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Supporting Information

Acyl Migration versus Epoxidation in Gold Catalysis: Facile, Switchable, and Atom-Economic Synthesis of Acylindoles and Quinoline Derivatives

Xianhai Tian[+], Lina Song[+], Kaveh Farshadfar, Matthias Rudolph, Frank Rominger, Thomas Oeser, Alireza Ariafard, and A. Stephen K. Hashmi**

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Contents

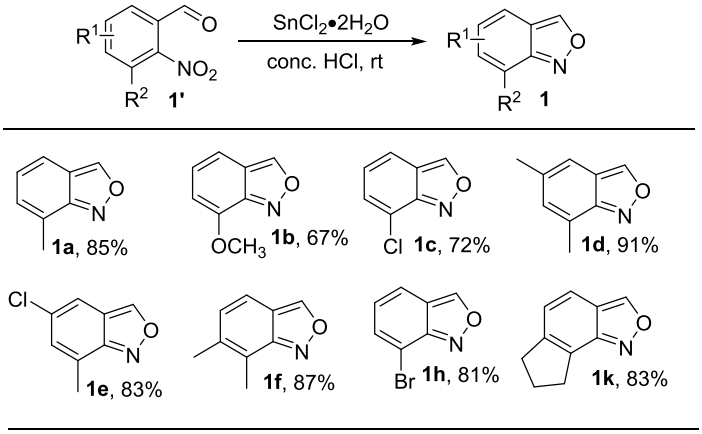
1. General Methods

Chemicals were purchased from commercial suppliers and used as delivered. The reagents **1**,[1] **2**[2] have been prepared according to the literature. Dry solvents were dispensed from the solvent purification system MB SPS-800. Deuterated solvents were bought from Euriso-Top. NMR spectra were, if not mentioned otherwise, recorded at room temperature on the following spectrometers: Bruker Avance-III-300, Bruker Avance III 400, and Bruker Avance-III-500. Chemical shifts are given in ppm and coupling constants in Hz. The following abbreviations were used for ^{1}H NMR spectra to indicate the signal multiplicity: s (singlet), brs (broad singlet), d (doublet), t (triplet), q (quartet), quint (quintet), sext (sextet), sept (septet) and m (multiplet) as well as combinations of them. When combinations of multiplicities are given the first character noted refers to the biggest coupling constant. All ^{13}C NMR spectra were measured with ^{1}H-decoupling. The multiplicities mentioned in these spectra [s (singlet, quaternary carbon), d (doublet, CH-group), t (triplet, CH_2-group), q (quartet, CH_3-group)] were determined by DEPT135 spectra. Mass spectra (MS and HRMS) were determined at the chemistry department of the University of Heidelberg under the direction of Dr. J. Gross. EI^+-spectra were measured on a JOEL JMS-700 spectrometer. For EI^+-, ESI^+-, ESI^-- or $DART^+$-spectra a Bruker Apex-Qu FT-ICR-MS spectrometer was applied. Infrared Spectroscopy (IR) was processed on an FT-IR Bruker (IF528), IR Perkin Elmer (283) or FT-IR Bruker Vector 22. The solvent or matrix is denoted in brackets. For the most significant bands the wave number ν (cm^{-1}) is given. X-ray crystal structure analyses were measured at the chemistry department of the University of Heidelberg under the direction of Dr. F. Rominger and T. Oeser on a Bruker Smart CCD or Bruker APEX-II CCD instrument using Mo-Kα-radiation. Diffraction intensities were corrected for Lorentz and polarization effects. An empirical absorption correction was applied using SADABS based on the Laue symmetry of reciprocal space. Heavy atom diffractions were solved by direct methods and refined against F2 with full matrix least square algorithm. Hydrogen atoms were either isotropically refined or calculated. The structures were solved and refined by Dr. F. Rominger and T. Oeser using the SHELXTL software package. Gas Chromatography / Mass Spectrometry (GC/MS) spectra were measured on two different hardware systems: 1. HP 5972 Mass Selective Detector, coupled with a HP 5890 SERIES II plus gas chromatograph. 2. Agilent 5975C Mass Selective Detector, coupled with an Agilent 7890A gas chromatograph. In both cases, as a capillary column, an OPTIMA 5 cross-linked Methyl Silicone column (30 m x 0.32 mm, 0.25 µm) was employed and helium was used as the carrier gas. Gas Chromatography (GC) was carried out on a HP 5890 SERIES II plus gas chromatograph. As a capillary column, an OPTIMA 5 cross-linked Methyl Silicone column (30 m x 0.32 mm, 0.25 µm) was employed and nitrogen was used as the carrier gas. Melting Points were measured in open glass capillaries in a Büchi melting point apparatus (according to Dr. Tottoli) and were not calibrated. Flash Column Chromatography was accomplished using Silica gel 60 (0.04 - 0.063 mm / 230 - 400 mesh ASTM) purchased from Aldrich or Aluminium oxide (neutral or basic) purchased from Aldrich. As eluents, mixtures of petroleum ether (PE), ethyl acetate (EA) were used. Analytical Thin Layer Chromatography (TLC) was carried out on precoated Macherey-Nagel POLYGRAM® SIL G/UV254 or POLYGRAM® ALOX N/UV254 plastic sheets. Detection was accomplished using UV-light (254 nm), $KMnO_4$ (in 1.5 M Na_2CO_3 (aq.)), molybdatophosphoric acid (5% in ethanol), vanillin/H_2SO_4 (in ethanol) or

anisaldehyde/HOAc (in ethanol). IUPAC names of the compounds described in the experimental section were determined with the program ACDLabs 12.0®

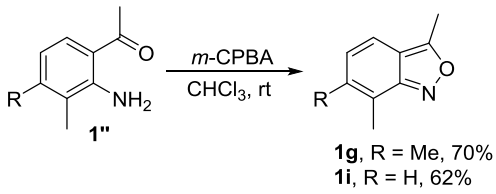
2. Experiment Procedures

General procedure 1: Synthesis of substituted anthranils 1a-1k (**1j** is commercially available)
Condition A[1a]:



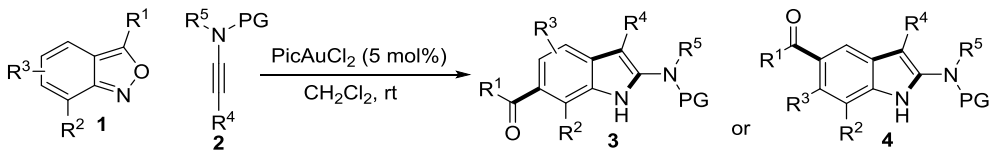
A round bottom flask equipped with a magnetic stirrer bar was charged with the substituted 2-nitroacylbenzene (1.00 mmol) in conc. HCl (3 ml). $SnCl_2{\cdot}2H_2O$ (4 mmol) was added and the reaction was stirred at 10 °C for 30 min. The reaction was quenched with saturated $NaHCO_3$ (20 ml), and filtered. The aqueous phase was extracted with EtOAc (3 × 10 mL) and the organic portions were combined, washed with H_2O (20 mL), saturated aqueous NaCl (20 mL), dried over Na_2SO_4, filtered and concentrated. The residue was purified by column chromatography (Silica gel, PE/EtOAc) to provide the title compound in 67-91% yield.

Condition B[1b]:



At room temperature, to a solution of substituted 2-acetylaniline **1"** (1 mmol) in chloroform (15 mL) was added *m*-CPBA (493 mg of 70% purity, 2 mmol) slowly. After a four-hour stirring, the resulting mixture was washed with 0.1 M $NaHCO_3$ (2 × 10 mL). The organic layer was dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by column chromatography (Silica gel, PE/EtOAc) to give the desired product in 62-70% yield.

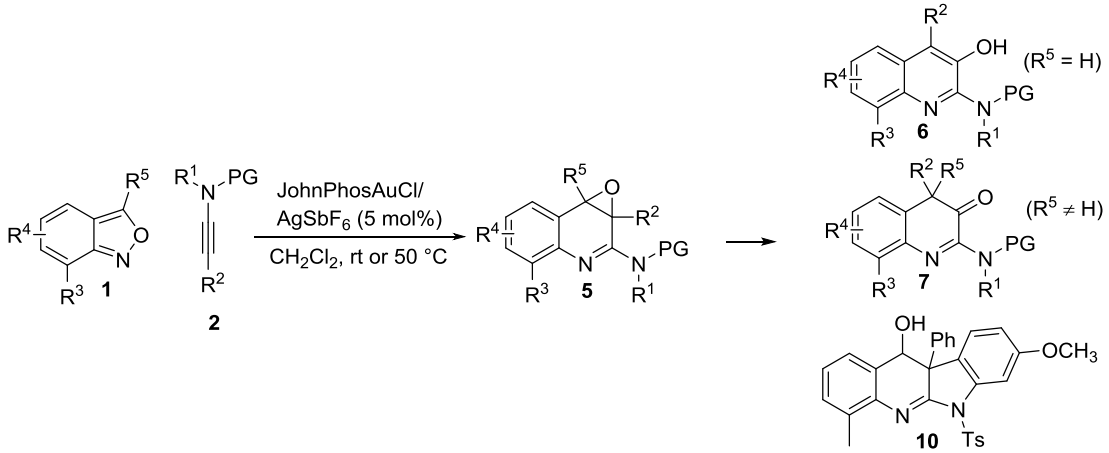
General procedure 2: Gold(III)-catalyzed [3+2] annulations with divergent acyl migrations for the synthesis of 3 and 4



A small glass vial (3 mL in volume) equipped with a magnetic stirrer bar was charged with **1** (0.2 mmol) and **2** (0.24 mmol), and to this mixture was added dry DCM (2.0 mL) and $PicAuCl_2$ (5 mol%,

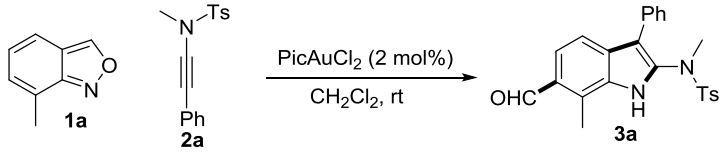
3.9 mg). The vial was then sealed with a plastic screw cap. The reaction mixture was stirred at room temperature for 12 h (for product **3ab**, the reaction temperature is 50 ºC). The solvent was removed under reduced pressure, and the residue was purified by column chromatography (Silica gel, PE/EtOAc) to give **3** or **4**.

General procedure 3: Gold(I)-catalyzed epoxidations for the synthesis of 5, 6, 7 and 10



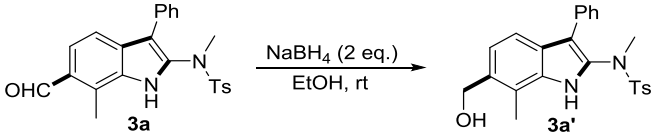
A small glass vial (3 mL in volume) equipped with a magnetic stirrer bar was charged with JohnPhosAuCl (5 mol%, 5.3 mg) and $AgSbF_6$ (5 mol%, 3.4 mg), and to this mixture was added dry DCM (0.5 mL). The resulting mixture was stirred at room temperature for 5 min. Then **1** (0.24 mmol) and **2** (0.20 mmol) dissolved in dry DCM (1.5 mL) were added slowly. The vial was then sealed with a plastic screw cap. The reaction mixture was stirred at room temperature for 12 h (for product **5c**, **5h-j**, **6c** and **7a-b**, the reaction temperature is 50 ºC, 10.6 mg JohnPhosAuCl, 6.8 mg $AgSbF_6$). The solvent was removed under reduced pressure, and the residue was purified by column chromatography (Silica gel, PE/EtOAc) to give compound **5**, **6, 7 or 10**.

Procedure 4: Gram-scale synthesis of 3a



A round-bottom flask (50 mL in volume) equipped with a magnetic stirrer bar was charged with **1a** (532 mg, 4.0 mmol) and **2a** (1.37 g, 4.8 mmol), and to this mixture was added dry DCM (20 mL). $PicAuCl_2$ (32 mg, 2 mol%) was slowly added to this mixture. The reaction mixture was stirred at room temperature for 12 h. The solvent was removed under reduced pressure, and the residue was purified by column chromatography (Silica gel, PE/EtOAc) to give **3a** (1.39 g, 83%).

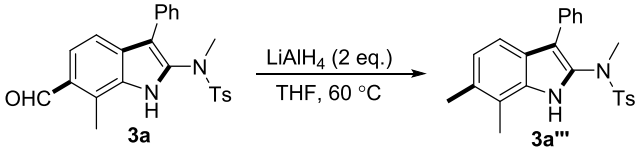
Procedure 5: $NaBH_4$-Mediated reduction of 3a



A sealed tube equipped with a magnetic stirrer bar was charged with **3a** (84 mg, 0.2 mmol) and 2 mL EtOH. After $NaBH_4$ (7.6 mg, 0.4 mmol) was added, the reaction was stirred at room temperature for 2 h and then quenched by H_2O (5 ml). The resulting mixture was extracted with EtOAc (3 × 5 mL) and the organic portions were combined, washed with saturated aqueous NaCl (10 mL), dried

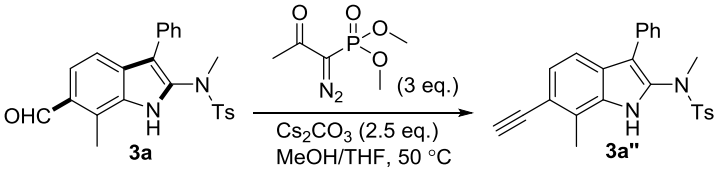
over $NaSO_4$, filtered and reduced in vacuo. The residue was purified by column chromatography (Silica gel, hexane/EtOAc) to provide compound **3a'**.

Procedure 6: $LiAlH_4$-Mediated reduction of 3a



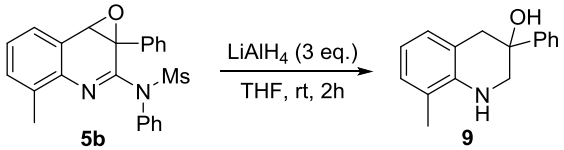
At 0 ºC, to a solution of **3a** (84 mg, 0.2 mmol) in 2 mL THF was added $LiAlH_4$ (7.6 mg, 0.4 mmol) and the reaction was heated to 60 ºC. After being stirred at this temperature for 24 h, the reaction was cooled down to 0 ºC again and then quenched by H_2O (5 ml, dropwisely added). The resulting mixture was extracted with EtOAc (3 × 5 mL). The organic portions were combined, washed with H_2O (10 mL), saturated aqueous NaCl (10 mL), dried over $NaSO_4$, filtered and reduced in vacuo. The residue was purified by column chromatography (Silica gel, hexane/EtOAc) to give compound **3a'''**.

Procedure 7: Seyferth-Gilbert homologation of 3a



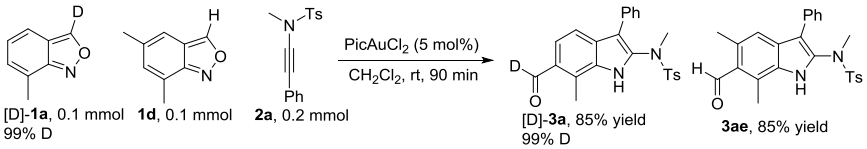
To the mixture of **3a** (84 mg, 0.2 mmol), Cs_2CO_3 (163 mg, 0.5 mmol), MeOH (1 ml) and THF (1 ml) was added dropwise the dimethyl (1-diazo-2-oxopropyl)phosphonate (114 mg, 0.6 mmol) at 0 ºC. Then, the reaction was stirred 6 h at room temperature. The mixture was washed with H_2O (10 mL), and extracted with EtOAc (3 × 5 mL). The organic portions were combined and washed with saturated aqueous NaCl (10 mL), dried over $NaSO_4$, filtered and reduced in vacuo. The residue was purified by column chromatography (SiO_2, hexane/EtOAc) to provide **3a''**.

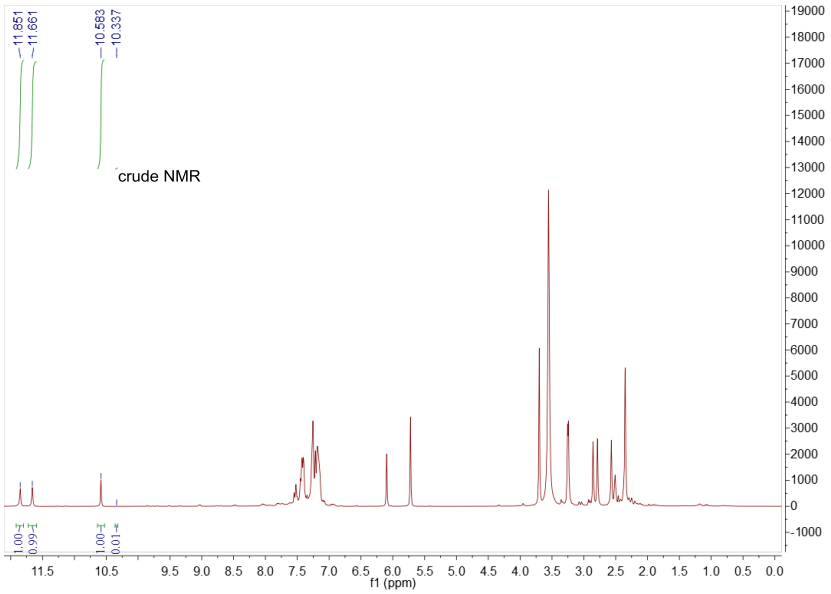
Procedure 8: $LiAlH_4$-Mediated reduction and deamination of 5b

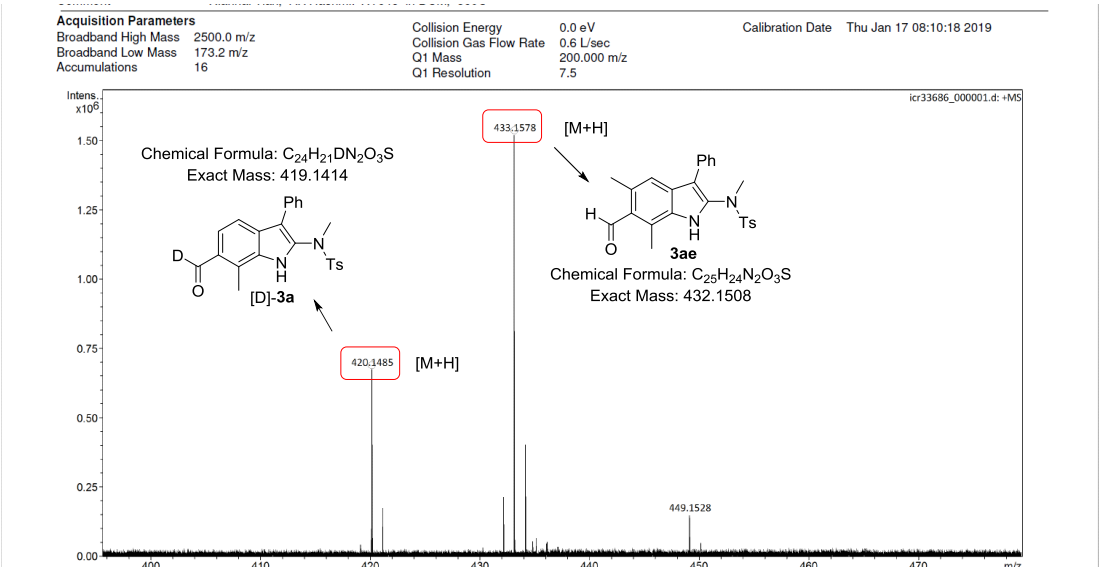


At 0 ºC, to a solution of **5b** (81 mg, 0.2 mmol) in 2 mL THF was added $LiAlH_4$ (11.4 mg, 0.6 mmol) and the reaction was then moved to room temperature. After being stirred for 2 h, the reaction was cooled down to 0 °C again and then quenched by H_2O (5 ml, dropwisely added). The resulting mixture was extracted with EtOAc (3 × 5 mL). The organic portions were combined, washed with H_2O (10 mL), saturated aqueous NaCl (10 mL), dried over $NaSO_4$, filtered and reduced in vacuo. The residue was purified by column chromatography (Silica gel, hexane/EtOAc) to give compound **9**.

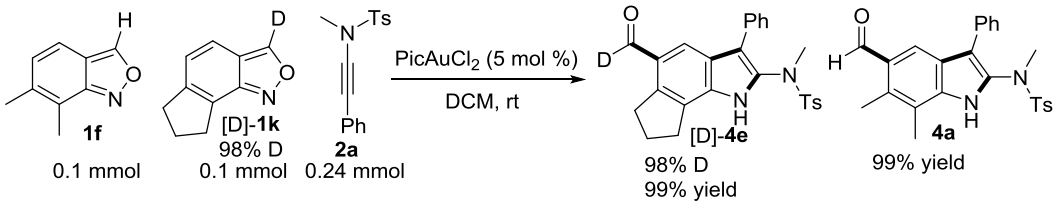
3. Mechanistic Study





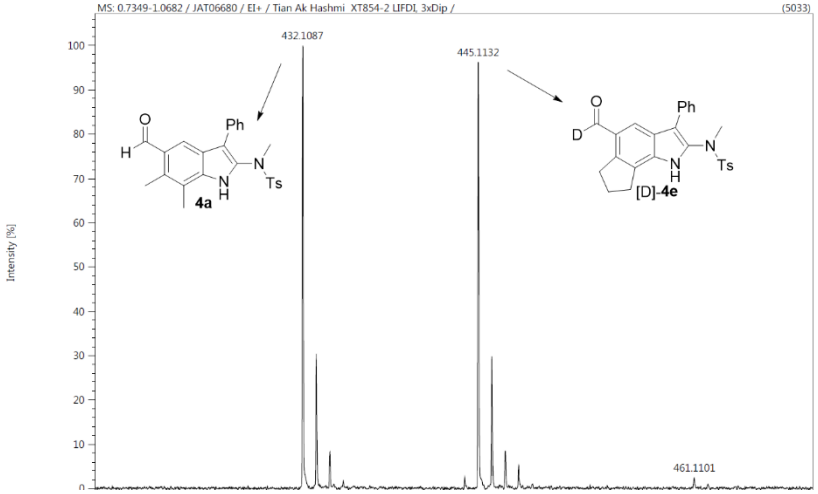


MS: [D]-**3a**: calcd.: 419 (100%), 420 (26%), 421 (4.5%); found: 419 (100%), 420 (26%), 421 (n.d.)
3ae: calcd.: 432 (100%), 433 (27%), 434 (4.5%); found: 432 (100%), 433 (26.5%), 434 (3.6%)

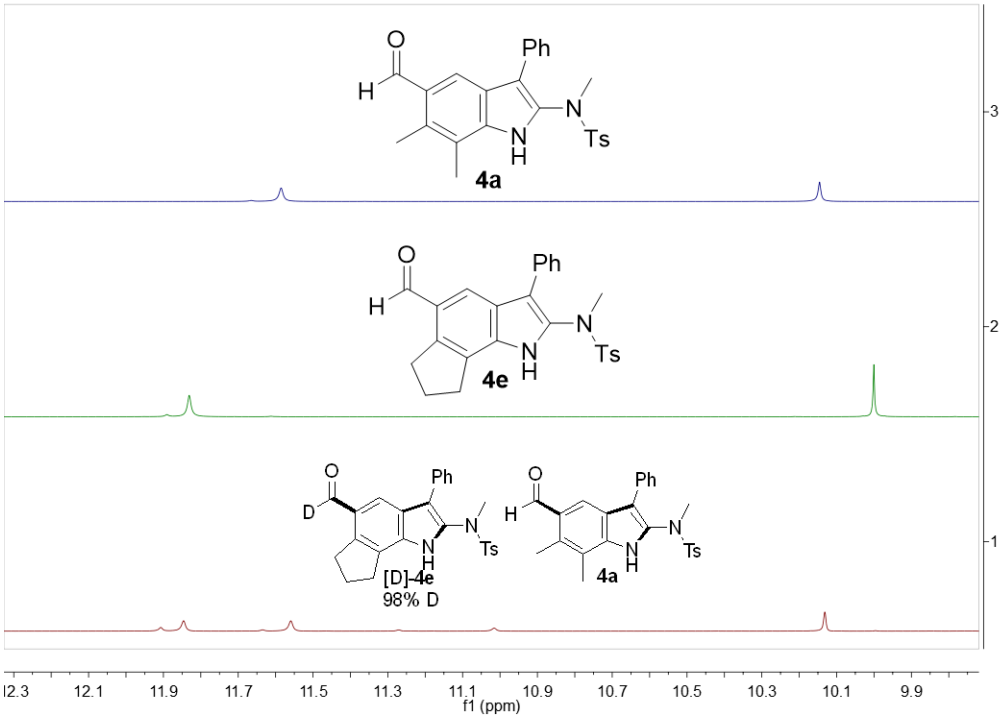


MS: [D]-**4e**: calcd.: 445 (100%), 446 (28.1%), 447 (4.5%); found: 445 (100%), 446 (28.9%), 447 (4.3%)

4a: calcd.: 432 (100%), 433 (27%), 434 (4.5%); found: 432 (100%), 433 (27%), 434 (5.0%)

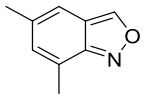


Crude ^{1}H NMR of this crossover experiment:



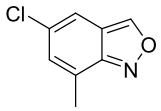
4. Characterization Data

Compounds **1a**-**c** were characterized in our previous report[3]



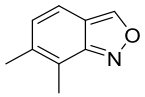
5,7-dimethylbenzo[c]isoxazole (1d)

Yield: 134 mg, 91%; colorless oil; R_f = 0.40 (EA/PE = 1/20); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.88 (s, 1H), 7.03 (s, 1H), 6.80 (s, 1H), 2.47 (s, 3H), 2.24 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.5 (s), 153.0 (d), 134.4 (s), 132.6 (d), 125.2 (s), 118.7 (s), 114.0 (d), 21.8 (q), 17.0 (q) ppm; IR (reflection) $\tilde{v}$ = 3127, 3096, 3017, 2975, 2944, 2917, 2859, 2737, 2202, 1646, 1557, 1472, 1445, 1403, 1378, 1327, 1233, 1155, 1108, 1037, 1019, 977, 921, 876, 844, 793, 754, 613 cm^{-1}; HRMS (EI) (*m/z*) C_9H_9NO calcd for 147.0684, found 147.0680.



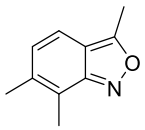
5-chloro-7-methylbenzo[c]isoxazole (1e)

Yield: 139 mg, 83%; colorless oil; R_f = 0.42 (EA/PE = 1/20); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.97 (s, 1H), 7.29 (s, 1H), 6.88 (d, J = 1.5 Hz, 1H), 2.48 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6 (s), 154.0 (d), 130.7 (d), 130.4 (s), 127.9 (s), 118.3 (s), 115.0 (d), 16.9 (q) ppm; IR (reflection) $\tilde{v}$ = 3135, 3107, 2983, 2963, 2913, 2208, 1732, 1715, 1635, 1544, 1463, 1439, 1408, 1377, 1345, 1318, 1263, 1218, 1183, 1111, 1069, 1034, 985, 924, 895, 872, 856, 810, 759, 613 cm^{-1}; HRMS (EI) (*m/z*) $C_8H_6{}^{35}ClNO$ calcd for 167.0138, found 167.0126.



6,7-dimethylbenzo[c]isoxazole (1f)

Yield: 128 mg, 87%; light yellow oil; R_f = 0.36 (EA/PE = 1/20); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.93 (s, 1H), 7.21 (d, J = 9.0 Hz, 1H), 6.75 (d, J = 9.0 Hz, 1H), 2.41 (s, 3H), 2.24 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 157.8 (s), 154.0 (d), 136.6 (s), 129.4 (d), 121.3 (s), 117.3 (s), 115.9 (d), 19.1 (q), 13.2 (q) ppm; IR (reflection) $\tilde{v}$ = 3115, 3049, 2922, 2861, 1637, 1533, 1448, 1379, 1309, 1252, 1205, 1175, 1113, 1015, 979, 922, 894, 851, 814, 755, 657 cm^{-1}; HRMS (EI) (*m/z*) C_9H_9NO calcd for 147.0684, found 147.0680.

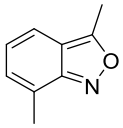


3,6,7-trimethylbenzo[c]isoxazole (1g)

Yield: 113 mg, 70%; colorless oil; R_f = 0.48 (EA/PE = 1/20); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.09 (d, J = 9.0 Hz, 1H), 6.68 (d, J = 8.5 Hz, 1H), 2.67 (s, 3H), 2.37 (s, 3H), 2.23 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.2 (s), 158.7 (s), 136.5 (s), 127.8 (d), 121.1 (s), 116.2 (d), 114.7 (s), 19.1 (q), 13.1 (q), 12.0 (q) ppm; IR (reflection) $\tilde{v}$ = 2920, 1724, 1640, 1531, 1450, 1376, 1248, 1202, 1172, 1158, 1098, 1019, 903, 860, 797, 760, 662, 615 cm^{-1}; HRMS (EI) (*m/z*) $C_{10}H_{11}NO$ calcd for 161.0841, found 161.0826.

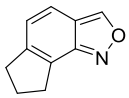
7-bromobenzo[c]isoxazole (1h)

Yield: 160 mg, 81%; colorless oil; R_f = 0.21 (EA/PE = 1/20); ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.20 (s, 1H), 7.49 (d, *J* = 5.0 Hz, 2H), 6.84 (dd, *J* = 7.0, 8.0 Hz, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2 (s), 155.6 (s), 133.7 (d), 125.2 (d), 119.1 (d), 119.0 (s), 108.8 (d) ppm; IR (reflection) $\tilde{\nu}$ = 3126, 3097, 1634, 1548, 1500, 1439, 1401, 1380, 1315, 1209, 1150, 1114, 1019, 952, 916, 874, 810, 774, 738, 670, 614 cm^{-1}; HRMS (EI) (*m/z*) $C_7H_4{}^{79}BrNO$ calcd for 196.9476, found 196.9484.



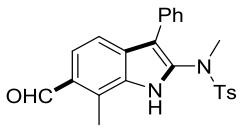
3,7-dimethylbenzo[c]isoxazole (1i)[1b]

Yield: 91 mg, 62%; light yellow oil; R_f = 0.36 (EA/PE = 1/20); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (d, *J* = 8.5 Hz, 1H), 6.92 (dt, *J* = 6.5, 1.0 Hz, 1H), 6.77 (dd, *J* = 6.5, 9.0 Hz, 1H), 2.70 (s, 3H), 2.45 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.6 (s), 157.9 (s), 129.0 (d), 125.5 (s), 123.3 (d), 117.1 (d), 115.6 (s), 17.0 (q), 12.1 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3470, 3055, 3029, 2975, 2924, 2854, 2736, 2540, 1915, 1697, 1645, 1568, 1547, 1450, 1405, 1378, 1273, 1225, 1162, 1056, 1037, 974, 896, 851, 780, 748, 715, 663 cm^{-1}; HRMS (EI) (*m/z*) C_9H_9NO calcd for 147.0684, found 147.0681.



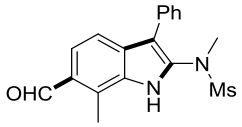
7,8-dihydro-6*H*-indeno[4,5-*c*]isoxazole (1k)

Yield: 132 mg, 83%; white solid, mp 48-49 °C; R_f = 0.40 (EA/PE = 1/20); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.98 (s, 1H), 7.21 (d, *J* = 8.7 Hz, 1H), 6.89 (d, *J* = 8.7 Hz, 1H), 3.13-3.05 (m, 2H), 2.92-2.83 (m, 2H), 2.22-2.10 (m, 2H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.6 (s), 154.3 (d), 146.2 (s), 127.6 (s), 123.3 (d), 118.4 (s), 117.7 (d), 33.9 (t), 30.3 (t), 24.1 (t) ppm; IR (ATR) $\tilde{\nu}$ = 3125, 3038, 2917, 2860, 1646, 1531, 1451, 1360, 1297, 1257, 1211, 1166, 1107, 1019, 979, 921, 898, 851, 811, 757, 638 cm^{-1}; HRMS (EI) (*m/z*) $C_{10}H_9NO$ calcd for 159.0684, found 159.0674.



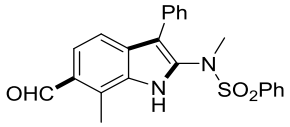
***N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3a)**

Yield: 73 mg, 87%; white solid, mp 216-218 °C; R_f = 0.27 (EA/PE = 1/4); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.86 (brs, 1H), 10.36 (s, 1H), 7.54 (d, *J* = 8.5 Hz, 1H), 7.44 (t, *J* = 8.0 Hz, 3H), 7.31-7.26 (m, 3H), 7.26-7.22 (m, 2H), 7.19-7.13 (m, 2H), 3.26 (s, 3H), 2.86 (s, 3H), 2.38 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 144.2 (s), 135.4 (s), 134.9 (s), 133.5 (s), 133.1 (s), 130.1 (d, 2C), 129.7 (s), 129.4 (d, 2C), 128.8 (d, 2C), 128.5 (s), 127.8 (d, 2C), 126.9 (d), 126.6 (s), 122.1 (d), 117.1 (d), 114.0 (s), 38.7 (q), 21.5 (q), 12.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3175, 3065, 1739, 1645, 1613, 1556, 1493, 1463, 1440, 1422, 1370, 1346, 1326, 1306, 1269, 1213, 1187, 1154, 1090, 1073, 1048, 1024, 988, 923, 911, 863, 813, 774, 763, 738, 698, 670, 654 cm^{-1}; HRMS (ESI) (*m/z*) $[M-H]^-$ $C_{24}H_{21}N_2O_3S$ calcd for 417.1278, found 417.1275.



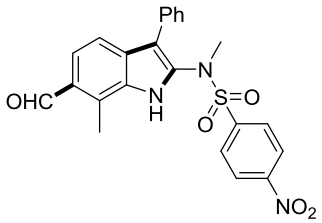
***N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-*N*-methylmethanesulfonamide (3b)**

Yield: 62 mg, 90%; light yellow solid, mp 246-248 °C; R_f = 0.14 (EA/PE = 1/2); ^{1}H NMR (500 MHz, Acetone-d_6) δ 10.85 (brs, 1H), 10.26 (s, 1H), 7.52-7.47 (m, 3H), 7.44 (d, J = 8.5 Hz, 1H), 7.39 (t, J = 7.5 Hz, 2H), 7.26 (t, J = 7.5 Hz, 1H), 3.24 (s, 3H), 2.76 (s, 3H), 2.70 (s, 3H) ppm; ^{13}C NMR (125 MHz, Acetone-d_6) δ 191.7 (d), 134.9 (s), 133.5 (s), 133.2 (s), 129.8 (s), 129.4 (d, 2C), 128.9 (s), 128.7 (d, 2C), 127.0 (d), 125.4 (s), 122.6 (d), 117.0 (d), 114.4 (s), 38.6 (q), 38.2 (q), 11.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3195, 3014, 2945, 2748, 1736, 1650, 1613, 1577, 1555, 1508, 1494, 1442, 1369, 1325, 1254, 1177, 1146, 1104, 1073, 1026, 966, 916, 867, 810, 783, 771, 760, 698, 648 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{18}H_{17}N_2O_3S$ calcd for 341.0965, found 341.0964.



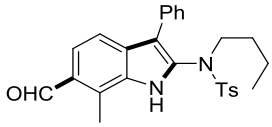
***N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-*N*-methylbenzenesulfonamide (3c)**

Yield: 76 mg, 94%; white solid, mp 265-267 °C; R_f = 0.14 (EA/PE = 1/5); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.87 (s, 1H), 10.36 (s, 1H), 7.66 (t, J = 7.5 Hz, 1H), 7.56 (dd, J = 12.0, 2.5 Hz, 3H), 7.47 (dd, J = 14.5, 7.5, 3H), 7.30-7.26 (m, 3H), 7.18 (d, J = 7.0 Hz, 2H), 3.27 (s, 3H), 2.85 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 138.3 (s), 134.8 (s), 133.7 (d), 133.5 (s), 133.1 (s), 129.7 (d, 2C; s, 1C), 129.4 (d, 2C), 128.9 (d, 2C), 128.6 (s), 127.8 (d, 2C), 127.1 (d), 126.6 (s), 122.1 (d), 117.1 (d), 114.0 (s), 38.8 (q), 12.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3152, 3116, 3065, 3018, 2947, 1737, 1649, 1612, 1554, 1512, 1492, 1446, 1423, 1351, 1331, 1271, 1213, 1188, 1161, 1092, 1074, 1049, 1025, 1002, 990, 924, 913, 867, 813, 777, 764, 741, 718, 688, 667, 605 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{23}H_{19}N_2O_3S$ calcd for 403.1122, found 403.1121.



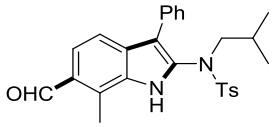
***N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-*N*-methyl-4-nitrobenzenesulfonamide (3d)**

Yield: 78 mg, 87%; yellow solid, mp 289-290 °C; R_f = 0.10 (EA/PE = 1/5); ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.01 (s, 1H), 10.36 (s, 1H), 8.12 (d, J = 9.0 Hz, 2H), 7.75 (d, J = 8.5 Hz, 2H), 7.55 (d, J = 8.5 Hz, 1H), 7.47 (d, J = 8.5 Hz, 1H), 7.25-7.21 (m, 4H), 7.19-7.16 (m, 1H), 3.50 (s, 3H), 2.84 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 150.2 (s), 144.2 (s), 133.9 (s), 133.7 (s), 132.9 (s), 129.34 (s), 129.25 (d, 2C), 129.1 (d, 2C), 128.9 (d, 2C), 128.8 (s), 126.8 (d), 126.7 (s), 124.7 (d, 2C), 122.1 (d), 117.3 (d), 114.5 (s), 39.9 (q), 12.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3172, 3103, 3065, 1738, 1647, 1614, 1555, 1526, 1492, 1462, 1440, 1422, 1371, 1350, 1310, 1270, 1215, 1189, 1160, 1105, 1088, 1073, 1048, 1027, 1013, 1002, 990, 916, 870, 853, 817, 777, 764, 740, 710, 699, 685, 667, 610 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{23}H_{18}N_3O_5S$ calcd for 448.0973, found 448.0974.



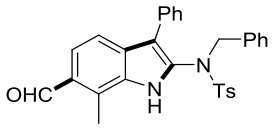
***N*-butyl-*N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-4-methylbenzenesulfonamide (3e)**

Yield: 83 mg, 90%; white solid, mp 144-146 °C; R_f = 0.26 (EA/PE = 1/5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.29 (s, 1H), 8.97 (brs, 1H), 7.52 (t, *J* = 8.0 Hz, 3H), 7.35 (d, *J* = 8.5 Hz, 1H), 7.23 (d, *J* = 8.5 Hz, 2H), 7.17-7.14 (m, 1H), 7.08 (t, *J* = 7.5 Hz, 2H), 6.53 (d, *J* = 7.5 Hz, 2H), 3.25 (t, *J* = 7.0 Hz, 2H), 2.80 (s, 3H), 2.38 (s, 3H), 1.28 (t, *J* = 7.5 Hz, 2H), 1.07-1.02 (m, 2H), 0.65 (t, *J* = 7.5 Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.5 (d), 144.4 (s), 135.3 (s), 133.0 (s), 132.3 (s), 132.0 (s), 130.4 (s), 130.0 (d, 2C), 129.2 (d, 2C), 128.6 (s), 128.4 (d, 2C), 127.4 (d, 2C), 127.3 (d), 124.5 (s), 123.7 (d), 117.0 (d), 113.1 (s), 49.5 (q), 30.9 (q), 21.6 (t), 19.5 (q), 13.5 (t), 12.8 (t) ppm; IR (reflection) $\tilde{\nu}$ = 3259, 3057, 2957, 2929, 2872, 2716, 1656, 1613, 1543, 1492, 1460, 1442, 1364, 1316, 1261, 1225, 1207, 1185, 1167, 1090, 1033, 1012, 953, 909, 884, 863, 811, 771, 733, 707, 695, 667 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{27}H_{27}N_2O_3S$ calcd for 459.1748, found 459.1748.



***N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-*N*-isobutyl-4-methylbenzenesulfonamide (3f)**

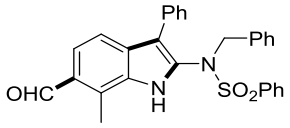
Yield: 70 mg, 76%; white solid, mp 221-224 °C; R_f = 0.34 (EA/PE = 1/5); ^{1}H NMR (500 MHz, DMSO-d_6) δ 10.29 (s, 1H), 8.96 (brs, 1H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.30 (d, *J* = 8.5 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.17 (t, *J* = 7.5 Hz, 1H), 7.07 (t, *J* = 8.0 Hz, 2H), 6.41 (d, *J* = 7.5 Hz, 2H), 2.99 (d, *J* = 7.0 Hz, 2H), 2.82 (s, 3H), 2.40 (s, 3H), 1.45 (hept, *J* = 7.0 Hz, 1H), 0.63 (d, *J* = 6.5 Hz, 6H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.4 (d), 144.5 (s), 135.2 (s), 132.8 (s), 132.3 (s), 132.1 (s), 130.6 (s), 130.1 (d, 2C), 129.3 (d, 2C), 128.6 (s), 128.4 (d, 2C), 127.41 (d, 2C), 127.40 (d), 124.4 (s), 123.7 (d), 116.9 (d), 112.6 (s), 56.1 (t), 27.3 (d), 21.7 (q), 19.7 (q), 12.8 (q, 2C) ppm; IR (reflection) $\tilde{\nu}$ = 3206, 3063, 2970, 2953, 2870, 2738, 1738, 1658, 1614, 1542, 1504, 1490, 1469, 1443, 1385, 1364, 1339, 1322, 1269, 1233, 1207, 1164, 1089, 1050, 1031, 1008, 936, 855, 824, 811, 769, 744, 703, 670, 657, 632 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{27}H_{27}N_2O_3S$ calcd for 459.1748, found 459.1749.



***N*-benzyl-*N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-4-methylbenzenesulfonamide (3g)**

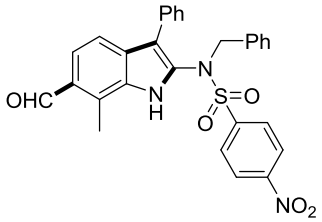
Yield: 82 mg, 83%; white solid, mp 231-233 °C; R_f = 0.21 (EA/PE = 1/5); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.85 (brs, 1H), 10.36 (s, 1H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 1H), 7.42 (d, *J* = 8.5 Hz, 2H), 7.30-7.25 (m, 2H), 7.21 (t, *J* = 7.5 Hz, 2H), 7.18-7.13 (m, 3H), 7.03-6.98 (m, 2H), 6.75 (d, *J* = 7.5 Hz, 2H), 4.65 (brs, 2H), 2.85 (s, 3H), 2.46 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.7 (d), 144.7 (s), 135.7 (s), 135.6 (s), 133.6 (s), 132.9 (s), 132.4 (s), 130.4 (d, 2C), 129.9 (s), 129.5 (d, 2C), 129.0 (d, 2C), 128.7 (d, 2C), 128.6 (d, 2C), 128.5 (s), 128.31 (d, 2C), 128.29 (d), 127.2 (d), 126.5 (s), 121.9 (d), 116.8 (d), 115.1 (s), 53.3 (t), 21.6 (q), 12.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3285, 3055, 2985, 2839, 2721, 1735, 1671, 1619, 1545, 1504, 1455, 1441, 1414, 1361, 1305,

1254, 1198, 1185, 1166, 1090, 1042, 970, 933, 917, 855, 844, 818, 805, 772, 755, 730, 707, 693, 660, 634 cm^{-1}; HRMS (ESI) (*m/z*) $[M-H]^-$ $C_{30}H_{25}N_2O_3S$ calcd for 493.1591, found 493.1592.



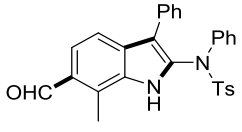
***N*-benzyl-*N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)benzenesulfonamide (3h)**

Yield: 76 mg, 79%; white solid, mp 215-218 °C; R_f = 0.15 (EA/PE = 1/5); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.75 (s, 1H), 10.33 (s, 1H), 7.80-7.78 (m, 3H), 7.63 (t, *J* = 7.5 Hz, 2H), 7.48 (d, *J* = 8.5 Hz, 1H), 7.28 (t, *J* = 7.5 Hz, 2H), 7.21 (t, *J* = 7.5 Hz, 2H), 7.19-7.13 (m, 3H), 7.00 (d, *J* = 7.0 Hz, 2H), 6.75 (d, *J* = 8.0 Hz, 2H), 4.67 (brs, 2H), 2.85 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.7 (d), 138.6 (s), 135.5 (s), 134.1 (d), 133.6 (s), 132.9 (s), 132.3 (s), 130.0 (d, 2C), 129.9 (s), 129.5 (d, 2C), 129.0 (d, 2C), 128.7 (d, 2C), 128.7 (d, 2C), 128.5 (s), 128.32 (d), 128.25 (d, 2C), 127.3 (d), 126.5 (s), 121.9 (d), 116.9 (d), 115.1 (s), 53.4 (t), 12.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3281, 3059, 3029, 2841, 2724, 1670, 1619, 1545, 1505, 1494, 1445, 1414, 1364, 1333, 1310, 1257, 1197, 1170, 1090, 1044, 1028, 999, 973, 914, 855, 831, 806, 774, 752, 733, 719, 706, 692, 650 cm^{-1}; HRMS (ESI) (*m/z*) $[M-H]^-$ $C_{29}H_{23}N_2O_3S$ calcd for 479.1435, found 479.1433.



***N*-benzyl-*N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-4-nitrobenzenesulfonamide (3i)**

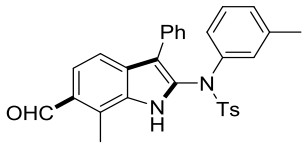
Yield: 95 mg, 90%; yellow solid, mp 206-207 °C; R_f = 0.28 (EA/PE = 1/4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.23 (s, 1H), 8.44 (s, 1H), 8.06 (d, *J* = 8.5 Hz, 2H), 7.70 (d, *J* = 8.5 Hz, 2H), 7.48 (d, *J* = 8.5 Hz, 1H), 7.35 (d, *J* = 8.5 Hz, 1H), 7.25-7.20 (m, 3H), 7.17-7.13 (m, 3H), 7.09 (t, *J* = 7.5 Hz, 2H), 6.65 (d, *J* = 7.5 Hz, 2H), 4.72 (s, 2H), 2.61 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.4 (d), 150.3 (s), 144.1 (s), 135.4 (s), 133.3 (s), 131.9 (s), 130.2 (s), 129.6 (s), 129.1 (s), 129.0 (d, 2C), 128.92 (d, 2C), 128.87 (d, 2C), 128.73 (d), 128.68 (d, 2C), 128.66 (d, 2C), 127.5 (d), 124.7 (s), 124.2 (d, 2C), 123.8 (d), 117.6 (d), 115.1 (s), 55.4 (t), 12.5 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3254, 3092, 3058, 3031, 2976, 2845, 2736, 1804, 1674, 1619, 1548, 1534, 1507, 1456, 1416, 1402, 1372, 1357, 1310, 1256, 1173, 1087, 1057, 1043, 1028, 971, 916, 850, 833, 806, 778, 756, 737, 709, 696, 649, 609 cm^{-1}; HRMS (ESI) (*m/z*) $[M-H]^-$ $C_{29}H_{22}N_3O_5S$ calcd for 524.1286, found 524.1290.



***N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (3j)**

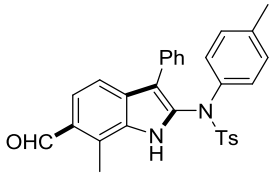
Yield: 45 mg, 47%; yellow solid, mp 118-120 °C; R_f = 0.17 (EA/PE = 1/5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.28 (s, 1H), 9.18 (s, 1H), 7.52 (t, *J* = 8.5 Hz, 3H), 7.37 (d, *J* = 8.0 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 3H), 7.11-7.05 (m, 5H), 7.00 (d, *J* = 8.5 Hz, 2H), 6.81 (d, *J* = 7.5 Hz, 2H), 2.81 (s, 3H), 2.35 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.6 (d), 144.7 (s), 140.5 (s), 136.0 (s), 133.4 (s), 133.0 (s), 131.9 (s), 130.3 (s), 129.8 (d, 2C), 129.5 (d, 2C), 129.03 (d, 2C), 128.95 (s), 128.1 (d, 2C), 127.8

(d, 2C), 127.2 (d), 127.1 (d), 126.5 (d, 2C), 124.8 (s), 123.9 (d), 117.7 (d), 115.8 (s), 21.7 (q), 12.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3323, 3064, 2927, 1672, 1597, 1556, 1491, 1441, 1362, 1246, 1215, 1186, 1163, 1090, 1020, 946, 873, 812, 776, 756, 734, 695, 658, 637, 619 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{29}H_{25}N_2O_3S$ calcd for 481.1580, found 481.1590.



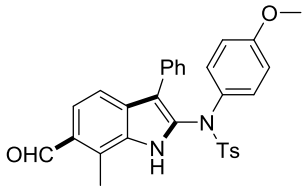
***N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-4-methyl-*N*-(*m*-tolyl)benzenesulfonamide (3k)**

Yield: 55 mg, 56%; light yellow solid, mp 170-173 °C; R_f = 0.23 (EA/PE = 1/5); ^{1}H NMR (300 MHz, $CDCl_3$) δ 10.29 (s, 1H), 9.07 (brs, 1H), 7.52 (d, *J* = 8.4 Hz, 3H), 7.35 (d, *J* = 8.4 Hz, 1H), 7.18-7.06 (m, 5H), 7.00-6.92 (m, 1H), 6.90-6.84 (m, 1H), 6.82-6.74 (m, 4H), 2.82 (s, 3H), 2.36 (s, 3H), 2.09 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.5 (d), 144.6 (s), 140.2 (s), 139.0 (s), 136.1 (s), 133.3 (s), 133.2 (s), 131.9 (s), 130.4 (s), 129.8 (d, 2C), 129.6 (d, 2C), 128.9 (s), 128.7 (d), 128.2 (d), 128.1 (d, 2C), 127.8 (d, 2C), 127.5 (d), 127.1 (d), 124.8 (s), 123.9 (d), 123.8 (d), 117.6 (d), 115.6 (s), 21.7 (q), 21.2 (q), 12.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3266, 3065, 2846, 2733, 1670, 1608, 1549, 1498, 1439, 1368, 1345, 1306, 1257, 1185, 1162, 1090, 1046, 1022, 972, 946, 893, 878, 839, 808, 789, 772, 761, 707, 657 cm^{-1}; HRMS (ESI) (*m/z*) $[M-H]^-$ $C_{30}H_{25}N_2O_3S$ calcd for 493.1591, found 493.1588.



***N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-4-methyl-*N*-(*p*-tolyl)benzenesulfonamide (3l)**

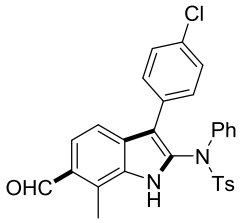
Yield: 64 mg, 65%; grey solid, mp 211-214 °C; R_f = 0.34 (EA/PE = 1/4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.27 (s, 1H), 9.15 (brs, 1H), 7.51 (t, *J* = 7.5 Hz, 3H), 7.36 (d, *J* = 8.5 Hz, 1H), 7.16-7.08 (m, 5H), 6.92-6.84 (m, 6H), 2.78 (s, 3H), 2.35 (s, 3H), 2.16 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.6 (d), 144.6 (s), 137.7 (s), 137.5 (s), 136.1 (s), 133.3 (s), 133.2 (s), 132.0 (s), 130.3 (s), 129.8 (d, 2C), 129.7 (d, 2C), 129.6 (d, 2C), 128.9 (s), 128.1 (d, 2C), 127.8 (d, 2C), 127.1 (d), 126.8 (d, 2C), 124.8 (s), 123.8 (d), 117.6 (d), 115.7 (s), 21.7 (q), 21.0 (q), 12.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3293, 3032, 2918, 2861, 2754, 1738, 1668, 1613, 1578, 1555, 1496, 1435, 1371, 1353, 1319, 1238, 1199, 1167, 1090, 1041, 1019, 952, 926, 884, 836, 812, 762, 713, 699, 663 cm^{-1}; HRMS (ESI) (*m/z*) $[M-H]^-$ $C_{30}H_{25}N_2O_3S$ calcd for 493.1591, found 493.1595.



***N*-(6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-*N*-(4-methoxyphenyl)-4-methylbenzenesulfonamide (3m)**

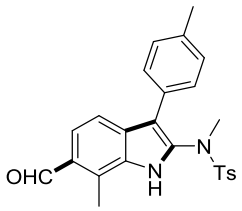
Yield: 41 mg, 40%; light yellow solid, mp 218-220 °C; R_f = 0.19 (EA/PE = 1/4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.27 (s, 1H), 9.09 (brs, 1H), 7.53 (d, *J* = 8.0 Hz, 2H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.19-7.16 (m, 3H), 7.13 (t, *J* = 7.5 Hz, 2H), 6.91-6.85 (m, 4H), 6.57 (d, *J* = 9.0

Hz, 2H), 3.64 (s, 3H), 2.79 (s, 3H), 2.37 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.6 (d), 158.9 (s), 144.6 (s), 136.0 (s), 133.5 (s), 133.2 (s), 132.7 (s), 132.1 (s), 130.4 (s), 129.8 (d, 2C), 129.7 (d, 2C), 129.0 (d, 2C), 128.8 (s), 128.2 (d, 2C), 127.9 (d, 2C), 127.1 (d), 124.7 (s), 123.9 (d), 117.6 (d), 115.4 (s), 114.2 (d, 2C), 55.4 (q), 21.7 (q), 12.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3276, 2844, 2754, 1751, 1668, 1609, 1578, 1554, 1500, 1462, 1437, 1370, 1349, 1318, 1303, 1245, 1198, 1164, 1118, 1090, 1029, 949, 924, 882, 838, 814, 774, 762, 717, 699, 663 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{30}H_{25}N_2O_4S$ calcd for 509.1541, found 509.1547.



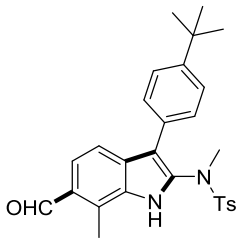
***N*-(3-(4-chlorophenyl)-6-formyl-7-methyl-1*H*-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (3n)**

Yield: 46 mg, 45%; white solid, mp 193-196 °C; R_f = 0.32 (EA/PE = 1/4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.28 (s, 1H), 9.18 (brs, 1H), 7.52 (d, *J* = 8.0 Hz, 3H), 7.33 (d, *J* = 8.5 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.14-7.08 (m, 3H), 7.07-7.04 (m, 2H), 7.02 (d, *J* = 7.0 Hz, 2H), 6.75 (d, *J* = 8.5 Hz, 2H), 2.80 (s, 3H), 2.37 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.5 (d), 144.9 (s), 140.5 (s), 136.0 (s), 133.4 (s), 133.13 (s), 133.05 (s), 130.7 (d, 2C), 130.4 (s), 130.0 (s), 129.9 (d, 2C), 129.2 (d, 2C), 129.1 (s), 128.4 (d, 2C), 127.7 (d, 2C), 127.3 (d), 126.2 (d, 2C), 124.9 (s), 124.1 (d), 117.4 (d), 114.4 (s), 21.7 (q), 12.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3356, 3170, 2978, 2714, 1727, 1686, 1616, 1597, 1552, 1489, 1447, 1382, 1352, 1333, 1242, 1216, 1186, 1163, 1089, 1037, 1011, 935, 873, 837, 812, 757, 740, 715, 693, 657, 638, 616 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{29}H_{22}{}^{35}ClN_2O_3S$ calcd for 513.1045, found 513.1051.



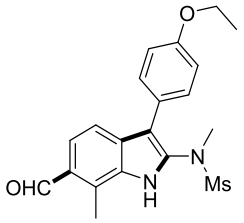
***N*-(6-formyl-7-methyl-3-(*p*-tolyl)-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3o)**

Yield: 79 mg, 92%; white solid, mp 250-253 °C; R_f = 0.16 (EA/PE = 1/5); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.83 (brs, 1H), 10.35 (s, 1H), 7.53 (d, *J* = 8.5 Hz, 1H), 7.42 (d, *J* = 8.0 Hz, 3H), 7.24 (d, *J* = 7.0 Hz, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 7.02 (d, *J* = 8.0 Hz, 2H), 3.26 (s, 3H), 2.85 (s, 3H), 2.38 (s, 3H), 2.33 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 144.1 (s), 136.2 (s), 135.6 (s), 134.8 (s), 133.5 (s), 130.1 (s), 130.0 (d, 2C), 129.8 (s), 129.4 (d, 2C), 129.2 (d, 2C), 128.5 (s), 127.7 (d, 2C), 126.6 (s), 121.9 (d), 117.1 (d), 113.9 (s), 38.8 (q), 21.5 (q), 21.3 (q), 12.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3353, 2946, 2918, 2708, 1911, 1739, 1679, 1617, 1561, 1510, 1452, 1420, 1405, 1378, 1364, 1345, 1327, 1305, 1256, 1211, 1154, 1105, 1090, 1048, 1020, 999, 916, 868, 829, 808, 763, 746, 716, 659, 642, 624 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{25}H_{23}N_2O_3S$ calcd for 431.1435, found 431.1434.



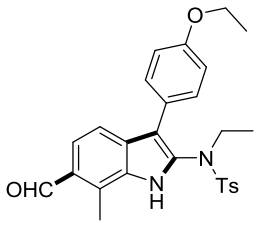
***N*-(3-(4-(*tert*-butyl)phenyl)-6-formyl-7-methyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3p)**

Yield: 94 mg, 99%; light yellow solid, mp 225-228 °C; R_f = 0.16 (EA/PE = 1/5); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.74 (brs, 1H), 10.33 (s, 1H), 7.56-7.43 (m, 2H), 7.42-7.36 (m, 2H), 7.33-7.27 (m, 2H), 7.24-7.18 (m, 2H), 7.15-7.10 (m, 2H), 3.27 (s, 3H), 2.86 (s, 3H), 2.36 (s, 3H), 1.32 (s, 9H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 149.2 (s), 143.9 (s), 135.5 (s), 134.7 (s), 133.6 (s), 130.1 (s), 129.9 (d, 2C), 129.8 (s), 129.0 (d, 2C), 128.5 (s), 127.9 (d, 2C), 126.6 (s), 125.5 (d, 2C), 121.9 (d), 117.2 (d), 114.1 (s), 38.7 (q), 34.7 (s), 31.6 (q), 21.6 (q), 12.9 (q, 3C) ppm; IR (reflection) $\tilde{\nu}$ = 3203, 2959, 2868, 1739, 1668, 1650, 1614, 1554, 1509, 1458, 1419, 1364, 1345, 1327, 1267, 1212, 1155, 1090, 1046, 1019, 994, 919, 867, 839, 811, 757, 739, 720, 659, 608 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{28}H_{29}N_2O_3S$ calcd for 473.1904, found 473.1904.



***N*-(3-(4-ethoxyphenyl)-6-formyl-7-methyl-1*H*-indol-2-yl)-*N*-methylmethanesulfonamide (3q)**

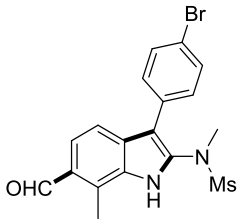
Yield: 77 mg, 99%; yellow solid, mp 247-249 °C; R_f = 0.13 (EA/PE = 1/2); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.86 (s, 1H), 10.35 (s, 1H), 7.55 (d, J = 8.5 Hz, 1H), 7.48 (d, J = 8.5 Hz, 1H), 7.46 (d, J = 8.0 Hz, 2H), 7.04 (d, J = 9.0 Hz, 2H), 4.07 (q, J = 7.0 Hz, 2H), 3.29 (s, 3H), 2.98 (s, 3H), 2.87 (s, 3H), 1.36 (t, J = 7.0 Hz, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 157.9 (s), 135.0 (s), 133.4 (s), 130.6 (d, 2C), 129.8 (s), 128.4 (s), 126.5 (s), 125.3 (s), 122.0 (d), 117.2 (d), 115.1 (d, 2C), 114.0 (s), 63.5 (t), 39.5 (q), 38.7 (q), 15.2 (q), 12.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3185, 3016, 2974, 2942, 2921, 2880, 1738, 1652, 1608, 1552, 1511, 1474, 1408, 1391, 1367, 1324, 1283, 1240, 1178, 1147, 1102, 1072, 1044, 1011, 994, 977, 960, 922, 868, 842, 809, 774, 743, 720, 673, 643, 605 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{20}H_{21}N_2O_4S$ calcd for 385.1228, found 385.1229.



***N*-(3-(4-ethoxyphenyl)-6-formyl-7-methyl-1*H*-indol-2-yl)-*N*-ethyl-4-methylbenzenesulfonamide (3r)**

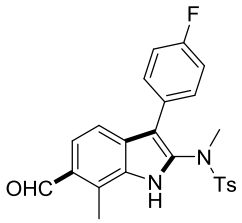
Yield: 91 mg, 96%; white solid, mp 208-210 °C; R_f = 0.33 (EA/PE = 1/4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.28 (s, 1H), 8.92 (brs, 1H), 7.51 (t, J = 8.0 Hz, 3H), 7.35 (d, J = 8.5 Hz, 1H), 7.21 (d, J = 8.0 Hz, 2H), 6.63-6.58 (m, 2H), 6.50-6.45 (m, 2H), 3.94 (q, J = 7.0 Hz, 2H), 3.37 (q, J = 7.0 Hz,

2H), 2.78 (s, 3H), 2.38 (s, 3H), 1.36 (t, J = 6.5 Hz, 3H), 0.96 (t, J = 7.5 Hz, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.5 (d), 158.2 (s), 144.4 (s), 135.5 (s), 133.0 (s), 131.4 (s), 130.6 (s), 130.2 (d, 2C), 129.9 (d, 2C), 128.6 (s), 127.4 (d, 2C), 124.4 (s), 124.3 (s), 123.5 (d), 117.1 (d), 114.3 (d, 2C), 113.1 (s), 63.4 (t), 45.1 (t), 21.6 (q), 14.9 (q), 14.6 (q), 12.7 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3251, 2980, 2923, 2875, 1917, 1655, 1608, 1554, 1507, 1478, 1454, 1392, 1377, 1355, 1326, 1308, 1280, 1245, 1202, 1174, 1158, 1115, 1090, 1044, 1020, 1000, 950, 920, 873, 842, 812, 800, 784, 768, 741, 727, 706, 695, 666, 648 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{27}H_{27}N_2O_4S$ calcd for 475.1697, found 475.1699.



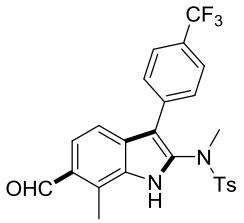
_N_-(3-(4-bromophenyl)-6-formyl-7-methyl-1_H_-indol-2-yl)-_N_-methylmethanesulfonamide (3s)

Yield: 60 mg, 71%; white solid, mp 252-255 °C; R_f = 0.10 (EA/PE = 1/2); ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.00 (s, 1H), 10.36 (s, 1H), 7.68 (d, J = 8.0 Hz, 2H), 7.57 (d, J = 8.0 Hz, 1H), 7.52 (t, J = 8.5 Hz, 3H), 3.32 (s, 3H), 3.07 (s, 3H), 2.88 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 135.4 (s), 133.6 (s), 132.7 (s), 132.1 (d, 2C), 131.4 (d, 2C), 129.2 (s), 128.6 (s), 126.7 (s), 122.4 (d), 120.4 (s), 117.0 (d), 113.1 (s), 39.3 (q), 38.6 (q), 13.0 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3176, 3070, 2942, 1649, 1613, 1553, 1510, 1488, 1414, 1390, 1341, 1323, 1262, 1212, 1180, 1148, 1096, 1071, 1043, 1009, 993, 965, 917, 865, 832, 807, 772, 727, 680, 652, 629 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{18}H_{16}{}^{79}BrN_2O_3S$ calcd for 419.0070, found 419.0071.



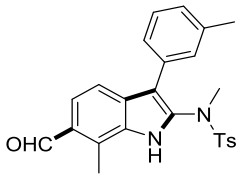
_N_-(3-(4-fluorophenyl)-6-formyl-7-methyl-1_H_-indol-2-yl)-_N_,4-dimethylbenzenesulfonamide (3t)

Yield: 75 mg, 86%; white solid, mp 273-276 °C; R_f = 0.23 (EA/PE = 1/4); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.90 (s, 1H), 10.35 (s, 1H), 7.54 (d, J = 8.5 Hz, 1H), 7.42 (d, J = 9.0 Hz, 3H), 7.24 (d, J = 8.0 Hz, 2H), 7.22-7.16 (m, 2H), 7.09 (t, J = 9.0 Hz, 2H), 3.31 (s, 3H), 2.85 (s, 3H), 2.38 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 162.5 (d, $J_{C\text{-}F}$ = 242.0 Hz), 144.1 (s), 135.6 (s), 134.9 (s), 133.5 (s), 131.2 (d, $J_{C\text{-}F}$ = 8.1 Hz, 2C), 130.0 (d, 2C), 129.5 (s), 129.4 (d, $J_{C\text{-}F}$ = 3.1 Hz), 128.6 (s), 127.7 (d, 2C), 126.7 (s), 122.1 (d), 117.0 (d), 115.7 (d, $J_{C\text{-}F}$ = 21.1 Hz, 2C), 113.1 (s), 39.0 (q), 21.5 (q), 12.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3154, 3114, 3067, 3018, 1895, 1646, 1602, 1556, 1502, 1466, 1424, 1393, 1372, 1344, 1327, 1272, 1214, 1188, 1157, 1106, 1089, 1045, 1011, 994, 921, 867, 838, 814, 754, 721, 692, 658, 614 cm^{-1}; HRMS (ESI) (*m/z*) [M+Na]$^+$ $C_{24}H_{21}FN_2NaO_3S$ calcd for 459.1149, found 459.1160.



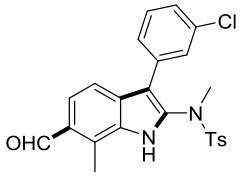
***N*-(6-formyl-7-methyl-3-(4-(trifluoromethyl)phenyl)-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3u)**

Yield: 49 mg, 50%; white solid, mp 273-276 °C; R_f = 0.20 (EA/PE = 1/4); ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.09 (s, 1H), 10.36 (s, 1H), 7.62-7.55 (m, 3H), 7.51 (d, J = 8.5 Hz, 1H), 7.43 (d, J = 8.0 Hz, 2H), 7.36 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 8.0 Hz, 2H), 3.42 (s, 3H), 2.86 (s, 3H), 2.32 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 144.0 (s), 137.6 (s), 135.7 (s), 135.5 (s), 133.7 (s), 129.9 (d, 2C), 129.8 (d, 2C), 129.1 (d), 128.8 (d), 127.6 (d, 2C), 127.1 (q, J_{C-F} = 31.5 Hz), 126.8 (s), 125.6 (q, J_{C-F} = 3.8 Hz, 2C), 124.9 (q, J_{C-F} = 270.3 Hz), 122.4 (d), 116.9 (d), 112.8 (s), 39.1 (q), 21.3 (q), 12.9 (q) ppm; ^{19}F NMR (471 MHz, DMSO-d_6) δ -60.78 (s, 3F) ppm; IR (reflection) $\tilde{\nu}$ = 3161, 3066, 1647, 1612, 1557, 1514, 1494, 1463, 1425, 1406, 1345, 1323, 1270, 1213, 1187, 1157, 1120, 1103, 1091, 1068, 1014, 993, 921, 868, 848, 816, 776, 760, 736, 703, 679, 657, 610 cm^{-1}; HRMS (ESI) (*m/z*) [M+Na]$^+$ $C_{25}H_{21}F_3N_2NaO_3S$ calcd for 509.1117, found 509.1124.



***N*-(6-formyl-7-methyl-3-(*m*-tolyl)-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3v)**

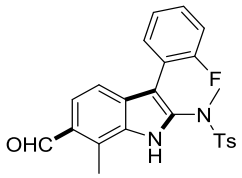
Yield: 78 mg, 90%; white solid, mp 231-233 °C; R_f = 0.34 (EA/PE = 1/4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.28 (s, 1H), 9.01 (brs, 1H), 7.51 (t, J = 8.5 Hz, 3H), 7.32 (d, J = 8.5 Hz, 1H), 7.25 (d, J = 8.0 Hz, 2H), 7.02 (t, J = 7.5 Hz, 1H), 6.96 (d, J = 7.5 Hz, 1H), 6.51 (d, J = 7.5 Hz, 1H), 6.13 (s, 1H), 2.94 (s, 3H), 2.81 (s, 3H), 2.39 (s, 3H), 2.06 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.5 (d), 144.6 (s), 137.8 (s), 134.1 (s), 133.9 (s), 132.6 (s), 132.3 (s), 130.6 (s), 130.1 (d, 2C), 130.0 (d), 128.6 (s), 128.2 (d), 128.0 (d), 127.6 (d, 2C), 126.5 (d), 124.3 (s), 123.7 (d), 117.0 (d), 111.7 (s), 38.1 (q), 21.7 (q), 21.3 (q), 12.7 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3168, 3116, 3067, 2915, 1738, 1643, 1614, 1586, 1554, 1512, 1484, 1425, 1391, 1371, 1343, 1326, 1305, 1270, 1212, 1182, 1156, 1108, 1090, 1058, 1008, 929, 905, 875, 842, 817, 801, 786, 764, 746, 710, 670, 653, 608 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{25}H_{25}N_2O_3S$ calcd for 431.1435, found 431.1438.



***N*-(3-(3-chlorophenyl)-6-formyl-7-methyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3w)**

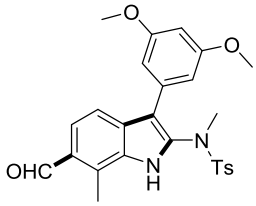
Yield: 63 mg, 70%; white solid, mp 249-251 °C; R_f = 0.28 (EA/PE = 1/4); ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.00 (s, 1H), 10.36 (s, 1H), 7.56 (d, J = 8.5 Hz, 1H), 7.45 (d, J = 8.5 Hz, 1H), 7.42 (d, J = 8.0 Hz, 2H), 7.35-7.27 (m, 2H), 7.25-7.19 (m, 3H), 7.08-7.05 (m, 1H), 3.33 (s, 3H), 2.85 (s, 3H),

2.38 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 144.2 (s), 135.4 (s), 135.3 (s), 135.2 (s), 133.6 (s), 133.5 (s), 130.7 (d), 130.1 (d, 2C), 129.3 (s), 128.74 (d), 128.67 (s), 128.0 (d), 127.6 (d, 2C), 126.8 (d), 126.7 (s), 122.3 (d), 116.9 (d), 112.5 (s), 38.9 (q), 21.5 (q), 12.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3153, 3116, 3061, 1739, 1645, 1613, 1597, 1553, 1511, 1479, 1425, 1393, 1371, 1344, 1325, 1271, 1211, 1188, 1157, 1109, 1090, 1075, 1052, 1020, 1001, 924, 888, 867, 816, 801, 786, 761, 698, 686, 662, 651, 610 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{24}H_{20}{}^{35}ClN_2O_3S$ calcd for 451.0889, found 451.0893.



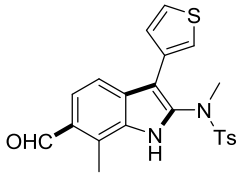
_N_-(3-(2-fluorophenyl)-6-formyl-7-methyl-1_H_-indol-2-yl)-_N_,4-dimethylbenzenesulfonamide (3x)

Yield: 44 mg, 50%; white solid, mp 159-161 °C; R_f = 0.26 (EA/PE = 1/5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.26 (s, 1H), 9.29 (brs, 1H), 7.49 (d, *J* = 8.5 Hz, 1H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.20-7.12 (m, 4H), 6.95 (t, *J* = 9.0 Hz, 1H), 6.78 (td, *J* = 7.5, 1.0 Hz, 1H), 6.23 (t, *J* = 7.5 Hz, 1H), 3.06 (s, 3H), 2.76 (s, 3H), 2.35 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.6 (d), 160.0 (d, J_{C-F} = 246.1 Hz), 144.5 (s), 135.2 (s), 134.1 (s), 132.7 (s), 132.1 (d, J_{C-F} = 3.1 Hz), 130.7 (s), 129.8 (d, 2C), 129.5 (d, J_{C-F} = 8.0 Hz), 128.6 (s), 127.5 (d, 2C), 124.7 (s), 123.8 (d, J_{C-F} = 3.4 Hz, 2C), 120.0 (d, J_{C-F} = 15.5 Hz), 117.3 (d, J_{C-F} = 1.9 Hz), 115.8 (d, J_{C-F} = 22.0 Hz), 105.9 (s), 38.0 (q), 21.6 (q), 12.7 (q) ppm; ^{19}F NMR (471 MHz, $CDCl_3$) δ -112.36 ppm; IR (reflection) $\tilde{\nu}$ = 3159, 3067, 2951, 1911, 1651, 1619, 1554, 1495, 1448, 1413, 1355, 1326, 1266, 1213, 1161, 1093, 1068, 1032, 1019, 994, 921, 867, 810, 757, 727, 715, 682, 665 cm^{-1}; HRMS (DART) (*m/z*) [M+H]$^+$ $C_{24}H_{22}FN_2O_3S$ calcd for 437.1330, found 437.1336.



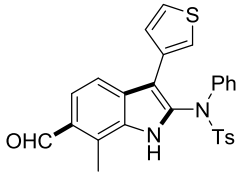
_N_-(3-(3,5-dimethoxyphenyl)-6-formyl-7-methyl-1_H_-indol-2-yl)-_N_,4-dimethylbenzenesulfonamide (3y)

Yield: 85 mg, 89%; light yellow solid, mp 188-190 °C; R_f = 0.18 (EA/PE = 1/4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.27 (s, 1H), 9.07 (brs, 1H), 7.50 (d, *J* = 8.5 Hz, 3H), 7.37 (d, *J* = 8.5 Hz, 1H), 7.19 (d, *J* = 8.5 Hz, 2H), 6.27 (t, *J* = 2.0 Hz, 1H), 5.83 (d, *J* = 2.0 Hz, 2H), 3.59 (s, 6H), 3.05 (s, 3H), 2.78 (s, 3H), 2.35 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.5 (d), 160.6 (s, 2C), 144.8 (s), 134.2 (s), 134.13 (s), 134.07 (s), 132.6 (s), 130.5 (s), 130.1 (d, 2C), 128.6 (s), 127.4 (d, 2C), 124.4 (s), 123.8 (d), 117.1 (d), 111.7 (s), 107.8 (d, 2C), 99.0 (d), 55.3 (q, 2C), 38.2 (q), 21.6 (q), 12.7 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3350, 2943, 2833, 2693, 1694, 1679, 1590, 1551, 1501, 1450, 1409, 1343, 1323, 1288, 1256, 1220, 1203, 1150, 1102, 1085, 1064, 1040, 1009, 935, 918, 866, 820, 796, 786, 764, 746, 718, 684, 668, 629 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{26}H_{25}N_2O_5S$ calcd for 477.1490, found 477.1492.



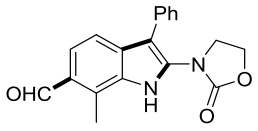
***N*-(6-formyl-7-methyl-3-(thiophen-3-yl)-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3z)**

Yield: 77 mg, 91%; white solid, mp 248-249 °C; R_f = 0.23 (EA/PE = 1/4); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.79 (s, 1H), 10.36 (s, 1H), 7.57 (q, *J* = 8.5 Hz, 2H), 7.53-7.48 (m, 3H), 7.35-7.30 (m, 3H), 7.07 (dd, *J* = 1.0, 5.0 Hz, 1H), 3.27 (s, 3H), 2.83 (s, 3H), 2.40 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 144.2 (s), 135.5 (s), 134.8 (s), 133.5 (s), 133.0 (s), 130.1 (d, 2C), 129.5 (s), 128.5 (s), 128.3 (d), 127.9 (d, 2C), 126.5 (s), 126.2 (d), 122.4 (d), 122.0 (d), 117.5 (d), 109.5 (s), 38.5 (q), 21.5 (q), 12.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3347, 2693, 1696, 1680, 1615, 1595, 1576, 1508, 1458, 1396, 1346, 1321, 1251, 1213, 1154, 1099, 1084, 100, 919, 867, 850, 815, 797, 783, 762, 741, 711, 688, 666, 638 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{22}H_{19}N_2O_3S_2$ calcd for 423.0843, found 423.0846.



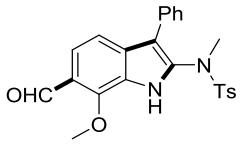
***N*-(6-formyl-7-methyl-3-(thiophen-3-yl)-1*H*-indol-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (3aa)**

Yield: 61 mg, 63%; yellow solid, mp 173-175 °C; R_f = 0.27 (EA/PE = 1/4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.29 (s, 1H), 9.04 (brs, 1H), 7.55 (d, *J* = 3.5 Hz, 1H), 7.53 (d, *J* = 4.0 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.17-7.12 (m, 4H), 7.11-7.05 (m, 4H), 6.73-6.69 (m, 1H), 6.67 (dd, *J* = 1.0, 5.0 Hz, 1H), 2.80 (s, 3H), 2.35 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.5 (d), 144.7 (s), 140.6 (s), 136.2 (s), 133.4 (s), 132.9 (s), 131.7 (s), 130.2 (s), 129.8 (d, 2C), 129.2 (d, 2C), 129.0 (s), 128.3 (d), 127.6 (d, 2C), 127.0 (d), 125.5 (d, 2C), 125.1 (d), 124.8 (s), 123.9 (d), 123.0 (d), 117.9 (d), 111.0 (s), 21.7 (q), 12.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3253, 2922, 1738, 1672, 1615, 1595, 1563, 1493, 1452, 1360, 1323, 1249, 1185, 1164, 1090, 1033, 955, 932, 875, 854, 811, 786, 761, 706, 693, 663, 621 cm^{-1}; HRMS (ESI) (*m/z*) [M-H]$^-$ $C_{27}H_{21}N_2O_3S_2$ calcd for 485.0999, found 485.1006.



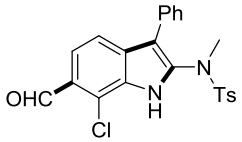
7-methyl-2-(2-oxooxazolidin-3-yl)-3-phenyl-1*H*-indole-6-carbaldehyde (3ab)

Yield: 42 mg, 66%; light yellow solid, mp 280-283 °C; R_f = 0.10 (EA/PE = 1/2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.28 (brs, 1H), 10.22 (s, 1H), 7.49 (d, *J* = 8.5 Hz, 1H), 7.41-7.31 (m, 5H), 7.21 (d, *J* = 8.5 Hz, 1H), 4.36 (t, *J* = 8.0 Hz, 2H), 3.65 (t, *J* = 8.5 Hz, 2H), 2.74 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 192.3 (d), 156.6 (s), 132.9 (s), 132.8 (s), 131.7 (s), 131.6 (s), 131.1 (d, 2C), 128.5 (d, 2C), 127.9 (s), 127.7 (d), 124.5 (d), 124.0 (s), 115.9 (d), 104.8 (s), 63.2 (t), 45.7 (t), 12.6 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3155, 3116, 3068, 3021, 2922, 1750, 1649, 1617, 1579, 1559, 1497, 1478, 1445, 1409, 1373, 1336, 1311, 1276, 1202, 1144, 1104, 1082, 1056, 1030, 973, 938, 887, 816, 783, 759, 715, 662, 646 cm^{-1}; HRMS (DART) (*m/z*) [M+H]$^+$ $C_{19}H_{17}N_2O_3$ calcd for 321.1234, found 321.1238.



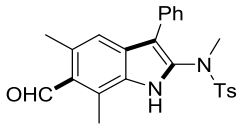
***N*-(6-formyl-7-methoxy-3-phenyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3ac)**

Yield: 48 mg, 55%; white solid, mp 169-171 °C; R_f = 0.18 (EA/PE = 1/5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.38 (s, 1H), 9.07 (brs, 1H), 7.52 (d, *J* = 8.5 Hz, 2H), 7.49 (d, *J* = 8.5 Hz, 1H), 7.26 (d, *J* = 8.5 Hz, 2H), 7.18-7.14 (m, 2H), 7.08 (t, *J* = 7.5 Hz, 2H), 6.51 (d, *J* = 7.5 Hz, 2H), 4.13 (s, 3H), 2.95 (s, 3H), 2.40 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.1 (d), 149.7 (s), 144.8 (s), 134.0 (s), 133.9 (s), 133.8 (s), 132.1 (s), 130.0 (d, 2C), 129.3 (d, 2C), 128.3 (d, 2C), 127.5 (d, 2C), 127.4 (d), 125.3 (s), 122.8 (s), 120.1 (d), 115.3 (d), 112.5 (s), 63.7 (q), 38.2 (q), 21.6 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3154, 3115, 3065, 2956, 2923, 2884, 1801, 1650, 1619, 1578, 1557, 1494, 1459, 1421, 1376, 1326, 1306, 1272, 1220, 1185, 1157, 1110, 1090, 1072, 1020, 965, 914, 878, 812, 782, 767, 745, 718, 698, 680, 661 cm^{-1}; HRMS (ESI) (*m/z*) $[M+H]^+$ $C_{24}H_{23}N_2O_4S$ calcd for 435.1373, found 435.1379.



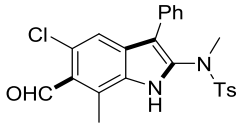
***N*-(7-chloro-6-formyl-3-phenyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3ad)**

Yield: 31 mg, 35%; white solid, mp 224-226 °C; R_f = 0.18 (EA/PE = 1/5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.48 (s, 1H), 9.14 (brs, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 8.0 Hz, 2H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 8.5 Hz, 2H), 7.18 (d, *J* = 8.5 Hz, 1H), 7.10 (d, *J* = 7.5 Hz, 2H), 6.51 (d, *J* = 7.0 Hz, 2H), 2.94 (s, 3H), 2.41 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 189.2 (d), 144.9 (s), 134.8 (s), 133.8 (s), 132.1 (s), 131.7 (s), 130.1 (d, 2C), 130.0 (s), 129.3 (d, 2C), 128.4 (d, 2C), 127.59 (d), 127.56 (d, 2C), 126.6 (s), 121.9 (s), 120.6 (d), 118.0 (d), 112.6 (s), 38.2 (q), 21.7 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3144, 3101, 3044, 2988, 2922, 1733, 1685, 1655, 1618, 1577, 1560, 1547, 1493, 1453, 1425, 1351, 1329, 1306, 1270, 1238, 1184, 1158, 1134, 1092, 1072, 1032, 1012, 985, 959, 913, 855, 811, 770, 753, 726, 692, 654 cm^{-1}; HRMS (ESI) (*m/z*) $[M-H]^-$ $C_{23}H_{18}{}^{35}ClN_2O_3S$ calcd for 437.0732, found 437.0733.



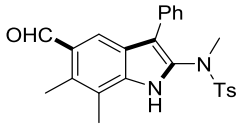
***N*-(6-formyl-5,7-dimethyl-3-phenyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3ae)**

Yield: 86 mg, 99%; white solid, mp 240-243 °C; R_f = 0.32 (EA/PE = 1/4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.62 (s, 1H), 8.83 (brs, 1H), 7.50 (d, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.16 (t, *J* = 7.0 Hz, 1H), 7.08 (t, *J* = 8.0 Hz, 2H), 7.05 (s, 1H), 6.51 (d, *J* = 7.5 Hz, 2H), 2.94 (s, 3H), 2.74 (s, 3H), 2.58 (s, 3H), 2.39 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 193.3 (d), 144.6 (s), 134.1 (s), 133.9 (s), 133.1 (s), 132.5 (s), 131.6 (s), 130.0 (d, 2C), 129.9 (s), 129.4 (d, 2C), 128.3 (d, 2C), 127.5 (d, 2C), 127.2 (s), 127.1 (d), 124.9 (s), 118.9 (d), 111.4 (s), 38.2 (q), 21.7 (q), 21.1 (q), 14.0 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3328, 2734, 1688, 1619, 1597, 1563, 1481, 1393, 1334, 1239, 1213, 1187, 1154, 1084, 998, 899, 876, 861, 825, 804, 787, 762, 754,731, 718, 672, 656, 638, 608 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{25}H_{25}N_2O_3S$ calcd for 433.1580, found 433.1585.



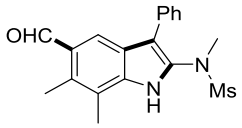
***N*-(5-chloro-6-formyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3af)**

Yield: 90 mg, 99%; white solid, mp 272-275 °C; R_f = 0.44 (EA/PE = 1/4); ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.03 (s, 1H), 10.58 (s, 1H), 7.43 (s, 1H), 7.41 (d, *J* = 3.0 Hz, 2H), 7.29 (t, *J* = 3.5 Hz, 3H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.15-7.12 (m, 2H), 3.24 (s, 3H), 2.76 (s, 3H), 2.39 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.8 (d), 170.9 (s), 144.3 (s), 136.1 (s), 135.2 (s), 132.6 (s), 132.4 (s), 130.1 (d, 2C), 129.3 (d, 2C), 129.0 (d, 2C), 128.8 (s), 127.8 (d, 2C), 127.6 (s), 127.2 (d), 124.4 (s), 117.9 (d), 113.6 (s), 38.6 (q), 21.5 (q), 15.0 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3323, 3065, 2919, 1670, 1613, 1580, 1551, 1498, 1475, 1371, 1347, 1328, 1302, 1250, 1154, 1121, 1088, 1060, 1034, 1017, 993, 934, 895, 852, 838, 814, 801, 780, 752, 715, 695, 660, 609 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{24}H_{22}{}^{35}ClN_2O_3S$ calcd for 453.1034, found 453.1041.



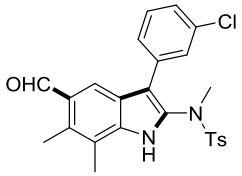
***N*-(5-formyl-6,7-dimethyl-3-phenyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (4a)**

Yield: 86 mg, 99%; white solid, mp 248-250 °C; R_f = 0.37 (EA/PE = 1/4); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.59 (s, 1H), 10.15 (s, 1H), 7.87 (s, 1H), 7.41 (d, *J* = 8.0 Hz, 2H), 7.32-7.26 (m, 3H), 7.22 (d, *J* = 8.0 Hz, 2H), 7.19 (d, *J* = 7.0 Hz, 2H), 3.27 (s, 3H), 2.63 (s, 3H), 2.46 (s, 3H), 2.37 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 194.0 (d), 144.1 (s), 137.0 (s), 135.5 (s), 133.1 (s), 132.1 (s), 131.9 (s), 130.0 (d, 2C), 129.3 (d, 2C), 128.9 (d, 2C), 128.6 (s), 127.8 (d, 2C), 126.9 (d), 124.8 (d), 123.5 (s), 120.9 (s), 114.8 (s), 38.8 (q), 21.5 (q), 14.7 (q), 13.7 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3350, 1686, 1617, 1599, 1565, 1494, 1473, 1417, 1341, 1310, 1243, 1206, 1155, 1122, 1086, 987, 894, 844, 813, 789, 759, 739, 713, 690, 665, 637 cm^{-1}; HRMS (ESI) (*m/z*) $[M-H]^-$ $C_{25}H_{23}N_2O_3S$ calcd for 431.1435, found 431.1442.



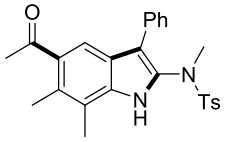
***N*-(5-formyl-6,7-dimethyl-3-phenyl-1*H*-indol-2-yl)-*N*-methylmethanesulfonamide (4b)**

Yield: 71 mg, 99%; light yellow solid, mp 215-218 °C; R_f = 0.10 (EA/PE = 1/4); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.68 (s, 1H), 10.17 (s, 1H), 7.96 (s, 1H), 7.60 (d, *J* = 8.0 Hz, 2H), 7.51 (t, *J* = 7.5 Hz, 2H), 7.37 (t, *J* = 7.5 Hz, 1H), 3.31 (s, 3H), 2.95 (s, 3H), 2.64 (s, 3H), 2.49 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 194.0 (d), 137.0 (s), 133.4 (s), 132.5 (s), 131.9 (s), 129.3 (d, 2C), 129.2 (d, 2C), 128.6 (s), 127.3 (d), 124.9 (d), 123.4 (s), 121.0 (s), 114.5 (s), 39.4 (q), 38.8 (q), 14.7 (q), 13.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3259, 3015, 2933, 1738, 1657, 1598, 1495, 1431, 1410, 1330, 1244, 1199, 1148, 1098, 1075, 1030, 1004, 991, 974, 964, 896, 847, 791, 776, 765, 741, 715, 701, 683, 663, 626 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{19}H_{21}N_2O_3S$ calcd for 357.1267, found 357.1273.



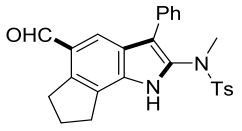
***N*-(3-(3-chlorophenyl)-5-formyl-6,7-dimethyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (4c)**

Yield: 69 mg, 74%; white solid, mp 228-231 °C; R_f = 0.36 (EA/PE = 1/4); ^{1}H NMR (500 MHz, DMSO-d_6) δ 11.72 (s, 1H), 10.16 (s, 1H), 7.86 (s, 1H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 8.0 Hz, 1H), 7.32-7.28 (m, 1H), 7.24 (d, *J* = 7.5 Hz, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.08 (s, 1H), 3.33 (s, 3H), 2.63 (s, 3H), 2.46 (s, 3H), 2.37 (s, 3H) ppm; ^{13}C NMR (125 MHz, DMSO-d_6) δ 194.0 (d), 144.1 (s), 137.0 (s), 135.6 (s), 135.3 (s), 133.6 (s), 132.6 (s), 132.2 (s), 130.7 (d), 130.0 (d, 2C), 128.8 (s), 128.6 (d), 128.0 (d), 127.5 (d, 2C), 126.8 (d), 124.4 (d), 123.2 (s), 121.1 (s), 113.2 (s), 39.0 (q), 21.5 (q), 14.7 (q), 13.7 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3331, 2921, 2731, 1690, 1619, 1596, 1563, 1480, 1392, 1334, 1310, 1270, 1239, 1213, 1186, 1155, 1084, 1021, 998, 899, 876, 861, 825, 803, 787, 762, 754, 731, 718, 674, 656, 638, 607 cm^{-1}; HRMS (DART) (*m/z*) [M+H]$^+$ $C_{25}H_{24}{}^{35}ClN_2O_3S$ calcd for 467.1191, found 467.1199.



***N*-(5-acetyl-6,7-dimethyl-3-phenyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (4d)**

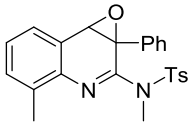
Yield: 37 mg, 42%; white solid, mp 249-251 °C; R_f = 0.38 (EA/PE = 1/4); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57 (brs, 1H), 7.57 (s, 1H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.16 (t, *J* = 7.5 Hz, 1H), 7.08 (t, *J* = 8.0 Hz, 2H), 6.54 (d, *J* = 7.0 Hz, 2H), 2.97 (s, 3H), 2.47 (s, 3H), 2.45 (s, 3H), 2.39 (s, 6H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 203.1 (s), 144.5 (s), 134.6 (s), 133.9 (s), 133.5 (s), 132.6 (s), 130.9 (s), 130.3 (s), 129.9 (d, 2C), 129.2 (d, 2C), 128.3 (d, 2C), 127.6 (d, 2C), 127.0 (d), 123.2 (s), 119.6 (s), 118.8 (d), 112.5 (s), 38.4 (q), 30.2 (q), 21.6 (q), 16.7 (q), 13.6 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3345, 2923, 1668, 1620, 1599, 1565, 1495, 1470, 1414, 1346, 1307, 1257, 1216, 1185, 1152, 1116, 1086, 1074, 1019, 987, 919, 875, 802, 789, 756, 712, 692, 672, 661, 633 cm^{-1}; HRMS (DART) (*m/z*) [M+H]$^+$ $C_{26}H_{27}N_2O_3S$ calcd for 447.1737, found 447.1740.



***N*-(5-formyl-3-phenyl-1,6,7,8-tetrahydrocyclopenta[*g*]indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (4e)**

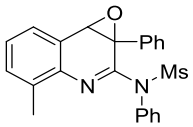
Yield: 88 mg, 99%; white solid, mp 215-217 °C; R_f = 0.35 (EA/PE = 1/4); ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.83 (s, 1H), 10.00 (s, 1H), 7.87 (s, 1H), 7.42 (d, *J* = 8.0 Hz, 2H), 7.32-7.26 (m, 3H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.21-7.18 (m, 2H), 3.27 (t, *J* = 7.6 Hz, 2H), 3.21 (s, 3H), 3.06-3.01 (m, 2H), 2.37 (s, 3H), 2.22-2.13 (m, 2H) ppm; ^{13}C NMR (75 MHz, DMSO-d_6) δ 193.3 (d), 144.2 (s), 140.0 (s), 135.2 (s), 134.0 (s), 133.3 (s), 132.0 (s), 130.1 (d, 2C), 129.3 (d, 2C), 128.9 (d, 2C), 127.9 (d), 127.8 (d, 2C), 127.0 (d), 126.7 (d), 125.0 (s), 124.7 (d), 115.0 (s), 32.4 (q), 30.0 (t), 29.8 (t), 25.4 (t), 21.5 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3323, 2946, 2733, 1741, 1672, 1636, 1599, 1576, 1497,

1476, 1454, 1435, 1422, 1378, 1336, 1305, 1252, 1185, 1156, 1089, 1074, 1028, 1002, 991, 949, 877, 862, 808, 774, 757, 739, 714, 695, 661, 643, 615 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{26}H_{25}N_2O_3S$ calcd for 445.1580, found 445.1581.



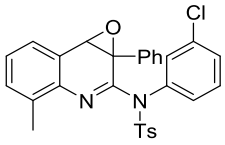
***N*,4-dimethyl-*N*-(4-methyl-1a-phenyl-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)benzenesulfonamide (5a)**

Yield: 74 mg, 88%; white solid, mp 100-102 °C; R_f = 0.26 (EA/PE = 1/10); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.1 Hz, 2H), 7.48-7.42 (m, 2H), 7.40-7.27 (m, 4H), 7.26-7.22 (m, 1H), 7.20-7.10 (m, 3H), 4.10 (s, 1H), 2.89 (s, 3H), 2.33 (s, 3H), 2.29 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.6 (s), 143.8 (s), 139.6 (s), 137.7 (s), 136.4 (s), 135.0 (s), 131.8 (d), 129.3 (d, 2C), 128.4 (d, 2C), 128.4 (d, 2C), 127.9 (d), 127.5 (d), 127.0 (d), 126.0 (d, 2C), 124.3 (s), 67.3 (d), 62.3 (s), 35.6 (q), 21.6 (q), 17.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 2920, 1599, 1579, 1495, 1450, 1351, 1292, 1251, 1160, 1089, 1073, 1021, 948, 898, 840, 808, 762, 731, 699, 682, 663, 620 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{24}H_{23}N_2O_3S$ calcd for 419.1424, found 419.1430.



***N*-(4-methyl-1a-phenyl-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)-*N*-phenylmethanesulfonamide (5b)**

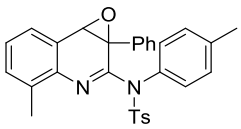
Yield: 65 mg, 81%; white solid, mp 185-187 °C; R_f = 0.19 (EA/PE = 1/15); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (d, *J* = 7.5 Hz, 2H), 7.20-7.17 (m, 1H), 7.15-7.11 (m, 2H), 7.10-7.02 (m, 4H), 6.93 (brs, 2H), 6.76 (d, *J* = 7.5 Hz, 2H), 4.10 (s, 1H), 3.42 (s, 3H), 2.57 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 154.3 (s), 139.5 (s), 137.2 (s), 135.9 (s), 134.7 (s), 132.1 (d), 129.4 (d, 2C), 128.6 (d, 2C), 128.2 (d), 128.0 (d, 2C), 127.9 (d), 127.3 (d), 127.1 (d), 125.6 (d, 2C), 124.3 (s), 66.4 (d), 62.3 (s), 40.3 (q), 18.5 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3032, 2923, 1738, 1612, 1580, 1492, 1473, 1449, 1351, 1316, 1278, 1205, 1163, 1152, 1111, 1077, 1030, 969, 940, 889, 858, 842, 810, 781, 768, 742, 691, 610 cm^{-1}; HRMS (ESI) (*m/z*) $[M+H]^+$ $C_{23}H_{21}N_2O_3S$ calcd for 405.1267, found 405.1260.



***N*-(3-chlorophenyl)-4-methyl-*N*-(4-methyl-1a-phenyl-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)benzenesulfonamide (5c)**

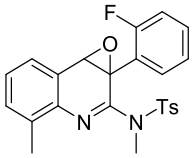
Yield: 58 mg, 56%; white solid, mp 166-169 °C; R_f = 0.28 (EA/PE = 1/15); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.5 Hz, 2H), 7.29 (d, *J* = 7.5 Hz, 2H), 7.22 (t, *J* = 7.5 Hz, 1H), 7.19-7.09 (m, 5H), 7.13-7.10 (m, 1H), 6.98 (t, *J* = 8.0 Hz, 3H), 6.69 (t, *J* = 2.0 Hz, 1H), 6.63 (dd, *J* = 1.0, 8.0 Hz, 1H), 4.07 (s, 1H), 2.42 (s, 3H), 2.34 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.3 (s), 143.9 (s), 139.7 (s), 137.7 (s), 137.5 (s), 137.0 (s), 134.9 (s), 134.0 (s), 132.1 (d), 130.3 (d), 129.1 (d, 2C), 129.0 (d), 128.5 (d, 2C), 128.2 (d, 4C), 128.1 (d), 127.8 (d), 127.3 (d), 127.1 (d), 125.6 (d), 124.4 (s), 66.3 (d), 62.4 (s), 21.6 (q), 19.0 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3030, 1609, 1572, 1495, 1466, 1448, 1432, 1363,

1289, 1251, 1203, 1168, 1092, 1079, 1042, 981, 953, 909, 889, 862, 845, 812, 783, 768, 752, 708, 699, 678, 666, 647 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{29}H_{24}{}^{35}ClN_2O_3S$ calcd for 515.1191, found 515.1200.



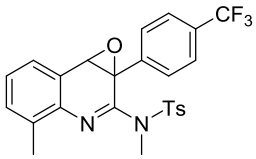
4-methyl-*N*-(4-methyl-1a-phenyl-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)-*N*-(p-tolyl)benzenesulfonamide (5e)

Yield: 54 mg, 60%; yellow solid, mp 190-191 °C; R_f = 0.33 (EA/PE = 1/10); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.5 Hz, 2H), 7.26 (d, *J* = 7.5 Hz, 2H), 7.18-7.09 (m, 6H), 6.99 (s, 2H), 6.81 (d, *J* = 8.0 Hz, 2H), 6.56 (d, *J* = 8.0 Hz, 2H), 4.01 (s, 1H), 2.41 (s, 3H), 2.32 (s, 3H), 2.22 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.7 (s), 143.5 (s), 139.9 (s), 138.1 (s), 137.5 (s), 137.3 (s), 135.4 (s), 133.6 (s), 132.0 (d), 129.8 (d, 2C), 128.93 (d, 2C), 128.88 (d, 2C), 128.6 (d, 2C), 128.0 (d, 2C), 127.8 (d), 127.01 (d), 126.98 (d), 125.7 (d, 2C), 124.3 (s), 66.3 (d), 62.4 (s), 21.6 (q), 21.2 (q), 19.0 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3032, 2951, 2925, 1896, 1609, 1576, 1506, 1466, 1449, 1348, 1320, 1299, 1279, 1255, 1209, 1162, 1090, 1077, 1045, 951, 903, 869, 843, 817, 764, 719, 696, 681, 665, 616 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{30}H_{27}N_2O_3S$ calcd for 495.1737, found 495.1744.



***N*-(1a-(2-fluorophenyl)-4-methyl-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)-*N*,4-dimethylbenzenesulfonamide (5f)**

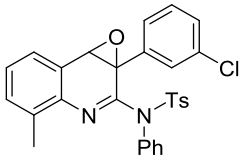
Yield: 67 mg, 77%; white solid, mp 173-175 °C; R_f = 0.24 (EA/PE = 1/10); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (t, *J* = 7.5 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.35 (d, *J* = 7.0 Hz, 1H), 7.31-7.26 (m, 1H), 7.24 (d, *J* = 7.5 Hz, 1H), 7.20-7.15 (m, 2H), 7.13 (d, *J* = 8.5 Hz, 2H), 6.95 (t, *J* = 10.0 Hz, 1H), 4.17 (s, 1H), 2.90 (s, 3H), 2.31 (s, 3H), 2.21 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 160.8 (d, J_{C-F} = 243.9 Hz), 155.2 (s), 144.0 (s), 139.5 (s), 137.9 (s), 133.0 (s), 131.7 (d), 129.9 (d, J_{C-F} = 8.0 Hz), 129.2 (d, 2C), 128.6 (d, 2C), 128.2 (d, J_{C-F} = 3.4 Hz), 127.7 (d), 127.0 (d), 124.8 (d, J_{C-F} = 13.1 Hz), 124.3 (s), 124.2 (d, J_{C-F} = 3.1 Hz), 114.6 (d, J_{C-F} = 20.3 Hz), 65.9 (d), 60.9 (s), 36.5 (q), 21.6 (q), 17.5 (q) ppm; ^{19}F NMR (471 MHz, $CDCl_3$) δ -12.14 ppm; IR (reflection) $\tilde{\nu}$ = 2946, 1929, 1736, 1596, 1579, 1491, 1458, 1420, 1341, 1319, 1296, 1260, 1249, 1233, 1211, 1188, 1177, 1156, 1115, 1103, 1085, 1018, 967, 953, 902, 882, 837, 807, 761, 726, 708, 660, 616 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{24}H_{22}FN_2O_3S$ calcd for 437.1330, found 437.1335.



***N*,4-dimethyl-*N*-(4-methyl-1a-(4-(trifluoromethyl)phenyl)-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)benzenesulfonamide (5g)**

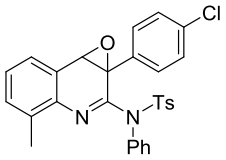
Yield: 94 mg, 97%; white solid, mp 136-139 °C; R_f = 0.31 (EA/PE = 1/10); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.7 Hz, 2H), 7.53 (dd, *J* = 2.4, 9.0 Hz, 4H), 7.33 (dd, *J* = 0.9, 7.2 Hz, 1H), 7.26 (d, *J* = 7.5 Hz, 1H), 7.19-7.12 (m, 3H), 4.09 (s, 1H), 2.93 (s, 3H), 2.32 (s, 3H), 2.27 (s, 3H)

ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 153.8 (s), 144.2 (s), 140.8 (q, J_{C-F} = 1.3 Hz), 139.4 (s), 137.9 (s), 133.9 (s), 132.0 (d), 129.9 (q, J_{C-F} = 32.2 Hz), 129.3 (d, 2C), 128.4 (d, 2C), 127.8 (d), 127.1 (d), 126.5 (d, 2C), 125.3 (q, J_{C-F} = 3.8 Hz, 2C), 124.1 (q, J_{C-F} = 270.0 Hz), 123.9 (s), 67.5 (d), 62.1 (s), 35.9 (q), 21.6 (q), 17.7 (q) ppm; IR (reflection) $\tilde{\nu}$ = 1609, 1598, 1578, 1461, 1409, 1385, 1324, 1279, 1232, 1185, 1164, 1152, 1117, 1106, 1087, 1065, 1023, 1014, 945, 898, 881, 849, 826, 809, 758, 744, 731, 711, 694, 659, 620, 610 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{25}H_{22}F_3N_2O_3S$ calcd for 487.1298, found 487.1304.



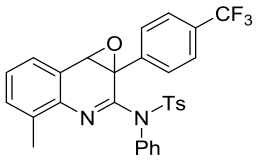
***N*-(1a-(3-chlorophenyl)-4-methyl-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (5h)**

Yield: 70 mg, 68%; white solid, mp 206-209 °C; R_f = 0.28 (EA/PE = 1/10); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 9.5 Hz, 2H), 7.29-7.25 (m, 2H), 7.19-7.10 (m, 6H), 7.09-6.98 (m, 3H), 6.73 (d, *J* = 8.0 Hz, 2H), 6.69 (brs, 1H), 4.03 (s, 1H), 2.41 (s, 3H), 2.32 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.9 (s), 143.7 (s), 139.8 (s), 137.7 (s), 137.4 (s), 137.1 (s), 136.3 (s), 134.2 (s), 132.3 (d), 130.0 (d, 2C), 129.4 (d), 129.0 (d, 2C), 128.53 (d, 2C), 128.47 (d, 2C), 128.2 (d), 128.0 (d), 127.2 (d), 127.1 (d), 125.3 (d), 124.6 (d), 123.9 (s), 66.2 (d), 61.8 (s), 21.6 (q), 19.0 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3071, 3042, 3026, 2954, 2921, 1923, 1879, 1810, 1611, 1597, 1573, 1490, 1476, 1424, 1360, 1302, 1281, 1255, 1237, 1202, 1189, 1166, 1111, 1092, 1079, 1032, 974, 947, 909, 893, 861, 838, 816, 784, 774, 757, 740, 708, 691, 667, 648 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{29}H_{24}{}^{35}ClN_2O_3S$ calcd for 515.1191, found 515.1206.



***N*-(1a-(4-chlorophenyl)-4-methyl-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (5i)**

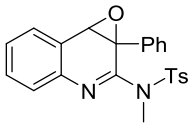
Yield: 75 mg, 73%; white solid, mp 179-180 °C; R_f = 0.47 (EA/PE = 1/10); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.5 Hz, 2H), 7.28 (d, *J* = 7.5 Hz, 2H), 7.17-7.13 (m, 4H), 7.12-7.09 (m, 2H), 7.07 (t, *J* = 8.0 Hz, 2H), 6.97-6.92 (m, 2H), 6.75 (d, *J* = 8.0 Hz, 2H), 4.01 (s, 1H), 2.40 (s, 3H), 2.32 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.1 (s), 143.7 (s), 139.8 (s), 137.7 (s), 137.1 (s), 136.3 (s), 133.91 (s), 133.88 (s), 132.2 (d), 129.8 (d, 2C), 129.0 (d, 2C), 128.9 (d), 128.5 (d, 4C), 128.2 (d, 2C), 128.1 (d), 127.2 (d), 127.0 (d, 2C), 124.1 (s), 66.4 (d), 62.0 (s), 21.6 (q), 19.0 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3052, 2952, 2919, 1611, 1596, 1580, 1490, 1455, 1402, 1378, 1360, 1309, 1291, 1269, 1255, 1199, 1168, 1111, 1089, 1044, 1013, 965, 942, 915, 899, 869, 843, 817, 773, 763, 745, 703, 692, 667, 649, 630, 613 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{29}H_{24}{}^{35}ClN_2O_3S$ calcd for 515.1191, found 515.1200.



4-methyl-*N*-(4-methyl-1a-(4-(trifluoromethyl)phenyl)-1a,7b-dihydrooxireno[2,3-c]quinolin-2-

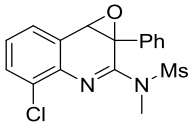
yl)-*N*-phenylbenzenesulfonamide (5j)

Yield: 86 mg, 78%; white solid, mp 147-149 °C; R_f = 0.36 (EA/PE = 1/10); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 7.0 Hz, 2H), 7.29 (dd, *J* = 2.5, 7.5 Hz, 2H), 7.25-7.06 (m, 6H), 7.03 (t, *J* = 8.0 Hz, 2H), 6.70 (d, *J* = 8.0 Hz, 2H), 4.05 (s, 1H), 2.41 (s, 3H), 2.32 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.6 (s), 143.8 (s), 139.8 (s), 139.2 (s), 137.8 (s), 137.1 (s), 136.3 (s), 132.3 (d), 130.1 (q, J_{C-F} = 32.3 Hz), 129.8 (d, 2C), 129.0 (d, 2C), 128.49 (d, 2C), 128.47 (d, 2C), 128.1 (d), 127.3 (d), 127.1 (d), 126.0 (d, 2C), 125.0 (q, J_{C-F} = 3.8 Hz, 2C), 124.0 (q, J_{C-F} = 270.5 Hz), 123.8 (s), 66.3 (d), 62.0 (s), 21.6 (q), 19.0 (q) ppm; IR (reflection) $\tilde{\nu}$ = 2924, 1619, 1595, 1575, 1491, 1469, 1412, 1361, 1323, 1279, 1250, 1165, 1115, 1092, 1066, 1043, 1017, 974, 943, 899, 868, 829, 811, 775, 763, 744, 722, 705, 696, 667, 650, 608 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{30}H_{24}FN_2O_3S$ calcd for 549.1454, found 549.1464.



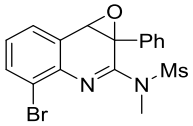
***N*,4-dimethyl-*N*-(1a-phenyl-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)benzenesulfonamide (5k)**

Yield: 39 mg, 48%; white solid, mp 172-175 °C; R_f = 0.20 (EA/PE = 1/10); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.8 Hz, 2H), 7.54-7.38 (m, 5H), 7.38-7.17 (m, 6H), 4.10 (s, 1H), 2.86 (s, 3H), 2.34 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.6 (s), 143.0 (s), 140.5 (s), 135.0 (s), 134.2 (s), 129.2 (d), 128.23 (d), 128.16 (d, 2C), 127.9 (d, 3C), 127.5 (d, 2C), 127.1 (d), 126.7 (d), 124.8 (d, 2C), 123.2 (s), 65.8 (d), 61.0 (s), 34.2 (q), 20.6 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3059, 3020, 2945, 2923, 1595, 1569, 1485, 1461, 1449, 1359, 1322, 1306, 1246, 1225, 1182, 1164, 1103, 1089, 1074, 1023, 956, 909, 886, 856, 816, 800, 766, 748, 698, 687, 665, 618 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{23}H_{21}N_2O_3S$ calcd for 405.1267, found 405.1268.



***N*-(4-chloro-1a-phenyl-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)-*N*-methylmethanesulfonamide (5l)**

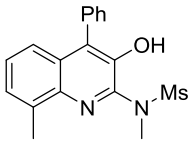
Yield: 71 mg, 98%; white solid, mp 192-194 °C; R_f = 0.13 (EA/PE = 1/15); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (dd, *J* = 1.0, 8.0 Hz, 1H), 7.50-7.47 (m, 2H), 7.41 (dd, *J* = 1.5, 7.5 Hz, 1H), 7.38-7.34 (m, 2H), 7.33-7.29 (m, 1H), 7.19 (dd, *J* = 8.0, 9.5 Hz, 1H), 4.16 (s, 1H), 3.45 (s, 3H), 2.85 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.7 (s), 138.0 (s), 134.4 (s), 133.6 (s), 131.4 (d), 128.9 (d, 2C), 128.8 (d), 127.94 (d), 127.87 (d), 125.8 (s), 125.7 (d, 2C), 66.6 (d), 61.9 (s), 41.1 (q), 34.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3059, 3020, 1965, 1602, 1561, 1494, 1450, 1347, 1310, 1285, 1238, 1192, 1164, 1124, 1068, 1035, 970, 878, 861, 836, 808, 782, 764, 755, 724, 698, 686, 670, 623 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{17}H_{16}{}^{35}ClN_2O_3S$ calcd for 363.0565, found 363.0569.



***N*-(4-bromo-1a-phenyl-1a,7b-dihydrooxireno[2,3-c]quinolin-2-yl)-*N*-**

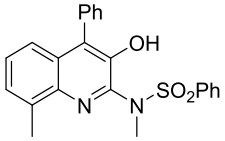
methylmethanesulfonamide (5m)

Yield: 65 mg, 80%; white solid, mp 189-191 °C; R_f = 0.12 (EA/PE = 1/2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 1.0, 8.0 Hz, 1H), 7.48 (d, *J* = 7.0 Hz, 2H), 7.45 (d, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 7.0 Hz, 2H), 7.33-7.30 (m, 1H), 7.12 (t, *J* = 8.0 Hz, 1H), 4.14 (s, 1H), 3.47 (s, 3H), 2.84 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 156.9 (s), 139.2 (s), 134.6 (d), 134.4 (s), 128.9 (d, 2C), 128.8 (d), 128.7 (d), 128.3(d), 125.8 (s), 125.6 (d, 2C), 124.5 (s), 66.7 (d), 62.0 (s), 41.0 (q), 34.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3057, 3019, 1963, 1600, 1557, 1494, 1446, 1347, 1310, 1238, 1188, 1163, 1128, 1068, 1034, 967, 912, 876, 862, 830, 805, 781, 764, 755, 722, 697, 685, 658, 621 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{17}H_{16}{}^{79}BrN_2O_3S$ calcd for 407.0060, found 407.0065.



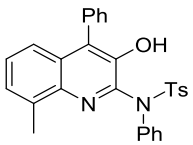
***N*-(3-hydroxy-8-methyl-4-phenylquinolin-2-yl)-*N*-methylmethanesulfonamide (6a)**

Yield: 66 mg, 97%; white solid, mp 195-197 °C; R_f = 0.25 (EA/PE = 1/5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (t, *J* = 7.0 Hz, 2H), 7.42-7.36 (m, 1H), 7.35 (d, *J* = 6.5 Hz, 3H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.24 (dd, *J* = 6.5 Hz, 8.0 Hz, 1H), 6.49 (s, 1H), 3.36 (s, 3H), 3.13 (s, 3H), 2.67 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.5 (s), 142.8 (s), 141.1 (s), 136.7 (s), 133.4 (s), 133.3 (s), 130.3 (d, 2C), 128.9 (s), 128.6 (d, 2C), 128.4 (d), 127.54 (d), 127.47 (d), 123.3 (d), 38.2 (q), 35.2 (q), 18.1 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3391, 1593, 1509, 1493, 1450, 1431, 1407, 1397, 1356, 1336, 1322, 1241, 1229, 1194, 1164, 1149, 1122, 1088, 1071, 1052, 972, 915, 857, 815, 790, 765, 748, 704, 684, 661, 644, 611 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{18}H_{19}N_2O_3S$ calcd for 343.1111, found 343.1115.



***N*-(3-hydroxy-8-methyl-4-phenylquinolin-2-yl)-*N*-methylbenzenesulfonamide (6b)**

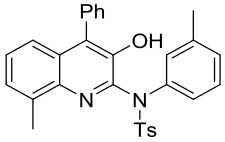
Yield: 77 mg, 96%; white solid, mp 206-207 °C; R_f = 0.21 (EA/PE = 1/10); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.5 Hz, 2H), 7.56 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.0 Hz, 2H), 7.43-7.36 (m, 5H), 7.31 (d, *J* = 8.5 Hz, 1H), 7.24 (d, *J* = 6.5 Hz, 1H), 7.20 (t, *J* = 8.5 Hz, 1H), 6.78 (s, 1H), 3.22 (s, 3H), 2.21 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 143.3 (s), 143.1 (s), 140.8 (s), 137.0 (s), 135.1 (s), 133.7 (s), 133.4 (d), 133.1 (s), 130.4 (d, 2C), 128.9 (d, 2C), 128.7 (d, 2C; s, 1C), 128.5 (d, 2C), 128.3 (d), 127.3 (d), 127.2 (d), 123.1 (d), 38.1 (q), 17.5 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3384, 3071, 2971, 2943, 1593, 1578, 1509, 1489, 1462, 1447, 1427, 1398, 1348, 1314, 1292, 1277, 1240, 1228, 1186, 1164, 1131, 1087, 1065, 1046, 1028, 999, 982, 910, 849, 826, 814, 782, 765, 756, 733, 718, 699, 687, 663, 646, 628 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{23}H_{21}N_2O_3S$ calcd for 405.1267, found 405.1274.



***N*-(3-hydroxy-8-methyl-4-phenylquinolin-2-yl)-4-methyl-*N*-phenylbenzenesulfonamide (6c)**

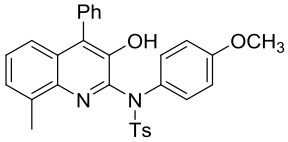
Yield: 73 mg, 76%; light yellow solid, mp 200-202 °C; R_f = 0.15 (EA/PE = 1/15); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 2H), 7.56-7.51 (m, 2H), 7.48-7.43 (m, 2H), 7.42-7.38 (m, 1H),

7.36-7.32 (m, 2H), 7.30 (t, J = 8.0 Hz, 2H), 7.26-7.22 (m, 4H), 7.20 (d, J = 8.5 Hz, 2H), 6.26 (s, 1H), 2.47 (s, 3H), 2.40 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.1 (s), 143.3 (s), 142.7 (s), 141.1 (s), 138.9 (s), 137.2 (s), 135.2 (s), 133.2 (s), 132.5 (s), 130.3 (d, 2C), 129.5 (d, 2C), 129.4 (d, 2C), 129.02 (d, 4C), 128.97 (s), 128.7 (d, 2C), 128.49 (d), 128.48 (d), 127.5 (d), 127.3 (d), 123.1 (d), 21.7 (q), 18.2 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3438, 3059, 2923, 1596, 1490, 1453, 1401, 1355, 1247, 1214, 1184, 1152, 1131, 1089, 1060, 1029, 1019, 980, 937, 913, 852, 812, 783, 766, 745, 732, 698, 672, 656, 634, 615 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{29}H_{25}N_2O_3S$ calcd for 481.1580, found 481.1588.



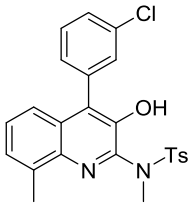
***N*-(4-hydroxy-8-methyl-3-phenylquinolin-2-yl)-4-methyl-*N*-(*m*-tolyl)benzenesulfonamide (6d)**

Yield: 64 mg, 65%; light yellow solid, mp 206-208 °C; R_f = 0.15 (EA/PE = 1/15); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 (d, J = 8.4 Hz, 2H), 7.48-7.26 (m, 9H), 7.21 (t, J = 7.8 Hz, 3H), 7.21 (t, J = 7.5 Hz, 1H), 7.03 (d, J = 7.5 Hz, 1H), 6.27 (s, 1H), 2.46 (s, 3H), 2.39 (s, 3H), 2.22 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.0 (s), 143.3 (s), 142.8 (s), 141.1 (s), 139.0 (s), 138.8 (s), 137.2 (s), 135.3 (s), 133.3 (s), 132.4 (s), 130.4 (d), 130.3 (d, 2C), 129.4 (d, 2C), 129.3 (d), 129.0 (d, 2C), 129.0 (s), 128.7 (d), 128.6 (d, 2C), 128.4 (d), 127.4 (d), 127.3 (d), 126.3 (d), 123.1 (d), 21.7 (q), 21.3 (q), 18.2 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3459, 3067, 3027, 2948, 2919, 1600, 1509, 1487, 1402, 1388, 1350, 1306, 1282, 1238, 1216, 1163, 1121, 1088, 1060, 1021, 978, 967, 907, 853, 828, 808, 769, 742, 728, 705, 695, 669, 646, 634, 615 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{30}H_{27}N_2O_3S$ calcd for 495.1737, found 495.1747.



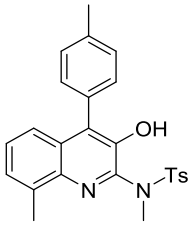
***N*-(3-hydroxy-8-methyl-4-phenylquinolin-2-yl)-*N*-(4-methoxyphenyl)-4-methylbenzenesulfonamide (6e)**

Yield: 77 mg, 76%; white solid, mp 209-211 °C; R_f = 0.25 (EA/PE = 1/5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, J = 8.0 Hz, 2H), 7.44 (t, J = 7.0 Hz, 4H), 7.38 (t, J = 7.5 Hz, 1H), 7.33 (d, J = 7.0 Hz, 2H), 7.28 (t, J = 6.5 Hz, 2H), 7.20 (t, J = 8.0 Hz, 3H), 6.73 (d, J = 9.0 Hz, 2H), 6.31 (s, 1H), 3.68 (s, 3H), 2.45 (s, 3H), 2.39 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 159.6 (s), 144.0 (s), 143.2 (s), 143.1 (s), 141.1 (s), 137.2 (s), 135.0 (s), 133.3 (s), 132.4 (s), 131.4 (s), 131.1 (d, 2C), 130.3 (d, 2C), 129.5 (d, 2C), 129.0 (d, 2C), 128.9 (s), 128.7 (d, 2C), 128.4 (d), 127.4 (d), 127.3 (d), 123.1 (d), 114.2 (d, 2C), 55.5 (q), 21.7 (q), 18.3 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3473, 2996, 2915, 2843, 1736, 1599, 1504, 1464, 1444, 1401, 1387, 1348, 1301, 1253, 1227, 1202, 1161, 1120, 1090, 1058, 1027, 967, 940, 914, 853, 836, 812, 798, 770, 741, 727, 706, 673, 652, 632, 617 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{30}H_{27}N_2O_4S$ calcd for 511.1686, found 511.1697.



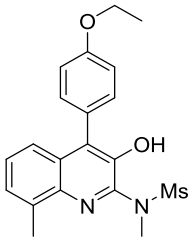
***N*-(4-(3-chlorophenyl)-3-hydroxy-8-methylquinolin-2-yl)-*N*,4-dimethylbenzenesulfonamide (6f)**

Yield: 85 mg, 94%; white solid, mp 187-189 °C; R_f = 0.21 (EA/PE = 1/10); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 (d, *J* = 8.4 Hz, 2H), 7.41-7.36 (m, 3H), 7.30-7.22 (m, 4H), 7.21-7.17 (m, 2H), 6.92 (s, 1H), 3.20 (s, 3H), 2.36 (s, 3H), 2.23 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.5 (s), 143.5 (s), 143.1 (s), 140.7 (s), 137.0 (s), 135.7 (s), 134.4 (s), 131.9 (s), 131.5 (s), 130.4 (d), 129.7 (d), 129.3 (d, 2C), 128.9 (d, 2C), 128.7 (d), 128.4 (d), 128.2 (s), 127.5 (d), 127.3 (d), 122.7 (d), 38.0 (q), 21.6 (q), 17.4 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3394, 1733, 1654, 1591, 1561, 1506, 1472, 1446, 1427, 1397, 1346, 1306, 1291, 1238, 1188, 1170, 1160, 1088, 1064, 1045, 1017, 915, 886, 865, 842, 813, 800, 787, 772, 739, 717, 700, 675, 648, 625 cm^{-1}; HRMS (ESI) (*m/z*) $[M+H]^+$ $C_{24}H_{22}ClN_2O_3S$ calcd for 453.1034, found 453.1041.



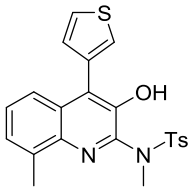
***N*-(3-hydroxy-8-methyl-4-(*p*-tolyl)quinolin-2-yl)-*N*,4-dimethylbenzenesulfonamide (6g)**

Yield: 69 mg, 80%; white solid, mp 186-188 °C; R_f = 0.18 (EA/PE = 1/15); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.50 (d, *J* = 5.1 Hz, 2H), 7.34 (dd, *J* = 1.5, 8.1 Hz, 1H), 7.28 (s, 4H), 7.24 (d, *J* = 5.7 Hz, 1H), 7.22-7.15 (m, 3H), 6.79 (s, 1H), 3.20 (s, 3H), 2.39 (s, 3H), 2.36 (s, 3H), 2.24 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.3 (s), 143.5 (s), 143.1 (s), 140.8 (s), 138.0 (s), 136.9 (s), 133.2 (s), 132.2 (s), 130.7 (s), 130.2 (d, 2C), 129.21 (d, 2C), 129.20 (d, 2C), 128.9 (d, 2C), 128.7 (s), 127.1 (d), 127.0 (d), 123.2 (d), 38.0 (q), 21.6 (q), 21.4 (q), 17.5 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3414, 2917, 1733, 1596, 1494, 1461, 1425, 1397, 1348, 1306, 1289, 1244, 1187, 1168, 1159, 1135, 1087, 1060, 1042, 1018, 980, 909, 850, 807, 777, 771, 756, 736, 720, 705, 679, 658, 635, 626 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{25}H_{25}N_2O_3S$ calcd for 433.1580, found 433.1585.



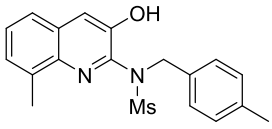
***N*-(4-(4-ethoxyphenyl)-3-hydroxy-8-methylquinolin-2-yl)-*N*-methylmethanesulfonamide (6h)**

Yield: 57 mg, 74%; white solid, mp 212-214 °C; R_f = 0.24 (EA/PE = 1/5); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.4 Hz, 1H), 7.34 (d, *J* = 6.6 Hz, 1H), 7.30-7.20 (m, 3H), 6.97 (d, *J* = 8.7 Hz, 2H), 6.44 (s, 1H), 4.04 (q, *J* = 7.2 Hz, 2H), 3.35 (s, 3H), 3.13 (s, 3H), 2.66 (s, 3H), 1.39 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 159.1 (s), 143.4 (s), 142.9 (s), 141.1 (s), 136.6 (s), 133.1 (s), 131.6 (d, 2C), 129.1 (s), 127.5 (d), 127.3 (d), 125.1 (s), 123.4 (d), 114.6 (d, 2C), 63.6 (t), 38.1 (q), 35.3 (q), 18.1 (q), 14.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3417, 3046, 2979, 2936, 2922, 1610, 1570, 1518, 1496, 1474, 1429, 1397, 1359, 1342, 1317, 1301, 1284, 1248, 1232, 1171, 1155, 1141, 1116, 1067, 1045, 952, 910, 832, 808, 786, 777, 744, 734, 722, 691, 656, 640, 621, 606 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{20}H_{23}N_2O_4S$ calcd for 387.1373, found 387.1377.



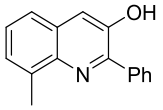
***N*-(3-hydroxy-8-methyl-4-(thiophen-3-yl)quinolin-2-yl)-*N*,4-dimethylbenzenesulfonamide (6i)**

Yield: 76 mg, 92%; white solid, mp 121-123 °C; R_f = 0.18 (EA/PE = 1/10); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55-7.51 (m, 1H), 7.50-7.40 (m, 4H), 7.28-7.22 (m, 3H), 7.19 (d, *J* = 8.0 Hz, 2H), 6.90 (s, 1H), 3.19 (s, 3H), 2.36 (s, 3H), 2.22 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 144.4 (s), 143.5 (s), 143.4 (s), 140.8 (s), 137.0 (s), 133.2 (s), 132.1 (s), 129.8 (d), 129.2 (d, 2C), 128.9 (d, 2C), 128.6 (s), 128.0 (s), 127.3 (d), 127.2 (d), 126.2 (d), 125.4 (d), 123.0 (d), 38.0 (q), 21.6 (q), 17.5 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3390, 3103, 1699, 1596, 1497, 1447, 1427, 1399, 1345, 1306, 1239, 1186, 1167, 1157, 1119, 1088, 1044, 1018,, 931, 900, 865, 844, 834, 811, 789, 774, 763, 743, 730, 704, 676, 655, 642, 626, 615 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{22}H_{21}N_2O_3S_2$ calcd for 425.0988, found 425.0093.



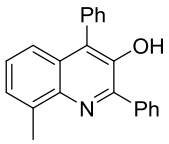
***N*-(3-hydroxy-8-methylquinolin-2-yl)-*N*-(4-methylbenzyl)methanesulfonamide (6j)**

Yield: 63 mg, 89% (according to procedure 3); 35 mg, 50% (according to procedure 2); light yellow solid, mp 276-278 °C; R_f = 0.27 (EA/PE = 1/5); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (s, 1H), 7.44 (d, *J* = 8.0 Hz, 1H), 7.35-7.32 (m, 1H), 7.30 (t, *J* = 7.5 Hz, 1H), 7.04 (d, *J* = 8.0 Hz, 2H), 6.91 (d, *J* = 8.0 Hz, 2H), 6.39 (s, 1H), 4.95 (s, 2H), 3.08 (s, 3H), 2.68 (s, 3H), 2.15 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 147.2 (s), 142.1 (s), 141.3 (s), 137.9 (s), 136.5 (s), 132.0 (s), 129.0 (s), 129.4 (d, 2C), 128.7 (d, 2C), 127.7 (d), 127.5 (d), 124.6 (d), 121.0 (d), 54.5 (t), 36.4 (q), 21.1 (q), 17.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3440, 3031, 2923, 1735, 1620, 1500, 1472, 1452, 1418, 1371, 1355, 1339, 1319, 1247, 1154, 1060, 1040, 1026, 956, 902, 869, 861, 838, 812, 782, 766, 743, 722, 708, 648, 638, 606 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{19}H_{21}N_2O_3S$ calcd for 357.1267, found 357.1273.



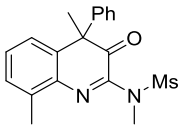
8-methyl-2-phenylquinolin-3-ol (6k)

Yield: 24 mg, 51%; light yellow oil; R_f = 0.53 (EA/PE = 1/5); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.87 (d, *J* = 7.2 Hz, 2H), 7.49 (s, 1H), 7.50-7.36 (m, 4H), 7.35-7.25 (m, 2H), 5.62 (brs, 1H), 2.73 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.4 (s), 147.5 (d), 142.1 (s), 136.8 (s), 136.7 (s), 129.4 (d), 129.3 (d, 2C), 129.0 (s), 128.9 (d, 2C), 127.5 (d), 127.0 (d), 124.2 (d), 119.0 (d), 18.0 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3053, 2967, 2928, 2867, 2757, 2223, 1690, 1600, 1491, 1464, 1441, 1411, 1396, 1351, 1325, 1276, 1174, 1155, 1140, 1106, 1072, 1034, 1010, 955, 905, 875, 841, 781, 760, 720, 694, 676, 623 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{16}H_{14}NO$ calcd for 236.1070, found 236.1070.



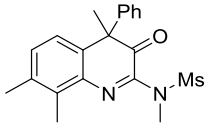
8-methyl-2,4-diphenylquinolin-3-ol (6l)

Yield: 37 mg, 60%; colorless oil; R_f = 0.41 (EA/PE = 1/10); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.15-8.05 (m, 2H), 7.59-7.51 (m, 2H), 7.51-7.32 (m, 7H), 7.25-7.19 (m, 1H), 7.17-7.12 (m, 1H), 5.26 (s, 1H), 2.81 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.8 (s), 143.9 (s), 142.5 (s), 138.1 (s), 137.7 (s), 132.7 (s), 130.5 (d, 2C), 129.8 (d, 2C), 129.7 (d, 2C), 129.6 (s), 129.1 (d), 128.9 (d), 128.3 (d, 2C), 127.6 (s), 127.0 (d), 126.7 (d), 122.6 (d), 18.2 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3516, 3058, 3028, 2955, 2920, 2870, 1589, 1559, 1485, 1463, 1443, 1409, 1382, 1321, 1288, 1258, 1224, 1171, 1133, 1074, 1029, 1015, 922, 856, 814, 766, 754, 725, 697, 636, 613 cm^{-1}; HRMS (EI) (*m/z*) $C_{22}H_{17}NO$ calcd for 311.1310, found 311.1312.



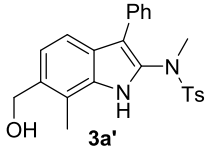
***N*-(4,8-dimethyl-3-oxo-4-phenyl-3,4-dihydroquinolin-2-yl)-*N*-methylmethanesulfonamide (7a)**

Yield: 59 mg, 83%; yellow solid, mp 163-166 °C; R_f = 0.17 (EA/PE = 1/15); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25-7.20 (m, 3H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.04 (t, *J* = 7.5 Hz, 1H), 7.01-6.98 (m, 2H), 6.75 (d, *J* = 7.5 Hz, 1H), 3.23 (s, 3H), 3.20 (s, 3H), 2.43 (s, 3H), 1.82 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.3 (s), 150.0 (s), 139.1 (s), 138.3 (s), 138.0 (s), 137.2 (s), 130.0 (d), 128.5 (d, 2C), 128.4 (d, 2C), 128.02 (d), 127.95 (d), 125.5 (d), 57.5 (s), 40.9 (q), 34.6 (q), 23.1 (q), 17.9 (q) ppm; IR (reflection) $\tilde{\nu}$ = 2990, 2945, 1721, 1600, 1572, 1490, 1474, 1446, 1414, 1352, 1328, 1283, 1259, 1241, 1182, 1150, 1091, 1029, 1001, 956, 917, 891, 829, 813, 788, 766, 758, 735, 723, 700, 641 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{19}H_{21}N_2O_3S$ calcd for 357.1267, found 357.1274.



***N*-methyl-*N*-(4,7,8-trimethyl-3-oxo-4-phenyl-3,4-dihydroquinolin-2-yl)methanesulfonamide (7b)**

Yield: 54 mg, 73%; yellow oil; R_f = 0.17 (EA/PE = 1/15); ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.25-7.20 (m, 3H), 7.02-6.98 (m, 2H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 3.23 (s, 3H), 3.19 (s, 3H), 2.38 (s, 3H), 2.25 (s, 3H), 1.81 (s, 3H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 195.5 (s), 149.9 (s), 139.3 (s), 137.7 (s), 137.3 (s), 135.9 (s), 135.8 (s), 129.5 (d), 128.43 (d, 2C), 128.40 (d, 2C), 127.9 (d), 124.6 (d), 57.3 (s), 40.8 (q), 34.6 (q), 23.2 (q), 20.3 (q), 13.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 2981, 2935, 2871, 2254, 1715, 1593, 1566, 1480, 1446, 1352, 1283, 1197, 1153, 1084, 1068, 960, 912, 852, 818, 784, 765, 734, 705, 685, 635 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{20}H_{23}N_2O_3S$ calcd for 371.1424, found 371.1430.

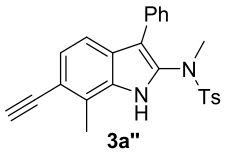


3a'

***N*-(6-(hydroxymethyl)-7-methyl-3-phenyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3a')**

Yield: 82 mg, 98%; white solid, mp 207-209 °C; R_f = 0.29 (EA/PE = 1/2); ^{1}H NMR (300 MHz, DMSO-d_6) δ 11.12 (brs, 1H), 7.42 (d, *J* = 8.1 Hz, 2H), 7.33-7.16 (m, 8H), 7.09 (d, *J* = 8.1 Hz, 1H),

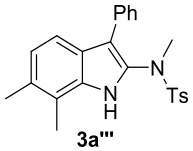
4.97 (brs, 1H), 4.61 (s, 2H), 3.26 (s, 3H), 2.46 (s, 3H), 2.37 (s, 3H) ppm; ^{13}C NMR (75 MHz, DMSO-d_6) δ 143.4 (s), 135.2 (s), 133.9 (s), 133.63 (s), 133.56 (s), 130.4 (s), 129.4 (d, 2C), 128.6 (d, 2C), 128.2 (d, 2C), 127.3 (d, 2C), 125.8 (d), 124.5 (s), 120.7 (d), 118.7 (s), 115.8 (d), 112.6 (s), 61.5 (t), 38.4 (q), 21.0 (q), 12.5 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3368, 2872, 1737, 1600, 1564, 1495, 1440, 1346, 1241, 1151, 1087, 1004, 988, 912, 861, 812, 777, 758, 730, 710, 695, 666, 608 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{24}H_{25}N_2O_3S$ calcd for 421.1580, found 421.1580.



3a"

***N*-(6-ethynyl-7-methyl-3-phenyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3a")**

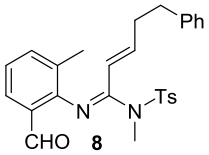
Yield: 73 mg, 87%; white solid, mp 196-198 °C; R_f = 0.43 (EA/PE = 1/4); ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.58 (brs, 1H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.24-7.15 (m, 4H), 7.14-7.09 (m, 1H), 7.09-6.99 (m, 2H), 6.53 (d, *J* = 6.9 Hz, 2H), 3.21 (s, 1H), 2.96 (s, 3H), 2.57 (s, 3H), 2.38 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.4 (s), 134.1 (s), 132.8 (s), 132.2 (s), 131.7 (s), 129.9 (d, 2C), 129.3 (d, 2C), 128.2 (d, 2C), 127.6 (d, 2C), 126.9 (d), 126.6 (s), 124.8 (d), 123.6 (s), 116.9 (d), 115.8 (s), 112.2 (s), 83.4 (s), 80.0 (d), 38.4 (q), 21.6 (q), 14.7 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3367, 3307, 3280, 3268, 3028, 2097, 1739, 1600, 1581, 1564, 1495, 1439, 1346, 1306, 1234, 1151, 1087, 1075, 1029, 986, 911, 861, 823, 812, 784, 758, 722, 709, 697, 683, 660, 627 cm^{-1}; HRMS (ESI) (*m/z*) $[M+H]^+$ $C_{25}H_{23}N_2O_2S$ calcd for 415.1475, found 415.1477.



3a'''

***N*-(6,7-dimethyl-3-phenyl-1*H*-indol-2-yl)-*N*,4-dimethylbenzenesulfonamide (3a''')**

Yield: 60 mg, 74%; white solid, mp 229-230 °C; R_f = 0.33 (EA/PE = 1/10); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37 (brs, 1H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.18-7.14 (m, 3H), 7.12-7.07 (m, 1H), 7.07-7.01 (m, 2H), 6.86 (d, *J* = 8.0 Hz, 1H), 6.63-6.57 (m, 2H), 2.99 (s, 3H), 2.35 (s, 3H), 2.34 (s, 3H), 2.33 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2 (s), 134.4 (s), 133.4 (s), 133.3 (s), 130.7 (s), 129.79 (s), 129.75 (d, 2C), 129.2 (d, 2C), 128.1 (d, 2C), 127.6 (d, 2C), 126.5 (d), 124.6 (s), 123.1 (d), 118.0 (s), 116.6 (d), 112.2 (s), 38.5 (q), 21.6 (q), 19.4 (q), 13.1 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3360, 3089, 3055, 2970, 2914, 2858, 1893, 1621, 1600, 1564, 1494, 1439, 1344, 1305, 1264, 1239, 1185, 1168, 1151, 1102, 1087, 1074, 1031, 1003, 990, 910, 864, 838, 810, 790, 771, 757, 726, 707, 693, 661, 609 cm^{-1}; HRMS (DRAT) (*m/z*) $[M+H]^+$ $C_{24}H_{25}N_2O_2S$ calcd for 405.1631, found 405.1628.

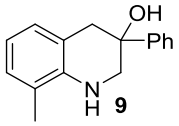


8

***N*'-(2-formyl-6-methylphenyl)-*N*-methyl-5-phenyl-*N*-tosylpent-2-enimidamide (8)**

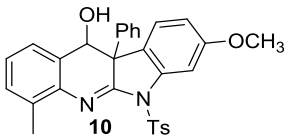
Yield: 36 mg, 39% ($PicAuCl_2$ as catalyst); 43 mg, 47% (JohnPhosAuCl/$AgSbF_6$ as catalyst), light yellow oil; R_f = 0.26 (EA/PE = 1/5); ^{1}H NMR (300 MHz, $CDCl_3$) δ 9.61 (s, 1H), 7.71 (d, *J* = 8.1 Hz, 2H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.29-7.21 (m, 3H), 7.18-7.12 (m, 2H), 7.12-7.06 (m, 1H), 7.02-6.92 (m, 3H), 6.28-6.12 (m, 1H), 5.64 (d, *J* = 15.9 Hz, 1H), 3.13 (s, 3H), 2.50 (t, *J* = 7.5 Hz, 2H), 2.37 (s, 3H), 2.33-2.23 (m, 2H), 1.85 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 190.9 (d), 156.2 (s),

149.6 (s), 145.8 (d), 144.3 (s), 140.5 (s), 136.3 (d), 135.1 (s), 129.6 (d, 2C), 128.4 (d, 2C), 128.2 (d, 2C), 128.1 (d, 2C; s, 1C), 126.9 (d), 126.1 (d), 125.2 (s), 123.3 (d), 121.4 (d), 36.4 (q), 34.20 (t), 34.18 (t), 21.6 (q), 17.6 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3064, 3027, 2925, 2858, 1692, 1677, 1649, 1591, 1496, 1455, 1353, 1290, 1240, 1162, 1088, 1040, 969, 920, 815, 780, 752, 700, 671, 627, 606 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{27}H_{29}N_2O_3S$ calcd for 461.1893, found 461.1895.



8-methyl-3-phenyl-1,2,3,4-tetrahydroquinolin-3-ol (9)

Yield: 30 mg, 63%; white solid, mp 118-119 °C; R_f = 0.43 (EA/PE = 1/4); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.53-7.43 (m, 2H), 7.33 (t, *J* = 7.5 Hz, 2H) 7.26-7.18 (m, 1H), 6.90 (d, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 7.5 Hz, 1H), 6.61 (t, *J* = 7.5 Hz, 1H), 3.87 (brs, 1H), 3.41 (d, *J* = 11.4 Hz, 1H), 3.32 (d, *J* = 16.8 Hz, 1H), 3.19 (dd, *J* = 11.4, 2.7 Hz, 1H), 3.00 (brs, 1H), 2.83 (dd, *J* = 16.8, 1.8 Hz, 1H), 2.11 (s, 3H) ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 144.8 (s), 140.7 (s), 128.6 (d), 128.4 (d, 2C), 128.3 (d), 127.2 (d), 125.0 (d, 2C), 121.7 (s), 119.5 (s), 118.1 (d), 68.7 (s), 52.7 (t), 41.6 (t), 17.2 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3346, 3057, 3010, 2931, 2899, 2829, 1906, 1597, 1479, 1456, 1424, 1382, 1355, 1273, 1233, 1201, 1130, 1098, 1068, 1054, 1028, 976, 947, 930, 905, 882, 859, 803, 767, 756, 734, 721, 700, 633 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{16}H_{18}NO$ calcd for 240.1383, found 240.1383.



8-methoxy-4-methyl-10b-phenyl-6-tosyl-10b,11-dihydro-6*H*-indolo[2,3-b]quinolin-11-ol (10)

Yield: 80 mg, 79%; white solid, mp 203-205 °C; R_f = 0.26 (EA/PE = 1/2); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 2.0 Hz, 1H), 7.32 (d, *J* = 8.0 Hz, 1H), 7.19 (d, *J* = 8.5 Hz, 2H), 7.09-7.07 (m, 2H), 7.04-6.98 (m, 4H), 6.85 (d, *J* = 6.0 Hz, 1H), 6.81 (t, *J* = 7.5 Hz, 1H), 6.60 (dd, *J* = 2.0, 8.0 Hz, 1H), 5.02 (s, 1H), 3.76 (s, 3H), 2.45 (s, 3H), 2.31 (s, 3H), 1.42 (brs, 1H) ppm; ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.4 (s), 160.6 (s), 145.0 (s), 142.7 (s), 140.8 (s), 137.4 (s), 135.7 (s), 134.5 (s), 131.8 (d), 129.4 (d, 2C), 128.9 (d, 2C), 128.5 (d, 2C), 127.6 (d), 126.5 (d), 126.0 (d), 125.6 (d, 2C), 124.7 (d), 124.4 (s), 121.8 (s), 109.8 (d), 101.4 (d), 72.5 (d), 55.69 (q), 55.68 (s), 21.7 (q), 17.8 (q) ppm; IR (reflection) $\tilde{\nu}$ = 3447, 3000, 2838, 1656, 1614, 1593, 1492, 1464, 1441, 1400, 1374, 1344, 1305, 1286, 1258, 1215, 1170, 1118, 1092, 1053, 997, 978, 946, 931, 880, 850, 820, 810, 781, 765, 752, 730, 695, 666, 650, 626, 613 cm^{-1}; HRMS (DART) (*m/z*) $[M+H]^+$ $C_{30}H_{27}N_2O_4S$ calcd for 511.1686, found 511.1693.

5. References

1. (a) Phillips, B. T.; Hartman, G. D. *J. Heterocycl. Chem*. **1986**, *23*, 897. (b) Wratten, S. J.; Fujiwara, H.; Solsten, R. T. *J. Agr. Food Chem*. **1987**, *35*, 484.

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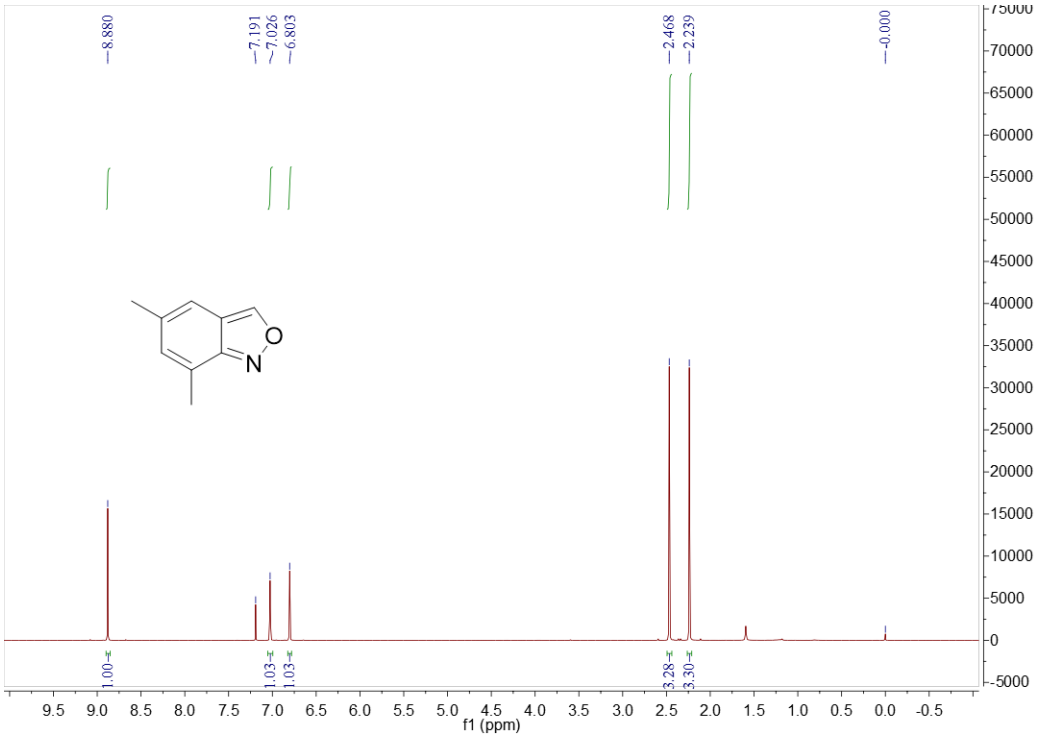
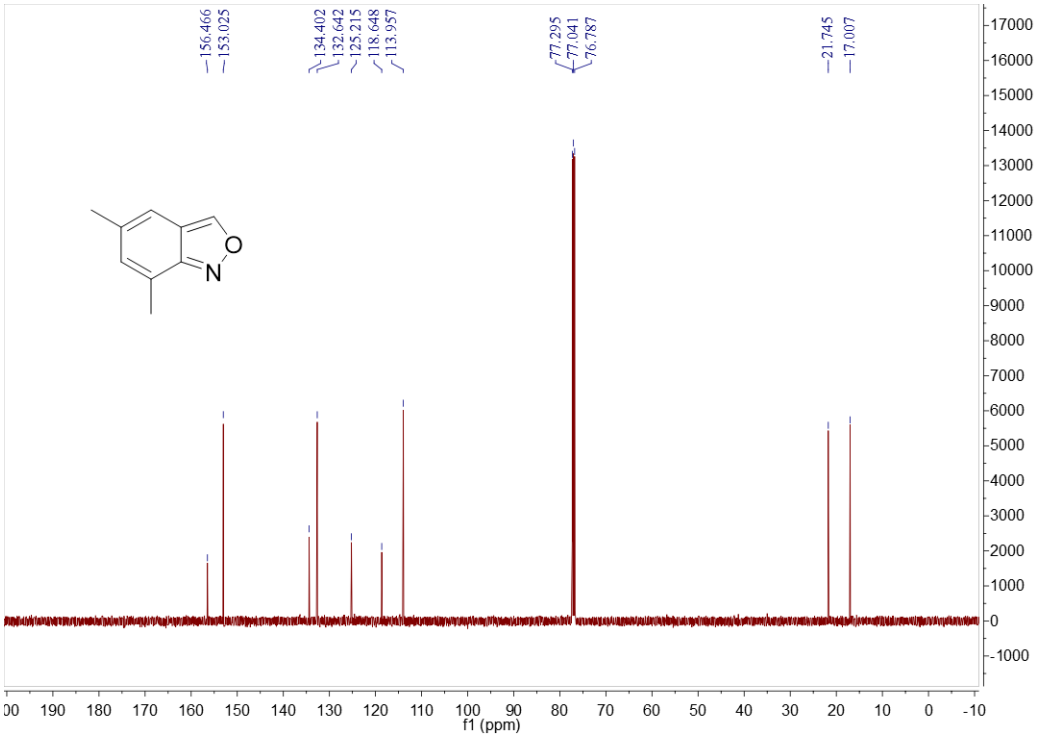
3. (a) Jin, H.; Huang, L.; Xie, J.; Rudolph, M.; Rominger, F.; Hashmi, A. S. K. *Angew. Chem., Int. Ed.* **2016**, *55*, 794. (b) Jin, H.; Tian, B.; Song, X.; Xie, J.; Rudolph, M.; Rominger, F.; Hashmi, A. S. K. *Angew. Chem., Int. Ed.* **2016**, *55*, 12688.

6. NMR Spectra

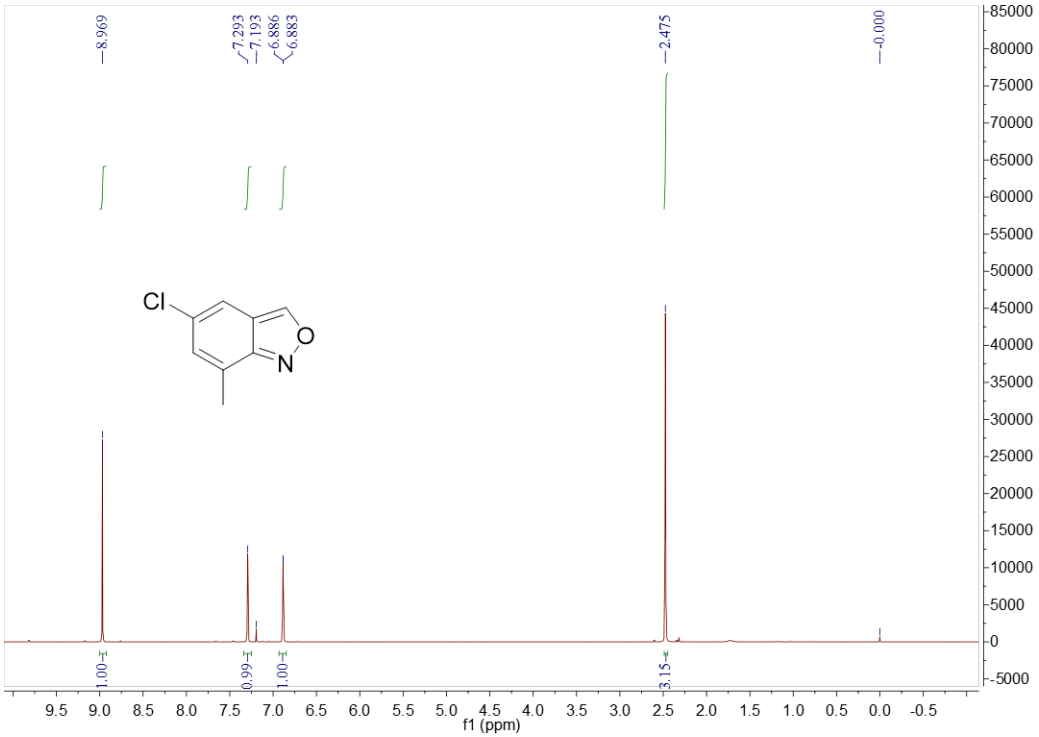
^{1}H NMR of compound **1a** in $CDCl_3$



^{13}C NMR of compound **1a** in $CDCl_3$



^{1}H NMR of compound **1e** in $CDCl_3$



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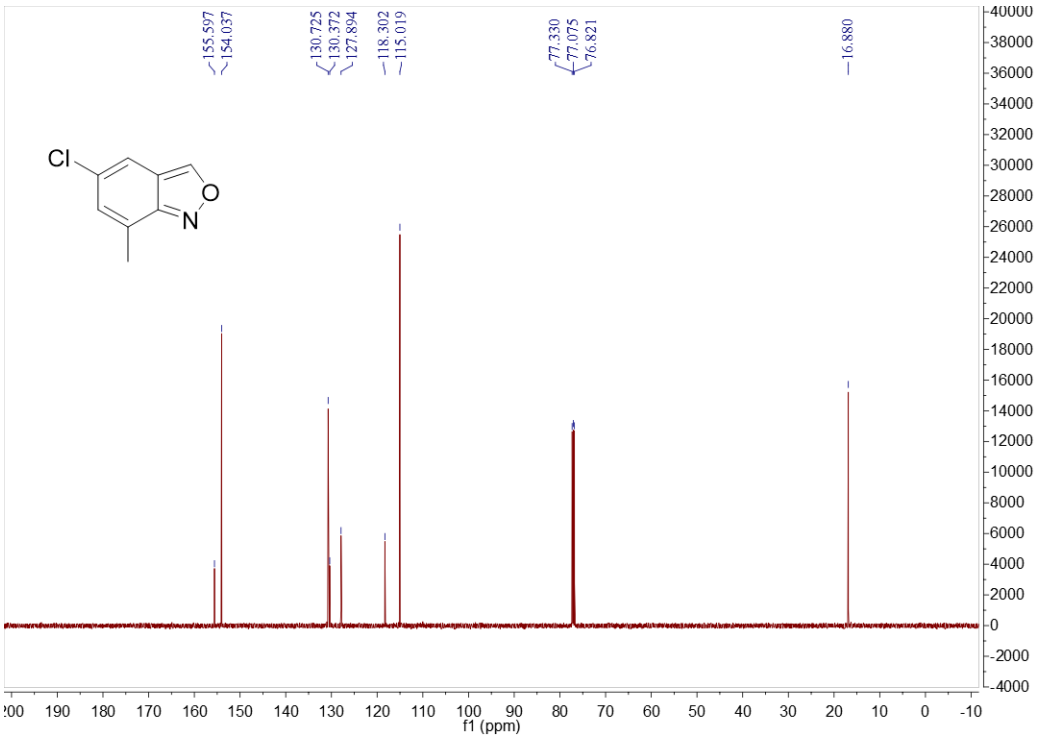
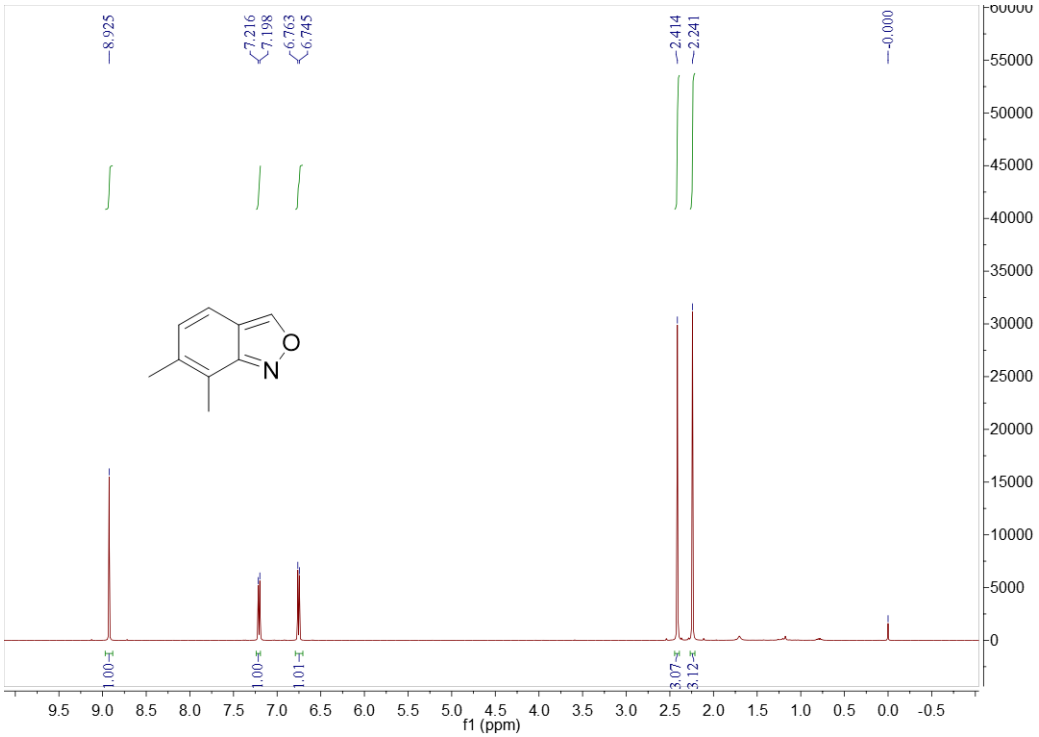
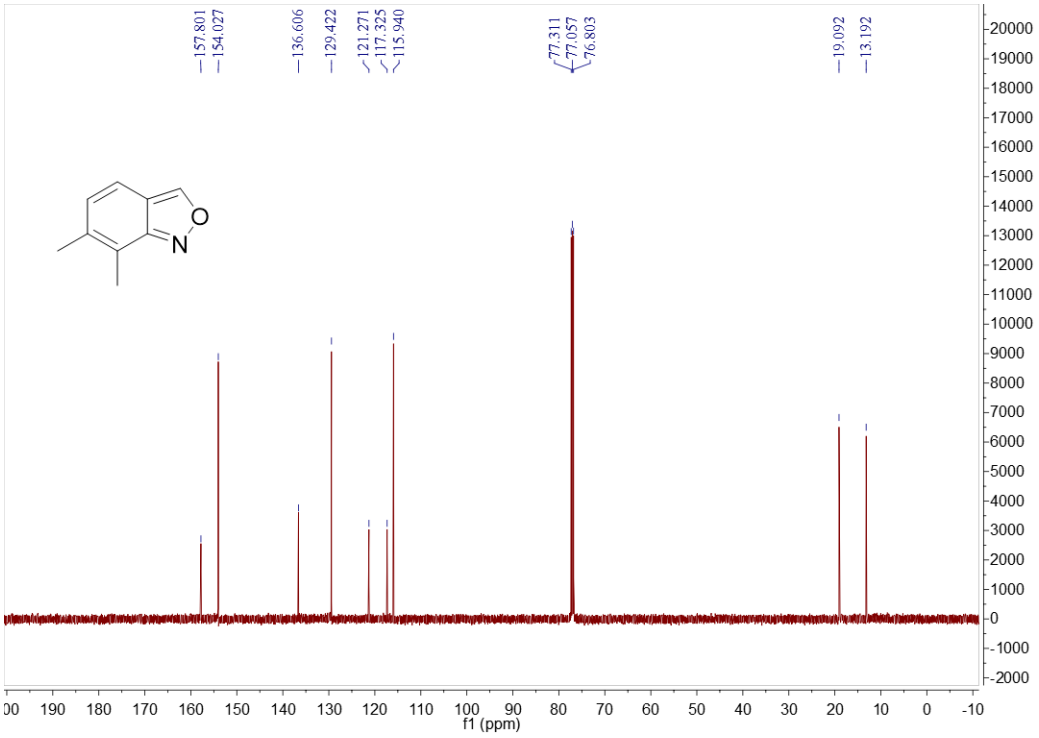


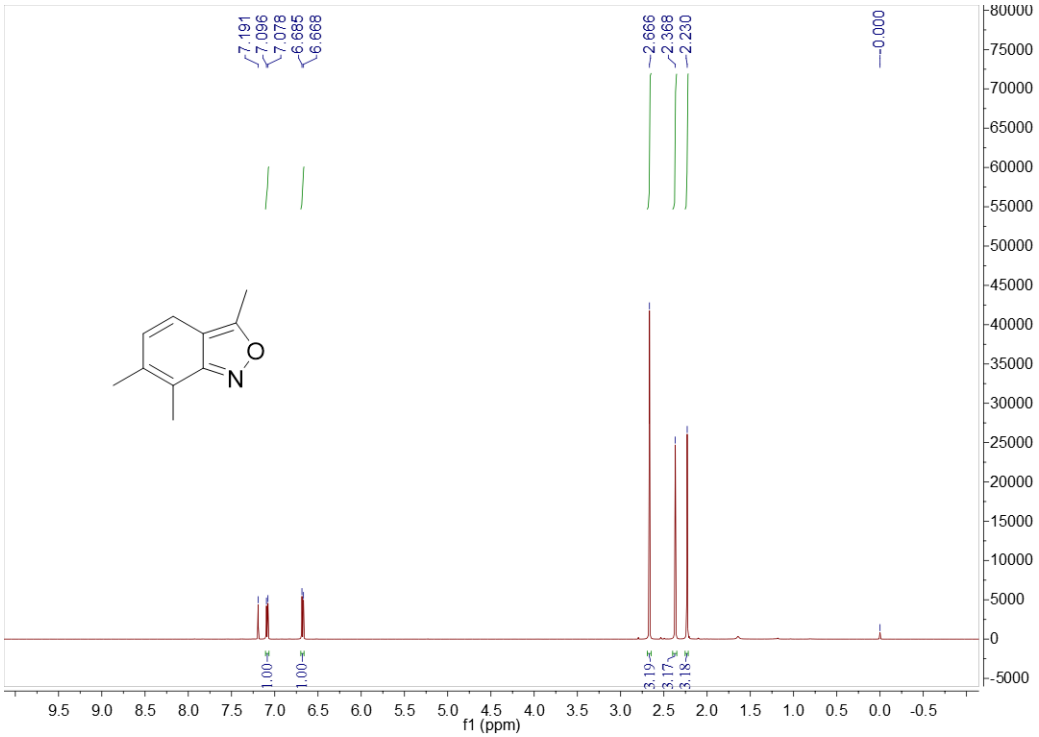
^{1}H NMR of compound **1f** in $CDCl_3$



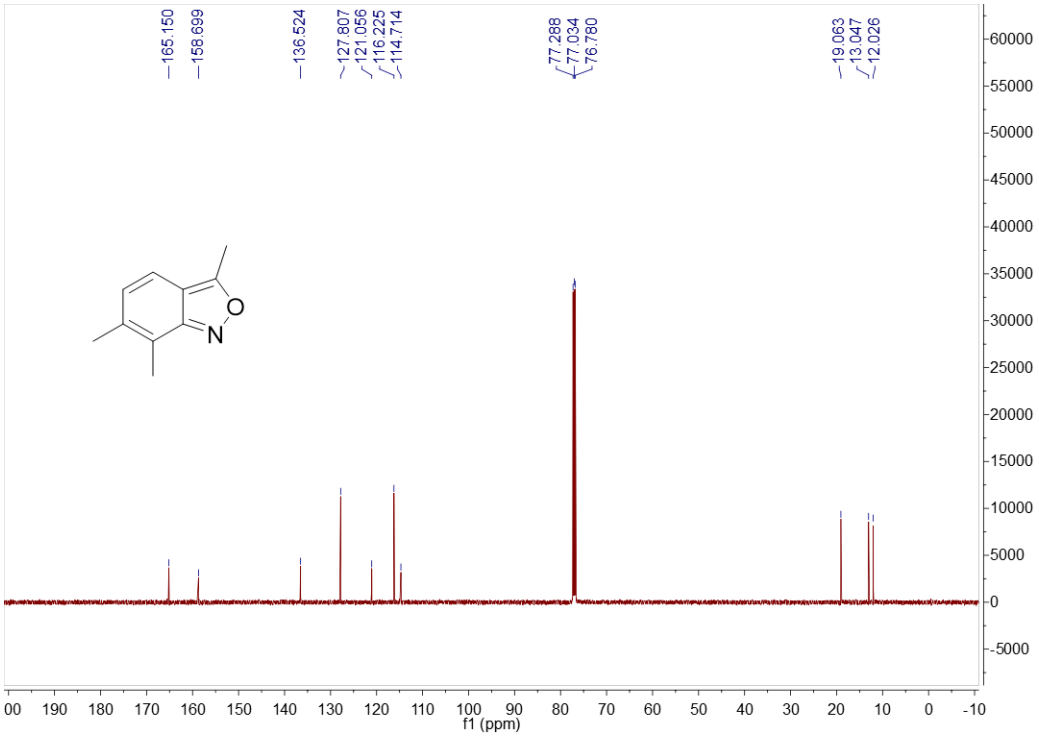
^{13}C NMR of compound **1f** in $CDCl_3$



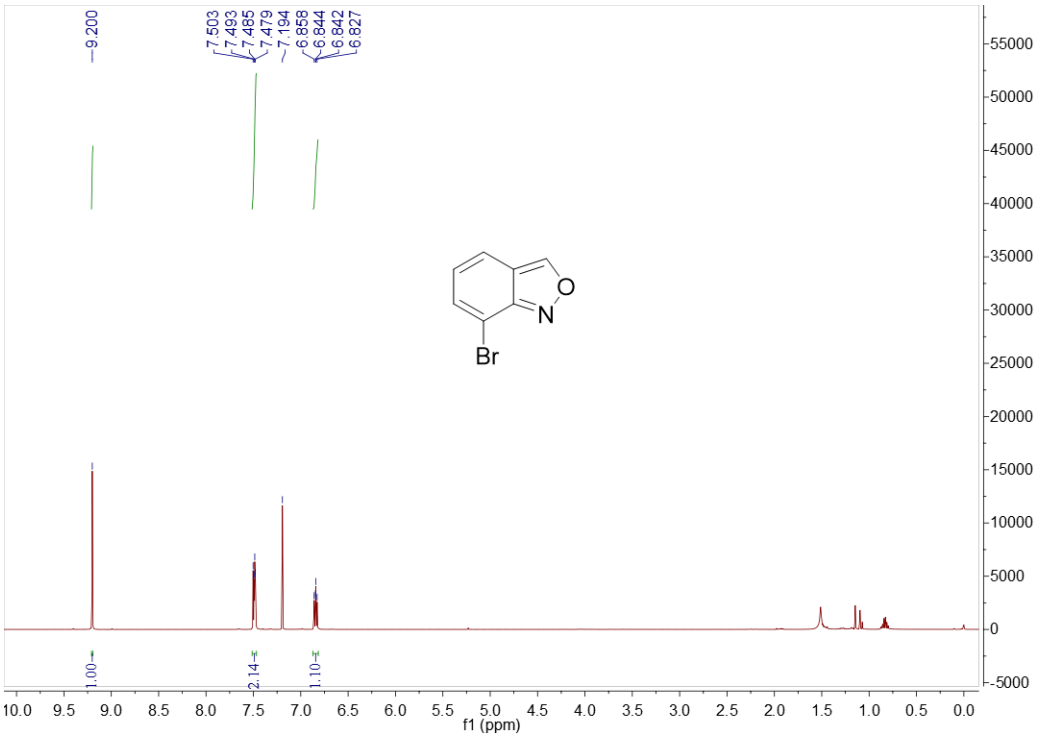
^{1}H NMR of compound **1g** in $CDCl_3$



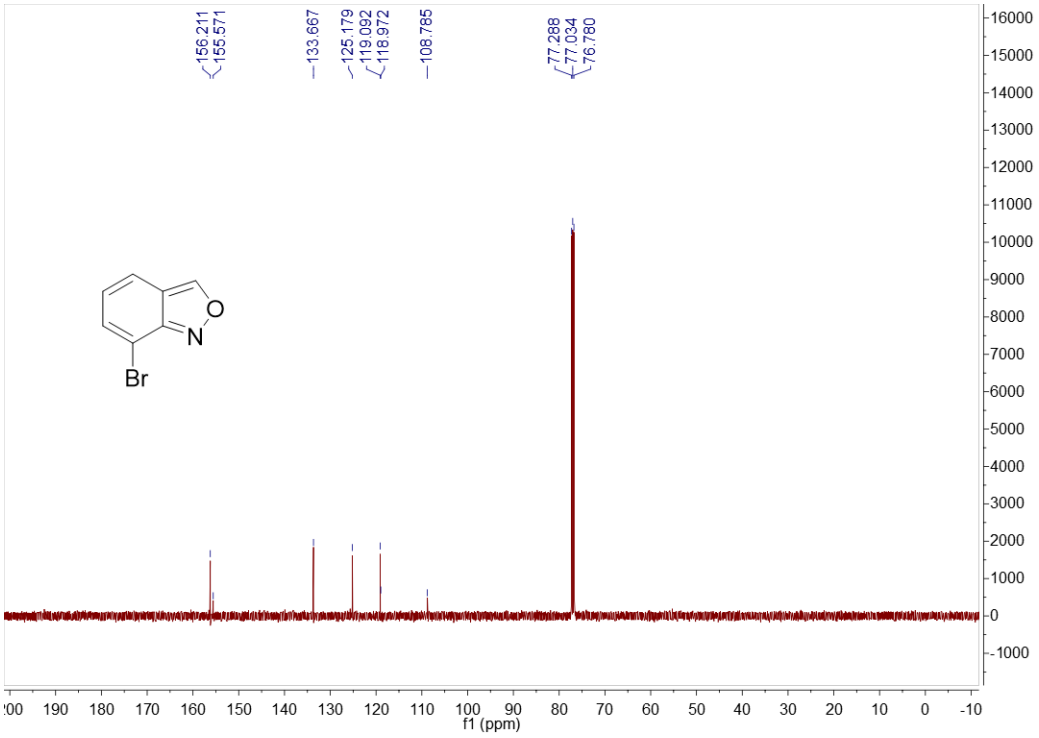
^{13}C NMR of compound **1g** in $CDCl_3$



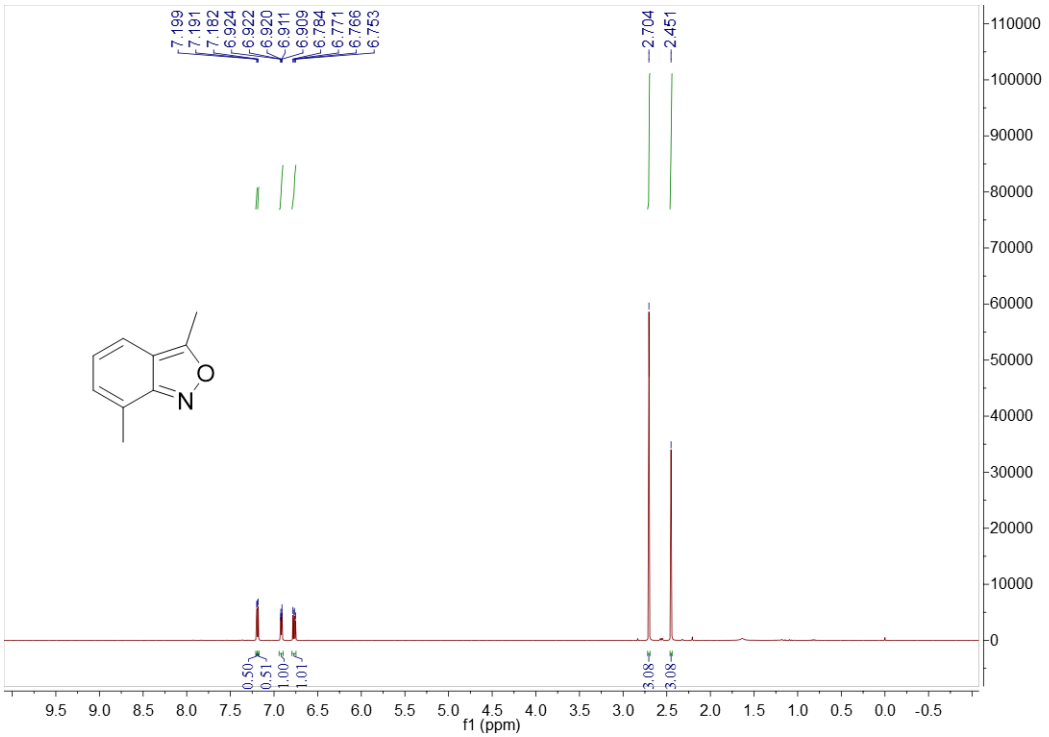
^{1}H NMR of compound **1h** in $CDCl_3$



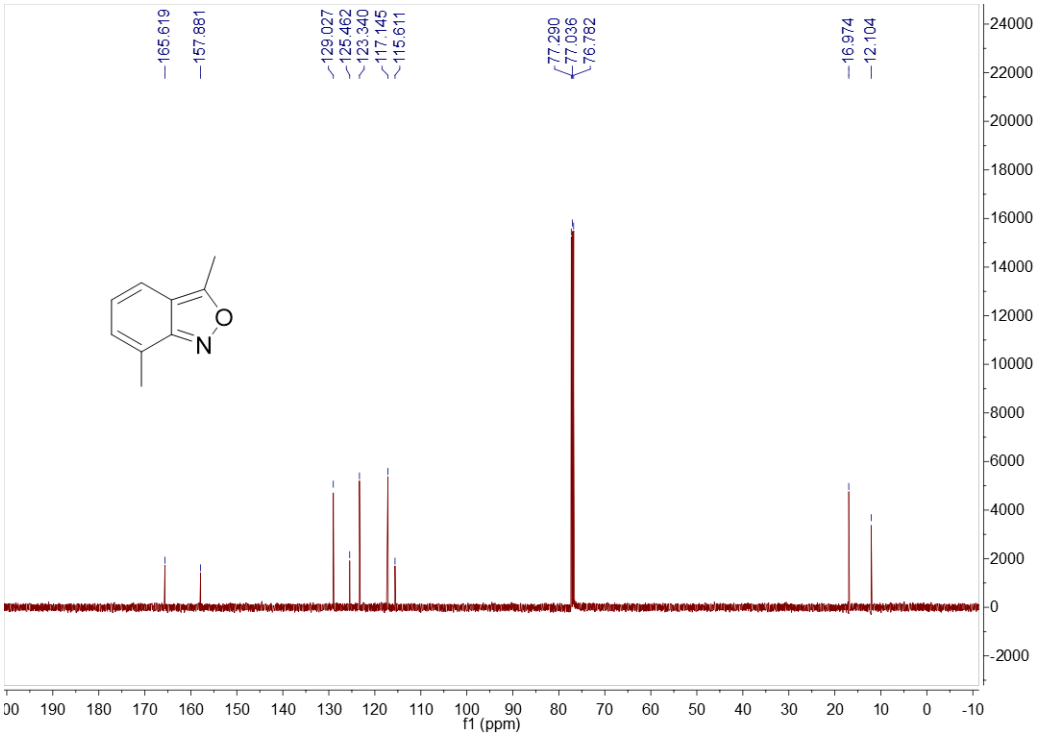
^{13}C NMR of compound **1h** in $CDCl_3$



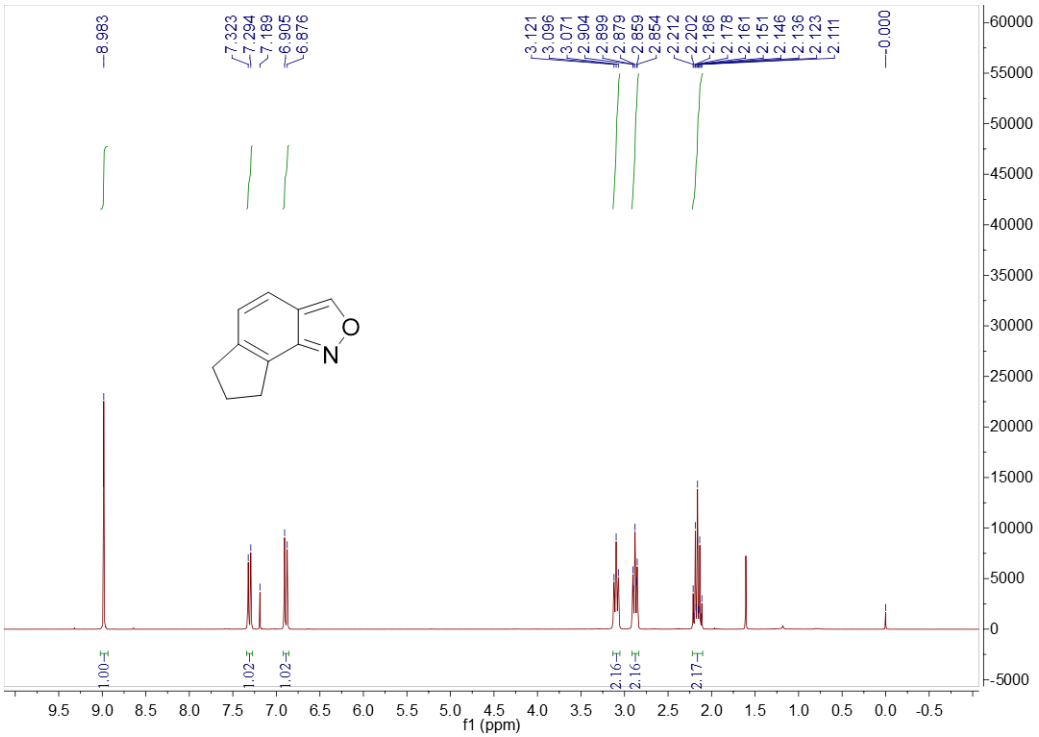
^{1}H NMR of compound **1i** in $CDCl_3$



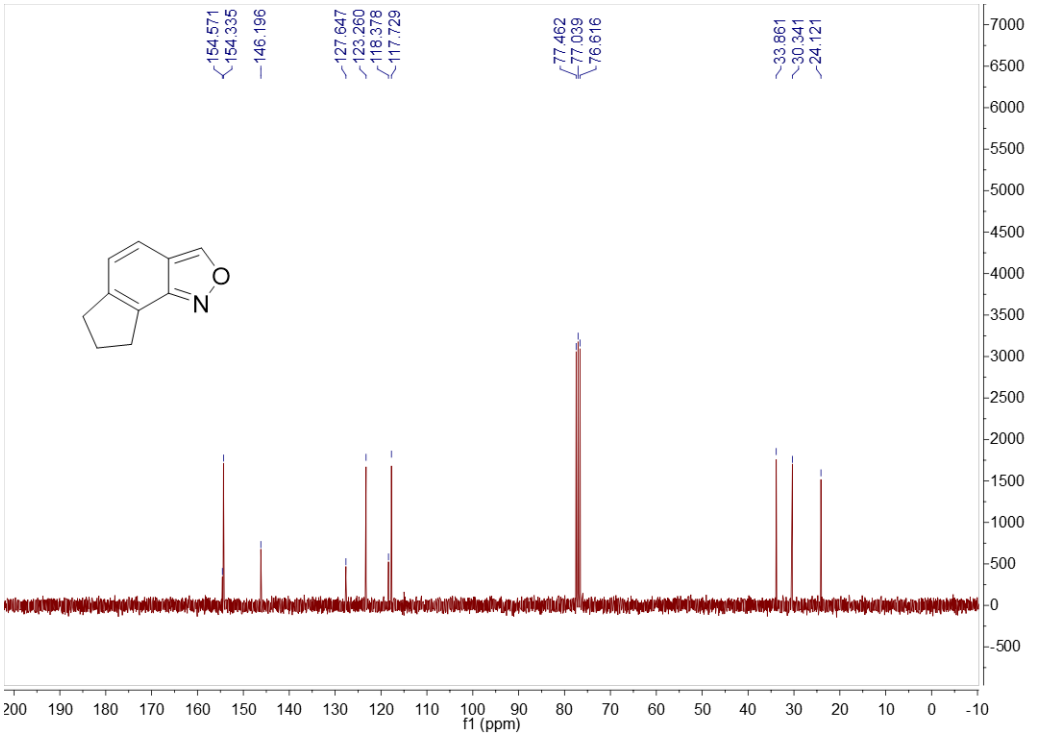
^{13}C NMR of compound **1i** in $CDCl_3$



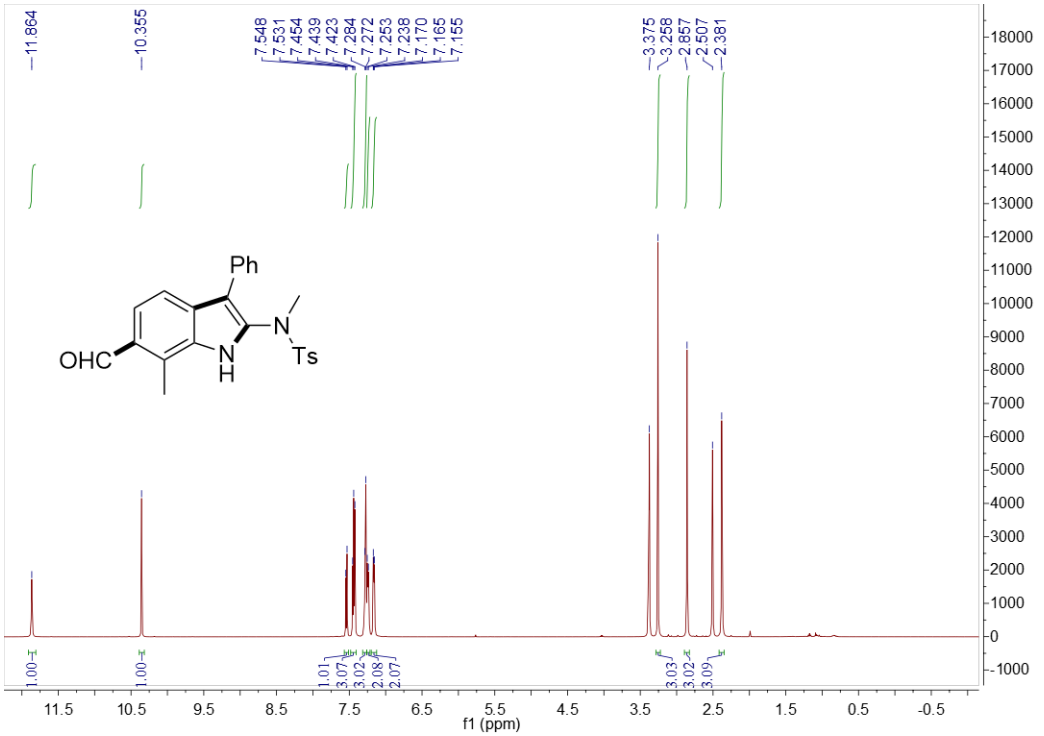
^{1}H NMR of compound **1k** in $CDCl_3$



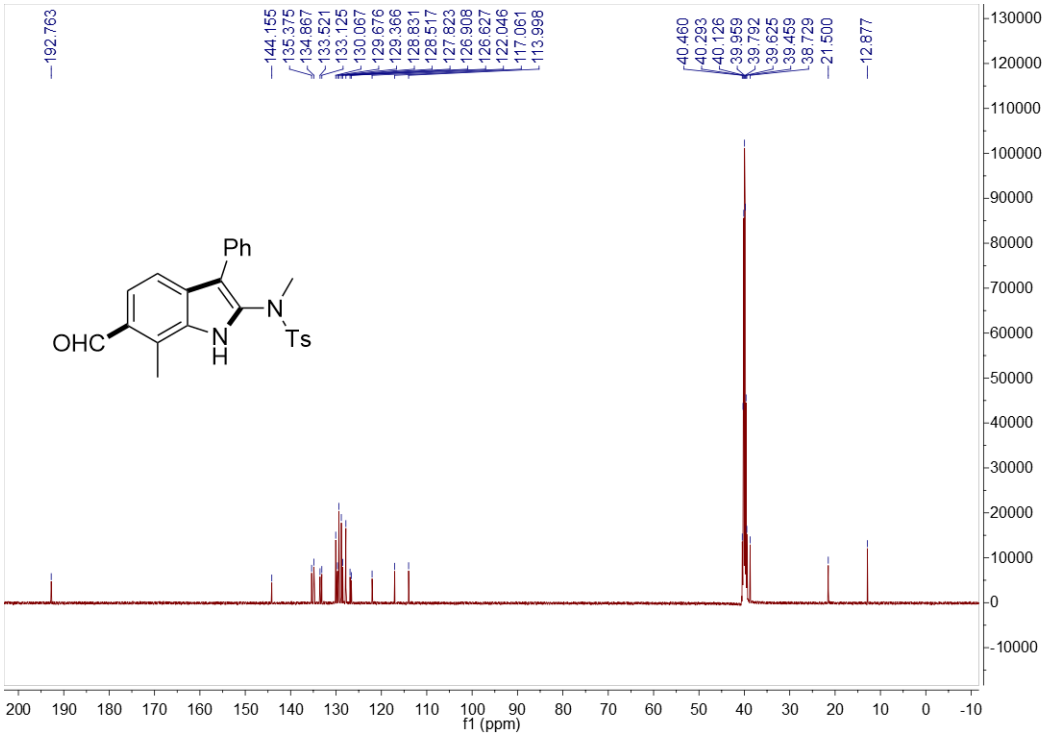
^{13}C NMR of compound **1k** in $CDCl_3$



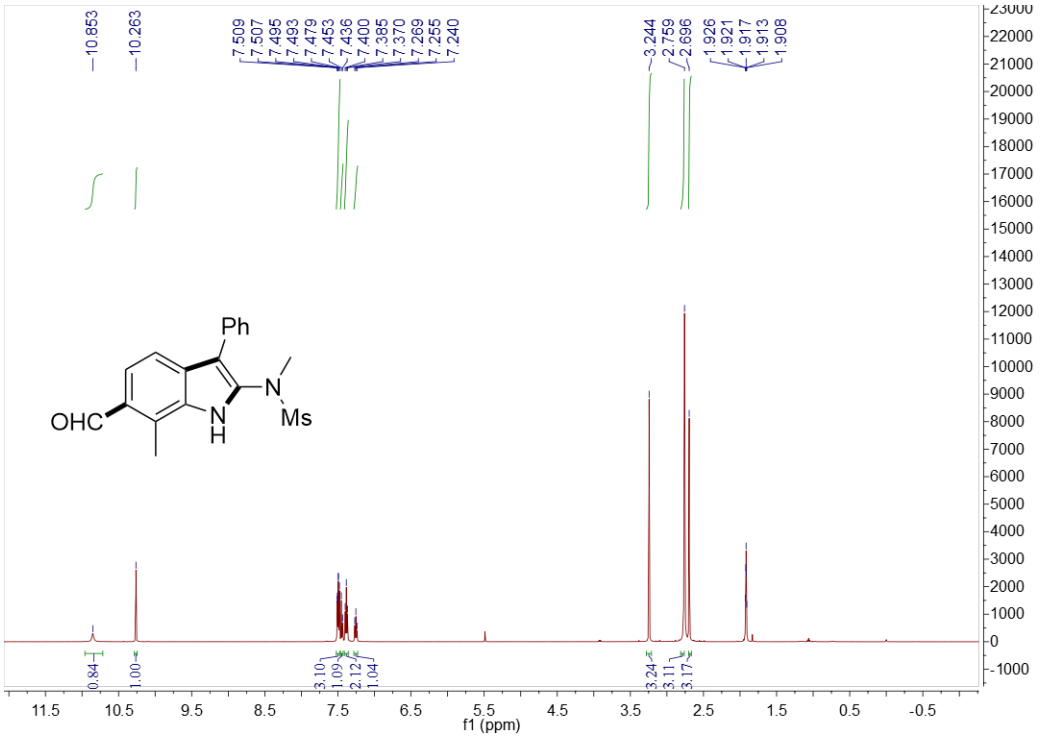
^{1}H NMR of compound **3a** in DMSO-d_6



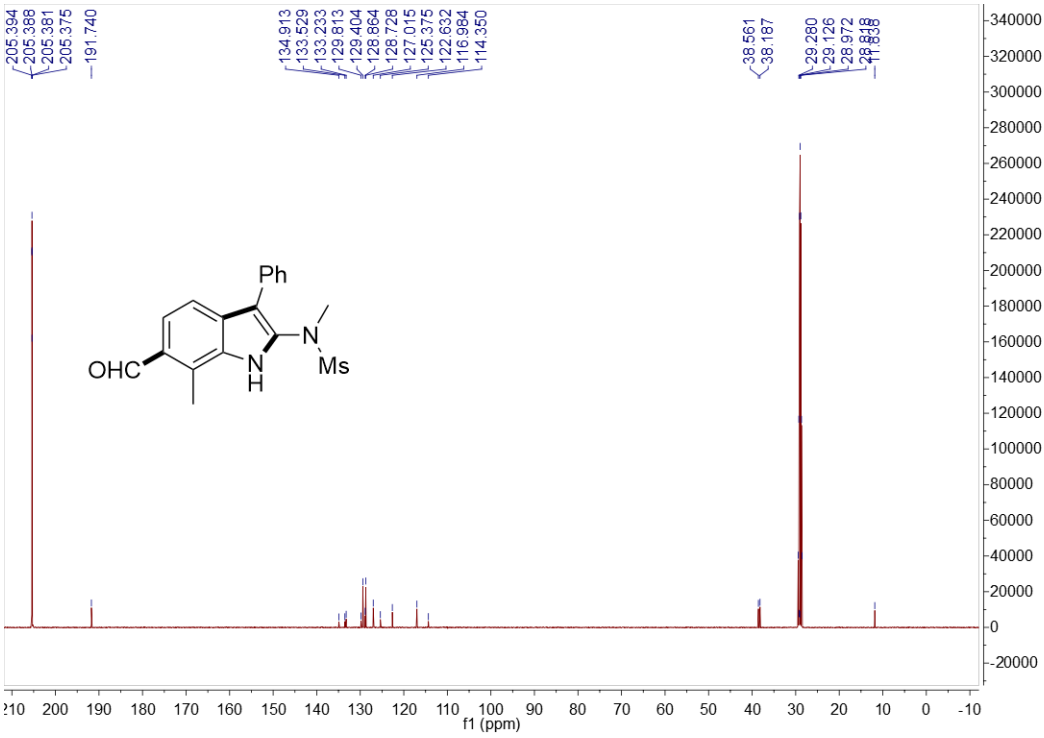
^{13}C NMR of compound **3a** in DMSO-d_6



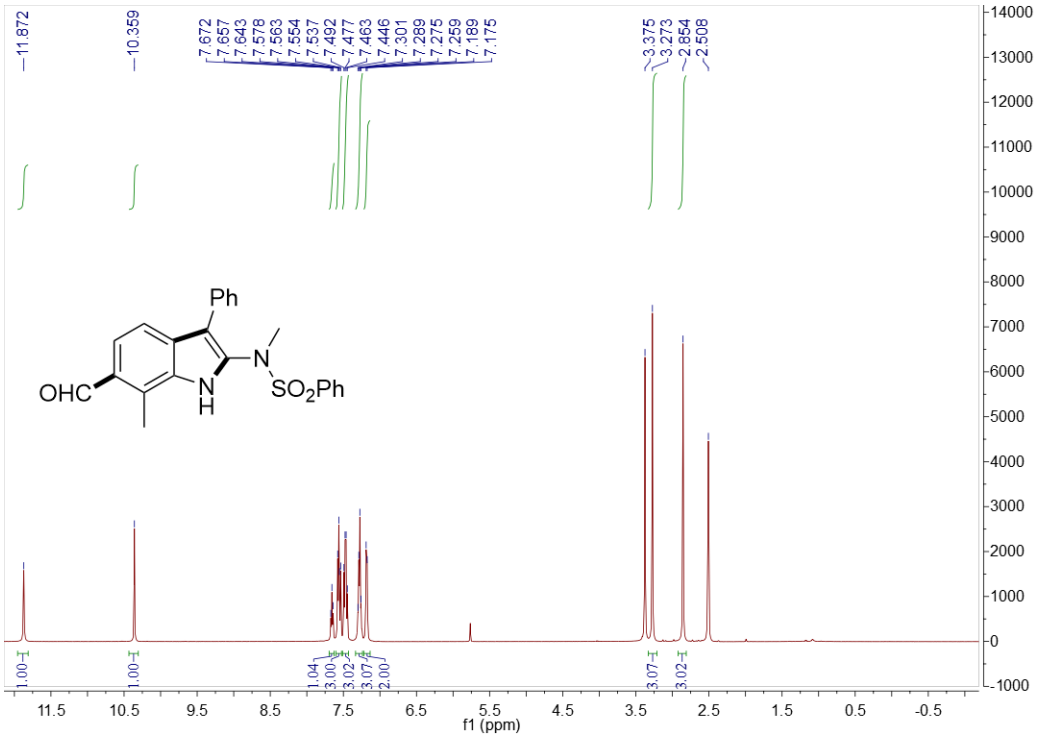
^{1}H NMR of compound **3b** in Acetone-d_6



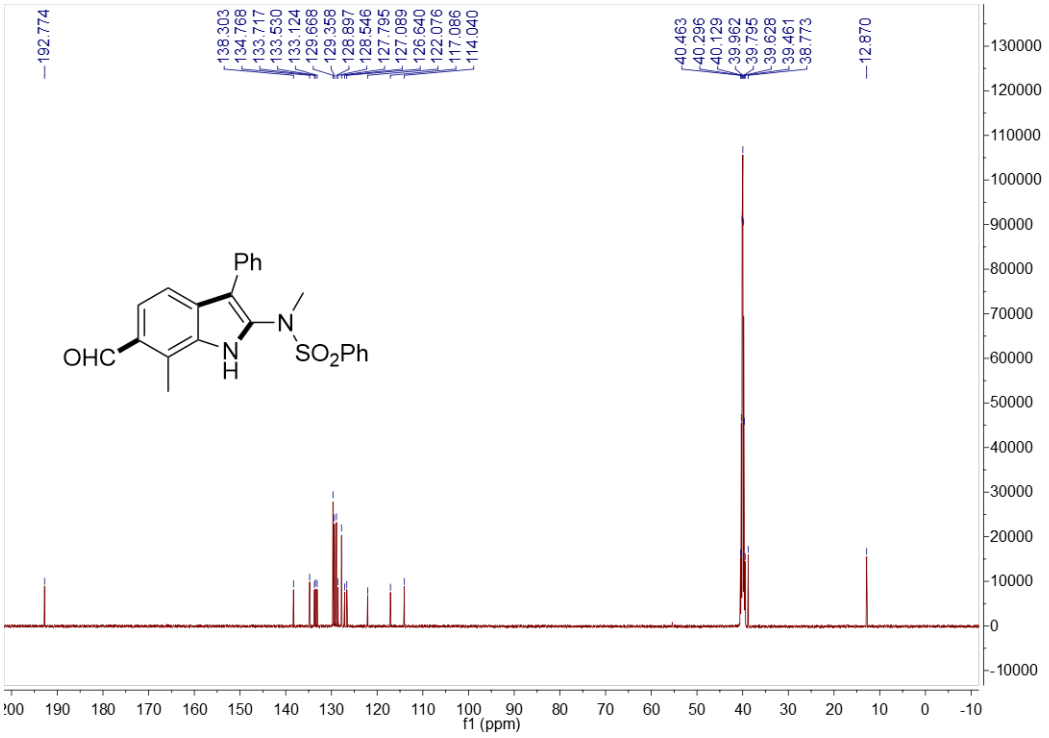
^{13}C NMR of compound **3b** in Acetone-d_6



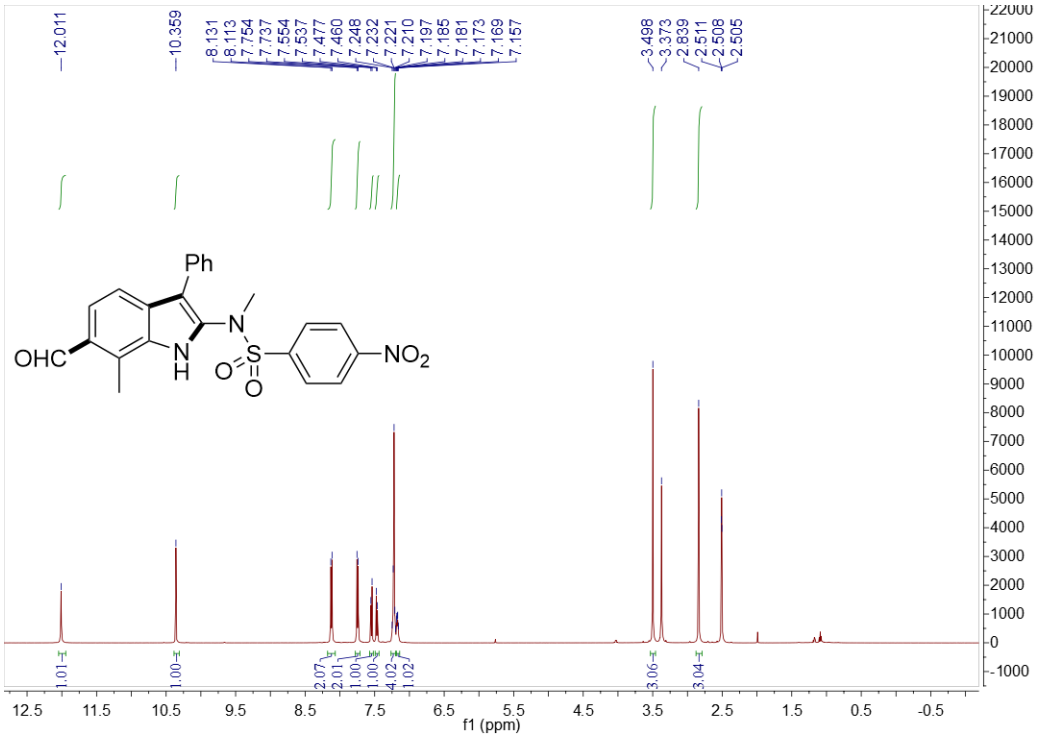
^{1}H NMR of compound **3c** in DMSO-d_6



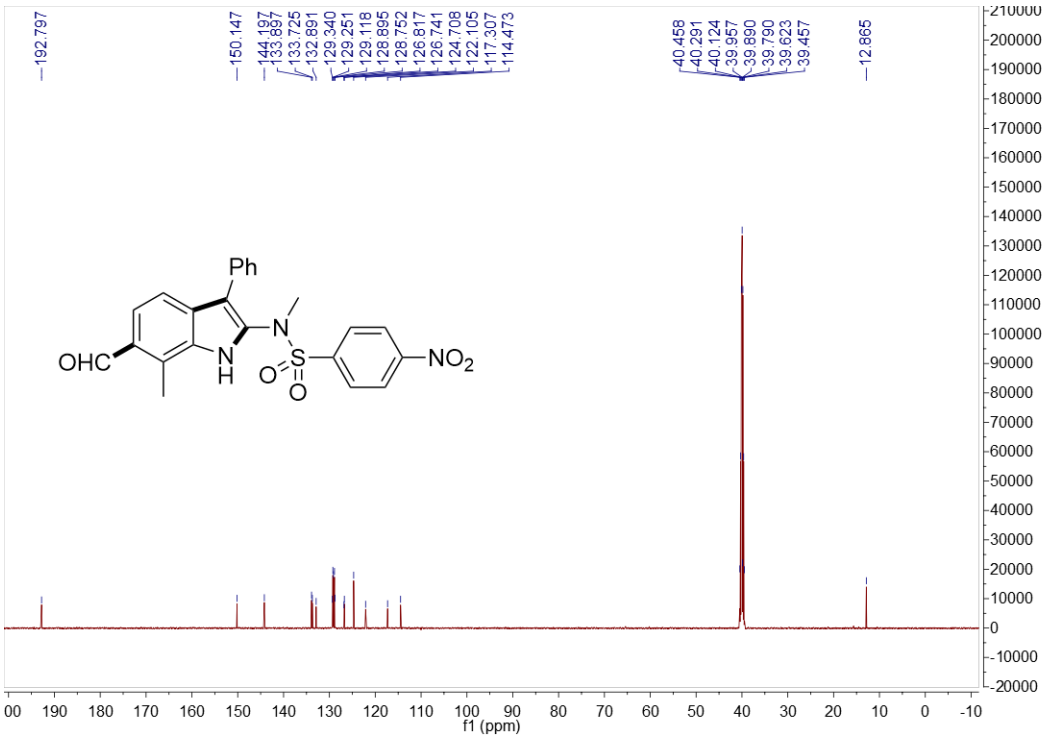
^{13}C NMR of compound **3c** in DMSO-d_6



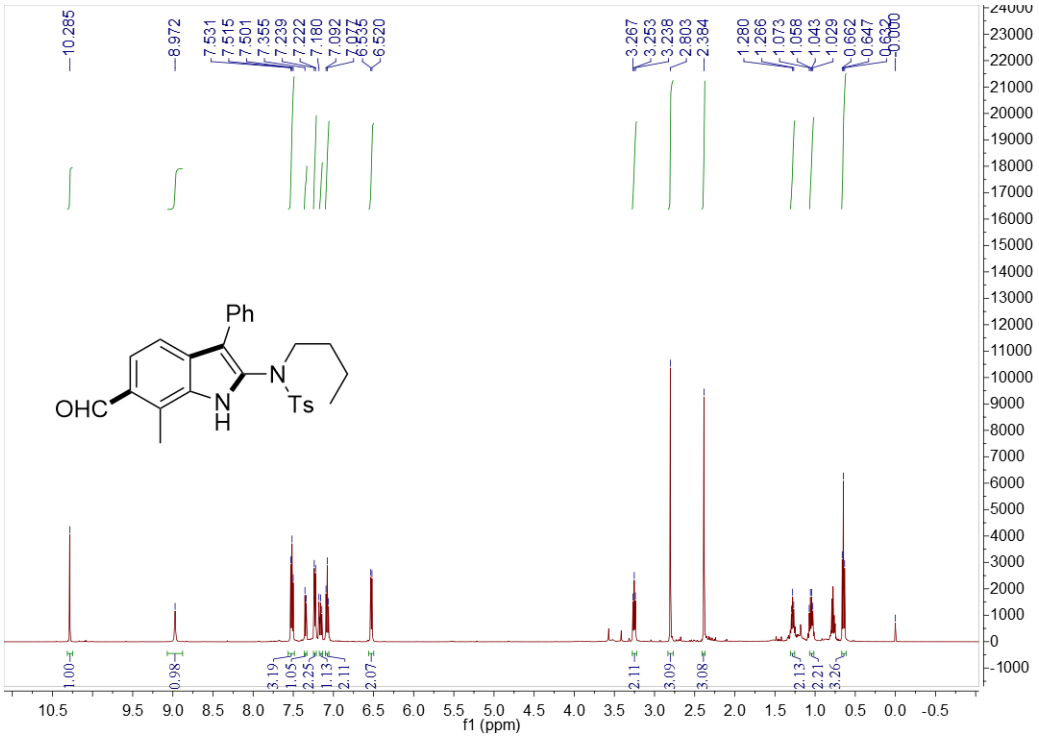
^{1}H NMR of compound **3d** in DMSO-d_6



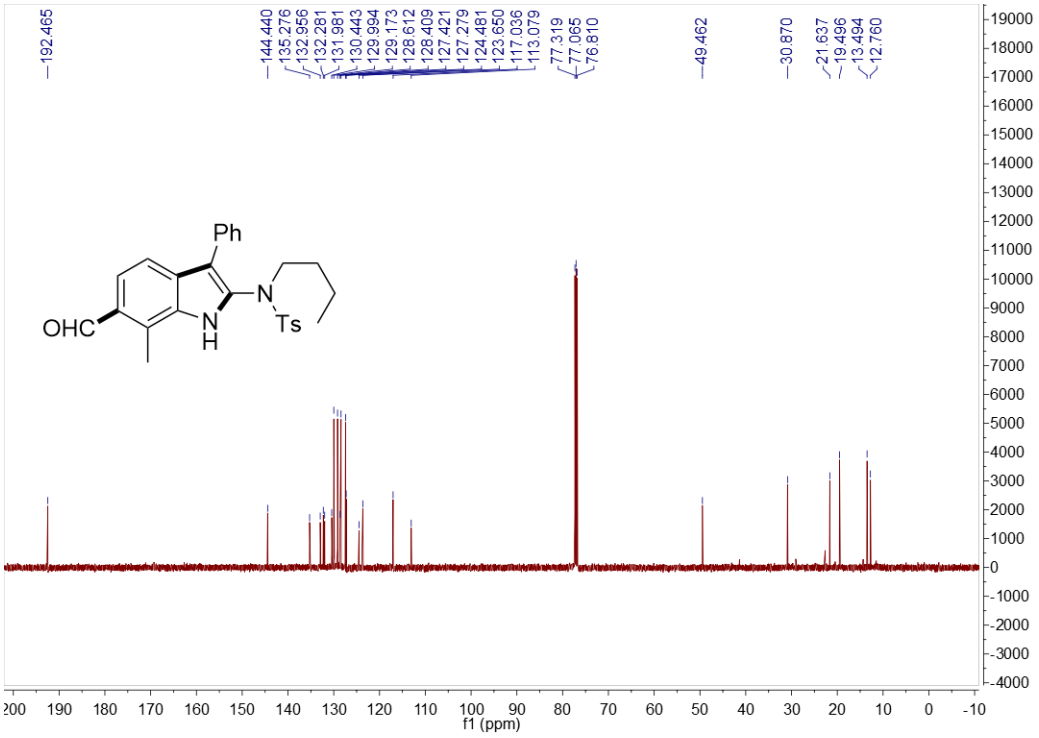
^{13}C NMR of compound **3d** in DMSO-d_6



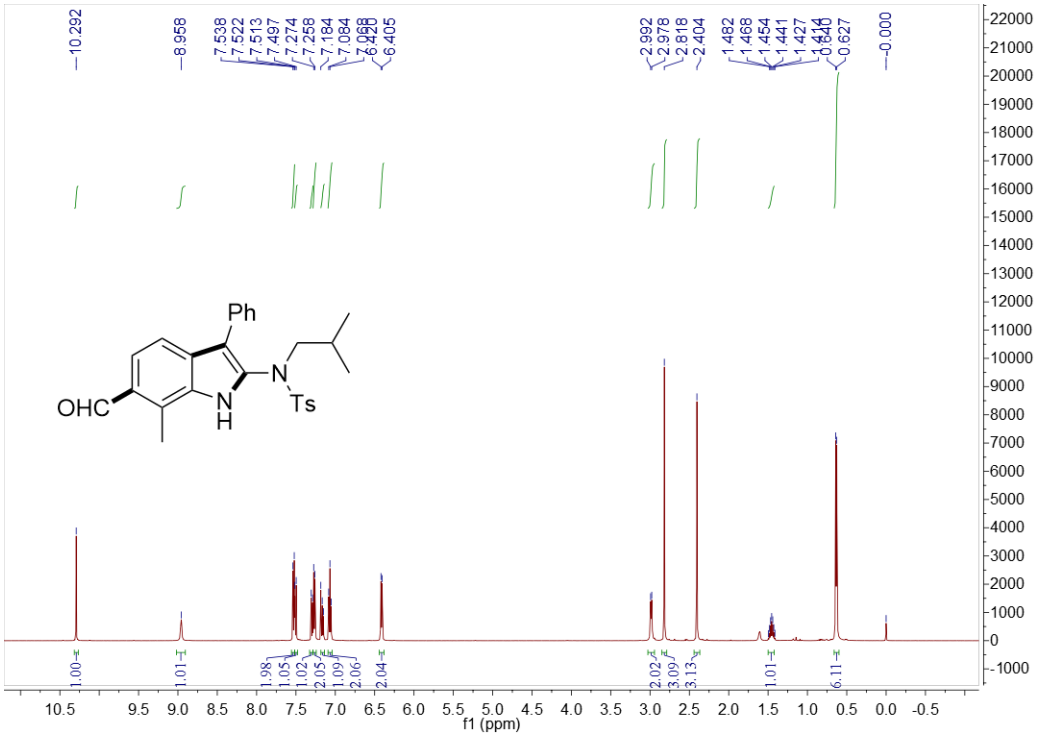
^{1}H NMR of compound **3e** in $CDCl_3$



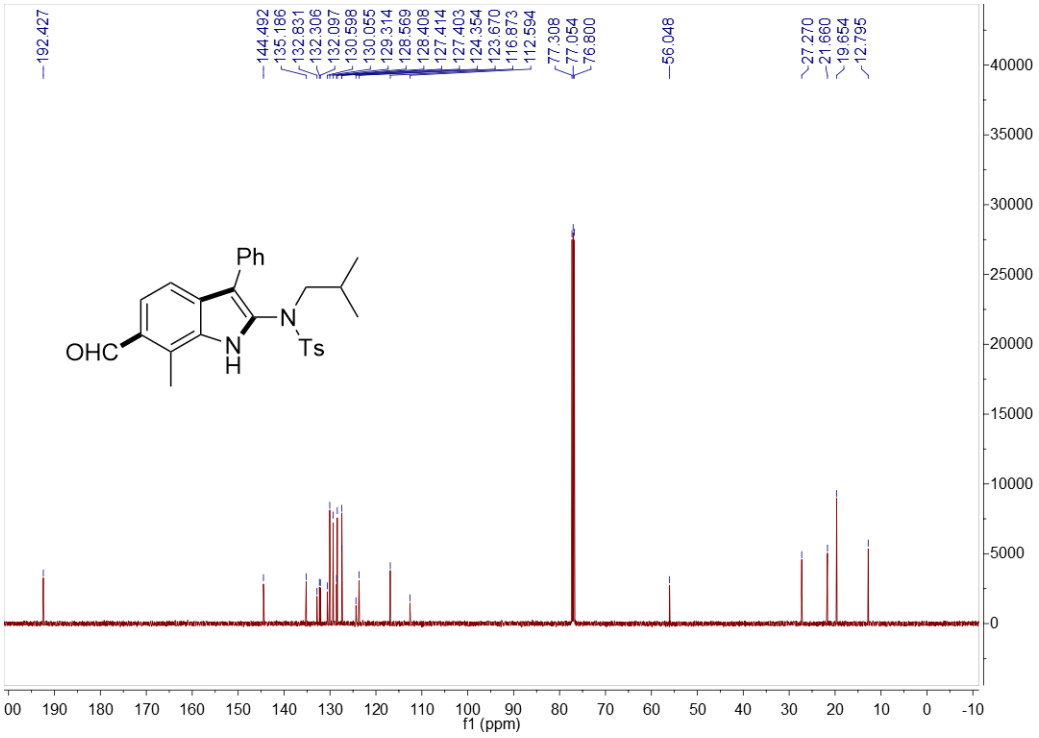
^{13}C NMR of compound **3e** in $CDCl_3$



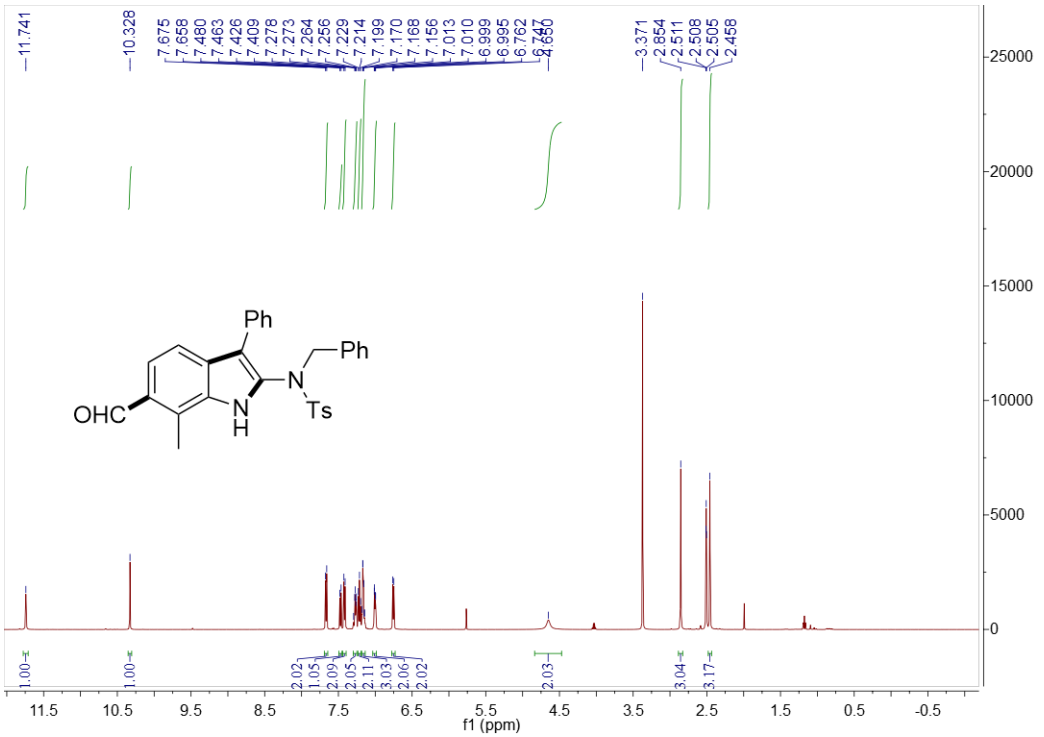
^{1}H NMR of compound **3f** in $CDCl_3$



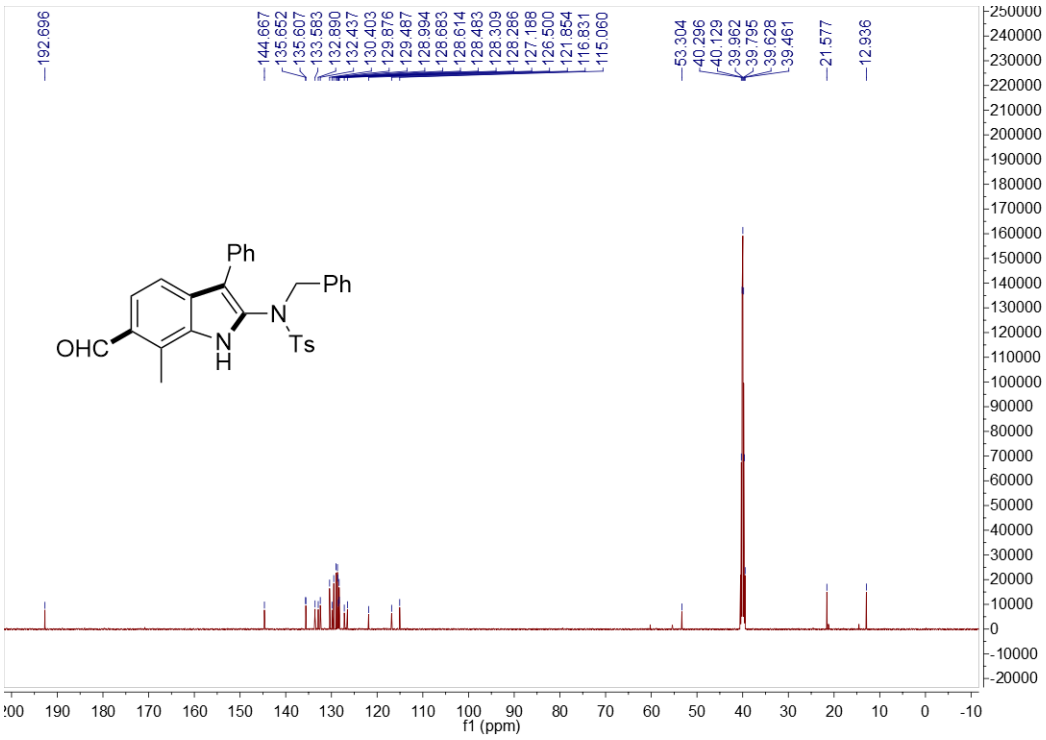
^{13}C NMR of compound **3f** in $CDCl_3$



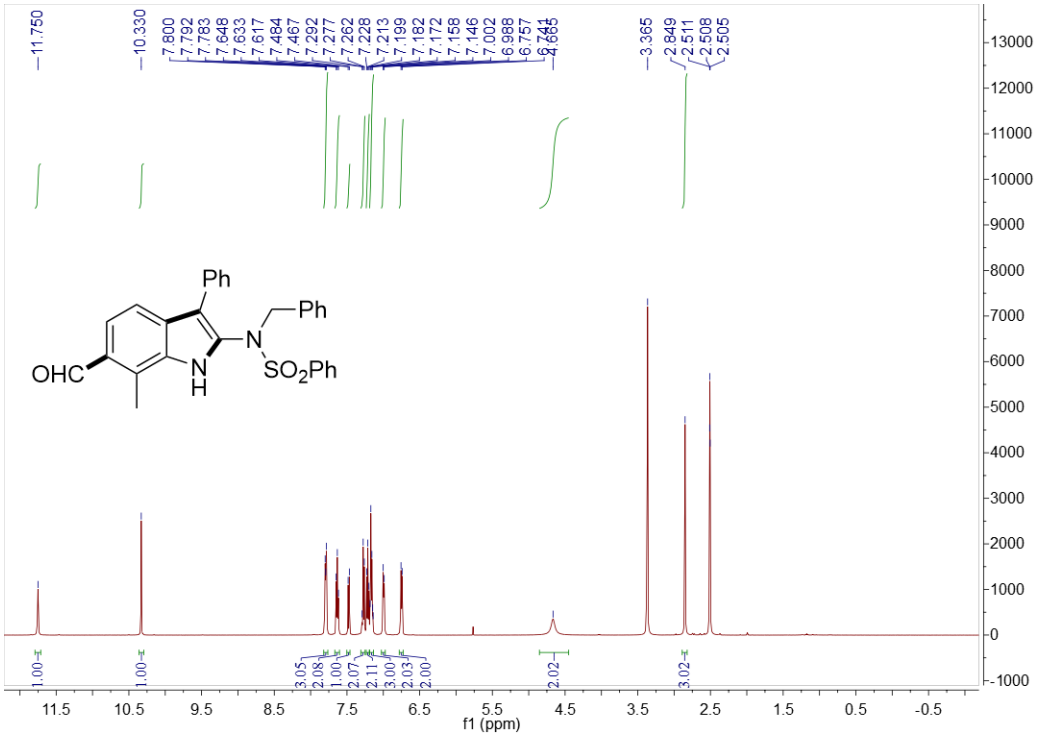
^{1}H NMR of compound **3g** in DMSO-d_6



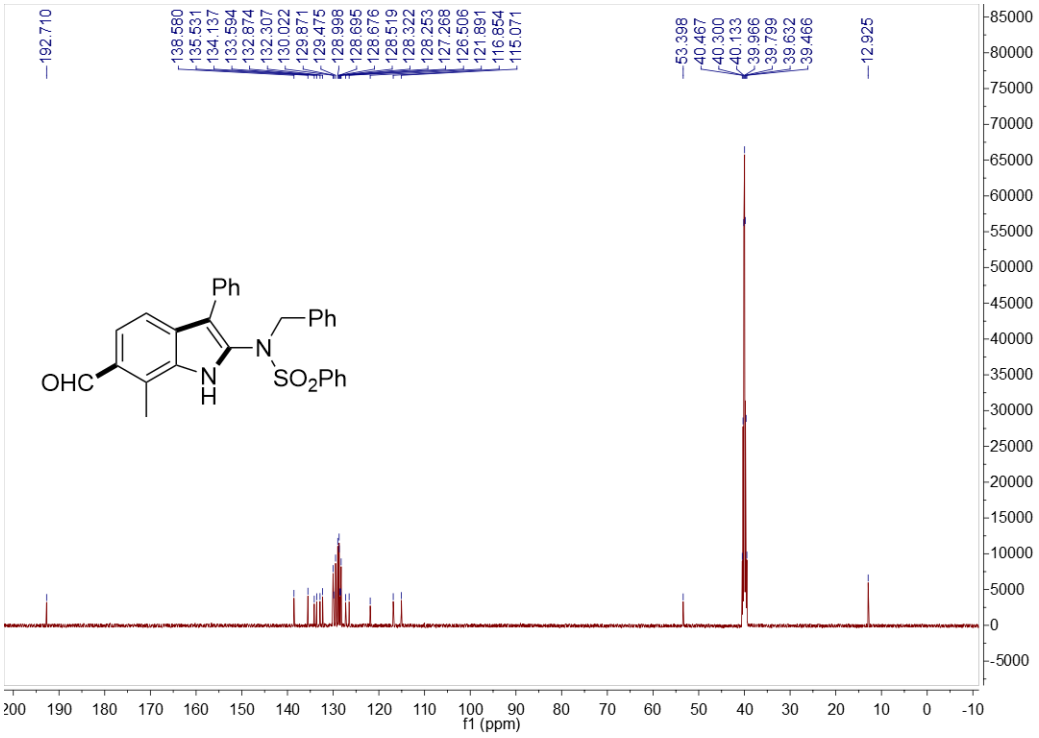
^{13}C NMR of compound **3g** in DMSO-d_6



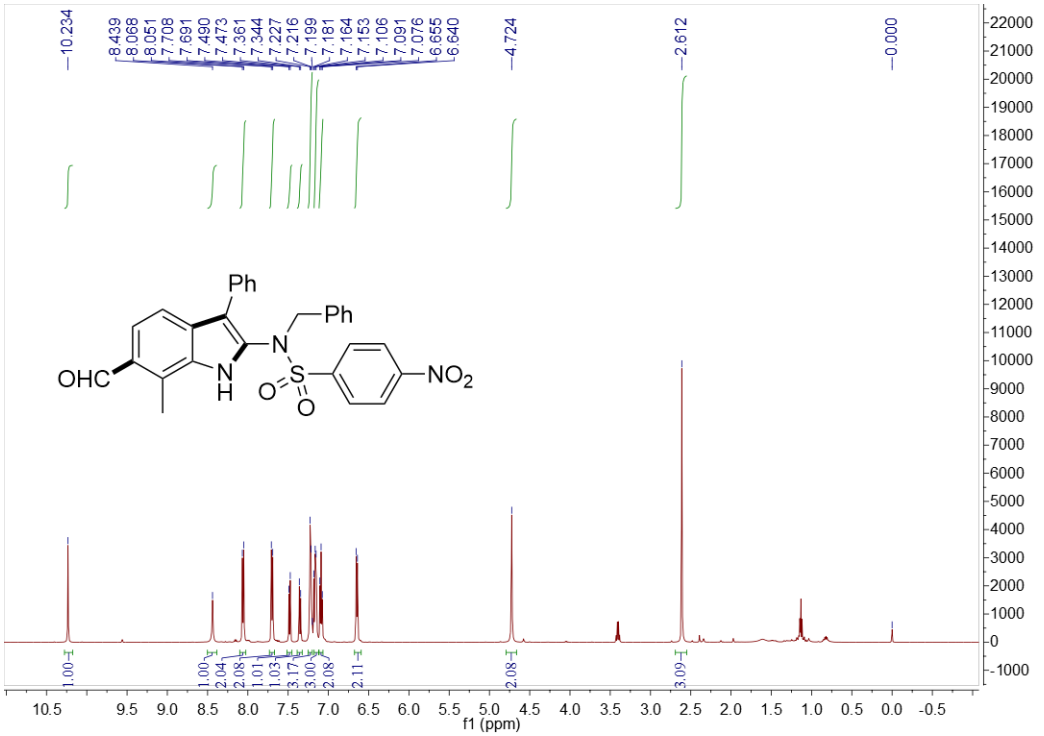
^{1}H NMR of compound **3h** in DMSO-d_6



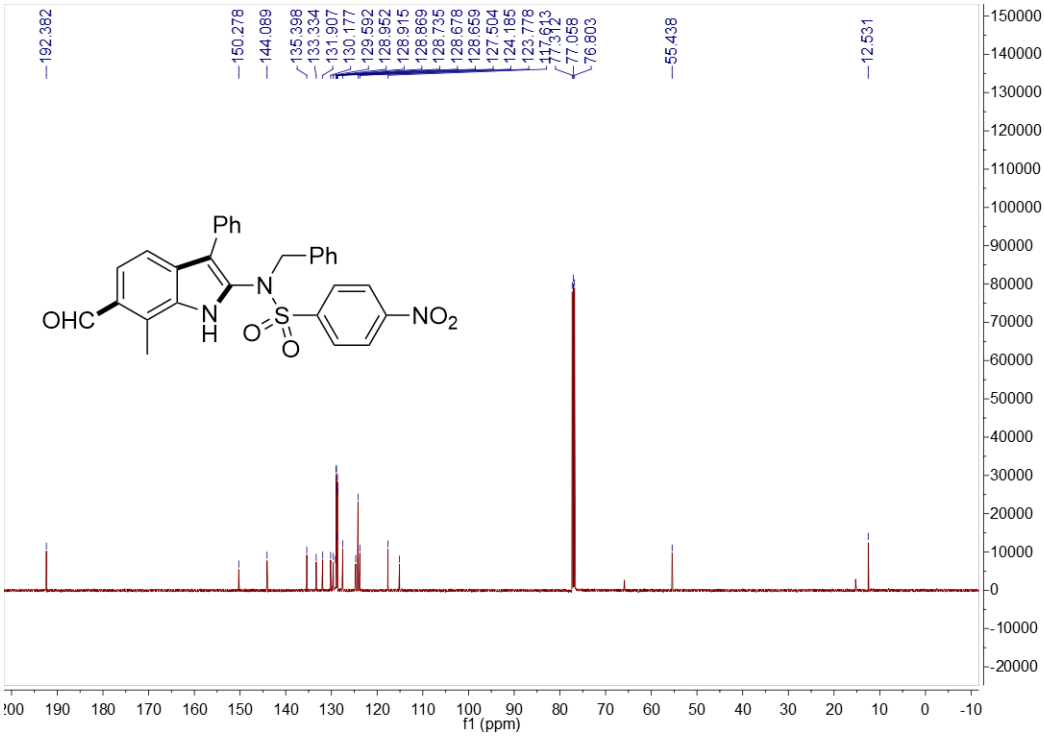
^{13}CNMR of compound **3h** in DMSO-d_6



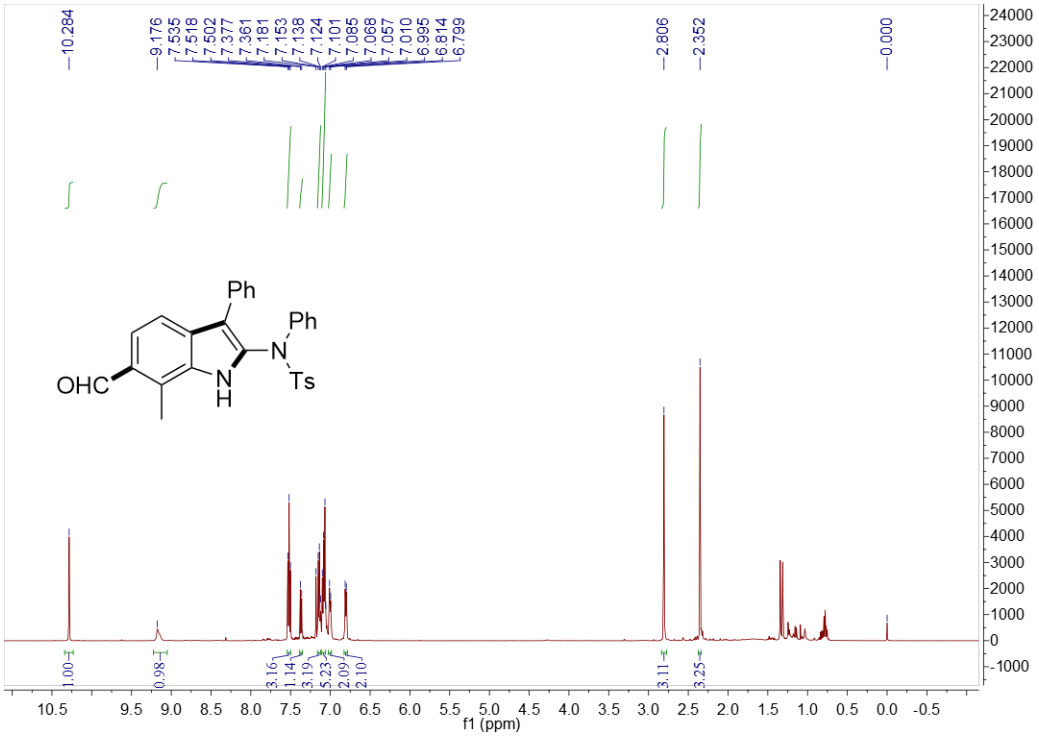
^{1}H NMR of compound **3i** in DMSO-d_6



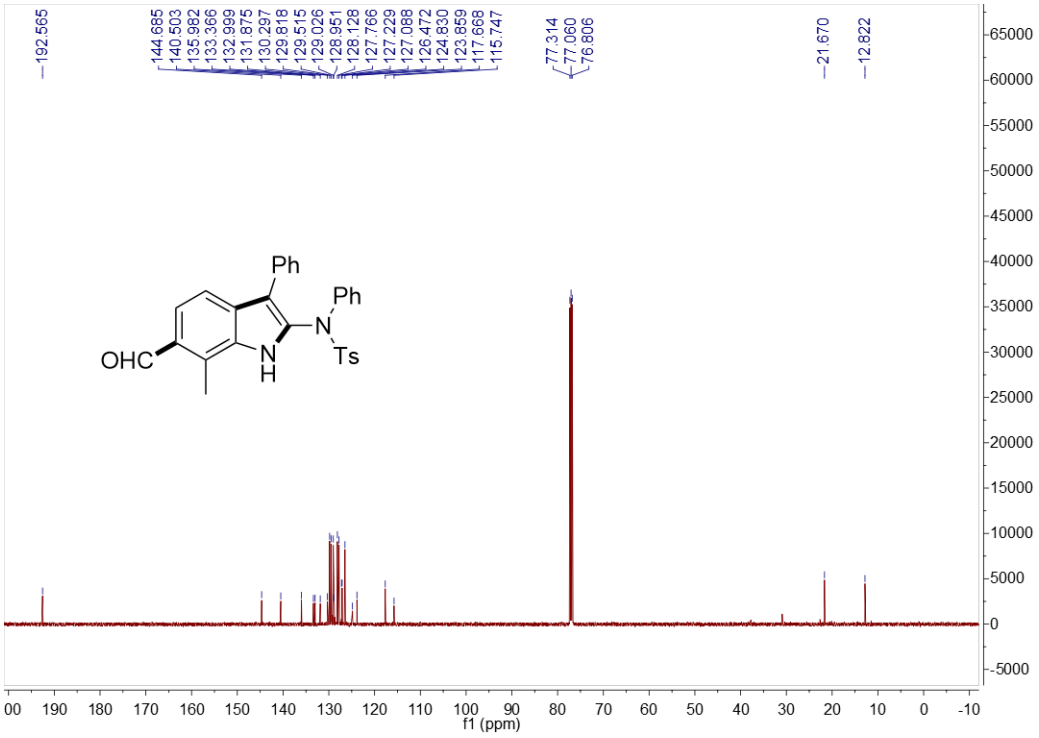
^{13}C NMR of compound **3i** in DMSO-d_6



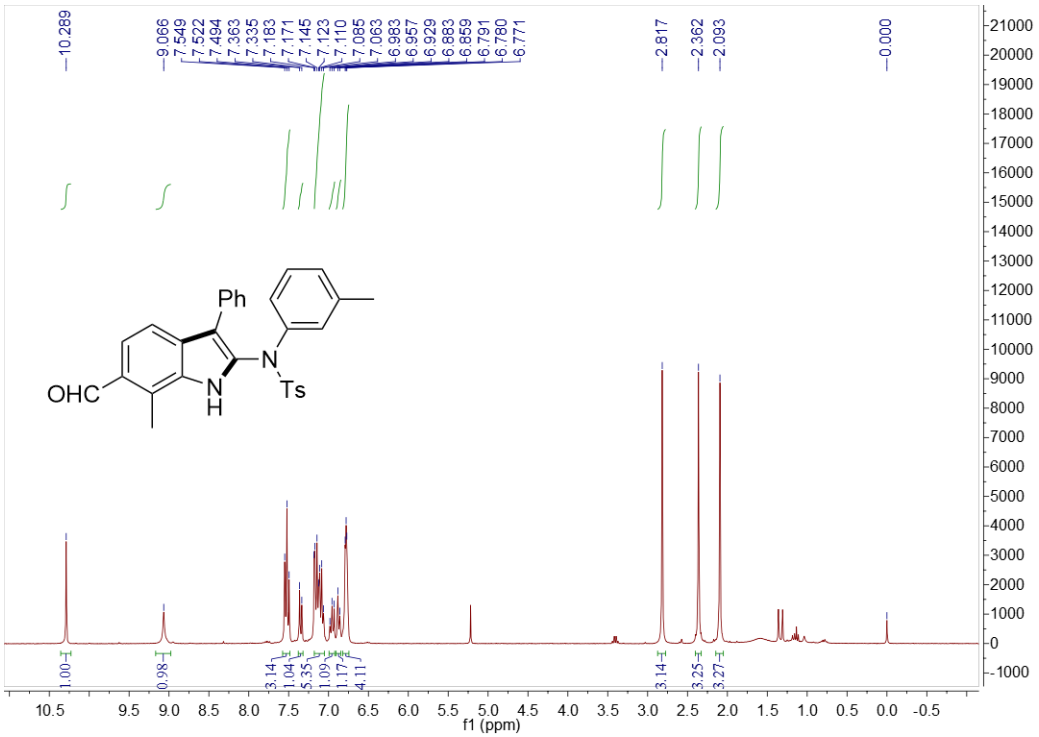
^{1}H NMR of compound **3j** in $CDCl_3$



^{13}C NMR of compound **3j** in $CDCl_3$



^{1}H NMR of compound **3k** in $CDCl_3$



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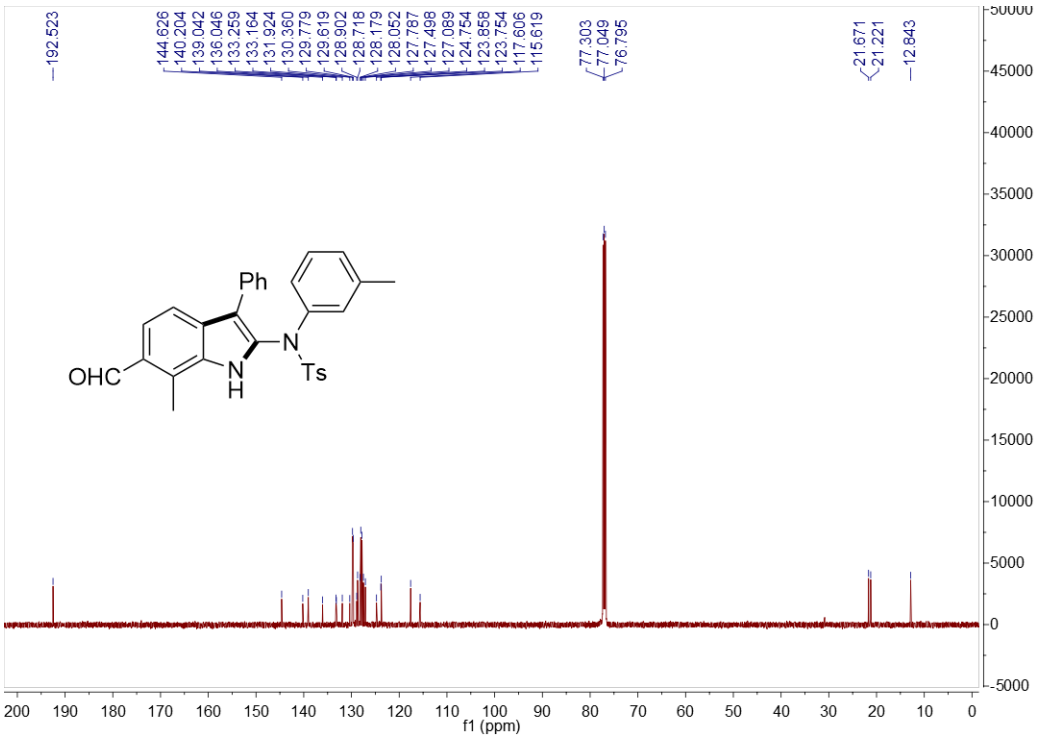
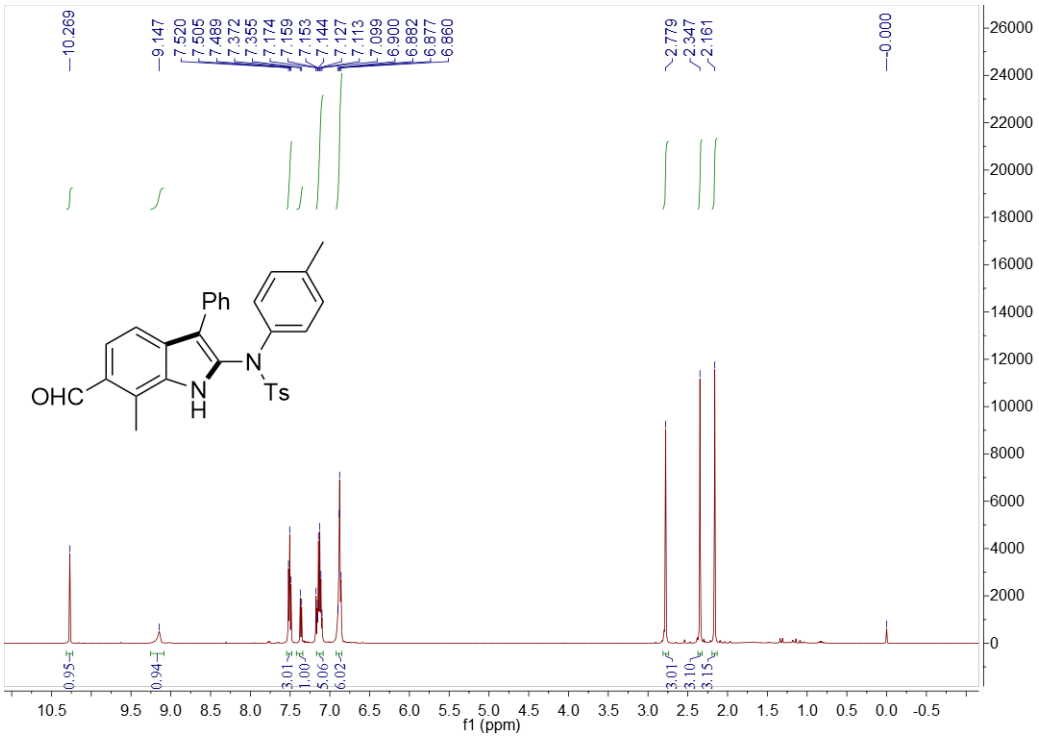
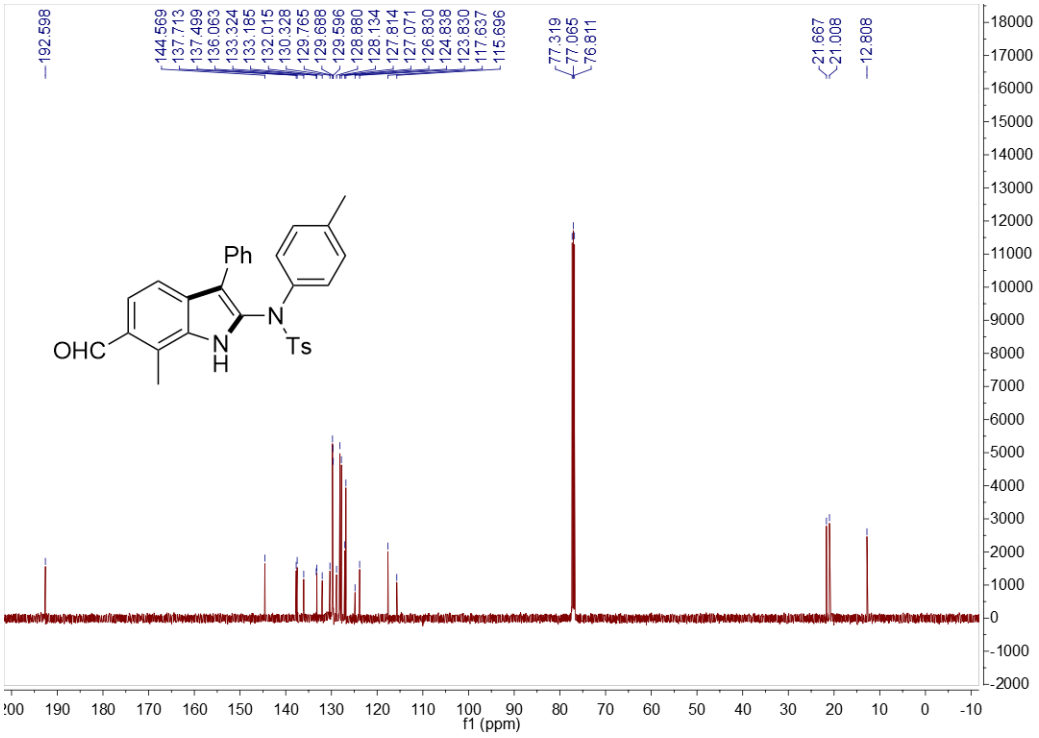


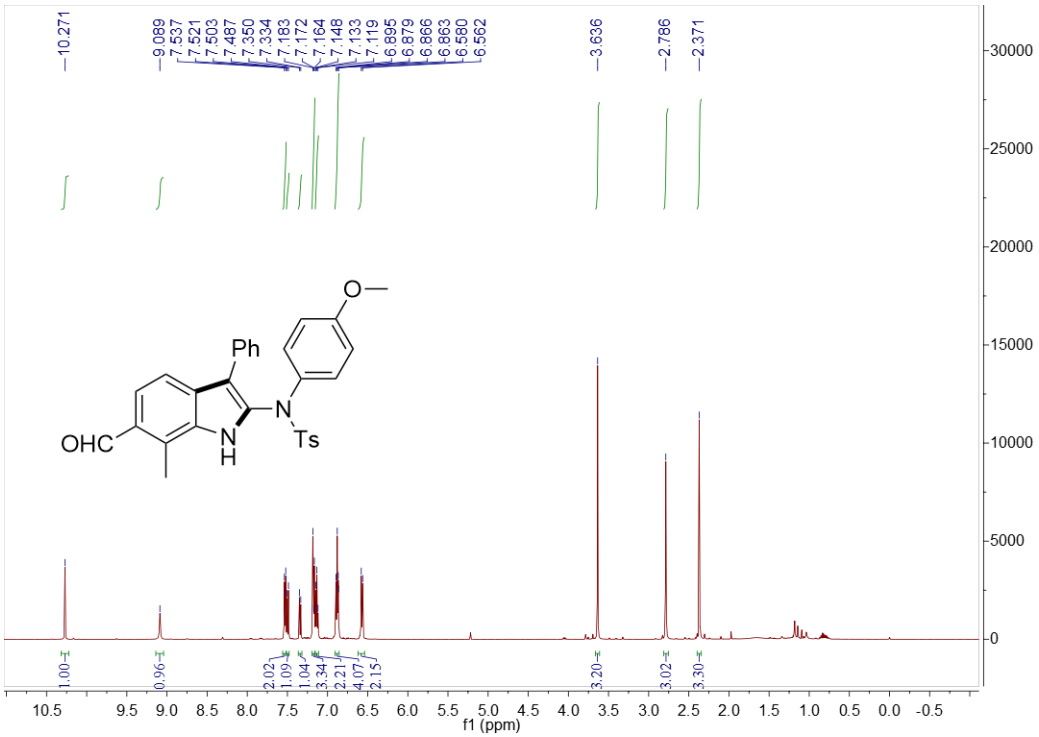
^{1}H NMR of compound **3l** in $CDCl_3$



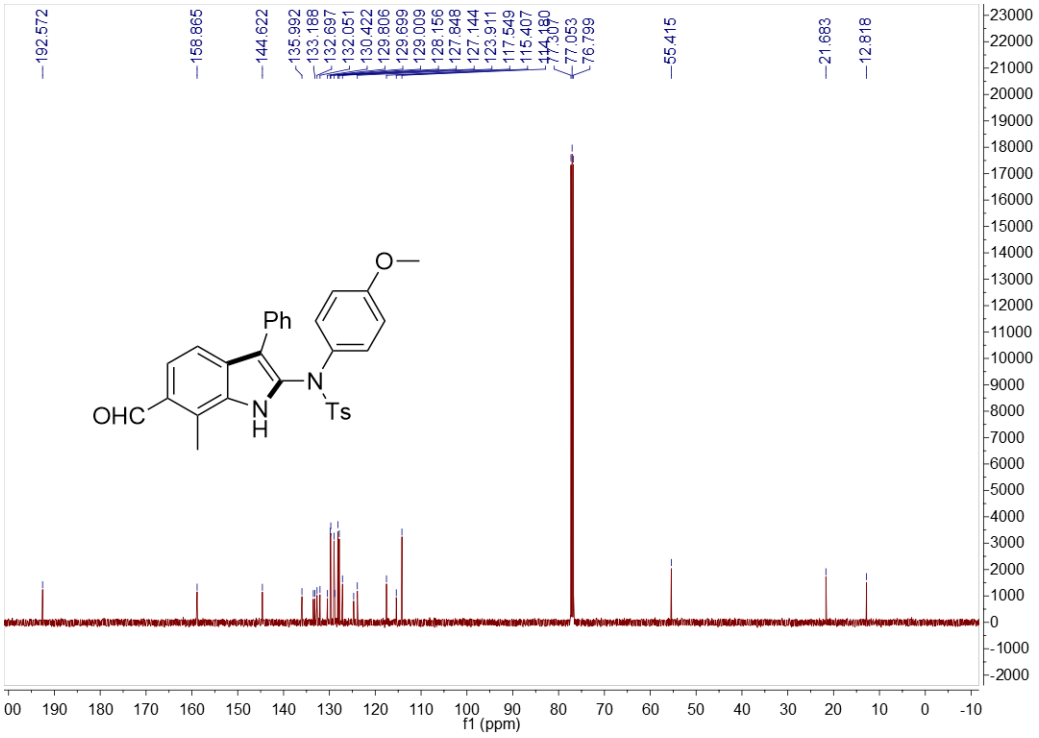
^{13}C NMR of compound **3l** in $CDCl_3$



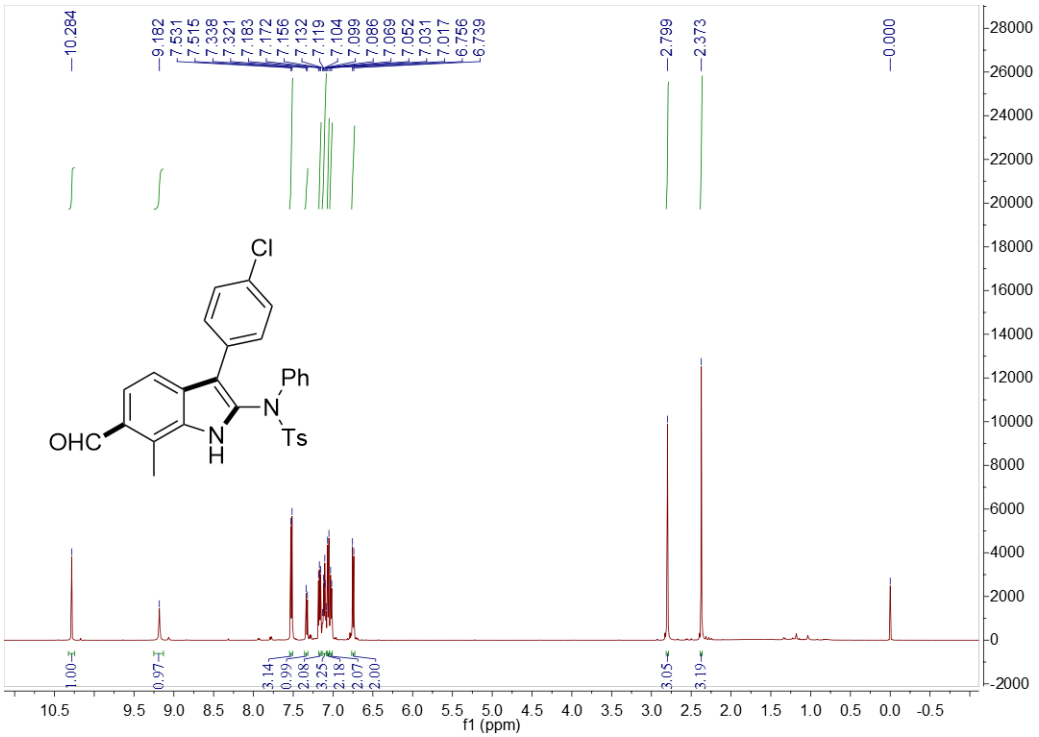
^{1}H NMR of compound **3m** in $CDCl_3$



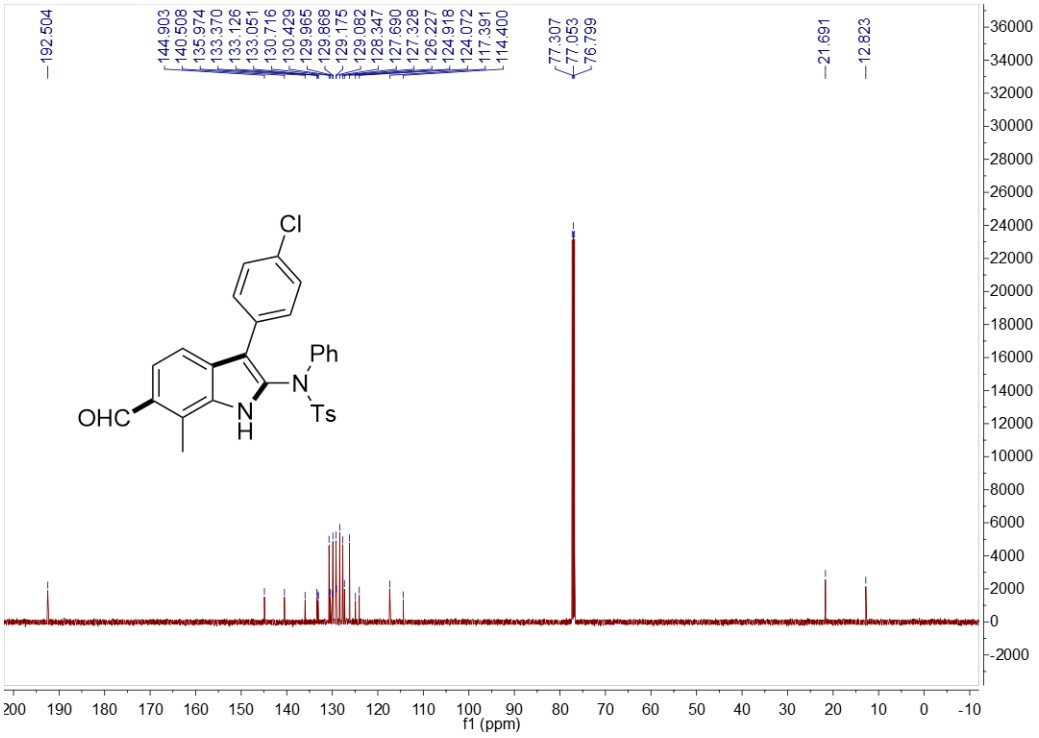
^{13}C NMR of compound **3m** in $CDCl_3$



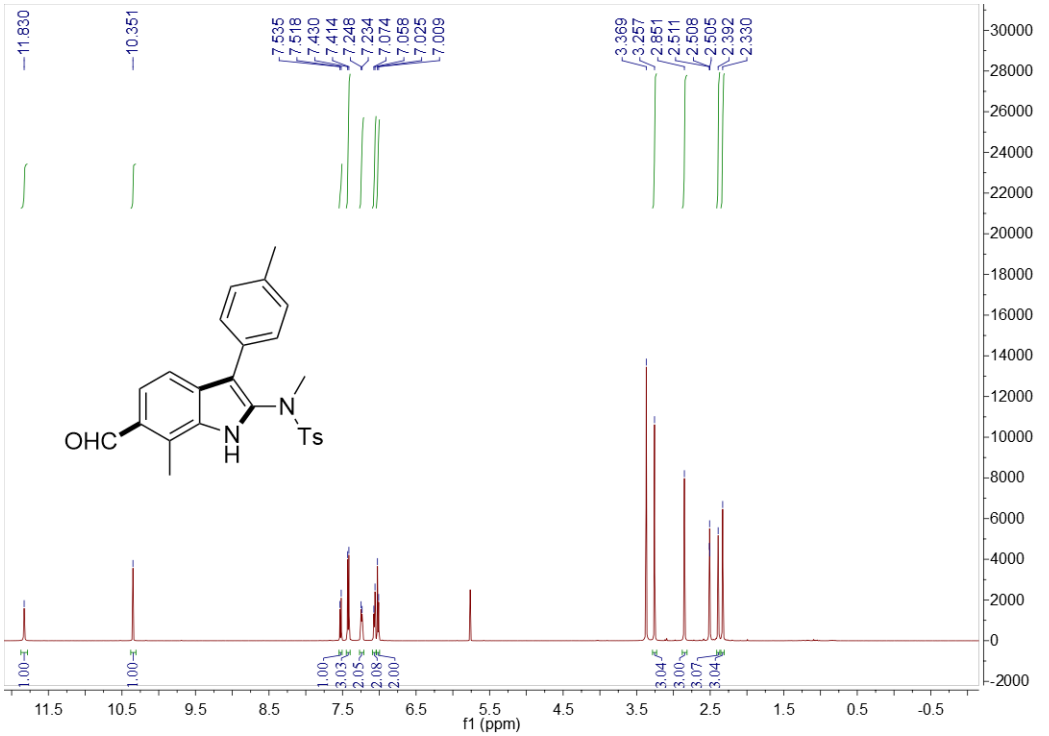
^{1}H NMR of compound **3n** in $CDCl_3$



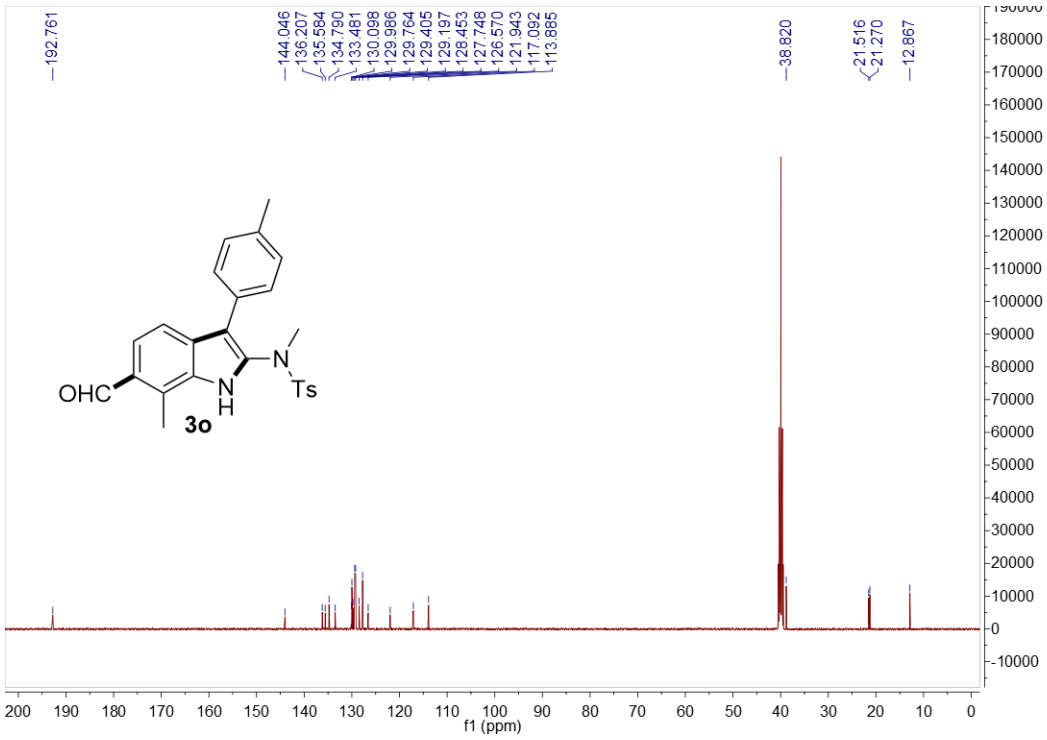
^{13}C NMR of compound **3n** in $CDCl_3$



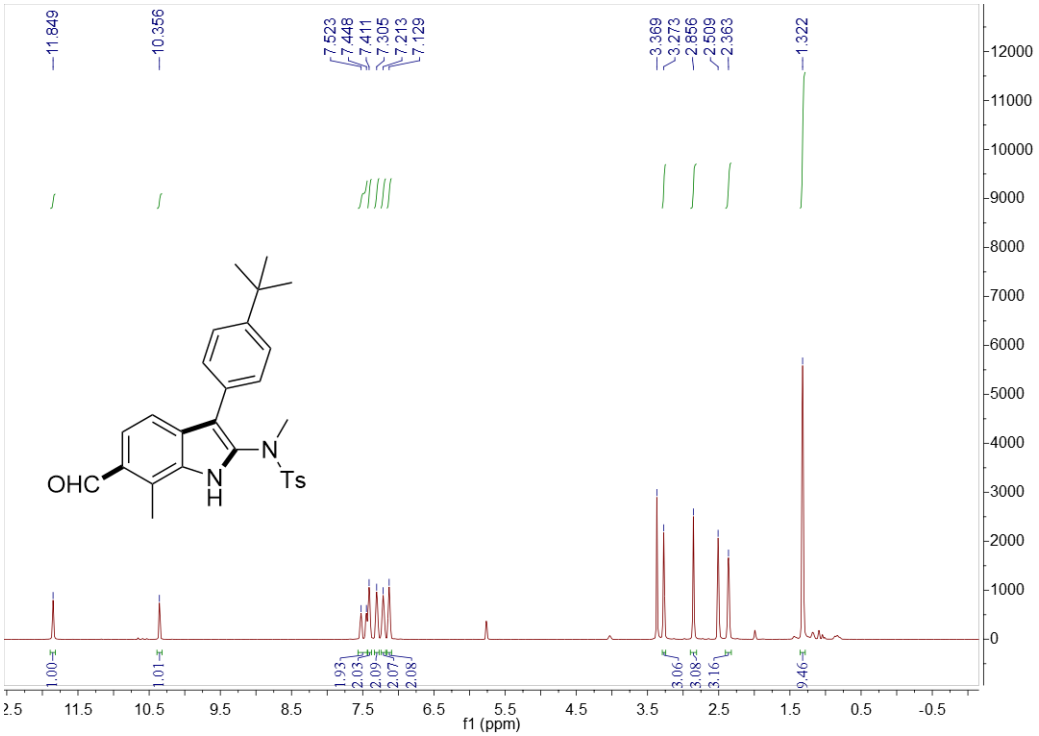
^{1}H NMR of compound **3o** in DMSO-d_6



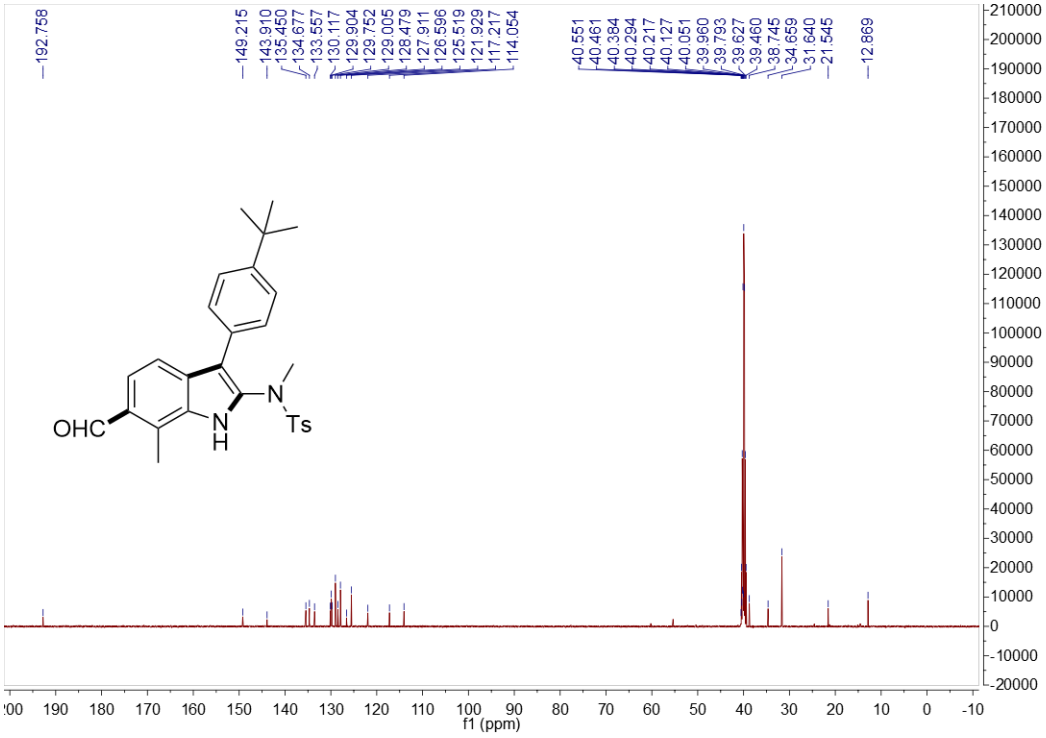
^{13}C NMR of compound **3o** in DMSO-d_6



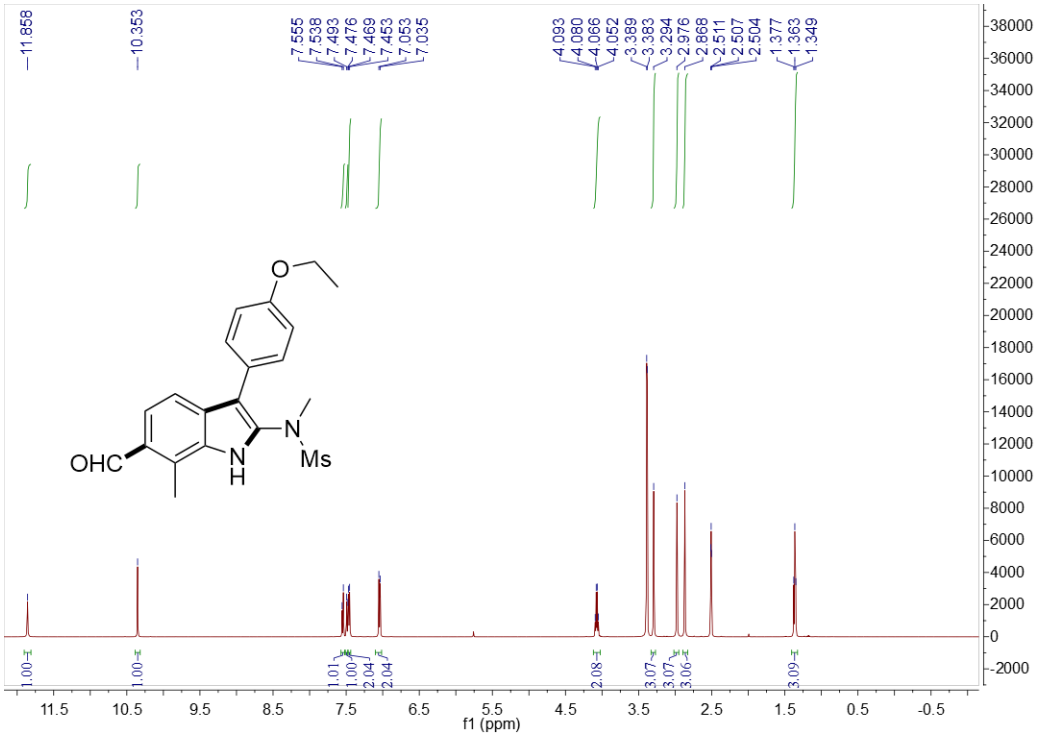
^{1}H NMR of compound **3p** in DMSO-d_6



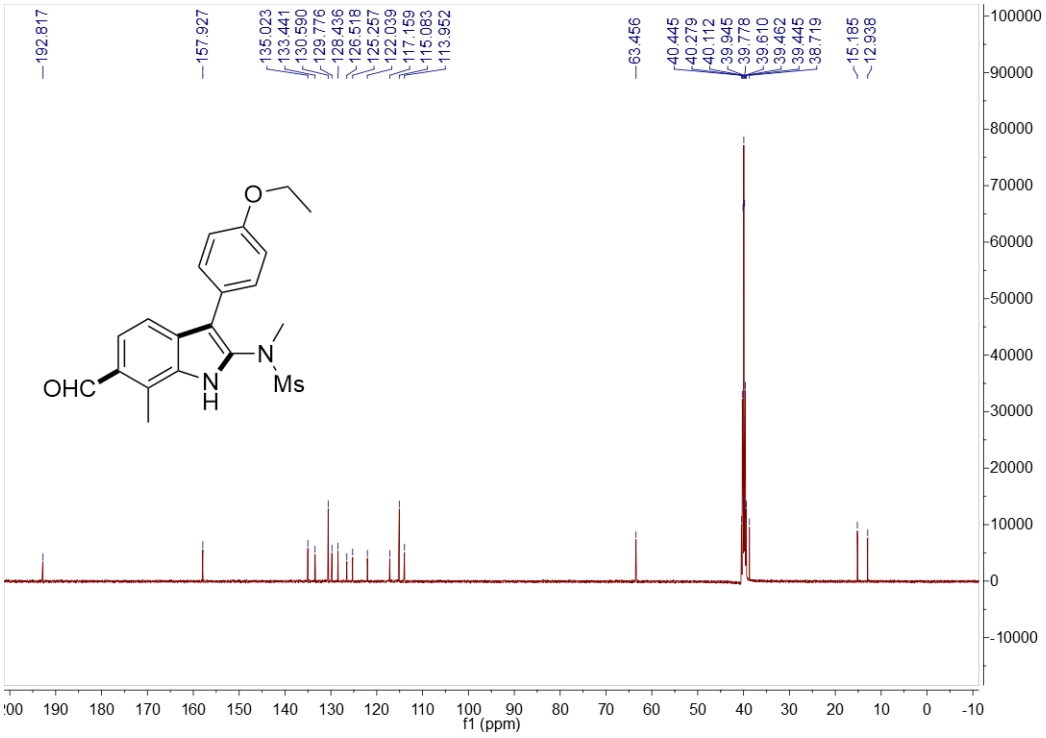
^{13}C NMR of compound **3p** in DMSO-d_6



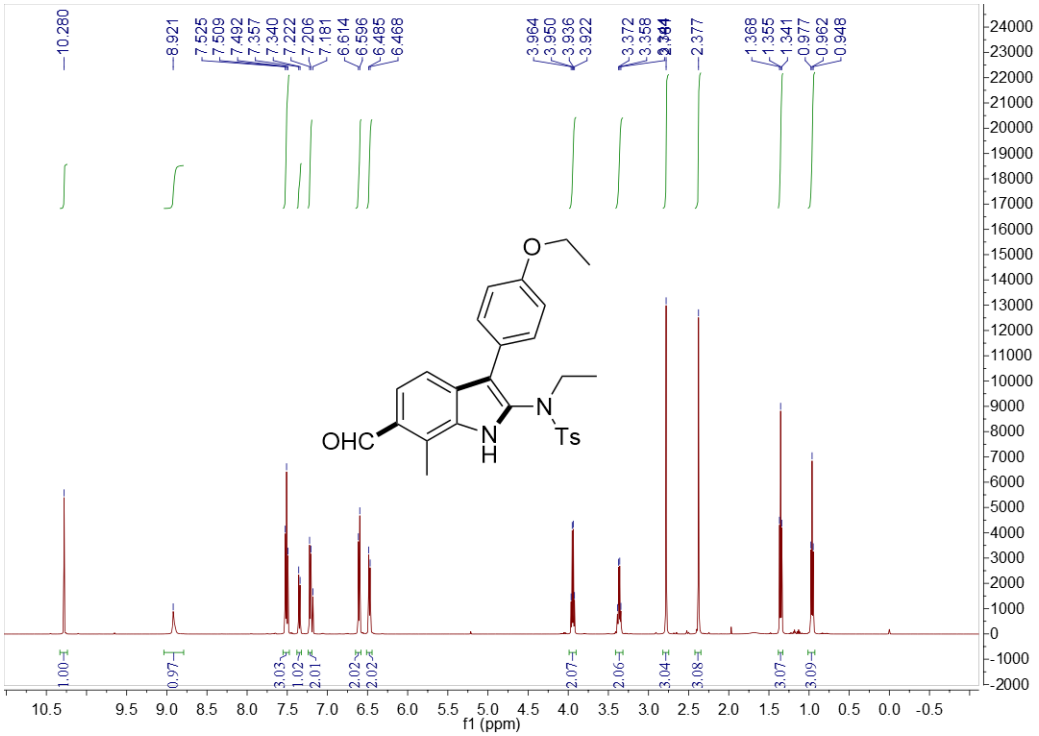
^{1}H NMR of compound **3q** in DMSO-d_6



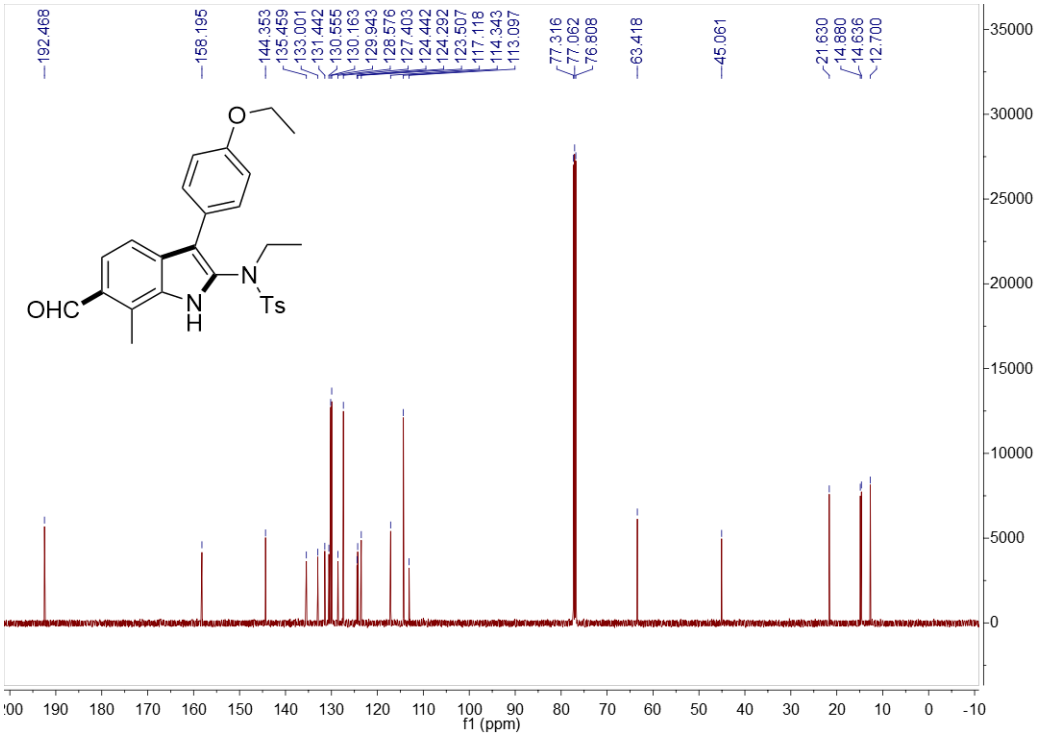
^{13}C NMR of compound **3q** in DMSO-d_6



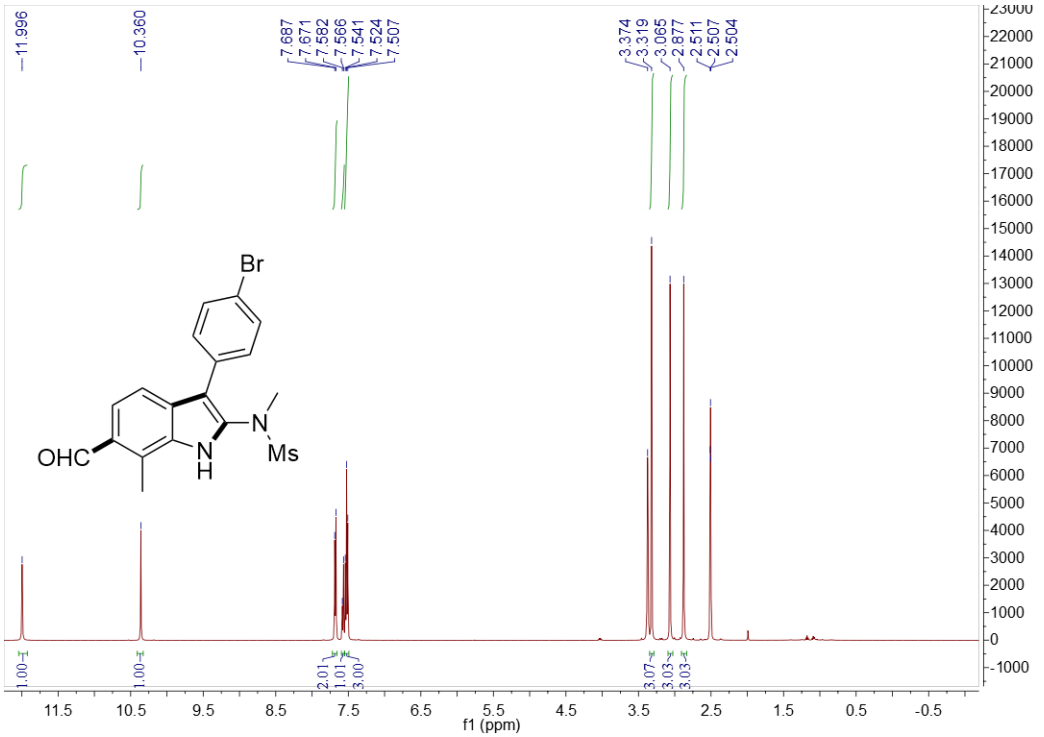
^{1}H NMR of compound **3r** in $CDCl_3$



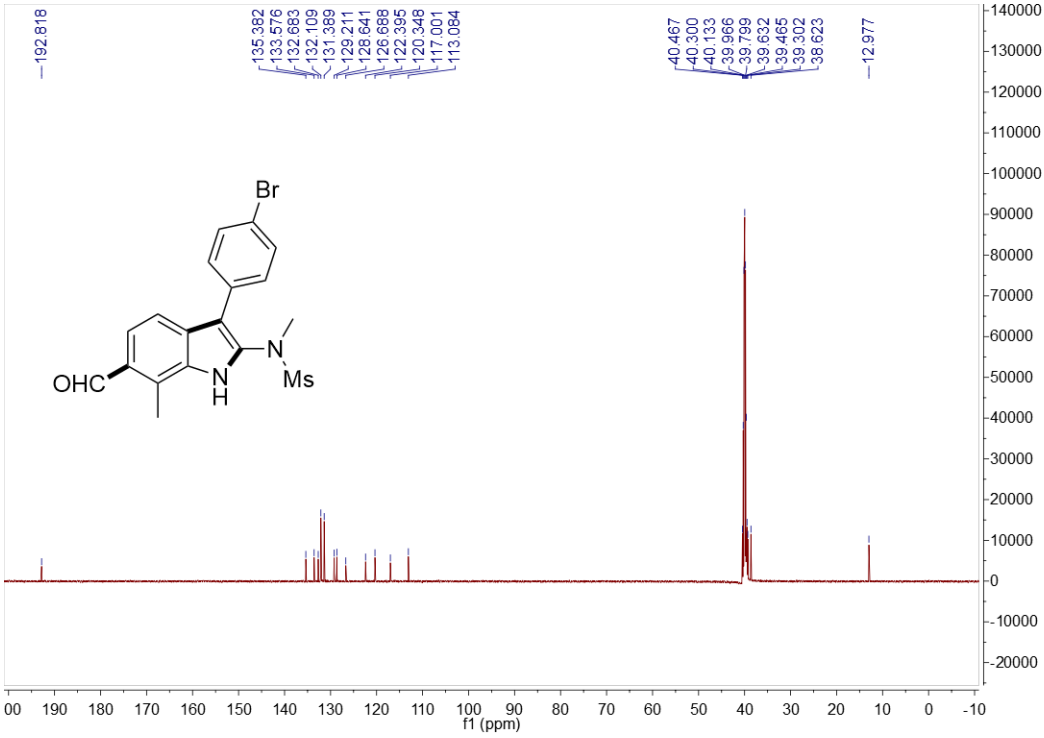
^{13}C NMR of compound **3r** in $CDCl_3$



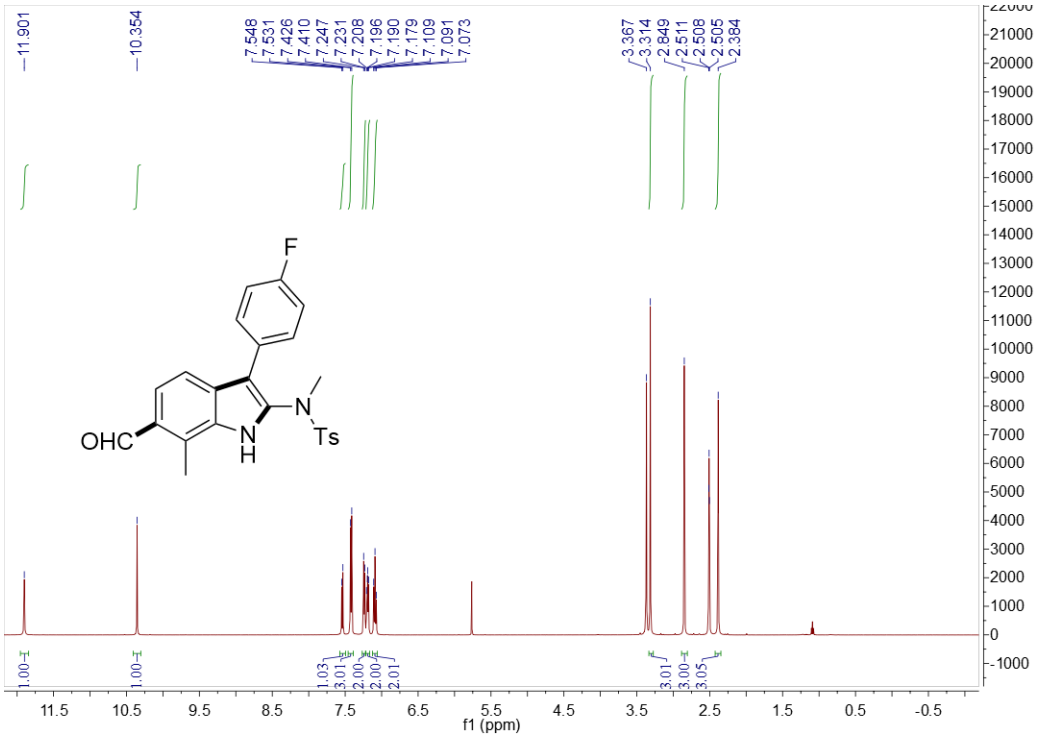
^{1}H NMR of compound **3s** in DMSO-d_6



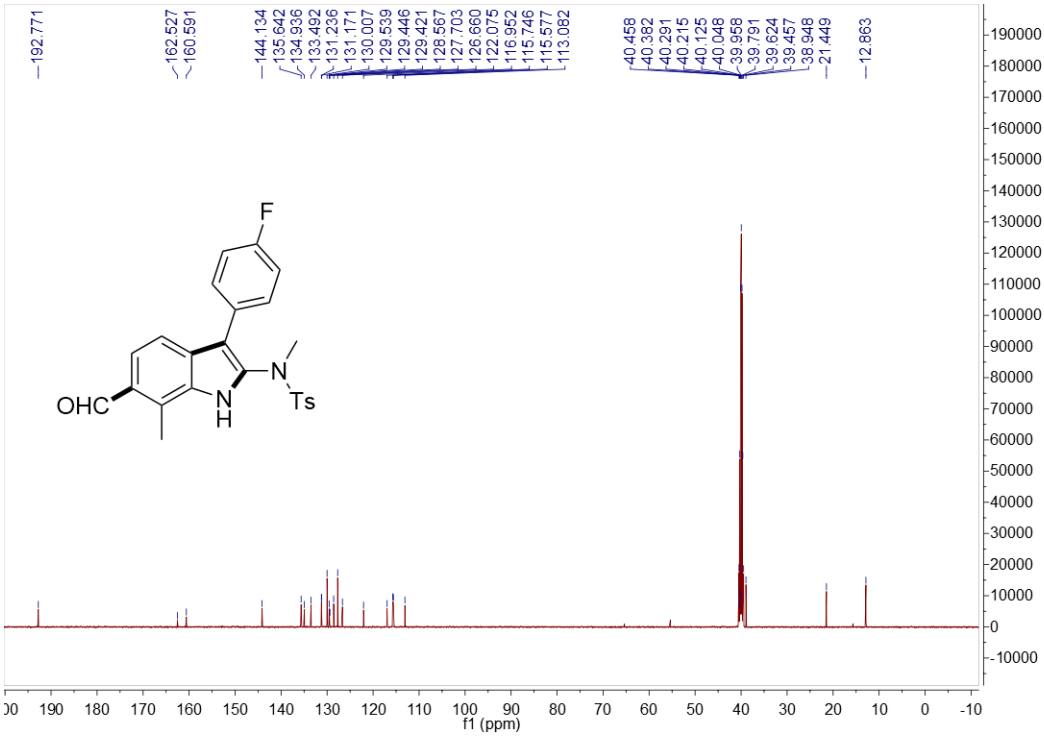
^{13}C NMR of compound **3s** in DMSO-d_6



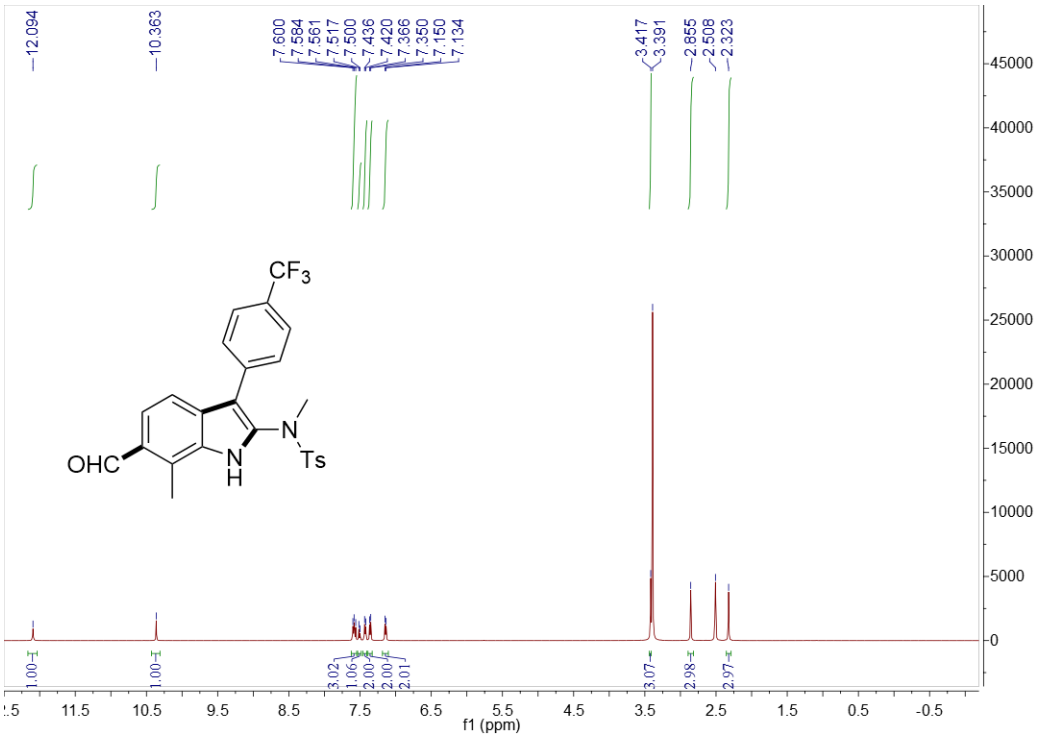
^{1}H NMR of compound **3t** in DMSO-d_6



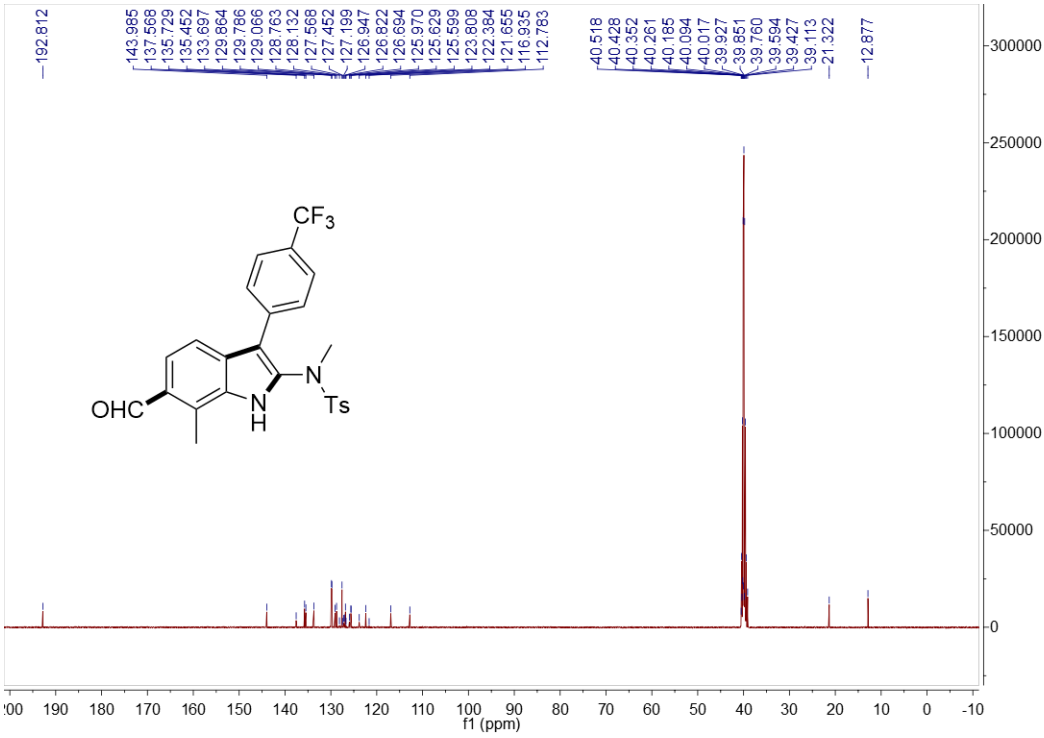
^{13}C NMR of compound **3t** in DMSO-d_6



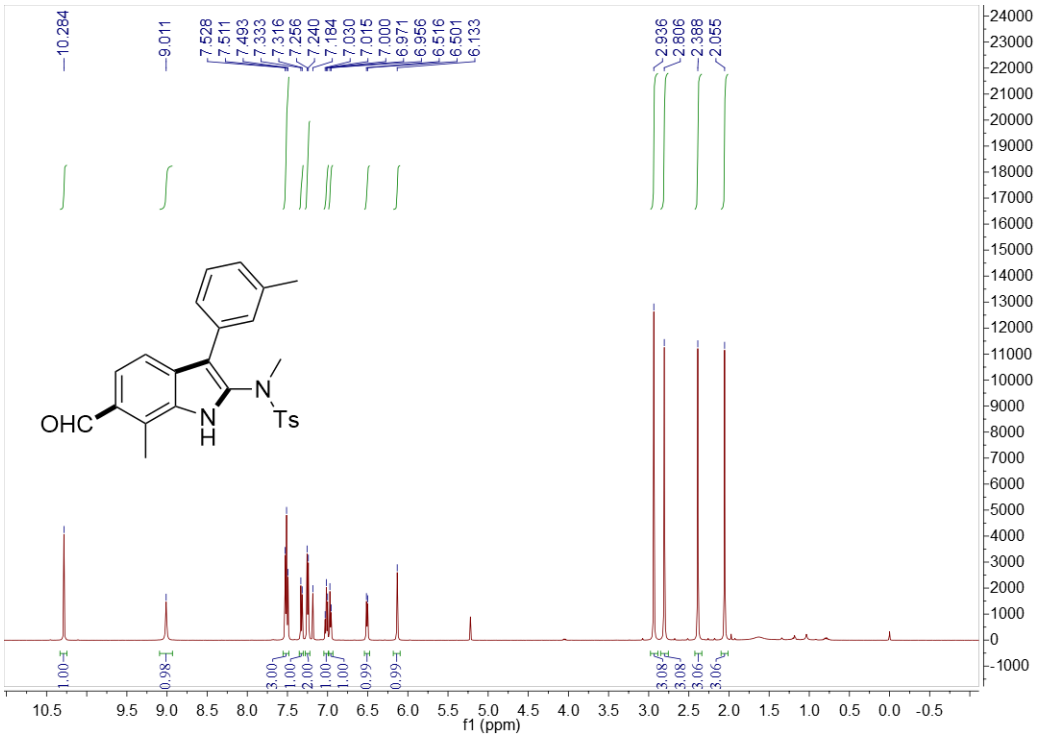
^{1}H NMR of compound **3u** in DMSO-d_6



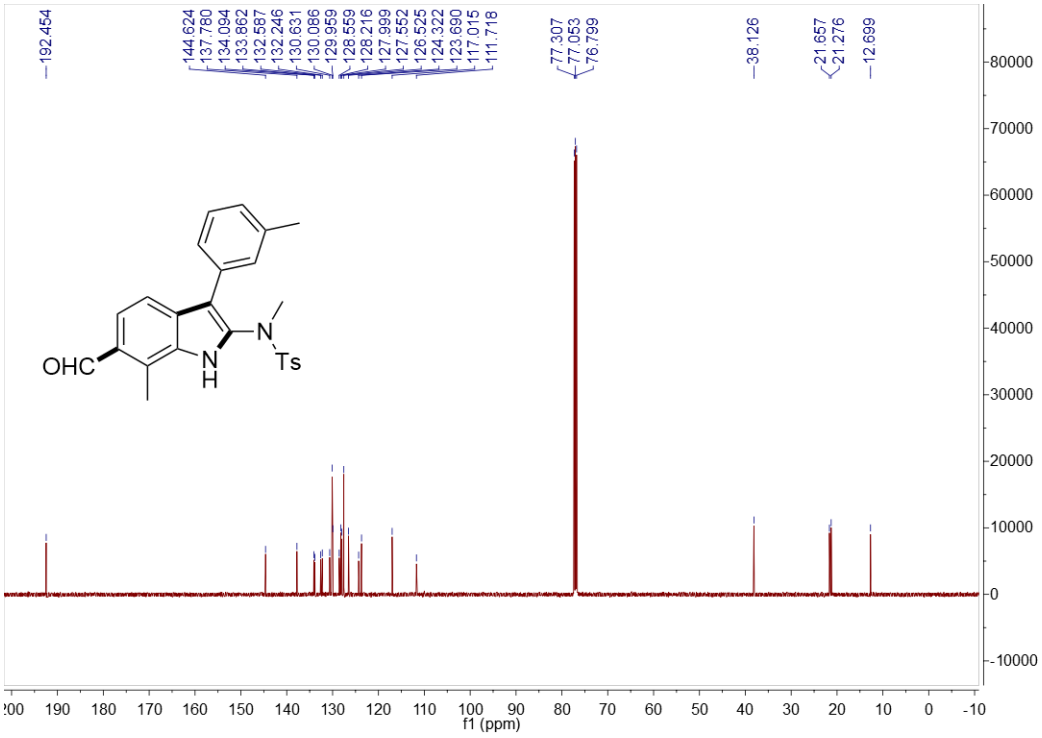
^{13}C NMR of compound **3u** in DMSO-d_6



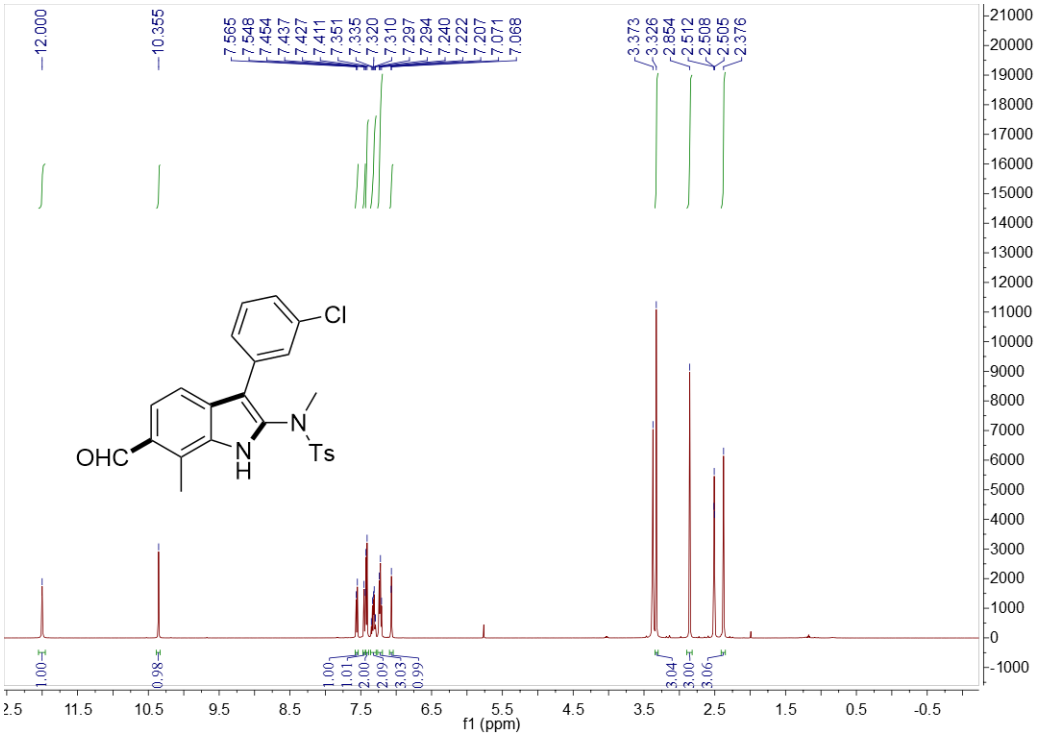
^{1}H NMR of compound **3v** in $CDCl_3$



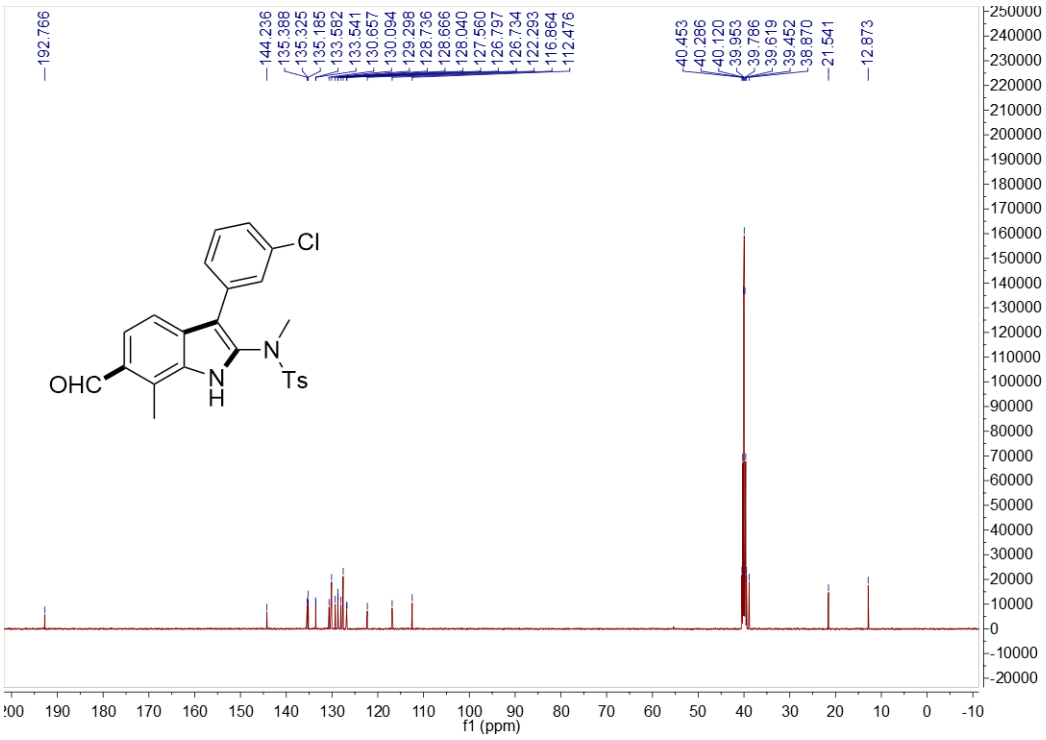
^{13}C NMR of compound **3v** in $CDCl_3$



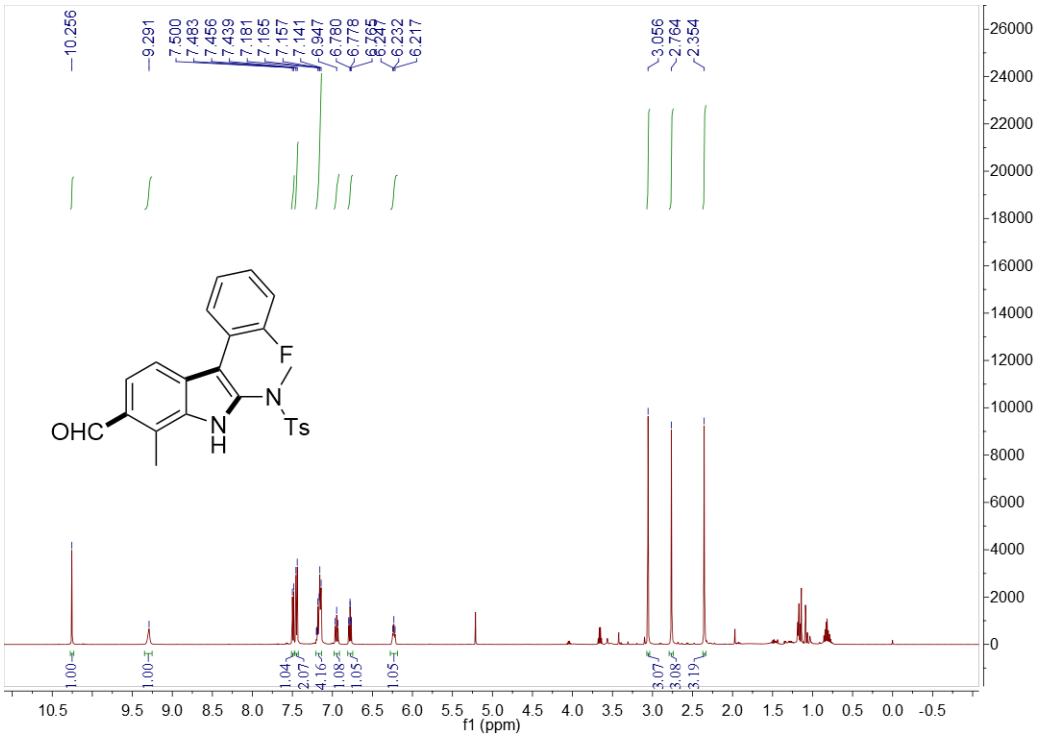
^{1}H NMR of compound **3w** in DMSO-d_6



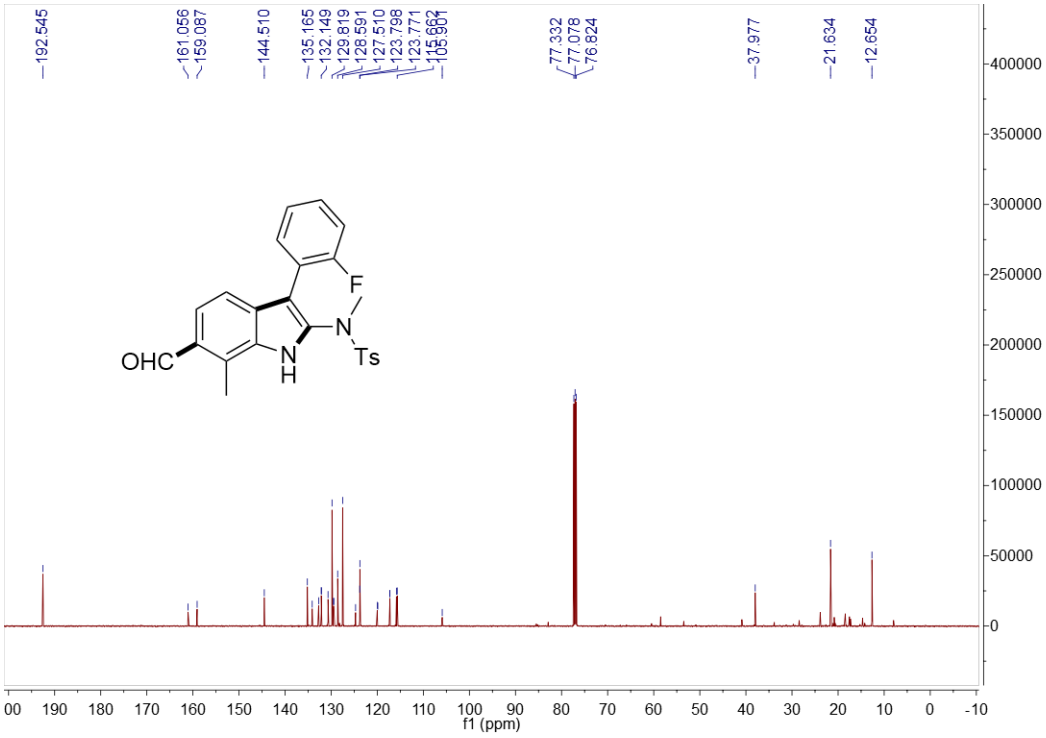
^{13}C NMR of compound **3w** in DMSO-d_6



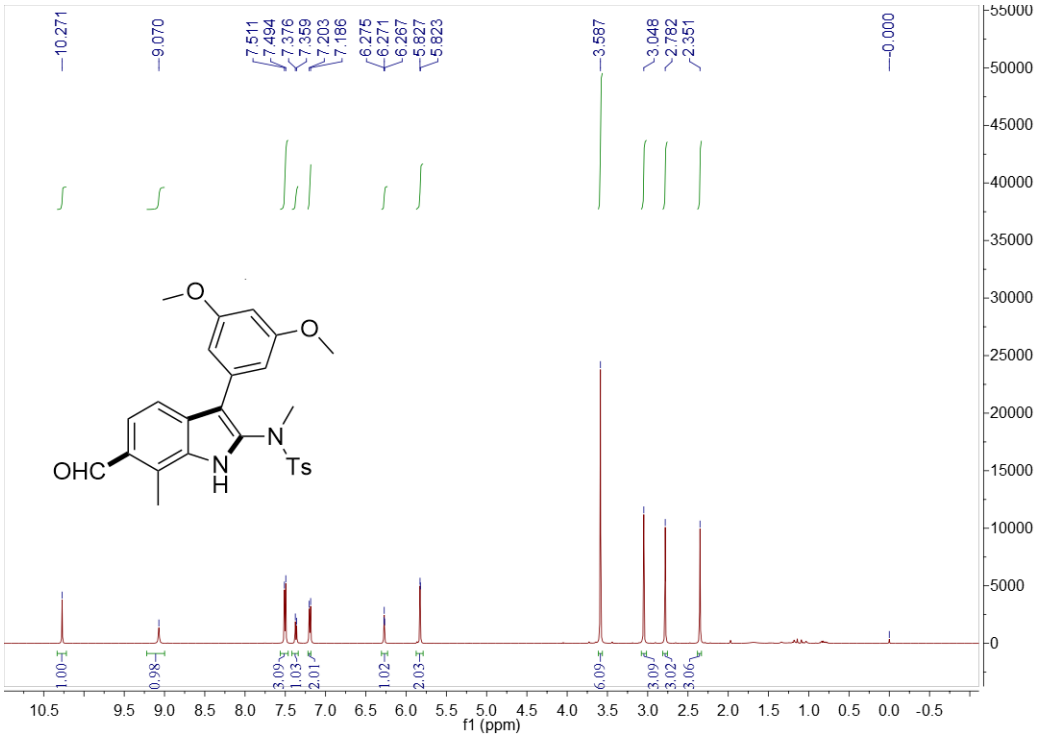
^{1}H NMR of compound **3x** in $CDCl_3$



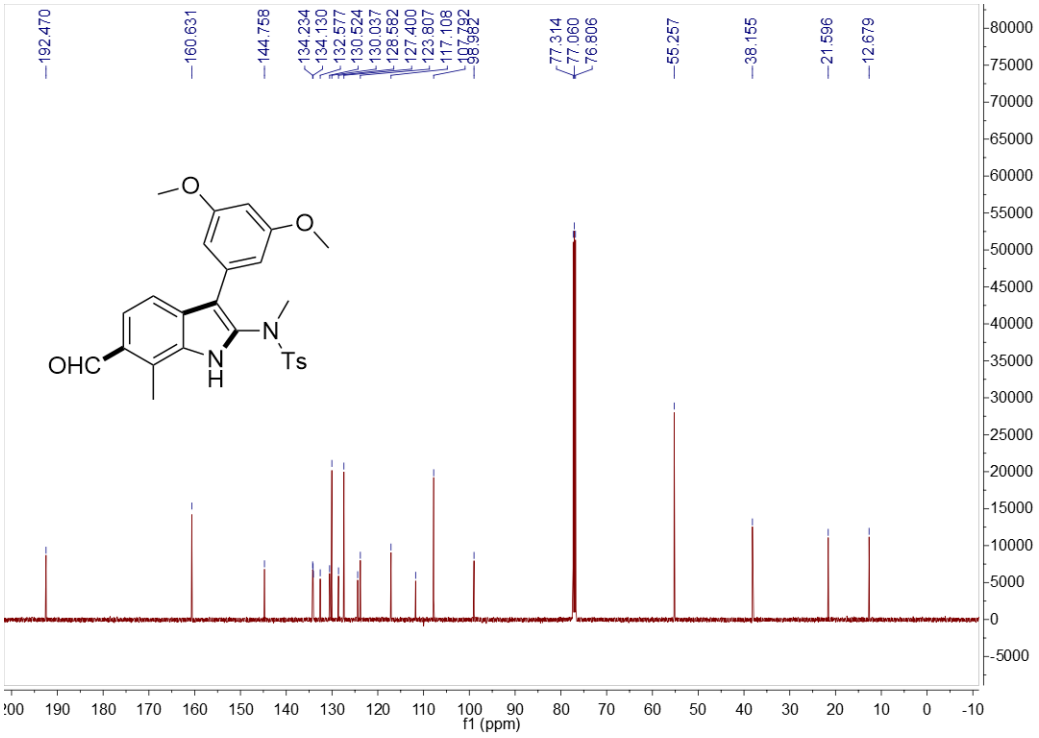
^{13}C NMR of compound **3x** in $CDCl_3$



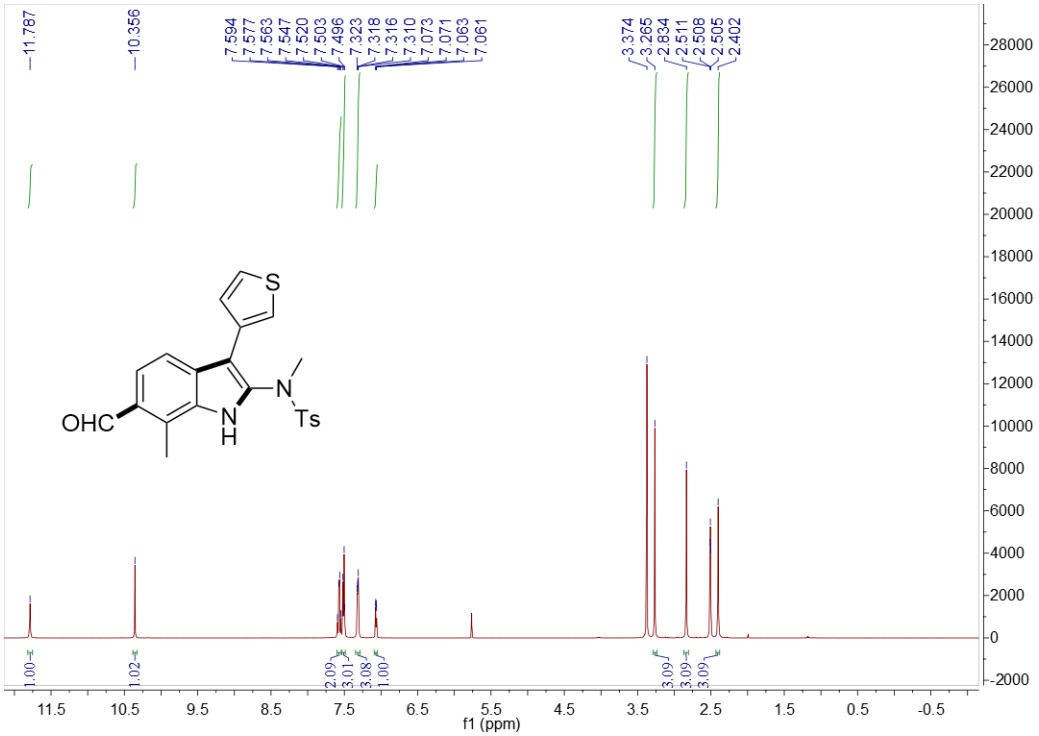
^{1}H NMR of compound **3y** in $CDCl_3$



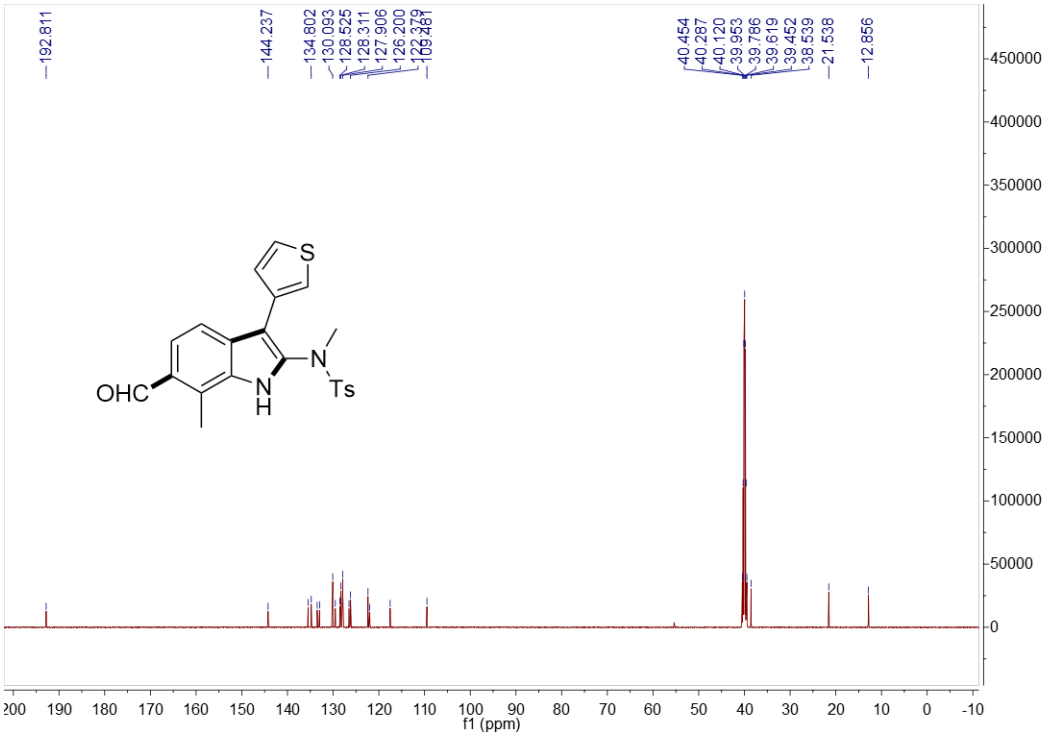
^{13}C NMR of compound **3y** in $CDCl_3$



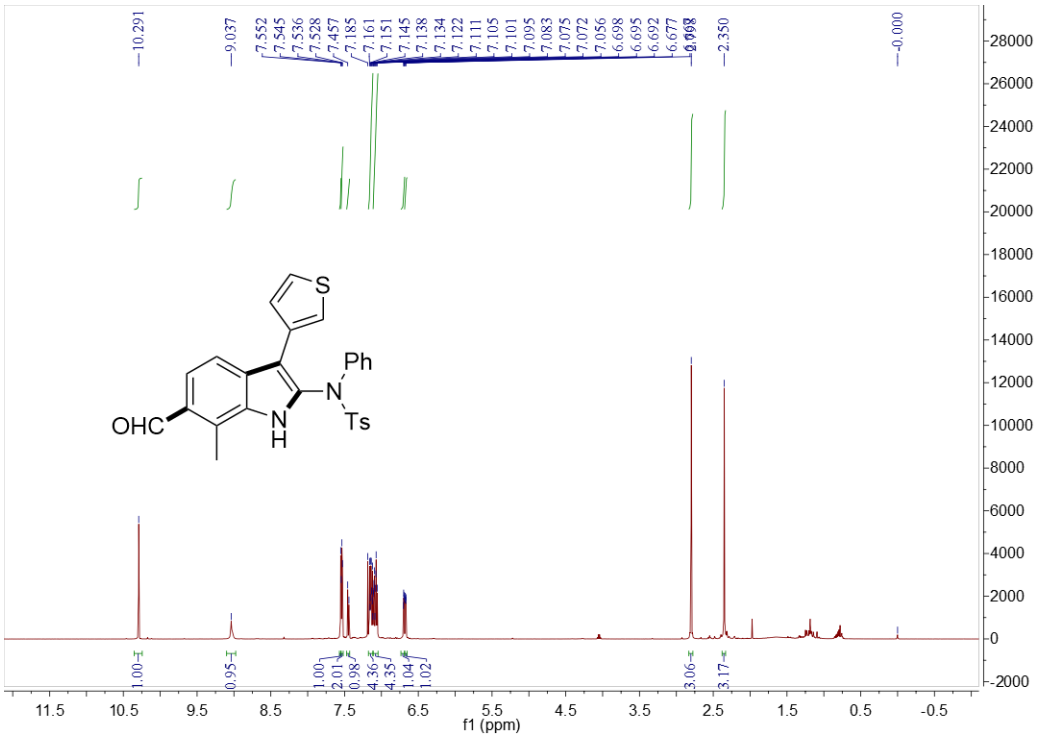
^{1}H NMR of compound **3z** in DMSO-d_6



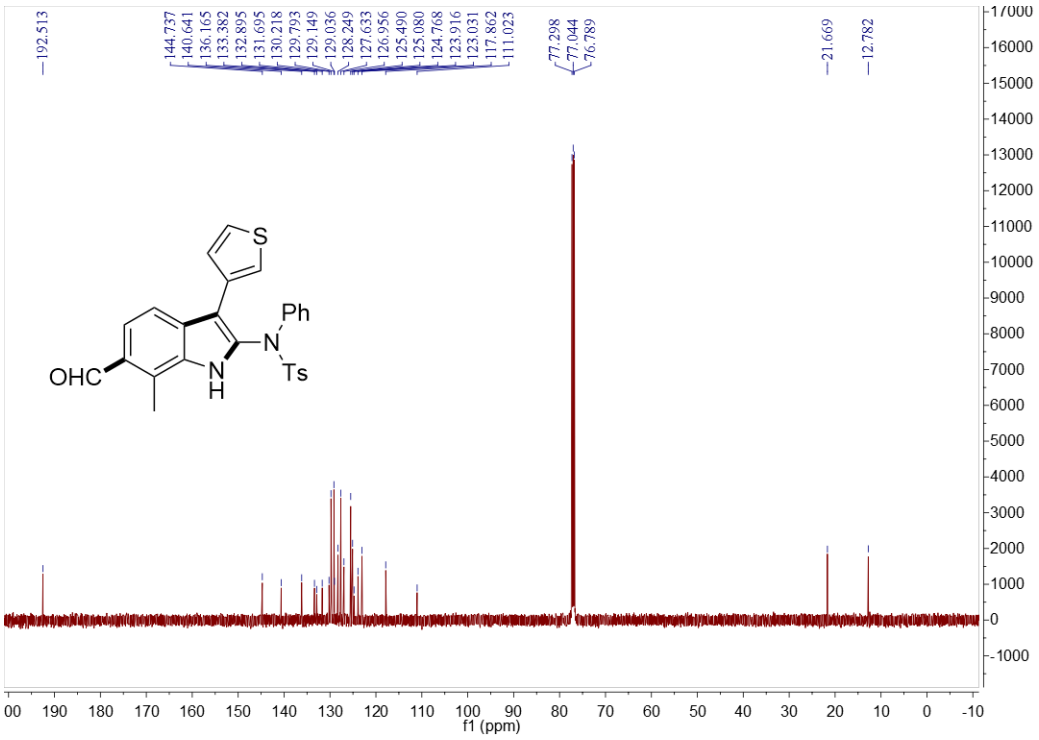
^{13}C NMR of compound **3z** in DMSO-d_6



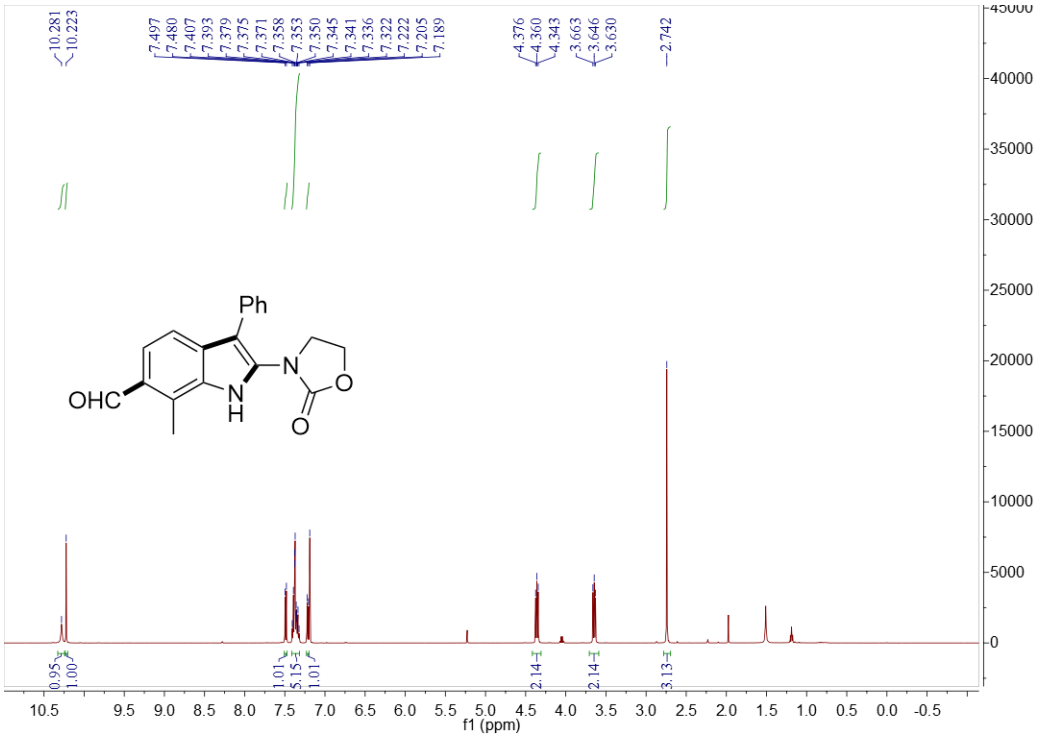
^{1}H NMR of compound **3aa** in $CDCl_3$



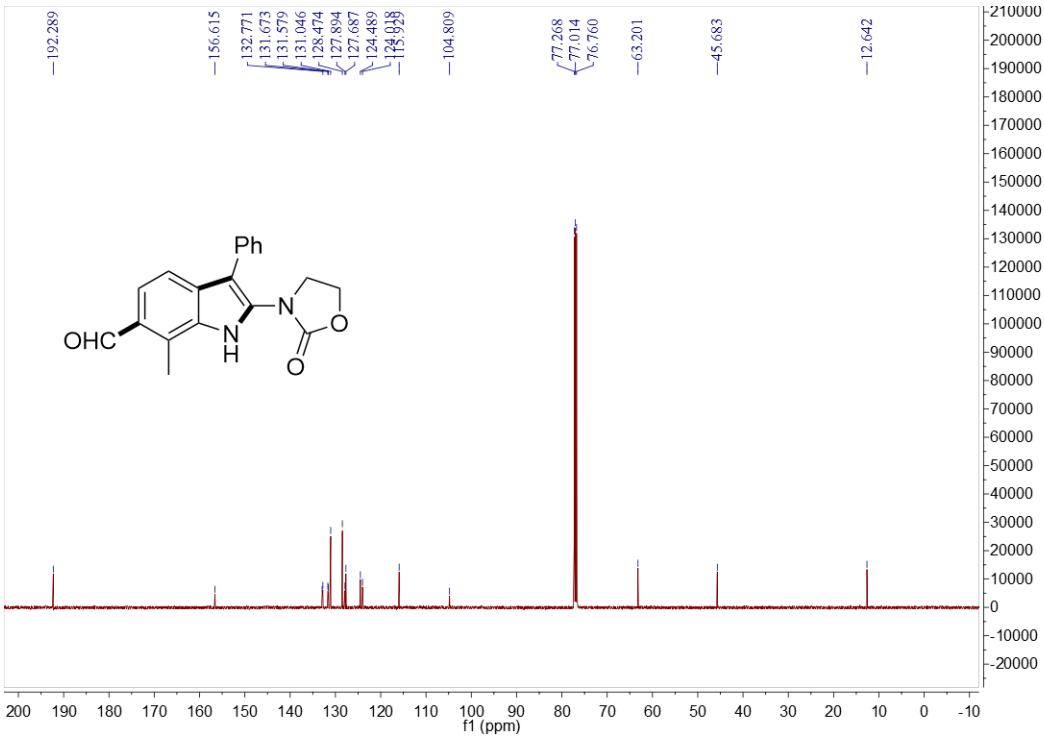
^{13}C NMR of compound **3aa** in $CDCl_3$



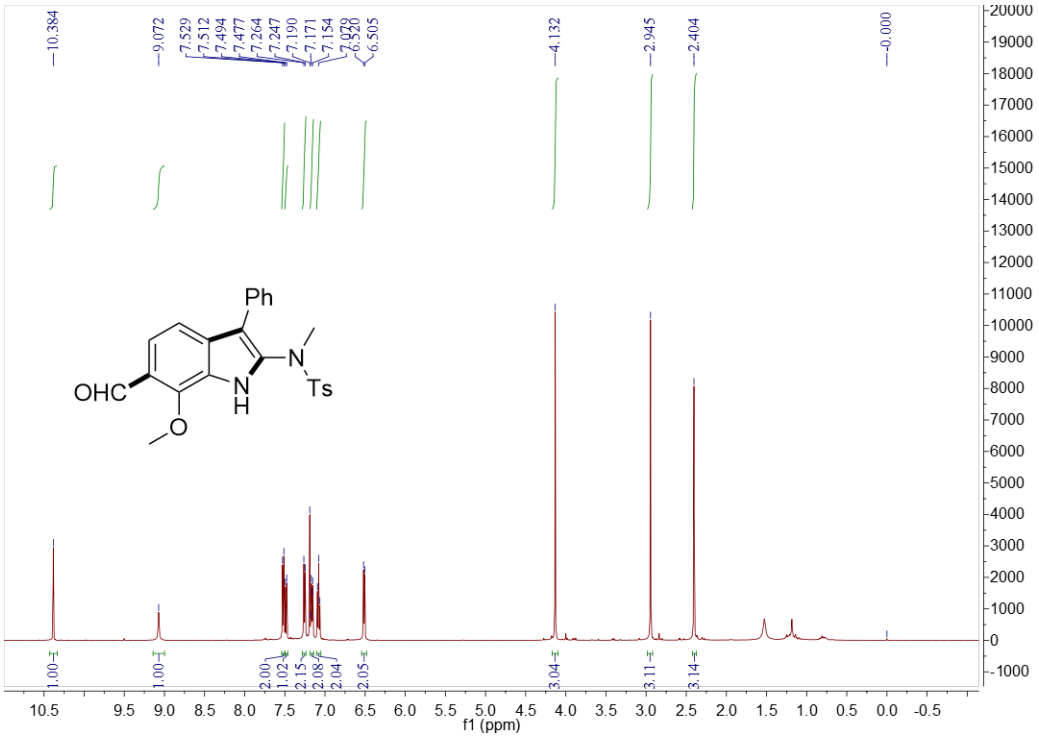
^{1}H NMR of compound **3ab** in $CDCl_3$



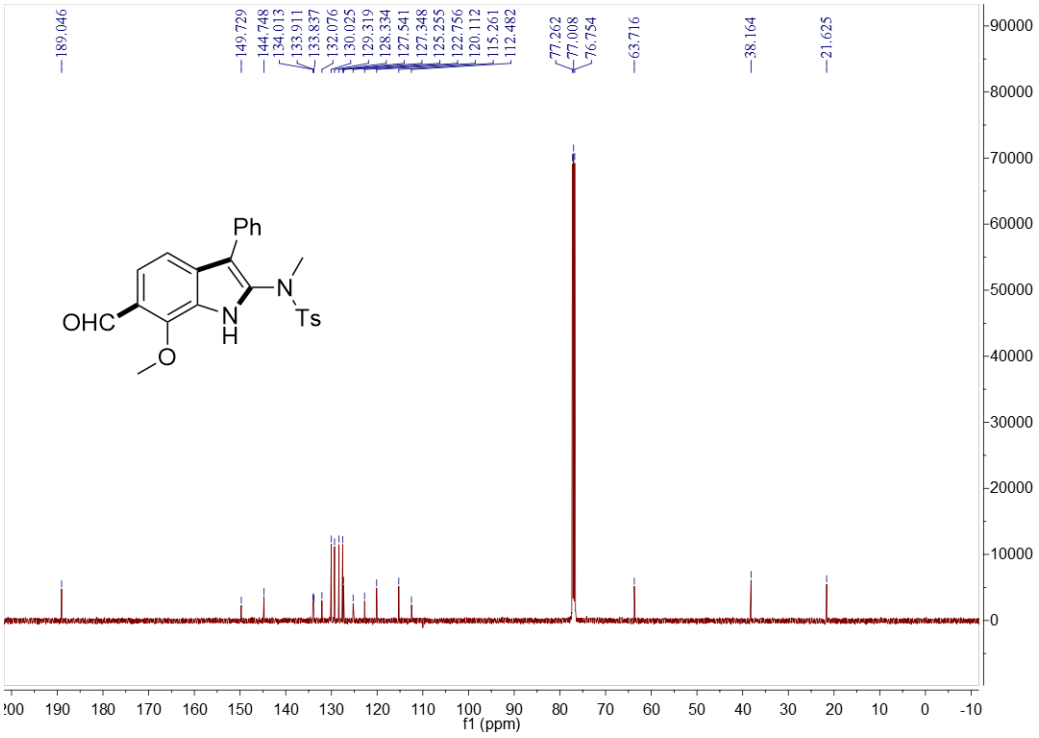
^{13}C NMR of compound **3ab** in $CDCl_3$



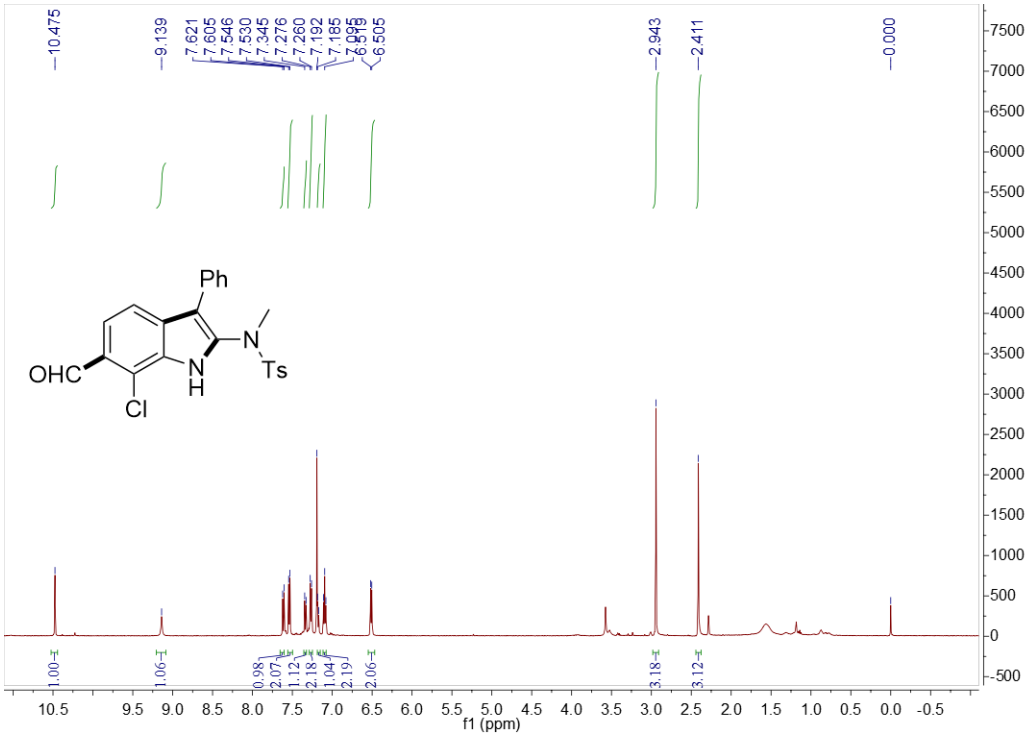
^{1}H NMR of compound **3ac** in $CDCl_3$



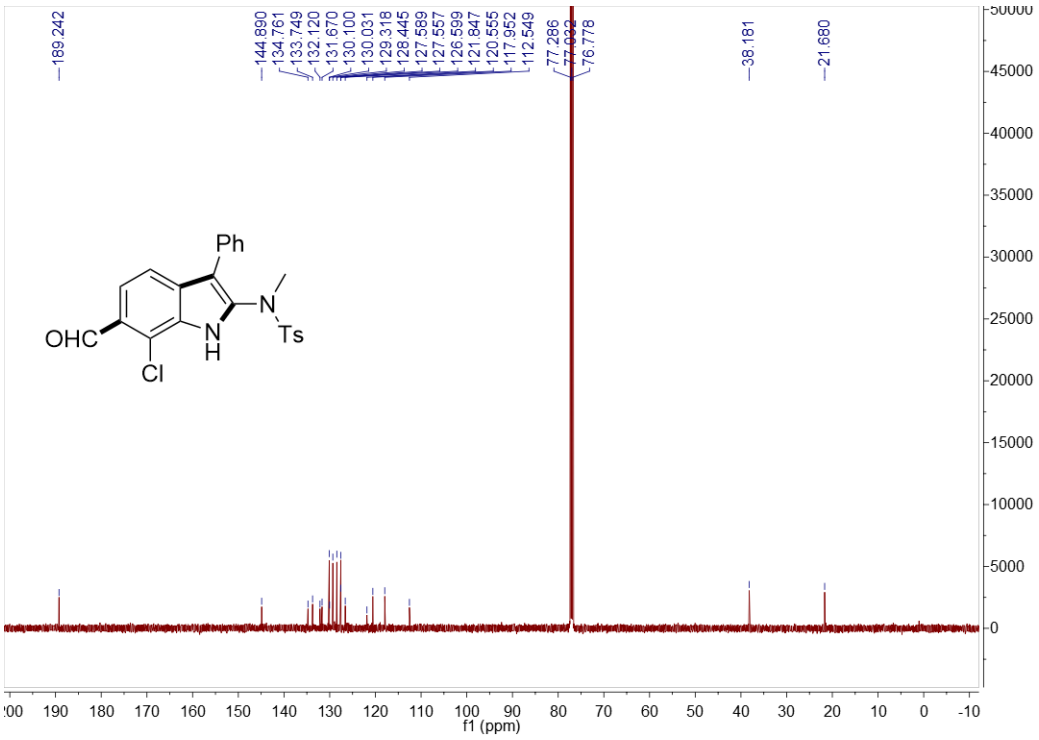
^{13}C NMR of compound **3ac** in $CDCl_3$



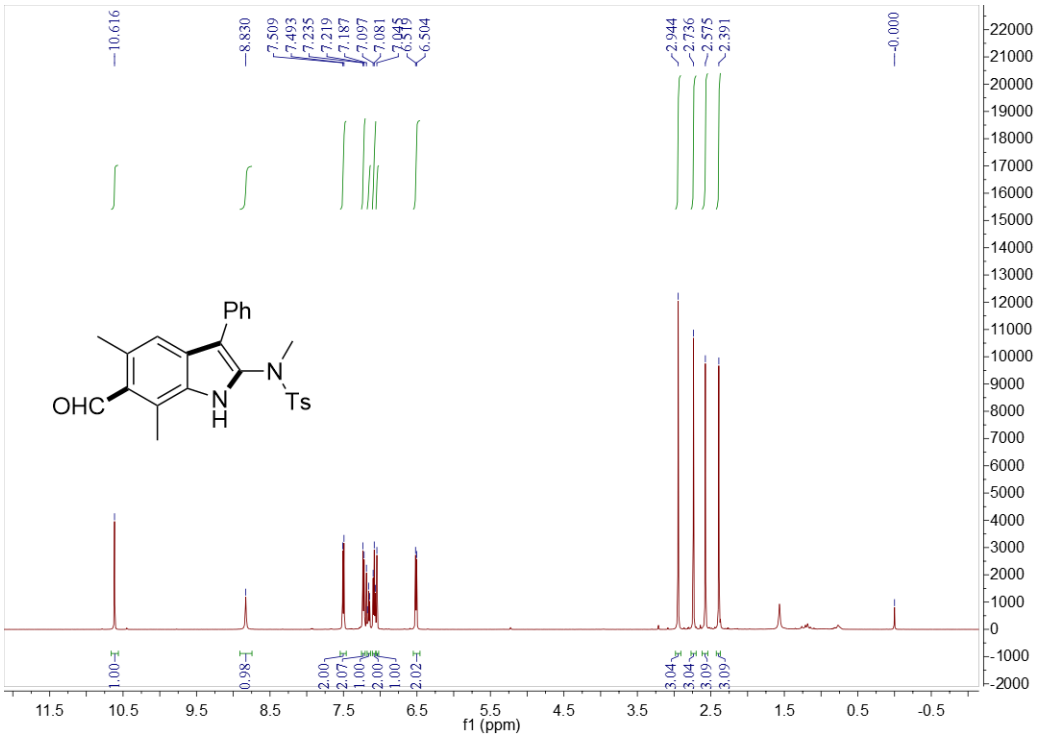
^{1}H NMR of compound **3ad** in $CDCl_3$



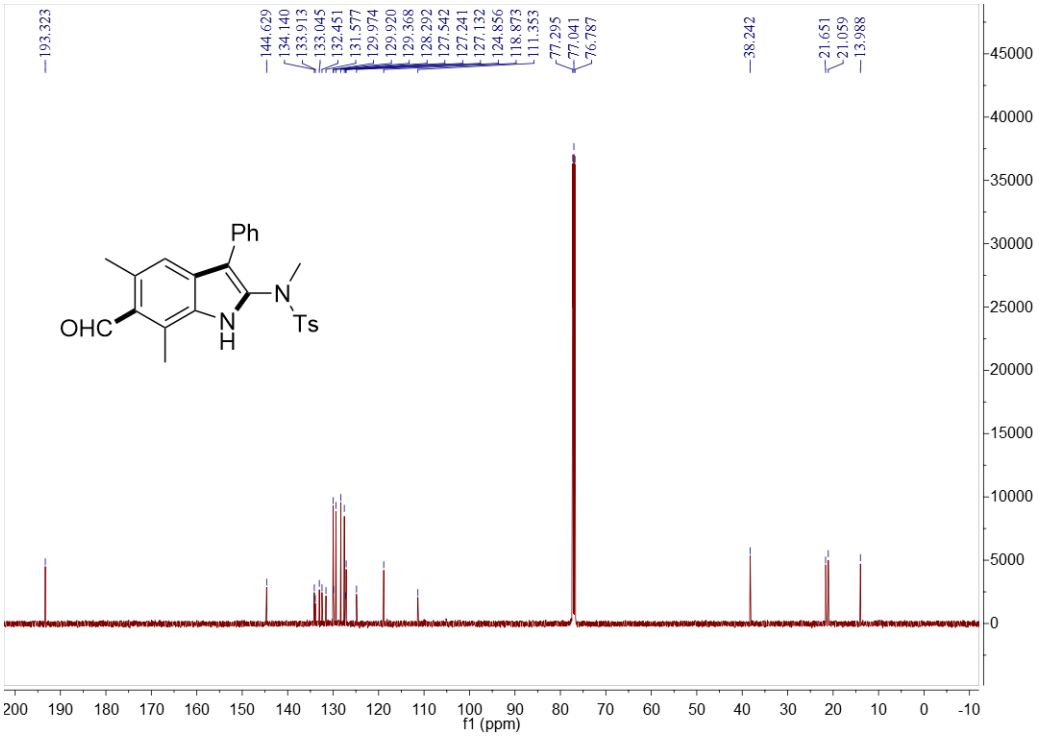
^{13}C NMR of compound **3ad** in $CDCl_3$



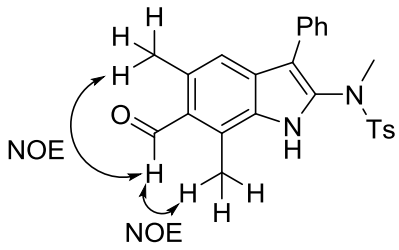
^{1}H NMR of compound **3ae** in $CDCl_3$

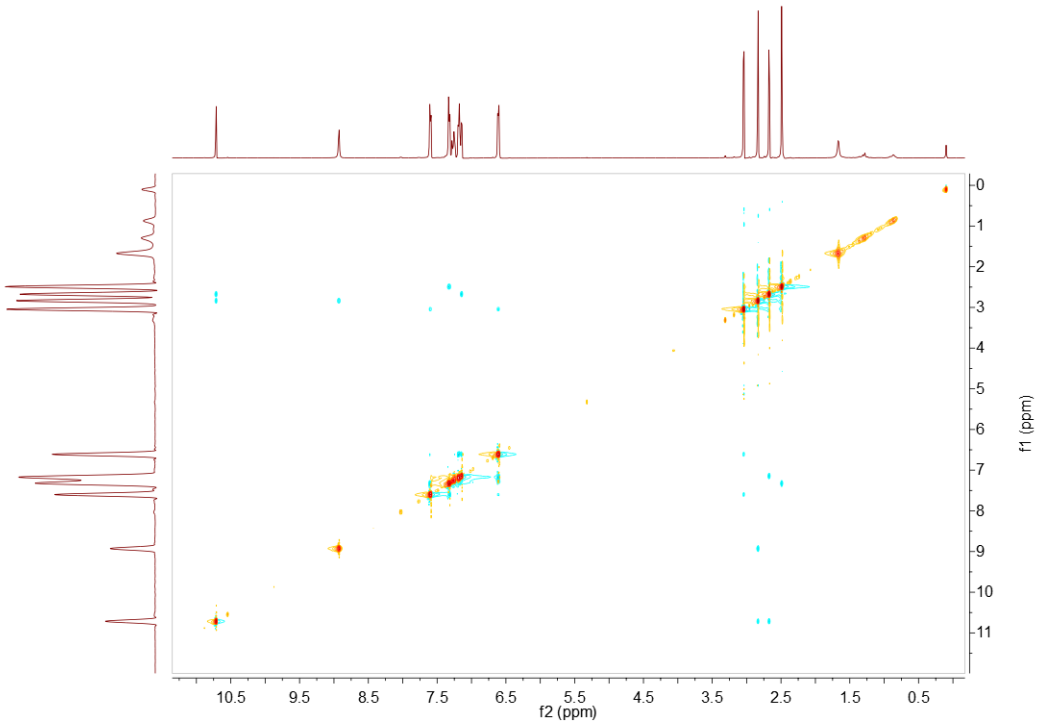


^{13}C NMR of compound **3ae** in $CDCl_3$

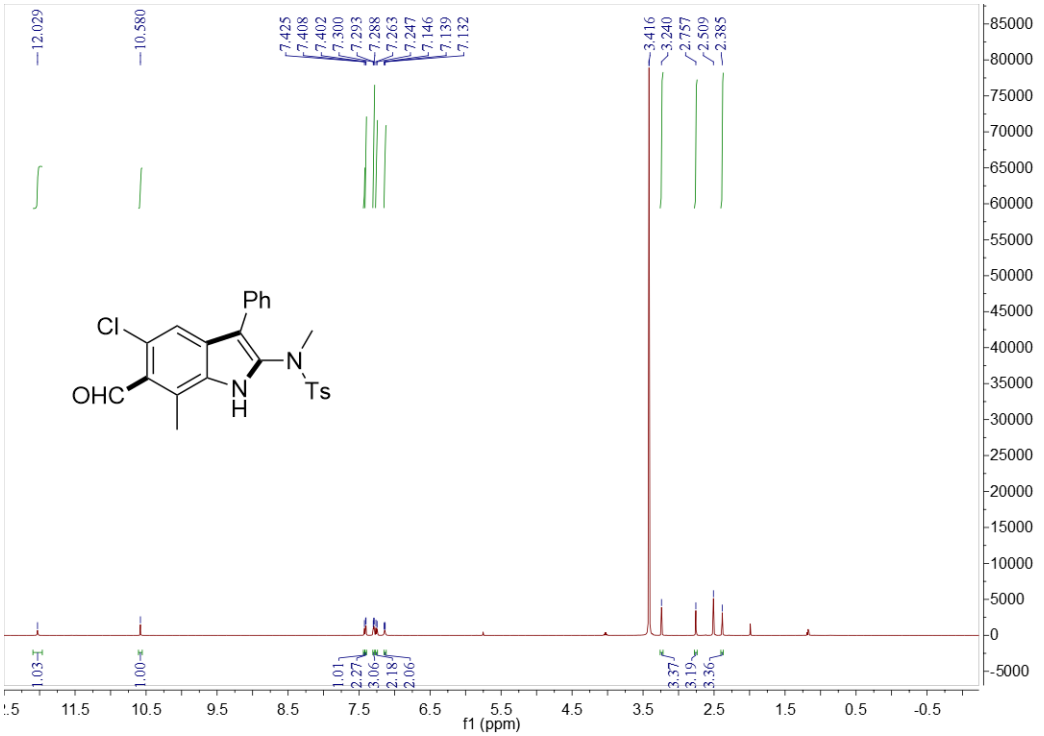


2D NOESY of **3ae** in $CDCl_3$

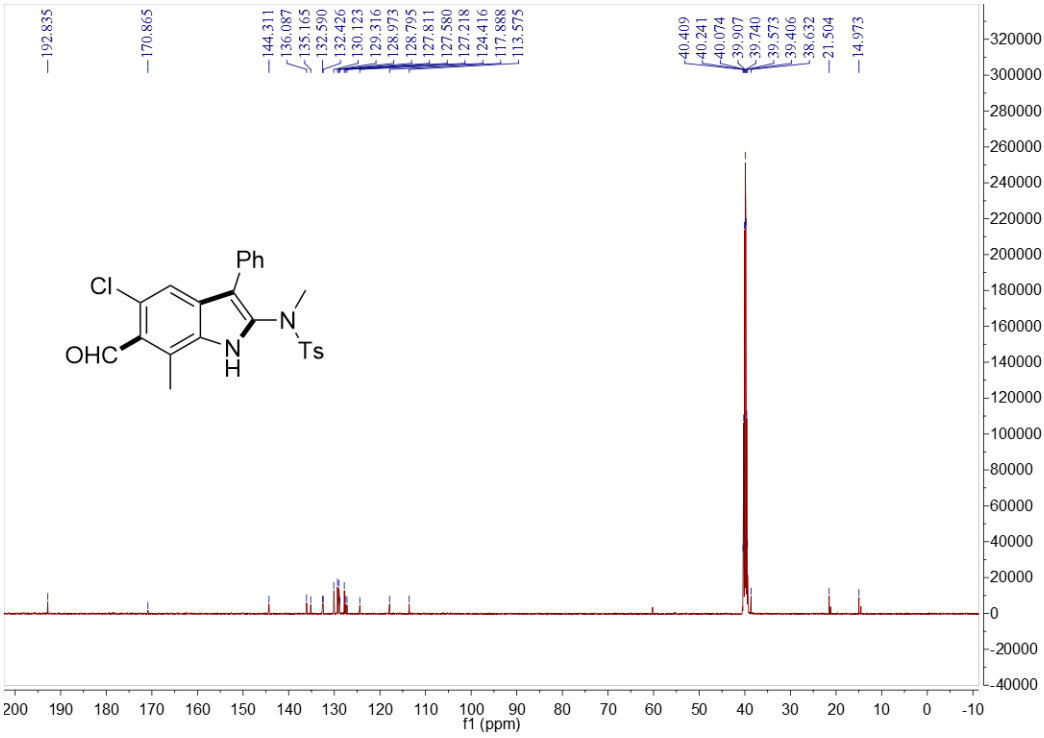




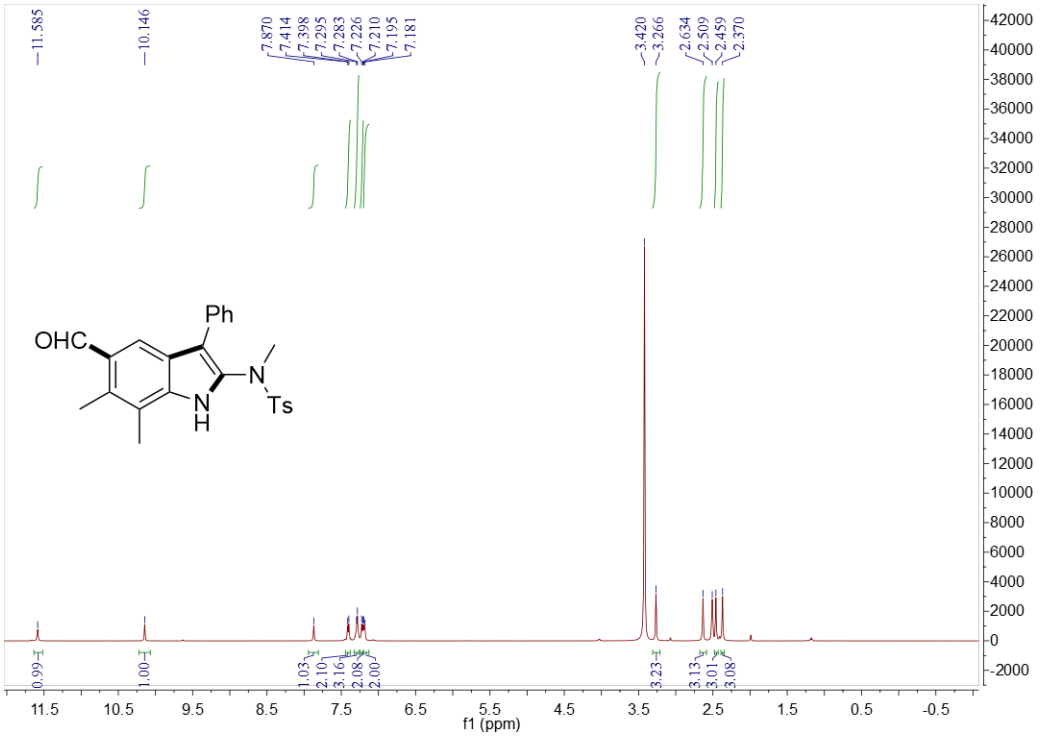
^{1}H NMR of compound **3af** in DMSO-d_6



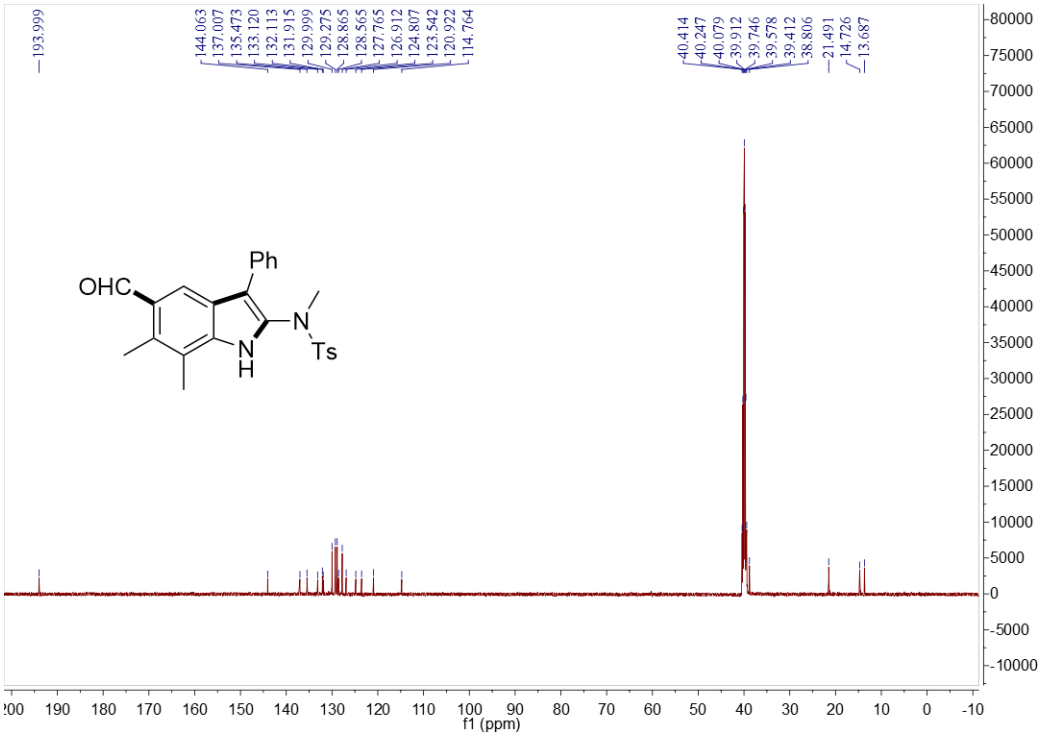
^{13}C NMR of compound **3af** in DMSO-d_6



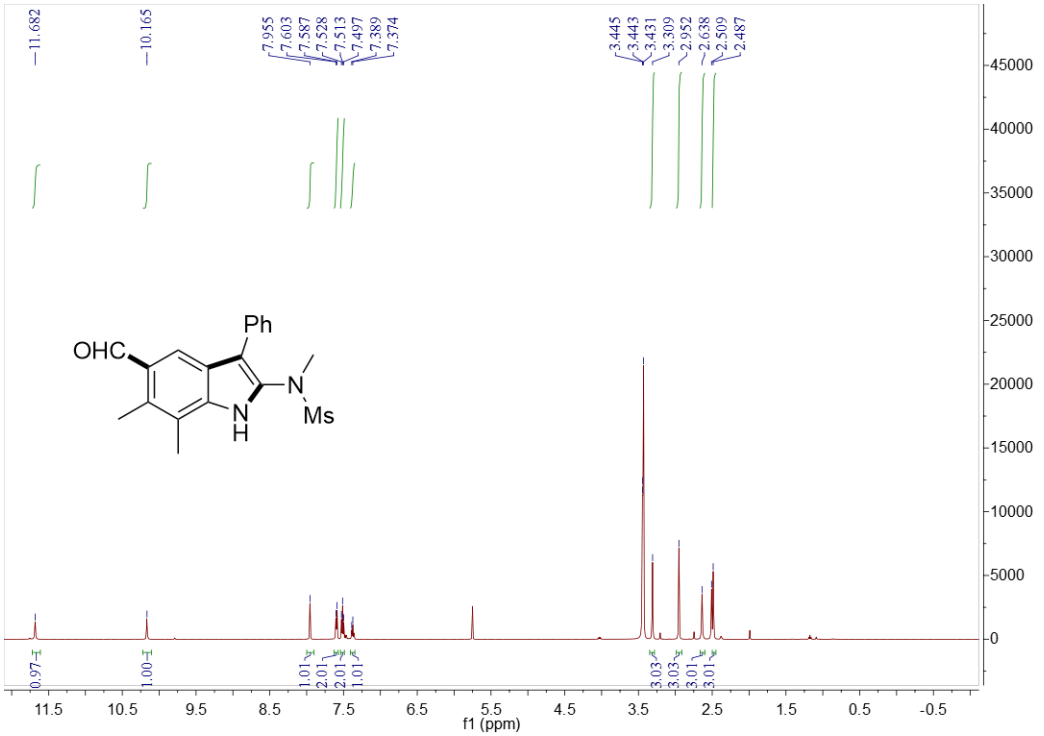
^{1}H NMR of compound **4a** in DMSO-d_6



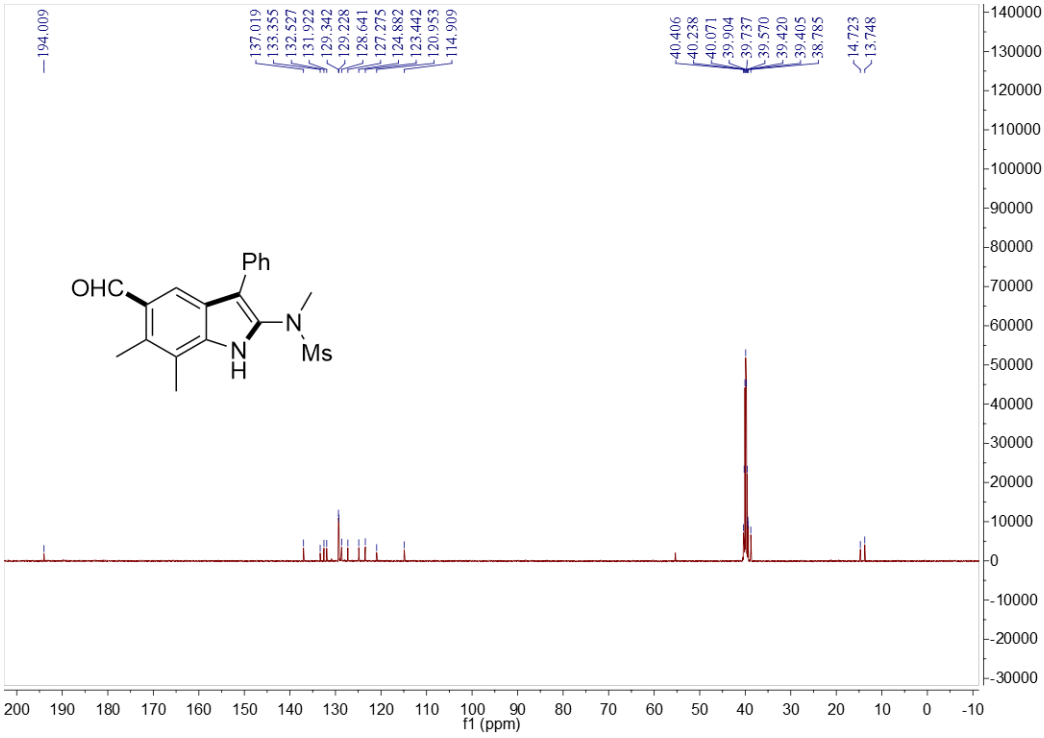
^{13}C NMR of compound **4a** in DMSO-d_6



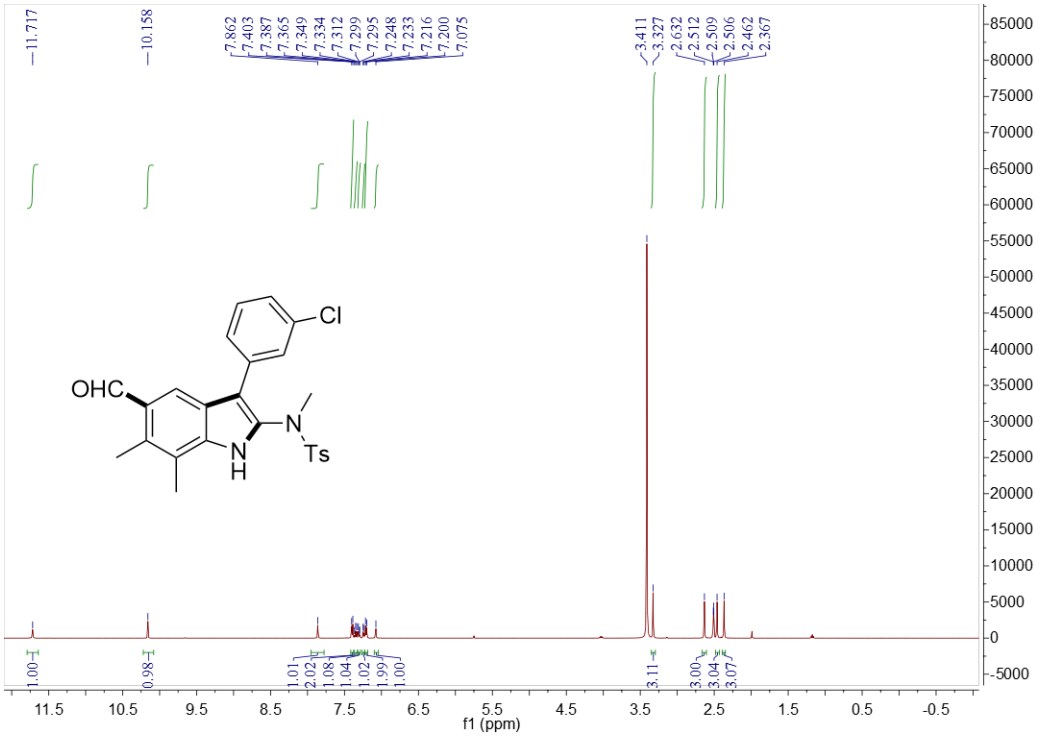
^{1}H NMR of compound **4b** in DMSO-d_6



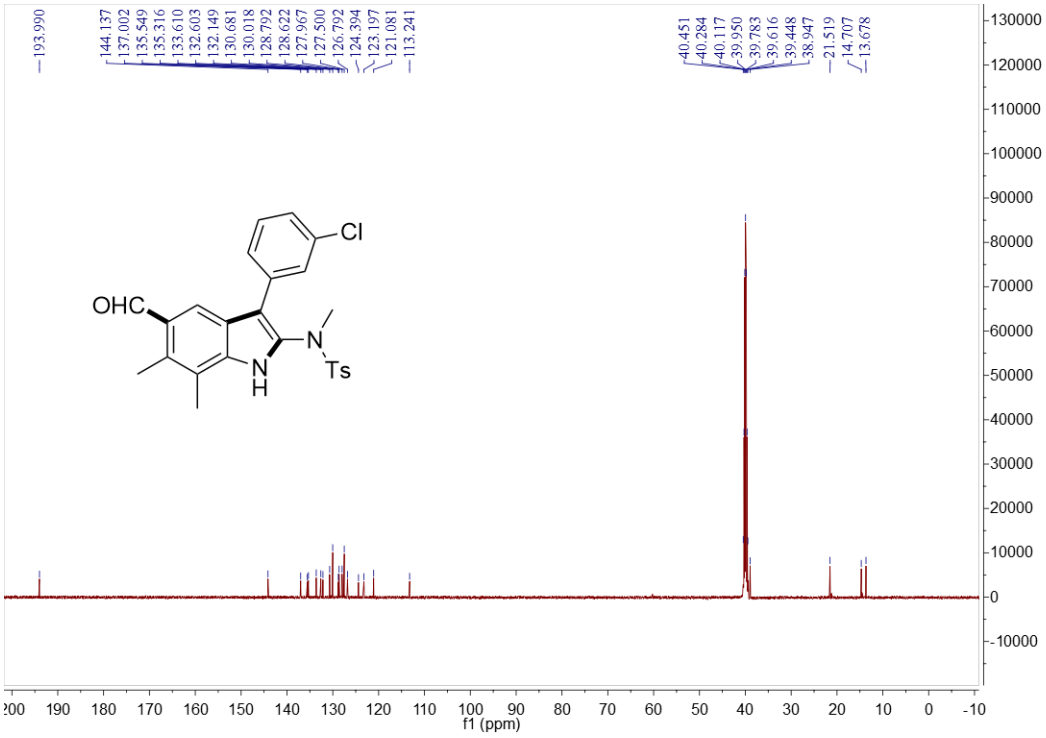
^{13}C NMR of compound **4b** in DMSO-d_6



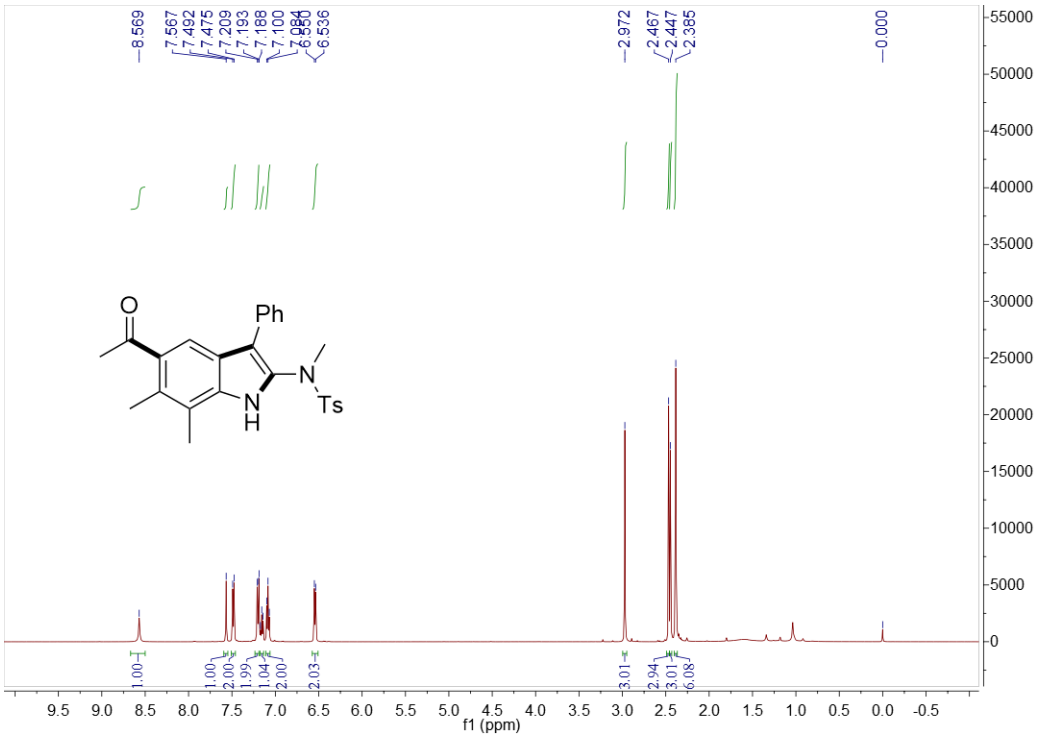
^{1}H NMR of compound **4c** in DMSO-d_6



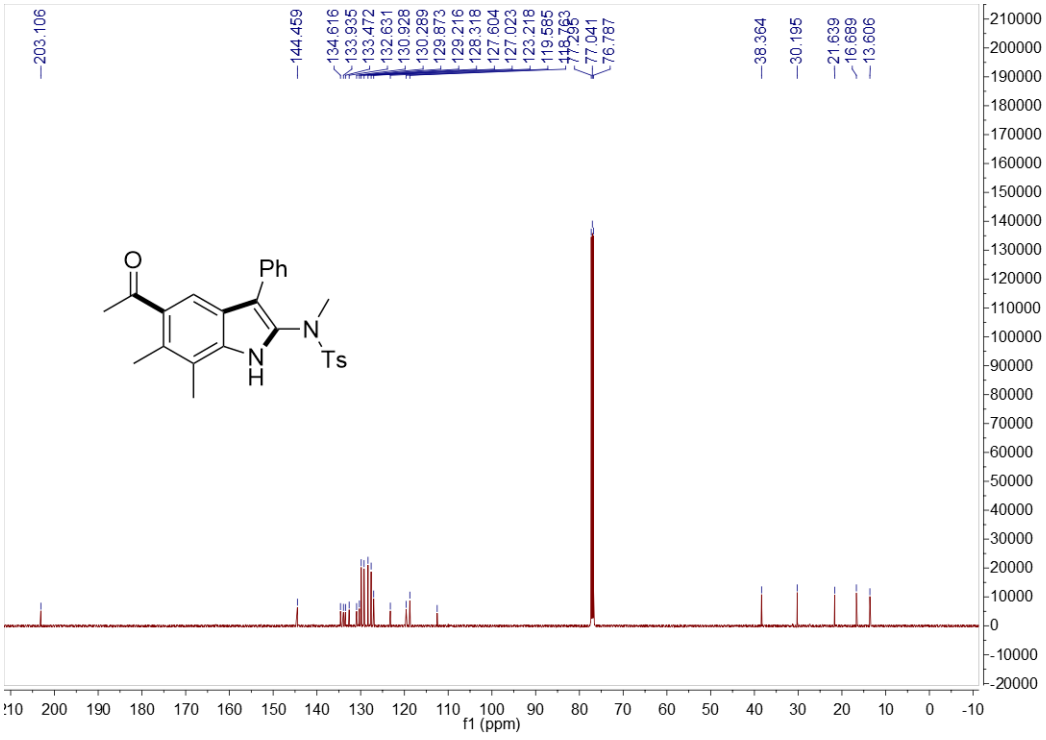
^{13}C NMR of compound **4c** in DMSO-d_6



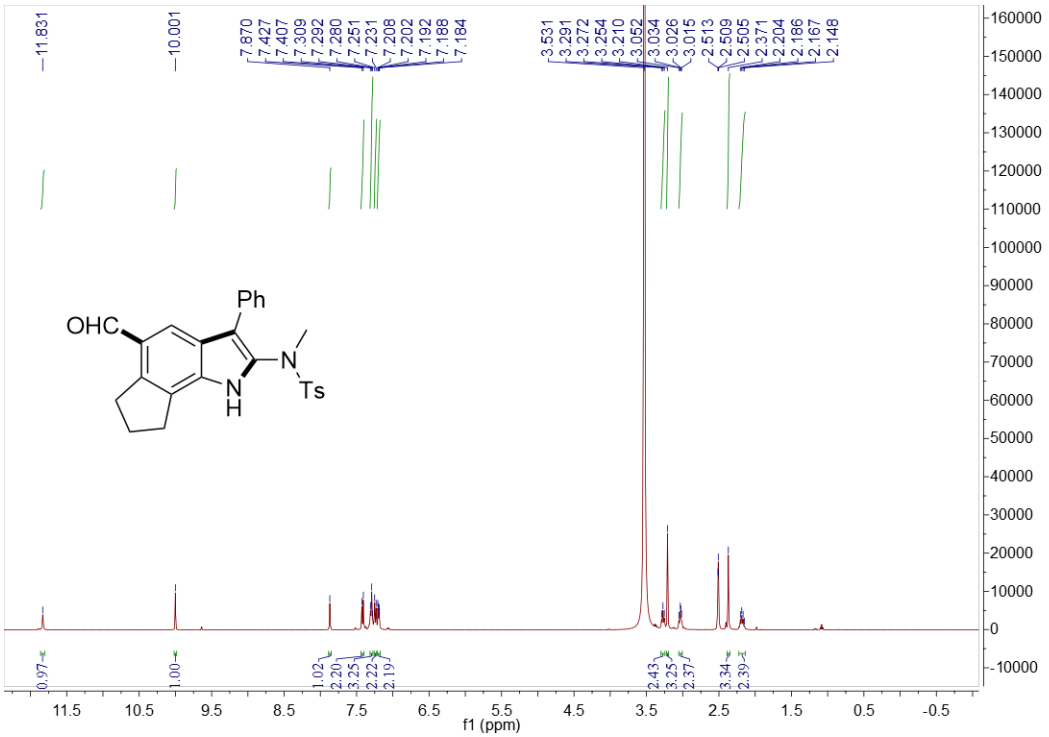
^{1}H NMR of compound **4d** in $CDCl_3$



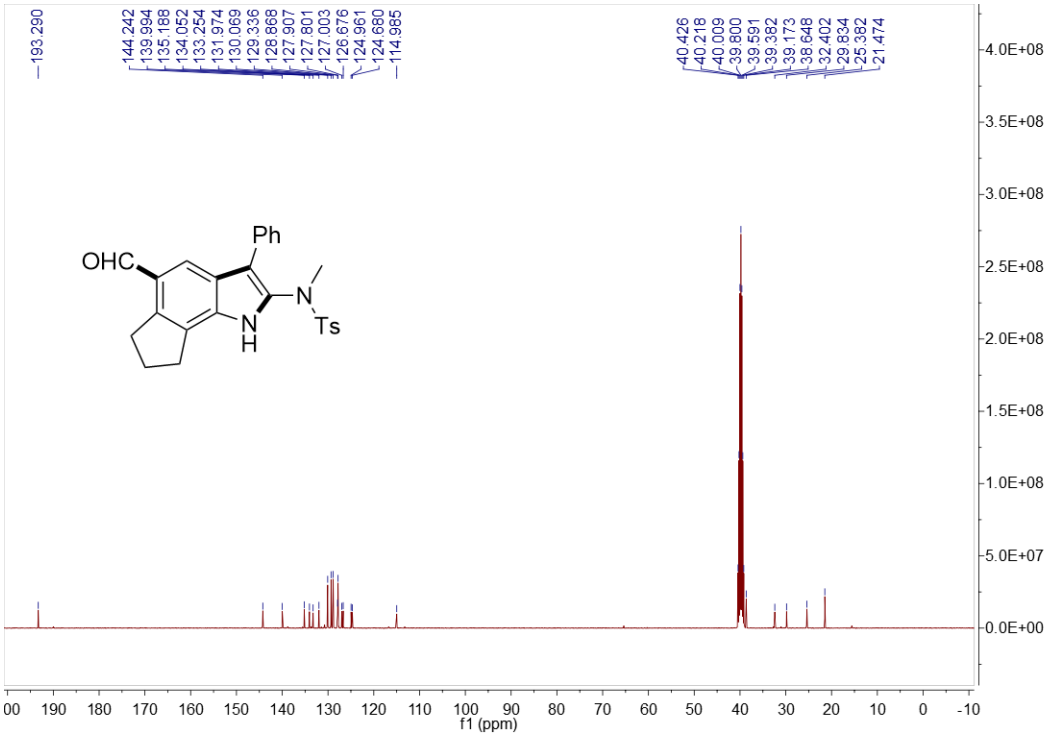
^{13}C NMR of compound **4d** in $CDCl_3$



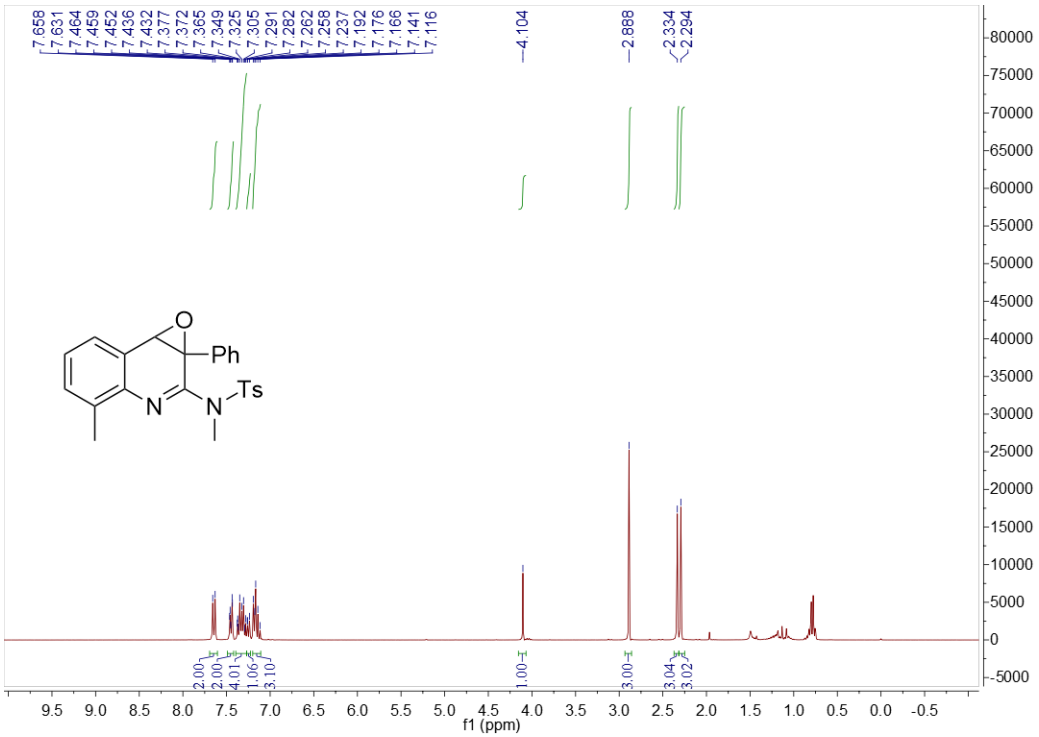
^{1}H NMR of compound **4e** in DMSO-d_6



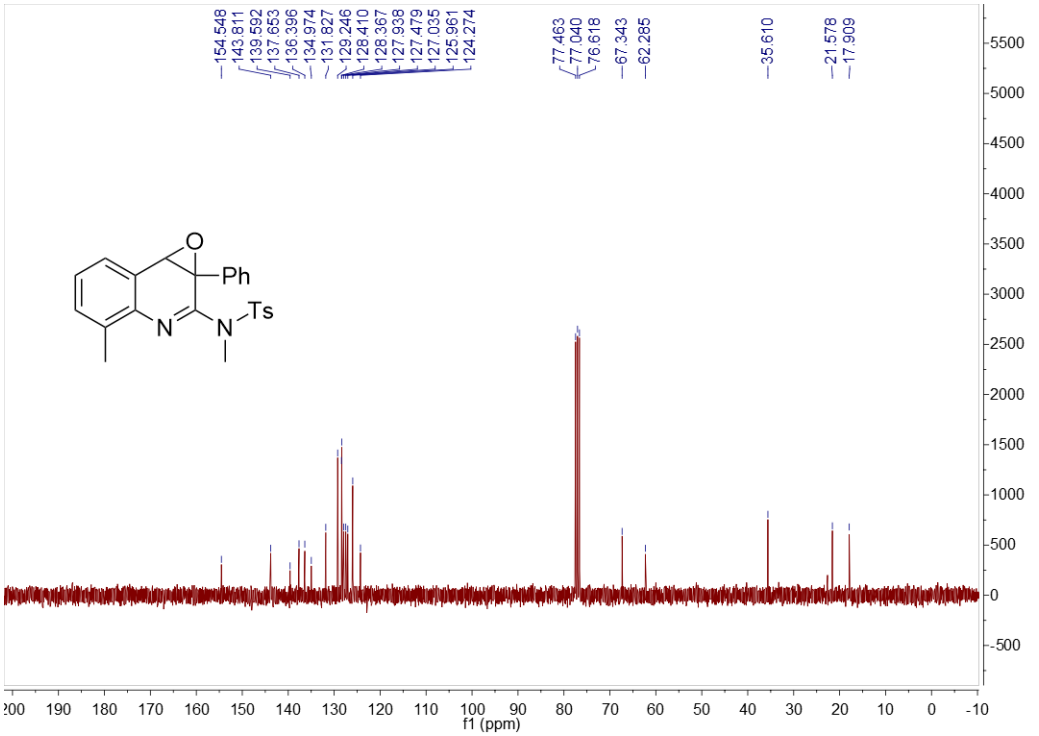
^{13}C NMR of compound **4e** in DMSO-d_6



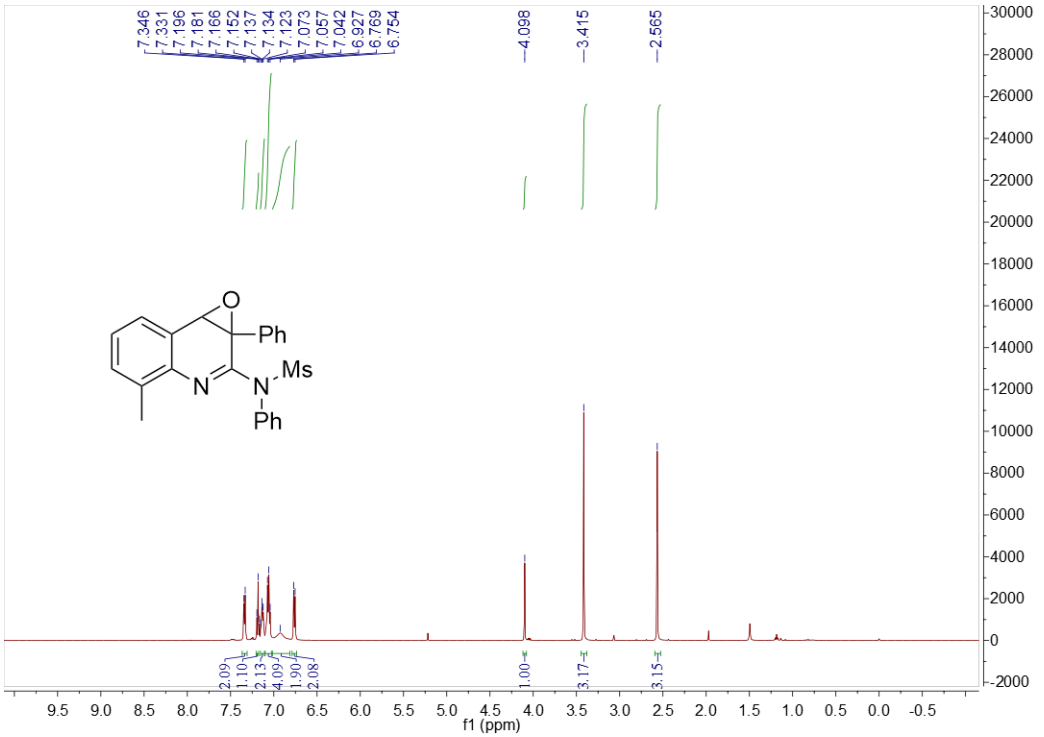
^{1}H NMR of compound **5a** in $CDCl_3$



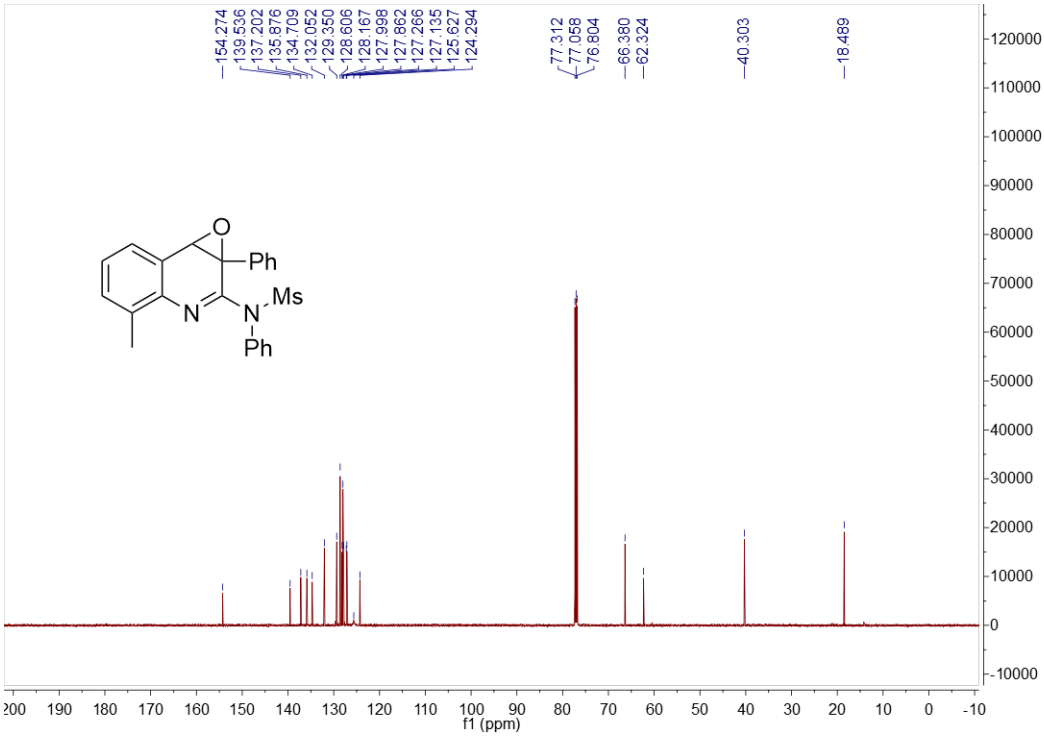
^{13}C NMR of compound **5a** in $CDCl_3$



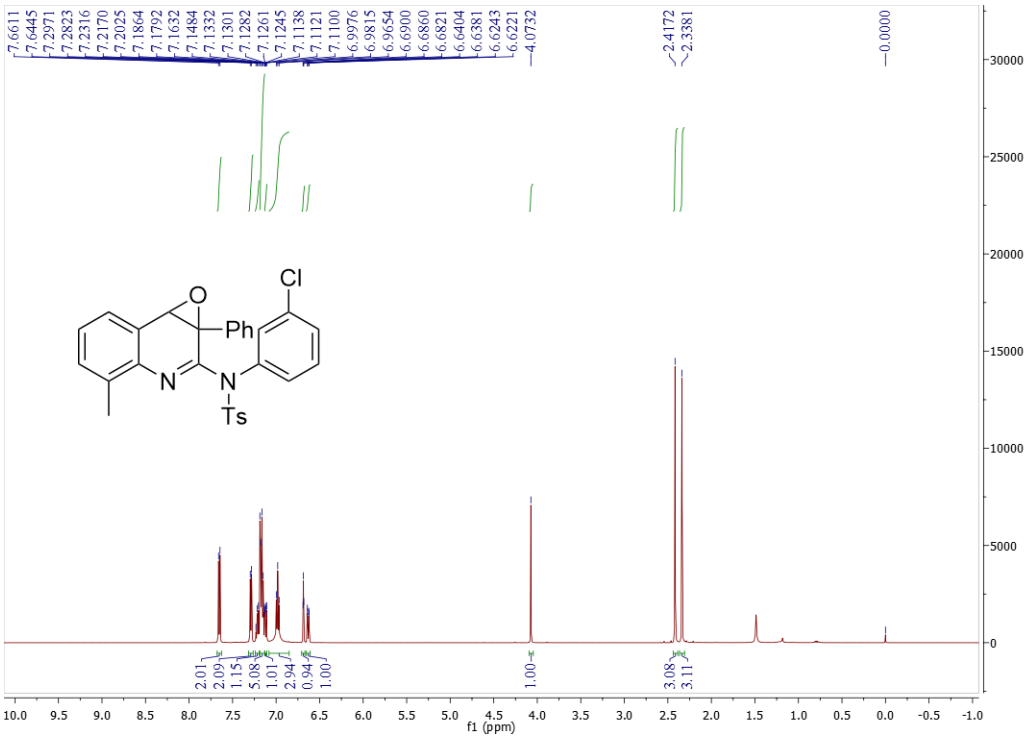
^{1}H NMR of compound **5b** in $CDCl_3$



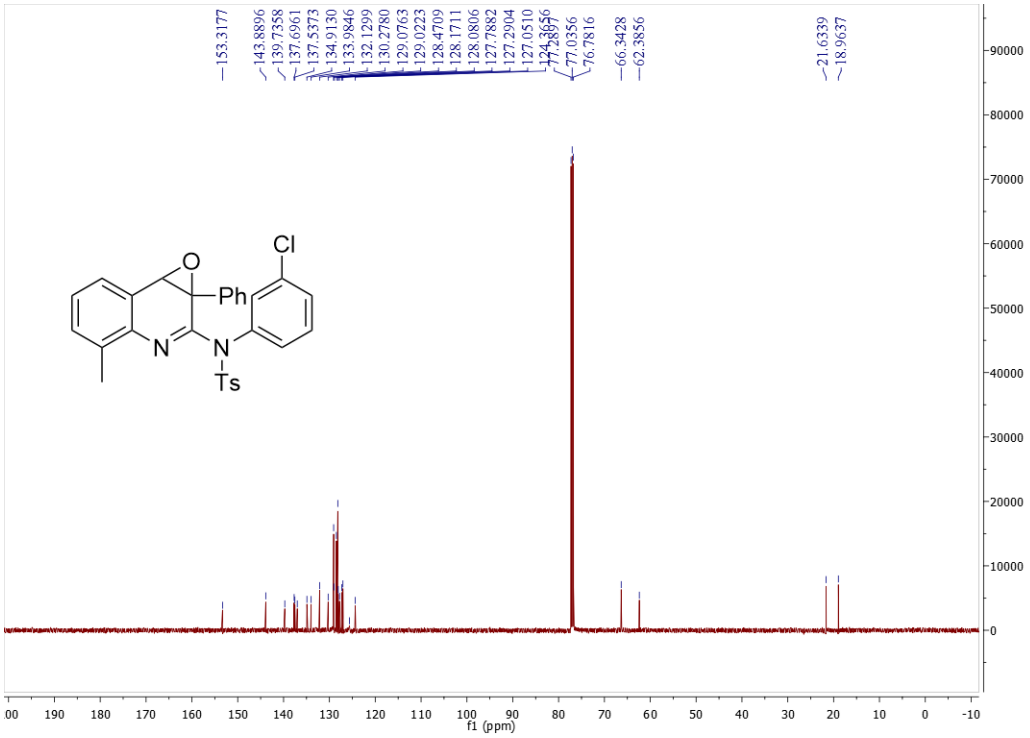
^{13}C NMR of compound **5b** in $CDCl_3$



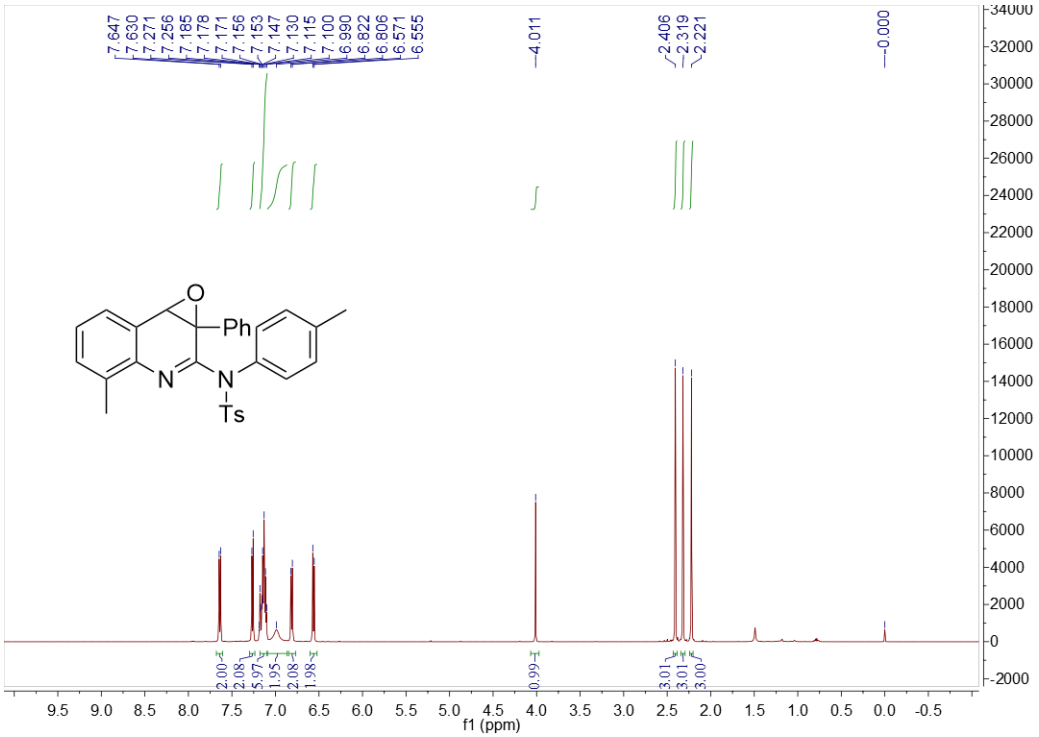
^{1}H NMR of compound **5c** in $CDCl_3$



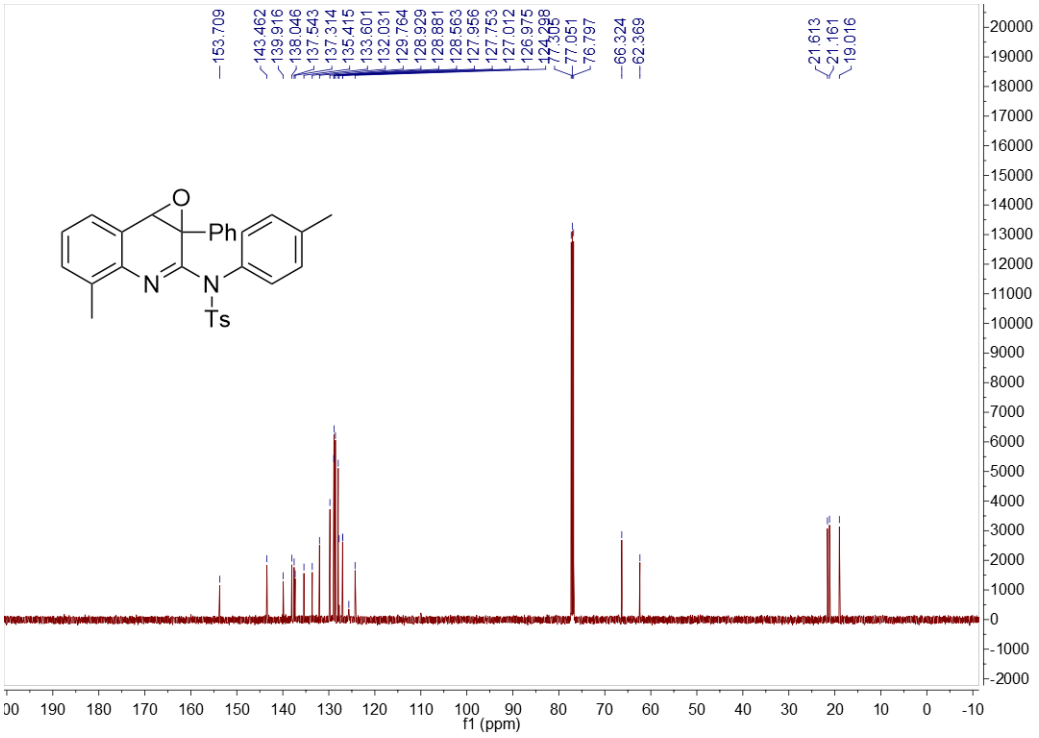
^{13}C NMR of compound **5c** in $CDCl_3$



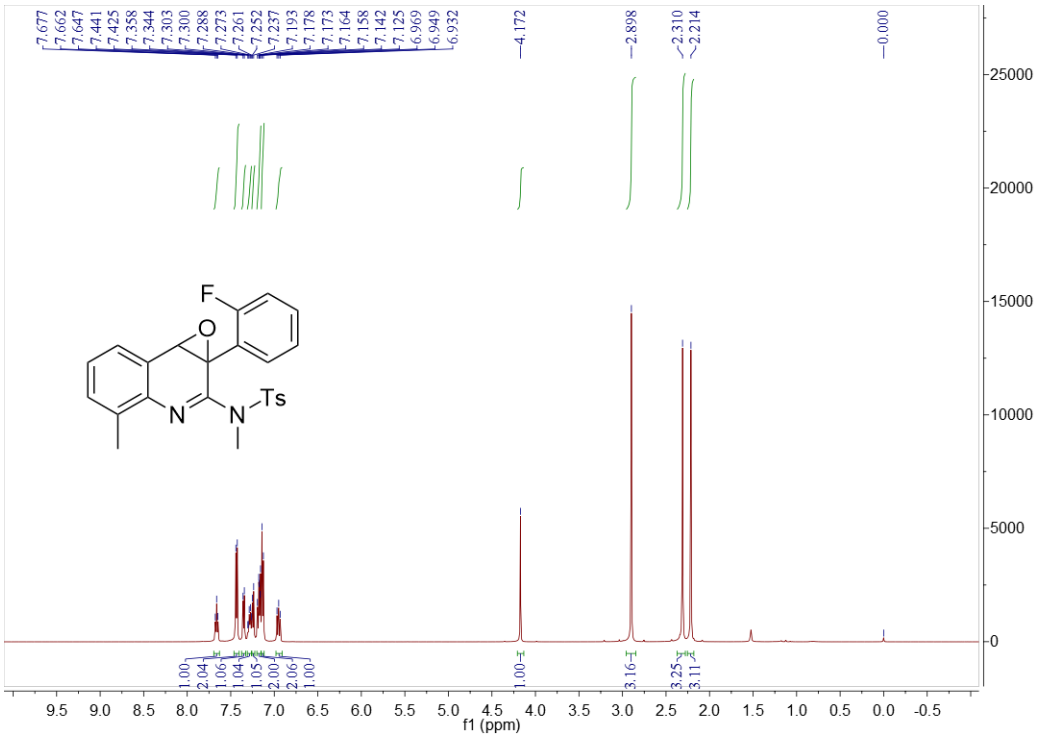
^{1}H NMR of compound **5e** in $CDCl_3$



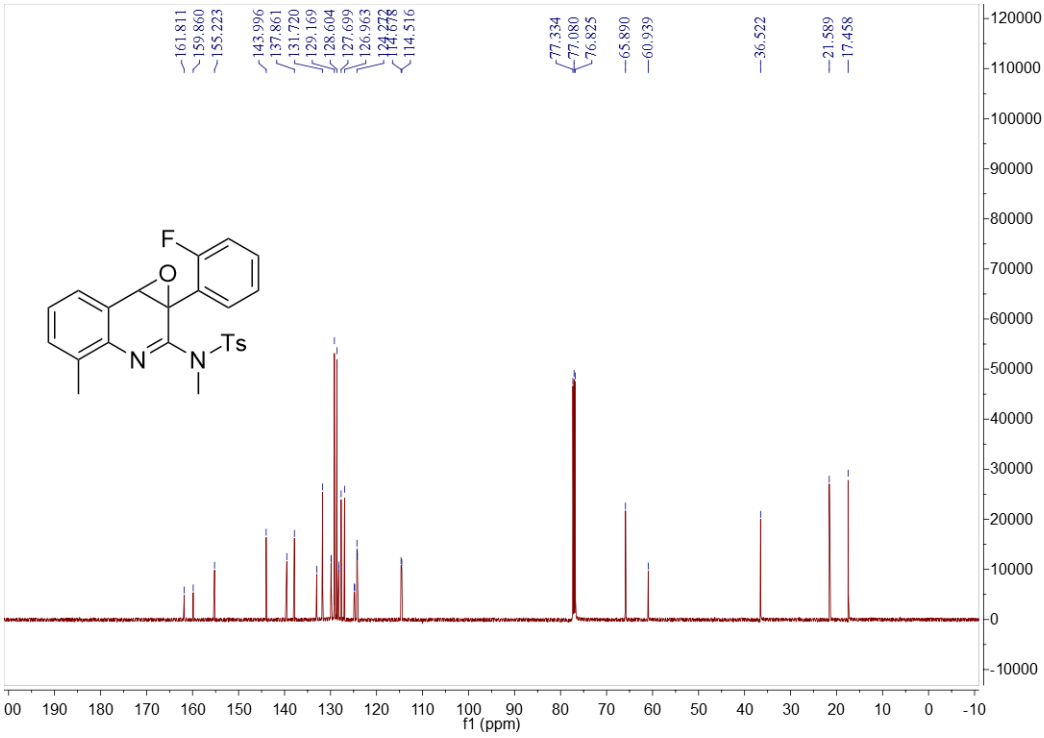
^{13}C NMR of compound **5e** in $CDCl_3$



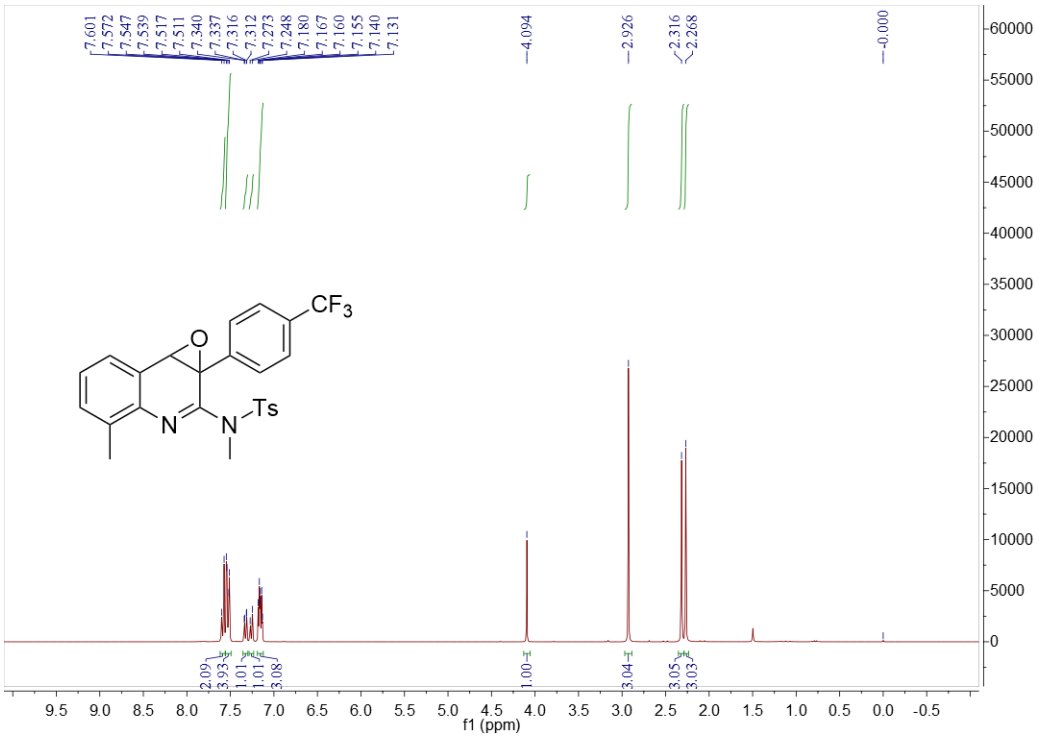
^{1}H NMR of compound **5f** in $CDCl_3$



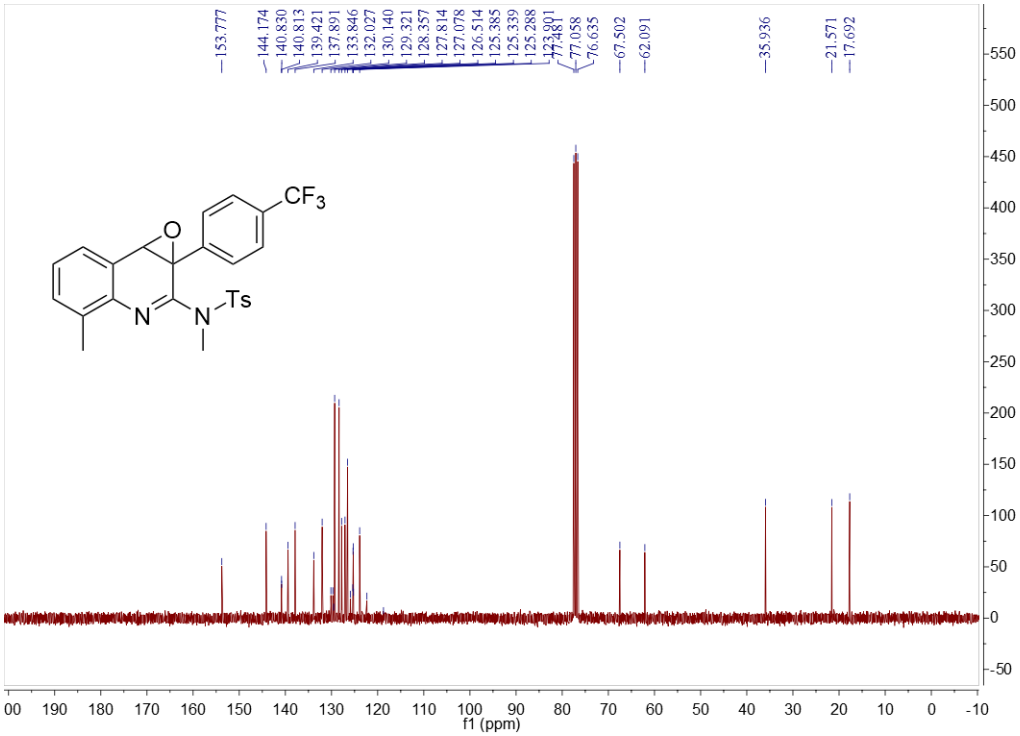
^{13}C NMR of compound **5f** in $CDCl_3$



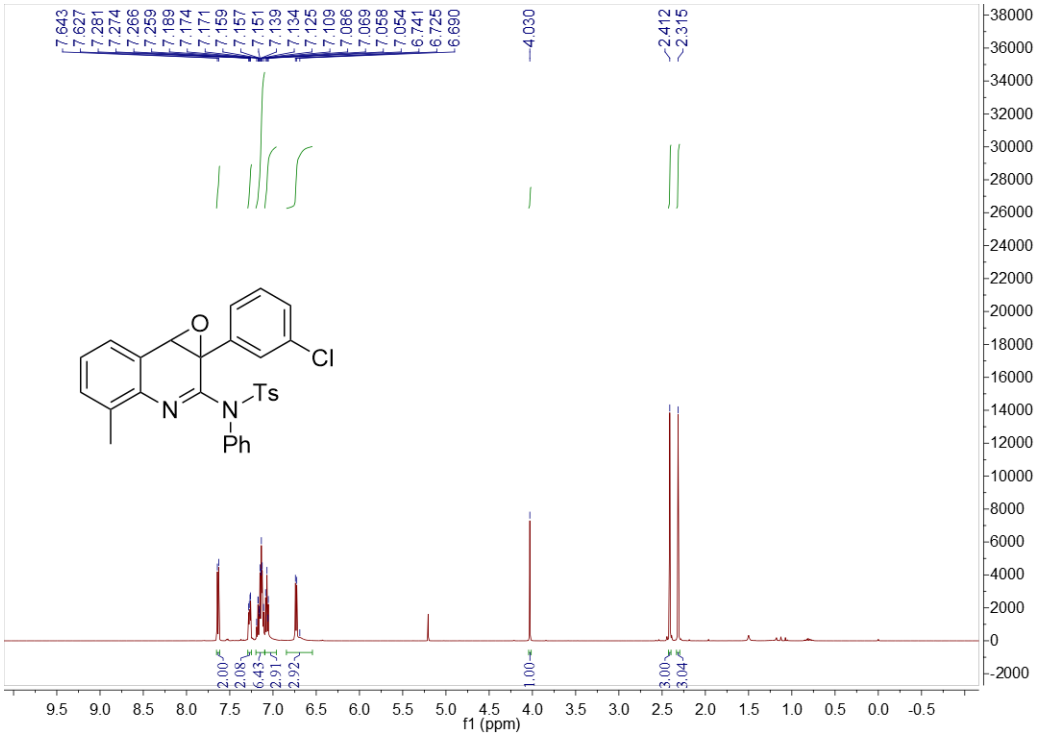
^{1}H NMR of compound **5g** in $CDCl_3$



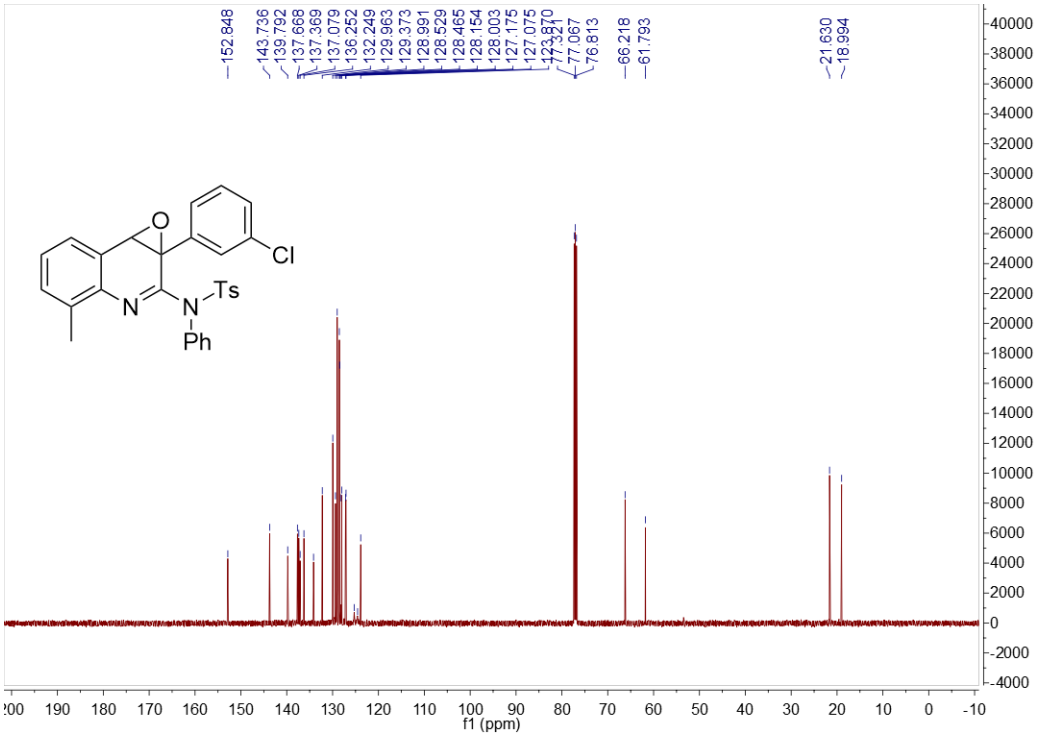
^{13}C NMR of compound **5g** in $CDCl_3$



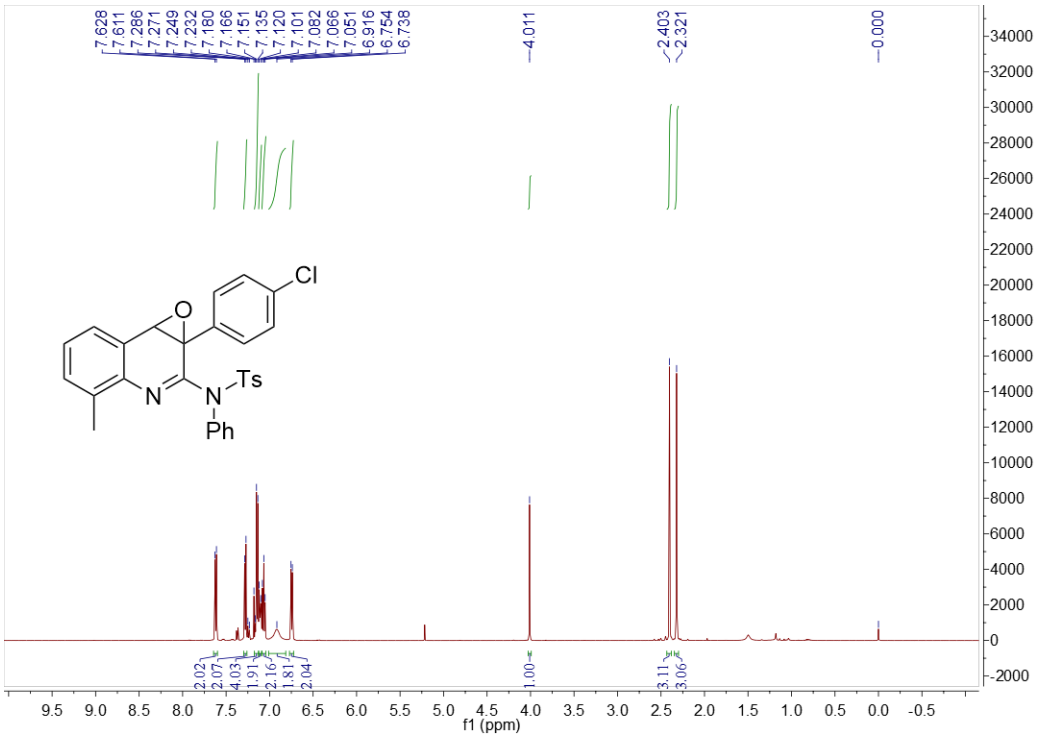
^{1}H NMR of compound **5h** in $CDCl_3$



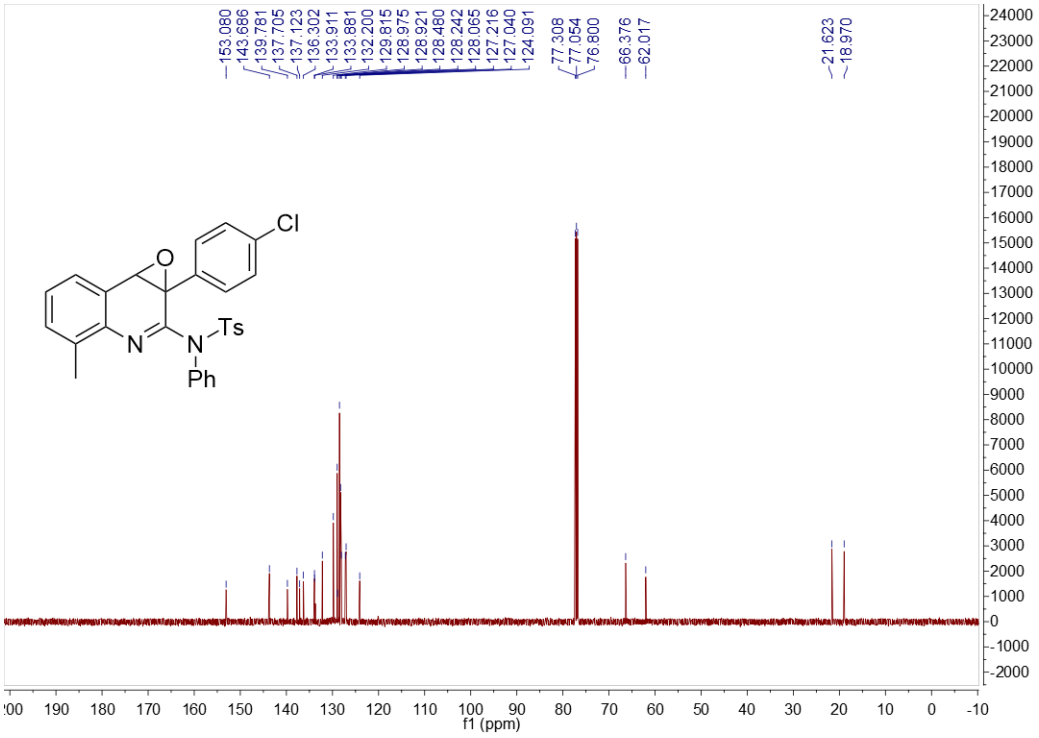
^{13}C NMR of compound **5h** in $CDCl_3$



^{1}H NMR of compound **5i** in $CDCl_3$



^{13}C NMR of compound **5i** in $CDCl_3$



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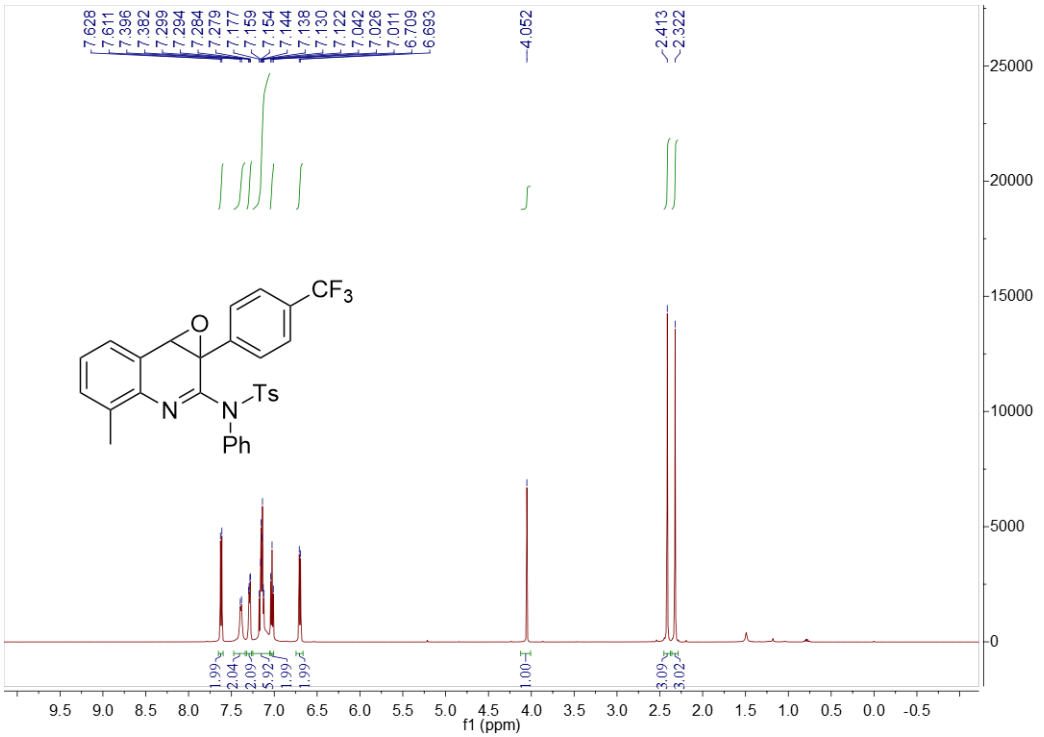

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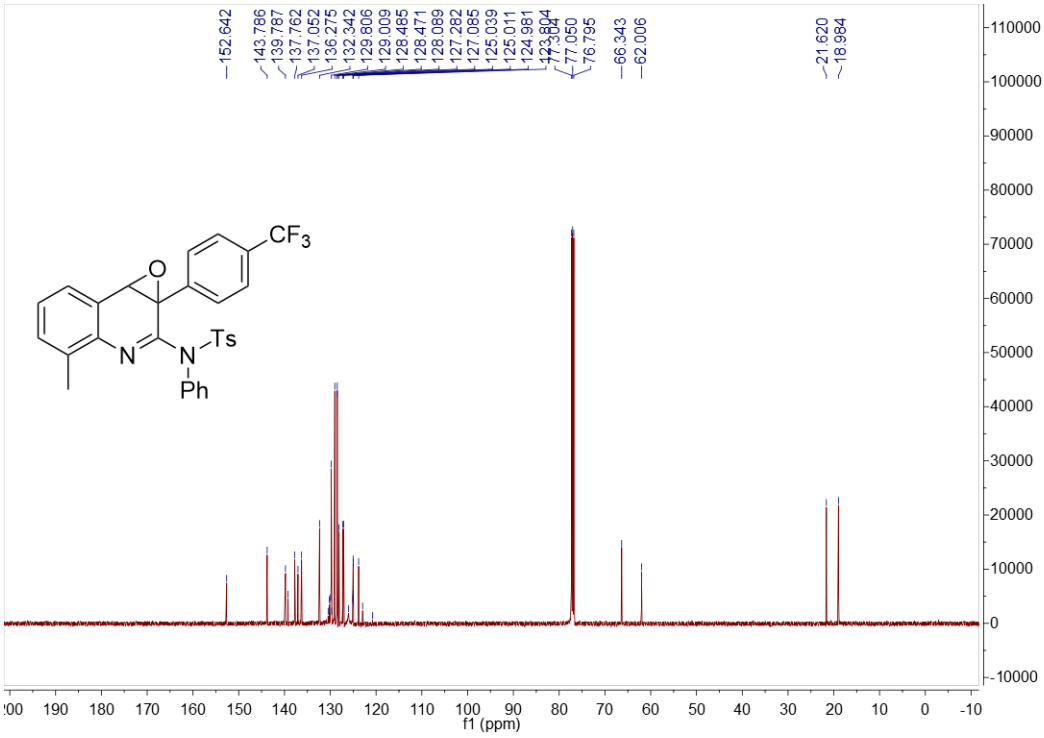
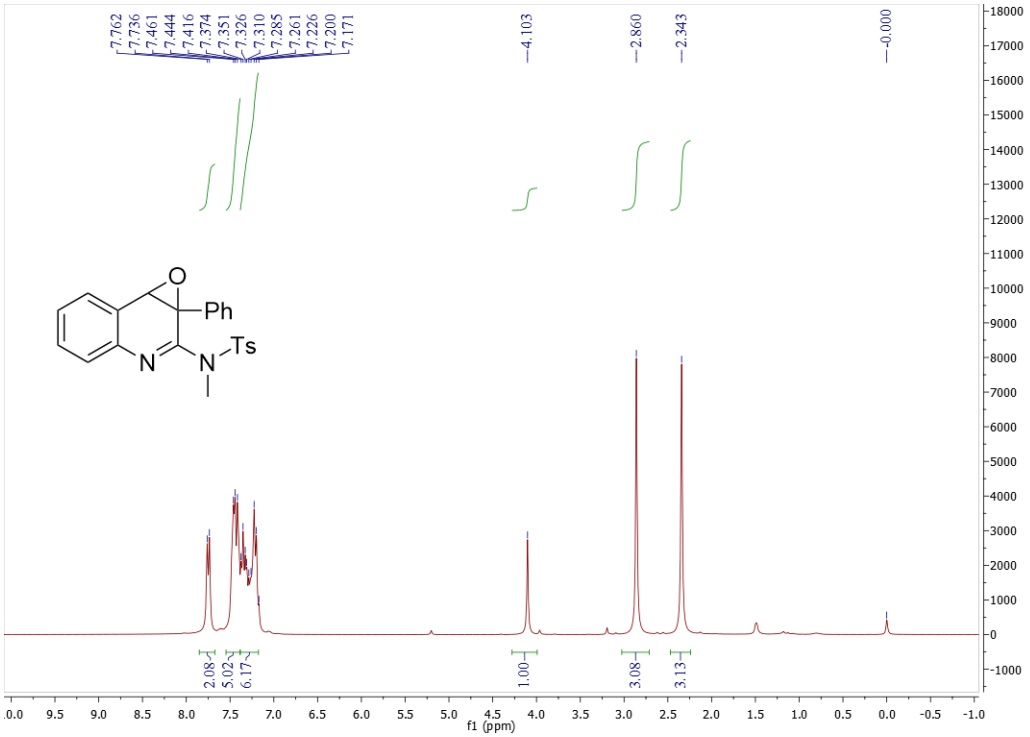


^{1}H NMR of compound **5k** in $CDCl_3$



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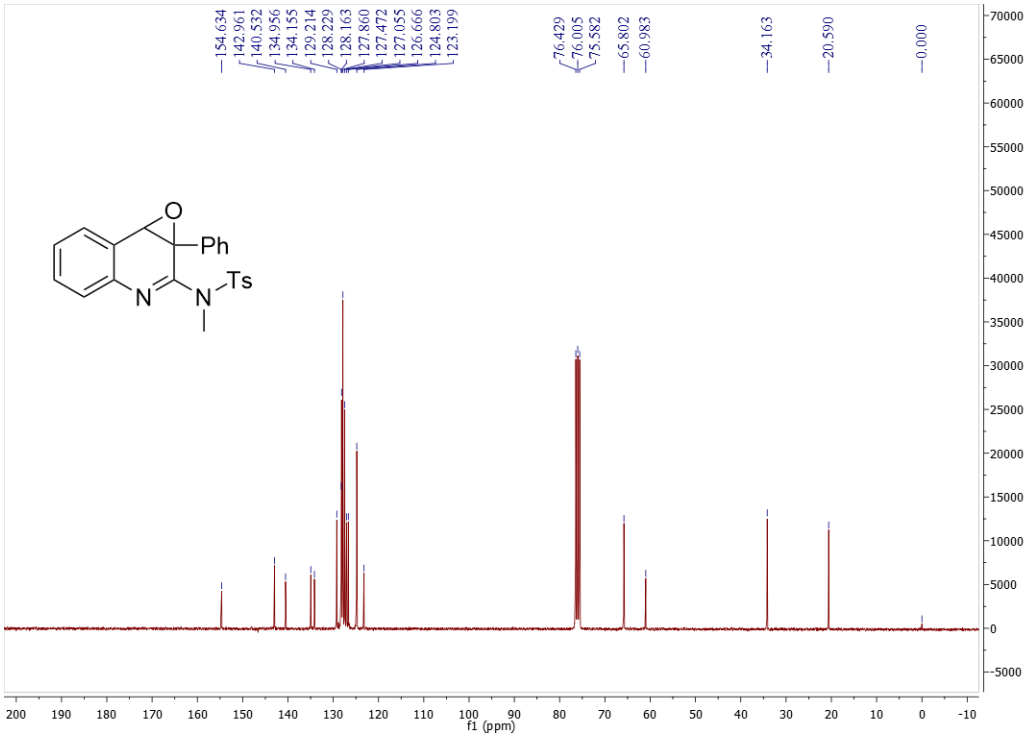
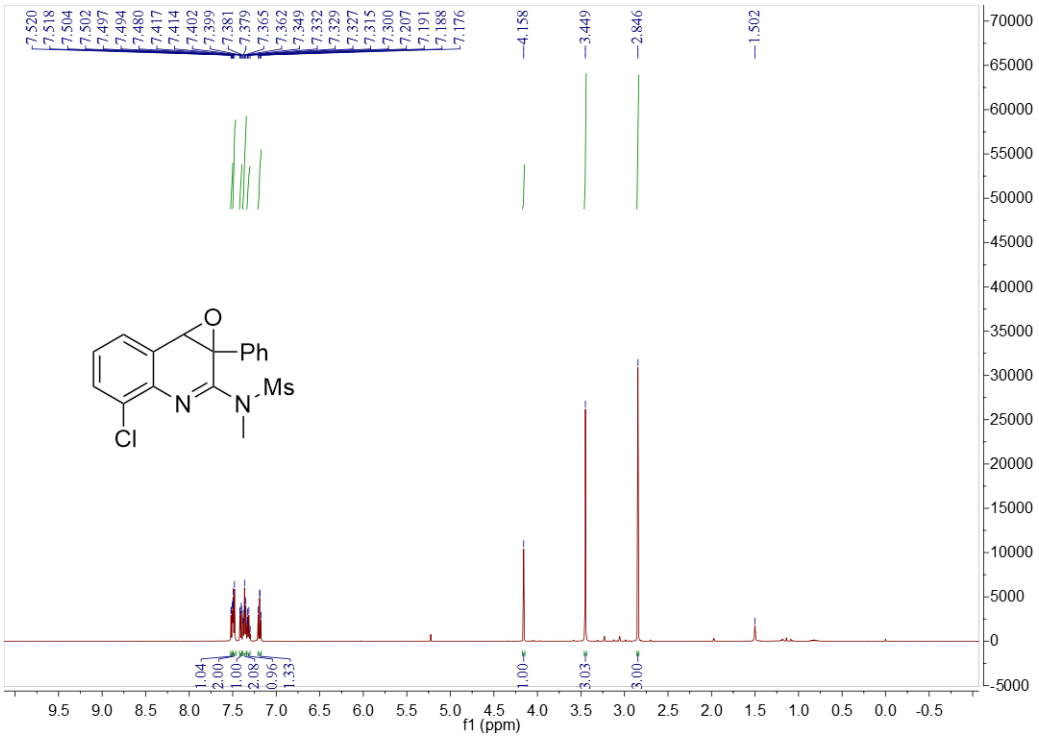
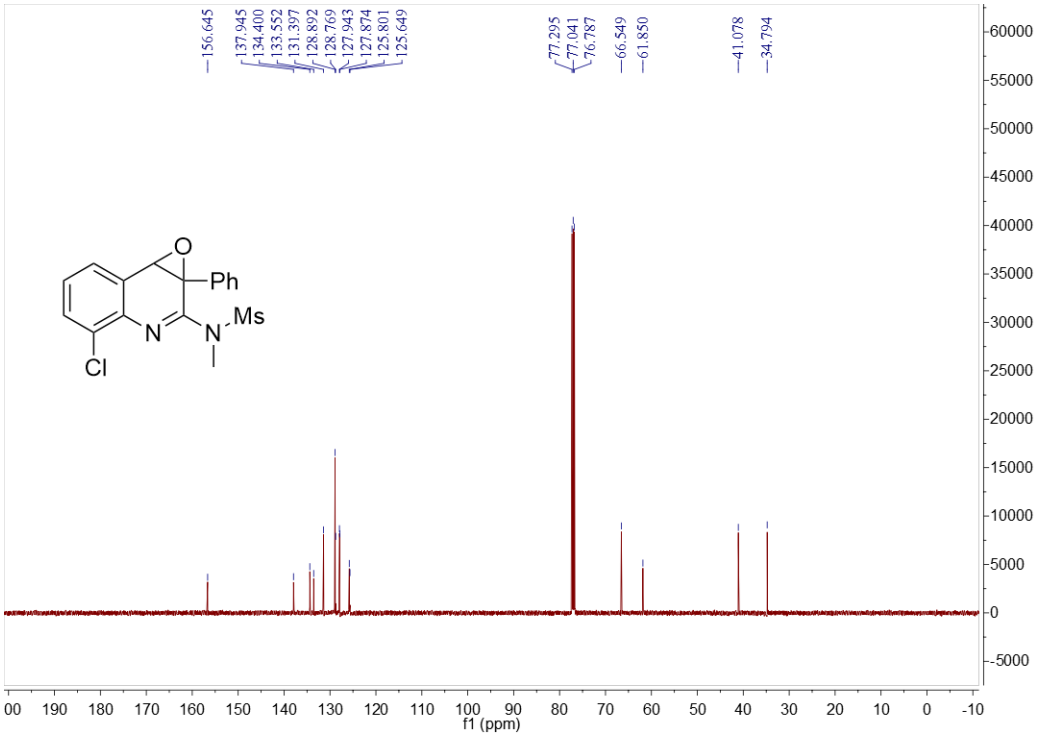


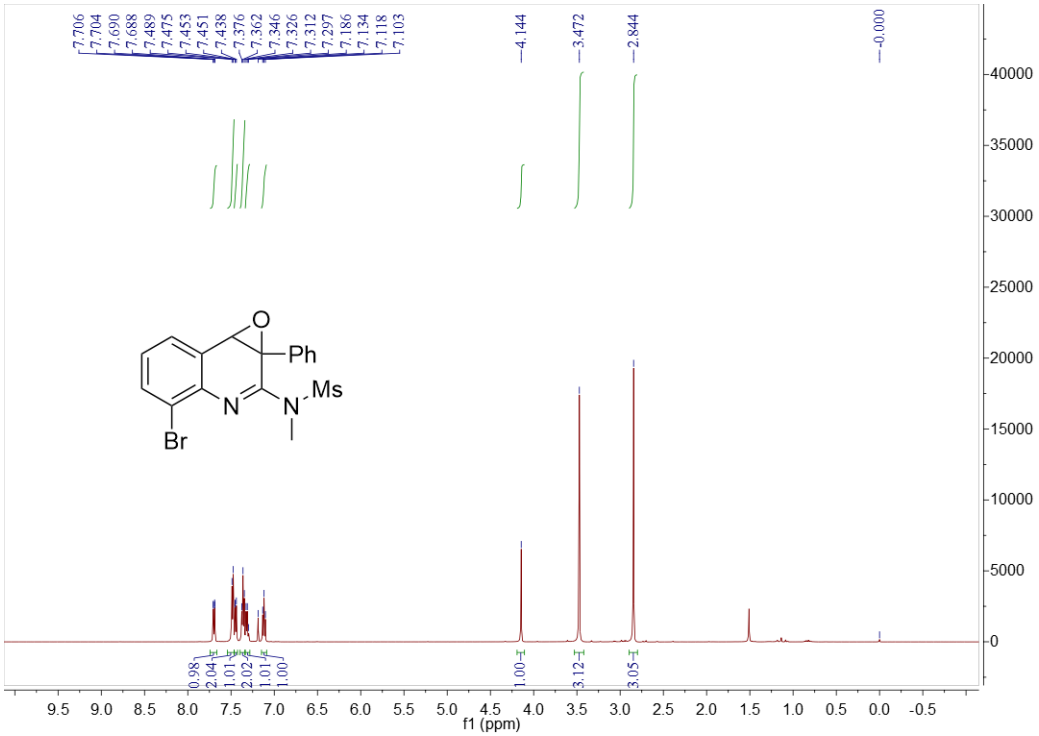
^{1}H NMR of compound **5l** in $CDCl_3$



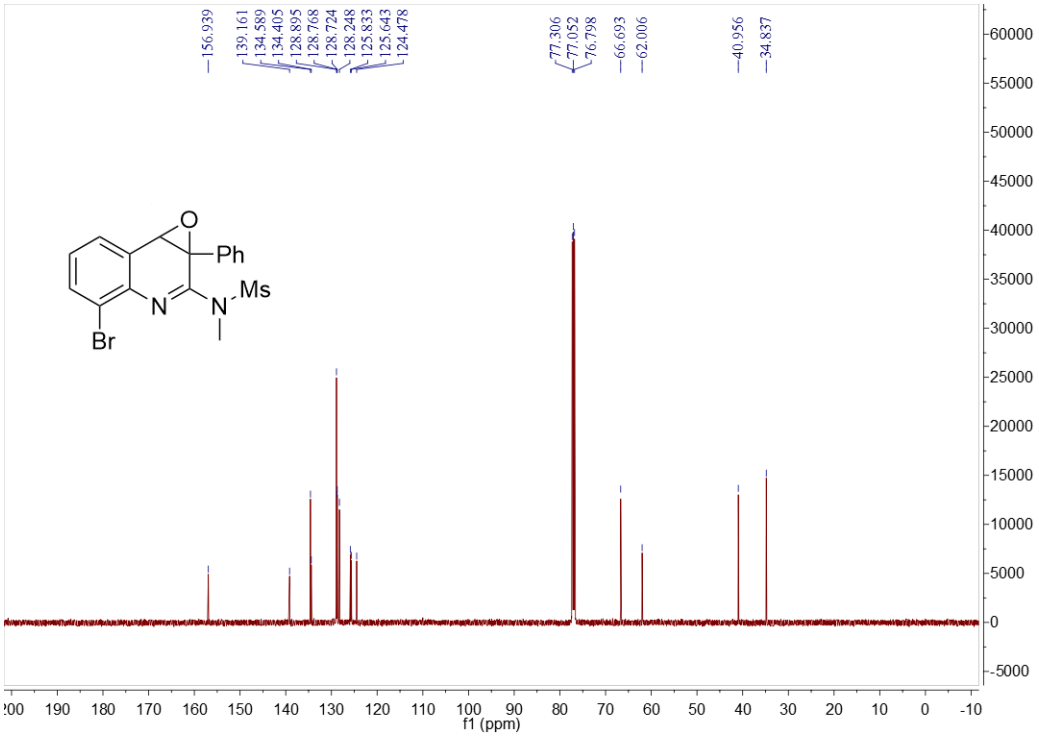
^{13}C NMR of compound **5l** in $CDCl_3$



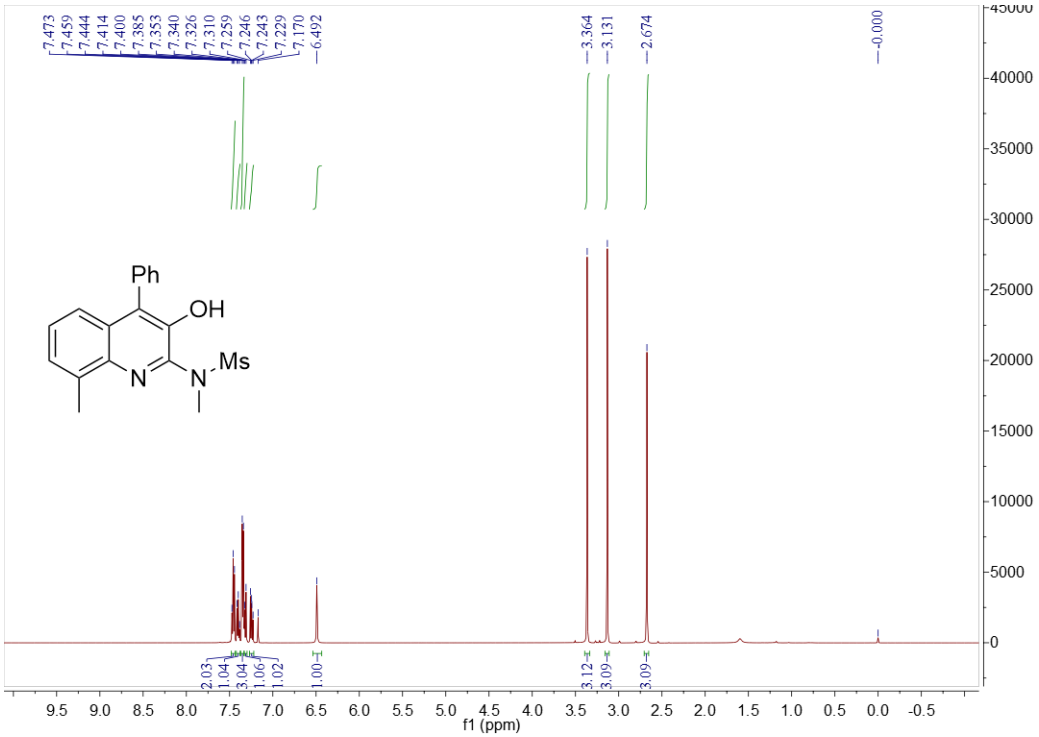
^{1}H NMR of compound **5m** in $CDCl_3$



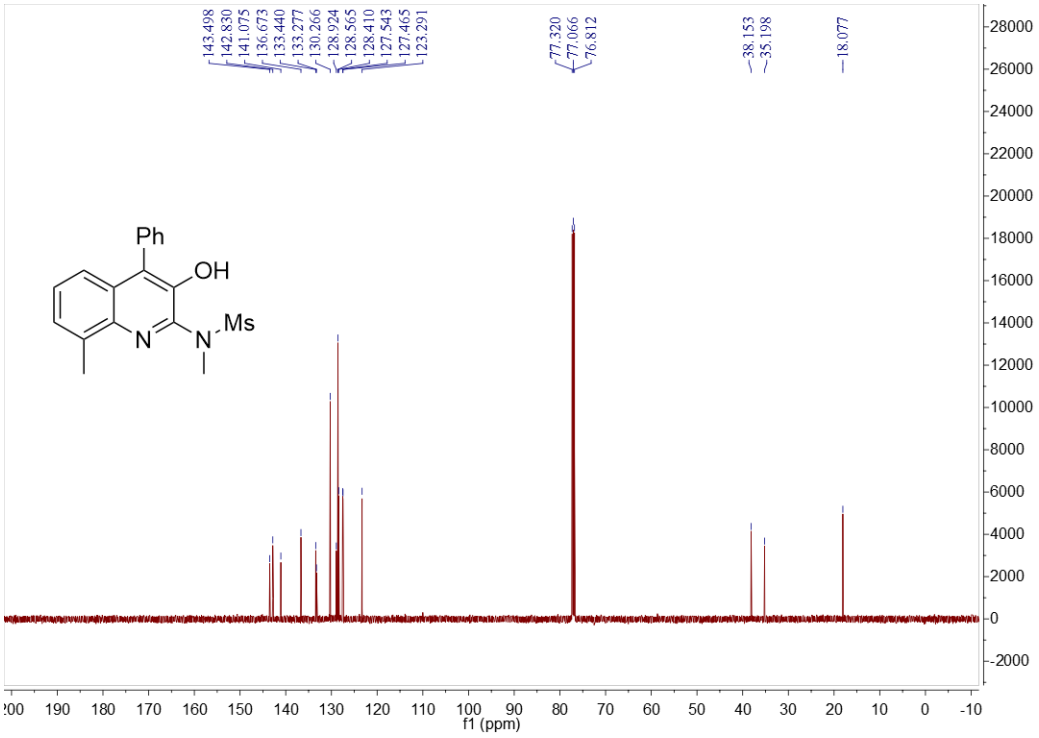
^{13}C NMR of compound **5m** in $CDCl_3$



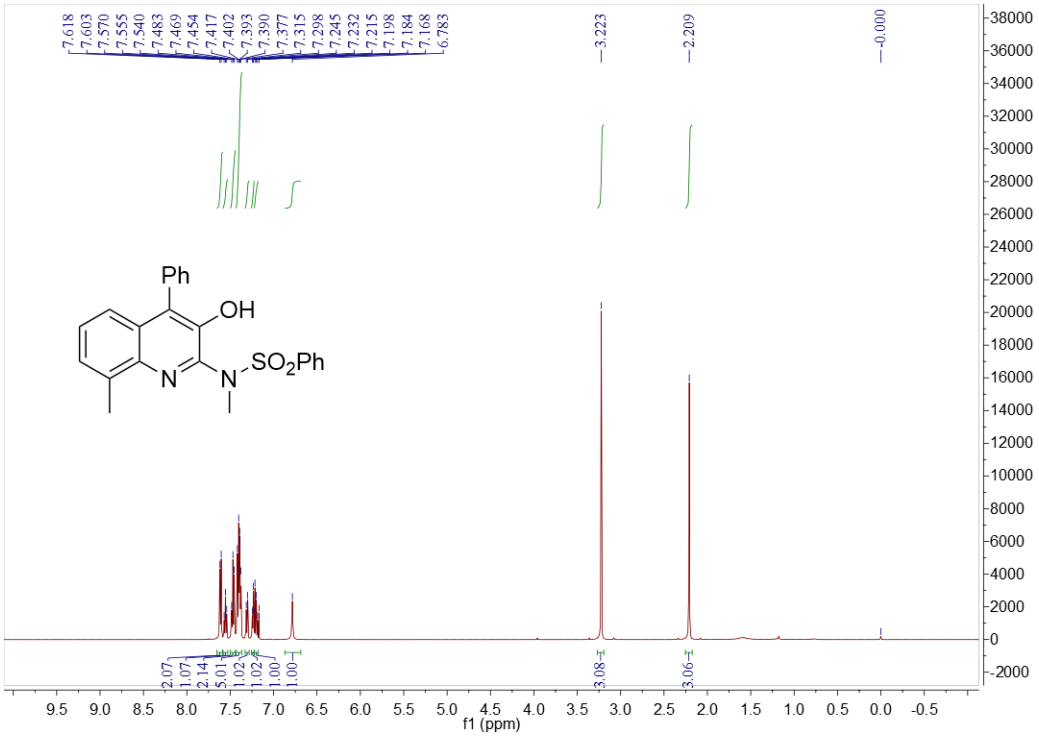
^{1}H NMR of compound **6a** in $CDCl_3$



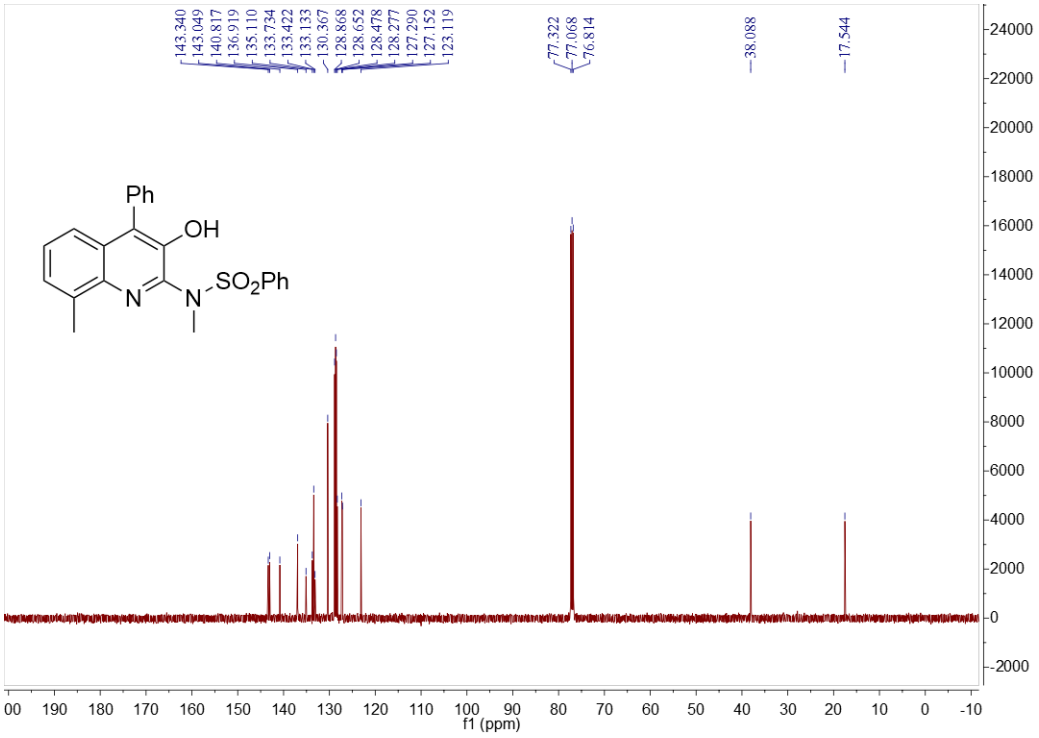
^{13}C NMR of compound **6a** in $CDCl_3$



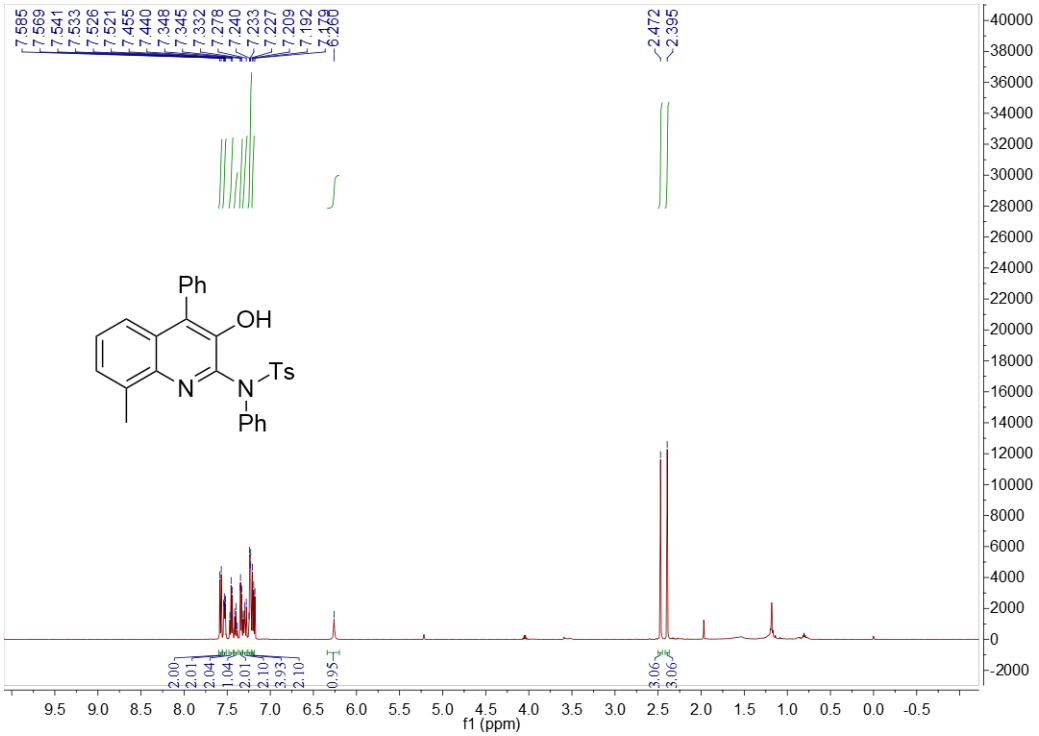
^{1}H NMR of compound **6b** in $CDCl_3$



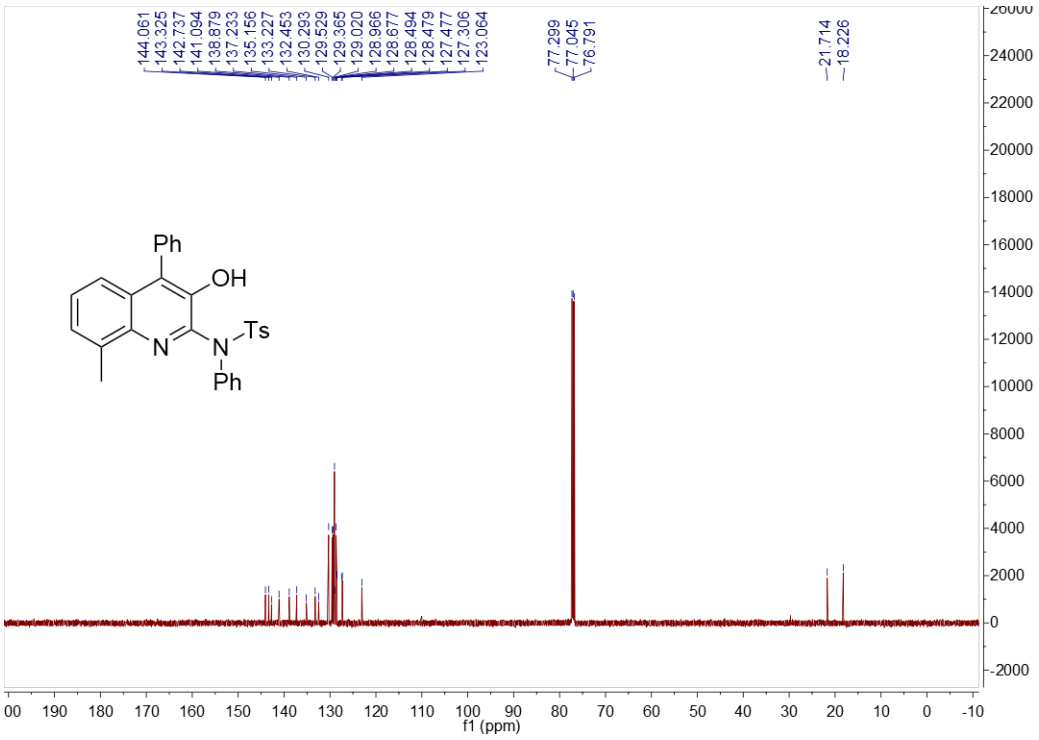
^{13}C NMR of compound **6b** in $CDCl_3$



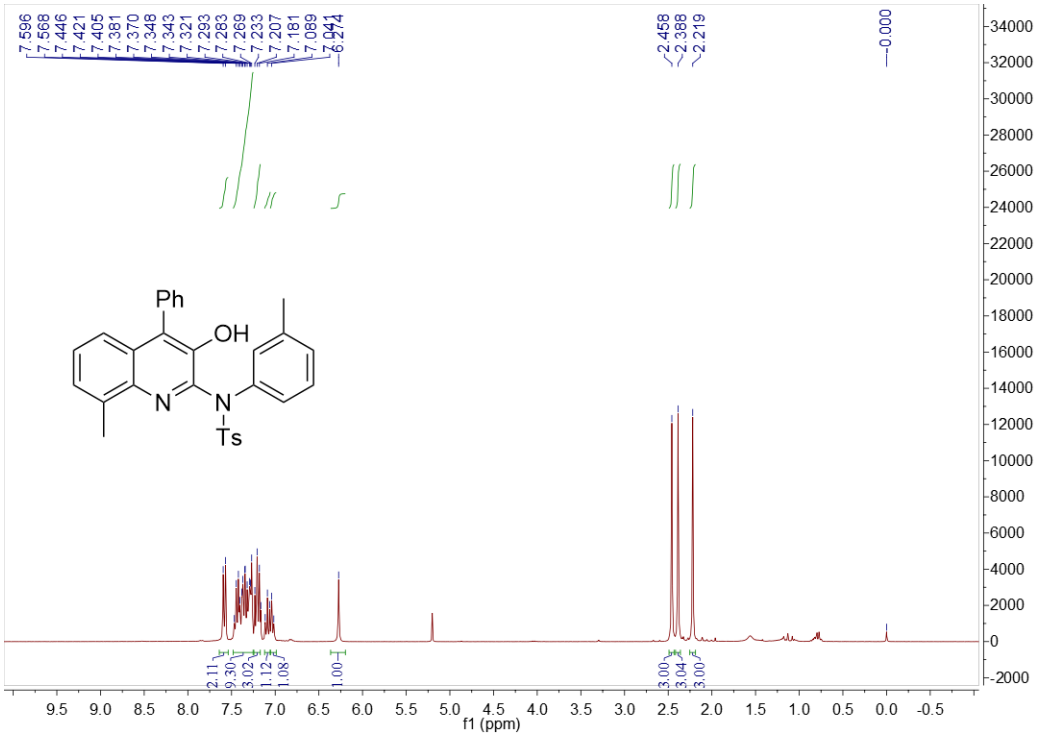
^{1}H NMR of compound **6c** in $CDCl_3$



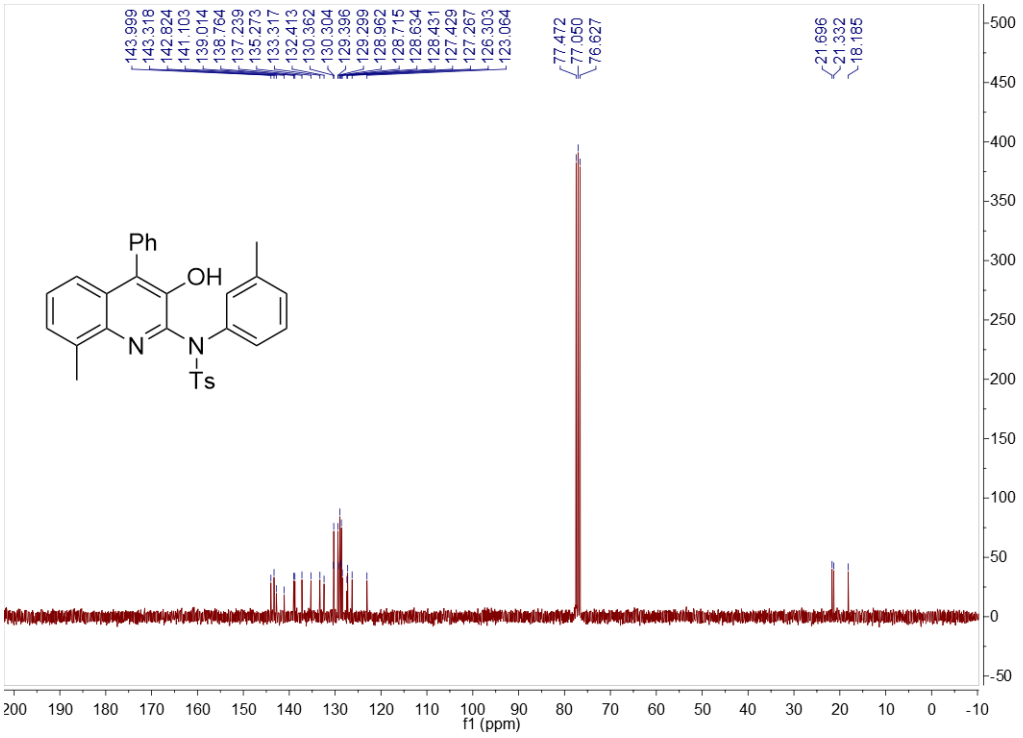
^{13}C NMR of compound **6c** in $CDCl_3$



^{1}H NMR of compound **6d** in $CDCl_3$



^{13}C NMR of compound **6d** in $CDCl_3$



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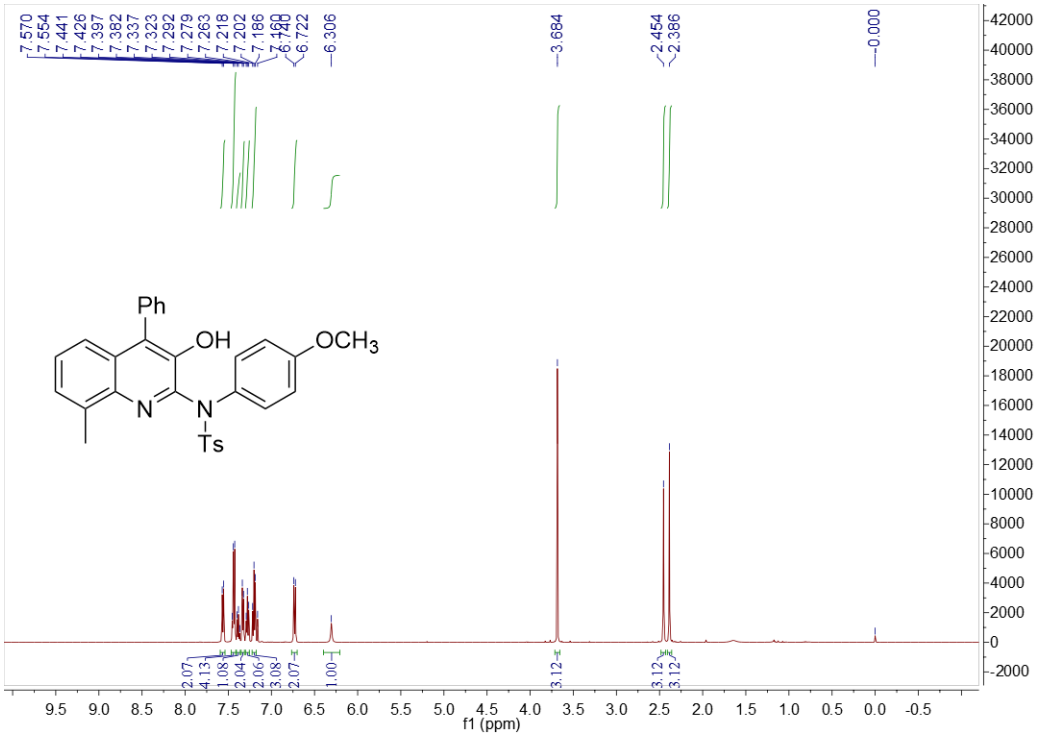

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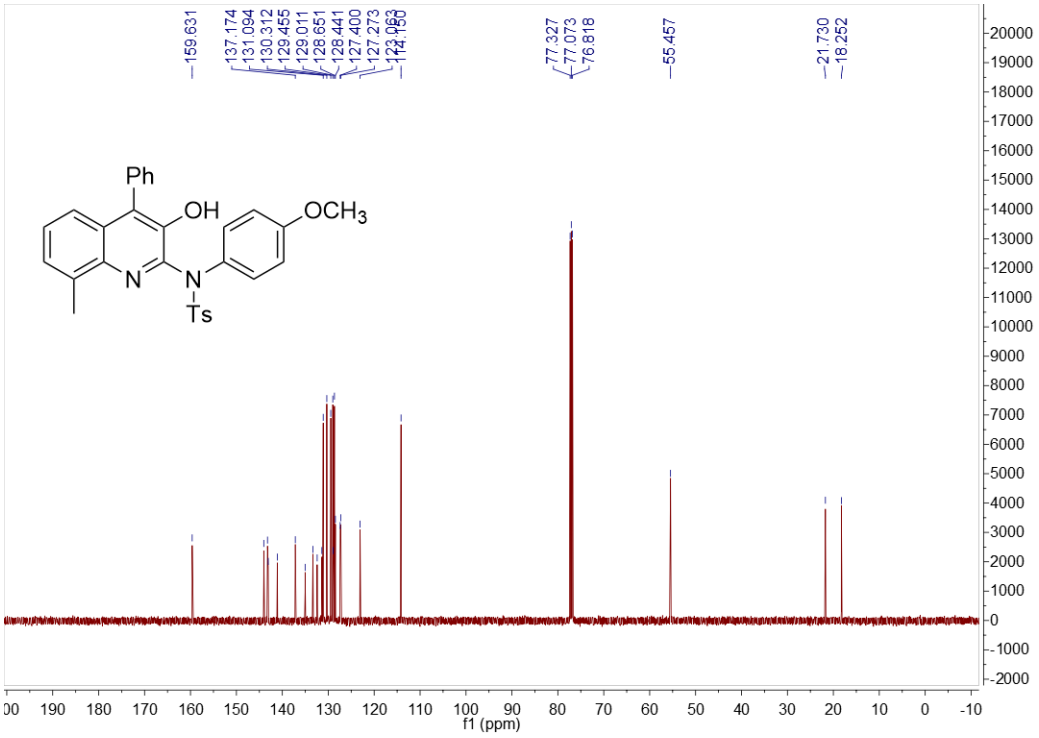
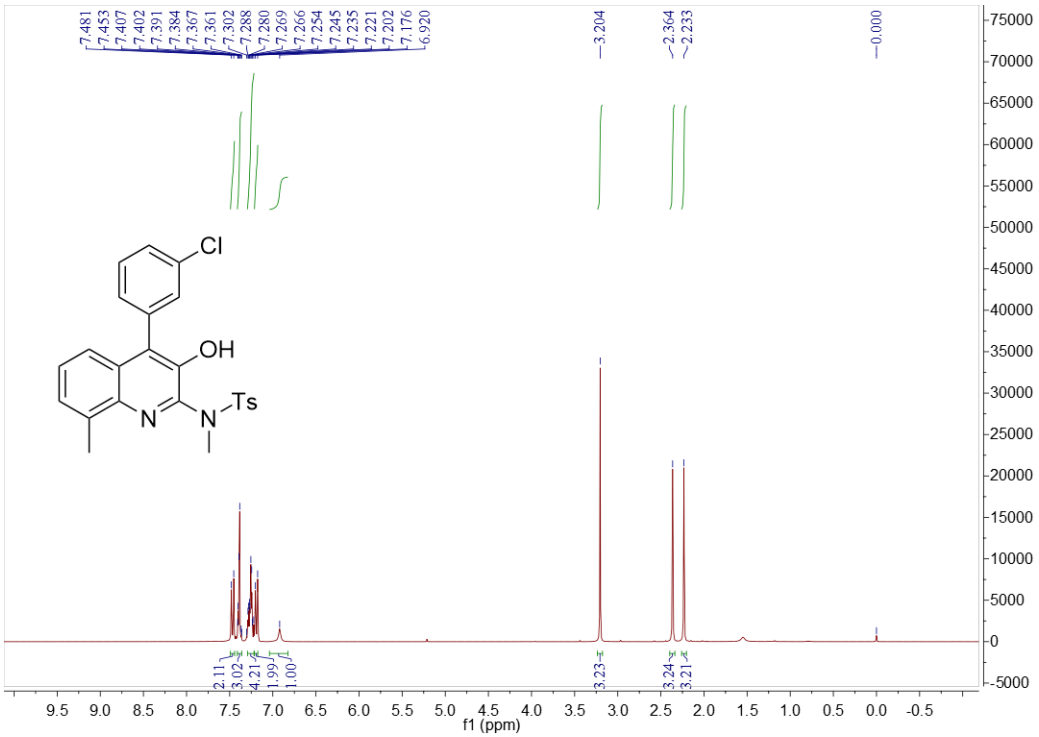


^{1}H NMR of compound **6f** in $CDCl_3$



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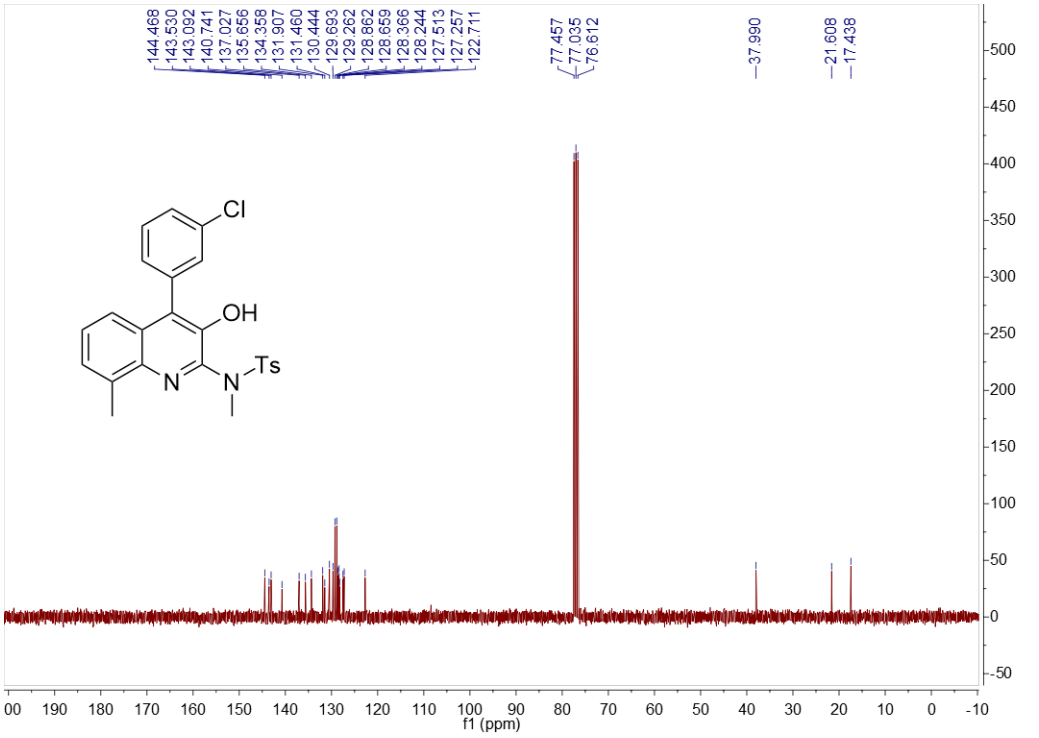
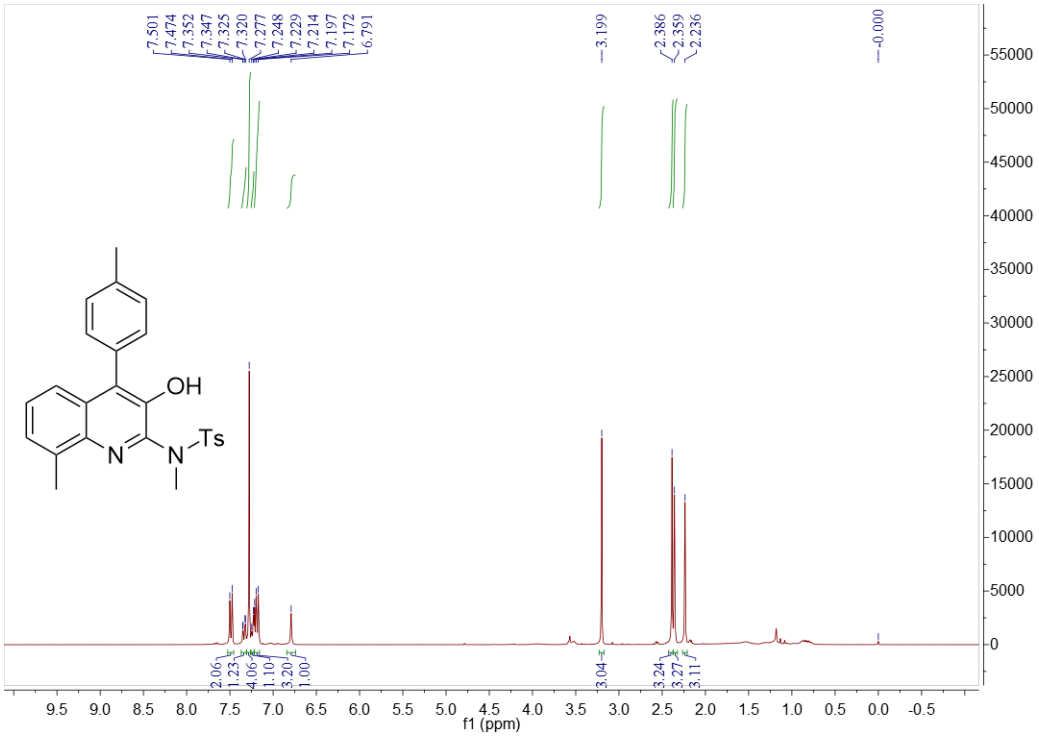
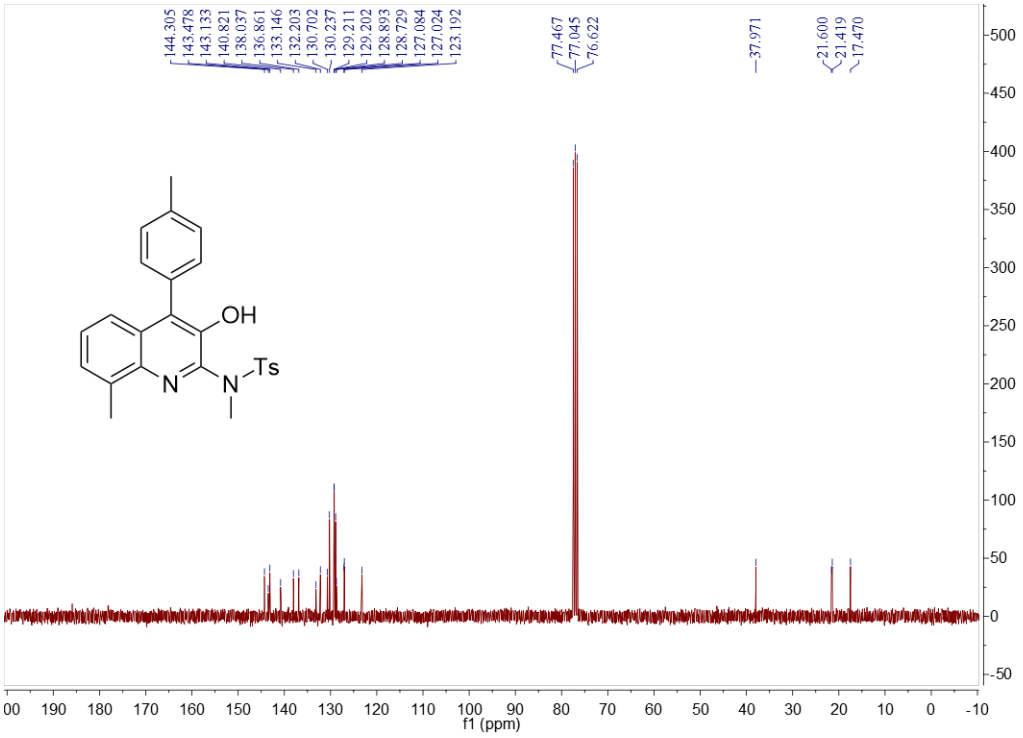


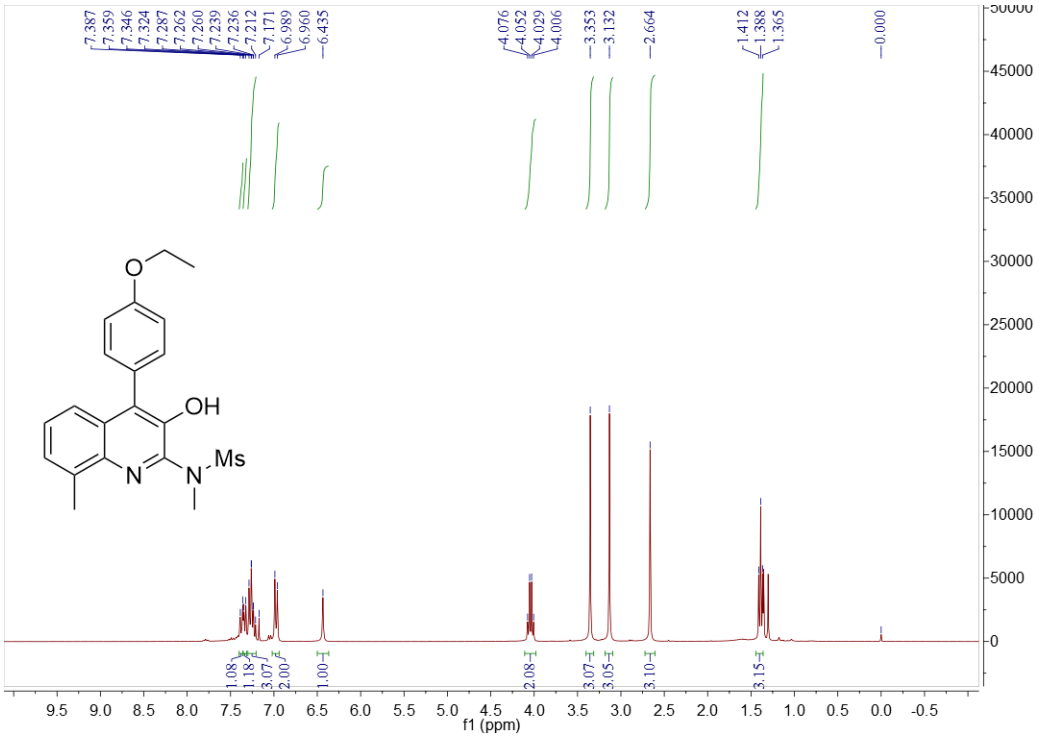
^{1}H NMR of compound **6g** in $CDCl_3$



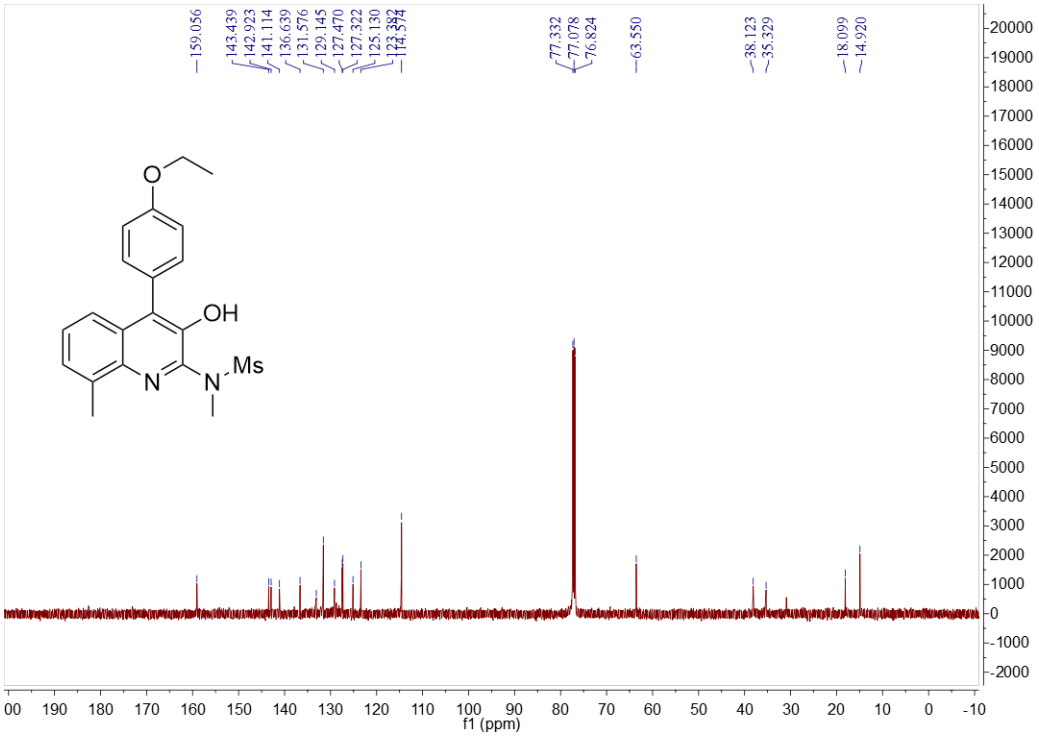
^{13}C NMR of compound **6g** in $CDCl_3$



^{1}H NMR of compound **6h** in $CDCl_3$



^{13}C NMR of compound **6h** in $CDCl_3$



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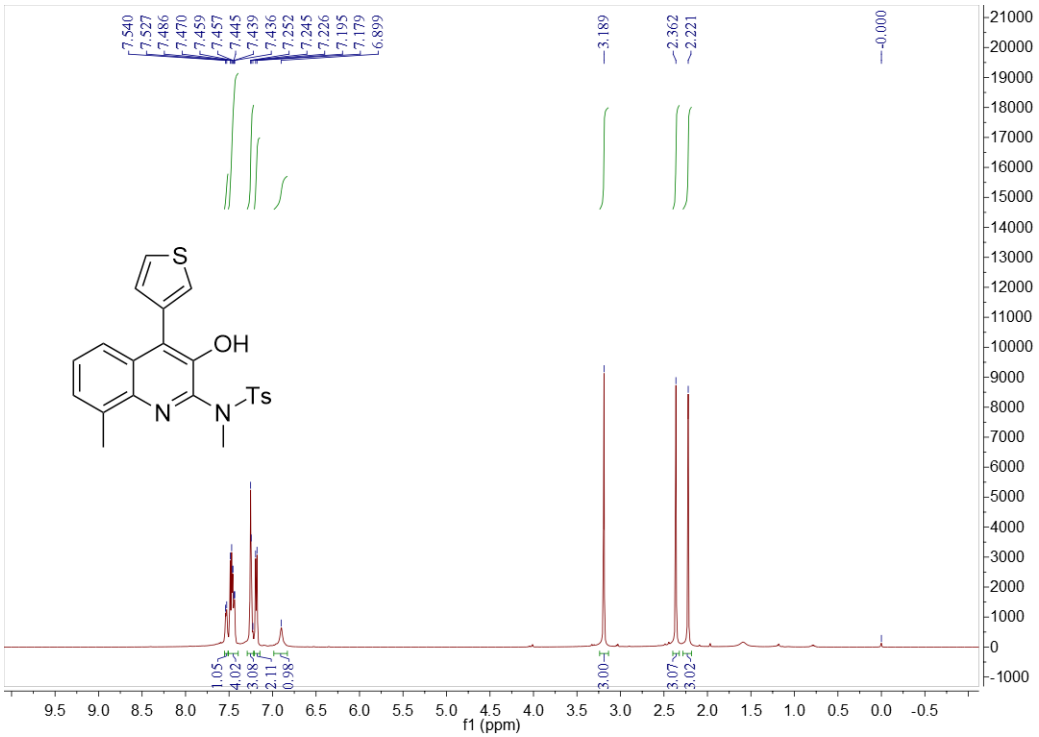
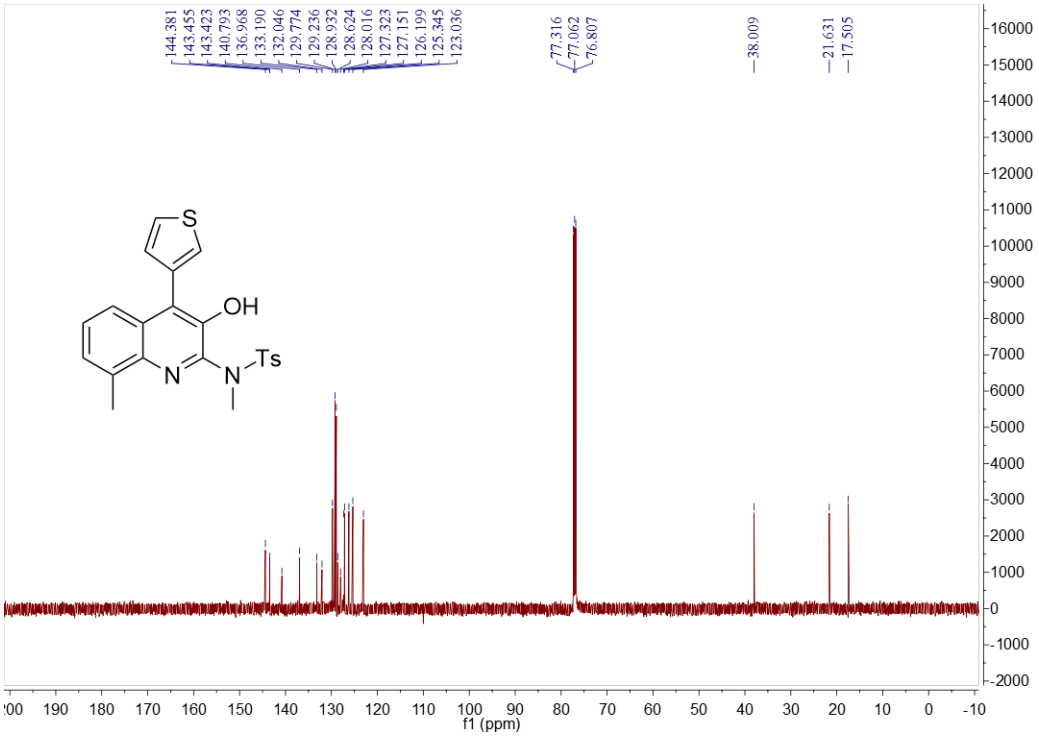


^{13}C NMR of compound **6i** in $CDCl_3$



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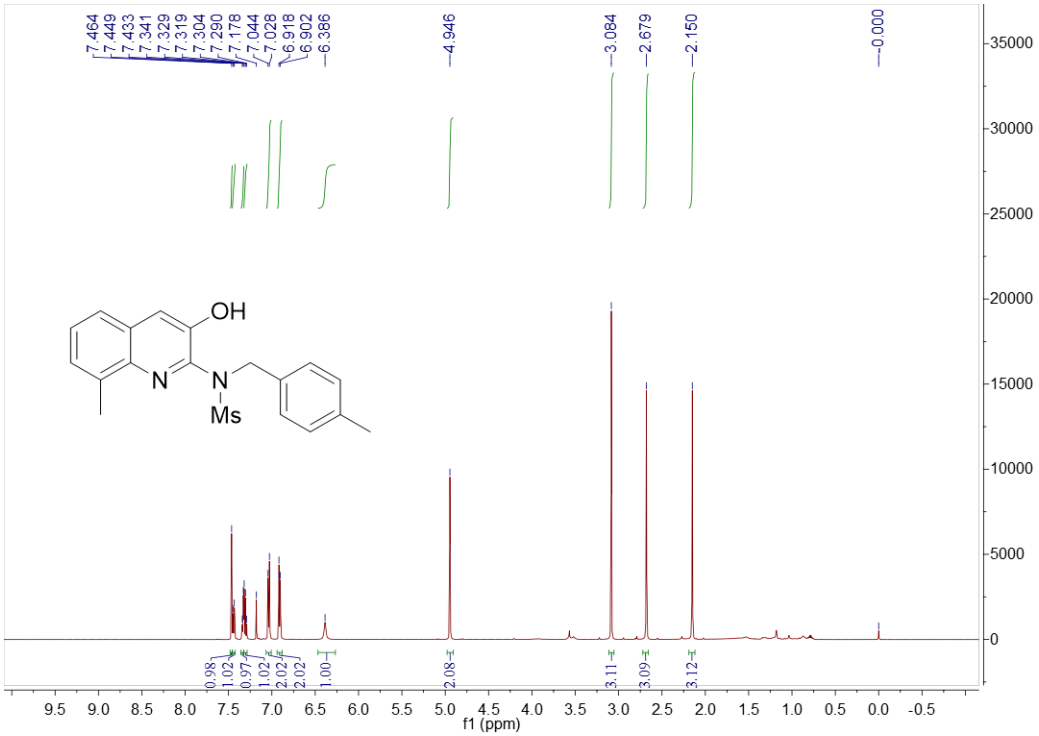

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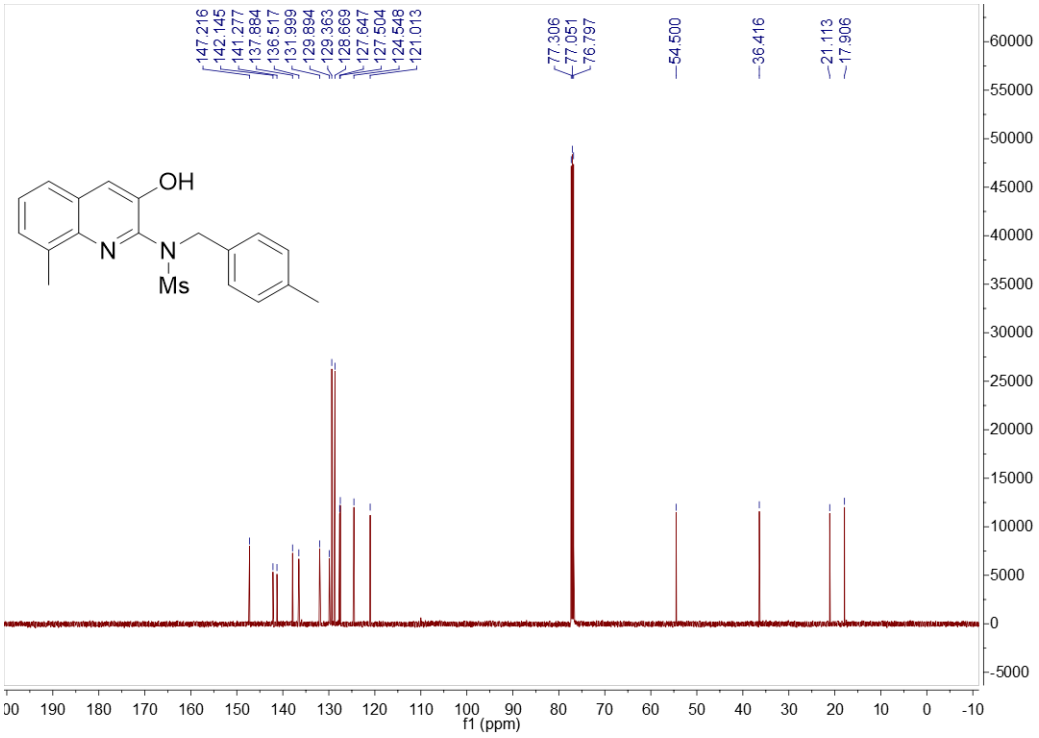

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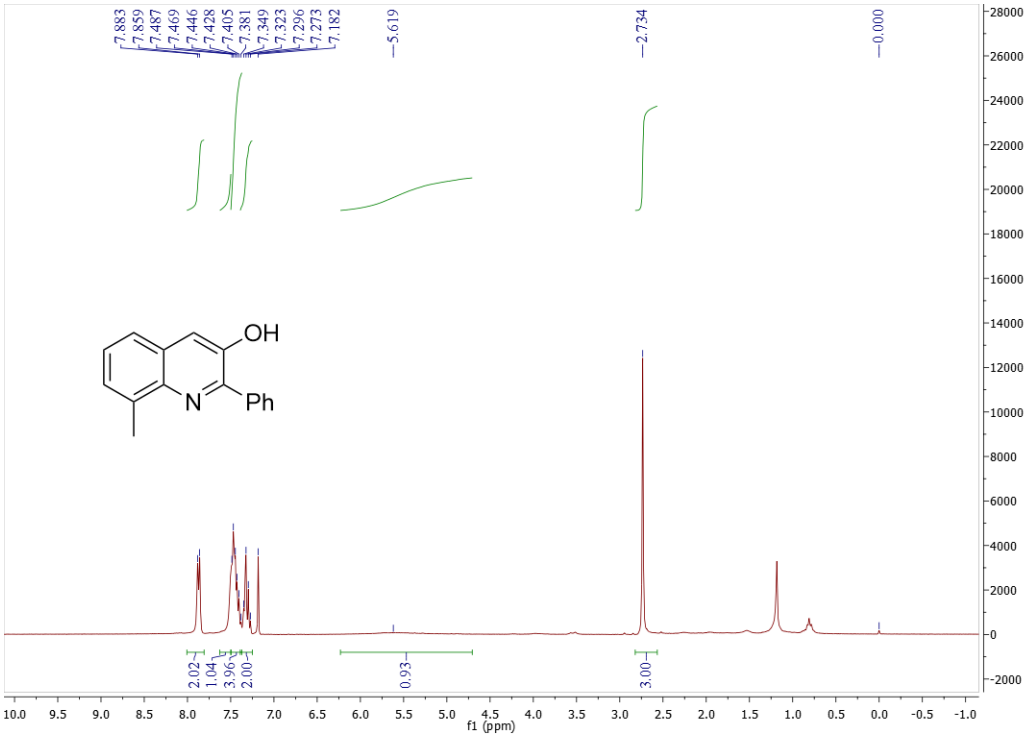
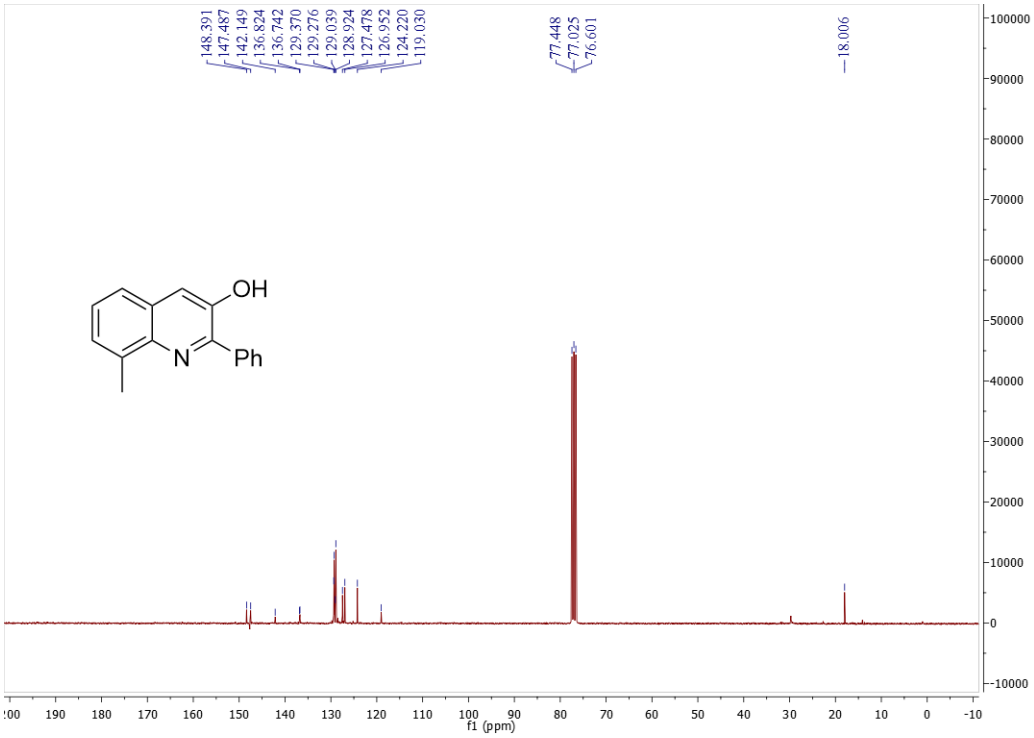


^{13}C NMR of compound **6k** in $CDCl_3$



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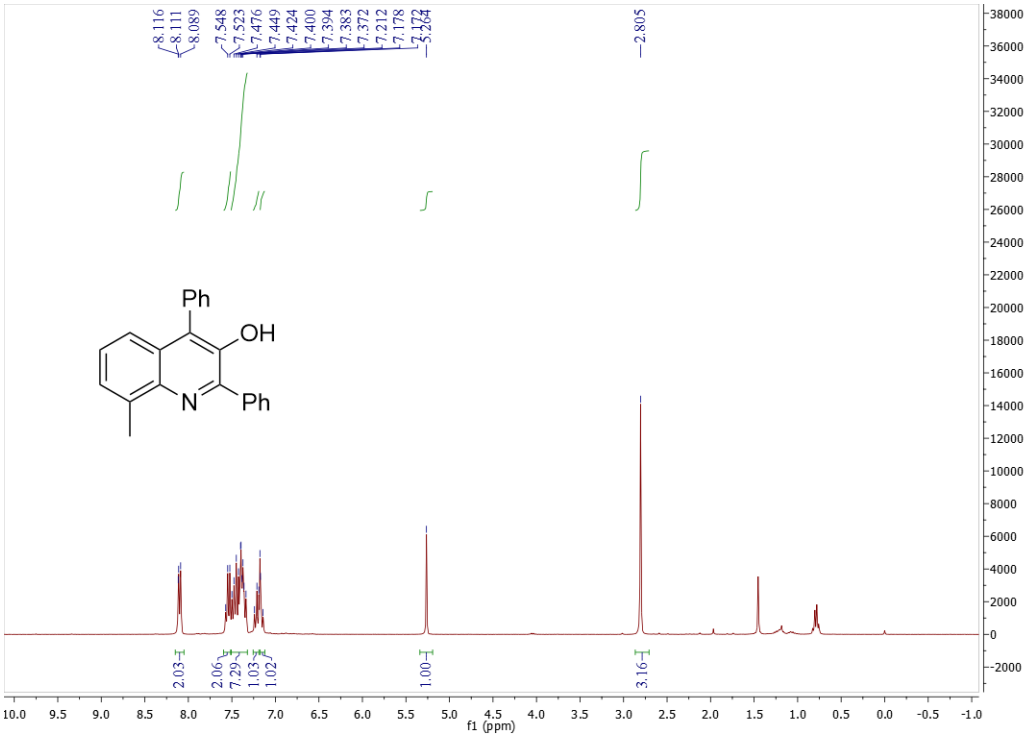
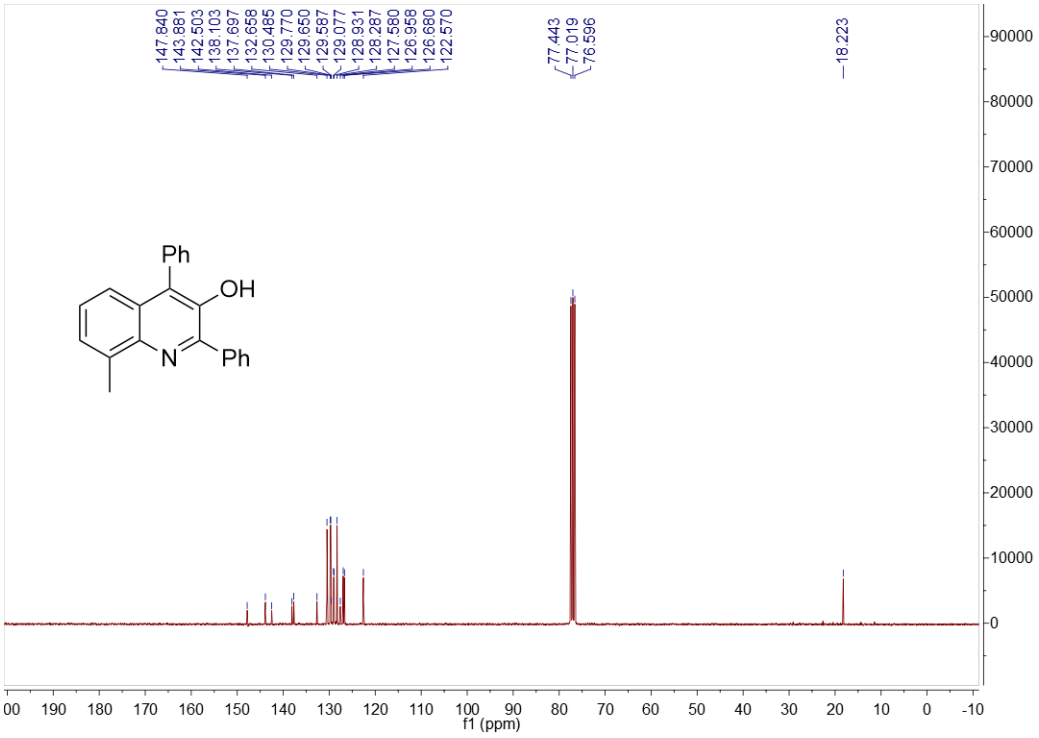


^{13}C NMR of compound **6l** in $CDCl_3$



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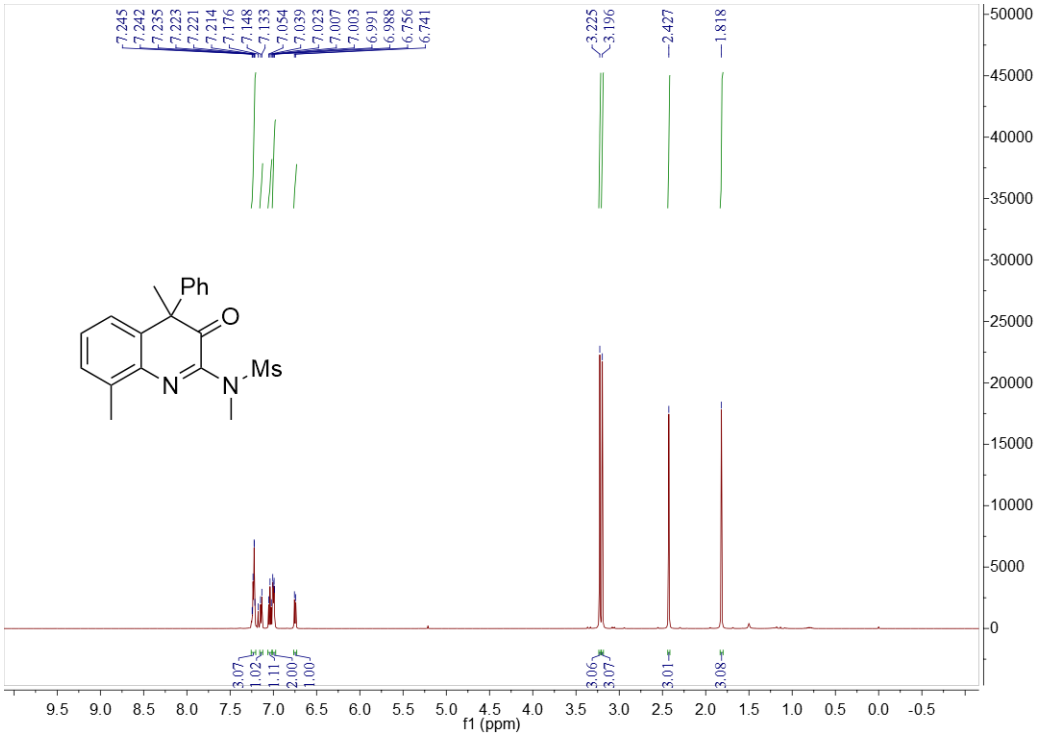
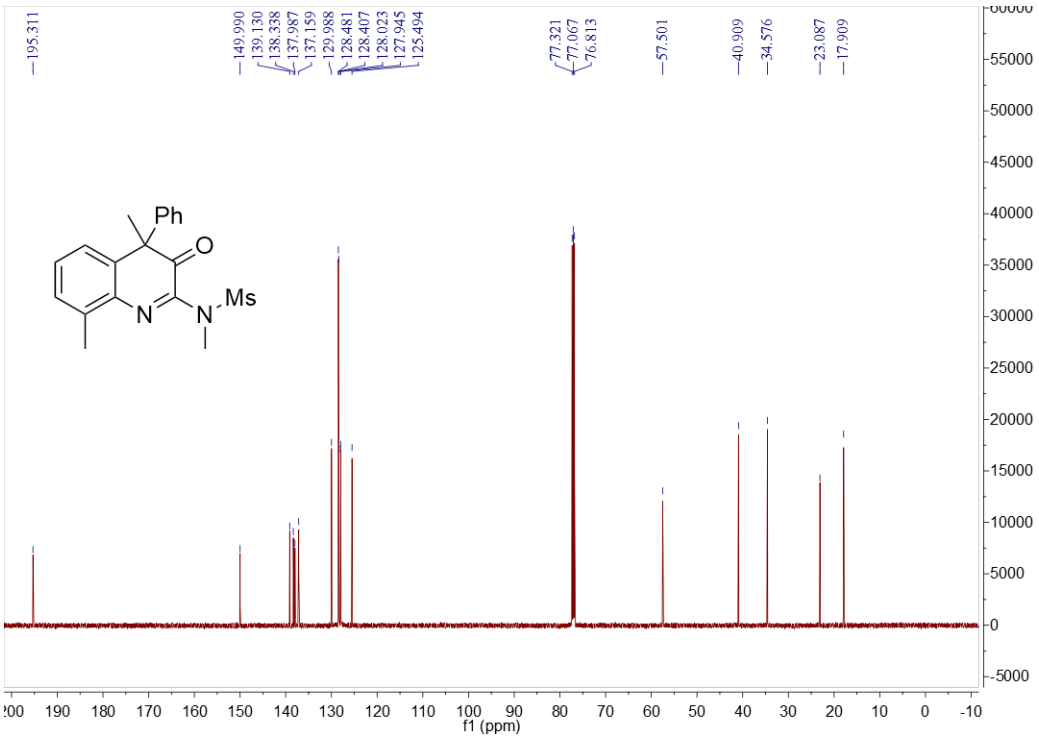
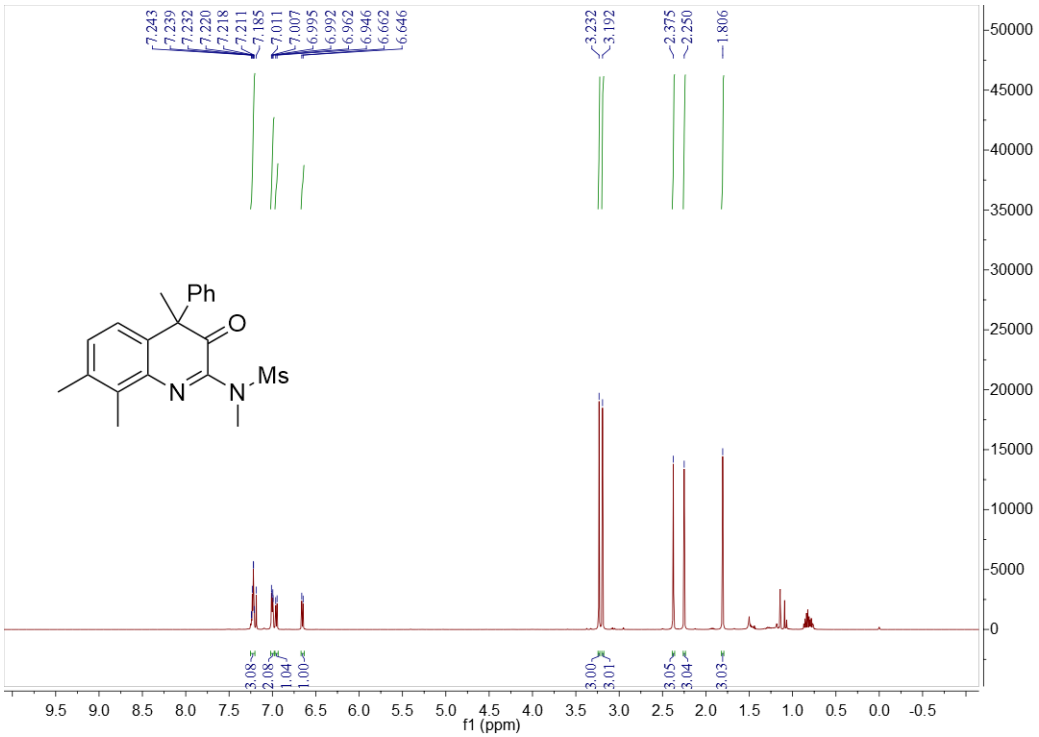


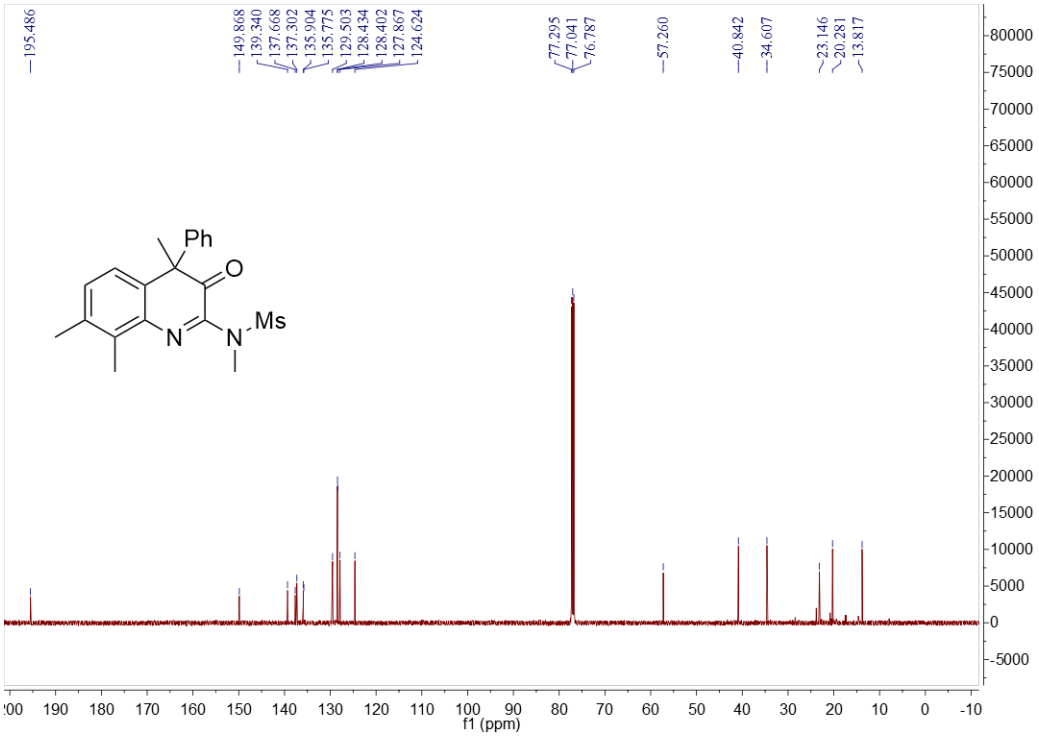
^{13}C NMR of compound **7a** in $CDCl_3$



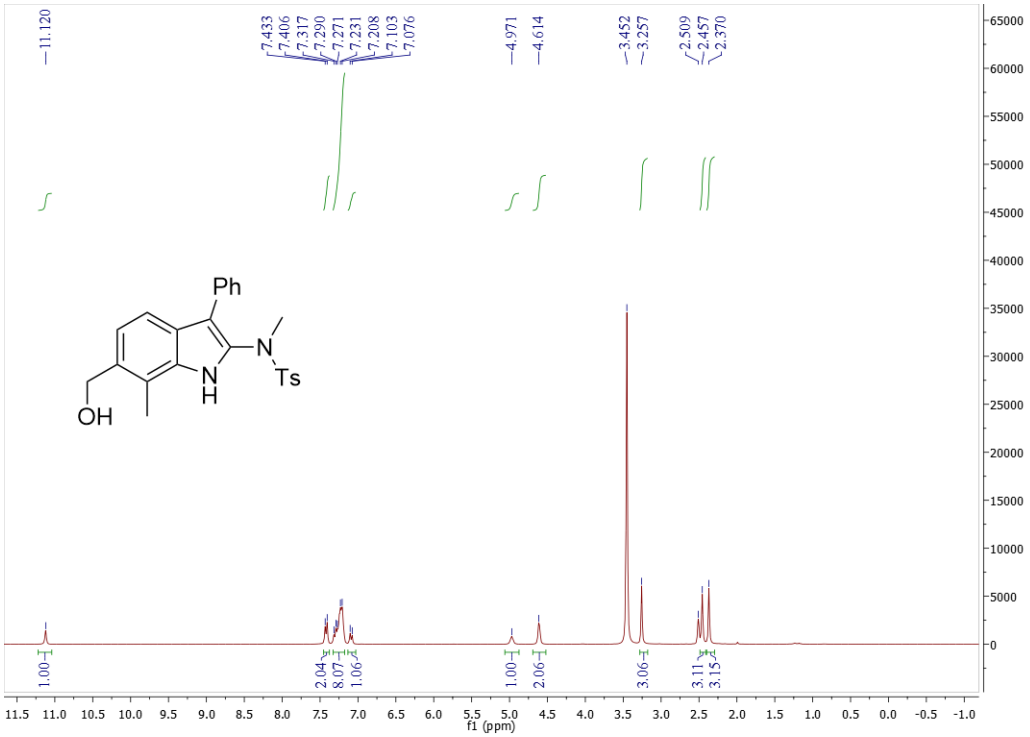
^{1}H NMR of compound **7b** in $CDCl_3$



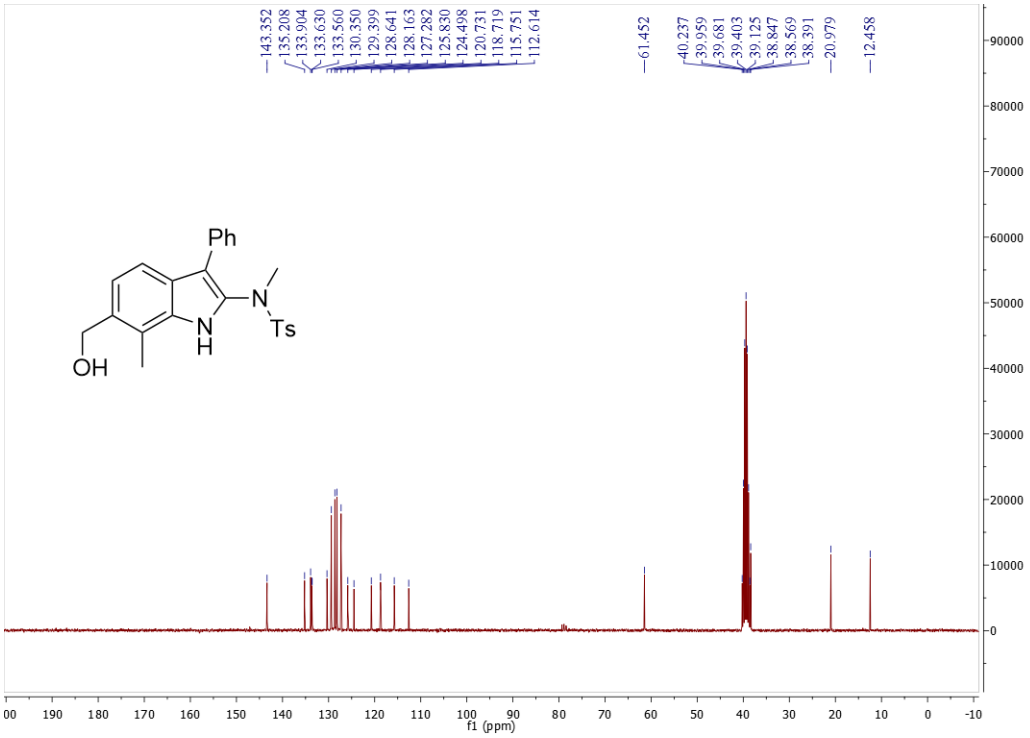
^{13}C NMR of compound **7b** in $CDCl_3$



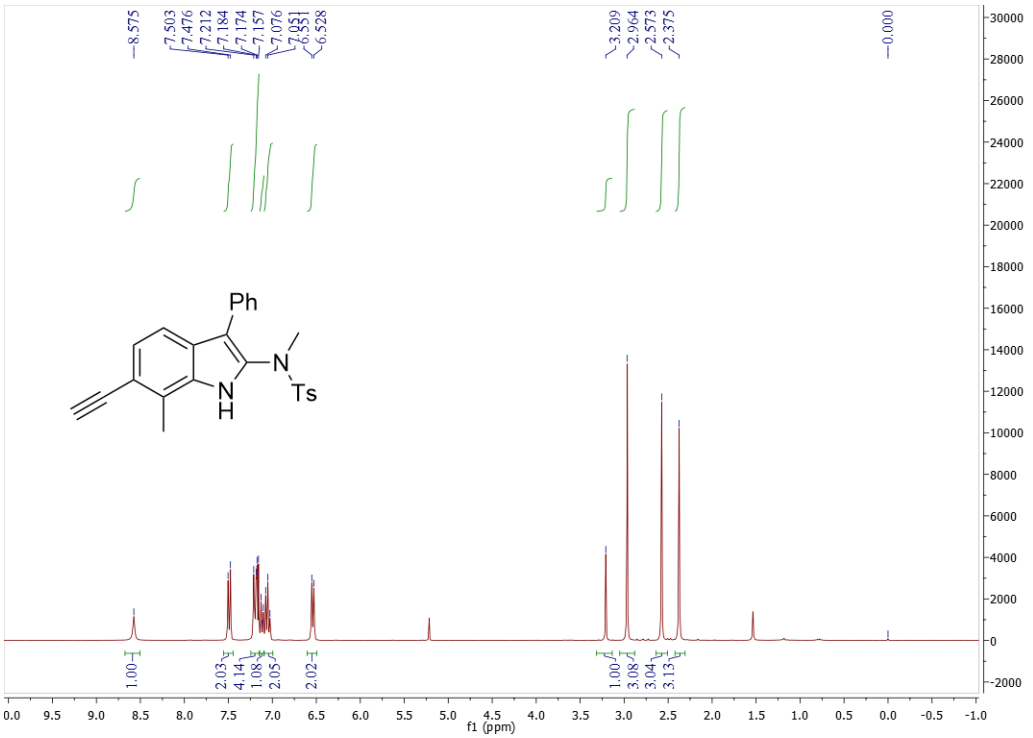
^{1}H NMR of compound **3a'** in DMSO-d_6



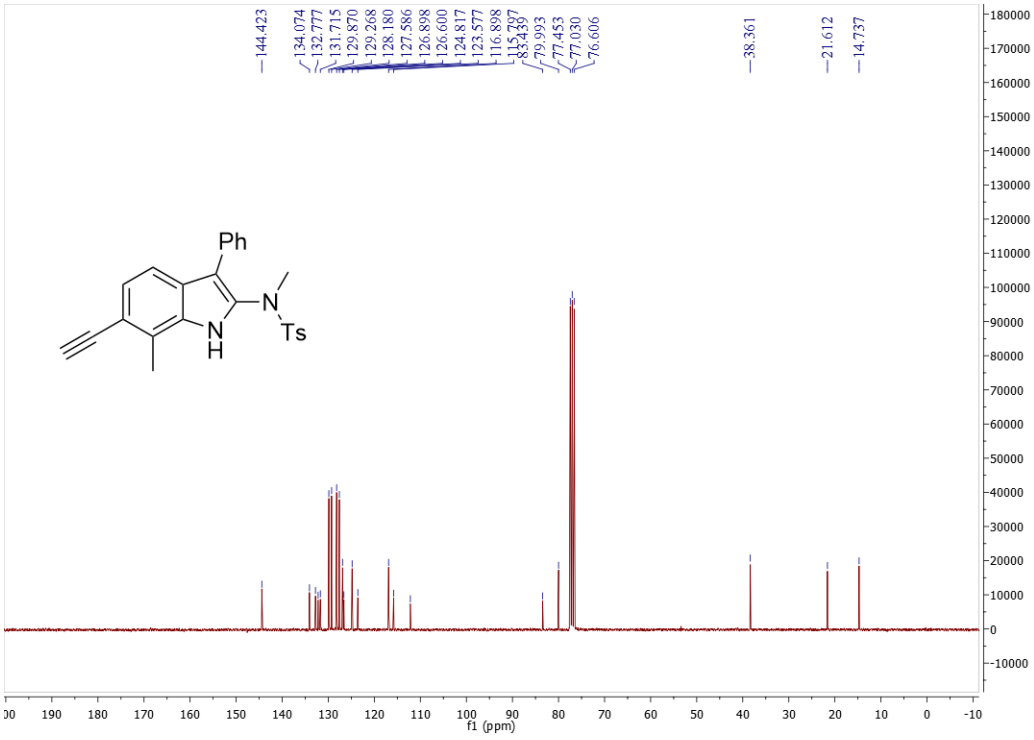
^{13}C NMR of compound **3a'** in DMSO-d_6



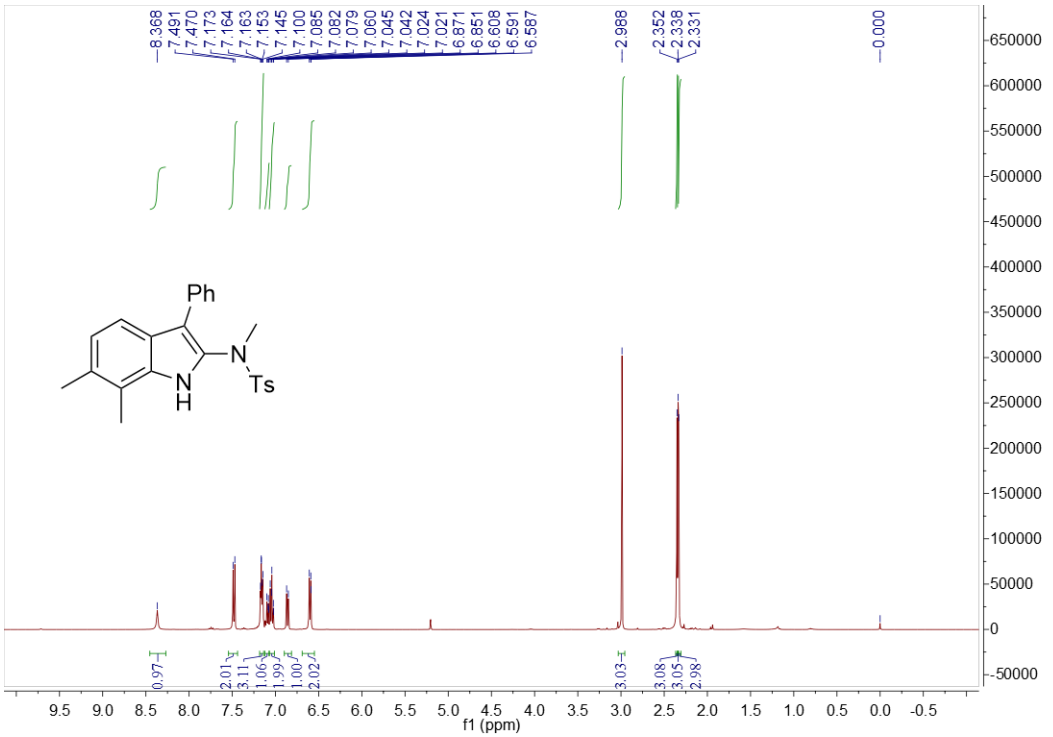
^{1}H NMR of compound **3a"** in $CDCl_3$



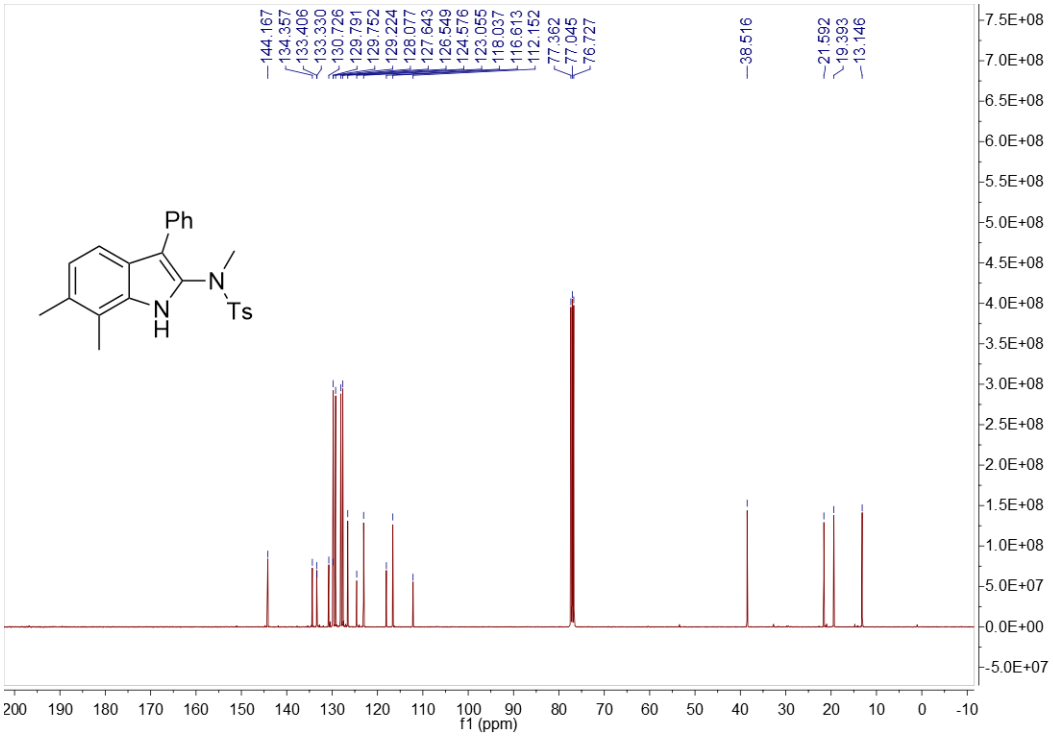
^{13}C NMR of compound **3a"** in $CDCl_3$



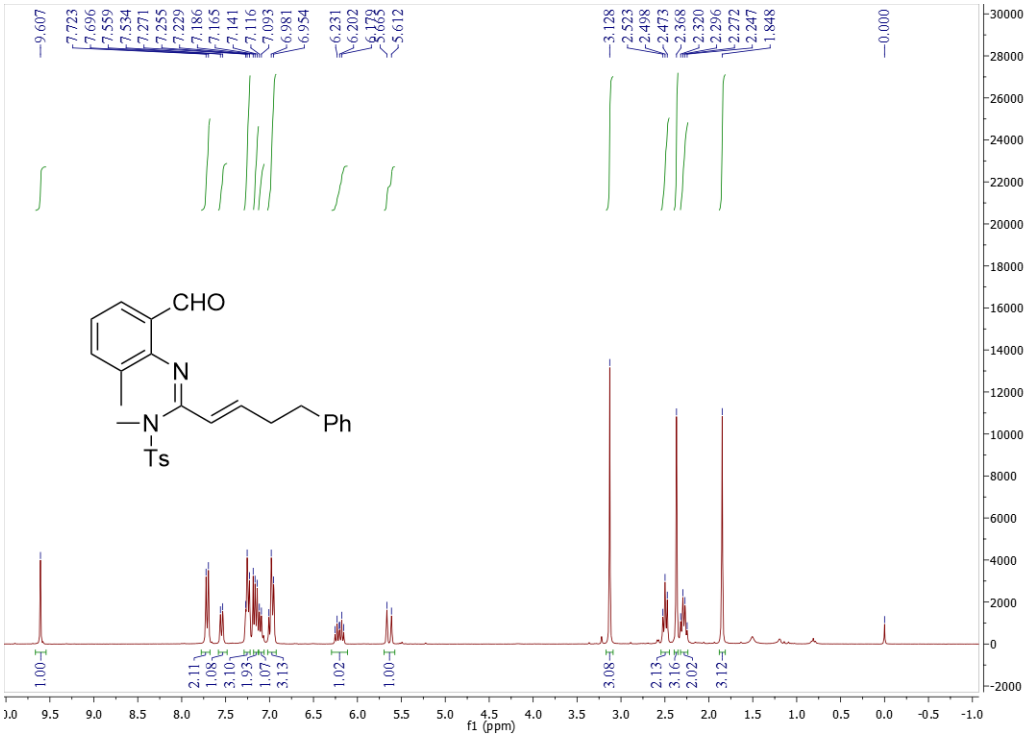
^{13}C NMR of compound **3a'''** in $CDCl_3$



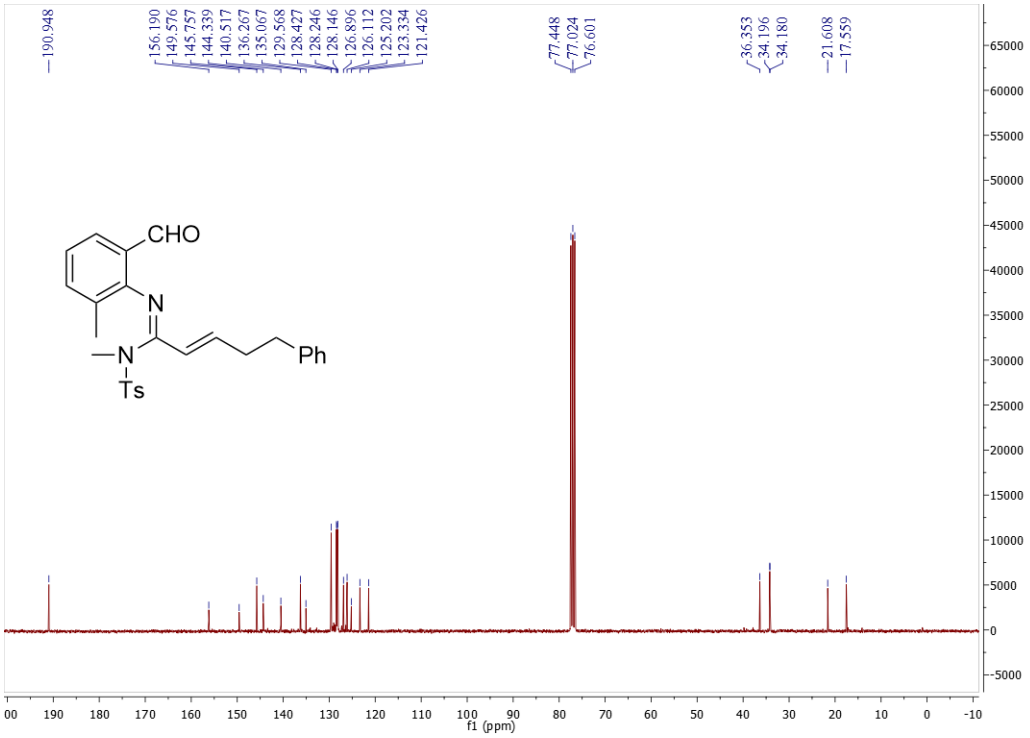
^{13}C NMR of compound **3a'''** in $CDCl_3$



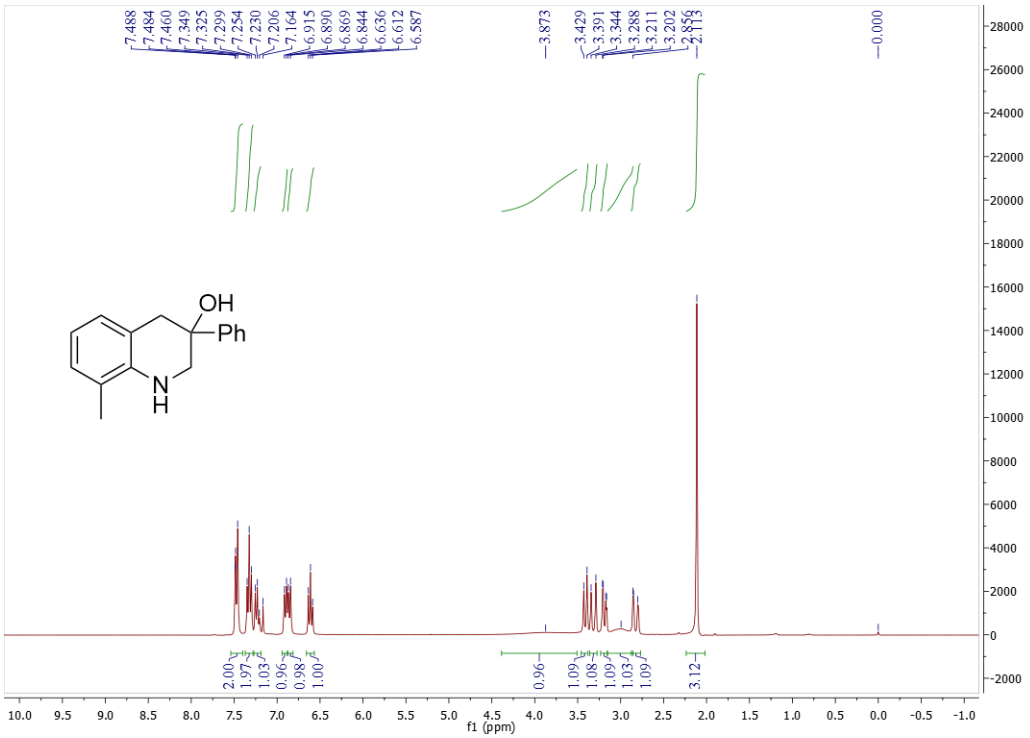
^{1}H NMR of compound **8** in $CDCl_3$



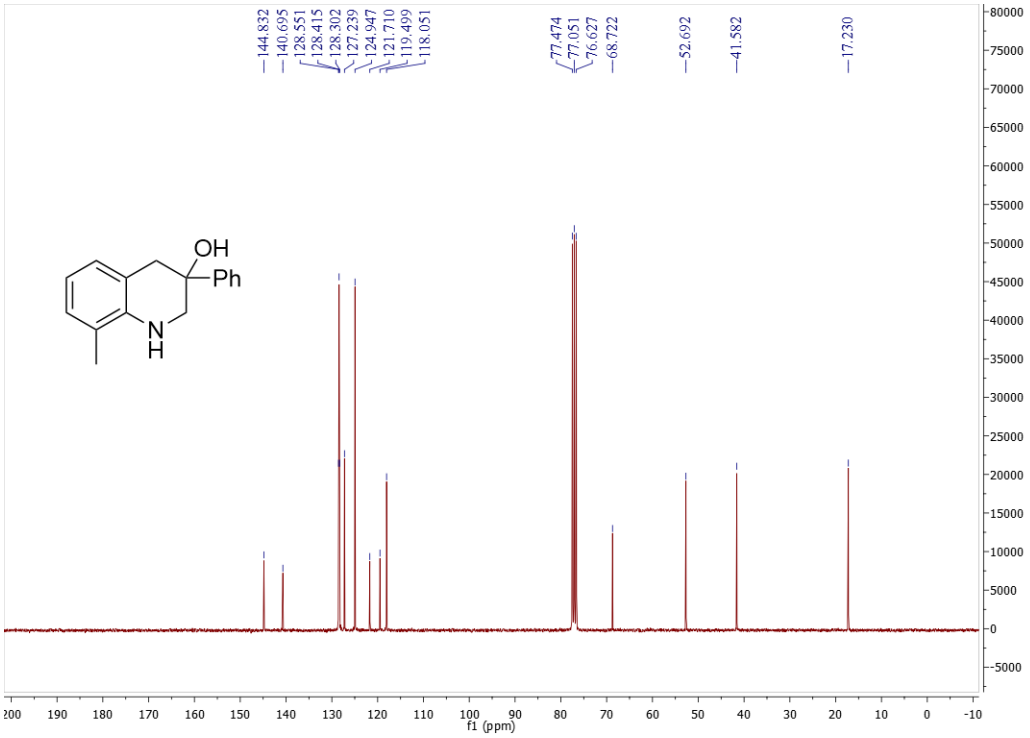
^{13}C NMR of compound **8** in $CDCl_3$



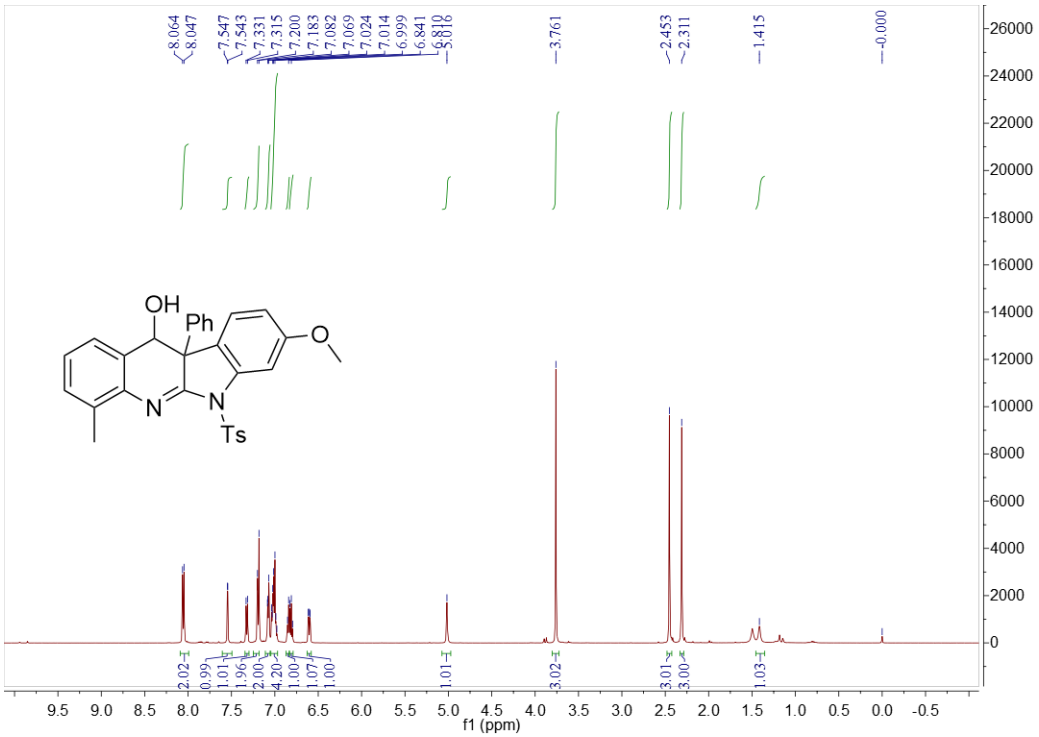
^{1}H NMR of compound **9** in $CDCl_3$



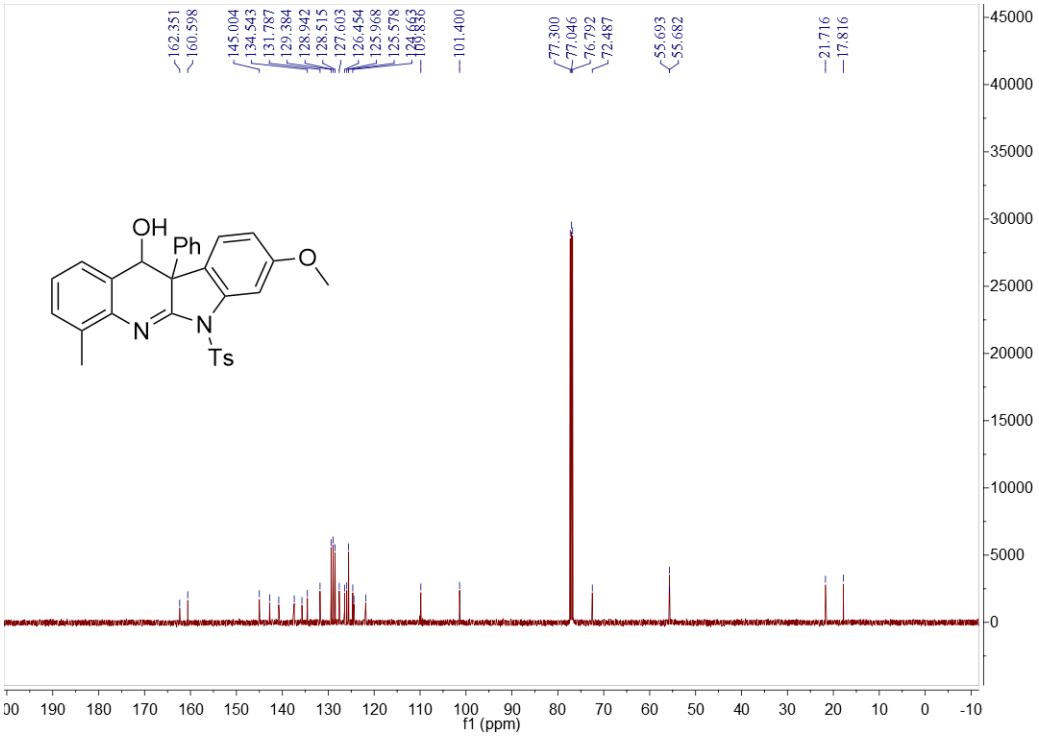
^{13}C NMR of compound **9** in $CDCl_3$



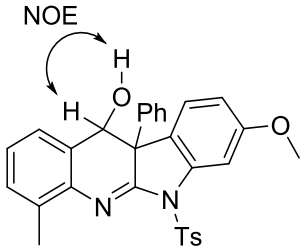
^{1}H NMR of compound **10** in $CDCl_3$

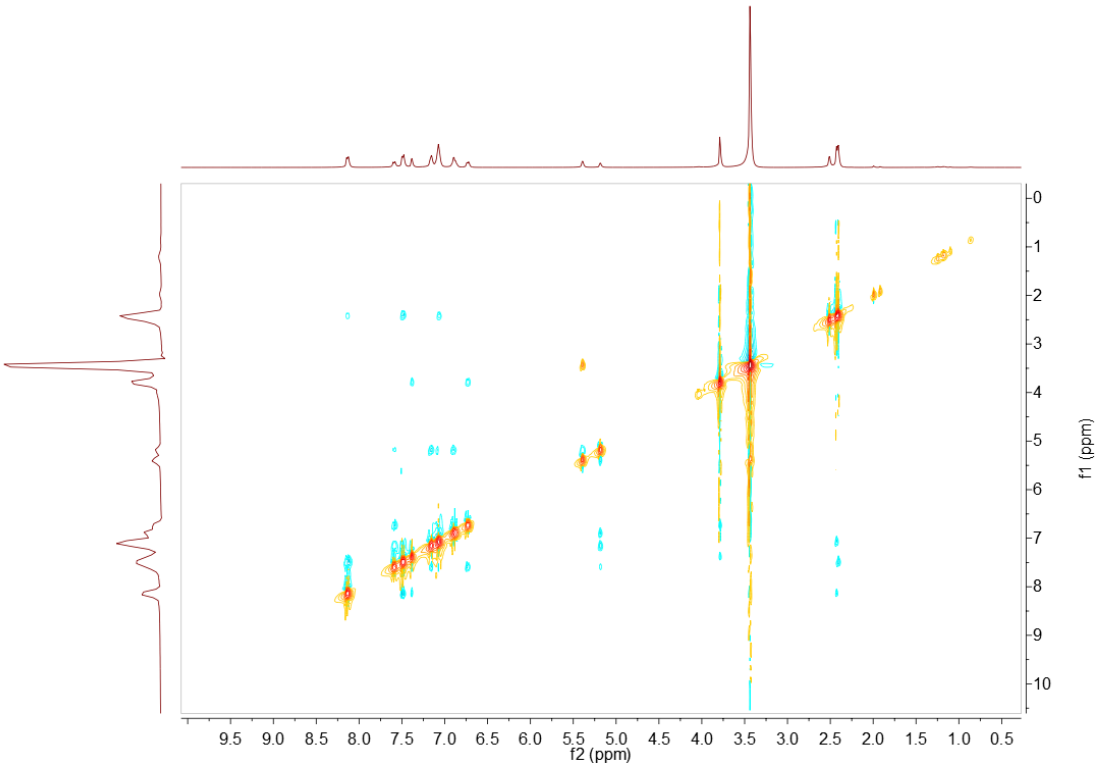


^{13}C NMR of compound **10** in $CDCl_3$

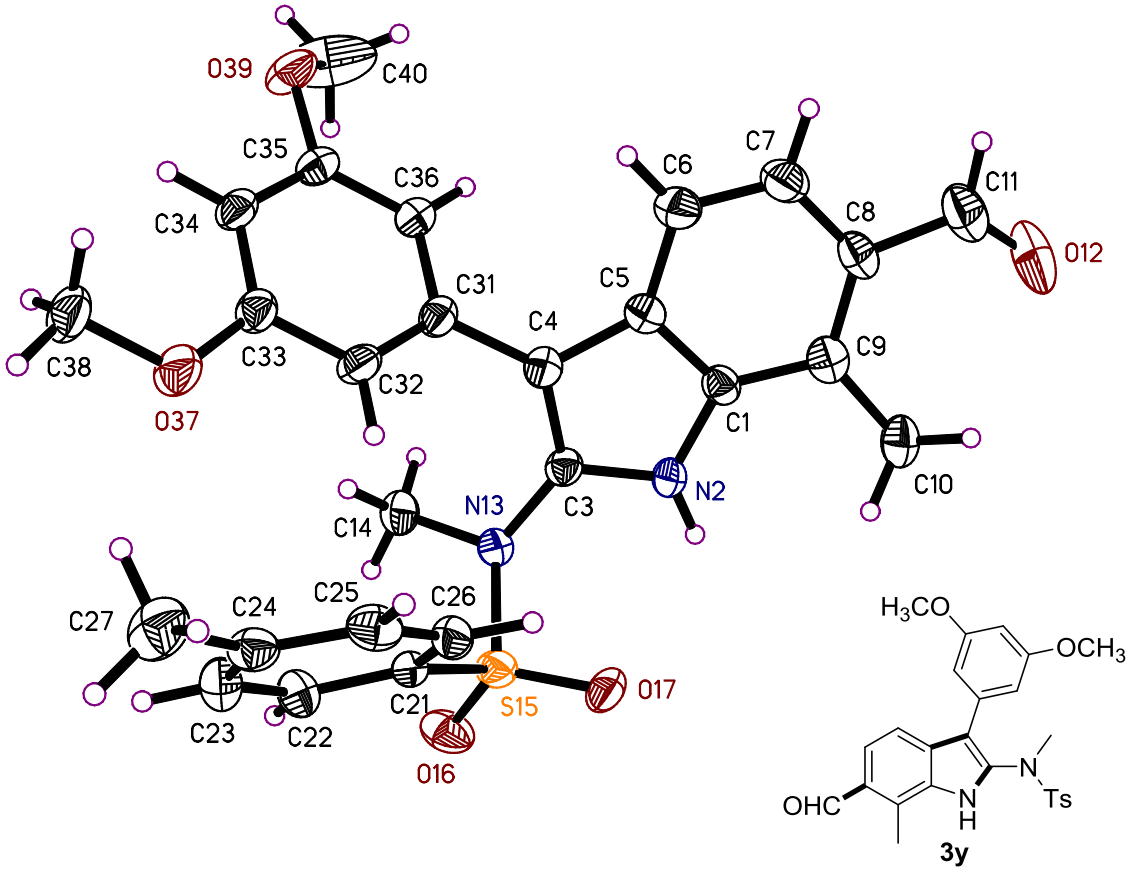


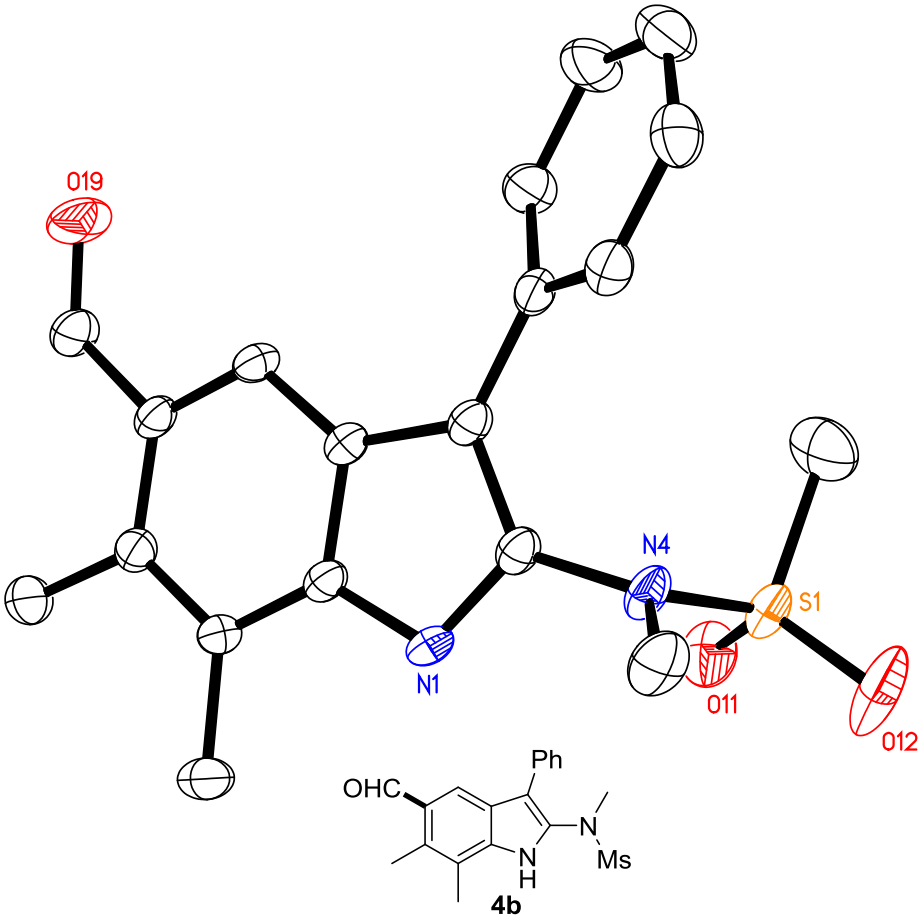
2D NOESY of **10** in DMSO-d_6



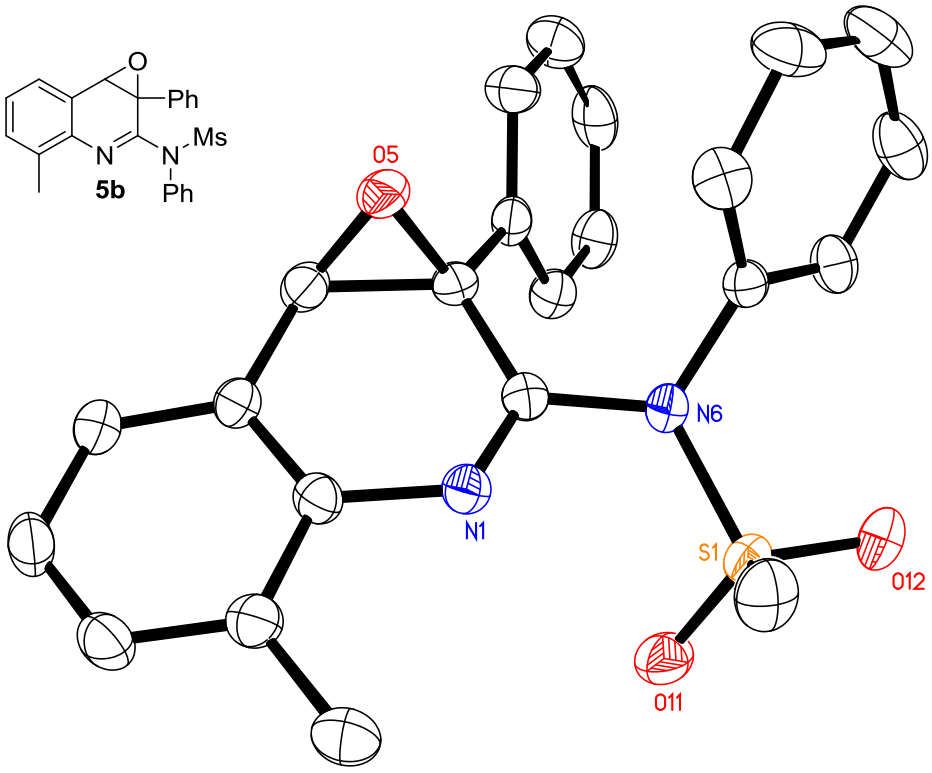


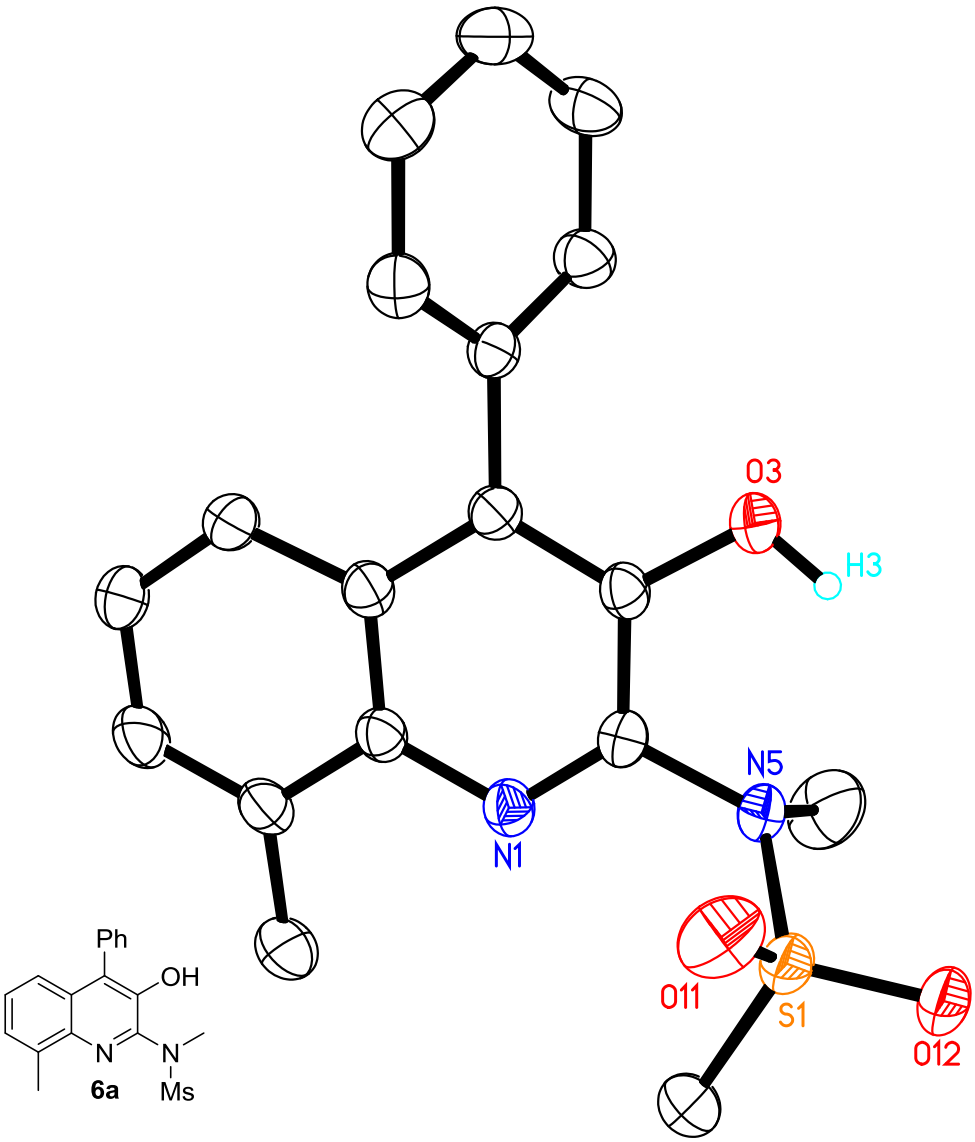
7. Solid state molecular structures of **3y**, **4b**, **5b**, **6a** and **6b**.

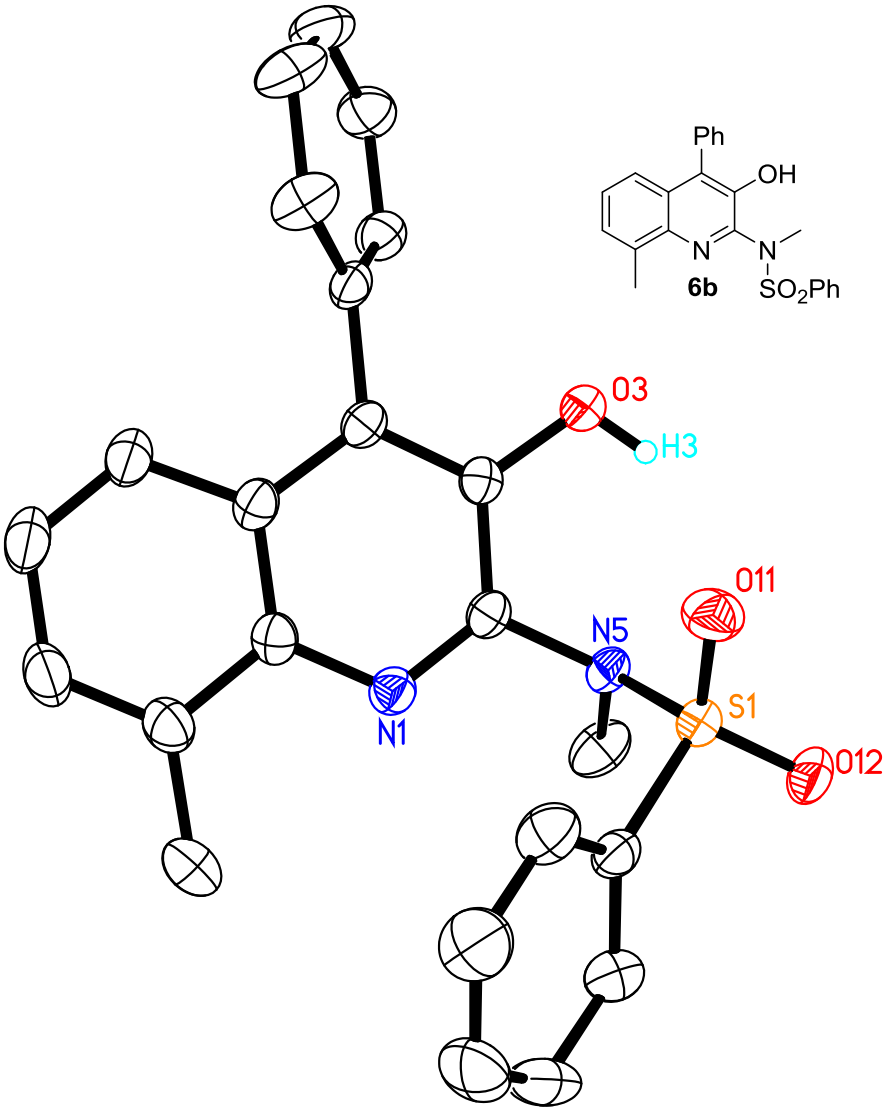




4b


O
Ph
Ms
N
N
Ph
5b
O5
N6
N1
S1
O12
O11


O3
H3
N5
N1
O11
S1
O12
Ph
OH
N
N
Ms
6a


Ph
OH
N
N
SO2Ph
6b
O3
H3
O11
N5
S1
N1
O12

8. Computational Details

Gaussian 09[1] was used to fully optimize all the structures reported in this paper at the M06 level of theory.[2] For all the calculations, solvent effects were considered using the CPCM solvation model with dichloromethane as the solvent.[3] The effective core potential of Hay and Wadt with a double-ξ valence basis set (LANL2DZ) was chosen to describe gold.[4] The 6-31G(d) basis set was used for other atoms.[5] A polarization function was also added for Au (ξ_d = 1.050).[6] This basis set combination will be referred to as BS1. Frequency calculations were carried out at the same level of theory as those for the structural optimization. Transition structures were located using the Berny algorithm. Intrinsic reaction coordinate (IRC) calculations were used to confirm the connectivity between transition structures and minima.[7] To further refine the energies obtained from the CPCM/M06/BS1 level, we carried out single-point energy calculations using the M06 functional method with SMD[8] solvation model in dichloromethane along with a larger basis set (BS2) for all the optimized structures. BS2 utilizes the def2-TZVP basis set[9] on all atoms. We also employed the D3 empirical dispersion correction for all the single point calculations. Tight convergence criterion and ultrafine integral grid were exploited to increase the accuracy of the single point calculations. In this work, the free energy for each species in solution was calculated using the following formula:

$$G = E(BS2) + G(BS1) - E(BS1) + \Delta G^{1atm \rightarrow 1M} \quad (1)$$

where $\Delta G^{1atm \rightarrow 1M}$ = 1.89 kcal/mol is the free-energy change for compression of 1 mol of an ideal gas from 1 atm to the 1 M solution phase standard state.[10]

[1] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L.

Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford CT, **2009**.

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[6] A. Höllwarth, M. Böhme, S. Dapprich, A. Ehlers, A. Gobbi, V. Jonas, K. Köhler, R. Stegmann, A. Veldkamp, G. Frenking, *Phys. Lett.* **1993**, *208*, 237.

[7] a) K. Fukui, *Acc. Chem. Res.* **1981**, *14*, 363; b) K. Fukui, *J. Phys. Chem.* **1970**, *74*, 4161.

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[9] F. Weigend, F. Furche, R. Ahlrichs, *J. Chem. Phys.* **2003**, *119*, 12753.

[10] J. Ochterski, W. Thermochemistry, Gaussian, Gaussian, Inc., Wallingford, CT, **2000**, pp. 1–19.

Table S1 Cartesian coordinates and total energies for all of the calculated structures.

i

E (M06-D3-CPCM/BS1) = -1491.79362436 au

H (M06-D3-CPCM/BS1) = -1491.684573 au

G (M06-D3-CPCM/BS1) = -1491.737094 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -1492.37326996 au

C	3.12286700	-1.96272700	0.00031900
C	3.97737400	-0.86696000	0.00059300
C	3.44117200	0.41794000	0.00025700
C	2.06861800	0.56321900	-0.00021700
C	1.74942200	-1.75590900	-0.00009900
H	3.50511100	-2.97891100	0.00037800
H	5.05456800	-1.01147200	0.00071600
H	4.05675100	1.31381000	0.00039500
H	1.02732200	-2.56897900	-0.00055900
C	1.39897500	1.90599800	-0.00047600
O	2.03777200	2.93612400	-0.00062000
O	0.08327800	1.88233800	-0.00026700
Au	-0.73214300	0.02523200	0.00006700
Cl	-2.89849700	0.89095900	0.00051600
Cl	-1.57965400	-2.15626400	-0.00059500
N	1.25788100	-0.51352200	-0.00000900

ii

E (M06-D3-CPCM/BS1) = -1221.37612478 au

H (M06-D3-CPCM/BS1) = -1221.082637 au

G (M06-D3-CPCM/BS1) = -1221.152862 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -1221.78985614 au

C	-5.39738900	-0.13623600	0.07642100
C	-4.20863100	-0.84071100	0.21705500
C	-2.97923500	-0.16541200	0.18573800
C	-2.96784000	1.22661500	0.00571000
C	-4.15945500	1.92323200	-0.14574800
C	-5.37578600	1.24462300	-0.10798000
H	-6.34662600	-0.66805200	0.10571500
H	-4.21692300	-1.92070400	0.35382700
H	-2.01235800	1.74929100	-0.01363900
H	-4.14030000	3.00206000	-0.28902400
H	-6.30901100	1.79312400	-0.22247000
C	-1.75043800	-0.87585800	0.33122600
C	-0.69168400	-1.45728100	0.45016300
S	1.64029100	-1.73986100	-0.63872300
O	2.79703900	-2.56705300	-0.32970400
O	0.93278100	-1.87258500	-1.90118200

C	2.04677700	-0.04195900	-0.37551500
C	3.11283800	0.28134800	0.46181200
C	1.24578300	0.94621900	-0.94822500
C	3.38156400	1.61935900	0.71699300
H	3.72775900	-0.50540800	0.89440600
C	1.53130700	2.27671000	-0.67683300
H	0.42220500	0.67354900	-1.60479800
C	2.59942500	2.63250900	0.15405800
H	4.21593500	1.88580600	1.36487200
H	0.91614700	3.05909400	-1.12065800
C	2.91418300	4.07373100	0.41195600
H	3.57615100	4.47300700	-0.36908500
H	2.00687200	4.68932100	0.41164400
H	3.42548600	4.20904700	1.37205300
N	0.48831700	-2.10042500	0.58303400
C	1.00787000	-2.27278500	1.94948700
H	0.22314600	-2.74883200	2.54347300
H	1.87986100	-2.92935700	1.91573400
H	1.27451100	-1.30873000	2.40546700

TS_i

E (M06-D3-CPCM/BS1) = -2713.17253935 au

H (M06-D3-CPCM/BS1) = -2712.769866 au

G (M06-D3-CPCM/BS1) = -2712.869265 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2714.1549846 au

C	4.63470900	-0.45331400	-1.42864500
C	4.28273600	0.03767900	-2.68082300
C	2.93909400	0.11972000	-3.02445700
C	1.97596300	-0.28406800	-2.11569200
C	3.63291400	-0.84323400	-0.55294200
H	5.67230800	-0.53518800	-1.11887500
H	5.05068900	0.35331700	-3.38283000
H	2.59657400	0.49478500	-3.98543700
H	3.84370400	-1.23838800	0.43806300
C	0.49667000	-0.20383400	-2.45352600
O	-0.30735700	-0.62278300	-1.54709800
O	0.18139700	0.23728400	-3.55305100
N	2.34376600	-0.75389200	-0.90725200
C	3.85055000	3.07525600	-0.11022100
C	2.54730100	2.59641400	-0.09204800
C	2.14078500	1.72225700	0.92750900
C	3.05567800	1.32590900	1.91441700
C	4.35202400	1.82323000	1.89320900
C	4.75333300	2.69407600	0.88155400

H	4.16267900	3.75315900	-0.90224100
H	1.83017000	2.88944900	-0.85864900
H	2.73762400	0.62790400	2.68871500
H	5.05608200	1.52229600	2.66636100
H	5.77267800	3.07444900	0.86402000
C	0.79216200	1.21843800	0.93242400
C	-0.41997200	1.48999600	1.06090200
S	-2.66352700	2.29116700	-0.11874500
O	-3.33411000	3.46029500	0.42285500
O	-1.73028800	2.38506400	-1.22267600
C	-3.82283700	0.99135500	-0.34261100
C	-5.12606000	1.16122300	0.12265000
C	-3.39628900	-0.18674600	-0.95592800
C	-6.02659600	0.11917000	-0.04498600
H	-5.42237800	2.09168800	0.60190600
C	-4.31775600	-1.21230400	-1.10486400
H	-2.36561700	-0.29874000	-1.30077500
C	-5.63838300	-1.07588800	-0.65961700
H	-7.05037000	0.23208500	0.30915400
H	-4.00903000	-2.14383700	-1.57834600
C	-6.62240800	-2.18588200	-0.85931200
H	-7.06391800	-2.13430400	-1.86431800
H	-6.14287100	-3.16767600	-0.76857700
H	-7.44526200	-2.13156500	-0.13748800
N	-1.68930200	1.67194900	1.22866000
C	-2.36112400	1.54808400	2.53270900
H	-2.60331400	2.54301900	2.91766400
H	-3.27459200	0.95618900	2.40901500
H	-1.68632300	1.02560500	3.21327100
Au	0.80542800	-1.21059700	0.38665400
Cl	-1.08308100	-1.65968100	1.69653700
Cl	2.02045900	-3.04068800	1.42436100

TS_{ii}

E (M06-D3-CPCM/BS1) = -2713.17067375 au

H (M06-D3-CPCM/BS1) = -2712.768298 au

G (M06-D3-CPCM/BS1) = -2712.869894 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2714.15336612 au

C	-4.84161100	-1.43608800	0.74392000
C	-4.62875100	-1.46163300	2.11755900
C	-3.33027100	-1.36853300	2.60777500
C	-2.29004500	-1.24933800	1.69928100
C	-3.74425300	-1.31672900	-0.10414000
H	-5.84181800	-1.50387600	0.32496400

H	-5.46862900	-1.55282300	2.80216500
H	-3.10343800	-1.38164500	3.67063300
H	-3.84829500	-1.28839500	-1.18811800
C	-0.86829900	-1.12643800	2.17190000
O	0.07309700	-1.01915300	1.25956600
O	-0.59954500	-1.13311000	3.35859200
N	-2.50768000	-1.22974900	0.37882500
C	-4.16411700	2.33565800	1.27623800
C	-2.82427600	2.04738900	1.05825400
C	-2.35965100	1.84291400	-0.25097200
C	-3.25086500	1.91877100	-1.33176500
C	-4.58790300	2.20961200	-1.09929000
C	-5.04760900	2.41691300	0.20071700
H	-4.52143800	2.49609500	2.29149200
H	-2.12275100	1.98501000	1.88996800
H	-2.88095000	1.74310600	-2.34023000
H	-5.27739800	2.27406200	-1.93857700
H	-6.09753800	2.64276800	0.37604000
C	-0.97711400	1.53724900	-0.45503000
C	0.22752600	1.80630500	-0.60236800
S	2.49138600	2.34236500	0.66997500
O	3.17747400	3.58702400	0.37121900
O	1.56028700	2.22932300	1.77553000
C	3.64264700	1.01664400	0.65175300
C	4.95581700	1.27232700	0.25822500
C	3.21570200	-0.25532700	1.03292300
C	5.86312800	0.22344700	0.26525600
H	5.25616300	2.27479300	-0.03801100
C	4.14438800	-1.28514400	1.02734100
H	2.17978500	-0.44420000	1.31904400
C	5.47435600	-1.06328600	0.65317600
H	6.89448000	0.40405000	-0.03480300
H	3.82932700	-2.28788300	1.31427900
C	6.46731800	-2.18269100	0.68739800
H	6.88238600	-2.29972700	1.69817300
H	6.00328600	-3.13852700	0.41711300
H	7.30754600	-1.99840000	0.00834300
N	1.50197700	2.01990200	-0.75813500
C	2.16972500	1.89711700	-2.06174500
H	2.99353300	2.61534300	-2.10858500
H	2.54314100	0.87330000	-2.19059500
H	1.44300600	2.12810400	-2.84438200
Au	-0.46598600	-0.91547800	-0.70567700
Cl	1.45503600	-2.25469500	-1.37426500

Cl	-1.18123000	-0.69911800	-2.92823800

TS_{iii}

E (M06-D3-CPCM/BS1) = -2713.16917053 au

H (M06-D3-CPCM/BS1) = -2712.766771 au

G (M06-D3-CPCM/BS1) = -2712.867156 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2714.14850584 au

C	4.09808200	-1.55152800	-1.37445300
C	3.64305300	-2.54550600	-2.23123300
C	2.32039300	-2.96807700	-2.14025200
C	1.48857100	-2.38194300	-1.20579500
C	3.21642300	-0.98877600	-0.46092200
H	5.12615900	-1.20219000	-1.40033200
H	4.31498000	-2.99502300	-2.95809500
H	1.90652900	-3.75186200	-2.76964200
H	3.51768000	-0.21564400	0.24391800
C	0.06680700	-2.84409400	-1.00352900
O	-0.55483600	-2.32547600	0.00645800
O	-0.41759800	-3.67596000	-1.75676800
N	1.94491300	-1.39593400	-0.40534600
C	3.88139100	2.24404500	-1.94848300
C	2.57608800	1.97402100	-1.56311600
C	2.23124400	1.99525600	-0.20181300
C	3.20635700	2.28266600	0.76458600
C	4.50870700	2.55598800	0.36410900
C	4.84994600	2.53316900	-0.98720000
H	4.14584700	2.22735000	-3.00382000
H	1.80974800	1.73989900	-2.30130200
H	2.93474300	2.26950000	1.81794100
H	5.26413600	2.78252800	1.11357500
H	5.87335900	2.74126700	-1.29267400
C	0.87620200	1.68311100	0.17429700
C	-0.28798100	2.14904800	0.13859800
S	-2.46366700	2.25387300	-1.36266500
O	-3.34698800	3.40184100	-1.43789900
O	-1.46727000	1.96594600	-2.37517700
C	-3.36043200	0.80966900	-0.93937700
C	-4.61485200	0.93705900	-0.34273600
C	-2.76759100	-0.43462600	-1.15580300
C	-5.28507400	-0.21767900	0.03299600
H	-5.06211100	1.91801900	-0.19642100
C	-3.46226500	-1.57307200	-0.77949200
H	-1.78654700	-0.51031900	-1.62127400
C	-4.72108800	-1.48159900	-0.17542300

H	-6.26972400	-0.13988600	0.49172600
H	-3.00564400	-2.54822500	-0.94316600
C	-5.43971500	-2.72140100	0.25645900
H	-5.02098500	-3.10070200	1.19887100
H	-6.50718800	-2.53620700	0.41981200
H	-5.33410800	-3.52234100	-0.48517300
N	-1.51208100	2.55065800	0.11570700
C	-2.20194300	3.18222200	1.25263100
H	-2.53207100	4.18288100	0.96291700
H	-3.05941600	2.56584900	1.54432100
H	-1.49859600	3.23529100	2.08572100
Au	0.52925300	-0.64569800	0.88924100
Cl	-1.25200500	-0.01899700	2.27656100
Cl	2.25910500	-0.39474200	2.80202700

TS_{iv}

E (M06-D3-CPCM/BS1) = -2713.16618552 au

H (M06-D3-CPCM/BS1) = -2712.763659 au

G (M06-D3-CPCM/BS1) = -2712.862911 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2714.14810723 au

C	-3.88682700	-1.14599100	-2.78417600
C	-2.68995900	-1.31450200	-2.10501000
C	-2.69052000	-1.42813700	-0.70472400
C	-3.89805500	-1.36442500	0.00295400
C	-5.08976900	-1.20105500	-0.69021500
C	-5.08906200	-1.08860900	-2.07939900
H	-3.88371400	-1.05954600	-3.86890700
H	-1.74311600	-1.36091600	-2.64223700
H	-3.88135800	-1.42745400	1.08880000
H	-6.02802000	-1.15613100	-0.14072300
H	-6.02700700	-0.95474100	-2.61484700
C	-1.42628600	-1.59407300	-0.04552700
C	-0.45871400	-2.33275000	0.21917000
S	1.74673500	-3.18575900	-0.89683100
O	2.59544100	-4.29330000	-0.49934200
O	0.91357600	-3.22933900	-2.08330600
C	2.64848900	-1.67840600	-0.86314500
C	3.86051500	-1.63303000	-0.17478200
C	2.13904100	-0.56853400	-1.53551600
C	4.57905900	-0.44841300	-0.17914000
H	4.23939200	-2.51774000	0.33248600
C	2.88088800	0.60592100	-1.52805000
H	1.19570100	-0.62838000	-2.07576800
C	4.10675900	0.68109100	-0.85974000

H	5.53500800	-0.39695000	0.34072900
H	2.50815100	1.47676600	-2.06866800
C	4.92129700	1.93711800	-0.87193900
H	5.07602900	2.31687100	0.14764600
H	5.91813200	1.75288900	-1.29330900
H	4.44489000	2.72644500	-1.46479300
N	0.61709500	-3.02325500	0.44539800
C	0.95345700	-3.64175500	1.73818800
H	0.92631700	-4.73058800	1.64713700
H	1.94971800	-3.31411100	2.05140400
H	0.21628100	-3.29875600	2.46788600
C	2.14850000	3.96803900	-0.02158000
C	1.41646100	4.64933900	-0.98766600
C	0.16380800	4.16982800	-1.35926100
C	-0.31329500	3.02394800	-0.74851100
C	1.62159500	2.80755300	0.53589300
H	3.12227200	4.32327100	0.30466700
H	1.81508800	5.55324500	-1.44140000
H	-0.46109900	4.66575100	-2.09769300
H	2.14949300	2.21804300	1.28463700
C	-1.68022400	2.47470600	-1.03930800
O	-2.04463400	1.42499900	-0.34037100
O	-2.40810200	2.99385600	-1.86278100
Au	-0.63248800	0.61898900	0.88948700
Cl	1.13138500	-0.20998600	2.19751100
Cl	-2.31129300	0.09455600	2.78015800
N	0.41888500	2.36746500	0.16570300

iii

E (M06-D3-CPCM/BS1) = -2713.1892791 au

H (M06-D3-CPCM/BS1) = -2712.785237 au

G (M06-D3-CPCM/BS1) = -2712.885953 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2714.17135705 au

C	-4.05991300	-0.15369000	2.91318600
C	-3.81478700	-1.45589800	3.33700800
C	-2.97546500	-2.26499600	2.58599400
C	-2.39507000	-1.77619400	1.42023400
C	-3.45657100	0.28960500	1.75007700
H	-4.70898900	0.51716300	3.46797800
H	-4.27543700	-1.83460800	4.24647600
H	-2.74210500	-3.28773100	2.86583800
H	-3.61783700	1.29578000	1.36927900
C	-1.45371000	-2.68055800	0.59774100
O	-1.22516200	-3.78839500	1.10244100

O	-0.99500900	-2.18615100	-0.46340700
Au	-1.86023300	0.23684500	-0.75889200
Cl	-1.03263500	1.25932900	-2.71294500
Cl	-3.91942500	-0.37340600	-1.83021600
C	-0.73283500	4.57570700	0.71524000
C	-0.90566200	3.26607200	0.28461200
C	0.01101300	2.27489900	0.65743800
C	1.10029600	2.62141300	1.47469500
C	1.26866600	3.92995000	1.89812900
C	0.35199300	4.91044400	1.51971400
H	-1.45084100	5.33717000	0.41883600
H	-1.74967300	3.01034400	-0.35468600
H	1.81204400	1.85554800	1.78319700
H	2.11592300	4.18679600	2.53028800
H	0.48397800	5.93668100	1.85641700
C	-0.14948200	0.88887200	0.22873500
C	0.66474800	-0.10033700	0.40640300
S	2.50480800	-1.50132900	-0.93718800
O	2.51340100	-2.94900300	-0.92087900
O	1.92736200	-0.71626500	-2.00502300
C	4.05375900	-0.85383600	-0.43457400
C	5.01357900	-1.71332000	0.09555200
C	4.26759800	0.52103600	-0.55201700
C	6.22358800	-1.17233200	0.50773600
H	4.81868200	-2.78088600	0.17084500
C	5.48173800	1.03404600	-0.12892100
H	3.50002500	1.16972300	-0.97143900
C	6.47473100	0.19895900	0.40186600
H	6.98983700	-1.82714900	0.91962300
H	5.67145800	2.10322900	-0.21232000
C	7.78972100	0.77236100	0.82642400
H	8.43279400	0.94828200	-0.04694800
H	7.66038300	1.73858000	1.32860900
H	8.32706700	0.09742800	1.50149500
N	1.46752700	-1.06399900	0.51857100
C	1.52470900	-2.00780200	1.65203200
H	2.57241200	-2.14801200	1.93624800
H	0.96884500	-1.57110900	2.48487700
H	1.07033000	-2.95479600	1.34344000
N	-2.64938000	-0.51464300	1.03775500

iv

E (M06-D3-CPCM/BS1) = -438.672231293 au

H (M06-D3-CPCM/BS1) = -438.530816 au

G (M06-D3-CPCM/BS1) = -438.57155 au
E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -438.847773279 au

C	-0.83442500	0.80867400	0.00027100
C	-0.19093500	-0.47118600	0.00022800
C	1.23539800	-0.58689000	0.00022700
C	1.92727000	0.59298000	0.00002500
C	1.29031200	1.87713300	-0.00018000
C	-0.06756100	2.00665100	-0.00001400
C	-2.16473400	0.47692200	0.00001200
H	1.91950700	2.76506300	-0.00048700
H	-0.55019100	2.98101100	-0.00004600
H	-3.08424000	1.04847100	0.00026100
C	1.87692500	-1.93438900	-0.00003600
H	1.57209700	-2.51774900	0.87991400
H	1.57159200	-2.51737400	-0.88007500
H	2.96973800	-1.85497900	-0.00030700
N	-1.06421900	-1.47083600	-0.00010400
O	-2.29995700	-0.84832000	-0.00020000
H	3.01719300	0.55860100	-0.00014100

TS_{iii-v}
E (M06-D3-CPCM/BS1) = -3151.87553508 au
H (M06-D3-CPCM/BS1) = -3151.329051 au
G (M06-D3-CPCM/BS1) = -3151.446092 au
E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.03077892 au

C	-4.83431200	2.21217900	0.45370200
C	-4.44068700	2.69633200	1.69943000
C	-3.43502200	2.04215700	2.39324900
C	-2.85553200	0.89940800	1.85168300
C	-4.21748100	1.07957200	-0.04417500
H	-5.60586100	2.70334500	-0.13168900
H	-4.90717200	3.58672400	2.11485100
H	-3.06316100	2.39882100	3.34981500
H	-4.47247600	0.66451600	-1.01680100
C	-1.70825000	0.17890700	2.56027400
O	-0.91768900	0.91994000	3.17051200
O	-1.68436800	-1.06707700	2.41218800
Au	-2.30374000	-1.20925800	-0.23642800
Cl	-1.29755400	-3.01396000	-1.35330800
Cl	-4.38644700	-2.42913800	0.00436500
C	-1.70311000	2.86982600	-2.63667900
C	-1.35843300	1.58552400	-2.23173600
C	-0.92498300	1.35988500	-0.92003300
C	-0.86637500	2.42436900	-0.01090600

C	-1.22917000	3.70193900	-0.42051700
C	-1.64150500	3.92814500	-1.73205900
H	-2.02851700	3.04297200	-3.66044800
H	-1.41418800	0.74722500	-2.92667800
H	-0.57046100	2.23783200	1.02379300
H	-1.18770800	4.52468700	0.29133900
H	-1.92297500	4.93057200	-2.04877400
C	-0.60808700	-0.00475400	-0.49448200
C	0.52762700	-0.55585200	-0.16182000
S	2.31722400	-2.45672300	-0.67593300
O	2.17215400	-3.82884800	-0.22525000
O	2.02049900	-2.04233200	-2.03145700
C	3.88269700	-1.83256800	-0.16345700
C	4.48647100	-2.36192800	0.97790500
C	4.47632900	-0.80419900	-0.89447300
C	5.69213300	-1.82301500	1.40307900
H	4.02928600	-3.19151900	1.51328300
C	5.68406600	-0.28577900	-0.45260400
H	4.00453900	-0.43161700	-1.79955100
C	6.30072800	-0.77426900	0.70466100
H	6.17694000	-2.22826200	2.29015500
H	6.16485700	0.51104400	-1.01862600
C	7.58429400	-0.17892300	1.19230100
H	8.18787500	0.20990100	0.36403400
H	7.38575000	0.66134700	1.87214700
H	8.18290600	-0.91061800	1.74692100
N	1.21078900	-1.52737500	0.35821000
C	1.22968300	-1.85035500	1.79767000
H	2.13929900	-1.45736600	2.26622500
H	0.32528500	-1.43029300	2.25588700
H	1.19925000	-2.94031200	1.88971300
N	-3.26480200	0.44287400	0.65816400
C	2.25416600	3.07141200	-1.32186100
C	2.19845900	2.10930600	-0.26839200
C	2.42904900	2.46886000	1.08856500
C	2.66862000	3.80313100	1.30458700
C	2.70503400	4.77933600	0.26225200
C	2.51455300	4.43828400	-1.04644300
C	1.98968500	2.32442000	-2.44500200
H	2.90447800	5.81436600	0.53028900
H	2.55899100	5.17191200	-1.84682000
H	1.91852900	2.55682200	-3.50044600
C	2.40986200	1.43746900	2.16667500
H	1.39204500	1.05623400	2.35649200

H	3.04667700	0.58166700	1.89247000
H	2.78494900	1.85064300	3.10951300
N	1.93159600	0.89080100	-0.75212400
O	1.79212200	1.05565500	-2.11812100
H	2.85091700	4.13529200	2.32657800

v

E (M06-D3-CPCM/BS1) = -3151.90623211 au

H (M06-D3-CPCM/BS1) = -3151.356901 au

G (M06-D3-CPCM/BS1) = -3151.471344 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.0623124 au

C	-5.01207200	2.31213800	0.20234000
C	-4.61839400	2.99347200	1.35201400
C	-3.57696500	2.48669300	2.11277100
C	-2.96260100	1.29639900	1.73611500
C	-4.35498100	1.14282400	-0.13345800
H	-5.81385500	2.67723900	-0.43264800
H	-5.11420700	3.91765700	1.64030500
H	-3.20601800	2.99194900	2.99997700
H	-4.61224500	0.57557400	-1.02509500
C	-1.80281700	0.72399800	2.54692500
O	-1.06161200	1.57140600	3.07783400
O	-1.73371800	-0.52732700	2.56221500
Au	-2.36890500	-1.07636100	-0.11195400
Cl	-1.43616100	-2.86199000	-1.33405100
Cl	-4.41921700	-2.32798900	0.34009800
C	-1.91956800	2.70472600	-2.89428200
C	-1.59558200	1.46584300	-2.35696400
C	-1.04968700	1.37694900	-1.06921100
C	-0.85020100	2.54430400	-0.32139000
C	-1.17852200	3.78149900	-0.86622700
C	-1.71043500	3.86503700	-2.15071700
H	-2.33635200	2.76572400	-3.89771600
H	-1.75199600	0.55173900	-2.93147800
H	-0.47567100	2.47174000	0.70210400
H	-1.02522800	4.68467100	-0.27842300
H	-1.96788300	4.83519500	-2.57133300
C	-0.70373200	0.05452700	-0.52673100
C	0.57083200	-0.32531100	-0.32413400
S	2.26697800	-2.35044700	-0.67832400
O	2.18253400	-3.72422800	-0.20819400
O	2.06307400	-2.00927100	-2.07911900
C	3.82081300	-1.66872100	-0.16293300
C	4.28506400	-1.93242900	1.12518700

C	4.52553600	-0.83488800	-1.02613200
C	5.44778900	-1.31199900	1.55954700
H	3.74990500	-2.61989200	1.77851400
C	5.69166400	-0.22859100	-0.57547300
H	4.16727800	-0.67615700	-2.04170000
C	6.15685400	-0.43953400	0.72545100
H	5.81711300	-1.50779000	2.56558900
H	6.25061400	0.42472400	-1.24519900
C	7.38035500	0.26599100	1.22258600
H	8.06951800	0.50377100	0.40396600
H	7.11000300	1.21564700	1.70655800
H	7.91783600	-0.33348500	1.96660100
N	1.13184300	-1.46832700	0.25052300
C	0.52209600	-2.17035800	1.38575600
H	1.31156200	-2.57580900	2.02792500
H	-0.07246100	-1.44868900	1.95735300
H	-0.12609800	-2.98893900	1.05168700
N	-3.36629500	0.65079800	0.63327400
C	2.99412600	2.30290900	-1.15726700
C	2.42599000	1.47407300	-0.14605200
C	2.76756600	1.60840000	1.21998400
C	3.72790800	2.57085800	1.46292300
C	4.32655700	3.38963600	0.46692800
C	3.96746700	3.28142900	-0.84654000
C	2.39710900	1.88964800	-2.32845700
H	5.07516700	4.11617000	0.77195800
H	4.40089800	3.90064000	-1.62608800
H	2.48787600	2.20039100	-3.36213400
C	2.15780000	0.79927300	2.31789900
H	1.07754600	0.98926800	2.43359900
H	2.29307100	-0.27482000	2.14200700
H	2.63764400	1.04755900	3.27064500
N	1.57757700	0.61408500	-0.76316100
O	1.56540700	0.89220900	-2.10970100
H	4.04206400	2.71424800	2.49634100

$TS_{v\text{-}vi}$

E (M06-D3-CPCM/BS1) = -3151.8806838 au

H (M06-D3-CPCM/BS1) = -3151.334648 au

G (M06-D3-CPCM/BS1) = -3151.454329 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.03084324 au

C	-4.59231600	0.17998600	2.69423600
C	-4.58734100	-1.05731500	3.32971300
C	-3.84771400	-2.09300200	2.78006000

C	-3.11531600	-1.88935900	1.61469400
C	-3.84337500	0.33378200	1.54132600
H	-5.16808300	1.01886600	3.07405200
H	-5.16289800	-1.21232500	4.23956100
H	-3.81285700	-3.08607200	3.21753900
H	-3.82097400	1.27861800	1.00074800
C	-2.33247500	-3.06473400	0.99605400
O	-2.42260600	-4.13227100	1.61711800
O	-1.69305700	-2.81011700	-0.05564000
Au	-2.11869800	-0.36784700	-0.81624500
Cl	-1.10039300	0.20435900	-2.87089400
Cl	-4.02593800	-1.42825100	-1.93530100
C	-3.00570700	4.00764400	-0.08878600
C	-2.33013000	2.87068200	-0.50909600
C	-1.46495700	2.19958800	0.37414800
C	-1.31703400	2.67724400	1.68875800
C	-2.01909200	3.79796600	2.10689900
C	-2.86011000	4.46740100	1.21963500
H	-3.65701000	4.53325100	-0.78349700
H	-2.44518300	2.50330000	-1.52845200
H	-0.67971300	2.13442700	2.38535700
H	-1.91246200	4.14954600	3.13077100
H	-3.40802600	5.34739800	1.54978600
C	-0.79552100	0.97101500	-0.01237900
C	0.57209800	0.80870100	0.08363600
S	2.09674000	-1.01352500	-1.22827700
O	1.39434600	-2.15540400	-1.79657700
O	2.39371600	0.15776500	-2.04218400
C	3.59198000	-1.60767400	-0.48825400
C	3.68575800	-2.94059800	-0.09402800
C	4.64998800	-0.72161000	-0.29812200
C	4.85488000	-3.37959900	0.51339200
H	2.85520900	-3.62246900	-0.26611500
C	5.80965200	-1.17956600	0.31038600
H	4.57134800	0.30966500	-0.63839800
C	5.92946000	-2.51044800	0.72494900
H	4.93764200	-4.41899600	0.82918500
H	6.64257300	-0.49309000	0.46384400
C	7.19587100	-3.00235200	1.35508100
H	7.71644700	-2.20064700	1.89191900
H	7.00383000	-3.82260900	2.05659600
H	7.88737000	-3.38418600	0.59114000
N	1.24268100	-0.43272000	0.11751000
C	0.80474100	-1.45692400	1.07764500

H	1.68341500	-1.91287200	1.55310500
H	0.21133700	-0.95895700	1.85330200
H	0.18500400	-2.22178600	0.59831600
N	-3.11828200	-0.67709100	1.03574700
C	3.30721500	2.89603400	-0.57164800
C	2.61130500	2.15464900	0.40812000
C	3.24775800	1.78805000	1.60787900
C	4.57682600	2.18415400	1.73090600
C	5.27962700	2.90321600	0.75083400
C	4.64477400	3.28018600	-0.41262300
C	2.40674600	3.17149800	-1.62470300
H	6.32007200	3.16565200	0.92194800
H	5.15002700	3.84889200	-1.18920200
H	2.61769300	3.80188100	-2.49470900
C	2.56703800	1.03353900	2.70440000
H	1.52004400	1.33608600	2.82651900
H	2.58079600	-0.04673700	2.50768700
H	3.07677200	1.20131000	3.65889800
N	1.27437500	1.97415300	0.11769400
O	1.25885900	2.68207500	-1.50210700
H	5.09529700	1.91461300	2.65096600

vi

E (M06-D3-CPCM/BS1) = -3151.92141169 au

H (M06-D3-CPCM/BS1) = -3151.373597 au

G (M06-D3-CPCM/BS1) = -3151.492578 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.07528497 au

C	-2.39093700	-3.56093200	2.42059300
C	-2.13190600	-4.57071100	1.49736300
C	-1.89311000	-4.23249700	0.17401900
C	-1.89759100	-2.89571500	-0.21321100
C	-2.39838000	-2.24877800	1.98358000
H	-2.59004200	-3.77810700	3.46576800
H	-2.12138500	-5.61212700	1.81050700
H	-1.69536900	-4.97183200	-0.59636200
H	-2.60597000	-1.42291000	2.66151100
C	-1.60108500	-2.51728300	-1.67864000
O	-1.55379400	-3.47181400	-2.46199400
O	-1.43154500	-1.29073800	-1.89582500
Au	-2.30134200	0.08716000	0.07713500
Cl	-2.61948800	2.40004900	-0.29219600
Cl	-4.56876700	-0.40877100	-0.56248700
C	-0.99950300	2.12187700	4.03766800
C	-1.26130600	1.59607700	2.79418400

C	-0.19251000	1.13186700	1.96739700
C	1.14538100	1.22635400	2.46228800
C	1.39159600	1.75367700	3.70923800
C	0.32294600	2.20188000	4.49310400
H	-1.81310300	2.47831800	4.66301400
H	-2.28366900	1.54307300	2.42476400
H	1.97416500	0.89182000	1.84144900
H	2.41039400	1.82334900	4.08040200
H	0.52246800	2.62262000	5.47657300
C	-0.42241200	0.51270200	0.73546200
C	0.70339500	0.21051500	-0.18148000
S	2.24014900	-1.70724900	-1.39824000
O	1.95172900	-3.13245000	-1.41536900
O	2.08098100	-0.90989100	-2.59745800
C	3.83936800	-1.45828800	-0.68952500
C	4.60490300	-2.56070300	-0.32330300
C	4.28552500	-0.15307000	-0.48793300
C	5.85421500	-2.34233600	0.24544300
H	4.22522200	-3.56767700	-0.48101700
C	5.52794800	0.03956000	0.09512100
H	3.65869800	0.69831000	-0.75023700
C	6.33263900	-1.04726800	0.46059100
H	6.46760700	-3.19463200	0.53544900
H	5.88120900	1.05479000	0.27562900
C	7.68560900	-0.81782500	1.06012700
H	8.42157800	-0.57946300	0.27979300
H	7.67520900	0.02768000	1.75880400
H	8.04761100	-1.70399300	1.59369100
N	1.19935300	-1.07972200	-0.16797700
C	1.08046100	-1.95808600	1.00051600
H	2.05771100	-2.08106400	1.48766500
H	0.39505900	-1.51505600	1.72680200
H	0.69363300	-2.93686600	0.70389100
N	-2.14289200	-1.94461800	0.69886300
C	1.33929700	3.54862100	-0.57408700
C	0.79915300	2.42578400	-1.24998300
C	-0.02410700	2.62506800	-2.37759600
C	-0.37546300	3.92880700	-2.72160300
C	0.06620700	5.03622400	-2.00261700
C	0.93389700	4.83787000	-0.94387900
C	2.42496500	3.48277500	0.40344900
H	-0.23868900	6.03918300	-2.29153000
H	1.34656200	5.68782000	-0.39991500
H	2.66236400	4.47397600	0.85525200

C	-0.51792400	1.46713200	-3.18163500
H	0.28902100	0.75410500	-3.39420300
H	-1.29037700	0.89284000	-2.65181300
H	-0.94644500	1.81293400	-4.12939400
N	1.16866900	1.13388000	-0.92020000
O	3.08786200	2.50529000	0.70614500
H	-1.02488900	4.07176200	-3.58542800

TS_{vi-vii}

E (M06-D3-CPCM/BS1) = -3151.91569182 au

H (M06-D3-CPCM/BS1) = -3151.369193 au

G (M06-D3-CPCM/BS1) = -3151.485008 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.06860366 au

C	1.35267200	1.76803500	3.50913800
C	0.70167700	0.91468200	4.39733000
C	0.46027100	-0.39680400	4.01913000
C	0.88372400	-0.84728000	2.77288100
C	1.72318000	1.28159700	2.26937400
H	1.57504800	2.80020300	3.76509600
H	0.39086500	1.27299400	5.37586700
H	-0.04823800	-1.10591600	4.66635600
H	2.23879700	1.89936900	1.53726900
C	0.71053300	-2.31864100	2.37725100
O	-0.32322100	-2.85987000	2.79196800
O	1.64905600	-2.78135500	1.68146800
Au	2.13694000	-0.71168100	0.05726900
Cl	3.01465300	-1.62992200	-1.92867300
Cl	4.37480800	-0.50949900	0.93362000
C	-0.74343400	-4.22540700	-1.13491000
C	-0.01000500	-3.09954400	-0.80176800
C	-0.50166100	-1.80967300	-1.11466600
C	-1.72018200	-1.70456700	-1.84347600
C	-2.42694700	-2.83395100	-2.19130000
C	-1.94643200	-4.09647200	-1.82502800
H	-0.37272300	-5.20980500	-0.86112300
H	0.90965500	-3.20488600	-0.22986200
H	-2.06183400	-0.72586400	-2.16768600
H	-3.35052500	-2.74312300	-2.75848400
H	-2.51231800	-4.98597600	-2.09491200
C	0.21028400	-0.63347100	-0.74091200
C	-0.49667900	0.66633100	-0.48787400
S	-2.85324200	1.87862500	-0.30662600
O	-2.68450000	2.86939800	0.74939200
O	-2.66792500	2.22729000	-1.70751900

C	-4.43328400	1.10875000	-0.11214200
C	-5.16455100	1.32992500	1.05061300
C	-4.92309000	0.30239300	-1.13938600
C	-6.40751900	0.72357100	1.18459600
H	-4.76103800	1.96552900	1.83617200
C	-6.16298800	-0.29655200	-0.98373700
H	-4.34858100	0.16117000	-2.05304700
C	-6.92178700	-0.09575900	0.17663500
H	-6.98971000	0.88735900	2.09046800
H	-6.55782700	-0.93077900	-1.77692600
C	-8.26784500	-0.73635200	0.31552000
H	-9.00841400	-0.22680500	-0.31607000
H	-8.24448400	-1.78568200	-0.00368900
H	-8.62997600	-0.69741300	1.34881000
N	-1.82041500	0.52257900	-0.02083400
C	-2.00317100	-0.12390700	1.28647400
H	-3.05664000	-0.38473000	1.42151500
H	-1.43317600	-1.05880100	1.32806500
H	-1.67664300	0.53938700	2.10198500
N	1.47594800	0.00666000	1.92123800
C	1.91009200	1.74033100	-2.20466400
C	1.20400500	2.27102400	-1.09507300
C	1.71605100	3.42138100	-0.45053400
C	2.97868600	3.88562500	-0.81245200
C	3.70416900	3.32218400	-1.86286400
C	3.13788400	2.29444200	-2.59266000
C	1.34971800	0.73028300	-3.07620900
H	4.67929000	3.72024400	-2.13135700
H	3.64410100	1.88469900	-3.46654400
H	1.76181800	0.69896000	-4.10284600
C	0.89836200	4.15039700	0.57259500
H	0.02350700	4.61371600	0.09526500
H	0.49532900	3.49196500	1.35078700
H	1.48786200	4.94094500	1.04996400
N	-0.02182100	1.84481100	-0.61423000
O	0.44705500	-0.05520500	-2.79075000
H	3.38854300	4.74233700	-0.27843000

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E (M06-D3-CPCM/BS1) = -3151.93603726 au

H (M06-D3-CPCM/BS1) = -3151.389368 au

G (M06-D3-CPCM/BS1) = -3151.501422 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.08718236 au

C	0.11712000	0.69502700	3.61811000

C	-0.34021400	-0.44882900	4.26262400
C	-0.13180800	-1.68322900	3.66561800
C	0.50858100	-1.76917400	2.43468800
C	0.74443600	0.55724200	2.39298100
H	-0.00151400	1.68441500	4.05052100
H	-0.84126100	-0.37776700	5.22522400
H	-0.44367800	-2.61786100	4.12194200
H	1.13379500	1.41753200	1.85685800
C	0.76584600	-3.15958500	1.81760800
O	0.33161800	-4.11086500	2.47793700
O	1.38881900	-3.16595500	0.72629000
Au	2.05606200	-0.77966900	0.03009100
Cl	3.52231600	-0.96442300	-1.80800300
Cl	3.94901000	-1.05908800	1.55960900
C	-0.81422300	-3.57129600	-2.53880500
C	-0.02739200	-2.62340900	-1.88643000
C	-0.35044100	-1.27231200	-1.97681800
C	-1.43751200	-0.87721200	-2.77216000
C	-2.21853000	-1.82413100	-3.41747100
C	-1.91155100	-3.17875300	-3.29483400
H	-0.56072100	-4.62571100	-2.44935200
H	0.80718800	-2.94895200	-1.27021200
H	-1.67530300	0.18146800	-2.88080600
H	-3.06664000	-1.50347700	-4.01973500
H	-2.52559200	-3.92438300	-3.79637400
C	0.45428400	-0.17213300	-1.32846400
C	-0.32900400	0.88276100	-0.56607400
S	-2.63180400	1.89106700	0.33242900
O	-2.35377400	2.20022100	1.72818300
O	-2.53934700	2.90752300	-0.70184800
C	-4.20493700	1.10204600	0.20515100
C	-4.90353400	0.76652800	1.35946900
C	-4.71146000	0.82905600	-1.06601800
C	-6.13890300	0.14354800	1.23224100
H	-4.48181500	0.98811500	2.33772200
C	-5.94011000	0.19774500	-1.16920700
H	-4.14763700	1.10425900	-1.95616300
C	-6.67139000	-0.15074100	-0.02544200
H	-6.69918400	-0.12535600	2.12670500
H	-6.34786600	-0.03071800	-2.15331800
C	-8.00855400	-0.81027300	-0.15935600
H	-8.77915800	-0.07439500	-0.42743700
H	-8.00169300	-1.56899500	-0.95135300
H	-8.31943700	-1.28826700	0.77620100

N	-1.60616400	0.56001000	-0.15760100
C	-1.98814000	-0.75312200	0.38648700
H	-2.81774100	-1.19118500	-0.17833100
H	-1.13804800	-1.43364300	0.34072000
H	-2.26922700	-0.63947600	1.44243400
N	0.90210000	-0.64240800	1.80974900
C	2.19625600	2.36585500	-1.59126000
C	1.28755300	2.68300100	-0.53470600
C	1.58491700	3.80004500	0.28385500
C	2.77746400	4.48269100	0.07855200
C	3.68031900	4.15492100	-0.94558200
C	3.37064400	3.13097800	-1.80266400
C	1.90179200	1.40391400	-2.55913300
H	4.59203100	4.73162900	-1.07385800
H	4.01994400	2.87644100	-2.63881400
H	2.40287000	1.43969100	-3.52932500
C	0.60955300	4.25439600	1.32407600
H	-0.37208100	4.44946500	0.87419600
H	0.43643000	3.49648900	2.09829400
H	0.96421200	5.16695500	1.81438300
N	0.10408100	2.06014900	-0.26187300
O	1.01899300	0.47442000	-2.50972300
H	3.00257100	5.32987800	0.72563000

TS_{vi-ix}

E (M06-D3-CPCM/BS1) = -3151.90341325 au

H (M06-D3-CPCM/BS1) = -3151.357196 au

G (M06-D3-CPCM/BS1) = -3151.471857 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.05341021 au

C	-0.99662600	2.98921700	-3.14744400
C	-1.06388800	4.08732600	-2.29355600
C	-1.44293000	3.89414900	-0.97403100
C	-1.74862100	2.61530500	-0.51810700
C	-1.28134000	1.73595100	-2.63758100
H	-0.72356300	3.09191400	-4.19342700
H	-0.83440900	5.08474400	-2.66121200
H	-1.53713300	4.71032000	-0.26405700
H	-1.23546200	0.84217300	-3.25745500
C	-2.29773600	2.41539600	0.90703600
O	-2.22587300	3.41265500	1.63940700
O	-2.77376600	1.28061800	1.15126300
Au	-2.16245400	-0.38205700	-0.70552700
Cl	-2.87129000	-2.61296200	-0.38615800
Cl	-4.32114000	0.10824100	-1.68942300

C	0.68919100	-3.06525200	-3.04307900
C	-0.04056400	-2.28306200	-2.16377400
C	0.57742100	-1.64028000	-1.06413600
C	1.97405800	-1.84028100	-0.90098400
C	2.69529200	-2.62927400	-1.77586400
C	2.05670800	-3.24620400	-2.85199000
H	0.18600300	-3.53824800	-3.88280200
H	-1.10707400	-2.16364400	-2.33404700
H	2.49911800	-1.36487600	-0.07883400
H	3.76468300	-2.75837000	-1.62232600
H	2.62699700	-3.86287300	-3.54342400
C	-0.16849600	-0.81364000	-0.13364000
C	0.50110600	0.25438500	0.66139300
S	2.76634900	1.74102900	1.11351000
O	2.76942900	3.13275300	0.69285600
O	2.55752300	1.36645100	2.49557400
C	4.23040100	0.94754600	0.52119200
C	5.02671600	1.58887100	-0.42385500
C	4.55995400	-0.31122000	1.02627900
C	6.17400800	0.94852500	-0.87378100
H	4.75132000	2.57375200	-0.79571200
C	5.70846500	-0.93214200	0.55797200
H	3.92295600	-0.79749600	1.76544600
C	6.53097300	-0.31426700	-0.39233000
H	6.80638100	1.43789500	-1.61339700
H	5.97978700	-1.91584200	0.93968800
C	7.78372400	-0.98654400	-0.86090200
H	8.61311500	-0.78376900	-0.16915100
H	7.66187300	-2.07523400	-0.90688000
H	8.08874200	-0.62795000	-1.85054400
N	1.53829700	0.97275000	0.12194000
C	1.72699600	1.23008000	-1.30706100
H	2.66775300	0.79633700	-1.66834300
H	0.91226100	0.78122800	-1.87342300
H	1.72725000	2.31191200	-1.48147900
N	-1.62351400	1.56916600	-1.34707900
C	-0.49522200	-1.78012700	1.95680200
C	-0.63875800	-0.42264100	2.44165800
C	-1.56879200	-0.11358800	3.46917400
C	-2.47624700	-1.10058000	3.80038100
C	-2.45965300	-2.38529200	3.21305800
C	-1.47814800	-2.73499000	2.31890100
C	0.84829900	-2.40146500	1.82208000
H	-3.18712000	-3.12552300	3.53810600

H	-1.37347400	-3.76301000	1.97726700
H	0.80512100	-3.42224000	1.38019700
C	-1.58336500	1.23496900	4.10511600
H	-0.56467300	1.55360600	4.36061000
H	-1.99669400	1.99032400	3.42169500
H	-2.18683700	1.21865600	5.01977300
N	0.08502000	0.55038500	1.87155200
O	1.89218400	-1.90501900	2.18227700
H	-3.23552400	-0.87848500	4.54960900

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E (M06-D3-CPCM/BS1) = -3151.94162062 au

H (M06-D3-CPCM/BS1) = -3151.395214 au

G (M06-D3-CPCM/BS1) = -3151.508921 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.09258636 au

C	3.60343100	3.18284400	-1.08157800
C	4.63653200	3.18731700	-0.15065600
C	4.82862600	2.06552200	0.64060500
C	3.97592200	0.97314500	0.52371900
C	2.79869100	2.06093300	-1.17112300
H	3.42110500	4.02508100	-1.74242500
H	5.29040500	4.05107900	-0.05494800
H	5.63143400	1.99177200	1.36811700
H	2.00754300	1.99959900	-1.91276200
C	4.18457900	-0.24085000	1.44492200
O	5.26814500	-0.27353000	2.03760500
O	3.21620800	-1.04572100	1.51220100
Au	1.76028900	-0.73604300	-0.62337600
Cl	0.61255700	-2.74020800	-1.11279400
Cl	3.63961400	-1.50020500	-1.99666300
C	1.43948700	2.93377800	2.32213500
C	1.17442900	1.65403100	1.85675900
C	0.20369200	1.42857500	0.86947200
C	-0.53596400	2.52690600	0.41455700
C	-0.27243700	3.80986500	0.88261000
C	0.72400000	4.02267800	1.82830400
H	2.21520100	3.07972100	3.07169600
H	1.76731400	0.81866300	2.22616600
H	-1.36398500	2.38477600	-0.27597100
H	-0.86374600	4.64398400	0.51037000
H	0.93441800	5.02758200	2.18838900
C	-0.05360400	0.01970700	0.42179300
C	-1.20632100	-0.25234400	-0.51869200
S	-3.08066500	0.16614400	-2.41966800

O	-3.09697900	1.20898200	-3.43293800
O	-3.24379600	-1.22153100	-2.80393200
C	-4.16500700	0.61613300	-1.10612700
C	-4.27969100	1.96719500	-0.78201900
C	-4.87518800	-0.36704900	-0.42375300
C	-5.11489500	2.32934400	0.26415500
H	-3.73016000	2.72170600	-1.34273700
C	-5.70882100	0.01974000	0.61539300
H	-4.76407600	-1.41140100	-0.70353100
C	-5.83769200	1.36534600	0.97631200
H	-5.21235800	3.37986900	0.53451600
H	-6.27046900	-0.73707100	1.16221200
C	-6.75581300	1.77070300	2.08676800
H	-7.76415500	1.97370600	1.69993100
H	-6.85050300	0.97954000	2.83948200
H	-6.40866100	2.68436400	2.58290900
N	-1.47938000	0.40000900	-1.66493300
C	-0.47027000	1.08691300	-2.46804800
H	-0.96573900	1.55103300	-3.32239600
H	0.00577700	1.87793600	-1.88223200
H	0.27248300	0.36324200	-2.83061200
N	2.96850400	1.00199000	-0.36552700
C	-0.41450900	-0.97280400	1.54613100
C	-1.49292600	-1.78551000	0.95568700
C	-1.94574900	-2.96304800	1.59112200
C	-1.14504500	-3.43792600	2.61031700
C	0.09434600	-2.83704900	2.99409400
C	0.51675000	-1.67455100	2.43418000
C	-1.49290500	-0.24772700	2.57898600
H	0.71389200	-3.34919300	3.72570000
H	1.48442000	-1.24046200	2.67147800
H	-1.53664000	-0.76848500	3.55561700
C	-3.15724200	-3.67203200	1.08679400
H	-4.05807500	-3.06163800	1.23691100
H	-3.07324600	-3.86015700	0.00832000
H	-3.30044100	-4.62847500	1.59944600
N	-2.01994700	-1.23651500	-0.13888700
O	-2.14631200	0.68970100	2.25314700
H	-1.44160800	-4.36096400	3.10834900

TS_{ix}

E (M06-D3-CPCM/BS1) = -3151.91478887 au

H (M06-D3-CPCM/BS1) = -3151.368951 au

G (M06-D3-CPCM/BS1) = -3151.48708 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.06522416 au

C	-1.28635000	-4.39094300	0.45820700
C	-2.62211400	-4.62483500	0.76692200
C	-3.55006500	-3.62445900	0.52247000
C	-3.13580300	-2.39520800	0.02063900
C	-0.93326900	-3.15745800	-0.05937000
H	-0.52275600	-5.15015000	0.59896500
H	-2.93560600	-5.58291800	1.17508100
H	-4.61266500	-3.75497900	0.70446700
H	0.09029700	-2.95453000	-0.36191500
C	-4.18178000	-1.29148800	-0.21633300
O	-5.35406600	-1.67859500	-0.25788800
O	-3.72460100	-0.11951700	-0.31052900
Au	-1.24689500	-0.33135700	-1.13380500
Cl	-0.62903200	1.55119600	-2.41781600
Cl	-1.92669700	-1.46761600	-3.19844900
C	-1.92057600	-1.55559100	3.43389500
C	-1.80436500	-0.72226800	2.33108300
C	-0.54862400	-0.26240800	1.89477400
C	0.58188000	-0.64076700	2.63281700
C	0.46184600	-1.47925700	3.73748500
C	-0.78359000	-1.94610400	4.13966300
H	-2.90511100	-1.90808400	3.73561000
H	-2.69426000	-0.45320800	1.76396200
H	1.56913400	-0.27365800	2.35950800
H	1.35622100	-1.76107100	4.28925000
H	-0.87164800	-2.60464900	5.00102500
C	-0.46350100	0.66762900	0.71976500
C	0.90075500	1.22764100	0.33520700
S	3.47739100	1.36067500	-0.32188500
O	3.31894000	1.72399400	-1.72217900
O	3.73377200	2.35975500	0.69938100
C	4.69687000	0.09458700	-0.18225900
C	5.18468800	-0.51659000	-1.33306500
C	5.14570700	-0.26455300	1.08843600
C	6.14662000	-1.50943300	-1.20117200
H	4.81085300	-0.21939800	-2.31065800
C	6.09980900	-1.26399500	1.19641100
H	4.74783800	0.22910300	1.97358700
C	6.61528900	-1.89651800	0.05760500
H	6.53965100	-1.99799300	-2.09177300
H	6.45823800	-1.56253800	2.18087400
C	7.66689800	-2.95344700	0.19134000
H	7.50761600	-3.56652600	1.08638300

H	7.68969100	-3.61347300	-0.68313200
H	8.66277800	-2.49871800	0.28534200
N	2.03534200	0.47627600	0.16585700
C	1.94772900	-0.91101100	-0.28831000
H	2.83782200	-1.46642400	0.01581100
H	1.09814600	-1.37481900	0.21367800
H	1.82291700	-0.97006900	-1.38044100
N	-1.83353800	-2.17680600	-0.23092400
C	-1.23919300	1.95760600	0.79207400
C	-0.34219100	2.97764900	0.38149100
C	-0.77103700	4.28784500	0.14254600
C	-2.13963600	4.54650900	0.27885000
C	-3.05766200	3.56433000	0.64106700
C	-2.63063500	2.26563500	0.93371400
C	-1.69014900	2.43618900	2.68149900
H	-4.10994100	3.81173600	0.74856400
H	-3.35195400	1.47124800	1.11636800
H	-1.92206600	1.46759300	3.15312500
C	0.20079900	5.32141000	-0.30920100
H	1.03812800	5.40800900	0.39465800
H	0.63578600	5.03090400	-1.27572700
H	-0.27451600	6.30101300	-0.41944500
N	0.93344500	2.52312200	0.18236100
O	-1.36040100	3.46698000	3.12802000
H	-2.49673200	5.55592100	0.07909600

TS_{ix-x}

E (M06-D3-CPCM/BS1) = -3151.92784731 au

H (M06-D3-CPCM/BS1) = -3151.382429 au

G (M06-D3-CPCM/BS1) = -3151.499312 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.07604059 au

C	0.94076900	-4.14504200	-0.65775500
C	0.39894000	-4.83585600	0.42240300
C	-0.71930000	-4.32143600	1.05991400
C	-1.28450600	-3.12811900	0.62043500
C	0.34833700	-2.95768300	-1.04722500
H	1.80962700	-4.51262600	-1.19575800
H	0.84348200	-5.77033700	0.75747700
H	-1.19660400	-4.81639600	1.90060200
H	0.73010800	-2.37557600	-1.88346600
C	-2.55570500	-2.58933000	1.30744100
O	-2.93059700	-3.23138000	2.29515100
O	-3.07213100	-1.56813100	0.78108700
Au	-1.55344600	-0.65412900	-1.11185900

Cl	-2.38905600	1.27352100	-2.21554300
Cl	-2.48757300	-2.04051000	-2.89676100
C	-0.14336700	-1.32982300	3.76596500
C	-0.67676900	-0.49016700	2.79418600
C	-0.03297100	-0.30779300	1.56077500
C	1.17091300	-0.99838800	1.34085300
C	1.69592500	-1.84173800	2.30832000
C	1.04318200	-2.01261700	3.52854100
H	-0.66944700	-1.45180700	4.71026200
H	-1.61290400	0.01784400	3.01095900
H	1.68460300	-0.89041500	0.38879800
H	2.62127700	-2.37882800	2.10083500
H	1.45675300	-2.67663700	4.28463400
C	-0.62550400	0.58483800	0.51929300
C	0.26509300	1.52376400	-0.23532500
S	2.76902800	2.15252500	-0.03611900
O	3.00542100	3.34105600	-0.84508300
O	2.36808500	2.28665100	1.36606200
C	4.17936600	1.09933600	-0.14935900
C	5.06247500	1.26091000	-1.21473700
C	4.39032800	0.13317900	0.83320000
C	6.16481200	0.42096600	-1.30058300
H	4.89141700	2.03710400	-1.95782400
C	5.49830000	-0.69366700	0.72771800
H	3.69907700	0.03725500	1.66842300
C	6.39849600	-0.56420600	-0.33670600
H	6.86130000	0.53354200	-2.13042300
H	5.67477900	-1.45359300	1.48857000
C	7.60600800	-1.44511100	-0.42110700
H	7.40958600	-2.43752200	0.00129200
H	7.94419200	-1.56796600	-1.45638700
H	8.44163600	-1.01161700	0.14576800
N	1.54231300	1.17235400	-0.73720000
C	1.60829400	1.09669300	-2.20747800
H	2.60374500	0.74566500	-2.49974600
H	0.87183200	0.35995200	-2.54816600
H	1.39448500	2.06719300	-2.67456100
N	-0.72506600	-2.46874500	-0.40300100
C	-1.73334900	1.51436600	0.88418800
C	-1.40057000	2.77850200	0.29360300
C	-2.28804500	3.87752700	0.29134100
C	-3.48835200	3.67597800	0.95024000
C	-3.84222900	2.42864500	1.50764900
C	-3.00879100	1.32844500	1.44777600

C	-0.68546200	2.72891700	2.28736200
H	-4.82217100	2.32599600	1.96828400
H	-3.33058400	0.34111700	1.77274900
H	0.37861500	2.49843900	2.04157100
C	-1.93201000	5.13473100	-0.42237100
H	-0.95227900	5.51302500	-0.10512800
H	-1.86058700	4.94528400	-1.50290500
H	-2.68362600	5.91248200	-0.25506000
N	-0.18158000	2.73474100	-0.37156300
O	-1.27575100	3.19231000	3.16808400
H	-4.20356400	4.49557900	1.00172200

x

E (M06-D3-CPCM/BS1) = -3151.93304872 au

H (M06-D3-CPCM/BS1) = -3151.386175 au

G (M06-D3-CPCM/BS1) = -3151.504241 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.08220195 au

C	0.96860400	-4.19376700	-0.52320700
C	0.38396100	-4.87287400	0.54160000
C	-0.75792700	-4.35011100	1.12848300
C	-1.30204100	-3.15978600	0.65492700
C	0.39205900	-3.01153000	-0.95025400
H	1.85781500	-4.56755800	-1.02225500
H	0.81336600	-5.80424300	0.90397000
H	-1.26825800	-4.83459900	1.95568400
H	0.80904100	-2.44442900	-1.77966400
C	-2.59678600	-2.61264800	1.28515200
O	-2.99211500	-3.21874700	2.28747100
O	-3.11198100	-1.62252400	0.70063500
Au	-1.50306900	-0.70135000	-1.12108300
Cl	-2.25020500	1.25945300	-2.24249300
Cl	-2.34891500	-2.09033200	-2.95473400
C	-0.25561900	-1.20908400	3.83776400
C	-0.77710100	-0.41998100	2.81841900
C	-0.10132600	-0.28123900	1.59763100
C	1.12180800	-0.95530600	1.43828200
C	1.63898700	-1.74087500	2.45712600
C	0.95193500	-1.87470000	3.66315200
H	-0.80298000	-1.30020200	4.77352100
H	-1.72076600	0.09311900	2.98803000
H	1.65939800	-0.87660900	0.49621700
H	2.58165300	-2.26480600	2.30078000
H	1.35737900	-2.49500400	4.45981500
C	-0.66738800	0.56197000	0.50015200

C	0.27238300	1.53717700	-0.17919600
S	2.79221200	2.20307100	-0.09076500
O	3.01794300	3.30817600	-1.01425900
O	2.44838100	2.46506900	1.30438300
C	4.18008600	1.11353000	-0.16055000
C	5.06471900	1.20418700	-1.23140400
C	4.37009800	0.18936600	0.86659800
C	6.15092900	0.33882300	-1.27605900
H	4.90558100	1.94526500	-2.01208500
C	5.46007200	-0.66421700	0.80179800
H	3.67504100	0.14606600	1.70352600
C	6.36414600	-0.60320200	-0.26652500
H	6.84916700	0.39726900	-2.10999300
H	5.62046800	-1.39210500	1.59697900
C	7.54984400	-1.51666700	-0.30386900
H	8.34607200	-1.14625500	0.35654500
H	7.28939000	-2.52407500	0.04283300
H	7.96912100	-1.59479900	-1.31318400
N	1.54308000	1.17341100	-0.67646200
C	1.59761400	0.94591700	-2.13021200
H	2.57779400	0.53332900	-2.39180900
H	0.83147800	0.21069200	-2.40054000
H	1.41217100	1.87380100	-2.68843600
N	-0.70552000	-2.51287400	-0.35629400
C	-1.80769400	1.46082100	0.79992500
C	-1.35288600	2.81284800	0.49248700
C	-2.31655500	3.86869500	0.25165100
C	-3.58011800	3.64662800	0.75323800
C	-3.93089300	2.39661800	1.29264300
C	-3.08720800	1.27691200	1.27354800
C	-0.81002600	3.22042300	2.11489200
H	-4.94256300	2.26973800	1.67423100
H	-3.45906100	0.28177400	1.51408000
H	0.29869600	3.25397400	2.04736900
C	-1.88628800	5.11181600	-0.42762200
H	-0.99355000	5.54189000	0.04742700
H	-1.59373200	4.87791100	-1.46201500
H	-2.68248200	5.86155900	-0.43884900
N	-0.12348100	2.75789300	-0.22693500
O	-1.51585300	3.38839500	3.03835200
H	-4.33204600	4.43034200	0.69025100

$TS_{x\text{-}xi}$

E (M06-D3-CPCM/BS1) = -3151.92605241 au

H (M06-D3-CPCM/BS1) = -3151.380591 au
G (M06-D3-CPCM/BS1) = -3151.498344 au
E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.07947379 au

C	0.35033100	-4.39277100	-0.20234400
C	-0.30647900	-4.87207900	0.92718900
C	-1.36185900	-4.14304000	1.45312200
C	-1.74532600	-2.94485200	0.85743400
C	-0.06741400	-3.19367800	-0.74980400
H	1.17301800	-4.93393200	-0.66045800
H	-0.00150600	-5.81043200	1.38508500
H	-1.92378700	-4.46808300	2.32374200
H	0.40476000	-2.77930000	-1.63814400
C	-2.95239100	-2.16860000	1.41339800
O	-3.40801200	-2.59164900	2.48235200
O	-3.34793300	-1.20262900	0.70771200
Au	-1.60152800	-0.65436600	-1.15591500
Cl	-1.96513700	1.28555900	-2.47587800
Cl	-2.66058500	-2.06770000	-2.86251000
C	-0.39825000	-0.95528000	3.79303300
C	-0.83678000	-0.19689200	2.71352100
C	-0.13746000	-0.19306500	1.49711400
C	1.02483900	-0.97874300	1.41254700
C	1.46519000	-1.72995400	2.49199900
C	0.75377400	-1.72524800	3.69077300
H	-0.96843000	-0.93902000	4.71944100
H	-1.73622600	0.40116600	2.83248300
H	1.58814100	-1.02590800	0.48513600
H	2.36703000	-2.33205600	2.38818300
H	1.09679000	-2.31846500	4.53589900
C	-0.62703300	0.61963500	0.33211900
C	0.45975600	1.47028900	-0.31770200
S	3.05173300	2.01310700	-0.45863300
O	3.32407400	2.81511000	-1.64289000
O	2.82593600	2.63878300	0.83520000
C	4.29701600	0.77408600	-0.29374600
C	5.18313700	0.53870800	-1.34023000
C	4.35590900	0.04558700	0.89444900
C	6.14431500	-0.45286400	-1.18828800
H	5.11769700	1.12314900	-2.25567200
C	5.31872000	-0.94280400	1.02188300
H	3.65607300	0.25248700	1.70288500
C	6.22588000	-1.20480900	-0.01312400
H	6.84479500	-0.64931200	-1.99893800
H	5.37566600	-1.52321900	1.94246600

C	7.27783600	-2.25693000	0.15265000
H	6.89551600	-3.12143900	0.70851300
H	7.65688300	-2.60548800	-0.81462100
H	8.13347700	-1.86345200	0.71874100
N	1.67914700	0.99964600	-0.75275600
C	1.81678500	0.05922500	-1.87216700
H	2.41450500	-0.81595800	-1.59000000
H	0.82135500	-0.26093400	-2.19563000
H	2.28611100	0.56691400	-2.72427100
N	-1.07786700	-2.49022700	-0.21201700
C	-1.62986700	1.68528100	0.63469800
C	-1.01354300	2.91774100	0.28620800
C	-1.67587300	4.17333700	0.42118300
C	-2.98677600	4.13143800	0.94674300
C	-3.56718100	2.93165700	1.30385000
C	-2.91056800	1.69119700	1.13438500
C	-0.47541600	3.70181200	2.05238500
H	-4.57566400	2.93205000	1.71111100
H	-3.42237500	0.75157000	1.34687600
H	0.49856400	4.13459000	1.75487700
C	-1.07162900	5.41718500	-0.13628800
H	0.00859300	5.47795400	0.04658600
H	-1.19277200	5.41387700	-1.22830000
H	-1.55657200	6.31160600	0.26634300
N	0.22714000	2.75260900	-0.30524700
O	-0.93888900	3.35659200	3.06302200
H	-3.52961300	5.06599900	1.07070100

xi

E (M06-D3-CPCM/BS1) = -3151.94495538 au

H (M06-D3-CPCM/BS1) = -3151.396872 au

G (M06-D3-CPCM/BS1) = -3151.515944 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.093973 au

C	-1.96381300	-4.14266100	1.23587800
C	-3.34504300	-4.17437100	1.39842000
C	-4.10859300	-3.16182600	0.83895900
C	-3.49146300	-2.11449400	0.16275400
C	-1.40525700	-3.09074800	0.53221400
H	-1.32078900	-4.92239700	1.63318700
H	-3.81841500	-4.98750900	1.94391700
H	-5.19228800	-3.14164900	0.90453900
H	-0.33502700	-3.05197600	0.34599100
C	-4.35435900	-0.97650600	-0.40930700
O	-5.56192900	-1.22386200	-0.49669100

O	-3.73458900	0.08410400	-0.69263800
Au	-1.22576600	-0.53394700	-1.08393300
Cl	-0.09647600	1.01456600	-2.47208700
Cl	-1.83191400	-1.90319200	-3.03460400
C	-2.45049500	-0.88712300	3.53155900
C	-2.15457500	-0.22518400	2.35101100
C	-0.82642100	-0.05603200	1.92812000
C	0.19500000	-0.53145900	2.76179400
C	-0.10408700	-1.18657000	3.95311300
C	-1.42473600	-1.37818900	4.33860500
H	-3.49070100	-1.02145000	3.82254600
H	-2.96625300	0.12789300	1.71887300
H	1.24183100	-0.37357200	2.51046800
H	0.70903300	-1.54225900	4.58251900
H	-1.65672500	-1.89793600	5.26584400
C	-0.55303900	0.65301300	0.62879200
C	0.90003700	1.05087900	0.40594100
S	3.55783400	1.04933100	0.04456000
O	3.51732800	1.68459800	-1.25835800
O	3.79729300	1.79716700	1.26314000
C	4.62922100	-0.34114900	-0.01132700
C	4.93255000	-0.91337400	-1.24541800
C	5.14146400	-0.84514100	1.18425500
C	5.76970800	-2.01874900	-1.27267800
H	4.51725400	-0.49949600	-2.16204000
C	5.97411000	-1.95202100	1.13011200
H	4.88802500	-0.37761700	2.13351500
C	6.29980500	-2.55215000	-0.09270400
H	6.01798700	-2.48062100	-2.22710900
H	6.38354900	-2.36211100	2.05227800
C	7.22115800	-3.73016500	-0.13617900
H	8.26780600	-3.39818500	-0.17859700
H	7.11641700	-4.35542400	0.75803500
H	7.04004300	-4.35130300	-1.02060000
N	1.95175500	0.24182900	0.28202100
C	1.83074700	-1.19085500	0.02499600
H	2.67189400	-1.72904800	0.46664700
H	0.92405600	-1.55191800	0.51147000
H	1.78529900	-1.38378500	-1.05601500
N	-2.15384800	-2.09108700	0.04099300
C	-1.18805800	2.00973400	0.50884800
C	-0.11865800	2.92932900	0.38944700
C	-0.32781800	4.37775500	0.19633100
C	-1.74829000	4.78795900	0.32242300

C	-2.74416400	3.88370100	0.42156100
C	-2.47512000	2.47225400	0.49226300
C	0.61886300	5.21585600	1.07043000
H	-3.78087800	4.20857200	0.45487800
H	-3.31275100	1.77676600	0.48420800
H	1.57981300	4.70935000	1.30643900
C	0.15105400	4.70832200	-1.26009000
H	1.20692900	4.43258300	-1.37111900
H	-0.44397600	4.13092500	-1.97723800
H	0.02069100	5.77979400	-1.44660000
N	1.09050800	2.37880800	0.35651500
O	0.36844800	6.34267400	1.40356800
H	-1.94968200	5.85699100	0.28586400

TS_{xi-xii}

E (M06-D3-CPCM/BS1) = -3151.91938638 au

H (M06-D3-CPCM/BS1) = -3151.37418 au

G (M06-D3-CPCM/BS1) = -3151.489179 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.07225723 au

C	-1.56261200	-4.02059700	1.55841300
C	-2.92754300	-4.15986200	1.78636800
C	-3.80249600	-3.27565800	1.17473100
C	-3.31271600	-2.25388300	0.36795800
C	-1.13175700	-2.99695200	0.73359800
H	-0.83449100	-4.69344000	2.00176600
H	-3.30220900	-4.95420800	2.42794400
H	-4.87965000	-3.33946600	1.29616400
H	-0.07409500	-2.86557100	0.51837300
C	-4.29881500	-1.25741800	-0.26430100
O	-5.48788000	-1.59325100	-0.22134900
O	-3.78685600	-0.20232300	-0.72586200
Au	-1.24718200	-0.63170100	-1.15572200
Cl	-0.31295300	0.87088200	-2.72821000
Cl	-1.86407000	-2.21289400	-2.93947900
C	-2.05838400	-0.68004100	3.58206100
C	-1.89463700	-0.06248500	2.35285500
C	-0.62613900	0.05022700	1.75824300
C	0.47535600	-0.45735900	2.46278100
C	0.30899600	-1.07100900	3.70071900
C	-0.95523200	-1.19288000	4.26361700
H	-3.05603000	-0.76486900	4.00864100
H	-2.77353900	0.30092700	1.82615700
H	1.48206900	-0.36208700	2.06372500
H	1.18244300	-1.45197200	4.22606400

H	-1.08321300	-1.67749300	5.22934900
C	-0.49218200	0.70100600	0.40870600
C	0.91584400	1.19569900	0.06431200
S	3.54553400	1.27839100	-0.34096700
O	3.54331300	1.66974600	-1.74226000
O	3.71724700	2.25169400	0.72216800
C	4.71074800	-0.02220500	-0.09563700
C	5.29725600	-0.63530800	-1.19789800
C	5.02211100	-0.40237900	1.21003400
C	6.21619300	-1.65404800	-0.98116300
H	5.03432900	-0.31825800	-2.20498900
C	5.93458900	-1.42729300	1.40209200
H	4.55229100	0.09607300	2.05661500
C	6.54542900	-2.06421000	0.31363600
H	6.68531900	-2.14403600	-1.83327000
H	6.18557200	-1.74252500	2.41423700
C	7.54998800	-3.15009100	0.54292500
H	7.25810000	-3.79473000	1.38072800
H	7.68043600	-3.77512900	-0.34750100
H	8.53113000	-2.72324700	0.79289800
N	2.03698300	0.42073100	-0.03043900
C	2.00435700	-0.97359000	-0.47520400
H	2.72196700	-1.57747100	0.08682300
H	1.00718300	-1.37292700	-0.29148400
H	2.20292300	-1.04541500	-1.55362700
N	-1.98906500	-2.12871600	0.17564300
C	-1.24281200	1.99091900	0.26436100
C	-0.26860100	2.98340900	0.06206100
C	-0.61246400	4.34697800	-0.00646200
C	-2.01709000	4.65539200	0.08419500
C	-2.98265400	3.64323700	0.16345400
C	-2.59978700	2.31093200	0.27174300
C	-1.19658600	4.81477400	1.82196000
H	-4.03481100	3.91273000	0.18058600
H	-3.35364300	1.52531400	0.28262100
H	-0.92564100	5.88070900	1.89350700
C	0.40562600	5.38730200	-0.33576800
H	1.33572300	5.23272200	0.22201100
H	0.64966900	5.31934200	-1.40448300
H	0.02803100	6.40064300	-0.15410100
N	1.00212200	2.49404800	-0.06803100
O	-1.34361200	4.00793300	2.66202600
H	-2.32353500	5.69020400	-0.07488000

xii

E (M06-D3-CPCM/BS1) = -3151.93301301 au

H (M06-D3-CPCM/BS1) = -3151.38556 au

G (M06-D3-CPCM/BS1) = -3151.507434 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.08475425 au

C	-0.82774800	-4.45037600	1.09507600
C	-2.14615600	-4.79253000	1.37653900
C	-3.16238300	-3.96278600	0.92944200
C	-2.85693000	-2.79028700	0.24659600
C	-0.58242800	-3.28427500	0.39235700
H	0.00559200	-5.07685600	1.39897100
H	-2.37573500	-5.70316200	1.92507400
H	-4.21325900	-4.18567300	1.08800900
H	0.43111600	-3.00599300	0.11719300
C	-4.00029000	-1.86656100	-0.20683300
O	-5.12577500	-2.37664400	-0.19565300
O	-3.66026300	-0.69081300	-0.50784600
Au	-1.13198000	-0.71138800	-1.12979000
Cl	-0.58615800	1.06528600	-2.58594000
Cl	-1.56380300	-2.16421100	-3.04841200
C	-1.72327100	-1.46022700	3.56516700
C	-1.70315200	-0.71246700	2.39859500
C	-0.49435100	-0.24220400	1.85878600
C	0.69017000	-0.52554500	2.55495300
C	0.66573800	-1.27267400	3.72841600
C	-0.53642000	-1.74836500	4.23727500
H	-2.67448200	-1.82513400	3.94815400
H	-2.63689800	-0.53602400	1.87236000
H	1.64540200	-0.15105100	2.19500400
H	1.60030400	-1.47681600	4.24691800
H	-0.55250600	-2.33669100	5.15233900
C	-0.48286000	0.56314800	0.59031000
C	0.82162400	1.25962500	0.20011600
S	3.39357900	1.64584000	-0.35887000
O	3.29428400	1.95989900	-1.77771600
O	3.47617800	2.69407600	0.64267600
C	4.73999800	0.53317200	-0.10003800
C	5.40665000	-0.00576000	-1.19553700
C	5.11524800	0.23210000	1.20894600
C	6.47379600	-0.86548200	-0.96817800
H	5.08739300	0.24292300	-2.20551400
C	6.17743700	-0.63457300	1.41238000
H	4.58040600	0.66979400	2.05041500
C	6.87247500	-1.19161000	0.33108500

H	7.00625800	-1.29622700	-1.81514300
H	6.48072300	-0.88613000	2.42809700
C	8.03566600	-2.10322100	0.57051500
H	8.94737900	-1.52367800	0.77127400
H	7.86664900	-2.74768000	1.44155100
H	8.23622800	-2.73936400	-0.29892900
N	2.03983700	0.62290100	0.06353300
C	2.09265300	-0.74252300	-0.46032700
H	3.06681400	-1.18781700	-0.24723000
H	1.35252400	-1.33783000	0.07708500
H	1.89354200	-0.77520600	-1.54124200
N	-1.57459200	-2.46426200	0.01288000
C	-1.41455500	1.71657500	0.52772900
C	-0.62119600	2.85610300	0.23328500
C	-1.14983500	4.12042300	0.15625300
C	-2.60717600	4.26587000	0.35454200
C	-3.37995200	3.04989400	0.64942900
C	-2.81073700	1.81790700	0.72124600
C	-2.99966200	5.43390500	1.30368500
H	-4.44794500	3.17788600	0.81064600
H	-3.42737200	0.93526600	0.84944100
H	-2.22080100	6.21474600	1.41859500
C	-0.30751100	5.30598500	-0.12857500
H	-0.02825200	5.81301600	0.80937400
H	0.62360300	5.00677900	-0.61871600
H	-0.83085600	6.04299400	-0.74952200
N	0.71223300	2.53794700	0.03452000
O	-4.06941800	5.49903400	1.83716600
H	-3.00877100	4.65589900	-0.60984700

$TS_{xi\text{-}xii'}$

E (M06-D3-CPCM/BS1) = -3151.89949985 au

H (M06-D3-CPCM/BS1) = -3151.35285 au

G (M06-D3-CPCM/BS1) = -3151.470777 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.05000491 au

C	-1.49797500	-4.40497600	0.65924500
C	-2.84957300	-4.59010300	0.93040200
C	-3.73929200	-3.57231000	0.62420000
C	-3.27452300	-2.37598700	0.08767700
C	-1.09389100	-3.20359400	0.10505800
H	-0.76114100	-5.17747100	0.85828000
H	-3.20356300	-5.52275200	1.36374900
H	-4.80933600	-3.66196200	0.78560900
H	-0.05240400	-3.03511400	-0.15630100

C	-4.27526800	-1.24431700	-0.20482400
O	-5.46375800	-1.58469500	-0.21834900
O	-3.77164900	-0.10053800	-0.36617500
Au	-1.27846600	-0.41550500	-1.07462100
Cl	-0.47344200	1.43543300	-2.31365200
Cl	-1.97646900	-1.52547700	-3.15590900
C	-1.90305900	-1.67671800	3.51667600
C	-1.80117700	-0.79300500	2.45448200
C	-0.55077600	-0.43581400	1.92173400
C	0.59546400	-0.97779300	2.52199800
C	0.49092800	-1.85891600	3.59411600
C	-0.75477000	-2.21850800	4.09312000
H	-2.88754800	-1.94707600	3.89408200
H	-2.70979300	-0.41290100	1.99509400
H	1.58774000	-0.70167600	2.17276100
H	1.39787500	-2.26054900	4.04155600
H	-0.83416100	-2.91232800	4.92747200
C	-0.47647400	0.51866000	0.76515600
C	0.90185400	1.09361200	0.44015500
S	3.49689100	1.27282300	-0.12816100
O	3.39942800	1.85669900	-1.45765500
O	3.73019900	2.09471600	1.04581500
C	4.69041500	-0.02532900	-0.14727600
C	5.20901400	-0.46047300	-1.36281600
C	5.08380800	-0.59078400	1.06534100
C	6.14459700	-1.48664600	-1.35671900
H	4.87748400	-0.00429700	-2.29324500
C	6.01239200	-1.61958700	1.04659000
H	4.66384300	-0.23122300	2.00339900
C	6.55668800	-2.07933200	-0.15964100
H	6.56071100	-1.83979200	-2.29932300
H	6.32718000	-2.07829300	1.98319000
C	7.57870100	-3.17312000	-0.15938300
H	8.58100600	-2.76640900	0.03405100
H	7.37464000	-3.91219400	0.62445800
H	7.61617000	-3.69066900	-1.12458100
N	2.02498800	0.35617300	0.16657200
C	1.92415200	-0.93738900	-0.50969100
H	2.80848200	-1.54356500	-0.30168300
H	1.06816900	-1.46957100	-0.09405300
H	1.79352900	-0.81437000	-1.59470600
N	-1.96121100	-2.21029800	-0.14196100
C	-1.24882600	1.79394200	0.91225600
C	-0.31807600	2.81693700	0.76282400

C	-0.70012900	4.18163600	0.84695800
C	-2.08143800	4.47330500	1.08505600
C	-3.00494600	3.41062500	1.26329100
C	-2.60031400	2.09582000	1.16191500
C	0.33658500	5.24787600	1.03876100
H	-4.04232600	3.64972000	1.47794100
H	-3.34346300	1.30655000	1.22078400
H	1.34557000	4.86545100	1.28779500
C	-1.68980300	4.63141900	-0.71523900
H	-0.79829400	5.11193600	-1.12440300
H	-1.89622200	3.66260600	-1.17155500
H	-2.51580900	5.34031500	-0.81752900
N	0.95689300	2.39724200	0.48609600
O	0.07577400	6.42266000	0.94575200
H	-2.34166000	5.48878000	1.37679600

xii'

E (M06-D3-CPCM/BS1) = -3151.93490443 au

H (M06-D3-CPCM/BS1) = -3151.38668 au

G (M06-D3-CPCM/BS1) = -3151.506293 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.08450227 au

C	-1.23971200	-4.50180000	0.51896400
C	-2.57800900	-4.76936300	0.78738200
C	-3.52333000	-3.79207900	0.51772100
C	-3.12627000	-2.55482300	0.02214700
C	-0.90305300	-3.26213900	0.00589900
H	-0.46103900	-5.23957800	0.68800700
H	-2.87857800	-5.73443800	1.18873400
H	-4.58665100	-3.94520500	0.67665700
H	0.12548500	-3.03069900	-0.25649500
C	-4.18783800	-1.47031000	-0.23185800
O	-5.35462200	-1.87403500	-0.26867200
O	-3.74494000	-0.29507200	-0.34181000
Au	-1.25698600	-0.44051600	-1.06159300
Cl	-0.62086000	1.51419200	-2.22598700
Cl	-1.84043600	-1.52046900	-3.16561900
C	-1.76689500	-1.92343200	3.47889300
C	-1.71991200	-1.00110900	2.44574000
C	-0.49338400	-0.53294000	1.94652600
C	0.68408700	-1.00410800	2.54622200
C	0.63295500	-1.92794700	3.58521200
C	-0.58832300	-2.39690700	4.05321300
H	-2.73282100	-2.27979100	3.83174200
H	-2.65046400	-0.68111700	1.98582500

H	1.65592900	-0.64183100	2.21920200
H	1.56217700	-2.27650600	4.03110100
H	-0.62515900	-3.12350400	4.86212400
C	-0.45296300	0.46785300	0.82817000
C	0.88923300	1.11312300	0.48472700
S	3.45748600	1.41306400	-0.14082400
O	3.30455400	1.97471900	-1.47438400
O	3.66599300	2.25779600	1.02095000
C	4.71749000	0.17953300	-0.16603400
C	5.25922400	-0.22005000	-1.38369700
C	5.15370700	-0.35661400	1.04536900
C	6.26433400	-1.17832100	-1.38082000
H	4.89439800	0.21270400	-2.31282000
C	6.15153700	-1.31817900	1.02314700
H	4.71501900	-0.02530400	1.98524200
C	6.72287400	-1.73843400	-0.18504900
H	6.70074600	-1.50155300	-2.32492700
H	6.50178900	-1.75276500	1.95866100
C	7.82239700	-2.75419900	-0.18776400
H	8.79127200	-2.27575000	0.01174600
H	7.67114300	-3.51091700	0.59122400
H	7.90094800	-3.26177400	-1.15576600
N	2.03754700	0.42519800	0.18925700
C	1.97644000	-0.86374600	-0.50162900
H	2.90346100	-1.41910700	-0.34422100
H	1.17467300	-1.45223500	-0.05318500
H	1.78953500	-0.73683700	-1.57807000
N	-1.82463800	-2.30914900	-0.20184200
C	-1.29001300	1.67602800	0.96694600
C	-0.40941400	2.80229500	0.77732300
C	-0.86668000	4.08711500	0.87258100
C	-2.31090100	4.33539500	1.04826200
C	-3.12431000	3.14649400	1.31127200
C	-2.64812400	1.86205900	1.25791700
C	0.05748700	5.22675700	0.77644200
H	-4.18745100	3.31068000	1.48394500
H	-3.33100200	1.02519600	1.34304600
H	1.11902100	4.96339500	0.60176800
C	-2.89892100	4.98871200	-0.25149800
H	-2.36553000	5.92546600	-0.43567900
H	-2.76415400	4.31078900	-1.10207200
H	-3.96463400	5.19789400	-0.11820300
N	0.88011600	2.41242500	0.50919100
O	-0.31334200	6.37974000	0.88987900

H	-2.46857400	5.08353200	1.84444200

TS_{xii}

E (M06-D3-CPCM/BS1) = -3151.9244875 au

H (M06-D3-CPCM/BS1) = -3151.378334 au

G (M06-D3-CPCM/BS1) = -3151.494583 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.07734639 au

C	0.96103200	-4.28709700	0.10291900
C	0.25193300	-4.80539800	1.18239900
C	-0.93081300	-4.19323200	1.56705400
C	-1.39237300	-3.07454800	0.87891300
C	0.46157500	-3.16903500	-0.53917400
H	1.88640600	-4.73679300	-0.24495300
H	0.61672500	-5.68280100	1.71175900
H	-1.53514700	-4.55289900	2.39457300
H	0.97198500	-2.73058800	-1.39394500
C	-2.73258000	-2.43476000	1.27827500
O	-3.21673600	-2.83542800	2.34327200
O	-3.19230000	-1.58690300	0.46639200
Au	-1.33450100	-0.87327700	-1.23890200
Cl	-1.83756700	0.93010600	-2.69219100
Cl	-1.99487800	-2.50002300	-2.96038400
C	-0.59900200	-0.86215600	3.75443000
C	-1.02448100	-0.19683000	2.61045200
C	-0.19941800	-0.09571400	1.48040100
C	1.07261600	-0.69009100	1.54768500
C	1.49650300	-1.35250100	2.68989400
C	0.66273100	-1.44234000	3.80328600
H	-1.26880800	-0.92851700	4.60916000
H	-2.01944600	0.23961900	2.60747400
H	1.73718300	-0.65653900	0.68883700
H	2.48499700	-1.81012100	2.70404700
H	0.99467400	-1.96469600	4.69814900
C	-0.67125700	0.60317400	0.23652100
C	0.35765300	1.56567700	-0.35114300
S	2.90386900	2.35055400	-0.38563000
O	3.16646700	3.14345900	-1.57889500
O	2.56819200	2.98459400	0.87782400
C	4.24509500	1.22967400	-0.12866900
C	5.18267700	1.01901500	-1.13509700
C	4.32904000	0.56918900	1.09703700
C	6.21634300	0.11945900	-0.90622700
H	5.10175700	1.55219800	-2.08017200
C	5.36548900	-0.32777700	1.30256000

H	3.59274300	0.76059200	1.87618900
C	6.32215800	-0.56540600	0.30757900
H	6.95615700	-0.05694400	-1.68602800
H	5.44156300	-0.85349500	2.25415300
C	7.45103800	-1.51734500	0.55486500
H	7.13278100	-2.36442800	1.17416900
H	7.86317300	-1.90769100	-0.38260000
H	8.27016400	-1.01701600	1.08982600
N	1.64288000	1.21756000	-0.71714800
C	1.92253100	0.27284600	-1.80653800
H	2.51514300	-0.58271400	-1.45870600
H	0.97698300	-0.07630500	-2.23167500
H	2.46182900	0.78888200	-2.61032700
N	-0.67799800	-2.57920200	-0.14140500
C	-1.81656700	1.54790400	0.40924900
C	-1.32412300	2.83678300	0.08349200
C	-2.10628900	3.98781700	0.15636400
C	-3.41693900	3.80159700	0.63318100
C	-3.93793600	2.49308500	0.91209700
C	-3.13830400	1.35262800	0.76619900
C	-3.34819100	3.47136500	2.52819000
H	-4.99669900	2.39335600	1.14711100
H	-3.53785500	0.34818500	0.91935500
H	-4.26377200	3.93256000	2.92405000
C	-1.56178100	5.32644700	-0.19723800
H	-2.31190500	6.11321500	-0.06998000
H	-0.68740600	5.56693800	0.42158600
H	-1.21792300	5.33538500	-1.23956100
N	-0.02054500	2.80996600	-0.36727700
O	-2.34366700	3.17913800	3.05983400
H	-4.10624500	4.64745100	0.63424600

$TS_{xii\text{-}xiv}$

E (M06-D3-CPCM/BS1) = -3590.62497477 au

H (M06-D3-CPCM/BS1) = -3589.93832 au

G (M06-D3-CPCM/BS1) = -3590.073818 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3591.95031494 au

C	-1.68471300	4.88019000	-0.42902200
C	-0.68385500	5.79673300	-0.12518800
C	0.62333400	5.34816400	-0.01689300
C	0.91225400	3.99707100	-0.17606400
C	-1.33599900	3.55175500	-0.59664100
H	-2.72178400	5.18012700	-0.54733200
H	-0.92137600	6.84917100	0.01225700

H	1.45535000	6.01419600	0.19131700
H	-2.08487900	2.81286500	-0.86903100
C	2.36064400	3.51379100	-0.00792300
O	3.22415500	4.39678700	-0.05205400
O	2.49452200	2.27545700	0.18705000
Au	0.40164100	1.06372000	-0.80738000
Cl	0.80708100	-1.15984400	-1.48459000
Cl	1.00673100	1.86285100	-3.05334400
C	-0.73555800	3.48372700	3.16267800
C	-0.16607400	2.45300400	2.43254100
C	-0.94395400	1.38769500	1.94804000
C	-2.31356700	1.38538300	2.25395600
C	-2.88147100	2.41849100	2.99326500
C	-2.10047800	3.47439800	3.44655300
H	-0.10811900	4.30478500	3.50483700
H	0.89065200	2.50513100	2.18690200
H	-2.95028100	0.56540000	1.93045200
H	-3.94614700	2.38840100	3.21617400
H	-2.54826100	4.28418400	4.01893000
C	-0.30996300	0.28417400	1.15020500
C	-1.15202300	-0.96734300	0.90187600
S	-3.17676700	-2.53130400	0.18312500
O	-2.54052000	-3.26607300	-0.90232900
O	-3.26322800	-3.09051800	1.52112300
C	-4.80072200	-2.05170500	-0.31783000
C	-5.19635300	-2.23972700	-1.63814100
C	-5.65788400	-1.50038900	0.63375300
C	-6.48217300	-1.86627400	-2.00736100
H	-4.50317200	-2.66654300	-2.36003300
C	-6.93378400	-1.12691600	0.24149400
H	-5.32614200	-1.36578000	1.66214800
C	-7.36494900	-1.30703400	-1.07911300
H	-6.80746600	-2.00687100	-3.03741600
H	-7.61503600	-0.68915100	0.97030000
C	-8.75643100	-0.92643300	-1.47961300
H	-9.46294300	-1.73328700	-1.24023100
H	-9.09716300	-0.03145600	-0.94553300
H	-8.82884600	-0.73741500	-2.55667500
N	-2.40518900	-0.96990000	0.31636600
C	-2.72196600	-0.01515700	-0.74667800
H	-3.80445000	0.09300200	-0.84495500
H	-2.33185100	0.95983400	-0.45091000
H	-2.28158800	-0.31290700	-1.70916700
N	-0.07378200	3.12453500	-0.44231400

C	0.90650600	-0.34611000	1.74555300
C	0.62969300	-1.73011900	1.84401800
C	1.52752900	-2.63212000	2.38064900
C	2.84559700	-2.10783300	2.71734300
C	3.05154400	-0.67512900	2.71417200
C	2.12438800	0.18796200	2.19320900
C	3.73542600	-2.88806100	3.65735800
H	4.01703700	-0.31690700	3.06695700
H	2.36510900	1.23834600	2.07515100
H	3.40904700	-3.92608000	3.87359900
C	1.20745500	-4.08027400	2.47967500
H	1.14890000	-4.39920300	3.53039300
H	0.24502400	-4.28783400	2.00443100
H	1.97856200	-4.69558000	1.99732100
N	-0.61687000	-2.06213700	1.33396800
O	4.74552800	-2.42988100	4.12960200
H	3.36228600	-2.31613700	1.63837800
C	3.62660300	-2.92608600	-2.18326900
C	4.02599400	-2.07867500	-1.10171900
C	4.62652900	-0.80575000	-1.32919700
C	4.77563000	-0.45805300	-2.64605300
C	4.37030500	-1.29154300	-3.73654000
C	3.80593900	-2.51635600	-3.53169300
C	3.09260400	-4.01806000	-1.54878200
H	4.52787200	-0.92855200	-4.74985400
H	3.50075900	-3.15596700	-4.35558300
H	2.64446800	-4.94231400	-1.89032700
C	5.02221900	0.07262200	-0.18880800
H	4.15977400	0.64745100	0.18467300
H	5.43214000	-0.51408100	0.64488500
H	5.78061300	0.79969400	-0.50207900
N	3.75315500	-2.64915300	0.06927800
O	3.16017600	-3.85953400	-0.23023800
H	5.22978400	0.50589700	-2.87729800

xiii

E (M06-D3-CPCM/BS1) = -439.091933076 au

H (M06-D3-CPCM/BS1) = -438.937242 au

G (M06-D3-CPCM/BS1) = -438.979156 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -439.277365218 au

H	1.19461700	-2.35299200	-0.00025300
C	0.77451600	0.85057500	-0.00020700
C	0.15527300	-0.43342600	-0.00011600
C	-1.24359300	-0.61658700	-0.00002300

C	-1.96123900	0.55892800	0.00010300
C	-1.37081700	1.85646600	0.00006100
C	-0.01589900	2.02733800	-0.00007900
C	2.12567200	0.58376300	0.00011500
H	-2.02721300	2.72249200	0.00019800
H	0.44770500	3.00898900	-0.00023900
H	3.01270300	1.20432200	0.00010500
C	-1.85576800	-1.97841400	0.00001800
H	-1.55308500	-2.55413600	-0.88518300
H	-1.55384100	-2.55371700	0.88576400
H	-2.94801100	-1.91139900	-0.00043900
N	1.14421400	-1.33924800	-0.00012400
O	2.35216300	-0.72145200	0.00019100
H	-3.04854800	0.49093200	0.00016000

xiv

E (M06-D3-CPCM/BS1) = -3151.55534713 au

H (M06-D3-CPCM/BS1) = -3151.018746 au

G (M06-D3-CPCM/BS1) = -3151.135951 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3152.69726132 au

C	-2.27382000	3.71444700	-0.29279200
C	-1.80939900	4.57098700	0.70129000
C	-0.51752400	4.41178200	1.17758800
C	0.29619300	3.40564700	0.66285300
C	-1.42593900	2.72783100	-0.76210000
H	-3.27505400	3.80346500	-0.70442100
H	-2.44989900	5.35776600	1.09413900
H	-0.09300600	5.04996100	1.94677600
H	-1.73679400	2.03342900	-1.54021700
C	1.74614300	3.26916600	1.16666400
O	2.03648600	3.99271200	2.12974400
O	2.47145900	2.45639800	0.53841100
Au	1.03698100	1.06626100	-1.15617300
Cl	2.18291200	-0.57108300	-2.44671200
Cl	1.29053700	2.70683600	-3.02177600
C	0.11303500	1.29216000	3.83222700
C	0.75145900	0.66015000	2.77102600
C	0.04312600	0.27738000	1.62240500
C	-1.33651100	0.54920200	1.58587900
C	-1.97298900	1.17520600	2.64701700
C	-1.25098000	1.55457000	3.77788700
H	0.69292200	1.58039500	4.70693500
H	1.81577500	0.45752200	2.84593800
H	-1.90805300	0.28520600	0.69945600

H	-3.04092200	1.38443800	2.58145600
H	-1.74977800	2.05152300	4.60783700
C	0.73616400	-0.39264700	0.48064600
C	0.02965900	-1.59214600	-0.11650800
S	-2.27304600	-2.84002000	0.08320900
O	-2.27318500	-3.99491900	-0.81045800
O	-1.86158000	-2.98396500	1.47334800
C	-3.88501700	-2.10727100	0.03688300
C	-4.74440500	-2.37957200	-1.02338700
C	-4.27259300	-1.27666800	1.08766000
C	-6.00256800	-1.78884100	-1.03667400
H	-4.43297000	-3.05069900	-1.82152100
C	-5.53157500	-0.69711800	1.05611800
H	-3.59448100	-1.09645500	1.92008500
C	-6.41279700	-0.94190000	-0.00408300
H	-6.68186700	-1.99158700	-1.86397800
H	-5.84405400	-0.04469300	1.87159000
C	-7.77878000	-0.32754400	-0.00987000
H	-8.46218400	-0.89002600	0.64131600
H	-7.75560800	0.70320000	0.36448400
H	-8.21449800	-0.32068300	-1.01544600
N	-1.31830900	-1.57746400	-0.56456000
C	-1.47519600	-1.41822200	-2.01847200
H	-2.53714900	-1.29599900	-2.25840600
H	-0.94688700	-0.50982500	-2.32826600
H	-1.05885700	-2.27556000	-2.56552200
N	-0.18114200	2.58142400	-0.27957300
C	2.08707300	-0.98089000	0.71442500
C	2.00474100	-2.33582500	0.35189500
C	3.08274600	-3.21096200	0.43925100
C	4.29268400	-2.64996100	0.90196800
C	4.38561200	-1.29075900	1.23064000
C	3.29431600	-0.43635600	1.13852500
C	5.50272500	-3.47503000	1.03883900
H	5.35394400	-0.91673800	1.55861600
H	3.38565200	0.63222700	1.32909300
H	5.38832300	-4.54416600	0.75498400
C	2.92900300	-4.64867800	0.04295300
H	3.15245000	-5.32925600	0.87478100
H	1.90160200	-4.83883800	-0.28125400
H	3.59814200	-4.91702400	-0.78504600
N	0.73569100	-2.66588800	-0.15244000
O	6.57815200	-3.06210500	1.43254300

xv

E (M06-D3-CPCM/BS1) = -3590.68005358 au

H (M06-D3-CPCM/BS1) = -3589.986629 au

G (M06-D3-CPCM/BS1) = -3590.123840 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3592.00730159 au

Au	1.86591500	-0.80938500	-1.29388000
Cl	0.17170000	-2.33160700	-1.97912000
Cl	2.96135300	-1.01157500	-3.51265200
C	3.16216900	0.86209200	3.27762500
C	2.44107500	-0.04611000	2.51195200
C	1.58382100	0.38623100	1.48836900
C	1.47374900	1.77057200	1.27241800
C	2.19107000	2.67654700	2.03964000
C	3.04267200	2.22782800	3.04745400
H	3.82441800	0.49192100	4.05761100
H	2.54934700	-1.10675300	2.71889200
H	0.83733800	2.14985100	0.47729600
H	2.08801600	3.74229300	1.83979600
H	3.60915500	2.93912800	3.64521200
C	0.83757600	-0.60270800	0.65003700
C	-0.62908200	-0.27705600	0.40447300
S	-2.43270600	1.71127500	0.66485600
O	-3.57371500	1.68180000	-0.24648600
O	-2.54668300	1.14111800	1.99820300
C	-1.86923100	3.38001100	0.78779500
C	-2.18448700	4.29428600	-0.21523300
C	-1.12152300	3.75230100	1.90416200
C	-1.72917900	5.60033500	-0.09552200
H	-2.78587700	3.98991400	-1.06920400
C	-0.68102500	5.06362200	2.00480700
H	-0.89619500	3.02622300	2.68283900
C	-0.97513100	6.00376700	1.01081900
H	-1.96702400	6.32445800	-0.87374700
H	-0.09784500	5.36803200	2.87369100
C	-0.51543400	7.42208400	1.14647900
H	-1.24158800	8.01134300	1.72354300
H	0.44338900	7.48479900	1.67439100
H	-0.40680400	7.90595700	0.16904600
N	-1.12905300	0.92200200	-0.10691100
C	-0.82623800	1.38882300	-1.46443200
H	-0.17461400	2.27369400	-1.45994700
H	-0.34490300	0.57787500	-2.02070200
H	-1.76015200	1.63404300	-1.98349100
C	0.71276900	-1.99972000	1.16584100

C	-0.65532000	-2.27889900	1.27405300
C	-1.15933800	-3.49191400	1.73555500
C	-0.19709900	-4.46958600	2.05980800
C	1.17352000	-4.20615900	1.92369100
C	1.64933900	-2.98203000	1.47593000
C	-0.58651200	-5.81395500	2.52101200
H	1.86642500	-5.00697900	2.17488500
H	2.71179300	-2.80869000	1.31049200
H	-1.67841200	-6.01077900	2.57899200
C	-2.64166900	-3.68856900	1.84135100
H	-2.92750600	-4.35490500	2.66067700
H	-3.13240700	-2.72566300	2.02384000
H	-3.06139500	-4.10499600	0.91421600
N	-1.43294800	-1.21477000	0.79256300
O	0.20350500	-6.68930900	2.81966000
H	-2.99321900	-1.29607600	0.04756900
C	-5.38276700	-0.50504800	-2.02187200
C	-5.03597500	-0.82451600	-0.67891400
C	-5.92977900	-0.66608900	0.40310700
C	-7.17339200	-0.20012000	0.04679400
C	-7.55614100	0.09968400	-1.29429200
C	-6.68529600	-0.04100000	-2.33671800
C	-4.22186100	-0.72496500	-2.72976900
H	-8.56673300	0.45670200	-1.47546500
H	-6.96192200	0.19413900	-3.36012800
H	-3.95193200	-0.63384900	-3.77430000
C	-5.50620800	-0.97025300	1.80084700
H	-5.32675300	-2.04630400	1.93562600
H	-4.57521800	-0.44079300	2.05627900
H	-6.27603300	-0.66796000	2.51817900
N	-3.76938300	-1.25992600	-0.67254300
O	-3.25502500	-1.14738100	-1.93171100
H	-7.90738400	-0.04526100	0.83699500
C	3.91437700	3.01345400	-1.47485800
C	5.05146200	2.86010900	-0.68669200
C	5.27836100	1.64292700	-0.06415400
C	4.37441100	0.59682700	-0.23006800
C	3.04654000	1.94368300	-1.59616500
H	3.69760200	3.94261400	-1.99394600
H	5.75542200	3.68100500	-0.56848400
H	6.14944800	1.45445300	0.55637700
H	2.15040300	2.00797500	-2.21007400
C	4.66897600	-0.76988500	0.41117100
O	5.59666600	-0.78219600	1.23080000

O	3.94692300	-1.72088600	0.01298400
N	3.27377200	0.77597200	-0.97234600

xvi

E (M06-D3-CPCM/BS1) = -3152.00005161 au

H (M06-D3-CPCM/BS1) = -3151.450133 au

G (M06-D3-CPCM/BS1) = -3151.566574 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -3153.15531895 au

Au	-1.75743100	-0.77359900	-0.90107000
Cl	-2.25658200	1.12844900	-2.23095400
Cl	-3.39917000	-2.13243600	-2.10474200
C	1.08185700	-0.95909800	3.35758400
C	0.33986800	-0.20668400	2.45384900
C	0.53923300	-0.33343500	1.07123700
C	1.51889000	-1.24119900	0.63506800
C	2.25819400	-1.99117500	1.53649700
C	2.04320800	-1.85514900	2.90704800
H	0.89610500	-0.84121300	4.42302200
H	-0.40148400	0.48664600	2.83990300
H	1.70022800	-1.39467100	-0.42349500
H	3.00364700	-2.69144400	1.16225300
H	2.61831400	-2.44845700	3.61551400
C	-0.28428300	0.48342500	0.10303900
C	0.60079700	1.20297200	-0.90516800
S	3.04923000	1.46622700	-2.08239200
O	3.48802300	0.92481700	-3.35063300
O	2.85646700	2.89682600	-1.89265200
C	3.99074700	0.79943200	-0.75945100
C	4.75733800	-0.34139900	-0.98837300
C	3.87938000	1.37609900	0.50782900
C	5.42703900	-0.91183700	0.08543800
H	4.83851500	-0.76220300	-1.98835200
C	4.54789900	0.77946600	1.56350600
H	3.29188100	2.27934500	0.66242300
C	5.32145500	-0.37266000	1.37112600
H	6.04118100	-1.79661400	-0.07559900
H	4.47176100	1.21214300	2.56030000
C	5.99699200	-1.02745300	2.53377500
H	6.40098200	-0.28649100	3.23373100
H	5.27679800	-1.64028700	3.09510500
H	6.81145300	-1.68613600	2.21294800
N	1.48389900	0.69970700	-1.80030900
C	1.24453200	-0.49439900	-2.62224800
H	2.00883300	-1.26098600	-2.45246600

H	0.25572900	-0.89039500	-2.38091600
H	1.24975800	-0.20398000	-3.67634700
C	-1.03201700	1.63666700	0.71262100
C	-0.48412100	2.83048100	0.24019500
C	-0.88641400	4.10321100	0.62116900
C	-1.95599700	4.12720000	1.53851500
C	-2.53859000	2.94439900	2.00760000
C	-2.09471200	1.69074200	1.60824000
C	-2.51269400	5.40628900	2.02396900
H	-3.36837000	3.03540000	2.70570600
H	-2.57779400	0.77512600	1.94747400
H	-2.04861500	6.32619900	1.60901100
C	-0.23499300	5.34144300	0.08032000
H	0.07067700	6.02080700	0.88418300
H	0.66840800	5.11870500	-0.49650000
H	-0.91312300	5.89596700	-0.58088300
N	0.49320500	2.50580500	-0.71337500
O	-3.42419500	5.48760600	2.82257600
H	1.02120300	3.17243300	-1.27568300
C	0.07543300	-4.67649900	-0.34207800
C	-0.18850600	-5.01511400	0.98188700
C	-0.93576800	-4.14651500	1.76210700
C	-1.40335000	-2.95376400	1.21861200
C	-0.40344800	-3.47200700	-0.82537500
H	0.64086600	-5.33081100	-0.99912300
H	0.17743000	-5.95277000	1.39429200
H	-1.18992200	-4.35683200	2.79682900
H	-0.23374500	-3.17093000	-1.85725500
C	-2.30566800	-2.03629300	2.05652700
O	-2.35415900	-2.29102900	3.26555500
O	-2.91337000	-1.14554700	1.40421800
N	-1.10703400	-2.63270600	-0.04764200

xvii

E (M06-D3-CPCM/BS1) = -2914.5683151 au

H (M06-D3-CPCM/BS1) = -2913.688456 au

G (M06-D3-CPCM/BS1) = -2913.827206 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2915.83431854 au

C	-0.35588000	4.80950300	-0.45345000
C	-0.08213700	3.49023700	-0.15754000
C	-1.00488100	2.46599700	-0.51004000
C	-2.20170500	2.82412700	-1.19243800
C	-2.44607200	4.14115700	-1.52018400
C	-1.52972200	5.12959400	-1.14291600

H	0.34018200	5.59423100	-0.16788900
H	0.83224900	3.21000100	0.36519700
H	-2.91735000	2.04614500	-1.45907200
H	-3.35007800	4.41388100	-2.05871600
H	-1.73558400	6.16930600	-1.39035700
C	-0.69053300	1.12319500	-0.24529400
C	-1.74011600	0.08750500	-0.26086900
S	-2.15980400	-2.53566600	-0.66697100
O	-1.66505600	-3.40652700	-1.72525800
O	-1.77460500	-2.77255300	0.71620600
C	-3.92005600	-2.44715000	-0.79167200
C	-4.50640600	-2.62277300	-2.04297200
C	-4.68841900	-2.20125500	0.34449600
C	-5.88881700	-2.54301000	-2.15095600
H	-3.89278300	-2.83472800	-2.91639400
C	-6.06710900	-2.13719100	0.21571900
H	-4.20789700	-2.06392400	1.31021700
C	-6.68640000	-2.30271600	-1.02864100
H	-6.35994900	-2.67714200	-3.12401200
H	-6.68076800	-1.95032800	1.09673100
C	-8.17849900	-2.25031300	-1.14512100
H	-8.62457100	-3.21758500	-0.87488600
H	-8.60692100	-1.49973400	-0.46998100
H	-8.49616700	-2.01792200	-2.16798900
N	-1.54403800	-1.00238000	-1.10413200
C	-1.07107100	-0.80797500	-2.47566100
H	-1.88979100	-0.92950600	-3.19583400
H	-0.68715100	0.21525000	-2.56079300
H	-0.26116200	-1.50260600	-2.71494400
C	-4.27975800	1.69372300	1.39036400
C	-3.09200000	0.94478400	1.57338900
C	-2.44560000	0.95904800	2.82616800
C	-2.95532900	1.78005000	3.82952500
C	-4.09890600	2.55638500	3.64656000
C	-4.76221400	2.49232600	2.43484500
C	-5.08776700	1.64025300	0.16920900
H	-4.47320800	3.18155600	4.45361400
H	-5.67842400	3.06112200	2.27345500
H	-6.05123200	2.19479600	0.26396000
C	-1.25230400	0.08976900	3.06356700
H	-1.43289200	-0.93711500	2.71289700
H	-0.36838200	0.45456100	2.51409500
H	-0.98898500	0.05828200	4.12716100
N	-2.68529200	0.06369100	0.59178600

O	-4.81288300	1.07056800	-0.87188700
H	-2.44273500	1.79544700	4.79170700
Au	1.17101900	0.35965500	0.22321500
P	3.16252800	-0.83326200	0.84537500
C	3.82246400	-0.13564700	2.48121700
C	2.60761800	-2.64476500	0.92103600
C	2.63687000	0.22440600	3.38056600
H	3.02445100	0.66754100	4.30957500
H	1.97889700	0.96690200	2.90708800
H	2.02862600	-0.64489400	3.65833200
C	4.55337900	1.15974900	2.11935200
H	3.90237800	1.84963600	1.56112700
H	4.85399700	1.66672200	3.04769500
H	5.45860800	0.97959100	1.52569100
C	4.76014900	-1.06139100	3.25200200
H	5.66080300	-1.32618000	2.68609700
H	5.09600500	-0.53829200	4.15942200
H	4.26159500	-1.98324400	3.57773000
C	1.55597700	-2.78683300	2.02255200
H	0.74843200	-2.04589800	1.93012000
H	1.09235500	-3.78052900	1.93835700
H	1.99386500	-2.71469300	3.02688300
C	1.95087200	-2.92556200	-0.43556300
H	1.63811300	-3.97979500	-0.46860600
H	1.05194300	-2.31110500	-0.59223300
H	2.64110600	-2.75418500	-1.27434700
C	3.70942300	-3.68007000	1.14125500
H	4.28996300	-3.50852900	2.05603600
H	3.23402500	-4.66698800	1.23806600
H	4.39873800	-3.73655100	0.29079700
C	4.55993100	-0.76849100	-0.34863200
C	4.52462700	0.00905200	-1.52363500
C	5.71565800	-1.52092300	-0.07996600
C	5.62427900	-0.02444300	-2.39113500
C	6.80106100	-1.53233600	-0.94463000
H	5.77500200	-2.12022600	0.82390900
C	6.75153600	-0.78474200	-2.11519300
H	5.58347600	0.57650500	-3.29905000
H	7.67893700	-2.12711800	-0.70180800
H	7.59020300	-0.78643900	-2.80850800
C	3.42366900	0.92227600	-1.94286200
C	3.43237900	2.26054000	-1.53406300
C	2.48633100	0.51162100	-2.89629800
C	2.51342700	3.16513200	-2.05738000

H	4.18547600	2.59473100	-0.81945000
C	1.57031400	1.42013900	-3.42375900
H	2.49399000	-0.52409400	-3.23870300
C	1.57895800	2.74738100	-3.00348800
H	2.53872000	4.20620800	-1.73791600
H	0.86155000	1.09198300	-4.18327900
H	0.86310500	3.45855500	-3.41509900

$TS_{xvii\text{-}xviii}$

E (M06-D3-CPCM/BS1) = -2913.670018 au

H (M06-D3-CPCM/BS1) = -2913.670018 au

G (M06-D3-CPCM/BS1) = -2913.807679 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2915.81432087 au

C	1.59244000	-1.61840100	3.66804000
C	0.97631000	-0.89678300	2.65885100
C	1.69765600	-0.46890800	1.52228400
C	3.06844900	-0.80489500	1.44810400
C	3.67223600	-1.56253400	2.43682500
C	2.93756500	-1.96727100	3.55161700
H	1.02219900	-1.92313500	4.54306600
H	-0.07756300	-0.62491500	2.74500400
H	3.66753500	-0.45606800	0.61118900
H	4.72591900	-1.82146900	2.34735300
H	3.41719000	-2.54894200	4.33622600
C	1.02559800	0.38434400	0.56369700
C	1.69012600	0.93578700	-0.64676900
S	3.73606600	0.56237000	-2.44783700
O	3.56737400	-0.13157600	-3.71450600
O	3.86360000	2.00298900	-2.38608000
C	5.06395000	-0.17722100	-1.54874500
C	5.42263600	-1.49749200	-1.80724000
C	5.66772700	0.56027200	-0.52893400
C	6.40166100	-2.08905300	-1.01765500
H	4.95067600	-2.05000200	-2.61727600
C	6.64309000	-0.05055400	0.24362800
H	5.35779200	1.58488700	-0.33354500
C	7.02049400	-1.38087000	0.01557500
H	6.69325000	-3.12075900	-1.20916100
H	7.12486700	0.51115900	1.04348200
C	8.07049000	-2.01860600	0.87143400
H	8.23534100	-3.06665600	0.59903100
H	9.02772800	-1.48880500	0.77881400
H	7.78935500	-1.98137700	1.93242100
N	2.36633900	0.08106600	-1.48874500

C	2.02717800	-1.34052800	-1.55592900
H	2.65439400	-1.95791600	-0.89688900
H	0.97837000	-1.46439200	-1.26300400
H	2.13490800	-1.67939200	-2.59025000
C	1.18727100	2.49608900	1.37974600
C	0.95573500	2.89971500	0.02252900
C	0.03818600	3.93830200	-0.27252800
C	-0.73271900	4.41906100	0.76983300
C	-0.60873900	3.94110500	2.09387600
C	0.34173000	3.00100500	2.40235400
C	2.56343200	2.17071700	1.85863700
H	-1.24328100	4.35865000	2.87273500
H	0.51455800	2.69450800	3.43432000
H	2.57508800	1.82410800	2.91807800
C	-0.13790000	4.39997500	-1.68317800
H	0.81493200	4.73942100	-2.10877100
H	-0.49470100	3.58351900	-2.32614200
H	-0.86037100	5.22195700	-1.73878000
N	1.51188500	2.19001400	-0.98651400
O	3.58328600	2.29928800	1.22247200
H	-1.48355600	5.18009100	0.55352800
Au	-1.06796100	0.20342200	0.30144600
P	-3.43703300	0.17177000	-0.12691700
C	-4.30397300	0.85578200	1.41880400
C	-3.64412800	1.24244200	-1.68384000
C	-3.47089100	2.00648600	1.98980200
H	-3.92903700	2.33440000	2.93463900
H	-2.43731600	1.70093400	2.21030700
H	-3.43256300	2.87677300	1.32387500
C	-4.29983900	-0.28302900	2.44141600
H	-3.27719100	-0.62473100	2.66164100
H	-4.73385900	0.08488700	3.38235200
H	-4.89440100	-1.14544900	2.11238700
C	-5.73380000	1.34924000	1.20667200
H	-6.42202800	0.54816400	0.91503200
H	-6.10532400	1.75446900	2.15930300
H	-5.79507300	2.15782400	0.46698700
C	-3.23434500	2.67554900	-1.34985700
H	-2.26919100	2.71943300	-0.82593500
H	-3.13154200	3.24182900	-2.28760800
H	-3.98667200	3.19269000	-0.73942700
C	-2.65590900	0.65902300	-2.70203700
H	-2.77607000	1.18776000	-3.65906000
H	-1.60995500	0.78097000	-2.38125700

H	-2.83523800	-0.41065400	-2.88714300
C	-5.02978300	1.26703600	-2.32736000
H	-5.81862100	1.60937700	-1.64599100
H	-4.99801800	1.97693500	-3.16679700
H	-5.31662100	0.29259000	-2.73861500
C	-4.26466300	-1.42400300	-0.53688500
C	-3.59128400	-2.65949400	-0.63296300
C	-5.63342300	-1.38895500	-0.85416000
C	-4.29352300	-3.77780800	-1.10467500
C	-6.32048100	-2.51349100	-1.28835700
H	-6.18282300	-0.45594900	-0.78091300
C	-5.63907300	-3.71547900	-1.43461400
H	-3.76005100	-4.72458700	-1.18167100
H	-7.38081900	-2.44230400	-1.52073900
H	-6.15492400	-4.60554300	-1.78915900
C	-2.19580600	-2.93555700	-0.20306100
C	-1.88193700	-2.98970400	1.15941700
C	-1.23783400	-3.34674700	-1.13460300
C	-0.63533100	-3.44062700	1.58008900
H	-2.64029500	-2.71552600	1.89334500
C	0.01256000	-3.79104700	-0.71189400
H	-1.48653300	-3.33312900	-2.19637200
C	0.31959500	-3.83432500	0.64581100
H	-0.41427900	-3.49908400	2.64437300
H	0.74753000	-4.11379900	-1.44884000
H	1.29757300	-4.18202800	0.97791700

xviii

E (M06-D3-CPCM/BS1) = -2914.58386114 au

H (M06-D3-CPCM/BS1) = -2913.702079 au

G (M06-D3-CPCM/BS1) = -2913.841027 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2915.84998539 au

C	-0.80400700	4.16078800	2.62383900
C	-0.56965700	2.84322500	2.24713000
C	-1.37240300	2.21398200	1.28804500
C	-2.43285500	2.94078300	0.72990100
C	-2.65303000	4.26708600	1.08702000
C	-1.83968100	4.88162400	2.03505300
H	-0.16638400	4.62943100	3.37187400
H	0.25918500	2.28975000	2.69248300
H	-3.11203000	2.45543800	0.02676100
H	-3.47626500	4.81589100	0.63370700
H	-2.01817500	5.91639800	2.32065300
C	-1.16222900	0.76251800	0.99212400

C	-1.65570700	0.10861300	-0.20692100
S	-2.53225100	-0.26976800	-2.73810700
O	-2.59254000	0.71674100	-3.80552300
O	-1.85343300	-1.53336300	-2.96146600
C	-4.14750200	-0.51095000	-2.07639100
C	-4.98414200	0.59798000	-1.97414400
C	-4.55706500	-1.78121700	-1.68013400
C	-6.25820300	0.42293800	-1.45082100
H	-4.64770700	1.57990800	-2.30526500
C	-5.83500200	-1.93285300	-1.16529400
H	-3.87776500	-2.62547700	-1.77014200
C	-6.69904100	-0.83795400	-1.03790800
H	-6.92504300	1.27937500	-1.36308400
H	-6.17473800	-2.91979200	-0.85142100
C	-8.07148900	-1.02896700	-0.47118100
H	-8.62564500	-0.08540400	-0.42202500
H	-8.65329000	-1.73389000	-1.07951000
H	-8.02305000	-1.44896400	0.54203700
N	-1.72358000	0.62257600	-1.45635900
C	-1.03149300	1.84645700	-1.85735900
H	-1.70728400	2.70921800	-1.88131400
H	-0.21977300	2.03730900	-1.14695000
H	-0.59490500	1.70459000	-2.85015800
C	-1.69304100	-0.23538800	2.07258700
C	-1.96194400	-1.44095000	1.25578900
C	-2.06447500	-2.74021300	1.84025500
C	-1.61223300	-2.85496100	3.12413000
C	-1.08310900	-1.74596300	3.88444400
C	-1.05963000	-0.49356500	3.38453900
C	-3.10353800	0.39431400	2.41572300
H	-0.69816600	-1.94458500	4.88223400
H	-0.70546200	0.35099000	3.97536800
H	-3.06234100	1.10237200	3.26898300
C	-2.55149900	-3.88457800	1.01526300
H	-3.58964600	-3.71954100	0.69505400
H	-1.95373900	-3.99331700	0.09964000
H	-2.50785900	-4.82428300	1.57569600
N	-2.05309500	-1.19185900	-0.03055300
O	-4.10451500	0.16994300	1.79540900
H	-1.61954700	-3.83805200	3.59492100
Au	0.95359800	0.15582500	0.59023500
P	2.86661800	-1.14147300	-0.00144000
C	3.41156700	-2.10286900	1.54676200
C	2.23010100	-2.25359300	-1.40412000

C	2.16677300	-2.35599400	2.40441500
H	2.46495600	-2.91768000	3.30226700
H	1.70340700	-1.41715700	2.73925300
H	1.39944500	-2.94476100	1.88443100
C	4.35023300	-1.18242400	2.32919500
H	3.88655500	-0.20580200	2.53163000
H	4.57287500	-1.64777100	3.30029100
H	5.30186500	-1.01225900	1.81115200
C	4.09183800	-3.44928300	1.29687800
H	5.02296800	-3.37468300	0.72455200
H	4.35576800	-3.88383500	2.27211800
H	3.42889000	-4.16571000	0.79581300
C	1.07683000	-3.11479700	-0.88779000
H	0.28506300	-2.51343300	-0.41705900
H	0.62036700	-3.63707400	-1.74185500
H	1.40823500	-3.88091800	-0.17412900
C	1.69780500	-1.30353800	-2.48221000
H	1.35400400	-1.89913600	-3.34040000
H	0.83691200	-0.71661400	-2.12921200
H	2.47205900	-0.61171600	-2.84325900
C	3.28918700	-3.15213300	-2.04199400
H	3.75226900	-3.84667000	-1.33157700
H	2.79987600	-3.75811300	-2.81822500
H	4.08044700	-2.57320200	-2.53285400
C	4.34790700	-0.31208500	-0.71285500
C	4.36746100	1.04032800	-1.11576100
C	5.48042100	-1.10153600	-0.97081400
C	5.49406300	1.52362000	-1.79633800
C	6.59840000	-0.59733400	-1.61955200
H	5.49084800	-2.14588900	-0.67206500
C	6.59878800	0.72430100	-2.04962500
H	5.49769400	2.56748200	-2.10795600
H	7.45777400	-1.24062800	-1.79548500
H	7.45999900	1.13585800	-2.57202200
C	3.30717600	2.04698900	-0.85027800
C	3.06927600	2.50615000	0.45112500
C	2.64746900	2.66649600	-1.91528500
C	2.18793600	3.55844400	0.67813500
H	3.61159200	2.05758300	1.28441000
C	1.75567100	3.71165500	-1.68518000
H	2.84387400	2.32829100	-2.93326300
C	1.52027900	4.15797900	-0.38786700
H	2.02991900	3.91964600	1.69272000
H	1.24471100	4.17972200	-2.52573500

H	0.82314400	4.97496700	-0.20447400

$TS_{xvii-xix}$

E (M06-D3-CPCM/BS1) = -2914.55624978 au

H (M06-D3-CPCM/BS1) = -2913.67547 au

G (M06-D3-CPCM/BS1) = -2913.816002 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2915.81849928 au

C	1.18412800	-3.14129500	2.77476600
C	0.67649500	-2.13573600	1.96815400
C	1.45162700	-0.99741900	1.65016200
C	2.73501600	-0.87509000	2.24387100
C	3.22719600	-1.86611900	3.06698800
C	2.45876000	-3.00806300	3.32095000
H	0.58483400	-4.02415700	2.98601300
H	-0.32183100	-2.23074100	1.54130200
H	3.31427100	0.02868300	2.07166400
H	4.20910100	-1.75750300	3.52243800
H	2.85586000	-3.79177000	3.96328500
C	0.91569600	-0.01817800	0.75197900
C	1.84375400	0.90068900	0.03038700
S	4.34495800	1.38739900	-0.77470700
O	4.20829000	1.85965000	-2.14824400
O	4.45212400	2.32908600	0.33041400
C	5.69934900	0.25403700	-0.69916800
C	6.28308900	-0.20132900	-1.87703700
C	6.14987600	-0.17198600	0.54985200
C	7.33774700	-1.10155600	-1.79594800
H	5.91231200	0.14580400	-2.83924700
C	7.19896900	-1.07624000	0.60873700
H	5.69180100	0.20775500	1.46172900
C	7.80875900	-1.55114400	-0.55923900
H	7.80428100	-1.46617000	-2.71033000
H	7.55925800	-1.42085200	1.57747800
C	8.96262000	-2.50182000	-0.47978900
H	9.90909000	-1.95364600	-0.37288800
H	8.87614800	-3.16773600	0.38678200
H	9.04271900	-3.11564800	-1.38423700
N	3.06003700	0.31951400	-0.37513200
C	3.03867100	-0.96196400	-1.09307100
H	3.78523000	-1.65312500	-0.68544200
H	2.04770100	-1.41093100	-0.97997800
H	3.21193400	-0.80806100	-2.16713400
C	0.13699900	3.34936400	1.27740100
C	0.60668100	3.00411600	-0.01317600

C	0.16454700	3.76130800	-1.12483300
C	-0.69195300	4.83535100	-0.91434900
C	-1.11524600	5.21035400	0.36278200
C	-0.69058100	4.47192000	1.44910400
C	0.47324400	2.61632800	2.48086500
H	-1.76638600	6.07090600	0.49578800
H	-1.00310200	4.73846700	2.45920400
H	0.25969000	3.15267300	3.42940500
C	0.63683900	3.40012800	-2.49733200
H	1.73410000	3.35938500	-2.53846100
H	0.28297800	2.40086800	-2.79144200
H	0.27803000	4.11993600	-3.24123500
N	1.62236100	2.11256600	-0.29365500
O	0.93200200	1.48017000	2.53873500
H	-1.02229300	5.41072200	-1.77949500
Au	-1.07596500	-0.03237200	0.18651000
P	-3.48301000	0.09750000	-0.05462400
C	-4.11810300	0.33841500	1.72653500
C	-3.93057500	1.51811500	-1.22008600
C	-3.13895000	1.24431900	2.48372300
H	-3.51379800	1.38077400	3.50867000
H	-2.13702200	0.79738100	2.55434600
H	-3.03636200	2.23961400	2.03323600
C	-4.08586200	-1.04689400	2.37919000
H	-3.10693200	-1.53740500	2.25838000
H	-4.26756200	-0.93311700	3.45771300
H	-4.85603300	-1.71635500	1.97654700
C	-5.51768300	0.93655400	1.85590700
H	-6.29489500	0.32327400	1.38698400
H	-5.76843100	1.00152600	2.92491100
H	-5.57669500	1.95439400	1.44920500
C	-3.42991400	2.81682600	-0.59467000
H	-2.37298300	2.75256800	-0.30331400
H	-3.51566900	3.62548000	-1.33586900
H	-4.01828400	3.11656400	0.28288100
C	-3.15201700	1.25633900	-2.51222100
H	-3.33881700	2.08188900	-3.21464800
H	-2.06698100	1.20304700	-2.33936200
H	-3.47658400	0.32769500	-3.00318700
C	-5.40856200	1.66428600	-1.57662700
H	-6.05096900	1.81957800	-0.70142700
H	-5.51641800	2.55072500	-2.21874800
H	-5.78535200	0.80587400	-2.14506500
C	-4.35813300	-1.40034300	-0.67907300

C	-3.70689900	-2.60459200	-1.02355800
C	-5.76314400	-1.38117500	-0.68273600
C	-4.48751900	-3.73091500	-1.32401900
C	-6.51812300	-2.50164600	-0.99801100
H	-6.29201100	-0.47018200	-0.42096200
C	-5.87330000	-3.69148500	-1.31290800
H	-3.97627800	-4.65453200	-1.59262500
H	-7.60424000	-2.44183400	-0.98864400
H	-6.44525800	-4.58446100	-1.55658900
C	-2.24044500	-2.81225200	-1.13226200
C	-1.63164300	-3.81525000	-0.36919500
C	-1.47564200	-2.14203800	-2.09482900
C	-0.29439700	-4.14615400	-0.56578500
H	-2.22273400	-4.34608000	0.37781700
C	-0.13825400	-2.47661600	-2.29552200
H	-1.94442700	-1.38515100	-2.72322300
C	0.45338100	-3.48359000	-1.53605200
H	0.16169500	-4.93246800	0.03369800
H	0.43586700	-1.95925700	-3.06353000
H	1.49338400	-3.75911400	-1.70690100

xix

E (M06-D3-CPCM/BS1) = -2914.572727 au

H (M06-D3-CPCM/BS1) = -2913.690711 au

G (M06-D3-CPCM/BS1) = -2913.828516 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2915.83484904 au

C	-1.41323500	-3.65426600	-1.31730500
C	-0.88149100	-2.42059000	-0.95344900
C	-1.52021500	-1.22976200	-1.31195900
C	-2.68704800	-1.30539700	-2.08265800
C	-3.20734100	-2.53560900	-2.46698600
C	-2.57790500	-3.71579200	-2.07593300
H	-0.90739900	-4.56837400	-1.00994900
H	0.02751100	-2.38365500	-0.35005100
H	-3.19612800	-0.38859800	-2.37637000
H	-4.11658800	-2.57247800	-3.06501200
H	-2.99217200	-4.67918600	-2.36726000
C	-1.00626500	0.08850800	-0.79820400
C	-1.83413900	0.68624500	0.34279900
S	-4.32840900	1.27986000	0.99016700
O	-4.40679700	1.50238900	2.42874000
O	-4.12837600	2.39526300	0.07493300
C	-5.73374600	0.34431500	0.47572200
C	-6.57519500	-0.21918600	1.42910400

C	-5.95737700	0.17217300	-0.89023200
C	-7.66235300	-0.96984200	0.99891800
H	-6.37722500	-0.07131100	2.48869100
C	-7.04304100	-0.58618100	-1.29776500
H	-5.29291000	0.63382200	-1.61869000
C	-7.91060400	-1.16513300	-0.36224900
H	-8.33051100	-1.41666200	1.73405000
H	-7.22966300	-0.73259400	-2.36119400
C	-9.09469700	-1.95814800	-0.82099400
H	-9.91961500	-1.29178500	-1.10878000
H	-8.85268900	-2.56675000	-1.70064000
H	-9.46781700	-2.62090200	-0.03219100
N	-3.08204600	0.14782600	0.62941400
C	-3.27798200	-1.21462800	1.14118800
H	-3.99417100	-1.76937200	0.52442300
H	-2.31907400	-1.73731900	1.13304100
H	-3.62892700	-1.16875000	2.18123900
C	-0.44625100	3.03646000	-0.88536400
C	-0.55260800	2.66634900	0.48975600
C	0.15846200	3.41682700	1.45524700
C	0.88889900	4.51511000	1.03041300
C	0.92787300	4.93428000	-0.31189200
C	0.24664600	4.21620700	-1.26113900
C	-1.00623900	2.27546100	-1.92413200
H	1.49064500	5.82246700	-0.58678100
H	0.26174500	4.50924300	-2.30992600
H	-1.17214600	2.73324700	-2.90225300
C	0.09971900	3.01969300	2.89364500
H	-0.93240600	2.80497300	3.20057200
H	0.68018500	2.10139700	3.06931900
H	0.50995300	3.80211900	3.54053100
N	-1.49446300	1.77674200	0.92502200
O	-1.31678700	1.03586100	-1.90770400
H	1.43106400	5.09366500	1.77853300
Au	1.12304800	0.05608200	-0.44110200
P	3.52291700	-0.06284900	-0.54953400
C	3.88957400	-0.94048500	-2.19932100
C	4.19465600	1.70536400	-0.43866000
C	2.87582500	-0.47322700	-3.24957000
H	3.08798700	-0.99323100	-4.19532000
H	1.84320800	-0.71646000	-2.96048500
H	2.92981200	0.60463500	-3.44592000
C	3.65390200	-2.43159400	-1.93950700
H	2.66632200	-2.61909000	-1.49014300

H	3.68800100	-2.96706400	-2.89946100
H	4.41810000	-2.86743400	-1.28349700
C	5.29319400	-0.73297100	-2.76312600
H	6.08367200	-1.07897800	-2.08772100
H	5.38611000	-1.32029200	-3.68862300
H	5.48467700	0.31518800	-3.02704800
C	3.59069800	2.51807400	-1.58504800
H	2.49902800	2.39978600	-1.65353800
H	3.79749200	3.58485700	-1.41220900
H	4.03263300	2.25384900	-2.55510400
C	3.67577300	2.24399200	0.89770900
H	4.00225300	3.28863300	1.01472700
H	2.57773000	2.23130800	0.94955000
H	4.07442600	1.67422300	1.74945500
C	5.71308900	1.87864900	-0.45743100
H	6.18997800	1.44364100	-1.34381400
H	5.93143700	2.95670300	-0.46731400
H	6.18749500	1.46468500	0.43967100
C	4.42412700	-1.05400300	0.71610000
C	3.77718900	-1.83328600	1.69961600
C	5.82174400	-1.14847500	0.60712200
C	4.55332200	-2.67544700	2.50972900
C	6.57390500	-1.97674800	1.42784000
H	6.34531100	-0.57183500	-0.14868000
C	5.93222400	-2.75267100	2.38519600
H	4.04584300	-3.27145800	3.26728700
H	7.65456000	-2.01842200	1.30982100
H	6.50121400	-3.41415700	3.03535000
C	2.31885300	-1.86279700	1.98748500
C	1.62891500	-3.07468800	1.86970000
C	1.65014800	-0.75734000	2.52667900
C	0.31014300	-3.18838100	2.29924900
H	2.14511400	-3.93941200	1.45150400
C	0.33100300	-0.87112400	2.96039200
H	2.18705300	0.18478300	2.64862800
C	-0.33506500	-2.09042300	2.86254900
H	-0.20882600	-4.14155200	2.20830700
H	-0.17284600	-0.01051100	3.40052900
H	-1.35074200	-2.18822100	3.24192200

TS_{xix-xx}

E (M06-D3-CPCM/BS1) = -2914.54986084 au

H (M06-D3-CPCM/BS1) = -2913.668875 au

G (M06-D3-CPCM/BS1) = -2913.808286 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2915.8135703 au

C	1.36837600	-1.10645700	4.80098000
C	0.79397200	-0.29598500	3.83342200
C	1.50317800	0.05463600	2.67681500
C	2.80606000	-0.42695400	2.51286600
C	3.37963000	-1.23864400	3.48842700
C	2.66815600	-1.58062800	4.63241700
H	0.79913100	-1.36746000	5.69108800
H	-0.22163900	0.07181400	3.98007100
H	3.39268200	-0.13833200	1.64487500
H	4.39976800	-1.59198700	3.35120800
H	3.12363800	-2.21141500	5.39325700
C	0.91078600	1.10078000	1.78460500
C	1.38186300	1.51445700	0.43637600
S	3.23914200	1.44617700	-1.48284800
O	2.48733300	1.40972000	-2.73349400
O	3.76016800	2.69910300	-0.95884700
C	4.57485300	0.29159800	-1.59505100
C	4.65035100	-0.57557300	-2.67917500
C	5.53927900	0.28685300	-0.58741700
C	5.71468900	-1.46669900	-2.74927100
H	3.88449300	-0.55109800	-3.45168100
C	6.58907000	-0.61397700	-0.67305300
H	5.46773800	0.98454300	0.24570500
C	6.69385100	-1.49980800	-1.75347300
H	5.78680200	-2.15187800	-3.59303900
H	7.34914100	-0.63206000	0.10744600
C	7.85033100	-2.44673900	-1.84240300
H	8.75796500	-1.92198400	-2.17105800
H	8.07614300	-2.89486800	-0.86698600
H	7.65819900	-3.25379300	-2.55818200
N	2.32921000	0.69112500	-0.22185000
C	1.97815100	-0.70697500	-0.50688900
H	2.87137700	-1.34108000	-0.47513800
H	1.29289000	-1.07195000	0.26229500
H	1.48549100	-0.80511000	-1.48570100
C	-0.97803000	3.19339400	1.12677500
C	0.00404500	3.45708800	0.13319400
C	-0.19113400	4.54723700	-0.75360900
C	-1.34710100	5.29974900	-0.62972800
C	-2.33969600	4.99560200	0.31660300
C	-2.17207400	3.93440000	1.18042500
C	-0.66699700	2.19795900	2.10769200
H	-3.23451000	5.61104900	0.37662300

H	-2.91280000	3.70845000	1.94644600
H	-1.39607400	1.88364700	2.86275500
C	0.80577600	4.81027300	-1.83543900
H	1.82911700	4.85611600	-1.44416300
H	0.79695000	3.98991400	-2.56782600
H	0.57985800	5.74550300	-2.35938700
N	1.02594800	2.59883400	-0.16660400
O	0.63117100	2.23826600	2.55625900
H	-1.50036800	6.13864600	-1.30796200
Au	-1.11566200	0.16513400	0.83041300
P	-2.86848500	-0.52214800	-0.69676700
C	-4.54204700	-0.11170900	0.11723700
C	-2.51380700	0.49633800	-2.26758300
C	-4.37756300	1.14537700	0.97402600
H	-5.34379900	1.37944300	1.44365200
H	-3.65070200	0.98997500	1.78432000
H	-4.07028300	2.02376100	0.39299700
C	-4.88550500	-1.27706200	1.04609900
H	-4.10893500	-1.42867300	1.80929600
H	-5.81912800	-1.03981900	1.57606300
H	-5.03585800	-2.21978700	0.50551400
C	-5.69589200	0.12292100	-0.85864200
H	-5.95387300	-0.76490500	-1.44574600
H	-6.58964300	0.38119600	-0.27260500
H	-5.50848600	0.95938700	-1.54309400
C	-2.68021400	1.98250800	-1.95434400
H	-2.13747100	2.28512900	-1.04996000
H	-2.26690900	2.56532800	-2.79136400
H	-3.73267300	2.27501600	-1.84197600
C	-1.04623600	0.22102400	-2.61188100
H	-0.81284900	0.68533100	-3.58111900
H	-0.36222500	0.65836200	-1.87072300
H	-0.83093200	-0.85518200	-2.69721000
C	-3.36097600	0.15077400	-3.49207900
H	-4.43856600	0.25751800	-3.32005200
H	-3.09059300	0.85390300	-4.29299500
H	-3.15991500	-0.85944400	-3.86625300
C	-2.96666500	-2.27237300	-1.26823700
C	-2.05245600	-3.29045400	-0.91971000
C	-3.98495700	-2.58088400	-2.18653500
C	-2.16382500	-4.53765500	-1.55392600
C	-4.09491900	-3.82935600	-2.78059700
H	-4.70931500	-1.82354900	-2.46614200
C	-3.16193400	-4.81233600	-2.47515900

H	-1.45808000	-5.31924800	-1.27654700
H	-4.90215900	-4.02387000	-3.48312600
H	-3.22085600	-5.79574500	-2.93691100
C	-1.00619500	-3.21343300	0.12726700
C	-1.34427800	-2.95501700	1.46193100
C	0.30649600	-3.59431500	-0.17213000
C	-0.39424000	-3.08244300	2.47056300
H	-2.37672600	-2.71654200	1.71629000
C	1.25669800	-3.71860600	0.83680700
H	0.57758200	-3.80118700	-1.20802500
C	0.90707200	-3.46858700	2.16057700
H	-0.67841100	-2.89916500	3.50545300
H	2.27433100	-4.01582100	0.58711000
H	1.64762500	-3.56851500	2.95212100

xx

E (M06-D3-CPCM/BS1) = -2914.58879435 au

H (M06-D3-CPCM/BS1) = -2913.705316 au

G (M06-D3-CPCM/BS1) = -2913.846012 au

E (M06-D3-SMD/BS2//M06-D3-CPCM/BS1) = -2915.85250094 au

C	0.08733100	-1.03998400	-3.57872400
C	-0.12703400	0.16423700	-2.87901700
C	-1.33887100	0.37442800	-2.17331700
C	-2.31556000	-0.61717800	-2.21593100
C	-2.09524200	-1.80199100	-2.91934900
C	-0.89541800	-2.02829800	-3.58214500
H	1.00575900	-1.16594400	-4.15054900
H	0.55219100	1.00333200	-3.05127100
H	-3.25878500	-0.46540800	-1.69633200
H	-2.87876100	-2.55678900	-2.94576600
H	-0.73332000	-2.95720200	-4.12429500
C	-1.55565500	1.65737200	-1.43449100
C	-1.86327400	1.64690200	0.03546500
S	-4.03285800	0.99934600	1.38144600
O	-3.76364400	1.04224800	2.81578800
O	-4.56559800	2.16860100	0.69529600
C	-5.07546000	-0.39132800	1.04915600
C	-5.28856200	-1.35216100	2.03134200
C	-5.68000200	-0.48646400	-0.20478300
C	-6.11681900	-2.43186900	1.74433200
H	-4.81502600	-1.25004000	3.00577600
C	-6.50035000	-1.57062300	-0.47167700
H	-5.51689800	0.28912200	-0.95217100
C	-6.73155300	-2.55691800	0.49688100

H	-6.29143600	-3.19126800	2.50553400
H	-6.98044300	-1.65697000	-1.44607400
C	-7.63981400	-3.70873400	0.19510100
H	-8.68801300	-3.38130400	0.16468400
H	-7.41500000	-4.14747000	-0.78517100
H	-7.55978900	-4.49692100	0.95197100
N	-2.63469000	0.54416000	0.51360800
C	-1.88427400	-0.55556200	1.12244900
H	-2.55229300	-1.41196600	1.27522800
H	-1.09520600	-0.87310900	0.42781300
H	-1.42882200	-0.26264800	2.08056300
C	-0.57153900	3.94389900	-0.94038500
C	-0.91972400	3.74650400	0.40677600
C	-0.56013700	4.69246600	1.38357100
C	0.16235500	5.81392700	0.97586600
C	0.53039800	5.99824400	-0.35468000
C	0.16574100	5.06104600	-1.31573300
C	-0.96407100	2.91893500	-1.92388300
H	1.09584200	6.88190200	-0.64354500
H	0.44167000	5.19934100	-2.36081300
H	-0.40629300	2.91367700	-2.86365200
C	-0.92329800	4.48424100	2.82070700
H	-1.99059100	4.26074500	2.93905800
H	-0.38027300	3.62979400	3.24851100
H	-0.68099600	5.37033500	3.41790600
N	-1.59167500	2.60123100	0.83697600
O	-2.35317400	2.64413100	-2.09468000
H	0.44514500	6.55667500	1.72140400
Au	1.33442000	-0.53507600	-1.16650800
P	3.18047300	-0.13672900	0.26925600
C	4.66018300	0.19722100	-0.87975800
C	2.71317600	1.33573700	1.36381200
C	4.15971200	0.93788400	-2.12570200
H	5.02264400	1.15134400	-2.77283800
H	3.45455100	0.32916500	-2.70921800
H	3.67608100	1.89433500	-1.89248500
C	5.19856300	-1.16652900	-1.31533500
H	4.41701600	-1.78288800	-1.78269300
H	5.98516000	-1.00989100	-2.06730800
H	5.63623200	-1.73174000	-0.48344300
C	5.78678600	1.02359400	-0.25805400
H	6.24922800	0.54741100	0.61331400
H	6.57959700	1.13866400	-1.01115900
H	5.46164500	2.03296900	0.02226500

C	2.48630600	2.56275000	0.48169400
H	1.79850600	2.35684400	-0.35312300
H	2.02698300	3.35483300	1.09317900
H	3.42164600	2.96695900	0.07316700
C	1.39100000	0.94936700	2.03087400
H	1.11443900	1.73260900	2.75302400
H	0.57545500	0.87594600	1.29918400
H	1.45664200	-0.00217500	2.57942700
C	3.72525800	1.67190600	2.45887300
H	4.72279500	1.90888300	2.07118200
H	3.36266200	2.56310600	2.99102400
H	3.81616700	0.86657400	3.19726100
C	3.64295900	-1.48864700	1.42572600
C	2.86222600	-2.64572200	1.64048000
C	4.79524600	-1.30417300	2.20735500
C	3.24297000	-3.53285200	2.65697900
C	5.17121500	-2.20957200	3.18880200
H	5.41498100	-0.42432500	2.06109100
C	4.37894700	-3.32640800	3.42558000
H	2.63331900	-4.42086000	2.81933200
H	6.07407300	-2.03354300	3.76921500
H	4.64940700	-4.04228800	4.19899900
C	1.67091100	-3.04967900	0.85129100
C	1.79407800	-3.41635300	-0.49576800
C	0.43317400	-3.20562900	1.48088300
C	0.69944200	-3.91464200	-1.19718800
H	2.76841600	-3.35079900	-0.98116500
C	-0.66080300	-3.70594000	0.77852100
H	0.33236100	-2.93608800	2.53300200
C	-0.53260700	-4.05685800	-0.56200600
H	0.81871400	-4.21028100	-2.23838000
H	-1.61619200	-3.83038300	1.28602200
H	-1.38530800	-4.45668700	-1.10842600