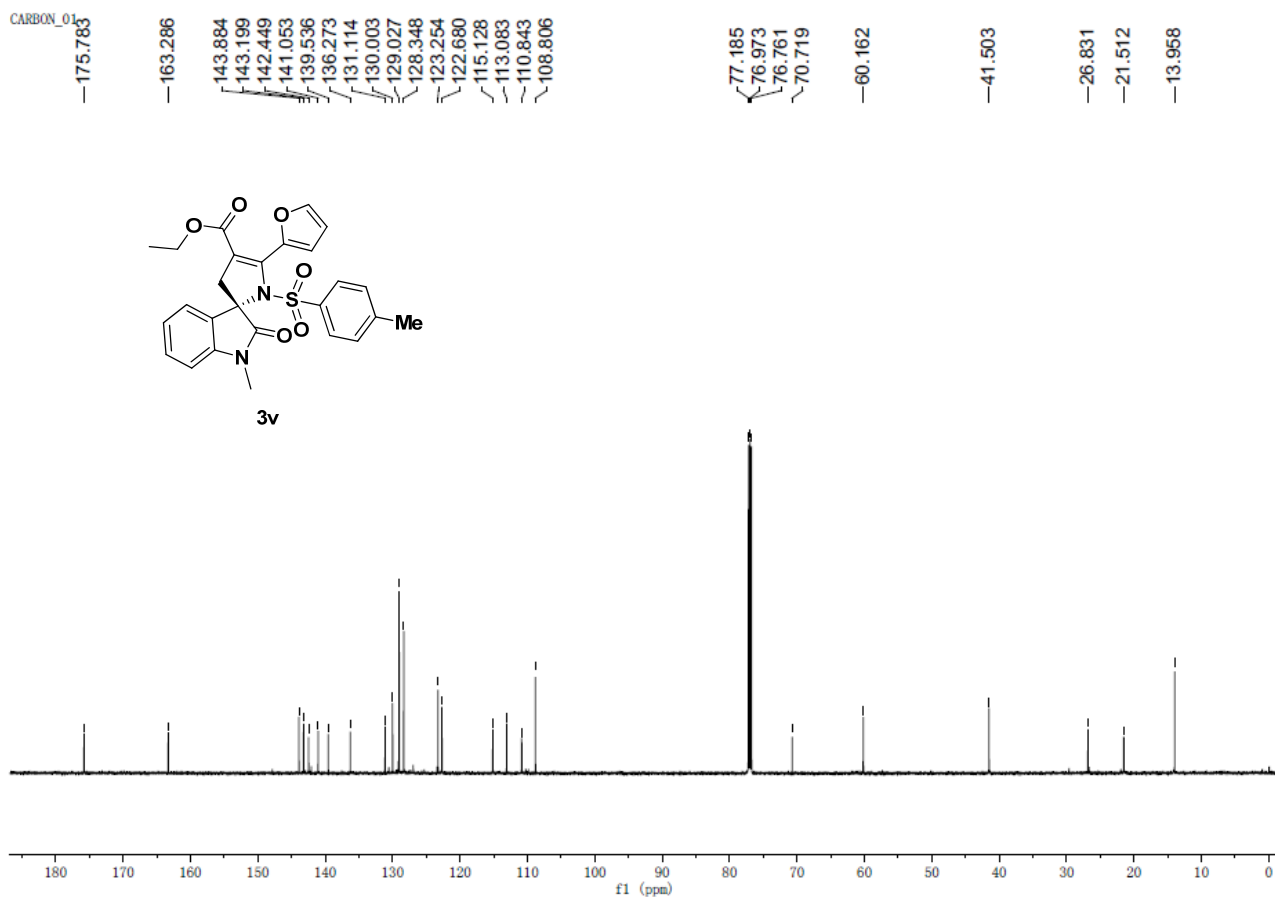
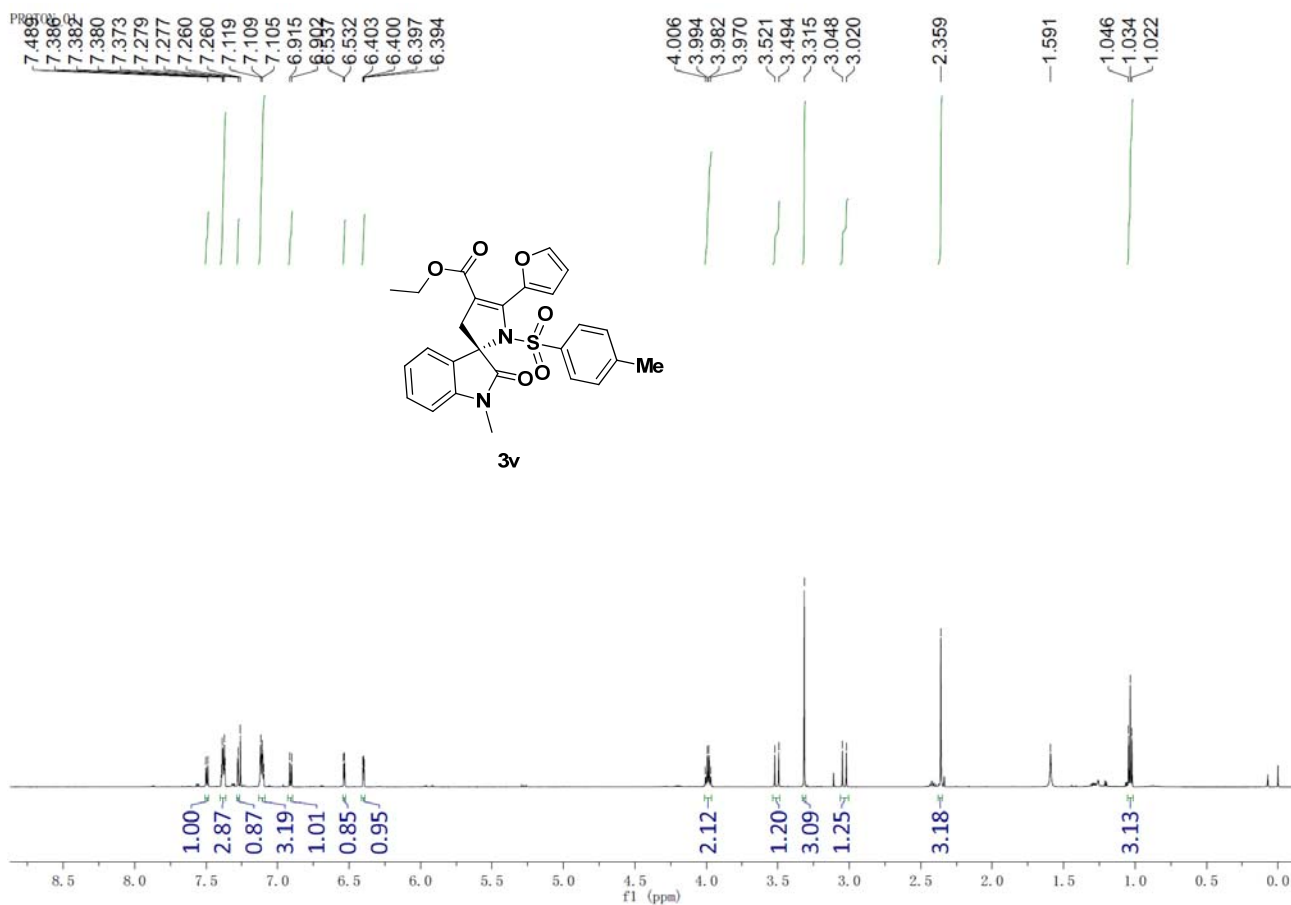
Peak Results

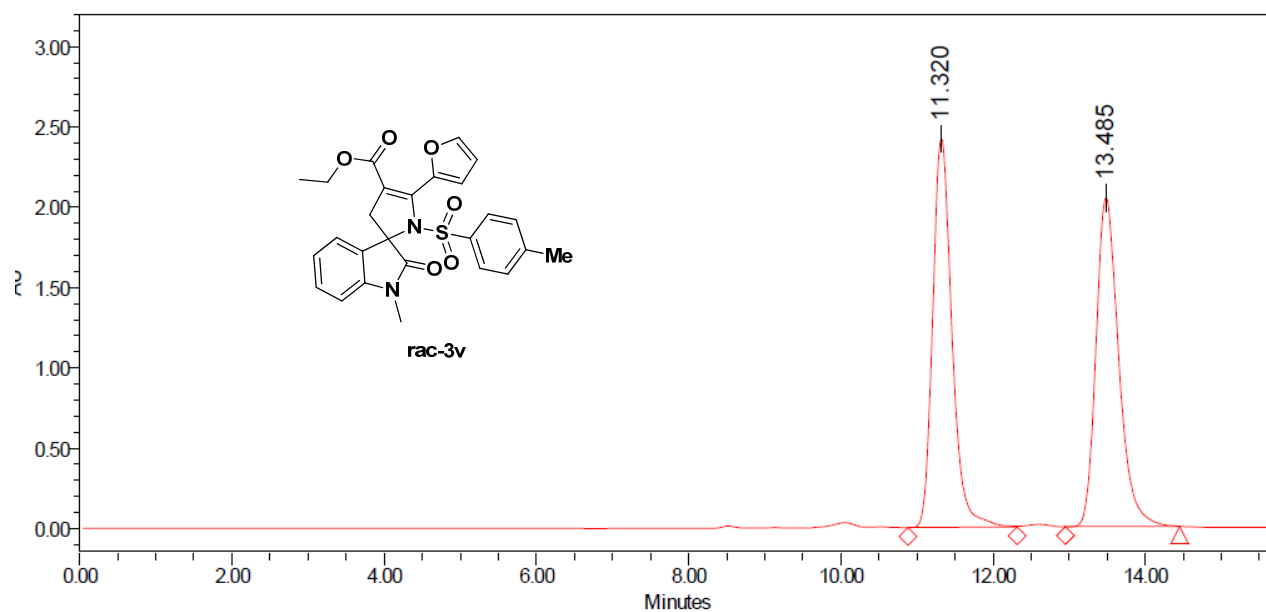
	Name	RT	Area	Height	% Area
1		24.117	5708352	93021	49.26
2		34.325	5880512	88855	50.74



Peak Results

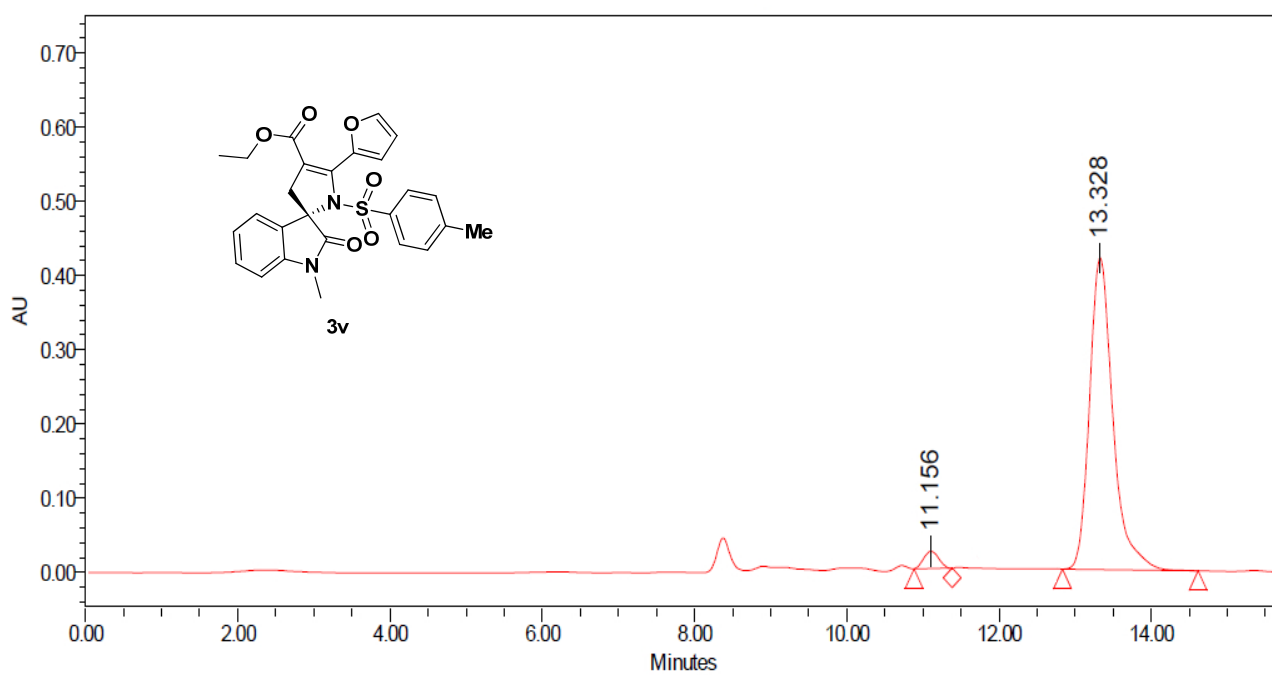
	Name	RT	Area	Height	% Area
1		24.808	295406	5556	4.18
2		34.358	6772037	102636	95.82





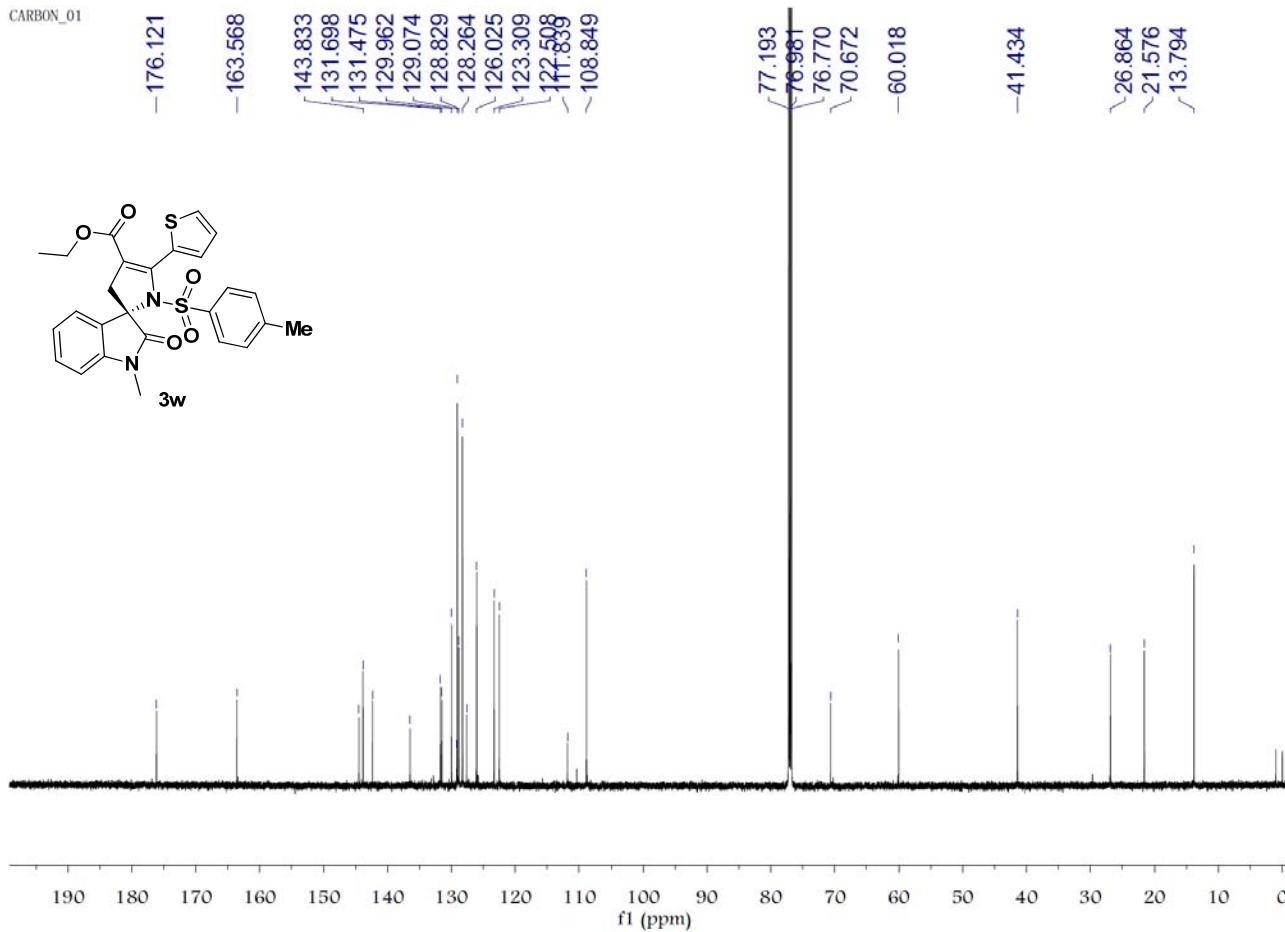
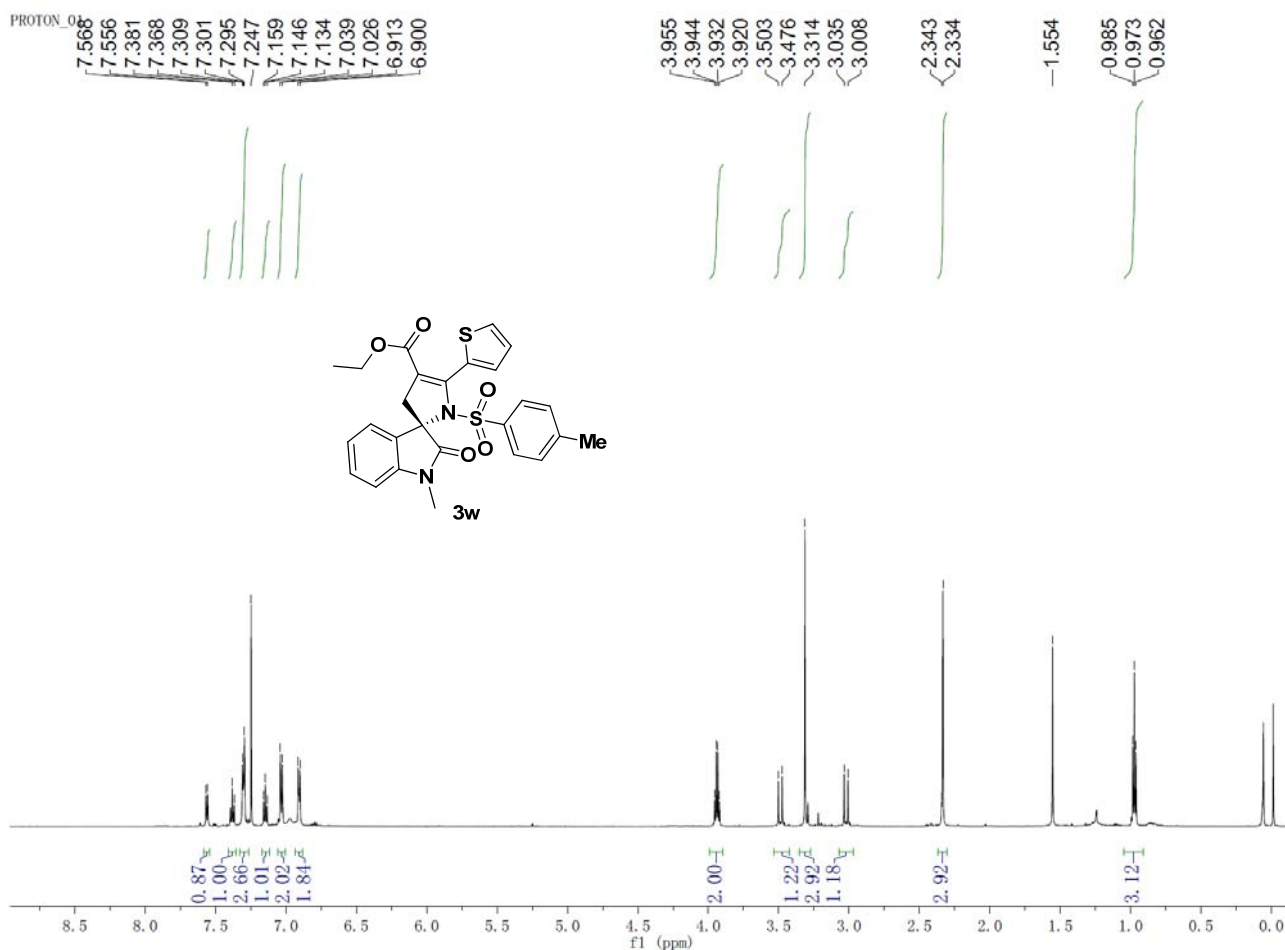
Peak Results

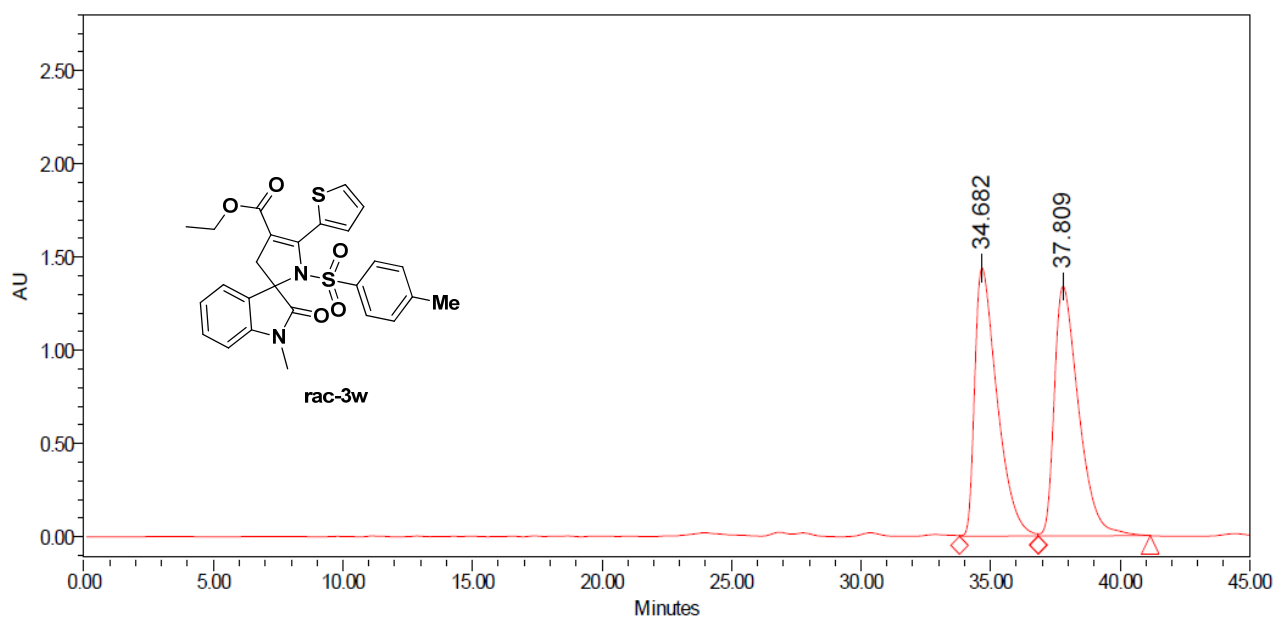
	Name	RT	Area	Height	% Area
1		11.320	42484948	2424486	49.97
2		13.485	42542447	2049580	50.03



Peak Results

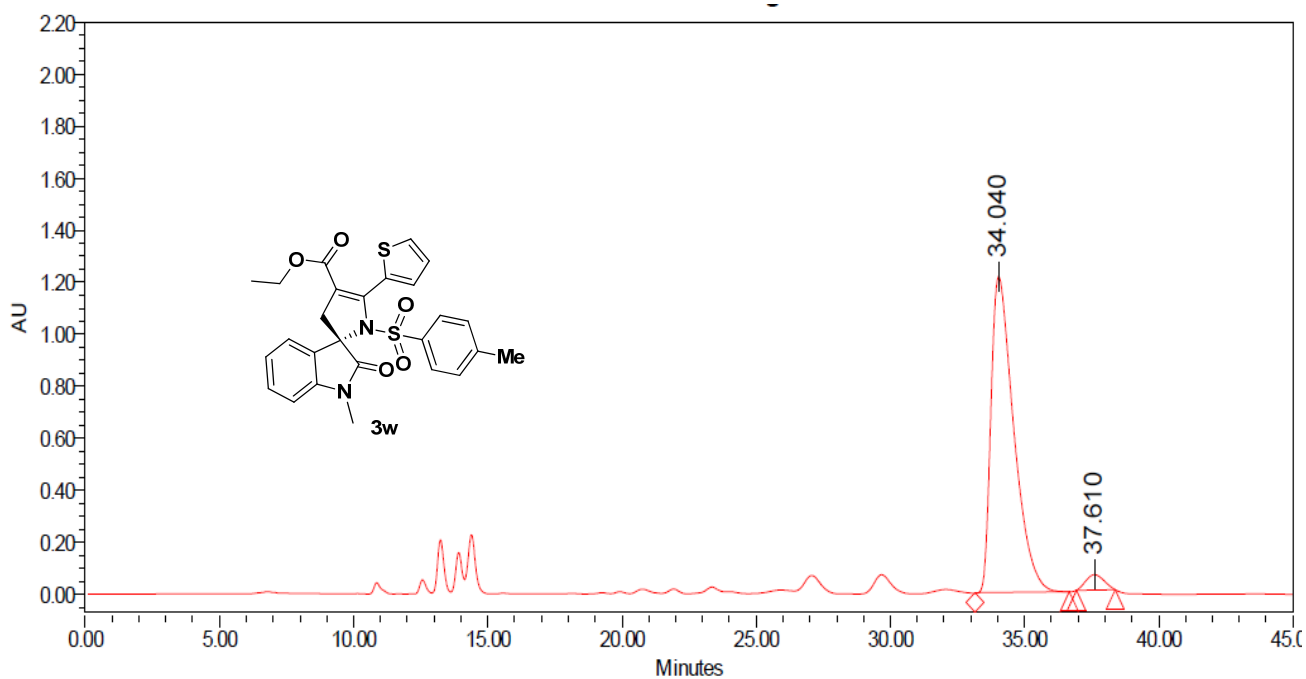
	Name	RT	Area	Height	% Area
1		11.156	314529	23032	3.38
2		13.328	8988945	420351	96.62





Peak Results

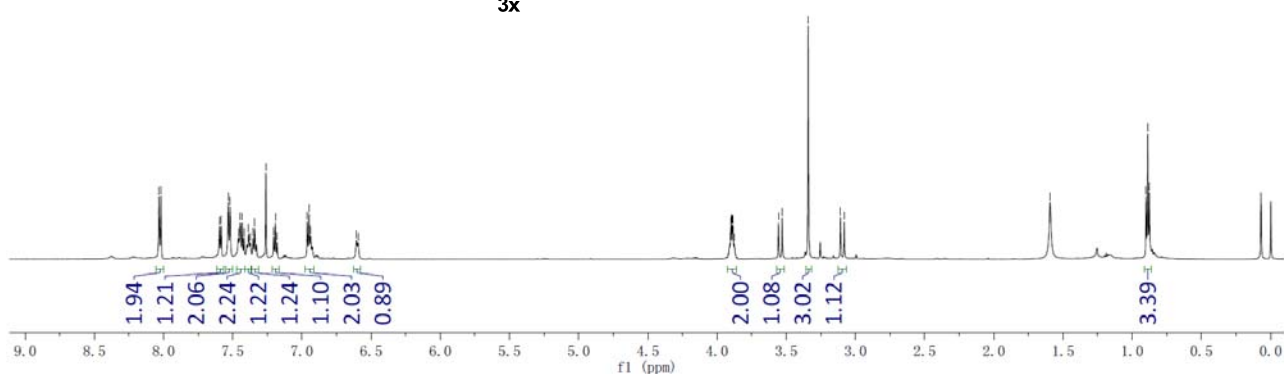
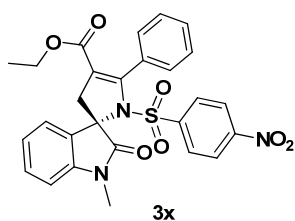
	Name	RT	Area	Height	% Area
1		34.682	86385792	1438122	49.78
2		37.809	87160453	1339547	50.22



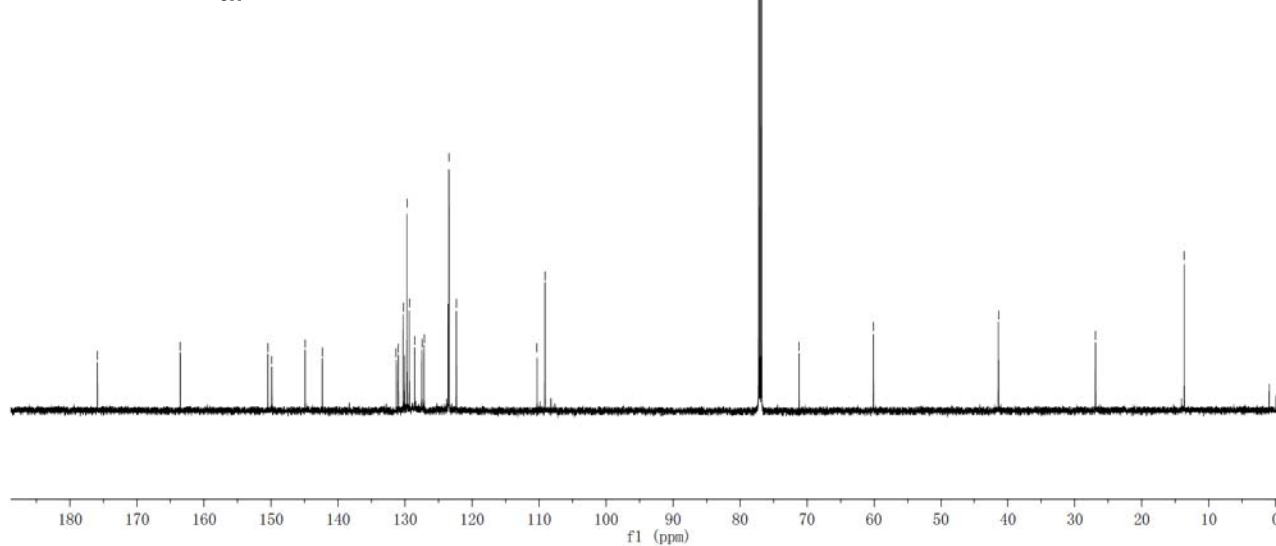
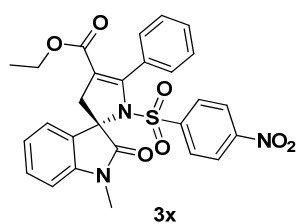
Peak Results

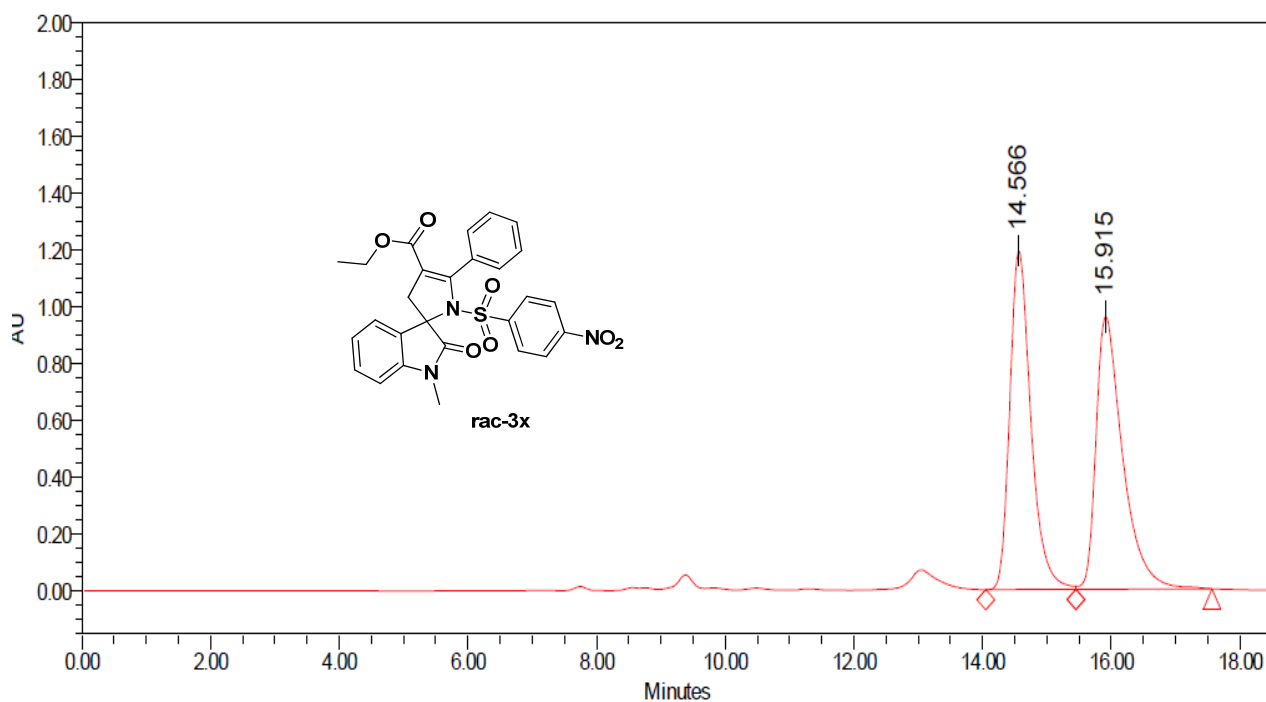
	Name	RT	Area	Height	% Area
1		34.040	71980732	1216067	96.27
2		37.610	2788848	58895	3.73

PROTON_01



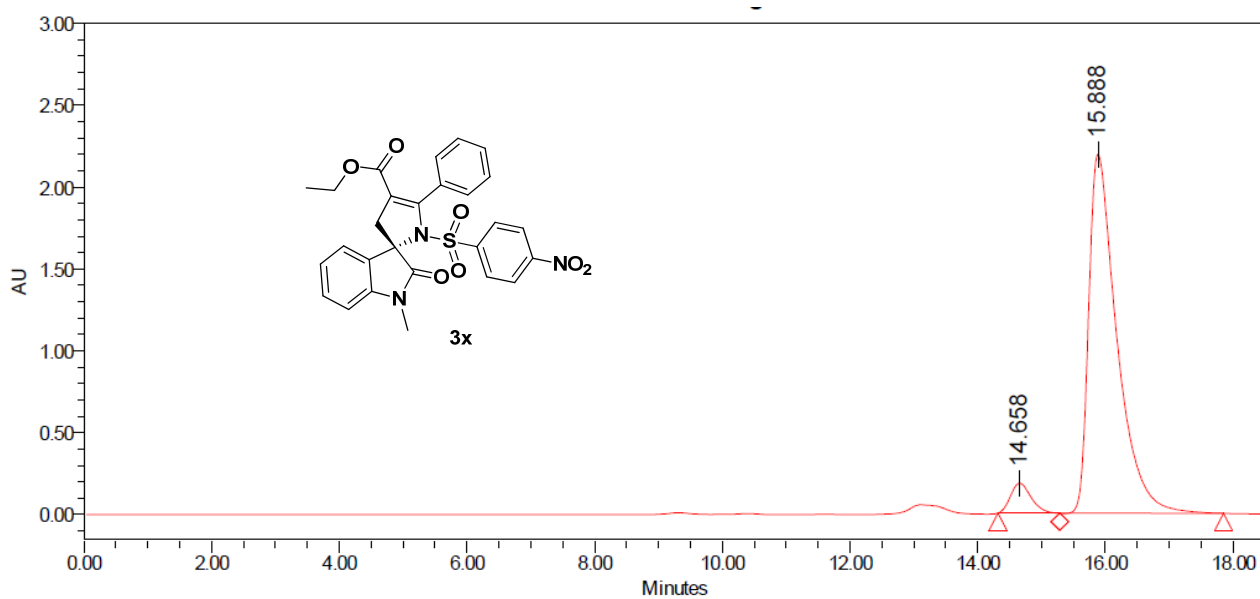
CARBON_01





Peak Results

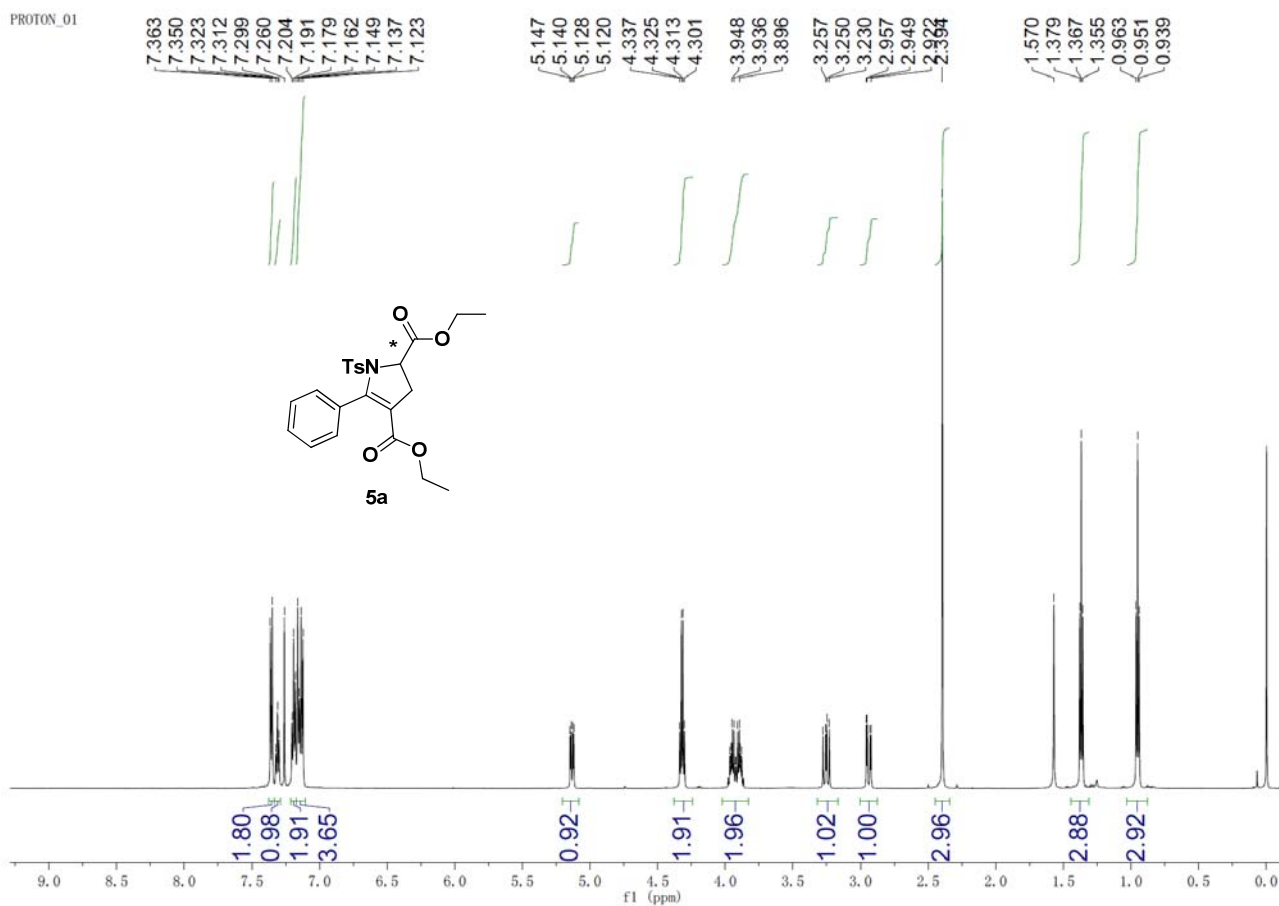
	Name	RT	Area	Height	% Area
1		14.566	27238954	1193204	49.64
2		15.915	27638695	959490	50.36



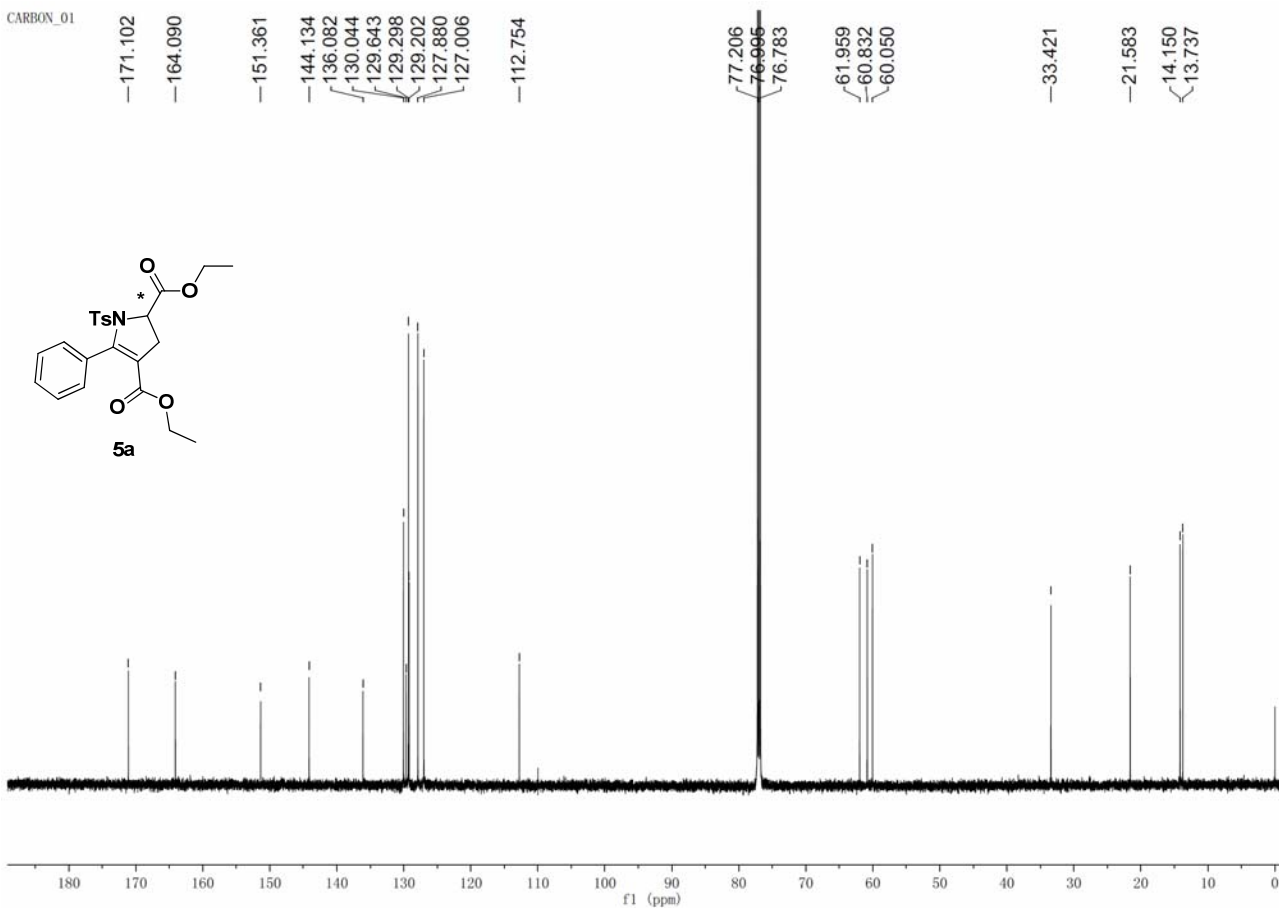
Peak Results

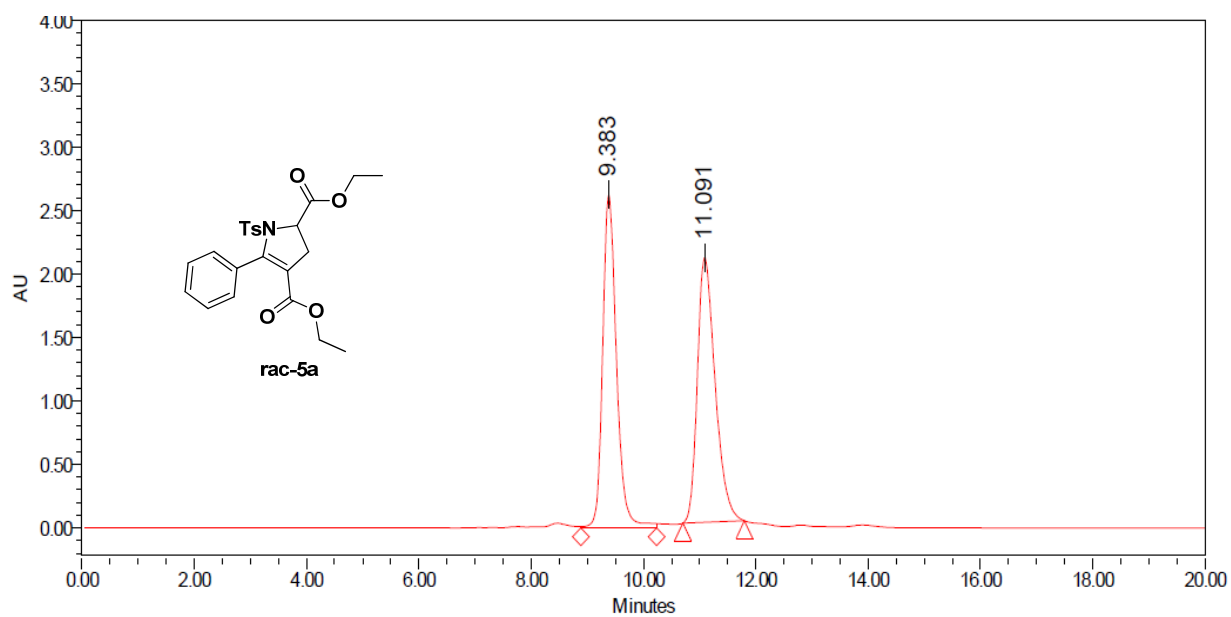
	Name	RT	Area	Height	% Area
1		14.658	4087543	183006	5.73
2		15.888	67268180	2194360	94.27

PROTON_01



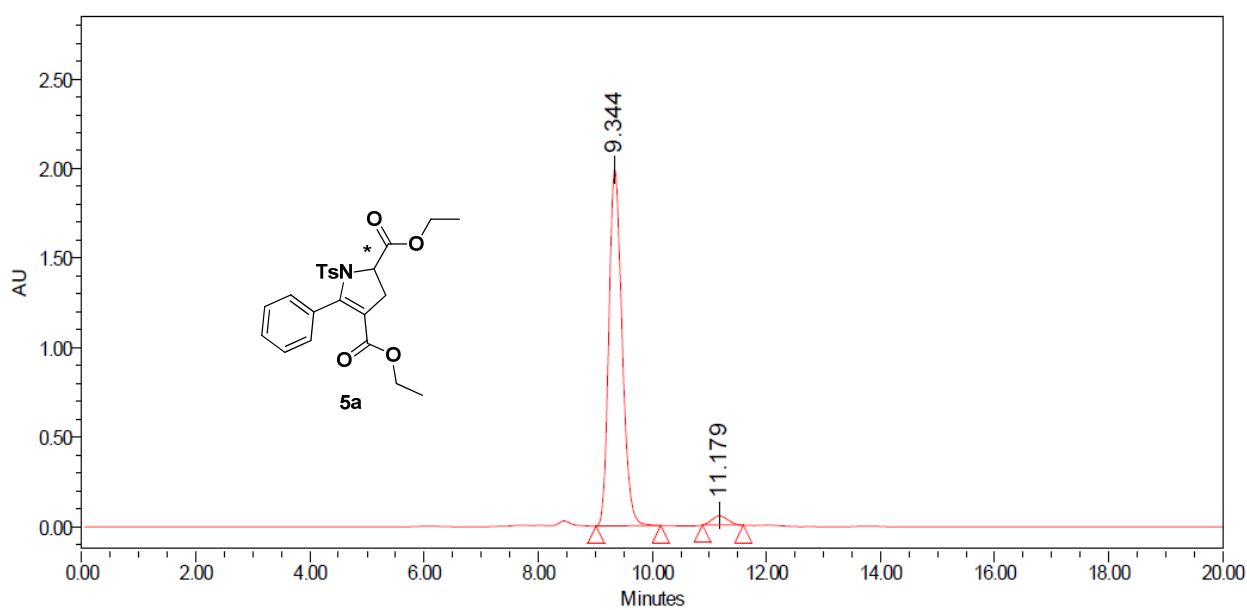
CARBON_01





Peak Results

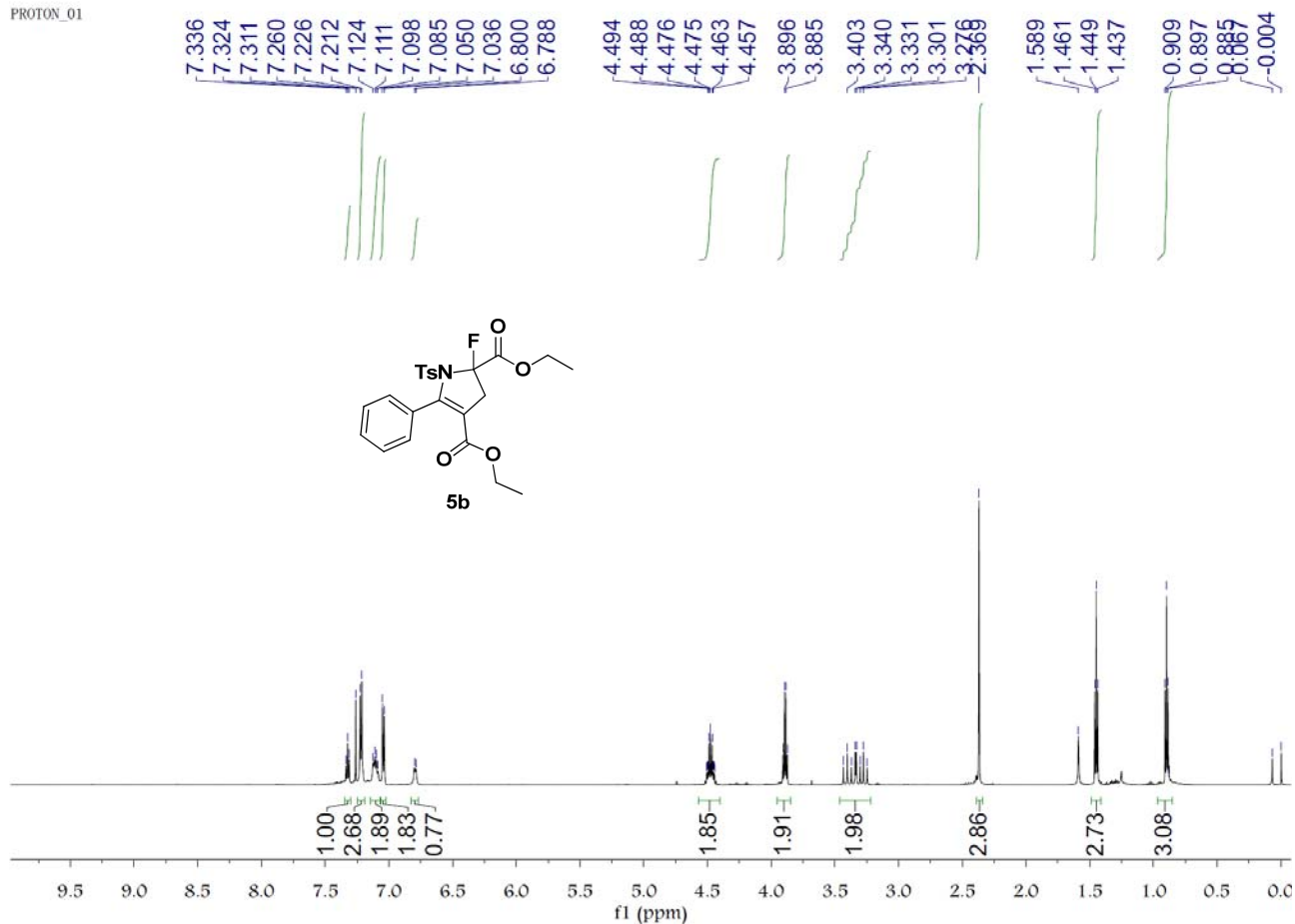
	Name	RT	Area	Height	%Area
1		9.383	44913115	2627916	49.51
2		11.091	45806541	2089565	50.49



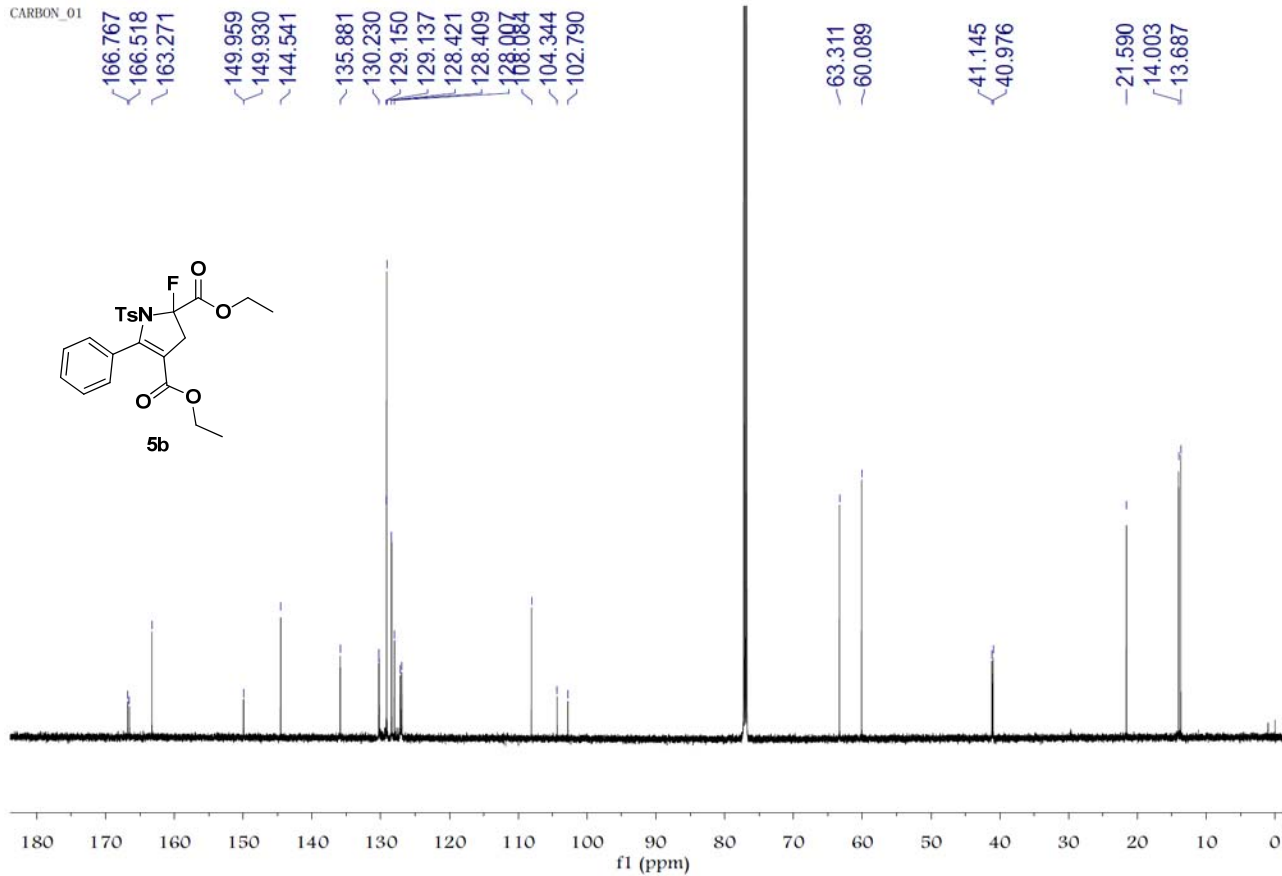
Peak Results

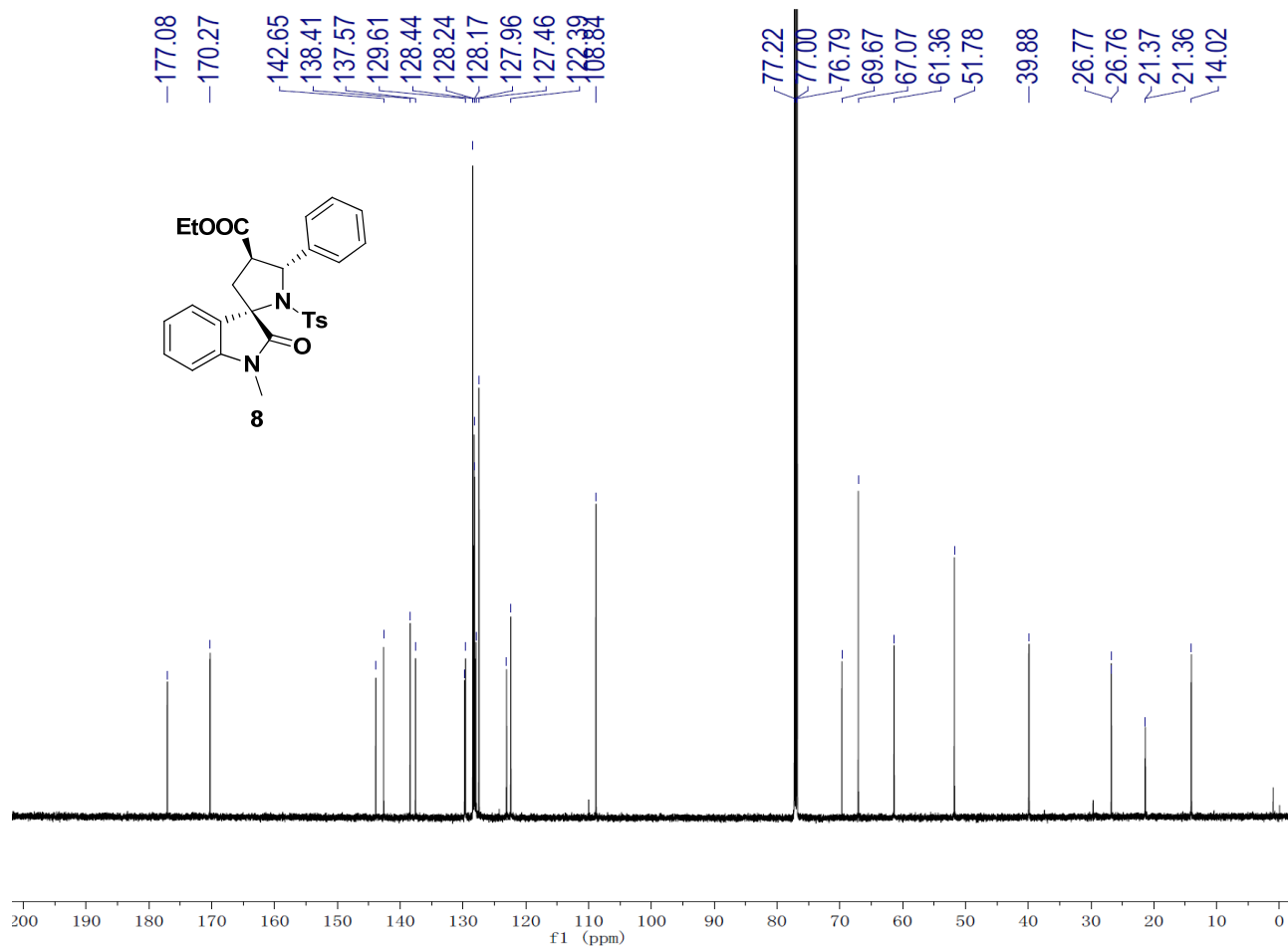
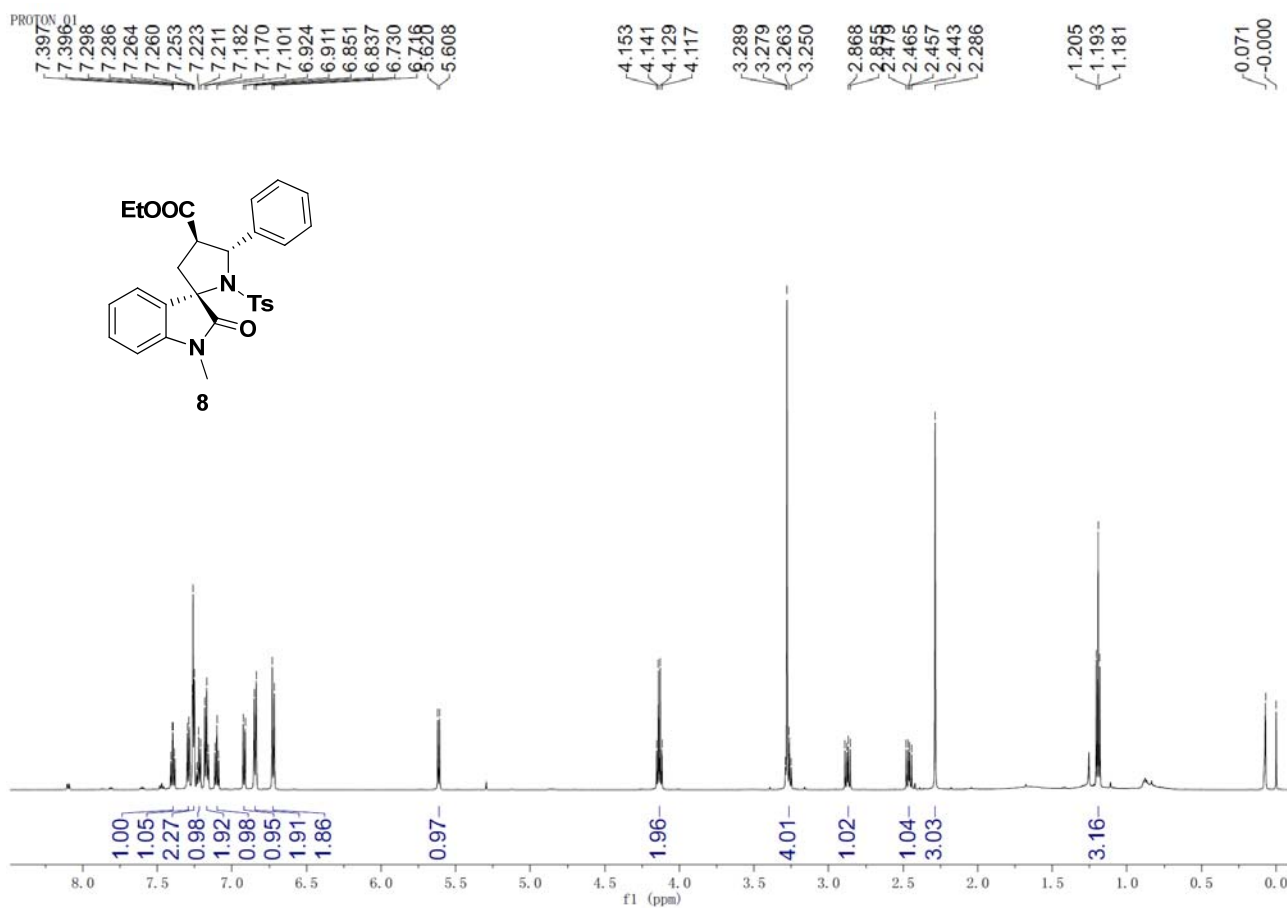
	Name	RT	Area	Height	%Area
1		9.344	31950565	1990683	96.99
2		11.179	989913	50988	3.01

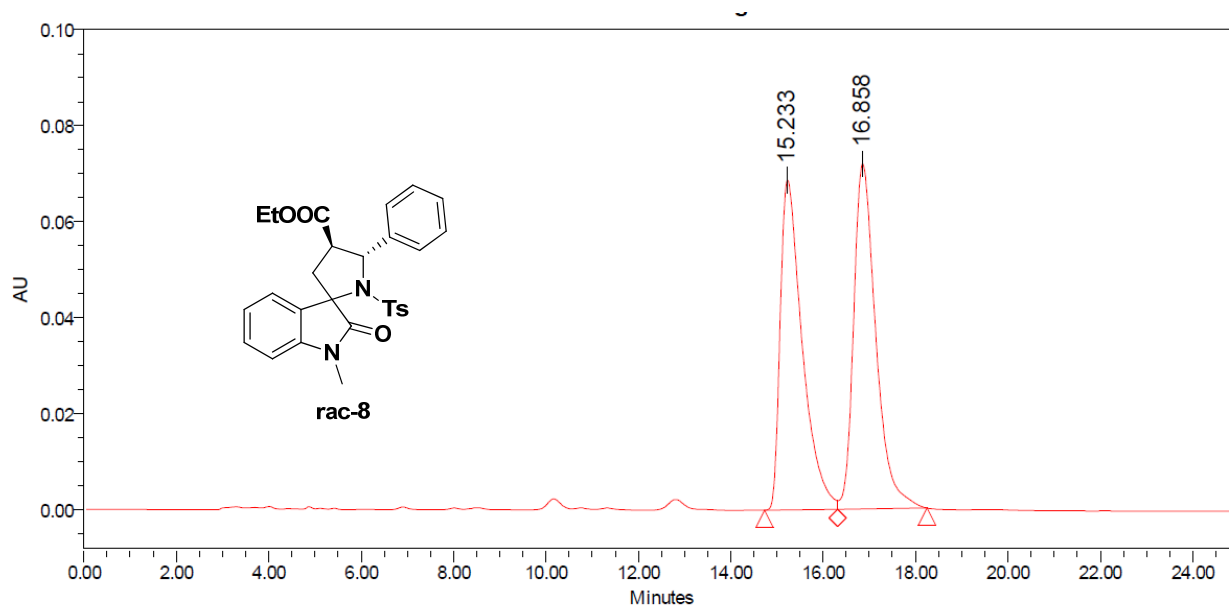
PROTON_01



CARBON_01

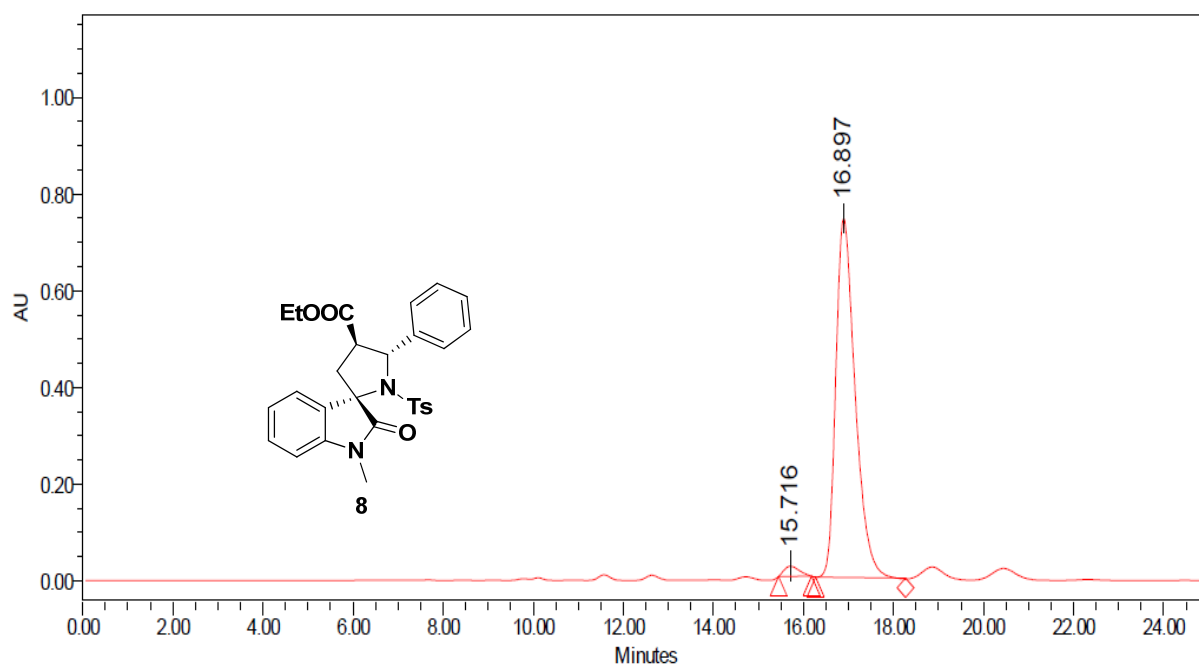






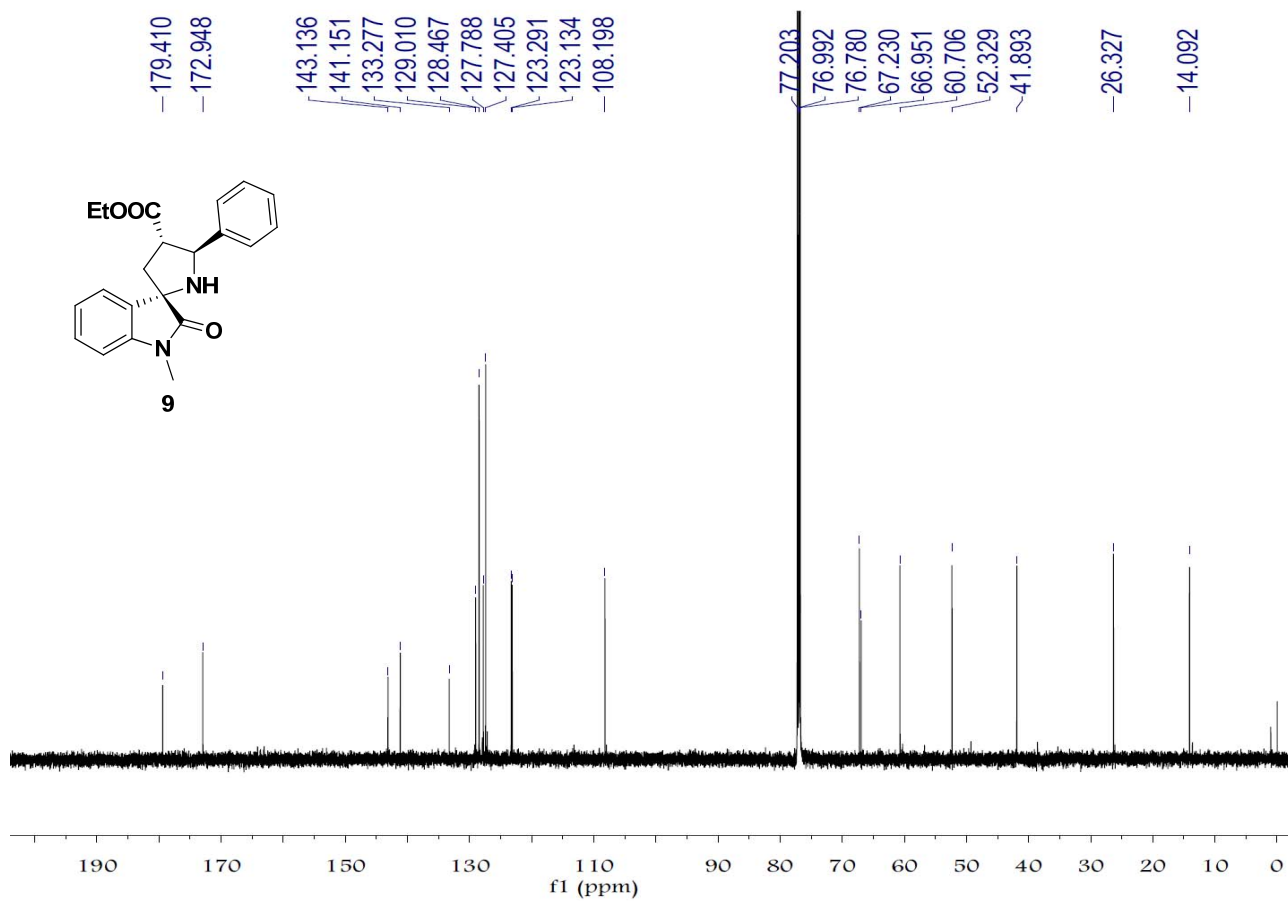
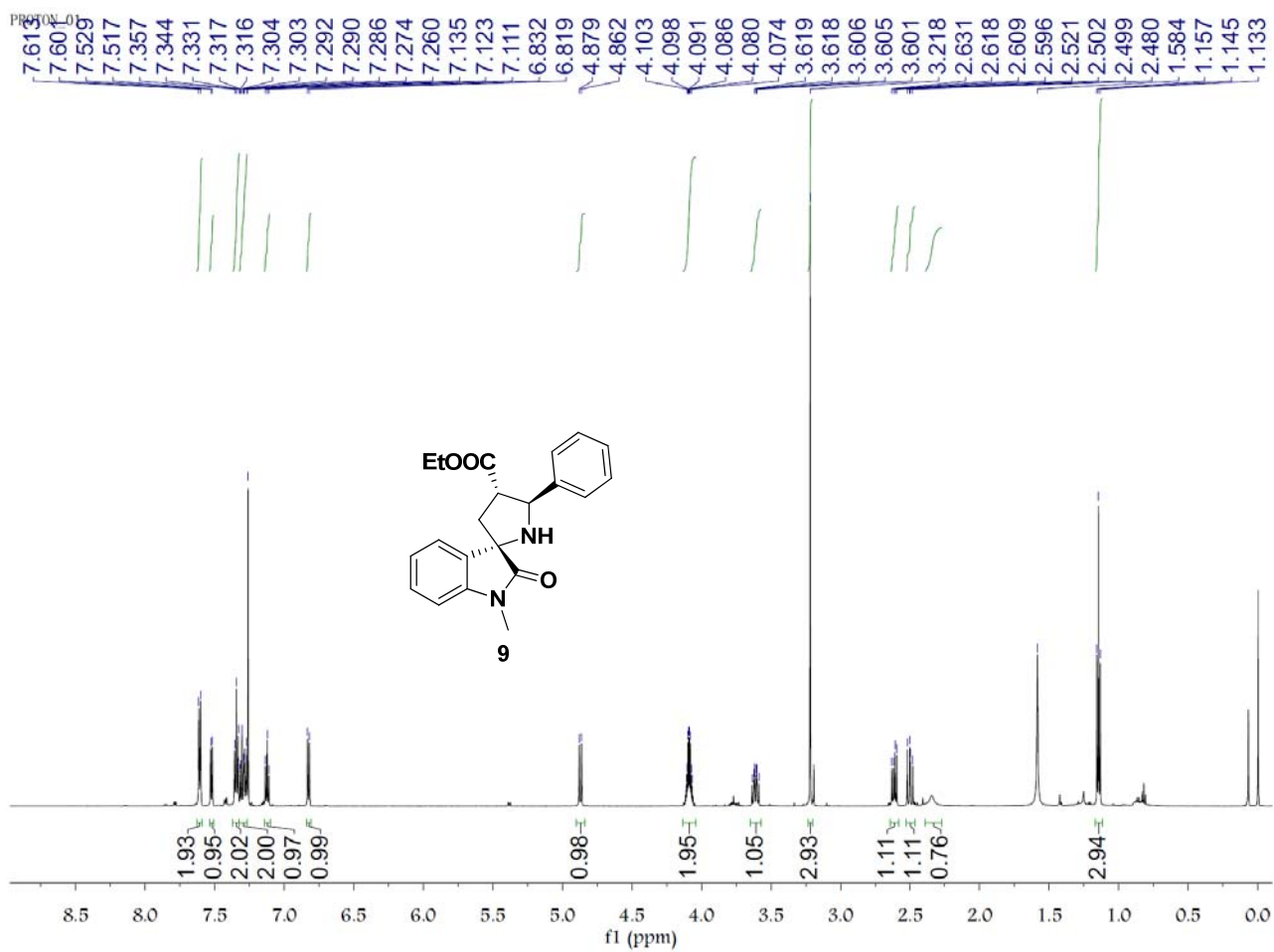
Peak Results

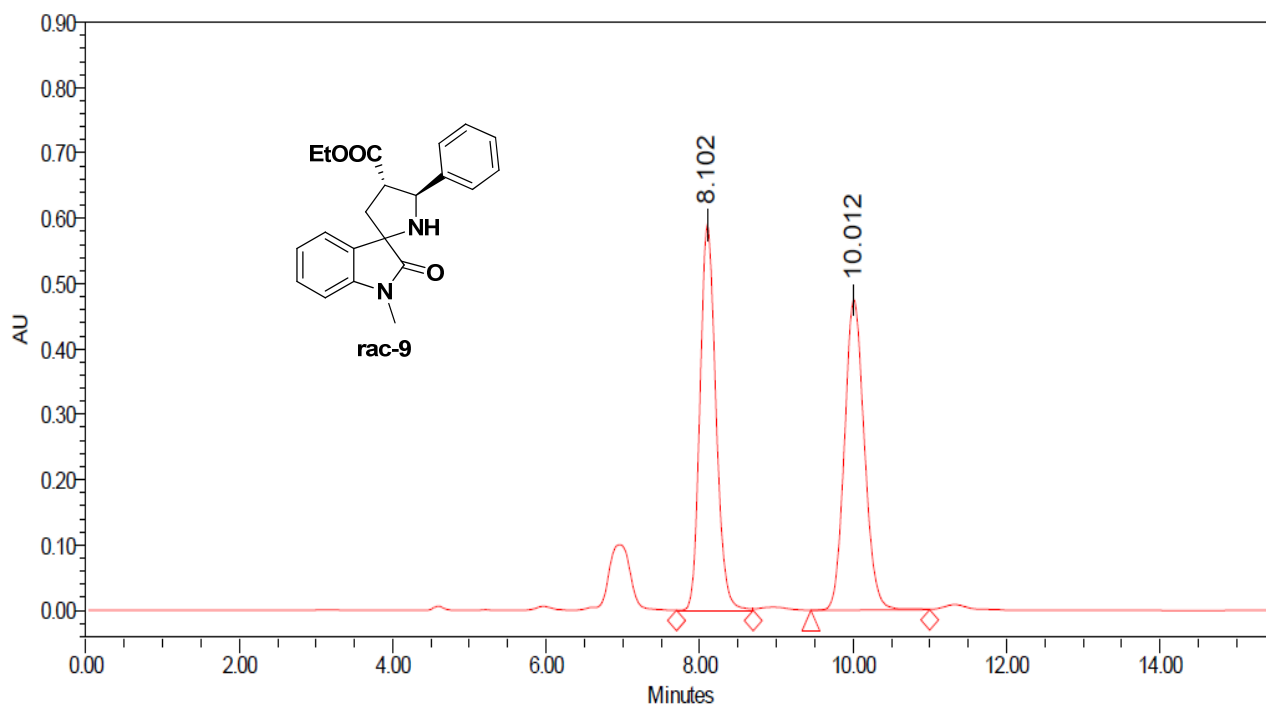
	Name	RT	Area	Height	% Area
1		15.233	2277694	68765	48.65
2		16.858	2404563	72011	51.35



Peak Results

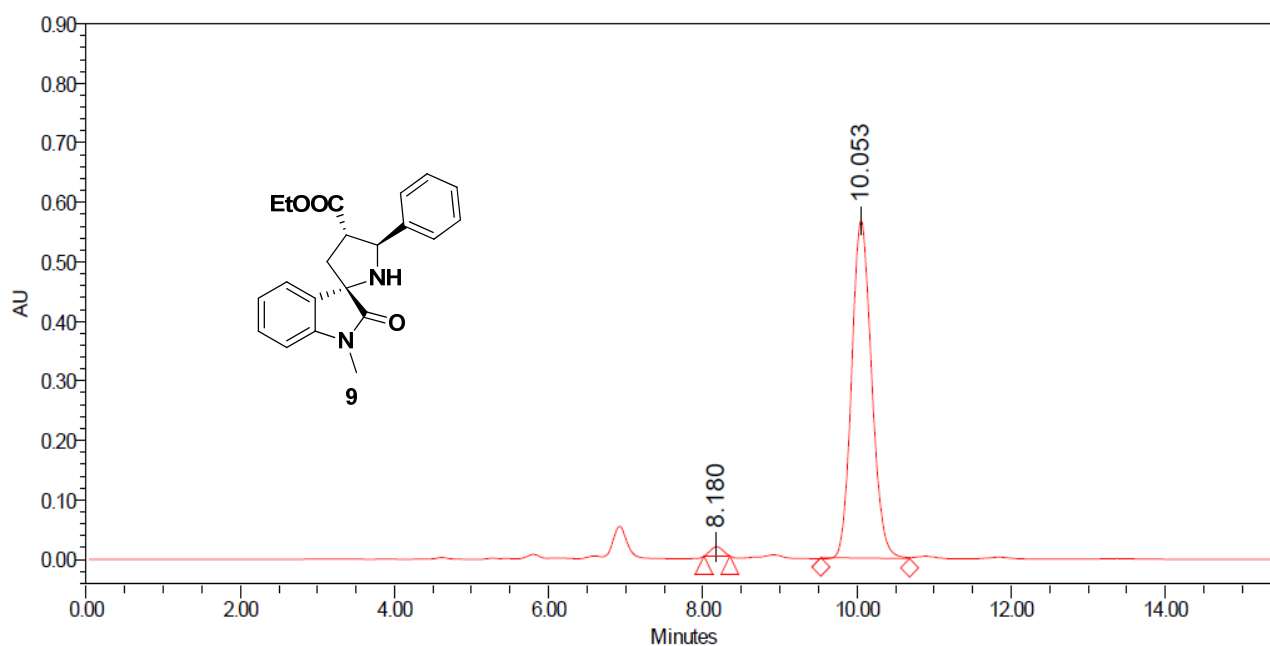
	Name	RT	Area	Height	% Area
1		15.716	495243	21139	2.19
2		16.897	22102060	742028	97.81





Peak Results

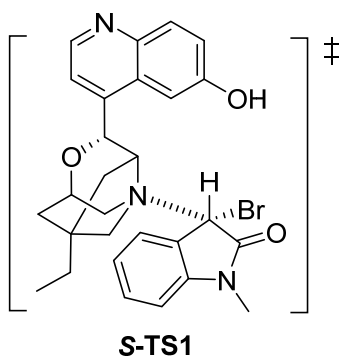
	Name	RT	Area	Height	% Area
1		8.102	8495909	590655	49.80
2		10.012	8562664	474802	50.20



Peak Results

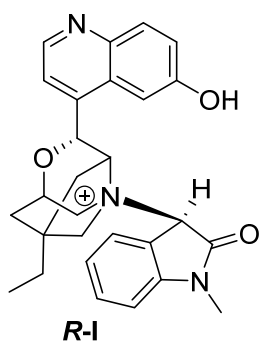
	Name	RT	Area	Height	% Area
1		8.180	175319	15720	1.69
2		10.053	10201003	567454	98.31

11. Computational Data



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.143455	1.380414	0.897483
2	6	0	5.424976	0.969298	0.462372
3	6	0	3.082970	0.524013	0.754147
4	6	0	3.309751	-0.768287	0.189059
5	6	0	4.633122	-1.053366	-0.241752
6	7	0	5.673097	-0.188265	-0.099063
7	6	0	2.295162	-1.749614	0.025648
8	6	0	2.579064	-2.944495	-0.597964
9	6	0	3.899525	-3.223828	-1.042303
10	6	0	4.894741	-2.307948	-0.856194
11	8	0	1.662195	-3.907512	-0.815715
12	6	0	0.838657	1.092783	-0.143784
13	8	0	1.662093	2.152296	1.838850
14	6	0	-1.091530	2.350223	-0.648481
15	6	0	-0.720288	1.728523	1.640363
16	7	0	-0.618144	1.260695	0.233921
17	6	0	1.229146	2.367011	-0.925604
18	6	0	0.369987	2.773730	1.868195
19	6	0	0.081863	3.340466	-0.623863
20	6	0	-0.044621	4.508845	-1.605558
21	6	0	0.251302	3.879530	0.809817
22	6	0	-0.421590	4.136762	-3.040484
23	6	0	1.678997	0.920877	1.122199
24	6	0	-4.907814	0.569288	-1.525949
25	6	0	-5.588263	0.345088	-0.330313
26	6	0	-4.938121	-0.151889	0.802123
27	6	0	-3.580896	-0.405841	0.696678
28	6	0	-2.881512	-0.175466	-0.499994
29	6	0	-3.541551	0.302039	-1.620244
30	7	0	-2.717106	-0.907972	1.666199
31	6	0	-1.439249	-1.062680	1.171234
32	6	0	-1.487149	-0.541470	-0.249452

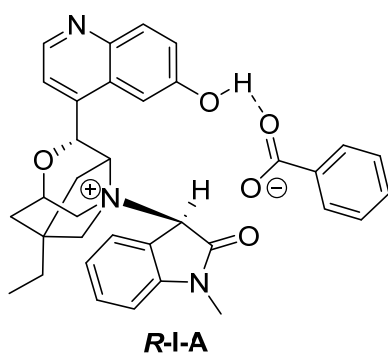
33	8	0	-0.471427	-1.396853	1.828318
34	6	0	-3.120192	-1.411585	2.959299
35	1	0	3.997735	2.357072	1.337678
36	1	0	6.268466	1.642480	0.578608
37	1	0	1.304271	-1.609434	0.439442
38	1	0	4.082411	-4.177773	-1.518801
39	1	0	5.910964	-2.498924	-1.174815
40	1	0	0.756450	-3.587821	-0.638237
41	1	0	0.941084	0.208840	-0.767416
42	1	0	-2.046234	2.740382	-0.294217
43	1	0	-1.231686	1.944291	-1.652767
44	1	0	-1.714859	2.150738	1.786082
45	1	0	-0.594434	0.893164	2.324584
46	1	0	1.285295	2.150729	-1.993153
47	1	0	2.198169	2.748003	-0.603383
48	1	0	0.266391	3.206821	2.864054
49	1	0	0.908692	5.046478	-1.605955
50	1	0	-0.790403	5.208719	-1.215046
51	1	0	1.143113	4.509369	0.862309
52	1	0	-0.611695	4.506590	1.062019
53	1	0	0.269057	3.410303	-3.471797
54	1	0	-0.398423	5.024333	-3.673726
55	1	0	-1.430063	3.722966	-3.098059
56	1	0	1.248540	0.124894	1.733770
57	1	0	-5.445090	0.937396	-2.389384
58	1	0	-6.649904	0.549668	-0.277241
59	1	0	-5.479570	-0.341512	1.719221
60	1	0	-3.013303	0.437468	-2.555443
61	1	0	-2.221652	-1.762607	3.460745
62	1	0	-3.819035	-2.241294	2.839590
63	1	0	-3.585343	-0.620854	3.550046
64	1	0	-0.708339	-0.658434	-0.974064
65	35	0	-1.706516	-2.980321	-0.821536



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-3.382778	1.469762	-1.343868
2	6	0	-4.764901	1.555977	-1.059179
3	6	0	-2.656404	0.408586	-0.861279
4	6	0	-3.336673	-0.598457	-0.117337
5	6	0	-4.723675	-0.392240	0.125270
6	7	0	-5.416870	0.677718	-0.339460
7	6	0	-2.719389	-1.774948	0.376102
8	6	0	-3.455237	-2.693046	1.087335
9	6	0	-4.828792	-2.477903	1.361160
10	6	0	-5.441585	-1.355266	0.884921
11	8	0	-2.924914	-3.846707	1.562622
12	6	0	-0.409660	0.634493	0.215024
13	8	0	-0.813203	1.306588	-2.075337
14	6	0	1.638932	1.867023	0.662659
15	6	0	1.444912	0.709225	-1.469355
16	7	0	1.153516	0.594120	0.003735
17	6	0	-0.681217	2.069716	0.698536
18	6	0	0.524763	1.784175	-2.033209
19	6	0	0.562032	2.872108	0.295851
20	6	0	0.700641	4.219673	1.015409
21	6	0	0.619210	3.085629	-1.227063
22	6	0	0.884521	4.161745	2.532618
23	6	0	-1.158025	0.335601	-1.097355
24	6	0	5.654986	-0.028763	0.978528
25	6	0	6.047194	-1.106345	0.189564
26	6	0	5.107108	-1.954735	-0.398285
27	6	0	3.771160	-1.664584	-0.186073
28	6	0	3.352813	-0.562082	0.568346
29	6	0	4.301006	0.243122	1.184163
30	7	0	2.661111	-2.411365	-0.617755
31	6	0	1.500952	-1.888132	-0.151606
32	6	0	1.843106	-0.594979	0.629380
33	8	0	0.381868	-2.328518	-0.328726
34	6	0	2.737620	-3.654386	-1.365439
35	1	0	-2.908225	2.233501	-1.942325
36	1	0	-5.336441	2.394873	-1.441098
37	1	0	-1.681299	-1.986443	0.161408
38	1	0	-5.363102	-3.226589	1.930024
39	1	0	-6.492151	-1.163681	1.056061
40	1	0	-2.012916	-3.931878	1.256249
41	1	0	-0.641707	-0.130512	0.952100
42	1	0	2.636322	2.097509	0.293540
43	1	0	1.668608	1.682900	1.737398
44	1	0	2.499720	0.956360	-1.581063
45	1	0	1.244006	-0.249200	-1.943941

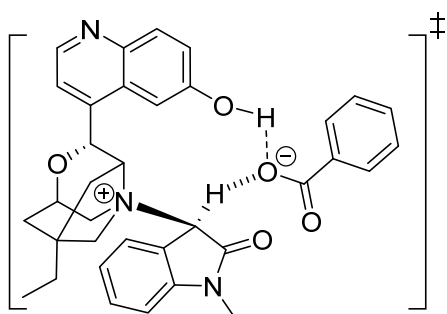
46	1	0	-0.808589	2.083854	1.780955
47	1	0	-1.592678	2.457552	0.247139
48	1	0	0.810689	1.973825	-3.067712
49	1	0	-0.192495	4.803766	0.777476
50	1	0	1.544272	4.759021	0.574841
51	1	0	-0.196816	3.736815	-1.546750
52	1	0	1.559093	3.589559	-1.475511
53	1	0	0.074466	3.628054	3.031692
54	1	0	0.898082	5.173803	2.936403
55	1	0	1.830726	3.694422	2.814169
56	1	0	-0.897740	-0.664452	-1.450651
57	1	0	6.402632	0.595536	1.447700
58	1	0	7.100360	-1.305761	0.043419
59	1	0	5.415328	-2.811295	-0.982201
60	1	0	4.014475	1.062126	1.830427
61	1	0	1.720959	-4.001928	-1.528239
62	1	0	3.294824	-4.398968	-0.796523
63	1	0	3.226104	-3.483013	-2.324333
64	1	0	1.453454	-0.669802	1.646333



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.258466	-3.820086	0.690660
2	6	0	3.656468	-4.038230	0.664871
3	6	0	1.723677	-2.799545	-0.053584
4	6	0	2.604697	-1.994793	-0.835829
5	6	0	3.996692	-2.275690	-0.741784
6	7	0	4.505439	-3.300679	-0.006132
7	6	0	2.173405	-0.918480	-1.643061
8	6	0	3.088075	-0.064771	-2.215714
9	6	0	4.474913	-0.347235	-2.136091
10	6	0	4.910031	-1.438224	-1.434461
11	8	0	2.693439	1.056287	-2.859774
12	6	0	-0.042544	-1.112934	0.533391

13	8	0	-0.404140	-3.490733	0.790597
14	6	0	-1.859198	-0.235144	1.862180
15	6	0	-2.335958	-2.103867	0.387154
16	7	0	-1.579977	-0.811828	0.491030
17	6	0	0.336031	-1.015866	2.017630
18	6	0	-1.667041	-3.104524	1.320402
19	6	0	-0.996876	-1.099625	2.770079
20	6	0	-0.916771	-0.575759	4.208491
21	6	0	-1.536035	-2.538041	2.740779
22	6	0	-0.748098	0.941265	4.333260
23	6	0	0.236442	-2.511130	-0.030155
24	6	0	-5.151523	2.179687	0.223369
25	6	0	-5.864340	1.820683	-0.916053
26	6	0	-5.307518	0.980051	-1.881978
27	6	0	-4.034067	0.492495	-1.641673
28	6	0	-3.319422	0.798651	-0.476358
29	6	0	-3.862174	1.685582	0.439868
30	7	0	-3.253402	-0.300997	-2.491076
31	6	0	-2.014473	-0.528875	-1.960953
32	6	0	-1.951728	0.173878	-0.595364
33	8	0	-1.138603	-1.193451	-2.479427
34	6	0	-3.647843	-0.747870	-3.808992
35	1	0	1.620702	-4.449767	1.293316
36	1	0	4.075704	-4.855370	1.243703
37	1	0	1.126562	-0.725984	-1.822139
38	1	0	5.164442	0.327163	-2.626676
39	1	0	5.961277	-1.680468	-1.351869
40	1	0	1.873694	1.371955	-2.406251
41	1	0	0.420311	-0.326936	-0.053832
42	1	0	-2.930882	-0.284411	2.051495
43	1	0	-1.491846	0.788006	1.832764
44	1	0	-3.373130	-1.904364	0.656131
45	1	0	-2.288189	-2.465160	-0.637185
46	1	0	0.812623	-0.053654	2.194316
47	1	0	1.018817	-1.818750	2.297529
48	1	0	-2.272611	-4.011520	1.345574
49	1	0	-0.078944	-1.085988	4.692821
50	1	0	-1.817657	-0.882980	4.749257
51	1	0	-0.879811	-3.200799	3.309908
52	1	0	-2.523292	-2.558288	3.216620
53	1	0	0.029287	1.329622	3.673607
54	1	0	-0.490646	1.206423	5.359187
55	1	0	-1.674376	1.463273	4.083527
56	1	0	-0.141042	-2.577903	-1.051772
57	1	0	-5.588109	2.863247	0.938920
58	1	0	-6.858771	2.218129	-1.072805

59	1	0	-5.844512	0.735441	-2.788577
60	1	0	-3.291176	2.013956	1.297351
61	1	0	-2.814116	-1.311259	-4.220705
62	1	0	-3.864139	0.108243	-4.449750
63	1	0	-4.529858	-1.386864	-3.744966
64	1	0	-1.146293	0.920043	-0.615226
65	6	0	3.666244	4.661429	-0.362003
66	6	0	2.748486	3.648721	-0.624192
67	6	0	1.729030	3.377344	0.287492
68	6	0	1.636800	4.126609	1.460841
69	6	0	2.548793	5.143170	1.719278
70	6	0	3.566273	5.411935	0.806300
71	1	0	4.460151	4.863983	-1.070280
72	1	0	2.830751	3.056894	-1.524911
73	1	0	0.839154	3.893393	2.153259
74	1	0	2.469597	5.724811	2.629741
75	1	0	4.280312	6.201712	1.006308
76	6	0	0.717298	2.282924	0.033434
77	8	0	0.710026	1.710464	-1.097367
78	8	0	-0.071430	2.000717	0.971898

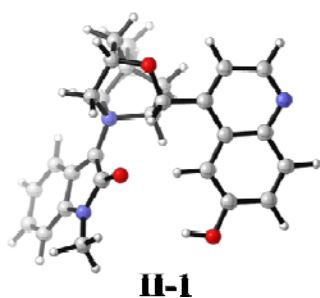


R-TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.572583	-2.913048	-0.197435
2	6	0	4.932662	-2.521306	-0.147687
3	6	0	2.638755	-2.022295	-0.657650
4	6	0	3.078215	-0.734180	-1.084321
5	6	0	4.456453	-0.431067	-0.928969
6	7	0	5.371615	-1.331616	-0.477223
7	6	0	2.203705	0.257598	-1.588908
8	6	0	2.651845	1.540706	-1.789353
9	6	0	4.025851	1.853041	-1.635296
10	6	0	4.904102	0.881091	-1.239647
11	8	0	1.804183	2.539860	-2.137716
12	6	0	0.427752	-1.407223	0.296314

13	8	0	0.951087	-3.688196	-0.258371
14	6	0	-1.567552	-1.665207	1.595671
15	6	0	-1.358953	-2.970042	-0.440889
16	7	0	-1.110686	-1.609094	0.160148
17	6	0	0.758668	-1.733741	1.759893
18	6	0	-0.380681	-3.955329	0.185054
19	6	0	-0.475669	-2.483235	2.274529
20	6	0	-0.593047	-2.500732	3.802716
21	6	0	-0.484328	-3.914279	1.715040
22	6	0	-0.922151	-1.150719	4.444772
23	6	0	1.163099	-2.338852	-0.670449
24	6	0	-5.262116	0.646329	0.655856
25	6	0	-5.786042	0.939893	-0.599014
26	6	0	-5.025286	0.730562	-1.747853
27	6	0	-3.755563	0.197988	-1.593030
28	6	0	-3.203745	-0.128141	-0.335564
29	6	0	-3.970209	0.135517	0.797395
30	7	0	-2.831725	-0.079926	-2.595400
31	6	0	-1.682762	-0.616177	-2.068034
32	6	0	-1.793557	-0.516326	-0.597498
33	8	0	-0.738023	-1.032750	-2.742473
34	6	0	-3.035703	0.129580	-4.009288
35	1	0	3.271511	-3.897372	0.131591
36	1	0	5.675716	-3.230750	0.202763
37	1	0	1.175845	0.025807	-1.834505
38	1	0	4.346971	2.867854	-1.828910
39	1	0	5.959511	1.085127	-1.117221
40	1	0	0.915220	2.294602	-1.820444
41	1	0	0.606079	-0.366395	0.069598
42	1	0	-2.568789	-2.093150	1.630522
43	1	0	-1.556852	-0.638632	1.952550
44	1	0	-2.396589	-3.228339	-0.230764
45	1	0	-1.210234	-2.900595	-1.514107
46	1	0	0.898665	-0.803438	2.306576
47	1	0	1.665419	-2.334995	1.830645
48	1	0	-0.622803	-4.957923	-0.170652
49	1	0	0.354288	-2.880088	4.197336
50	1	0	-1.358517	-3.228999	4.089569
51	1	0	0.348012	-4.485310	2.133757
52	1	0	-1.413655	-4.412306	2.014141
53	1	0	-0.275765	-0.349968	4.082780
54	1	0	-0.809619	-1.214122	5.527705
55	1	0	-1.953390	-0.854855	4.240743
56	1	0	0.783091	-2.189274	-1.682179
57	1	0	-5.853821	0.833585	1.542426
58	1	0	-6.784900	1.347031	-0.686551

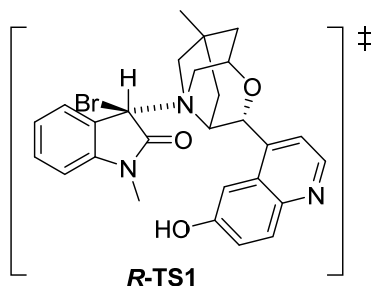
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62	1	0	-3.209459	1.186583	-4.217234
63	1	0	-3.888189	-0.452969	-4.363781
64	1	0	-1.075653	0.695963	-0.450094
65	6	0	0.735785	5.691555	0.408216
66	6	0	0.272187	4.414424	0.112573
67	6	0	0.241821	3.439247	1.108613
68	6	0	0.669898	3.747169	2.400200
69	6	0	1.138300	5.021595	2.692501
70	6	0	1.171430	5.994278	1.695439
71	1	0	0.758872	6.448503	-0.365279
72	1	0	-0.073223	4.173532	-0.882439
73	1	0	0.626598	2.974110	3.155510
74	1	0	1.476377	5.258412	3.693315
75	1	0	1.536093	6.988472	1.922165
76	6	0	-0.256657	2.055362	0.836117
77	8	0	-0.469703	1.759367	-0.420656
78	8	0	-0.442516	1.258488	1.756601



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.682184	1.537474	0.480341
2	6	0	4.942923	1.338420	-0.131507
3	6	0	2.771214	0.512044	0.491528
4	6	0	3.150831	-0.735418	-0.082382
5	6	0	4.435957	-0.815255	-0.683086
6	7	0	5.315258	0.222331	-0.707942
7	6	0	2.316979	-1.877825	-0.061742
8	6	0	2.748480	-3.050494	-0.629981
9	6	0	4.014775	-3.135923	-1.259189
10	6	0	4.834586	-2.041582	-1.278341
11	8	0	1.991047	-4.178308	-0.609767

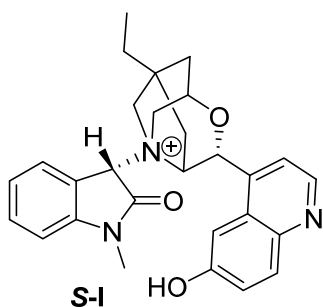
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14	6	0	-1.704564	2.057939	-0.210333
15	6	0	-0.988213	1.265697	1.976521
16	7	0	-1.098744	0.895024	0.517823
17	6	0	0.538650	2.151854	-0.816611
18	6	0	0.053707	2.368711	2.115278
19	6	0	-0.569630	3.065617	-0.272726
20	6	0	-0.871134	4.283886	-1.152836
21	6	0	-0.249025	3.528777	1.159078
22	6	0	-1.429387	3.988261	-2.545824
23	6	0	1.386486	0.684002	1.071451
24	6	0	-5.409472	-0.283333	-1.230492
25	6	0	-5.665786	-1.638493	-1.030147
26	6	0	-4.712562	-2.440302	-0.407118
27	6	0	-3.521515	-1.857467	-0.003032
28	6	0	-3.221306	-0.475553	-0.204334
29	6	0	-4.210231	0.301167	-0.828703
30	7	0	-2.462255	-2.458820	0.642754
31	6	0	-1.455753	-1.530179	0.891950
32	6	0	-1.901818	-0.310504	0.343442
33	8	0	-0.390086	-1.813399	1.501333
34	6	0	-2.393803	-3.833834	1.063795
35	1	0	3.441495	2.485390	0.940511
36	1	0	5.661081	2.152230	-0.143025
37	1	0	1.352885	-1.856819	0.436574
38	1	0	4.310379	-4.078811	-1.699658
39	1	0	5.814520	-2.074267	-1.735601
40	1	0	1.181252	-3.988230	-0.114327
41	1	0	0.366854	-0.055552	-0.702092
42	1	0	-2.598487	2.381657	0.322023
43	1	0	-1.970784	1.696928	-1.201327
44	1	0	-1.978532	1.587849	2.294502
45	1	0	-0.712127	0.360240	2.512225
46	1	0	0.405768	1.995055	-1.887229
47	1	0	1.534587	2.561439	-0.654082
48	1	0	0.050159	2.730667	3.144348
49	1	0	0.055786	4.858222	-1.243979
50	1	0	-1.577560	4.926915	-0.618310
51	1	0	0.614553	4.198273	1.151997
52	1	0	-1.104873	4.094073	1.544463
53	1	0	-0.774111	3.334609	-3.123336
54	1	0	-1.536379	4.918177	-3.105230
55	1	0	-2.416075	3.523199	-2.498351
56	1	0	1.131771	-0.189905	1.671498
57	1	0	-6.156094	0.337342	-1.710179

58	1	0	-6.604272	-2.068770	-1.354183
59	1	0	-4.892649	-3.494595	-0.236951
60	1	0	-4.077714	1.358337	-1.009723
61	1	0	-1.463801	-3.948294	1.617248
62	1	0	-2.399666	-4.510765	0.205994
63	1	0	-3.234407	-4.081295	1.715758



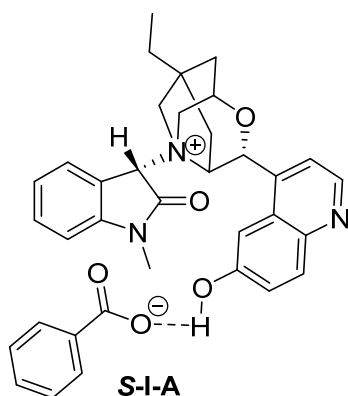
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.033450	1.548365	-0.927292
2	6	0	-5.345454	1.190328	-0.541342
3	6	0	-3.021814	0.633163	-0.793949
4	6	0	-3.327494	-0.664046	-0.281666
5	6	0	-4.681026	-0.902930	0.082562
6	7	0	-5.670263	0.020437	-0.049240
7	6	0	-2.376034	-1.703450	-0.117515
8	6	0	-2.745455	-2.918663	0.415176
9	6	0	-4.097901	-3.152841	0.782008
10	6	0	-5.032717	-2.172998	0.614089
11	8	0	-1.888181	-3.934864	0.614873
12	6	0	-0.725841	1.108099	0.078594
13	8	0	-1.555559	2.189681	-1.899463
14	6	0	1.262358	2.304331	0.537442
15	6	0	0.812465	1.710199	-1.742564
16	7	0	0.726494	1.241898	-0.343493
17	6	0	-1.048888	2.387720	0.879080
18	6	0	-0.251090	2.782898	-1.946860
19	6	0	0.116577	3.330109	0.545067
20	6	0	0.304781	4.491465	1.524819
21	6	0	-0.078846	3.877547	-0.882747
22	6	0	0.707916	4.101936	2.947980
23	6	0	-1.602274	0.973333	-1.164620
24	6	0	4.629723	-0.360748	-2.327023
25	6	0	5.472481	-0.221554	-1.225853
26	6	0	4.981389	-0.252441	0.081779
27	6	0	3.616026	-0.416955	0.246713

28	6	0	2.755181	-0.544701	-0.855596
29	6	0	3.256701	-0.532431	-2.146183
30	7	0	2.890588	-0.486341	1.432112
31	6	0	1.542647	-0.672859	1.195345
32	6	0	1.401382	-0.690142	-0.314892
33	8	0	0.675365	-0.676446	2.043420
34	6	0	3.461122	-0.497982	2.759074
35	1	0	-3.827363	2.528608	-1.333446
36	1	0	-6.148315	1.912875	-0.646569
37	1	0	-1.340798	-1.579539	-0.398273
38	1	0	-4.350859	-4.121395	1.192104
39	1	0	-6.069891	-2.324453	0.881967
40	1	0	-0.970411	-3.671800	0.403185
41	1	0	-0.810753	0.228794	0.710474
42	1	0	2.217591	2.666887	0.154398
43	1	0	1.404191	1.888347	1.536047
44	1	0	1.814246	2.101109	-1.917209
45	1	0	0.659464	0.875087	-2.427156
46	1	0	-1.067368	2.154580	1.943982
47	1	0	-2.016828	2.803421	0.598156
48	1	0	-0.159775	3.221716	-2.941224
49	1	0	-0.631608	5.057566	1.552276
50	1	0	1.060601	5.170167	1.116111
51	1	0	-0.956598	4.528560	-0.909993
52	1	0	0.790875	4.485944	-1.156633
53	1	0	0.006281	3.396457	3.395360
54	1	0	0.732650	4.987859	3.583586
55	1	0	1.702384	3.652724	2.976220
56	1	0	-1.227533	0.154662	-1.792151
57	1	0	5.043813	-0.352101	-3.326057
58	1	0	6.536201	-0.097206	-1.383482
59	1	0	5.646824	-0.162799	0.930013
60	1	0	2.600017	-0.679855	-2.994229
61	1	0	2.635889	-0.589443	3.461174
62	1	0	4.005210	0.428734	2.951040
63	1	0	4.134921	-1.348574	2.874617
64	1	0	0.509140	-0.904391	-0.863152
65	35	0	1.396637	-3.168000	-0.172777



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.655313	1.874922	-0.650419
2	6	0	-5.005428	1.690057	-0.271484
3	6	0	-2.824044	0.786492	-0.726408
4	6	0	-3.349968	-0.503880	-0.425369
5	6	0	-4.716262	-0.561859	-0.034683
6	7	0	-5.523803	0.527308	0.033153
7	6	0	-2.602478	-1.708221	-0.469372
8	6	0	-3.170881	-2.895938	-0.074038
9	6	0	-4.534073	-2.958000	0.307155
10	6	0	-5.283514	-1.817467	0.314106
11	8	0	-2.477067	-4.058317	-0.028493
12	6	0	-0.455809	0.592476	0.050400
13	8	0	-1.138867	2.299159	-1.498799
14	6	0	1.747929	1.360191	0.690537
15	6	0	1.134707	1.511598	-1.656485
16	7	0	1.035772	0.637707	-0.429314
17	6	0	-0.527040	1.609406	1.198793
18	6	0	0.224482	2.709361	-1.450054
19	6	0	0.744648	2.454701	1.055607
20	6	0	1.128118	3.241769	2.314023
21	6	0	0.584614	3.415057	-0.136269
22	6	0	1.521644	2.405495	3.532530
23	6	0	-1.372344	0.952846	-1.116534
24	6	0	5.250876	-0.341142	-2.000993
25	6	0	5.852127	-1.026333	-0.949258
26	6	0	5.093156	-1.590150	0.078450
27	6	0	3.721752	-1.418434	0.021893
28	6	0	3.099417	-0.699196	-1.005504
29	6	0	3.863708	-0.181862	-2.041435
30	7	0	2.761598	-1.953291	0.899314
31	6	0	1.500896	-1.684800	0.473309
32	6	0	1.613344	-0.724739	-0.745340
33	8	0	0.466120	-2.121790	0.939630
34	6	0	3.057756	-2.877873	1.980634

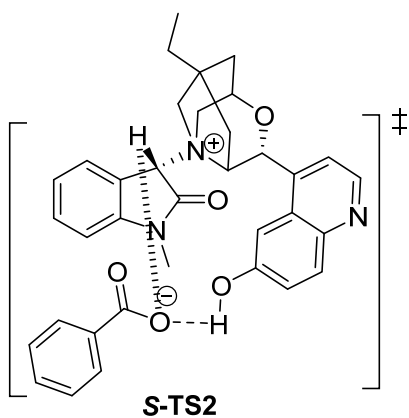
35	1	0	-3.289354	2.862879	-0.887544
36	1	0	-5.666851	2.547751	-0.218468
37	1	0	-1.573340	-1.723992	-0.803945
38	1	0	-4.944065	-3.917423	0.591549
39	1	0	-6.326926	-1.823639	0.599055
40	1	0	-1.531833	-3.870148	-0.099066
41	1	0	-0.637207	-0.417422	0.395316
42	1	0	2.720814	1.700546	0.338616
43	1	0	1.878271	0.651999	1.509546
44	1	0	2.173469	1.815071	-1.759457
45	1	0	0.839468	0.928241	-2.527074
46	1	0	-0.540399	1.084238	2.153591
47	1	0	-1.434943	2.208145	1.123745
48	1	0	0.361414	3.399289	-2.282723
49	1	0	0.276874	3.879998	2.566280
50	1	0	1.952255	3.915491	2.061799
51	1	0	-0.193780	4.148175	0.084778
52	1	0	1.520109	3.964468	-0.285828
53	1	0	0.747636	1.689311	3.813174
54	1	0	1.681013	3.059920	4.389154
55	1	0	2.453389	1.860198	3.368553
56	1	0	-1.172328	0.283142	-1.964606
57	1	0	5.858398	0.057274	-2.801581
58	1	0	6.927377	-1.144837	-0.934996
59	1	0	5.561884	-2.150916	0.875683
60	1	0	3.407310	0.314842	-2.887755
61	1	0	2.113049	-3.167505	2.432932
62	1	0	3.688581	-2.391080	2.723790
63	1	0	3.564413	-3.760805	1.589730
64	1	0	1.016736	-1.124546	-1.567767



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.125399	3.055593	-1.217465

2	6	0	3.548971	4.302310	-0.695260
3	6	0	1.993162	2.474336	-0.709786
4	6	0	1.266665	3.160099	0.305231
5	6	0	1.791417	4.398957	0.759462
6	7	0	2.928455	4.952718	0.259210
7	6	0	0.064379	2.662313	0.849669
8	6	0	-0.611287	3.368762	1.820066
9	6	0	-0.080586	4.599721	2.295311
10	6	0	1.083689	5.095689	1.776247
11	8	0	-1.772596	2.942016	2.342079
12	6	0	1.864073	0.068152	-0.118437
13	8	0	2.069038	0.771517	-2.407851
14	6	0	2.223035	-2.323401	-0.352621
15	6	0	0.744127	-1.215682	-1.926254
16	7	0	1.148988	-1.272511	-0.470298
17	6	0	3.357784	-0.286465	-0.148460
18	6	0	1.905241	-0.611948	-2.710832
19	6	0	3.442646	-1.610204	-0.929667
20	6	0	4.758668	-2.369975	-0.726445
21	6	0	3.206813	-1.370549	-2.429729
22	6	0	5.019233	-2.899436	0.684834
23	6	0	1.488861	1.129264	-1.160603
24	6	0	-2.579331	-4.030288	-0.979805
25	6	0	-2.508546	-4.939345	0.070537
26	6	0	-1.682229	-4.710278	1.173634
27	6	0	-0.910165	-3.562148	1.157548
28	6	0	-0.924990	-2.664694	0.083024
29	6	0	-1.801512	-2.868378	-0.970550
30	7	0	-0.066336	-3.087564	2.172053
31	6	0	0.490822	-1.886542	1.838107
32	6	0	-0.035800	-1.504085	0.439797
33	8	0	1.302374	-1.269799	2.502001
34	6	0	0.145809	-3.735068	3.447137
35	1	0	3.679205	2.578665	-2.014694
36	1	0	4.446058	4.766070	-1.092936
37	1	0	-0.381591	1.743475	0.500996
38	1	0	-0.631101	5.129405	3.061669
39	1	0	1.498932	6.036263	2.113688
40	1	0	-2.040199	2.107208	1.887516
41	1	0	1.521730	0.350816	0.871675
42	1	0	1.899937	-3.222031	-0.878468
43	1	0	2.377060	-2.539384	0.701112
44	1	0	0.545500	-2.236571	-2.246501
45	1	0	-0.167287	-0.624305	-1.992673
46	1	0	3.712701	-0.425429	0.872624
47	1	0	3.936745	0.509248	-0.615690

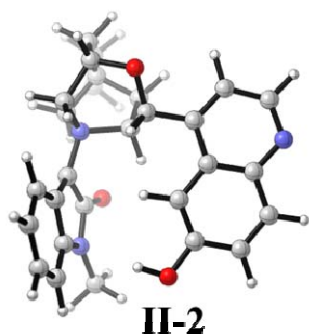
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49	1	0	5.568442	-1.695732	-1.020331
50	1	0	4.787367	-3.207430	-1.430511
51	1	0	4.034858	-0.796572	-2.851951
52	1	0	3.175771	-2.338335	-2.942493
53	1	0	4.947891	-2.115779	1.440261
54	1	0	6.023741	-3.319692	0.742202
55	1	0	4.320588	-3.693778	0.954268
56	1	0	0.401539	1.179756	-1.260518
57	1	0	-3.262015	-4.208037	-1.799623
58	1	0	-3.125804	-5.828272	0.051205
59	1	0	-1.664417	-5.393469	2.012240
60	1	0	-1.914672	-2.117039	-1.740243
61	1	0	0.826612	-3.108350	4.017702
62	1	0	0.585836	-4.723205	3.303500
63	1	0	-0.799622	-3.832932	3.982422
64	1	0	-0.613857	-0.572245	0.496470
65	6	0	-4.931321	1.095030	0.375690
66	6	0	-6.262031	1.352131	0.063942
67	6	0	-6.669817	1.393240	-1.267255
68	6	0	-5.744959	1.176964	-2.286543
69	6	0	-4.415223	0.918555	-1.973504
70	1	0	-4.591365	1.057947	1.401833
71	1	0	-6.980431	1.522212	0.856325
72	1	0	-7.705813	1.596153	-1.510095
73	1	0	-6.061492	1.213582	-3.321796
74	1	0	-3.674312	0.751706	-2.743688
75	6	0	-4.004169	0.877307	-0.642070
76	6	0	-2.559153	0.593764	-0.307571
77	8	0	-1.779354	0.330971	-1.259269
78	8	0	-2.221487	0.622799	0.912566



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	2.592373	3.528299	-1.031967
2	6	0	2.673395	4.836307	-0.490556
3	6	0	1.587198	2.698281	-0.612330
4	6	0	0.652496	3.195940	0.338816
5	6	0	0.831875	4.517610	0.818258
6	7	0	1.845019	5.324230	0.400613
7	6	0	-0.433367	2.427142	0.803156
8	6	0	-1.317291	2.938096	1.720435
9	6	0	-1.142701	4.256379	2.215948
10	6	0	-0.096214	5.019334	1.771406
11	8	0	-2.366727	2.215981	2.174449
12	6	0	1.868259	0.293239	-0.021759
13	8	0	2.205304	1.078495	-2.272033
14	6	0	2.738661	-1.957868	-0.186874
15	6	0	1.279191	-1.149884	-1.947446
16	7	0	1.487442	-1.152865	-0.455264
17	6	0	3.394695	0.258882	0.142702
18	6	0	2.378195	-0.304665	-2.582084
19	6	0	3.849455	-1.003859	-0.610205
20	6	0	5.258119	-1.478118	-0.235164
21	6	0	3.761773	-0.783572	-2.129138
22	6	0	5.435630	-1.978157	1.199442
23	6	0	1.423835	1.283206	-1.104706
24	6	0	-1.714376	-4.521165	-1.363365
25	6	0	-2.012473	-5.193230	-0.182425
26	6	0	-1.545878	-4.717476	1.042925
27	6	0	-0.753058	-3.581733	1.033371
28	6	0	-0.411311	-2.896637	-0.152381
29	6	0	-0.938041	-3.359692	-1.354399
30	7	0	-0.192119	-2.930560	2.128299
31	6	0	0.563669	-1.854371	1.721697
32	6	0	0.292898	-1.661332	0.276409
33	8	0	1.306230	-1.203124	2.455324
34	6	0	-0.276486	-3.368786	3.500468
35	1	0	3.304445	3.197517	-1.775346
36	1	0	3.469700	5.495569	-0.820870
37	1	0	-0.600969	1.428408	0.438470
38	1	0	-1.854022	4.633646	2.938559
39	1	0	0.056929	6.029464	2.127629
40	1	0	-2.349332	1.344698	1.736900
41	1	0	1.362321	0.468654	0.920058
42	1	0	2.671700	-2.897029	-0.736648
43	1	0	2.776225	-2.144394	0.882851
44	1	0	1.345910	-2.182367	-2.283423
45	1	0	0.280607	-0.765098	-2.144585

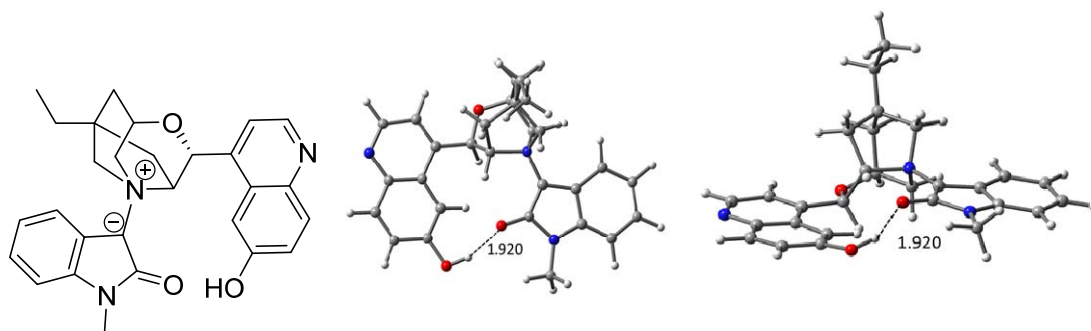
46	1	0	3.633088	0.172777	1.202267
47	1	0	3.853741	1.165473	-0.251175
48	1	0	2.294430	-0.391531	-3.666094
49	1	0	5.941822	-0.644245	-0.421319
50	1	0	5.550971	-2.274228	-0.926994
51	1	0	4.500417	-0.042857	-2.444890
52	1	0	3.995820	-1.725226	-2.638159
53	1	0	5.104100	-1.245246	1.936093
54	1	0	6.488830	-2.185529	1.391928
55	1	0	4.884256	-2.903496	1.374537
56	1	0	0.367744	1.123702	-1.340700
57	1	0	-2.106591	-4.886886	-2.303285
58	1	0	-2.627172	-6.083650	-0.208749
59	1	0	-1.796075	-5.216317	1.970274
60	1	0	-0.785327	-2.821588	-2.278486
61	1	0	0.315828	-2.675724	4.093177
62	1	0	0.125602	-4.378450	3.606637
63	1	0	-1.312094	-3.355804	3.843891
64	1	0	-0.856960	-0.791045	0.328074
65	6	0	-4.677902	0.260062	0.289729
66	6	0	-6.015463	0.626168	0.190146
67	6	0	-6.525796	1.073688	-1.025545
68	6	0	-5.700753	1.151907	-2.145726
69	6	0	-4.364851	0.784494	-2.048994
70	1	0	-4.272199	-0.100553	1.225308
71	1	0	-6.658213	0.563401	1.058815
72	1	0	-7.567073	1.361568	-1.100507
73	1	0	-6.099557	1.500460	-3.089902
74	1	0	-3.700710	0.834175	-2.901138
75	6	0	-3.850809	0.342228	-0.830274
76	6	0	-2.405841	-0.035255	-0.758560
77	8	0	-1.709823	-0.079375	-1.771989
78	8	0	-1.949388	-0.282808	0.443652



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	1.186591	3.518678	-0.844655
2	6	0	0.654914	4.753802	-0.399009
3	6	0	0.420328	2.391090	-0.729339
4	6	0	-0.893816	2.495965	-0.181124
5	6	0	-1.310753	3.782510	0.246088
6	7	0	-0.533964	4.894438	0.133140
7	6	0	-1.778894	1.394828	-0.046165
8	6	0	-3.024901	1.571053	0.504898
9	6	0	-3.440793	2.851791	0.950517
10	6	0	-2.603910	3.924672	0.818203
11	8	0	-3.910571	0.555321	0.652073
12	6	0	1.217586	0.207460	0.120707
13	8	0	2.039375	1.050496	-1.961076
14	6	0	2.511210	-1.801409	0.414660
15	6	0	1.610585	-1.336656	-1.784080
16	7	0	1.290223	-1.286867	-0.317995
17	6	0	2.577225	0.526456	0.747851
18	6	0	2.635839	-0.250986	-2.090416
19	6	0	3.485452	-0.628554	0.295374
20	6	0	4.756120	-0.788386	1.135744
21	6	0	3.858504	-0.414062	-1.180933
22	6	0	4.538658	-1.244110	2.579416
23	6	0	0.895031	1.024422	-1.121073
24	6	0	-2.709108	-2.813990	-2.524675
25	6	0	-3.743814	-2.910367	-1.598334
26	6	0	-3.479215	-2.730210	-0.238931
27	6	0	-2.180564	-2.427888	0.148841
28	6	0	-1.099170	-2.289082	-0.783926
29	6	0	-1.401971	-2.521017	-2.134785
30	7	0	-1.709111	-2.202791	1.423459
31	6	0	-0.356540	-1.864865	1.385045
32	6	0	0.046005	-1.974803	0.024659
33	8	0	0.291337	-1.474525	2.378208
34	6	0	-2.499892	-2.150303	2.628520
35	1	0	2.176506	3.465127	-1.277169
36	1	0	1.254350	5.654063	-0.488194
37	1	0	-1.501177	0.398846	-0.369579
38	1	0	-4.428297	2.948509	1.381426
39	1	0	-2.896770	4.915109	1.140000
40	1	0	-3.560205	-0.254949	0.244185
41	1	0	0.428337	0.259810	0.858267
42	1	0	2.827932	-2.734365	-0.051369
43	1	0	2.192045	-1.967600	1.441103
44	1	0	1.989458	-2.332975	-2.005441
45	1	0	0.700510	-1.179022	-2.347029

46	1	0	2.467315	0.524051	1.831453
47	1	0	2.954307	1.498208	0.425523
48	1	0	2.940033	-0.340667	-3.133894
49	1	0	5.277819	0.173897	1.125749
50	1	0	5.418498	-1.500979	0.633376
51	1	0	4.488293	0.473620	-1.281660
52	1	0	4.438089	-1.273691	-1.536004
53	1	0	3.825513	-0.610323	3.108016
54	1	0	5.481694	-1.210578	3.126145
55	1	0	4.168495	-2.269196	2.624740
56	1	0	0.063729	0.552318	-1.653288
57	1	0	-2.914928	-2.976790	-3.575084
58	1	0	-4.749302	-3.139600	-1.924898
59	1	0	-4.262811	-2.832958	0.502662
60	1	0	-0.637236	-2.506688	-2.899453
61	1	0	-1.817277	-1.896336	3.436676
62	1	0	-2.967929	-3.115688	2.830609
63	1	0	-3.272392	-1.381194	2.550792



II

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.698754	1.486540	-1.063579
2	6	0	-5.051355	1.177101	-0.770987
3	6	0	-2.745628	0.514053	-0.907813
4	6	0	-3.163339	-0.772823	-0.469296
5	6	0	-4.534677	-0.956233	-0.151876
6	7	0	-5.468149	0.018825	-0.320849
7	6	0	-2.258717	-1.832205	-0.281798
8	6	0	-2.652908	-2.988020	0.346963
9	6	0	-4.022724	-3.191711	0.656809
10	6	0	-4.937079	-2.206259	0.391127
11	8	0	-1.752550	-3.934174	0.689063
12	6	0	-0.465281	0.732933	0.153659

13	8	0	-1.142376	2.050570	-1.760863
14	6	0	1.520966	1.910891	0.844290
15	6	0	1.194406	1.496074	-1.534950
16	7	0	1.061340	0.880206	-0.162605
17	6	0	-0.801617	1.938909	1.047000
18	6	0	0.167948	2.603949	-1.674361
19	6	0	0.372977	2.910995	0.866701
20	6	0	0.487866	3.973893	1.964992
21	6	0	0.281281	3.594461	-0.508655
22	6	0	0.804279	3.455364	3.368594
23	6	0	-1.274874	0.772408	-1.153987
24	6	0	5.560227	0.065523	-1.016831
25	6	0	5.919012	-1.260161	-0.778001
26	6	0	4.967632	-2.171491	-0.325542
27	6	0	3.669267	-1.724510	-0.133168
28	6	0	3.263587	-0.386406	-0.395294
29	6	0	4.252549	0.508535	-0.828428
30	7	0	2.584268	-2.425536	0.338765
31	6	0	1.455680	-1.608174	0.419865
32	6	0	1.859989	-0.345038	-0.083886
33	8	0	0.363177	-2.040542	0.880483
34	6	0	2.604169	-3.798464	0.776600
35	1	0	-3.427211	2.475061	-1.404885
36	1	0	-5.808053	1.943116	-0.906987
37	1	0	-1.217714	-1.735270	-0.538355
38	1	0	-4.314191	-4.127039	1.116176
39	1	0	-5.987353	-2.333099	0.618285
40	1	0	-0.873993	-3.497343	0.696728
41	1	0	-0.565812	-0.220715	0.663269
42	1	0	2.491925	2.297870	0.537474
43	1	0	1.625046	1.379160	1.788264
44	1	0	2.205429	1.875538	-1.634662
45	1	0	1.054666	0.702461	-2.263556
46	1	0	-0.876445	1.617680	2.085711
47	1	0	-1.755143	2.380240	0.756145
48	1	0	0.339079	3.128577	-2.615229
49	1	0	-0.455176	4.528565	1.982963
50	1	0	1.260058	4.691481	1.670401
51	1	0	-0.587223	4.256797	-0.537539
52	1	0	1.174146	4.211276	-0.659943
53	1	0	0.079898	2.713111	3.706872
54	1	0	0.782260	4.280647	4.080931
55	1	0	1.798274	3.007912	3.419836
56	1	0	-0.902198	-0.003770	-1.831615
57	1	0	6.309455	0.771182	-1.353108
58	1	0	6.939874	-1.582458	-0.935538

59	1	0	5.231807	-3.201852	-0.123049
60	1	0	4.041883	1.555321	-1.009360
61	1	0	1.635952	-4.012368	1.221738
62	1	0	3.385092	-3.947558	1.525014
63	1	0	2.778133	-4.476635	-0.061521

II-TS1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.607477	-1.575144	-0.913522
2	6	0	4.956634	-1.459457	-0.497618
3	6	0	2.756261	-0.510740	-0.748846
4	6	0	3.290187	0.681443	-0.184373
5	6	0	4.653135	0.680792	0.217368
6	7	0	5.474174	-0.391238	0.057437
7	6	0	2.515893	1.842170	-0.009736
8	6	0	3.051623	2.955142	0.586721
9	6	0	4.405131	2.968879	1.004819
10	6	0	5.181823	1.856518	0.813868
11	8	0	2.302959	4.067888	0.792926
12	6	0	0.375977	-0.655465	0.098753
13	8	0	1.143129	-1.788721	-1.917726
14	6	0	-1.620967	-1.931140	0.565534
15	6	0	-1.198217	-1.279998	-1.737389
16	7	0	-1.136711	-0.800753	-0.311761
17	6	0	0.672710	-1.909563	0.938117
18	6	0	-0.155850	-2.368772	-1.919167
19	6	0	-0.447542	-2.892360	0.587949
20	6	0	-0.610021	-4.053256	1.575518
21	6	0	-0.271536	-3.451353	-0.836966
22	6	0	-0.952709	-3.672712	3.016684
23	6	0	1.288595	-0.602317	-1.143198
24	6	0	-5.782566	-0.125998	0.065298
25	6	0	-6.106500	1.227105	0.136157
26	6	0	-5.097501	2.187061	0.099059
27	6	0	-3.783675	1.757620	-0.003167
28	6	0	-3.414473	0.381084	-0.047078
29	6	0	-4.459041	-0.554758	-0.026175
30	7	0	-2.644817	2.523521	-0.096011
31	6	0	-1.513917	1.716206	-0.223416
32	6	0	-1.977608	0.383608	-0.127181
33	8	0	-0.366640	2.199566	-0.390084
34	6	0	-2.600611	3.962059	-0.143035

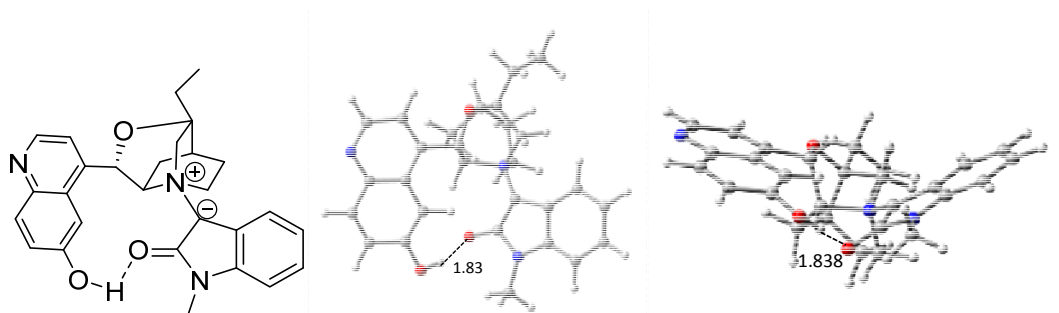
35	1	0	3.257676	-2.493480	-1.361797
36	1	0	5.623094	-2.305612	-0.632312
37	1	0	1.487231	1.873036	-0.334804
38	1	0	4.798929	3.865261	1.465240
39	1	0	6.221372	1.834094	1.113399
40	1	0	1.397454	3.866712	0.504446
41	1	0	0.442779	0.276967	0.648561
42	1	0	-2.527158	-2.350237	0.140321
43	1	0	-1.837264	-1.493445	1.538416
44	1	0	-2.217163	-1.621211	-1.916043
45	1	0	-0.999145	-0.422541	-2.376053
46	1	0	0.639131	-1.662051	1.999050
47	1	0	1.662865	-2.303427	0.711904
48	1	0	-0.278289	-2.824299	-2.902400
49	1	0	0.321460	-4.627303	1.561958
50	1	0	-1.387071	-4.722097	1.191570
51	1	0	0.624140	-4.075107	-0.888780
52	1	0	-1.132570	-4.088564	-1.068037
53	1	0	-0.199625	-3.020443	3.460605
54	1	0	-1.006396	-4.572144	3.631033
55	1	0	-1.920476	-3.173406	3.087535
56	1	0	1.020914	0.275396	-1.738363
57	1	0	-6.571797	-0.867356	0.080670
58	1	0	-7.140896	1.535440	0.213075
59	1	0	-5.328073	3.244334	0.141194
60	1	0	-4.280109	-1.619060	-0.089120
61	1	0	-1.566811	4.242844	-0.328775
62	1	0	-2.934689	4.397832	0.801229
63	1	0	-3.229874	4.339377	-0.952160

II-TS2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.721707	0.726389	-1.334828
2	6	0	-4.969705	0.092054	-1.123939
3	6	0	-2.571018	0.056185	-1.014285
4	6	0	-2.670331	-1.262776	-0.479038
5	6	0	-3.976847	-1.784726	-0.286483
6	7	0	-5.109585	-1.107419	-0.617276
7	6	0	-1.550327	-2.049740	-0.110050
8	6	0	-1.730479	-3.265808	0.501007
9	6	0	-3.030641	-3.796751	0.689023
10	6	0	-4.120708	-3.074808	0.291165

11	8	0	-0.689646	-4.012387	0.949157
12	6	0	-0.542715	0.900465	0.154410
13	8	0	-1.308921	1.917935	-1.876021
14	6	0	1.182678	2.391100	0.880359
15	6	0	1.076635	1.844093	-1.486870
16	7	0	0.949542	1.269961	-0.105719
17	6	0	-1.135455	2.074365	0.941511
18	6	0	-0.131807	2.723823	-1.750958
19	6	0	-0.108803	3.203494	0.774532
20	6	0	-0.225535	4.326459	1.809338
21	6	0	-0.248340	3.781475	-0.644821
22	6	0	0.096327	3.932338	3.251453
23	6	0	-1.210536	0.674288	-1.190836
24	6	0	4.756895	-0.671167	-2.290550
25	6	0	5.202584	-1.791623	-1.592998
26	6	0	4.542866	-2.197718	-0.434228
27	6	0	3.446044	-1.466677	-0.008019
28	6	0	2.958735	-0.318768	-0.705118
29	6	0	3.652791	0.064293	-1.862363
30	7	0	2.661404	-1.685409	1.107191
31	6	0	1.682340	-0.693138	1.215027
32	6	0	1.825620	0.118562	0.062986
33	8	0	0.865763	-0.624021	2.162323
34	6	0	2.898031	-2.666322	2.136307
35	1	0	-3.674665	1.723229	-1.749245
36	1	0	-5.882928	0.616809	-1.385237
37	1	0	-0.537616	-1.706650	-0.284478
38	1	0	-3.126518	-4.767021	1.157511
39	1	0	-5.127676	-3.448123	0.420934
40	1	0	0.104178	-3.458090	0.967278
41	1	0	-0.510986	0.013192	0.771857
42	1	0	2.105953	2.906616	0.615394
43	1	0	1.279164	1.908576	1.852217
44	1	0	2.002949	2.414186	-1.519040
45	1	0	1.146048	1.021164	-2.191969
46	1	0	-1.226487	1.785415	1.988198
47	1	0	-2.120313	2.350542	0.562208
48	1	0	-0.006347	3.219947	-2.713918
49	1	0	-1.245697	4.718994	1.753593
50	1	0	0.435620	5.145431	1.507917
51	1	0	-1.213354	4.284815	-0.743219
52	1	0	0.533591	4.531342	-0.809780
53	1	0	-0.505305	3.088055	3.590664
54	1	0	-0.105826	4.770362	3.919385
55	1	0	1.147477	3.664838	3.370651
56	1	0	-0.603196	-0.028188	-1.775012

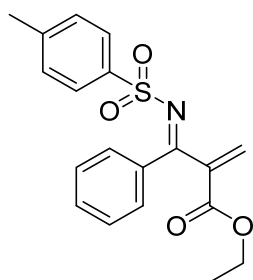
57	1	0	5.277474	-0.356375	-3.186485
58	1	0	6.062496	-2.345809	-1.945587
59	1	0	4.877599	-3.062765	0.125146
60	1	0	3.361913	0.930396	-2.440477
61	1	0	2.141672	-2.504751	2.902575
62	1	0	3.891225	-2.542588	2.574162
63	1	0	2.812907	-3.681855	1.741314



β -II

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.843297	5.088889	-0.182318
2	6	0	-0.744624	4.268319	-0.855741
3	6	0	-0.376525	2.961653	-0.168591
4	6	0	-0.025287	3.085590	1.344819
5	6	0	-1.252557	2.775364	2.222716
6	6	0	-1.603478	1.283244	2.041923
7	8	0	0.760823	2.463936	-0.896173
8	6	0	-1.457240	1.892260	-0.283775
9	7	0	-1.079092	0.814698	0.702345
10	6	0	0.473249	0.786454	0.769901
11	6	0	0.979827	1.068930	-0.651554
12	6	0	2.445446	0.743280	-0.811206
13	6	0	3.383907	1.698394	-1.101894
14	6	0	4.748288	1.320317	-1.175758
15	7	0	5.197528	0.113124	-0.933475
16	6	0	4.281126	-0.843767	-0.623351
17	6	0	4.739923	-2.141932	-0.270499
18	6	0	3.867634	-3.109627	0.152895
19	6	0	2.473512	-2.843698	0.186027
20	8	0	1.635020	-3.768353	0.703121
21	6	0	1.997248	-1.643637	-0.284515
22	6	0	2.883940	-0.595046	-0.601145
23	6	0	0.958448	1.948937	1.635502
24	6	0	-4.812237	-0.657547	-1.825054

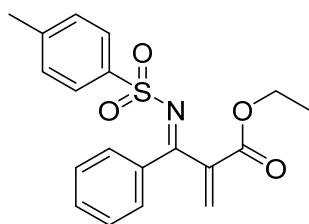
25	6	0	-4.963552	-2.041319	-1.748224
26	6	0	-4.062507	-2.800870	-1.007999
27	6	0	-3.025921	-2.145516	-0.359928
28	6	0	-2.826691	-0.736768	-0.439970
29	6	0	-3.762824	-0.002795	-1.185118
30	7	0	-2.050835	-2.687667	0.448134
31	6	0	-1.200559	-1.696472	0.924224
32	6	0	-1.633800	-0.486013	0.329031
33	8	0	-0.244242	-1.952263	1.713068
34	6	0	-1.918601	-4.080581	0.800546
35	1	0	-2.034016	5.992046	-0.762348
36	1	0	-1.556766	5.399399	0.823771
37	1	0	-2.786415	4.541972	-0.115940
38	1	0	0.176142	4.854516	-0.907644
39	1	0	-1.022808	4.033966	-1.886429
40	1	0	0.390838	4.068630	1.567890
41	1	0	-1.004761	2.964083	3.268425
42	1	0	-2.106929	3.404171	1.973520
43	1	0	-2.675474	1.097442	2.019912
44	1	0	-1.150096	0.626767	2.782487
45	1	0	-1.481055	1.467320	-1.282881
46	1	0	-2.449860	2.247428	-0.019696
47	1	0	0.730838	-0.189269	1.165515
48	1	0	0.409887	0.468436	-1.370242
49	1	0	3.089619	2.725752	-1.262357
50	1	0	5.491083	2.070907	-1.426242
51	1	0	5.807138	-2.316938	-0.304984
52	1	0	4.213448	-4.079415	0.485720
53	1	0	0.868660	-3.269073	1.075329
54	1	0	0.929888	-1.504772	-0.349698
55	1	0	1.976414	2.189733	1.331275
56	1	0	0.976335	1.699023	2.696849
57	1	0	-5.522116	-0.072310	-2.395985
58	1	0	-5.782754	-2.527441	-2.261445
59	1	0	-4.164840	-3.876299	-0.936536
60	1	0	-3.701013	1.071139	-1.284420
61	1	0	-1.508190	-4.665543	-0.025116
62	1	0	-2.890893	-4.485990	1.083706
63	1	0	-1.245413	-4.139579	1.652752



D1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.091453	2.006858	-0.462569
2	6	0	0.659016	2.698291	-1.604897
3	6	0	1.083201	4.005676	-1.829011
4	6	0	1.928083	4.640658	-0.916951
5	6	0	2.363159	3.958143	0.220827
6	6	0	1.961324	2.642760	0.438594
7	6	0	0.686453	0.600326	-0.197450
8	7	0	-0.484901	0.060777	-0.278227
9	6	0	1.761420	-0.335251	0.277214
10	6	0	3.034410	-0.362098	-0.510450
11	8	0	4.032090	-0.997338	0.139800
12	6	0	5.271586	-1.133878	-0.595923
13	8	0	3.145095	0.107225	-1.624251
14	6	0	1.552703	-1.147681	1.322693
15	6	0	6.251608	-1.871718	0.296035
16	16	0	-1.911552	0.958120	-0.595812
17	8	0	-1.981472	2.183251	0.212050
18	8	0	-2.094862	1.009741	-2.054346
19	6	0	-3.103716	-0.201733	0.070459
20	6	0	-3.693895	0.060577	1.304654
21	6	0	-4.638296	-0.834654	1.808389
22	6	0	-5.001459	-1.982856	1.094221
23	6	0	-4.391963	-2.218105	-0.148882
24	6	0	-3.449936	-1.335729	-0.667934
25	6	0	-6.043062	-2.936199	1.629970
26	1	0	0.005411	2.209266	-2.318298
27	1	0	0.750476	4.529646	-2.720396
28	1	0	2.250073	5.663368	-1.093947
29	1	0	3.018795	4.447743	0.935583
30	1	0	2.303763	2.111324	1.322183
31	1	0	5.069901	-1.675351	-1.525647
32	1	0	5.629505	-0.135412	-0.865725
33	1	0	2.326206	-1.822325	1.672147
34	1	0	0.598717	-1.148016	1.839877
35	1	0	7.206658	-1.994114	-0.226166

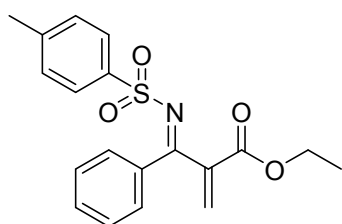
36	1	0	6.434276	-1.316298	1.221547
37	1	0	5.873299	-2.865167	0.557767
38	1	0	-3.420208	0.956022	1.852290
39	1	0	-5.102642	-0.633775	2.770778
40	1	0	-4.663999	-3.103403	-0.718901
41	1	0	-2.991342	-1.515233	-1.634608
42	1	0	-6.220359	-2.777940	2.698231
43	1	0	-7.002259	-2.802809	1.112839
44	1	0	-5.742368	-3.980063	1.486009



D2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.540548	0.175422	-1.812513
2	6	0	2.505722	0.824551	-3.057699
3	6	0	3.633725	1.493821	-3.527757
4	6	0	4.798132	1.539619	-2.759131
5	6	0	4.839886	0.898378	-1.519026
6	6	0	3.725050	0.204103	-1.056360
7	6	0	1.361962	-0.575151	-1.295679
8	7	0	0.120485	-0.218627	-1.283089
9	6	0	1.602062	-1.958710	-0.778163
10	6	0	0.822039	-2.486172	0.397995
11	8	0	0.598985	-3.665767	0.581259
12	8	0	0.474149	-1.504491	1.247384
13	6	0	2.465129	-2.795566	-1.372678
14	16	0	-0.429131	1.332427	-1.738309
15	8	0	0.430541	2.403417	-1.216536
16	8	0	-0.765217	1.275945	-3.169882
17	6	0	-1.958205	1.358552	-0.806127
18	6	0	-2.023796	2.099546	0.374386
19	6	0	-3.221576	2.135988	1.084460
20	6	0	-4.355351	1.444909	0.631473
21	6	0	-4.259900	0.714705	-0.561043
22	6	0	-3.070269	0.667573	-1.285693
23	6	0	-5.646592	1.495978	1.413629
24	6	0	-0.284567	-1.894069	2.417952
25	6	0	0.633011	-2.301559	3.560760
26	1	0	1.601548	0.799653	-3.656551

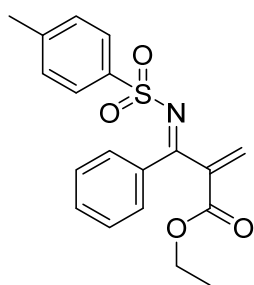
27	1	0	3.599086	1.984606	-4.496113
28	1	0	5.672126	2.070812	-3.126269
29	1	0	5.742327	0.933479	-0.915159
30	1	0	3.760645	-0.302289	-0.096731
31	1	0	2.554894	-3.819709	-1.024975
32	1	0	3.071552	-2.486813	-2.217486
33	1	0	-1.150369	2.644580	0.715781
34	1	0	-3.279580	2.716897	2.002181
35	1	0	-5.130863	0.179966	-0.931463
36	1	0	-3.006173	0.112445	-2.215541
37	1	0	-5.989421	2.529076	1.547666
38	1	0	-6.443560	0.941052	0.909656
39	1	0	-5.521978	1.066720	2.415593
40	1	0	-0.866940	-1.003339	2.664975
41	1	0	-0.960904	-2.706404	2.142213
42	1	0	0.037997	-2.513081	4.456717
43	1	0	1.194689	-3.203486	3.301574
44	1	0	1.338789	-1.499039	3.799023



D3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.072538	1.334963	-0.817413
2	6	0	3.081688	2.385859	-1.749620
3	6	0	4.039149	3.393478	-1.655700
4	6	0	4.982482	3.376491	-0.626788
5	6	0	4.976964	2.337474	0.306543
6	6	0	4.040005	1.312681	0.202300
7	6	0	2.076205	0.233022	-0.907137
8	7	0	0.807249	0.308273	-1.130688
9	6	0	2.575477	-1.172724	-0.781169
10	6	0	1.686457	-2.150634	-0.062124
11	8	0	1.858135	-3.409195	-0.517390
12	8	0	0.947494	-1.852333	0.852771
13	6	0	3.760392	-1.556011	-1.279444
14	16	0	-0.073734	1.768772	-1.170383
15	8	0	0.318208	2.647733	-0.060682
16	8	0	-0.079911	2.287394	-2.548571
17	6	0	-1.697496	1.096109	-0.824860

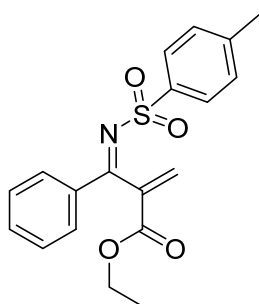
18	6	0	-1.892619	0.258546	0.277298
19	6	0	-3.179383	-0.186960	0.561685
20	6	0	-4.276344	0.197112	-0.227294
21	6	0	-4.046910	1.034740	-1.324326
22	6	0	-2.762693	1.488152	-1.630920
23	6	0	-5.668836	-0.279486	0.112152
24	6	0	1.094603	-4.446410	0.149797
25	6	0	-0.299484	-4.569676	-0.445568
26	1	0	2.343387	2.411013	-2.543771
27	1	0	4.043002	4.196878	-2.386681
28	1	0	5.721116	4.170062	-0.552529
29	1	0	5.704791	2.322688	1.112945
30	1	0	4.038939	0.503535	0.925982
31	1	0	4.076924	-2.592137	-1.233593
32	1	0	4.431207	-0.845508	-1.751619
33	1	0	-1.049568	-0.063949	0.879851
34	1	0	-3.336340	-0.847824	1.411102
35	1	0	-4.881725	1.335525	-1.952570
36	1	0	-2.582621	2.127443	-2.488489
37	1	0	-6.042139	0.207156	1.022507
38	1	0	-6.375577	-0.059543	-0.693928
39	1	0	-5.688706	-1.360271	0.294475
40	1	0	1.682092	-5.354005	-0.009068
41	1	0	1.053811	-4.221068	1.218086
42	1	0	-0.830129	-5.404912	0.025981
43	1	0	-0.247184	-4.758521	-1.522554
44	1	0	-0.874294	-3.655221	-0.275288



D4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.091086	1.842770	-0.445457
2	6	0	0.658891	2.520462	-1.596692
3	6	0	1.127340	3.804023	-1.866540
4	6	0	2.017992	4.430039	-0.992018
5	6	0	2.453684	3.761416	0.153526
6	6	0	2.006370	2.468916	0.417129
7	6	0	0.645426	0.456555	-0.133782

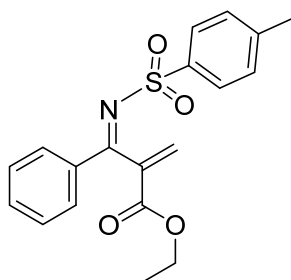
8	7	0	-0.539580	-0.055030	-0.200134
9	6	0	1.692348	-0.489153	0.377694
10	6	0	2.984632	-0.680327	-0.362563
11	8	0	3.957242	-1.244542	0.096264
12	6	0	4.087351	-0.322099	-2.445544
13	8	0	2.908711	-0.185920	-1.612848
14	6	0	1.493477	-1.200027	1.495753
15	16	0	-1.943404	0.858777	-0.565374
16	8	0	-1.990592	2.124643	0.179129
17	8	0	-2.115472	0.843911	-2.026868
18	6	0	-3.164018	-0.240180	0.149559
19	6	0	-3.785544	0.117872	1.343128
20	6	0	-4.755098	-0.728941	1.882721
21	6	0	-5.109541	-1.923529	1.245442
22	6	0	-4.470961	-2.253223	0.038299
23	6	0	-3.504209	-1.421014	-0.515487
24	6	0	-6.151437	-2.843888	1.835631
25	6	0	4.108476	-1.667691	-3.154034
26	1	0	-0.030767	2.039510	-2.281429
27	1	0	0.791657	4.317595	-2.762975
28	1	0	2.373792	5.434716	-1.204109
29	1	0	3.145016	4.243217	0.839254
30	1	0	2.350559	1.948400	1.306152
31	1	0	4.008711	0.505819	-3.153786
32	1	0	4.973252	-0.185958	-1.820834
33	1	0	2.267424	-1.867249	1.861701
34	1	0	0.567172	-1.119060	2.054280
35	1	0	-3.518510	1.049624	1.829946
36	1	0	-5.246718	-0.452023	2.811980
37	1	0	-4.741157	-3.172619	-0.475908
38	1	0	-3.023480	-1.673812	-1.454648
39	1	0	-6.639028	-2.392813	2.705109
40	1	0	-6.928451	-3.088727	1.101889
41	1	0	-5.704527	-3.792714	2.158829
42	1	0	4.965796	-1.713021	-3.835441
43	1	0	3.195089	-1.813601	-3.739560
44	1	0	4.201166	-2.482731	-2.430883



D5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.015281	1.617298	0.087994
2	6	0	1.372799	2.679621	-0.573668
3	6	0	2.108200	3.757008	-1.053828
4	6	0	3.496136	3.794312	-0.882355
5	6	0	4.143038	2.746594	-0.226747
6	6	0	3.408715	1.663744	0.254967
7	6	0	1.220389	0.472565	0.602112
8	7	0	-0.066929	0.585481	0.575110
9	6	0	1.959404	-0.721730	1.135785
10	6	0	2.508121	-1.727218	0.167753
11	8	0	3.141811	-2.710233	0.488492
12	6	0	2.600773	-2.317512	-2.137649
13	8	0	2.207724	-1.385375	-1.100029
14	6	0	2.131424	-0.924100	2.446276
15	16	0	-1.053519	-0.706711	1.114408
16	8	0	-0.664047	-1.973082	0.474427
17	8	0	-1.162280	-0.611630	2.577227
18	6	0	-2.611826	-0.190986	0.399748
19	6	0	-3.056508	-0.790024	-0.777442
20	6	0	-4.282243	-0.399145	-1.315223
21	6	0	-5.067558	0.580380	-0.693692
22	6	0	-4.598671	1.157012	0.496908
23	6	0	-3.378608	0.778044	1.049509
24	6	0	-6.381112	1.018903	-1.296220
25	6	0	1.567918	-3.422284	-2.298807
26	1	0	0.296942	2.638479	-0.702926
27	1	0	1.601196	4.570402	-1.565604
28	1	0	4.068850	4.637494	-1.259207
29	1	0	5.220169	2.770793	-0.087556
30	1	0	3.918591	0.858925	0.773941
31	1	0	2.676202	-1.699244	-3.035339
32	1	0	3.585347	-2.721935	-1.890215
33	1	0	2.668317	-1.805373	2.784059
34	1	0	1.731093	-0.245528	3.191657
35	1	0	-2.455207	-1.558765	-1.250478
36	1	0	-4.637058	-0.868630	-2.229465
37	1	0	-5.202723	1.907158	1.001693
38	1	0	-3.028925	1.213036	1.979852
39	1	0	-6.800258	0.247417	-1.949886
40	1	0	-7.120820	1.247920	-0.521662
41	1	0	-6.253279	1.926736	-1.900754
42	1	0	1.843765	-4.065440	-3.142623

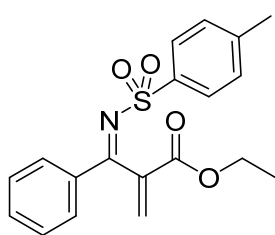
43	1	0	0.576562	-3.000238	-2.489143
44	1	0	1.516346	-4.036536	-1.396100



D6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.919530	1.137420	-0.501142
2	6	0	-0.238492	0.998094	-1.287182
3	6	0	-0.530193	1.926276	-2.279880
4	6	0	0.325486	3.009976	-2.503447
5	6	0	1.475733	3.158301	-1.728014
6	6	0	1.773269	2.227103	-0.734475
7	6	0	1.215687	0.147869	0.564119
8	7	0	0.271882	-0.670167	0.893178
9	6	0	2.575829	0.176845	1.207455
10	6	0	3.673293	-0.411396	0.380416
11	8	0	4.856499	-0.421721	1.021182
12	6	0	5.956336	-1.026226	0.300339
13	8	0	3.504010	-0.829280	-0.747616
14	6	0	2.765408	0.689687	2.428507
15	6	0	7.165785	-1.003641	1.215148
16	16	0	0.539826	-1.873144	2.084004
17	8	0	0.279737	-1.262087	3.396220
18	8	0	1.790175	-2.607678	1.838820
19	6	0	-0.820764	-2.966930	1.689229
20	6	0	-0.585732	-4.090979	0.899377
21	6	0	-1.648505	-4.944032	0.603830
22	6	0	-2.937776	-4.691809	1.090150
23	6	0	-3.141950	-3.554126	1.886499
24	6	0	-2.093447	-2.691373	2.192554
25	6	0	-4.078578	-5.635426	0.791837
26	1	0	-0.892508	0.152201	-1.106922
27	1	0	-1.424457	1.805210	-2.884974
28	1	0	0.095595	3.733948	-3.280632
29	1	0	2.143140	3.998980	-1.895481
30	1	0	2.664089	2.354968	-0.128552
31	1	0	5.669886	-2.043785	0.018300

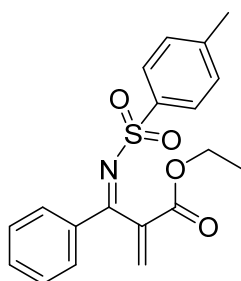
32	1	0	6.124860	-0.460091	-0.621658
33	1	0	3.752603	0.697780	2.877433
34	1	0	1.940738	1.086339	3.011665
35	1	0	8.024354	-1.453131	0.704426
36	1	0	7.429430	0.022038	1.493145
37	1	0	6.972970	-1.571827	2.130558
38	1	0	0.414567	-4.291697	0.531080
39	1	0	-1.471335	-5.821959	-0.012492
40	1	0	-4.135779	-3.344621	2.275079
41	1	0	-2.251552	-1.820009	2.819184
42	1	0	-3.866185	-6.258140	-0.082816
43	1	0	-4.263123	-6.309787	1.638487
44	1	0	-5.010483	-5.090933	0.604048



D7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.173733	0.828489	-1.386041
2	6	0	-1.087570	0.479805	-1.901629
3	6	0	-1.577979	1.104674	-3.042285
4	6	0	-0.821048	2.089218	-3.685953
5	6	0	0.430468	2.443676	-3.181543
6	6	0	0.926902	1.816153	-2.040250
7	6	0	0.683073	0.164137	-0.160926
8	7	0	-0.156189	-0.536568	0.526747
9	6	0	2.125846	0.368739	0.214932
10	6	0	3.103046	-0.418543	-0.597287
11	8	0	4.372917	-0.252460	-0.184227
12	6	0	5.370239	-1.026817	-0.891559
13	8	0	2.775016	-1.126199	-1.528588
14	6	0	2.484309	1.192592	1.206232
15	6	0	6.708251	-0.755532	-0.231019
16	16	0	0.355541	-1.372579	1.932547
17	8	0	0.280540	-0.430301	3.059243
18	8	0	1.583671	-2.143357	1.686364
19	6	0	-0.997617	-2.535257	2.075902
20	6	0	-0.839268	-3.830513	1.586188
21	6	0	-1.894217	-4.734000	1.710072

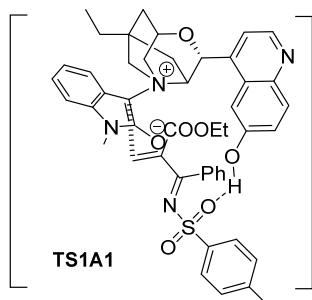
22	6	0	-3.099484	-4.362440	2.319665
23	6	0	-3.227014	-3.052222	2.806764
24	6	0	-2.184920	-2.136596	2.692659
25	6	0	-4.227544	-5.354026	2.478017
26	1	0	-1.663777	-0.287116	-1.396079
27	1	0	-2.551066	0.822964	-3.435026
28	1	0	-1.206362	2.575819	-4.578003
29	1	0	1.022187	3.209044	-3.675807
30	1	0	1.896406	2.104638	-1.647961
31	1	0	5.090563	-2.083344	-0.840996
32	1	0	5.362025	-0.730287	-1.945601
33	1	0	3.529213	1.323788	1.465300
34	1	0	1.745987	1.730121	1.792259
35	1	0	7.494083	-1.324369	-0.739850
36	1	0	6.964413	0.307674	-0.283754
37	1	0	6.691623	-1.055915	0.821351
38	1	0	0.097521	-4.121196	1.123093
39	1	0	-1.776742	-5.745501	1.329197
40	1	0	-4.154620	-2.747585	3.285643
41	1	0	-2.281629	-1.128572	3.081859
42	1	0	-4.129442	-6.188918	1.777130
43	1	0	-4.241392	-5.775739	3.491722
44	1	0	-5.202188	-4.882308	2.311504



D8

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.824361	0.096368	-0.977232
2	6	0	1.385673	1.399630	-1.276542
3	6	0	2.301072	2.401034	-1.578747
4	6	0	3.672542	2.125678	-1.574316
5	6	0	4.119983	0.840627	-1.268487
6	6	0	3.203897	-0.169912	-0.977216
7	6	0	0.825015	-0.957620	-0.638765
8	7	0	-0.348009	-0.531897	-0.303221
9	6	0	1.262783	-2.390953	-0.746927
10	6	0	1.232413	-3.301965	0.449768

11	8	0	1.530711	-4.476611	0.413986
12	8	0	0.874616	-2.627010	1.553732
13	6	0	1.704132	-2.891670	-1.906941
14	16	0	-1.658897	-1.552513	0.082814
15	8	0	-1.504574	-2.923660	-0.431625
16	8	0	-1.953696	-1.325679	1.501956
17	6	0	-2.923632	-0.744944	-0.895421
18	6	0	-3.373116	-1.349500	-2.067217
19	6	0	-4.372945	-0.722665	-2.812310
20	6	0	-4.926434	0.495977	-2.402275
21	6	0	-4.456776	1.078539	-1.213176
22	6	0	-3.463464	0.467303	-0.455745
23	6	0	-6.008790	1.172772	-3.209308
24	6	0	0.671019	-3.392257	2.768545
25	6	0	1.959813	-3.500993	3.567932
26	1	0	0.320802	1.603831	-1.270541
27	1	0	1.947165	3.399688	-1.819546
28	1	0	4.386873	2.910643	-1.807734
29	1	0	5.183865	0.620997	-1.254831
30	1	0	3.562975	-1.164401	-0.737932
31	1	0	1.982343	-3.939355	-1.965372
32	1	0	1.767392	-2.290093	-2.808227
33	1	0	-2.951814	-2.299357	-2.378522
34	1	0	-4.730859	-1.192178	-3.725184
35	1	0	-4.881997	2.020599	-0.874743
36	1	0	-3.114417	0.911202	0.470644
37	1	0	-6.921558	1.306483	-2.615945
38	1	0	-5.692914	2.169632	-3.540936
39	1	0	-6.269292	0.590735	-4.098293
40	1	0	-0.100387	-2.832823	3.300475
41	1	0	0.284560	-4.376276	2.494413
42	1	0	1.764197	-4.015924	4.515641
43	1	0	2.711079	-4.073146	3.015575
44	1	0	2.364072	-2.508806	3.794282

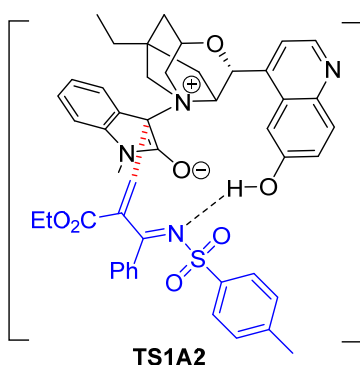


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	4.160288	2.046776	-2.641557
2	6	0	4.179047	3.450190	-2.812976
3	6	0	2.976071	1.416956	-2.353279
4	6	0	1.785865	2.202349	-2.277949
5	6	0	1.936916	3.610092	-2.428539
6	7	0	3.124896	4.218122	-2.692827
7	6	0	0.497102	1.657572	-2.050954
8	6	0	-0.587667	2.495608	-1.922454
9	6	0	-0.437243	3.901101	-2.033108
10	6	0	0.791747	4.438384	-2.293894
11	8	0	-1.838143	2.038109	-1.692683
12	6	0	2.658799	-0.282381	-0.571045
13	8	0	4.184907	-0.650155	-2.406535
14	6	0	3.388568	-1.980109	0.968509
15	6	0	3.146696	-2.581469	-1.369213
16	7	0	2.509529	-1.801743	-0.240485
17	6	0	3.870878	0.181740	0.259615
18	6	0	4.446963	-1.896701	-1.764054
19	6	0	4.595803	-1.108281	0.659490
20	6	0	5.551044	-0.929933	1.845708
21	6	0	5.349013	-1.701030	-0.541123
22	6	0	4.885847	-0.641358	3.193457
23	6	0	2.927694	-0.066582	-2.068812
24	6	0	0.656353	-5.266875	2.389317
25	6	0	-0.452451	-5.800337	1.739531
26	6	0	-0.953931	-5.199973	0.585043
27	6	0	-0.296670	-4.084461	0.093306
28	6	0	0.847818	-3.529419	0.720145
29	6	0	1.293227	-4.122859	1.903548
30	7	0	-0.617770	-3.337240	-1.026602
31	6	0	0.281720	-2.309514	-1.193737
32	6	0	1.120151	-2.278942	0.007067
33	8	0	0.376539	-1.621362	-2.214916
34	6	0	-1.676904	-3.634766	-1.960695
35	1	0	5.072374	1.473901	-2.728602
36	1	0	5.117322	3.945844	-3.041195
37	1	0	0.340352	0.585270	-1.995052
38	1	0	-1.318816	4.519136	-1.922821
39	1	0	0.936852	5.504857	-2.406704
40	1	0	-1.825278	1.062126	-1.596295
41	1	0	1.719163	0.176827	-0.281448
42	1	0	3.598240	-3.039915	1.097335
43	1	0	2.840419	-1.586561	1.822633
44	1	0	3.304795	-3.595319	-1.003008
45	1	0	2.443334	-2.594672	-2.196512

46	1	0	3.528483	0.702674	1.149333
47	1	0	4.507200	0.846942	-0.322450
48	1	0	4.955779	-2.519471	-2.501606
49	1	0	6.233801	-0.114562	1.587677
50	1	0	6.168908	-1.829103	1.936381
51	1	0	6.176961	-1.046300	-0.823804
52	1	0	5.773226	-2.670333	-0.255292
53	1	0	4.165244	0.175312	3.137100
54	1	0	5.643817	-0.374054	3.930890
55	1	0	4.360842	-1.520259	3.574267
56	1	0	2.129793	-0.521845	-2.652572
57	1	0	1.025095	-5.731383	3.294669
58	1	0	-0.941118	-6.679223	2.139486
59	1	0	-1.833596	-5.585829	0.087386
60	1	0	2.122239	-3.717553	2.466571
61	1	0	-1.677768	-2.841771	-2.703496
62	1	0	-2.633586	-3.647735	-1.438789
63	1	0	-1.502037	-4.599861	-2.442303
64	6	0	-1.879647	2.133760	2.258334
65	6	0	-2.560063	3.182577	1.638787
66	6	0	-2.782345	4.365496	2.332737
67	6	0	-2.356866	4.494694	3.654386
68	6	0	-1.695845	3.440635	4.277884
69	6	0	-1.445830	2.264382	3.577620
70	6	0	-1.676345	0.848637	1.517097
71	7	0	-2.807975	0.399544	1.039201
72	6	0	-0.349974	0.276564	1.581067
73	6	0	0.798284	1.178759	1.841143
74	8	0	1.790494	0.862063	2.479889
75	6	0	1.718676	3.327022	1.375325
76	8	0	0.679187	2.344100	1.199721
77	6	0	-0.055026	-1.078860	1.636091
78	16	0	-2.946741	-0.870978	0.015778
79	8	0	-2.079895	-0.662178	-1.165302
80	8	0	-2.863596	-2.172800	0.690526
81	6	0	-4.622767	-0.661222	-0.521330
82	6	0	-5.566045	-1.615232	-0.173476
83	6	0	-6.873789	-1.462166	-0.627500
84	6	0	-7.235268	-0.372946	-1.417830
85	6	0	-6.257799	0.570993	-1.754781
86	6	0	-4.950246	0.435906	-1.315101
87	6	0	-8.652435	-0.198919	-1.900111
88	6	0	1.535957	4.076698	2.680227
89	1	0	-2.883622	3.060141	0.613174
90	1	0	-3.294498	5.186327	1.846651
91	1	0	-2.544417	5.413254	4.196193

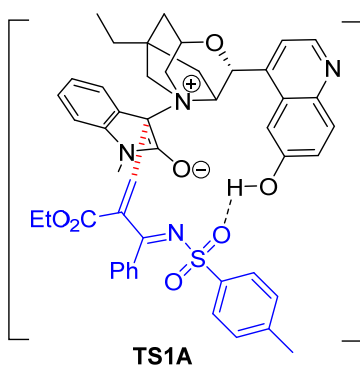
92	1	0	-1.372428	3.533432	5.306966
93	1	0	-0.929177	1.441168	4.056814
94	1	0	2.686447	2.830465	1.329167
95	1	0	1.607407	3.980344	0.513316
96	1	0	0.811865	-1.352529	2.218048
97	1	0	-0.840785	-1.818465	1.568647
98	1	0	-5.272945	-2.456246	0.440143
99	1	0	-7.621476	-2.200426	-0.363252
100	1	0	-6.528577	1.419295	-2.372505
101	1	0	-4.197203	1.167799	-1.580723
102	1	0	-9.112721	0.676919	-1.437393
103	1	0	-8.681024	-0.053002	-2.981517
104	1	0	-9.260784	-1.069567	-1.655981
105	1	0	2.286986	4.865170	2.759370
106	1	0	1.649851	3.399018	3.526367
107	1	0	0.543969	4.527077	2.720228



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.743110	-5.098158	-0.378229
2	6	0	1.696176	-5.924403	0.256997
3	6	0	0.758846	-3.742785	-0.157410
4	6	0	1.776954	-3.204998	0.686145
5	6	0	2.688930	-4.136555	1.262251
6	7	0	2.632829	-5.478518	1.056016
7	6	0	1.946319	-1.820434	0.939221
8	6	0	3.016722	-1.378561	1.688873
9	6	0	3.907797	-2.310367	2.285876
10	6	0	3.739719	-3.648821	2.083510
11	8	0	3.303790	-0.079405	1.893611
12	6	0	-1.358636	-2.458498	0.193614
13	8	0	-0.861098	-3.582792	-1.893363
14	6	0	-3.749205	-2.116809	-0.063542
15	6	0	-2.298271	-1.644359	-1.962482

16	7	0	-2.424921	-1.495329	-0.468475
17	6	0	-2.181656	-3.679016	0.641285
18	6	0	-2.144798	-3.122664	-2.289015
19	6	0	-3.487859	-3.607612	-0.156997
20	6	0	-4.621004	-4.475851	0.402594
21	6	0	-3.250389	-3.959814	-1.634948
22	6	0	-5.120979	-4.115254	1.802286
23	6	0	-0.275331	-2.851090	-0.817989
24	6	0	-5.528001	1.879429	-1.185014
25	6	0	-5.508983	2.804937	-0.145628
26	6	0	-4.533968	2.732968	0.850528
27	6	0	-3.603595	1.710084	0.773820
28	6	0	-3.593075	0.761160	-0.273960
29	6	0	-4.568637	0.867225	-1.264088
30	7	0	-2.577760	1.423154	1.659187
31	6	0	-1.880128	0.302534	1.262758
32	6	0	-2.407416	-0.067331	-0.048738
33	8	0	-0.928002	-0.165541	1.899591
34	6	0	-2.266824	2.195286	2.844111
35	6	0	1.088542	2.816989	1.566454
36	6	0	1.452240	4.164131	1.578779
37	6	0	1.830842	4.769469	2.769713
38	6	0	1.856711	4.034826	3.953195
39	6	0	1.509790	2.689242	3.937331
40	6	0	1.131709	2.075330	2.745551
41	6	0	0.796638	2.127039	0.263467
42	7	0	1.815268	1.388374	-0.122450
43	6	0	-0.447368	2.278675	-0.454055
44	6	0	-1.255211	3.513511	-0.343740
45	8	0	-1.179185	4.361635	0.522442
46	6	0	-2.845102	4.870395	-1.421836
47	8	0	-2.102199	3.640695	-1.387058
48	6	0	-0.933878	1.226874	-1.217081
49	16	0	2.090122	0.928934	-1.711227
50	8	0	1.625547	-0.452943	-1.936071
51	8	0	1.670287	1.963421	-2.656131
52	6	0	3.859366	0.884279	-1.684816
53	6	0	4.504334	-0.261975	-1.235260
54	6	0	5.892335	-0.276178	-1.206853
55	6	0	6.632690	0.832600	-1.624737
56	6	0	5.953869	1.962334	-2.086474
57	6	0	4.565292	1.998824	-2.118897
58	6	0	8.137861	0.814995	-1.557458
59	6	0	-3.661309	4.854321	-2.695480
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61	1	0	1.671185	-6.995829	0.085726

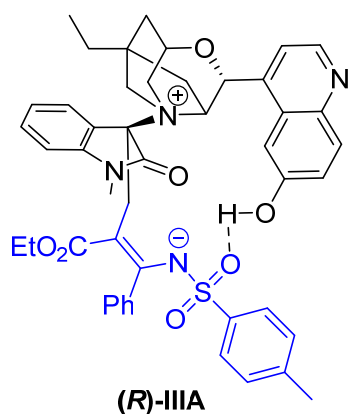
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65	1	0	2.795206	0.491957	1.277405
66	1	0	-0.923638	-1.905216	1.019155
67	1	0	-4.535773	-1.732160	-0.709462
68	1	0	-3.933484	-1.793505	0.960115
69	1	0	-3.189789	-1.222587	-2.418398
70	1	0	-1.429901	-1.086468	-2.298878
71	1	0	-2.388083	-3.607464	1.709404
72	1	0	-1.632298	-4.601998	0.464100
73	1	0	-2.191226	-3.241184	-3.372338
74	1	0	-4.270008	-5.512139	0.395462
75	1	0	-5.462851	-4.432756	-0.295614
76	1	0	-2.977308	-5.013210	-1.732517
77	1	0	-4.185006	-3.807414	-2.186360
78	1	0	-4.321427	-4.134995	2.543901
79	1	0	-5.876805	-4.834488	2.119314
80	1	0	-5.583739	-3.127130	1.826034
81	1	0	0.233729	-1.966106	-1.205430
82	1	0	-6.289338	1.947261	-1.951641
83	1	0	-6.252425	3.590892	-0.108961
84	1	0	-4.500076	3.453401	1.657312
85	1	0	-4.610311	0.183911	-2.102807
86	1	0	-1.513385	1.645479	3.400269
87	1	0	-3.165518	2.307789	3.453529
88	1	0	-1.872161	3.173415	2.565895
89	1	0	1.425396	4.737075	0.662052
90	1	0	2.107176	5.816249	2.772941
91	1	0	2.153456	4.509692	4.880071
92	1	0	1.541041	2.106505	4.849331
93	1	0	0.855329	1.029851	2.727912
94	1	0	-3.472660	4.928642	-0.533620
95	1	0	-2.141499	5.702561	-1.396267
96	1	0	-1.714252	1.416447	-1.938645
97	1	0	-0.307651	0.365966	-1.380979
98	1	0	3.928405	-1.124807	-0.927099
99	1	0	6.408272	-1.162770	-0.857990
100	1	0	6.519775	2.821222	-2.427082
101	1	0	4.030031	2.865039	-2.483908
102	1	0	8.479178	1.116204	-0.563936
103	1	0	8.528077	-0.184357	-1.752904
104	1	0	8.572835	1.503465	-2.282340
105	1	0	-4.244453	5.773243	-2.775574
106	1	0	-4.343207	4.004058	-2.692870
107	1	0	-3.007865	4.778967	-3.565065



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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2	6	0	2.199113	-5.933453	2.738755
3	6	0	0.940407	-4.504834	1.259385
4	6	0	2.000636	-3.552116	1.361961
5	6	0	3.094182	-3.907077	2.205824
6	7	0	3.181949	-5.080975	2.884656
7	6	0	2.028141	-2.309156	0.675394
8	6	0	3.096069	-1.453091	0.843223
9	6	0	4.178671	-1.803025	1.692893
10	6	0	4.174407	-2.996974	2.350562
11	8	0	3.210154	-0.264286	0.220240
12	6	0	-1.173986	-3.167119	1.113715
13	8	0	-1.029050	-5.457751	0.318285
14	6	0	-3.585058	-2.934550	1.312714
15	6	0	-2.681858	-4.009863	-0.671544
16	7	0	-2.479783	-2.866202	0.288489
17	6	0	-1.695399	-3.640066	2.480195
18	6	0	-2.422957	-5.307689	0.079968
19	6	0	-3.143826	-4.067585	2.221956
20	6	0	-4.014689	-4.204051	3.475560
21	6	0	-3.205967	-5.369132	1.400398
22	6	0	-3.973720	-3.026034	4.451761
23	6	0	-0.304002	-4.235230	0.432243
24	6	0	-5.915496	-0.014316	-1.267091
25	6	0	-5.450623	0.771095	-2.320435
26	6	0	-4.096411	0.774334	-2.650552
27	6	0	-3.245582	-0.052800	-1.934551
28	6	0	-3.694518	-0.895429	-0.876038
29	6	0	-5.049706	-0.823586	-0.528700
30	7	0	-1.896027	-0.264273	-2.144792
31	6	0	-1.443304	-1.294273	-1.337265

32	6	0	-2.508980	-1.581260	-0.416945
33	8	0	-0.319976	-1.814181	-1.425144
34	6	0	-1.067580	0.414647	-3.112088
35	1	0	0.287072	-6.441807	1.861619
36	1	0	2.284895	-6.873013	3.275396
37	1	0	1.244242	-2.040638	-0.023414
38	1	0	4.992361	-1.096731	1.790389
39	1	0	4.986401	-3.296628	2.999630
40	1	0	2.375223	-0.001987	-0.211974
41	1	0	-0.612750	-2.243383	1.155684
42	1	0	-4.520270	-3.130899	0.792300
43	1	0	-3.629339	-1.964563	1.808962
44	1	0	-3.698991	-3.928879	-1.052158
45	1	0	-1.977249	-3.876975	-1.489539
46	1	0	-1.674329	-2.812662	3.190689
47	1	0	-1.076674	-4.445313	2.874898
48	1	0	-2.712797	-6.147162	-0.553216
49	1	0	-3.711270	-5.116802	3.997112
50	1	0	-5.046249	-4.370379	3.146923
51	1	0	-2.808515	-6.203513	1.982913
52	1	0	-4.257041	-5.589232	1.181306
53	1	0	-3.007397	-2.956975	4.952731
54	1	0	-4.729662	-3.165818	5.225775
55	1	0	-4.169649	-2.069217	3.964662
56	1	0	-0.011828	-3.870545	-0.552802
57	1	0	-6.965355	0.007806	-1.002322
58	1	0	-6.136923	1.398879	-2.873806
59	1	0	-3.716340	1.397405	-3.449755
60	1	0	-5.452394	-1.380064	0.304501
61	1	0	-0.066471	0.003301	-3.014864
62	1	0	-1.037403	1.483745	-2.894759
63	1	0	-1.443192	0.252094	-4.124737
64	6	0	-3.084667	3.355019	0.060792
65	6	0	-2.809709	4.709803	-0.152610
66	6	0	-3.827303	5.579456	-0.519599
67	6	0	-5.125173	5.101508	-0.693787
68	6	0	-5.398584	3.751097	-0.499641
69	6	0	-4.384000	2.881139	-0.117389
70	6	0	-1.977216	2.435604	0.438562
71	7	0	-0.822448	2.806385	-0.034978
72	6	0	-2.267157	1.240716	1.237715
73	6	0	-3.346916	1.199357	2.251657
74	8	0	-3.827768	0.162389	2.680688
75	6	0	-4.757596	2.428716	3.688644
76	8	0	-3.691125	2.403603	2.719095
77	6	0	-1.540376	0.089714	1.157445

78	16	0	0.640204	2.143624	0.368911
79	8	0	0.786898	1.788141	1.779801
80	8	0	0.939574	1.101692	-0.639838
81	6	0	1.686170	3.534201	0.048286
82	6	0	2.562499	3.945990	1.040481
83	6	0	3.424036	5.006433	0.772990
84	6	0	3.415923	5.643467	-0.466552
85	6	0	2.519486	5.202372	-1.447766
86	6	0	1.654939	4.147800	-1.201561
87	6	0	4.366605	6.774185	-0.762847
88	6	0	-6.108595	2.323873	3.005994
89	1	0	-1.797166	5.064834	-0.016861
90	1	0	-3.610678	6.629602	-0.668459
91	1	0	-5.917759	5.779888	-0.984422
92	1	0	-6.398961	3.365155	-0.652042
93	1	0	-4.598103	1.828232	0.014077
94	1	0	-4.603160	1.617560	4.396939
95	1	0	-4.637774	3.384528	4.192769
96	1	0	-0.648635	-0.010990	0.561075
97	1	0	-1.718837	-0.655001	1.918197
98	1	0	2.559986	3.442831	1.997642
99	1	0	4.112270	5.341074	1.539680
100	1	0	2.503872	5.694232	-2.413282
101	1	0	0.957061	3.805946	-1.954563
102	1	0	3.859894	7.584281	-1.289518
103	1	0	4.798010	7.176296	0.153592
104	1	0	5.186435	6.429312	-1.397505
105	1	0	-6.904707	2.376510	3.751075
106	1	0	-6.189571	1.374141	2.476724
107	1	0	-6.236874	3.139311	2.294491

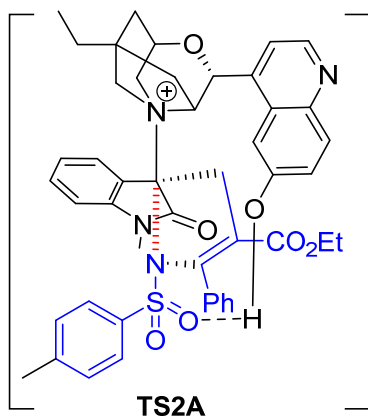


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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2	6	0	6.952292	0.268307	0.475155
3	6	0	4.624557	0.306713	-0.149540
4	6	0	4.403451	1.244465	0.906597
5	6	0	5.550522	1.607436	1.674723
6	7	0	6.799201	1.119239	1.458103
7	6	0	3.146080	1.827766	1.219462
8	6	0	3.039509	2.723036	2.267067
9	6	0	4.188078	3.087675	3.021563
10	6	0	5.403135	2.544657	2.731253
11	8	0	1.895505	3.319910	2.635115
12	6	0	2.533364	-1.075947	-0.276731
13	8	0	4.073554	-0.881122	-2.142408
14	6	0	1.312085	-3.076683	-0.961386
15	6	0	1.770261	-1.389179	-2.626928
16	7	0	1.358607	-1.579940	-1.192741
17	6	0	3.212897	-2.367956	0.203150
18	6	0	3.220410	-1.837501	-2.755460
19	6	0	2.776323	-3.442339	-0.797825
20	6	0	2.976733	-4.886445	-0.324941
21	6	0	3.451674	-3.235735	-2.164723
22	6	0	2.388292	-5.231315	1.045504
23	6	0	3.498474	-0.166771	-1.050896
24	6	0	-2.745569	-3.094774	-2.623026
25	6	0	-3.242370	-2.087435	-3.444401
26	6	0	-2.694883	-0.805037	-3.422126
27	6	0	-1.624981	-0.578665	-2.571133
28	6	0	-1.102634	-1.580579	-1.743353
29	6	0	-1.685547	-2.839773	-1.748279
30	7	0	-0.924891	0.618036	-2.407467
31	6	0	0.013844	0.497407	-1.428792
32	6	0	-0.013215	-0.957913	-0.891850
33	8	0	0.813286	1.346816	-1.088687
34	6	0	-1.369148	1.898592	-2.918916
35	6	0	-4.076750	-0.427634	0.890890
36	6	0	-4.885920	0.506379	1.541962
37	6	0	-6.265671	0.333319	1.563891
38	6	0	-6.849815	-0.746759	0.906763
39	6	0	-6.047291	-1.660010	0.227868
40	6	0	-4.666143	-1.502347	0.223228
41	6	0	-2.603204	-0.201235	0.842914
42	7	0	-2.237766	1.045030	0.359461
43	6	0	-1.674232	-1.184263	1.052968
44	6	0	-1.933213	-2.538100	1.550351
45	8	0	-1.183558	-3.488010	1.321926
46	6	0	-3.360937	-3.988347	2.753380
47	8	0	-3.018326	-2.661983	2.317521

48	6	0	-0.244070	-0.952840	0.649259
49	16	0	-1.619885	2.153783	1.304982
50	8	0	-2.476164	2.490911	2.455160
51	8	0	-0.188269	1.925664	1.686072
52	6	0	-1.610828	3.536279	0.185844
53	6	0	-0.428545	4.195808	-0.113804
54	6	0	-0.463658	5.278177	-0.991256
55	6	0	-1.662723	5.706821	-1.558959
56	6	0	-2.842670	5.028811	-1.230058
57	6	0	-2.824479	3.951145	-0.356707
58	6	0	-1.699165	6.899100	-2.480719
59	6	0	-2.593088	-4.356390	4.008842
60	1	0	6.097175	-0.857496	-1.161089
61	1	0	7.955764	-0.109361	0.307325
62	1	0	2.262658	1.617918	0.629595
63	1	0	4.053166	3.797889	3.826414
64	1	0	6.293914	2.800069	3.289509
65	1	0	1.103608	2.848160	2.284684
66	1	0	2.089088	-0.507139	0.529696
67	1	0	0.834167	-3.541073	-1.821343
68	1	0	0.716266	-3.269085	-0.070767
69	1	0	1.088815	-1.969991	-3.245831
70	1	0	1.683382	-0.336855	-2.885997
71	1	0	2.854936	-2.618486	1.202137
72	1	0	4.294378	-2.241849	0.247879
73	1	0	3.485812	-1.842291	-3.813136
74	1	0	4.051651	-5.090124	-0.319624
75	1	0	2.544514	-5.548524	-1.082628
76	1	0	4.530430	-3.387858	-2.085936
77	1	0	3.060551	-3.985360	-2.861590
78	1	0	2.915996	-4.719149	1.850585
79	1	0	2.486648	-6.302451	1.225421
80	1	0	1.327915	-4.981961	1.123202
81	1	0	2.953429	0.704534	-1.416892
82	1	0	-3.199788	-4.076657	-2.637354
83	1	0	-4.077914	-2.293352	-4.100892
84	1	0	-3.096923	-0.013191	-4.039104
85	1	0	-1.363307	-3.602417	-1.053201
86	1	0	-0.673087	2.655908	-2.566306
87	1	0	-2.362402	2.118788	-2.526004
88	1	0	-1.382440	1.884036	-4.009368
89	1	0	-4.419326	1.350125	2.036119
90	1	0	-6.886830	1.048538	2.088628
91	1	0	-7.925868	-0.870462	0.914646
92	1	0	-6.497419	-2.490163	-0.302984
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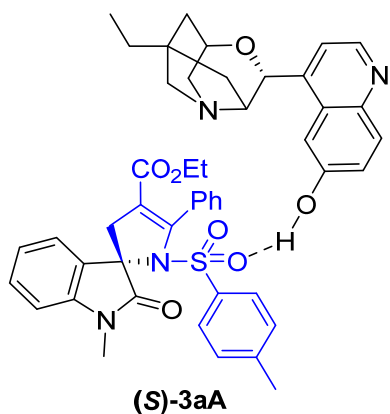
94	1	0	-4.432184	-3.939963	2.937181
95	1	0	-3.158231	-4.689975	1.945890
96	1	0	0.359185	-1.737264	1.102833
97	1	0	0.102126	0.006352	1.030124
98	1	0	0.502061	3.862925	0.323196
99	1	0	0.456478	5.796703	-1.234262
100	1	0	-3.781864	5.355796	-1.661851
101	1	0	-3.730193	3.413156	-0.105742
102	1	0	-0.721670	7.081180	-2.928022
103	1	0	-2.424701	6.755674	-3.282880
104	1	0	-1.987592	7.799493	-1.932701
105	1	0	-2.924478	-5.328813	4.378116
106	1	0	-2.764611	-3.611389	4.785925
107	1	0	-1.526952	-4.407682	3.792849



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.958734	0.827331	-0.087861
2	6	0	-6.881297	0.956448	-1.149849
3	6	0	-4.620361	1.014865	-0.326673
4	6	0	-4.202125	1.360580	-1.648447
5	6	0	-5.222784	1.446396	-2.636540
6	7	0	-6.542688	1.243339	-2.382118
7	6	0	-2.853933	1.619647	-2.016315
8	6	0	-2.538685	1.925504	-3.323064
9	6	0	-3.557576	1.997511	-4.310563
10	6	0	-4.858733	1.769070	-3.971346
11	8	0	-1.290493	2.181530	-3.757366
12	6	0	-2.791625	-0.444174	0.558102
13	8	0	-4.275765	0.758719	2.031870
14	6	0	-1.770468	-1.976222	2.071297
15	6	0	-2.016203	0.297945	2.754012

16	7	0	-1.688753	-0.570992	1.598457
17	6	0	-3.659780	-1.711807	0.724251
18	6	0	-3.504046	0.137389	3.063610
19	6	0	-3.276940	-2.241289	2.111866
20	6	0	-3.636361	-3.705432	2.381785
21	6	0	-3.878197	-1.343728	3.209667
22	6	0	-3.211685	-4.709109	1.307002
23	6	0	-3.605900	0.836155	0.777806
24	6	0	2.266139	-2.167358	3.359997
25	6	0	2.567160	-1.047020	4.131975
26	6	0	2.118014	0.229356	3.780339
27	6	0	1.357542	0.338949	2.627898
28	6	0	1.047915	-0.781552	1.840106
29	6	0	1.503491	-2.041560	2.196452
30	7	0	0.793731	1.481344	2.073199
31	6	0	0.088920	1.184120	0.929047
32	6	0	0.263114	-0.301439	0.694976
33	8	0	-0.599589	1.969374	0.308763
34	6	0	0.846671	2.802490	2.655637
35	6	0	3.741182	-1.446315	-1.178400
36	6	0	4.162180	-1.977574	-2.397041
37	6	0	5.497148	-2.313858	-2.581750
38	6	0	6.416219	-2.131735	-1.550605
39	6	0	5.999668	-1.597708	-0.334758
40	6	0	4.667891	-1.241427	-0.153295
41	6	0	2.335645	-1.046779	-0.922440
42	7	0	2.124539	0.228512	-0.372515
43	6	0	1.219084	-1.815902	-0.969021
44	6	0	1.125303	-3.280278	-1.058333
45	8	0	0.227752	-3.912483	-0.517504
46	6	0	2.112584	-5.306332	-1.767004
47	8	0	2.108785	-3.864532	-1.744261
48	6	0	-0.035372	-1.082041	-0.552492
49	16	0	2.269600	1.447839	-1.457247
50	8	0	3.416317	1.233915	-2.340233
51	8	0	0.977708	1.731808	-2.113531
52	6	0	2.627744	2.835209	-0.405364
53	6	0	1.855238	3.984341	-0.494497
54	6	0	2.226467	5.103023	0.247819
55	6	0	3.357576	5.081930	1.064406
56	6	0	4.112946	3.905275	1.139871
57	6	0	3.759167	2.782101	0.404138
58	6	0	3.780122	6.311230	1.827713
59	6	0	1.163186	-5.829532	-2.827613
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61	1	0	-7.939275	0.807364	-0.958468

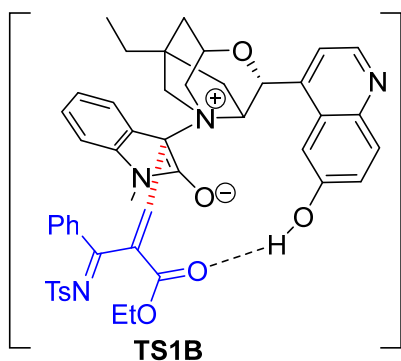
62	1	0	-2.060996	1.624787	-1.279487
63	1	0	-3.263580	2.242652	-5.322499
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65	1	0	-0.618091	2.038270	-3.066475
66	1	0	-2.343624	-0.392469	-0.427956
67	1	0	-1.271722	-2.073250	3.036001
68	1	0	-1.272039	-2.633759	1.356233
69	1	0	-1.392495	0.001027	3.597793
70	1	0	-1.805190	1.339060	2.516281
71	1	0	-3.395742	-2.441325	-0.043209
72	1	0	-4.721680	-1.484507	0.629022
73	1	0	-3.749440	0.670755	3.983493
74	1	0	-4.719800	-3.770652	2.524194
75	1	0	-3.186757	-3.986623	3.340552
76	1	0	-4.968742	-1.419474	3.202712
77	1	0	-3.528718	-1.700567	4.185711
78	1	0	-3.791159	-4.583169	0.391783
79	1	0	-3.384042	-5.725981	1.662745
80	1	0	-2.154559	-4.625338	1.047169
81	1	0	-2.929770	1.694938	0.764468
82	1	0	2.629983	-3.140610	3.660008
83	1	0	3.164999	-1.163444	5.027175
84	1	0	2.363674	1.095124	4.380727
85	1	0	1.260220	-2.906020	1.592468
86	1	0	0.242848	3.455961	2.031368
87	1	0	1.873291	3.169834	2.670531
88	1	0	0.442875	2.782641	3.670820
89	1	0	3.444298	-2.104198	-3.194971
90	1	0	5.823753	-2.710141	-3.534897
91	1	0	7.455600	-2.396987	-1.698807
92	1	0	6.711991	-1.452241	0.467762
93	1	0	4.328045	-0.815638	0.783614
94	1	0	3.145894	-5.563645	-1.988883
95	1	0	1.845219	-5.673536	-0.777979
96	1	0	-0.824244	-1.812483	-0.396939
97	1	0	-0.341325	-0.377292	-1.328814
98	1	0	0.978161	3.987788	-1.126833
99	1	0	1.631501	6.006770	0.185432
100	1	0	4.993736	3.878277	1.771159
101	1	0	4.347163	1.873380	0.443081
102	1	0	4.497322	6.894473	1.244851
103	1	0	2.926783	6.954685	2.043376
104	1	0	4.260104	6.045467	2.770455
105	1	0	1.233744	-6.917309	-2.884704
106	1	0	1.418578	-5.413343	-3.802478
107	1	0	0.137905	-5.558773	-2.580100



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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2	6	0	6.737087	-0.392018	1.998446
3	6	0	4.621309	0.338838	1.114463
4	6	0	4.024086	-0.096698	2.336063
5	6	0	4.888120	-0.686489	3.299034
6	7	0	6.229134	-0.831895	3.122896
7	6	0	2.640511	0.037546	2.630812
8	6	0	2.142672	-0.421376	3.829334
9	6	0	3.001774	-1.026221	4.784068
10	6	0	4.335427	-1.148573	4.523389
11	8	0	0.843013	-0.331658	4.187982
12	6	0	2.954498	-0.166194	-0.700896
13	8	0	4.605103	1.575553	-0.931187
14	6	0	2.120848	-0.361813	-2.884071
15	6	0	2.462898	1.820063	-2.010492
16	7	0	1.991010	0.467603	-1.670655
17	6	0	3.874166	-1.096107	-1.534818
18	6	0	3.974716	1.797106	-2.200324
19	6	0	3.628865	-0.636498	-2.978358
20	6	0	4.054303	-1.639950	-4.053477
21	6	0	4.352821	0.705239	-3.212080
22	6	0	3.282794	-2.960656	-4.075504
23	6	0	3.768738	0.918441	0.015182
24	6	0	-1.995744	-0.093464	-4.229873
25	6	0	-1.792851	1.242757	-4.552363
26	6	0	-1.321749	2.154779	-3.601432
27	6	0	-1.068347	1.672039	-2.329440
28	6	0	-1.276824	0.332578	-1.985774
29	6	0	-1.742577	-0.558598	-2.932307
30	7	0	-0.541993	2.366571	-1.237677

31	6	0	-0.248679	1.509883	-0.207022
32	6	0	-0.966985	0.172637	-0.510744
33	8	0	0.418016	1.789492	0.768222
34	6	0	-0.205001	3.770017	-1.238197
35	6	0	-3.994235	-1.792841	0.251618
36	6	0	-4.426734	-2.787638	1.128657
37	6	0	-5.764032	-3.158989	1.147377
38	6	0	-6.674217	-2.545566	0.289298
39	6	0	-6.245610	-1.549432	-0.582955
40	6	0	-4.910717	-1.163612	-0.594184
41	6	0	-2.586358	-1.364631	0.187611
42	7	0	-2.326799	0.063801	0.161012
43	6	0	-1.437966	-2.051350	0.026719
44	6	0	-1.201091	-3.495182	-0.163819
45	8	0	-0.082229	-3.949667	-0.271877
46	6	0	-2.126658	-5.652137	-0.398688
47	8	0	-2.316510	-4.230859	-0.237174
48	6	0	-0.261273	-1.113470	-0.107311
49	16	0	-2.546055	0.743641	1.723313
50	8	0	-3.855347	0.293392	2.165651
51	8	0	-1.384517	0.484553	2.572832
52	6	0	-2.627654	2.472351	1.359031
53	6	0	-1.825279	3.353083	2.071734
54	6	0	-1.984911	4.718008	1.856788
55	6	0	-2.927667	5.198166	0.946089
56	6	0	-3.714494	4.282053	0.237666
57	6	0	-3.579785	2.916823	0.445617
58	6	0	-3.115312	6.679131	0.743034
59	6	0	-1.809976	-6.305216	0.933030
60	1	0	6.457336	0.545148	0.059527
61	1	0	7.809703	-0.503946	1.874508
62	1	0	1.965883	0.525373	1.938038
63	1	0	2.564564	-1.372439	5.711179
64	1	0	5.016991	-1.596754	5.234183
65	1	0	0.299316	0.050040	3.479948
66	1	0	2.395738	-0.734249	0.039513
67	1	0	1.689681	0.153793	-3.745989
68	1	0	1.570740	-1.296579	-2.742326
69	1	0	1.958630	2.141575	-2.924623
70	1	0	2.195253	2.519625	-1.218102
71	1	0	3.569186	-2.135766	-1.404515
72	1	0	4.919579	-1.010293	-1.237202
73	1	0	4.344995	2.763069	-2.549866
74	1	0	5.121952	-1.843938	-3.921089
75	1	0	3.955247	-1.159187	-5.032755
76	1	0	5.435772	0.554983	-3.172805

77	1	0	4.108171	1.070099	-4.217065
78	1	0	3.319445	-3.472900	-3.113023
79	1	0	3.710726	-3.631960	-4.821666
80	1	0	2.233951	-2.807656	-4.334955
81	1	0	3.076048	1.637368	0.464153
82	1	0	-2.353868	-0.781610	-4.983866
83	1	0	-1.997512	1.588358	-5.557645
84	1	0	-1.157854	3.193773	-3.855702
85	1	0	-1.911784	-1.597900	-2.681022
86	1	0	0.271196	3.990385	-0.285687
87	1	0	-1.113010	4.367481	-1.337041
88	1	0	0.479693	4.006460	-2.054921
89	1	0	-3.716442	-3.249238	1.800489
90	1	0	-6.099539	-3.921439	1.838598
91	1	0	-7.716491	-2.838040	0.307448
92	1	0	-6.951294	-1.068600	-1.248368
93	1	0	-4.563516	-0.384714	-1.262336
94	1	0	-3.073509	-6.002037	-0.802986
95	1	0	-1.330958	-5.818214	-1.122158
96	1	0	0.433816	-1.445620	-0.872383
97	1	0	0.278119	-1.000171	0.836813
98	1	0	-1.084665	2.968730	2.759015
99	1	0	-1.366714	5.419275	2.404132
100	1	0	-4.446558	4.645960	-0.473447
101	1	0	-4.194607	2.201902	-0.086384
102	1	0	-2.214695	7.231112	1.011798
103	1	0	-3.365369	6.906413	-0.293973
104	1	0	-3.931799	7.048204	1.368445
105	1	0	-1.739711	-7.387105	0.807997
106	1	0	-2.597207	-6.090488	1.656723
107	1	0	-0.859278	-5.938155	1.317129

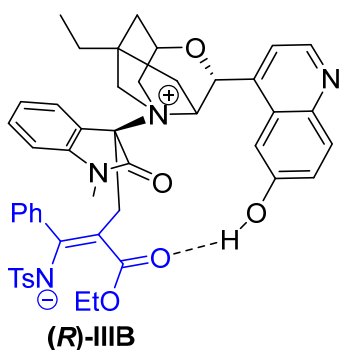


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

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3	6	0	-5.391822	-0.075240	-0.346472
4	6	0	-5.104784	1.174177	-0.976958
5	6	0	-5.921187	1.536257	-2.083502
6	7	0	-6.974849	0.794836	-2.518339
7	6	0	-4.056094	2.042717	-0.572328
8	6	0	-3.783088	3.183134	-1.294035
9	6	0	-4.583304	3.533556	-2.413576
10	6	0	-5.629506	2.738088	-2.782929
11	8	0	-2.776478	4.037142	-1.002657
12	6	0	-3.129515	-0.958733	0.164385
13	8	0	-5.083043	-1.774110	1.322152
14	6	0	-1.501991	-2.660217	0.719220
15	6	0	-2.951485	-1.803254	2.484576
16	7	0	-2.128425	-1.407284	1.281624
17	6	0	-3.209011	-2.158742	-0.791596
18	6	0	-4.147819	-2.612913	1.999784
19	6	0	-2.670844	-3.341101	0.021607
20	6	0	-2.271564	-4.563265	-0.812812
21	6	0	-3.693841	-3.764488	1.093208
22	6	0	-1.193037	-4.342083	-1.874637
23	6	0	-4.499359	-0.605442	0.754087
24	6	0	2.372517	-1.557195	2.793070
25	6	0	2.737214	-0.344754	3.384675
26	6	0	1.856910	0.731484	3.366127
27	6	0	0.611767	0.546290	2.776915
28	6	0	0.216577	-0.670799	2.157095
29	6	0	1.142028	-1.723527	2.164449
30	7	0	-0.442973	1.439038	2.746485
31	6	0	-1.553806	0.845739	2.174178
32	6	0	-1.112021	-0.413054	1.645003
33	8	0	-2.686087	1.365469	2.163294
34	6	0	-0.488338	2.720619	3.406318
35	6	0	3.202543	1.095953	-0.881874
36	6	0	4.168186	1.050003	0.122726
37	6	0	5.416335	1.615891	-0.101856
38	6	0	5.699636	2.233910	-1.319439
39	6	0	4.730577	2.282503	-2.316637
40	6	0	3.476919	1.715975	-2.098316
41	6	0	1.848951	0.497564	-0.668107
42	7	0	1.553439	-0.743790	-0.851809
43	6	0	0.707297	1.357434	-0.315422
44	6	0	0.766974	2.750571	0.172756
45	8	0	-0.216078	3.462782	0.308945
46	6	0	2.125756	4.580250	0.779685

47	8	0	1.997319	3.182534	0.455983
48	6	0	-0.542166	0.849901	-0.482717
49	16	0	2.458681	-1.959604	-1.541823
50	8	0	1.988862	-3.162258	-0.849736
51	8	0	2.292196	-1.832756	-2.988258
52	6	0	4.192940	-1.825542	-1.187428
53	6	0	5.042589	-1.288068	-2.148287
54	6	0	6.395136	-1.185636	-1.858346
55	6	0	6.902560	-1.612008	-0.627200
56	6	0	6.028936	-2.174733	0.304938
57	6	0	4.671460	-2.291822	0.029853
58	6	0	8.366918	-1.445798	-0.314471
59	6	0	3.608312	4.861748	0.888793
60	1	0	-6.713629	-1.745096	-0.325457
61	1	0	-8.085339	-0.892320	-2.224925
62	1	0	-3.502972	1.850969	0.339859
63	1	0	-4.341800	4.443912	-2.945785
64	1	0	-6.265561	2.987208	-3.621945
65	1	0	-2.162647	3.682080	-0.335962
66	1	0	-2.704068	-0.079652	-0.292733
67	1	0	-1.072920	-3.230902	1.540503
68	1	0	-0.711851	-2.352536	0.031595
69	1	0	-2.297763	-2.376083	3.140970
70	1	0	-3.256389	-0.886318	2.983125
71	1	0	-2.577289	-1.983215	-1.662787
72	1	0	-4.231676	-2.314343	-1.134445
73	1	0	-4.673537	-3.015303	2.866934
74	1	0	-3.183541	-4.940623	-1.286445
75	1	0	-1.938993	-5.347044	-0.124078
76	1	0	-4.579974	-4.188527	0.615159
77	1	0	-3.245546	-4.547826	1.714763
78	1	0	-1.489476	-3.593489	-2.611032
79	1	0	-1.023598	-5.273516	-2.416642
80	1	0	-0.237164	-4.039608	-1.445743
81	1	0	-4.371258	0.165153	1.513385
82	1	0	3.059459	-2.393347	2.824989
83	1	0	3.703711	-0.242278	3.861927
84	1	0	2.115852	1.679755	3.819860
85	1	0	0.947592	-2.659829	1.664368
86	1	0	0.256868	3.395693	2.986336
87	1	0	-0.316639	2.606395	4.479139
88	1	0	-1.480028	3.130950	3.232712
89	1	0	3.934256	0.572186	1.065924
90	1	0	6.171492	1.572113	0.673433
91	1	0	6.674558	2.673897	-1.489736
92	1	0	4.946861	2.759490	-3.264207

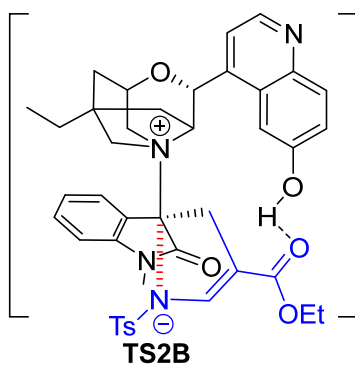
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94	1	0	1.599249	4.778613	1.713242
95	1	0	1.648578	5.165079	-0.006062
96	1	0	-1.395687	1.497379	-0.356514
97	1	0	-0.662909	-0.096376	-0.987109
98	1	0	4.639700	-0.960140	-3.096357
99	1	0	7.068647	-0.761492	-2.593932
100	1	0	6.417208	-2.531665	1.251541
101	1	0	3.987235	-2.740317	0.735703
102	1	0	8.598141	-0.394701	-0.122235
103	1	0	8.650974	-2.019878	0.567344
104	1	0	8.986882	-1.770818	-1.151407
105	1	0	3.770279	5.913196	1.130379
106	1	0	4.106844	4.631815	-0.053098
107	1	0	4.055762	4.247608	1.670848



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	6.628269	-0.320056	-0.541103
2	6	0	7.728317	0.491352	-0.184004
3	6	0	5.367695	0.224093	-0.598204
4	6	0	5.213997	1.612259	-0.296689
5	6	0	6.397033	2.323731	0.062714
6	7	0	7.633103	1.762453	0.114111
7	6	0	3.978245	2.301944	-0.325935
8	6	0	3.911354	3.631795	0.036943
9	6	0	5.090690	4.341851	0.382731
10	6	0	6.296626	3.702174	0.387420
11	8	0	2.754528	4.317161	0.076287
12	6	0	3.212143	-0.815263	0.197720
13	8	0	4.702734	-1.927334	-1.370787
14	6	0	1.931576	-2.725063	0.993682
15	6	0	2.380905	-2.564221	-1.375327
16	7	0	2.001590	-1.756211	-0.164763
17	6	0	3.884303	-1.515264	1.390028

18	6	0	3.819178	-3.025090	-1.203746
19	6	0	3.394339	-2.966961	1.328574
20	6	0	3.607278	-3.762927	2.621536
21	6	0	4.034738	-3.715913	0.148328
22	6	0	2.883011	-3.243258	3.864549
23	6	0	4.186595	-0.656198	-0.982101
24	6	0	-2.061163	-3.790328	-0.765986
25	6	0	-2.354484	-3.541778	-2.103005
26	6	0	-1.738748	-2.496826	-2.798443
27	6	0	-0.788128	-1.758879	-2.114737
28	6	0	-0.421133	-2.043619	-0.796491
29	6	0	-1.102962	-3.024603	-0.095974
30	7	0	-0.071047	-0.651124	-2.584907
31	6	0	0.785042	-0.172302	-1.637928
32	6	0	0.638512	-1.048272	-0.363281
33	8	0	1.582010	0.727852	-1.809440
34	6	0	-0.246855	-0.034488	-3.880721
35	6	0	-3.234617	1.503374	0.774166
36	6	0	-3.755672	1.814302	-0.481896
37	6	0	-4.783240	2.740148	-0.601177
38	6	0	-5.283340	3.376400	0.534072
39	6	0	-4.761897	3.069042	1.786880
40	6	0	-3.742833	2.127552	1.910847
41	6	0	-2.145197	0.481663	0.901810
42	7	0	-2.392411	-0.763371	1.300035
43	6	0	-0.809827	0.803709	0.606231
44	6	0	-0.279871	2.124602	0.392458
45	8	0	0.931986	2.377806	0.467646
46	6	0	-0.650505	4.432339	0.028460
47	8	0	-1.162298	3.094447	0.113190
48	6	0	0.240964	-0.241476	0.887478
49	16	0	-3.817053	-1.331061	1.853860
50	8	0	-3.676295	-2.792344	1.816776
51	8	0	-4.205691	-0.705896	3.124358
52	6	0	-5.078610	-0.913640	0.661010
53	6	0	-6.174403	-0.156300	1.049837
54	6	0	-7.142802	0.161451	0.104137
55	6	0	-7.026279	-0.267958	-1.218763
56	6	0	-5.921829	-1.045346	-1.577897
57	6	0	-4.948983	-1.375496	-0.643503
58	6	0	-8.059656	0.126247	-2.243240
59	6	0	-1.854557	5.335515	-0.135183
60	1	0	6.784334	-1.361604	-0.777222
61	1	0	8.721021	0.054248	-0.145410
62	1	0	3.068634	1.819510	-0.652062
63	1	0	4.995975	5.387168	0.645343

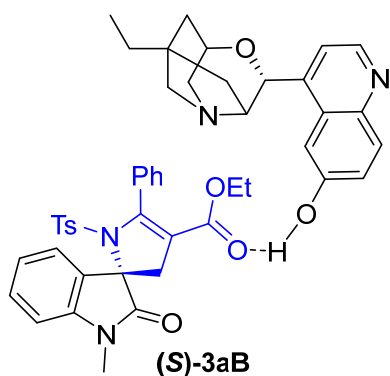
64	1	0	7.213709	4.213235	0.648438
65	1	0	2.005208	3.677942	0.102377
66	1	0	2.795470	0.154429	0.442226
67	1	0	1.373067	-3.605468	0.681385
68	1	0	1.415275	-2.229984	1.811192
69	1	0	1.681312	-3.394084	-1.452061
70	1	0	2.291182	-1.937619	-2.260679
71	1	0	3.564202	-1.046882	2.321141
72	1	0	4.968968	-1.434244	1.321349
73	1	0	4.054309	-3.723162	-2.008217
74	1	0	4.684475	-3.790308	2.811125
75	1	0	3.301906	-4.798209	2.439903
76	1	0	5.110800	-3.820632	0.304729
77	1	0	3.606387	-4.723060	0.100970
78	1	0	3.149402	-2.211732	4.098079
79	1	0	3.155895	-3.851296	4.727372
80	1	0	1.797977	-3.300948	3.761750
81	1	0	3.663334	-0.193406	-1.820739
82	1	0	-2.617969	-4.533287	-0.213330
83	1	0	-3.107641	-4.136892	-2.604015
84	1	0	-2.006087	-2.266934	-3.821302
85	1	0	-0.956529	-3.171443	0.965014
86	1	0	-1.272554	0.320666	-3.991416
87	1	0	-0.021682	-0.747411	-4.675694
88	1	0	0.440363	0.806024	-3.935588
89	1	0	-3.350704	1.322360	-1.357948
90	1	0	-5.194183	2.967497	-1.577398
91	1	0	-6.081600	4.102579	0.441446
92	1	0	-5.153148	3.554360	2.672360
93	1	0	-3.355574	1.858887	2.884229
94	1	0	0.031117	4.504469	-0.821061
95	1	0	-0.088153	4.660727	0.934619
96	1	0	1.113026	0.257234	1.306554
97	1	0	-0.174470	-0.934387	1.619137
98	1	0	-6.244379	0.184989	2.073493
99	1	0	-7.998087	0.760660	0.395308
100	1	0	-5.827955	-1.396181	-2.599759
101	1	0	-4.089833	-1.973825	-0.917230
102	1	0	-7.870799	1.138157	-2.611904
103	1	0	-8.045095	-0.548899	-3.099492
104	1	0	-9.062705	0.114792	-1.814460
105	1	0	-1.537852	6.378250	-0.186044
106	1	0	-2.535970	5.206848	0.706258
107	1	0	-2.395271	5.083949	-1.047743



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.500010	-0.131852	3.243182
2	6	0	-5.394454	0.756420	3.868460
3	6	0	-3.929199	0.171957	2.026307
4	6	0	-4.265970	1.436602	1.441245
5	6	0	-5.202534	2.245078	2.161976
6	7	0	-5.752891	1.905830	3.354416
7	6	0	-3.765025	1.955191	0.218096
8	6	0	-4.171750	3.176344	-0.268076
9	6	0	-5.116991	3.959548	0.439524
10	6	0	-5.608837	3.497150	1.623305
11	8	0	-3.700375	3.690634	-1.426361
12	6	0	-2.588491	-0.899567	0.024542
13	8	0	-3.650994	-2.152736	1.795743
14	6	0	-2.189431	-2.648661	-1.551787
15	6	0	-1.708960	-3.088646	0.736847
16	7	0	-1.638766	-2.045258	-0.309776
17	6	0	-3.820707	-1.115104	-0.880781
18	6	0	-3.177520	-3.293934	1.086733
19	6	0	-3.700163	-2.581355	-1.327882
20	6	0	-4.552327	-2.946089	-2.547387
21	6	0	-4.028391	-3.537721	-0.165874
22	6	0	-4.227782	-2.203345	-3.844520
23	6	0	-2.981671	-0.917431	1.502103
24	6	0	1.635791	-4.781216	-1.801109
25	6	0	2.086180	-5.139353	-0.532065
26	6	0	1.969145	-4.276952	0.560497
27	6	0	1.387559	-3.042219	0.332838
28	6	0	0.915772	-2.674999	-0.938579
29	6	0	1.047877	-3.534821	-2.014188
30	7	0	1.162260	-2.012445	1.244892
31	6	0	0.524443	-0.948588	0.644327

32	6	0	0.356859	-1.331459	-0.819419
33	8	0	0.115562	0.046931	1.207211
34	6	0	1.443937	-2.061474	2.661011
35	6	0	2.611664	2.191222	-0.901467
36	6	0	2.525662	2.629890	0.419762
37	6	0	3.229895	3.760592	0.821914
38	6	0	4.025586	4.446358	-0.092347
39	6	0	4.111767	4.001772	-1.410872
40	6	0	3.402903	2.876874	-1.819904
41	6	0	1.825189	0.975179	-1.262528
42	7	0	2.286925	-0.275773	-0.987919
43	6	0	0.528040	0.986674	-1.693213
44	6	0	-0.344397	2.130569	-1.840615
45	8	0	-1.557076	2.025389	-2.058618
46	6	0	-0.565392	4.491125	-1.768686
47	8	0	0.258716	3.311857	-1.734417
48	6	0	-0.061445	-0.383598	-1.909051
49	16	0	3.860589	-0.720229	-1.131972
50	8	0	3.853905	-2.176750	-1.260439
51	8	0	4.519181	0.097729	-2.151701
52	6	0	4.666033	-0.372554	0.419517
53	6	0	5.240008	0.873241	0.648534
54	6	0	5.855514	1.115164	1.870567
55	6	0	5.915822	0.129135	2.858038
56	6	0	5.357503	-1.122894	2.590024
57	6	0	4.734418	-1.380991	1.374112
58	6	0	6.565165	0.415938	4.187508
59	6	0	0.380762	5.665418	-1.644285
60	1	0	-4.278343	-1.075602	3.719460
61	1	0	-5.830485	0.490828	4.826058
62	1	0	-3.043752	1.423628	-0.372626
63	1	0	-5.415993	4.911725	0.022024
64	1	0	-6.324191	4.062719	2.205224
65	1	0	-2.980596	3.119398	-1.766562
66	1	0	-2.036027	0.011123	-0.179064
67	1	0	-1.792578	-3.655776	-1.680803
68	1	0	-1.898146	-2.046870	-2.412110
69	1	0	-1.240985	-3.996226	0.356722
70	1	0	-1.165442	-2.771145	1.624778
71	1	0	-3.775357	-0.444594	-1.741296
72	1	0	-4.747058	-0.914222	-0.340742
73	1	0	-3.283205	-4.137642	1.770943
74	1	0	-5.599628	-2.771989	-2.281702
75	1	0	-4.456957	-4.022573	-2.723267
76	1	0	-5.079445	-3.444144	0.118232
77	1	0	-3.866125	-4.566569	-0.506993

78	1	0	-4.307500	-1.121579	-3.731090
79	1	0	-4.927509	-2.501653	-4.626153
80	1	0	-3.223303	-2.433988	-4.204025
81	1	0	-2.065201	-0.846460	2.095430
82	1	0	1.759100	-5.467362	-2.627756
83	1	0	2.548253	-6.107485	-0.387546
84	1	0	2.335291	-4.559578	1.538864
85	1	0	0.714040	-3.240797	-3.001488
86	1	0	2.517259	-2.124826	2.839959
87	1	0	0.943287	-2.917569	3.120070
88	1	0	1.063762	-1.138800	3.093715
89	1	0	1.904158	2.080897	1.117604
90	1	0	3.161595	4.100537	1.847805
91	1	0	4.578388	5.323765	0.219888
92	1	0	4.734014	4.530782	-2.121683
93	1	0	3.477592	2.513329	-2.835098
94	1	0	-1.276836	4.450558	-0.944842
95	1	0	-1.124624	4.508001	-2.704646
96	1	0	-1.140151	-0.273269	-1.971133
97	1	0	0.289487	-0.808588	-2.855294
98	1	0	5.213808	1.632746	-0.121845
99	1	0	6.302726	2.084836	2.056346
100	1	0	5.429545	-1.907329	3.335273
101	1	0	4.331415	-2.357913	1.137974
102	1	0	5.864798	0.919778	4.858525
103	1	0	6.889890	-0.504119	4.674194
104	1	0	7.432708	1.065975	4.067865
105	1	0	-0.182294	6.599511	-1.638936
106	1	0	1.081263	5.678103	-2.479408
107	1	0	0.953559	5.587467	-0.719898

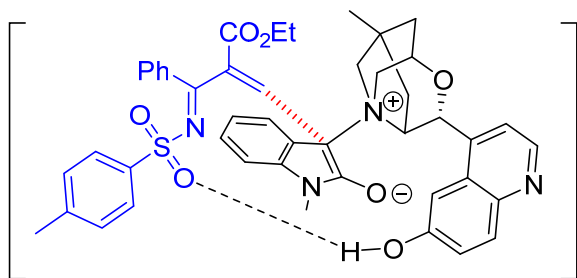


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.198955	1.032831	1.000698

2	6	0	6.536897	0.579952	1.074150
3	6	0	4.289936	0.333638	0.248766
4	6	0	4.731786	-0.848950	-0.414474
5	6	0	6.097062	-1.209992	-0.266749
6	7	0	6.988001	-0.490823	0.468002
7	6	0	3.873593	-1.678194	-1.178182
8	6	0	4.351391	-2.832198	-1.758634
9	6	0	5.719928	-3.183914	-1.630148
10	6	0	6.564083	-2.389265	-0.906526
11	8	0	3.563363	-3.684216	-2.452383
12	6	0	2.586752	1.419869	-1.260820
13	8	0	2.559467	1.720644	1.137335
14	6	0	1.073021	3.036613	-2.000616
15	6	0	0.479033	1.769335	-0.088226
16	7	0	1.118971	1.686891	-1.411904
17	6	0	3.309540	2.788692	-1.387890
18	6	0	1.391348	2.518871	0.868023
19	6	0	2.166144	3.800142	-1.234346
20	6	0	2.479635	5.208046	-1.746844
21	6	0	1.764828	3.875979	0.254309
22	6	0	2.727028	5.329717	-3.251272
23	6	0	2.859343	0.786093	0.109616
24	6	0	-5.320475	-2.907531	-2.386402
25	6	0	-6.033365	-2.069422	-3.237609
26	6	0	-5.650287	-0.740612	-3.443002
27	6	0	-4.529982	-0.291502	-2.766062
28	6	0	-3.800705	-1.125230	-1.915851
29	6	0	-4.187110	-2.435327	-1.716013
30	7	0	-3.961892	0.989450	-2.786944
31	6	0	-2.917919	1.084419	-1.911094
32	6	0	-2.628103	-0.338397	-1.386302
33	8	0	-2.297073	2.094494	-1.643141
34	6	0	-4.564954	2.140091	-3.418419
35	6	0	-1.183198	-1.741075	1.804836
36	6	0	-0.089216	-1.195149	2.480161
37	6	0	0.196605	-1.596973	3.780125
38	6	0	-0.598719	-2.553425	4.405678
39	6	0	-1.682320	-3.107574	3.728478
40	6	0	-1.976876	-2.702739	2.431151
41	6	0	-1.453431	-1.329663	0.402537
42	7	0	-2.450590	-0.394806	0.078771
43	6	0	-0.775536	-1.672234	-0.716482
44	6	0	0.320115	-2.625814	-0.846708
45	8	0	0.926762	-2.779229	-1.899286
46	6	0	1.651808	-4.275617	0.221729
47	8	0	0.572106	-3.317182	0.261288

48	6	0	-1.256214	-0.856578	-1.891428
49	16	0	-3.705652	0.129774	1.088253
50	8	0	-4.538558	0.925208	0.195207
51	8	0	-4.264537	-0.991310	1.828768
52	6	0	-2.870735	1.204570	2.214915
53	6	0	-2.585088	0.770098	3.501706
54	6	0	-1.899630	1.630287	4.353564
55	6	0	-1.511287	2.902224	3.931727
56	6	0	-1.830742	3.313118	2.631335
57	6	0	-2.507877	2.471413	1.761652
58	6	0	-0.738896	3.818035	4.844968
59	6	0	1.571535	-5.048456	1.519767
60	1	0	4.887243	1.916386	1.539327
61	1	0	7.255493	1.139856	1.664544
62	1	0	2.833764	-1.421141	-1.319221
63	1	0	6.060458	-4.091480	-2.110910
64	1	0	7.610868	-2.634638	-0.785129
65	1	0	2.634236	-3.390039	-2.388116
66	1	0	2.906307	0.736681	-2.047756
67	1	0	0.067152	3.450515	-1.913093
68	1	0	1.328061	2.969914	-3.062061
69	1	0	-0.478424	2.269779	-0.207315
70	1	0	0.259798	0.769144	0.285696
71	1	0	3.773419	2.877310	-2.371703
72	1	0	4.089149	2.916057	-0.635847
73	1	0	0.912992	2.671450	1.838037
74	1	0	3.354250	5.581303	-1.203219
75	1	0	1.647589	5.866633	-1.474682
76	1	0	2.582323	4.314288	0.835578
77	1	0	0.896840	4.539905	0.353568
78	1	0	3.531370	4.673449	-3.587260
79	1	0	3.011165	6.352557	-3.503730
80	1	0	1.831511	5.086267	-3.824960
81	1	0	2.214807	-0.095613	0.219035
82	1	0	-5.645572	-3.928713	-2.239811
83	1	0	-6.908487	-2.448722	-3.749497
84	1	0	-6.216021	-0.090826	-4.097489
85	1	0	-3.628800	-3.078565	-1.046494
86	1	0	-5.556056	2.324371	-2.998943
87	1	0	-4.645907	1.982413	-4.494605
88	1	0	-3.920052	2.992313	-3.219960
89	1	0	0.536958	-0.454004	1.999240
90	1	0	1.042652	-1.164593	4.298603
91	1	0	-0.372837	-2.869222	5.416468
92	1	0	-2.300430	-3.854849	4.209077
93	1	0	-2.826468	-3.118910	1.908239

94	1	0	2.591500	-3.732144	0.129455
95	1	0	1.527494	-4.912774	-0.653379
96	1	0	-0.568757	-0.021115	-2.070338
97	1	0	-1.367812	-1.439237	-2.804178
98	1	0	-2.884103	-0.220241	3.819576
99	1	0	-1.660706	1.304259	5.358442
100	1	0	-1.541565	4.304002	2.300070
101	1	0	-2.748274	2.773411	0.749464
102	1	0	0.315261	3.843929	4.556930
103	1	0	-1.121129	4.838287	4.790562
104	1	0	-0.796169	3.482596	5.880129
105	1	0	2.383054	-5.775094	1.570637
106	1	0	0.619902	-5.575578	1.590960
107	1	0	1.652494	-4.367439	2.367472

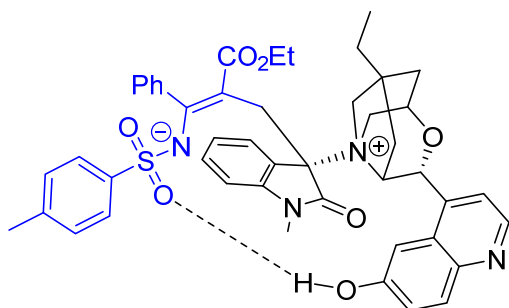


TS1C

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.841542	1.858416	-2.658702
2	6	0	5.135240	3.134840	-3.191595
3	6	0	3.683790	1.672148	-1.948350
4	6	0	2.806085	2.786455	-1.766300
5	6	0	3.212085	4.021327	-2.345304
6	7	0	4.363625	4.182864	-3.050309
7	6	0	1.583310	2.737628	-1.048556
8	6	0	0.818181	3.869163	-0.882456
9	6	0	1.218410	5.096337	-1.471203
10	6	0	2.380862	5.162209	-2.183715
11	8	0	-0.327547	3.891496	-0.168491
12	6	0	3.289065	0.341378	0.129095
13	8	0	4.303563	-0.642849	-1.815210
14	6	0	3.723334	-1.302088	1.822476
15	6	0	3.004722	-2.089484	-0.352878
16	7	0	2.767356	-1.019366	0.682357

17	6	0	4.685248	0.524901	0.744388
18	6	0	4.345936	-1.824876	-1.013840
19	6	0	5.072673	-0.868353	1.255230
20	6	0	6.212046	-0.875345	2.279943
21	6	0	5.444218	-1.758055	0.056569
22	6	0	5.910585	-0.198873	3.618095
23	6	0	3.335595	0.308660	-1.391495
24	6	0	-0.170388	-4.379887	2.104710
25	6	0	-1.006222	-3.888276	3.103596
26	6	0	-1.010684	-2.530320	3.416216
27	6	0	-0.147914	-1.699766	2.720323
28	6	0	0.707136	-2.166567	1.690306
29	6	0	0.669046	-3.528794	1.383417
30	7	0	0.048361	-0.341312	2.899473
31	6	0	1.024253	0.123685	2.047364
32	6	0	1.353567	-0.979013	1.140529
33	8	0	1.505090	1.264521	2.117101
34	6	0	-0.493548	0.460144	3.972055
35	1	0	5.516143	1.030689	-2.821261
36	1	0	6.050220	3.277512	-3.757368
37	1	0	1.243693	1.827554	-0.580672
38	1	0	0.585560	5.961717	-1.326822
39	1	0	2.717620	6.083536	-2.639866
40	1	0	-0.482141	3.045634	0.292003
41	1	0	2.608743	1.086253	0.514124
42	1	0	3.621529	-2.347458	2.112553
43	1	0	3.416981	-0.656461	2.644328
44	1	0	3.028873	-3.040989	0.171108
45	1	0	2.177132	-2.118677	-1.055651
46	1	0	4.616210	1.233959	1.569279
47	1	0	5.391285	0.910038	0.007984
48	1	0	4.559726	-2.642817	-1.702195
49	1	0	7.075414	-0.393214	1.811199
50	1	0	6.503535	-1.914117	2.464951
51	1	0	6.361366	-1.387121	-0.407399
52	1	0	5.639937	-2.776396	0.410380
53	1	0	5.575498	0.831505	3.492174
54	1	0	6.810536	-0.178390	4.233624
55	1	0	5.144697	-0.737168	4.178889
56	1	0	2.355687	0.036655	-1.793241
57	1	0	-0.181361	-5.435973	1.864782
58	1	0	-1.666145	-4.560874	3.636274
59	1	0	-1.669703	-2.128025	4.173628
60	1	0	1.246209	-3.941286	0.568714
61	1	0	-0.191235	1.486785	3.781331
62	1	0	-0.090816	0.131643	4.934032

63	1	0	-1.577901	0.389193	3.974741
64	6	0	-3.429076	-1.586855	-1.969807
65	6	0	-4.780405	-1.836901	-1.728026
66	6	0	-5.573413	-2.398022	-2.720870
67	6	0	-5.030314	-2.684710	-3.971788
68	6	0	-3.688979	-2.412474	-4.224657
69	6	0	-2.887114	-1.873692	-3.224409
70	6	0	-2.591245	-0.952341	-0.902392
71	7	0	-3.220375	0.019134	-0.308822
72	6	0	-1.209201	-1.409615	-0.833046
73	6	0	-0.882039	-2.810815	-1.186684
74	8	0	0.181524	-3.161944	-1.673855
75	6	0	-1.636618	-5.049423	-1.172019
76	8	0	-1.858913	-3.663514	-0.862382
77	6	0	-0.127813	-0.566414	-0.756134
78	16	0	-2.738272	0.815775	1.052985
79	8	0	-2.935634	-0.056263	2.212356
80	8	0	-1.440213	1.504325	0.901260
81	6	0	-3.973069	2.085800	1.113923
82	6	0	-3.733464	3.311056	0.503978
83	6	0	-4.721542	4.286917	0.561028
84	6	0	-5.930750	4.052862	1.218562
85	6	0	-6.138839	2.811290	1.824523
86	6	0	-5.164697	1.822771	1.779056
87	6	0	-6.980246	5.130997	1.301981
88	6	0	-1.990241	-5.337282	-2.618775
89	1	0	-5.189762	-1.594234	-0.756775
90	1	0	-6.617058	-2.606345	-2.522241
91	1	0	-5.652563	-3.112423	-4.747891
92	1	0	-3.265449	-2.620273	-5.199122
93	1	0	-1.842805	-1.663055	-3.420669
94	1	0	-0.597775	-5.292967	-0.957271
95	1	0	-2.286175	-5.586085	-0.484186
96	1	0	0.756148	-0.895142	-1.269097
97	1	0	-0.266984	0.485069	-0.576938
98	1	0	-2.794450	3.503474	0.001813
99	1	0	-4.548338	5.247133	0.090035
100	1	0	-7.073084	2.619960	2.339195
101	1	0	-5.312021	0.862551	2.255132
102	1	0	-7.982046	4.701878	1.338668
103	1	0	-6.842447	5.732027	2.204312
104	1	0	-6.923343	5.801539	0.444223
105	1	0	-1.883693	-6.404482	-2.823174
106	1	0	-1.324834	-4.786433	-3.283467
107	1	0	-3.018636	-5.038197	-2.823221

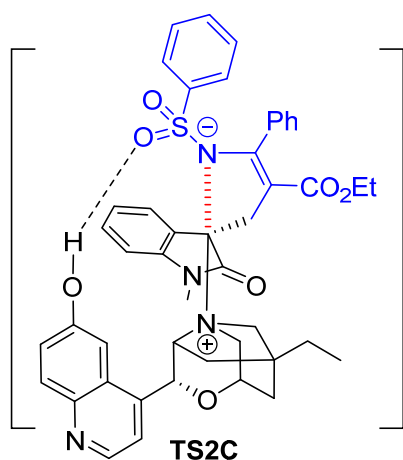


(S)-IIIC

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.653567	-0.591478	-0.927869
2	6	0	6.713770	0.279403	-1.252282
3	6	0	4.351226	-0.177833	-1.082545
4	6	0	4.106525	1.134389	-1.594535
5	6	0	5.264024	1.926097	-1.867278
6	7	0	6.540390	1.498888	-1.695734
7	6	0	2.820977	1.687460	-1.837422
8	6	0	2.694908	2.983905	-2.304407
9	6	0	3.854518	3.767639	-2.561100
10	6	0	5.095677	3.250092	-2.353312
11	8	0	1.531641	3.595291	-2.549464
12	6	0	2.477309	-0.591014	0.536846
13	8	0	3.812958	-2.393830	-0.399335
14	6	0	1.554848	-1.687186	2.502866
15	6	0	1.627016	-2.949914	0.448351
16	7	0	1.345152	-1.580984	1.008109
17	6	0	3.395104	-0.466405	1.763603
18	6	0	3.120151	-3.195482	0.543536
19	6	0	3.072010	-1.688765	2.629636
20	6	0	3.572690	-1.590638	4.075139
21	6	0	3.620996	-2.969669	1.977235
22	6	0	2.968258	-0.470120	4.922691
23	6	0	3.228444	-1.127779	-0.688434
24	6	0	-2.567990	-3.913953	1.724733
25	6	0	-3.312367	-3.138211	2.607987
26	6	0	-2.992019	-1.800480	2.837368
27	6	0	-1.890756	-1.279427	2.176768
28	6	0	-1.119996	-2.045406	1.291724
29	6	0	-1.481021	-3.361479	1.041417
30	7	0	-1.391319	0.019915	2.279605
31	6	0	-0.331984	0.201179	1.441869

32	6	0	-0.081934	-1.130416	0.672889
33	8	0	0.357476	1.198030	1.361562
34	6	0	-2.113012	1.134031	2.862668
35	6	0	-4.081293	-0.634818	-1.256978
36	6	0	-4.946778	0.309919	-1.812801
37	6	0	-6.307613	0.037417	-1.900080
38	6	0	-6.818256	-1.156360	-1.397215
39	6	0	-5.960684	-2.084995	-0.813038
40	6	0	-4.597091	-1.827531	-0.749185
41	6	0	-2.638406	-0.292460	-1.101473
42	7	0	-2.418113	0.914005	-0.454770
43	6	0	-1.612129	-1.155684	-1.383239
44	6	0	-1.808119	-2.390200	-2.153676
45	8	0	-2.748002	-2.708198	-2.842756
46	6	0	-0.801942	-4.421638	-2.840605
47	8	0	-0.712917	-3.226973	-2.050943
48	6	0	-0.227486	-0.869330	-0.855437
49	16	0	-1.842606	2.161356	-1.238166
50	8	0	-0.396357	2.035800	-1.623075
51	8	0	-2.693404	2.612813	-2.351542
52	6	0	-1.903588	3.389460	0.043511
53	6	0	-0.741481	3.999812	0.488240
54	6	0	-0.828516	4.958505	1.495896
55	6	0	-2.058108	5.311130	2.050248
56	6	0	-3.216065	4.683533	1.575237
57	6	0	-3.146825	3.729736	0.570573
58	6	0	-2.150364	6.371859	3.117607
59	6	0	0.468314	-5.209656	-2.594669
60	1	0	5.868047	-1.584111	-0.563177
61	1	0	7.738413	-0.056142	-1.129636
62	1	0	1.918172	1.112077	-1.684349
63	1	0	3.704288	4.773472	-2.929946
64	1	0	5.994911	3.818979	-2.548253
65	1	0	0.757143	3.027781	-2.316618
66	1	0	1.984450	0.345698	0.306779
67	1	0	1.042094	-2.575201	2.869453
68	1	0	1.127804	-0.799716	2.965357
69	1	0	1.073087	-3.665169	1.050472
70	1	0	1.273119	-3.007343	-0.577478
71	1	0	3.152864	0.454351	2.294362
72	1	0	4.441983	-0.429944	1.464196
73	1	0	3.316606	-4.228042	0.252534
74	1	0	4.659386	-1.471934	4.033873
75	1	0	3.387664	-2.549515	4.569384
76	1	0	4.712902	-2.941986	1.958118
77	1	0	3.322483	-3.829819	2.586590

78	1	0	3.107189	0.511749	4.468807
79	1	0	3.449961	-0.448676	5.900597
80	1	0	1.900236	-0.618870	5.091935
81	1	0	2.541904	-1.228224	-1.534334
82	1	0	-2.849607	-4.941573	1.538026
83	1	0	-4.167257	-3.570298	3.111825
84	1	0	-3.589333	-1.187550	3.498259
85	1	0	-0.964969	-3.944693	0.291647
86	1	0	-1.499741	2.023144	2.735065
87	1	0	-2.293235	0.954188	3.922923
88	1	0	-3.052237	1.269753	2.324888
89	1	0	-4.539316	1.243870	-2.180335
90	1	0	-6.971716	0.763351	-2.352535
91	1	0	-7.880718	-1.359553	-1.454118
92	1	0	-6.354219	-3.009670	-0.408739
93	1	0	-3.926237	-2.545498	-0.295002
94	1	0	-1.692652	-4.977740	-2.548106
95	1	0	-0.913713	-4.146043	-3.888802
96	1	0	0.477035	-1.486367	-1.401195
97	1	0	0.032008	0.171665	-1.031062
98	1	0	0.209553	3.716556	0.059567
99	1	0	0.074337	5.439493	1.853708
100	1	0	-4.178067	4.953379	1.996136
101	1	0	-4.036003	3.235053	0.200034
102	1	0	-1.188574	6.520665	3.609075
103	1	0	-2.455500	7.327769	2.684831
104	1	0	-2.887549	6.104433	3.876407
105	1	0	0.466301	-6.123968	-3.189245
106	1	0	0.552721	-5.489878	-1.541683
107	1	0	1.344674	-4.621259	-2.871984

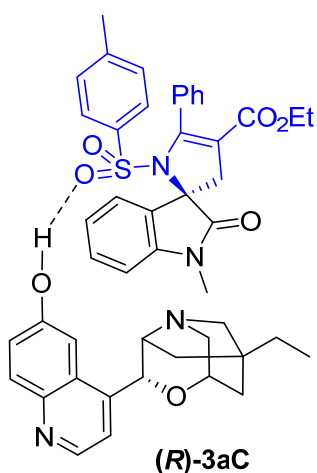


Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	5.828617	0.075949	-1.452397
2	6	0	6.636577	0.941880	-2.219674
3	6	0	4.476008	0.237421	-1.440503
4	6	0	3.915470	1.286478	-2.240525
5	6	0	4.827412	2.091991	-2.952391
6	7	0	6.167208	1.910188	-2.931357
7	6	0	2.521427	1.567017	-2.358270
8	6	0	2.078791	2.612770	-3.115413
9	6	0	3.009716	3.423891	-3.821271
10	6	0	4.332530	3.165787	-3.742531
11	8	0	0.802314	2.967484	-3.262661
12	6	0	2.918368	-0.000580	0.565102
13	8	0	4.412441	-1.745003	-0.115250
14	6	0	2.283776	-0.715739	2.720063
15	6	0	2.403688	-2.361238	1.016785
16	7	0	2.000268	-0.968529	1.290997
17	6	0	3.939474	0.487950	1.620220
18	6	0	3.920800	-2.432682	1.014746
19	6	0	3.806935	-0.533211	2.755140
20	6	0	4.381421	-0.093325	4.109645
21	6	0	4.472957	-1.860308	2.326949
22	6	0	3.792717	1.169499	4.744188
23	6	0	3.608883	-0.698829	-0.610879
24	6	0	-1.755263	-3.279777	3.192648
25	6	0	-2.097429	-2.334637	4.162198
26	6	0	-1.829956	-0.982531	4.015676
27	6	0	-1.192684	-0.585081	2.853792
28	6	0	-0.841061	-1.519213	1.867583
29	6	0	-1.136466	-2.871690	2.031301
30	7	0	-0.814802	0.687629	2.481190
31	6	0	-0.232051	0.665276	1.238563
32	6	0	-0.267509	-0.797334	0.773836
33	8	0	0.269249	1.578557	0.677929
34	6	0	-1.068649	1.899985	3.231605
35	6	0	-3.995175	-1.446705	-1.523601
36	6	0	-4.259221	-1.817199	-2.834222
37	6	0	-5.547847	-2.127606	-3.223955
38	6	0	-6.582981	-2.095295	-2.302057
39	6	0	-6.325176	-1.733451	-0.991507
40	6	0	-5.037700	-1.395156	-0.609141
41	6	0	-2.626206	-1.053999	-1.061640
42	7	0	-2.464150	0.164503	-0.440095
43	6	0	-1.526174	-1.856269	-1.098329
44	6	0	-1.540037	-3.280170	-1.461540

45	8	0	-2.464908	-3.921845	-1.853176
46	6	0	-0.221071	-5.222193	-1.687602
47	8	0	-0.336097	-3.863467	-1.283004
48	6	0	-0.216096	-1.206930	-0.667735
49	16	0	-2.699699	1.492255	-1.286635
50	8	0	-1.459965	1.898228	-1.928516
51	8	0	-3.844879	1.435950	-2.155102
52	6	0	-3.028555	2.707707	-0.035867
53	6	0	-2.235396	3.834872	0.056524
54	6	0	-2.554502	4.824372	0.977938
55	6	0	-3.661130	4.702590	1.804357
56	6	0	-4.450685	3.557488	1.694338
57	6	0	-4.145261	2.570537	0.778817
58	6	0	-4.035828	5.796255	2.776478
59	6	0	1.210339	-5.655974	-1.446736
60	1	0	6.287844	-0.710042	-0.889046
61	1	0	7.704991	0.805029	-2.221282
62	1	0	1.795789	0.969576	-1.844438
63	1	0	2.623619	4.233331	-4.411994
64	1	0	5.052835	3.761271	-4.271373
65	1	0	0.174961	2.435515	-2.775252
66	1	0	2.320717	0.817615	0.212342
67	1	0	1.904148	-1.524286	3.331767
68	1	0	1.790486	0.197373	3.023222
69	1	0	1.981945	-3.001607	1.779540
70	1	0	2.023342	-2.701299	0.067196
71	1	0	3.662058	1.478642	1.958051
72	1	0	4.941383	0.550011	1.218508
73	1	0	4.251071	-3.457898	0.902113
74	1	0	5.452899	0.044656	3.987173
75	1	0	4.265961	-0.916386	4.811736
76	1	0	5.544658	-1.722720	2.224994
77	1	0	4.319675	-2.603848	3.107074
78	1	0	3.914833	2.043391	4.114531
79	1	0	4.297235	1.375086	5.682512
80	1	0	2.735813	1.061563	4.966702
81	1	0	2.853043	-1.113420	-1.271229
82	1	0	-1.992373	-4.315055	3.347487
83	1	0	-2.593721	-2.666258	5.056643
84	1	0	-2.115717	-0.278160	4.772901
85	1	0	-0.877905	-3.578134	1.266620
86	1	0	-0.660082	2.726580	2.674532
87	1	0	-0.591705	1.849606	4.203794
88	1	0	-2.132516	2.053402	3.353598
89	1	0	-3.459911	-1.849925	-3.549589
90	1	0	-5.744699	-2.398518	-4.245745

91	1	0	-7.584105	-2.344596	-2.606713
92	1	0	-7.123781	-1.703372	-0.271275
93	1	0	-4.837409	-1.094980	0.403331
94	1	0	-0.919323	-5.823926	-1.122617
95	1	0	-0.487645	-5.303572	-2.731809
96	1	0	0.588630	-1.898883	-0.821082
97	1	0	-0.029199	-0.317194	-1.248720
98	1	0	-1.385577	3.936211	-0.589436
99	1	0	-1.934810	5.701520	1.041640
100	1	0	-5.320255	3.448061	2.319767
101	1	0	-4.770947	1.702868	0.685883
102	1	0	-4.953242	6.286942	2.463285
103	1	0	-4.205262	5.400392	3.772840
104	1	0	-3.262395	6.551941	2.840133
105	1	0	1.341278	-6.687485	-1.756993
106	1	0	1.467015	-5.585560	-0.394449
107	1	0	1.901881	-5.040863	-2.011839

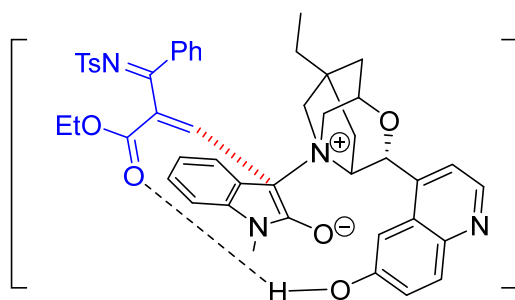


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.816401	0.531173	-1.681361
2	6	0	-6.602619	-0.343211	-2.468995
3	6	0	-4.455973	0.366141	-1.645887
4	6	0	-3.880890	-0.675783	-2.433715
5	6	0	-4.770821	-1.510190	-3.161749
6	7	0	-6.120449	-1.335687	-3.175282
7	6	0	-2.488108	-0.917661	-2.503177
8	6	0	-1.998932	-1.991124	-3.210428
9	6	0	-2.886187	-2.833402	-3.929907
10	6	0	-4.230843	-2.588777	-3.911734
11	8	0	-0.684407	-2.302519	-3.275416
12	6	0	-3.033162	0.466233	0.436803

13	8	0	-4.313520	2.359169	-0.334808
14	6	0	-2.393278	1.139849	2.583513
15	6	0	-2.231660	2.733796	0.831262
16	7	0	-2.027299	1.313555	1.168115
17	6	0	-4.177413	0.164353	1.441279
18	6	0	-3.726187	3.028003	0.790952
19	6	0	-3.928473	1.170979	2.572236
20	6	0	-4.604563	0.830434	3.902608
21	6	0	-4.376793	2.572707	2.107442
22	6	0	-4.133188	-0.458905	4.578544
23	6	0	-3.573386	1.230727	-0.781129
24	6	0	2.618981	0.714826	4.145344
25	6	0	1.778840	-0.208082	4.760734
26	6	0	0.874417	-0.974627	4.019998
27	6	0	0.846465	-0.772756	2.650386
28	6	0	1.673620	0.158654	2.020053
29	6	0	2.572660	0.902869	2.759349
30	7	0	0.047967	-1.419249	1.700445
31	6	0	0.293568	-0.953772	0.441720
32	6	0	1.398784	0.125027	0.535010
33	8	0	-0.307281	-1.293053	-0.558941
34	6	0	-0.917360	-2.454796	1.990605
35	6	0	4.567142	1.305034	-1.023357
36	6	0	4.944010	1.994801	-2.174708
37	6	0	6.290640	2.141242	-2.482698
38	6	0	7.262895	1.612132	-1.639495
39	6	0	6.888592	0.924429	-0.487387
40	6	0	5.544704	0.760983	-0.185152
41	6	0	3.149914	1.150832	-0.652512
42	7	0	2.694365	-0.127830	-0.182780
43	6	0	2.169489	2.073488	-0.556058
44	6	0	2.274435	3.519760	-0.809663
45	8	0	3.260325	4.144140	-1.126872
46	6	0	1.034801	5.520522	-0.879715
47	8	0	1.066973	4.102506	-0.635115
48	6	0	0.894285	1.452427	-0.053698
49	16	0	2.849597	-1.420113	-1.305630
50	8	0	1.872828	-1.293399	-2.384294
51	8	0	4.261154	-1.496681	-1.639634
52	6	0	2.416421	-2.788067	-0.270140
53	6	0	1.475188	-3.706347	-0.723931
54	6	0	1.194639	-4.810000	0.071169
55	6	0	1.834076	-4.997691	1.300263
56	6	0	2.771202	-4.053102	1.728104
57	6	0	3.080112	-2.950472	0.941720
58	6	0	1.529104	-6.211355	2.139348

59	6	0	-0.388648	5.977204	-0.644573
60	1	0	-6.280479	1.325067	-1.113784
61	1	0	-7.679344	-0.208125	-2.496893
62	1	0	-1.790064	-0.286501	-1.975640
63	1	0	-2.464224	-3.657808	-4.489604
64	1	0	-4.928705	-3.208554	-4.459088
65	1	0	-0.157542	-1.720678	-2.699210
66	1	0	-2.544397	-0.448588	0.105065
67	1	0	-1.928205	1.913003	3.199828
68	1	0	-2.026249	0.170349	2.929693
69	1	0	-1.738903	3.344288	1.590724
70	1	0	-1.758841	2.976220	-0.121966
71	1	0	-4.093212	-0.860054	1.809542
72	1	0	-5.161720	0.276929	0.985707
73	1	0	-3.919083	4.091580	0.636779
74	1	0	-5.684750	0.776286	3.732569
75	1	0	-4.446013	1.665449	4.593392
76	1	0	-5.463372	2.592144	1.981994
77	1	0	-4.122732	3.302697	2.885486
78	1	0	-4.265657	-1.329250	3.933115
79	1	0	-4.707939	-0.637491	5.488563
80	1	0	-3.080220	-0.401940	4.862135
81	1	0	-2.727125	1.565292	-1.391902
82	1	0	3.312980	1.291833	4.741778
83	1	0	1.825605	-0.340507	5.834094
84	1	0	0.226633	-1.697015	4.499427
85	1	0	3.228709	1.615685	2.274417
86	1	0	-1.350467	-2.767800	1.043330
87	1	0	-1.703727	-2.077559	2.647892
88	1	0	-0.420836	-3.303106	2.464552
89	1	0	4.184673	2.409665	-2.821597
90	1	0	6.579791	2.669588	-3.381754
91	1	0	8.311501	1.730596	-1.881694
92	1	0	7.643223	0.507116	0.166773
93	1	0	5.239953	0.210181	0.696108
94	1	0	1.740627	6.007501	-0.207199
95	1	0	1.363379	5.706290	-1.902059
96	1	0	0.399266	2.040561	0.712271
97	1	0	0.176953	1.273352	-0.860353
98	1	0	0.954776	-3.539159	-1.658100
99	1	0	0.460294	-5.532917	-0.263596
100	1	0	3.267101	-4.185315	2.682052
101	1	0	3.808583	-2.218109	1.265779
102	1	0	0.476825	-6.488083	2.062900
103	1	0	2.120064	-7.065953	1.801183
104	1	0	1.767338	-6.036388	3.188670

105	1	0	-0.468651	7.051164	-0.817215
106	1	0	-0.692356	5.767102	0.381808
107	1	0	-1.072267	5.464896	-1.322397

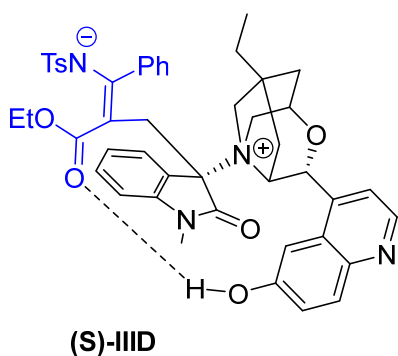


TS1D

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.002644	-2.327971	-1.883780
2	6	0	5.996650	-2.112311	-2.862304
3	6	0	4.063917	-1.357719	-1.630013
4	6	0	4.127298	-0.141311	-2.380929
5	6	0	5.172517	-0.045655	-3.346968
6	7	0	6.091212	-1.019850	-3.576065
7	6	0	3.233428	0.952738	-2.237792
8	6	0	3.368214	2.078472	-3.023544
9	6	0	4.407094	2.164370	-3.986150
10	6	0	5.281376	1.130082	-4.136330
11	8	0	2.559153	3.152109	-2.938281
12	6	0	3.143116	-0.709739	0.622727
13	8	0	3.105529	-2.987190	-0.182996
14	6	0	2.774345	-1.039302	2.986602
15	6	0	1.438367	-2.344469	1.438747
16	7	0	2.012764	-0.977032	1.677440
17	6	0	4.452933	-0.983459	1.378828
18	6	0	2.579208	-3.285337	1.105486
19	6	0	4.038906	-1.799357	2.611624
20	6	0	5.097144	-1.845537	3.719012
21	6	0	3.660785	-3.230413	2.193046
22	6	0	5.417138	-0.510265	4.392568
23	6	0	2.987157	-1.627839	-0.589081
24	6	0	-2.388454	-0.764624	3.408707
25	6	0	-2.690926	0.542773	3.781485
26	6	0	-1.810578	1.579581	3.478187
27	6	0	-0.636127	1.266874	2.812383
28	6	0	-0.285682	-0.060314	2.449256

29	6	0	-1.205096	-1.074043	2.739246
30	7	0	0.368665	2.134273	2.403714
31	6	0	1.431376	1.414816	1.867950
32	6	0	0.965407	0.057141	1.719163
33	8	0	2.549362	1.901869	1.639699
34	6	0	0.501147	3.514619	2.800533
35	1	0	4.970174	-3.263889	-1.347728
36	1	0	6.732546	-2.886424	-3.054299
37	1	0	2.446319	0.948100	-1.498641
38	1	0	4.475717	3.066756	-4.578785
39	1	0	6.087181	1.161954	-4.857337
40	1	0	1.867559	3.011194	-2.264150
41	1	0	3.053807	0.337347	0.364001
42	1	0	2.128800	-1.495511	3.737324
43	1	0	2.996780	-0.008004	3.253350
44	1	0	0.934335	-2.647130	2.352331
45	1	0	0.707540	-2.298238	0.635544
46	1	0	4.887850	-0.031022	1.680669
47	1	0	5.167357	-1.513885	0.749259
48	1	0	2.184872	-4.299339	1.036317
49	1	0	6.008971	-2.264541	3.282317
50	1	0	4.767157	-2.557593	4.482148
51	1	0	4.544183	-3.758348	1.825470
52	1	0	3.293352	-3.771736	3.071991
53	1	0	5.719981	0.251953	3.673671
54	1	0	6.237291	-0.639844	5.099601
55	1	0	4.562446	-0.125708	4.951522
56	1	0	2.009810	-1.474420	-1.058301
57	1	0	-3.088405	-1.561441	3.626495
58	1	0	-3.618527	0.761817	4.293897
59	1	0	-2.043701	2.604298	3.737735
60	1	0	-1.053864	-2.092258	2.414818
61	1	0	1.460895	3.859655	2.422558
62	1	0	0.478875	3.608693	3.889252
63	1	0	-0.299013	4.126469	2.379087
64	6	0	-3.360503	2.010572	0.324733
65	6	0	-4.756962	1.964017	0.333966
66	6	0	-5.491721	3.028898	0.839721
67	6	0	-4.839947	4.151371	1.344064
68	6	0	-3.448315	4.202560	1.343104
69	6	0	-2.714133	3.137690	0.836798
70	6	0	-2.590256	0.852079	-0.209248
71	7	0	-3.251911	-0.262999	-0.227762
72	6	0	-1.191725	1.051949	-0.618010
73	6	0	-0.721137	2.282369	-1.277197
74	8	0	0.451377	2.631972	-1.256014

75	6	0	-1.249101	4.144473	-2.629727
76	8	0	-1.664227	2.938324	-1.949883
77	6	0	-0.242074	0.088865	-0.478041
78	16	0	-2.747252	-1.664622	-0.975952
79	8	0	-2.140563	-1.437118	-2.288226
80	8	0	-2.013535	-2.493872	-0.004520
81	6	0	-4.333470	-2.410160	-1.229499
82	6	0	-4.720423	-2.742578	-2.517655
83	6	0	-5.950721	-3.368279	-2.706120
84	6	0	-6.780648	-3.659416	-1.625588
85	6	0	-6.359788	-3.310282	-0.335743
86	6	0	-5.138768	-2.689560	-0.127807
87	6	0	-8.105536	-4.348583	-1.826836
88	6	0	-1.158362	5.306436	-1.659016
89	1	0	-5.250037	1.087545	-0.063299
90	1	0	-6.573325	2.985562	0.835678
91	1	0	-5.413338	4.981962	1.736332
92	1	0	-2.934300	5.069198	1.741262
93	1	0	-1.632582	3.166036	0.866403
94	1	0	-0.298646	3.956501	-3.125934
95	1	0	-2.023526	4.305056	-3.375213
96	1	0	-0.501224	-0.896628	-0.136518
97	1	0	0.711866	0.237188	-0.952523
98	1	0	-4.067797	-2.508867	-3.347847
99	1	0	-6.267871	-3.631950	-3.707862
100	1	0	-7.001169	-3.530400	0.509778
101	1	0	-4.808019	-2.412071	0.864978
102	1	0	-8.906978	-3.810070	-1.317917
103	1	0	-8.357077	-4.416918	-2.884930
104	1	0	-8.079214	-5.361827	-1.419397
105	1	0	-0.911292	6.220280	-2.201952
106	1	0	-0.378320	5.123296	-0.920082
107	1	0	-2.111574	5.446332	-1.148699

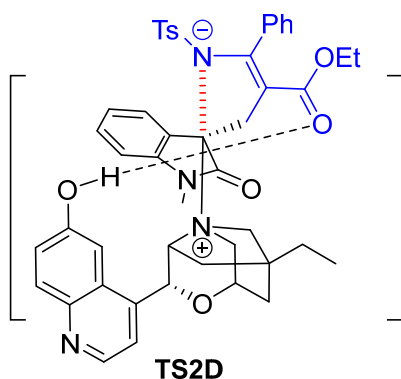


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	5.024027	-2.941732	-0.432459
2	6	0	6.123126	-3.120297	-1.302153
3	6	0	4.038678	-2.041432	-0.753989
4	6	0	4.156750	-1.313731	-1.979682
5	6	0	5.317254	-1.570668	-2.766181
6	7	0	6.281811	-2.464117	-2.423861
7	6	0	3.215448	-0.365141	-2.449485
8	6	0	3.421704	0.320928	-3.627298
9	6	0	4.579871	0.060592	-4.407081
10	6	0	5.492705	-0.861296	-3.985082
11	8	0	2.572088	1.247146	-4.100461
12	6	0	2.888047	-0.428291	0.774174
13	8	0	2.967540	-2.790612	1.246604
14	6	0	2.242217	0.456092	2.936747
15	6	0	1.107213	-1.527853	2.146993
16	7	0	1.649303	-0.186504	1.705048
17	6	0	4.103076	-0.199837	1.686720
18	6	0	2.290737	-2.430144	2.447137
19	6	0	3.553836	-0.301410	3.115080
20	6	0	4.470970	0.293849	4.189281
21	6	0	3.239465	-1.768005	3.453791
22	6	0	4.711756	1.802118	4.108447
23	6	0	2.864997	-1.842178	0.191372
24	6	0	-2.451487	0.975735	3.479516
25	6	0	-2.438285	2.359329	3.605071
26	6	0	-1.490240	3.134454	2.933900
27	6	0	-0.556062	2.465178	2.164312
28	6	0	-0.529802	1.070305	2.051755
29	6	0	-1.507462	0.318011	2.684285
30	7	0	0.452305	3.035598	1.378958
31	6	0	1.214427	2.082111	0.769639
32	6	0	0.564079	0.695509	1.068919
33	8	0	2.244845	2.294994	0.163294
34	6	0	0.710202	4.452346	1.253753
35	1	0	4.954970	-3.519071	0.477219
36	1	0	6.895790	-3.836914	-1.043136
37	1	0	2.309557	-0.150217	-1.909161
38	1	0	4.705848	0.611384	-5.329639
39	1	0	6.383657	-1.084292	-4.556852
40	1	0	1.851919	1.423165	-3.456879
41	1	0	2.837810	0.320709	-0.003726
42	1	0	1.529186	0.378348	3.756010
43	1	0	2.430237	1.504187	2.710165
44	1	0	0.505702	-1.356693	3.036286
45	1	0	0.463922	-1.957450	1.385997

46	1	0	4.505838	0.795448	1.498066
47	1	0	4.881982	-0.935434	1.486393
48	1	0	1.907121	-3.360881	2.865030
49	1	0	5.427433	-0.233282	4.125693
50	1	0	4.053195	0.053058	5.171764
51	1	0	4.164411	-2.348179	3.491326
52	1	0	2.778356	-1.812723	4.446543
53	1	0	5.093798	2.107571	3.133451
54	1	0	5.448413	2.098622	4.855670
55	1	0	3.800940	2.369065	4.310019
56	1	0	1.936144	-2.007458	-0.364850
57	1	0	-3.218759	0.396743	3.975352
58	1	0	-3.188245	2.851143	4.210954
59	1	0	-1.501928	4.214467	2.995832
60	1	0	-1.585530	-0.748928	2.522230
61	1	0	1.549117	4.568437	0.572221
62	1	0	0.959648	4.884949	2.224436
63	1	0	-0.167263	4.958400	0.847320
64	6	0	-3.368237	1.846085	-0.657806
65	6	0	-4.713818	1.616863	-0.946880
66	6	0	-5.610822	2.677793	-1.010896
67	6	0	-5.175868	3.977011	-0.765884
68	6	0	-3.837201	4.211283	-0.458071
69	6	0	-2.941497	3.151487	-0.405315
70	6	0	-2.425435	0.690971	-0.539480
71	7	0	-3.028336	-0.373720	-0.000345
72	6	0	-1.065785	0.841525	-0.874771
73	6	0	-0.592224	1.645457	-1.969271
74	8	0	0.611580	1.776475	-2.238975
75	6	0	-1.073250	3.094343	-3.775968
76	8	0	-1.535485	2.203162	-2.751031
77	6	0	0.018396	0.030880	-0.213883
78	16	0	-2.488931	-1.894554	-0.162526
79	8	0	-1.767582	-2.168348	-1.413746
80	8	0	-1.800238	-2.352451	1.075823
81	6	0	-4.034697	-2.764961	-0.235389
82	6	0	-4.196398	-3.740881	-1.206272
83	6	0	-5.384795	-4.467197	-1.240702
84	6	0	-6.400723	-4.225926	-0.318744
85	6	0	-6.209760	-3.231641	0.648683
86	6	0	-5.033720	-2.499727	0.698351
87	6	0	-7.686563	-5.011744	-0.352716
88	6	0	-0.696529	4.443363	-3.188618
89	1	0	-5.039868	0.600238	-1.121758
90	1	0	-6.649989	2.490139	-1.250619
91	1	0	-5.875956	4.802275	-0.809272

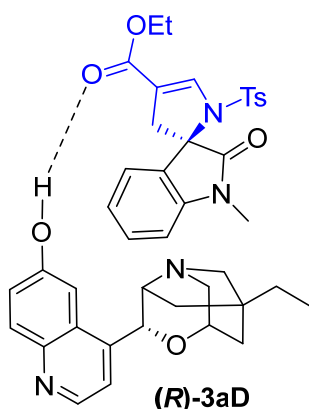
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93	1	0	-1.899406	3.321426	-0.166033
94	1	0	-0.234333	2.640464	-4.300504
95	1	0	-1.918318	3.181355	-4.455254
96	1	0	-0.323725	-0.959744	0.047207
97	1	0	0.833778	-0.082627	-0.917897
98	1	0	-3.405176	-3.912365	-1.923455
99	1	0	-5.523267	-5.228987	-1.998726
100	1	0	-6.997874	-3.030317	1.365458
101	1	0	-4.887998	-1.716145	1.430019
102	1	0	-7.814587	-5.587805	0.566420
103	1	0	-8.547760	-4.347079	-0.446724
104	1	0	-7.700325	-5.706555	-1.192264
105	1	0	-0.408336	5.133677	-3.983597
106	1	0	0.146465	4.328408	-2.506828
107	1	0	-1.545984	4.864193	-2.648574



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	6.018942	0.563536	-1.568536
2	6	0	6.896443	1.651212	-1.772488
3	6	0	4.705009	0.786018	-1.231792
4	6	0	4.280199	2.144023	-1.082890
5	6	0	5.253907	3.157795	-1.322931
6	7	0	6.544566	2.906406	-1.666523
7	6	0	2.973275	2.544064	-0.708732
8	6	0	2.661381	3.875178	-0.536240
9	6	0	3.621106	4.878833	-0.814235
10	6	0	4.880758	4.521858	-1.199703
11	8	0	1.446557	4.289960	-0.106763
12	6	0	3.183614	-0.582340	0.324739
13	8	0	4.529199	-1.564018	-1.428009
14	6	0	2.678837	-2.465202	1.665872
15	6	0	2.567453	-2.727449	-0.706561

16	7	0	2.270905	-1.799628	0.402428
17	6	0	4.312917	-0.831048	1.353338
18	6	0	4.072306	-2.799467	-0.881624
19	6	0	4.204788	-2.330436	1.650630
20	6	0	4.905090	-2.781656	2.935348
21	6	0	4.752704	-3.131745	0.454069
22	6	0	4.336943	-2.218238	4.238904
23	6	0	3.768006	-0.408850	-1.086925
24	6	0	-0.230049	0.464811	-2.857265
25	6	0	-0.466870	-0.689314	-3.607226
26	6	0	-0.542417	-1.955355	-3.019000
27	6	0	-0.365073	-2.031730	-1.644197
28	6	0	-0.101694	-0.874678	-0.882566
29	6	0	-0.050863	0.379071	-1.476362
30	7	0	-0.396888	-3.152325	-0.831187
31	6	0	-0.194367	-2.808648	0.490581
32	6	0	0.005894	-1.301317	0.498271
33	8	0	-0.118017	-3.561575	1.431846
34	6	0	-0.779996	-4.481000	-1.252996
35	6	0	-3.432330	0.989871	1.270229
36	6	0	-3.637168	1.790224	0.145333
37	6	0	-4.759092	2.605551	0.067855
38	6	0	-5.675880	2.629209	1.117965
39	6	0	-5.469017	1.830971	2.238844
40	6	0	-4.349022	1.007398	2.317227
41	6	0	-2.211769	0.127990	1.326627
42	7	0	-2.199872	-1.144493	0.867322
43	6	0	-0.975810	0.592975	1.705664
44	6	0	-0.579450	1.974841	1.814172
45	8	0	0.580577	2.348810	1.593871
46	6	0	-1.240120	4.235314	2.044657
47	8	0	-1.546629	2.830778	2.138915
48	6	0	0.104632	-0.461448	1.718350
49	16	0	-3.557983	-2.050634	0.653224
50	8	0	-3.095188	-3.302589	0.051798
51	8	0	-4.357675	-2.097491	1.877837
52	6	0	-4.529521	-1.209947	-0.580752
53	6	0	-5.836842	-0.843217	-0.291462
54	6	0	-6.579123	-0.185534	-1.265394
55	6	0	-6.028967	0.110341	-2.514020
56	6	0	-4.714704	-0.283179	-2.780781
57	6	0	-3.961138	-0.946341	-1.821446
58	6	0	-6.833415	0.865802	-3.540770
59	6	0	-2.469255	4.969818	2.533205
60	1	0	6.380450	-0.444095	-1.697483
61	1	0	7.929494	1.455611	-2.042185

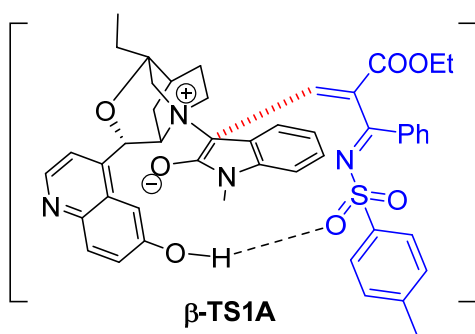
62	1	0	2.198613	1.814229	-0.537339
63	1	0	3.329595	5.912930	-0.687307
64	1	0	5.646619	5.258039	-1.404313
65	1	0	1.063667	3.600798	0.476304
66	1	0	2.600645	0.295303	0.591783
67	1	0	2.300170	-3.484835	1.697089
68	1	0	2.251361	-1.913436	2.505101
69	1	0	2.149725	-3.703364	-0.460609
70	1	0	2.102178	-2.373393	-1.627532
71	1	0	4.134474	-0.243493	2.255021
72	1	0	5.286588	-0.548594	0.950521
73	1	0	4.332755	-3.557912	-1.621511
74	1	0	5.962809	-2.512030	2.850598
75	1	0	4.870269	-3.874915	2.979826
76	1	0	5.827116	-2.957383	0.348313
77	1	0	4.610175	-4.200431	0.650997
78	1	0	4.319656	-1.127204	4.242145
79	1	0	4.952683	-2.537018	5.080830
80	1	0	3.322490	-2.575062	4.423487
81	1	0	2.942714	-0.282516	-1.799868
82	1	0	-0.182588	1.427091	-3.348301
83	1	0	-0.600459	-0.604444	-4.678368
84	1	0	-0.744308	-2.837150	-3.611961
85	1	0	0.114486	1.263578	-0.874450
86	1	0	-0.048160	-4.883913	-1.956825
87	1	0	-1.772626	-4.451369	-1.699591
88	1	0	-0.818957	-5.098615	-0.359603
89	1	0	-2.921260	1.758991	-0.668016
90	1	0	-4.920897	3.217163	-0.811274
91	1	0	-6.551379	3.263914	1.058740
92	1	0	-6.181537	1.844372	3.053888
93	1	0	-4.191710	0.367466	3.174663
94	1	0	-1.012539	4.476917	1.005042
95	1	0	-0.358178	4.447461	2.647991
96	1	0	1.071374	0.034240	1.777899
97	1	0	-0.017691	-1.128921	2.576011
98	1	0	-6.245148	-1.058053	0.686477
99	1	0	-7.598391	0.112854	-1.048863
100	1	0	-4.277949	-0.065473	-3.748728
101	1	0	-2.939996	-1.241947	-2.027013
102	1	0	-7.860954	0.501285	-3.580042
103	1	0	-6.870575	1.929865	-3.293059
104	1	0	-6.396529	0.768602	-4.534766
105	1	0	-2.312795	6.046915	2.461367
106	1	0	-2.675715	4.712745	3.572183
107	1	0	-3.335117	4.693224	1.930998



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.699881	0.031230	1.322618
2	6	0	-7.839521	0.844034	1.128398
3	6	0	-5.452220	0.533067	1.050058
4	6	0	-5.352160	1.879928	0.587760
5	6	0	-6.567417	2.604265	0.438864
6	7	0	-7.795215	2.082089	0.703370
7	6	0	-4.123235	2.523287	0.291632
8	6	0	-4.110260	3.830755	-0.142210
9	6	0	-5.321172	4.554622	-0.285725
10	6	0	-6.513427	3.952614	-0.002305
11	8	0	-2.971631	4.493831	-0.448845
12	6	0	-3.590678	-0.783405	-0.064582
13	8	0	-4.566494	-1.442644	2.040209
14	6	0	-2.358201	-2.679049	-0.656163
15	6	0	-2.253528	-1.961972	1.607876
16	7	0	-2.293266	-1.491893	0.213803
17	6	0	-4.516686	-1.807589	-0.773999
18	6	0	-3.620395	-2.520241	1.976955
19	6	0	-3.813896	-3.147706	-0.521745
20	6	0	-4.234445	-4.284190	-1.457096
21	6	0	-4.046236	-3.574209	0.943158
22	6	0	-3.866192	-4.104057	-2.930681
23	6	0	-4.216252	-0.310188	1.253928
24	6	0	1.428364	-2.425837	2.548017
25	6	0	1.221066	-3.751639	2.178765
26	6	0	1.067065	-4.122371	0.837409
27	6	0	1.138157	-3.117810	-0.116567
28	6	0	1.363965	-1.784157	0.243413
29	6	0	1.499565	-1.426776	1.569350

30	7	0	1.001142	-3.228959	-1.498387
31	6	0	1.209261	-2.019720	-2.122244
32	6	0	1.396268	-0.958017	-1.017112
33	8	0	1.172478	-1.808810	-3.310369
34	6	0	0.860654	-4.468864	-2.222984
35	6	0	3.449223	2.183739	-0.680639
36	6	0	3.666686	2.694191	0.600602
37	6	0	4.655576	3.646419	0.813649
38	6	0	5.424673	4.098916	-0.255991
39	6	0	5.200686	3.599060	-1.536490
40	6	0	4.214588	2.641561	-1.753060
41	6	0	2.367949	1.189357	-0.875956
42	7	0	2.628934	-0.154208	-1.186099
43	6	0	1.033362	1.380128	-0.767944
44	6	0	0.293918	2.616638	-0.564027
45	8	0	-0.930821	2.628497	-0.546251
46	6	0	0.322176	4.956631	-0.250706
47	8	0	1.034564	3.711526	-0.412567
48	6	0	0.290772	0.115368	-1.107524
49	16	0	4.141083	-0.905161	-1.313974
50	8	0	3.797553	-2.298552	-1.564099
51	8	0	4.935680	-0.127871	-2.248803
52	6	0	4.926906	-0.815479	0.271384
53	6	0	5.804727	0.230059	0.542190
54	6	0	6.425237	0.272113	1.783758
55	6	0	6.185681	-0.715101	2.743705
56	6	0	5.316287	-1.763549	2.432099
57	6	0	4.685116	-1.826781	1.196734
58	6	0	6.847407	-0.642555	4.095239
59	6	0	1.375029	6.027821	-0.071923
60	1	0	-6.804536	-0.975397	1.700160
61	1	0	-8.824092	0.439504	1.341577
62	1	0	-3.180485	2.002601	0.395719
63	1	0	-5.263845	5.579601	-0.627395
64	1	0	-7.455072	4.475676	-0.103991
65	1	0	-2.223992	3.865005	-0.454474
66	1	0	-3.389364	0.075297	-0.705390
67	1	0	-1.617368	-3.419461	-0.345317
68	1	0	-2.136213	-2.379582	-1.685393
69	1	0	-1.475453	-2.722267	1.693372
70	1	0	-1.976610	-1.146783	2.278351
71	1	0	-4.565580	-1.592690	-1.842794
72	1	0	-5.532399	-1.783891	-0.377821
73	1	0	-3.617924	-2.966725	2.973377
74	1	0	-5.317443	-4.417381	-1.364980
75	1	0	-3.782457	-5.214005	-1.094108

76	1	0	-5.104422	-3.805849	1.098240
77	1	0	-3.477684	-4.491669	1.138759
78	1	0	-4.265352	-3.175621	-3.341621
79	1	0	-4.271494	-4.926054	-3.522721
80	1	0	-2.784286	-4.096465	-3.075992
81	1	0	-3.481225	0.299786	1.792243
82	1	0	1.541165	-2.166972	3.592417
83	1	0	1.173357	-4.517452	2.942878
84	1	0	0.904942	-5.155459	0.559220
85	1	0	1.679254	-0.393652	1.842234
86	1	0	-0.054649	-4.985105	-1.924920
87	1	0	1.722290	-5.115014	-2.043227
88	1	0	0.810556	-4.216008	-3.279525
89	1	0	3.057039	2.340509	1.422722
90	1	0	4.824544	4.034439	1.810139
91	1	0	6.195218	4.841904	-0.093104
92	1	0	5.794177	3.952108	-2.369769
93	1	0	4.047206	2.238666	-2.741791
94	1	0	-0.338557	4.876956	0.612715
95	1	0	-0.291584	5.126040	-1.135889
96	1	0	-0.540034	-0.124693	-0.443745
97	1	0	-0.082153	0.167067	-2.135387
98	1	0	6.004712	0.981366	-0.210455
99	1	0	7.111992	1.079901	2.007192
100	1	0	5.138158	-2.545608	3.160353
101	1	0	4.028910	-2.648683	0.943487
102	1	0	7.848288	-0.216641	4.019706
103	1	0	6.267907	-0.010125	4.772546
104	1	0	6.926275	-1.630980	4.547854
105	1	0	0.898150	7.002933	0.031552
106	1	0	2.041528	6.048934	-0.934372
107	1	0	1.972095	5.830257	0.818592

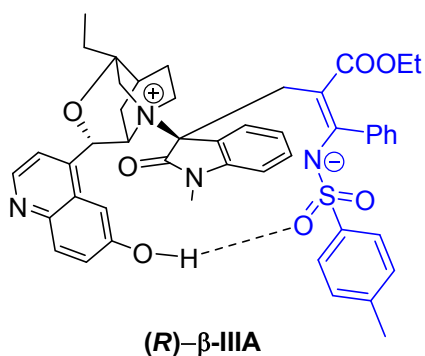


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	-6.199848	-3.151816	-1.789365
2	6	0	-5.577560	-1.804217	-2.150126
3	6	0	-4.836524	-1.092080	-1.027610
4	6	0	-5.653724	-0.902221	0.286295
5	6	0	-5.350210	-2.031400	1.284063
6	6	0	-3.887446	-1.867351	1.738391
7	8	0	-4.484107	0.187741	-1.570806
8	6	0	-3.529914	-1.773896	-0.641698
9	7	0	-3.105130	-1.137971	0.658327
10	6	0	-3.599249	0.343554	0.638401
11	6	0	-3.485758	0.866254	-0.796483
12	6	0	-3.719098	2.361036	-0.908656
13	6	0	-4.811677	2.829919	-1.595938
14	6	0	-4.991931	4.220443	-1.763880
15	7	0	-4.160231	5.123992	-1.311111
16	6	0	-3.071645	4.683053	-0.627618
17	6	0	-2.168087	5.667506	-0.147294
18	6	0	-1.053407	5.315546	0.554196
19	6	0	-0.785727	3.948010	0.827161
20	8	0	0.334297	3.719406	1.540633
21	6	0	-1.634871	2.964931	0.369883
22	6	0	-2.793648	3.309041	-0.373953
23	6	0	-5.096583	0.358936	0.955980
24	6	0	-0.322039	-4.872325	0.416103
25	6	0	0.704299	-4.776813	1.354589
26	6	0	0.888038	-3.603069	2.080674
27	6	0	0.009427	-2.551652	1.853556
28	6	0	-1.041788	-2.615770	0.904492
29	6	0	-1.178490	-3.798442	0.171373
30	7	0	-0.022570	-1.327424	2.489061
31	6	0	-1.056628	-0.550915	2.009277
32	6	0	-1.650804	-1.293729	0.897887
33	8	0	-1.350348	0.560114	2.475721
34	6	0	0.870722	-0.901100	3.540774
35	6	0	3.482843	-1.087456	-0.499071
36	6	0	4.280052	-1.863305	0.341515
37	6	0	5.527989	-2.292504	-0.097412
38	6	0	5.985608	-1.943655	-1.366563
39	6	0	5.184921	-1.175447	-2.208172
40	6	0	3.929926	-0.758939	-1.779777
41	6	0	2.127708	-0.608425	-0.089795
42	7	0	1.885763	0.284512	0.824600
43	6	0	0.974148	-1.063822	-0.855338
44	6	0	0.930262	-2.290708	-1.686271
45	8	0	0.046426	-2.527333	-2.489460

46	6	0	1.961628	-4.327364	-2.246962
47	8	0	1.941007	-3.132047	-1.452086
48	6	0	-0.184874	-0.340083	-0.826291
49	16	0	3.059182	1.081837	1.709170
50	8	0	2.281768	2.019583	2.523282
51	8	0	3.965338	0.150474	2.386922
52	6	0	3.993254	2.034036	0.540313
53	6	0	3.440362	3.216417	0.052385
54	6	0	4.163135	3.950839	-0.877110
55	6	0	5.422344	3.524589	-1.313871
56	6	0	5.953318	2.344410	-0.792824
57	6	0	5.245651	1.589798	0.136791
58	6	0	6.181704	4.329638	-2.336971
59	6	0	3.166174	-5.120538	-1.789771
60	1	0	-6.694607	-3.572337	-2.665060
61	1	0	-6.950634	-3.053744	-1.003438
62	1	0	-5.452859	-3.877964	-1.461231
63	1	0	-6.357047	-1.115342	-2.485443
64	1	0	-4.881294	-1.918396	-2.984750
65	1	0	-6.719964	-0.825296	0.070141
66	1	0	-6.007945	-1.939709	2.150061
67	1	0	-5.512672	-3.019614	0.854870
68	1	0	-3.382888	-2.820270	1.879730
69	1	0	-3.773374	-1.270616	2.641926
70	1	0	-2.756087	-1.624942	-1.391211
71	1	0	-3.644769	-2.838305	-0.461288
72	1	0	-2.982096	0.870744	1.357597
73	1	0	-2.497532	0.650186	-1.206091
74	1	0	-5.518383	2.137277	-2.027604
75	1	0	-5.858584	4.583707	-2.306897
76	1	0	-2.407561	6.700837	-0.360044
77	1	0	-0.358247	6.052122	0.934720
78	1	0	0.465971	2.789034	1.799192
79	1	0	-1.423990	1.943401	0.647742
80	1	0	-5.515041	1.272753	0.537383
81	1	0	-5.300211	0.362919	2.027133
82	1	0	-0.451745	-5.787624	-0.147632
83	1	0	1.364231	-5.618512	1.522456
84	1	0	1.677934	-3.513477	2.815290
85	1	0	-1.906851	-3.895669	-0.620414
86	1	0	1.906671	-1.068230	3.246448
87	1	0	0.660869	-1.443176	4.465903
88	1	0	0.716320	0.164085	3.691011
89	1	0	3.924319	-2.122879	1.327534
90	1	0	6.145121	-2.897414	0.554674
91	1	0	6.961909	-2.273469	-1.699282

92	1	0	5.535195	-0.902035	-3.195264
93	1	0	3.297671	-0.164442	-2.428570
94	1	0	1.026941	-4.864480	-2.090074
95	1	0	2.023289	-4.047976	-3.299437
96	1	0	-0.934754	-0.595122	-1.557825
97	1	0	-0.202629	0.631572	-0.359272
98	1	0	2.477701	3.556670	0.415268
99	1	0	3.751082	4.875813	-1.263406
100	1	0	6.931693	2.009625	-1.116238
101	1	0	5.651732	0.673996	0.546030
102	1	0	6.161980	5.392439	-2.090596
103	1	0	7.222085	4.010055	-2.396054
104	1	0	5.735973	4.213146	-3.327808
105	1	0	3.251749	-6.043511	-2.365365
106	1	0	3.066361	-5.370290	-0.732616
107	1	0	4.076257	-4.533662	-1.920386

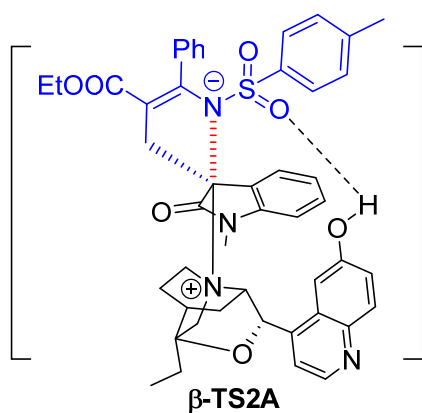


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.669165	-3.974112	-0.572763
2	6	0	-5.331728	-2.668349	-1.289985
3	6	0	-4.541170	-1.646171	-0.484292
4	6	0	-5.153937	-1.281438	0.899862
5	6	0	-4.530424	-2.145799	2.001178
6	6	0	-3.064391	-1.705996	2.144565
7	8	0	-4.502245	-0.481215	-1.316525
8	6	0	-3.093688	-2.073230	-0.243725
9	7	0	-2.573006	-1.141172	0.822161
10	6	0	-3.283284	0.248994	0.608375
11	6	0	-3.550102	0.500393	-0.887762
12	6	0	-4.131991	1.886964	-1.125230
13	6	0	-5.408973	1.997655	-1.622289

14	6	0	-5.972617	3.272188	-1.838282
15	7	0	-5.351023	4.394592	-1.575970
16	6	0	-4.085409	4.310226	-1.093142
17	6	0	-3.425665	5.535509	-0.808708
18	6	0	-2.150781	5.552477	-0.331449
19	6	0	-1.443094	4.335842	-0.120998
20	8	0	-0.195660	4.477850	0.333848
21	6	0	-2.058178	3.125913	-0.382957
22	6	0	-3.394910	3.082759	-0.860110
23	6	0	-4.683079	0.142931	1.226324
24	6	0	0.348505	-4.717250	1.038431
25	6	0	1.005081	-4.570883	2.256469
26	6	0	0.966115	-3.365874	2.958590
27	6	0	0.240588	-2.322397	2.405670
28	6	0	-0.429681	-2.452099	1.181411
29	6	0	-0.364712	-3.650257	0.485708
30	7	0	0.052054	-1.052182	2.948391
31	6	0	-0.620213	-0.249179	2.075675
32	6	0	-1.023145	-1.101913	0.836551
33	8	0	-0.942318	0.906693	2.256753
34	6	0	0.816907	-0.519842	4.058849
35	6	0	3.345863	-0.690340	-1.028604
36	6	0	4.444865	-1.073501	-0.259172
37	6	0	5.710857	-1.139693	-0.830204
38	6	0	5.888702	-0.810751	-2.171479
39	6	0	4.796723	-0.413961	-2.941447
40	6	0	3.530997	-0.355894	-2.372122
41	6	0	2.007107	-0.558887	-0.393787
42	7	0	1.898949	0.030976	0.836768
43	6	0	0.844324	-1.025620	-0.957186
44	6	0	0.696297	-2.061392	-1.970873
45	8	0	-0.390999	-2.405541	-2.432642
46	6	0	1.705552	-3.702454	-3.328721
47	8	0	1.829260	-2.683418	-2.327689
48	6	0	-0.456472	-0.463926	-0.455839
49	16	0	2.269035	1.563538	1.099143
50	8	0	1.539781	2.414924	0.117067
51	8	0	2.062950	1.829873	2.526053
52	6	0	3.994825	1.893305	0.790349
53	6	0	4.414749	2.341350	-0.457044
54	6	0	5.774008	2.489381	-0.697445
55	6	0	6.716332	2.201209	0.293225
56	6	0	6.267134	1.784976	1.547242
57	6	0	4.909384	1.627118	1.801880
58	6	0	8.188951	2.319609	-0.004337
59	6	0	3.111331	-4.179578	-3.626086

60	1	0	-6.220626	-4.629188	-1.247534
61	1	0	-6.296099	-3.803647	0.304231
62	1	0	-4.775146	-4.515722	-0.255844
63	1	0	-6.252869	-2.166011	-1.595698
64	1	0	-4.768816	-2.871547	-2.204354
65	1	0	-6.240899	-1.365331	0.874504
66	1	0	-5.043386	-1.966850	2.947512
67	1	0	-4.597657	-3.212284	1.790144
68	1	0	-2.415665	-2.541344	2.392208
69	1	0	-2.930828	-0.919930	2.883683
70	1	0	-2.499103	-1.983660	-1.151758
71	1	0	-2.999240	-3.087227	0.136848
72	1	0	-2.647714	0.996979	1.067637
73	1	0	-2.647727	0.411816	-1.489990
74	1	0	-5.979594	1.109299	-1.847291
75	1	0	-6.979519	3.351715	-2.235119
76	1	0	-3.981405	6.445650	-0.990800
77	1	0	-1.632064	6.475551	-0.110012
78	1	0	0.310612	3.635300	0.376410
79	1	0	-1.494633	2.221204	-0.211021
80	1	0	-5.307981	0.903018	0.763843
81	1	0	-4.687107	0.327078	2.300658
82	1	0	0.406501	-5.655168	0.502563
83	1	0	1.566259	-5.401377	2.665571
84	1	0	1.489125	-3.246081	3.897588
85	1	0	-0.817267	-3.748480	-0.491853
86	1	0	1.879660	-0.576388	3.821425
87	1	0	0.590157	-1.075287	4.969913
88	1	0	0.549816	0.527105	4.166099
89	1	0	4.292319	-1.306481	0.786860
90	1	0	6.559593	-1.434887	-0.225822
91	1	0	6.876917	-0.852936	-2.613345
92	1	0	4.934868	-0.140219	-3.980250
93	1	0	2.676730	-0.034297	-2.954899
94	1	0	1.071182	-4.503390	-2.944918
95	1	0	1.217275	-3.282302	-4.208260
96	1	0	-1.156765	-0.605597	-1.269710
97	1	0	-0.325430	0.600221	-0.266536
98	1	0	3.679601	2.565732	-1.217715
99	1	0	6.111371	2.826405	-1.670950
100	1	0	6.988305	1.583047	2.330978
101	1	0	4.550670	1.312990	2.773297
102	1	0	8.415892	3.262318	-0.505106
103	1	0	8.782219	2.265076	0.908684
104	1	0	8.510461	1.509873	-0.665066
105	1	0	3.092572	-4.953912	-4.394626

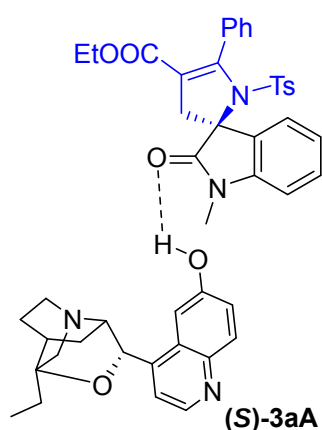
106	1	0	3.571213	-4.586757	-2.725500
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.462376	-4.295912	0.553016
2	6	0	5.303584	-2.931659	1.221815
3	6	0	4.594676	-1.871199	0.393970
4	6	0	5.189350	-1.628078	-1.025940
5	6	0	4.410115	-2.436626	-2.074795
6	6	0	2.979750	-1.838570	-2.136267
7	8	0	4.701578	-0.664485	1.173090
8	6	0	3.093003	-2.116773	0.205561
9	7	0	2.662107	-1.169012	-0.851608
10	6	0	3.501254	0.088357	-0.744593
11	6	0	3.791633	0.355644	0.741556
12	6	0	4.409321	1.714840	0.997411
13	6	0	5.704230	1.815209	1.441472
14	6	0	6.259767	3.088135	1.700986
15	7	0	5.611392	4.215366	1.546022
16	6	0	4.325741	4.139723	1.111214
17	6	0	3.620610	5.361465	0.941884
18	6	0	2.328719	5.375565	0.505039
19	6	0	1.657563	4.157170	0.211209
20	8	0	0.392705	4.284337	-0.223176
21	6	0	2.311554	2.954762	0.374624
22	6	0	3.657547	2.916947	0.819740
23	6	0	4.887189	-0.163936	-1.370031
24	6	0	-0.590424	-4.473017	-1.280886
25	6	0	-0.760153	-4.324442	-2.660418
26	6	0	-0.550909	-3.106841	-3.311261
27	6	0	-0.162578	-2.028460	-2.530129

28	6	0	-0.006922	-2.164016	-1.135225
29	6	0	-0.216832	-3.381983	-0.500153
30	7	0	0.153383	-0.740417	-2.927681
31	6	0	0.489918	0.034897	-1.838228
32	6	0	0.368209	-0.867701	-0.627703
33	8	0	0.863645	1.186967	-1.858002
34	6	0	-0.001633	-0.203468	-4.261595
35	6	0	-3.471301	-0.483377	1.220921
36	6	0	-4.463293	-1.126056	0.479011
37	6	0	-5.775472	-1.144596	0.937660
38	6	0	-6.105385	-0.507978	2.131579
39	6	0	-5.120155	0.147489	2.867275
40	6	0	-3.807050	0.158083	2.414755
41	6	0	-2.078091	-0.443018	0.707521
42	7	0	-1.851569	-0.125077	-0.617412
43	6	0	-0.969976	-0.793417	1.424732
44	6	0	-0.880923	-1.671579	2.594723
45	8	0	0.161150	-2.214909	2.934297
46	6	0	-1.985343	-2.831004	4.322093
47	8	0	-2.034618	-1.888881	3.237562
48	6	0	0.346786	-0.420949	0.784559
49	16	0	-2.282920	1.334398	-1.225162
50	8	0	-1.708905	2.406066	-0.384154
51	8	0	-1.952264	1.292632	-2.652197
52	6	0	-4.047954	1.535299	-1.144755
53	6	0	-4.623949	2.240945	-0.095362
54	6	0	-6.007116	2.339074	-0.034822
55	6	0	-6.814647	1.746594	-1.009098
56	6	0	-6.206950	1.072007	-2.069579
57	6	0	-4.823929	0.961699	-2.144613
58	6	0	-8.314969	1.814853	-0.892670
59	6	0	-3.388854	-2.905239	4.884036
60	1	0	5.963259	-4.984637	1.234124
61	1	0	6.065708	-4.232967	-0.354241
62	1	0	4.498927	-4.739146	0.292355
63	1	0	6.287470	-2.525113	1.470521
64	1	0	4.759600	-3.033129	2.164371
65	1	0	6.257260	-1.851258	-1.044720
66	1	0	4.891624	-2.336234	-3.049463
67	1	0	4.376762	-3.499672	-1.836366
68	1	0	2.239170	-2.619594	-2.307795
69	1	0	2.884929	-1.098599	-2.930652
70	1	0	2.586121	-1.948637	1.155012
71	1	0	2.854007	-3.128594	-0.120476
72	1	0	2.961243	0.903794	-1.217905
73	1	0	2.871588	0.294117	1.329148

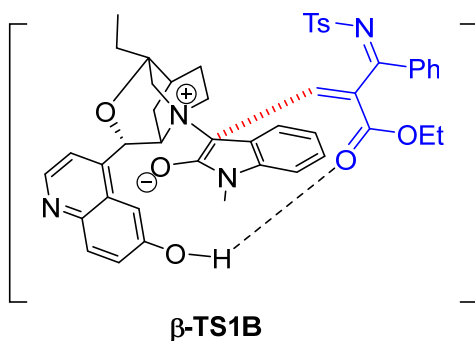
74	1	0	6.289326	0.922044	1.604011
75	1	0	7.284108	3.160460	2.052532
76	1	0	4.154827	6.273715	1.172184
77	1	0	1.780451	6.298097	0.367639
78	1	0	-0.051081	3.431694	-0.393883
79	1	0	1.789195	2.050985	0.106323
80	1	0	5.602686	0.528836	-0.930340
81	1	0	4.894518	-0.006621	-2.449728
82	1	0	-0.760191	-5.436536	-0.820289
83	1	0	-1.061654	-5.182367	-3.248308
84	1	0	-0.683871	-3.012578	-4.380446
85	1	0	-0.084782	-3.465942	0.572094
86	1	0	-1.040729	-0.289251	-4.576382
87	1	0	0.656517	-0.724496	-4.959902
88	1	0	0.258002	0.850191	-4.210810
89	1	0	-4.193835	-1.599776	-0.456382
90	1	0	-6.541114	-1.645631	0.358646
91	1	0	-7.129453	-0.516078	2.484586
92	1	0	-5.376706	0.652708	3.790142
93	1	0	-3.031648	0.664462	2.974781
94	1	0	-1.642648	-3.792512	3.938651
95	1	0	-1.260390	-2.485636	5.058654
96	1	0	1.130074	-0.897266	1.362797
97	1	0	0.478926	0.661470	0.806949
98	1	0	-3.990703	2.699970	0.651254
99	1	0	-6.469427	2.877113	0.784575
100	1	0	-6.824017	0.630784	-2.843591
101	1	0	-4.342188	0.449121	-2.966561
102	1	0	-8.797906	1.566455	-1.837823
103	1	0	-8.668388	1.107517	-0.137273
104	1	0	-8.642097	2.810535	-0.589748
105	1	0	-3.427907	-3.623500	5.704148
106	1	0	-4.090618	-3.212768	4.108315
107	1	0	-3.700286	-1.928913	5.255812



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.142641	-3.335635	-2.763587
2	6	0	-5.801407	-1.863945	-2.536241
3	6	0	-5.010773	-1.566133	-1.273190
4	6	0	-5.642536	-2.105955	0.049068
5	6	0	-5.009008	-3.452639	0.450563
6	6	0	-3.518867	-3.166253	0.791419
7	8	0	-4.947145	-0.123843	-1.205944
8	6	0	-3.555454	-2.043921	-1.279338
9	7	0	-3.073793	-1.936036	0.118373
10	6	0	-3.762133	-0.768374	0.755604
11	6	0	-3.894955	0.307486	-0.335865
12	6	0	-4.193660	1.688842	0.178004
13	6	0	-5.397485	2.302944	-0.050217
14	6	0	-5.598054	3.630738	0.395820
15	7	0	-4.692872	4.344267	1.018262
16	6	0	-3.490344	3.751722	1.255932
17	6	0	-2.498816	4.515338	1.927843
18	6	0	-1.275610	3.980975	2.221424
19	6	0	-0.975310	2.643637	1.851982
20	8	0	0.244944	2.184803	2.205901
21	6	0	-1.900824	1.887346	1.169350
22	6	0	-3.180424	2.420342	0.868867
23	6	0	-5.209005	-1.125684	1.148467
24	6	0	2.212822	-4.908693	-1.372421
25	6	0	1.630434	-5.686398	-0.376931
26	6	0	0.919428	-5.107631	0.679385
27	6	0	0.819054	-3.727851	0.696650
28	6	0	1.394753	-2.936460	-0.300613
29	6	0	2.091744	-3.514229	-1.340737
30	7	0	0.184278	-2.916311	1.646812
31	6	0	0.371952	-1.599275	1.366363
32	6	0	1.055169	-1.503425	-0.014516
33	8	0	0.005901	-0.658039	2.052610
34	6	0	-0.377804	-3.388775	2.891037
35	6	0	2.667675	1.826079	-0.726224
36	6	0	3.617235	1.725343	-1.744215
37	6	0	4.526332	2.756760	-1.955272
38	6	0	4.490096	3.886658	-1.144372
39	6	0	3.544089	3.982841	-0.125005
40	6	0	2.629384	2.957592	0.088625
41	6	0	1.713559	0.697934	-0.572899
42	7	0	2.178314	-0.540095	-0.049055

43	6	0	0.472662	0.556059	-1.067867
44	6	0	-0.377276	1.544744	-1.740021
45	8	0	-1.375226	1.225139	-2.358074
46	6	0	-0.884769	3.819544	-2.046834
47	8	0	0.016462	2.804340	-1.558482
48	6	0	0.031575	-0.880616	-0.997833
49	16	0	3.232802	-0.549398	1.295830
50	8	0	3.052353	0.663558	2.078211
51	8	0	3.021710	-1.867782	1.886041
52	6	0	4.836692	-0.515738	0.556618
53	6	0	5.584825	0.651546	0.605952
54	6	0	6.847521	0.653409	0.022705
55	6	0	7.355639	-0.488606	-0.596361
56	6	0	6.572436	-1.648922	-0.629189
57	6	0	5.312096	-1.674505	-0.052096
58	6	0	8.736046	-0.489021	-1.199735
59	6	0	-0.331757	5.145299	-1.573229
60	1	0	-6.688306	-3.451564	-3.700960
61	1	0	-6.772065	-3.730267	-1.963990
62	1	0	-5.246317	-3.956234	-2.827378
63	1	0	-6.721762	-1.276050	-2.479259
64	1	0	-5.231530	-1.472170	-3.382901
65	1	0	-6.728231	-2.179029	-0.040582
66	1	0	-5.531558	-3.855184	1.321390
67	1	0	-5.092023	-4.193096	-0.346141
68	1	0	-2.873093	-3.988452	0.473592
69	1	0	-3.377740	-3.033469	1.866042
70	1	0	-2.967451	-1.421816	-1.957284
71	1	0	-3.449998	-3.078970	-1.606625
72	1	0	-3.167993	-0.429615	1.602760
73	1	0	-2.962254	0.377888	-0.901787
74	1	0	-6.173557	1.780088	-0.590432
75	1	0	-6.552930	4.113757	0.213356
76	1	0	-2.760060	5.527581	2.207349
77	1	0	-0.519019	4.543526	2.753069
78	1	0	0.304765	1.219265	2.068870
79	1	0	-1.637703	0.876445	0.891174
80	1	0	-5.817578	-0.221865	1.170857
81	1	0	-5.272602	-1.595005	2.132521
82	1	0	2.758861	-5.384289	-2.176295
83	1	0	1.729868	-6.763624	-0.414842
84	1	0	0.478099	-5.718033	1.456065
85	1	0	2.542504	-2.895682	-2.108060
86	1	0	0.398650	-3.852087	3.502498
87	1	0	-1.172697	-4.108909	2.695365
88	1	0	-0.783668	-2.524561	3.411067

89	1	0	3.644258	0.835389	-2.361722
90	1	0	5.260498	2.673909	-2.746528
91	1	0	5.195832	4.692177	-1.305476
92	1	0	3.517323	4.860867	0.507757
93	1	0	1.899173	3.011784	0.884257
94	1	0	-0.933535	3.749720	-3.133544
95	1	0	-1.876911	3.619730	-1.642280
96	1	0	0.121808	-1.351144	-1.981067
97	1	0	-0.989602	-1.033491	-0.644193
98	1	0	5.175059	1.537338	1.073795
99	1	0	7.441474	1.558990	0.044346
100	1	0	6.961541	-2.539900	-1.107577
101	1	0	4.703630	-2.570544	-0.062088
102	1	0	9.074703	0.525485	-1.409187
103	1	0	9.452603	-0.946326	-0.513102
104	1	0	8.758434	-1.060082	-2.128792
105	1	0	-0.961808	5.960000	-1.932663
106	1	0	0.683072	5.290600	-1.945237
107	1	0	-0.314315	5.172137	-0.483488

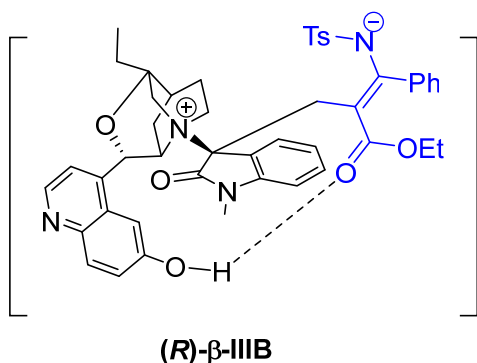


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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3	6	0	3.649665	-2.814103	0.654457
4	6	0	4.771250	-2.747212	-0.425799
5	6	0	4.242934	-3.211411	-1.793193
6	6	0	3.216000	-2.168111	-2.271269
7	8	0	3.826935	-1.754272	1.605509
8	6	0	2.331439	-2.540902	-0.059306
9	7	0	2.626084	-1.456242	-1.065285
10	6	0	3.739086	-0.548563	-0.451872
11	6	0	3.516035	-0.464723	1.062839
12	6	0	4.409707	0.568680	1.725061

13	6	0	5.383255	0.165895	2.605966
14	6	0	6.193447	1.130220	3.245546
15	7	0	6.080092	2.420874	3.057547
16	6	0	5.121290	2.843356	2.192440
17	6	0	4.999419	4.243931	1.991521
18	6	0	4.058050	4.756565	1.147441
19	6	0	3.182562	3.885981	0.447569
20	8	0	2.286996	4.470502	-0.367209
21	6	0	3.282465	2.520893	0.609488
22	6	0	4.246346	1.967404	1.487454
23	6	0	5.084121	-1.259511	-0.622140
24	6	0	-1.538193	-2.987830	-2.492188
25	6	0	-2.162592	-2.048422	-3.312359
26	6	0	-1.590495	-0.796021	-3.515432
27	6	0	-0.388322	-0.521686	-2.876269
28	6	0	0.252243	-1.442332	-2.017284
29	6	0	-0.346384	-2.693332	-1.838239
30	7	0	0.383299	0.629682	-2.969507
31	6	0	1.554635	0.492253	-2.249470
32	6	0	1.401189	-0.728879	-1.467254
33	8	0	2.484850	1.311047	-2.299803
34	6	0	0.148634	1.725366	-3.878551
35	1	0	3.582599	-6.240311	1.389502
36	1	0	4.481774	-5.510600	0.064279
37	1	0	2.711340	-5.481436	0.067648
38	1	0	4.524296	-4.056485	2.113061
39	1	0	2.772246	-4.032889	2.159094
40	1	0	5.644244	-3.320036	-0.110935
41	1	0	5.068332	-3.255787	-2.505700
42	1	0	3.794683	-4.203591	-1.751950
43	1	0	2.373551	-2.616492	-2.793233
44	1	0	3.643910	-1.386073	-2.896134
45	1	0	1.563251	-2.196892	0.628501
46	1	0	1.960544	-3.403212	-0.602799
47	1	0	3.667736	0.402708	-0.968244
48	1	0	2.475501	-0.216819	1.288682
49	1	0	5.518968	-0.883565	2.820225
50	1	0	6.960180	0.804505	3.941194
51	1	0	5.681688	4.879735	2.539916
52	1	0	3.949806	5.821079	0.987506
53	1	0	1.636778	3.817829	-0.684280
54	1	0	2.650858	1.897127	-0.003605
55	1	0	5.763473	-0.872122	0.134970
56	1	0	5.536140	-1.074057	-1.596915
57	1	0	-2.015457	-3.941879	-2.314274
58	1	0	-3.106047	-2.292084	-3.783064

59	1	0	-2.060370	-0.058326	-4.153720
60	1	0	0.042230	-3.423580	-1.143785
61	1	0	-0.872426	2.087141	-3.759797
62	1	0	0.303407	1.414508	-4.914799
63	1	0	0.855035	2.511942	-3.622957
64	6	0	-3.584530	0.708689	-0.216565
65	6	0	-3.906216	1.675855	0.737807
66	6	0	-5.149749	2.294026	0.708408
67	6	0	-6.063646	1.969404	-0.293008
68	6	0	-5.732137	1.020535	-1.256484
69	6	0	-4.497179	0.379669	-1.217285
70	6	0	-2.250768	0.039470	-0.131657
71	7	0	-2.067216	-1.210987	0.145201
72	6	0	-1.036492	0.855430	-0.231664
73	6	0	-0.974319	2.187945	-0.853001
74	8	0	-0.015600	2.939810	-0.762769
75	6	0	-2.143524	3.893857	-1.991052
76	8	0	-2.062232	2.522694	-1.556890
77	6	0	0.143079	0.389439	0.289321
78	16	0	-3.282543	-2.307155	0.500786
79	8	0	-4.164227	-2.534078	-0.646314
80	8	0	-2.567544	-3.438789	1.084506
81	6	0	-4.242365	-1.542748	1.788489
82	6	0	-5.580459	-1.246458	1.562714
83	6	0	-6.304110	-0.612055	2.563951
84	6	0	-5.705176	-0.270106	3.778677
85	6	0	-4.362732	-0.597208	3.984337
86	6	0	-3.625458	-1.239552	2.996966
87	6	0	-6.497236	0.453330	4.837485
88	6	0	-3.483574	4.043673	-2.677253
89	1	0	-3.186675	1.923912	1.509278
90	1	0	-5.405178	3.027768	1.462754
91	1	0	-7.031196	2.455281	-0.321610
92	1	0	-6.439513	0.770800	-2.037366
93	1	0	-4.238171	-0.375194	-1.945803
94	1	0	-2.052575	4.538871	-1.116776
95	1	0	-1.307802	4.108406	-2.656519
96	1	0	0.949677	1.089157	0.425350
97	1	0	0.127683	-0.521560	0.868799
98	1	0	-6.026880	-1.496924	0.610325
99	1	0	-7.346911	-0.368004	2.396816
100	1	0	-3.893687	-0.350858	4.929518
101	1	0	-2.588084	-1.505515	3.157212
102	1	0	-5.961285	0.475199	5.786211
103	1	0	-6.690018	1.485678	4.535175
104	1	0	-7.463224	-0.027459	5.000234

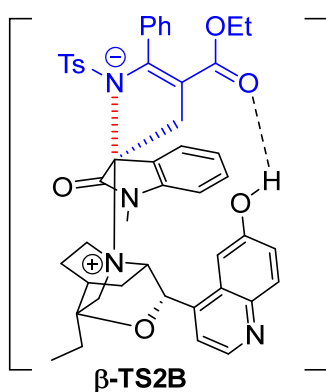
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107	1	0	-3.548752	3.373403	-3.535766



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.018506	-5.538565	0.123590
2	6	0	3.118550	-4.349625	1.077689
3	6	0	3.220557	-2.976377	0.428137
4	6	0	4.343809	-2.829205	-0.638071
5	6	0	3.783081	-3.087757	-2.042436
6	6	0	2.831655	-1.926563	-2.376905
7	8	0	3.474285	-2.073106	1.514292
8	6	0	1.912337	-2.533607	-0.228447
9	7	0	2.272265	-1.346603	-1.089387
10	6	0	3.433343	-0.591016	-0.355264
11	6	0	3.241722	-0.703091	1.164598
12	6	0	4.215378	0.185000	1.924072
13	6	0	5.151887	-0.390804	2.746663
14	6	0	6.022111	0.426497	3.502036
15	7	0	5.992920	1.735143	3.483946
16	6	0	5.072711	2.329040	2.679996
17	6	0	5.036399	3.749572	2.679336
18	6	0	4.140285	4.437793	1.913939
19	6	0	3.228724	3.731004	1.086773
20	8	0	2.377256	4.468930	0.355362
21	6	0	3.250786	2.352458	1.054471
22	6	0	4.154385	1.613285	1.857570
23	6	0	4.736027	-1.345918	-0.643290
24	6	0	-1.822470	-2.648932	-2.824637
25	6	0	-2.010193	-1.932598	-4.000112
26	6	0	-1.216736	-0.822924	-4.307205
27	6	0	-0.233315	-0.477414	-3.397517
28	6	0	-0.010659	-1.200863	-2.220291

29	6	0	-0.825503	-2.279440	-1.916210
30	7	0	0.662630	0.597635	-3.484090
31	6	0	1.533505	0.608941	-2.441339
32	6	0	1.051437	-0.466842	-1.423501
33	8	0	2.533465	1.297644	-2.359147
34	6	0	0.703888	1.564864	-4.557134
35	1	0	2.935807	-6.460627	0.699022
36	1	0	3.903081	-5.625445	-0.509983
37	1	0	2.137404	-5.481133	-0.519078
38	1	0	4.006625	-4.452856	1.706278
39	1	0	2.258698	-4.332242	1.751935
40	1	0	5.184807	-3.482942	-0.405383
41	1	0	4.596496	-3.094815	-2.769696
42	1	0	3.269284	-4.044989	-2.118228
43	1	0	1.978561	-2.252594	-2.967414
44	1	0	3.331557	-1.107969	-2.888282
45	1	0	1.184173	-2.248000	0.525012
46	1	0	1.471474	-3.288653	-0.873776
47	1	0	3.429616	0.423989	-0.729127
48	1	0	2.231013	-0.427395	1.468109
49	1	0	5.208987	-1.465943	2.831002
50	1	0	6.760283	-0.036252	4.149053
51	1	0	5.748565	4.256320	3.316933
52	1	0	4.100020	5.518881	1.911021
53	1	0	1.753169	3.896448	-0.140592
54	1	0	2.569147	1.878272	0.370183
55	1	0	5.442126	-1.099957	0.147333
56	1	0	5.188485	-1.055068	-1.591594
57	1	0	-2.485203	-3.462870	-2.567875
58	1	0	-2.800484	-2.221244	-4.680798
59	1	0	-1.377069	-0.249369	-5.210561
60	1	0	-0.763713	-2.800406	-0.971181
61	1	0	-0.265580	2.056934	-4.644833
62	1	0	0.954924	1.082745	-5.503758
63	1	0	1.465776	2.297111	-4.301969
64	6	0	-3.341912	1.053731	-0.452144
65	6	0	-4.058481	1.612870	0.602265
66	6	0	-5.247839	2.293035	0.352665
67	6	0	-5.728334	2.400816	-0.948336
68	6	0	-5.017044	1.826212	-2.001416
69	6	0	-3.824237	1.159242	-1.755495
70	6	0	-2.050161	0.350440	-0.172918
71	7	0	-2.010351	-0.870645	0.368975
72	6	0	-0.824888	0.972023	-0.439904
73	6	0	-0.607857	2.360708	-0.743953
74	8	0	0.526654	2.836321	-0.910879

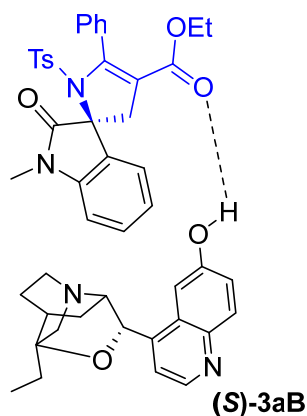
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76	8	0	-1.690078	3.145604	-0.831506
77	6	0	0.436053	0.193768	-0.166381
78	16	0	-3.255241	-1.922903	0.358552
79	8	0	-4.146405	-1.769641	-0.799417
80	8	0	-2.632811	-3.238471	0.575907
81	6	0	-4.227322	-1.588700	1.813060
82	6	0	-5.494402	-1.039490	1.680446
83	6	0	-6.233405	-0.764531	2.828447
84	6	0	-5.718102	-1.030820	4.096231
85	6	0	-4.439372	-1.590724	4.199940
86	6	0	-3.691837	-1.873760	3.066446
87	6	0	-6.512046	-0.720685	5.339859
88	6	0	-2.816711	5.194727	-1.126283
89	1	0	-3.681222	1.519949	1.613396
90	1	0	-5.799393	2.730596	1.175854
91	1	0	-6.656290	2.924272	-1.142849
92	1	0	-5.397774	1.895632	-3.012968
93	1	0	-3.265982	0.699684	-2.561821
94	1	0	-0.809343	4.948509	-0.327346
95	1	0	-0.933834	4.628569	-2.057546
96	1	0	1.165243	0.859417	0.276162
97	1	0	0.169643	-0.588662	0.541978
98	1	0	-5.881115	-0.832408	0.691439
99	1	0	-7.225558	-0.338174	2.735947
100	1	0	-4.033933	-1.811276	5.181022
101	1	0	-2.709743	-2.322609	3.138520
102	1	0	-7.529138	-0.417539	5.091330
103	1	0	-6.565999	-1.591385	5.996249
104	1	0	-6.046760	0.089423	5.906435
105	1	0	-2.716937	6.259418	-1.342803
106	1	0	-3.309763	5.072374	-0.161793
107	1	0	-3.446413	4.731165	-1.885984



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	6.547072	-2.461923	1.717465
2	6	0	6.011563	-1.032407	1.770141
3	6	0	4.961353	-0.667637	0.730885
4	6	0	5.353931	-0.954163	-0.746962
5	6	0	4.845051	-2.336194	-1.162155
6	6	0	3.301871	-2.237814	-1.187753
7	8	0	4.780744	0.750759	0.877085
8	6	0	3.582934	-1.323860	0.968697
9	7	0	2.826896	-1.148060	-0.292156
10	6	0	3.219561	0.205821	-0.866409
11	6	0	3.547149	1.181529	0.300347
12	6	0	3.681668	2.620311	-0.151055
13	6	0	4.876303	3.116913	-0.611933
14	6	0	4.931540	4.418327	-1.161412
15	7	0	3.897415	5.215967	-1.264342
16	6	0	2.725052	4.782772	-0.730542
17	6	0	1.619033	5.674802	-0.756581
18	6	0	0.439149	5.358802	-0.144407
19	6	0	0.313866	4.126100	0.546135
20	8	0	-0.835474	3.904948	1.222808
21	6	0	1.342744	3.212907	0.532268
22	6	0	2.563314	3.507308	-0.119284
23	6	0	4.548616	0.028843	-1.620407
24	6	0	0.621984	-4.522628	2.166403
25	6	0	0.579007	-5.433190	1.105955
26	6	0	0.528075	-5.025444	-0.228025
27	6	0	0.523476	-3.660523	-0.474685
28	6	0	0.572457	-2.732814	0.588007
29	6	0	0.609990	-3.155088	1.911576
30	7	0	0.491350	-3.003007	-1.690683
31	6	0	0.485192	-1.638640	-1.507740
32	6	0	0.532082	-1.423551	-0.004927
33	8	0	0.539976	-0.785180	-2.366951
34	6	0	0.431428	-3.638544	-2.987018
35	6	0	-3.512110	-0.325983	1.088400
36	6	0	-3.904693	1.011720	0.981284
37	6	0	-5.200124	1.386485	1.313081
38	6	0	-6.106121	0.429110	1.766447
39	6	0	-5.711900	-0.901281	1.882308
40	6	0	-4.419334	-1.283481	1.536739
41	6	0	-2.109108	-0.681909	0.713428
42	7	0	-1.800106	-1.500135	-0.311393

43	6	0	-1.042796	-0.076862	1.347459
44	6	0	-1.126969	0.746750	2.526980
45	8	0	-0.304273	1.629505	2.802201
46	6	0	-2.437077	1.464237	4.351733
47	8	0	-2.154004	0.480928	3.340881
48	6	0	0.303022	-0.119990	0.654476
49	16	0	-2.904661	-1.979542	-1.447002
50	8	0	-2.116006	-2.535994	-2.547799
51	8	0	-3.959776	-2.818583	-0.875446
52	6	0	-3.648107	-0.473491	-2.025258
53	6	0	-2.820064	0.512613	-2.556768
54	6	0	-3.392005	1.703747	-2.978435
55	6	0	-4.773375	1.912655	-2.885203
56	6	0	-5.574502	0.900815	-2.357533
57	6	0	-5.019146	-0.298558	-1.921719
58	6	0	-5.376276	3.208038	-3.364947
59	6	0	-3.711832	1.019732	5.035036
60	1	0	7.268292	-2.613884	2.521163
61	1	0	7.057123	-2.666587	0.774810
62	1	0	5.755620	-3.203504	1.845648
63	1	0	6.834152	-0.325349	1.635575
64	1	0	5.583705	-0.825478	2.754821
65	1	0	6.431163	-0.844807	-0.882668
66	1	0	5.211933	-2.587239	-2.159304
67	1	0	5.175932	-3.122910	-0.484725
68	1	0	2.858901	-3.168560	-0.836684
69	1	0	2.930132	-2.032254	-2.189798
70	1	0	3.083848	-0.836575	1.808131
71	1	0	3.648221	-2.388116	1.193523
72	1	0	2.404143	0.566824	-1.491250
73	1	0	2.769685	1.131740	1.060626
74	1	0	5.775518	2.519847	-0.553923
75	1	0	5.874335	4.792170	-1.547511
76	1	0	1.765845	6.625268	-1.252182
77	1	0	-0.398716	6.043125	-0.129902
78	1	0	-0.703570	3.130615	1.806390
79	1	0	1.215649	2.312790	1.111488
80	1	0	5.032515	0.992617	-1.737125
81	1	0	4.400654	-0.376874	-2.622060
82	1	0	0.648904	-4.885530	3.184534
83	1	0	0.577329	-6.493603	1.324570
84	1	0	0.477956	-5.745862	-1.032771
85	1	0	0.612416	-2.431110	2.716755
86	1	0	-0.450969	-4.272207	-3.045709
87	1	0	1.341491	-4.217168	-3.165640
88	1	0	0.337556	-2.846737	-3.724843

89	1	0	-3.194266	1.748390	0.622791
90	1	0	-5.503001	2.421089	1.212365
91	1	0	-7.117002	0.718836	2.025940
92	1	0	-6.413410	-1.646554	2.235132
93	1	0	-4.115995	-2.318265	1.601400
94	1	0	-1.592435	1.522664	5.037395
95	1	0	-2.553101	2.436736	3.870241
96	1	0	0.395889	0.662099	-0.104339
97	1	0	1.069566	0.031151	1.414944
98	1	0	-1.750947	0.344974	-2.627327
99	1	0	-2.762006	2.486325	-3.385148
100	1	0	-6.643517	1.056589	-2.272949
101	1	0	-5.624179	-1.079927	-1.481583
102	1	0	-5.390130	3.246263	-4.456892
103	1	0	-6.401709	3.319329	-3.012376
104	1	0	-4.796641	4.063083	-3.013275
105	1	0	-3.990731	1.737043	5.808339
106	1	0	-3.574157	0.042154	5.497818
107	1	0	-4.520061	0.948048	4.306620

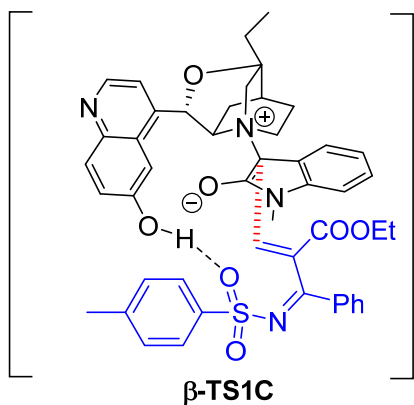


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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3	6	0	4.885976	-1.014054	1.149052
4	6	0	5.672729	-0.149774	0.113577
5	6	0	5.064635	-0.300928	-1.295514
6	6	0	3.641552	0.322520	-1.238538
7	8	0	4.859668	-0.322427	2.421683
8	6	0	3.434949	-1.041401	0.666894
9	7	0	3.143194	0.312809	0.146816
10	6	0	3.931322	1.301563	0.945031

11	6	0	3.961387	0.789499	2.395338
12	6	0	4.408176	1.829346	3.389474
13	6	0	5.639189	1.762448	3.989649
14	6	0	6.017798	2.759051	4.918688
15	7	0	5.258054	3.768174	5.264652
16	6	0	4.027083	3.845961	4.689798
17	6	0	3.192098	4.928946	5.072718
18	6	0	1.940096	5.072498	4.547596
19	6	0	1.453063	4.131432	3.604153
20	8	0	0.202053	4.345008	3.135646
21	6	0	2.233963	3.068232	3.208780
22	6	0	3.539045	2.905896	3.741783
23	6	0	5.406608	1.313884	0.496710
24	6	0	1.231275	-3.897874	0.264380
25	6	0	2.086512	-4.267291	-0.768717
26	6	0	2.103901	-3.576585	-1.986508
27	6	0	1.230131	-2.511033	-2.124538
28	6	0	0.376420	-2.121871	-1.087507
29	6	0	0.363230	-2.810911	0.107602
30	7	0	1.030323	-1.696274	-3.245503
31	6	0	-0.001848	-0.818692	-3.041166
32	6	0	-0.414811	-0.929177	-1.559361
33	8	0	-0.464371	-0.043865	-3.851273
34	6	0	1.626613	-1.923040	-4.541310
35	6	0	-3.737464	-0.252086	0.091536
36	6	0	-4.594069	0.744408	-0.379853
37	6	0	-5.925297	0.758916	0.016131
38	6	0	-6.400290	-0.212784	0.894274
39	6	0	-5.543587	-1.201141	1.370138
40	6	0	-4.211873	-1.226193	0.968040
41	6	0	-2.319599	-0.231152	-0.344667
42	7	0	-1.874762	-1.043684	-1.394355
43	6	0	-1.319012	0.581187	0.058061
44	6	0	-1.355329	1.606750	1.089549
45	8	0	-0.416792	2.370720	1.275907
46	6	0	-2.573634	2.643248	2.831222
47	8	0	-2.475624	1.630423	1.807868
48	6	0	-0.102113	0.396392	-0.811986
49	16	0	-2.690295	-2.377993	-2.033145
50	8	0	-1.786290	-2.850595	-3.074801
51	8	0	-3.124282	-3.276500	-0.971601
52	6	0	-4.110422	-1.616129	-2.754066
53	6	0	-3.912443	-0.628583	-3.716725
54	6	0	-5.029506	-0.023370	-4.272391
55	6	0	-6.322214	-0.397177	-3.884854
56	6	0	-6.479496	-1.393292	-2.920690

57	6	0	-5.375334	-2.013475	-2.346408
58	6	0	-7.521760	0.257528	-4.518850
59	6	0	-3.935258	2.468744	3.466275
60	1	0	6.188056	-4.208937	0.558763
61	1	0	6.507563	-2.786026	-0.428848
62	1	0	4.870763	-3.449138	-0.332497
63	1	0	6.424136	-2.186861	2.005546
64	1	0	4.821483	-2.888163	2.144876
65	1	0	6.736072	-0.397259	0.127381
66	1	0	5.688289	0.228432	-2.019575
67	1	0	5.017928	-1.345485	-1.608478
68	1	0	2.940558	-0.236677	-1.862555
69	1	0	3.641705	1.354579	-1.593583
70	1	0	2.775593	-1.306491	1.494428
71	1	0	3.259453	-1.768350	-0.125886
72	1	0	3.457223	2.279447	0.872660
73	1	0	2.956188	0.460004	2.681377
74	1	0	6.305436	0.943355	3.759938
75	1	0	6.994730	2.704754	5.388723
76	1	0	3.591682	5.628802	5.794658
77	1	0	1.292344	5.892723	4.827565
78	1	0	-0.014459	3.677107	2.455591
79	1	0	1.833394	2.366646	2.487796
80	1	0	6.040377	1.658576	1.312859
81	1	0	5.577525	1.973260	-0.356614
82	1	0	1.232110	-4.457257	1.190224
83	1	0	2.749426	-5.112999	-0.635673
84	1	0	2.758869	-3.881509	-2.792240
85	1	0	-0.317214	-2.523071	0.900002
86	1	0	1.359857	-2.914598	-4.912010
87	1	0	2.712383	-1.833682	-4.479803
88	1	0	1.233490	-1.164148	-5.213155
89	1	0	-4.212570	1.493661	-1.062083
90	1	0	-6.590116	1.526078	-0.359854
91	1	0	-7.436885	-0.199534	1.206873
92	1	0	-5.910607	-1.956127	2.053428
93	1	0	-3.546335	-2.002917	1.318500
94	1	0	-1.761517	2.505976	3.544372
95	1	0	-2.456792	3.623283	2.368143
96	1	0	-0.036711	1.215495	-1.534613
97	1	0	0.839642	0.343607	-0.262796
98	1	0	-2.907364	-0.333422	-3.998327
99	1	0	-4.901064	0.753169	-5.017068
100	1	0	-7.475775	-1.680368	-2.607041
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102	1	0	-7.721734	-0.179921	-5.500016

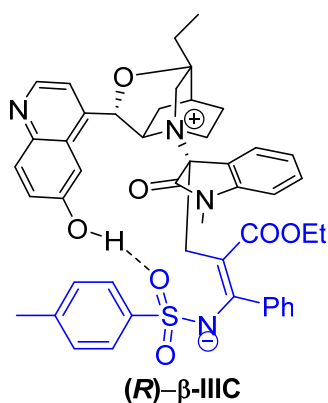
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104	1	0	-7.355347	1.325935	-4.662411
105	1	0	-4.080172	3.216478	4.246579
106	1	0	-4.022590	1.476032	3.907983
107	1	0	-4.718610	2.580317	2.716158



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	-2.569060	1.629539	1.088227
2	8	0	-2.873762	1.432981	2.504965
3	7	0	-3.303844	0.421975	0.266565
4	8	0	-2.350550	-3.394801	-0.698497
5	8	0	-1.163117	1.907490	0.723261
6	6	0	-2.929587	-0.639587	-0.384367
7	8	0	-0.704304	-2.906026	-2.140922
8	6	0	-1.634929	-1.149712	-0.806566
9	6	0	-4.136410	-1.369668	-0.908316
10	6	0	-5.638668	4.135945	0.449234
11	6	0	-3.534314	2.997061	0.501188
12	6	0	-3.747987	5.030707	-0.736398
13	6	0	-5.087885	5.130587	-0.367503
14	6	0	-0.468497	-0.433899	-0.930763
15	6	0	-4.870370	3.070471	0.889636
16	6	0	-2.958811	3.966465	-0.306958
17	6	0	-4.213286	-1.763314	-2.245797
18	6	0	-5.355804	-2.395473	-2.723274
19	6	0	-6.354289	-2.243987	-0.535391
20	6	0	-1.515528	-2.549363	-1.303621
21	6	0	-5.219895	-1.594887	-0.061133
22	6	0	-2.417530	-4.717815	-1.253775
23	6	0	-3.540457	-5.428921	-0.532223
24	6	0	-6.425564	-2.645707	-1.866930
25	6	0	-5.929376	6.298248	-0.813649

26	1	0	-6.680043	4.203472	0.741748
27	1	0	-3.309002	5.796458	-1.364525
28	1	0	0.227537	-0.793479	-1.668311
29	1	0	-0.387527	0.589819	-0.600891
30	1	0	-5.288114	2.300163	1.524231
31	1	0	-1.915991	3.905277	-0.584910
32	1	0	-3.381367	-1.571301	-2.913592
33	1	0	-5.412527	-2.687752	-3.764340
34	1	0	-7.185212	-2.431451	0.133056
35	1	0	-5.155704	-1.264544	0.967074
36	1	0	-2.606675	-4.633704	-2.325146
37	1	0	-1.453832	-5.205151	-1.109673
38	1	0	-3.646417	-6.446281	-0.912358
39	1	0	-4.479153	-4.894150	-0.682914
40	1	0	-3.329376	-5.470381	0.536701
41	1	0	-7.312852	-3.143244	-2.237805
42	1	0	-5.471346	6.812853	-1.658276
43	1	0	-6.044794	7.021066	-0.002271
44	1	0	-6.927452	5.971403	-1.109132
45	8	0	1.482684	0.682533	1.776123
46	7	0	-0.136516	-0.869702	2.315614
47	6	0	0.542953	-2.631390	1.021282
48	6	0	-0.341835	-2.210446	2.049524
49	6	0	0.926489	-0.399119	1.559534
50	6	0	-1.195940	-3.076808	2.716612
51	6	0	0.586538	-4.005670	0.744594
52	6	0	-1.147870	-4.428368	2.391260
53	6	0	-0.248199	-4.885948	1.429784
54	6	0	-0.552862	-0.210078	3.538065
55	6	0	1.195277	-1.413656	0.561234
56	6	0	6.101968	-3.980982	0.103962
57	6	0	6.060852	-2.521615	0.553132
58	6	0	4.887672	-1.693999	0.044517
59	6	0	4.687433	-1.711182	-1.497252
60	6	0	3.680697	-2.801833	-1.882892
61	6	0	2.309068	-2.307997	-1.416825
62	8	0	5.169441	-0.359145	0.475327
63	6	0	3.553624	-2.082415	0.678622
64	7	0	2.481455	-1.443749	-0.172187
65	6	0	3.078354	-0.075146	-0.665767
66	6	0	4.040537	0.526937	0.383958
67	6	0	4.556308	1.895960	-0.053873
68	6	0	5.891470	2.048401	-0.344988
69	6	0	6.381102	3.293327	-0.798014
70	7	0	5.633040	4.351555	-0.981714
71	6	0	4.313045	4.235032	-0.680542

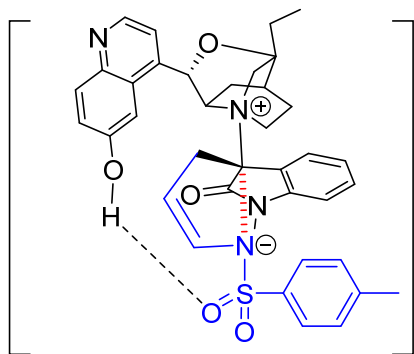
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73	6	0	2.178076	5.378827	-0.548999
74	6	0	1.587042	4.198505	-0.031872
75	8	0	0.276247	4.279557	0.288593
76	6	0	2.329696	3.051879	0.134397
77	6	0	3.709040	3.039827	-0.190327
78	6	0	3.991449	-0.389144	-1.863894
79	1	0	-1.858565	-2.706647	3.487585
80	1	0	1.272573	-4.430357	0.023856
81	1	0	-1.793457	-5.128201	2.906292
82	1	0	-0.189393	-5.944308	1.207765
83	1	0	-0.080055	-0.685435	4.402014
84	1	0	-1.634230	-0.238231	3.632480
85	1	0	-0.240869	0.827655	3.466270
86	1	0	6.971343	-4.473180	0.540475
87	1	0	6.185285	-4.068175	-0.980665
88	1	0	5.219030	-4.537361	0.426204
89	1	0	6.964354	-2.005846	0.218139
90	1	0	6.055216	-2.460952	1.644519
91	1	0	5.644404	-1.827147	-2.007056
92	1	0	3.655268	-2.927609	-2.966717
93	1	0	3.924150	-3.770544	-1.447678
94	1	0	1.607303	-3.095004	-1.191039
95	1	0	1.834262	-1.685107	-2.165275
96	1	0	3.472782	-1.669453	1.682105
97	1	0	3.352489	-3.151066	0.714720
98	1	0	2.235657	0.574893	-0.878879
99	1	0	3.548387	0.612665	1.350332
100	1	0	6.567443	1.214062	-0.235885
101	1	0	7.437364	3.397800	-1.025183
102	1	0	3.997791	6.276715	-1.237830
103	1	0	1.554345	6.255129	-0.666984
104	1	0	-0.053565	3.429353	0.637057
105	1	0	1.867028	2.187343	0.590833
106	1	0	4.699461	0.428853	-1.966380
107	1	0	3.456948	-0.474396	-2.809562



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	-2.171380	1.418964	0.624606
2	8	0	-1.748753	0.367224	1.578050
3	7	0	-2.788564	0.841759	-0.731145
4	8	0	-2.415279	-3.172958	-1.521347
5	8	0	-1.183193	2.496035	0.376042
6	6	0	-2.474775	-0.363933	-1.235430
7	8	0	-0.237892	-3.014384	-2.025786
8	6	0	-1.331166	-1.137666	-1.052597
9	6	0	-3.519181	-0.785335	-2.228418
10	6	0	-5.594818	2.071429	2.636989
11	6	0	-3.580587	2.219826	1.350680
12	6	0	-4.915295	4.175680	1.693585
13	6	0	-5.830737	3.435266	2.443312
14	6	0	0.012953	-0.572172	-0.673412
15	6	0	-4.472627	1.457154	2.096091
16	6	0	-3.786162	3.577147	1.144891
17	6	0	-3.167550	-1.207192	-3.512220
18	6	0	-4.149057	-1.557477	-4.432721
19	6	0	-5.850515	-1.044323	-2.806143
20	6	0	-1.263208	-2.480827	-1.596786
21	6	0	-4.867924	-0.680298	-1.891934
22	6	0	-2.485781	-4.369218	-2.306822
23	6	0	-3.931348	-4.817804	-2.277754
24	6	0	-5.494467	-1.486171	-4.078229
25	6	0	-7.036476	4.100300	3.057014
26	1	0	-6.299213	1.487325	3.217979
27	1	0	-5.088934	5.233911	1.536697
28	1	0	0.661041	-0.831077	-1.512190
29	1	0	-0.028867	0.517148	-0.632178
30	1	0	-4.279004	0.402852	2.246878
31	1	0	-3.068913	4.145078	0.567930

32	1	0	-2.120380	-1.251956	-3.788920
33	1	0	-3.864916	-1.874898	-5.428475
34	1	0	-6.895325	-0.973962	-2.529877
35	1	0	-5.131716	-0.310922	-0.909377
36	1	0	-2.150049	-4.147054	-3.321089
37	1	0	-1.811821	-5.117831	-1.885792
38	1	0	-4.054426	-5.731699	-2.861487
39	1	0	-4.569102	-4.038832	-2.696912
40	1	0	-4.248171	-5.011464	-1.252414
41	1	0	-6.260563	-1.758354	-4.793780
42	1	0	-7.381069	4.931885	2.441382
43	1	0	-6.797662	4.496966	4.047174
44	1	0	-7.858970	3.393486	3.171850
45	8	0	1.126958	1.226462	1.508102
46	7	0	0.463558	-0.445028	2.922838
47	6	0	0.143799	-2.186593	1.445179
48	6	0	-0.011163	-1.746688	2.767494
49	6	0	0.781319	0.083280	1.705109
50	6	0	-0.582190	-2.528885	3.757332
51	6	0	-0.329288	-3.450771	1.110440
52	6	0	-1.024506	-3.802446	3.402951
53	6	0	-0.902152	-4.257956	2.095789
54	6	0	0.110070	0.407748	4.039978
55	6	0	0.744947	-1.045930	0.633048
56	6	0	5.682914	-3.457607	2.111336
57	6	0	5.596170	-1.937706	1.987005
58	6	0	4.578534	-1.388414	0.994294
59	6	0	4.678470	-1.959547	-0.444207
60	6	0	3.755992	-3.166442	-0.586304
61	6	0	2.313833	-2.645293	-0.509668
62	8	0	4.838678	0.017673	0.954770
63	6	0	3.129497	-1.565045	1.477469
64	7	0	2.256303	-1.335804	0.269499
65	6	0	2.987103	-0.211651	-0.559090
66	6	0	3.767284	0.760320	0.358347
67	6	0	4.347012	1.903682	-0.460821
68	6	0	5.708064	1.999796	-0.625458
69	6	0	6.247242	3.018593	-1.439600
70	7	0	5.520519	3.894672	-2.087680
71	6	0	4.173870	3.832242	-1.922812
72	6	0	3.391826	4.789287	-2.622808
73	6	0	2.035029	4.817967	-2.495373
74	6	0	1.377864	3.896392	-1.635419
75	8	0	0.045869	4.032059	-1.549114
76	6	0	2.103305	2.942430	-0.950299
77	6	0	3.514352	2.877709	-1.093609

78	6	0	4.071861	-0.906176	-1.387935
79	1	0	-0.695233	-2.155412	4.765963
80	1	0	-0.267312	-3.820164	0.097073
81	1	0	-1.479093	-4.435127	4.154612
82	1	0	-1.267340	-5.239952	1.827144
83	1	0	0.563181	0.034338	4.958352
84	1	0	-0.975936	0.447026	4.135269
85	1	0	0.487813	1.402317	3.818539
86	1	0	6.424071	-3.718545	2.867319
87	1	0	5.992588	-3.923227	1.174485
88	1	0	4.735008	-3.904010	2.419790
89	1	0	6.564103	-1.537415	1.675797
90	1	0	5.375938	-1.490591	2.960108
91	1	0	5.715324	-2.189607	-0.691856
92	1	0	3.902259	-3.637705	-1.559432
93	1	0	3.935610	-3.924683	0.174485
94	1	0	1.691063	-3.340717	0.033527
95	1	0	1.853683	-2.480106	-1.476712
96	1	0	2.913158	-0.822820	2.241799
97	1	0	2.903889	-2.555782	1.867977
98	1	0	2.246739	0.316613	-1.146053
99	1	0	3.135337	1.173506	1.138264
100	1	0	6.362981	1.289968	-0.142081
101	1	0	7.323173	3.089439	-1.564183
102	1	0	3.922396	5.491989	-3.251487
103	1	0	1.425095	5.543015	-3.017679
104	1	0	-0.347875	3.401549	-0.910656
105	1	0	1.586185	2.297688	-0.252702
106	1	0	4.794014	-0.152162	-1.689633
107	1	0	3.681486	-1.369658	-2.294216



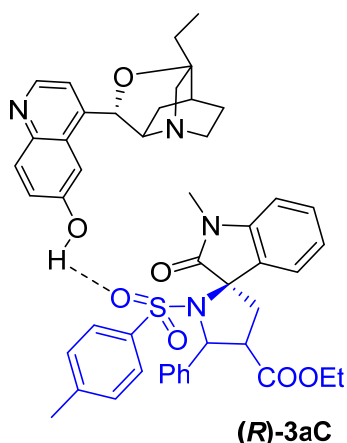
β -TS2C

Center	Atomic	Atomic	Coordinates (Angstroms)		
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Number	Number	Type	X	Y	Z
1	16	0	1.886951	1.065565	-1.657220
2	8	0	1.511591	0.718119	-3.028791
3	7	0	1.737420	-0.294984	-0.769312
4	8	0	2.681468	-0.471989	3.425218
5	8	0	1.189590	2.191312	-0.999557
6	6	0	2.231747	-0.291274	0.539048
7	8	0	0.578999	-1.237067	3.562229
8	6	0	1.294427	-0.285256	1.517173
9	6	0	3.689574	-0.559641	0.696364
10	6	0	5.877751	0.964558	-2.146907
11	6	0	3.605501	1.514640	-1.641120
12	6	0	5.358987	2.997474	-0.969131
13	6	0	6.309540	2.135084	-1.512019
14	6	0	-0.132263	-0.139097	1.038877
15	6	0	4.530563	0.651164	-2.221603
16	6	0	4.001879	2.690932	-1.021854
17	6	0	4.549976	0.301141	1.375781
18	6	0	5.909721	0.016703	1.440424
19	6	0	5.555022	-2.004888	0.175571
20	6	0	1.467778	-0.701591	2.919740
21	6	0	4.200466	-1.706543	0.082425
22	6	0	2.918192	-0.985511	4.749785
23	6	0	4.364890	-0.685175	5.075922
24	6	0	6.413487	-1.139833	0.849545
25	6	0	7.782255	2.427828	-1.394052
26	8	0	-1.251324	0.522844	-1.858339
27	7	0	-0.466929	-1.573707	-2.411005
28	6	0	0.120384	-2.369529	-0.342487
29	6	0	0.052277	-2.657066	-1.718340
30	6	0	-0.735802	-0.530513	-1.554294
31	6	0	0.489528	-3.872093	-2.220186
32	6	0	0.643893	-3.291861	0.553350
33	6	0	1.000327	-4.797826	-1.306282
34	6	0	1.078989	-4.522295	0.059227
35	6	0	-0.512874	-1.435818	-3.850820
36	6	0	-0.344548	-1.000014	-0.167408
37	6	0	-5.724491	-4.109631	-1.118884
38	6	0	-5.718163	-2.601644	-1.361637
39	6	0	-4.756038	-1.790383	-0.506384
40	6	0	-4.879539	-2.012263	1.028981
41	6	0	-3.879884	-3.077634	1.491065
42	6	0	-2.466554	-2.477759	1.294698
43	8	0	-5.068032	-0.420024	-0.805287
44	6	0	-3.274253	-1.981145	-0.877008

45	7	0	-2.495150	-1.415388	0.254233
46	6	0	-3.274464	-0.211904	0.767894
47	6	0	-4.018729	0.471054	-0.403448
48	6	0	-4.622815	1.793007	0.019509
49	6	0	-5.972295	1.904004	0.248161
50	6	0	-6.507254	3.126481	0.710683
51	7	0	-5.788275	4.194253	0.952598
52	6	0	-4.454641	4.116559	0.701893
53	6	0	-3.678974	5.283236	0.936311
54	6	0	-2.341701	5.302454	0.670817
55	6	0	-1.701114	4.150391	0.139977
56	8	0	-0.389920	4.287896	-0.129364
57	6	0	-2.415257	2.990901	-0.075510
58	6	0	-3.805656	2.948431	0.209552
59	6	0	-4.391521	-0.716619	1.698754
60	1	0	6.610644	0.290413	-2.574691
61	1	0	5.682102	3.913548	-0.488820
62	1	0	-0.785440	-0.442222	1.852541
63	1	0	-0.346462	0.896115	0.766144
64	1	0	4.190916	-0.256559	-2.703442
65	1	0	3.255040	3.342906	-0.589860
66	1	0	4.150115	1.192694	1.839447
67	1	0	6.575981	0.699336	1.953663
68	1	0	5.942438	-2.904146	-0.287067
69	1	0	3.524343	-2.351343	-0.466434
70	1	0	2.226617	-0.503221	5.440118
71	1	0	2.707673	-2.054846	4.752803
72	1	0	4.609501	-1.062831	6.069662
73	1	0	4.543009	0.390434	5.057757
74	1	0	5.022640	-1.155556	4.344798
75	1	0	7.471728	-1.362791	0.909896
76	1	0	7.957228	3.450024	-1.058831
77	1	0	8.290354	2.287228	-2.349534
78	1	0	8.244533	1.749856	-0.671451
79	1	0	0.450181	-4.092847	-3.278275
80	1	0	0.697611	-3.056211	1.609493
81	1	0	1.348395	-5.755230	-1.673263
82	1	0	1.484348	-5.262515	0.735473
83	1	0	-1.174104	-2.187640	-4.285215
84	1	0	0.492306	-1.524492	-4.261804
85	1	0	-0.886755	-0.437717	-4.061648
86	1	0	-6.427277	-4.589630	-1.800782
87	1	0	-6.035279	-4.352630	-0.101487
88	1	0	-4.743967	-4.558395	-1.292238
89	1	0	-6.714931	-2.193583	-1.175127
90	1	0	-5.486505	-2.387661	-2.408476

91	1	0	-5.906965	-2.259628	1.300838
92	1	0	-4.038984	-3.304047	2.546969
93	1	0	-3.982414	-4.011040	0.937937
94	1	0	-1.773829	-3.245742	0.961551
95	1	0	-2.071358	-2.051049	2.216672
96	1	0	-3.072199	-1.442763	-1.801813
97	1	0	-2.984556	-3.023733	-1.011189
98	1	0	-2.593539	0.484682	1.249517
99	1	0	-3.342059	0.643084	-1.239329
100	1	0	-6.619657	1.055982	0.076817
101	1	0	-7.573865	3.205972	0.895467
102	1	0	-4.198190	6.151504	1.319871
103	1	0	-1.738179	6.185995	0.831214
104	1	0	-0.012823	3.482264	-0.530737
105	1	0	-1.915346	2.143042	-0.526173
106	1	0	-5.166483	0.042980	1.765847
107	1	0	-4.036143	-0.914375	2.711319

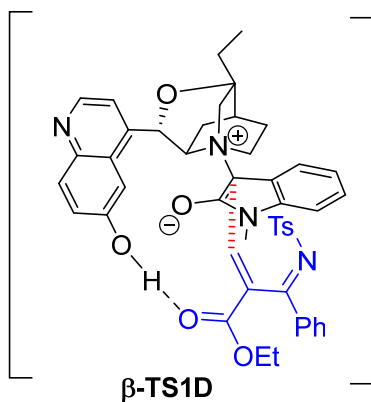


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
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2	8	0	2.060710	-2.529506	0.474100
3	7	0	1.891644	-0.060205	0.639445
4	8	0	0.875120	4.018278	0.194862
5	8	0	0.912075	-1.299885	-1.418501
6	6	0	1.553176	1.249374	0.242410
7	8	0	0.172355	3.853072	2.327254
8	6	0	1.095636	1.951582	1.292582
9	6	0	1.822763	1.711260	-1.141396
10	6	0	5.902777	-1.212872	-1.154611
11	6	0	3.517246	-1.163412	-1.239649
12	6	0	4.769645	-0.662269	-3.207694

13	6	0	5.960423	-0.859470	-2.508642
14	6	0	1.046623	1.110482	2.538065
15	6	0	4.685848	-1.372349	-0.510682
16	6	0	3.536940	-0.812909	-2.581840
17	6	0	0.818562	1.659650	-2.107707
18	6	0	1.082148	2.131724	-3.389811
19	6	0	3.333910	2.704321	-2.733930
20	6	0	0.673078	3.351998	1.340006
21	6	0	3.078255	2.233064	-1.451186
22	6	0	0.418720	5.382606	0.171710
23	6	0	0.709866	5.901033	-1.219952
24	6	0	2.335671	2.653333	-3.703692
25	6	0	7.292143	-0.722495	-3.198901
26	8	0	-0.673492	-1.277085	1.629750
27	7	0	0.768400	-2.222014	3.165759
28	6	0	2.622677	-0.898451	2.896314
29	6	0	2.102151	-2.023785	3.541327
30	6	0	0.387846	-1.316952	2.215117
31	6	0	2.870018	-2.782148	4.408201
32	6	0	3.928559	-0.506641	3.107324
33	6	0	4.193952	-2.381899	4.613069
34	6	0	4.723479	-1.264129	3.975549
35	6	0	-0.015818	-3.392796	3.490925
36	6	0	1.532836	-0.291180	2.058599
37	6	0	-4.080423	3.748399	2.764818
38	6	0	-4.319316	2.259196	2.517222
39	6	0	-3.889001	1.747649	1.152755
40	6	0	-4.521237	2.487021	-0.068195
41	6	0	-3.573359	3.580175	-0.598158
42	6	0	-2.323737	2.850735	-1.164384
43	8	0	-4.308319	0.363036	1.120416
44	6	0	-2.375635	1.740113	0.911460
45	7	0	-2.180182	1.525779	-0.539803
46	6	0	-3.285773	0.640736	-1.017172
47	6	0	-3.585967	-0.358980	0.117082
48	6	0	-4.383782	-1.541189	-0.355372
49	6	0	-5.718272	-1.683785	-0.077463
50	6	0	-6.417175	-2.805200	-0.583009
51	7	0	-5.872982	-3.743421	-1.317941
52	6	0	-4.543447	-3.628892	-1.588824
53	6	0	-3.937403	-4.647562	-2.371046
54	6	0	-2.604615	-4.608135	-2.667876
55	6	0	-1.800426	-3.542497	-2.187500
56	8	0	-0.487591	-3.586342	-2.514051
57	6	0	-2.353257	-2.533603	-1.433052
58	6	0	-3.738154	-2.554480	-1.125764

59	6	0	-4.587862	1.446829	-1.198225
60	1	0	6.823830	-1.370594	-0.606224
61	1	0	4.803420	-0.380631	-4.252957
62	1	0	1.709681	1.499236	3.312460
63	1	0	0.038733	1.065112	2.953503
64	1	0	4.632677	-1.658585	0.532824
65	1	0	2.609235	-0.643589	-3.112059
66	1	0	-0.150578	1.260916	-1.832109
67	1	0	0.306017	2.093892	-4.143927
68	1	0	4.309196	3.107447	-2.975449
69	1	0	3.847882	2.264331	-0.689420
70	1	0	-0.646500	5.400955	0.407154
71	1	0	0.944333	5.942882	0.944889
72	1	0	0.390321	6.940034	-1.309347
73	1	0	0.183356	5.303032	-1.964866
74	1	0	1.778024	5.839678	-1.429602
75	1	0	2.533227	3.021986	-4.702653
76	1	0	7.200932	-0.149239	-4.121176
77	1	0	7.692128	-1.706815	-3.453862
78	1	0	8.019439	-0.227753	-2.553847
79	1	0	2.467744	-3.655920	4.903193
80	1	0	4.328544	0.364400	2.600573
81	1	0	4.818082	-2.958461	5.283721
82	1	0	5.751278	-0.977918	4.154941
83	1	0	-0.162513	-3.464550	4.569026
84	1	0	0.483494	-4.291509	3.124411
85	1	0	-0.977292	-3.284247	2.995276
86	1	0	-4.400214	4.012979	3.773814
87	1	0	-4.648596	4.366682	2.067227
88	1	0	-3.023768	4.011599	2.677003
89	1	0	-5.383367	2.029563	2.624132
90	1	0	-3.793183	1.665530	3.269747
91	1	0	-5.503911	2.888813	0.187771
92	1	0	-4.076190	4.149704	-1.383465
93	1	0	-3.291791	4.286324	0.184781
94	1	0	-1.408162	3.414695	-0.974892
95	1	0	-2.399327	2.712845	-2.245702
96	1	0	-1.907849	0.944205	1.490776
97	1	0	-1.907042	2.680380	1.200308
98	1	0	-2.972159	0.128810	-1.926854
99	1	0	-2.649040	-0.727974	0.538126
100	1	0	-6.223079	-0.945569	0.529812
101	1	0	-7.475249	-2.914421	-0.365566
102	1	0	-4.573888	-5.452225	-2.714950
103	1	0	-2.127149	-5.378463	-3.259043
104	1	0	-0.028944	-2.826639	-2.116998

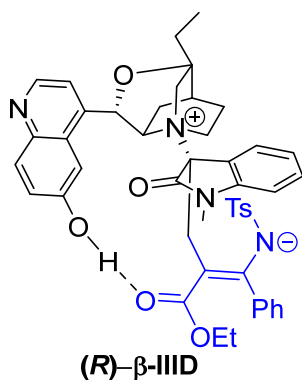
105	1	0	-1.713312	-1.741830	-1.062623
106	1	0	-5.449127	0.785686	-1.112964
107	1	0	-4.642773	1.938726	-2.171862



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	4.445659	1.757160	-0.039531
2	8	0	4.199666	1.838800	-1.485527
3	7	0	3.062975	1.443280	0.821888
4	8	0	-0.055808	3.681049	1.810616
5	8	0	5.207100	2.833742	0.602509
6	8	0	-1.119082	0.477110	-1.055777
7	6	0	1.949214	2.095791	0.651646
8	8	0	-1.503999	1.961873	1.906470
9	7	0	1.017152	-0.261794	-1.525534
10	6	0	0.773990	1.555637	1.336361
11	6	0	1.240303	-1.996518	-0.057151
12	6	0	1.769133	3.311373	-0.195052
13	6	0	1.863644	-1.273194	-1.099589
14	6	0	7.012447	-1.279442	-0.531234
15	6	0	-0.177879	-0.293715	-0.833557
16	6	0	5.333223	0.244195	0.245705
17	6	0	6.022078	-1.576602	1.637489
18	6	0	6.917601	-2.007764	0.655925
19	6	0	0.733386	0.239104	1.754676
20	6	0	6.220661	-0.157411	-0.745901
21	6	0	3.122480	-1.586140	-1.581570
22	6	0	5.233133	-0.449685	1.445739
23	6	0	0.645899	3.397526	-1.026767
24	6	0	1.928715	-3.078436	0.492678
25	6	0	0.434285	4.533097	-1.797205
26	6	0	2.428897	5.528224	-0.881717
27	6	0	-0.372271	2.393348	1.680353

28	6	0	2.655293	4.387635	-0.117805
29	6	0	3.779539	-2.683850	-1.024471
30	6	0	-1.123575	4.638845	1.928452
31	6	0	-0.468676	5.999776	2.011116
32	6	0	3.188908	-3.420944	-0.004267
33	6	0	1.325613	5.602435	-1.725738
34	6	0	1.269628	0.581925	-2.677400
35	6	0	7.738894	-3.254136	0.864351
36	6	0	-0.015364	-1.292526	0.219369
37	1	0	7.710007	-1.597373	-1.297586
38	1	0	5.943034	-2.132025	2.565005
39	1	0	-0.043692	-0.025723	2.455081
40	1	0	1.651594	-0.329649	1.774525
41	1	0	6.277300	0.401420	-1.670935
42	1	0	3.586941	-0.981551	-2.349315
43	1	0	4.537506	-0.115902	2.202724
44	1	0	-0.059661	2.574747	-1.064773
45	1	0	1.511906	-3.680251	1.291370
46	1	0	-0.429723	4.585311	-2.447716
47	1	0	3.119363	6.359091	-0.814048
48	1	0	3.510881	4.339347	0.540254
49	1	0	4.768359	-2.945201	-1.376212
50	1	0	-1.762774	4.555731	1.050073
51	1	0	-1.714905	4.407430	2.814804
52	1	0	-1.233008	6.773645	2.092154
53	1	0	0.127241	6.180600	1.116068
54	1	0	0.183743	6.057039	2.882640
55	1	0	3.714535	-4.265173	0.423592
56	1	0	1.157077	6.490110	-2.322780
57	1	0	1.503813	-0.045902	-3.540122
58	1	0	2.097731	1.262939	-2.483222
59	1	0	0.359554	1.141683	-2.874825
60	1	0	7.160548	-4.144804	0.603298
61	1	0	8.045415	-3.353510	1.906360
62	1	0	8.634026	-3.244933	0.242102
63	6	0	-2.331740	-6.361631	0.469909
64	6	0	-2.944700	-5.271061	-0.406712
65	6	0	-2.717343	-3.838963	0.057905
66	6	0	-3.135081	-3.552414	1.529789
67	6	0	-1.915426	-3.672646	2.457162
68	6	0	-0.993298	-2.485262	2.139472
69	8	0	-3.488588	-3.033975	-0.834410
70	6	0	-1.281346	-3.370878	-0.102131
71	7	0	-1.179749	-2.084527	0.690317
72	6	0	-2.569126	-1.369341	0.606706
73	6	0	-3.177760	-1.620568	-0.784288

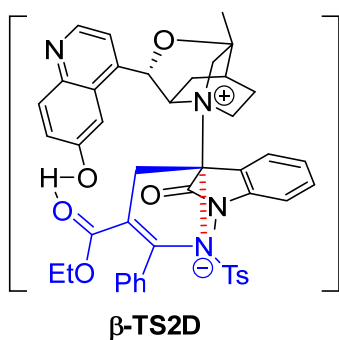
74	6	0	-4.503999	-0.910079	-1.087522
75	6	0	-5.409097	-1.626232	-1.839006
76	6	0	-6.693163	-1.108845	-2.103217
77	7	0	-7.131346	0.028328	-1.626261
78	6	0	-6.258186	0.765521	-0.894028
79	6	0	-6.756181	1.982343	-0.355097
80	6	0	-5.968746	2.792740	0.407608
81	6	0	-4.611832	2.443785	0.621088
82	8	0	-3.879769	3.292477	1.374923
83	6	0	-4.078410	1.300144	0.070597
84	6	0	-4.902269	0.389342	-0.638252
85	6	0	-3.526771	-2.069613	1.581531
86	1	0	-2.543768	-7.340467	0.039336
87	1	0	-2.747158	-6.350899	1.479059
88	1	0	-1.245819	-6.269695	0.544224
89	1	0	-4.027851	-5.404072	-0.462623
90	1	0	-2.566560	-5.349875	-1.429146
91	1	0	-3.949642	-4.208273	1.837645
92	1	0	-2.231478	-3.602958	3.499305
93	1	0	-1.393213	-4.621428	2.337263
94	1	0	0.059931	-2.701379	2.285514
95	1	0	-1.246810	-1.611287	2.731231
96	1	0	-1.062711	-3.147927	-1.143779
97	1	0	-0.529775	-4.058722	0.272943
98	1	0	-2.359498	-0.335935	0.840455
99	1	0	-2.459916	-1.374357	-1.566295
100	1	0	-5.157818	-2.611150	-2.200054
101	1	0	-7.386629	-1.687064	-2.705283
102	1	0	-7.789195	2.222215	-0.568731
103	1	0	-6.338420	3.710325	0.845632
104	1	0	-3.029559	2.861829	1.604070
105	1	0	-3.010469	1.159100	0.121629
106	1	0	-4.540653	-1.902642	1.221134
107	1	0	-3.469019	-1.674986	2.596192



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	4.040056	1.164174	-0.445721
2	8	0	3.662319	0.947196	-1.858332
3	7	0	2.750507	1.011264	0.543668
4	8	0	-0.133787	3.785897	1.459290
5	8	0	4.898487	2.321354	-0.160275
6	8	0	-1.203334	0.634339	-1.069841
7	6	0	1.762374	1.913839	0.530397
8	8	0	-1.661121	2.155025	1.711896
9	7	0	0.647788	-0.481797	-1.846813
10	6	0	0.560918	1.567847	1.155776
11	6	0	1.323260	-1.649618	0.011481
12	6	0	1.858854	3.211754	-0.218241
13	6	0	1.571439	-1.405199	-1.340994
14	6	0	6.631585	-1.907284	-0.512816
15	6	0	-0.267468	-0.126549	-0.907994
16	6	0	4.987534	-0.256465	0.062192
17	6	0	5.882887	-1.695298	1.758966
18	6	0	6.693648	-2.331943	0.815375
19	6	0	0.283735	0.147329	1.576281
20	6	0	5.785228	-0.871254	-0.893894
21	6	0	2.590080	-2.028968	-2.037677
22	6	0	5.036577	-0.655127	1.392759
23	6	0	0.973348	3.437181	-1.274653
24	6	0	2.176308	-2.492753	0.708863
25	6	0	1.027851	4.624231	-1.995608
26	6	0	2.833443	5.384404	-0.593506
27	6	0	-0.496290	2.497417	1.437504
28	6	0	2.790040	4.192092	0.120394
29	6	0	3.384213	-2.936882	-1.338717
30	6	0	-1.169215	4.778093	1.480605
31	6	0	-0.474256	6.122193	1.461049
32	6	0	3.192175	-3.158923	0.020569
33	6	0	1.959760	5.601803	-1.655453
34	6	0	0.761533	0.156733	-3.145981
35	6	0	7.640596	-3.429238	1.231437
36	6	0	0.082163	-0.868132	0.410742
37	1	0	7.255295	-2.391852	-1.255817
38	1	0	5.922687	-2.014931	2.794559
39	1	0	-0.626452	0.184526	2.172258
40	1	0	1.098935	-0.236633	2.194558
41	1	0	5.723068	-0.544283	-1.923928
42	1	0	2.785190	-1.792092	-3.073992
43	1	0	4.403391	-0.161701	2.117696

44	1	0	0.226555	2.687849	-1.508686
45	1	0	2.103814	-2.624601	1.780908
46	1	0	0.341644	4.788038	-2.817383
47	1	0	3.558026	6.141979	-0.322994
48	1	0	3.479884	4.016388	0.932262
49	1	0	4.193065	-3.439045	-1.852212
50	1	0	-1.806009	4.646810	0.605126
51	1	0	-1.778312	4.645252	2.375632
52	1	0	-1.214354	6.923723	1.471019
53	1	0	0.139096	6.211427	0.564341
54	1	0	0.170747	6.227604	2.333846
55	1	0	3.865786	-3.810080	0.560261
56	1	0	2.005112	6.528036	-2.215148
57	1	0	0.719101	-0.595542	-3.934862
58	1	0	1.703773	0.703623	-3.186154
59	1	0	-0.081190	0.835472	-3.247885
60	1	0	7.231512	-4.012680	2.057648
61	1	0	8.593295	-3.009973	1.564434
62	1	0	7.849481	-4.106158	0.402186
63	6	0	-1.666344	-6.208305	-0.012500
64	6	0	-2.416869	-5.108121	-0.760327
65	6	0	-2.389786	-3.720710	-0.130553
66	6	0	-2.841220	-3.664666	1.355389
67	6	0	-1.615980	-3.770965	2.267865
68	6	0	-0.826218	-2.463956	2.105795
69	8	0	-3.265778	-2.940219	-0.937408
70	6	0	-1.023024	-3.053511	-0.227624
71	7	0	-1.067077	-1.883381	0.723937
72	6	0	-2.548567	-1.332815	0.698292
73	6	0	-3.184825	-1.522595	-0.702821
74	6	0	-4.621141	-0.992396	-0.821145
75	6	0	-5.565626	-1.842111	-1.351713
76	6	0	-6.912135	-1.435979	-1.461521
77	7	0	-7.360802	-0.279099	-1.047385
78	6	0	-6.452570	0.582513	-0.522484
79	6	0	-6.954915	1.823923	-0.050276
80	6	0	-6.129814	2.747556	0.519396
81	6	0	-4.738499	2.486828	0.609332
82	8	0	-3.984603	3.433442	1.196237
83	6	0	-4.206296	1.316750	0.108154
84	6	0	-5.052672	0.310757	-0.417364
85	6	0	-3.386735	-2.248979	1.602304
86	1	0	-1.743616	-7.143271	-0.567730
87	1	0	-2.085344	-6.382319	0.979967
88	1	0	-0.602770	-5.984663	0.096281
89	1	0	-3.472131	-5.376672	-0.851392

90	1	0	-2.031251	-5.012375	-1.778593
91	1	0	-3.582229	-4.436580	1.563576
92	1	0	-1.929563	-3.861125	3.309063
93	1	0	-0.993224	-4.633814	2.036651
94	1	0	0.239084	-2.624214	2.201413
95	1	0	-1.129205	-1.711240	2.825282
96	1	0	-0.863936	-2.687031	-1.240382
97	1	0	-0.189875	-3.690591	0.053613
98	1	0	-2.493446	-0.298650	1.019837
99	1	0	-2.578890	-1.063236	-1.480872
100	1	0	-5.289680	-2.833212	-1.673002
101	1	0	-7.638760	-2.117412	-1.892258
102	1	0	-8.019261	1.989639	-0.150397
103	1	0	-6.498284	3.688006	0.907118
104	1	0	-3.097006	3.053899	1.398136
105	1	0	-3.131954	1.215754	0.087060
106	1	0	-4.425854	-2.150118	1.294311
107	1	0	-3.331734	-1.980890	2.657482

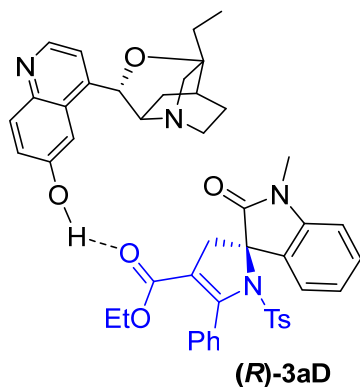


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	3.538345	0.508418	-1.311591
2	8	0	3.118397	-0.235773	-2.506370
3	7	0	2.228354	0.728015	-0.360173
4	8	0	0.414587	3.998228	1.514735
5	8	0	4.329855	1.722436	-1.491147
6	8	0	-0.769385	0.666334	-1.227774
7	6	0	1.825277	1.888408	0.208273
8	8	0	-1.176721	2.509132	2.065554
9	7	0	0.424301	-1.211076	-1.874678
10	6	0	0.863845	1.724047	1.174510
11	6	0	1.371725	-1.821728	0.128886
12	6	0	2.274596	3.211834	-0.314256
13	6	0	1.254312	-2.128577	-1.238613

14	6	0	5.953337	-2.534908	-0.226460
15	6	0	-0.015325	-0.254286	-0.989662
16	6	0	4.515821	-0.621407	-0.338151
17	6	0	5.535239	-1.227129	1.745789
18	6	0	6.167553	-2.315211	1.133377
19	6	0	0.513166	0.297220	1.539091
20	6	0	5.129891	-1.692697	-0.969068
21	6	0	1.878472	-3.240201	-1.782554
22	6	0	4.716684	-0.375761	1.017396
23	6	0	1.779559	3.634587	-1.544871
24	6	0	2.150643	-2.609926	0.965609
25	6	0	2.163453	4.869966	-2.055137
26	6	0	3.555428	5.237969	-0.119802
27	6	0	-0.049391	2.754724	1.620601
28	6	0	3.157905	4.014062	0.401679
29	6	0	2.622569	-4.045933	-0.921045
30	6	0	-0.487002	5.087741	1.791632
31	6	0	0.350616	6.347549	1.755567
32	6	0	2.764813	-3.741701	0.434329
33	6	0	3.055487	5.669834	-1.346802
34	6	0	0.244876	-1.107397	-3.307744
35	6	0	7.081739	-3.212046	1.928586
36	6	0	0.568698	-0.628543	0.362986
37	1	0	6.433477	-3.377311	-0.711179
38	1	0	5.694225	-1.045961	2.802840
39	1	0	-0.492223	0.321165	1.953199
40	1	0	1.190764	-0.091267	2.307000
41	1	0	4.945583	-1.865189	-2.020834
42	1	0	1.803016	-3.465883	-2.837431
43	1	0	4.226203	0.465919	1.491916
44	1	0	1.091817	2.996188	-2.087295
45	1	0	2.296237	-2.340218	2.004228
46	1	0	1.773601	5.202988	-3.008642
47	1	0	4.251395	5.858212	0.431057
48	1	0	3.525794	3.677258	1.362819
49	1	0	3.120980	-4.919599	-1.321924
50	1	0	-1.264241	5.103719	1.029343
51	1	0	-0.953585	4.922199	2.762512
52	1	0	-0.280980	7.218074	1.938006
53	1	0	0.828349	6.450815	0.781004
54	1	0	1.129071	6.310584	2.518232
55	1	0	3.382991	-4.365935	1.064852
56	1	0	3.364174	6.625983	-1.750710
57	1	0	-0.213036	-2.017041	-3.700243
58	1	0	1.211074	-0.926004	-3.777055
59	1	0	-0.417694	-0.263557	-3.485526

60	1	0	8.067415	-2.754054	2.041281
61	1	0	7.217145	-4.174554	1.434653
62	1	0	6.686432	-3.390903	2.929733
63	6	0	-2.319644	-6.097553	0.461050
64	6	0	-2.954419	-4.976719	-0.360024
65	6	0	-2.738920	-3.567699	0.171092
66	6	0	-3.159220	-3.349575	1.654538
67	6	0	-1.932909	-3.487816	2.569458
68	6	0	-0.995379	-2.297122	2.246271
69	8	0	-3.518086	-2.728371	-0.693950
70	6	0	-1.308097	-3.057404	0.027972
71	7	0	-1.238582	-1.827547	0.857703
72	6	0	-2.596585	-1.140410	0.825065
73	6	0	-3.228999	-1.322431	-0.567288
74	6	0	-4.551718	-0.585217	-0.787541
75	6	0	-5.603755	-1.312467	-1.295665
76	6	0	-6.858660	-0.706079	-1.509493
77	7	0	-7.123870	0.541149	-1.219003
78	6	0	-6.106581	1.285671	-0.712934
79	6	0	-6.422226	2.627294	-0.371565
80	6	0	-5.488717	3.452035	0.181006
81	6	0	-4.168191	2.978940	0.381731
82	8	0	-3.306611	3.844190	0.958110
83	6	0	-3.805326	1.706070	-0.002272
84	6	0	-4.777942	0.801041	-0.504576
85	6	0	-3.564402	-1.875059	1.775999
86	1	0	-2.516740	-7.059485	-0.013227
87	1	0	-2.729962	-6.139229	1.471407
88	1	0	-1.235724	-5.986576	0.535847
89	1	0	-4.035911	-5.125720	-0.416877
90	1	0	-2.580196	-5.002533	-1.386883
91	1	0	-3.964216	-4.028935	1.938197
92	1	0	-2.242658	-3.435475	3.614829
93	1	0	-1.416284	-4.436993	2.428398
94	1	0	0.049174	-2.592561	2.324254
95	1	0	-1.168646	-1.462579	2.923453
96	1	0	-1.128758	-2.832564	-1.020443
97	1	0	-0.545936	-3.756977	0.368720
98	1	0	-2.447722	-0.101021	1.096527
99	1	0	-2.527502	-1.020792	-1.349252
100	1	0	-5.478918	-2.359573	-1.519165
101	1	0	-7.671634	-1.296051	-1.920777
102	1	0	-7.439289	2.949320	-0.550744
103	1	0	-5.717565	4.466936	0.477631
104	1	0	-2.543673	3.355568	1.334121
105	1	0	-2.759598	1.439589	0.046335

106	1	0	-4.584727	-1.693553	1.441197
107	1	0	-3.486492	-1.530261	2.808054



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	16	0	3.743410	-0.845862	-1.217508
2	8	0	3.631332	-2.290712	-1.058828
3	7	0	2.592632	-0.233835	-0.121622
4	8	0	0.473631	3.417823	0.022957
5	8	0	3.589849	-0.209573	-2.514788
6	8	0	0.528941	-1.669299	-1.736929
7	6	0	2.073692	1.069409	-0.207738
8	8	0	-0.944318	2.271666	1.344341
9	7	0	0.940073	-3.339217	-0.191939
10	6	0	0.871801	1.135418	0.395515
11	6	0	2.068091	-2.164586	1.424559
12	6	0	2.894350	2.184634	-0.743837
13	6	0	1.636845	-3.430856	1.018059
14	6	0	6.981372	-0.586428	1.136798
15	6	0	0.958006	-2.051282	-0.671762
16	6	0	5.280984	-0.320824	-0.519975
17	6	0	7.164041	1.147707	-0.524000
18	6	0	7.689324	0.489872	0.588255
19	6	0	0.482551	-0.193195	0.982586
20	6	0	5.777446	-1.002084	0.588827
21	6	0	1.909098	-4.564026	1.765454
22	6	0	5.958004	0.748065	-1.090339
23	6	0	2.769092	2.605667	-2.067218
24	6	0	2.785728	-2.007753	2.591971
25	6	0	3.520331	3.683791	-2.519715
26	6	0	4.515773	3.923400	-0.334625
27	6	0	0.052715	2.315496	0.634612
28	6	0	3.766181	2.843696	0.121807
29	6	0	2.643116	-4.397479	2.944082

30	6	0	-0.297464	4.619697	0.232698
31	6	0	0.414387	5.712531	-0.533301
32	6	0	3.080512	-3.142889	3.356628
33	6	0	4.392406	4.344070	-1.655391
34	6	0	0.562989	-4.470964	-1.006374
35	6	0	9.010415	0.907183	1.179896
36	6	0	1.572102	-1.156379	0.428183
37	1	0	7.385162	-1.104872	1.998389
38	1	0	7.701567	1.984456	-0.953349
39	1	0	-0.526998	-0.510019	0.707028
40	1	0	0.534119	-0.160256	2.073792
41	1	0	5.229342	-1.840711	1.000116
42	1	0	1.576211	-5.543699	1.449058
43	1	0	5.540490	1.256924	-1.949507
44	1	0	2.098621	2.077749	-2.731074
45	1	0	3.122832	-1.024495	2.899551
46	1	0	3.425296	4.009000	-3.547711
47	1	0	5.193513	4.431423	0.339568
48	1	0	3.856903	2.505753	1.146919
49	1	0	2.873436	-5.267138	3.546160
50	1	0	-1.312804	4.453915	-0.126024
51	1	0	-0.343326	4.826861	1.301837
52	1	0	-0.109987	6.659770	-0.403873
53	1	0	0.448165	5.469738	-1.595401
54	1	0	1.438269	5.819520	-0.173604
55	1	0	3.645529	-3.044013	4.273991
56	1	0	4.973498	5.185007	-2.012663
57	1	0	-0.222859	-5.053430	-0.520406
58	1	0	1.430838	-5.107754	-1.189270
59	1	0	0.198855	-4.077449	-1.953209
60	1	0	9.288044	1.910104	0.856351
61	1	0	9.802374	0.222342	0.867414
62	1	0	8.973812	0.893397	2.270071
63	6	0	-3.544871	-4.744869	-2.551424
64	6	0	-4.152737	-3.343420	-2.574716
65	6	0	-4.009246	-2.550997	-1.286260
66	6	0	-4.549602	-3.262228	-0.005142
67	6	0	-3.403761	-3.953620	0.759348
68	6	0	-2.466983	-2.825799	1.278003
69	8	0	-4.770146	-1.340608	-1.512213
70	6	0	-2.590817	-2.087348	-0.954213
71	7	0	-2.623911	-1.618027	0.449765
72	6	0	-3.975025	-1.029764	0.713313
73	6	0	-4.424817	-0.317634	-0.575147
74	6	0	-5.607222	0.596191	-0.372501
75	6	0	-6.850763	0.264561	-0.846616

76	6	0	-7.938590	1.141466	-0.631083
77	7	0	-7.847475	2.283482	0.003494
78	6	0	-6.619506	2.638568	0.469679
79	6	0	-6.511295	3.882420	1.146169
80	6	0	-5.312616	4.316602	1.633983
81	6	0	-4.148364	3.523352	1.466792
82	8	0	-3.001023	4.031526	1.972747
83	6	0	-4.214817	2.309514	0.819072
84	6	0	-5.453831	1.840044	0.311192
85	6	0	-5.019616	-2.142104	0.935157
86	1	0	-3.674123	-5.223788	-3.522858
87	1	0	-4.024078	-5.378976	-1.803369
88	1	0	-2.473625	-4.718110	-2.339379
89	1	0	-5.222793	-3.408847	-2.791133
90	1	0	-3.704738	-2.752564	-3.377858
91	1	0	-5.351378	-3.959651	-0.256107
92	1	0	-3.815872	-4.525442	1.593954
93	1	0	-2.859321	-4.655389	0.125089
94	1	0	-1.419482	-3.134032	1.244958
95	1	0	-2.695350	-2.562609	2.312158
96	1	0	-2.278305	-1.298121	-1.637735
97	1	0	-1.851957	-2.883310	-1.038326
98	1	0	-3.906912	-0.338053	1.551899
99	1	0	-3.593951	0.279405	-0.967729
100	1	0	-6.989036	-0.658436	-1.390835
101	1	0	-8.921280	0.872058	-1.005288
102	1	0	-7.416306	4.465465	1.254153
103	1	0	-5.213286	5.261388	2.151945
104	1	0	-2.267322	3.406055	1.813002
105	1	0	-3.310071	1.725372	0.707955
106	1	0	-6.014334	-1.773612	0.688365
107	1	0	-5.043733	-2.491469	1.969356
