Supporting Information

Synthesis of Chiral Polycyclic *N*-Heterocycles *via* Gold(I)-Catalyzed 1,6-Enyne Cyclization/Intramolecular Nucleophilic Addition

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I. General information

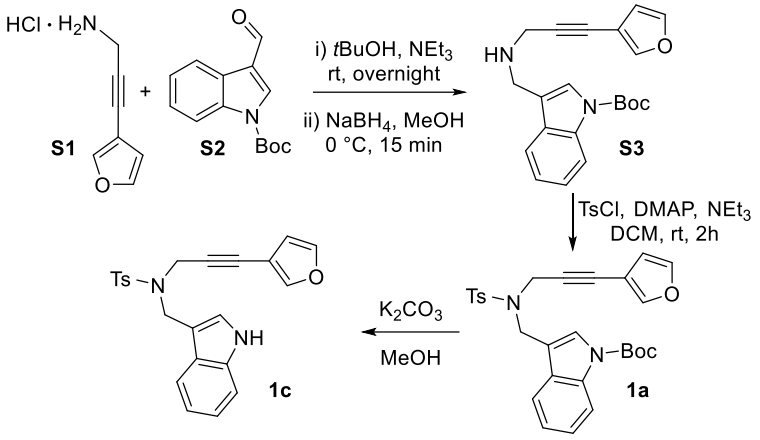
Reactions were performed using oven dried glassware under an atmosphere of argon. All purifications were carried out under flash-chromatographic conditions on silica gel (Redi Sep prepacked column, 230–400 mesh) at medium pressure (20 psi) with use of a CombiFlash Companion. Reactions were monitored by thin-layer chromatography on Merck silica gel plates (60 F254 aluminum sheets) which were rendered visible by ultraviolet and spraying with vanillin (15%) + sulfuric acid (2.5%) in EtOH followed by heating. Reagent-grade chemicals were obtained from diverse commercial suppliers and used as received. ^{1}H NMR (500 or 300 MHz) and ^{13}C NMR (125 or 75 MHz) spectra were recorded on Brüker Avance spectrometers at 298 K unless otherwise stated. Chemical shifts are given in ppm (δ) and are referenced to the internal solvent signal. Multiplicities are declared as follow: s (singlet), bs (broad singlet), d (doublet), t (triplet), q (quadruplet), dd (doublet of doublet), ddd (doublet of doublet of doublet), dt (doublet of triplet), m (multiplet). Coupling constants *J* are given in Hz. Carbon multiplicities were determined by DEPT135 experiment. Infrared spectra (IR) were recorded on a Perkin-Elmer FT-IR system using diamond window Dura SamplIR II and the data are reported in reciprocal centimeters (cm^{-1}). High-resolution mass spectrometry (HRMS) was performed using electrospray ionization (ESI) and time-of-flight (TOF) analyzer, in positive-ion or negative-ion detection mode. Supercritical fluid chromatography (SFC) separation was performed on an Investigator SFC System (Waters) equipped with a diode array UV detector. Data are reported as follows: column type, temperature, eluent, flow rate, pressure in column, retention times. Substrates **S1**[1] and **S2**[2] were synthesized according to the literature procedures. 1-Methylindole-3-carboxaldehyde substrate is commercially available.

[1] H. Deng, X. Yang, Z. Tong, Z. Li and H. Zhai, *Org. Lett.*, 2008, **10**, 1791.

[2] N. Netz and T. Opatz, *J. Org. Chem.*, 2016, **81**, 1723.

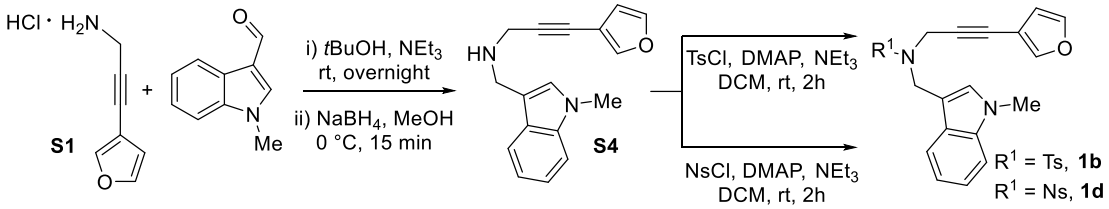
II. Experimental procedures

1. Synthesis of substrates **1a** and **1c**.



Substrate **S1**[1] (561 mg, 3.58 mmol, 1.4 equiv) was dissolved in *t*BuOH (13 mL) and aldehyde **S2**[2] (628 mg, 2.56 mmol, 1.0 equiv) and triethylamine (364 µL, 2.61 mmol, 1.02 equiv) were added successively. The resultant mixture was stirred at rt overnight, concentrated under reduced pressure, and diluted with MeOH (13 mL). $NaBH_4$ (135 mg, 3.58 mmol, 1.4 equiv) was added at 0 °C and the stirring was continued for 15 min. Then the mixture was quenched with saturated aqueous $NaHCO_3$ solution and extracted with diethyl ether. The combined organic layers were washed with brine, dried ($MgSO_4$), filtered, and concentrated to give a crude secondary amine **S3**, which was directly used into next step without purification. **S3** was dissolved in dichloromethane and *p*-toluenesulfonyl chloride (1.7 equiv.) and 4-dimethylaminopyridine (DMAP) (10 mol%) were added sequentially. The mixture was stirred 2 hours at room temperature. Then the mixture was washed with saturated aqueous $NaHCO_3$ solution and extracted with diethyl ether. The combined organic layers were washed with brine, dried ($MgSO_4$), filtered, and concentrated *in vacuo*. The crude residue was purified by flash chromatography to give compound **1a** (1.08 g, 84% over three steps). Deprotection of the Boc group of **1a** (200 mg, 0.4 mmol, 1.0 equiv) occurred with K_2CO_3 (0.8 mmol, 2 equiv) in MeOH (2 mL). The solution was stirred at reflux for 1 h.[3] After purification, compound **1c** was isolated (105 mg, 65% yield).

2. Synthesis of substrates **1b** and **1d**.

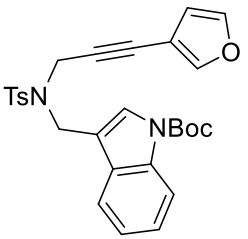


Substrate **S1**[1] (328 mg, 2.1 mmol, 1.4 equiv) was dissolved in *t*BuOH (7.5 mL) and 1-methylindole-3-carboxaldehyde (239 mg, 1.5 mmol, 1.0 equiv) and triethylamine (213 µL, 1.53 mmol, 1.02 equiv) were added successively. The resultant mixture was stirred at rt overnight, concentrated under reduced pressure, and diluted with MeOH (7.5 mL). $NaBH_4$ (79 mg, 2.1 mmol, 1.4 equiv) was added at 0 °C and the stirring was continued for 15 min. Then the mixture was quenched with saturated aqueous $NaHCO_3$ solution and

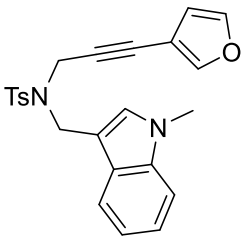
[3] A. K. Banala, P. Zhang, P. Plenge, G. Cyriac, T. Kopajtic, J. L. Katz, C. J. Loland and A. H. Newman, *J. Med. Chem.*, 2013, **56**, 9709.

extracted with diethyl ether. The combined organic layers were washed with brine, dried ($MgSO_4$), filtered, and concentrated to give a crude secondary amine **S4**, which was directly used into next step without purification. **S4** was dissolved in dichloromethane and *p*-toluenesulfonyl chloride (1.7 equiv.) and 4-dimethylaminopyridine (DMAP) (10 mol%) were added sequentially. The mixture was stirred 2 hours at room temperature, and then the mixture was washed with saturated aqueous $NaHCO_3$ solution and extracted with diethyl ether. The combined organic layers were washed with brine, dried ($MgSO_4$), filtered, and concentrated under vacuum. The crude residue was purified by flash chromatography to give compound **1b** (356 mg, 57% over three steps). The same procedure was used for the synthesis of **1d**, starting from 4-nitrobenzenesulfonyl chloride (270 mg, 40% yield over three steps).

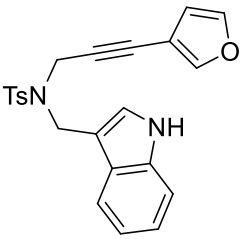
II.1. *tert*-Butyl 3-(((*N*-(3-(furan-3-yl)prop-2-yn-1-yl)-4-methylphenyl)sulfonamido)methyl)-1*H*-indole-1-carboxylate (1a) Colorless oil; R_f 0.46 (35% EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.10 (d, J = 8.1 Hz, 1H), 7.90-7.82 (m, 3H), 7.57 (s, 1H), 7.39-7.23 (m, 6H), 6.14 (s, 1H), 4.54 (s, 2H), 4.14 (s, 2H), 2.42 (s, 3H), 1.67 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.8 (CH), 143.7 (C), 142.8 (CH), 135.9 (C), 135.8 (C), 129.7 (CH), 128.2 (CH), 125.9 (CH), 125.0 (CH), 123.1 (CH), 120.2 (CH), 115.3 (CH), 114.2 (C), 112.4 (CH), 84.2 (C), 83.6 (C), 41.9 (CH_2), 36.6 (CH_2), 28.3 (CH_3), 21.6 (CH_3); IR: ν_{max} = 2984, 1732, 1454, 1371, 1350, 1259, 1230, 1160, 1087, 904, 872, 725, 665; HRMS (ESI) calcd. for $C_{28}H_{28}N_2NaO_5S$ $[M+Na]^+$: 527.1617, found: 527.1606.



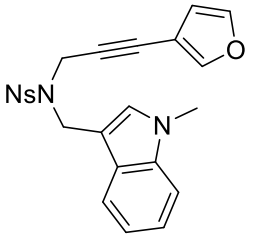
II.2. *N*-(3-(Furan-3-yl)prop-2-yn-1-yl)-4-methyl-*N*-((1-methyl-1*H*-indol-3-yl)methyl)benzenesulfonamide (1b). White solid; R_f 0.52 (30% EtOAc/*n*-heptane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.82-7.74 (m, 3H), 7.28-7.21 (m, 5H), 7.18 (t, J = 7.5 Hz, 1H), 7.07 (t, J = 7.3 Hz, 1H), 6.96 (s, 1H), 6.08 (s, 1H), 4.51 (s, 2H), 4.05 (s, 2H), 3.69 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 179.9 (C), 145.7 (CH), 143.4 (C), 142.8 (CH), 129.6 (CH), 129.3 (CH), 128.2 (CH), 122.3 (CH), 119.8 (CH), 112.4 (CH), 109.4 (CH), 107.9 (C), 84.2 (C), 41.9 (CH_2), 36.2 (CH_2), 33.0 (CH_3), 21.6 (CH_3); IR: ν_{max} = 3055, 2987, 1556, 1475, 1344, 1330, 1264, 1158, 1092, 1003, 890, 871, 733, 704, 662; HRMS (ESI) calcd. for $C_{24}H_{22}N_2NaO_3S$ $[M+Na]^+$: 441.1249, found: 441.1229.



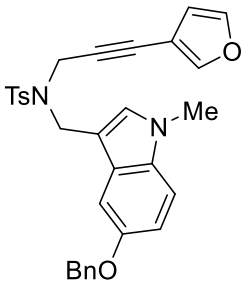
II.3. *N*-((1*H*-Indol-3-yl)methyl)-*N*-(3-(furan-3-yl)prop-2-yn-1-yl)- 4-methyl-benzenesulfonamide (1c). Light yellow foam; R_f 0.39 (40% EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (bs, 1H), 7.86 (d, J = 8.0 Hz, 2H+1H), 7.39-7.30 (m, 5H), 7.28-7.15 (m, 3H), 6.14 (s, 1H), 4.60 (s, 2H), 4.11 (s, 2H), 2.41 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 145.7 (CH), 143.4 (C), 142.8 (CH), 136.6 (C), 136.2 (C), 129.8 (C), 129.6 (CH), 128.2 (CH), 127.1 (C), 124.7 (CH), 122.8 (CH), 120.3 (CH), 119.8 (CH), 112.4 (CH), 111.3 (CH), 109.6 (C), 106.9 (C), 84.1 (C), 42.0 (CH_2), 36.2 (CH_2), 21.6 (CH_3); IR: ν_{max} = 3403, 3055, 1598, 1493, 1457, 1422, 1341, 1265, 1159, 1091, 1003, 893, 872, 791, 776, 728, 703, 662 cm^{-1}; HRMS (ESI) calcd. for $C_{23}H_{21}N_2O_3S$ $[M+H]^+$: 405.1273, found: 405.1255.



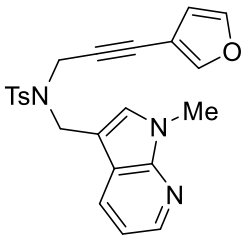
II.4. *N*-(3-(Furan-3-yl)prop-2-yn-1-yl)-*N*-((1-methyl-1*H*-indol-3-yl)methyl)-4-nitrobenzenesulfonamide (1d). Yellow solid; R_f 0.55 (100% CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.30 (d, J = 8.2 Hz, 2H), 8.13 (d, J = 8.2 Hz, 2H), 7.82 (d, J = 7.9 Hz, 1H), 7.38-7.27 (m, 4H), 7.20-7.10 (m, 1H), 7.07 (s, 1H), 6.12 (d, J = 1.4 Hz, 1H), 4.63 (s, 2H), 4.18 (s, 2H), 3.78 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.1 (C), 145.8 (CH), 145.1 (C), 143.3 (CH), 137.4 (C), 129.5 (CH), 129.3 (CH), 127.4 (C), 124.0 (CH), 122.5 (CH), 120.0 (CH), 119.6 (CH), 112.0 (CH), 109.6 (CH), 107.0 (C), 106.4 (C), 83.6 (C), 77.6 (C), 42.3 (CH_2), 36.4 (CH_2), 33.0 (CH_3); IR: ν_{max} = 3106, 2933, 1606, 1529, 1476, 1348, 1312, 1261, 1200, 1161, 1132, 1090, 1004, 908, 891, 855, 792, 772, 739, 687 cm^{-1}; HRMS (ESI) calcd. for $C_{23}H_{20}N_3O_5S$ $[M+H]^+$: 450.1124, found: 450.1140.



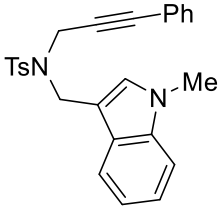
II.5. *N*-((5-(Benzyloxy)-1-methyl-1*H*-indol-3-yl)methyl)-*N*-(3-(furanyl)prop-2-yn-1-yl)-4-methylbenzenesulfonamide (1e). Following the same general procedure as for isolation of **1b**, substrate **1e** was isolated in 11% yield over two steps (300 mg). Light yellow solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.87 (d, J = 8.2 Hz, 2H), 7.48 (d, J = 7.4 Hz, 2H), 7.42 (d, J = 1.8 Hz, 1H), 7.38 (t, J = 7.5 Hz, 2H), 7.35-7.28 (m, 5H), 7.20 (d, J = 8.8 Hz, 1H), 7.02 (s, 1H), 6.98 (dd, J = 8.8, 2.0 Hz, 1H), 6.17 (d, J = 1.5 Hz, 1H), 5.09 (s, 2H), 4.55 (s, 2H), 4.13 (s, 2H), 3.73 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.5 (C), 145.7 (CH), 143.4 (C), 142.8 (CH), 137.7 (C), 136.4 (C), 132.8 (C), 129.8 (CH), 129.6 (CH), 128.6 (CH), 128.2 (CH), 128.0 (CH), 127.9 (CH), 113.4 (CH), 112.4 (CH), 110.2 (CH), 107.3 (C), 106.9 (C), 102.6 (CH), 84.3 (C), 77.0 (C), 70.8 (CH_2), 41.9 (CH_2), 36.1 (CH_2), 33.1 (CH_3), 21.6 (CH_3); IR: ν_{max} = 2922, 1623, 1579, 1490, 1426, 1344, 1327, 1264, 1206, 1158, 1091, 1003, 888, 872, 794, 737, 698, 662 cm^{-1}; HRMS (ESI) calcd. for $C_{31}H_{28}N_2NaO_4S$ $[M+Na]^+$: 547.1667, found: 547.1654.



II.6. *N*-(3-(Furan-3-yl)prop-2-yn-1-yl)-4-methyl-*N*-((1-methyl-1*H*-pyrrolo[2,3-*b*]pyridin-3-yl)methyl)benzenesulfonamide (1f). Following the same general procedure as for isolation of **1b**, substrate **1f** was isolated in 29% yield over two steps (320 mg). White solid; R_f 0.46 (10% EtOAc/CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.34 (dd, J = 4.7, 1.3 Hz, 1H), 8.15 (dd, J = 7.9, 1.3 Hz, 1H), 7.83 (d, J = 8.2 Hz, 2H), 7.34-7.25 (m, 4H), 7.14 (s, 1H), 7.07 (dd, J = 7.9, 4.7 Hz, 1H), 6.13 (d, J = 0.8 Hz, 1H), 4.54 (s, 2H), 4.10 (s, 2H), 3.84 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.3 (C), 145.7 (CH), 143.6 (CH), 143.5 (C), 142.8 (CH), 136.1 (C), 129.6 (CH), 129.1 (CH), 128.2 (CH), 128.1 (CH), 119.9 (C), 115.9 (CH), 112.4 (CH), 106.8 (C),106.6 (C), 83.8 (C), 42.1 (CH_2), 36.3 (CH_2), 31.3 (CH_3), 21.6 (CH_3); IR: ν_{max} = 3055, 2923, 1600, 1544, 1461, 1409, 1341, 1297, 1265, 1158, 1092, 1003, 889, 871, 736, 704, 660 cm^{-1}; HRMS (ESI) calcd. for $C_{23}H_{22}N_3O_3S$ $[M+H]^+$: 420.1382, found: 420.1381.

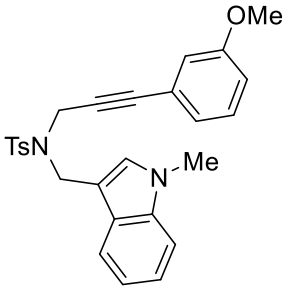


II.7. 4-Methyl-*N*-((1-methyl-1*H*-indol-3-yl)methyl)-*N*-(3-phenylprop-2-yn-1-yl)benzenesulfonamide (S5). Starting from 3-phenylprop-2-yn-1-amine, substrate **S5** was isolated in 26% yield over two steps (200 mg). White solid; R_f 0.55 (25% EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.87 (d, J = 8.0 Hz, 2H+1H), 7.36-7.21 (m, 7H), 7.15 (t, J = 7.2 Hz, 1H), 7.07 (d, J = 8.7 Hz, 2H+1H), 4.62 (s, 2H), 4.16 (s, 2H), 3.76 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.5 (C), 137.4 (C), 136.2 (C), 131.6 (CH), 129.6 (CH), 129.3 (CH), 128.5 (CH), 128.3 (CH), 128.1 (CH), 127.7 (C), 122.6 (C), 122.3



(CH), 119.84 (CH), 119.80 (CH), 109.4 (CH), 107.9 (C), 85.9 (C), 82.3 (C), 41.9 (CH_2), 36.2 (CH_2), 33.0 (CH_3), 21.6 (CH_3); IR: ν_{max} = 3058, 2924, 1712, 1598, 1491, 1444, 1372, 1352, 1189, 1175, 1164, 1093, 1058, 1005, 917, 815, 785, 758, 716, 693, 662 cm^{-1}; HRMS (ESI) calcd. for $C_{26}H_{24}N_2NaO_2S$ $[M+Na]^+$: 451.1456, found: 451.1451.

II.8. *N*-(3-(3-Methoxyphenyl)prop-2-yn-1-yl)-4-methyl-*N*-((1-methyl-1*H*-indol-3-yl)methyl)benzenesulfonamide (S6). Starting from 3-(3-methoxyphenyl)prop-2-yn-1-amine, substrate **S6** was isolated in 67% yield over two steps (209 mg). Colorless oil; R_f 0.71 (100% CH_2Cl_2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88-7.84 (m, 3H), 7.33-7.23 (m, 4H), 7.17 (d, J = 7.6 Hz, 1H), 7.15 (d, J = 7.6 Hz, 1H), 7.05 (s, 1H), 6.85 (dd, J = 8.2, 2.1 Hz, 1H), 6.66 (d, J = 7.6 Hz, 1H), 6.61 (bs, 1H), 4.61 (s, 2H), 4.15 (s, 2H), 3.80 (s, 3H), 3.76 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.3 (C), 143.6 (C), 137.3 (C), 136.1 (C), 129.65 (CH), 129.3 (CH), 128.1 (CH), 127.6 (C), 124.1 (CH), 123.5 (C), 122.3 (CH), 119.85 (CH), 119.78 (CH), 117.2 (CH), 114.3 (CH), 109.4 (CH), 107.7 (CH), 85.8 (C), 82.1 (C), 55.4 (CH_3), 41.9 (CH_2), 36.2 (CH_2), 33.0 (CH_3), 21.6 (CH_3); IR: ν_{max} = 2972, 1598, 1482, 1346, 1332, 1289, 1161, 1091, 1045, 905, 836, 728, 694, 653 cm^{-1}; HRMS (ESI) calcd. for $C_{27}H_{26}N_2NaO_3S$ $[M+Na]^+$: 481.1562, found: 481.1585.



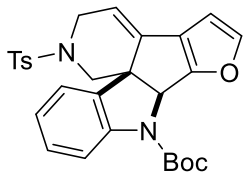
3. General Procedure I for the synthesis of racemic mixture of compounds **2a-g** and **3b.**

In a Schlenk tube, substrates **1a-g** or **S5-6** (0.10 mmol or 0.05 mmol, 1.0 equiv), gold catalyst [Au(MeCN)(P*t*Bu$_2$C$_6$H$_4$-2-Ph)][BF_4] (5 mol%) and distilled dichloromethane (0.5 M) were added. The reaction mixture was then stirred 17 h at 20 °C. The crude reaction mixture was concentrated and purified by automatic flash chromatography using 4g silica gel pre-packed column and EtOAc/*n*-heptane as eluent (5-10% EtOAc/*n*-heptane). Alternatively, preparative TLC (5-10% EtOAc/*n*-heptane) can be used for purification.

4. General Procedure II for asymmetric synthesis of compounds **2a-g** and **3b.**

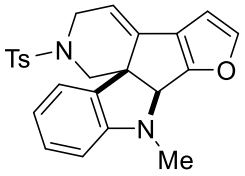
In a Schlenk tube, chiral gold catalyst DTBM-MeO-BIPHEP(AuCl)$_2$ (**I**) or DTBM-SEGPHOS(AuCl)$_2$ (**II**) (5 mol%), $AgNTf_2$ (5 or 10 mol%) and distilled dichloromethane (0.125 M) were stirred 15 minutes at 20 °C. After filtration, this mixture was added in a Schlenk tube containing substrates **1a-g** or **S5-6** (0.10 mmol or 0.05 mmol, 1.0 equiv). Then, the reaction mixture was stirred 40 h at 10 °C. The crude reaction mixture was concentrated and purified by automatic flash chromatography using 4g silica gel pre-packed column and EtOAc/*n*-heptane as eluent (10-35 % EtOAc/*n*-heptane). Alternatively, preparative TLC (10-35 % EtOAc/*n*-heptane or 100% CH_2Cl_2) can be used for purification.

III.9. *tert*-Butyl3-tosyl-2,3,4,9a-tetrahydro-9*H*-furo[3',2':4,5]pyrido[3',4':2,3]cyclopenta[1,2-*b*]indole-9 –carboxylate (2a) (*General Procedure I*: 27 mg, 54% yield, *General Procedure II*: 20 mg, 40% yield, 38% ee). Colorless oil; R_f 0.41 (35% EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$, *mixture of rotamers*) δ 7.85 (bs, 1H), 7.65 (d, J = 8.3 Hz, 2H), 7.43 (bs, 1H), 7.37-7.34 (m, 1H), 7.30 (d, J = 8.0 Hz, 2H), 7.28-7.20 (m, 1H), 6.97 (bs, 1H), 6.27 (d, J = 1.9 Hz, 1H), 5.63 (t, J = 3.3 Hz, 1H), 5.50-5.40 (m, 1H), 4.48 (dd, J = 17.1, 2.8 Hz, 1H), 4.00 (d, J = 10.5 Hz, 1H), 3.55-3.48 (m, 1H), 2.90-2.80 (m, 1H), 2.42 (s, 3H), 1.64 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$, *mixture of rotamers*) δ 159.6 (C), 149.1 (C), 143.9 (C), 134.4 (C), 129.8 (CH), 129.5 (CH), 127.7 (CH), 125.7 (CH), 122.9 (CH), 115.0 (CH), 110.4 (CH), 105.1 (CH), 63.4 (CH),

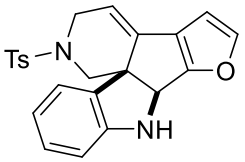


50.4 (CH_2), 44.8 (CH_2), 28.5 (CH_3), 21.6 (CH_3); IR: ν_{max} = 2980, 1705, 1480, 1463, 1388, 1370, 1316, 1261, 1161, 1151, 1047, 1021, 907, 730; HRMS (ESI) calcd. for $C_{30}H_{31}N_3NaO_5S$ $[M+Na+CH_3CN]^+$: 568.1882, found: 568.1855.

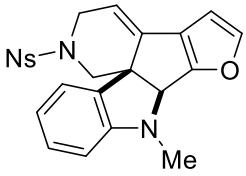
II.10. 9-Methyl-3-tosyl-3,4,9,9a-tetrahydro-2*H*-furo[3',2':4,5]pyrido[3',4':2,3]cyclopenta[1,2-*b*]indole (2b) (*General Procedure I*: 31 mg, 74% yield, *General Procedure II*: 41.5 mg, 99% yield, 93% ee). White solid; R_f 0.65 (100% CH_2Cl_2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, J = 8.2 Hz, 2H), 7.32 (d, J = 1.5 Hz, 1H), 7.29 (d, J = 8.0 Hz, 2H), 7.25 (d, J = 7.5 Hz, 1H), 7.15 (t, J = 7.6 Hz, 1H), 6.68 (t, J = 7.4 Hz, 1H), 6.45 (d, J = 7.8 Hz, 1H), 6.26 (d, J = 1.7 Hz, 1H), 5.58 (t, J = 3.2 Hz, 1H), 4.65 (s, 1H), 4.44 (dd, J = 16.9, 3.1 Hz, 1H), 4.04 (d, J = 10.4 Hz, 1H), 3.49 (dd, J = 16.9, 3.3 Hz, 1H), 3.05 (s, 3H), 2.85 (d, J = 10.4 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.9 (C), 150.0 (C), 148.7 (CH), 143.7 (C), 135.2 (C), 132.1 (C), 129.8 (CH), 129.4 (CH), 127.8 (CH), 127.7 (C), 125.6 (CH), 118.3 (CH), 109.4 (CH), 107.4 (CH), 105.2 (CH), 68.7 (CH), 50.0 (CH_2), 44.8 (CH_2), 33.2 (CH_3), 21.6 (CH_3); IR: ν_{max} = 2947, 2889, 1603, 1483, 1351, 1222, 1165, 1116, 963, 909, 733, 719, 655 cm^{-1}; HRMS (ESI) calcd. for $C_{24}H_{23}NO_3S$ $[M+H]^+$: 419.1429, found: 419.1429; SFC Analysis: 93% ee [CHIRALPAK® IA, 30 °C, 30% MeOH, 4.0 mL/min, 100 bar, retention times: 3.3 min (major) and 4.3 min (minor)].



II.11. 3-Tosyl-3,4,9,9a-tetrahydro-2*H*-furo[3',2':4,5]pyrido[3',4':2,3]cyclopenta[1,2-*b*]indole (2c) (*General Procedure I*: 12 mg, 30% yield, *General Procedure II*: 8 mg, 20% yield, 62% ee). Light yellow oil; R_f 0.31 (40% EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.66 (d, J = 8.1 Hz, 2H), 7.35 (d, J = 7.5 Hz, 1H), 7.32 (d, J = 2.1 Hz, 1H), 7.29 (d, J = 8.1 Hz, 2H), 7.10 (td, J = 7.7, 0.9 Hz, 1H), 6.77 (td, J = 7.8, 0.9 Hz, 1H), 6.67 (d, J = 7.8 Hz, 1H), 6.27 (d, J = 1.9 Hz, 1H), 5.59 (t, J = 3.3 Hz, 1H), 4.74 (s, 1H), 4.46 (dd, J = 16.9, 3.1 Hz, 1H), 4.06 (d, J = 10.4 Hz, 1H), 3.49 (dd, J = 16.9, 3.3 Hz, 1H), 2.85 (d, J = 10.4 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 161.4 (C), 148.4 (CH), 143.7 (C), 135.5 (C), 133.9 (C), 132.0 (C), 129.8 (CH), 129.3 (CH), 128.3 (C), 127.9 (C), 127.8 (CH), 125.9 (CH), 120.0 (CH), 111.0 (CH), 109.6 (CH), 105.3 (CH), 62.9 (C), 62.2 (CH), 50.2 (CH_2), 44.9 (CH_2), 21.7 (CH_3); IR: ν_{max} = 2902, 1601, 1482, 1464, 1353, 1329, 1259, 1224, 1166, 1122, 1096, 1019, 973, 903, 815, 727, 671 cm^{-1}; HRMS (ESI) calcd. for $C_{23}H_{21}N_2O_3S$ $[M+H]^+$: 405.1273, found: 405.1264; SFC Analysis: 62% ee [CHIRALPAK® IB, 30 °C, 20% MeOH, 4.0 mL/min, 100 bar, retention times: 7.3 min (major) and 10.4 min (minor)].

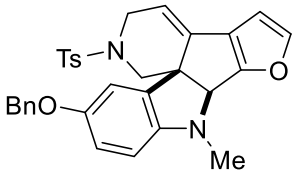


II.12. 9-Methyl-3-((4-nitrophenyl)sulfonyl)-3,4,9,9a-tetrahydro-2*H*-furo[3',2':4,5]pyrido[3',4':2,3]cyclopenta[1,2-*b*]indole (2d) (*General Procedure I*: 34 mg, 76% yield, *General Procedure II*: 22 mg, 50% yield, 45% ee). Yellow solid; R_f 0.60 (100% CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.33 (d, J = 8.1 Hz, 2H), 7.94 (d, J = 8.1 Hz, 2H), 7.34 (d, J = 1.8 Hz, 1H), 7.15-7.10 (m, 2H), 6.65 (t, J = 7.4 Hz, 1H), 6.45 (d, J = 7.8 Hz, 1H), 6.28 (d, J = 1.9 Hz, 1H), 5.60 (t, J = 3.2 Hz, 1H), 4.68 (s, 1H), 4.50 (dd, J = 16.9, 3.1 Hz, 1H), 4.08 (d, J = 10.7 Hz, 1H), 3.63 (dd, J = 16.9, 3.4 Hz, 1H), 3.05 (s, 3H), 3.01 (d, J = 10.7 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.0 (C), 148.9 (CH), 131.6 (C), 129.6 (CH), 128.7 (CH), 125.1 (CH), 124.4 (CH), 118.2 (CH), 108.7 (CH), 107.6 (CH), 105.2 (CH), 68.6 (CH), 50.0 (CH_2), 44.8 (CH_2), 33.2 (CH_3); IR: ν_{max} = 3051, 2892, 1604, 1530, 1483, 1350, 1312, 1265, 1170, 1116, 965, 906, 737, 708 cm^{-1}; HRMS (ESI) calcd. for $C_{23}H_{20}N_3O_5S$ $[M+H]^+$: 450.1124, found: 450.1131; SFC Analysis:

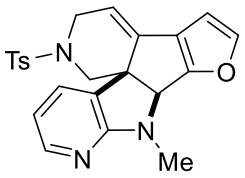


45% ee [CHIRALPAK® IA, 30 °C, 30% MeOH, 4.0 mL/min, 100 bar, retention times: 4.6 min (major) and 7.6 min (minor)].

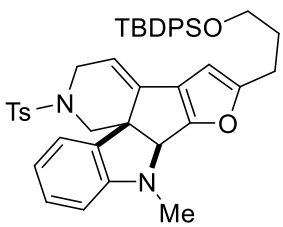
II.13. 6-(Benzyloxy)-9-methyl-3-tosyl-3,4,9α-tetrahydro-2*H*-furo[3',2':4,5]pyrido[3',4':2,3]cyclopenta[1,2-*b*]indole (2e) (*General Procedure I*: 24 mg, 92% yield, *General Procedure II*: < 5% yield). White solid; R_f 0.30 (100% CH_2Cl_2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (d, J = 8.1 Hz, 2H), 7.48 (d, J = 7.4 Hz, 2H), 7.40 (t, J = 7.5 Hz, 2H), 7.36 (s, 1H), 7.34-7.28 (m, 3H), 7.06 (d, J = 2.3 Hz, 1H), 6.81 (dd, J = 8.4, 2.4 Hz, 1H), 6.39 (d, J = 8.4 Hz, 1H), 6.29 (d, J = 1.6 Hz, 1H), 5.59 (s, 1H), 5.05-4.96 (m, 2H), 4.67 (s, 1H), 4.42 (dd, J = 16.9, 3.1 Hz, 1H), 4.11 (d, J = 10.5 Hz, 1H), 3.51 (dd, J = 16.9, 3.1 Hz, 1H), 3.03 (s, 3H), 2.90 (d, J = 10.5 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.3 (C), 148.8 (CH), 144.8 (C), 143.7 (C), 137.9 (C), 134.0 (C), 133.6 (C), 129.8 (CH), 128.6 (CH), 127.9 (CH), 127.8 (CH), 115.9 (CH), 113.9 (CH), 109.5 (CH), 108.0 (CH), 105.1 (CH), 71.4 (CH_2), 69.3 (CH), 49.8 (CH_2), 44.8 (CH_2), 34.2 (CH_3), 21.6 (CH_3); IR: ν_{max} = 2919, 2853, 1677, 1597, 1489, 1455, 1350, 1251, 1184, 1166, 1096, 1020, 965, 922, 815, 735, 714, 698, 656 cm^{-1}; HRMS (ESI) calcd. for $C_{31}H_{29}N_2O_4S$ $[M+H]^+$: 525.1848, found: 525.1838.



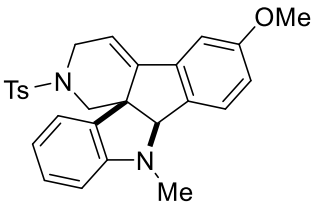
II.14. Compound 2f (*General Procedure I*: 8 mg, 40% yield, *General Procedure II*: <10% yield). White solid; R_f 0.33 (10% EtOAc/CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.98 (dd, J = 5.3, 1.6 Hz, 1H), 7.65 (d, J = 8.2 Hz, 2H), 7.47 (dd, J = 7.2, 1.6 Hz, 1H), 7.36 (d, J = 1.7 Hz, 1H), 7.31 (d, J = 8.0 Hz, 2H), 6.52 (dd, J = 7.2, 5.3 Hz, 1H), 6.29 (d, J = 1.9 Hz, 1H), 5.60 (t, J = 3.2 Hz, 1H), 4.68 (s, 1H), 4.45 (dd, J = 17.0, 3.1 Hz, 1H), 4.00 (d, J = 10.5 Hz, 1H), 3.46 (dd, J = 17.0, 3.3 Hz, 1H), 3.22 (s, 3H), 2.81 (d, J = 10.5 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 160.6 (C), 160.3 (C), 149.1 (CH), 148.0 (CH), 143.9 (C), 134.8 (C), 133.8 (C), 132.9 (CH), 129.9 (CH), 129.4 (C), 127.7 (CH), 125.7 (C), 113.5 (CH), 109.9 (CH), 105.1 (CH), 65.5 (CH), 58.9 (C), 50.0 (CH_2), 44.9 (CH_2), 30.7 (CH_3), 21.7 (CH_3); IR: ν_{max} = 3058, 2850, 1603, 1486, 1406, 1351, 1247, 1163, 1122, 1095, 1001, 964, 920, 893, 816, 773, 735, 718, 656 cm^{-1}; HRMS (ESI) calcd. for $C_{23}H_{22}N_3O_3S$ $[M+H]^+$: 420.1382, found: 420.1381.



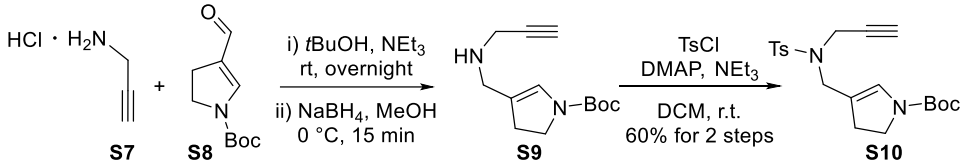
II.15. (4α*R*,9α*S*)-11-(3-((*tert*-Butyldiphenylsilyl)oxy)propyl)-9-methyl-3-tosyl-3,4,9,9a-tetrahydro-2*H*-furo[3',2':4,5]pyrido[3',4':2,3]cyclopenta[1,2-*b*]indole (2g) (*General Procedure I*: 29.5 mg, 83% yield, *General Procedure II*: 31.5 mg, 88% yield, 45% ee). White solid; R_f 0.36 (30% EtOAc/*n*-heptane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.70-7.58 (m, 6H), 7.41-7.27 (m, 9H), 7.14 (td, J = 7.7, 1.3 Hz, 1H), 6.68 (td, J = 7.5, 0.9 Hz, 1H), 6.44 (d, J = 7.8 Hz, 1H), 5.82 (s, 1H), 5.49 (t, J = 3.2 Hz, 1H), 4.61 (s, 1H), 4.43 (dd, J = 16.9, 3.1 Hz, 1H), 4.03 (d, J = 10.4 Hz, 1H), 3.67 (t, J = 6.1 Hz, 2H), 3.50 (dd, J = 16.9, 3.3 Hz, 1H), 3.01 (s, 3H), 2.83 (d, J = 10.4 Hz, 1H), 2.66 (t, J = 7.5 Hz, 2H), 2.42 (s, 3H), 1.88-1.75 (m, 2H), 1.03 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 163.2 (C), 159.0 (C), 150.1 (C), 143.6 (C), 135.7 (CH), 134.0 (C), 132.3 (C), 130.0 (C), 129.7 (CH), 129.3 (CH), 127.9 (C), 127.8 (CH), 125.5 (CH), 118.2 (CH), 108.5 (CH), 107.4 (CH), 100.5 (CH), 68.9 (CH), 62.9 (CH_2), 50.1 (CH_2), 44.9 (CH_2), 33.3 (CH_3), 30.8 (CH_2), 27.0 (CH_3), 25.3 (CH_2), 21.7 (CH_3); IR: ν_{max} = 2929, 2857, 1603, 1484, 1428, 1351, 1331, 1264, 1221, 1167, 1105, 1091, 963, 916, 815, 733, 719, 701, 677, 655 cm^{-1}; HRMS (ESI) calcd. for $C_{43}H_{47}N_2O_4SSi$ $[M+H]^+$: 715.3026, found: 715.3021; SFC Analysis: 45% ee [CHIRALPAK® IA, 30 °C, 30% MeOH, 4.0 mL/min, 100 bar, retention times: 6.8 min (major) and 9.7 min (minor)].



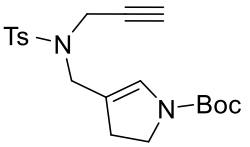
II.16. 12-Methoxy-9-methyl-3-tosyl-3,4,9,9a-tetrahydro-2*H*-pyrido[3',4':2,3]indeno[1,2-*b*]indole (3b) (*General Procedure I*: 31 mg, 67% yield, *General Procedure II*: 16 mg, 35% yield, 19% ee). White solid; R_f 0.55 (100% CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.71 (d, J = 8.2 Hz, 2H), 7.33-7.28 (m, 3H), 7.08 (t, J = 7.6 Hz, 1H), 6.93 (d, J = 7.3 Hz, 1H), 6.71 (dd, J = 8.4, 2.6 Hz, 1H), 6.57 (t, J = 7.4 Hz, 1H), 6.40 (d, J = 2.6 Hz, 1H), 6.38 (d, J = 7.3 Hz, 1H), 6.16 (bs, 1H), 4.50 (s, 1H), 4.45 (dd, J = 14.0, 2.5 Hz, 1H), 4.05 (d, J = 14.0 Hz, 1H), 3.75 (s, 3H), 3.68 (d, J = 8.4 Hz, 1H), 3.14 (d, J = 8.4 Hz, 1H), 3.04 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.5 (C), 150.0 (C), 143.9 (C), 136.3 (C), 134.0 (C), 133.6 (C), 133.4 (C), 129.9 (CH), 129.3 (CH), 128.8 (CH), 127.7 (CH), 125.3 (C), 123.0 (CH), 121.1 (CH), 118.7 (CH), 113.1 (CH), 112.7 (CH), 107.9 (CH), 69.6 (CH), 59.6 (CH_2), 55.4 (CH_3), 54.6 (C), 50.9 (CH_2), 36.2 (CH_3), 21.7 (CH_3); IR: ν_{max} = 2956, 2922, 2851, 1676, 1624, 1598, 1464, 1332, 1289, 1234, 1161, 1093, 1028, 921, 815, 740, 708, 665 cm^{-1}; HRMS (ESI) calcd. for $C_{27}H_{27}N_2O_3S$ $[M+H]^+$: 459.1742, found: 459.1738.



5. Synthesis of substrates **S10**.



II.17. *tert*-Butyl4-(((4-methyl-*N*-(prop-2-yn-1-yl)phenyl)sulfonamido)methyl)-2,3-dihydro-1*H*-pyrrole-1-carboxylate (S10). Using the same procedure as for the synthesis of substrates **1a-d** and starting from compounds **S7** and **S8**,[4] compound **S10** was isolated in 60% overall yield over three steps (264 mg). Colorless oil; R_f 0.50 (30% EtOAc/*n*-heptane); ^{1}H NMR (500 MHz, $CDCl_3$, *mixture of rotamers*) δ 7.73 (d, J = 8.1 Hz, 2H), 7.29 (d, J = 8.1 Hz, 2H), 6.59 (s, 0.5H), 6.42 (s, 0.5H), 4.05 (bs, 2H), 3.87 (s, 2H), 3.78-3.70 (m, 2H), 3.48 (s, 1H), 2.62-2.54 (m, 2H), 2.42 (s, 3H), 1.46 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$, *mixture of rotamers*) δ 133.8 (C), 129.7 (C), 129.6 (CH), 127.9 (CH), 74.1 (CH), 45.7 (CH_2), 44.7 (CH_2), 35.6 (CH_2), 29.7 (CH_2), 28.5 (CH_3), 21.7 (CH_3); IR: ν_{max} =3302, 2980, 1693, 1420, 1393, 1366, 1349, 1265, 1160, 1092, 1041, 895, 815, 733, 703, 661 cm^{-1}; HRMS (ESI) calcd. for $C_{20}H_{26}N_2NaO_4S$ $[M+Na]^+$: 413.1511, found: 413.1515.

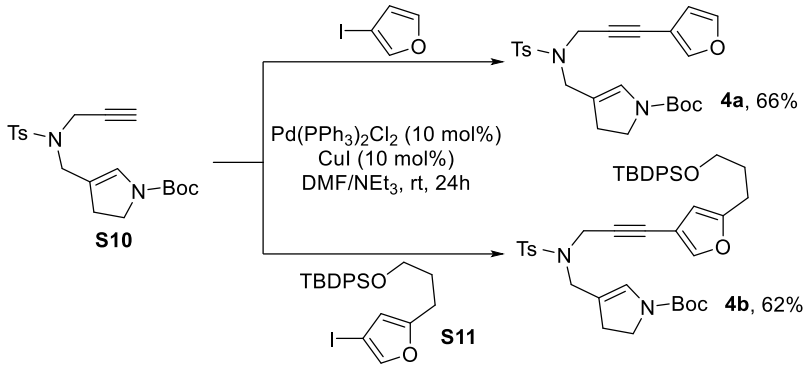


6. Synthesis of substrates **4a-b**.

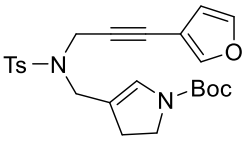
To **S10** (1.0 equiv.) in DMF (2 mL) and triethylamine (2 mL), were added 3-iodofuran or **S11**[5] (1.2 equiv.), $Pd(PPh_3)_2Cl_2$ (10 mol%) and CuI (10 mol%) at -20 °C. The solution was then stirred 24 h at room temperature. The crude reaction mixture was concentrated and purified by automatic flash chromatography using 4g silica gel pre-packed column and EtOAc/*n*-heptane as eluent (20-35 % EtOAc/*n*-heptane).

[4] T. J. Greshock and R. L. Funk, *J. Am. Chem. Soc.*, 2006, **128**, 4946.

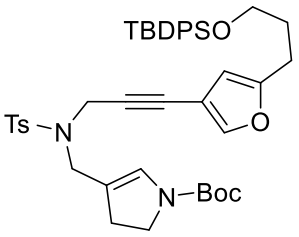
[5] B. Cheng, F. Wu, X. Yang, Y. Zhou, X. Wan and H. Zhai, *Chem. Eur. J.*, 2011, **17**, 12569.



II.18. *tert*-Butyl 4-(((*N*-(3-(furan-3-yl)prop-2-yn-1-yl)-4-methylphenyl)sulfonamido)methyl)-2,3-dihydro-1*H*-pyrrole-1-carboxylate (4a) (83 mg, 66%). R_f = 0.31 (20% EtOAc/*n*-heptane); ^{1}H NMR (500 MHz, $CDCl_3$, *mixture of rotamers*) δ 7.75 (d, *J* = 8.0 Hz, 2H), 7.33-7.29 (m, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 6.60 (bs, 0.5H), 6.43 (bs, 0.5H), 6.13 (s, 1H), 4.22-4.20 (m, 2H), 3.89 (s, 2H), 3.80-3.71 (m, 2H), 2.68-2.57 (m, 2H), 2.38 (s, 3H), 1.46 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$, *mixture of rotamers*) *δ* 152.2 (C), 151.4 (C), 145.9 (CH), 145.8 (CH), 143.6 (C), 142.84 (CH), 142.78 (CH), 136.1 (C), 129.8 (CH), 129.6 (CH), 129.5 (CH), 128.0 (CH), 115.5 (C), 115.4 (C), 112.4 (CH), 106.7 (C), 83.8 (C), 83.5 (C), 80.6 (C), 80.5 (C), 77.4 (C), 46.2 (CH_2), 45.7 (CH_2), 45.1 (CH_2), 44.9 (CH_2), 36.8 (CH_2), 36.5 (CH_2), 30.6 (CH_2), 29.7 (CH_2), 28.5 (CH_3), 21.6 (CH_3); IR: ν_{max} = 2970, 2928, 1760, 1421, 1366, 1351, 1265, 1229, 1217, 1161, 1093, 907, 732, 703 cm^{-1}; HRMS (ESI) calcd. for $C_{24}H_{28}N_2NaO_5S$ $[M+Na]^+$: 479.1617, found: 479.1618.



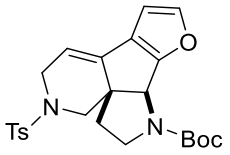
II.19. *tert*-Butyl4-(((*N*-(3-(5-(3-((tert-butyldiphenylsilyl)oxy)propyl)furan-3-yl)prop-2-yn-1-yl)-4-methylphenyl)sulfonamido)methyl)-2,3-dihydro-1*H*-pyrrole-1-carboxylate (4b) (46 mg, 62%). Light yellow foam; R_f0.44 (100% CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, *mixture of rotamers*) *δ* 7.75 (d, *J* = 8.2 Hz, 2H), 7.70-7.61 (m, 4H), 7.49-7.32 (m, 6H), 7.26 (d, *J* = 8.1 Hz, 2H), 7.17 (s, 1H), 6.61 (bs, 0.5H), 6.44 (bs, 0.5H), 5.70 (s, 1H), 4.22 (bs, 2H), 3.90 (s, 2H), 3.80-3.70 (m, 2H), 3.69 (t, *J* = 6.1 Hz, 2H), 2.71-2.55 (m, 4H), 2.37 (s, 3H), 1.85 (quint, *J* = 6.9 Hz, 2H), 1.47 (s, 9H), 1.06 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$, *mixture of rotamers*) *δ* 144.3 (CH), 143.5 (C), 136.3 (C), 135.7 (CH), 134.0 (C), 129.8 (CH), 129.6 (CH), 128.0 (CH), 127.8 (CH), 115.5 (C), 107.6 (CH), 62.9 (CH_2), 45.7 (CH_2), 44.9 (CH_2), 36.6 (CH_2), 30.8 (CH_2), 29.8 (CH_2), 28.5 (CH_3), 27.0 (CH_3), 24.4 (CH_2), 21.6 (CH_3); IR: ν_{max} = 3053, 2931, 2860, 1698, 1427, 1394, 1368, 1264, 1163, 1091, 896, 817, 735, 703 cm^{-1}; HRMS (ESI) calcd. for $C_{43}H_{52}N_2NaO_6SSi$ $[M+Na]^+$: 775.3213, found: 775.3210.



7. General Procedure III for asymmetric synthesis of compounds **5a-b**.

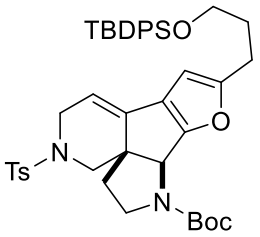
In a Schlenk tube, chiral gold catalyst DTBM-SEGPHOS$(AuCl)_2$ (**II**) (5 mol%), $AgNTf_2$ (5 mol%) and distilled dichloromethane (0.125 M) were stirred 15 minutes at 20 °C. After filtration, this mixture was added in a Schlenk tube containing substrates **4a-b** (0.05 mmol, 1.0 equiv). Then, the reaction mixture was stirred 18-40 h at -20 °C. The crude reaction mixture was concentrated and purified by automatic flash chromatography using 4g silica gel pre-packed column and EtOAc/*n*-heptane as eluent (10-35 % EtOAc/*n*-heptane). Alternatively, preparative TLC (10-35 % EtOAc/*n*-heptane or 100% CH_2Cl_2) can be used for purification.

II.20. *tert*-Butyl 5-tosyl-2,3,4,5,6,10b-hexahydro-1*H*-furo[3',2':3,4]pyrrolo[3',2':1,5]cyclopenta[1,2-*c*]pyridine-1-carboxylate (5a) (*General Procedure III*: 14.5 mg, 63% yield, 49% ee).



^{1}H NMR (300 MHz, $CDCl_3$, *mixture of rotamers*) δ 7.74-7.65 (m, 2H), 7.40-7.35 (m, 1H), 7.33 (d, *J* = 8.1 Hz, 2H), 6.28 (bs, 1H), 5.42 (bs, 1H), 4.82 (bs, 0.5H), 4.68 (bs, 0.5H), 4.27 (dd, *J* = 17.1, 3.3 Hz, 1H), 3.94 (d, *J* = 10.8 Hz, 1H), 3.64-3.50 (m, 2H), 3.40-3.30 (m, 1H), 2.69-2.59 (m, 1H), 2.43 (s, 3H), 2.52-3.35 (m, 1H), 2.05-1.95 (m, 1H), 1.52 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$, *mixture of rotamers*) *δ* 161.9 (C), 161.8 (C), 155.1 (C), 154.3 (C), 148.7 (CH), 148.4 (CH), 143.93 (C), 143.88 (C), 134.8 (C), 134.7 (C), 133.8 (C), 133.5 (C), 129.9 (CH), 127.6 (CH), 126.1 (C), 109.5 (CH), 105.1 (CH), 105.0 (CH), 80.3 (C), 61.4 (CH), 61.3 (CH), 60.0 (C), 58.8 (C), 48.62 (CH_2), 48.56 (CH_2), 46.3 (CH_2), 45.7 (CH_2), 44.7 (CH_2), 44.6 (CH_2), 34.5 (CH_2), 33.7 (CH_2), 28.5 (CH_3), 21.7 (CH_3); HRMS (ESI) calcd. for $C_{24}H_{29}N_2O_5S$ $[M+H]^+$: 457.1792, found: 457.1770; SFC Analysis: 49% e.e. [CHIRALPAK® IA, 30 °C, 15% MeOH, 4.0 mL/min, 100 bar, retention times: 3.8 min (major) and 5.0 min (minor)].

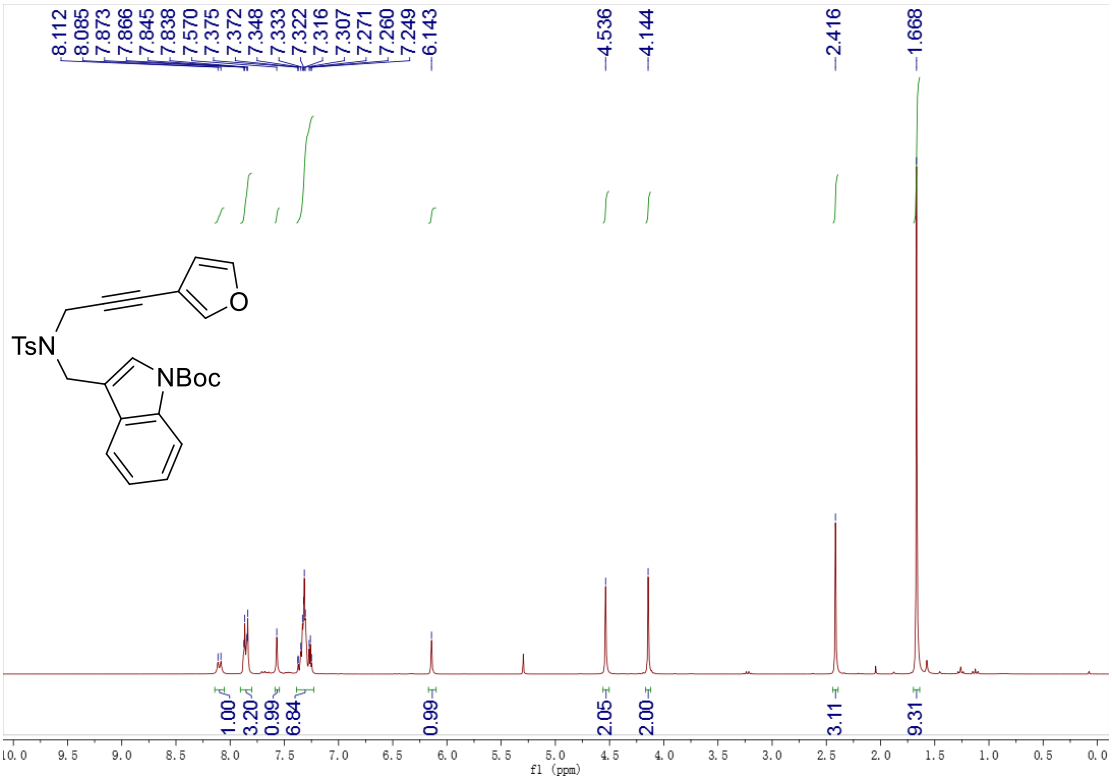
II.21. *tert*-Butyl(3*α*S,10*β*S)-9-(3-((tert-butyldiphenylsilyl)oxy)propyl)-5-tosyl-2,3,4,5,6,10b-hexahydro-1H-furo[3',2':3,4]pyrrolo[3',2':1,5]cyclopenta[1,2-c]pyridine-1-carboxylate (5b) (*General Procedure III*: 28.1 mg, 75% yield, 41% ee). Colorless oil; R_f 0.29 (100% CH_2Cl_2); ^{1}H NMR (300 MHz, $CDCl_3$, *mixture of rotamers*) *δ* 7.72-7.59 (m, 6H), 7.44-7.28 (m, 8H), 5.85 (bs, 1H), 5.33 (bs, 1H), 4.82 (bs, 0.4H), 4.63 (bs, 0.6H), 4.26 (dd, *J* = 16.7, 3.0 Hz, 1H), 3.93 (d, *J* = 10.7 Hz, 1H), 3.68 (t, *J* = 5.7 Hz, 2H), 3.62-3.48 (m, 2H), 3.37-3.25 (m, 1H), 2.72 (t, *J* = 7.3 Hz, 2H), 2.62 (d, *J* = 10.8 Hz, 1H), 2.43 (s, 3H), 2.40-2.30 (m, 1H), 2.05-1.95 (m, 1H), 1.87 (quint, *J* = 7.2 Hz, 2H), 1.52 (s, 9H), 1.04 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$, *mixture of rotamers*) *δ* 162.4 (C), 159.9 (C), 154.2 (C), 143.7 (C), 135.5 (CH), 133.8 (C), 129.7 (CH), 129.6 (CH), 127.6 (CH), 127.5 (CH), 108.6 (CH), 100.3 (CH), 80.0 (C), 62.8 (CH_2), 61.5 (CH), 59.4 (C), 48.5 (CH_2), 45.5 (CH_2), 44.5 (CH_2), 33.5 (CH_2), 30.8 (CH_2), 28.4 (CH_3), 26.8 (CH_3), 25.3 (CH_2), 21.5 (CH_3), 19.2 (C); IR: ν_{max} = 2931, 2859, 1694, 1457, 1428, 1392, 1365, 1265, 1165, 1104, 1020, 977, 920, 816, 734, 701, 660 cm^{-1}; HRMS (ESI) calcd. for $C_{43}H_{52}N_2NaO_6SSi$ $[M+Na]^+$: 775.3213, found: 775.3221; SFC Analysis: 41% *e.e.* [CHIRALPAK® IA, 30 °C, 30% MeOH, 4.0 mL/min, 100 bar, retention times: 3.5 min (major) and 5.1 min (minor)].



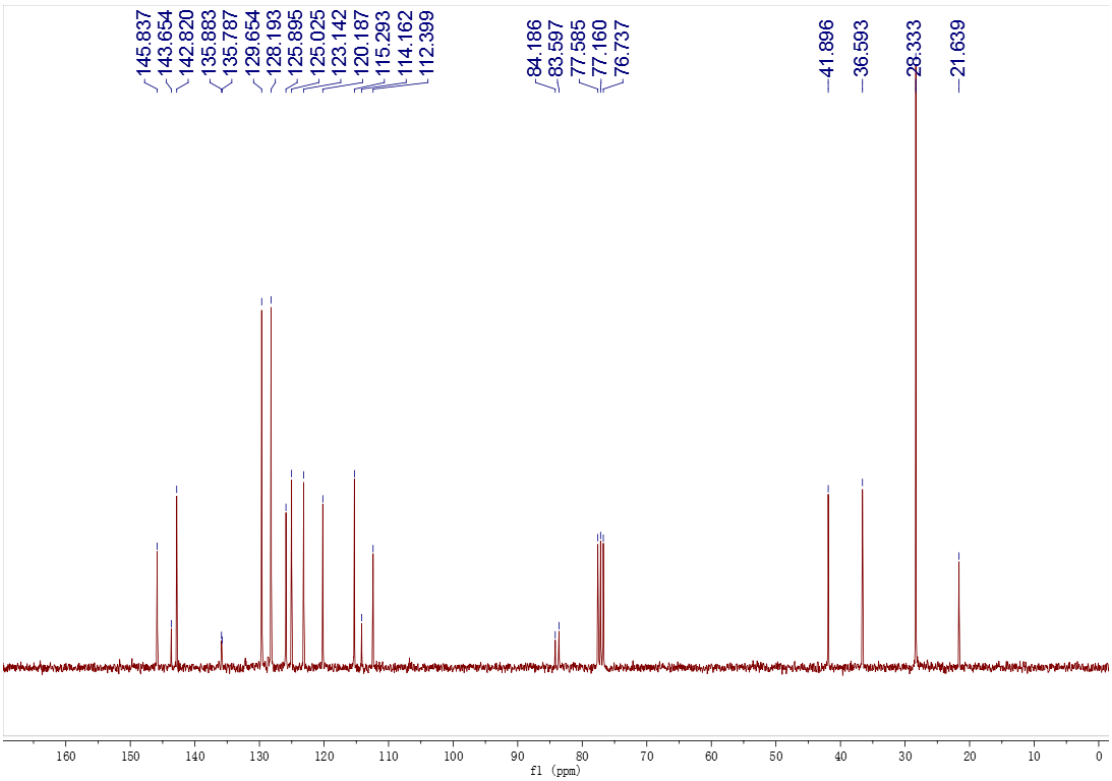
III. NMR Spectra (^{1}H and ^{13}C NMR)

III.1. Compound 1a.

^{1}H NMR ($CDCl_3$, 300 MHz)

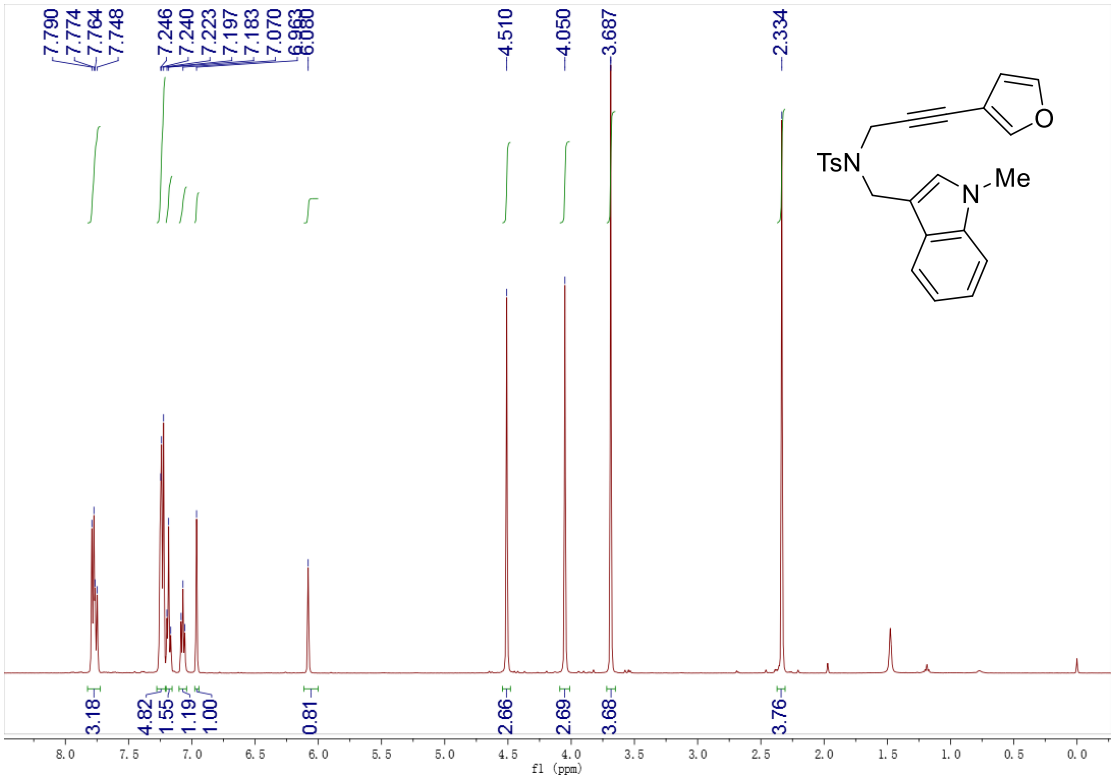


^{13}C NMR ($CDCl_3$, 75 MHz)

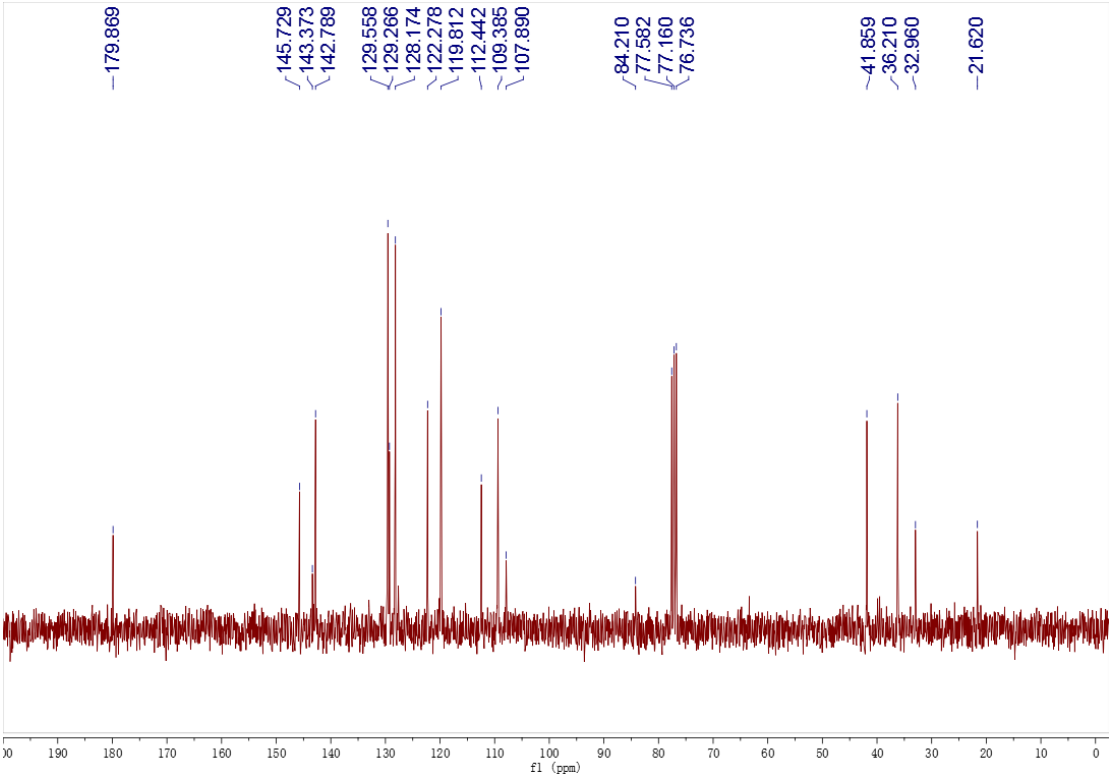


III.2. Compound 1b.

^{1}H NMR ($CDCl_3$, 500 MHz)

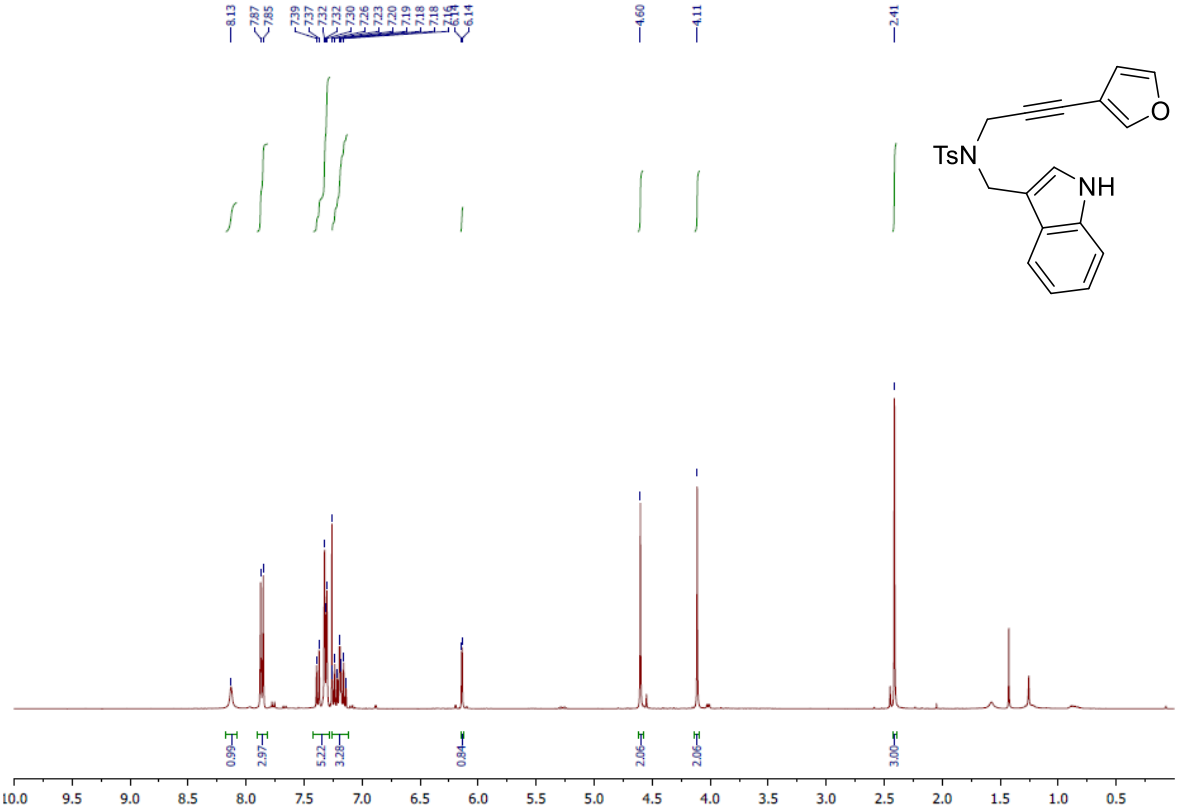


^{13}C NMR ($CDCl_3$, 75 MHz)

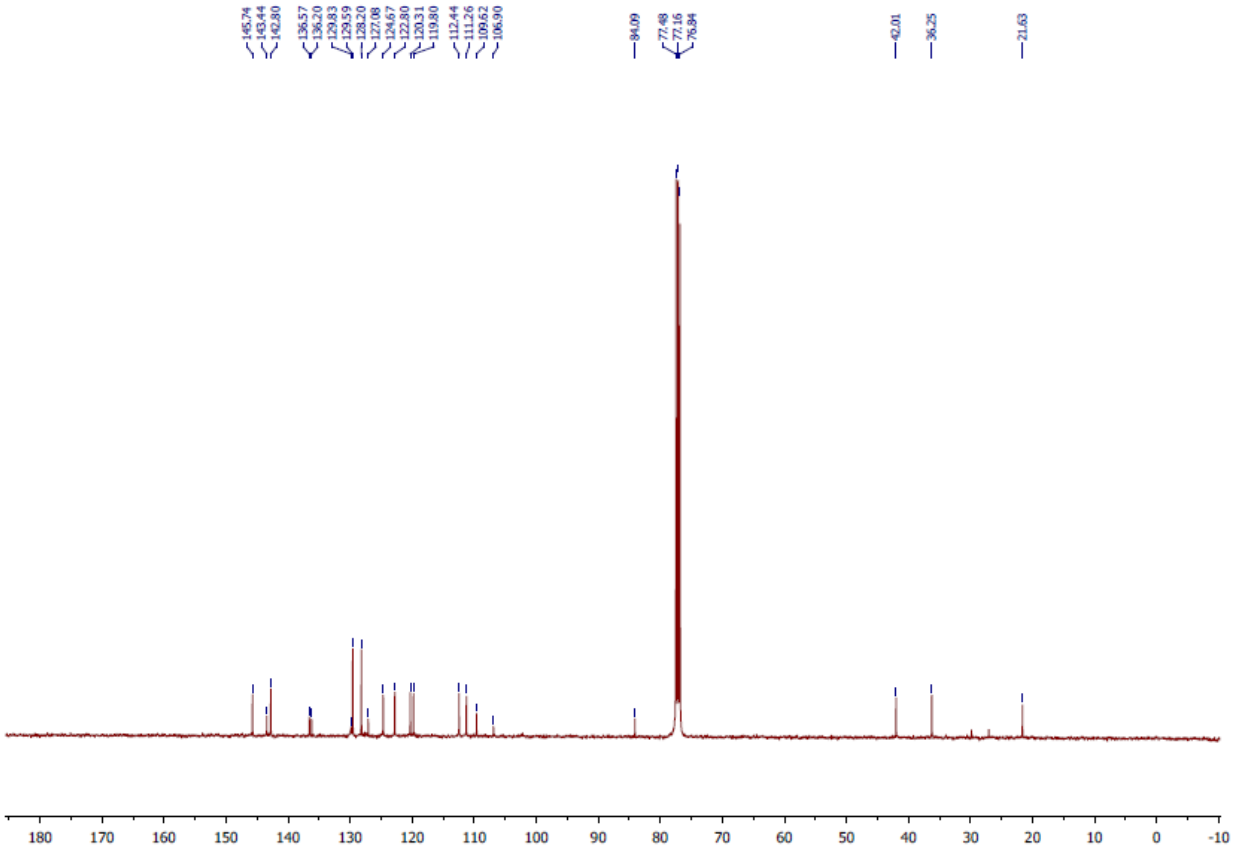


III.3. Compound 1c.

^{1}H NMR ($CDCl_3$, 300 MHz)

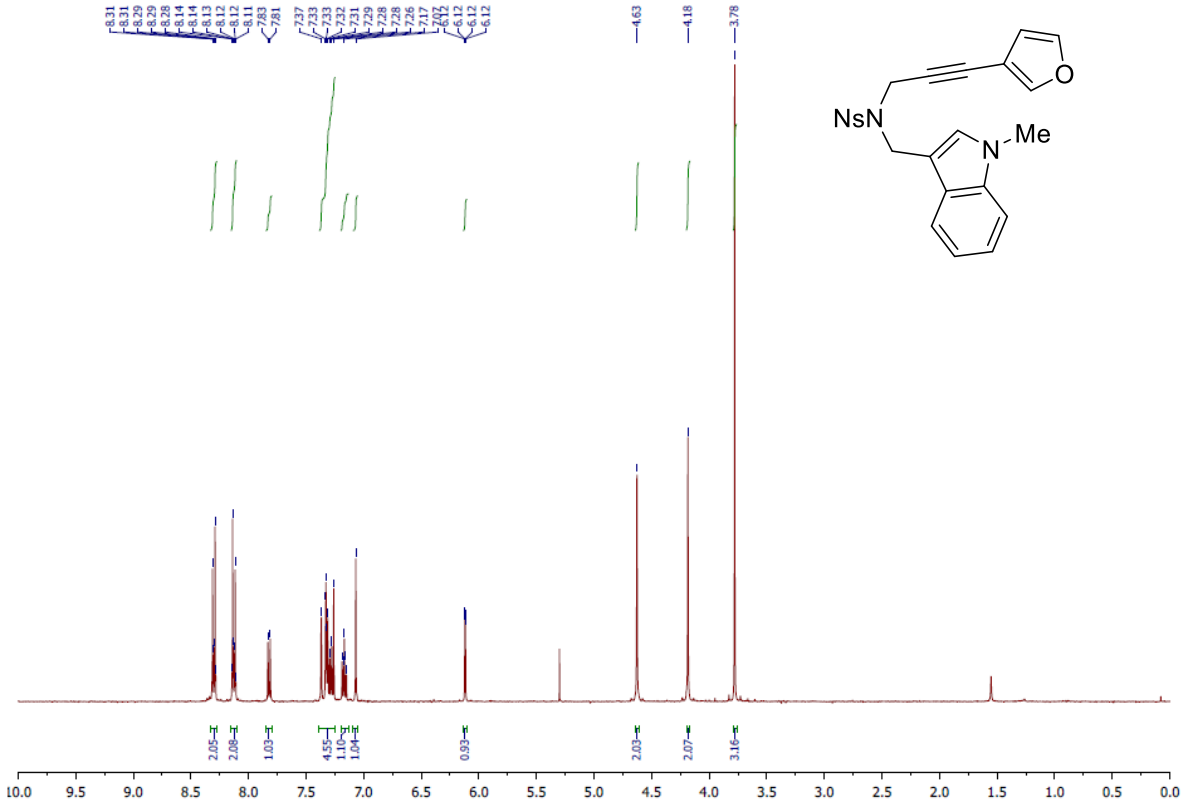


^{13}C NMR ($CDCl_3$, 75 MHz)

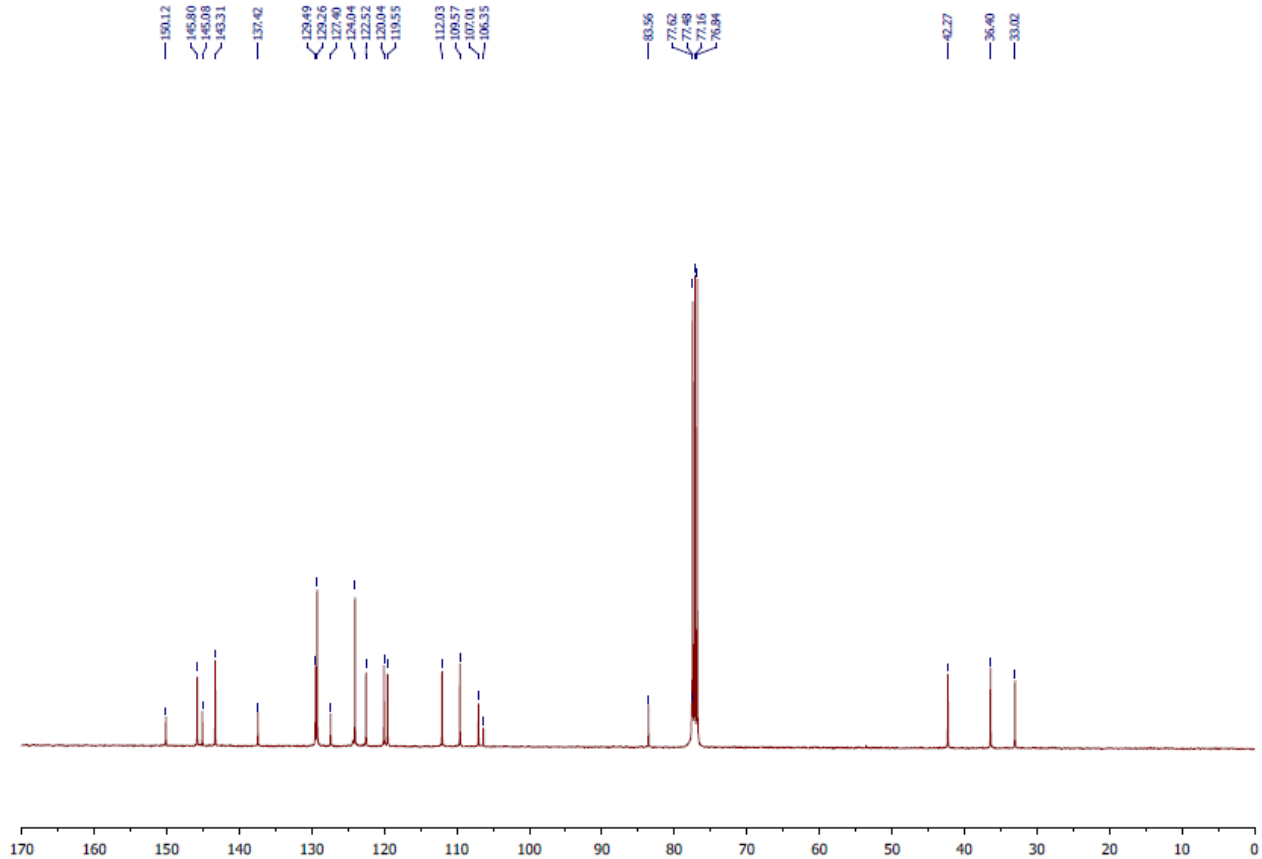


III.4. Compound 1d.

^{1}H NMR ($CDCl_3$, 300 MHz)

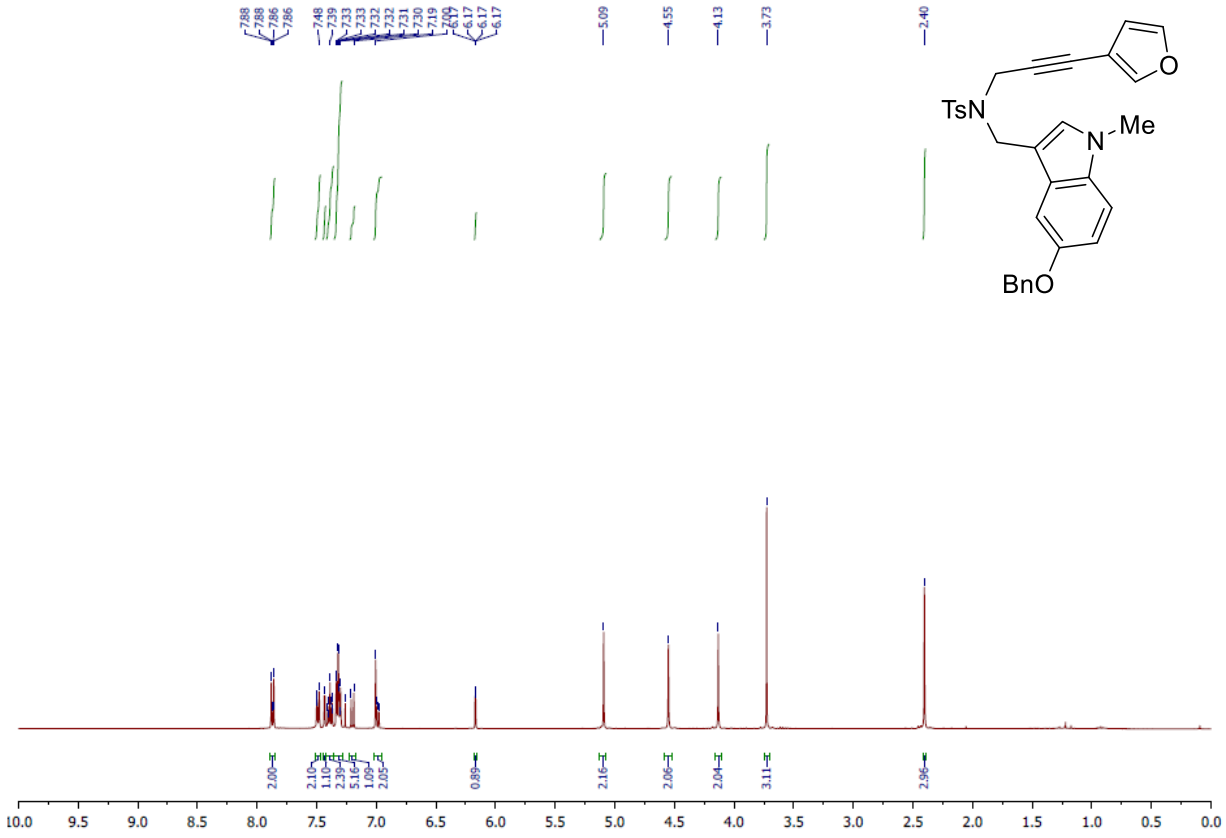


^{13}C NMR ($CDCl_3$, 75 MHz)

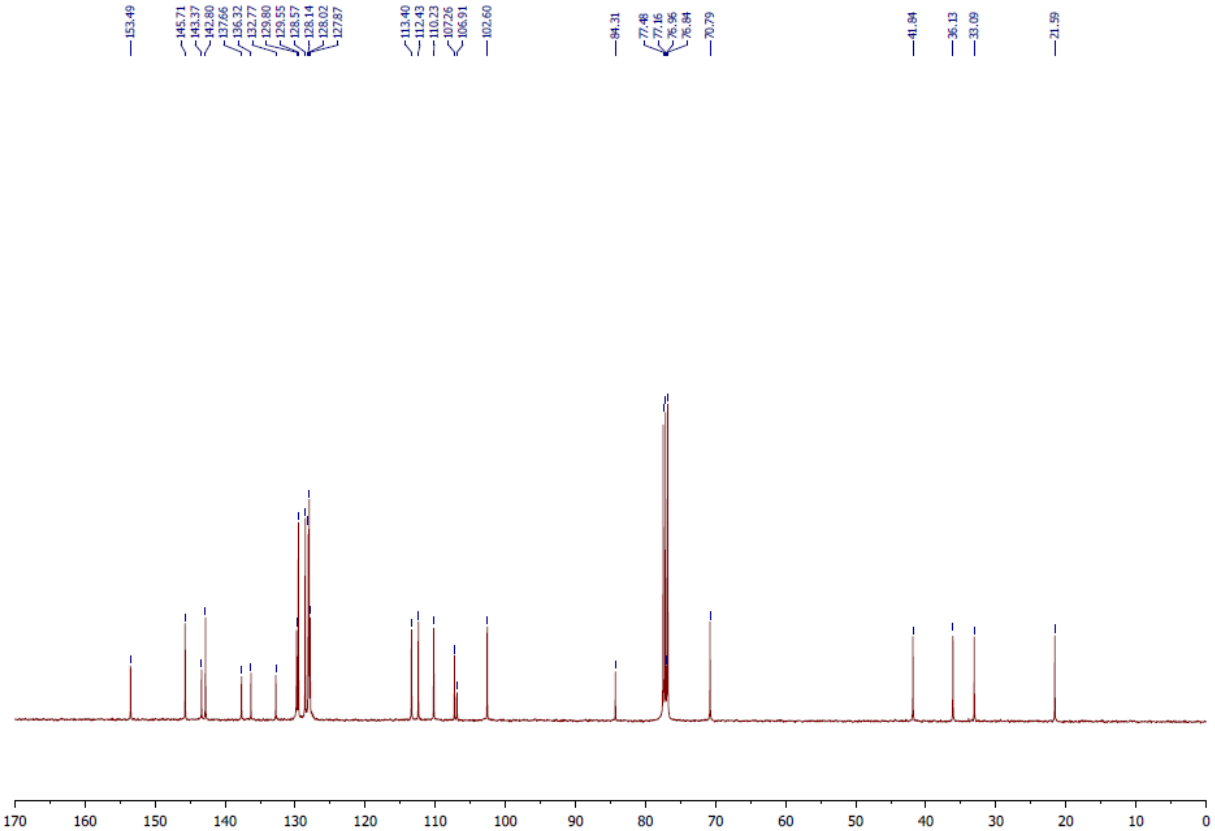


III.5. Compound 1e.

^{1}H NMR ($CDCl_3$, 500 MHz)

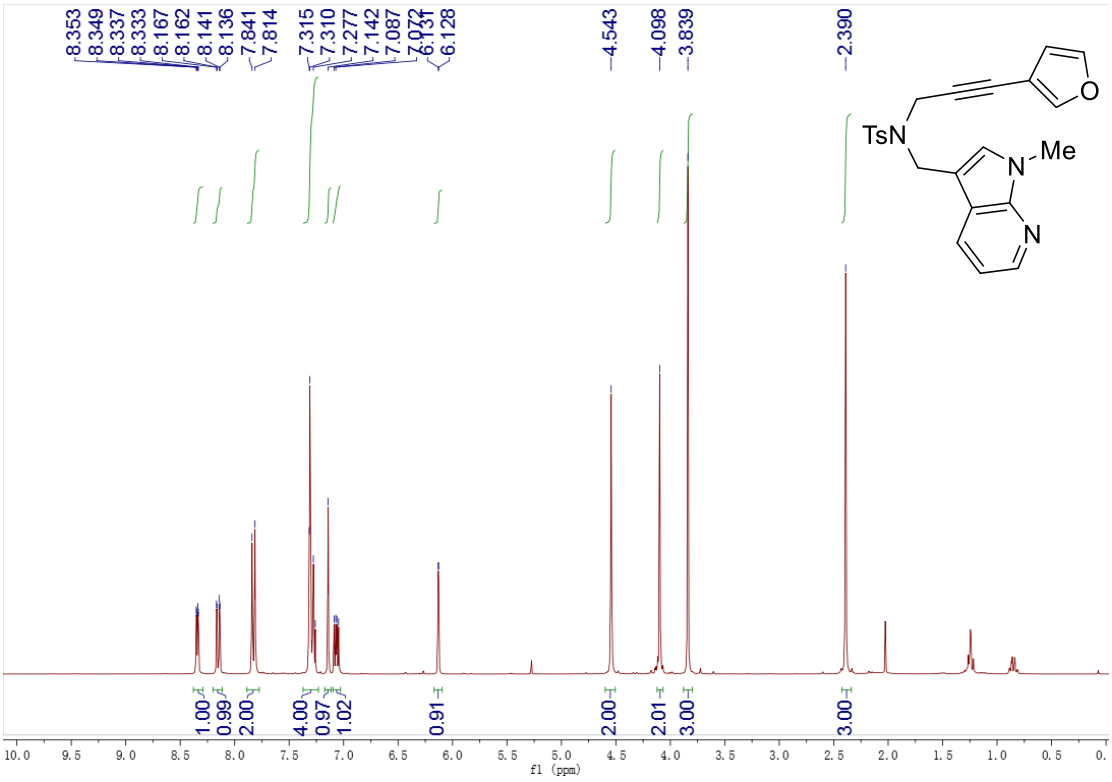


^{13}C NMR ($CDCl_3$, 75 MHz)

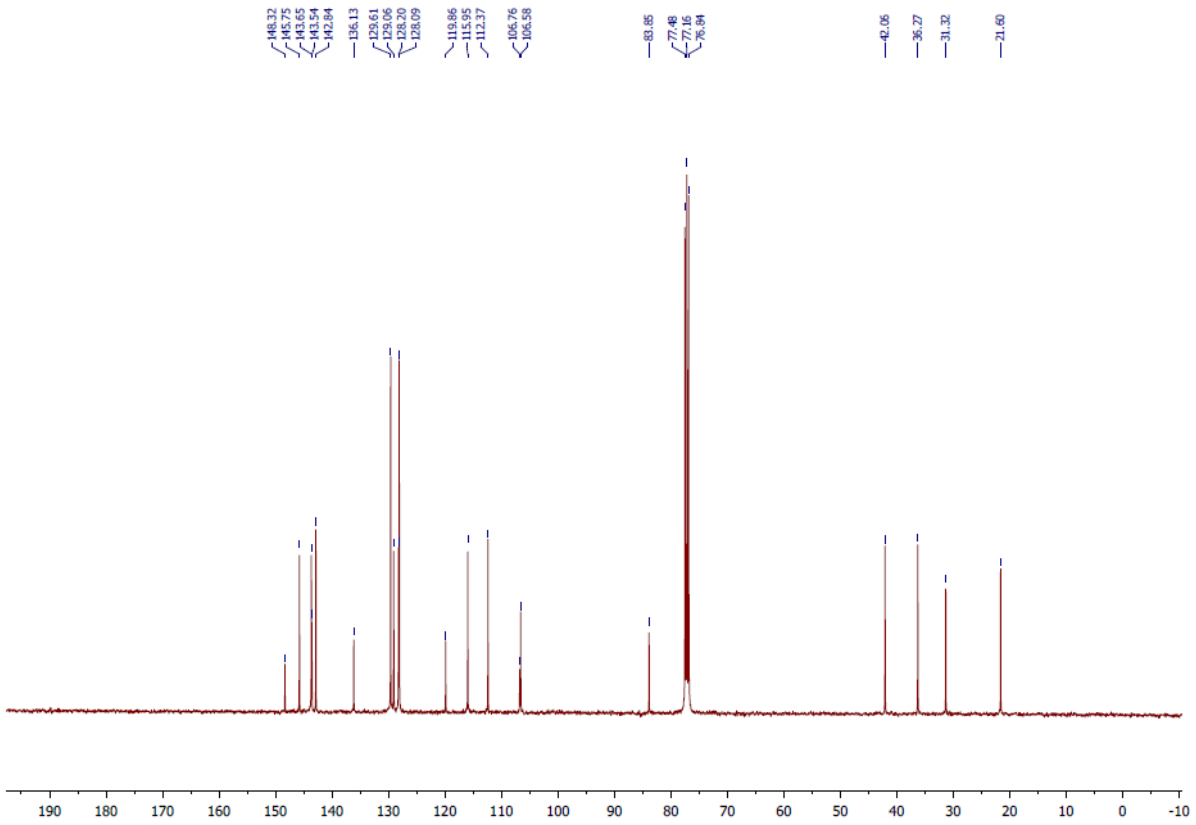


III.6. Compound 1f.

^{1}H NMR ($CDCl_3$, 300 MHz)

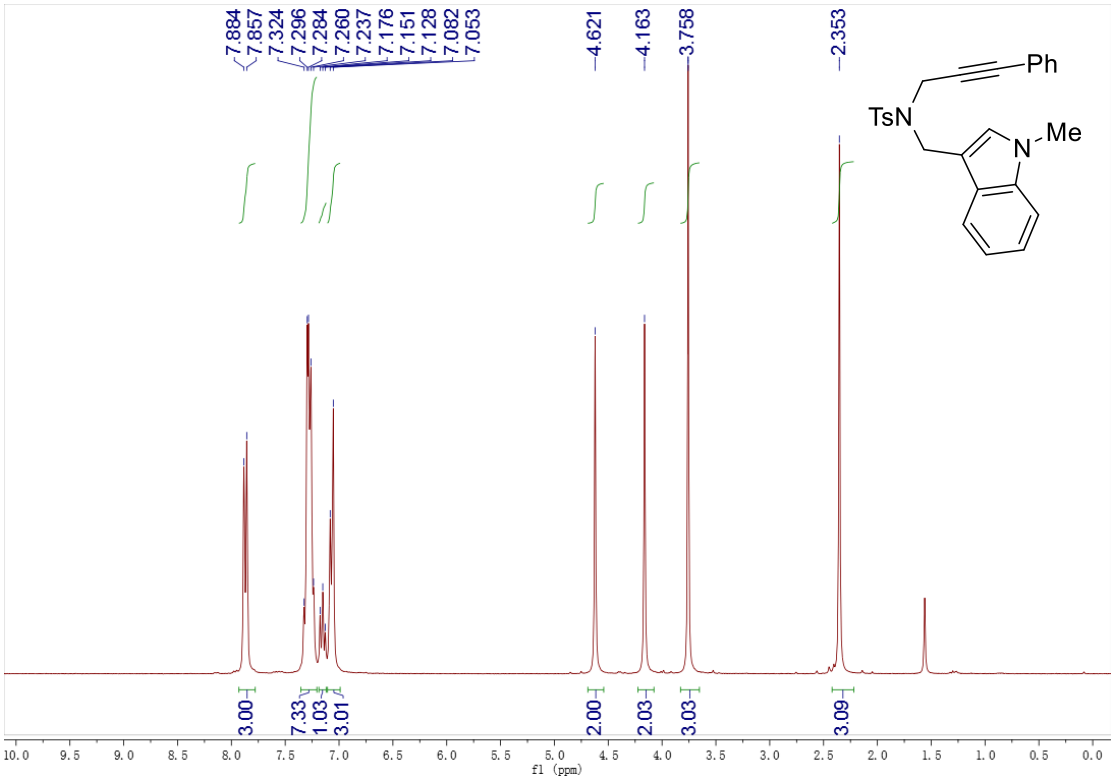


^{13}C NMR ($CDCl_3$, 75 MHz)

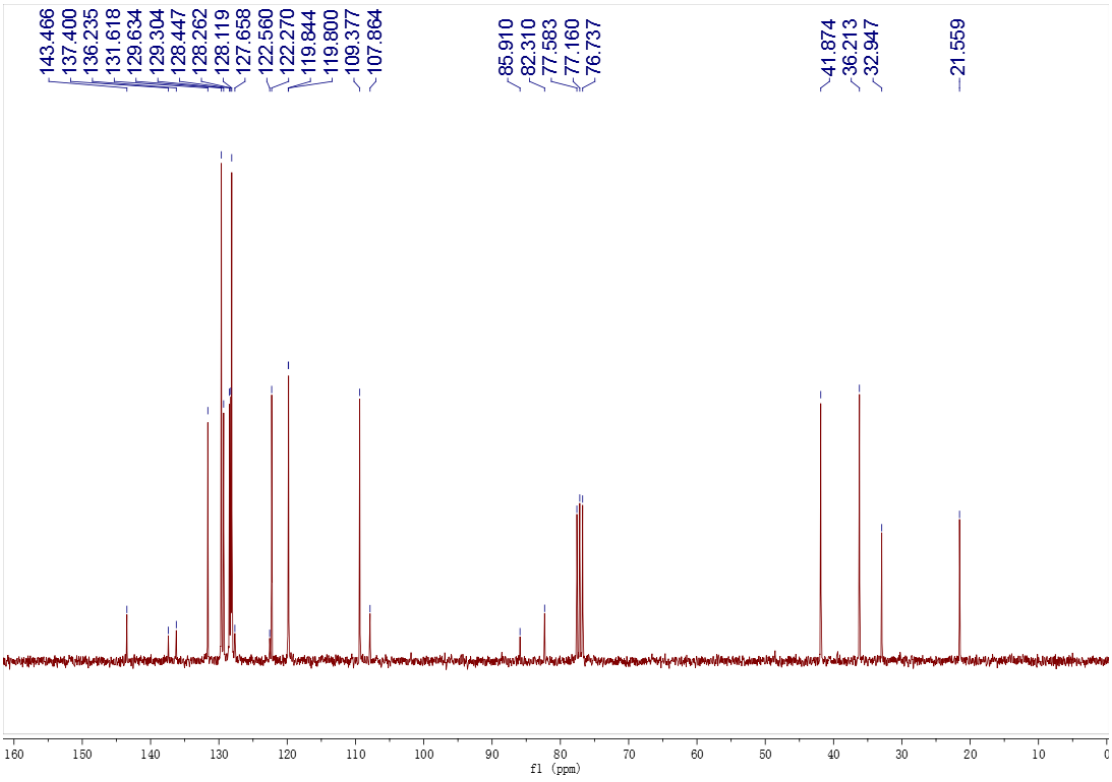


III.7. Compound S5.

^{1}H NMR ($CDCl_3$, 300 MHz)

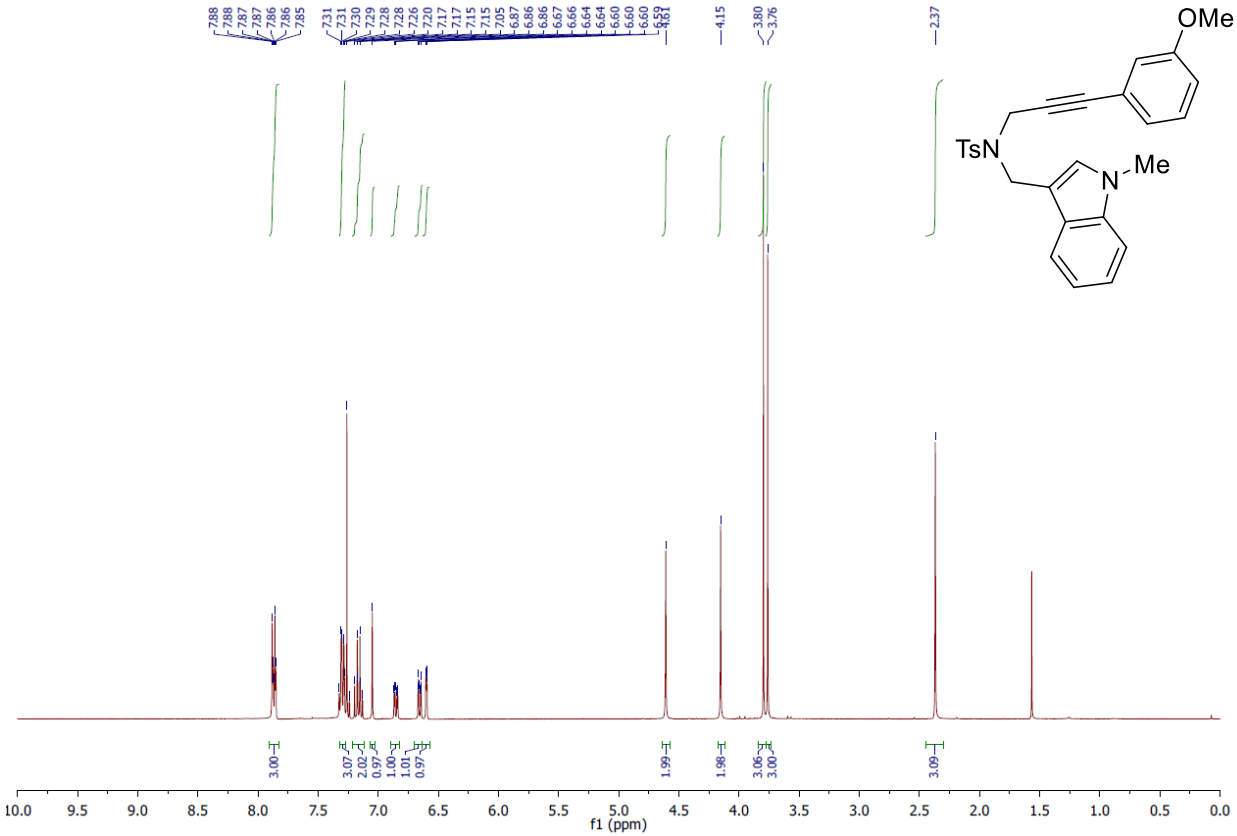


^{13}C NMR ($CDCl_3$, 75 MHz)

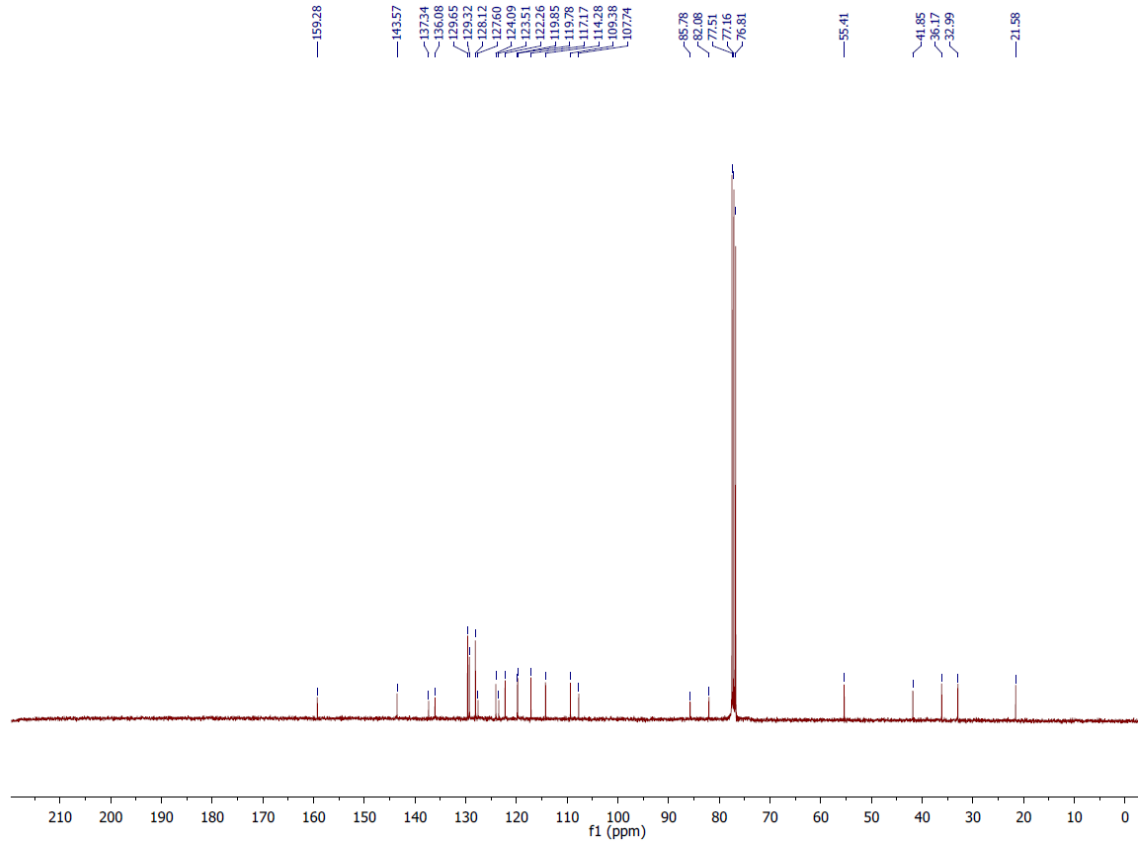


III.8. Compound (S6).

^{1}H NMR ($CDCl_3$, 500 MHz)

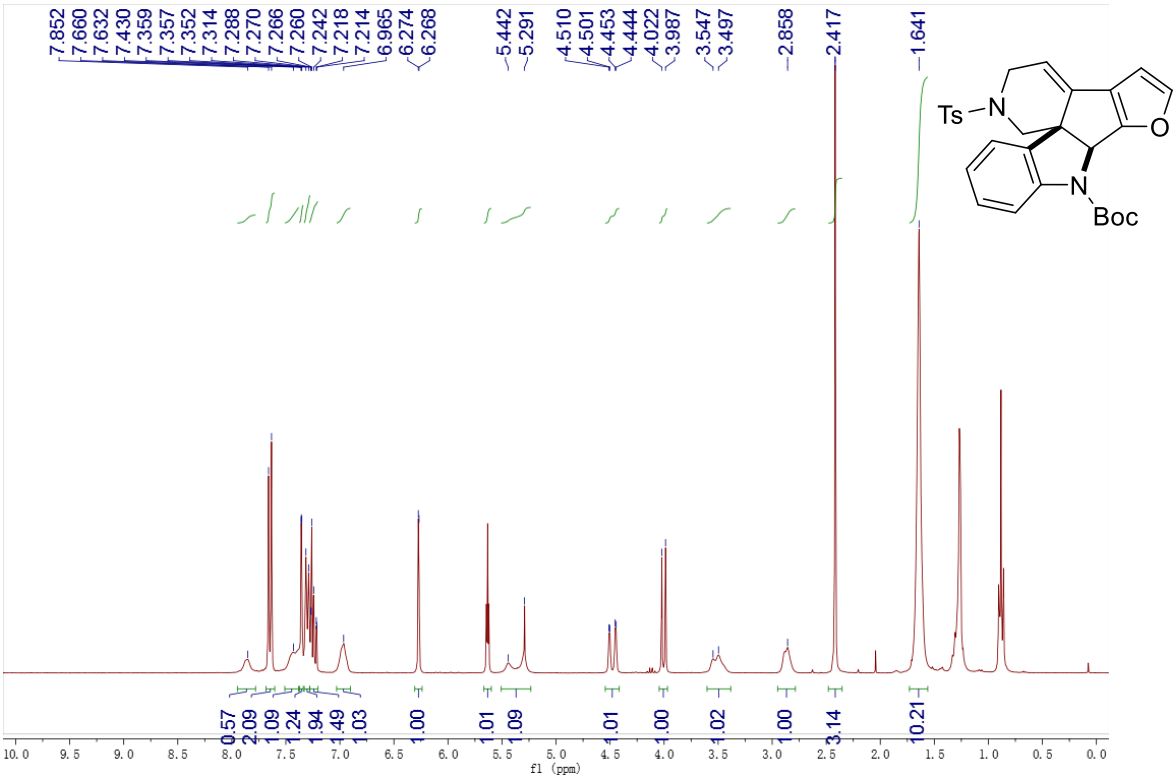


^{13}C NMR ($CDCl_3$, 75 MHz)

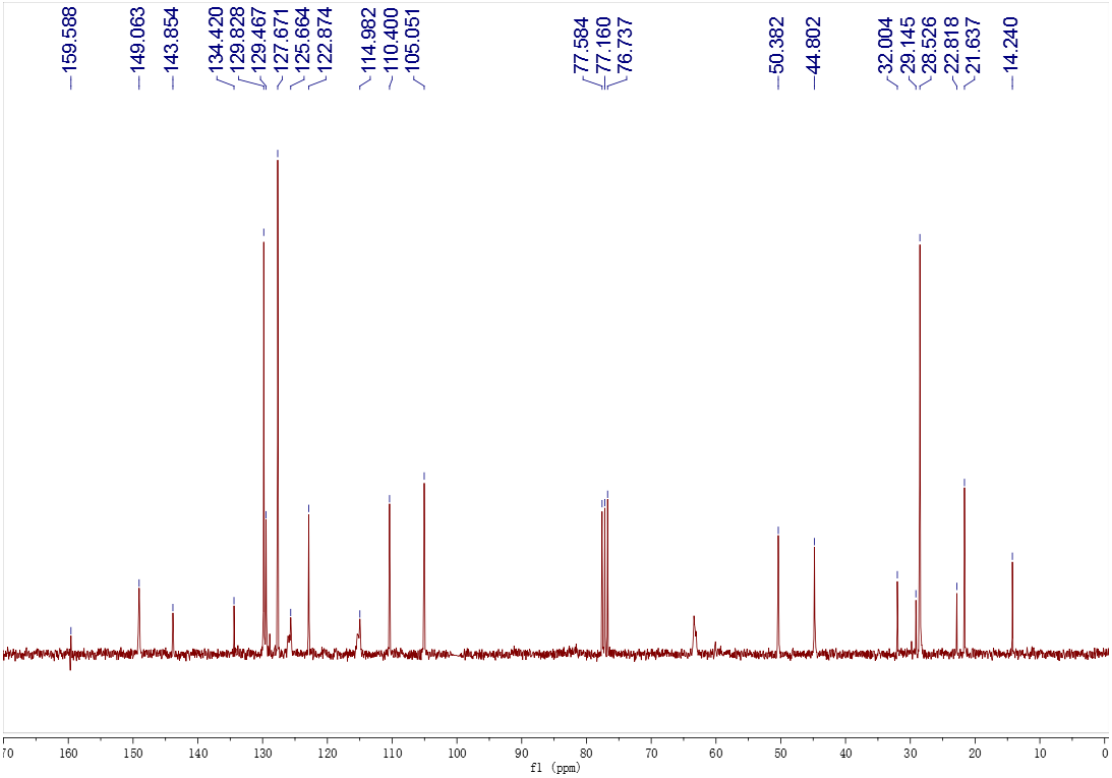


III.9. Compound 2a (*mixture of rotamers*).

^{1}H NMR ($CDCl_3$, 300 MHz)

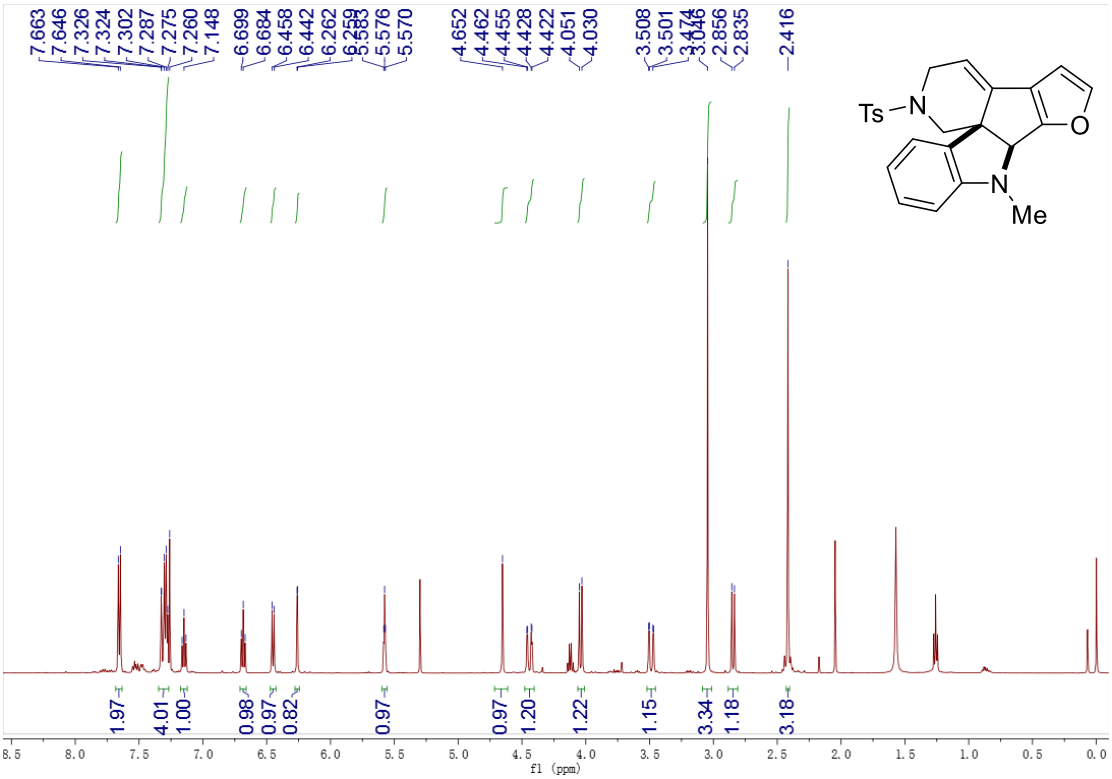


^{13}C NMR ($CDCl_3$, 75 MHz)

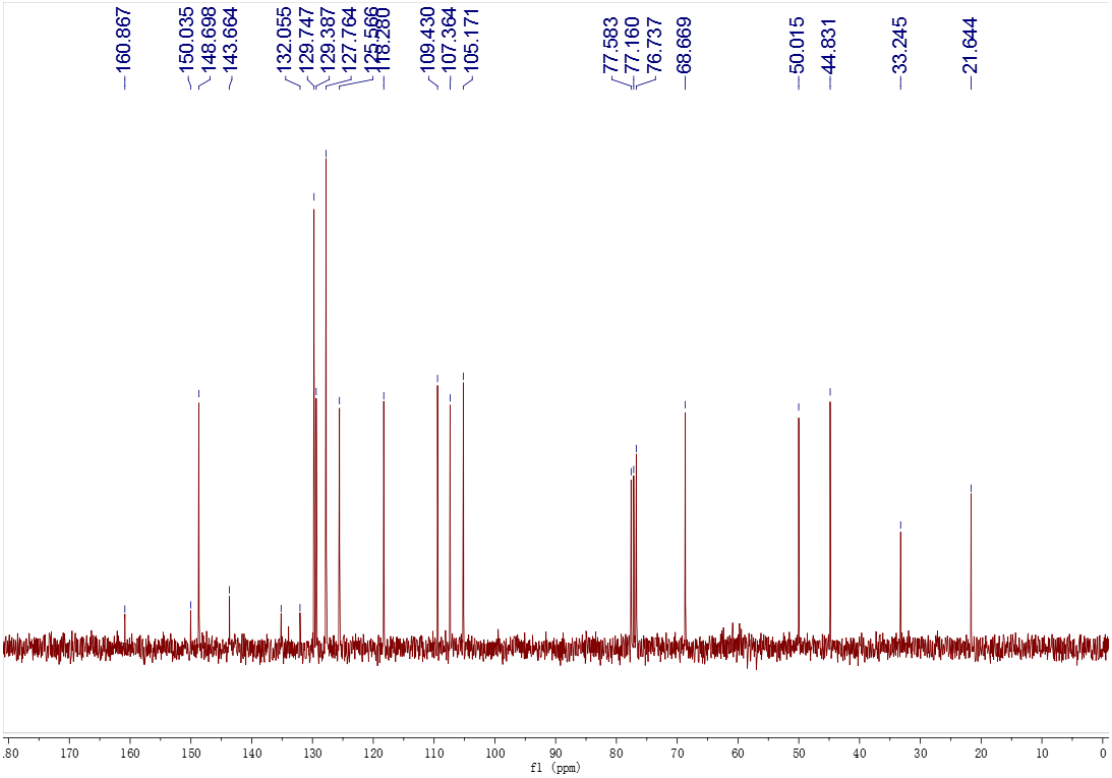


III.10. Compound 2b.

^{1}H NMR ($CDCl_3$, 500 MHz)

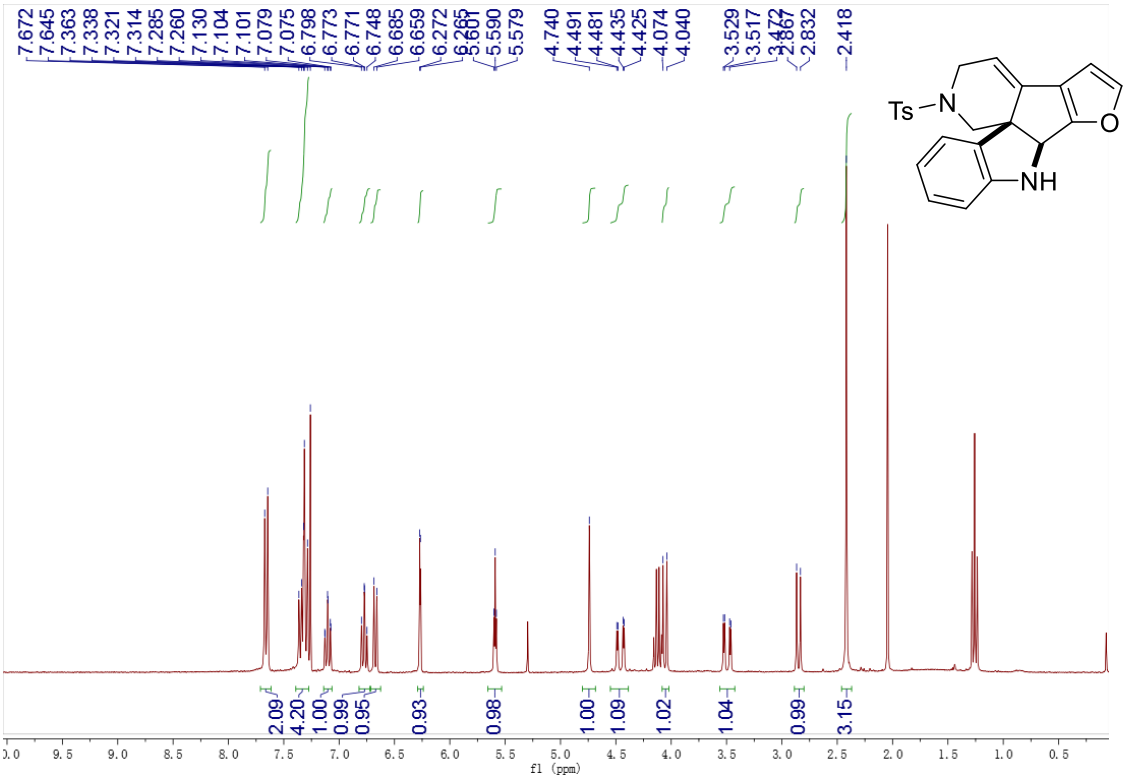


^{13}C NMR ($CDCl_3$, 75 MHz)

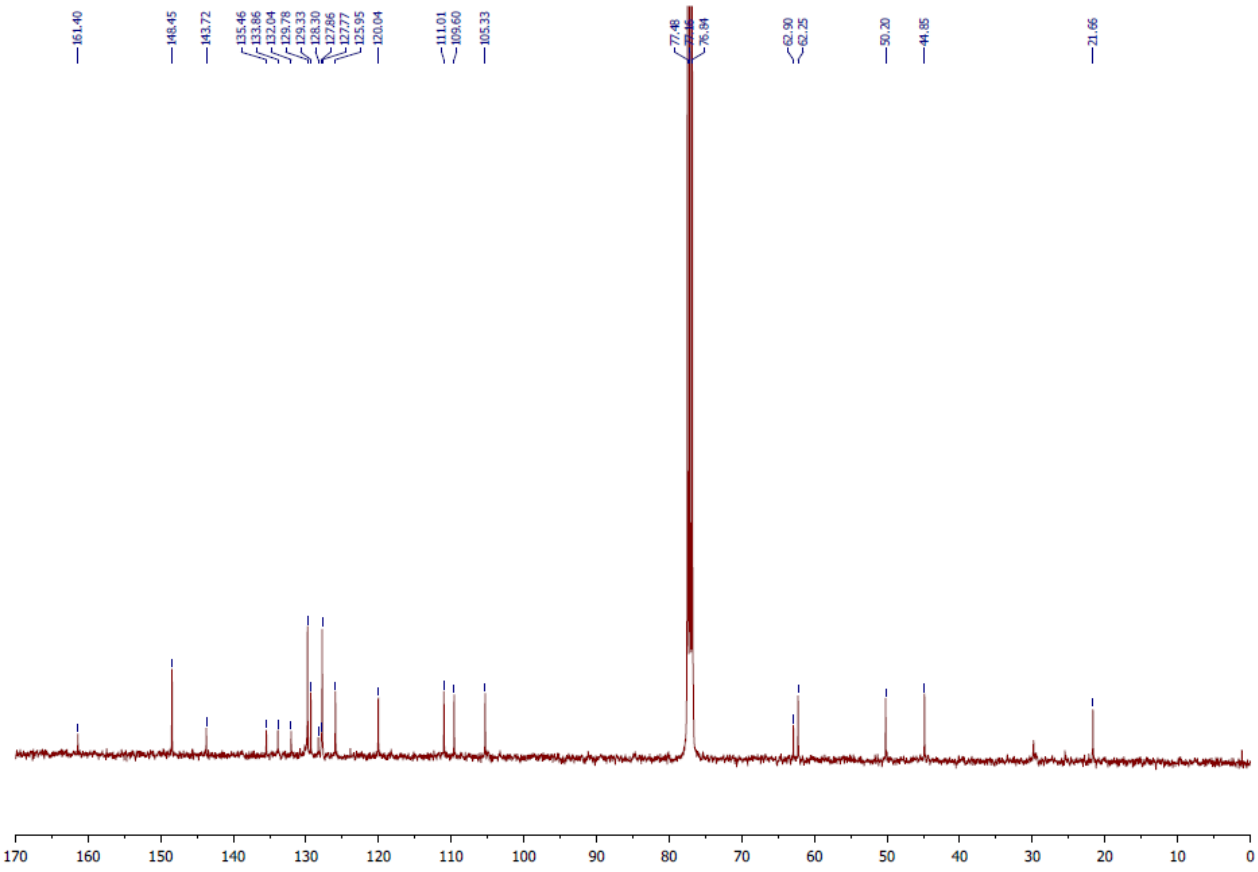


III.11. Compound 2c.

^{1}H NMR ($CDCl_3$, 300 MHz)

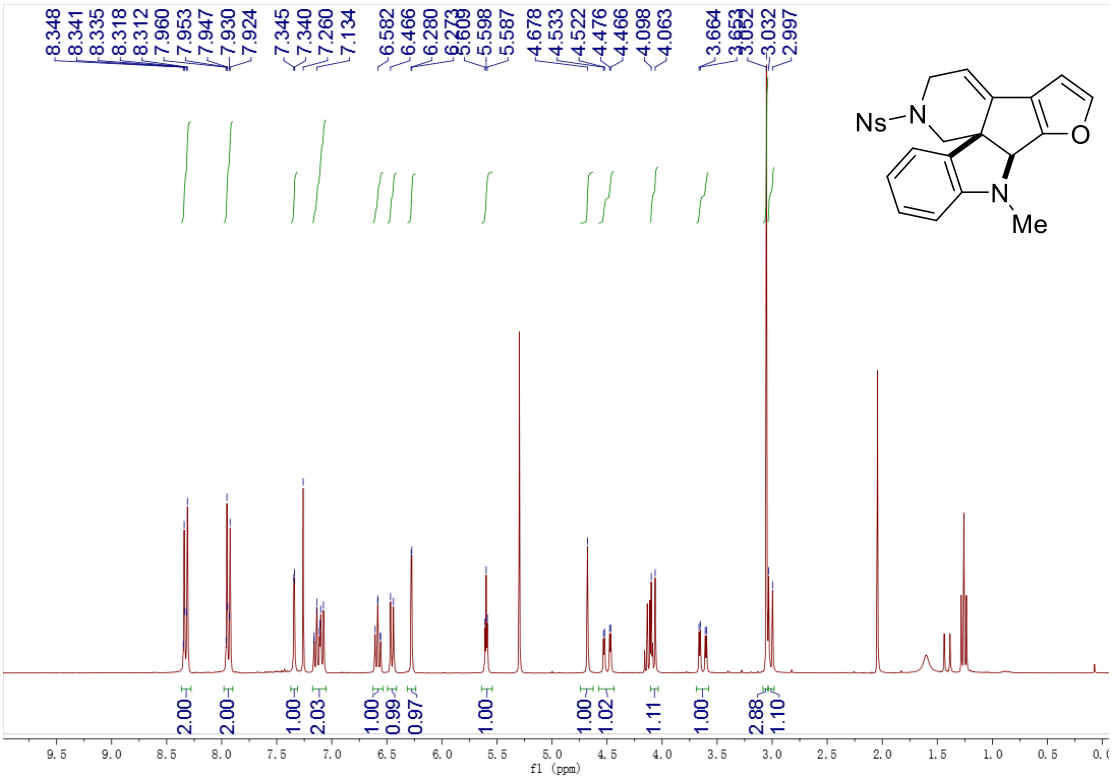


^{13}C NMR ($CDCl_3$, 75 MHz)

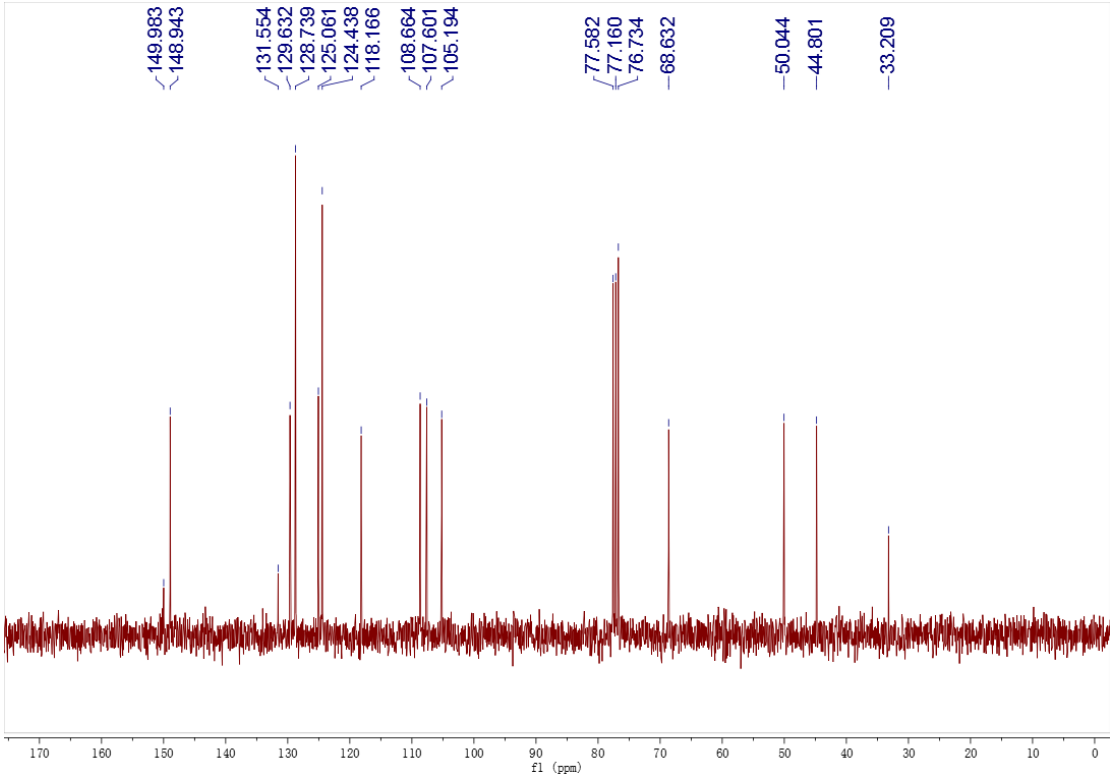


III.12. Compound 2d.

^{1}H NMR ($CDCl_3$, 300 MHz)

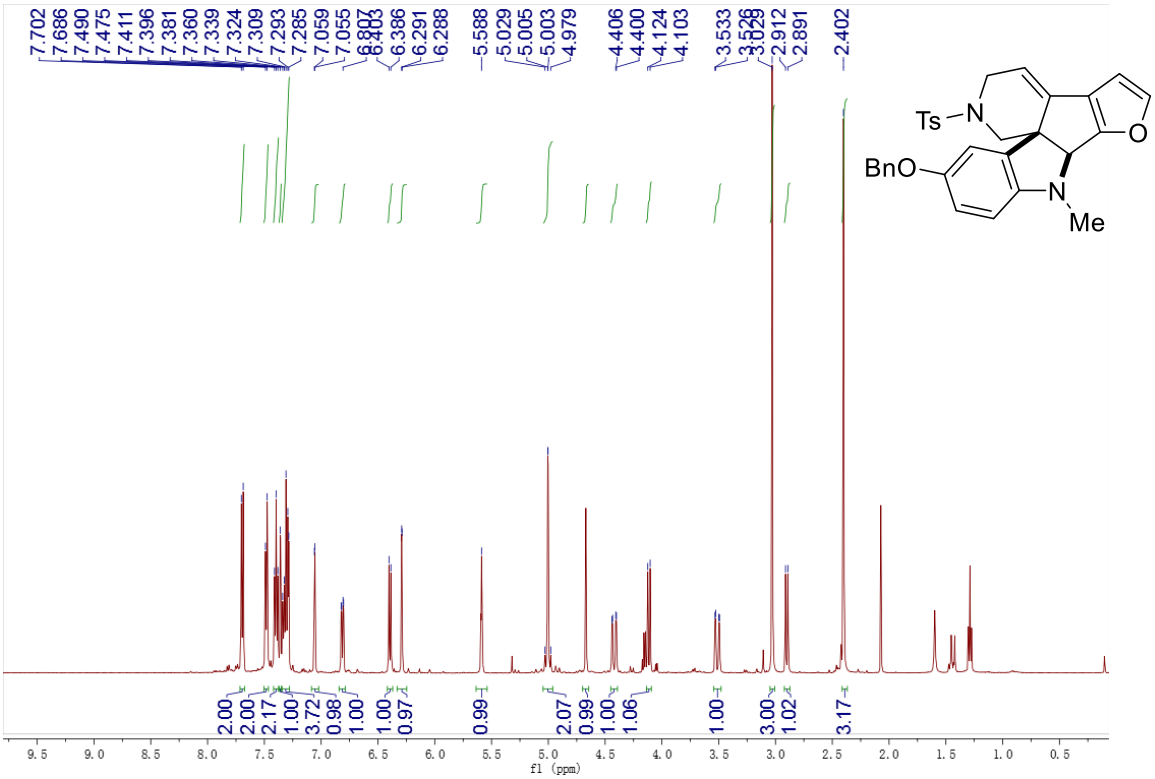


^{13}C NMR ($CDCl_3$, 75 MHz)

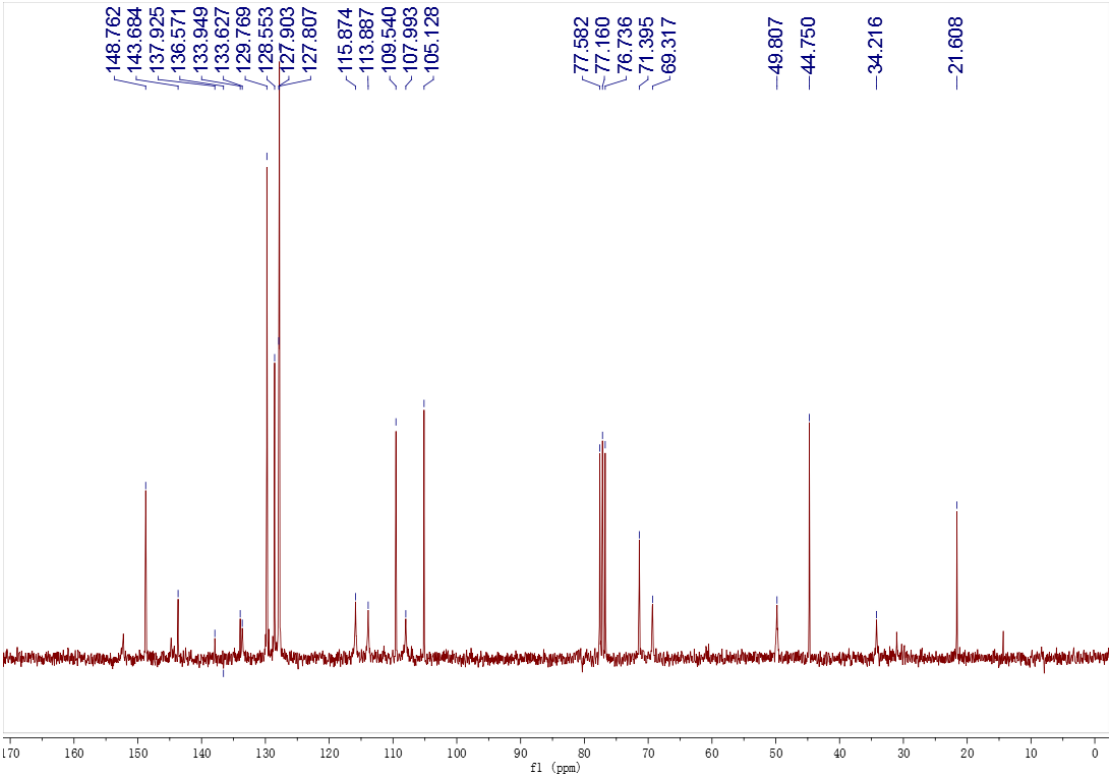


III.13. Compound 2e.

^{1}H NMR ($CDCl_3$, 500 MHz)

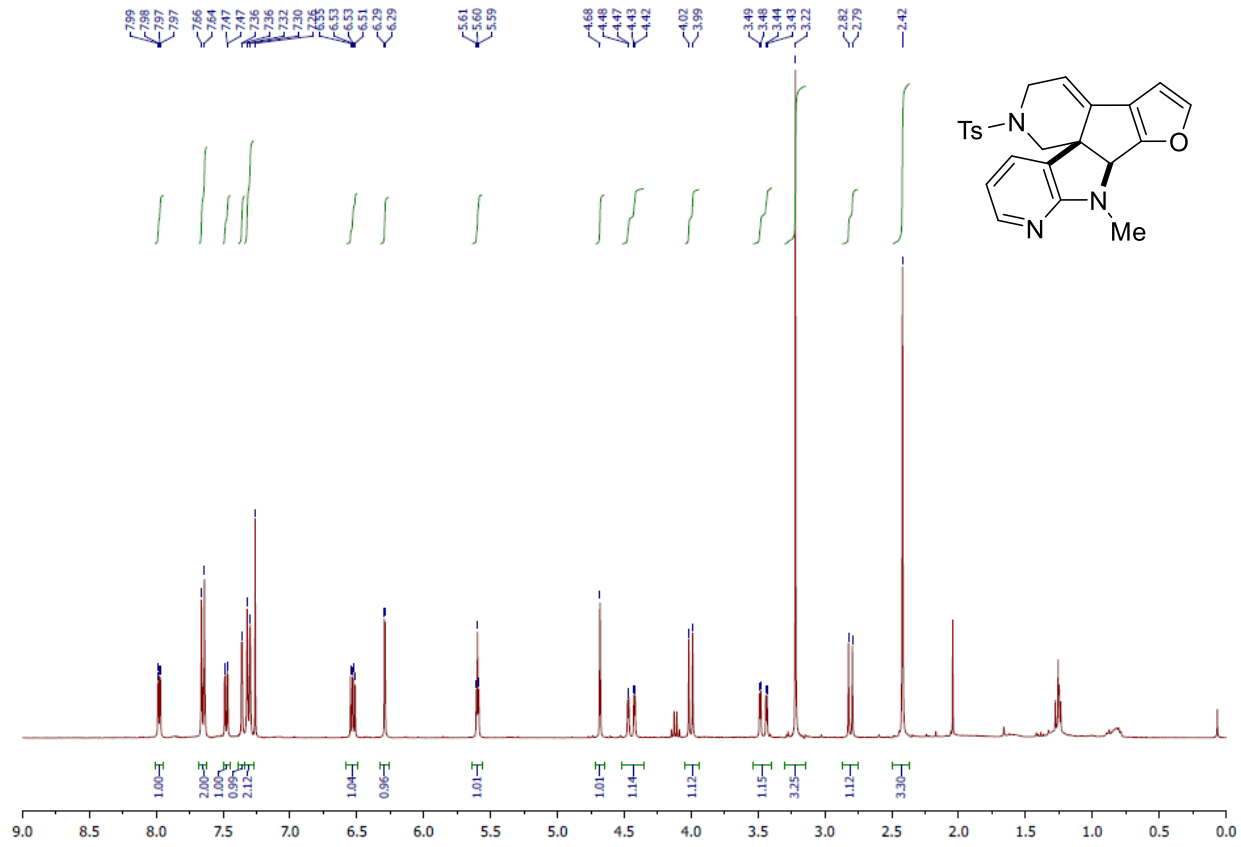


^{13}C NMR ($CDCl_3$, 75 MHz)

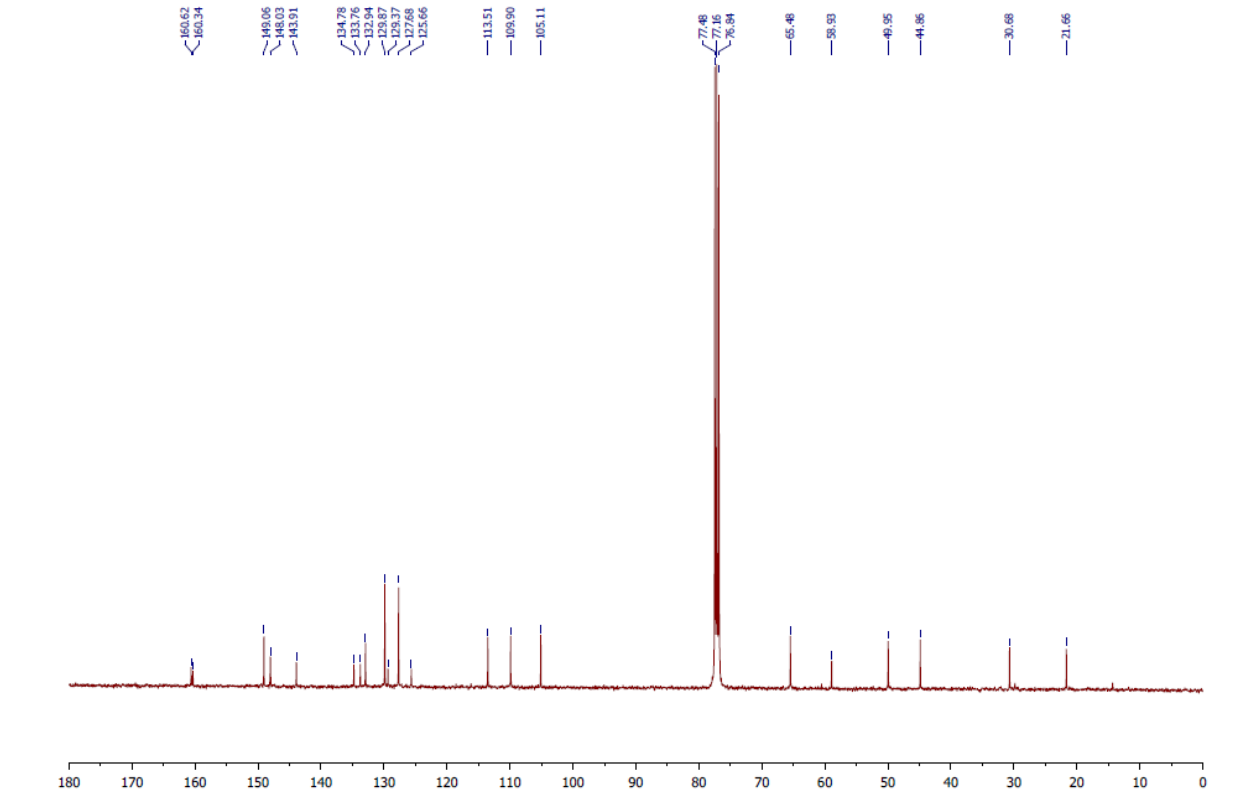


III.14. Compound 2f.

^{1}H NMR ($CDCl_3$, 300 MHz)

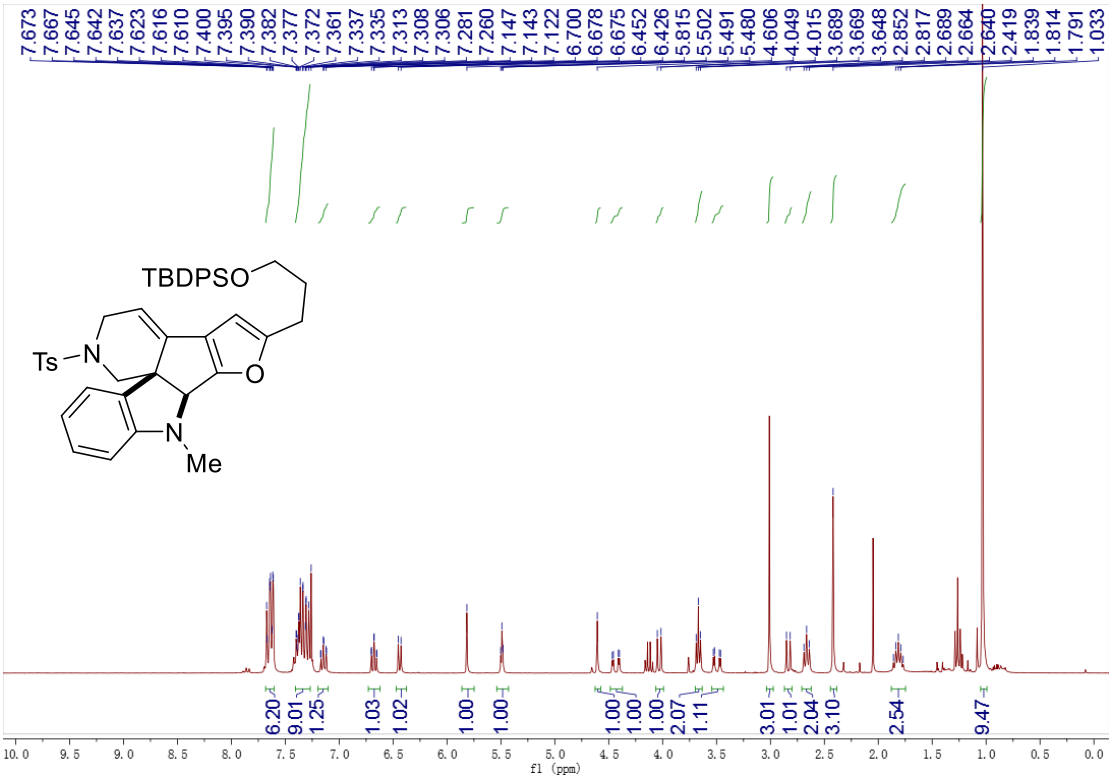


^{13}C NMR ($CDCl_3$, 75 MHz)

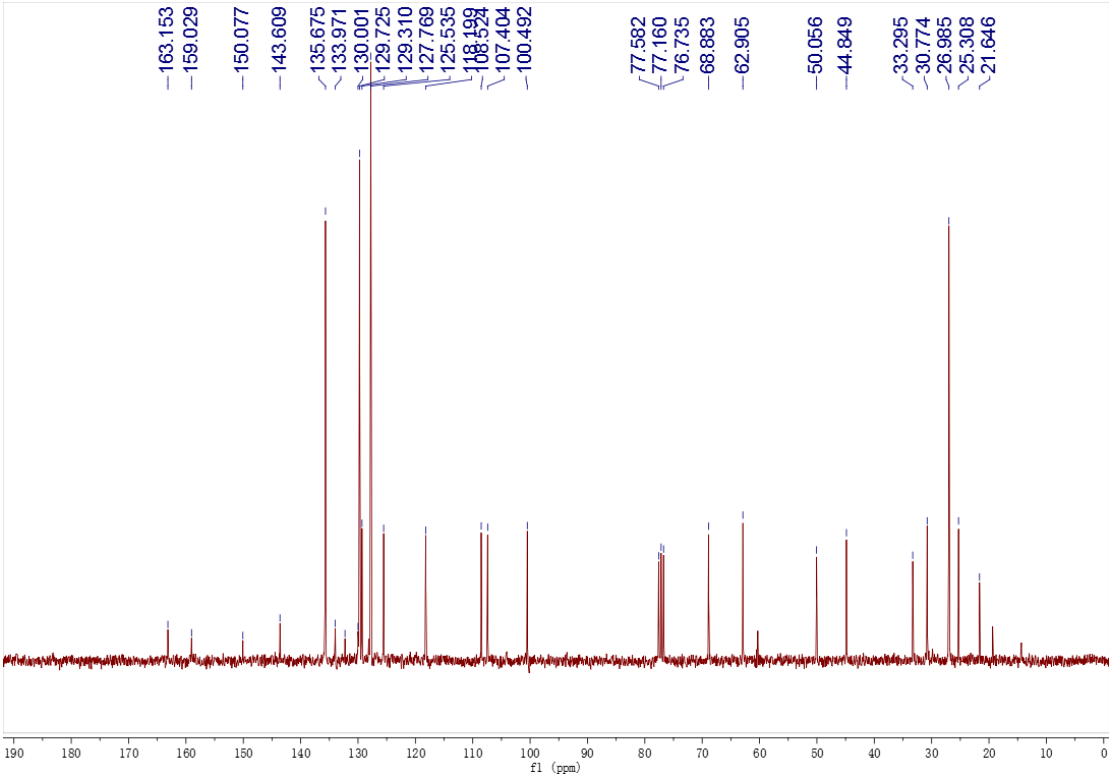


III.14. Compound 2g.

^{1}H NMR ($CDCl_3$, 300 MHz)

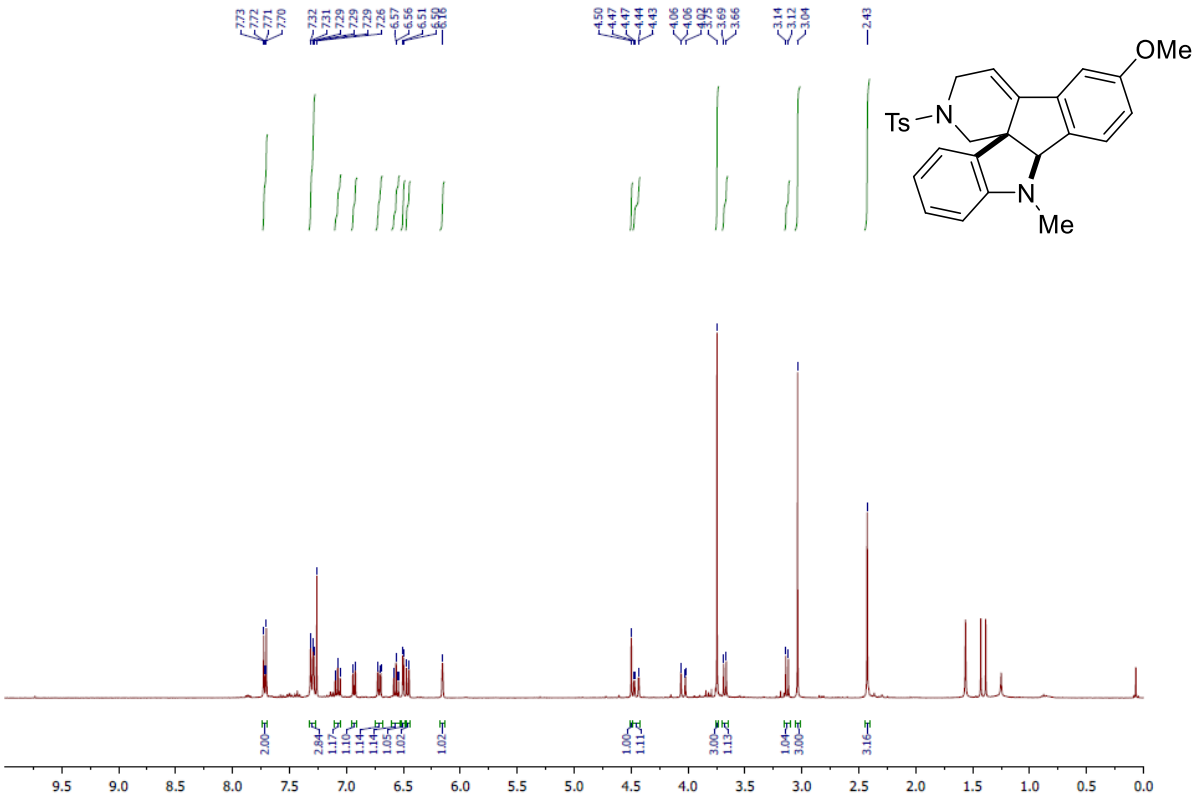


^{13}C NMR ($CDCl_3$, 75 MHz)

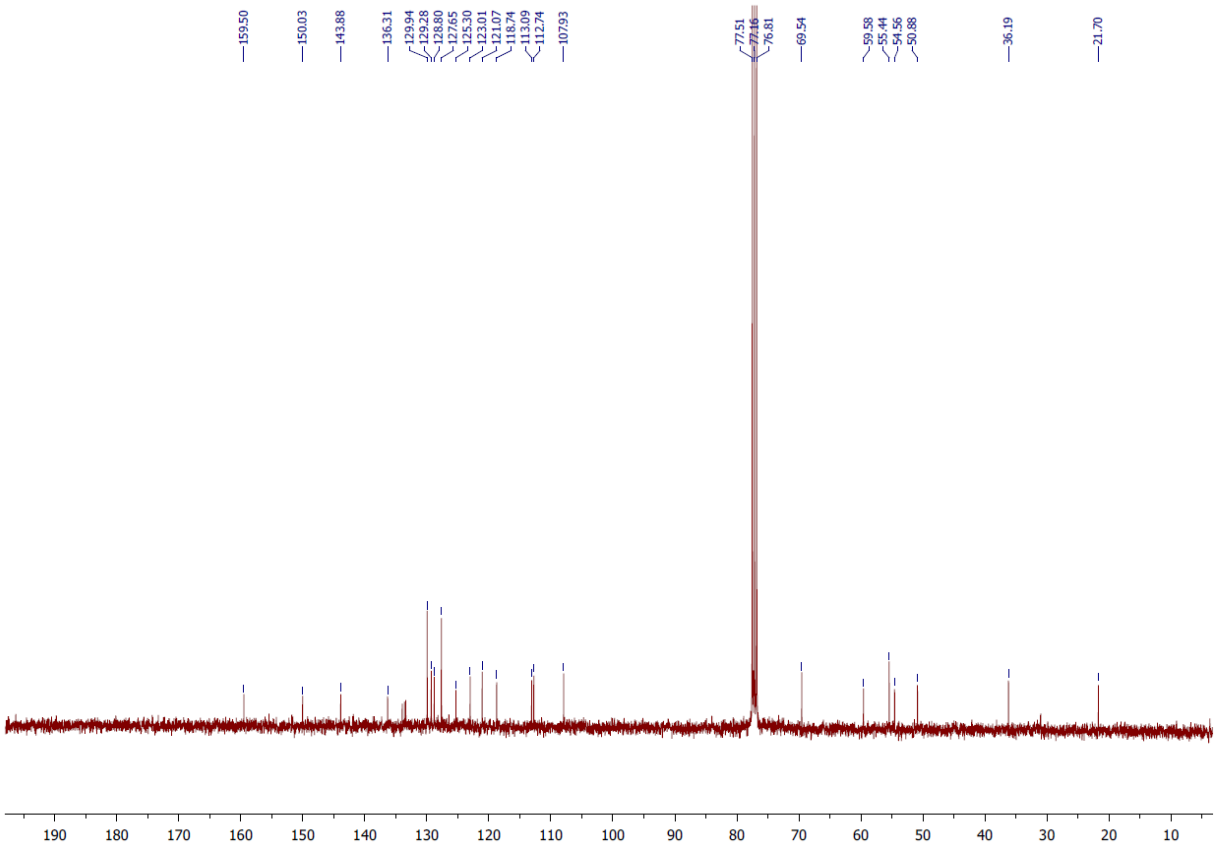


III.15. Compound 3b.

^{1}H NMR ($CDCl_3$, 500 MHz)

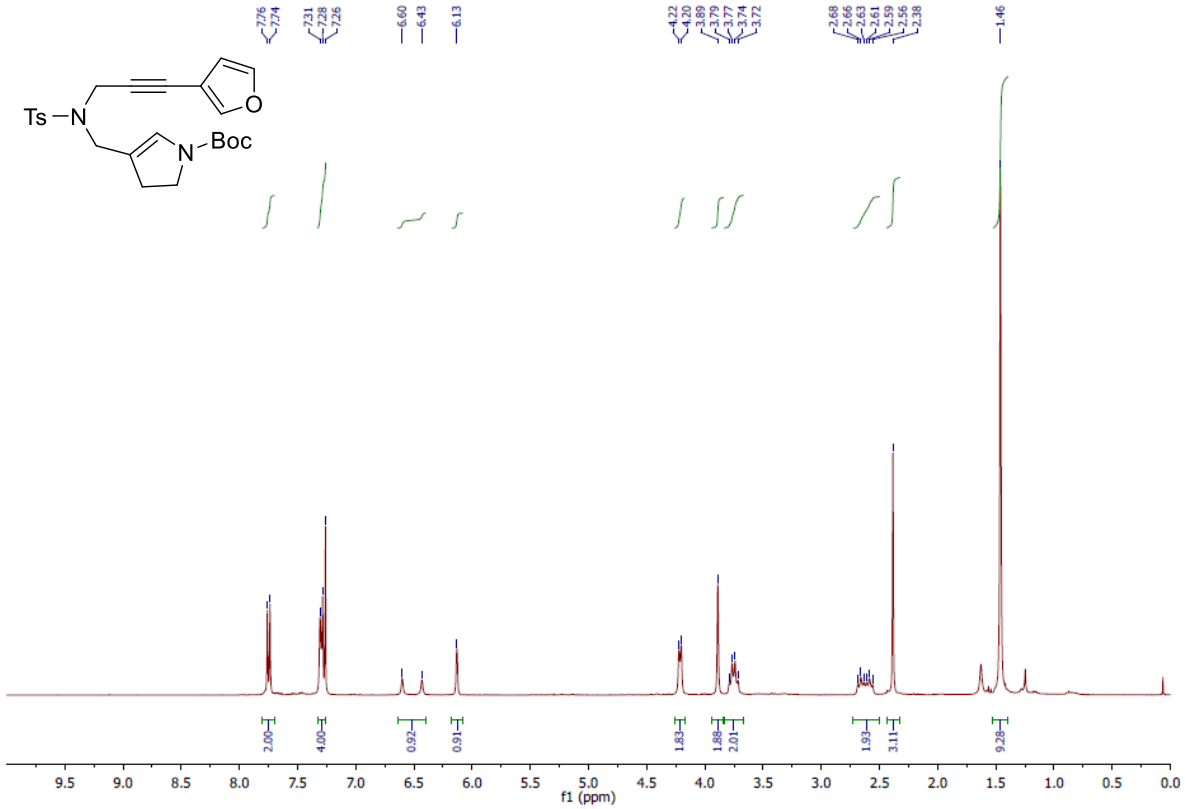


^{13}C NMR ($CDCl_3$, 75 MHz)

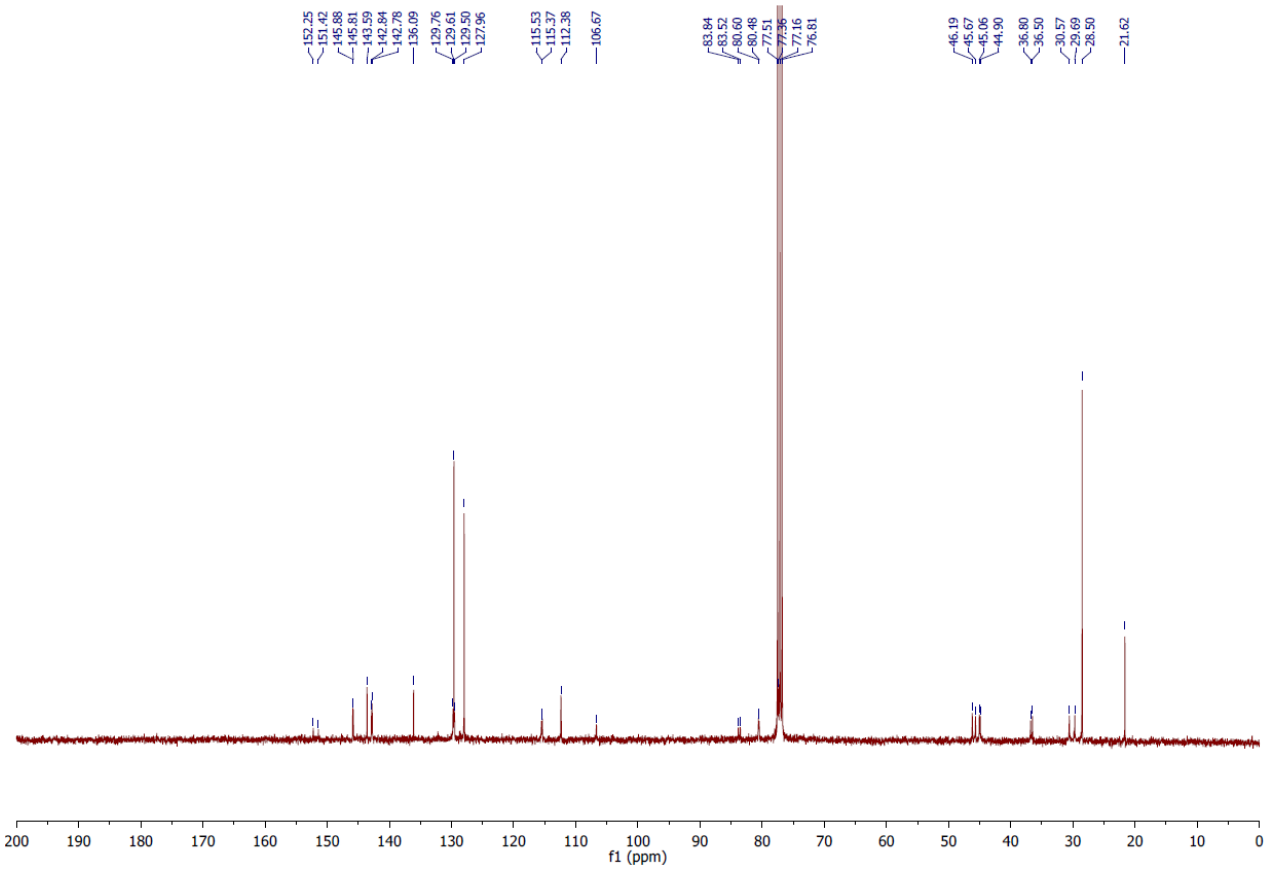


III.16. Compound 4a (*mixture of rotamers*).

^{1}H NMR ($CDCl_3$, 300 MHz)

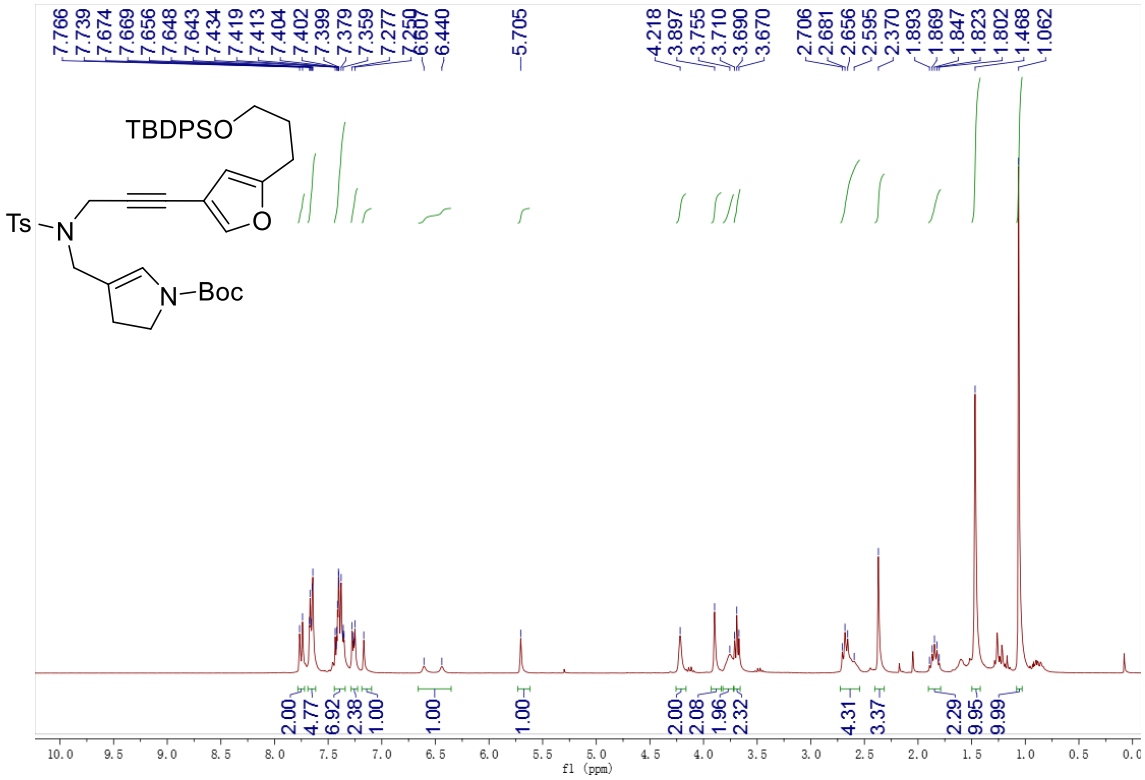


^{13}C NMR ($CDCl_3$, 75 MHz)

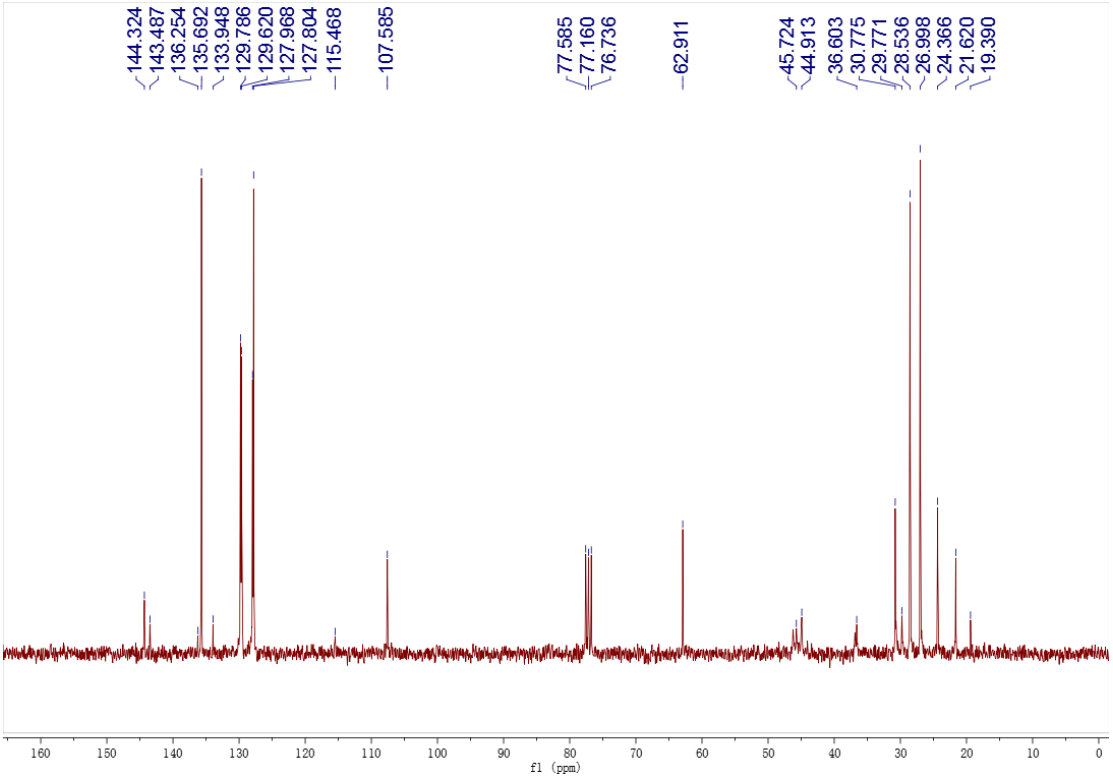


III.17. Compound 4b (*mixture of rotamers*).

^{1}H NMR ($CDCl_3$, 300 MHz)

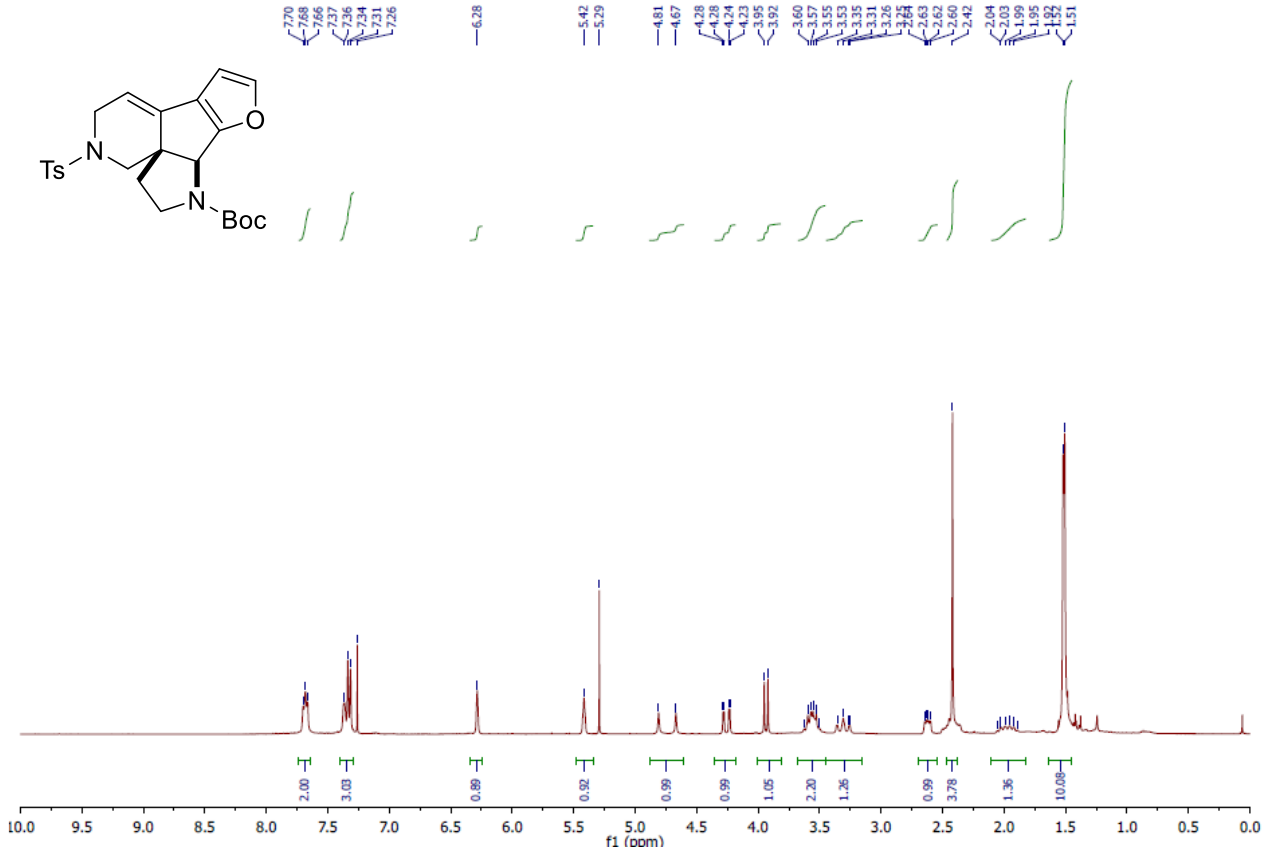


^{13}C NMR ($CDCl_3$, 75 MHz)

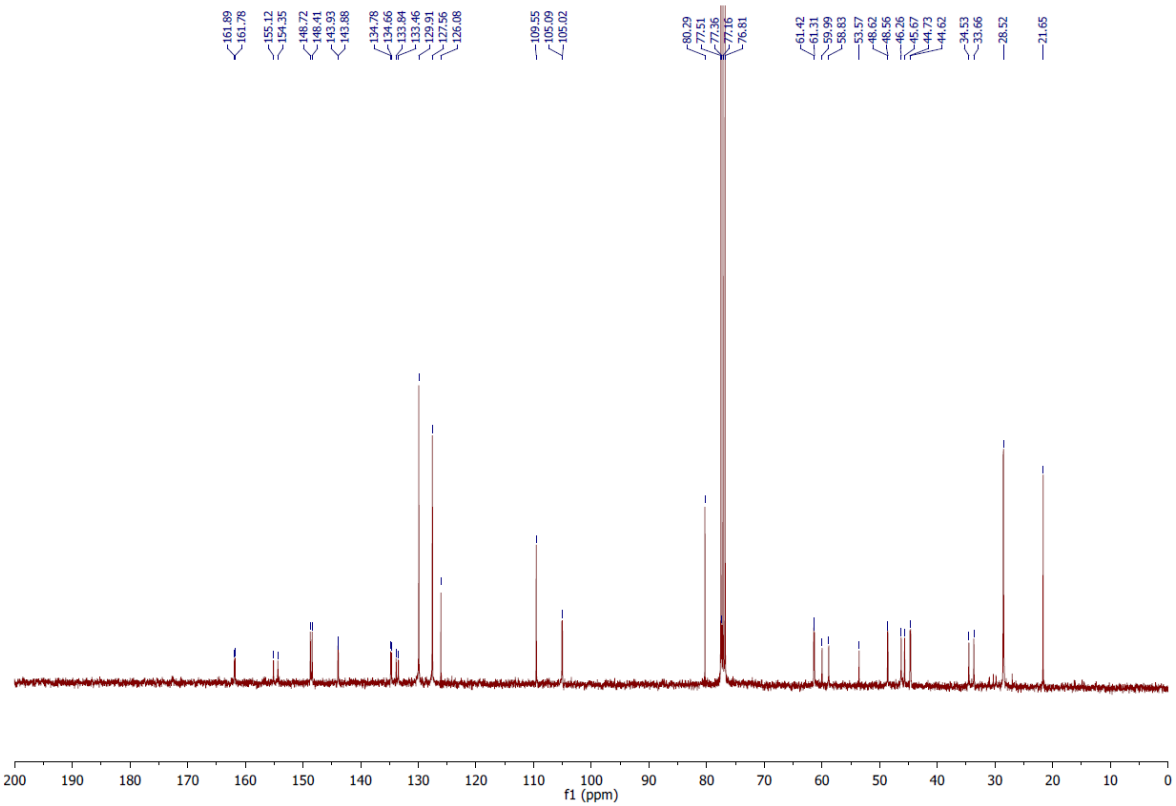


III.18. Compound 5a (*mixture of rotamers*).

^{1}H NMR ($CDCl_3$, 300 MHz)

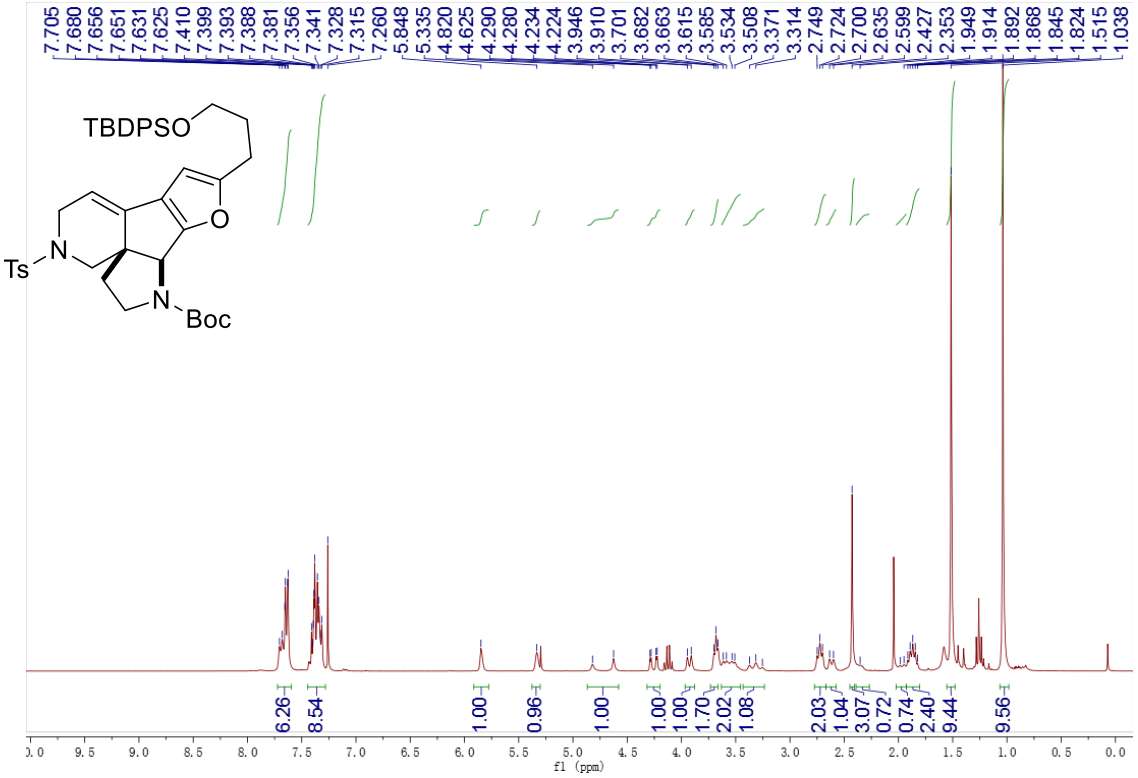


^{13}C NMR ($CDCl_3$, 75 MHz)

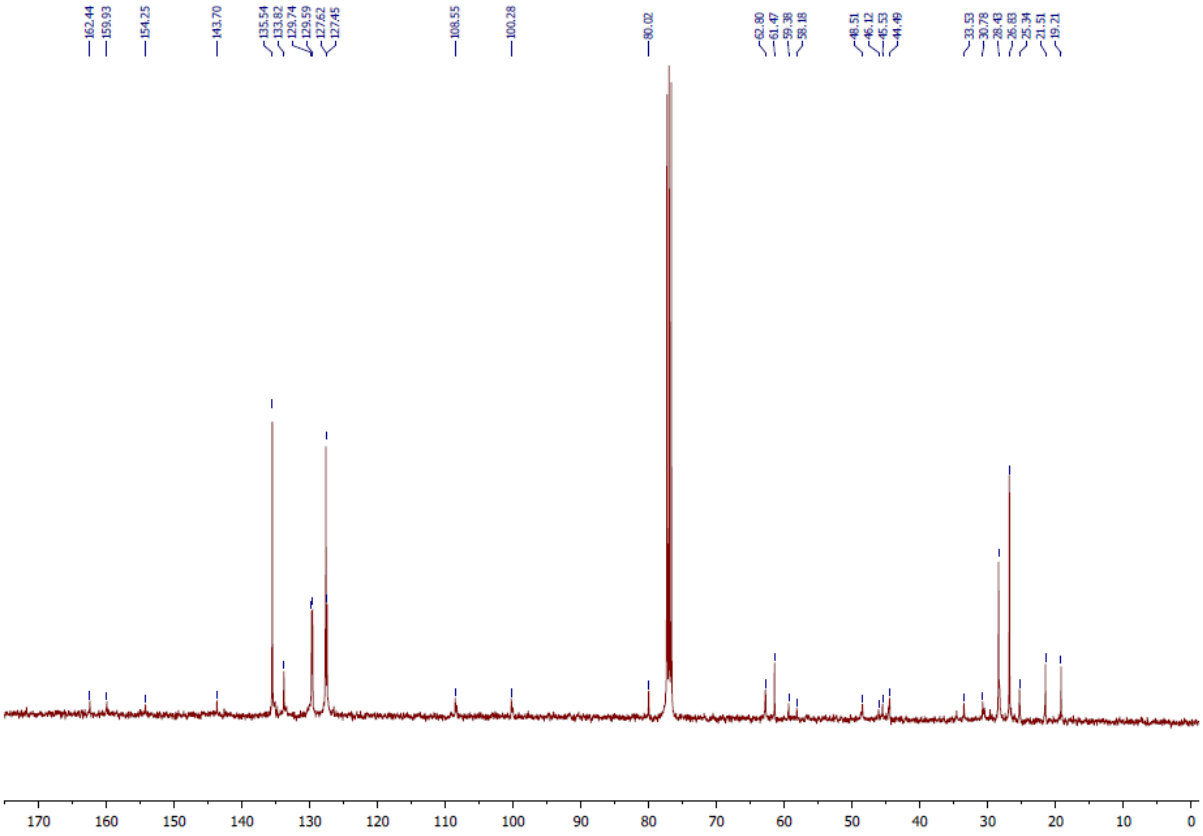


III.19. Compound 5b (*mixture of rotamers*).

^{1}H NMR ($CDCl_3$, 300 MHz)



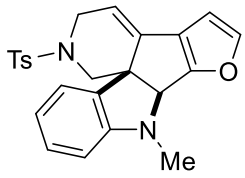
^{13}C NMR ($CDCl_3$, 75 MHz)

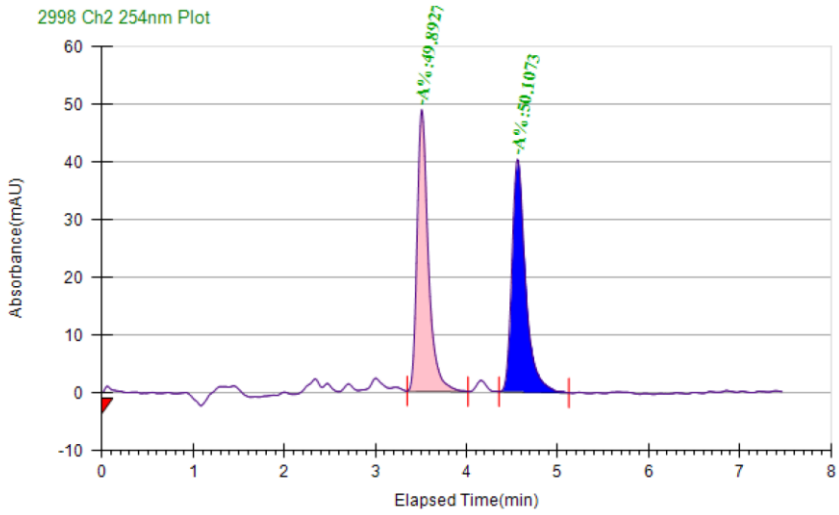


IV. SFC Data

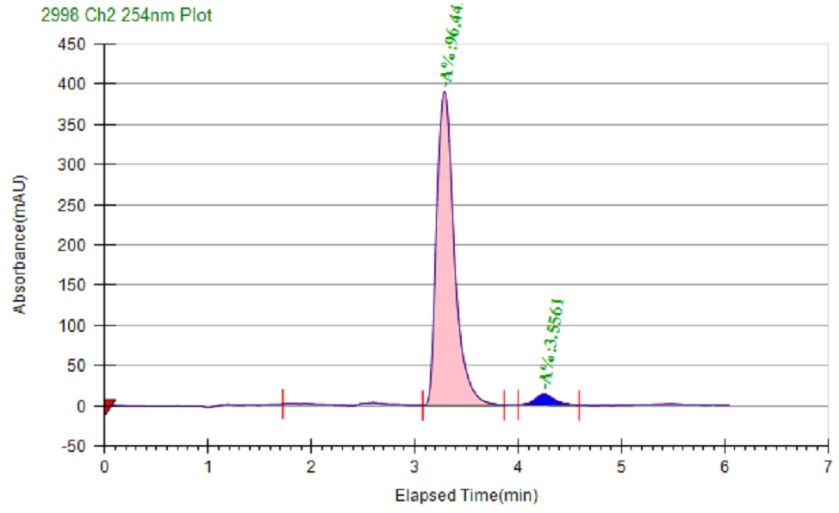
IV.1. Compound (2b)

SFC Analysis: 93% *e.e.* [CHIRALPAK® IA, 30 °C, 30% MeOH, 4.0 mL/min, 100 bar, retention times: 3.3 min (major) and 4.3 min (minor)].





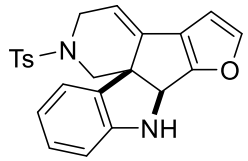
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.8927	3.51 min	48.7511	0.675 min	5009.7711	3507.3333	1.5417	0	4.7818
50.1073	4.56 min	40.288	0.775 min	5735.7019	4557.3333	1.5667	-4.7818	0

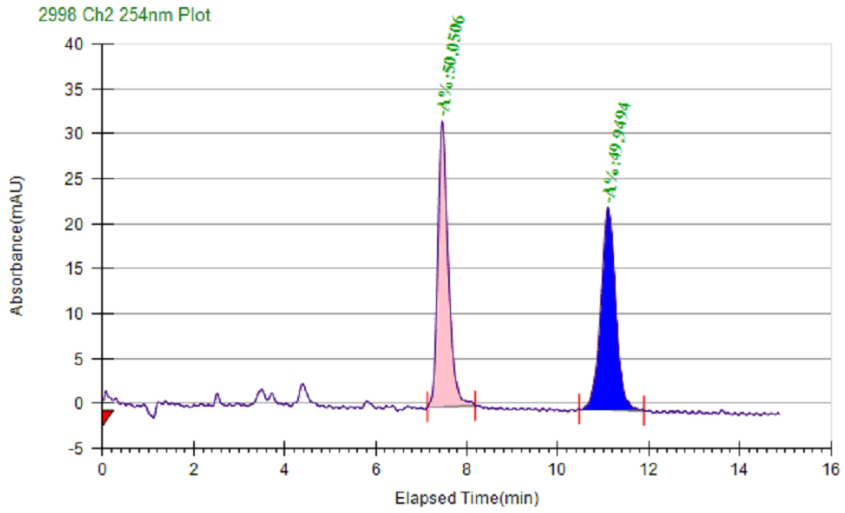


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
96.4439	3.29 min	390.199	0.8 min	2160.9462	3290.6667	1.4412	0	3.2213
3.5561	4.25 min	13.3013	0.6 min	2977.1777	4249	1.2045	-3.2213	0

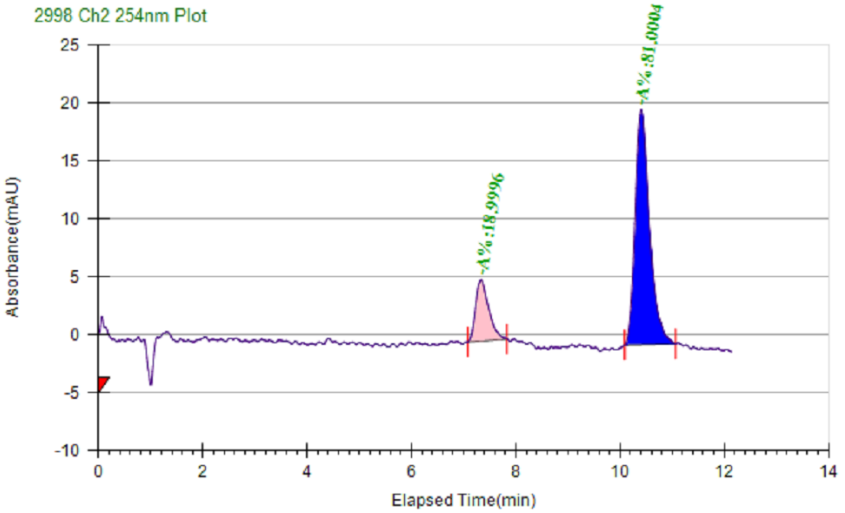
IV.2. Compound (2c)

SFC Analysis: 62% *e.e.* [CHIRALPAK® IB, 30 °C, 20% MeOH, 4.0 mL/min, 100 bar, retention times: 7.3 min (major) and 10.4 min (minor)].





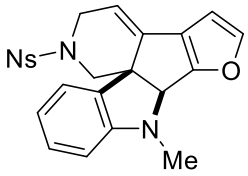
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.0506	7.46 min	31.7086	1.0583 min	6087.3505	7457.3333	1.36	0	7.7897
49.9494	11.1 min	22.5401	1.4417 min	6462.328	11099	1.0543	-7.7897	0

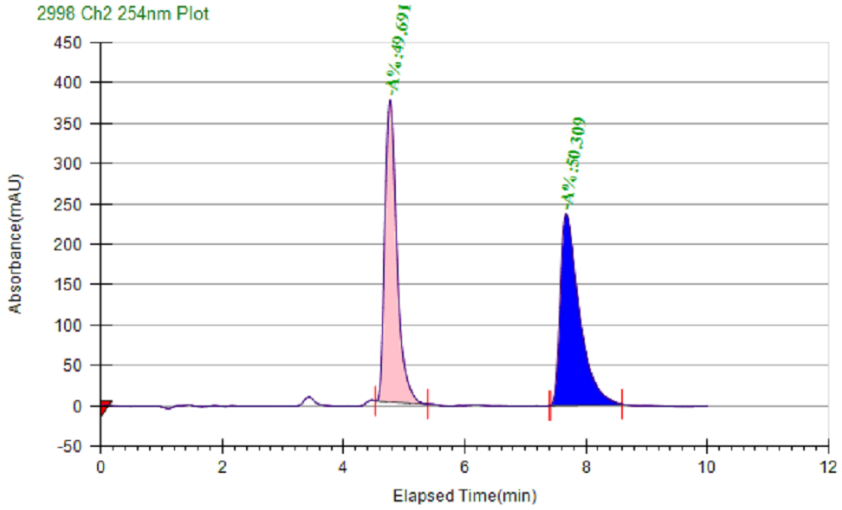


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
18.9996	7.33 min	5.2707	0.75 min	4766.8622	7332.3333	1.4375	0	6.8908
81.0004	10.41 min	20.2872	0.9833 min	7936.0932	10407.3333	1.3667	-6.8908	0

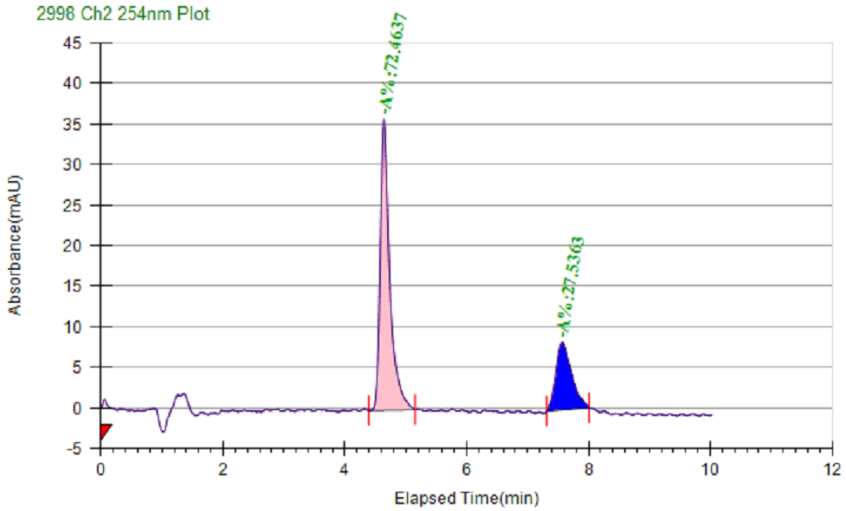
IV.3. Compound (2d)

SFC Analysis: 45% *e.e.* [CHIRALPAK® IA, 30 °C, 30% MeOH, 4.0 mL/min, 100 bar, retention times: 4.6 min (major) and 7.6 min (minor)].





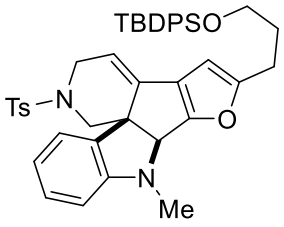
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.691	4.77 min	374.1	0.875 min	3146.8739	4765.6667	1.5526	0	6.6224
50.309	7.68 min	236.3588	1.2 min	3254.3318	7674	2.087	-6.6224	0

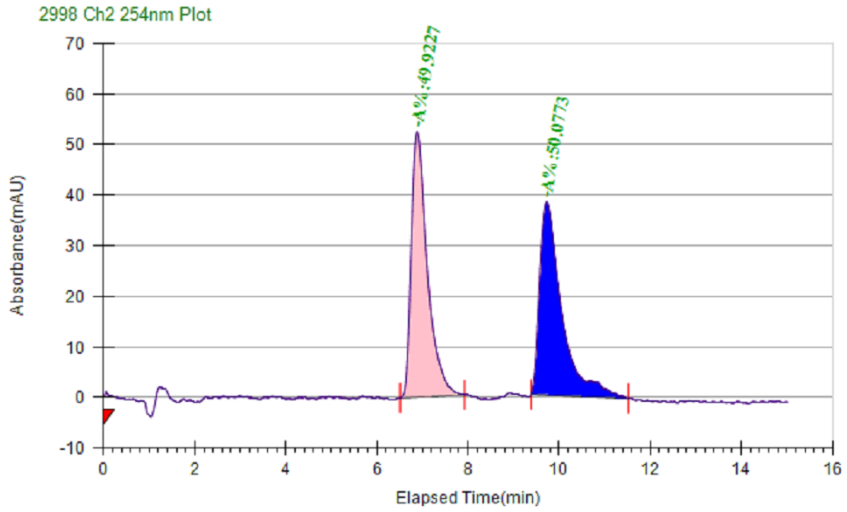


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
72.4637	4.64 min	35.9331	0.7667 min	5947.3338	4640.6667	1.7333	0	8.4274
27.5363	7.57 min	8.2946	0.7 min	4460.4791	7565.6667	1.4038	-8.4274	0

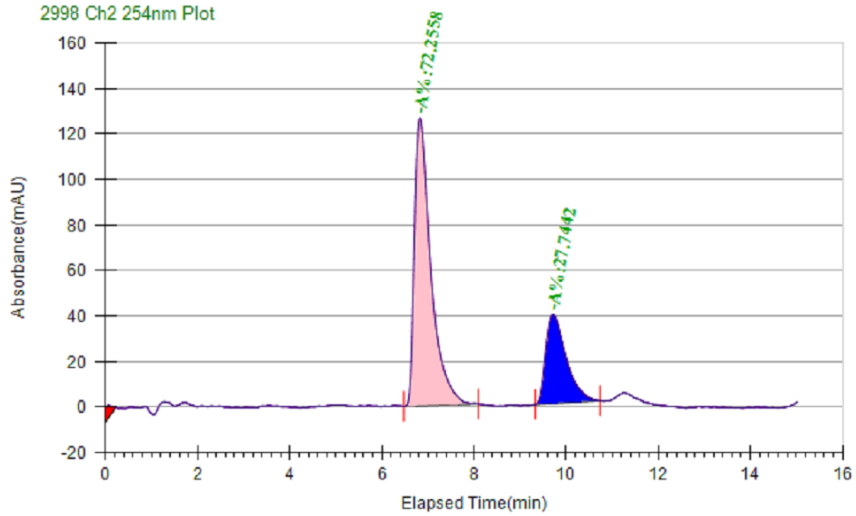
IV.4. Compound (2g)

SFC Analysis: 45% *e.e.* [CHIRALPAK® IA, 30 °C, 30% MeOH, 4.0 mL/min, 100 bar, retention times: 6.8 min (major) and 9.7 min (minor)].





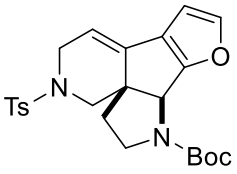
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.9227	6.88 min	52.4485	1.425 min	2142.7489	6882.3333	1.75	0	4.148
50.0773	9.73 min	38.1801	2.15 min	2498.4466	9732.3333	2.625	-4.148	0

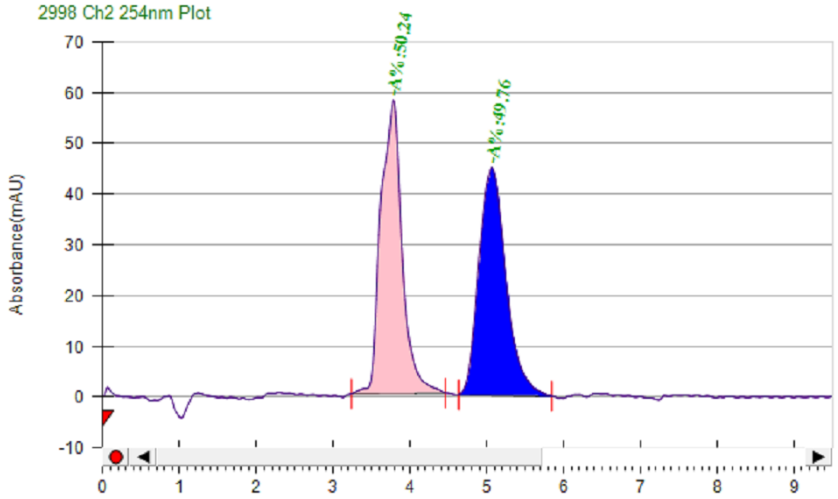


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
72.2558	6.82 min	126.4721	1.625 min	2106.585	6824	2.0556	0	4.2525
27.7442	9.72 min	39.02	1.4167 min	2582.9699	9715.6667	1.6757	-4.2525	0

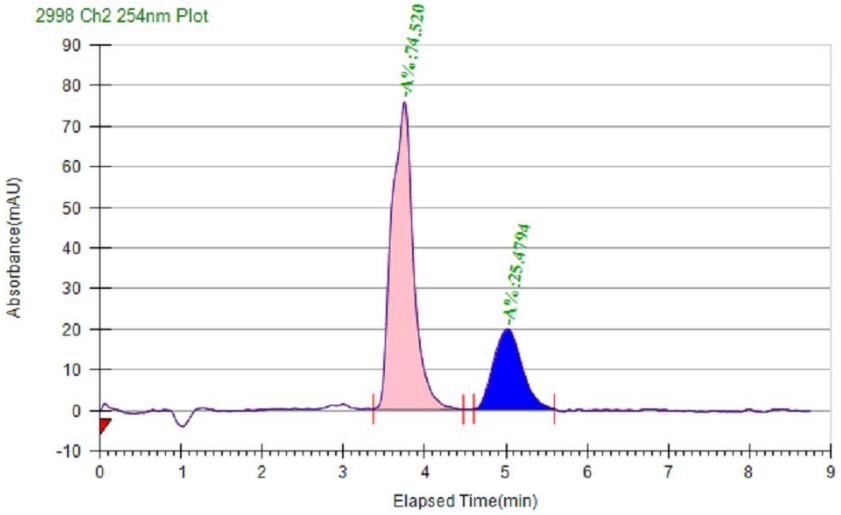
IV.5. Compound (5a)

SFC Analysis: 49% *e.e.* [CHIRALPAK® IA, 30 °C, 15% MeOH, 4.0 mL/min, 100 bar, retention times: 3.8 min (major) and 5.0 min (minor)].





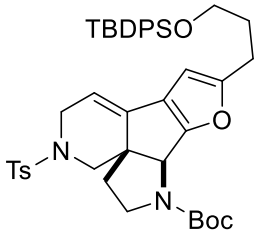
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
50.24	3.78 min	57.8004	1.2333 min	932.1491	3782.3333	1.1029	0	2.2647
49.76	5.07 min	44.8875	1.2167 min	1011.3277	5065.6667	1.25	-2.2647	0

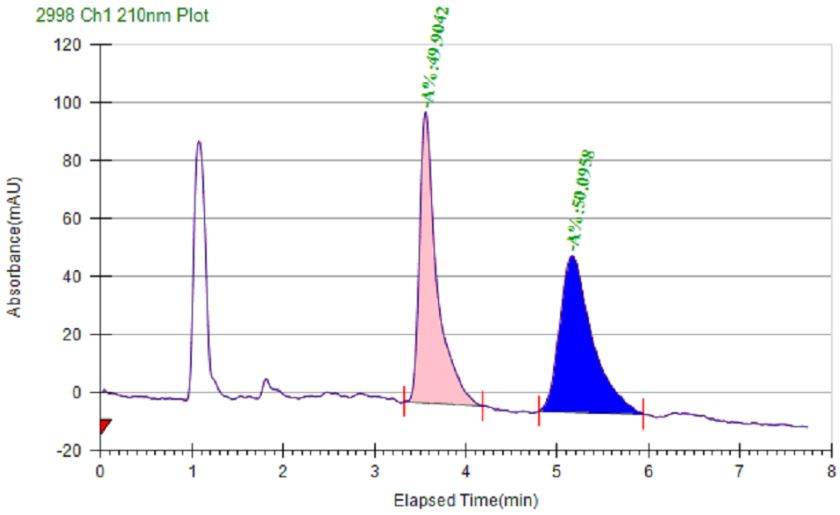


Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
74.5206	3.75 min	75.7118	1.1167 min	970.4585	3749	1.1212	0	2.25
25.4794	5.03 min	19.7444	1 min	951.982	5024	1.1463	-2.25	0

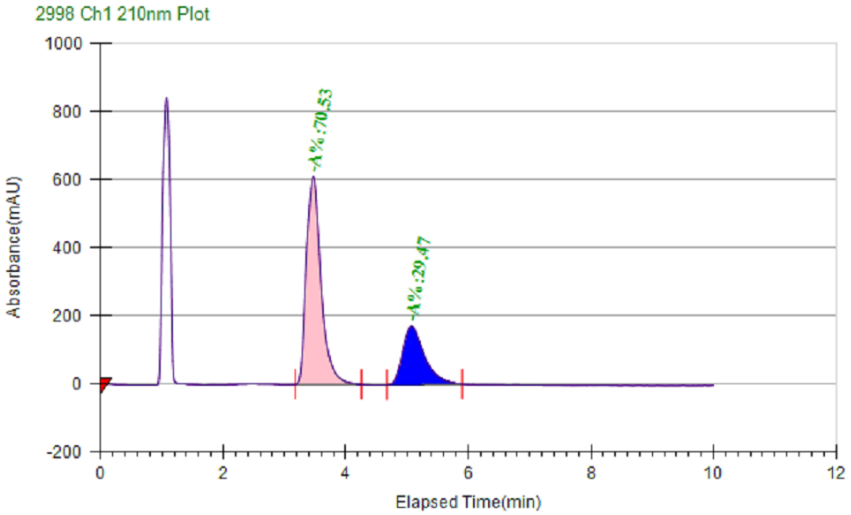
IV.6. Compound (5b)

SFC Analysis: 41% *e.e.* [CHIRALPAK® IA, 30 °C, 30% MeOH, 4.0 mL/min, 100 bar, retention times: 3.5 min (major) and 5.1 min (minor)].





Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
49.9042	3.56 min	100.1808	0.8667 min	2525.2567	3557.3333	2.0938	0	3.5854
50.0958	5.16 min	53.7891	1.15 min	1148.0324	5157.3333	1.6324	-3.5854	0



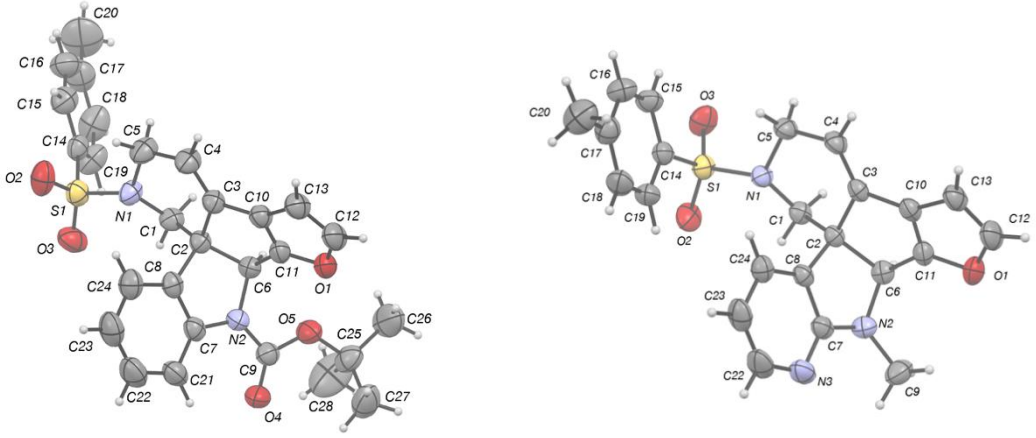
Area %	Ret. Time	Height	Peak Base Width	Theoretical Plates	Capacity Factor	Tailing Factor	ResolutionPeak1	ResolutionPeak2
70.53	3.47 min	610.9225	1.0833 min	1139.9884	3465.6667	1.38	0	3.1373
29.47	5.07 min	172.7617	1.2333 min	1107.5925	5065.6667	1.5441	-3.1373	0

V. X-ray crystal structure determination

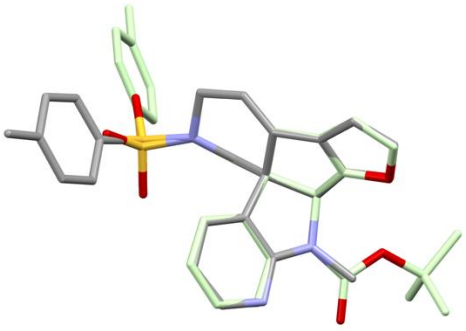
Crystallographic data collection, structure determination and refinement for **2a** and **2f**.

Small crystals suitable to single crystal X-ray diffraction (SCXRD) analyses were obtained by slow evaporation of a saturated dichloromethane solution both for **2a** and **2f**. X-ray diffraction data were measured at room temperature using a RIGAKU *XtaLabPro* diffractometer equipped with a Mo microfocus sealed tube *MM003* generator coupled to a double-bounce confocal Max-Flux® multilayer optic and a HPAD *PILATUS3R 200K* detector. *CrysAlisPro 1.171.39.46*[6] was employed for the data processing, with *SCALE3 ABSPACK* scaling algorithm implemented for the empirical absorption correction using spherical harmonics. Both structures were readily solved by intrinsic phasing methods (*SHELXT* program),[7] then refined by full-matrix least-squares methods on F^2 using *SHELX-L*.[8] All non-hydrogen atoms of the molecules of interest improved by anisotropic refinement. Most of their H atoms were clearly identified in difference maps but were positioned geometrically or allowed as rigid groups to rotate but not tip regarding the methyl H atoms, and refined with U_{iso} set to $1.2U_{eq}$(C) of the parent carbon atom (or 1.5 for the methyl). Crystal data, data collection and structure refinement details are summarized in Table S1.

CCDC 2056092 (compound **2a**) and CCDC 2127769 (compound **2f**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



Ortep views of ***2a*** and ***2f***. Ellipsoids are drawn at 50% of probability.



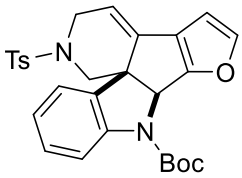
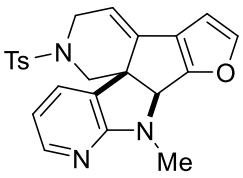
Overlay of both structures over their common central moiety. Carbons in pale green refer to ***2a***.

[6] Rigaku OD (2015). CrysAlis PRO. Rigaku Oxford Diffraction, Yarnton, Oxfordshire, England.

[7] Sheldrick, G. M. *Acta Cryst.* 2015, **C71**, 3-8.

[8] Sheldrick, G. M. *Acta Cryst.* 2015, **A71**, 3-8.

Table S1 Crystal data, data collection and structure refinement details for **2a** and **2f**.

Compound		**2a**	**2f**
			
Empirical formula		$C_{28}H_{28}N_2O_5S$	$C_{23}H_{21}N_3O_3S$
Formula weight		504.58	419.49
Temperature (K)		293(2)	293(2)
Wavelength (Å)		0.71073	0.71073
Crystal system, space group		Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$
Unit cell dimensions	a | (Å) b c α | ° β γ	9.4255 (5) 34.4504 (18) 8.2876 (5) 90 102.801 (6) 90	11.1095 (3) 8.1293 (2) 22.4667 (6) 90 103.438 (2) 90
Volume ($Å^3$)		2624.2 (3)	1973.47 (9)
Z, Calculated density (Mg/m^3)		4, 1.277	4, 1.412
Absorption coefficient (mm^{-1})		0.164	0.196
F(000)		1064	880
Crystal size (mm)		0.13 x 0.09 x 0.02	0.17 x 0.15 x 0.14
θ range for data collection (°)		2.365 to 25.350	2.673 to 26.732
Limiting indices		-11 ≤ k ≤ 11 -41 ≤ k ≤ 38 -8 ≤ l ≤ 9	-14 ≤ k ≤ 14 -9 ≤ k ≤ 10 -28 ≤ l ≤ 28
Reflections collected / unique R(int)		17083 / 4793 0.067	41286 / 4183 0.032
Completeness to θ_{full} (%)		99.3	99.9
Absorption correction		Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission		1.000 and 0.512	1.000 and 0.374
Refinement method		Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters		4775 / 0 / 329	4182 / 0 / 273
Goodness-of-fit on F^2		1.023	1.029
Final R indices [$I>2\sigma(I)$]	R1, wR2	0.0541, 0.1223	0.0368, 0.0984
R indices (all data)	R1, wR2	0.0842, 0.1347	0.0422, 0.1013
Largest Δ peak and hole ($e.Å^{-3}$)		0.206 and -0.298	0.241 and -0.338
CCDC deposit number		2056092	2127769

VI. Computational details

VI.1. Introduction.

All optimizations were performed at the B3LYP level of theory[9] using the Gaussian 16 package.[10] The Au atom was described by the LANL2DZ basis set, which includes a double-valence basis set with the Hay and Wadt effective core potential.[11] The 6-31G(d,p) Pople basis set was used for the other atoms (C, H, O, N and P). Vibrational frequency calculations were performed at the same level for all intermediates and transition states to confirm minima (no imaginary frequency) and first order saddle points (one imaginary frequency representing the desired reaction coordinate), respectively. Single point energies were calculated on the optimized structures at 298 K and 1 atm at the M06 level of theory.[12] The Gaussian basis set def2-QZVP[13] was used for Au and 6-311+G(2d,p) for the other atoms. Solvent effects were assessed through the conductor-like polarizable continuum model (CPCM)[14] method with the parameters for dichloromethane.

VI.2. Results and discussion.

Several pathways were envisaged to account for the formation of the polycyclic products in the dihydropyrrole series, all starting from the Johnphos alkyne gold complex **A** selected as reference of the free energies (Scheme S1). We also evaluated the possibility of a 7-*endo*-dig cyclization/ring contraction as alternate mechanism. However, the formation of the 7-membered complex **E'** from **A'** faces an unsurmountable barrier to reach $\mathbf{TS_{A'E'}}$ (32.3 kcal/mol). Of note, **E'** is not the expected cation, but a spontaneous 1,2-H shift occurs during optimization to directly give a *N*-stabilized carbocation. Besides, manifold efforts failed to connect rotamers **E** and **E'** to the spiro intermediates **B** and **B'**. Thus, it is the blue pathway that is supported by the computations.

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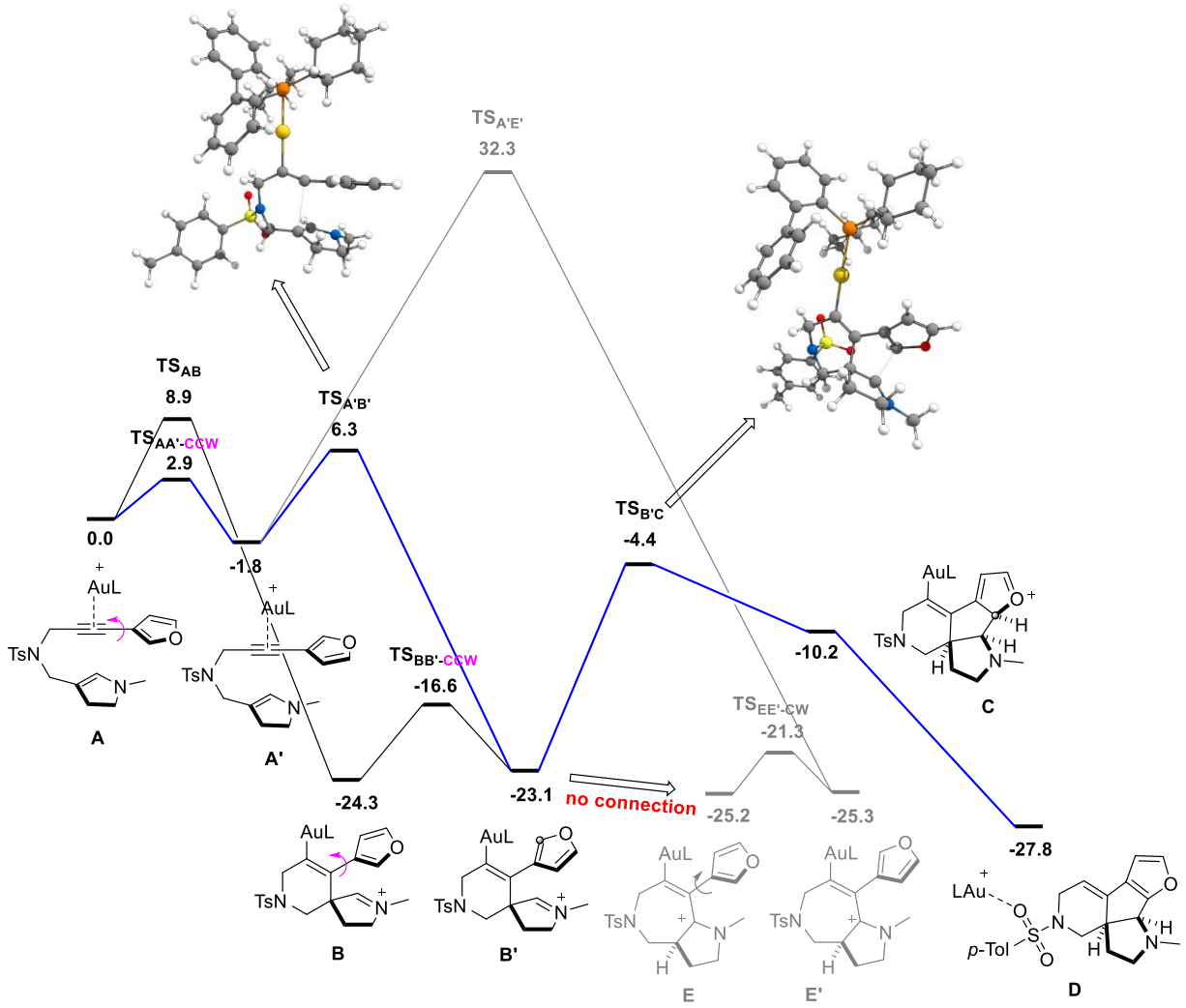

Scheme S1. Free Energy Profile in the Dihydropyrrole Series (ΔG_{298}, kcal/mol; L = CyJohnPhos ((2-Biphenyl)dicyclohexylphosphine)

Thermal corrections to the Gibbs free energies (Hartree), SCRF energies (Hartree), imaginary frequencies (cm^{-1}) and Cartesian coordinates (x,y,z) for all the intermediates and transition states

A Thermal correction to Gibbs Free Energy= 0.785374 E(RM06) = -2917.91041724				**A'** Thermal correction to Gibbs Free Energy= 0.784663 E(RM06) = -2917.91263581			
C	4.477422	2.086765	0.670298	C	4.924597	-3.098699	-0.749876
C	0.919582	2.272315	0.282581	C	0.90653	-2.072456	0.955371
C	4.851893	2.538031	-0.546197	C	4.972663	-1.757339	-0.612016
C	4.516616	0.664891	1.137688	C	4.221225	-0.933817	0.37417
H	5.241935	0.08637	0.559648	H	3.736078	-1.567797	1.128648
H	4.859131	0.624151	2.179747	H	4.89993	-0.259364	0.908841
N	3.254469	-0.141537	1.114331	N	3.21365	-0.051181	-0.29519
S	2.962934	-1.091837	-0.257064	S	2.694389	1.279091	0.649959
O	1.647755	-1.713471	-0.004229	O	1.581074	1.878908	-0.107029
O	3.173576	-0.337284	-1.500552	O	2.480968	0.876149	2.050463
N	4.977639	3.915681	-0.620016	N	5.68516	-3.583372	-1.805831
C	4.808878	4.627993	-1.871208	C	6.261061	-4.915725	-1.749008
H	5.248754	5.626789	-1.790714	H	6.583914	-5.220532	-2.748833
H	3.749192	4.740348	-2.158495	H	5.506711	-5.630376	-1.40827
H	5.330302	4.095222	-2.670963	H	7.131059	-4.976544	-1.073686
C	4.345727	4.473458	0.586825	C	6.573191	-2.480262	-2.227543
H	3.309453	4.775067	0.355639	H	6.721701	-2.489899	-3.311167
C	4.353742	3.296974	1.591712	C	5.869876	-1.202791	-1.707942
H	3.460049	3.305089	2.226657	H	5.278095	-0.722819	-2.500184
C	2.069919	0.373272	1.79774	C	2.12475	-0.743276	-0.992164
H	2.422884	0.923179	2.676526	H	2.59061	-1.529032	-1.595243
H	1.469735	-0.465574	2.149879	H	1.625958	-0.04058	-1.656106
C	1.214785	1.296166	0.982534	C	1.140777	-1.380406	-0.049091
C	0.644133	3.375863	-0.557566	C	0.686397	-2.764608	2.161536
C	0.180952	4.612598	-0.170257	C	0.961102	-2.243442	3.409881
O	0.059507	5.418547	-1.240251	O	0.693169	-3.153807	4.357882
H	-0.09335	5.024176	0.788269	H	1.347338	-1.28428	3.721768
C	0.448523	4.704736	-2.344779	C	0.232922	-4.286917	3.732009
H	0.403312	5.234844	-3.282896	H	-0.023842	-5.10709	4.383351
C	0.81713	3.447887	-1.992704	C	0.208289	-4.110841	2.388406
H	1.17914	2.658514	-2.634273	H	-0.103328	-4.821465	1.638281
C	4.242672	-2.334231	-0.147224	C	4.112762	2.360952	0.592092
C	4.289598	-3.187013	0.961134	C	4.501425	2.922117	-0.629163
H	3.581381	-3.070089	1.774388	H	3.966324	2.677994	-1.540413

C	5.257587	-4.183527	1.003727	C	5.583114	3.794858	-0.653
H	5.299797	-4.848769	1.861815	H	5.893732	4.232052	-1.597971
C	6.18077	-4.348224	-0.044179	C	6.280336	4.124154	0.522907
C	6.102613	-3.484673	-1.144208	C	5.863697	3.548635	1.730293
H	6.802597	-3.601037	-1.966601	H	6.390604	3.791121	2.648664
C	5.13902	-2.477512	-1.206194	C	4.781692	2.669173	1.776587
H	5.073946	-1.813612	-2.060888	H	4.454484	2.228707	2.711757
C	7.238333	-5.421216	0.030431	C	7.435339	5.093461	0.480745
H	6.821092	-6.366988	0.389686	H	8.043356	5.034107	1.386744
H	7.699597	-5.599274	-0.943969	H	8.083568	4.904251	-0.38034
H	8.034987	-5.134536	0.727342	H	7.073163	6.124714	0.391803
Au	-0.79529	0.473934	0.270098	Au	-0.931721	-0.559254	0.028673
P	-2.544199	-0.949881	-0.384597	P	-2.811205	0.849627	-0.076513
C	-3.970175	-1.099596	0.772569	C	-4.038508	0.48992	-1.402538
C	-4.855697	-2.17621	0.560243	C	-4.973999	1.500233	-1.70594
H	-4.705671	-2.836747	-0.283904	H	-4.979176	2.417781	-1.131857
C	-5.926645	-2.425748	1.41275	C	-5.899957	1.358193	-2.734826
H	-6.588522	-3.263663	1.217896	H	-6.60613	2.1565	-2.940253
C	-6.133253	-1.596673	2.513854	C	-5.905454	0.190209	-3.495343
H	-6.960873	-1.777827	3.192737	H	-6.617598	0.063106	-4.304899
C	-5.271857	-0.526956	2.738126	C	-4.99235	-0.82003	-3.208051
H	-5.436228	0.127046	3.588823	H	-5.001133	-1.735513	-3.791378
C	-4.189226	-0.24933	1.884734	C	-4.054424	-0.70309	-2.167148
C	-3.37138	0.951465	2.248377	C	-3.157215	-1.885255	-1.965652
C	-3.557199	2.177103	1.591194	C	-3.417566	-2.82442	-0.956304
H	-4.24996	2.237346	0.757306	H	-4.240469	-2.655905	-0.268302
C	-2.894194	3.32608	2.028016	C	-2.655716	-3.990736	-0.856295
H	-3.069825	4.271285	1.522366	H	-2.886003	-4.71712	-0.082169
C	-2.037295	3.266572	3.129333	C	-1.625381	-4.236942	-1.766417
H	-1.541222	4.164759	3.486044	H	-1.046472	-5.153641	-1.702162
C	-1.84602	2.051897	3.79211	C	-1.360511	-3.311128	-2.778112
H	-1.196078	2.001413	4.660897	H	-0.572554	-3.503564	-3.500437
C	-2.513048	0.904257	3.359104	C	-2.124179	-2.14658	-2.880771
H	-2.382601	-0.033803	3.891075	H	-1.930916	-1.438473	-3.681513
C	-3.155615	-0.432451	-2.086774	C	-3.667454	0.883006	1.598095
H	-2.338135	-0.77608	-2.73873	H	-2.979376	1.499879	2.195913
C	-4.47351	-1.0908	-2.551393	C	-5.067161	1.535949	1.618875
H	-5.283655	-0.783783	-1.878872	H	-5.745929	0.948605	0.988561
H	-4.412093	-2.180936	-2.495888	H	-5.038865	2.544979	1.198432
C	-4.823436	-0.672424	-3.991441	C	-5.628456	1.595331	3.051765
H	-4.06087	-1.065357	-4.678136	H	-5.003063	2.265246	3.65799
H	-5.771691	-1.138943	-4.280611	H	-6.628828	2.041589	3.027552
C	-4.907573	0.851795	-4.137225	C	-5.673979	0.208109	3.704101
H	-5.110045	1.123115	-5.179001	H	-6.031667	0.285866	4.736537

H	-5.754094	1.227464	-3.54588	H	-6.397937	-0.421824	3.168785
C	-3.613838	1.520814	-3.655403	C	-4.293811	-0.460654	3.668589
H	-3.703404	2.611959	-3.705033	H	-4.346678	-1.47429	4.081841
H	-2.788004	1.244174	-4.325708	H	-3.598643	0.101236	4.307895
C	-3.254085	1.104093	-2.219336	C	-3.724882	-0.520964	2.241106
H	-2.309743	1.572303	-1.920486	H	-2.726806	-0.972685	2.254902
H	-4.024368	1.476126	-1.530508	H	-4.358936	-1.1732	1.625778
C	-1.692437	-2.624269	-0.537656	C	-2.039818	2.541949	-0.381533
H	-0.720638	-2.32098	-0.950044	H	-1.148573	2.475334	0.257814
C	-1.4241	-3.223295	0.860849	C	-1.544658	2.655874	-1.84036
H	-2.376569	-3.503794	1.327926	H	-2.407702	2.687872	-2.517368
H	-0.959528	-2.471415	1.509981	H	-0.960141	1.768301	-2.111114
C	-2.287666	-3.678325	-1.494446	C	-2.815103	3.805349	0.046449
H	-2.433633	-3.257659	-2.494597	H	-3.127307	3.735005	1.093437
H	-3.267937	-4.016223	-1.137271	H	-3.7233	3.92402	-0.556622
C	-1.352698	-4.899703	-1.585113	C	-1.935161	5.056037	-0.142679
H	-1.797499	-5.64585	-2.25308	H	-2.505142	5.945715	0.147796
H	-0.404148	-4.591448	-2.045156	H	-1.076358	4.996344	0.539507
C	-1.078005	-5.507813	-0.203266	C	-1.433682	5.18433	-1.587363
H	-2.012942	-5.915897	0.206102	H	-2.289893	5.357527	-2.254565
H	-0.38482	-6.351389	-0.294465	H	-0.783232	6.060768	-1.683228
C	-0.511278	-4.45769	0.762104	C	-0.686844	3.918715	-2.030576
H	-0.379408	-4.890184	1.760756	H	-0.391351	3.999601	-3.083061
H	0.479851	-4.135056	0.420381	H	0.236287	3.807604	-1.448382
H	5.100265	1.939183	-1.416059	H	4.348433	-3.800114	-0.153639
H	5.220997	3.359835	2.26638	H	6.584843	-0.453115	-1.351202
H	4.883639	5.358525	0.939461	H	7.558792	-2.600565	-1.748061
B				**B'**			
Thermal correction to Gibbs Free Energy= 0.792824				Thermal correction to Gibbs Free Energy= 0.793895			
E(RM06) = -2917.95662652				E(RM06) = -2917.95577488			
C	-3.059386	2.270506	-0.484113	C	3.046458	2.27198	0.574124
C	-1.548311	1.907897	-0.32611	C	1.536868	1.911562	0.407939
C	-3.457453	2.851297	0.824423	C	3.410557	2.891717	-0.727377
C	-3.862612	1.002699	-0.866687	C	3.857594	0.997757	0.90658
H	-4.935849	1.200092	-0.822333	H	4.929475	1.203954	0.86892
H	-3.609828	0.765574	-1.908003	H	3.608081	0.715189	1.937315
N	-3.528354	-0.137889	-0.039955	N	3.530219	-0.108985	0.030991
S	-4.521292	-0.517287	1.271573	S	4.533259	-0.431886	-1.287577
O	-3.701681	-1.298961	2.199406	O	3.726365	-1.191814	-2.244331
O	-5.17234	0.735625	1.710291	O	5.171095	0.841994	-1.682767
N	-3.63666	4.1343	0.790385	N	3.549631	4.178737	-0.667447
C	-3.906313	4.999121	1.937419	C	3.768418	5.077473	-1.799466
H	-4.820917	5.568643	1.754483	H	4.672627	5.666029	-1.625073

H	-3.072424	5.694807	2.068538	H	2.914326	5.753887	-1.895105
H	-4.026783	4.391649	2.834411	H	3.88237	4.49416	-2.713167
C	-2.104083	-0.522462	-0.054594	C	3.38815	4.707296	0.711765
H	-1.923232	-1.195797	-0.905365	H	4.223319	5.376133	0.93686
H	-1.90309	-1.099373	0.849877	C	3.356244	3.43145	1.570609
C	-1.135894	0.630304	-0.152033	H	4.338878	3.262807	2.023039
C	-0.593742	3.048277	-0.375166	C	2.107622	-0.500613	0.021191
C	0.129306	3.465236	-1.458443	H	1.926016	-1.21633	0.836025
O	0.919349	4.529206	-1.141445	H	1.91257	-1.033731	-0.911258
H	0.208832	3.098956	-2.470351	C	1.132647	0.640255	0.172067
C	0.698466	4.810038	0.17275	C	0.575877	3.046039	0.484771
H	1.268057	5.630009	0.58255	C	0.010721	3.70879	-0.569922
C	-0.215393	3.945386	0.693788	O	-0.832114	4.689182	-0.140898
H	-0.547076	3.906035	1.72226	H	0.080485	3.578724	-1.639361
C	-5.802284	-1.565586	0.60302	C	-0.812883	4.658843	1.2217
C	-5.512944	-2.909453	0.344527	H	-1.446415	5.377209	1.718831
H	-4.530562	-3.311225	0.56877	C	0.027503	3.683001	1.661946
C	-6.509612	-3.724102	-0.181095	H	0.211785	3.412307	2.692069
H	-6.291728	-4.769848	-0.379896	C	5.823743	-1.48609	-0.647059
C	-7.79483	-3.223113	-0.4501	C	5.548806	-2.840514	-0.431182
C	-8.055769	-1.874538	-0.174332	H	4.571815	-3.246049	-0.67166
H	-9.046143	-1.471492	-0.366367	C	6.552721	-3.659663	0.073055
C	-7.070547	-1.040263	0.354035	H	6.346176	-4.713495	0.23857
H	-7.284394	-0.004158	0.590796	C	7.831162	-3.152655	0.36275
C	-8.872563	-4.129219	-0.991561	C	8.077783	-1.7935	0.12941
H	-9.295417	-4.749507	-0.192159	H	9.062793	-1.385418	0.337667
H	-9.692799	-3.558622	-1.434331	C	7.08505	-0.954512	-0.377203
H	-8.477615	-4.809015	-1.752571	H	7.287925	0.090702	-0.581378
Au	0.8573	0.07885	-0.033722	C	8.916541	-4.06282	0.881685
P	3.15272	-0.523875	0.37812	H	9.339114	-4.665407	0.068762
C	3.887174	-1.940134	-0.558998	H	9.735439	-3.496208	1.331906
C	5.076593	-2.51521	-0.067478	H	8.528794	-4.759333	1.6313
H	5.567892	-2.075856	0.79033	Au	-0.858135	0.081226	0.051552
C	5.647172	-3.644651	-0.646932	P	-3.170553	-0.473323	-0.333901
H	6.564557	-4.057073	-0.238438	C	-3.860846	-2.034285	0.379647
C	5.027556	-4.237875	-1.745129	C	-5.083359	-2.510837	-0.135966
H	5.453762	-5.122471	-2.20855	H	-5.618388	-1.924181	-0.870817
C	3.858314	-3.681113	-2.253425	C	-5.632099	-3.725815	0.263429
H	3.383103	-4.127895	-3.121286	H	-6.576325	-4.057247	-0.157445
C	3.272074	-2.532308	-1.691161	C	-4.955982	-4.507667	1.198039
C	2.042325	-2.034079	-2.382595	H	-5.364389	-5.460976	1.519478
C	2.06749	-0.863818	-3.15635	C	-3.752796	-4.052487	1.72744
H	2.974044	-0.268295	-3.193889	H	-3.233318	-4.648625	2.471287
C	0.956515	-0.484474	-3.911805	C	-3.186792	-2.821251	1.347883

H	1.003669	0.412039	-4.523552	C	-1.913193	-2.45853	2.043287
C	-0.197721	-1.270117	-3.907247	C	-1.867571	-1.42137	2.987411
H	-1.054361	-0.985779	-4.511599	H	-2.753244	-0.819391	3.162429
C	-0.234566	-2.437885	-3.141939	C	-0.71159	-1.186034	3.733738
H	-1.121387	-3.065494	-3.146339	H	-0.702954	-0.391628	4.474396
C	0.878158	-2.819211	-2.390094	C	0.417982	-1.986009	3.55017
H	0.853613	-3.738043	-1.811312	H	1.310247	-1.816137	4.14591
C	4.278662	0.978618	0.204571	C	0.385305	-3.021383	2.613121
H	4.042073	1.547379	1.117231	H	1.253531	-3.659481	2.474223
C	5.797995	0.709379	0.174521	C	-0.772045	-3.258177	1.869315
H	6.038135	0.11129	-0.713212	H	-0.800137	-4.075655	1.154637
H	6.113997	0.123576	1.042098	C	-4.278111	0.969325	0.162014
C	6.596972	2.025175	0.132812	H	-4.064122	1.702311	-0.631392
H	6.437066	2.574257	1.071507	C	-5.798922	0.707228	0.191718
H	7.667942	1.797427	0.085648	H	-6.017692	-0.044282	0.960357
C	6.183617	2.908906	-1.050948	H	-6.149998	0.295875	-0.758427
H	6.731392	3.857634	-1.026225	C	-6.579912	1.996947	0.504879
H	6.463155	2.411227	-1.990057	H	-6.440324	2.712215	-0.317917
C	4.670878	3.164366	-1.04377	H	-7.651845	1.771903	0.541569
H	4.373378	3.747511	-1.922805	C	-6.121565	2.637899	1.820846
H	4.406552	3.770084	-0.165319	H	-6.656628	3.578746	1.991944
C	3.87229	1.851111	-1.004267	H	-6.381323	1.974056	2.657197
H	2.798853	2.064085	-0.974642	C	-4.606075	2.877601	1.817175
H	4.05973	1.290663	-1.930301	H	-4.279082	3.276688	2.784633
C	3.139308	-0.981765	2.21133	H	-4.357487	3.639115	1.064278
H	2.462181	-0.203929	2.594859	C	-3.825619	1.590452	1.503106
C	2.437091	-2.341556	2.420228	H	-2.750476	1.797331	1.484085
H	3.074372	-3.141813	2.023052	H	-3.996593	0.864299	2.309474
H	1.499143	-2.373408	1.852701	C	-3.253429	-0.608757	-2.217439
C	4.433634	-0.892684	3.045831	H	-2.586313	0.220461	-2.496269
H	4.905991	0.088031	2.928453	C	-2.579257	-1.915861	-2.689766
H	5.158943	-1.64366	2.711608	H	-3.20595	-2.769441	-2.402134
C	4.130434	-1.140501	4.535983	H	-1.614772	-2.047984	-2.18461
H	5.062687	-1.091579	5.110102	C	-4.585626	-0.372564	-2.958282
H	3.489326	-0.330958	4.912278	H	-5.036781	0.577374	-2.653955
C	3.43256	-2.48949	4.756812	H	-5.3047	-1.164602	-2.718539
H	4.120919	-3.301982	4.484815	C	-4.359631	-0.366243	-4.482361
H	3.196875	-2.624298	5.818367	H	-5.318317	-0.216026	-4.991701
C	2.156913	-2.599798	3.910417	H	-3.727138	0.492342	-4.748585
H	1.701885	-3.589464	4.031042	C	-3.691508	-1.66131	-4.963466
H	1.416853	-1.870691	4.268745	H	-4.375792	-2.505168	-4.797429
H	-3.565254	2.293053	1.747062	H	-3.511025	-1.615569	-6.043264
C	-3.355845	3.450821	-1.460829	C	-2.376724	-1.918679	-4.214503
C	-3.455478	4.702104	-0.570663	H	-1.940584	-2.875297	-4.523751

H	-2.582566	3.558871	-2.22098	H	-1.646311	-1.142248	-4.481897
H	-4.311251	3.274232	-1.965289	H	3.516455	2.358249	-1.664506
H	-2.542106	5.303816	-0.563404	H	2.624071	3.502391	2.373792
H	-4.305494	5.349466	-0.80262	H	2.455897	5.27749	0.752064
E Thermal correction to Gibbs Free Energy= 0.785374 E(RM06) = -2917.91041724				**E'** Thermal correction to Gibbs Free Energy= 0.795445 E(RM06) = -2917.96089647			
C	4.477422	2.086765	0.670298	C	0.514718	4.398679	-2.173483
C	0.919582	2.272315	0.282581	C	0.30244	3.608434	-1.072415
C	4.851893	2.538031	-0.546197	C	1.287957	2.736954	-0.406593
C	4.516616	0.664891	1.137688	C	2.676015	3.201969	-0.323392
H	5.241935	0.08637	0.559648	C	3.841439	2.412249	-0.884858
H	4.859131	0.624151	2.179747	C	3.606869	0.909899	-1.060243
N	3.254469	-0.141537	1.114331	H	2.828899	0.771145	-1.820551
S	2.962934	-1.091837	-0.257064	H	4.526304	0.460137	-1.447862
O	1.647755	-1.713471	-0.004229	N	3.250147	0.238644	0.196362
O	3.173576	-0.337284	-1.500552	S	3.074943	-1.466833	0.002548
N	4.977639	3.915681	-0.620016	O	2.412798	-1.939656	1.223117
C	4.808878	4.627993	-1.871208	O	2.505528	-1.764504	-1.320868
H	5.248754	5.626789	-1.790714	N	3.12583	4.29883	0.234632
H	3.749192	4.740348	-2.158495	C	2.325112	5.372038	0.820188
H	5.330302	4.095222	-2.670963	H	1.290076	5.049662	0.911351
C	4.345727	4.473458	0.586825	H	2.373464	6.259179	0.181437
H	3.309453	4.775067	0.355639	H	2.731918	5.617868	1.804077
C	4.353742	3.296974	1.591712	C	5.03211	2.931811	-0.057957
H	3.460049	3.305089	2.226657	C	2.18893	0.898286	0.997544
C	2.069919	0.373272	1.79774	H	2.686788	1.654547	1.622299
H	2.422884	0.923179	2.676526	H	1.805552	0.14919	1.68739
H	1.469735	-0.465574	2.149879	C	1.040836	1.52956	0.190756
C	1.214785	1.296166	0.982534	O	-0.608752	5.088493	-2.497137
C	0.644133	3.375863	-0.557566	H	1.360694	4.547871	-2.827988
C	0.180952	4.612598	-0.170257	C	-1.563733	4.742551	-1.586308
O	0.059507	5.418547	-1.240251	H	-2.523181	5.220421	-1.709143
H	-0.09335	5.024176	0.788269	C	-1.069825	3.846041	-0.691658
C	0.448523	4.704736	-2.344779	H	-1.586195	3.406081	0.148567
H	0.403312	5.234844	-3.282896	C	4.776908	-2.012548	0.003306
C	0.81713	3.447887	-1.992704	C	5.490879	-2.026412	1.205904
H	1.17914	2.658514	-2.634273	H	5.017544	-1.701696	2.126281
C	4.242672	-2.334231	-0.147224	C	6.805439	-2.479498	1.202475
C	4.289598	-3.187013	0.961134	H	7.365146	-2.496858	2.133675
H	3.581381	-3.070089	1.774388	C	7.41995	-2.925301	0.019217
C	5.257587	-4.183527	1.003727	C	6.677049	-2.903282	-1.168487
H	5.299797	-4.848769	1.861815	H	7.133091	-3.250239	-2.091416

C	6.18077	-4.348224	-0.044179	C	5.356144	-2.454042	-1.186736
C	6.102613	-3.484673	-1.144208	H	4.774091	-2.458549	-2.101752
H	6.802597	-3.601037	-1.966601	C	8.835837	-3.445565	0.040366
C	5.13902	-2.477512	-1.206194	H	9.284437	-3.431768	-0.956173
H	5.073946	-1.813612	-2.060888	H	9.468868	-2.856375	0.710595
C	7.238333	-5.421216	0.030431	H	8.861876	-4.481593	0.399028
H	6.821092	-6.366988	0.389686	Au	-0.709751	0.450967	0.087278
H	7.699597	-5.599274	-0.943969	P	-2.511631	-1.094119	-0.312805
H	8.034987	-5.134536	0.727342	C	-3.557653	-1.62501	1.116142
Au	-0.79529	0.473934	0.270098	C	-4.337663	-2.790002	0.971935
P	-2.544199	-0.949881	-0.384597	H	-4.342219	-3.316879	0.026865
C	-3.970175	-1.099596	0.772569	C	-5.107292	-3.296531	2.014973
C	-4.855697	-2.17621	0.560243	H	-5.694126	-4.197547	1.865491
H	-4.705671	-2.836747	-0.283904	C	-5.11137	-2.641336	3.244918
C	-5.926645	-2.425748	1.41275	H	-5.702193	-3.023276	4.071932
H	-6.588522	-3.263663	1.217896	C	-4.352264	-1.486389	3.407137
C	-6.133253	-1.596673	2.513854	H	-4.358774	-0.967324	4.360712
H	-6.960873	-1.777827	3.192737	C	-3.57353	-0.954909	2.363739
C	-5.271857	-0.526956	2.738126	C	-2.832685	0.305755	2.691898
H	-5.436228	0.127046	3.588823	C	-3.364201	1.559514	2.354497
C	-4.189226	-0.24933	1.884734	H	-4.281771	1.611909	1.776195
C	-3.37138	0.951465	2.248377	C	-2.750409	2.734903	2.793285
C	-3.557199	2.177103	1.591194	H	-3.190798	3.696794	2.545336
H	-4.24996	2.237346	0.757306	C	-1.597318	2.673535	3.579135
C	-2.894194	3.32608	2.028016	H	-1.134464	3.587461	3.94057
H	-3.069825	4.271285	1.522366	C	-1.060399	1.430962	3.921869
C	-2.037295	3.266572	3.129333	H	-0.174513	1.372653	4.547963
H	-1.541222	4.164759	3.486044	C	-1.675404	0.255898	3.485256
C	-1.84602	2.051897	3.79211	H	-1.267393	-0.709384	3.770394
H	-1.196078	2.001413	4.660897	C	-3.644322	-0.458128	-1.677958
C	-2.513048	0.904257	3.359104	H	-3.023796	-0.596249	-2.576783
H	-2.382601	-0.033803	3.891075	C	-4.97496	-1.215068	-1.876219
C	-3.155615	-0.432451	-2.086774	H	-5.583218	-1.113525	-0.968976
H	-2.338135	-0.77608	-2.73873	H	-4.804109	-2.285102	-2.021388
C	-4.47351	-1.0908	-2.551393	C	-5.760121	-0.657248	-3.077463
H	-5.283655	-0.783783	-1.878872	H	-5.194417	-0.848609	-4.000106
H	-4.412093	-2.180936	-2.495888	H	-6.706648	-1.200865	-3.175578
C	-4.823436	-0.672424	-3.991441	C	-6.017999	0.848479	-2.940398
H	-4.06087	-1.065357	-4.678136	H	-6.535137	1.228428	-3.828574
H	-5.771691	-1.138943	-4.280611	H	-6.688873	1.025362	-2.088043
C	-4.907573	0.851795	-4.137225	C	-4.705166	1.611225	-2.720057
H	-5.110045	1.123115	-5.179001	H	-4.902831	2.678427	-2.564074
H	-5.754094	1.227464	-3.54588	H	-4.084993	1.538819	-3.624604
C	-3.613838	1.520814	-3.655403	C	-3.91336	1.055513	-1.524658

H	-3.703404	2.611959	-3.705033	H	-2.968894	1.598368	-1.417419
H	-2.788004	1.244174	-4.325708	H	-4.485152	1.226901	-0.60218
C	-3.254085	1.104093	-2.219336	C	-1.611049	-2.611041	-0.988043
H	-2.309743	1.572303	-1.920486	H	-0.827549	-2.123905	-1.586362
H	-4.024368	1.476126	-1.530508	C	-0.89966	-3.372101	0.153142
C	-1.692437	-2.624269	-0.537656	H	-1.651604	-3.842201	0.799714
H	-0.720638	-2.32098	-0.950044	H	-0.328133	-2.67573	0.7771
C	-1.4241	-3.223295	0.860849	C	-2.353996	-3.579892	-1.931602
H	-2.376569	-3.503794	1.327926	H	-2.813401	-3.037188	-2.764324
H	-0.959528	-2.471415	1.509981	H	-3.161165	-4.096058	-1.398183
C	-2.287666	-3.678325	-1.494446	C	-1.383636	-4.640284	-2.485694
H	-2.433633	-3.257659	-2.494597	H	-1.93287	-5.328312	-3.138754
H	-3.267937	-4.016223	-1.137271	H	-0.630951	-4.144524	-3.114185
C	-1.352698	-4.899703	-1.585113	C	-0.680756	-5.408558	-1.358494
H	-1.797499	-5.64585	-2.25308	H	-1.425991	-5.990034	-0.797055
H	-0.404148	-4.591448	-2.045156	H	0.025314	-6.133263	-1.779718
C	-1.078005	-5.507813	-0.203266	C	0.045745	-4.448877	-0.406624
H	-2.012942	-5.915897	0.206102	H	0.496424	-5.000879	0.425894
H	-0.38482	-6.351389	-0.294465	H	0.868834	-3.955254	-0.938244
C	-0.511278	-4.45769	0.762104	H	3.944351	2.800108	-1.913868
H	-0.379408	-4.890184	1.760756	C	4.610906	4.382687	0.225117
H	0.479851	-4.135056	0.420381	H	5.122525	2.36473	0.873388
H	5.100265	1.939183	-1.416059	H	4.921916	5.075428	-0.566603
H	5.220997	3.359835	2.26638	H	5.981706	2.870923	-0.592218
H	4.883639	5.358525	0.939461	H	4.953763	4.779012	1.183598
$TS_{AA'\text{-}CCW}$ Thermal correction to Gibbs Free Energy= 0.788216 Frequency -25.4354 E(RM06) = -2917.90867397				**$TS_{BB'\text{-}CCW}$** Thermal correction to Gibbs Free Energy= 0.797023 Frequency -37.1847 E(RM06) = -2917.94861789			
C	-0.254524	4.946136	-0.822561	C	3.390961	-2.261424	-0.61597
C	0.163875	3.726213	-0.342909	C	1.907991	-2.08937	-0.176866
C	-0.37146	2.472878	-0.759876	C	4.264349	-2.507436	0.567191
Au	0.800437	0.48727	-0.330067	C	3.88423	-0.987715	-1.384164
C	-1.12327	1.620091	-1.206544	H	4.961458	-1.030937	-1.550049
C	-2.1664	0.775755	-1.843019	H	3.381504	-1.006526	-2.35715
N	-3.286597	0.350093	-1.010117	N	3.524928	0.263486	-0.757358
C	-4.380711	1.314479	-0.710874	S	4.474029	0.717939	0.579358
C	-4.042225	2.571891	0.041759	O	3.809308	0.369051	1.849225
C	-3.668643	2.689147	1.335702	O	5.798688	0.129018	0.307935
H	-5.153856	0.728042	-0.201405	N	5.074528	-3.504839	0.43563
H	-4.810224	1.581006	-1.684044	C	6.063323	-3.947265	1.419224
S	-3.005708	-0.909188	0.078468	H	7.060813	-3.887024	0.976312
O	-1.858302	-1.639854	-0.495625	H	5.856419	-4.983233	1.700706

O	-2.923498	-0.42799	1.464533	H	6.015109	-3.305265	2.298253
N	-3.682076	3.994306	1.802436	C	4.945566	-4.182422	-0.88019
C	-2.80307	4.416462	2.87532	H	5.881209	-4.039247	-1.429867
H	-3.165262	5.355958	3.303884	C	3.729441	-3.493311	-1.534885
H	-1.763042	4.571535	2.537598	H	3.975305	-3.160863	-2.545583
H	-2.801908	3.663215	3.667585	C	2.054043	0.387535	-0.627364
C	-3.808434	4.875603	0.630929	H	1.676503	0.793068	-1.575125
H	-2.805705	5.22475	0.326596	H	1.843595	1.146987	0.130204
C	-4.418319	3.963145	-0.457284	C	1.2975	-0.878069	-0.273058
H	-4.04063	4.204497	-1.458139	C	1.272854	-3.293333	0.416143
H	-2.588633	1.365773	-2.666004	C	1.827334	-4.536191	0.635255
H	-1.701246	-0.108713	-2.281073	O	0.967288	-5.370424	1.281817
O	0.396935	5.945032	-0.191819	H	2.778304	-4.989488	0.418259
H	-0.959811	5.230168	-1.587465	C	-0.172868	-4.658683	1.493423
C	1.241602	5.374262	0.718646	H	-0.966566	-5.179486	2.006336
H	1.830068	6.059436	1.308086	C	-0.048032	-3.402214	1.000145
C	1.145075	4.020723	0.672487	H	-0.789243	-2.621591	1.058588
H	1.688856	3.308449	1.272826	C	4.525162	2.492094	0.447818
C	-4.48033	-1.906718	-0.065136	C	4.064424	3.262152	1.515837
C	-4.769662	-2.542316	-1.277862	H	3.646738	2.777307	2.39098
H	-4.122405	-2.407264	-2.137878	C	4.155592	4.651568	1.431612
C	-5.89519	-3.353319	-1.36066	H	3.796363	5.257983	2.258061
H	-6.124432	-3.851757	-2.298508	C	4.705622	5.276597	0.305002
C	-6.739816	-3.543668	-0.252364	C	5.163513	4.471119	-0.752845
C	-6.418978	-2.900099	0.949677	H	5.591836	4.939928	-1.634439
H	-7.054988	-3.041272	1.818757	C	5.081675	3.085274	-0.690598
C	-5.293369	-2.082384	1.0547	H	5.439324	2.472419	-1.51084
H	-5.0405	-1.591794	1.987853	C	4.828949	6.77803	0.230582
C	-7.969319	-4.40959	-0.368388	H	4.194747	7.271044	0.971399
H	-7.75375	-5.336382	-0.908933	H	5.862865	7.091275	0.41867
H	-8.370357	-4.671727	0.613595	H	4.554233	7.152409	-0.760325
H	-8.760277	-3.88959	-0.922	Au	-0.717284	-0.388277	-0.076058
P	2.184473	-1.259867	0.46017	P	-3.006194	0.248632	0.338886
C	3.771693	-1.540347	-0.436089	C	-3.831474	1.472784	-0.776445
C	4.515323	-2.681856	-0.069184	C	-5.010134	2.090794	-0.311281
H	4.15758	-3.32566	0.723247	H	-5.435456	1.784841	0.635236
C	5.708908	-3.016091	-0.70101	C	-5.652123	3.096366	-1.027762
H	6.254099	-3.902009	-0.391004	H	-6.558724	3.546179	-0.634997
C	6.189433	-2.208295	-1.730016	C	-5.116944	3.517935	-2.243367
H	7.118454	-2.453171	-2.235595	H	-5.599857	4.303348	-2.816811
C	5.466539	-1.081963	-2.11048	C	-3.960135	2.915304	-2.726495
H	5.835409	-0.451317	-2.913343	H	-3.553551	3.224873	-3.68425
C	4.259061	-0.723511	-1.484934	C	-3.301624	1.887678	-2.025213
C	3.600517	0.510415	-2.02171	C	-2.098258	1.316974	-2.70486

C	3.861437	1.767981	-1.456547	C	-2.089266	0.003253	-3.198401
H	4.478643	1.835415	-0.565073	H	-2.943558	-0.640744	-3.019368
C	3.368546	2.930236	-2.053931	C	-1.015616	-0.468605	-3.955465
H	3.589568	3.897048	-1.612422	H	-1.036878	-1.483015	-4.342712
C	2.610505	2.851386	-3.223967	C	0.06646	0.36766	-4.236474
H	2.242321	3.757093	-3.696333	H	0.891212	0.007608	-4.844875
C	2.345394	1.604632	-3.794559	C	0.070308	1.677796	-3.751478
H	1.771431	1.536647	-4.714197	H	0.900418	2.341348	-3.977269
C	2.841111	0.441931	-3.200723	C	-1.004203	2.148687	-2.994953
H	2.657467	-0.524799	-3.660703	H	-1.004935	3.172897	-2.633233
C	2.543246	-0.919468	2.277576	C	-4.103516	-1.278664	0.479874
H	1.569869	-1.132191	2.745189	H	-3.769249	-1.710626	1.4364
C	3.620866	-1.799695	2.948913	C	-5.627515	-1.044175	0.555734
H	4.587564	-1.613539	2.466127	H	-5.966264	-0.591113	-0.384094
H	3.400191	-2.862547	2.822225	H	-5.88294	-0.34167	1.353323
C	3.739853	-1.480099	4.450572	C	-6.382602	-2.366901	0.783846
H	2.800456	-1.746526	4.95438	H	-6.116231	-2.76858	1.7717
H	4.518915	-2.11214	4.890967	H	-7.460125	-2.168845	0.810345
C	4.049614	0.001842	4.692547	C	-6.055152	-3.406694	-0.295225
H	4.084373	0.213201	5.766749	H	-6.56324	-4.352842	-0.078055
H	5.047082	0.234897	4.294948	H	-6.44256	-3.059043	-1.263031
C	3.006575	0.89557	4.009981	C	-4.540834	-3.62698	-0.406569
H	3.267303	1.953208	4.13238	H	-4.312477	-4.321956	-1.222747
H	2.031503	0.755799	4.496797	H	-4.170415	-4.097162	0.515558
C	2.866795	0.573924	2.512286	C	-3.789277	-2.304639	-0.632997
H	2.078948	1.196493	2.073923	H	-2.711347	-2.48796	-0.694496
H	3.801415	0.82677	1.992493	H	-4.095043	-1.884373	-1.60059
C	1.133087	-2.814511	0.309656	C	-2.897795	1.013926	2.065012
H	0.139273	-2.429144	0.568103	H	-2.167458	0.333559	2.527689
C	1.077784	-3.270139	-1.166314	C	-2.236885	2.408002	1.988584
H	2.073293	-3.607122	-1.481844	H	-2.928934	3.110001	1.506582
H	0.807933	-2.424476	-1.81032	H	-1.340077	2.36669	1.358447
C	1.433719	-3.998075	1.252814	C	-4.130466	1.035489	2.991962
H	1.41697	-3.67371	2.298216	H	-4.567547	0.03582	3.080507
H	2.430641	-4.408932	1.053152	H	-4.906873	1.69406	2.585204
C	0.394982	-5.117739	1.049817	C	-3.741603	1.547903	4.3921
H	0.633784	-5.95486	1.715472	H	-4.632352	1.574212	5.02994
H	-0.594467	-4.748249	1.350841	H	-3.046581	0.834144	4.856065
C	0.3447	-5.585867	-0.410338	C	-3.084295	2.933113	4.328742
H	1.304491	-6.051096	-0.676082	H	-3.819201	3.667202	3.969634
H	-0.420197	-6.360967	-0.531461	H	-2.786504	3.256766	5.332341
C	0.063079	-4.411003	-1.356536	C	-1.870744	2.928075	3.389051
H	0.089647	-4.746374	-2.39987	H	-1.447317	3.935739	3.305888
H	-0.944349	-4.020435	-1.170978	H	-1.082605	2.291304	3.814648

H	-3.412042	1.884657	2.015536	H	4.245607	-1.911631	1.476004
H	-5.511602	4.082892	-0.497149	H	2.880532	-4.170239	-1.613216
H	-4.416153	5.755501	0.861235	H	4.817843	-5.255967	-0.709611
$TS_{EE'\text{-}CCW}$ Thermal correction to Gibbs Free Energy= 0.796471 Frequency -41.1687 E(RM06) = -2917.95555971				**TS_{AB}** Thermal correction to Gibbs Free Energy= 0.787086 Frequency -200.6850 E(RM06) = -2917.89841641			
C	-0.28836	4.668981	-1.000022	C	3.808678	2.030848	0.923782
C	0.353396	3.480374	-1.224549	C	1.471807	1.701918	-0.002066
C	1.287699	2.722526	-0.350577	C	4.256888	2.693987	-0.196016
C	2.678387	3.194828	-0.232453	C	4.20524	0.614631	1.309295
C	3.839201	2.446763	-0.854861	H	5.218333	0.390576	0.961178
C	3.598065	0.948463	-1.068532	H	4.244954	0.5581	2.403553
H	2.81542	0.831601	-1.826926	N	3.35439	-0.511256	0.884495
H	4.513159	0.506524	-1.474951	S	3.664185	-1.136714	-0.675946
N	3.249295	0.239404	0.17254	O	2.5491	-2.04595	-0.959426
S	3.059039	-1.458013	-0.087178	O	3.988514	-0.050858	-1.620075
O	2.395869	-1.974086	1.114662	N	4.178146	4.035475	-0.100199
O	2.485974	-1.695814	-1.420829	C	4.589612	4.999809	-1.098247
N	3.125362	4.229442	0.427619	H	5.453722	5.579939	-0.749031
C	2.311966	5.210527	1.142738	H	3.775064	5.697437	-1.325236
H	1.347764	4.762685	1.38274	H	4.865107	4.478746	-2.016677
H	2.166806	6.103019	0.527468	C	3.842882	4.436715	1.278174
H	2.827062	5.489886	2.063867	H	3.011378	5.147424	1.275094
C	5.04182	2.920751	-0.015793	C	3.498308	3.095019	1.982231
C	2.197364	0.869546	1.014119	H	2.452504	3.070111	2.308722
H	2.70263	1.606451	1.655747	C	1.946961	-0.454488	1.264923
H	1.823795	0.09805	1.684055	H	1.903653	-0.255635	2.342412
C	1.045658	1.512275	0.22494	H	1.509052	-1.436467	1.097582
O	-1.050566	5.015831	-2.069276	C	1.126191	0.591644	0.531211
H	-0.340624	5.342185	-0.159256	C	1.332215	2.788475	-0.88968
C	-0.897086	4.037683	-3.006173	C	0.951276	4.0798	-0.594403
H	-1.445884	4.175122	-3.92479	O	0.938307	4.836249	-1.708871
C	-0.051004	3.076329	-2.551044	H	0.638	4.558661	0.320622
H	0.252582	2.176601	-3.066173	C	1.331196	4.032198	-2.754439
C	4.75668	-2.017378	-0.111545	H	1.36333	4.510849	-3.720596
C	5.473902	-2.081326	1.087477	C	1.588364	2.776705	-2.317234
H	5.005991	-1.786373	2.02057	H	1.924247	1.925707	-2.891147
C	6.78435	-2.545562	1.06369	C	5.161364	-2.075471	-0.40658
H	7.346385	-2.601744	1.991962	C	5.135106	-3.180342	0.451795
C	7.391642	-2.953641	-0.136786	H	4.224619	-3.443042	0.979475
C	6.645703	-2.881931	-1.320555	C	6.291139	-3.933651	0.616406
H	7.09602	-3.199374	-2.256828	H	6.27749	-4.791065	1.283767

C	5.328805	-2.420584	-1.318414	C	7.476277	-3.609476	-0.067757
H	4.744138	-2.386911	-2.231144	C	7.4702	-2.501664	-0.924166
C	8.802818	-3.487019	-0.138763	H	8.375317	-2.237473	-1.463574
H	9.248515	-3.442011	-1.135685	C	6.319684	-1.732102	-1.102796
H	9.443231	-2.927571	0.549706	H	6.311937	-0.882661	-1.776329
H	8.820573	-4.535265	0.183002	C	8.714236	-4.453578	0.107242
Au	-0.724922	0.473167	0.096257	H	9.597288	-3.964204	-0.31071
P	-2.624946	-0.945709	-0.291274	H	8.907233	-4.662679	1.164259
C	-3.531437	-1.636909	1.16387	H	8.599933	-5.420547	-0.396758
C	-4.421683	-2.707313	0.943055	Au	-0.925248	0.162143	0.183761
H	-4.601869	-3.053822	-0.066035	P	-3.113432	-0.545829	-0.422766
C	-5.080435	-3.347202	1.988744	C	-4.161596	-1.283452	0.906281
H	-5.758785	-4.168286	1.778441	C	-5.292754	-2.025035	0.508463
C	-4.854945	-2.928803	3.298813	H	-5.554115	-2.082771	-0.539842
H	-5.355442	-3.418693	4.128546	C	-6.092922	-2.699064	1.426024
C	-3.984536	-1.870112	3.538679	H	-6.95636	-3.259312	1.081176
H	-3.815984	-1.531872	4.556467	C	-5.77037	-2.651216	2.780904
C	-3.317809	-1.202443	2.495585	H	-6.378949	-3.174815	3.511822
C	-2.441067	-0.063623	2.915153	C	-4.663444	-1.917312	3.195634
C	-2.85388	1.266918	2.748698	H	-4.419961	-1.86214	4.252116
H	-3.788089	1.476647	2.236953	C	-3.848528	-1.217214	2.287636
C	-2.096855	2.317995	3.269646	C	-2.723194	-0.441711	2.897204
H	-2.44409	3.340261	3.149462	C	-2.770698	0.958227	2.985433
C	-0.916687	2.053981	3.967811	H	-3.603253	1.493294	2.539679
H	-0.34108	2.870347	4.39536	C	-1.783668	1.662757	3.676946
C	-0.495203	0.733527	4.138912	H	-1.848361	2.744393	3.752084
H	0.413098	0.51695	4.694215	C	-0.7354	0.978241	4.295804
C	-1.253836	-0.317594	3.620669	H	0.019773	1.525197	4.852858
H	-0.932857	-1.344264	3.77008	C	-0.679189	-0.415164	4.217991
C	-3.858495	-0.085561	-1.426479	H	0.121119	-0.957918	4.713206
H	-3.337175	-0.115463	-2.395963	C	-1.667476	-1.120001	3.52782
C	-5.24068	-0.752045	-1.591466	H	-1.631991	-2.204792	3.485499
H	-5.752712	-0.759666	-0.62138	C	-4.05205	0.851029	-1.267704
H	-5.142318	-1.79541	-1.903552	H	-3.574208	0.88094	-2.259061
C	-6.106456	0.005565	-2.614911	C	-5.569079	0.635066	-1.457639
H	-5.643149	-0.072431	-3.608591	H	-6.046971	0.564201	-0.472837
H	-7.08613	-0.479781	-2.690721	H	-5.773014	-0.306494	-1.974879
C	-6.267915	1.484567	-2.241913	C	-6.200647	1.796242	-2.247606
H	-6.846517	2.009717	-3.010154	H	-5.795132	1.801115	-3.269023
H	-6.84385	1.562498	-1.309207	H	-7.278569	1.623736	-2.342633
C	-4.901303	2.155214	-2.051032	C	-5.93029	3.15235	-1.584248
H	-5.025177	3.194801	-1.726054	H	-6.347804	3.96248	-2.192187
H	-4.374472	2.190666	-3.01533	H	-6.445712	3.191629	-0.614523
C	-4.030395	1.39976	-1.033626	C	-4.426647	3.368497	-1.369005

H	-3.051656	1.882981	-0.944687	H	-4.24597	4.311887	-0.840956
H	-4.503602	1.456032	-0.043611	H	-3.92668	3.455909	-2.343933
C	-1.870596	-2.38655	-1.249542	C	-3.791241	2.210656	-0.581212
H	-1.155882	-1.84497	-1.886448	H	-2.714134	2.376579	-0.46839
C	-1.044729	-3.285083	-0.301336	H	-4.215916	2.189454	0.431405
H	-1.726225	-3.817462	0.374705	C	-2.774499	-1.866004	-1.727782
H	-0.383052	-2.67569	0.32465	H	-1.953702	-1.384619	-2.279543
C	-2.755952	-3.231319	-2.188072	C	-2.200161	-3.139933	-1.069374
H	-3.305853	-2.591795	-2.886503	H	-2.988138	-3.63028	-0.483682
H	-3.49849	-3.794677	-1.610476	H	-1.399878	-2.876268	-0.367388
C	-1.894148	-4.232106	-2.981359	C	-3.862576	-2.216898	-2.763738
H	-2.540792	-4.83448	-3.629823	H	-4.236991	-1.31431	-3.257549
H	-1.216954	-3.675576	-3.644261	H	-4.717374	-2.698471	-2.274677
C	-1.070846	-5.133558	-2.05134	C	-3.299197	-3.184032	-3.822808
H	-1.752456	-5.770209	-1.469457	H	-4.088932	-3.436305	-4.539398
H	-0.442351	-5.810112	-2.641633	H	-2.511041	-2.673217	-4.393156
C	-0.206046	-4.301763	-1.094416	C	-2.725586	-4.455352	-3.182717
H	0.325682	-4.955079	-0.393315	H	-3.540028	-5.021738	-2.709482
H	0.563368	-3.761577	-1.660916	H	-2.300778	-5.107407	-3.95384
H	3.923843	2.873117	-1.86916	C	-1.661891	-4.115955	-2.129563
C	4.610633	4.333916	0.406327	H	-1.30623	-5.027761	-1.63683
H	5.164764	2.276277	0.859799	H	-0.788219	-3.666361	-2.620386
H	4.899509	5.102703	-0.320055	H	4.603472	2.230645	-1.112519
H	5.978046	2.922119	-0.576385	H	4.110715	2.953046	2.880614
H	4.962522	4.641231	1.393574	H	4.707013	4.943058	1.729579
$TS_{A'B'}$ Thermal correction to Gibbs Free Energy= 0.788946 Frequency -127.5747 E(RM06) = -2917.90394755				**$TS_{A'E'}$** Thermal correction to Gibbs Free Energy= 0.787559 Frequency -359.5036 E(RM06) = -2917.86116028			
C	-3.881054	2.300345	-0.373092	C	2.891374	3.430678	-0.382229
C	-1.247073	1.965261	-0.199293	C	1.269826	2.586154	-0.441122
C	-3.818325	2.819239	0.887217	C	3.919291	2.518034	-0.056299
C	-4.100939	0.853117	-0.726691	C	4.003871	1.143778	-0.629241
H	-5.175673	0.632983	-0.779289	H	3.502901	1.121875	-1.605296
H	-3.706463	0.645692	-1.730588	H	5.043286	0.823183	-0.754855
N	-3.463157	-0.07014	0.209657	N	3.338161	0.216075	0.326486
S	-4.372906	-0.795829	1.429337	S	3.021041	-1.349717	-0.338458
O	-3.402306	-1.469394	2.296714	O	2.143465	-1.998609	0.64196
O	-5.27919	0.239725	1.936427	O	2.61984	-1.226491	-1.747251
N	-3.78595	4.184276	0.90456	N	2.99761	4.578577	0.456065
C	-4.087231	4.97935	2.082292	C	2.589905	5.8698	-0.085386
H	-5.163735	5.185558	2.170252	H	1.584872	5.801411	-0.503913
H	-3.55686	5.935206	2.034633	H	3.276437	6.237161	-0.867655

H	-3.763517	4.445527	2.978602	H	2.57004	6.607066	0.721686
C	-4.146096	4.695664	-0.43434	C	4.803647	3.097424	1.004492
H	-5.156677	5.125474	-0.398033	C	2.20692	0.821854	1.060357
C	-4.082443	3.444369	-1.352732	H	2.648188	1.631466	1.663419
H	-5.005546	3.323848	-1.933062	H	1.815537	0.076466	1.748815
C	-2.083594	-0.459848	-0.027819	C	1.122452	1.459265	0.224748
H	-1.985081	-1.012907	-0.974523	C	0.368498	3.330774	-1.324739
H	-1.783766	-1.131616	0.776389	C	0.259862	3.218411	-2.685384
C	-1.114927	0.698568	-0.096229	O	-0.689976	4.062279	-3.158421
C	-0.907516	3.311774	-0.378871	H	0.752969	2.594305	-3.415181
C	-0.854397	4.289424	0.601439	C	-1.204883	4.734033	-2.088074
O	-0.521008	5.475944	0.067693	H	-1.983987	5.446502	-2.310053
H	-0.984169	4.253926	1.67095	C	-0.595757	4.335289	-0.93961
C	-0.363478	5.293029	-1.287958	H	-0.800235	4.679999	0.063311
H	-0.086308	6.173313	-1.846117	C	4.64233	-2.093681	-0.28228
C	-0.59247	4.000981	-1.619885	C	5.170066	-2.494541	0.949869
H	-0.531065	3.556385	-2.601952	H	4.602606	-2.347428	1.862394
C	-5.382268	-2.040793	0.63366	C	6.423386	-3.095358	0.979685
C	-4.83051	-3.294143	0.350725	H	6.839753	-3.411079	1.932275
H	-3.812246	-3.521584	0.647853	C	7.157763	-3.309427	-0.200033
C	-5.616124	-4.251393	-0.284052	C	6.599415	-2.900937	-1.418734
H	-5.193898	-5.229339	-0.498978	H	7.149974	-3.063882	-2.340835
C	-6.948233	-3.98224	-0.638867	C	5.343482	-2.296237	-1.471821
C	-7.476528	-2.719914	-0.335608	H	4.903577	-1.998538	-2.417238
H	-8.508609	-2.496789	-0.591379	C	8.502149	-3.991521	-0.151282
C	-6.706591	-1.74752	0.301655	H	9.081543	-3.804324	-1.058751
H	-7.128845	-0.783756	0.563642	H	9.090119	-3.654914	0.707817
C	-7.799075	-5.041964	-1.294151	H	8.381295	-5.077192	-0.05474
H	-8.240628	-5.705118	-0.540369	Au	-0.715548	0.455963	0.120582
H	-8.621513	-4.601229	-1.863682	P	-2.644964	-0.892635	-0.273709
H	-7.209619	-5.667773	-1.970509	C	-3.403307	-1.757853	1.170528
Au	0.954056	0.180675	-0.027429	C	-4.299234	-2.812873	0.903367
P	3.217213	-0.441815	0.365587	H	-4.566195	-3.042549	-0.119845
C	3.881583	-1.868728	-0.598897	C	-4.854115	-3.583916	1.920331
C	5.06588	-2.474536	-0.131683	H	-5.540995	-4.388097	1.675559
H	5.584756	-2.052229	0.718558	C	-4.514122	-3.317148	3.245283
C	5.596217	-3.614376	-0.728232	H	-4.932459	-3.910815	4.052382
H	6.510799	-4.051701	-0.340237	C	-3.636349	-2.27599	3.5308
C	4.939994	-4.185768	-1.81677	H	-3.380863	-2.05517	4.562562
H	5.334734	-5.078201	-2.292642	C	-3.073663	-1.476085	2.51994
C	3.775177	-3.597781	-2.299737	C	-2.175446	-0.375312	2.990381
H	3.272537	-4.028343	-3.160191	C	-2.600017	0.962064	2.981185
C	3.228429	-2.437723	-1.721576	H	-3.569491	1.211914	2.56168
C	1.998803	-1.904843	-2.386794	C	-1.806834	1.965635	3.540742

C	2.042133	-0.737273	-3.164587	H	-2.159547	2.992903	3.54007
H	2.965442	-0.170022	-3.22497	C	-0.578992	1.646489	4.124257
C	0.926641	-0.32646	-3.896753	H	0.027901	2.42506	4.577297
H	0.986516	0.567554	-4.510653	C	-0.148669	0.317769	4.144459
C	-0.249304	-1.079019	-3.866867	H	0.795556	0.056715	4.614325
H	-1.10948	-0.771027	-4.454063	C	-0.941685	-0.686153	3.584989
C	-0.303773	-2.244551	-3.098942	H	-0.610541	-1.720042	3.613866
H	-1.207351	-2.84757	-3.085991	C	-3.96757	0.105569	-1.168713
C	0.812372	-2.656257	-2.367727	H	-3.545182	0.188399	-2.182104
H	0.773636	-3.573633	-1.78742	C	-5.365097	-0.543296	-1.268263
C	4.354292	1.046326	0.165527	H	-5.777182	-0.662421	-0.258693
H	4.15019	1.615818	1.085333	H	-5.307071	-1.544137	-1.704743
C	5.866348	0.739929	0.100649	C	-6.32122	0.323274	-2.108587
H	6.071634	0.138023	-0.793069	H	-5.960001	0.358119	-3.145965
H	6.186993	0.145817	0.960762	H	-7.307659	-0.153034	-2.139411
C	6.693735	2.037284	0.042173	C	-6.431388	1.750531	-1.558024
H	6.567211	2.589519	0.983844	H	-7.07744	2.357358	-2.202109
H	7.75736	1.783623	-0.028115	H	-6.912174	1.722481	-0.570265
C	6.275462	2.929058	-1.133348	C	-5.04636	2.398061	-1.429777
H	6.844959	3.864807	-1.121456	H	-5.128822	3.393752	-0.978547
H	6.522406	2.424681	-2.077873	H	-4.616713	2.54309	-2.431104
C	4.769862	3.221397	-1.092473	C	-4.087164	1.53487	-0.593322
H	4.468614	3.808492	-1.967644	H	-3.100734	2.008501	-0.544793
H	4.540501	3.835863	-0.210481	H	-4.462865	1.476622	0.437203
C	3.939312	1.928393	-1.033421	C	-1.996603	-2.191795	-1.478375
H	2.871711	2.168069	-0.976551	H	-1.341205	-1.566358	-2.102049
H	4.087868	1.363719	-1.963494	C	-1.094716	-3.207759	-0.742365
C	3.212987	-0.899986	2.196603	H	-1.716963	-3.837196	-0.093314
H	2.565632	-0.103431	2.592276	H	-0.377466	-2.689927	-0.09625
C	2.479643	-2.241586	2.41623	C	-2.974545	-2.904095	-2.435074
H	3.088929	-3.057037	2.006542	H	-3.584898	-2.178579	-2.982741
H	1.530219	-2.250211	1.866788	H	-3.661494	-3.547987	-1.872964
C	4.526917	-0.846064	3.003798	C	-2.195893	-3.777193	-3.437937
H	5.022528	0.121917	2.877712	H	-2.90394	-4.290729	-4.098333
H	5.224117	-1.616414	2.654479	H	-1.584816	-3.127149	-4.079561
C	4.244816	-1.087132	4.499379	C	-1.289266	-4.790657	-2.726229
H	5.189412	-1.063749	5.054178	H	-1.913111	-5.510995	-2.178345
H	3.633985	-0.260511	4.888154	H	-0.721	-5.369654	-3.462946
C	3.515417	-2.417012	4.733022	C	-0.336266	-4.09347	-1.745478
H	4.176352	-3.247818	4.448864	H	0.257412	-4.833454	-1.197034
H	3.29585	-2.545125	5.798577	H	0.378209	-3.470796	-2.300657
C	2.221068	-2.492732	3.91167	H	2.807215	3.60508	-1.462233
H	1.742514	-3.470025	4.039464	C	4.344327	4.571897	1.066741
H	1.506934	-1.745274	4.283799	H	4.684183	2.569508	1.960274

H	-3.771621	2.260812	1.813594	H	5.030321	5.205209	0.48011
H	-3.264186	3.521793	-2.078419	H	5.861084	2.978599	0.736927
H	-3.456674	5.48882	-0.737882	H	4.312722	4.96948	2.084759
$TS_{B'C}$ Thermal correction to Gibbs Free Energy= 0.795068 Frequency -296.6986 E(RM06) = -2917.92719477				**C** Thermal correction to Gibbs Free Energy= 0.797261 E(RM06) = -2917.93882237			
C	-3.5102	3.561083	0.758796	C	3.545431	3.599035	-0.687242
C	-1.729465	3.796509	1.58896	C	2.171517	3.739585	-1.497142
N	-3.979969	4.608726	0.044308	N	3.948605	4.655086	0.185066
C	-3.563065	4.535108	-1.35995	C	3.311967	4.485423	1.482633
C	-3.457034	3.025458	-1.604806	C	3.410573	2.974548	1.692263
C	-3.172426	2.392245	-0.195142	C	3.218484	2.372779	0.262181
C	-4.02341	1.129177	0.017467	C	4.059212	1.105865	0.072368
H	-5.079039	1.325986	-0.176282	H	5.106917	1.288563	0.316055
H	-3.909936	0.756236	1.048307	H	3.992071	0.743179	-0.966901
N	-3.542063	0.167452	-0.969008	N	3.529376	0.129994	1.026279
S	-4.650463	-0.838114	-1.750909	S	4.587516	-0.947101	1.78704
C	-2.149095	-0.290631	-0.832866	C	2.12639	-0.278223	0.882879
O	-5.848453	-0.016533	-1.947333	O	5.811641	-0.184215	2.035129
O	-3.913245	-1.436026	-2.864423	O	3.802207	-1.558895	2.860417
C	-1.691603	1.999449	-0.036639	C	1.736337	2.002645	0.039016
C	-1.191234	0.785681	-0.379011	C	1.189493	0.791619	0.396575
H	-2.066162	-1.124429	-0.115422	H	2.014455	-1.121649	0.176684
H	-1.834003	-0.680902	-1.80484	H	1.78264	-0.654966	1.85269
H	-4.024532	3.369624	1.697711	H	4.328201	3.39453	-1.425234
C	-0.987174	3.096584	0.589446	C	1.13426	3.041391	-0.702993
O	-1.068507	5.016989	1.830287	O	1.577215	5.009093	-1.863449
C	0.004107	5.037758	1.026063	C	0.299036	4.932104	-1.496699
H	0.590589	5.947123	1.047407	H	-0.303636	5.8027	-1.730351
C	0.129208	3.898067	0.263246	C	-0.057755	3.772987	-0.833767
H	0.871195	3.711839	-0.498785	H	-1.024406	3.565972	-0.399649
C	-5.065895	-2.148555	-0.601809	C	4.968837	-2.226592	0.591847
C	-4.316732	-3.32825	-0.604034	C	4.203869	-3.395654	0.566468
H	-3.529058	-3.466009	-1.336694	H	3.423069	-3.544981	1.304262
C	-4.624855	-4.329922	0.315667	C	4.489545	-4.373676	-0.385836
H	-4.054067	-5.254712	0.307335	H	3.907785	-5.291593	-0.398145
C	-5.673169	-4.175993	1.235515	C	5.530299	-4.205803	-1.311696
C	-6.413294	-2.983777	1.209262	C	6.286689	-3.024472	-1.257463
H	-7.239214	-2.852888	1.903218	H	7.107505	-2.883674	-1.955484
C	-6.121257	-1.971915	0.297631	C	6.018323	-2.037307	-0.312319
H	-6.720188	-1.068471	0.260037	H	6.631443	-1.144522	-0.253457
C	-6.027667	-5.282858	2.197932	C	5.861368	-5.287679	-2.310171

H	-6.41772	-4.886419	3.139707	H	6.230815	-4.867242	-3.249902
H	-6.803117	-5.931531	1.77275	H	6.645691	-5.947238	-1.919511
H	-5.162913	-5.913257	2.422352	H	4.991129	-5.911593	-2.531251
C	-4.380987	5.864611	0.654276	C	4.163564	5.988847	-0.34183
H	-4.886644	5.669592	1.603057	H	4.771375	5.932088	-1.250352
H	-3.513941	6.511433	0.846038	H	3.232911	6.524557	-0.587575
H	-5.072846	6.388633	-0.009009	H	4.715736	6.581064	0.3937
H	-2.009898	3.326467	2.525905	H	2.320513	3.2085	-2.446143
Au	0.785697	0.216624	-0.231358	Au	-0.78316	0.238281	0.221042
P	3.13169	-0.354934	-0.269926	P	-3.129978	-0.326807	0.280133
C	3.838098	-1.285535	1.163964	C	-3.835954	-1.250262	-1.156088
C	5.237175	-1.278939	1.336036	C	-5.236243	-1.254933	-1.318086
H	5.865593	-0.806908	0.592724	H	-5.864033	-0.792274	-0.568103
C	5.848789	-1.860839	2.442448	C	-5.849052	-1.837152	-2.42366
H	6.929844	-1.835744	2.538119	H	-6.930803	-1.821836	-2.51267
C	5.061902	-2.466496	3.420248	C	-5.06261	-2.430821	-3.409261
H	5.519404	-2.920985	4.293722	H	-5.521634	-2.885466	-4.281798
C	3.679824	-2.497365	3.263363	C	-3.679055	-2.449055	-3.262348
H	3.064676	-2.989794	4.010122	H	-3.064498	-2.931218	-4.016238
C	3.04226	-1.928742	2.145591	C	-3.039821	-1.879592	-2.146211
C	1.556978	-2.10052	2.094713	C	-1.551875	-2.033296	-2.106128
C	0.96628	-3.002095	1.196131	C	-0.945203	-2.945939	-1.229229
H	1.589693	-3.526055	0.478785	H	-1.558274	-3.492813	-0.520062
C	-0.402681	-3.26969	1.251113	C	0.426912	-3.195069	-1.296831
H	-0.83887	-3.984698	0.559667	H	0.876166	-3.919381	-0.623806
C	-1.203933	-2.642783	2.208023	C	1.215419	-2.538619	-2.244765
H	-2.265569	-2.866476	2.258203	H	2.27894	-2.749937	-2.305918
C	-0.62678	-1.744093	3.108197	C	0.622391	-1.628918	-3.123508
H	-1.238795	-1.262309	3.865479	H	1.224013	-1.126021	-3.875348
C	0.742633	-1.479175	3.055723	C	-0.750115	-1.382044	-3.058472
H	1.191496	-0.79514	3.770261	H	-1.211701	-0.691355	-3.758419
C	3.561818	-1.250376	-1.872867	C	-3.535703	-1.236381	1.880406
H	3.568549	-0.425175	-2.601714	H	-3.534117	-0.417986	2.616823
C	4.934797	-1.954359	-1.9139	C	-4.908036	-1.941559	1.929907
H	4.948526	-2.755121	-1.16411	H	-4.92983	-2.734753	1.172364
H	5.741912	-1.265161	-1.650079	H	-5.718341	-1.249972	1.682713
C	5.212114	-2.553154	-3.305279	C	-5.168212	-2.554669	3.318384
H	5.303519	-1.738316	-4.037139	H	-5.250969	-1.747593	4.059699
H	6.179738	-3.067345	-3.291221	H	-6.135864	-3.068735	3.310201
C	4.099956	-3.512613	-3.747246	C	-4.050748	-3.51864	3.736292
H	4.297975	-3.882457	-4.759261	H	-4.236215	-3.89903	4.74665
H	4.096257	-4.392115	-3.088293	H	-4.055049	-4.391183	3.068209
C	2.727871	-2.828544	-3.688904	C	-2.679571	-2.833682	3.668986
H	1.933295	-3.536936	-3.949205	H	-1.881707	-3.544544	3.911501

H	2.686529	-2.025903	-4.438489	H	-2.629011	-2.039274	4.426603
C	2.447965	-2.232975	-2.299044	C	-2.416233	-2.222842	2.282397
H	1.475459	-1.728877	-2.293434	H	-1.443929	-1.718131	2.272389
H	2.385963	-3.048029	-1.566092	H	-2.361973	-3.02936	1.539471
C	3.996235	1.324107	-0.358186	C	-3.995846	1.349365	0.386223
H	3.314557	1.849994	-1.043832	H	-3.306758	1.876764	1.063191
C	3.924237	2.044609	1.005575	C	-3.949771	2.072451	-0.977247
H	4.573554	1.52704	1.72237	H	-4.613967	1.557535	-1.682006
H	2.905729	1.989474	1.409604	H	-2.940714	2.013792	-1.405353
C	5.407052	1.438676	-0.972835	C	-5.398458	1.455809	1.021072
H	5.441415	0.964542	-1.958612	H	-5.416528	0.97899	2.005891
H	6.144219	0.927956	-0.342943	H	-6.141703	0.943013	0.399912
C	5.820629	2.917075	-1.099822	C	-5.815028	2.932583	1.158634
H	6.830305	2.978015	-1.520863	H	-6.819696	2.988195	1.59188
H	5.154268	3.418239	-1.816114	H	-5.141888	3.432664	1.869061
C	5.758156	3.641185	0.251625	C	-5.771944	3.663432	-0.189998
H	6.505762	3.208011	0.930411	H	-6.527714	3.233023	-0.861363
H	6.024774	4.696923	0.129504	H	-6.037662	4.718086	-0.058735
C	4.366106	3.513352	0.885744	C	-4.388555	3.541144	-0.844398
H	4.351581	3.982996	1.876128	H	-4.389259	4.015651	-1.832561
H	3.6375	4.059915	0.268652	H	-3.653753	4.086621	-0.232925
H	-2.606137	5.059074	-1.503482	H	2.259488	4.831808	1.492811
H	-4.400496	2.633724	-1.99396	H	4.40324	2.710659	2.06735
H	-4.31021	5.023157	-1.992011	H	3.848048	5.057358	2.246374
H	-2.676039	2.774806	-2.322825	H	2.673358	2.588739	2.398744
D Thermal correction to Gibbs Free Energy= 0.798343 E(RM06) = -2917.96765532							
C	3.167189	1.150527	1.701031				
S	1.793261	1.694822	-0.533909				
C	4.064179	0.260744	-0.491903				
H	3.729701	0.056363	-1.50962				
H	4.873752	1.003064	-0.518746				
N	2.907678	0.773575	0.286421				
O	7.725167	-2.653061	1.068435				
O	1.552561	1.071581	-1.834241				
C	4.876253	-0.680398	1.652707				
O	0.642533	1.843012	0.428794				
C	4.527642	-1.024028	0.198901				
N	5.298435	-2.79542	-1.232039				
C	4.236146	0.288685	2.31878				
H	4.513133	0.555585	3.334981				
H	1.643343	4.113912	1.09149				

H	3.484744	2.20507	1.768296
H	2.220306	1.064803	2.243349
C	3.45769	-2.164625	0.079903
C	4.221955	-3.389941	-0.444275
C	5.815277	-1.686405	-0.435448
H	6.390196	-1.010556	-1.083658
C	6.055112	-1.464576	1.987752
C	6.566021	-1.99479	0.838727
C	7.951081	-2.540217	2.424203
H	8.840582	-3.03219	2.786041
C	6.970396	-1.81765	3.037395
H	6.918124	-1.588206	4.091735
C	2.406988	3.350287	-0.780519
C	2.22121	4.330421	0.200391
C	2.76612	5.595725	-0.004725
H	2.620529	6.363413	0.749772
C	3.49225	5.898386	-1.166795
C	3.660231	4.892293	-2.13147
H	4.212665	5.110067	-3.040992
C	3.125648	3.620063	-1.950551
H	3.241353	2.856626	-2.711899
C	4.050539	7.28091	-1.391197
H	4.980468	7.248478	-1.965337
H	3.339893	7.896255	-1.956282
H	4.246963	7.792846	-0.44564
C	6.29292	-3.728072	-1.743316
H	7.039021	-3.185539	-2.33262
H	6.820251	-4.288014	-0.953036
H	5.803467	-4.449593	-2.40498
Au	-1.264431	0.752175	0.311981
P	-3.363863	-0.19708	0.408187
C	-4.260898	-0.191555	-1.206884
C	-5.48349	0.500424	-1.277001
H	-5.863922	1.019067	-0.409657
C	-6.240711	0.538206	-2.445926
H	-7.178696	1.084087	-2.461314
C	-5.787287	-0.129688	-3.579267
H	-6.364912	-0.114219	-4.498288
H	-4.213278	-1.332751	-4.412487
C	-4.577522	-0.818359	-3.528726
C	-3.78874	-0.86069	-2.367768
C	-2.510965	-1.633782	-2.47031
C	-2.555695	-3.026524	-2.649712
H	-3.516513	-3.533358	-2.65661

C	-1.382631	-3.761403	-2.829319	
H	-1.437135	-4.837427	-2.965781	
C	-0.146327	-3.112111	-2.848666	
H	0.765813	-3.682143	-2.998296	
H	0.857561	-1.199876	-2.744825	
C	-0.090484	-1.724943	-2.702063	
C	-1.264831	-0.990492	-2.520858	
H	-1.212235	0.092444	-2.464932	
H	-3.502961	-1.717173	2.213957	
C	-3.322064	-1.926942	1.149429	
C	-4.457749	-2.841732	0.643208	
H	-4.315419	-3.03271	-0.42538	
H	-5.431301	-2.350609	0.744659	
H	-4.70684	-4.000157	2.458101	
C	-4.457232	-4.180167	1.403035	
H	-5.248676	-4.823411	1.002526	
H	-3.108638	-5.809919	1.892849	
C	-3.094891	-4.881064	1.312254	
H	-2.901761	-5.165579	0.268973	
H	-0.99418	-4.457742	1.689188	
C	-1.965924	-3.96482	1.804786	
H	-2.093566	-3.776602	2.880239	
C	-1.947315	-2.622404	1.053007	
H	-1.171957	-1.971266	1.472959	
H	-1.687738	-2.79009	0.003016	
C	-4.267075	0.810327	1.717796	
H	-3.559302	0.660325	2.548272	
C	-4.297898	2.331858	1.446082	
H	-4.95473	2.559985	0.599417	
H	-3.297826	2.681549	1.163888	
H	-5.570038	-0.783083	2.459622	
C	-5.636116	0.279267	2.205021	
H	-6.390477	0.362516	1.41551	
H	-7.09776	0.704944	3.742281	
C	-6.110984	1.070986	3.438289	
H	-5.431657	0.87044	4.278371	
H	-6.916184	2.792981	2.404205	
C	-6.154927	2.580614	3.167943	
H	-6.464482	3.116424	4.071695	
H	-4.8452	4.165934	2.455272	
C	-4.792009	3.096457	2.68673	
H	-4.0549	2.987638	3.494549	
H	2.965964	-2.359867	1.035157	
H	3.605313	-4.039136	-1.075404	

H	2.684709	-1.8638	-0.633311	
H	4.598879	-4.004716	0.393399	