Supplementary Information

Catalytic asymmetric inverse-electron-demand aza-Diels–Alder reaction of 1,3-diazadienes with 3-vinylindoles

Yu-Hang Miao, Yuan-Zhao Hua,* Hao-Jie Gao, Nan-Nan Mo, Min-Can Wang,* and Guang-Jian Mei*

Green Catalysis Center, and College of Chemistry, Zhengzhou University, Zhengzhou 450001, China.

E-mail: hyzh@gs.zzu.edu.cn; wangmincan@zzu.edu.cn; meigj@zzu.edu.cn.

Contents

1. General Information. 2

2. General Procedures for the Synthesis of Isothiourea 3. 3

3. Synthesis of Isothiourea 4. 4

4. Characterization of benzothiazolopyrimidines. 5

5. Crystallographic data collection for compound 3oa. 23

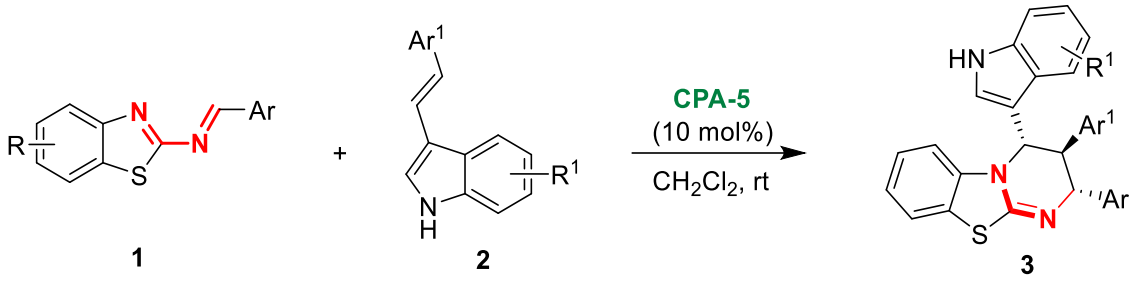
6. HPLC spectra of compounds. 25

7. NMR Spectra of compounds. 70

1. General Information.

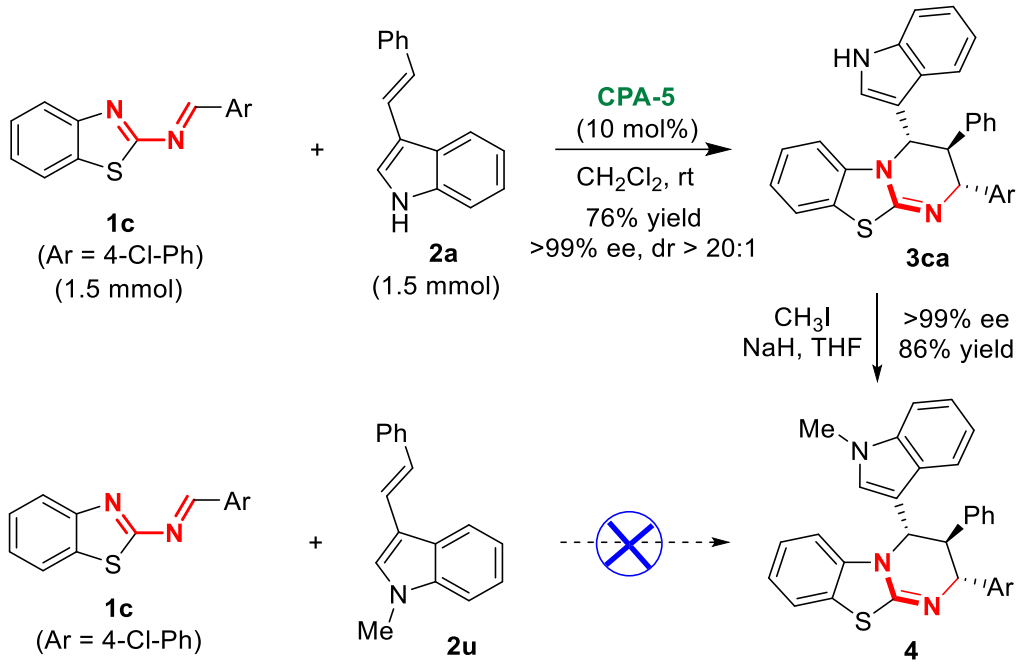
All reactions were carried out in oven-dried glassware with magnetic stirring. Reagents were obtained from commercial supplier and used without further purification unless otherwise noted. Solvents were dried with standard methods and freshly distilled prior to use if needed. All reactions sensitive to air or moisture were carried out under nitrogen using standard Schlenk and vacuum line techniques. NMR spectra were recorded on a 400 MHz NMR spectrometer with d_6-DMSO as the solvent and TMS as an internal standard (400 MHz for ^{1}H and 100 MHz for ^{13}C). HRMS were determined on a Q-TOF Micro LC/MS System ESI spectrometer. Enantiomeric excesses values were determined with HPLC (chiral column; mobile phase hexane/i-PrOH).

2. General Procedures for the Synthesis of Isothiourea 3.



To a solution of imine **1** (1 equiv) and catalyst CPA-5 (10 mol%) in dry DCM (1 mL), was added the 3-vinylindole **2** (1 equiv) in one portion. The reaction mixture was stirred for 12 h at rt. After completion (monitored by TLC), the solvent was removed under reduced pressure and the crude product was directly purified by flash chromatography on silica gel employing mixtures of DCM and ethyl acetate as eluents to afford the desired product **3**.

3. Synthesis of Isothiourea 4.

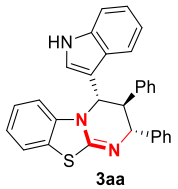


To a solution of imine **1c** (1.5 mol) and catalyst **CPA-5** (10 mol%) in dry DCM (0.1 M), was added the 3-vinylindole **2a** (1 equiv) in one portion. The reaction mixture was stirred for 24 h at rt. After completion (monitored by TLC), the solvent was removed under reduced pressure and the crude product was directly purified by flash chromatography on silica gel employing mixtures of DCM and ethyl acetate as eluents to afford the desired product **3ca**.

To a solution of **3ca** (0.1 mmol) in dry THF (0.1 M) at 0 °C was added NaH (0.12 mmol, 1.2 equiv). Reaction was stirred for 30 min. Then, add of CH_3I (0.12 mol, 1.2 equiv). The solution was stirred at rt for the necessary reaction time, and then quenched with aqueous NH_4Cl (5 mL), and extracted three times with ethyl acetate (3×5 mL). The combined organics was washed with brine before being dried by $MgSO_4$, filtered and concentrated in vacuo. The crude product was separated by flash column chromatography on silica gel (petroleum ether/ethyl acetate 5:1–2:1) to afford a compound **4** as a white solid.

4. Characterization of benzothiazolopyrimidines.

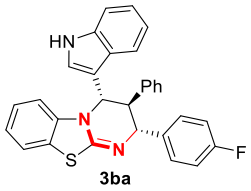
(*2R,3S,4S*)-4-(1H-indol-3-yl)-2,3-diphenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3aa**:



3aa

White solid, M.p.: 161-162 °C; yield: 65%; $[\alpha]^{20}_D$ = +26 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 18.75 min (major), t_2 = 21.58 min (minor), ee = 96%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.81 (s, 1H), 7.46-7.42 (m, 1H), 7.38-7.30 (m, 1H), 7.25-7.19 (m, 1H), 7.12-6.98 (m, 9H), 6.96-6.61 (m, 6H), 6.56 (d, *J* = 7.3 Hz, 1H), 5.70 (d, *J* = 10.0 Hz, 1H), 4.84 (d, *J* = 10.3 Hz, 1H), 3.22 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 157.8, 143.9, 140.5, 136.8, 129.2, 128.3, 128.1, 127.9, 126.8, 126.7, 125.7, 125.5, 125.0, 122.2, 122.1, 121.8, 121.5, 119.5, 118.2, 112.4, 112.0, 111.5, 64.7, 58.0, 53.6; HRMS (ESI) Calcd. For $C_{30}H_{24}N_3S$ $[M+H]^+$ 458.1685, found 458.1688.

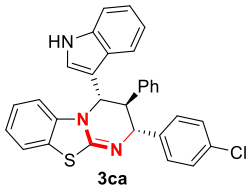
(*2R,3S,4S*)-2-(4-fluorophenyl)-4-(1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ba**:



3ba

White solid, M.p.: 182-183 °C; yield: 74%; $[\alpha]^{20}_D$ = +121 (*c* 0.23, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 8/92, flow rate 1.0 mL/min, λ = 254 nm), t_1= 33.64 min (minor), t_2 = 36.96 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.82 (s, 1H), 7.44-7.41 (m, 1H), 7.30 (d, J = 7.8 Hz, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.06-6.95 (m, 7H), 6.91-6.77 (m, 7H), 6.55 (d, *J* = 7.2 Hz, 1H), 5.71 (d, *J* = 10.0 Hz, 1H), 4.85 (d, *J* = 10.2 Hz, 1H), 3.18 (t, *J* = 10.1 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 161.1 (d, *J* = 240.2 Hz), 157.9, 140.5, 140.4, 140.1(d, *J* = 2.8 Hz), 136.8, 129.8 (d, *J* = 8.0 Hz), 129.2, 128.4, 126.9, 125.8, 125.5, 125.0, 122.2, 122.2, 121.8, 121.5, 119.5, 118.2, 114.6 (d, *J* = 21.0 Hz) 112.4, 112.1, 111.4, 63.9, 57.9, 53.8; ^{19}F NMR (376 MHz, d_6-DMSO) δ ppm: -111.98; HRMS (ESI) Calcd. For $C_{30}H_{23}FN_3S$ $[M+H]^+$ 476.1591, found 476.1595.

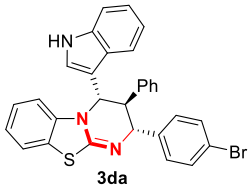
(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ca**:



3ca

White solid, M.p.: 154-155 °C; yield: 76%; $[\alpha]^{20}_D$ = +119 (c 0.28, CH_2Cl_2); HPLC (Chiralpak ID, i-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 26.81 min (minor), t_2 = 29.00 min (major), ee = >99%; ^{1}H NMR (400 M, d6-DMSO) δ ppm: 10.83 (s, 1H), 7.44-7.41 (m, 1H), 7.37-7.24 (m, 2H), 7.19-7.07 (m, 2H), 7.05-6.96 (m, 7H), 6.92-6.78 (m, 5H), 6.56 (d, *J* = 7.4 Hz, 1H), 5.71 (d, *J* = 10.0 Hz, 1H), 4.86 (d, *J* = 10.2 Hz, 1H), 3.18 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d6-DMSO) δ ppm: 158.1, 142.9, 140.5, 140.2, 136.8, 131.1, 129.9, 129.2, 128.4, 127.9, 127.0, 125.8, 125.6, 125.0, 122.2, 121.9, 121.5, 119.6, 118.2, 112.4, 112.1, 111.3, 63.9, 57.9, 53.6; HRMS (ESI) Calcd. For $C_{30}H_{23}ClN_3S$ $[M+H]^+$ 492.1296, found 492.1299.

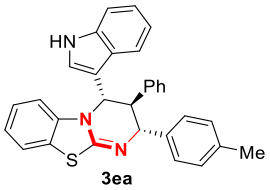
(*2R,3S,4S*)-2-(4-bromophenyl)-4-(1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3da**:



3da

White solid, M.p.: 182-183 °C; yield: 70%; $[\alpha]^{20}_D$ = +126 (*c* 0.18, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 28.64 min (minor), t_2 = 32.26 min (major), ee = 99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.82 (s, 1H), 7.44-7.42 (m, 1H), 7.30-7.23 (m, 4H), 7.07-7.02 (m, 3H), 6.99-6.95 (m, 4H), 6.91-6.76 (m, 5H), 6.55 (d, *J* = 7.3 Hz, 1H), 5.70 (d, *J* = 10.0 Hz, 1H), 4.85 (d, *J* = 10.3 Hz, 1H), 3.17 (t, *J* = 10.1 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.1, 143.4, 140.5, 140.3, 136.8, 130.8, 130.3, 129.2, 128.4, 127.0, 125.8, 125.0, 122.2, 122.2, 121.9, 121.5, 119.7, 119.5, 118.2, 112.4, 112.1, 111.3, 64.0, 57.9, 53.5; HRMS (ESI) Calcd. For $C_{30}H_{23}BrN_3S$ $[M+H]^+$ 536.0791, found 536.0795.

(*2R,3S,4S*)-4-(1H-indol-3-yl)-3-phenyl-2-(p-tolyl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ea**:

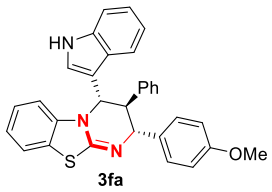


3ea

White solid, M.p.: 167-168 °C; yield: 60%; $[\alpha]^{20}_D$ = +60 (*c* 0.36, CH_2Cl_2); HPLC (Chiralpak IE, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1= 12.00 min (minor), t_2 = 13.02 min (major), ee = 98%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.83 (s, 1H), 7.43-7.41 (m, 1H), 7.32-7.24 (m, 2H), 7.03-6.88 (m, 10H), 6.82-6.77 (m, 4H), 6.55 (d, *J* = 7.0 Hz, 1H), 5.66 (d, *J* = 10.1 Hz, 1H), 4.80 (d, *J* = 10.4 Hz, 1H), 3.20

(t, *J* = 10.2 Hz, 1H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 157.7, 140.9, 140.6, 140.5, 136.8, 135.5, 129.3, 128.0, 126.8, 125.9, 125.7, 125.5, 125.0, 122.3, 122.1, 121.8, 121.5, 121.3, 119.5, 118.2, 112.4, 112.1, 111.5, 64.3, 58.1, 53.6, 21.1; HRMS (ESI) Calcd. For $C_{31}H_{26}N_3S$ $[M+H]^+$ 472.1842, found 472.1845.

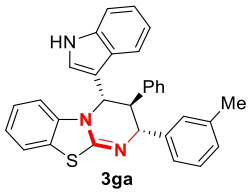
(*2R,3S,4S*)-4-(1H-indol-3-yl)-2-(4-methoxyphenyl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3fa**:



3fa

White solid, M.p.: 261-262 °C; yield: 55%; $[\alpha]^{20}_D$ = +55 (c 0.34, CH_2Cl_2); HPLC (Chiralpak ID, i-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1= 12.50 min (minor), t_2 = 17.62 min (major), ee = 99%; ^{1}H NMR (400 M, d6-DMSO) δ ppm: 10.66 (s, 1H), 7.47-7.42 (m, 1H), 7.23-7.14 (m, 3H), 7.10-7.01 (m, 6H), 6.88-6.78 (m, 6H), 6.61-6.59 (m, 2H), 5.67 (d, *J* = 10.0 Hz, 1H), 4.87 (d, *J* = 10.3 Hz, 1H), 3.71 (s, 3H), 3.19 (t, *J* = 10.1 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.3, 156.0, 143.1, 140.7, 140.4, 137.8, 131.3, 130.0, 129.4, 128.6, 128.0, 127.1, 125.7, 124.5, 122.4, 122.3, 122.1, 119.4, 118.9, 112.3, 111.5, 109.9, 95.6, 64.1, 58.2, 55.6, 53.9; HRMS (ESI) Calcd. For $C_{31}H_{26}N_3OS$ $[M+H]^+$ 488.1791, found 488.1789.

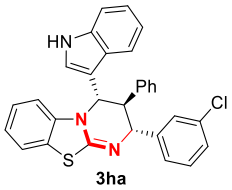
(*2R,3S,4S*)-4-(1H-indol-3-yl)-3-phenyl-2-(m-tolyl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ga**:



3ga

White solid, M.p.: 137-138 °C; yield: 52%; $[\alpha]^{20}_D$ = +58 (*c* 0.23, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 18.74 min (minor), t_2 = 21.28 min (major), ee = 98%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.85 (s, 1H), 7.46-7.43 (m, 1H), 7.34-7.26 (m, 2H), 7.15-7.01 (m, 7H), 7.00-6.81 (m, 6H), 6.80-6.74 (m, 2H), 6.59 (d, J = 7.2 Hz, 1H), 5.70 (d, *J* = 10.0 Hz, 1H), 4.82 (d, *J* = 10.2 Hz, 1H), 3.15 (t, *J* = 10.1 Hz, 1H), 2.11 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 157.7, 143.7, 140.6, 140.5, 136.8, 129.2, 128.6, 128.3, 127.7, 127.3, 126.8, 125.9, 125.7, 125.5, 125.3, 125.0, 122.2, 122.1, 121.8, 121.5, 121.3, 119.5, 118.2, 112.4, 112.0, 111.5, 64.6, 58.0, 53.4, 21.4; HRMS (ESI) Calcd. For $C_{31}H_{26}N_3S$ $[M+H]^+$ 472.1842, found 472.1843.

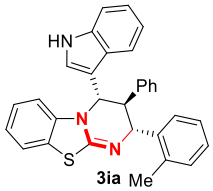
(*2R,3S,4S*)-2-(3-chlorophenyl)-4-(1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ha**:



3ha

White solid, M.p.: 152-153 °C; yield: 72%; $[\alpha]^{20}_D$ = +58 (*c* 0.23, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 23.34 min (major), t_2 = 27.44 min (minor), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.89 (s, 1H), 7.51-7.43 (m, 1H), 7.38-7.23 (m, 4H), 7.18-6.98 (m, 7H), 6.93-6.78 (m, 5H), 6.54 (d, *J* = 6.7 Hz, 1H), 5.69 (d, *J* = 10.1 Hz, 1H), 4.87 (d, *J* = 10.3 Hz, 1H), 3.20 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.3, 146.4, 140.5, 140.2, 136.8, 132.7, 129.7, 129.2, 128.5, 127.9, 127.0, 126.8, 126.7, 125.7, 125.6, 125.1, 122.2, 122.2, 121.9, 121.5, 119.6, 118.2, 112.4, 112.1, 111.4, 64.2, 57.9, 53.5; HRMS (ESI) Calcd. For $C_{30}H_{23}ClN_3S$ $[M+H]^+$ 492.1296, found 492.1299.

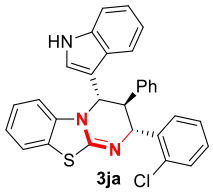
(*2R,3S,4S*)-4-(1H-indol-3-yl)-3-phenyl-2-(o-tolyl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ia**:



3ia

White solid, M.p.: 178-179 °C; yield: 62%; $[\alpha]^{20}_D$ = +20 (*c* 0.12, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 20.25 min (major), t_2 = 27.04 min (minor), ee = 94%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.86 (s, 1H), 7.85-7.67 (m, 1H), 7.53-7.43 (m, 1H), 7.38-7.21 (m, 3H), 7.20-7.04 (m, 2H), 7.02-6.72 (m, 9H), 6.64-6.62 (m, 2H), 5.66 (d, *J* = 10.2 Hz, 1H), 4.86 (d, *J* = 10.4 Hz, 1H), 3.53 (t, *J* = 10.4 Hz, 1H), 0.95 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.2, 142.9, 140.5, 139.2, 137.5, 136.8, 131.3, 129.9, 129.7, 128.1, 127.8, 126.7, 125.6, 125.3, 122.3, 122.3, 122.0, 121.7, 119.7, 118.0, 112.5, 112.3, 111.1, 64.2, 58.5, 47.8, 19.0; HRMS (ESI) Calcd. For $C_{31}H_{26}N_3S$ $[M+H]^+$ 472.1842, found 472.1845.

(*2R,3S,4S*)-2-(2-chlorophenyl)-4-(1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ja**:

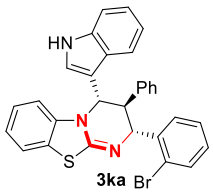


3ja

White solid, M.p.: 182-183 °C; yield: 72%; $[\alpha]^{20}_D$ = +20 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 19.45 min (major), t_2 = 26.79 min (minor), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.83 (s, 1H), 7.45-7.39 (m, 1H), 7.35-7.24 (m, 2H), 7.14-7.04 (m, 7H), 7.02-6.96 (m, 2H), 6.92-6.78 (m, 5H), 6.56 (d, *J* = 7.4 Hz, 1H), 5.72 (d, *J* = 10.0 Hz, 1H), 4.87 (d, *J*

= 10.3 Hz, 1H), 3.19 (t, *J* = 10.1 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.2, 143.0, 140.5, 140.3, 136.9, 131.2, 129.9, 129.3, 128.5, 127.9, 127.0, 125.8, 125.6, 125.0, 122.3, 122.2, 121.9, 121.6, 119.6, 118.2, 112.5, 112.1, 111.4, 64.0, 58.0, 53.6; HRMS (ESI) Calcd. For $C_{30}H_{23}ClN_3S$ $[M+H]^+$ 492.1296, found 492.1301.

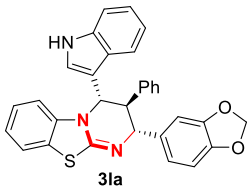
(*2R,3S,4S*)-2-(2-bromophenyl)-4-(1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ka**:



3ka

White solid, M.p.: 186-187 °C; yield: 70%; $[\alpha]^{20}_D$ = +116 (*c* 0.24, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 15/85, flow rate 1.0 mL/min, λ = 254 nm), t_1= 12.10 min (major), t_2 = 16.53 min (minor), ee = 98%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.83 (s, 1H), 7.46-7.37 (m, 3H), 7.34-7.11 (m, 3H), 7.05-6.82 (m, 11H), 6.80-6.59 (m, 1H), 5.82 (d, *J* = 7.4 Hz, 1H), 5.28 (d, *J* = 4.6 Hz, 1H), 3.54 (s, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.1, 142.5, 140.5, 139.8, 136.8, 132.2, 130.3, 129.2, 128.9, 128.3, 127.8, 127.0, 125.6, 125.0, 123.6, 122.2, 122.2, 121.9, 121.5, 119.5, 118.3, 112.3, 111.9, 111.5, 63.1, 57.5, 51.9; HRMS (ESI) Calcd. For $C_{30}H_{23}BrN_3S$ $[M+H]^+$ 536.0791, found 536.0794.

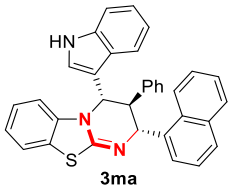
(*2R,3S,4S*)-2-(benzo[d][1,3]dioxol-5-yl)-4-(1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3la**:



3la

White solid, M.p.: 204-205 °C; yield: 70%; $[\alpha]^{20}_D$ = +98 (*c* 0.32, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 8/92, flow rate 1.0 mL/min, λ = 254 nm), t_1= 15.43 min (minor), t_2 = 17.06 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.81 (s, 1H), 7.45-7.39 (m, 1H), 7.35-7.21 (m, 2H), 7.08-6.95 (m, 5H), 6.92-6.76 (m, 5H), 6.61-6.46 (m, 4H), 5.86 (s, 2H), 5.66 (d, *J* = 10.0 Hz, 1H), 4.77 (d, *J* = 10.3 Hz, 1H), 3.19 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 157.6, 147.0, 145.8, 140.6, 140.5, 138.0, 136.8, 129.2, 128.3, 126.8, 125.7, 125.5, 125.0, 122.2, 122.1, 121.8, 121.5, 121.3, 119.5, 118.3, 112.4, 112.0, 111.5, 108.3, 107.7, 101.0, 64.3, 58.0, 53.6; HRMS (ESI) Calcd. For $C_{31}H_{24}N_3O_2S$ $[M+H]^+$ 502.1584, found 502.1585.

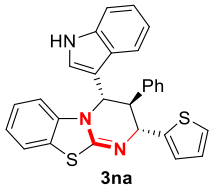
(*2R,3S,4S*)-4-(1H-indol-3-yl)-2-(naphthalen-1-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ma**:



3ma

White solid, M.p.: 215-216 °C; yield: 68%; $[\alpha]^{20}_D$ = +100 (*c* 0.31, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 15/85, flow rate 1.0 mL/min, λ = 254 nm), t_1= 20.43 min (major), t_2 = 23.18 min (minor), ee = 99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.86 (s, 1H), 7.57-7.21 (m, 4H), 7.17-7.00 (m, 11H), 6.97-6.79 (m, 5H), 6.61 (d, *J* = 7.3 Hz, 1H), 5.73 (d, *J* = 10.0 Hz, 1H), 4.89 (d, *J* = 10.3 Hz, 1H), 3.27 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.9, 143.8, 142.3, 141.1, 137.5, 132.4, 132.0, 131.2, 130.6, 130.6, 129.2, 128.7, 126.5, 126.3, 125.7, 122.9, 122.9, 122.6, 122.5, 122.3, 120.3, 118.8, 113.1, 112.8, 111.7, 64.5, 58.2, 54.1; HRMS (ESI) Calcd. For $C_{34}H_{26}N_3S$ $[M+H]^+$ 508.1842, found 508.1841.

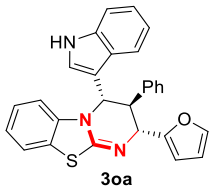
(*2R,3R,4S*)-4-(1H-indol-3-yl)-3-phenyl-2-(thiophen-2-yl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3na**:



3na

White solid, M.p.: 144-145 °C; yield: 70%; $[\alpha]^{20}_D$ = +67 (*c* 0.25, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 28.64 min (minor), t_2 = 30.18 min (major), ee = 97%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.83 (s, 1H), 7.45-7.32 (m, 1H), 7.26-7.18 (m, 3H), 7.15-7.02 (m, 3H), 7.00-6.78 (m, 7H), 6.66-6.64 (m, 1H), 6.55 (d, *J* = 7.6 Hz, 1H), 6.22 (d, *J* = 3.3 Hz, 1H), 5.69 (d, *J* = 10.0 Hz, 1H), 5.21 (d, *J* = 10.2 Hz, 1H), 3.17 (t, *J* = 10.1 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.0, 148.2, 140.6, 140.4, 136.8, 129.3, 128.5, 127.2, 126.5, 125.7, 125.6, 125.0, 124.4, 124.3, 122.2, 122.2, 122.0, 121.5, 119.5, 118.1, 112.4, 112.2, 111.2, 60.4, 58.0, 54.0; HRMS (ESI) Calcd. For $C_{28}H_{22}N_3S_2$ $[M+H]^+$ 464.1250, found 464.1254.

(*2R,3R,4S*)-2-(furan-2-yl)-4-(1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3oa**:

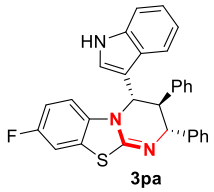


3oa

White solid, M.p.: 162-163 °C; yield: 73%; $[\alpha]^{20}_D$ = +73 (*c* 0.23, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 24.71 min (major), t_2 = 27.35 min (minor), ee = 91%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.90 (s, 1H), 7.40-7.28 (m, 3H), 7.10-6.92 (m, 11H), 6.81-6.73 (m, 3H), 5.74 (d, *J* =

10.2 Hz, 1H), 4.82 (d, *J* = 10.4 Hz, 1H), 3.24 (t, *J* = 10.3 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 157.8, 155.9, 141.8, 140.6, 140.4, 136.8, 128.8, 128.4, 127.0, 125.6, 125.6, 125.0, 122.2, 122.2, 121.9, 121.6, 119.5, 118.2, 112.4, 112.0, 111.3, 110.3, 106.8, 58.6, 57.7, 49.8; HRMS (ESI) Calcd. For $C_{28}H_{22}N_3OS$ $[M+H]^+$ 448.1478, found 448.1478.

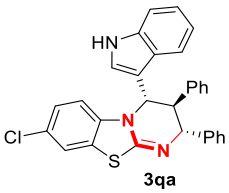
(*2R,3S,4S*)-8-fluoro-4-(1H-indol-3-yl)-2,3-diphenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3pa**:



3pa

White solid, M.p.: 136-137 °C; yield: 82%; $[\alpha]^{20}_D$ = +116 (*c* 0.27, CH_2Cl_2); HPLC (Chiralpak IE, *i*-propanol/hexane = 15/85, flow rate 1.0 mL/min, λ = 254 nm), t_1= 7.19 min (major), t_2 = 9.89 min (minor), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.84 (s, 1H), 7.38-7.29 (m, 1H), 7.19-7.15 (m, 1H), 7.12-6.88 (m, 10H), 6.79-6.57 (m, 5H), 6.45 (d, *J* = 7.2 Hz, 1H), 5.63 (d, *J* = 10.0 Hz, 1H), 4.79 (d, *J* = 10.2 Hz, 1H), 3.08 (t, *J* = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 159.0 (d, *J* = 233.2 Hz), 158.0, 142.8, 140.3, 140.1, 136.7, 136.6, 131.1, 129.8, 129.2, 128.4, 127.8, 127.0, 126.3, 125.6, 122.2, 122.1, 122.0, 121.8, 119.1, 111.8 (d, *J* = 35.9 Hz), 108.1 (d, *J* = 24.2 Hz), 98.5, 98.2, 63.8, 57.7, 53.6; ^{19}F NMR (376 MHz, d_6-DMSO) δ ppm: -122.4; HRMS (ESI) Calcd. For $C_{30}H_{23}FN_3S$ $[M+H]^+$ 476.1591, found 476.1593.

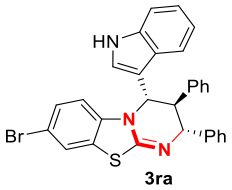
(*2R,3S,4S*)-8-chloro-4-(1H-indol-3-yl)-2,3-diphenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3qa**:



3qa

White solid, M.p.: 195-196 °C; yield: 82%; $[\alpha]^{20}_D$ = +84 (*c* 0.25, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 20.66 min (major), t_2 = 23.83 min (minor), ee = 98%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.87 (s, 1H), 7.70-7.53 (m, 1H), 7.37-7.20 (m, 2H), 7.10-6.90 (m, 11H), 6.84-6.82 (m, 3H), 6.51 (d, *J* = 8.2 Hz, 1H), 5.70 (d, *J* = 10.1 Hz, 1H), 4.85 (d, *J* = 10.4 Hz, 1H), 3.20 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.0, 142.8, 140.3, 140.1, 137.1, 131.2, 129.9, 129.2, 128.5, 127.9, 127.1, 126.8, 126.4, 125.6, 123.9, 122.3, 122.2, 122.0, 119.9, 119.5, 112.0, 112.0, 111.8, 63.9, 57.5, 53.7; HRMS (ESI) Calcd. For $C_{30}H_{23}ClN_3S$ $[M+H]^+$ 492.1296, found 492.1299.

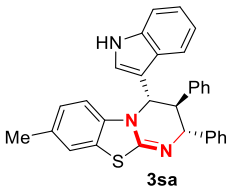
(*2R,3S,4S*)-8-bromo-4-(1H-indol-3-yl)-2,3-diphenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ra**:



3ra

White solid, M.p.: 172-173 °C; yield: 83%; $[\alpha]^{20}_D$ = +49 (*c* 0.32, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/92, flow rate 1.0 mL/min, λ = 254 nm), t_1= 22.24 min (major), t_2 = 28.70 min (minor), ee = 98%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.87 (s, 1H), 7.70-7.60 (m, 1H), 7.35-7.18 (m, 2H), 7.08-6.90 (m, 12H), 6.82 (s, 2H), 6.46 (d, *J* = 9.2 Hz, 1H), 5.70 (d, *J* = 10.1 Hz, 1H), 4.85 (d, *J* = 10.4 Hz, 1H), 3.20 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 157.9, 140.5, 140.4, 140.1, 140.1, 136.8, 129.8, 129.7, 129.2, 128.4, 126.9, 125.8, 125.5, 125.0, 122.2, 122.2, 121.8, 121.5, 119.5, 118.2, 114.7, 114.5, 112.4, 112.1, 111.4, 63.9, 57.9, 53.8; HRMS (ESI) Calcd. For $C_{30}H_{23}BrN_3S$ $[M+H]^+$ 536.0791, found 536.0795.

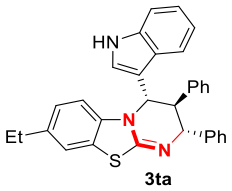
(*2R,3S,4S*)-4-(1H-indol-3-yl)-8-methyl-2,3-diphenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3sa**:



3sa

White solid, M.p.: 158-159 °C; yield: 72%; $[\alpha]^{20}_D$ = +104 (*c* 0.25, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 26.40 min (minor), t_2 = 29.47 min (major), ee = 98%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.81 (s, 1H), 7.32-7.23 (m, 3H), 7.10-6.97 (m, 9H), 6.94-6.81 (m, 4H), 6.59 (d, *J* = 7.6 Hz, 1H), 6.45 (d, *J* = 8.2 Hz, 1H), 5.66 (d, *J* = 10.1 Hz, 1H), 4.82 (d, *J* = 10.3 Hz, 1H), 3.21 (t, *J* = 10.2 Hz, 1H), 2.13 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.0, 143.8, 140.6, 138.4, 136.8, 131.0, 129.2, 128.3, 128.1, 127.9, 126.8, 126.7, 126.1, 125.8, 125.0, 122.4, 122.2, 121.5, 119.5, 118.2, 112.4, 111.9, 111.5, 64.6, 58.1, 53.6, 20.8; HRMS (ESI) Calcd. For $C_{31}H_{26}N_3S$ $[M+H]^+$ 472.1842, found 472.1845.

(*2R,3S,4S*)-8-ethyl-4-(1H-indol-3-yl)-2,3-diphenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ta**:

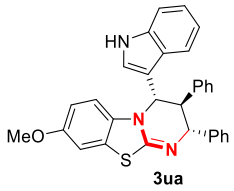


3ta

White solid, M.p.: 182-183 °C; yield: 80%; $[\alpha]^{20}_D$ = +121 (*c* 0.32, CH_2Cl_2); HPLC (Chiralpak IE, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 13.94 min (minor), t_2 = 15.93 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.81 (s, 1H), 7.32-7.21 (m, 2H), 7.09-6.97 (m, 10H), 6.94-6.80 (m, 4H), 6.45-6.34 (m,

2H), 5.63 (d, *J* = 10.0 Hz, 1H), 4.80 (d, *J* = 10.4 Hz, 1H), 3.86-3.81 (m, 2H), 3.20 (t, *J* = 10.2 Hz, 1H), 1.21 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.3, 154.0, 143.8, 140.5, 136.8, 134.4, 129.2, 128.3, 128.1, 127.9, 126.8, 126.7, 125.8, 125.0, 123.4, 121.5, 119.5, 118.3, 112.6, 112.4, 111.9, 111.5, 108.5, 64.6, 63.8, 58.1, 53.6, 15.1; HRMS (ESI) Calcd. For $C_{32}H_{28}N_3S$ $[M+H]^+$ 486.1998, found 486.1997.

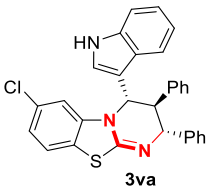
(*2R,3S,4S*)-4-(1H-indol-3-yl)-8-methoxy-2,3-diphenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ua**:



3ua

White solid, M.p.: 155-156 °C; yield: 72%; $[\alpha]^{20}_D$ = +115 (*c* 0.22, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 31.99 min (minor), t_2 = 34.79 min (major), ee = 99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.80 (s, 1H), 7.33-7.29 (m, 1H), 7.26-7.22 (m, 1H), 7.12-6.99 (m, 10H), 6.97-6.89 (m, 2H), 6.81 (d, *J* = 6.0 Hz, 2H), 6.47-6.37 (m, 2H), 5.64 (d, *J* = 10.0 Hz, 1H), 4.81 (d, *J* = 10.4 Hz, 1H), 3.60 (s, 3H), 3.19 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.0, 154.7, 143.9, 140.6, 136.8, 134.6, 129.2, 128.3, 128.1, 127.9,126.8, 126.7, 125.8, 125.1, 123.4, 121.5, 119.5, 118.5, 113.3, 112.5, 112.4, 111.6, 111.3, 108.1, 106.0, 64.7, 58.1, 55.8, 53.6; HRMS (ESI) Calcd. For $C_{31}H_{26}N_3OS$ $[M+H]^+$ 488.1791, found 488.1796.

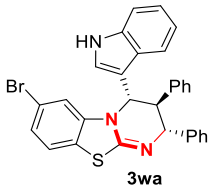
(*2R,3S,4S*)-7-chloro-4-(1H-indol-3-yl)-2,3-diphenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3va**:



3va

White solid, M.p.: 178-179 °C; yield: 80%; $[\alpha]^{20}_D$ = +87 (*c* 0.22, CH_2Cl_2); HPLC (Chiralpak IE, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1= 4.13 min (major), t_2 = 4.64 min (minor), ee = 98%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.88 (s, 1H), 7.66-7.54 (m, 1H), 7.35-7.21 (m, 2H), 7.10-6.99 (m, 9H), 6.96-6.83 (m, 5H), 6.51 (d, *J* = 8.2 Hz, 1H), 5.70 (d, *J* = 10.1 Hz, 1H), 4.85 (d, *J* = 10.4 Hz, 1H), 3.21 (t, *J* = 10.3 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.1, 143.0, 142.5, 140.3, 136.7, 131.6, 131.3, 130.4, 129.9, 128.5, 128.0, 125.8, 125.5, 124.9, 122.2, 122.1, 121.9, 121.7, 121.6, 119.6, 118.1, 112.4, 112.1, 111.0, 63.7, 57.5, 53.3; HRMS (ESI) Calcd. For $C_{30}H_{23}ClN_3S$ $[M+H]^+$ 492.1296, found 492.1301.

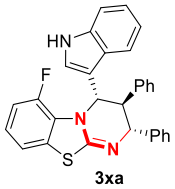
(*2R,3S,4S*)-7-bromo-4-(1H-indol-3-yl)-2,3-diphenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3wa**:



3wa

White solid, M.p.: 180-181 °C; yield: 72%; $[\alpha]^{20}_D$ = +68 (*c* 0.22, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1= 9.13 min (minor), t_2 = 9.82 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.86 (s, 1H), 7.44-7.42 (m, 1H), 7.33-7.26 (m, 3H), 7.12-6.88 (m, 9H), 6.85-6.77 (m, 2H), 6.53 (d, *J* = 7.6 Hz, 1H), 6.13-6.11 (m, 1H), 5.92 (d, *J* = 3.0 Hz, 1H), 5.00 (d, *J* = 10.2 Hz, 1H), 3.51 (t, *J* = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 157.9, 142.6, 140.1, 139.9, 135.0, 131.0, 129.8, 129.2, 128.4, 127.8, 127.2, 127.0, 126.1, 125.5, 123.9, 122.2, 122.1, 121.9, 121.5, 117.3, 113.8, 111.9, 111.4, 63.8, 57.3, 53.7; HRMS (ESI) Calcd. For $C_{30}H_{23}BrN_3S$ $[M+H]^+$ 536.0791, found 536.0793.

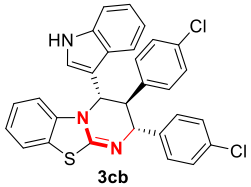
(*2R,3S,4S*)-6-fluoro-4-(1H-indol-3-yl)-2,3-diphenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3xa**:



3xa

White solid, M.p.: 145-146 °C; yield: 62%; $[\alpha]^{20}_D$ = +45 (*c* 0.12, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 15/85, flow rate 1.0 mL/min, λ = 254 nm), t_1= 10.12 (major), t_2 = 13.35 min (minor), ee = 71%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.82 (s, 1H), 7.50-7.23 (m, 1H), 7.17-7.08 (m, 1H), 7.04-6.87 (m, 9H), 6.78-6.53 (m, 6H), 6.44 (d, *J* = 7.2 Hz, 1H), 5.62 (d, *J* = 10.0 Hz, 1H), 4.78 (d, *J* = 10.2 Hz, 1H), 3.07 (t, *J* = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.9 (d, *J* = 233.1 Hz), 157.9, 142.6, 140.2, 140.0, 136.6, 136.5, 131.0, 129.7, 129.0, 128.3, 127.7, 126.9, 126.2, 125.5, 122.1, 122.0, 121.8, 121.7, 119.0, 118.9, 111.7 (d, *J* = 35.9 Hz), 107.9 (d, *J* = 24.1 Hz), 98.4, 98.1, 63.7, 57.6, 53.5; ^{19}F NMR (376 MHz, d_6-DMSO) δ ppm: -122.5; HRMS (ESI) Calcd. For $C_{30}H_{23}FN_3S$ $[M+H]^+$ 476.1591, found 476.1595.

(*2R,3S,4S*)-2,3-bis(4-chlorophenyl)-4-(1H-indol-3-yl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cb**:

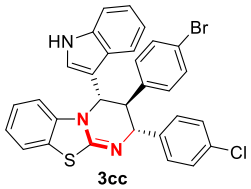


3cb

White solid, M.p.: 168-169 °C; yield: 78%; $[\alpha]^{20}_D$ = +80 (*c* 0.23, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 15.29 min (minor), t_2 = 17.06 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.88 (s, 1H), 7.47-7.42 (m, 1H), 7.36-7.21 (m, 2H), 7.17-6.98 (m, 8H), 6.93-6.77 (m,

5H), 6.54 (d, *J* = 7.3 Hz, 1H), 5.69 (d, *J* = 10.1 Hz, 1H), 4.87 (d, *J* = 10.4 Hz, 1H), 3.21 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.2, 142.7, 140.4, 139.3, 136.8, 131.5, 131.3, 131.0, 129.9, 128.4, 128.0, 125.8, 125.6, 124.9, 122.2, 121.9, 121.6, 119.6, 118.1, 112.5, 112.1, 111.1, 63.8, 57.8, 53.1; HRMS (ESI) Calcd. For $C_{30}H_{22}Cl_2N_3S$ $[M+H]^+$ 526.0906, found 526.0909.

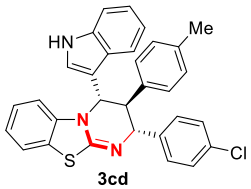
(*2R,3S,4S*)-3-(4-bromophenyl)-2-(4-chlorophenyl)-4-(1H-indol-3-yl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cc**:



3cc

White solid, M.p.: 195-196 °C; yield: 74%; $[\alpha]^{20}_D$ = +157 (*c* 0.22, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 16.88 min (minor), t_2 = 18.81 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.91 (s, 1H), 7.48-7.46 (m, 1H), 7.34-7.29 (m, 4H), 7.27-7.12 (m, 2H), 7.10-7.01 (m, 4H), 6.96-6.81 (m, 5H), 6.57 (d, *J* = 7.2 Hz, 1H), 5.72 (d, *J* = 10.1 Hz, 1H), 4.91 (d, *J* = 10.3 Hz, 1H), 3.23 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.1, 142.7, 140.4, 139.8, 136.8, 131.4, 131.3, 129.9, 128.1, 125.9, 125.6, 122.2, 121.9, 121.6, 120.1, 119.6, 118.1, 112.5, 112.1, 111.1, 63.7, 57.8, 53.1; HRMS (ESI) Calcd. For $C_{30}H_{22}BrClN_3S$ $[M+H]^+$ 570.0401, found 570.0402.

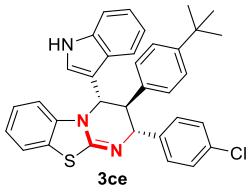
(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(1H-indol-3-yl)-3-(p-tolyl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cd**:



3cd

White solid, M.p.: 146-147 °C; yield: 64%; $[\alpha]^{20}_D$ = +107 (*c* 0.24, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 15.02 min (minor), t_2 = 20.43 min (major), ee = 99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.86 (s, 1H), 7.48-7.46 (m, 1H), 7.39-7.23 (m, 2H), 7.19-7.00 (m, 6H), 6.96-6.76 (m, 7H), 6.61 (d, *J* = 7.3 Hz, 1H), 5.69 (d, *J* = 10.0 Hz, 1H), 4.87 (d, *J* = 10.3 Hz, 1H), 3.21 (t, *J* = 10.1 Hz, 1H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.1, 143.0, 140.5, 137.2, 136.8, 135.8, 131.1, 129.9, 129.1, 129.0, 127.9, 125.9, 125.6, 124.9, 122.2, 122.2, 121.9, 121.5, 119.5, 118.2, 112.4, 112.1, 111.3, 63.9, 58.1, 52.9, 21.1; HRMS (ESI) Calcd. For $C_{31}H_{25}ClN_3S$ $[M+H]^+$ 506.1452, found 506.1450.

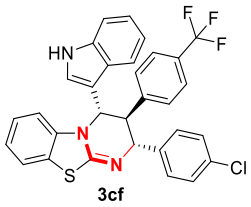
(*2R,3S,4S*)-3-(4-(tert-butyl)phenyl)-2-(4-chlorophenyl)-4-(1H-indol-3-yl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ce**:



3ce

White solid, M.p.: 189-190 °C; yield: 75%; $[\alpha]^{20}_D$ = -18 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 10.68 min (minor), t_2 = 13.27 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.83 (s, 1H), 7.46-7.44 (m, 1H), 7.28-7.21 (m, 2H), 7.11-6.96 (m, 7H), 6.93-6.81 (m, 6H), 6.58 (d, *J* = 7.3 Hz, 1H), 5.68 (d, *J* = 9.4 Hz, 1H), 4.84 (d, *J* = 9.7 Hz, 1H), 3.23 (t, *J* = 9.6 Hz, 1H), 1.17 (s, 9H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.4, 149.2, 142.8, 140.4, 137.3, 136.8, 131.1, 129.8, 128.8, 127.8, 125.7, 125.2, 124.9, 122.2, 122.0, 121.5, 119.5, 118.2, 112.3, 112.1, 111.5, 63.7, 57.8, 52.6, 34.5, 31.5; HRMS (ESI) Calcd. For $C_{34}H_{31}ClN_3S$ $[M+H]^+$ 548.1922, found 548.1917.

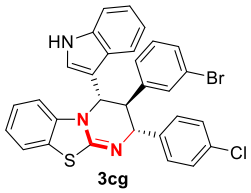
(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(1H-indol-3-yl)-3-(4-(trifluoromethyl)phenyl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cf**:



3cf

White solid, M.p.: 168-169 °C; yield: 74%; $[\alpha]^{20}_D$ = +117 (*c* 0.25, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 11.75 min (minor), t_2 = 17.72 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.86 (s, 1H), 7.42-7.36 (m, 3H), 7.32-7.22 (m, 2H), 7.12-6.97 (m, 8H), 6.91-6.76 (m, 3H), 6.54 (d, *J* = 7.2 Hz, 1H), 5.74 (d, *J* = 10.1 Hz, 1H), 4.87 (d, *J* = 10.3 Hz, 1H), 3.31 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.7, 145.0, 142.2, 140.2, 136.8, 131.4, 130.1, 129.8, 128.1, 127.6 (q, *J* = 31.7 Hz), 126.0, 125.8 (q, *J* = 15.4 Hz), 125.2, 124.8, 123.2, 122.2, 120.9 (q, *J* = 246.7 Hz), 118.1, 112.5, 112.2, 110.9, 63.6, 57.7, 53.5; ^{19}F NMR (376 MHz, d_6-DMSO) δ ppm: -60.8; HRMS (ESI) Calcd. For $C_{31}H_{22}F_3N_3S$ $[M+H]^+$ 560.1170, found 560.1173.

(*2R,3S,4S*)-3-(3-bromophenyl)-2-(4-chlorophenyl)-4-(1H-indol-3-yl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cg**:

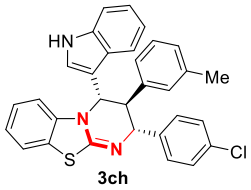


3cg

White solid, M.p.: 162-163 °C; yield: 81%; $[\alpha]^{20}_D$ = +85 (*c* 0.32, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 12.83 min (minor), t_2 = 20.45 min (major), ee = 99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm:

10.93 (s, 1H), 7.51-7.41 (m, 1H), 7.39-7.20 (m, 6H), 7.12-7.09 (m, 3H), 7.05-6.93 (m, 3H), 6.90-6.81 (m, 3H), 6.59 (d, *J* = 6.9 Hz, 1H), 5.78 (d, *J* = 10.1 Hz, 1H), 4.91 (d, *J* = 10.2 Hz, 1H), 3.25 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.2, 143.1, 142.6, 140.4, 136.8, 131.7, 131.3, 130.5, 129.9, 129.9, 128.5, 128.0, 125.8, 125.6, 125.0, 122.2, 122.2, 122.0, 121.8, 121.6, 119.6, 118.1, 112.5, 112.1, 111.0, 63.8, 57.5, 53.4; HRMS (ESI) Calcd. For $C_{30}H_{22}BrClN_3S$ $[M+H]^+$ 570.0401, found 570.0401.

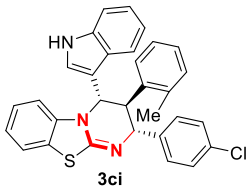
(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(1H-indol-3-yl)-3-(m-tolyl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ch**:



3ch

White solid, M.p.:137-138 °C; yield: 77%; $[\alpha]^{20}_D$ = +127 (*c* 0.26, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 23.49 min (minor), t_2 = 28.43 min (major), ee = 98%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.84 (s, 1H), 7.45-7.43 (m, 1H), 7.33-7.25 (m, 2H), 7.14-7.03 (m, 2H), 7.01-6.97 (m, 4H), 6.94-6.89 (m, 2H), 6.86-6,73 (m, 4H), 6.59 (d, *J* = 7.0 Hz, 1H), 5.70 (d, *J* = 9.9 Hz, 1H), 4.82 (d, *J* = 10.1 Hz, 1H), 3.17 (t, *J* = 10.0 Hz, 1H), 2.10 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.2, 142.9, 140.2, 137.3, 136.8, 131.1, 129.9, 129.7, 128.3, 127.8, 127.7, 126.4, 125.8, 125.6, 125.0, 122.2, 122.2, 121.9, 121.5, 119.5, 118.2, 112.4, 112.1, 111.4, 64.0, 57.9, 53.3, 21.4; HRMS (ESI) Calcd. For $C_{31}H_{25}ClN_3S$ $[M+H]^+$ 506.1452, found 506.1452.

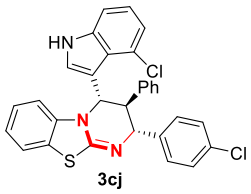
(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(1H-indol-3-yl)-3-(o-tolyl)-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ci**:



3ci

White solid, M.p.: 132-133 °C; yield: 64%; $[\alpha]^{20}_D$ = +109 (*c* 0.23, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 22.74 min (minor), t_2 = 24.95 min (major), ee = 95%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.87 (s, 1H), 7.77-7.68 (m, 1H), 7.62-7.43 (m, 1H), 7.41-7.21 (m, 3H), 7.17-7.05 (m, 2H), 7.03-6.81 (m, 8H), 6.64 (d, *J* = 7.6 Hz, 1H), 5.67 (d, *J* = 10.2 Hz, 1H), 4.87 (d, *J* = 10.5 Hz, 1H), 3.54 (t, *J* = 10.4 Hz, 1H), 0.96 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.2, 147.8, 140.4, 139.1, 137.4, 136.7, 131.2, 129.8, 129.6, 128.0, 127.7, 126.6, 125.5, 125.2, 122.2, 122.2, 121.9, 121.6, 119.7, 118.0, 112.4, 112.2, 111.0, 64.1, 58.4, 47.7, 18.9; HRMS (ESI) Calcd. For $C_{31}H_{25}ClN_3S$ $[M+H]^+$ 506.1452, found 506.1455.

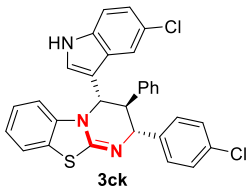
(*2R,3S,4S*)-4-(4-chloro-1H-indol-3-yl)-2-(4-chlorophenyl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cj**:



3cj

White solid, M.p.: 168-169 °C; yield: 75%; $[\alpha]^{20}_D$ = +40 (*c* 0.12, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1= 12.14 min (major), t_2 = 16.17 min (minor), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.83 (s, 1H), 7.77-7.45 (m, 1H), 7.31-7.23 (m, 2H), 7.14-6.98 (m, 8H), 6.95-6.91 (m, 3H), 6.88-6.78 (m, 2H), 6.42 (d, *J* = 8.2 Hz, 1H), 5.66 (d, *J* = 10.1 Hz, 1H), 4.81 (d, *J* = 10.4 Hz, 1H), 3.17 (t, *J* = 10.2 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 157.7, 142.5, 140.0, 139.8, 134.9, 130.9, 129.7, 129.0, 128.2, 127.6, 127.1, 126.8, 126.0, 125.4, 123.7, 122.1, 121.9, 121.8, 121.3, 117.2, 113.6, 111.7, 111.3, 63.7, 57.2, 53.5; HRMS (ESI) Calcd. For $C_{30}H_{22}Cl_2N_3S$ $[M+H]^+$ 526.0906, found 526.0906.

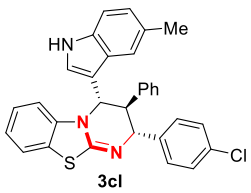
(*2R,3S,4S*)-4-(5-chloro-1H-indol-3-yl)-2-(4-chlorophenyl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ck**:



3ck

White solid, M.p.: 177-178 °C; yield: 76%; $[\alpha]^{20}_D$ = +97 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1= 12.51 min (minor), t_2 = 14.36 min (major), ee = 98%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 11.07 (s, 1H), 7.51-7.41 (m, 1H), 7.31-7.17 (m, 2H), 7.14-7.04 (m, 8H), 6.99-6.97 (m, 1H), 6.91-6.80 (m, 4H), 6.46 (d, *J* = 6.8 Hz, 1H), 5.73 (d, *J* = 10.0 Hz, 1H), 4.87 (d, *J* = 10.2 Hz, 1H), 3.11 (t, *J* = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.0, 142.7, 140.2, 140.0, 135.1, 131.2, 129.9, 129.3, 128.5, 127.9, 127.3, 127.1, 126.2, 125.6, 124.0, 122.3, 122.2, 122.0, 121.6, 117.4, 113.9, 112.0, 111.5, 63.9, 57.4, 53.8; HRMS (ESI) Calcd. For $C_{30}H_{22}Cl_2N_3S$ $[M+H]^+$ 526.0906, found 526.0909.

(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(5-methyl-1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cl**:

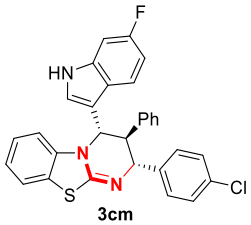


3cl

White solid, M.p.: 145-146 °C; yield: 64%; $[\alpha]^{20}_D$ = +175 (*c* 0.24, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1= 14.79

min (minor), t_2 = 16.59 min (major), ee = 99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.72 (s, 1H), 7.45-7.43 (m, 1H), 7.15-7.12 (dn, 3H), 7.07-6.99 (m, 6H), 6.89-6.74 (m, 6H), 6.56 (d, *J* = 7.0 Hz, 1H), 5.67 (d, *J* = 10.0 Hz, 1H), 4.86 (d, *J* = 10.2 Hz, 1H), 3.19 (t, *J* = 10.1 Hz, 1H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.2, 142.9, 140.5, 140.3, 135.2, 131.2, 129.9, 129.2, 128.4, 127.9, 127.8, 127.0, 125.7, 125.5, 125.3, 123.2, 122.2, 121.9, 117.9, 112.1, 112.1, 110.9, 64.0, 58.6, 53.5, 22.0; HRMS (ESI) Calcd. For $C_{31}H_{25}ClN_3S$ $[M+H]^+$ 506.1452, found 506.1457.

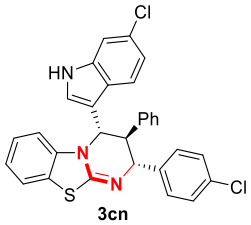
(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(6-fluoro-1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cm**:



3cm

White solid, M.p.: 177-178 °C; yield: 74%; $[\alpha]^{20}_D$ = +83 (*c* 0.21, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 21.18 min (minor), t_2 = 23.53 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.92 (s, 1H), 7.47-7.44 (m, 1H), 7.33-7.18 (m, 1H), 7.14-7.02 (m, 8H), 6.97-6.76 (m, 6H), 6.54 (d, *J* = 7.2 Hz, 1H), 5.72 (d, *J* = 10.0 Hz, 1H), 4.87 (d, *J* = 10.2 Hz, 1H), 3.17 (t, *J* = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 159.1 (d, *J* = 233.3 Hz), 158.1, 142.8, 140.4, 140.1, 136.7, 136.6, 131.2, 129.9, 129.2, 128.5, 127.9, 127.0, 126.3, 125.6, 122.3, 122.2, 122.0, 119.2, 119.1, 111.8 (d, *J* = 35.8 Hz), 108.1 (d, *J* = 24.3 Hz), 98.5, 98.3, 63.8, 57.7, 53.6; ^{19}F NMR (376 MHz, d_6-DMSO) δ ppm: -121. 83; HRMS (ESI) Calcd. For $C_{30}H_{22}ClFN_3S$ $[M+H]^+$ 510.1202, found 510.1199.

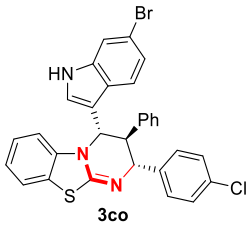
(*2R,3S,4S*)-4-(6-chloro-1H-indol-3-yl)-2-(4-chlorophenyl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cn**:



3cn

White solid, M.p.: 162-163 °C; yield: 80%; $[\alpha]^{20}_D$ = +122 (*c* 0.24, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 11.35 min (minor), t_2 = 12.65 min (major), ee = 99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 11.00 (s, 1H), 7.46-7.44 (m, 1H), 7.32-7.23 (m, 2H), 7.17-7.08 (m, 2H), 7.06-7.01 (m, 6H), 6.94-6.79 (m, 5H), 6.49 (d, *J* = 6.7 Hz, 1H), 5.72 (d, *J* = 10.0 Hz, 1H), 4.87 (d, *J* = 10.2 Hz, 1H), 3.14 (t, *J* = 10.1 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.0, 142.8, 140.3, 140.0, 133.5, 131.2, 129.9, 129.2, 128.5, 127.9, 127.1, 125.7, 122.3, 122.2, 122.0, 121.3, 121.2, 120.7, 117.3, 116.6, 112.9, 112.0, 63.8, 57.6, 53.6; HRMS (ESI) Calcd. For $C_{30}H_{22}Cl_2N_3S$ $[M+H]^+$ 526.0906, found 526.0911.

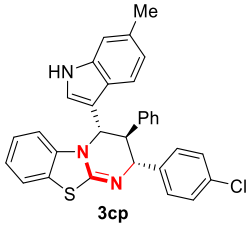
(*2R,3S,4S*)-4-(6-bromo-1H-indol-3-yl)-2-(4-chlorophenyl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3co**:



3co

White solid, M.p.: 196-197 °C; yield: 80%; $[\alpha]^{20}_D$ = +106 (*c* 0.28, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1= 11.80 min (minor), t_2 = 13.31 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 11.01 (s, 1H), 7.45-7.42 (m, 2H), 7.22-7.10 (m, 1H), 7.12-6.99 (m, 9H), 6.86-6.77 (m, 4H), 6.48 (d, J = 6.7 Hz, 1H), 5.70 (d, J = 10.0 Hz, 1H), 4.84 (d, J = 10.1 Hz, 1H), 3.14 (t, J = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.1, 142.7, 140.3, 140.0, 137.6, 131.2, 129.9, 129.2, 128.5, 127.9, 127.1, 126.7, 125.6, 124.1, 122.4, 122.2, 122.2, 122.1, 119.9, 115.0, 114.5, 112.0, 111.9, 63.9, 57.6, 53.6; HRMS (ESI) Calcd. For $C_{30}H_{22}BrClN_3S$ $[M+H]^+$ 570.0401, found 570.0405.

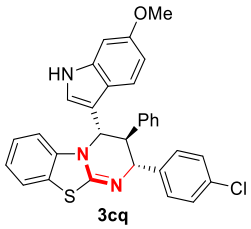
(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(6-methyl-1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cp**:



3cp

White solid, M.p.: 158-159 °C; yield: 72%; $[\alpha]^{20}_D$ = +154 (*c* 0.32, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1= 13.24 min (minor), t_2 = 15.68 min (major), ee = 98%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.79 (s, 1H), 7.42-7.12 (m, 2H), 7.09-6.96 (m, 9H), 6.93-6.67 (m, 4H), 6.58 (d, *J* = 7.6 Hz, 1H), 6.44 (d, *J* = 8.2 Hz, 1H), 5.65 (d, *J* = 10.0 Hz, 1H), 4.81 (d, *J* = 10.4 Hz, 1H), 3.20 (t, *J* = 10.2 Hz, 1H), 2.11 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.4, 142.8, 140.4, 140.1, 137.2, 131.2, 130.7, 129.8, 129.2, 128.4, 127.9, 127.0, 125.5, 125.0, 122.8, 122.2, 122.1, 122.0, 121.4, 117.9, 112.2, 63.9, 58.1, 21.7; HRMS (ESI) Calcd. For $C_{31}H_{25}ClN_3S$ $[M+H]^+$ 506.1452, found 506.1455.

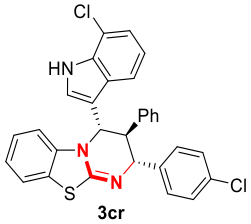
(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(6-methoxy-1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cq**:



3cq

White solid, M.p.: 152-153 °C; yield: 78%; $[\alpha]^{20}_D$ = +141 (*c* 0.34, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 20.39 min (minor), t_2 = 25.82 min (major), ee = 99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.64 (s, 1H), 7.45-7.39 (m, 1H), 7.18-7.12 (m, 3H), 7.08-7.01 (m, 5H), 6.86-6.76 (m, 6H), 6.59-6.56 (m, 2H), 5.65 (d, *J* = 10.0 Hz, 1H), 4.85 (d, *J* = 10.3 Hz, 1H), 3.69 (s, 3H), 3.17 (t, *J* = 10.1 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.1, 155.8, 142.9, 140.5, 137.6, 131.2, 129.8, 129.2, 128.4, 127.9, 127.0, 125.6, 124.4, 122.2, 122.2, 121.9, 119.3, 118.8, 112.1, 111.3, 109.7, 95.4, 64.0, 58.0, 55.4, 53.7; HRMS (ESI) Calcd. For $C_{31}H_{25}ClN_3OS$ $[M+H]^+$ 522.1401, found 522.1406.

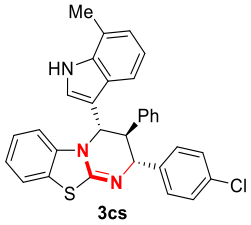
(*2R,3S,4S*)-4-(7-chloro-1H-indol-3-yl)-2-(4-chlorophenyl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cr**:



3cr

White solid, M.p.: 145-146 °C; yield: 64%; $[\alpha]^{20}_D$ = +120 (*c* 0.2, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1= 9.36 min (minor), t_2 = 11.36 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 11.29 (s, 1H), 7.50-7.45 (m, 1H), 7.30-7.22 (m, 1H), 7.17-7.04 (m, 9H), 6.98-6.83 (m, 5H), 6.56 (d, *J* = 6.0 Hz, 1H), 5.79 (d, *J* = 10.0 Hz, 1H), 4.91 (d, *J* = 10.2 Hz, 1H), 3.20 (t, *J* = 10.0 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.0, 142.8, 140.3, 140.0, 133.5, 131.2, 129.9, 129.2, 128.5, 127.9, 127.1, 125.7, 122.3, 122.2, 122.0, 121.3, 121.2, 120.7, 117.3, 116.6, 112.9, 112.0, 63.8, 57.6, 53.6; HRMS (ESI) Calcd. For $C_{30}H_{22}Cl_2N_3S$ $[M+H]^+$ 526.0906, found 526.0908.

(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(7-methyl-1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3cs**:

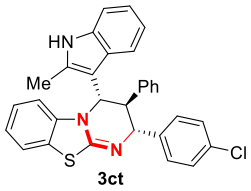


3cs

White solid, M.p.: 134-135 °C; yield: 74%; $[\alpha]^{20}_D$ = +174 (*c* 0.21, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 27.07

min (minor), t_2 = 30.78 min (major), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.82 (s, 1H), 7.45-7.42 (m, 1H), 7.19-7.11 (m, 3H), 7.08-6.96 (m, 6H), 6.85-6.78 (m, 6H), 6.59 (d, *J* = 6.9 Hz, 1H), 5.71 (d, *J* = 10.0 Hz, 1H), 4.84 (d, *J* = 10.2 Hz, 1H), 3.19 (t, *J* = 10.1 Hz, 1H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.2, 142.9, 140.5, 140.3, 136.4, 131.1, 129.9, 129.2, 128.5, 127.9, 127.0, 125.6, 124.6, 122.2, 122.2, 122.1, 121.9, 121.4, 119.8, 115.8, 112.1, 111.8, 64.0, 58.0, 53.6, 17.2; HRMS (ESI) Calcd. For $C_{31}H_{25}ClN_3S$ $[M+H]^+$ 506.1452, found 506.1456.

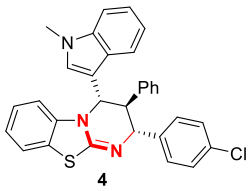
(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(2-methyl-1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **3ct**:



3ct

White solid, M.p.: 178-179 °C; yield: 62%; $[\alpha]^{20}_D$ = +123 (*c* 0.24, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 7.58 min (major), t_2 = 9.25 min (minor), ee = 96%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 10.86 (s, 1H), 7.48-7.44 (m, 1H), 7.38-7.21 (m, 2H), 7.13-6.99 (m, 4H), 6.97-6.90 (m, 5H), 6.86-6.79 (m, 4H), 6.58 (d, *J* = 7.4 Hz, 1H), 5.69 (d, *J* = 10.1 Hz, 1H), 4.83 (d, *J* = 10.4 Hz, 1H), 3.23 (t, *J* = 10.2 Hz, 1H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 157.6, 140.9, 140.7, 140.6, 136.8, 135.4, 129.3, 128.5, 128.3, 128.0, 126.8, 125.7, 125.5, 125.0, 122.3, 122.1, 121.8, 121.5, 119.5, 118.2, 112.4, 112.0, 111.5, 64.3, 58.1, 53.6, 21.1; HRMS (ESI) Calcd. For $C_{31}H_{25}ClN_3S$ $[M+H]^+$ 506.1452, found 506.1456.

(*2R,3S,4S*)-2-(4-chlorophenyl)-4-(1-methyl-1H-indol-3-yl)-3-phenyl-3,4-dihydro-2H-benzo[4,5]thiazolo[3,2-a]pyrimidine **4**:

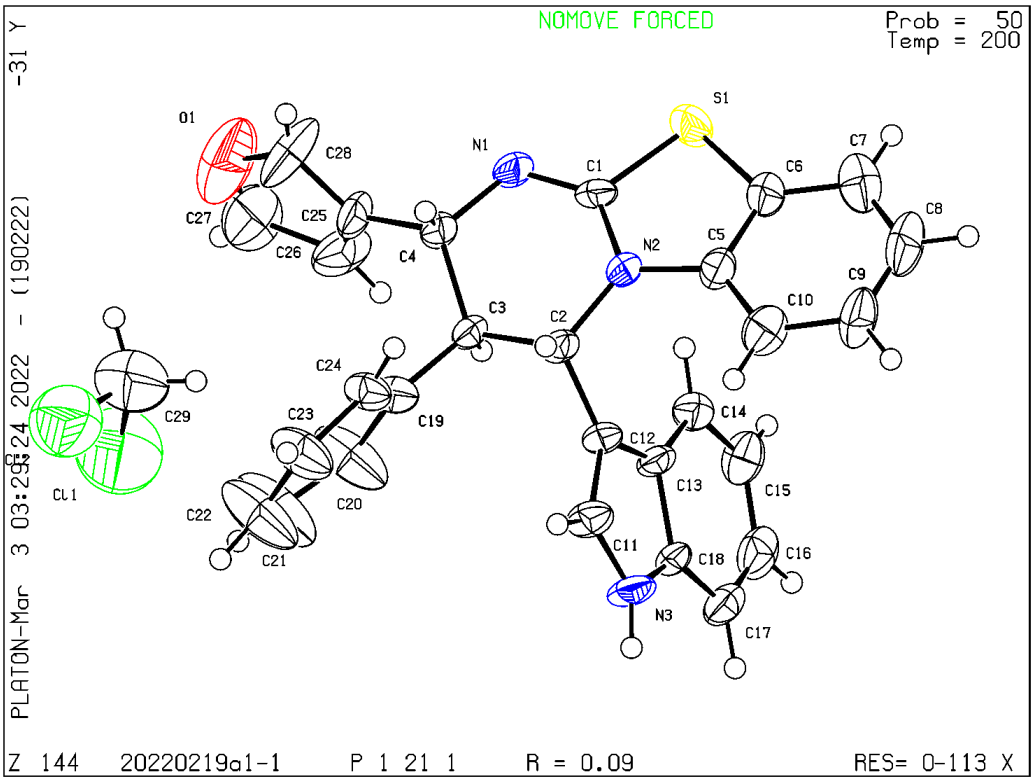


4

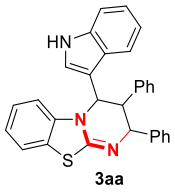
White solid, M.p.: 178-179 °C; yield: 86%; $[\alpha]^{20}_D$ = +123 (*c* 0.24, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1= 13.83 min (major), t_2 = 17.84 min (minor), ee = >99%; ^{1}H NMR (400 M, d_6-DMSO) δ ppm: 7.46-7.42 (m, 1H), 7.34-7.26 (m, 2H), 7.15-7.02 (m, 8H), 6.97-6.79 (m, 6H), 6.55 (d, *J* = 7.3 Hz, 1H), 5.72 (d, *J* = 9.4 Hz, 1H), 4.85 (d, *J* = 9.7 Hz, 1H), 3.54 (s, 3H), 3.23 (t, *J* = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, d_6-DMSO) δ ppm: 158.2, 155.9, 143.0, 140.6, 140.4, 137.7, 131.3, 130.0, 129.3, 128.5, 128.0, 127.1, 125.7, 124.5, 122.3, 122.2, 122.0, 119.4, 118.8, 112.2, 111.4, 109.8, 95.5, 64.1, 58.1, 55.5, 53.8; HRMS (ESI) Calcd. For $C_{31}H_{25}ClN_3S$ $[M+H]^+$ 506.1452, found 506.1453.

5. Crystallographic data collection for compound 3oa.

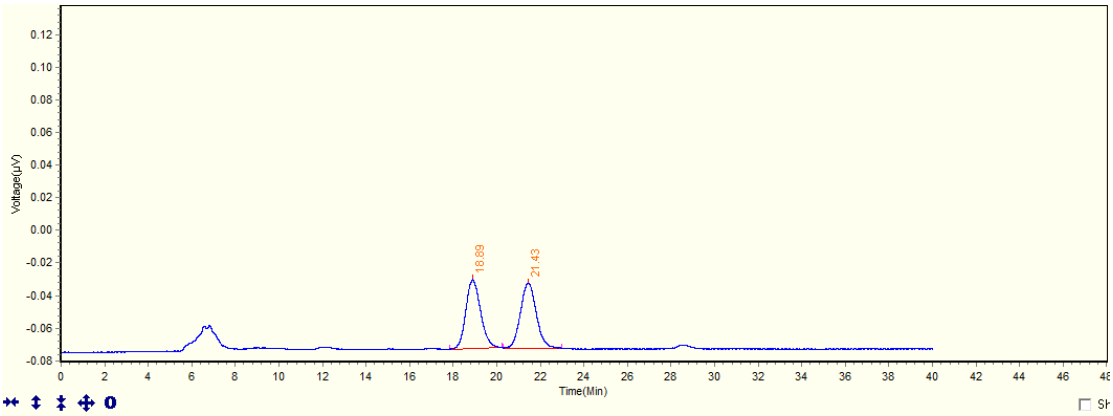
Bond precision: C-C = 0.0120 A Wavelength=1.54184
Cell: a=8.7321(2) b=15.7556(4) c=9.1821(2)
alpha=90 beta=100.916(2) gamma=90
Temperature: 200 K
Calculated Reported
Volume 1240.41(5) 1240.41(5)
Space group P 21 P 1 21 1
Hall group P 2yb P 2yb
Moiety formula C28 H21 N3 O S, C H2 Cl2 C28 H21 N3 O S, C H2 Cl2
Sum formula C29 H23 Cl2 N3 O S C29 H23 Cl2 N3 O S
Mr 532.46 532.46
Dx,g cm-3 1.426 1.426
Z 2 2
Mu (mm-1) 3.369 3.369
F000 552.0 552.0
F000’ 555.40
h,k,lmax 10,18,11 10,18,10
Nref 4544[2362] 4544
Tmin,Tmax 0.868,0.904 0.868,0.904
Tmin’ 0.859
Correction method= # Reported T Limits: Tmin=0.868 Tmax=0.904
AbsCorr = MULTI-SCAN
Data completeness= 1.92/1.00 Theta(max)= 68.217
R(reflections)= 0.0938(3103)
wR2(reflections)=
0.2506(3364)
S = 1.172 Npar= 325
The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.
Click on the hyperlinks for more details of the test.


NOMOVE FORCED
Prob = 50
Temp = 200
PLATON-Mar 3 03:29:24 2022 - (190222) -31 Y
Z 144 20220219a1-1 P 1 21 1 R = 0.09 RES= 0-113 X
O1
C28
N1
C1
S1
C7
C6
C27
C25
C26
C4
N2
C5
C8
C9
C3
C2
C10
C24
C29
C23
C19
C14
C12
C13
C15
Cl1
C22
C20
C11
C18
C16
C21
N3
C17

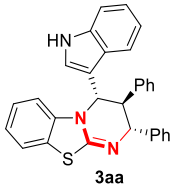
6. HPLC spectra of compounds.



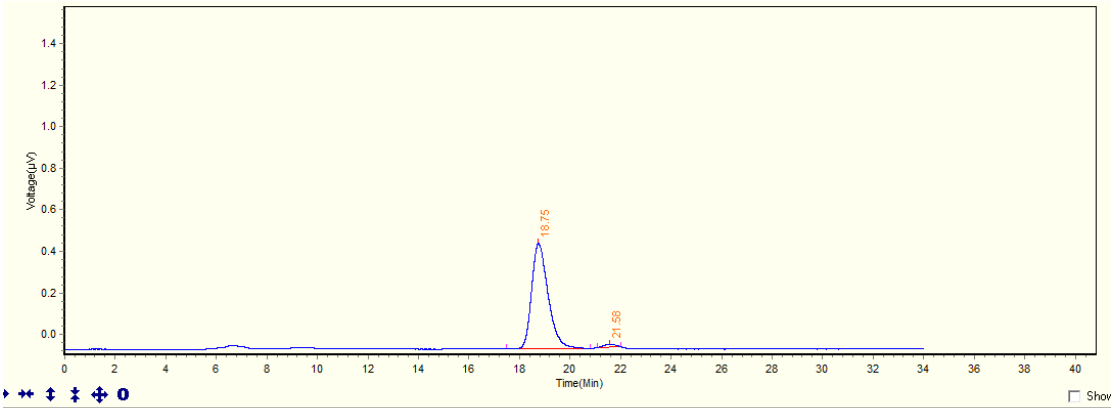
3aa



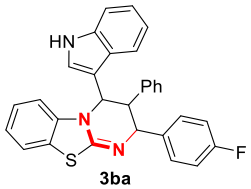
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	18.89	988777	21106	49.63%	2.404	BB
2	21.43	1003623	20003	50.37%	2.692	BB
		1,992,400	41,109	100.00%		



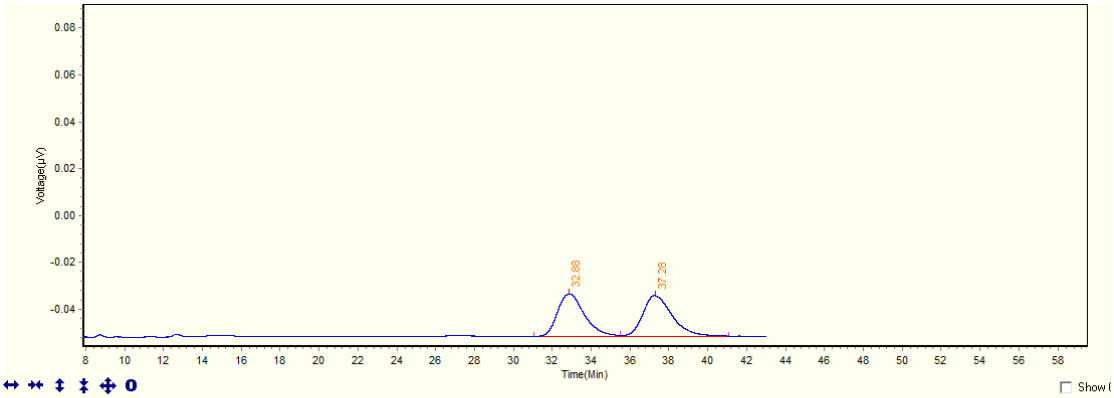
3aa



No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	18.75	11466427	253719	98.11%	3.318	BB
2	21.58	220741	6639	1.89%	0.93	BB
		11,687,168	260,358	100.00%		

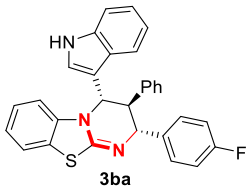


3ba

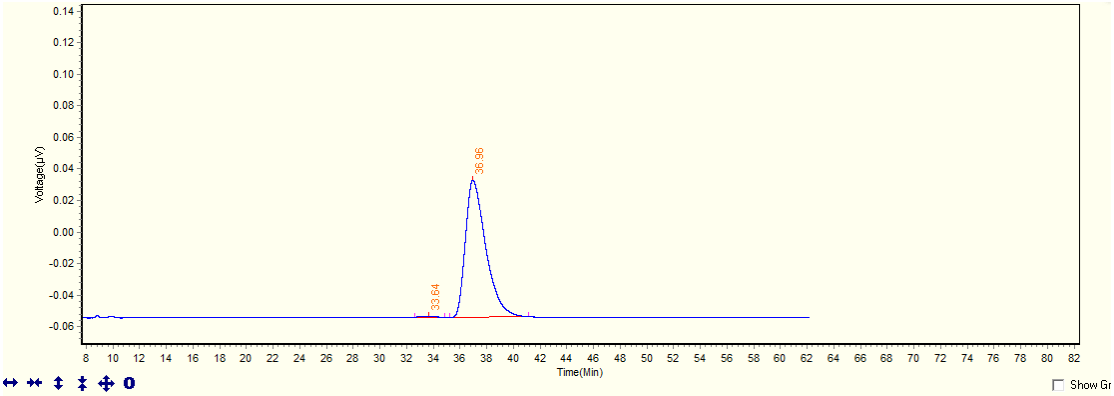


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	32.88	870963	9095	49.01%	4.443	BV
2	37.28	906022	8675	50.99%	5.579	VB
Total		1,776,985	17,770	100.00%		

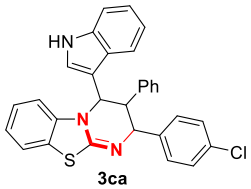


3ba

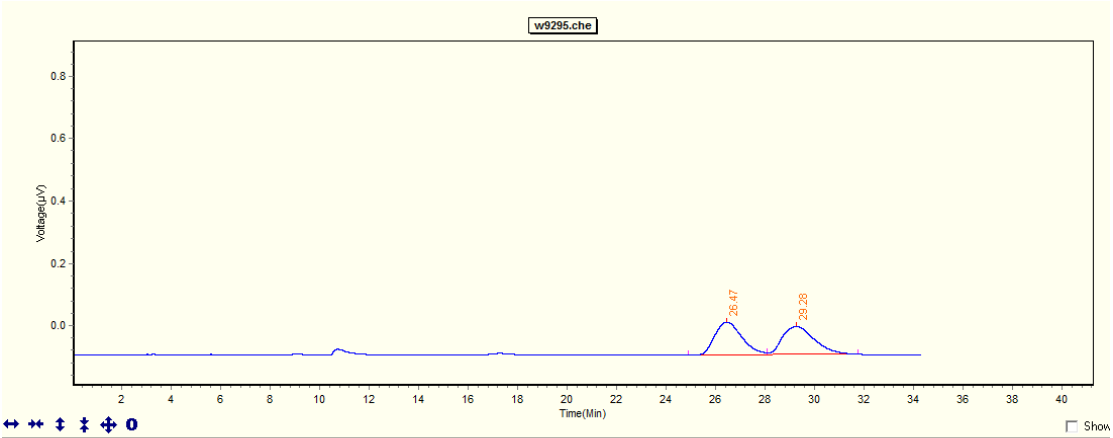


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	33.64	18985	272	0.41%	2.243	BB
2	36.96	4602569	43469	99.59%	5.907	BB
Total		4,621,554	43,741	100.00%		

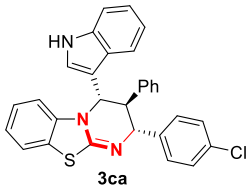


3ca

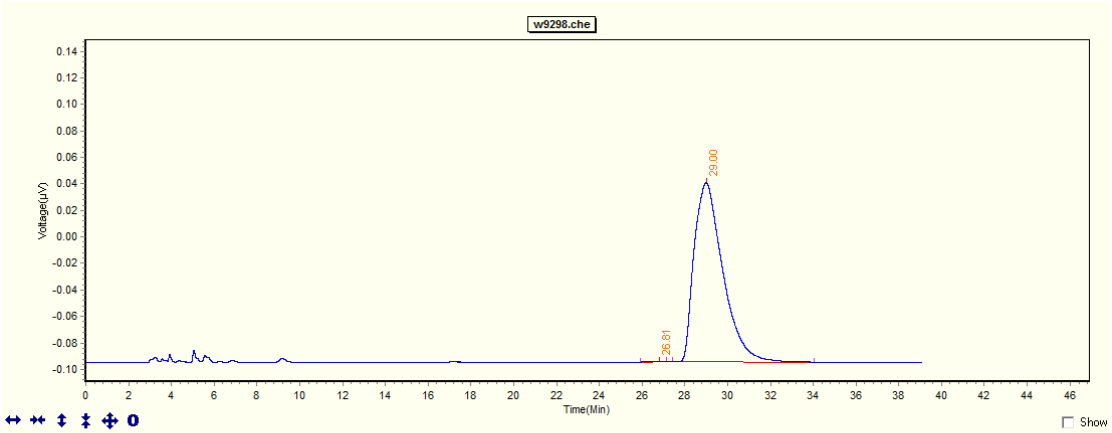


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	26.47	4034101	52822	49.61%	3.156	BV
2	29.28	4096994	44956	50.39%	3.688	VB
Total		8,131,095	97,778	100.00%		

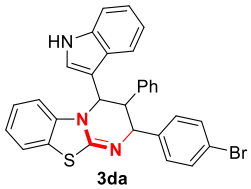


3ca

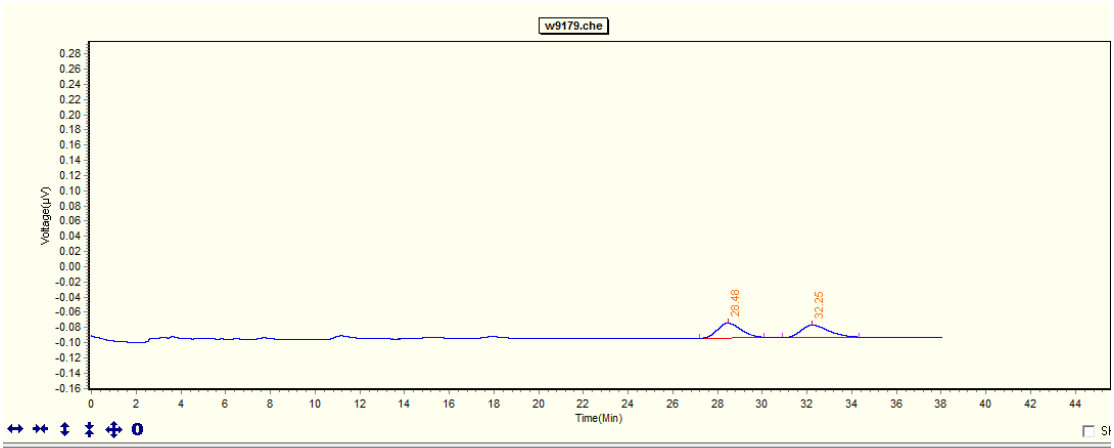


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	26.81	8953	209	0.14%	1.221	BB
2	29.00	6287037	67633	99.86%	6.621	BB
Total		6,295,990	67,842	100.00%		

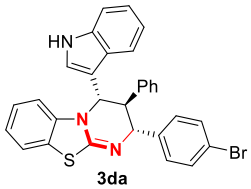


3da

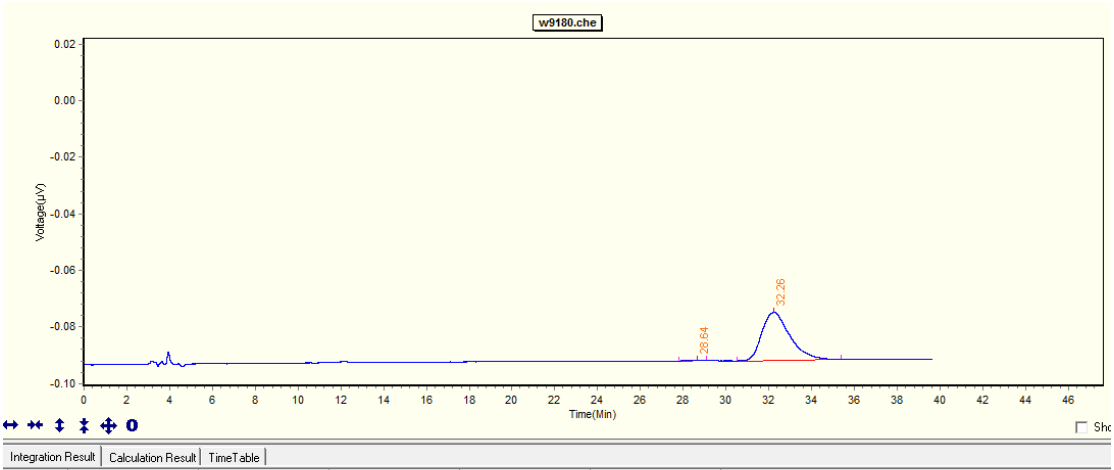


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	28.48	703024	9648	50.37%	2.88	BB
2	32.25	692686	8083	49.63%	3.428	BB
Total		1,395,710	17,731	100.00%		

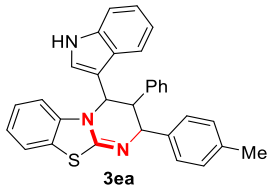


3da

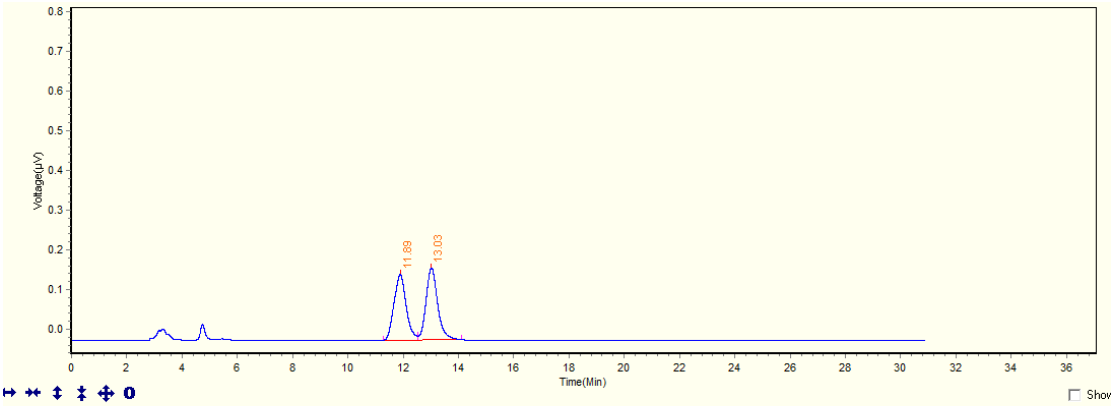


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	28.64	3604	117	0.47%	1.247	BB
2	32.26	766374	8496	99.53%	4.863	BB
Total		769,978	8,613	100.00%		

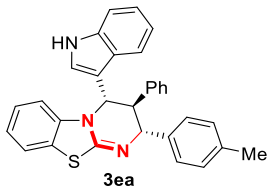


3ea

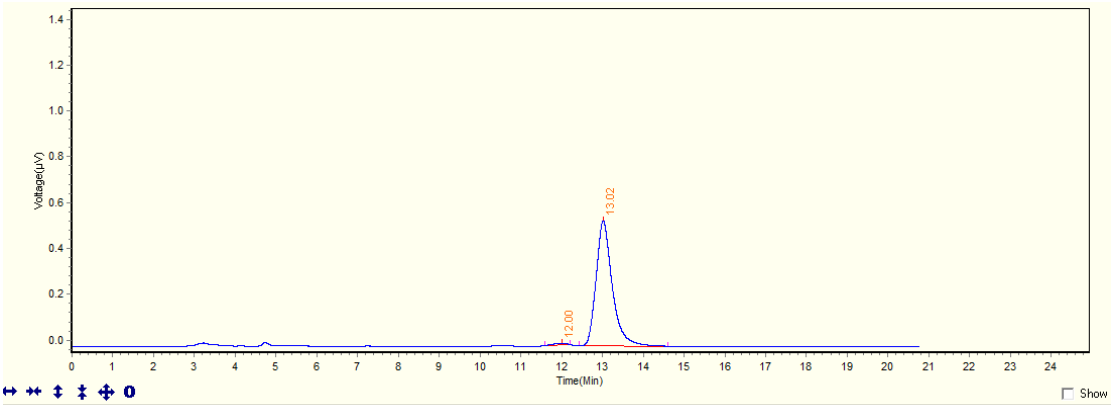


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.89	2531617	82478	48.91%	1.248	BV
2	13.03	2644687	90961	51.09%	1.581	VB
Total		5,176,304	173,439	100.00%		

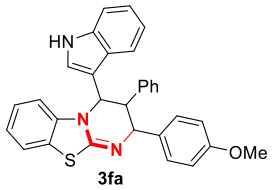


3ea

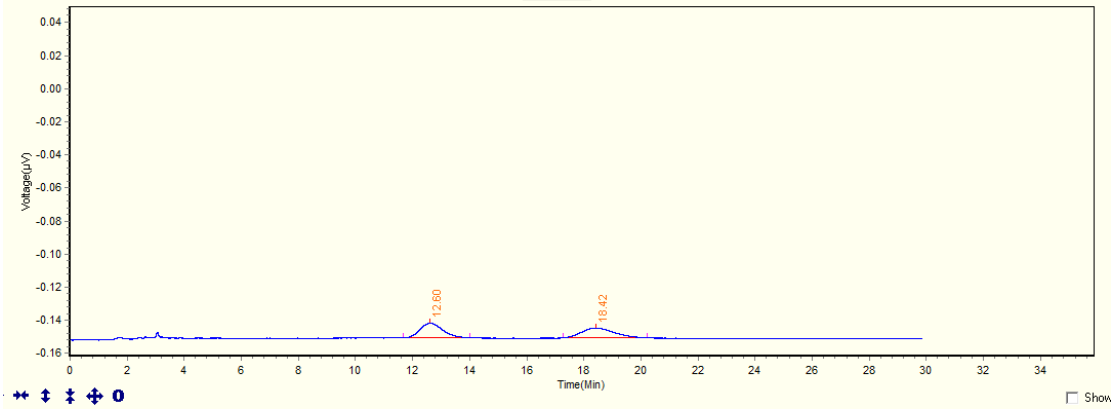


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.00	83344	3736	1.10%	0.618	BB
2	13.02	7489617	273499	98.90%	2.174	BB
Total		7,572,961	277,235	100.00%		

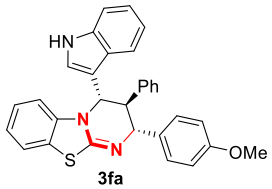


3fa

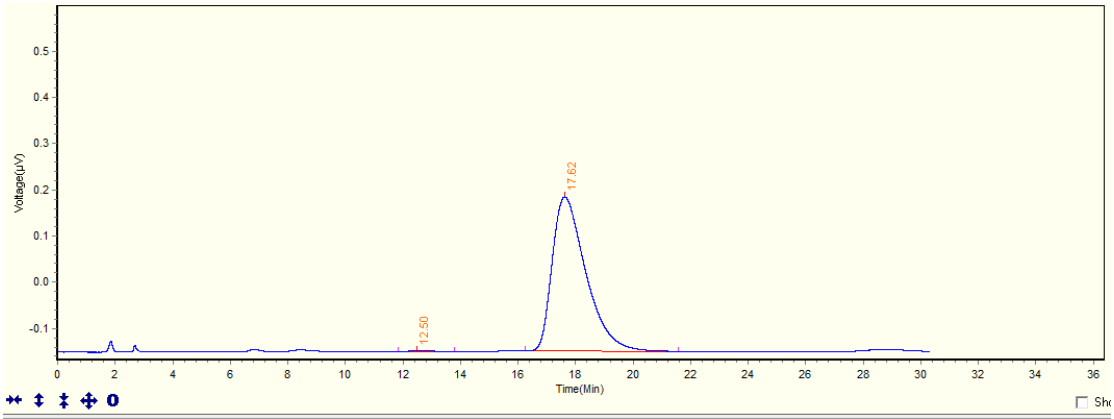


tegration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.60	238861	4385	50.42%	2.334	BB
2	18.42	234851	2996	49.58%	2.945	BB
tal		473,712	7,381	100.00%		

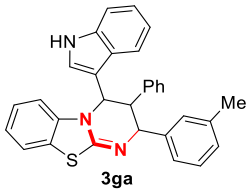


3fa

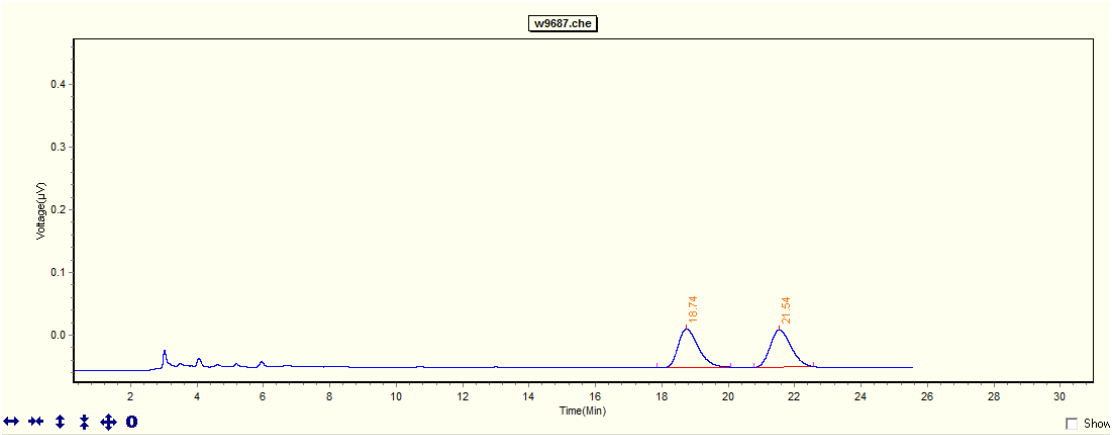


egration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.50	69710	1334	0.51%	1.967	BB
2	17.62	13522259	166542	99.49%	5.316	BB
al		13,591,969	167,876	100.00%		

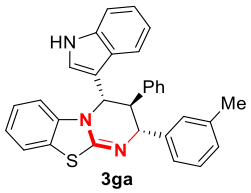


3ga

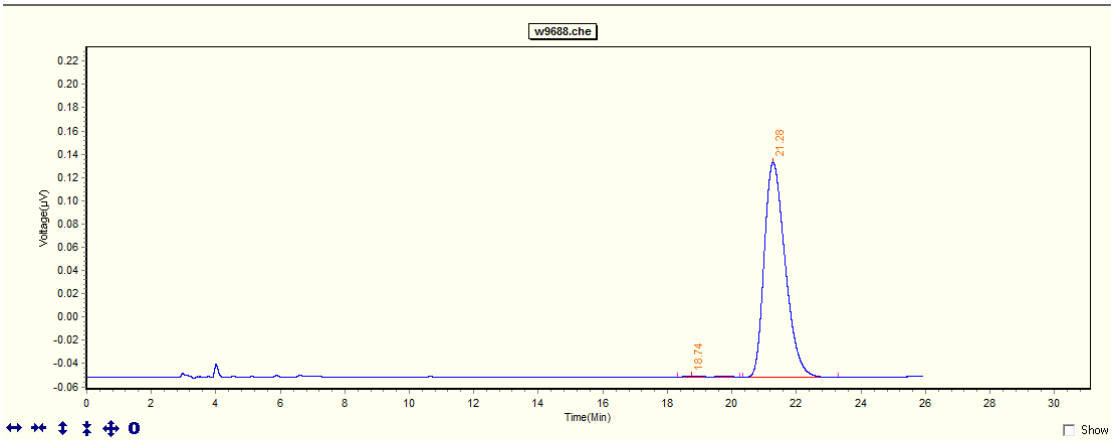


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	18.74	1280283	30706	49.95%	2.221	BB
2	21.54	1283036	29637	50.05%	1.794	BB
Total		2,563,319	60,343	100.00%		

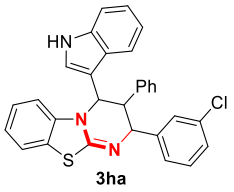


3ga

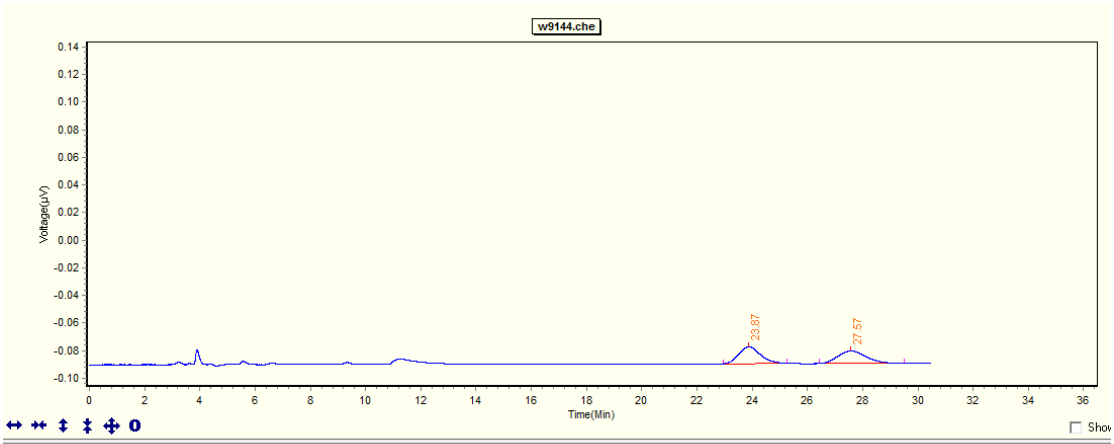


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	18.74	37655	652	0.89%	1.932	BB
2	21.28	4172035	92484	99.11%	2.959	BB
Total		4,209,690	93,136	100.00%		

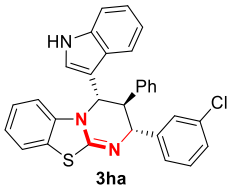


3ha

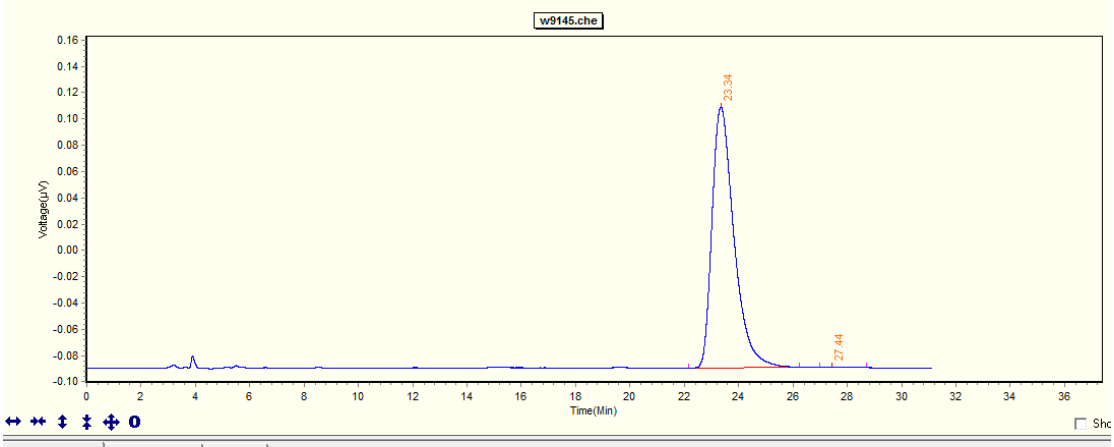


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	23.87	326276	6080	50.61%	2.307	BB
2	27.57	318367	4483	49.39%	3.075	BB
Total		644,643	10,563	100.00%		

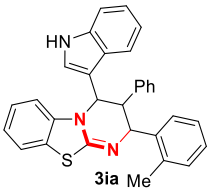


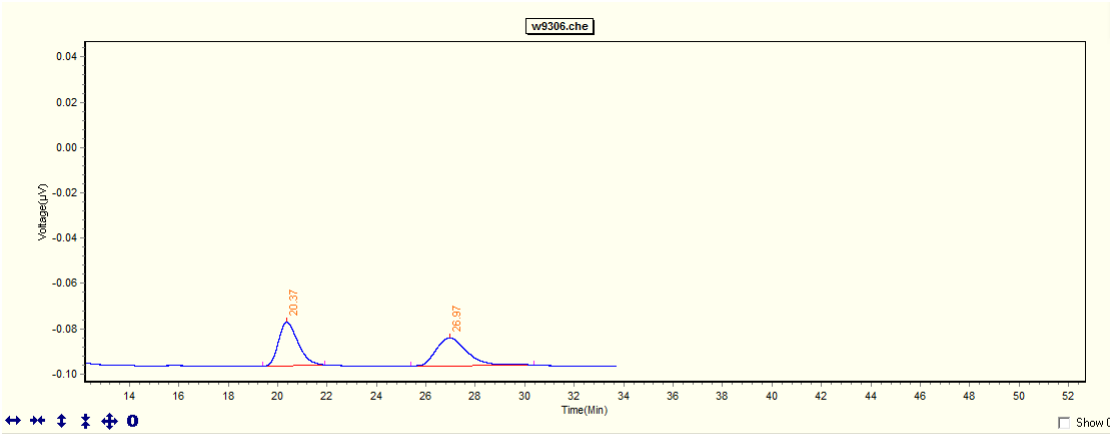
3ha



Integration Result | Calculation Result | TimeTable

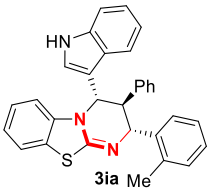
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	23.34	5562010	99076	99.79%	4.08	BB
2	27.44	11784	225	0.21%	1.722	BB
Total		5,573,794	99,301	100.00%		

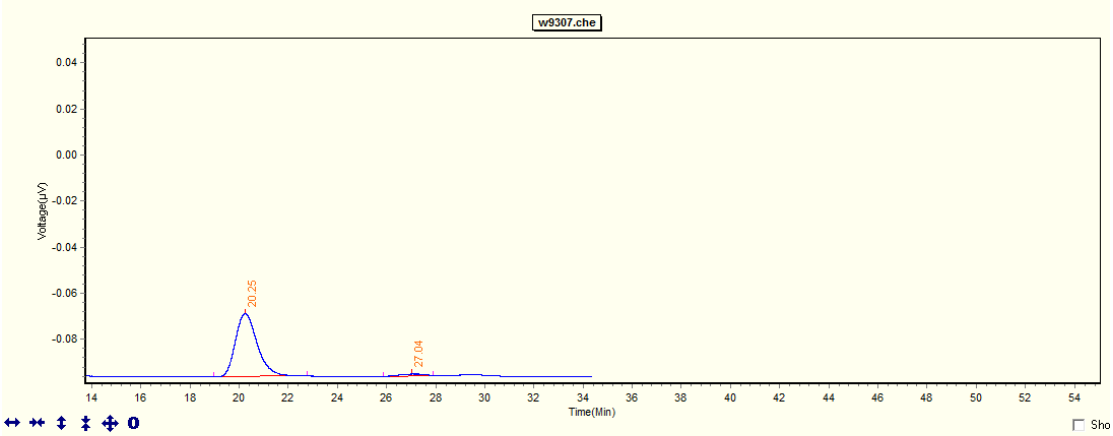




Integration Result | Calculation Result | TimeTable

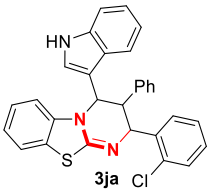
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	20.37	522089	9593	49.66%	2.51	BB
2	26.97	529262	6165	50.34%	4.981	BB
Total		1,051,351	15,758	100.00%		

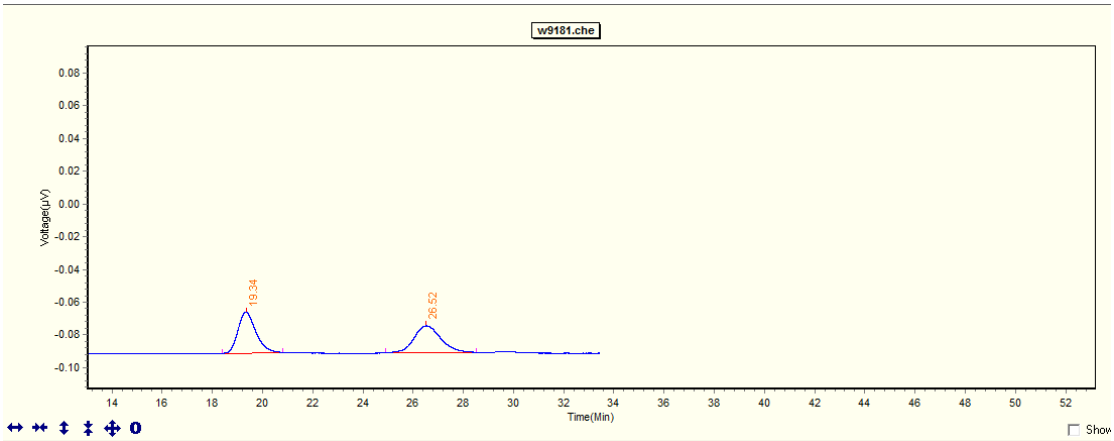




Integration Result | Calculation Result | TimeTable

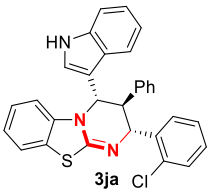
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	20.25	842797	13636	96.95%	3.803	BB
2	27.04	26554	410	3.05%	2.025	BB
Total		869,351	14,046	100.00%		

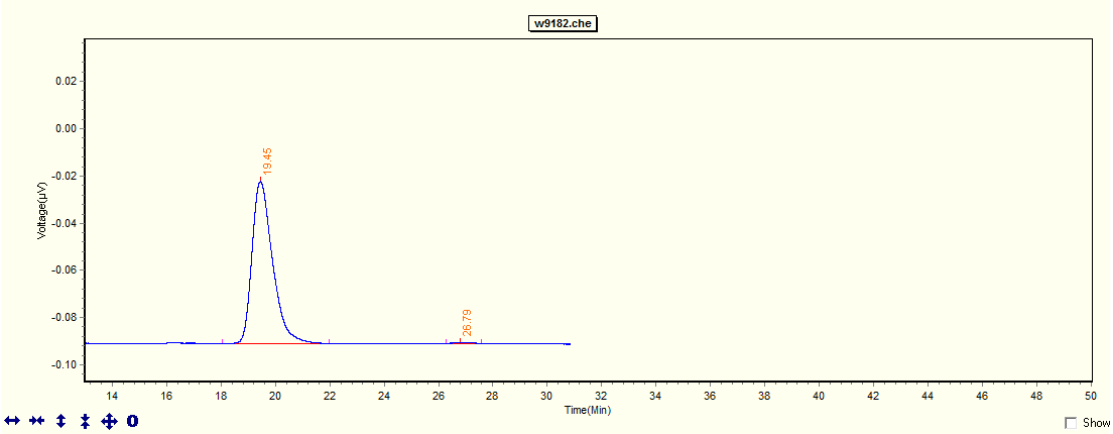




Integration Result | Calculation Result | TimeTable

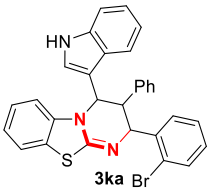
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	19.34	615300	12490	50.29%	2.41	BB
2	26.52	608290	8171	49.71%	3.615	BB
Total		1,223,590	20,661	100.00%		

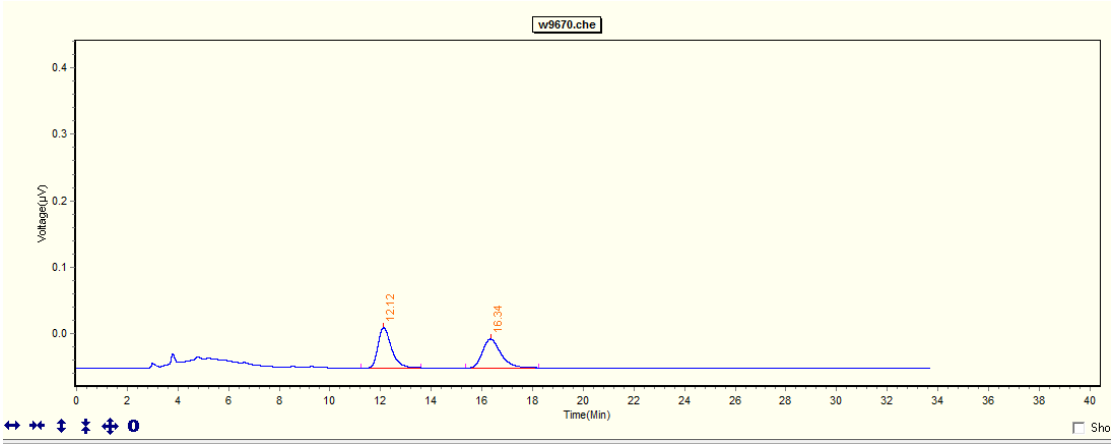




Integration Result | Calculation Result | TimeTable

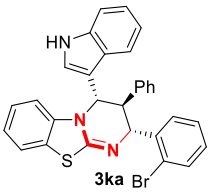
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	19.45	1795824	34291	99.66%	3.928	BB
2	26.79	6101	144	0.34%	1.298	BB
Total		1,801,925	34,435	100.00%		

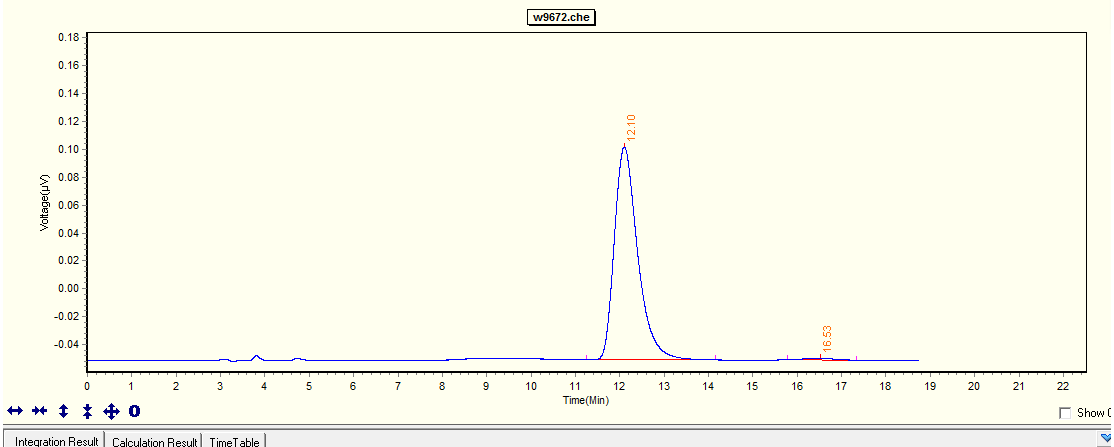




Integration Result | Calculation Result | TimeTable

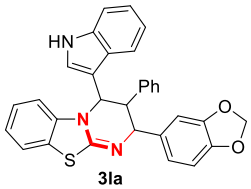
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.12	1102199	30323	50.57%	2.365	BB
2	16.34	1077385	21584	49.43%	2.886	BB
Total		2,179,584	51,907	100.00%		



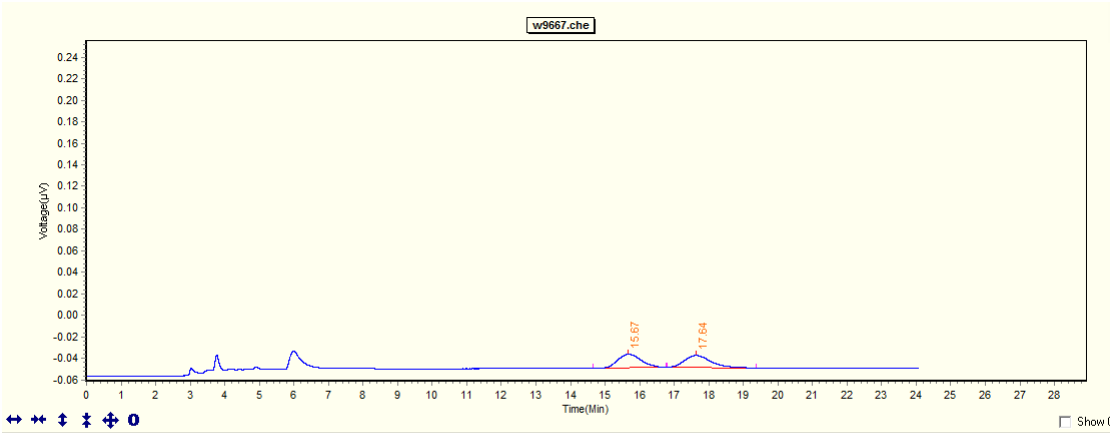


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.10	2784136	76165	98.95%	2.908	BB
2	16.53	29541	700	1.05%	1.555	BB
Total		2,813,677	76,865	100.00%		

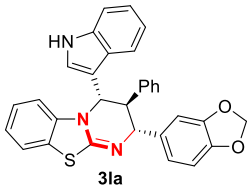


3la

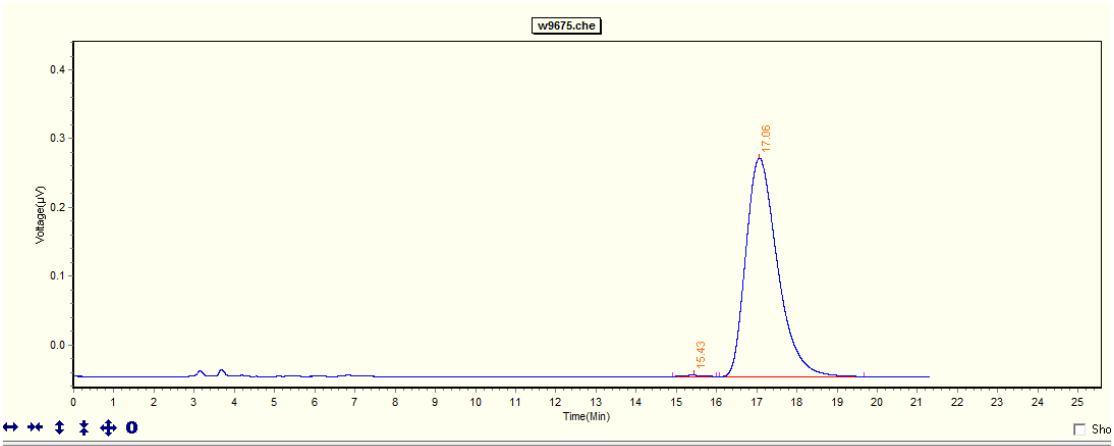


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	15.67	296564	6340	50.59%	2.114	BB
2	17.64	289677	5547	49.41%	2.577	BB
Total		586,241	11,887	100.00%		

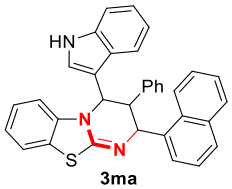


3la

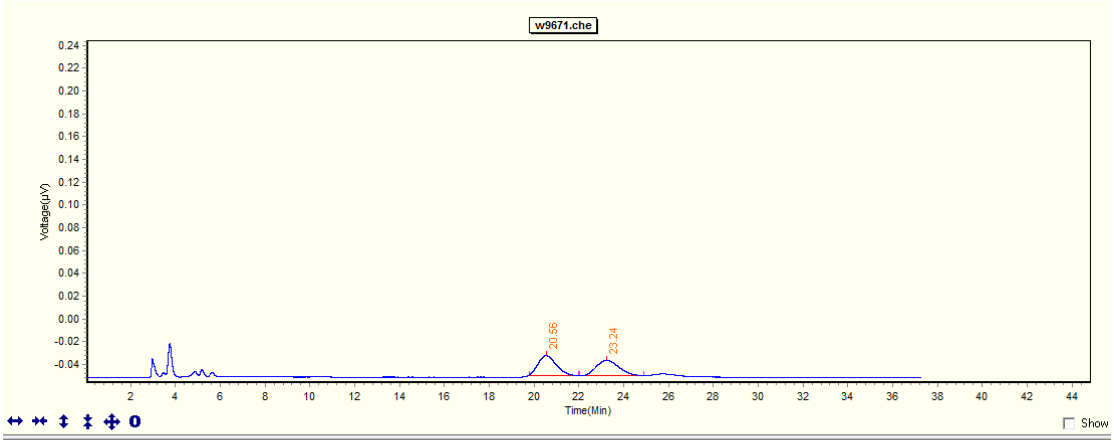


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	15.43	35738	988	0.41%	1.101	BB
2	17.06	8652109	158603	99.59%	3.584	BB
Total		8,687,847	159,591	100.00%		

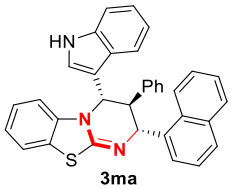


3ma

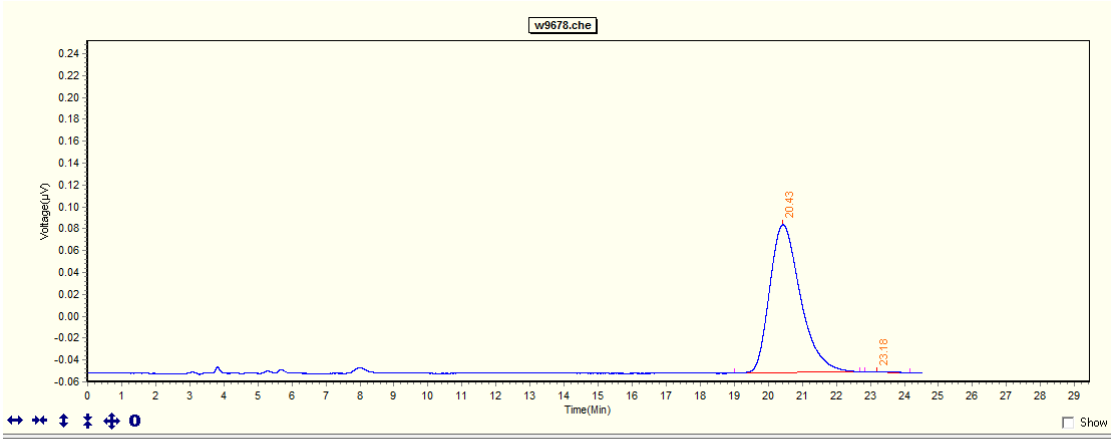


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	20.56	487315	8649	50.44%	2.194	BB
2	23.24	478758	6842	49.56%	2.866	BB
Total		966,073	15,491	100.00%		

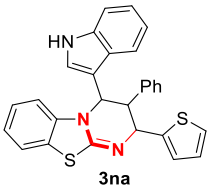


3ma

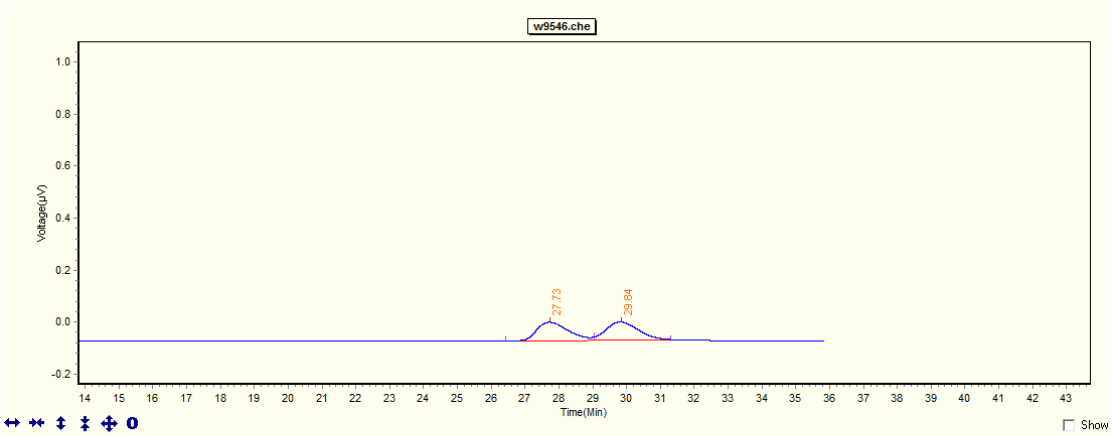


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	20.43	4256905	67592	99.82%	3.683	BB
2	23.18	7588	123	0.18%	1.326	BB
Total		4,264,493	67,715	100.00%		

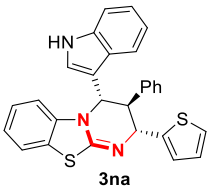


3na

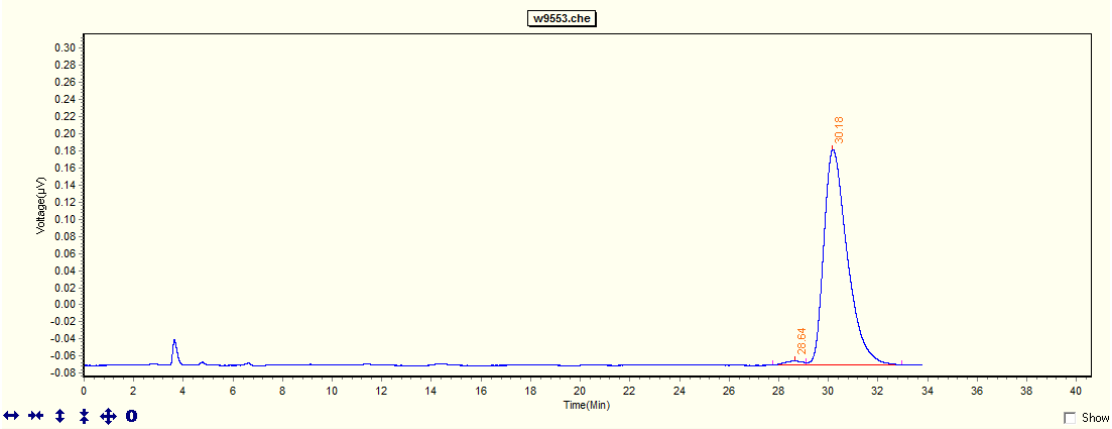


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	27.73	2240865	34979	49.93%	2.616	BV
2	29.84	2247453	34413	50.07%	2.26	VB
Total		4,488,318	69,392	100.00%		

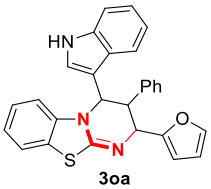


3na

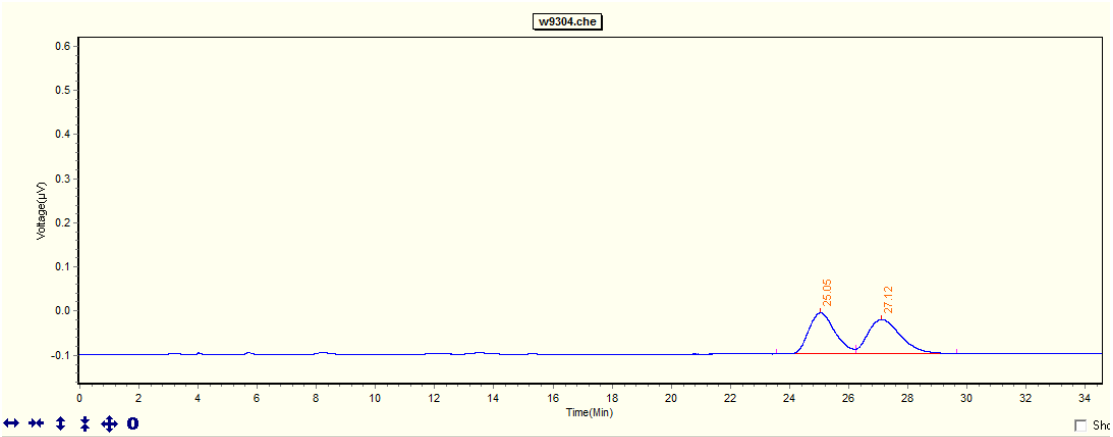


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	28.64	117582	2340	1.40%	1.34	BV
2	30.18	8274210	125911	98.60%	3.861	VB
Total		8,391,792	128,251	100.00%		

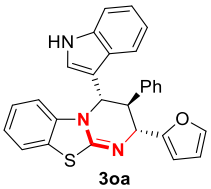


3oa

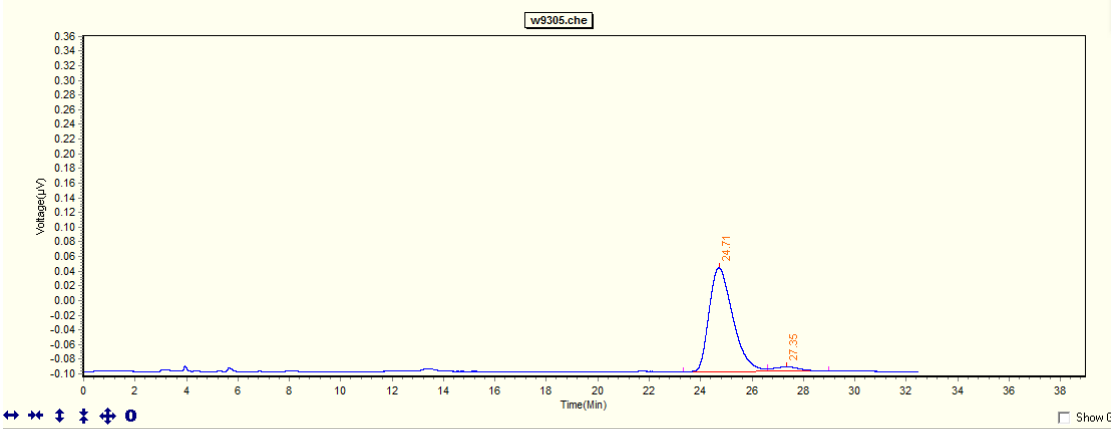


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	25.05	2854153	46308	48.95%	2.668	BV
2	27.12	2976941	38548	51.05%	3.429	VB
Total		5,831,094	84,856	100.00%		

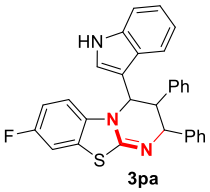


3oa

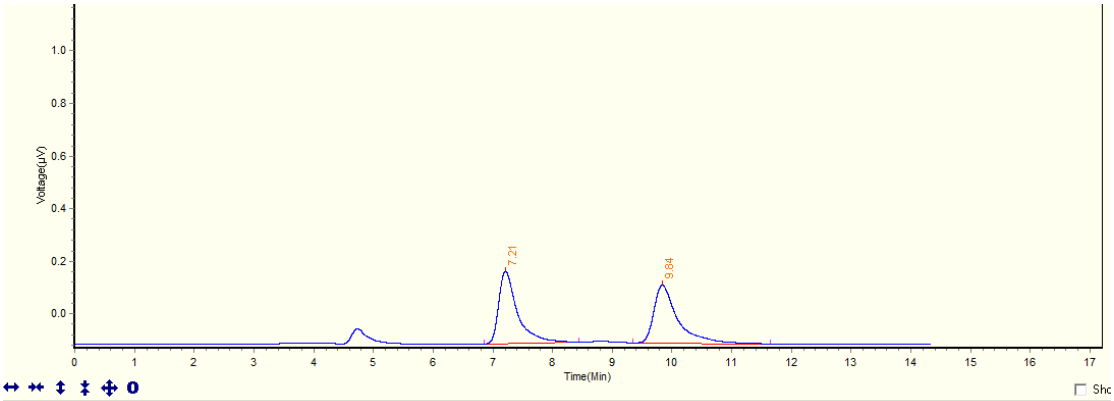


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	24.71	4522143	70616	95.45%	3.277	BV
2	27.35	215570	3005	4.55%	2.378	VB
Total		4,737,713	73,621	100.00%		

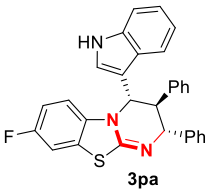


3pa

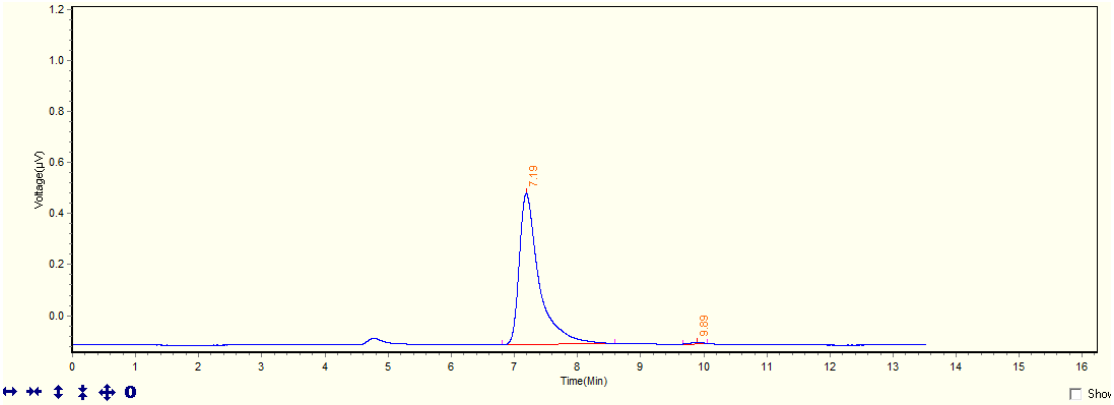


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.21	3012975	137409	49.75%	1.584	BB
2	9.84	3042911	109792	50.25%	2.291	BB
Total		6,055,886	247,201	100.00%		

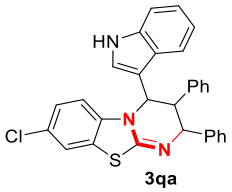


3pa

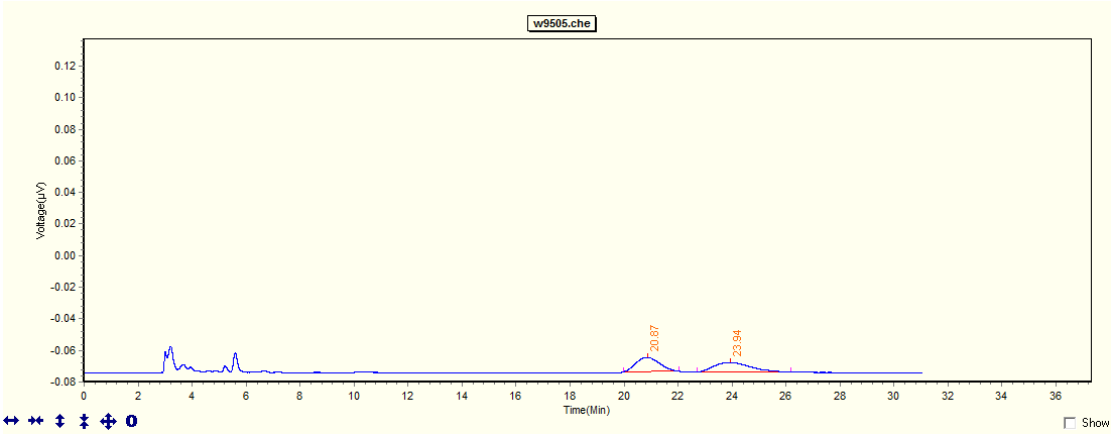


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.19	6454722	296388	99.55%	1.786	BB
2	9.89	29342	2146	0.45%	0.386	BB
Total		6,484,064	298,534	100.00%		

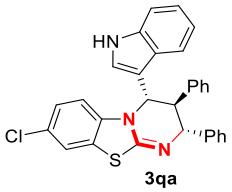


3qa

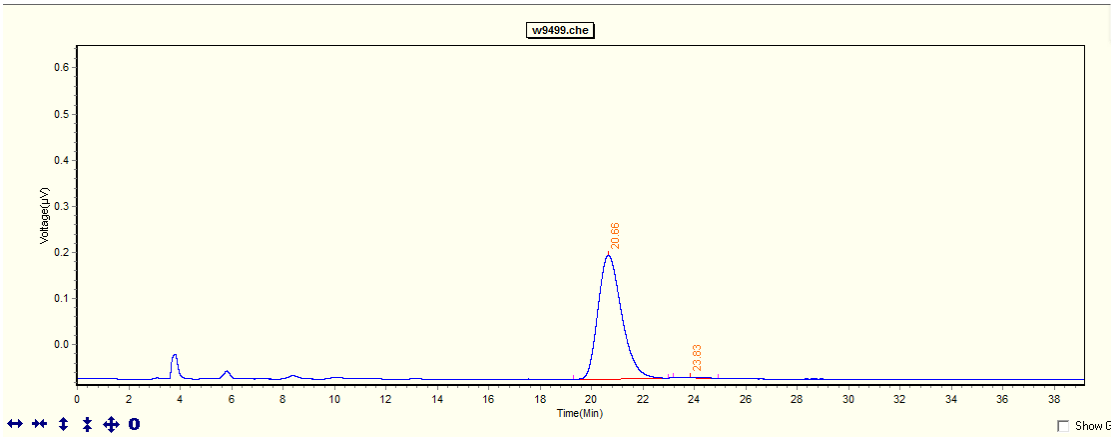


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	20.87	274273	4535	49.44%	2.054	BB
2	23.94	280477	3036	50.56%	3.473	BB
Total		554,750	7,571	100.00%		

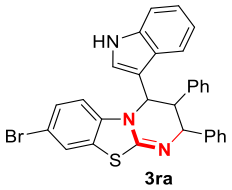


3qa

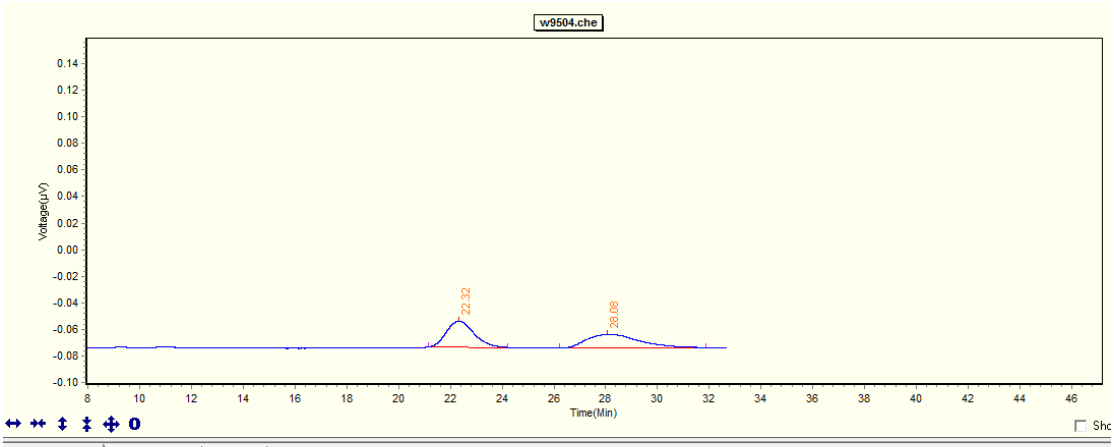


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	20.66	8489233	133950	99.24%	3.688	BB
2	23.83	65257	1041	0.76%	1.747	BB
Total		8,554,490	134,991	100.00%		

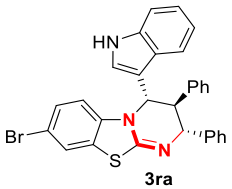


3ra

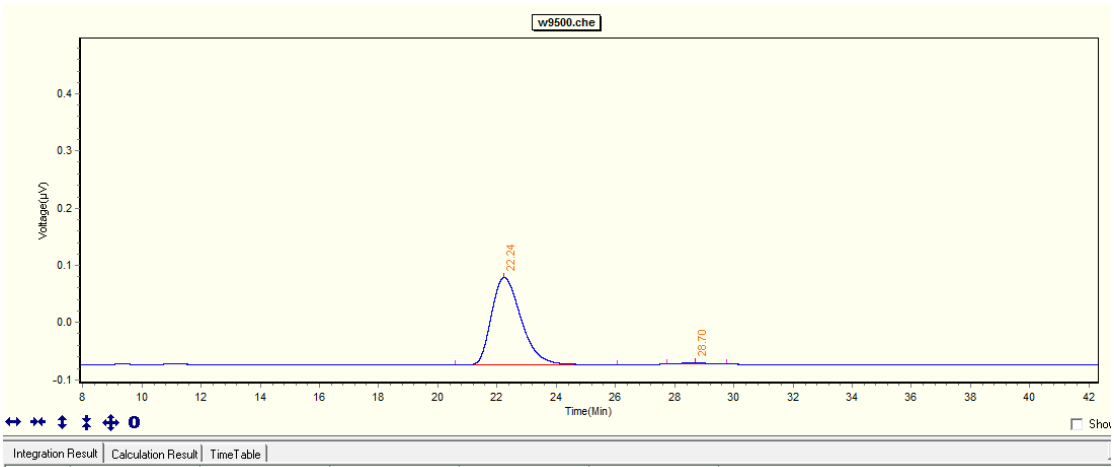


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	22.32	718722	9708	50.08%	3.061	BB
2	28.08	716289	5209	49.92%	5.652	BB
Total		1,435,011	14,917	100.00%		

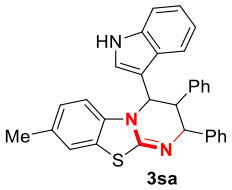


3ra

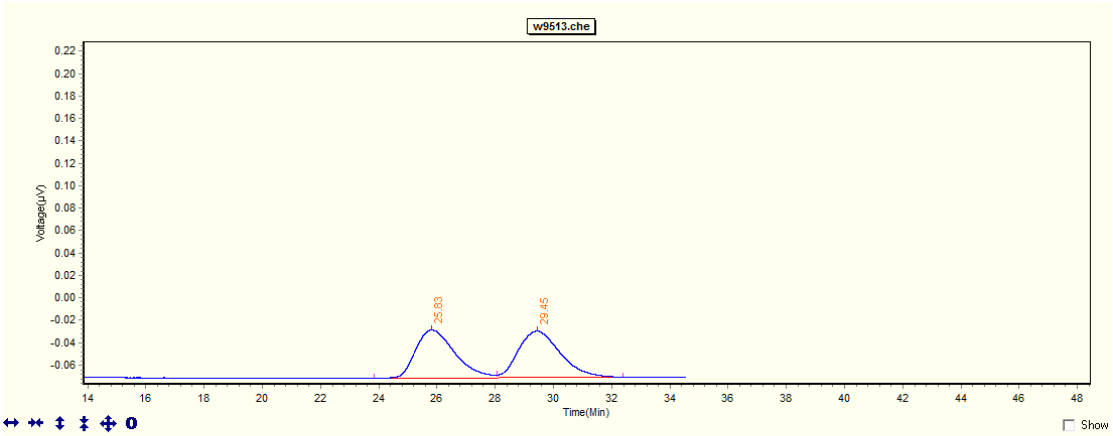


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	22.24	5309022	76279	99.00%	5.473	BB
2	28.70	53692	688	1.00%	2.023	BB
Total		5,362,714	76,967	100.00%		

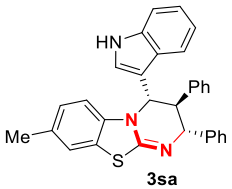


3sa

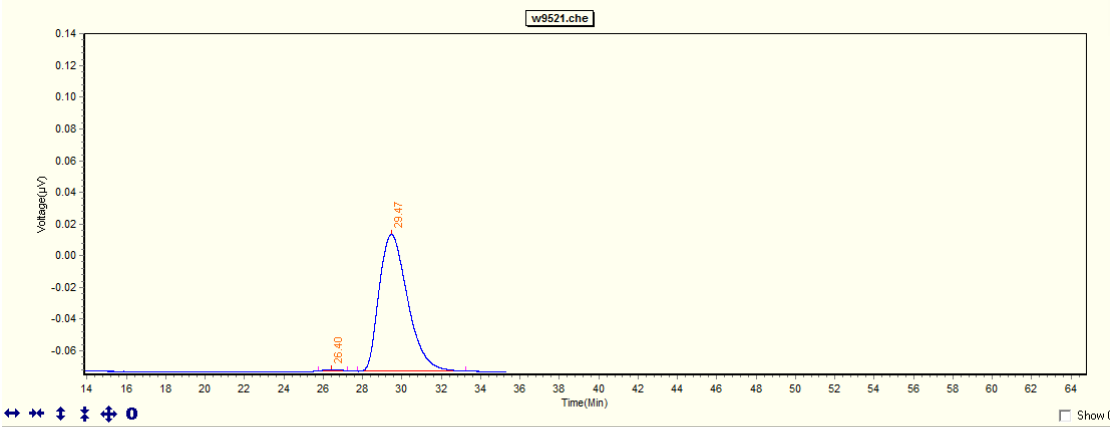


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	25.83	1961410	21291	48.96%	4.236	BV
2	29.45	2044552	20661	51.04%	4.318	VB
Total		4,005,962	41,952	100.00%		

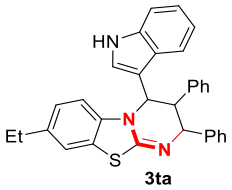


3sa

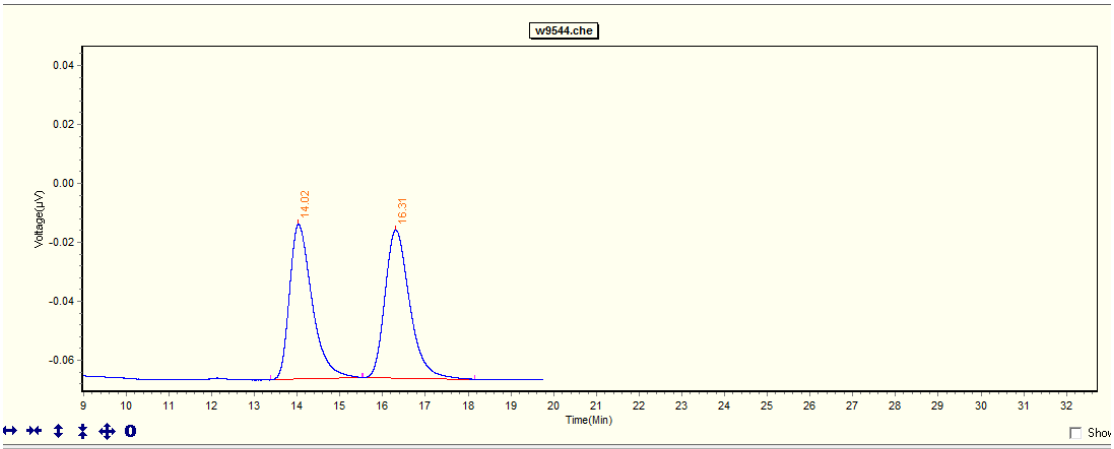


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	26.40	17357	338	0.40%	1.486	BB
2	29.47	4331893	43242	99.60%	5.52	BB
Total		4,349,250	43,580	100.00%		

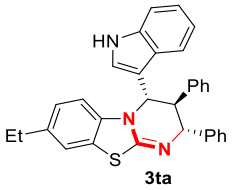


3ta

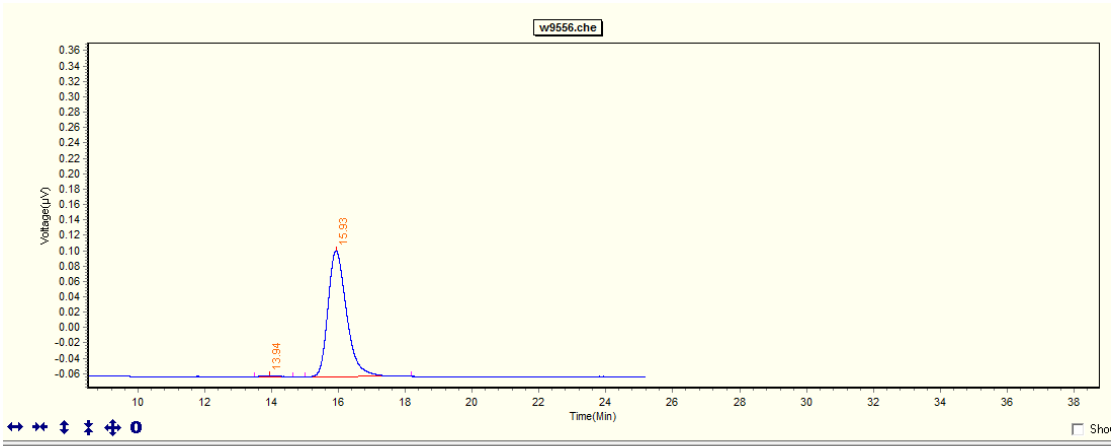


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	14.02	965007	26378	48.97%	2.139	BB
2	16.31	1005678	25114	51.03%	2.614	BB
Total		1,970,685	51,492	100.00%		

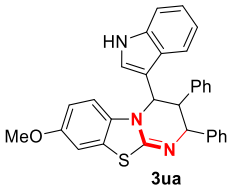


3ta

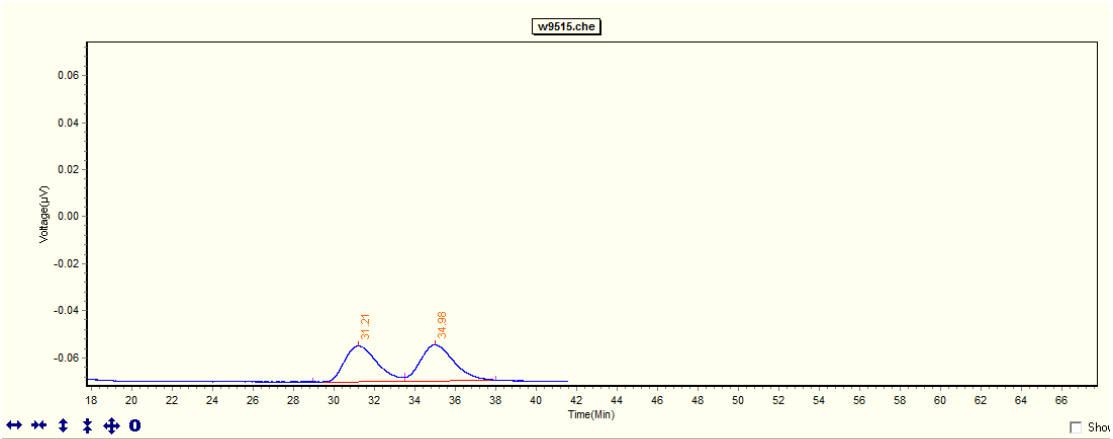


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	13.94	9777	306	0.31%	1.149	BB
2	15.93	3152618	81831	99.69%	3.176	BB
Total		3,162,395	82,137	100.00%		

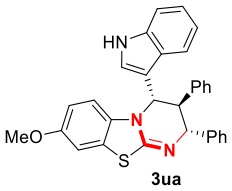


3ua

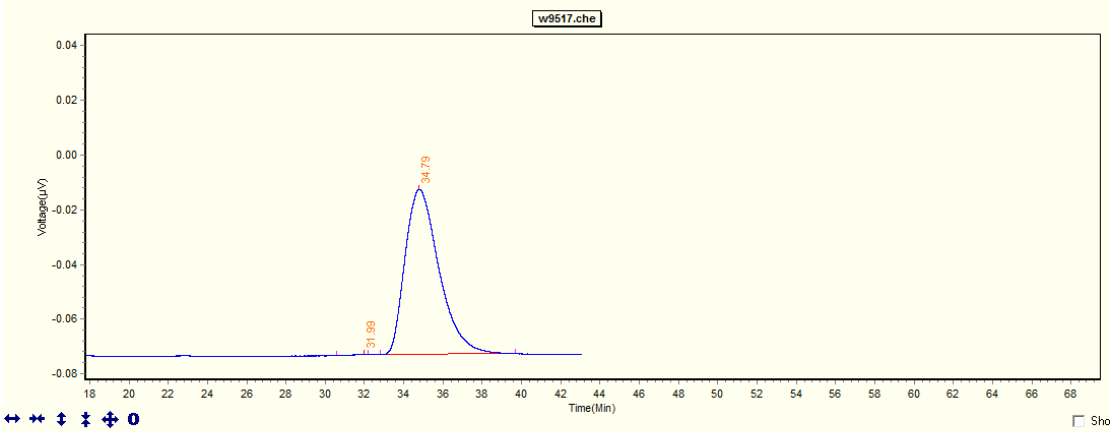


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	31.21	829623	7572	49.01%	4.549	BV
2	34.98	863247	7649	50.99%	4.5	VB
Total		1,692,870	15,221	100.00%		

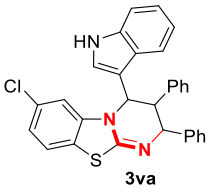


3ua

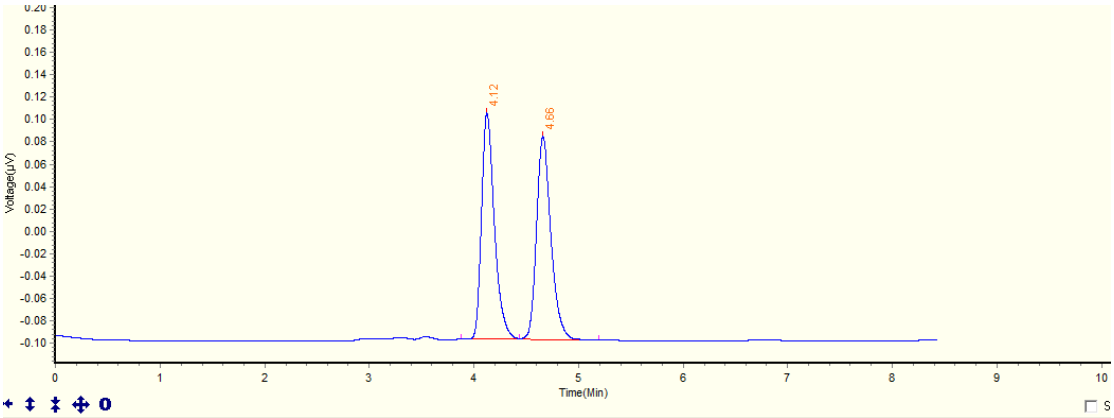


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	31.99	2727	47	0.07%	1.603	BB
2	34.79	3639352	30215	99.93%	6.882	BB
Total		3,642,079	30,262	100.00%		

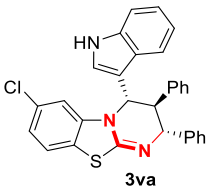


3va

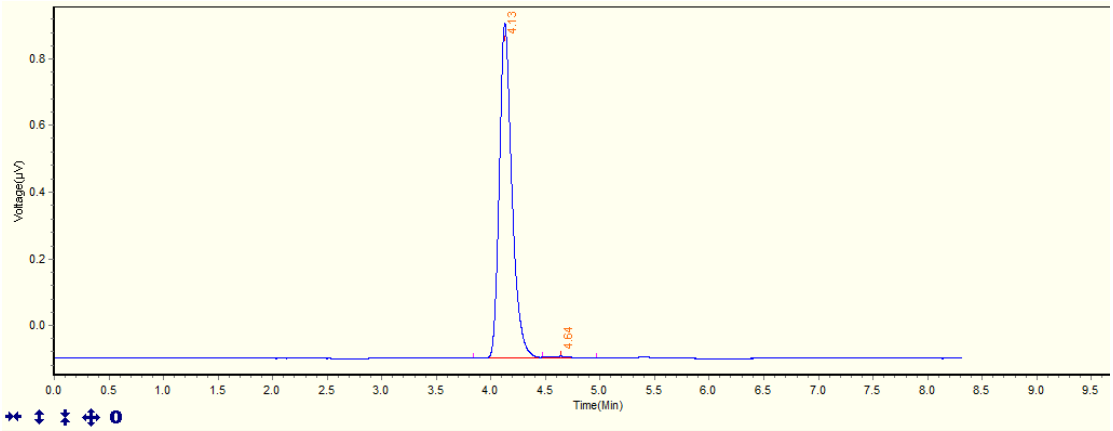


ration Result | Calculation Result | TimeTable

o.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	4.12	864694	100986	49.85%	0.557	BV
2	4.66	869927	90774	50.15%	0.758	VB

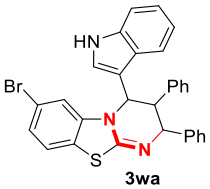


3va

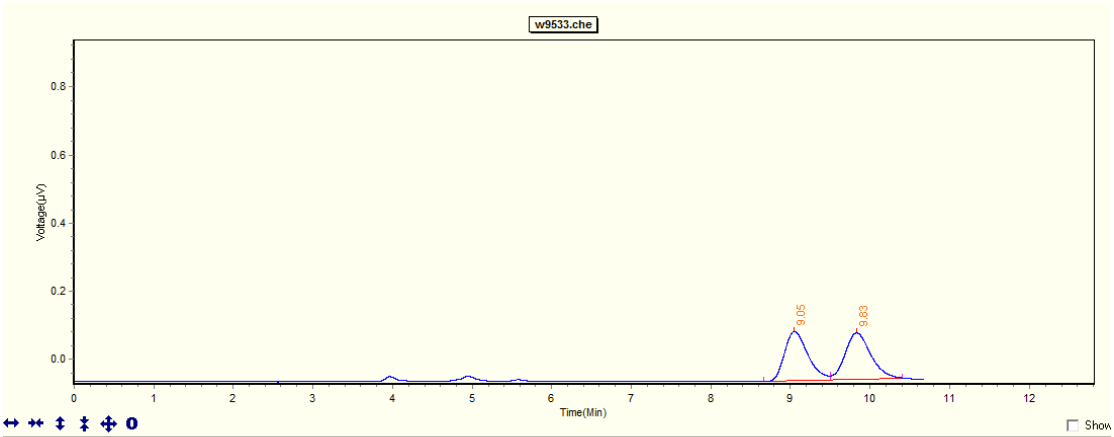


egration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	4.13	4022330	500626	99.08%	0.633	BV
2	4.64	37330	2897	0.92%	0.494	VB
al		4 059 660	503 523	100 00%		

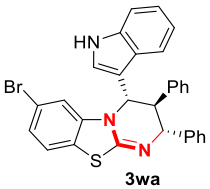


3wa

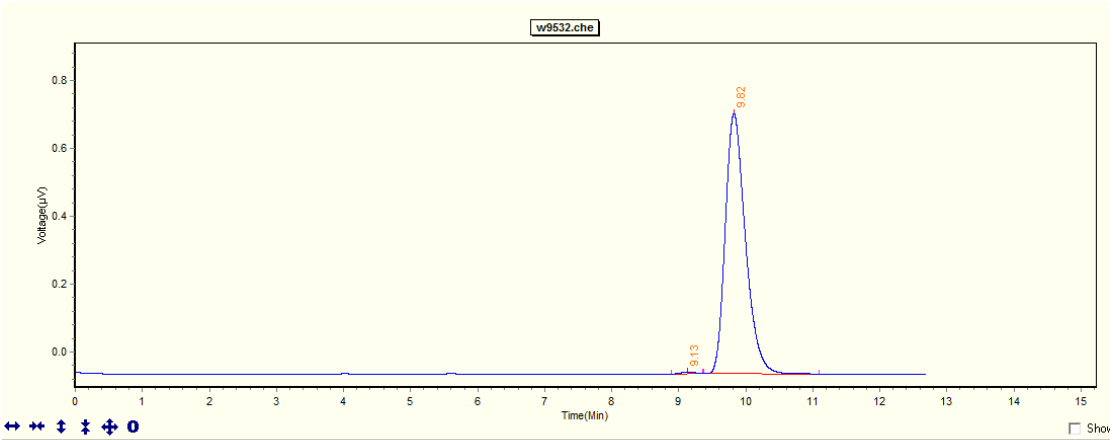


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.05	1480442	72887	49.33%	0.838	BV
2	9.83	1520519	67872	50.67%	0.901	VB
Total		3,000,961	140,759	100.00%		

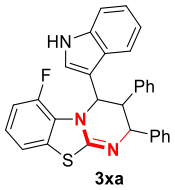


3wa

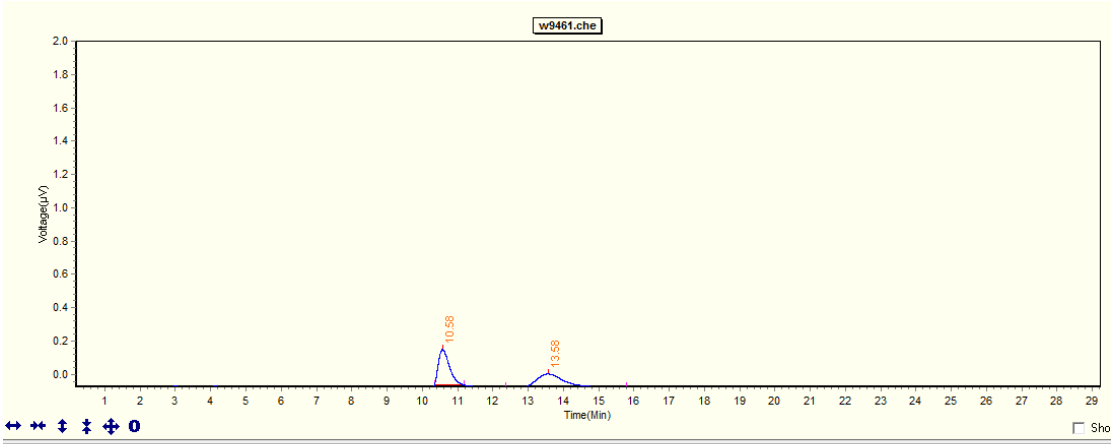


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.13	39617	2605	0.49%	0.469	BB
2	9.82	8012563	383586	99.51%	1.713	BB
Total		8,052,180	386,191	100.00%		

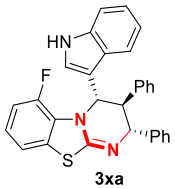


3xa

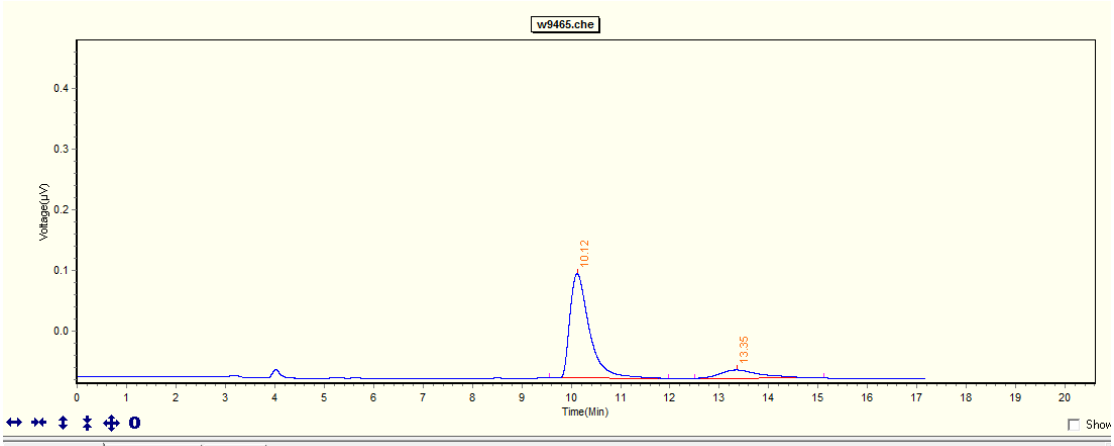


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.58	2257171	105375	51.99%	0.841	BB
2	13.58	2084722	39530	48.01%	3.424	BB
Total		4,341,893	144,905	100.00%		

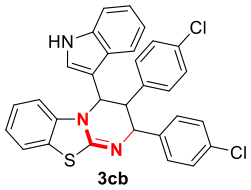


3xa

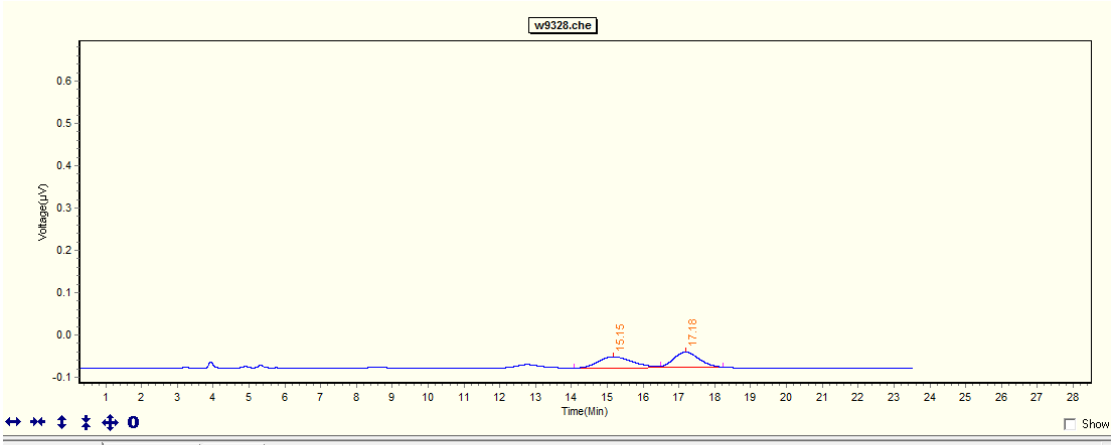


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.12	2341159	85970	85.56%	2.414	BB
2	13.35	395229	6783	14.44%	2.62	BB
Total		2,736,388	92,753	100.00%		

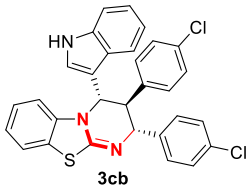


3cb

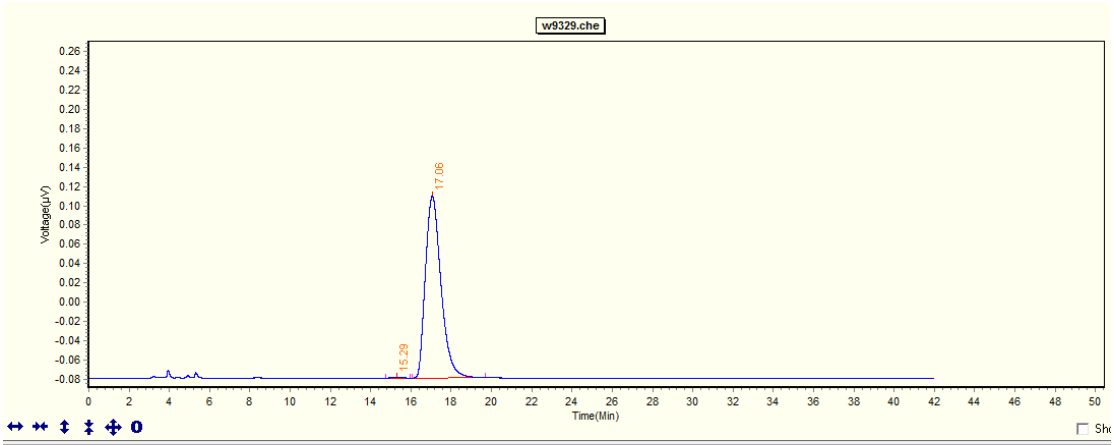


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	15.15	849863	13032	49.32%	2.415	BV
2	17.18	873150	17854	50.68%	1.742	VB
Total		1,723,013	30,886	100.00%		

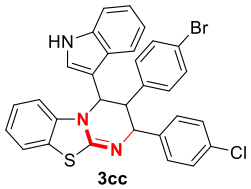


3cb

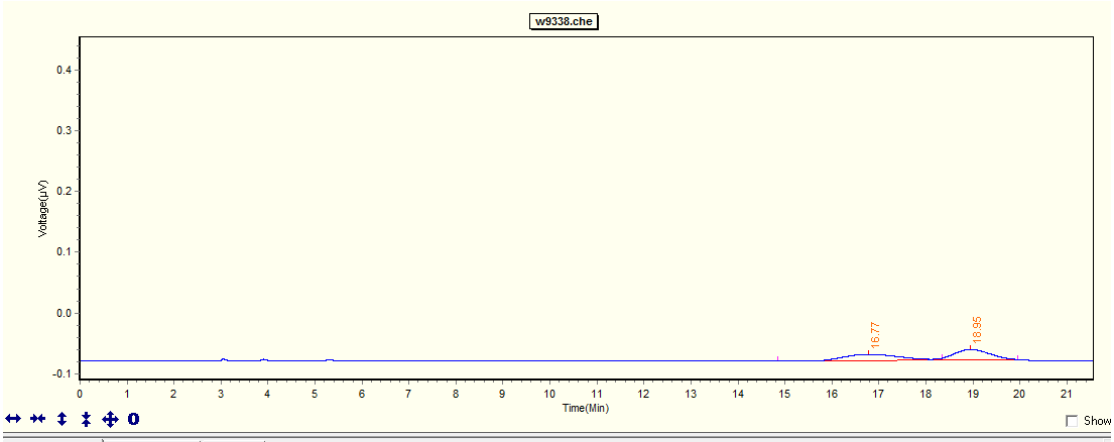


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	15.29	6328	167	0.12%	1.212	BB
2	17.06	5077700	94215	99.88%	3.635	BB
Total		5,084,028	94,382	100.00%		

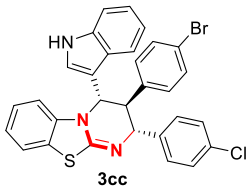


3cc

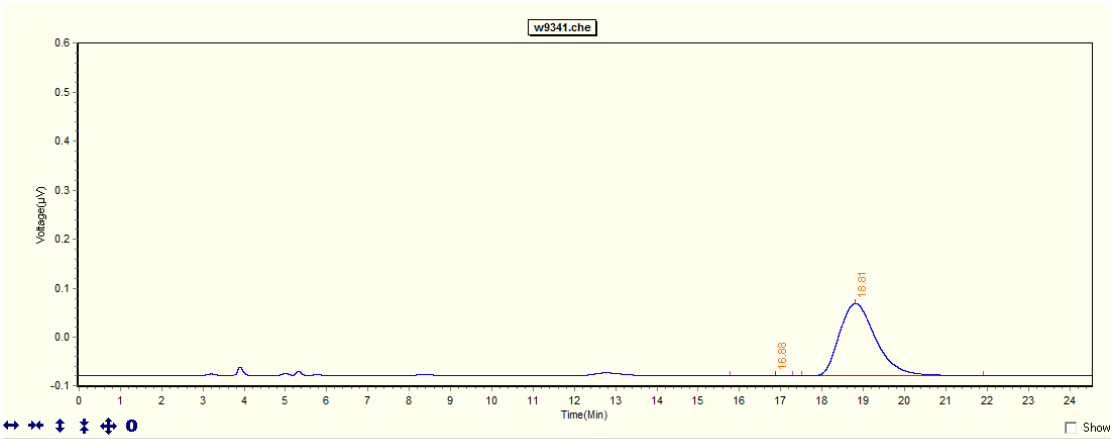


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	16.77	426244	5169	48.79%	3.48	BV
2	18.95	447379	8568	51.21%	1.616	VB
Total		873,623	13,737	100.00%		

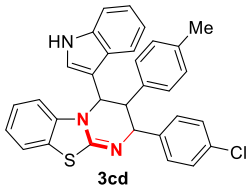


3cc

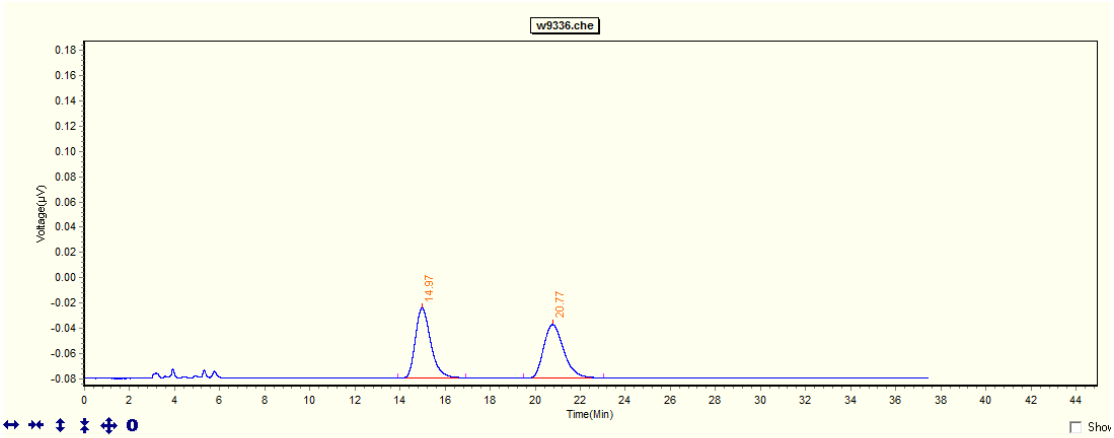


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	16.88	12335	291	0.28%	1.534	BB
2	18.81	4445334	73613	99.72%	4.398	BB
Total		4,457,669	73,904	100.00%		

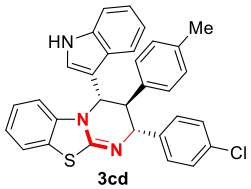


3cd

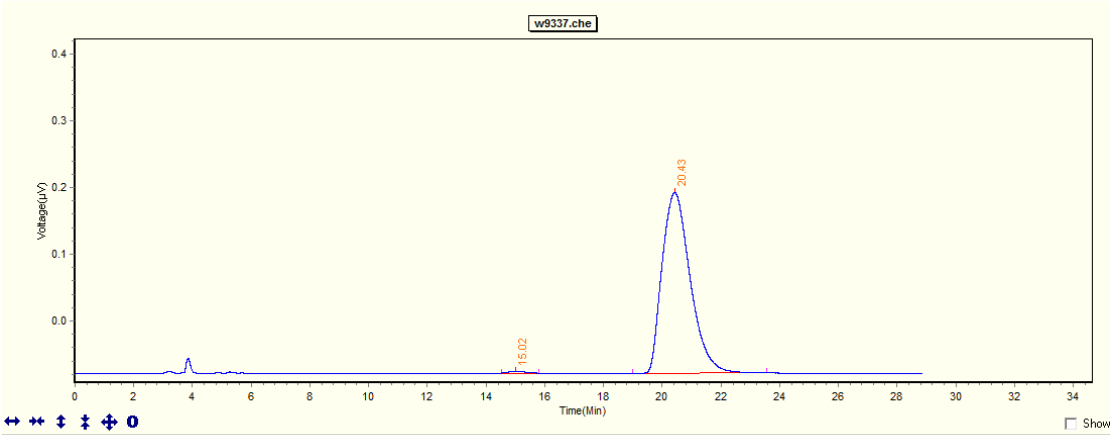


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	14.97	1309607	27756	50.13%	3.014	BB
2	20.77	1302902	21205	49.87%	3.554	BB
Total		2,612,509	48,961	100.00%		

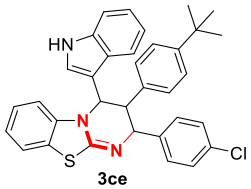


3cd

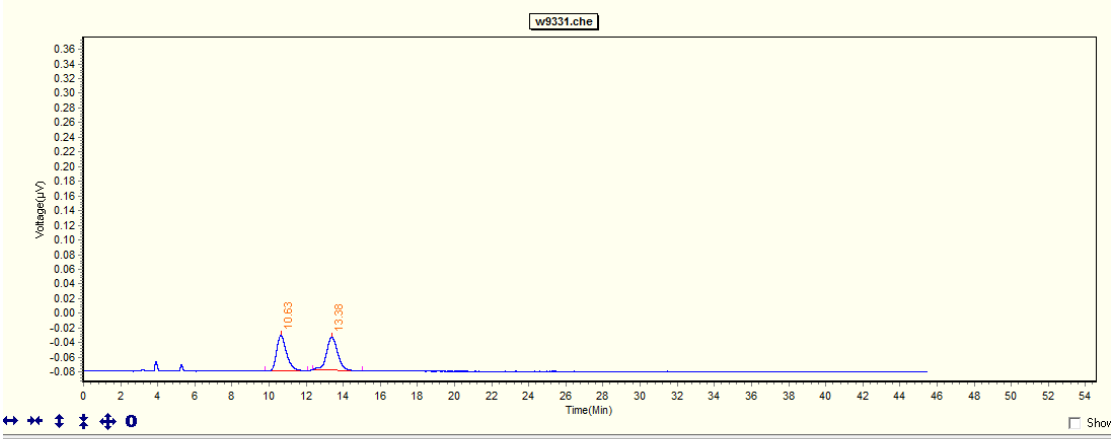


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	15.02	55221	1454	0.61%	1.271	BB
2	20.43	9024400	135524	99.39%	4.543	BB
Total		9,079,621	136,978	100.00%		

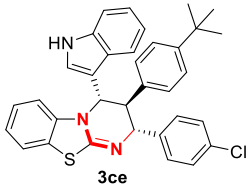


3ce

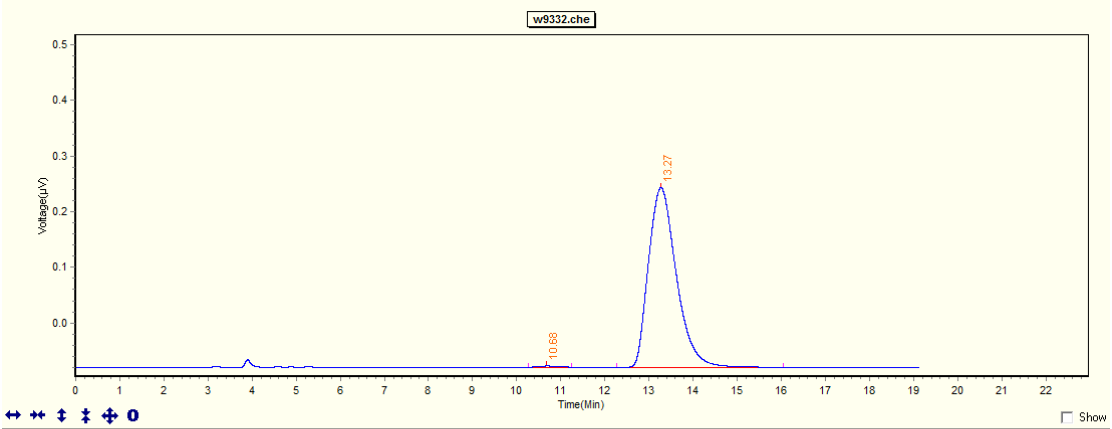


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.63	895954	24129	48.88%	2.294	BB
2	13.38	937084	22517	51.12%	2.677	BB
Total		1,833,038	46,646	100.00%		

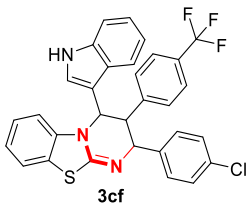


3ce

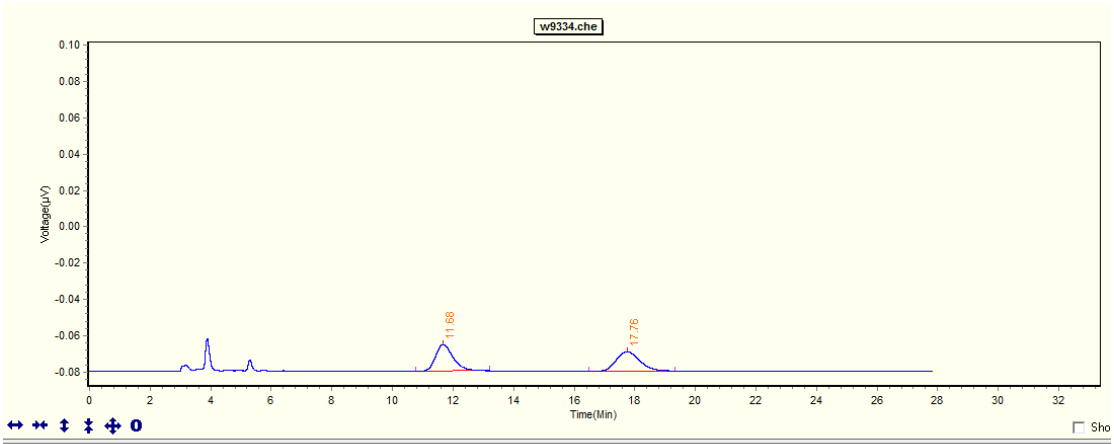


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.68	32774	1083	0.46%	0.966	BB
2	13.27	7064852	160988	99.54%	3.771	BB
Total		7,097,626	162,071	100.00%		

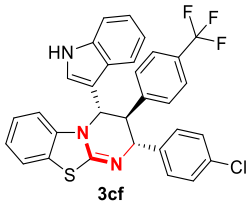


3cf

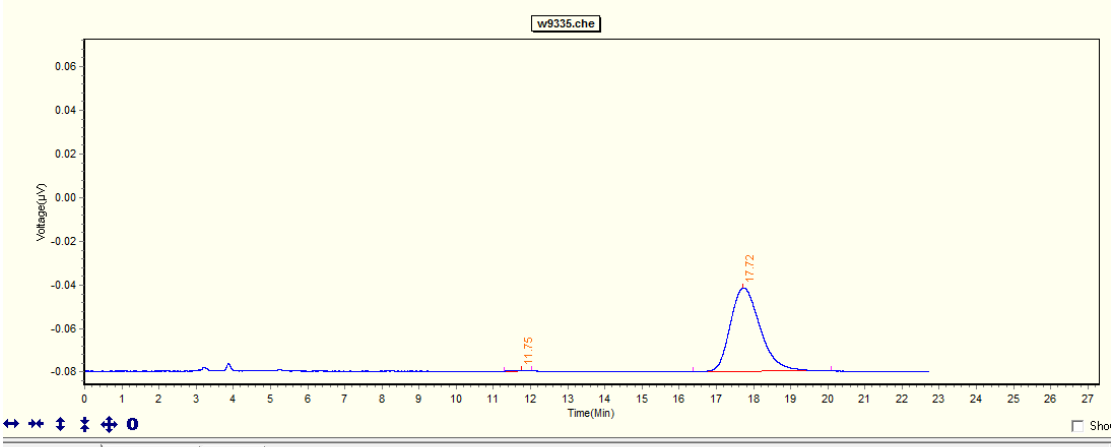


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.68	292835	7265	50.23%	2.441	BB
2	17.76	290173	5364	49.77%	2.842	BB
Total		583,008	12,629	100.00%		

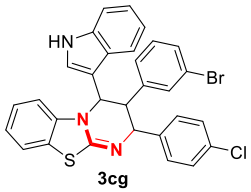


3cf

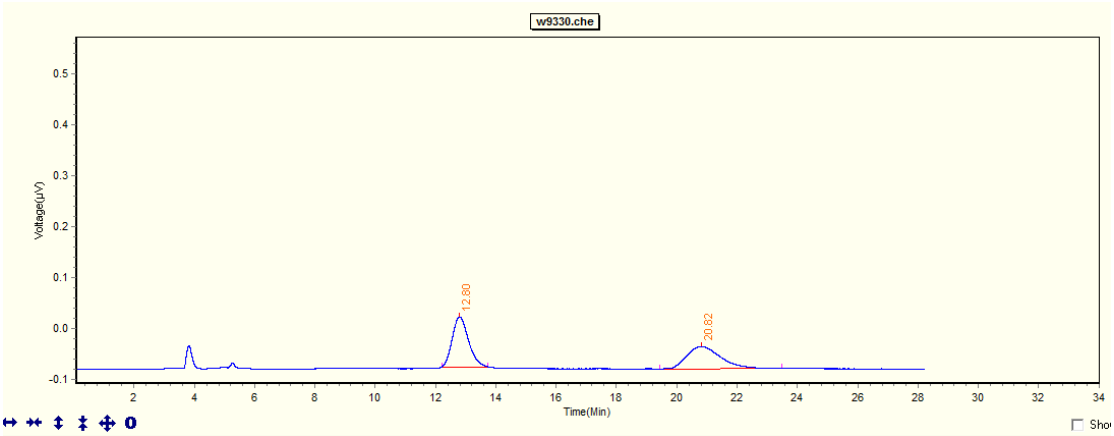


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.75	2071	94	0.19%	0.738	BB
2	17.72	1060192	19086	99.81%	3.718	BB
Total		1,062,263	19,180	100.00%		

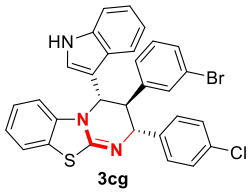


3cg

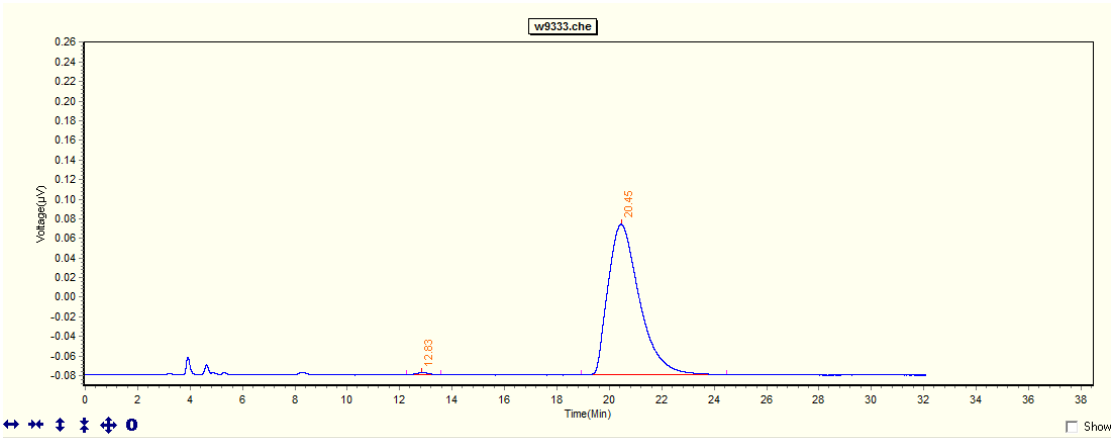


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.80	1822455	49004	51.67%	1.528	BB
2	20.82	1704821	21817	48.33%	4.039	BB
Total		3,527,276	70,821	100.00%		

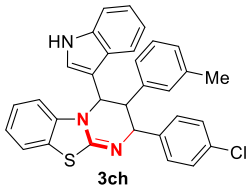


3cg

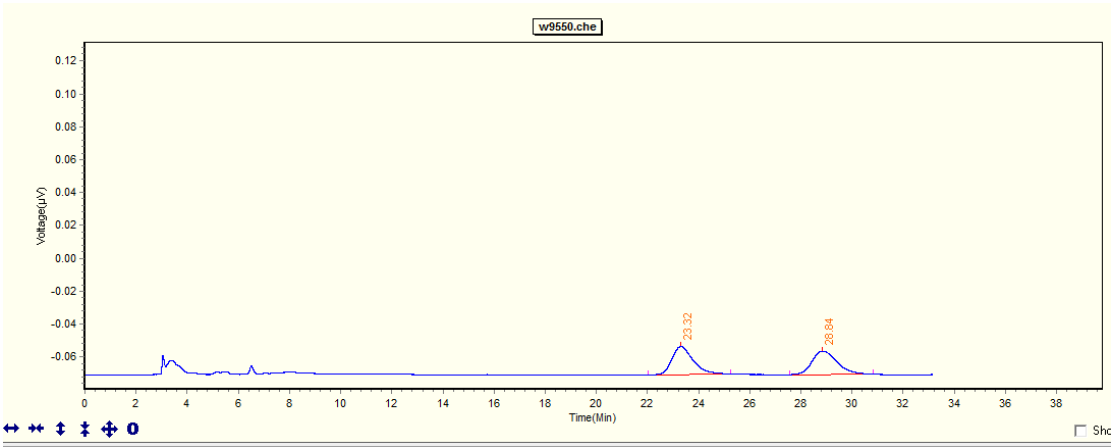


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.83	37797	1110	0.59%	1.31	BB
2	20.45	6342053	76587	99.41%	5.55	BB
Total		6,379,850	77,697	100.00%		

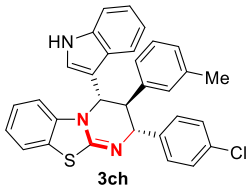


3ch

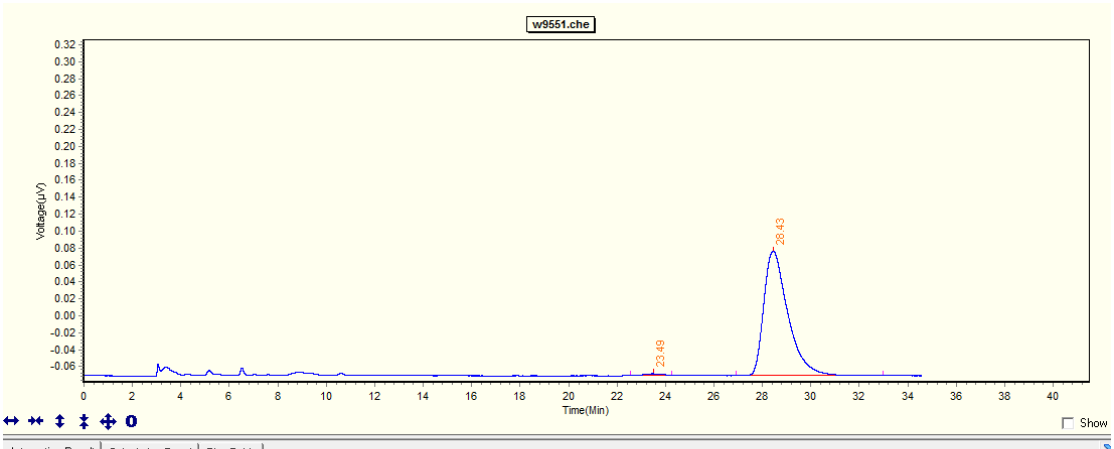


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	23.32	485992	8517	50.06%	3.226	BB
2	28.84	484836	7097	49.94%	3.266	BB
Total		970,828	15,614	100.00%		

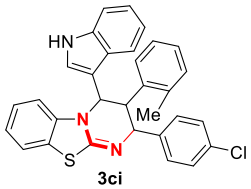


3ch

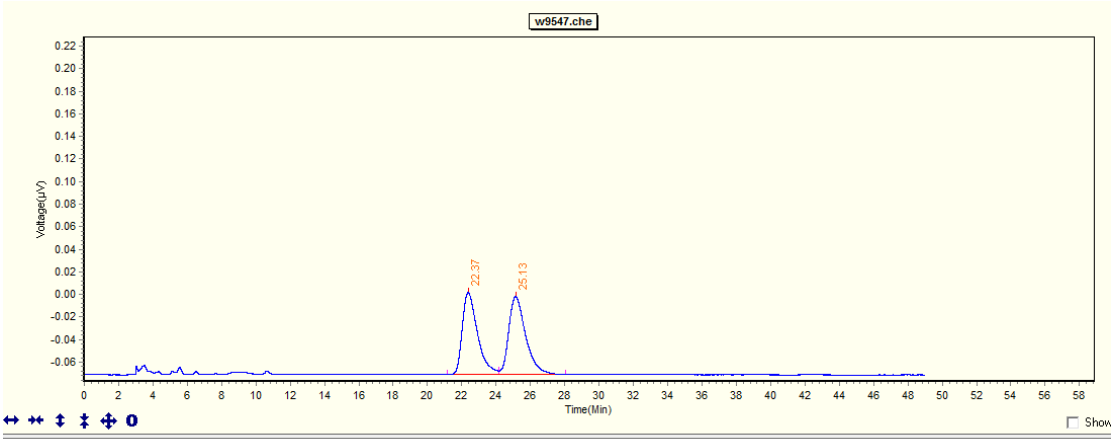


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	23.49	49936	1034	0.97%	1.702	BB
2	28.43	5079333	73627	99.03%	6.064	BB
Total		5,129,269	74,661	100.00%		

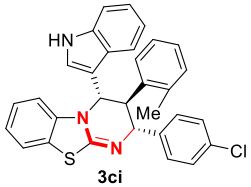


3ci

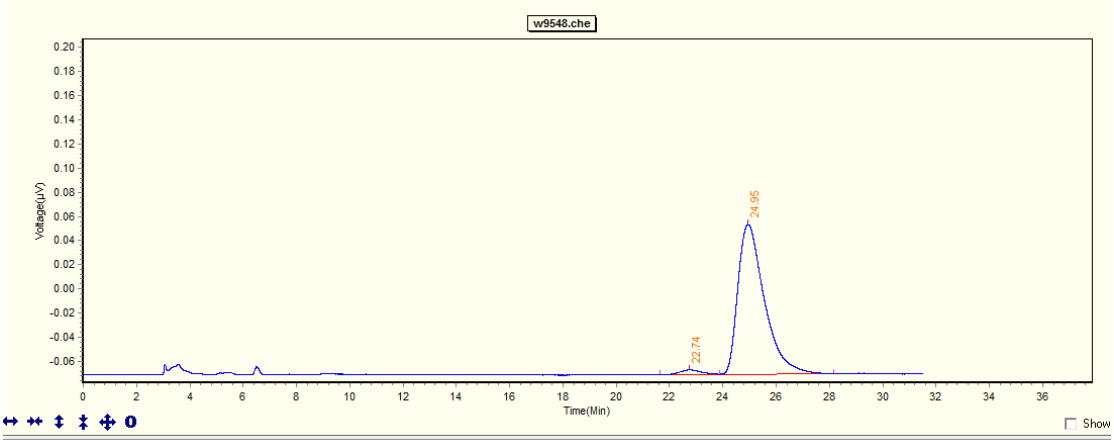


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	22.37	2244837	36284	48.60%	3.005	BV
2	25.13	2373889	34566	51.40%	3.888	VB
Total		4,618,726	70,850	100.00%		

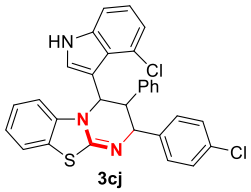


3ci

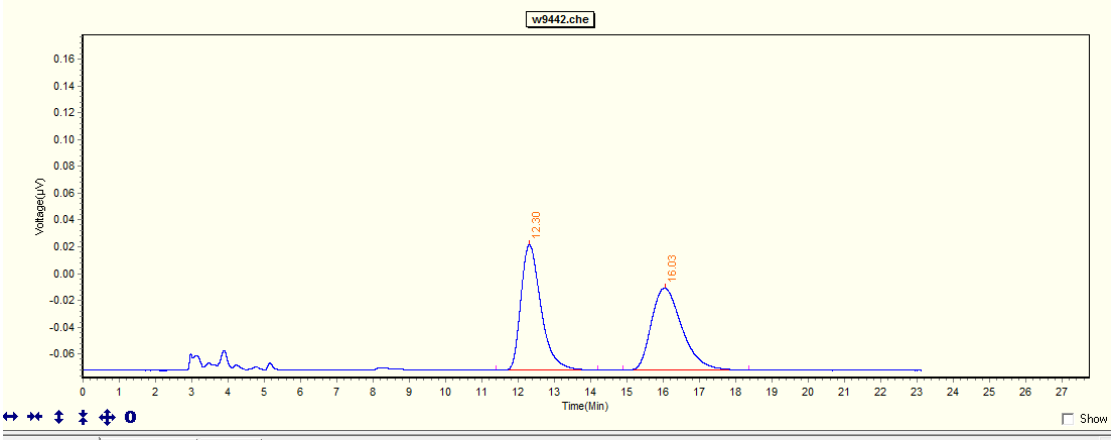


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	22.74	105681	1924	2.43%	2.236	BB
2	24.95	4245813	61885	97.57%	4.282	BB
Total		4,351,494	63,809	100.00%		

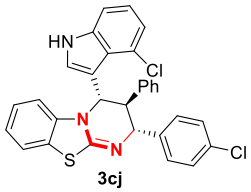


3cj

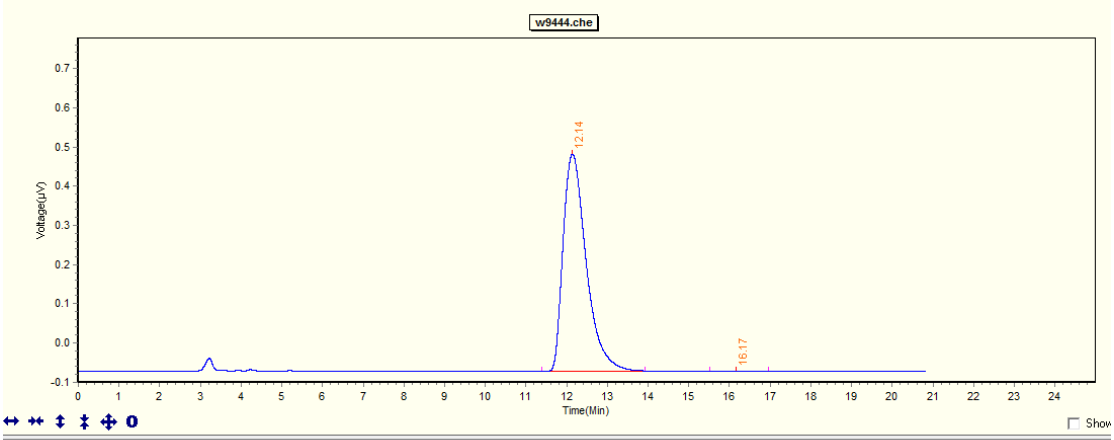


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.30	1798381	46726	50.06%	2.804	BB
2	16.03	1794069	30610	49.94%	3.47	BB
Total		3,592,450	77,336	100.00%		

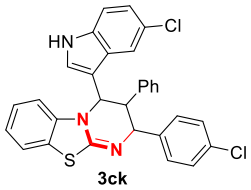


3cj

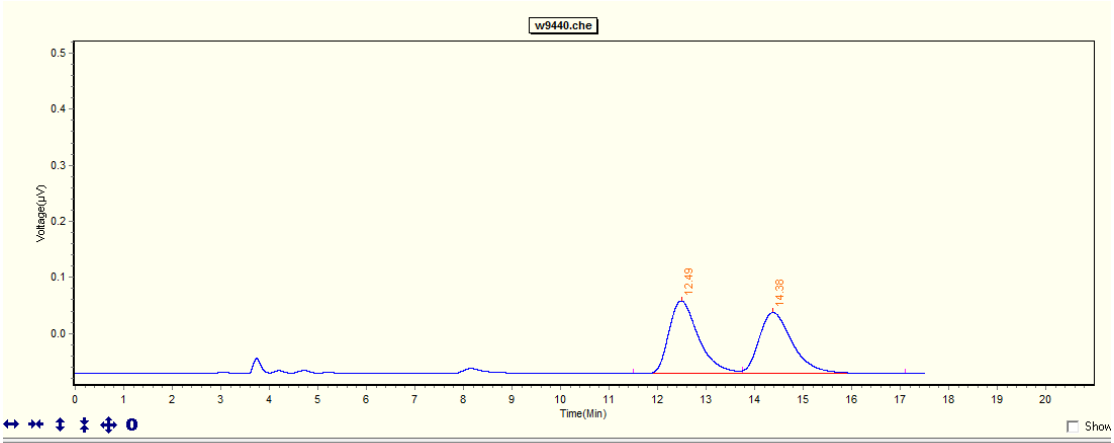


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.14	10927240	277320	99.75%	2.537	BB
2	16.17	27338	586	0.25%	1.451	BB
Total		10,954,578	277,906	100.00%		

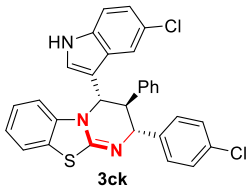


3ck

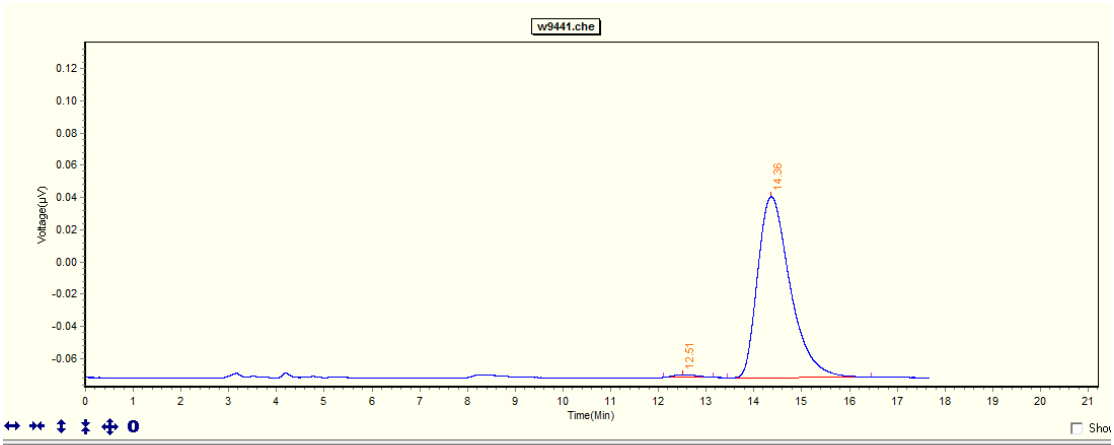


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.49	2735731	64795	51.41%	2.229	BV
2	14.38	2585956	54299	48.59%	3.365	VB
Total		5,321,687	119,094	100.00%		

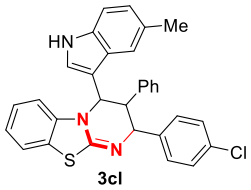


3ck

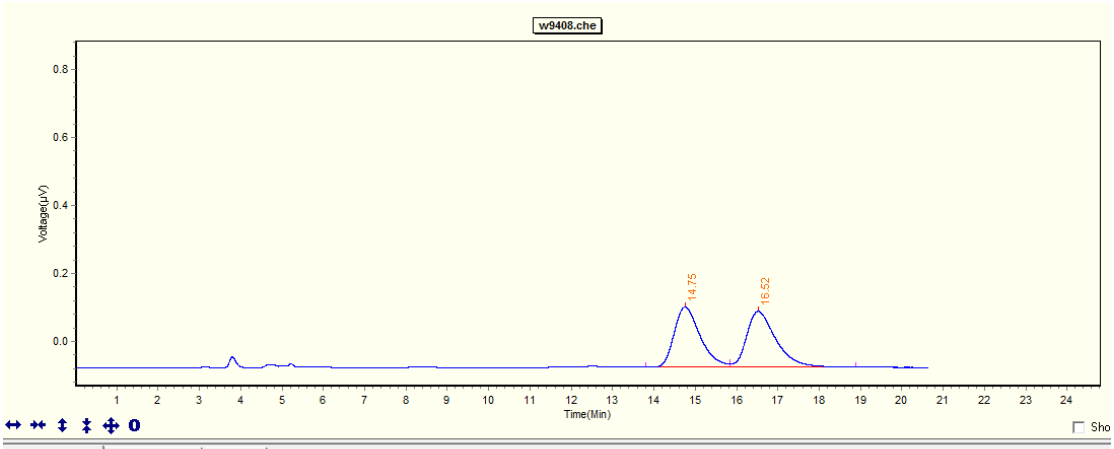


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.51	28339	881	1.06%	1.041	BB
2	14.36	2640748	56178	98.94%	3.015	BB
Total		2,669,087	57,059	100.00%		

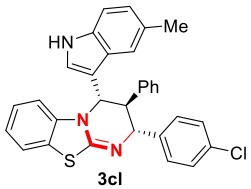


3cl

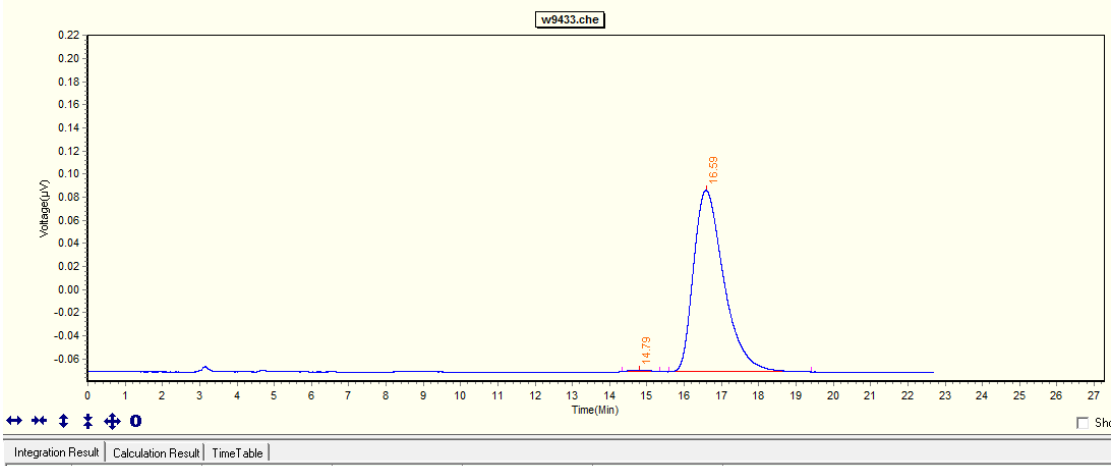


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	14.75	3871706	88216	48.99%	2.059	BV
2	16.52	4031829	82052	51.01%	3.025	VB
Total		7,903,535	170,268	100.00%		

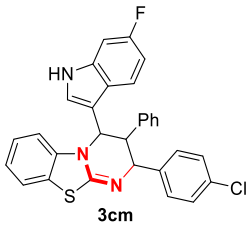


3cl

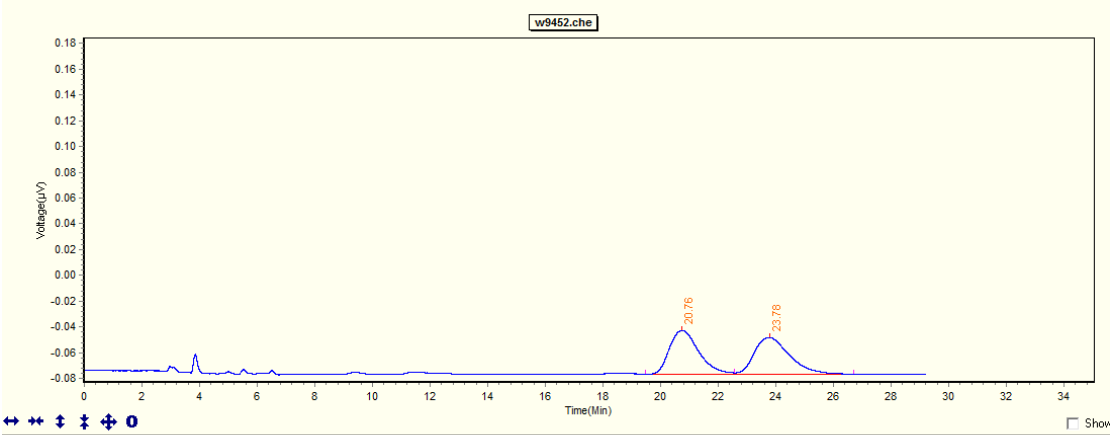


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	14.79	25513	733	0.57%	1.01	BB
2	16.59	4443968	78613	99.43%	3.822	BB
Total		4,469,481	79,346	100.00%		

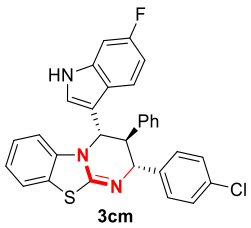


3cm

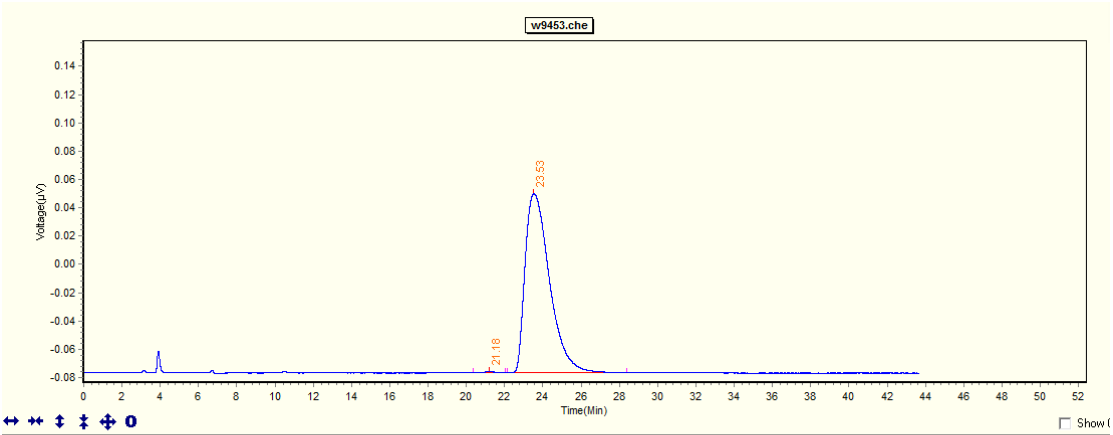


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	20.76	1190476	16956	49.83%	3.088	BV
2	23.78	1198814	14155	50.17%	4.141	VB
Total		2,389,290	31,111	100.00%		

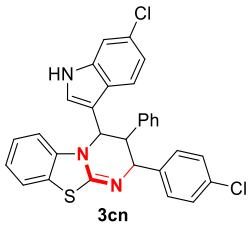


3cm

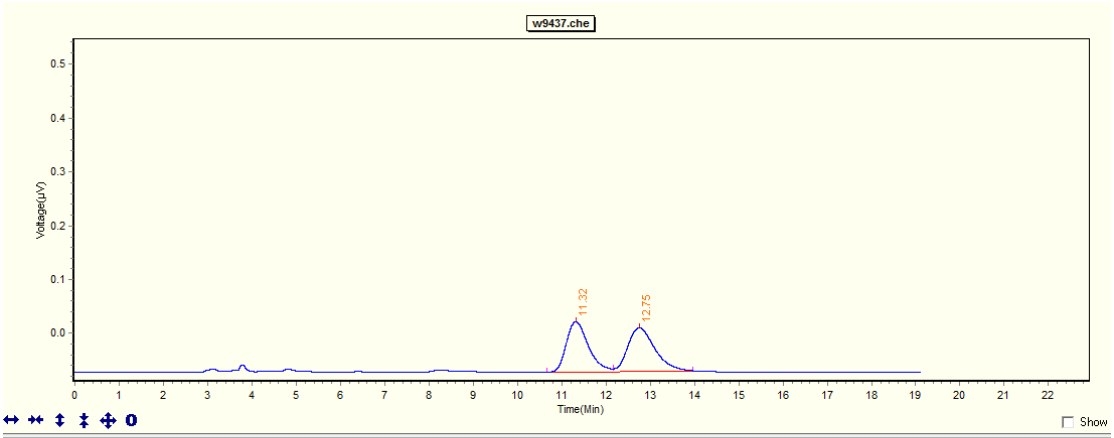


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	21.18	18541	367	0.33%	1.679	BB
2	23.53	5605547	63273	99.67%	6.243	BB
Total		5,624,088	63,640	100.00%		

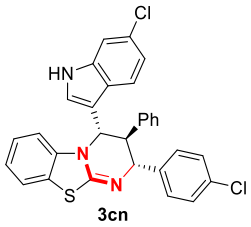


3cn

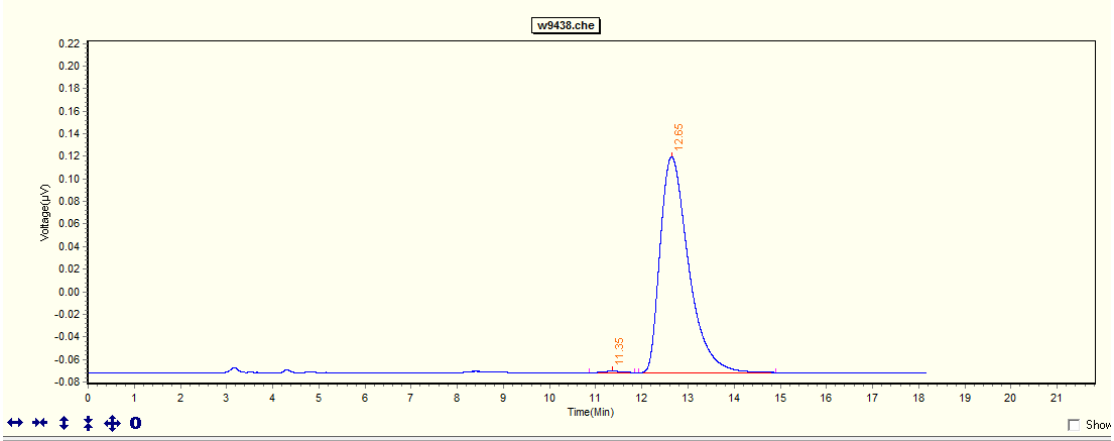


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.32	1601843	46495	48.42%	1.516	BV
2	12.75	1706327	40333	51.58%	1.791	VB
Total		3,308,170	86,828	100.00%		

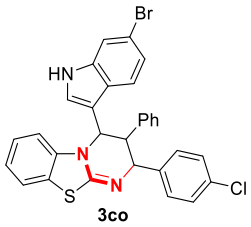


3cn

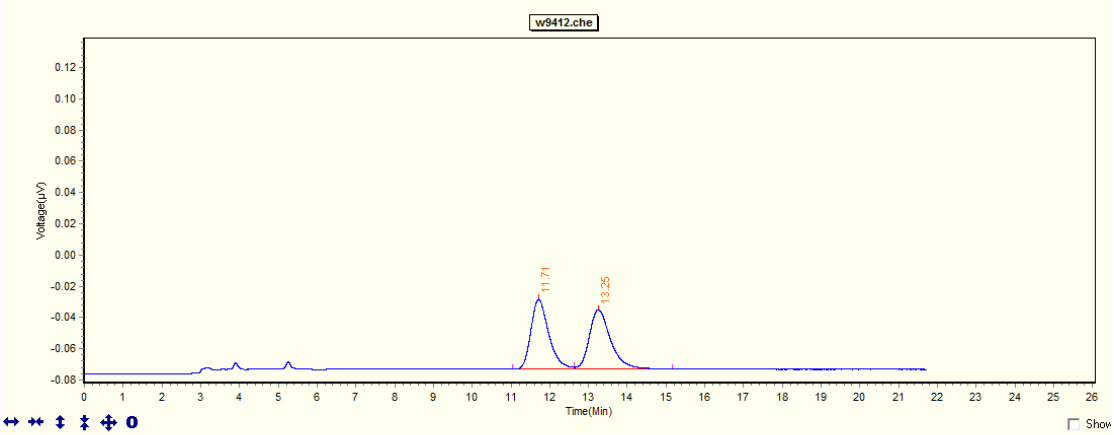


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.35	20938	683	0.51%	0.982	BB
2	12.65	4090830	95753	99.49%	2.972	BB
Total		4,111,768	96,436	100.00%		

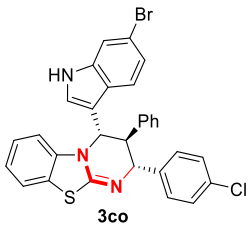


3co

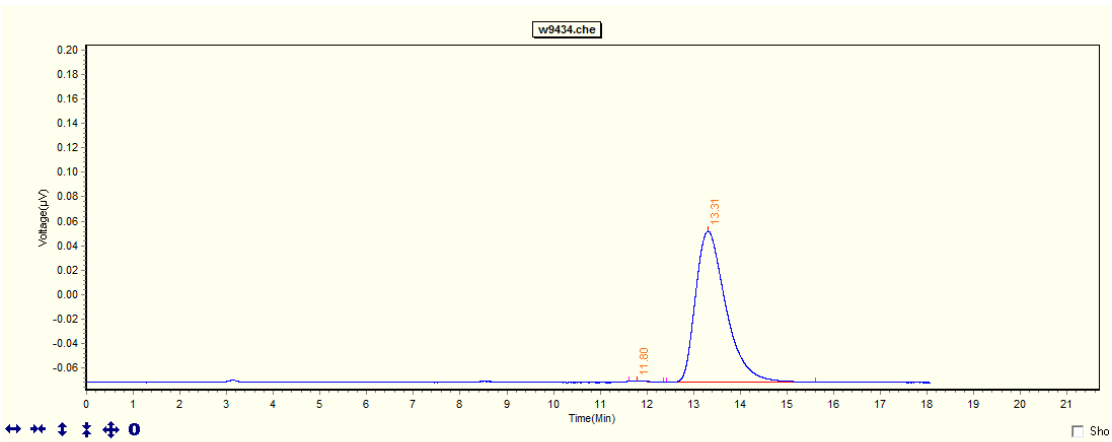


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.71	712353	22359	49.72%	1.592	BV
2	13.25	720275	19050	50.28%	2.53	VB
Total		1,432,628	41,409	100.00%		

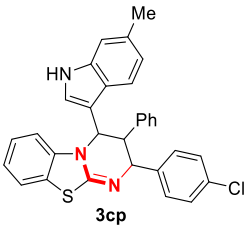


3co

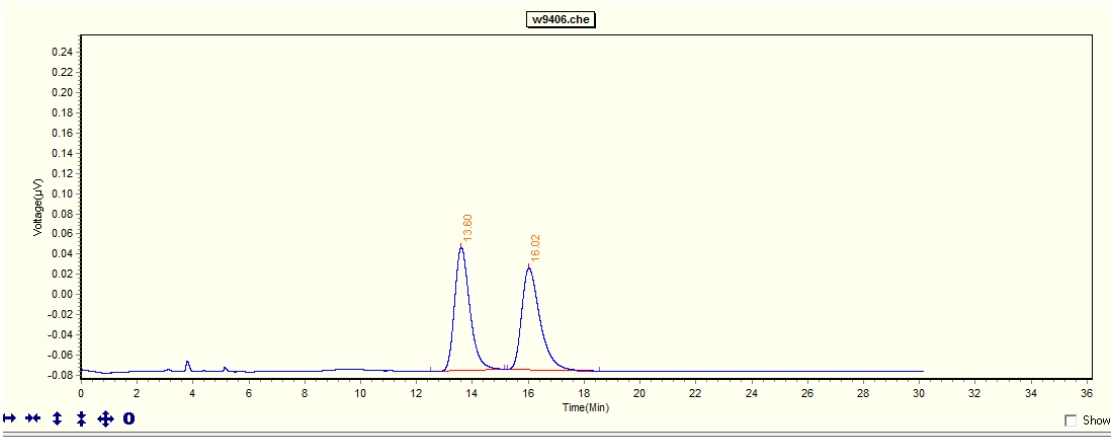


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.80	6920	331	0.25%	0.738	BB
2	13.31	2776046	61703	99.75%	3.192	BB
Total		2,782,966	62,034	100.00%		

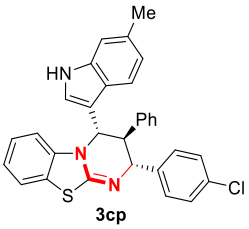


3cp

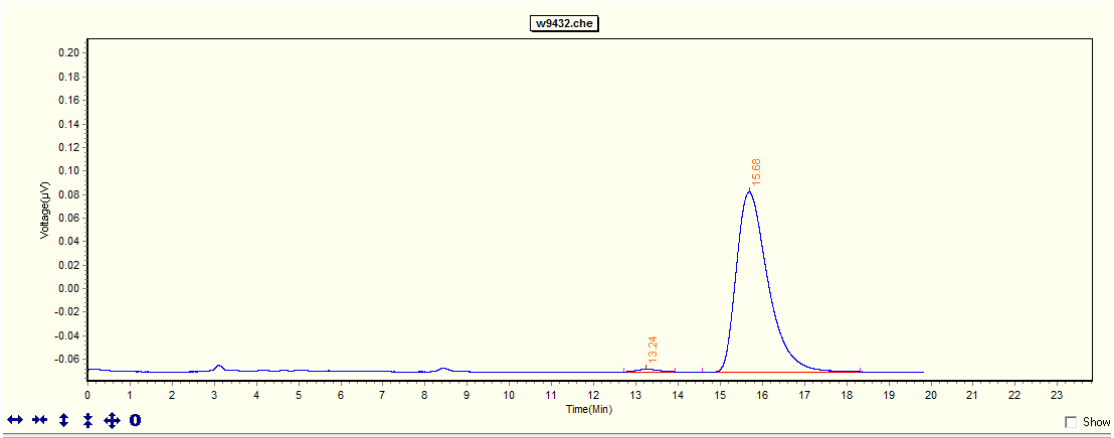


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	13.60	2278496	60810	50.04%	2.644	BB
2	16.02	2274453	50149	49.96%	3.297	BB
Total		4,552,949	110,959	100.00%		

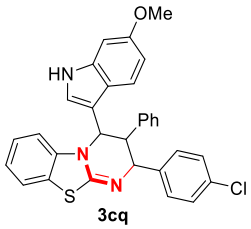


3cp

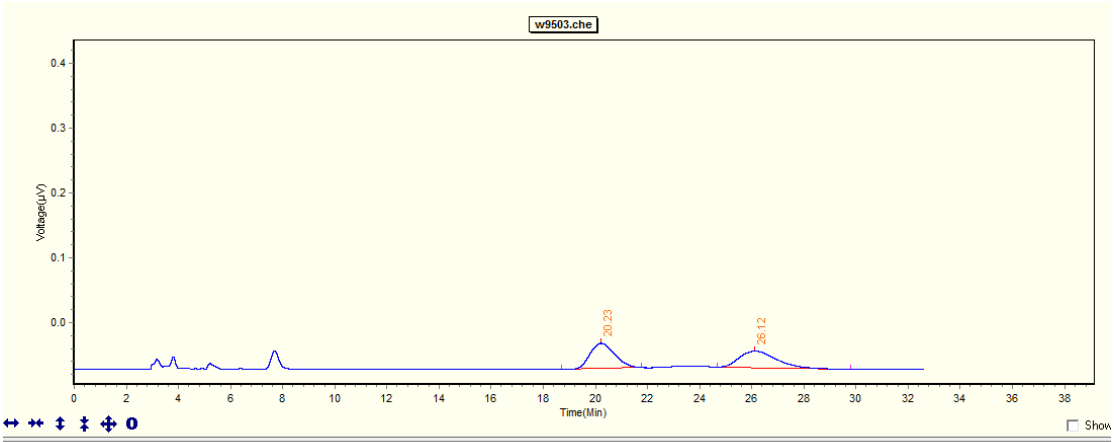


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	13.24	38396	1101	0.96%	1.216	BB
2	15.68	3972772	76436	99.04%	3.745	BB
Total		4,011,168	77,537	100.00%		

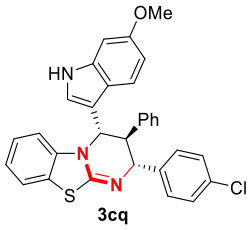


3cq

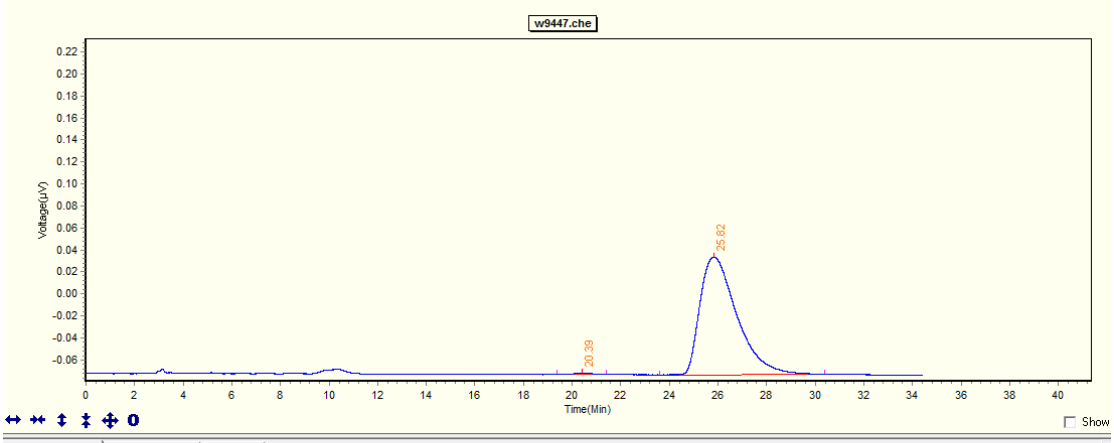


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	20.23	1274787	19398	50.71%	3.056	BB
2	26.12	1239170	12705	49.29%	5.093	BB
Total		2,513,957	32,103	100.00%		

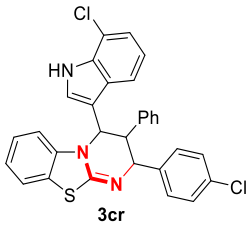


3cq

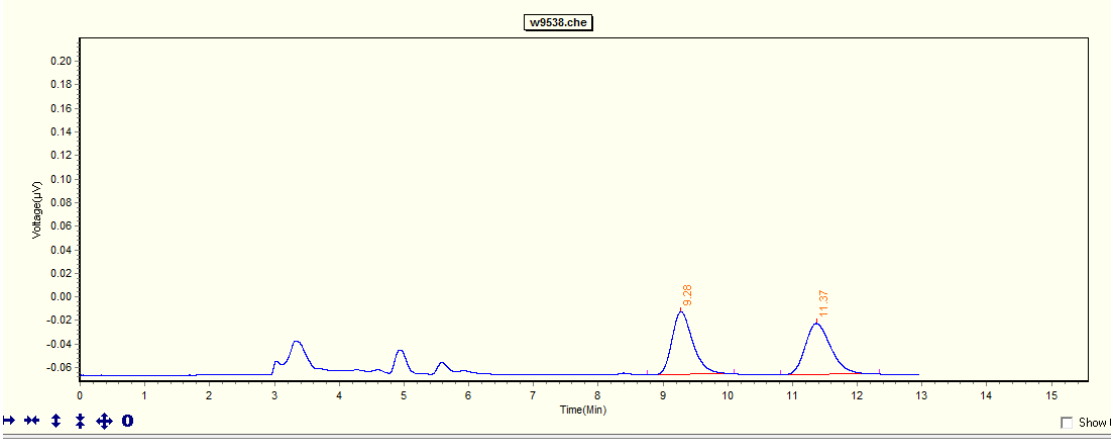


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	20.39	31117	545	0.55%	2.028	BB
2	25.82	5611315	53359	99.45%	6.789	BB
Total		5,642,432	53,904	100.00%		

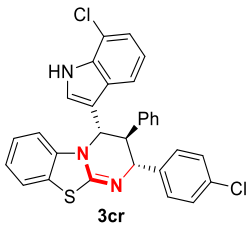


3cr

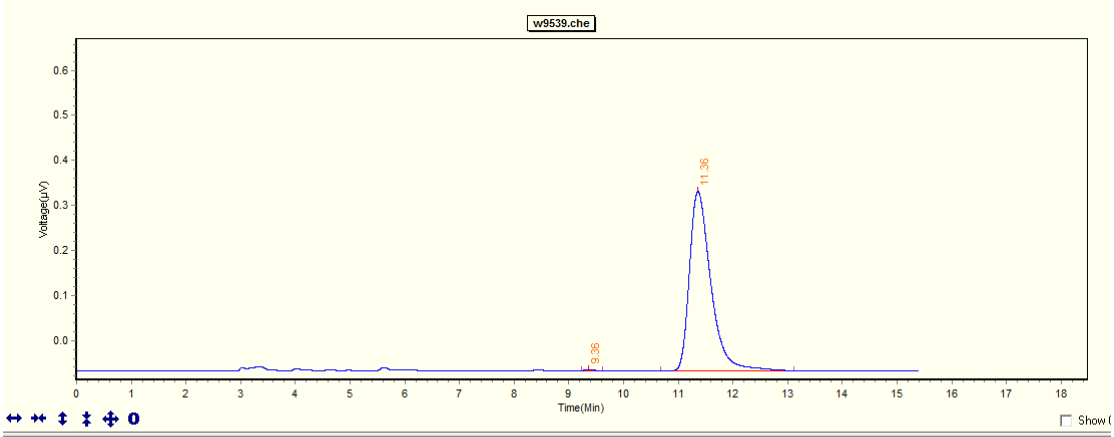


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.28	598266	26639	50.00%	1.34	BB
2	11.37	598304	21671	50.00%	1.528	BB
Total		1,196,570	48,310	100.00%		

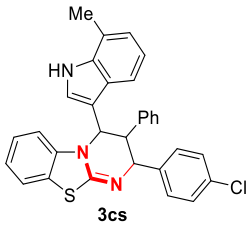


3cr

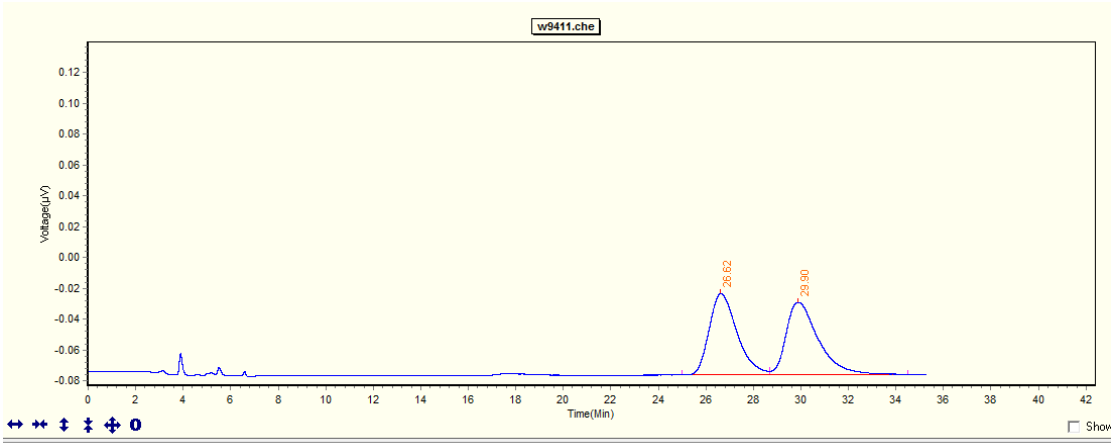


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	9.36	5026	368	0.09%	0.388	BB
2	11.36	5382653	198867	99.91%	2.443	BB
Total		5,387,679	199,235	100.00%		

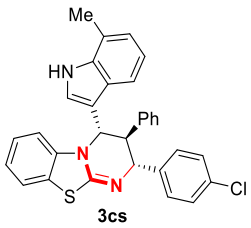


3cs

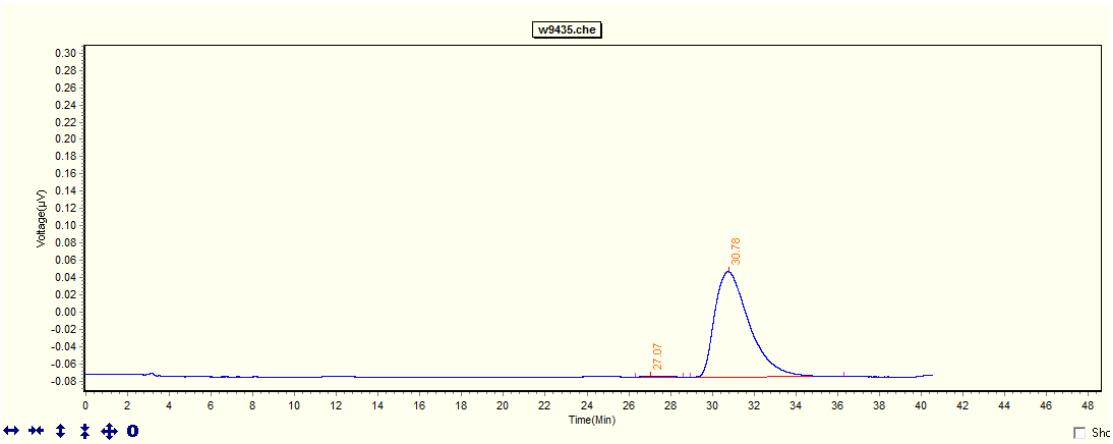


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	26.62	2150247	26376	49.33%	3.693	BV
2	29.90	2208744	23491	50.67%	5.813	VB
Total		4,358,991	49,867	100.00%		

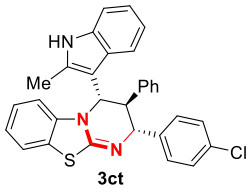


3cs

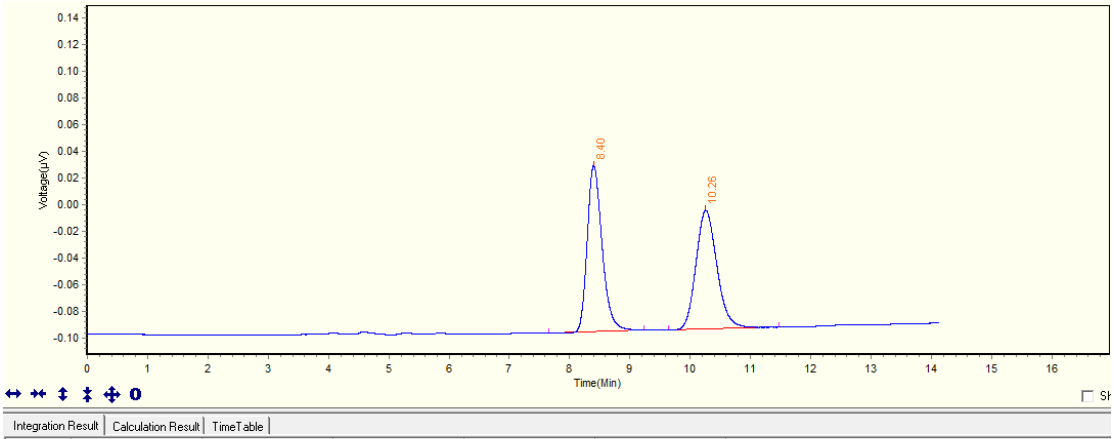


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	27.07	19776	268	0.28%	2.29	BB
2	30.78	6994835	60873	99.72%	7.358	BB
Total		7,014,611	61,141	100.00%		

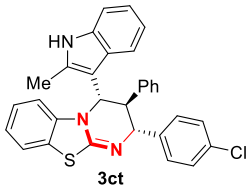


3ct

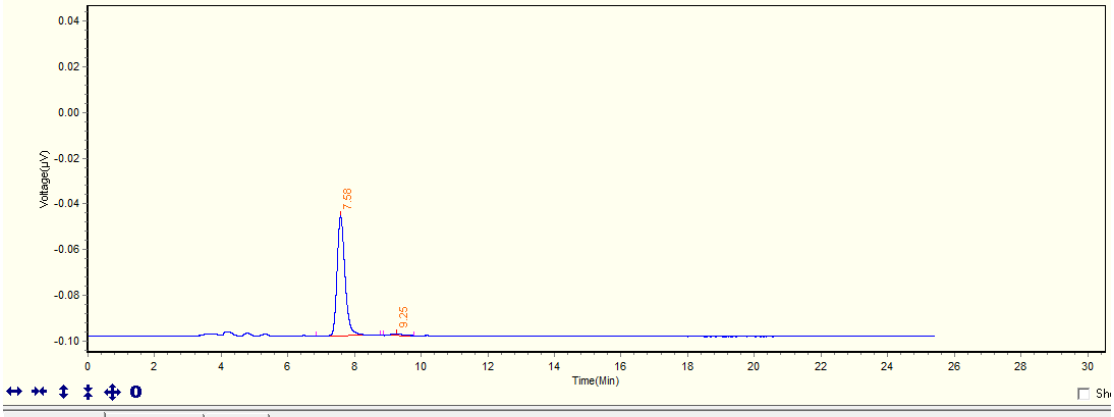


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	8.40	1069875	62196	49.76%	1.578	BB
2	10.26	1080269	44529	50.24%	1.833	BB
Total		2,150,144	106,725	100.00%		

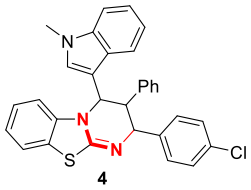


3ct

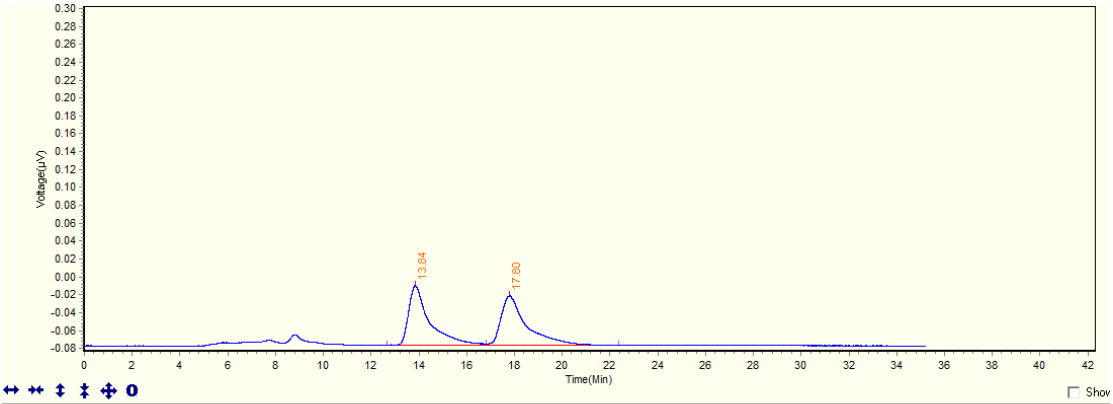


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.58	439079	26264	97.90%	1.926	BB
2	9.25	9413	445	2.10%	0.917	BB
Total		448,492	26,709	100.00%		

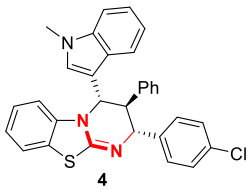


4

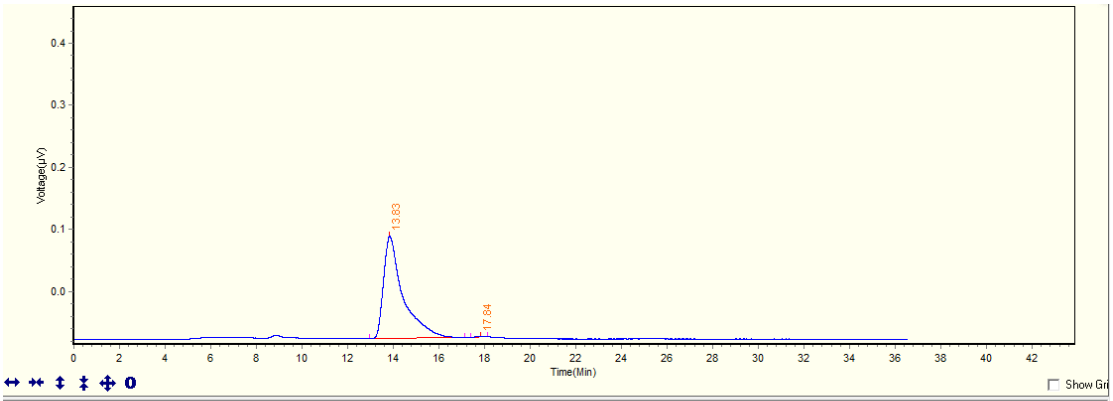


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	13.84	1998399	33016	49.50%	4.15	BV
2	17.80	2038543	27486	50.50%	5.547	VB
Total		4,036,942	60,502	100.00%		



4

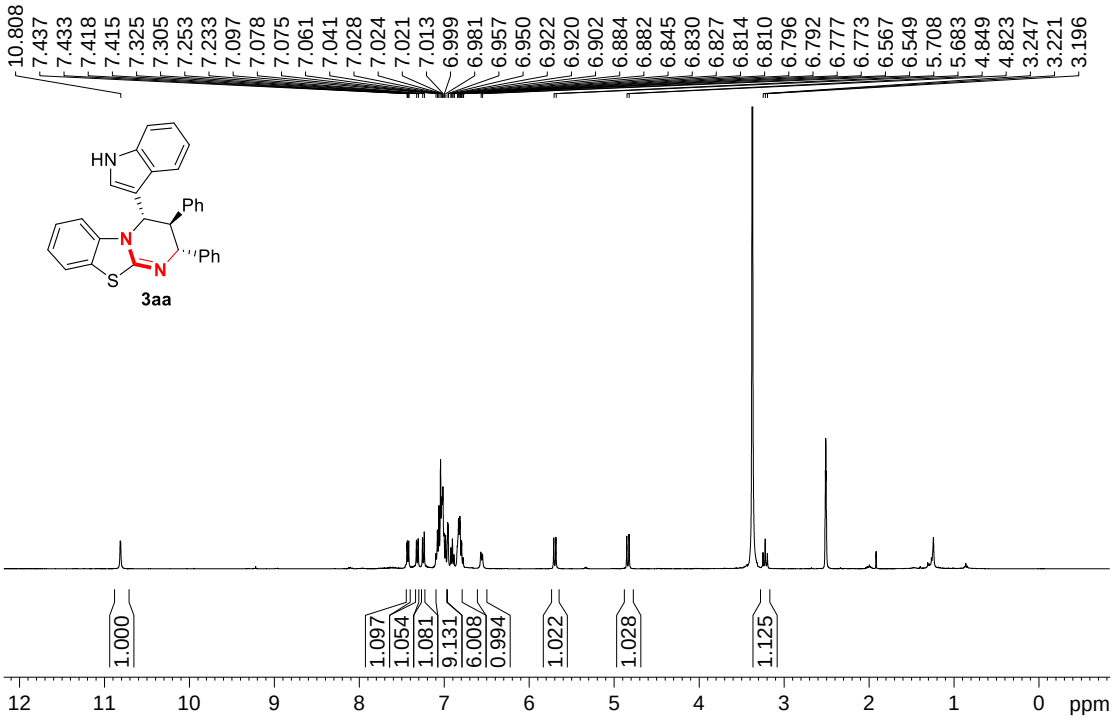


Integration Result | Calculation Result | TimeTable

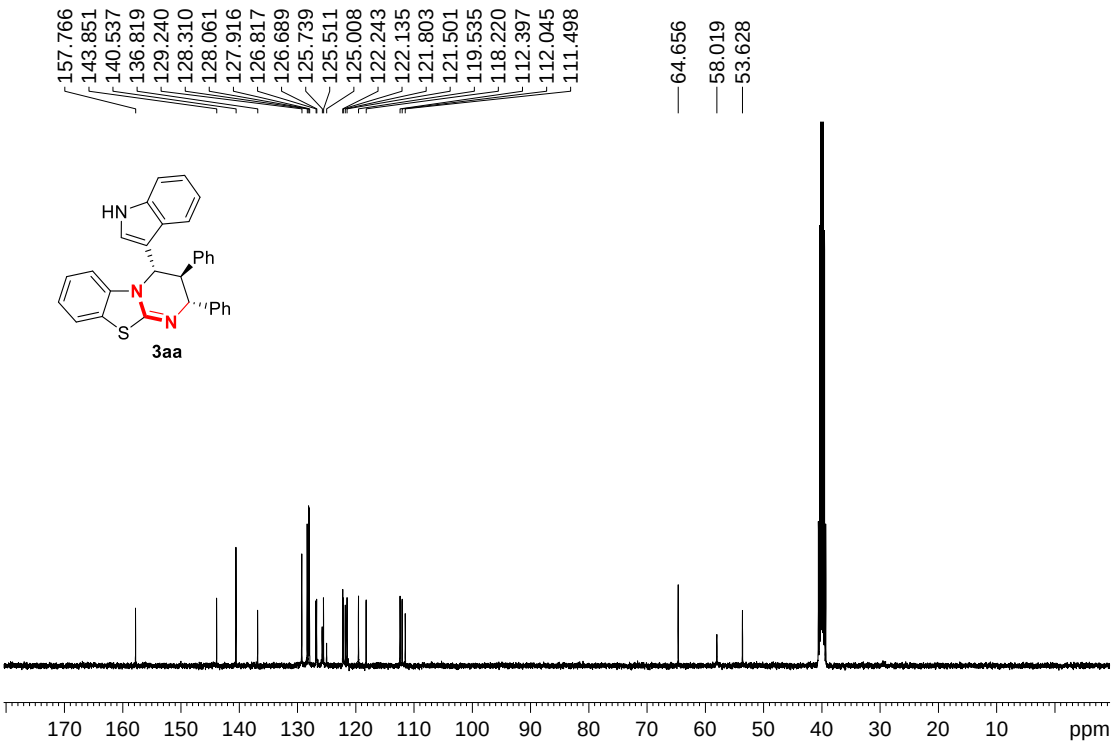
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	13.83	4884486	82280	99.67%	4.171	BB
2	17.84	16388	676	0.33%	0.746	BB
Total		4,900,874	82,956	100.00%		

7. NMR Spectra of compounds.

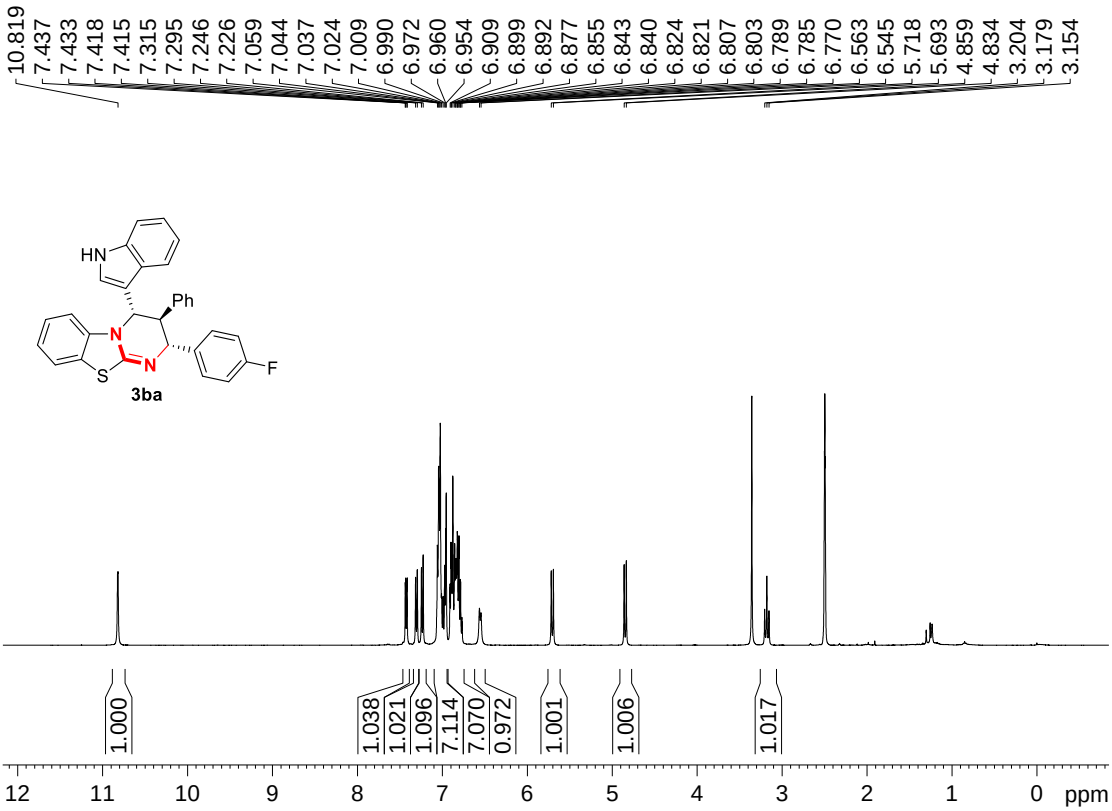
^{1}H NMR spectrum of compound **3aa** ($(CD_3)_2SO$, 400 MHz)



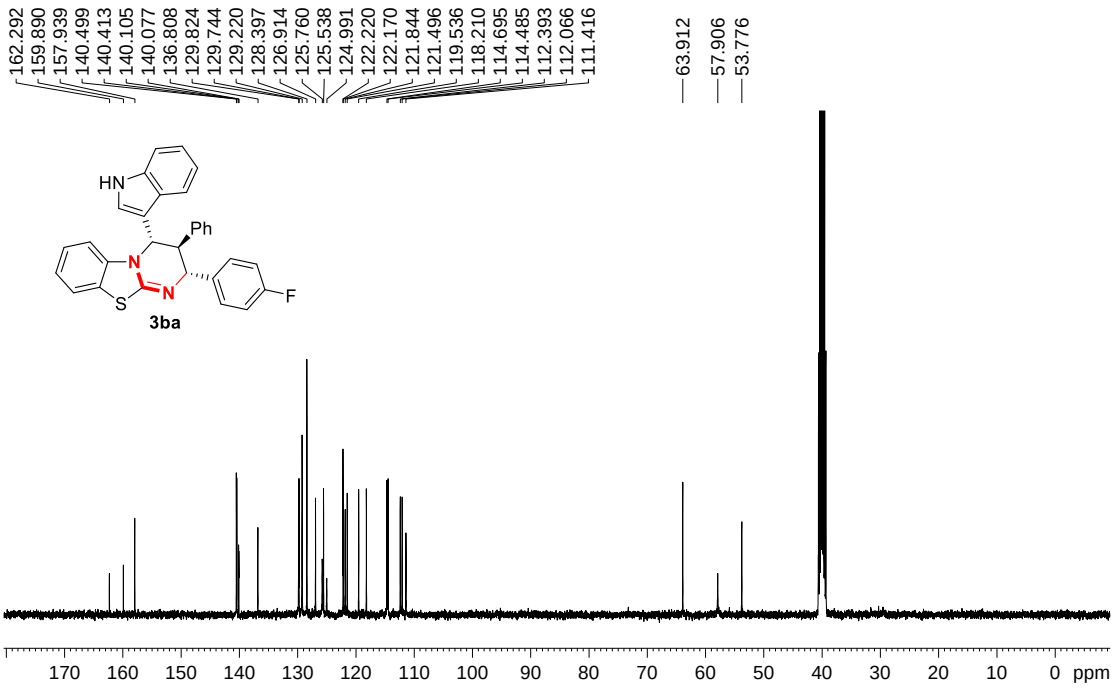
^{13}C NMR spectrum of compound **3aa** ($(CD_3)_2SO$, 100 MHz)



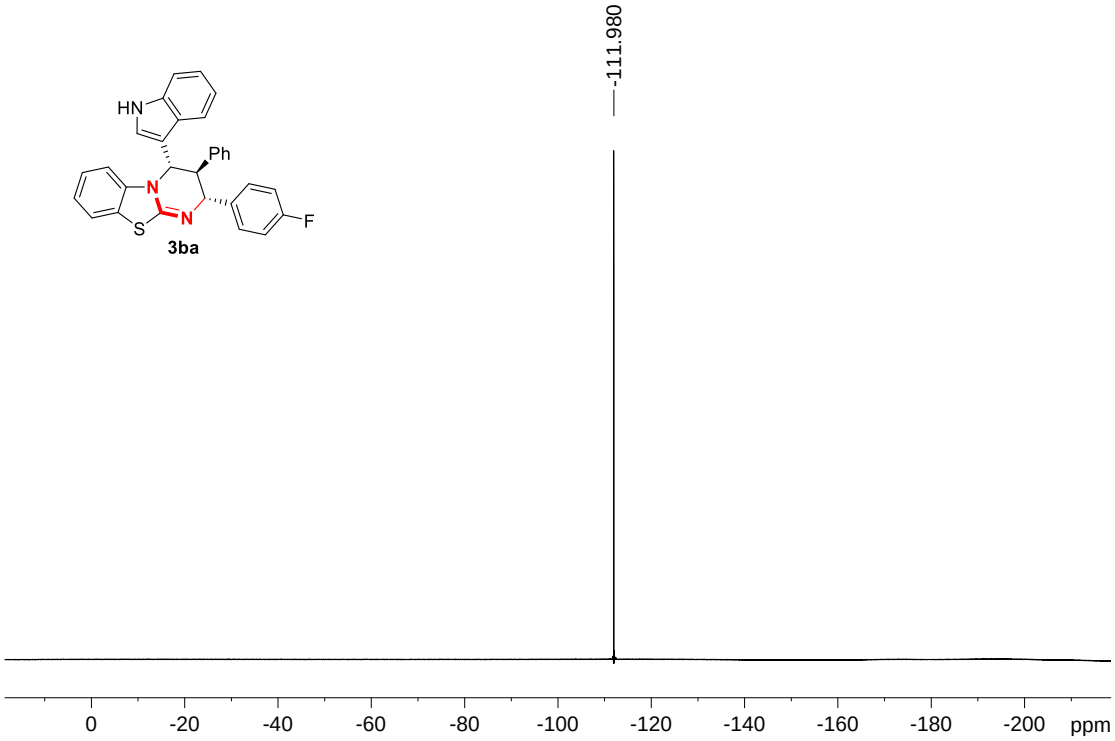
^{1}H NMR spectrum of compound **3ba** ($(CD_3)_2SO$, 400 MHz)



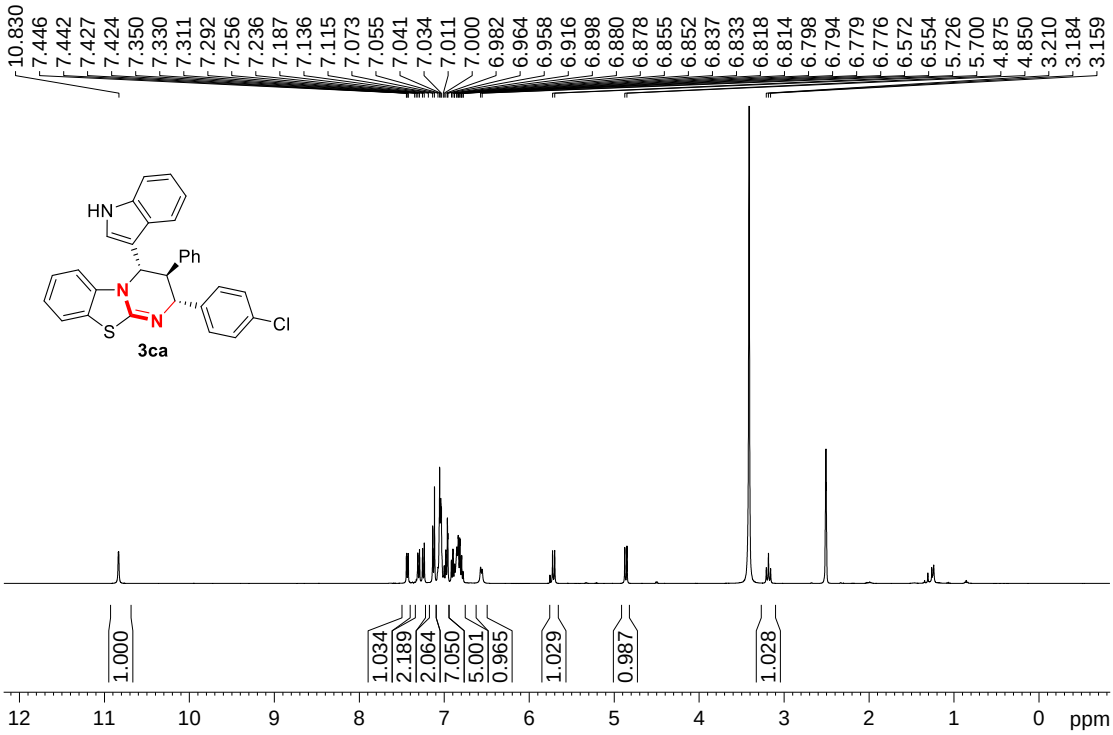
^{13}C NMR spectrum of compound **3ba** ($(CD_3)_2SO$, 100 MHz)



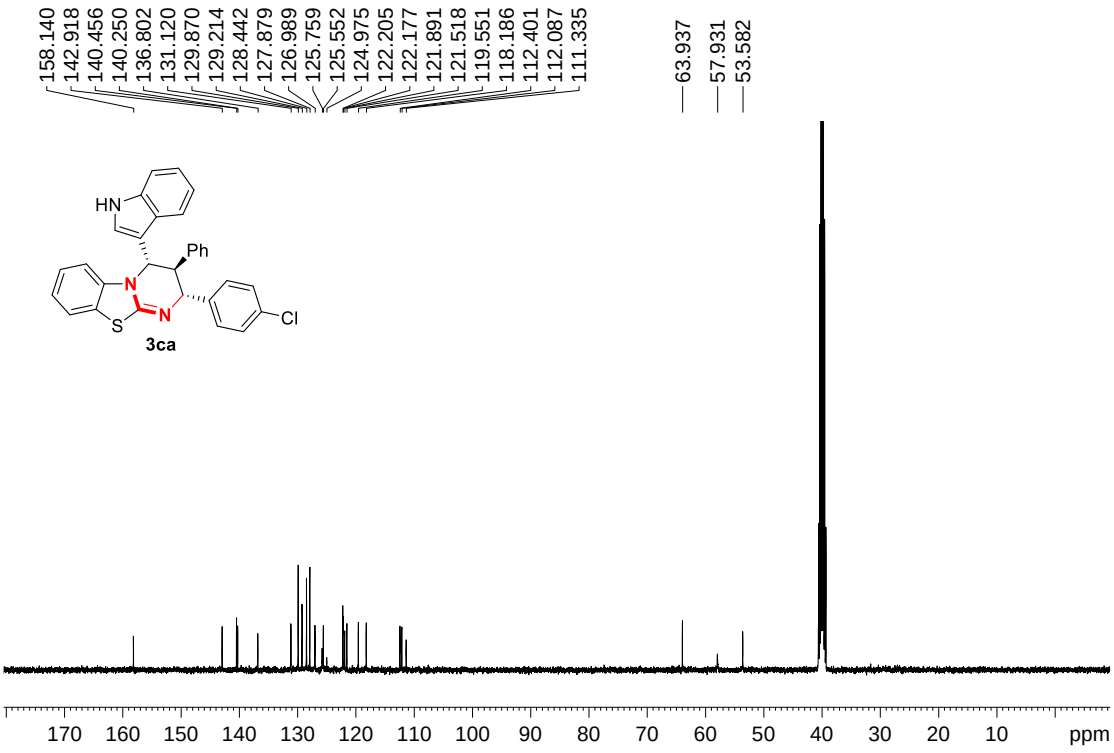
^{19}F NMR spectrum of compound **3ba** ($(CD_3)_2SO$, 376 MHz)



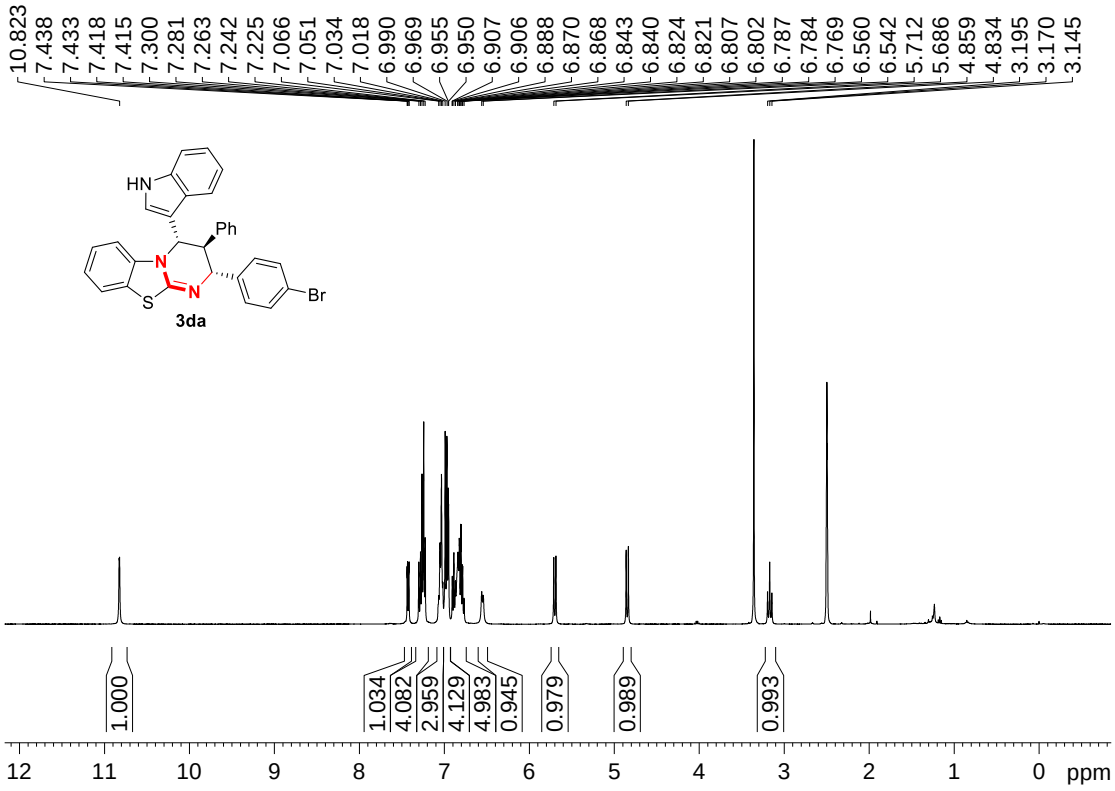
^{1}H NMR spectrum of compound **3ca** ($(CD_3)_2SO$, 400 MHz)



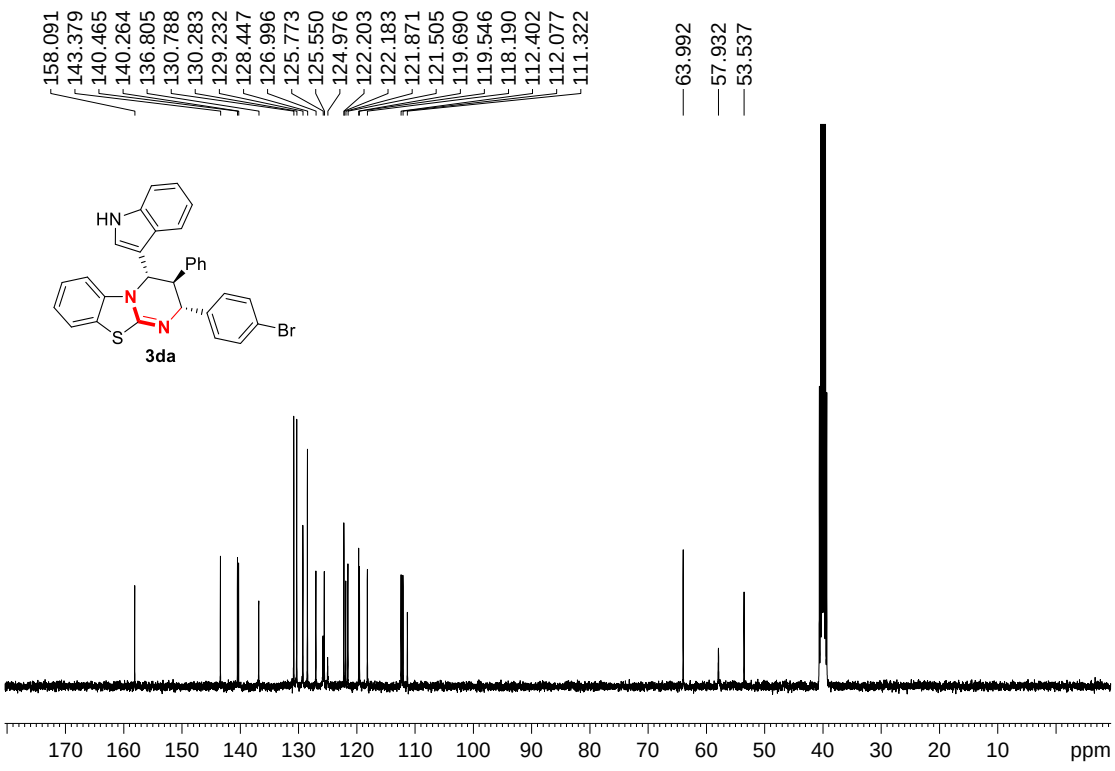
^{13}C NMR spectrum of compound **3ca** ($(CD_3)_2SO$, 100 MHz)



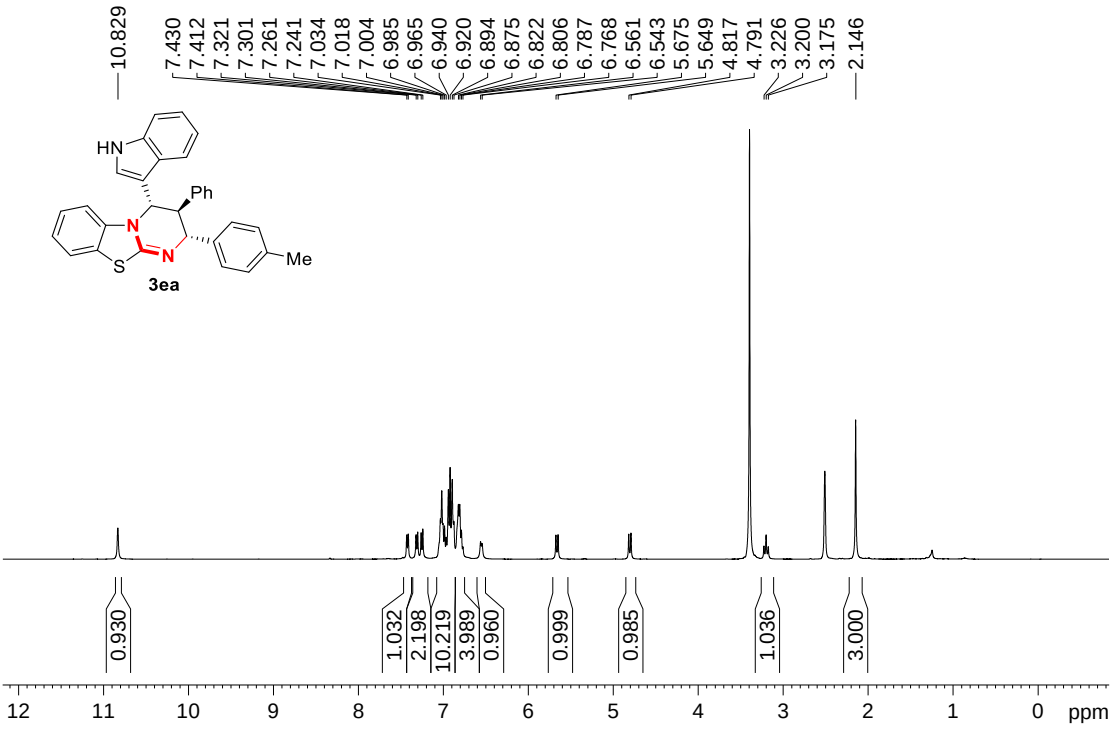
^{1}H NMR spectrum of compound **3da** ($(CD_3)_2SO$, 400 MHz)



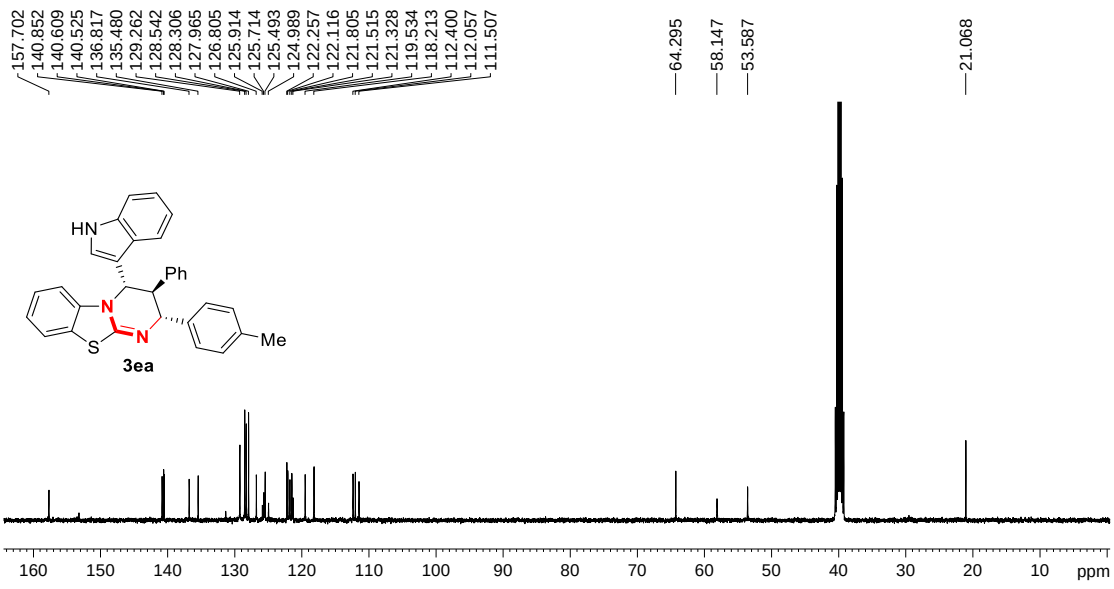
^{13}C NMR spectrum of compound **3da** ($(CD_3)_2SO$, 100 MHz)



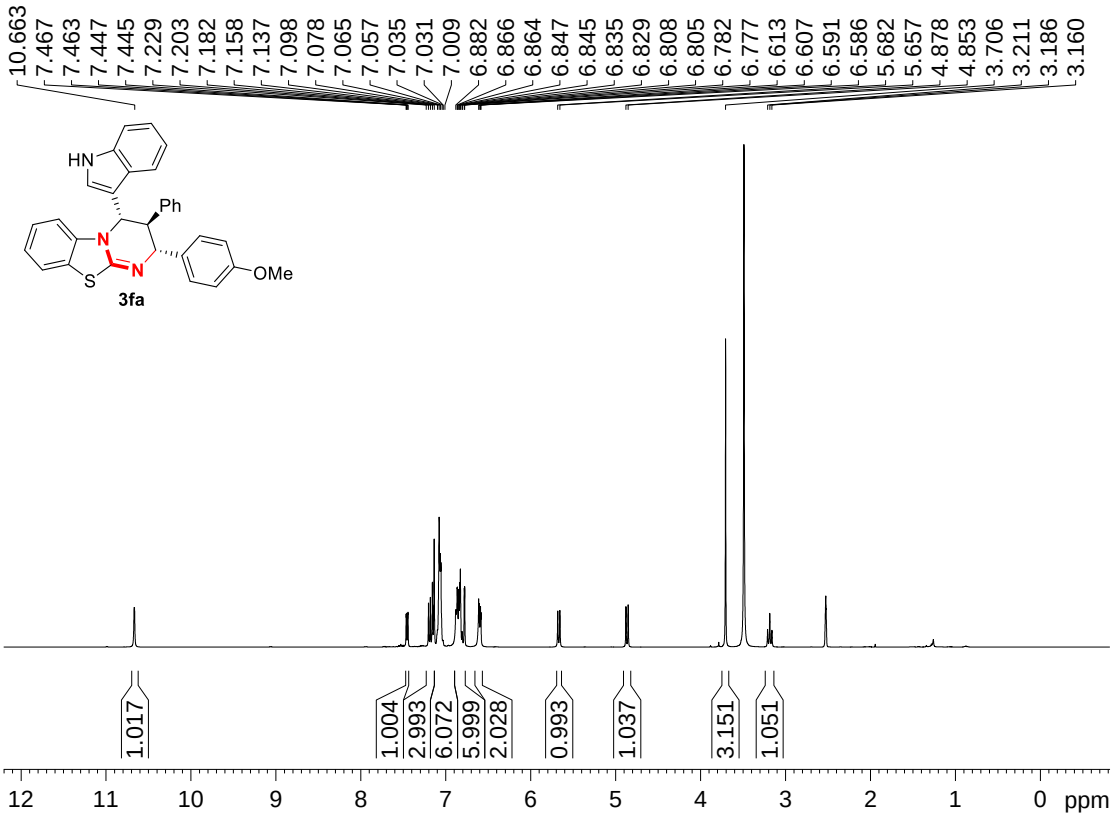
^{1}H NMR spectrum of compound **3ea** ($(CD_3)_2SO$, 400 MHz)



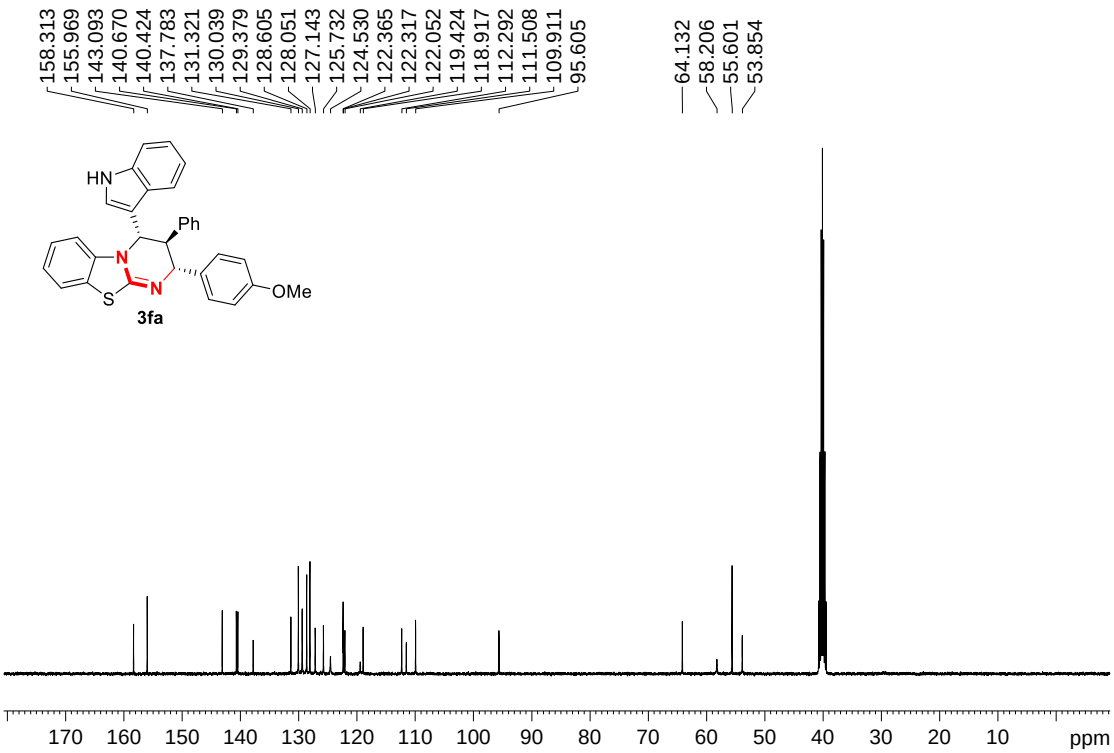
^{13}C NMR spectrum of compound **3ea** ($(CD_3)_2SO$, 100 MHz)



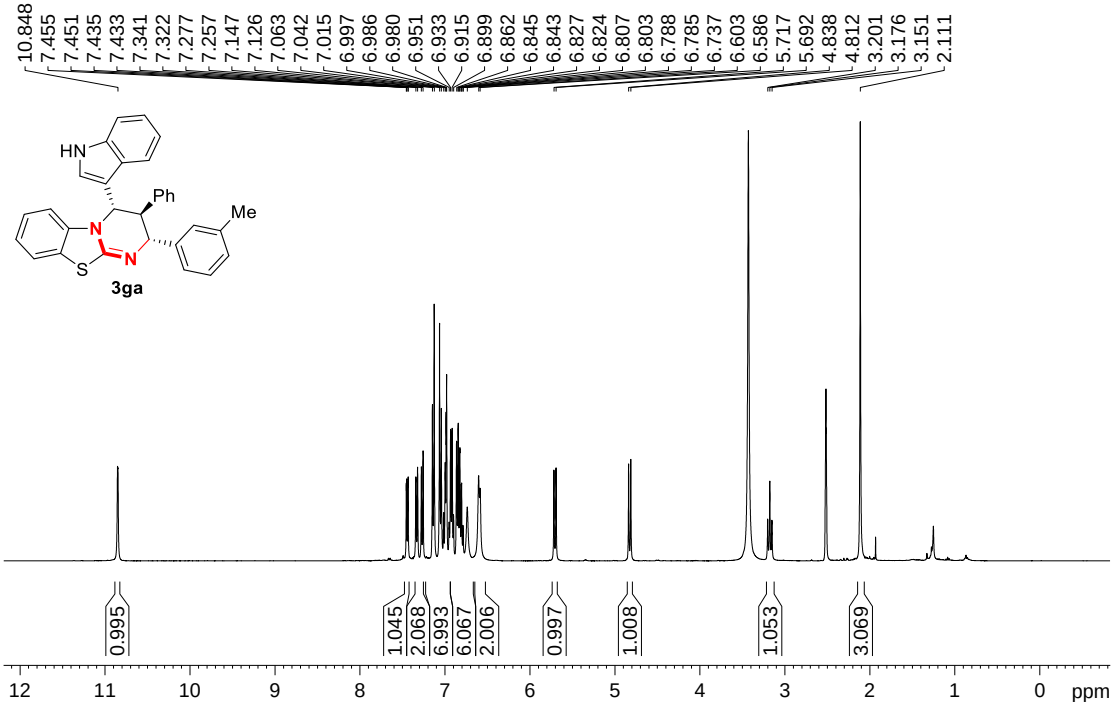
^{1}H NMR spectrum of compound **3fa** ($(CD_3)_2SO$, 400 MHz)



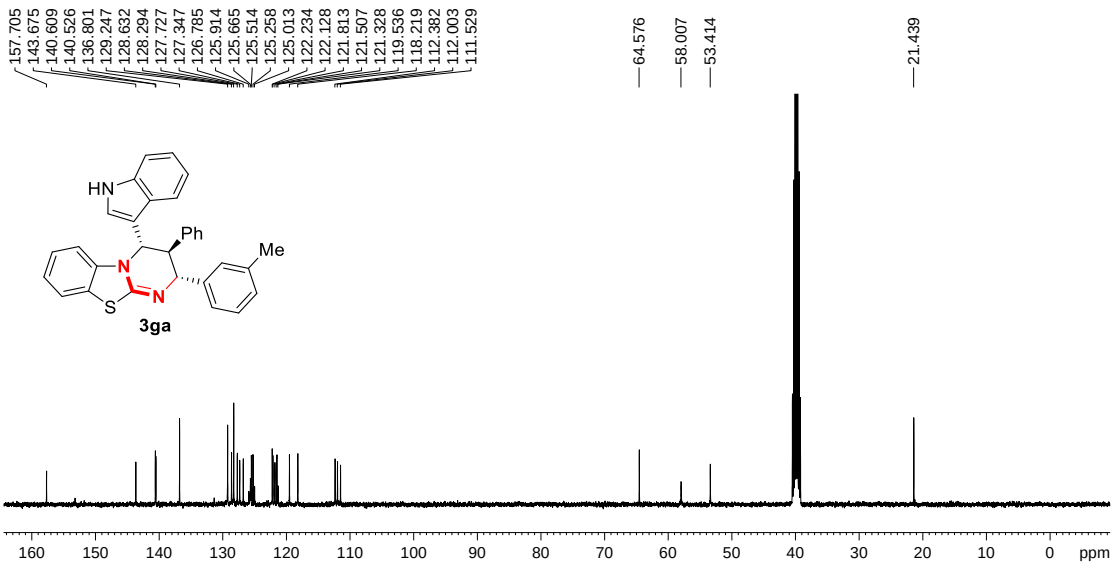
^{13}C NMR spectrum of compound **3fa** ($(CD_3)_2SO$, 100 MHz)



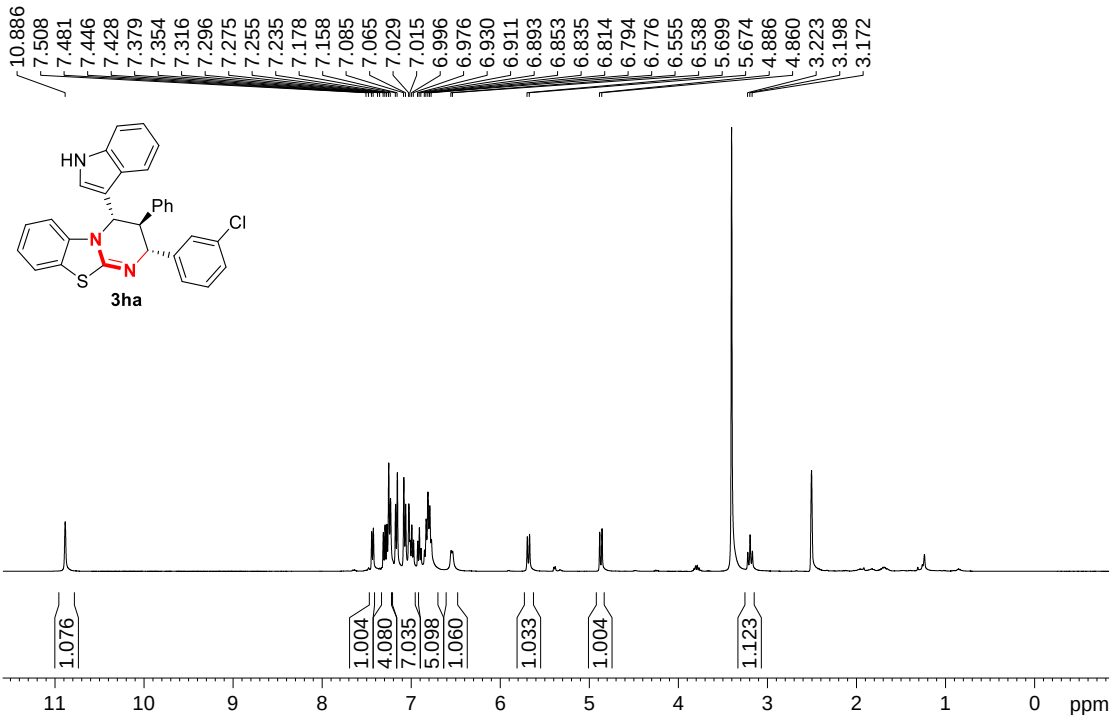
^{1}H NMR spectrum of compound **3ga** ($(CD_3)_2SO$, 400 MHz)



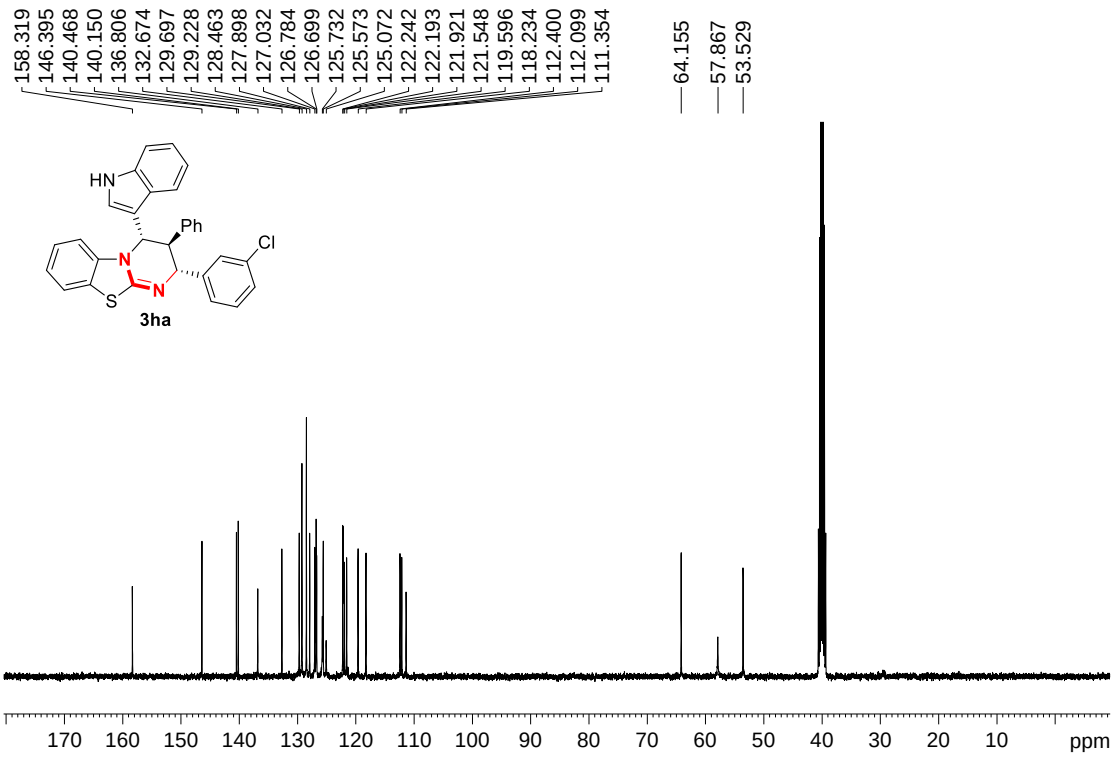
^{13}C NMR spectrum of compound **3ga** ($(CD_3)_2SO$, 100 MHz)



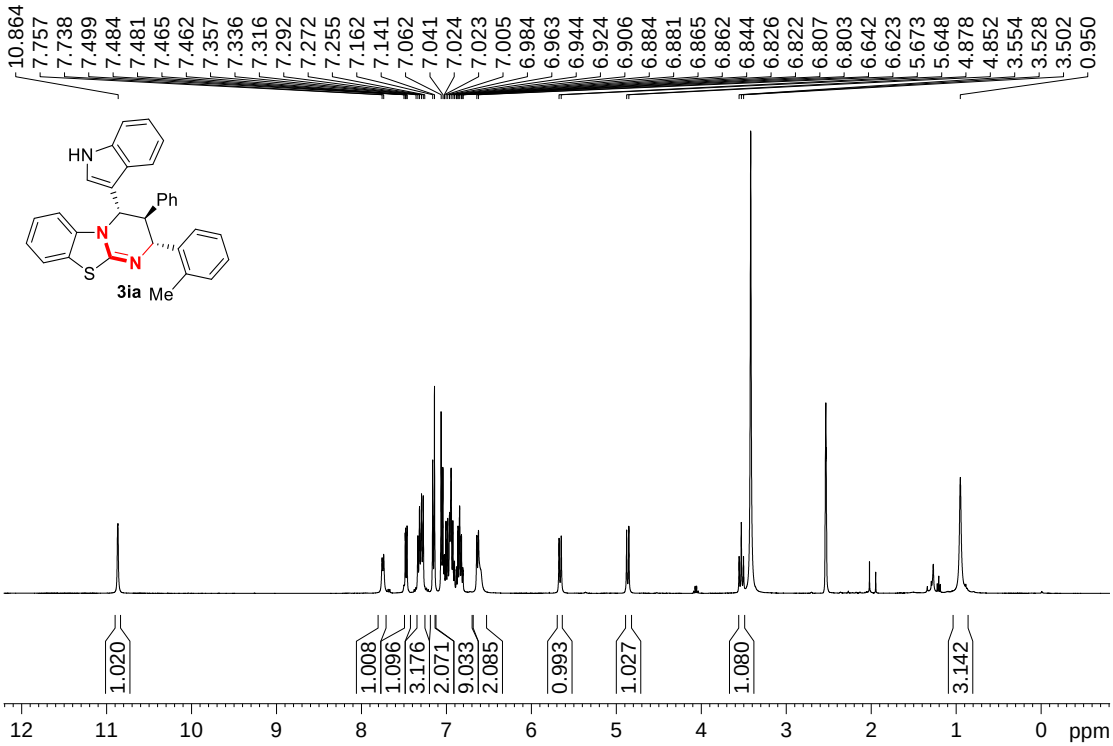
^{1}H NMR spectrum of compound **3ha** ($(CD_3)_2SO$, 400 MHz)



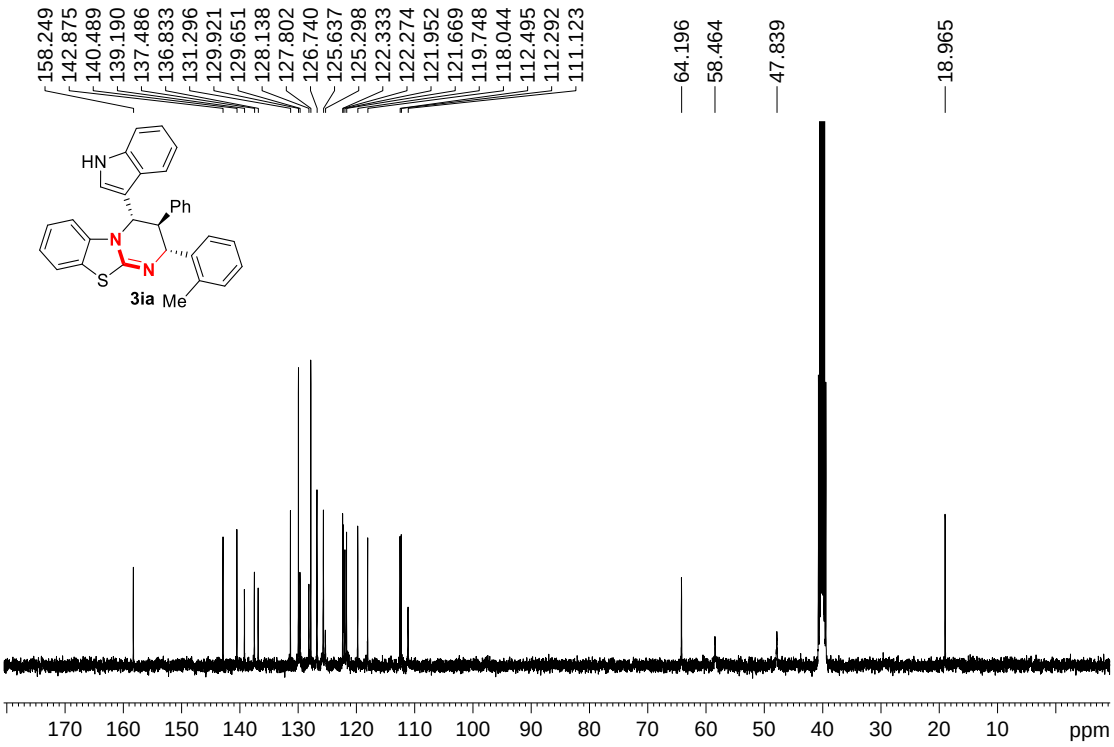
^{13}C NMR spectrum of compound **3ha** ($(CD_3)_2SO$, 100 MHz)



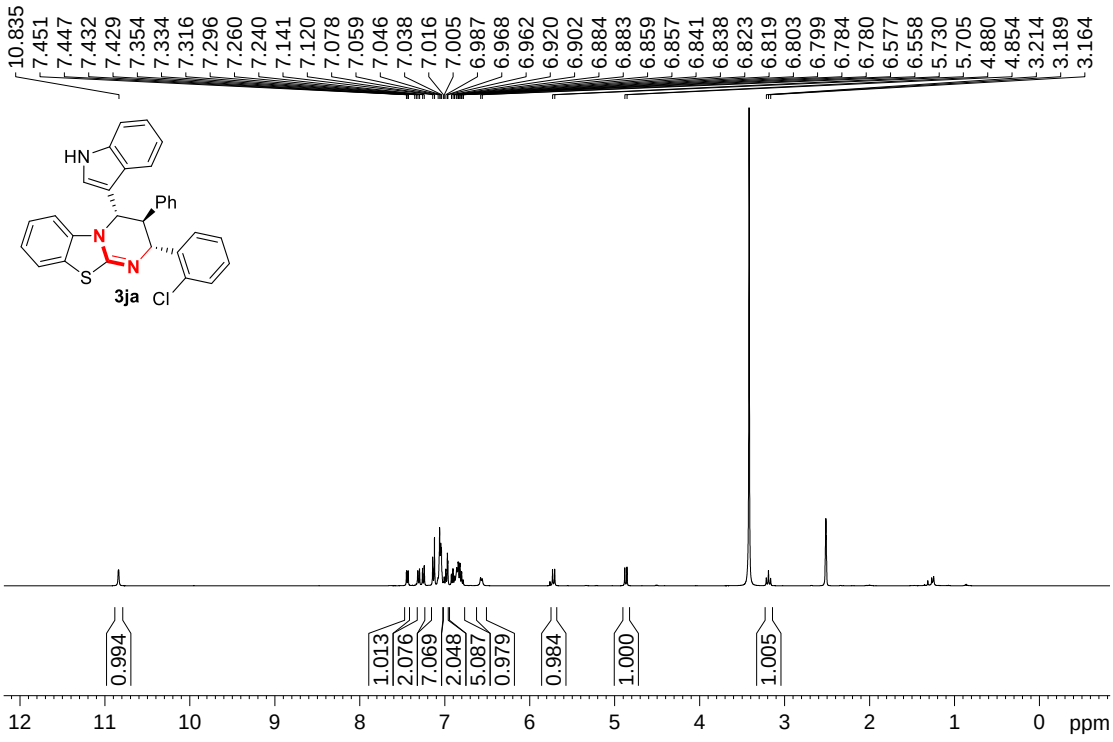
^{1}H NMR spectrum of compound **3ia** ($(CD_3)_2SO$, 400 MHz)



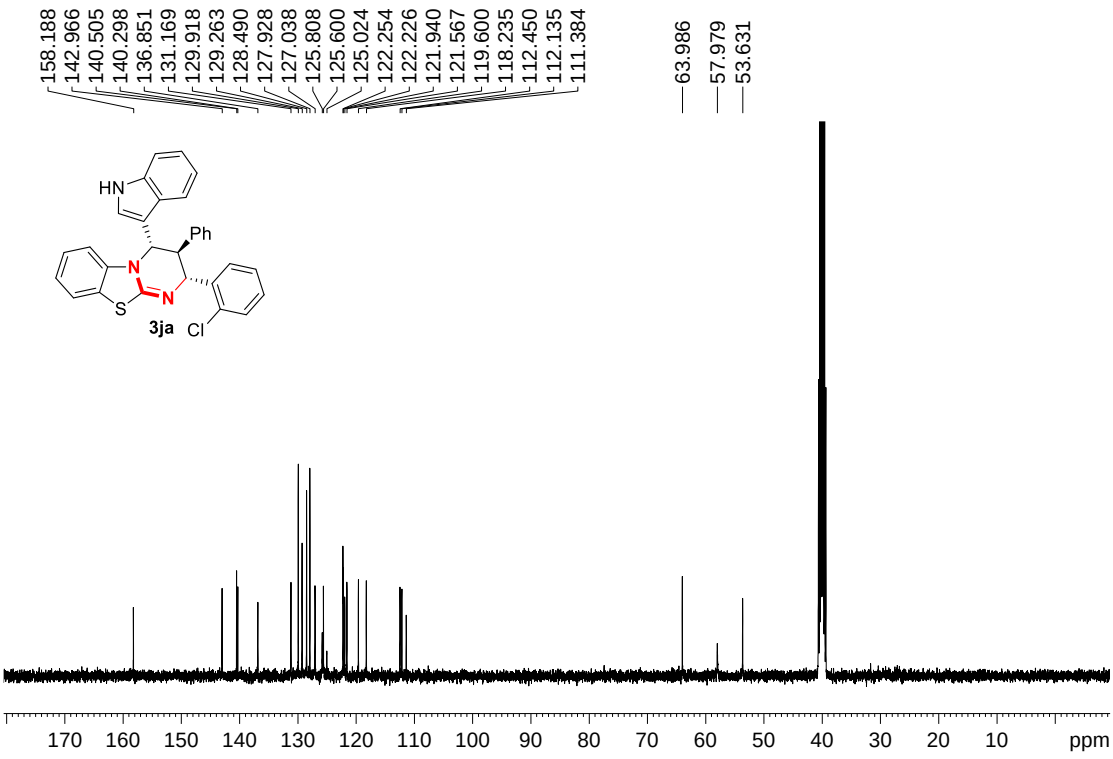
^{13}C NMR spectrum of compound **3ia** ($(CD_3)_2SO$, 100 MHz)



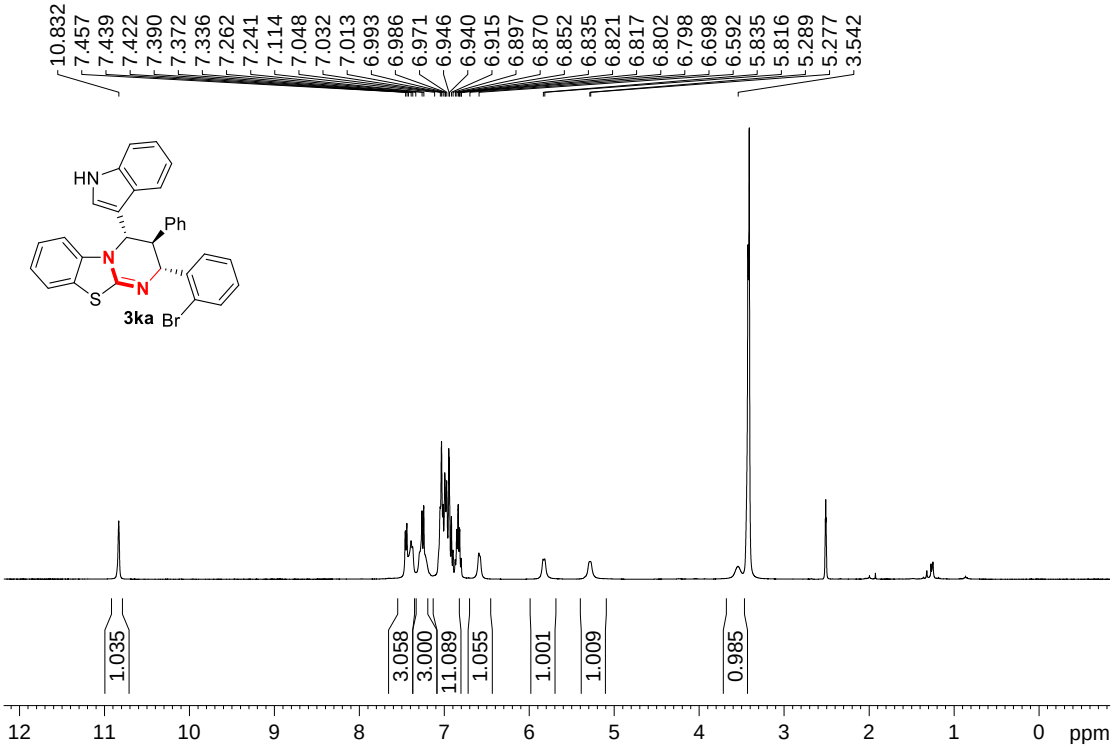
^{1}H NMR spectrum of compound **3ja** ($(CD_3)_2SO$, 400 MHz)



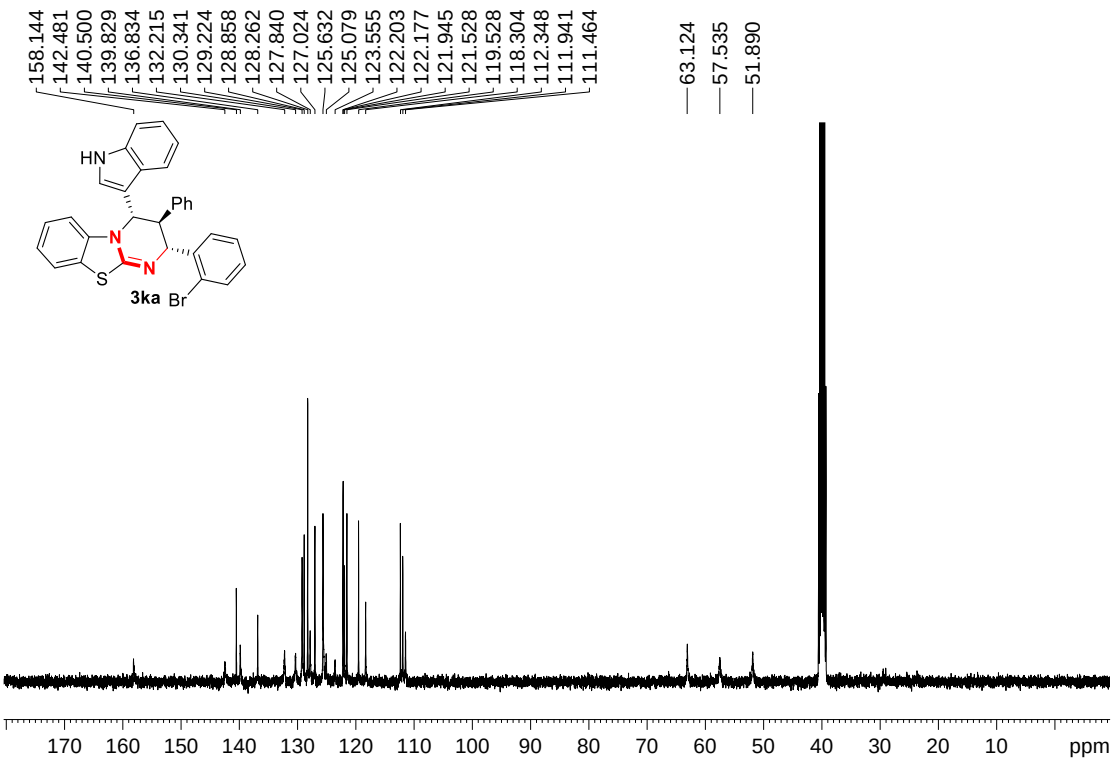
^{13}C NMR spectrum of compound **3ja** ($(CD_3)_2SO$, 100 MHz)



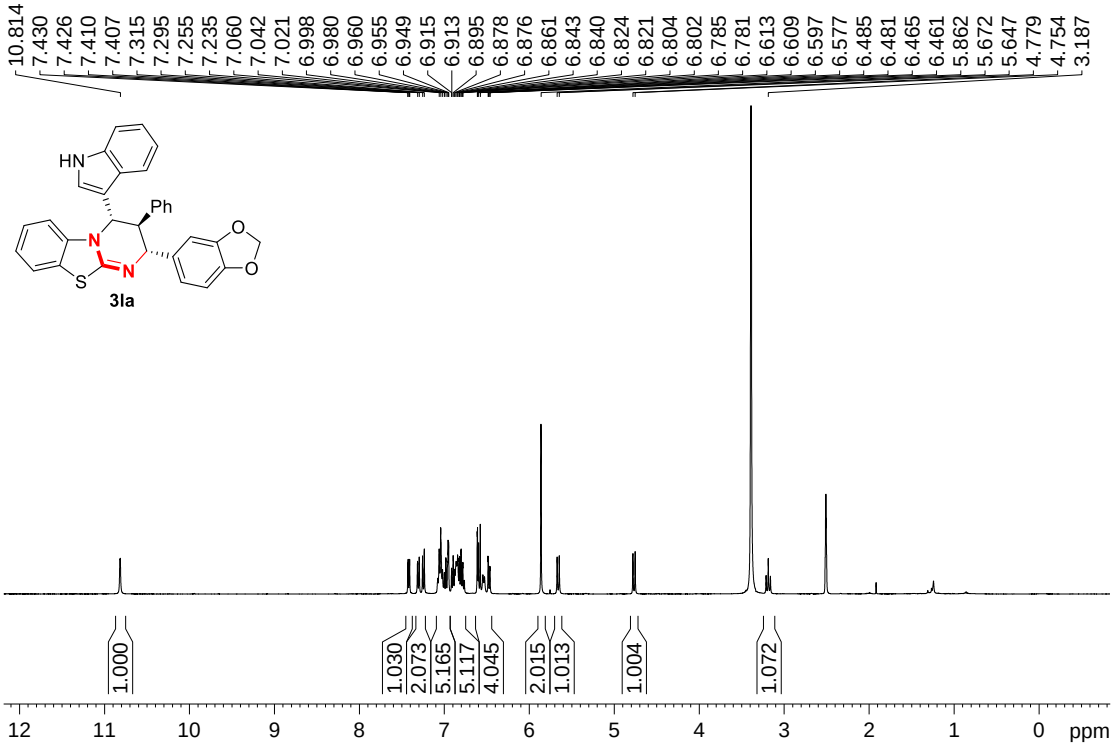
^{1}H NMR spectrum of compound **3ka** ($(CD_3)_2SO$, 400 MHz)



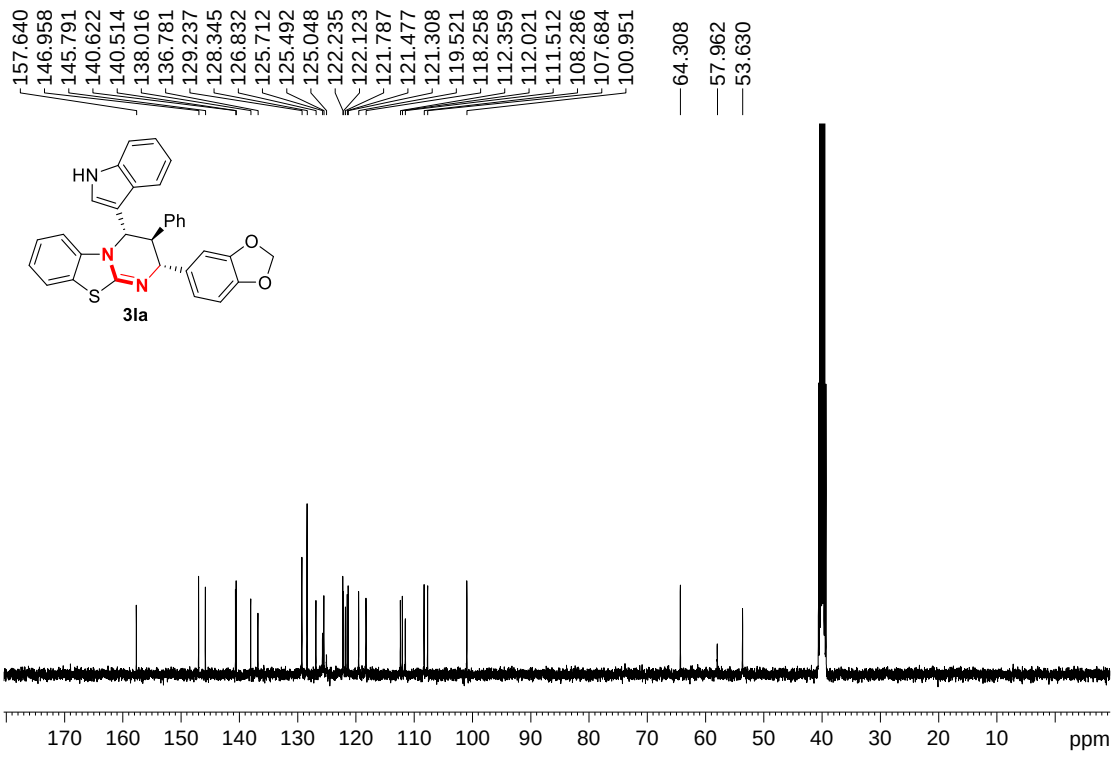
^{13}C NMR spectrum of compound **3ka** ($(CD_3)_2SO$, 100 MHz)



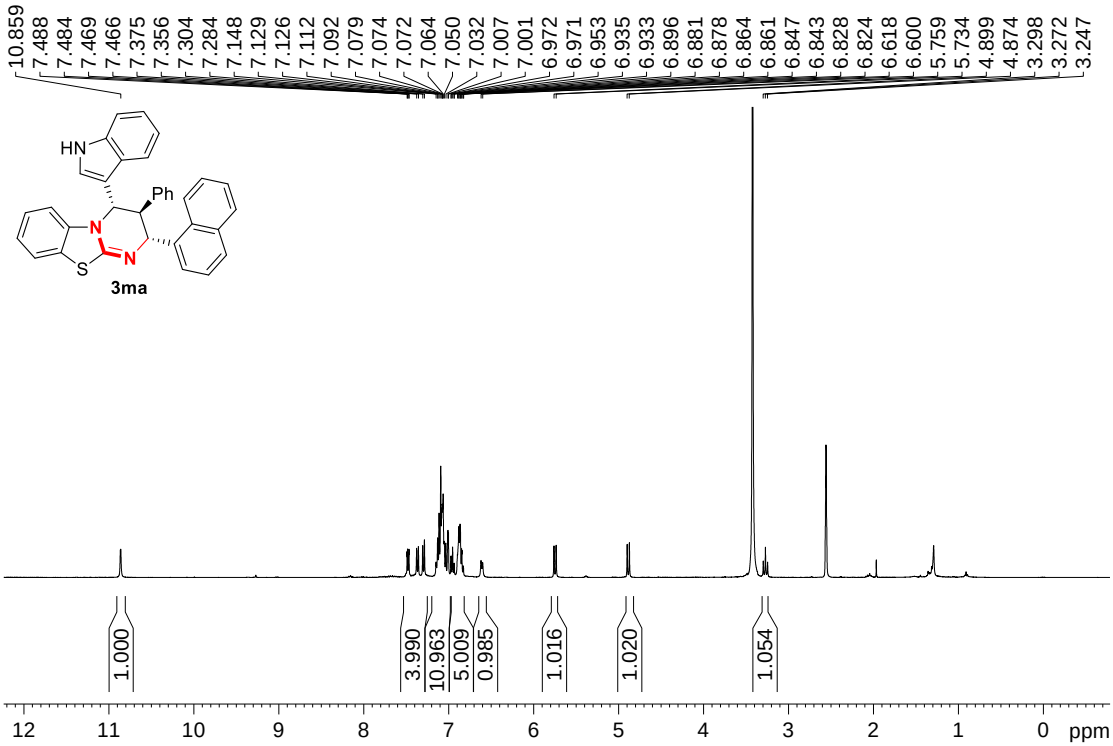
^{1}H NMR spectrum of compound **3la** ($(CD_3)_2SO$, 400 MHz)



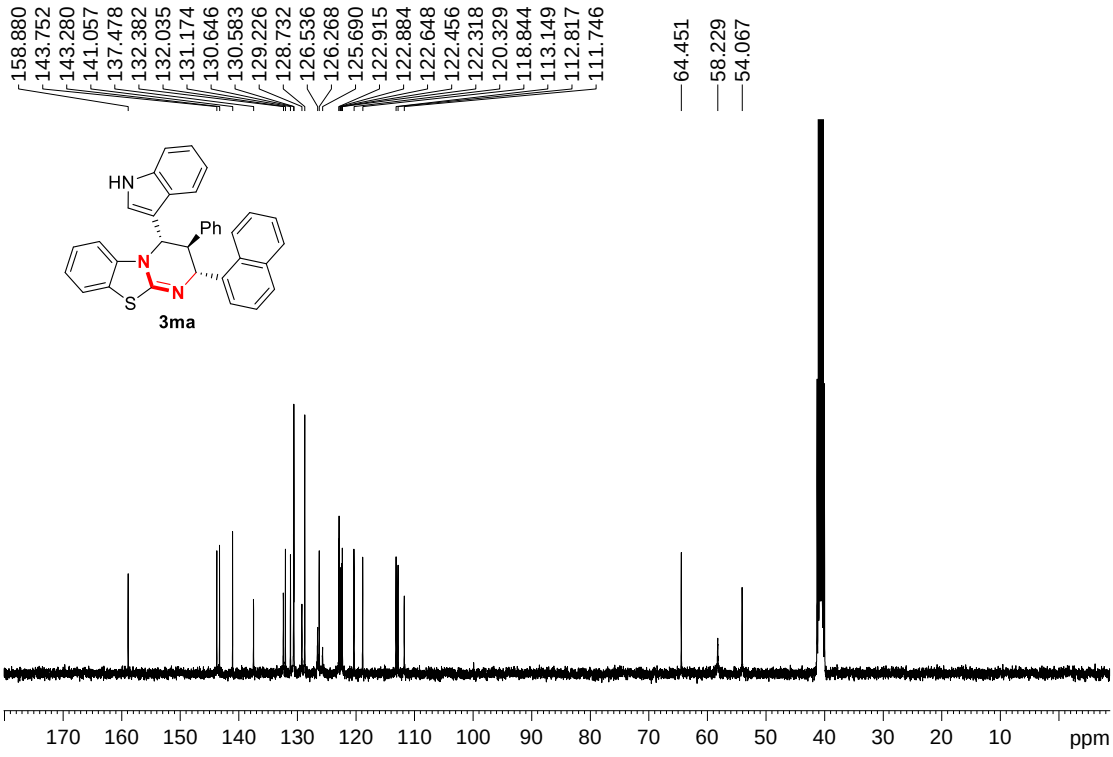
^{13}C NMR spectrum of compound **3la** ($(CD_3)_2SO$, 100 MHz)



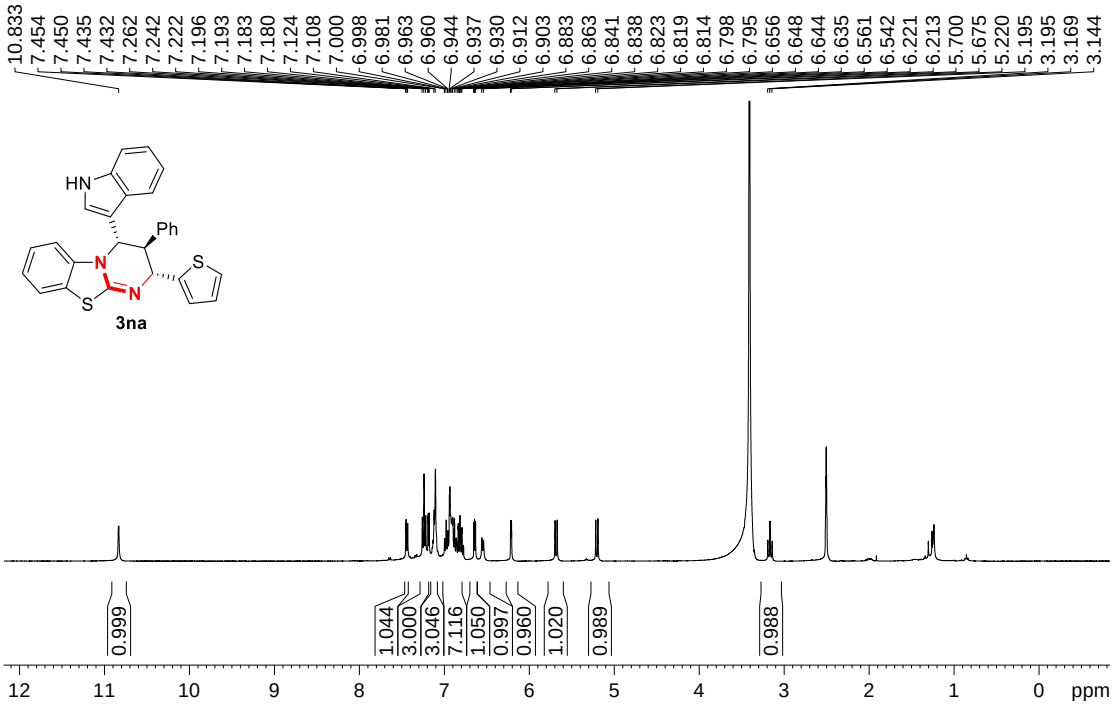
^{1}H NMR spectrum of compound **3ma** ($(CD_3)_2SO$, 400 MHz)



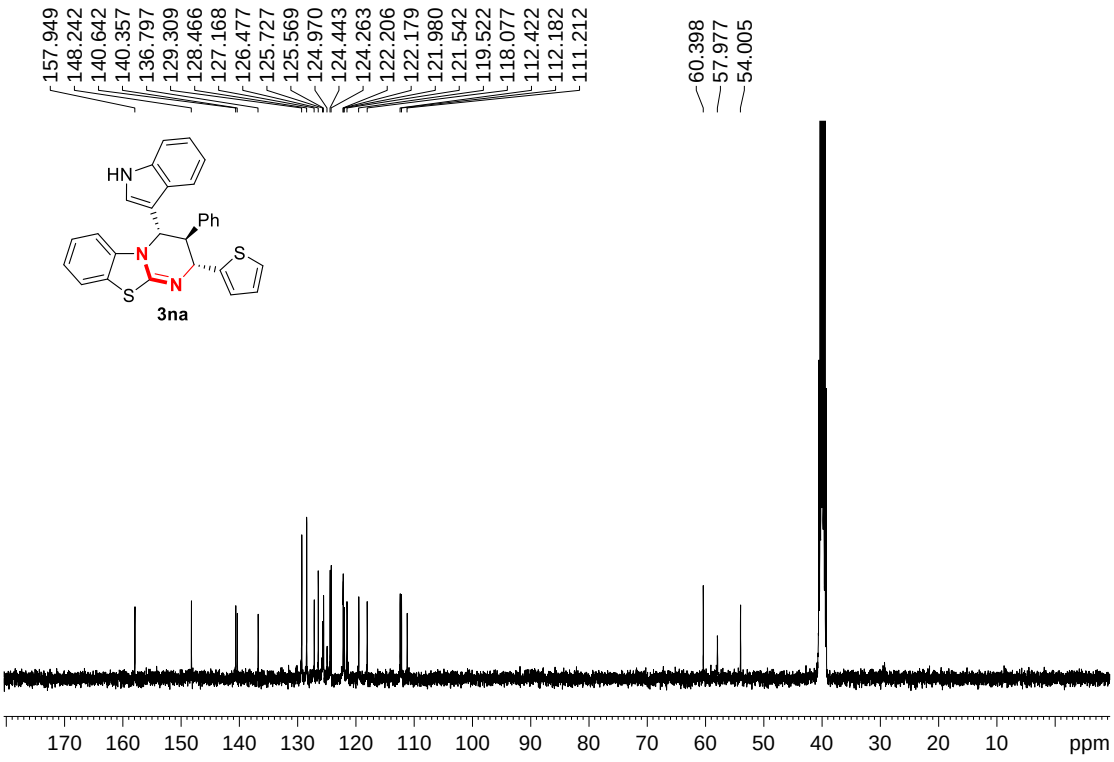
^{13}C NMR spectrum of compound **3ma** ($(CD_3)_2SO$, 100 MHz)



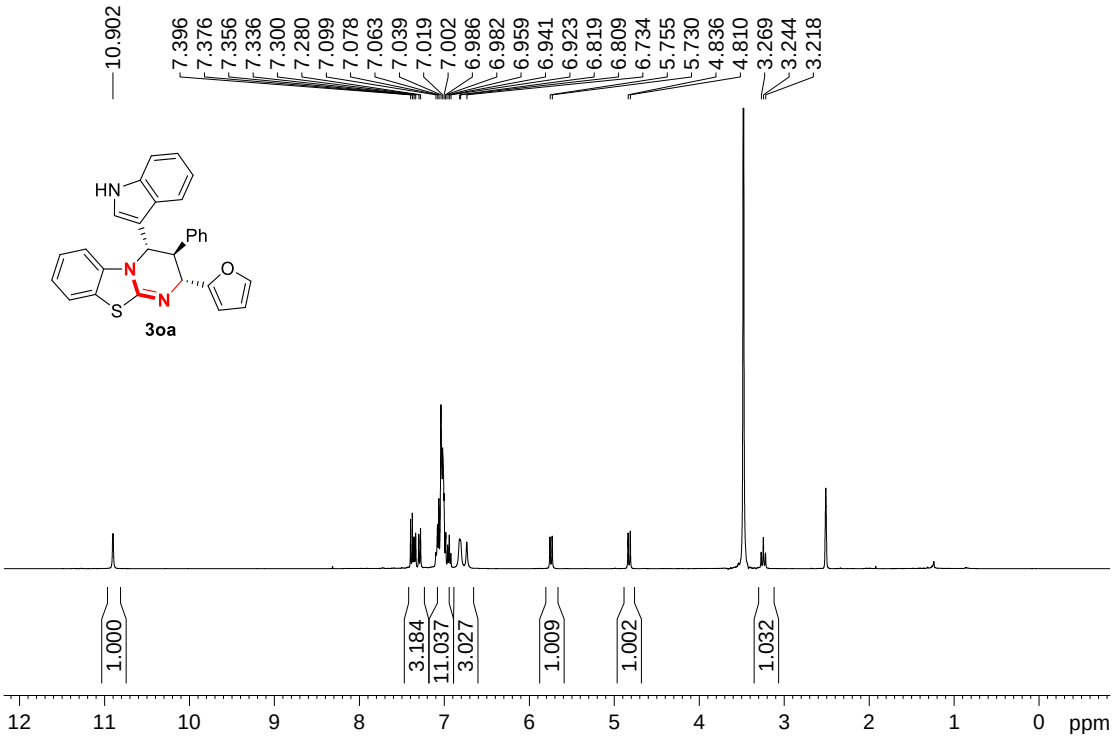
^{1}H NMR spectrum of compound **3na** ($(CD_3)_2SO$, 400 MHz)



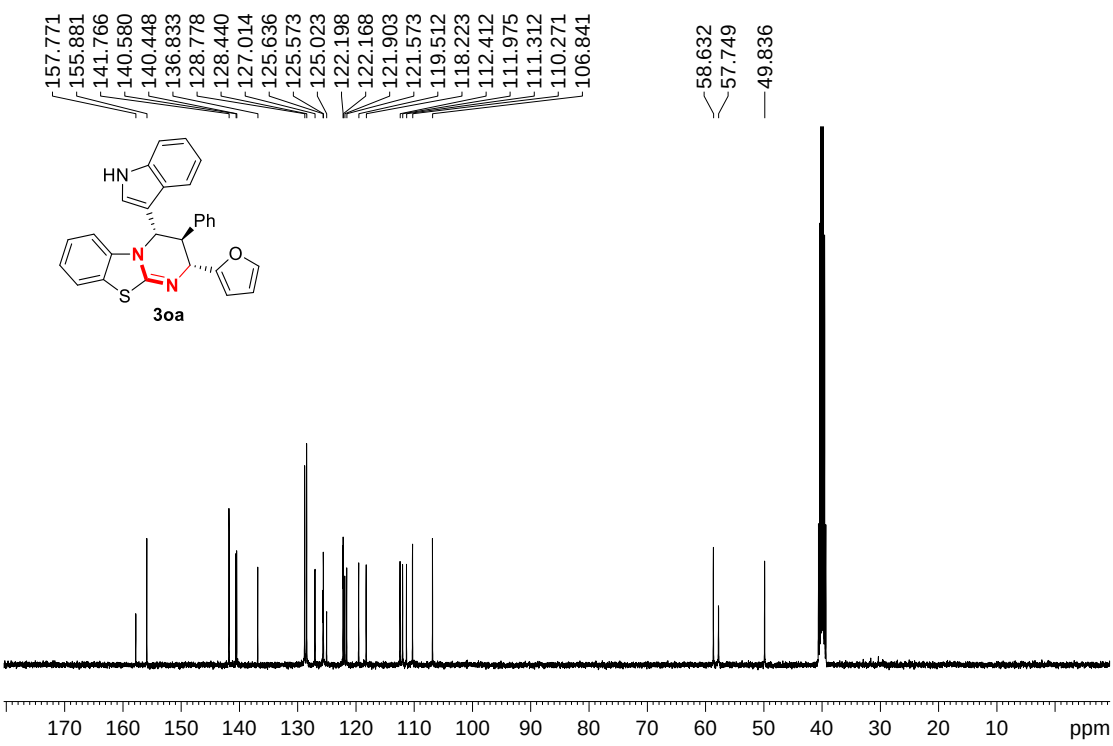
^{13}C NMR spectrum of compound **3na** ($(CD_3)_2SO$, 100 MHz)



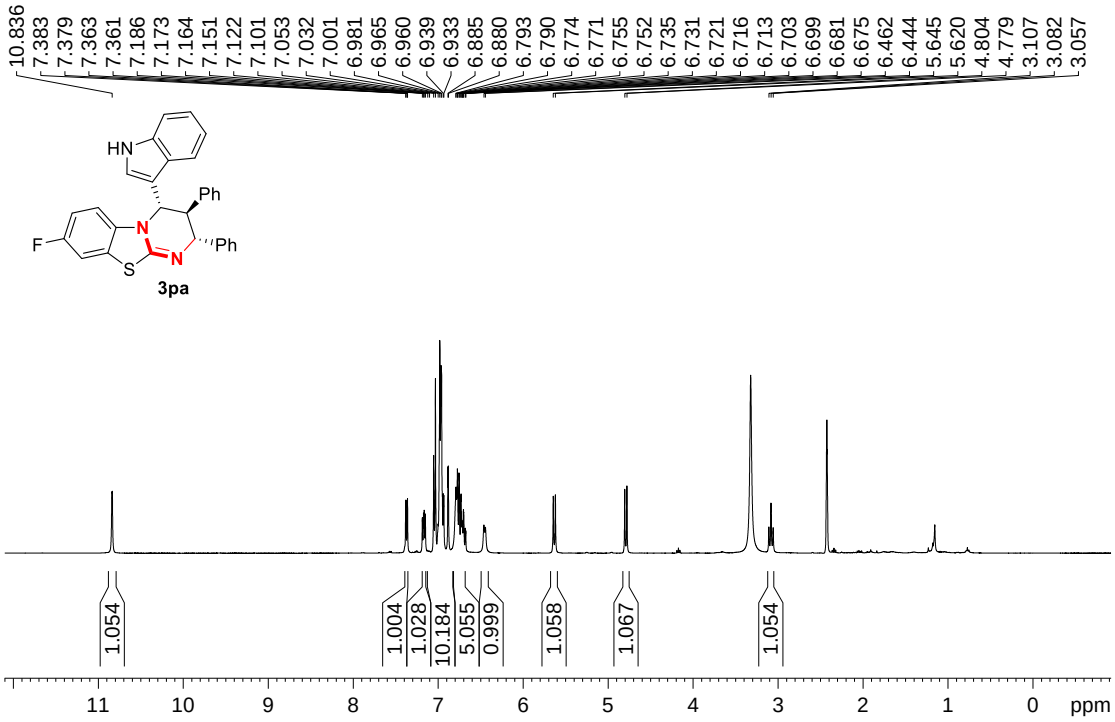
^{1}H NMR spectrum of compound **3oa** ($(CD_3)_2SO$, 400 MHz)



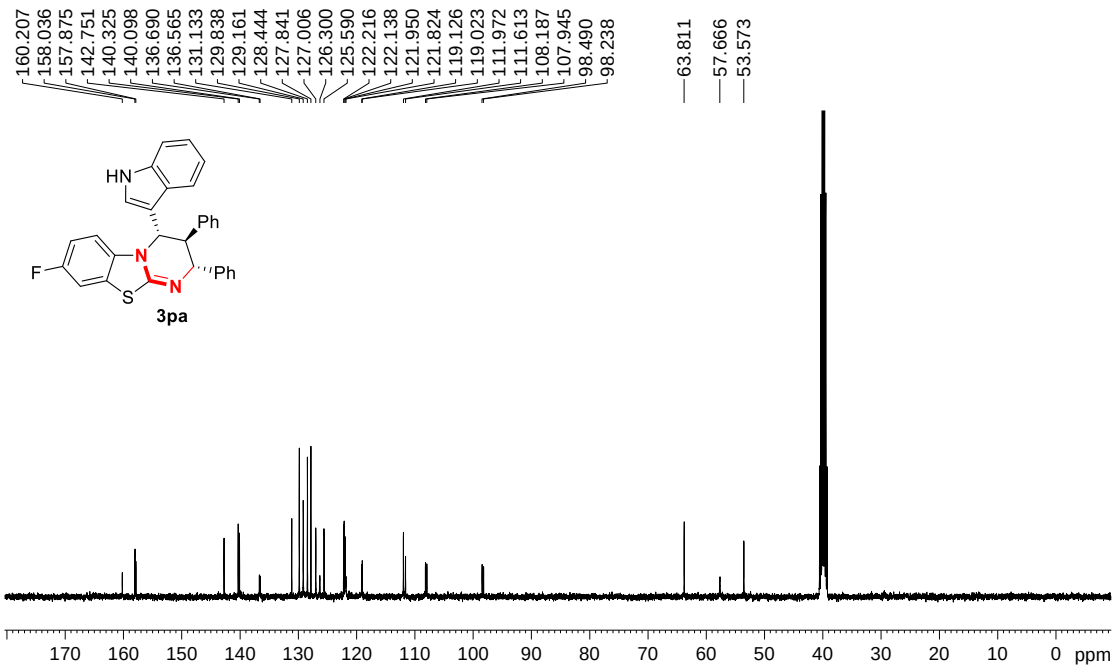
^{13}C NMR spectrum of compound **3oa** ($(CD_3)_2SO$, 100 MHz)



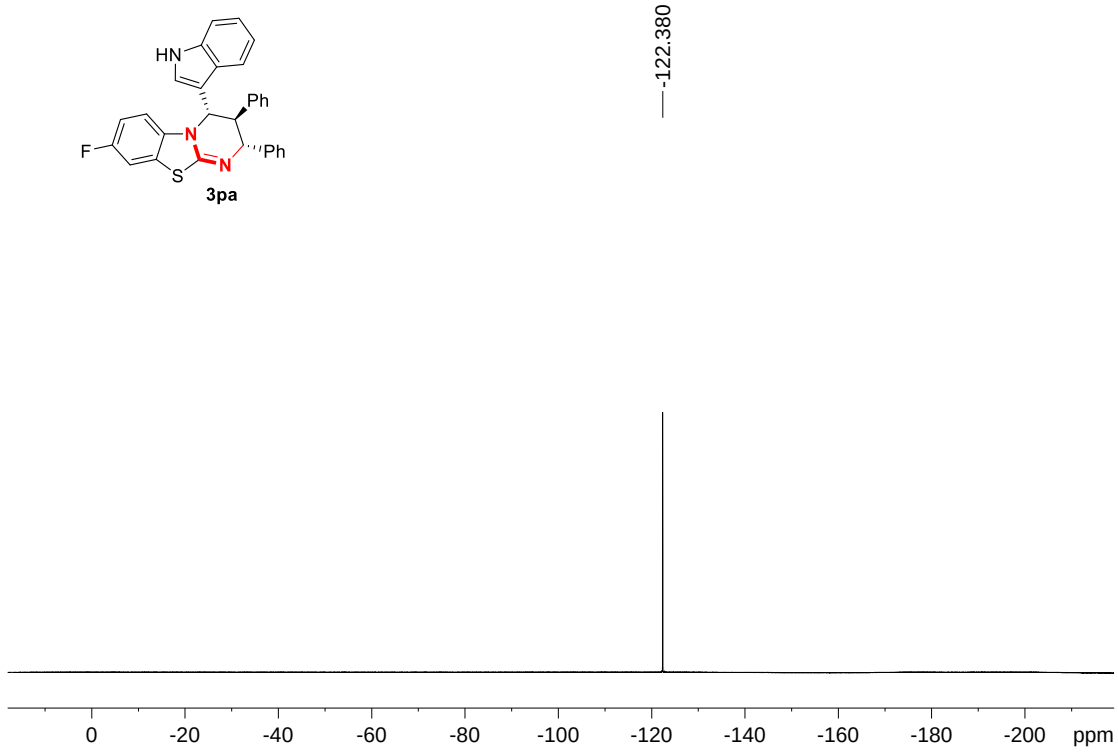
^{1}H NMR spectrum of compound **3pa** ($(CD_3)_2SO$, 400 MHz)



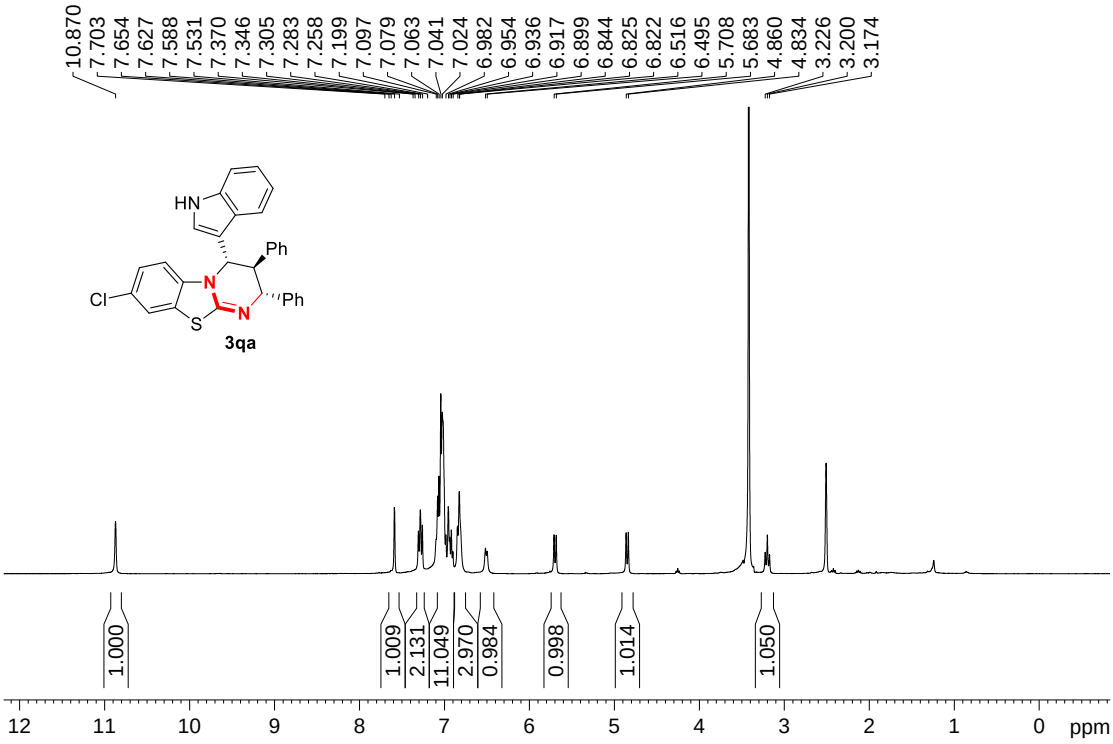
^{13}C NMR spectrum of compound **3pa** ($(CD_3)_2SO$, 100 MHz)



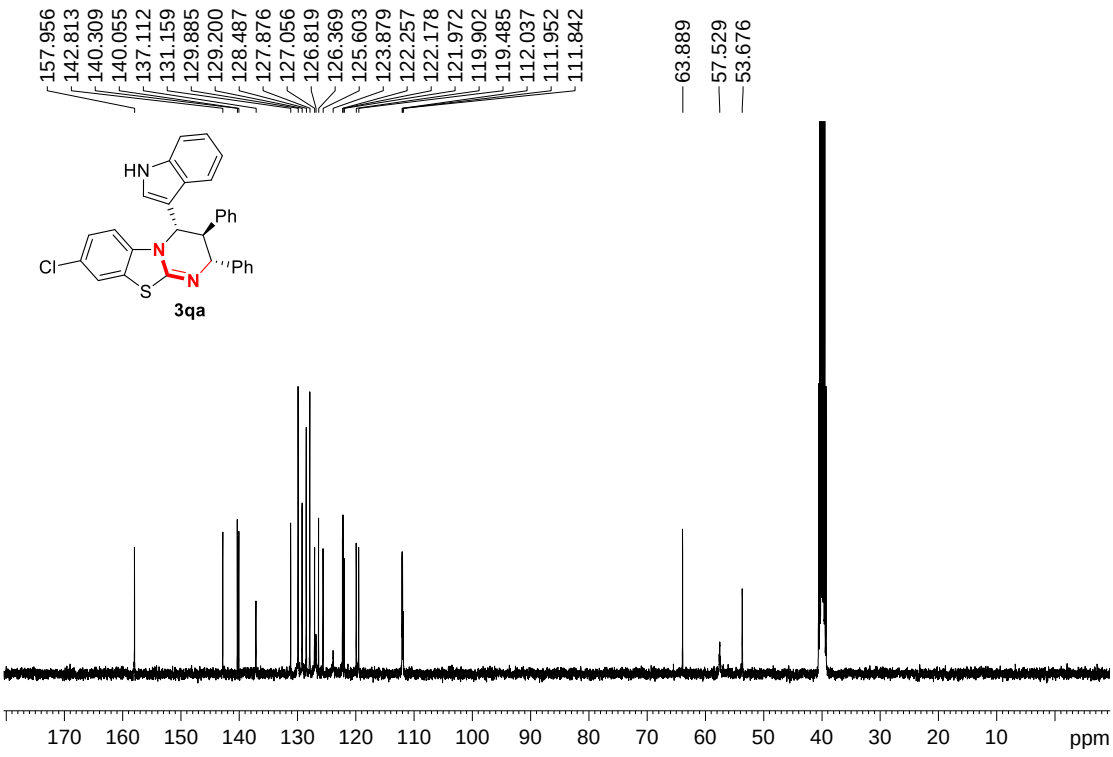
^{19}F NMR spectrum of compound **3pa** ($(CD_3)_2SO$, 376 MHz)



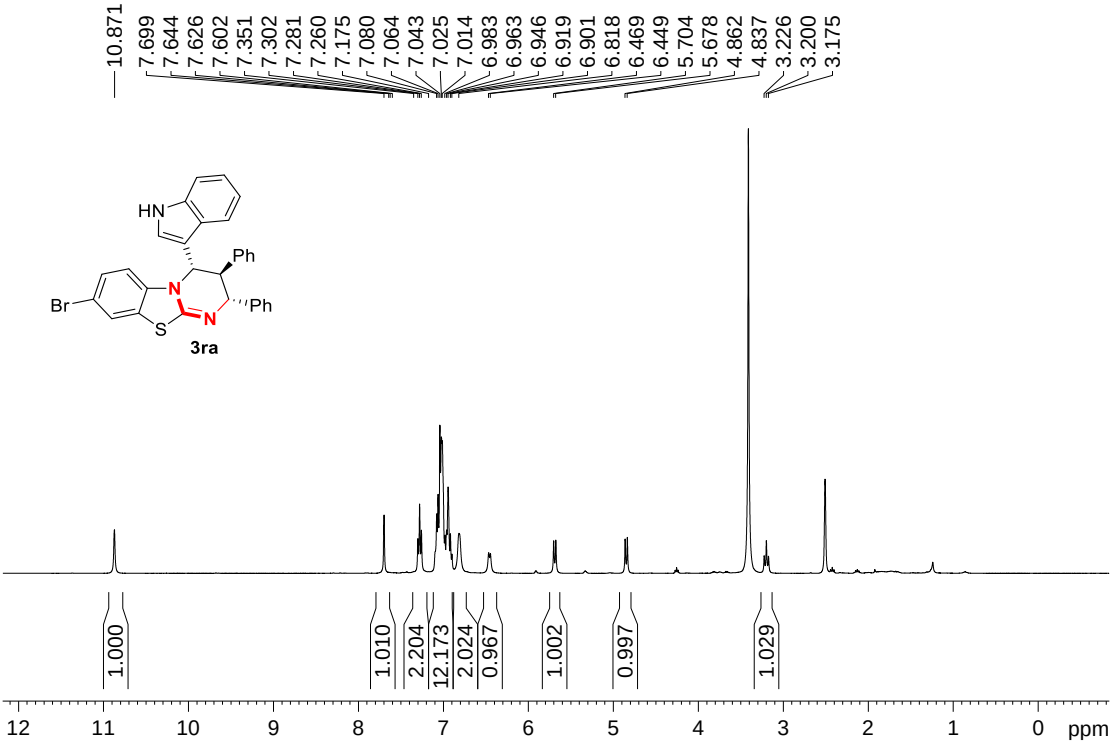
^{1}H NMR spectrum of compound **3qa** ($(CD_3)_2SO$, 400 MHz)



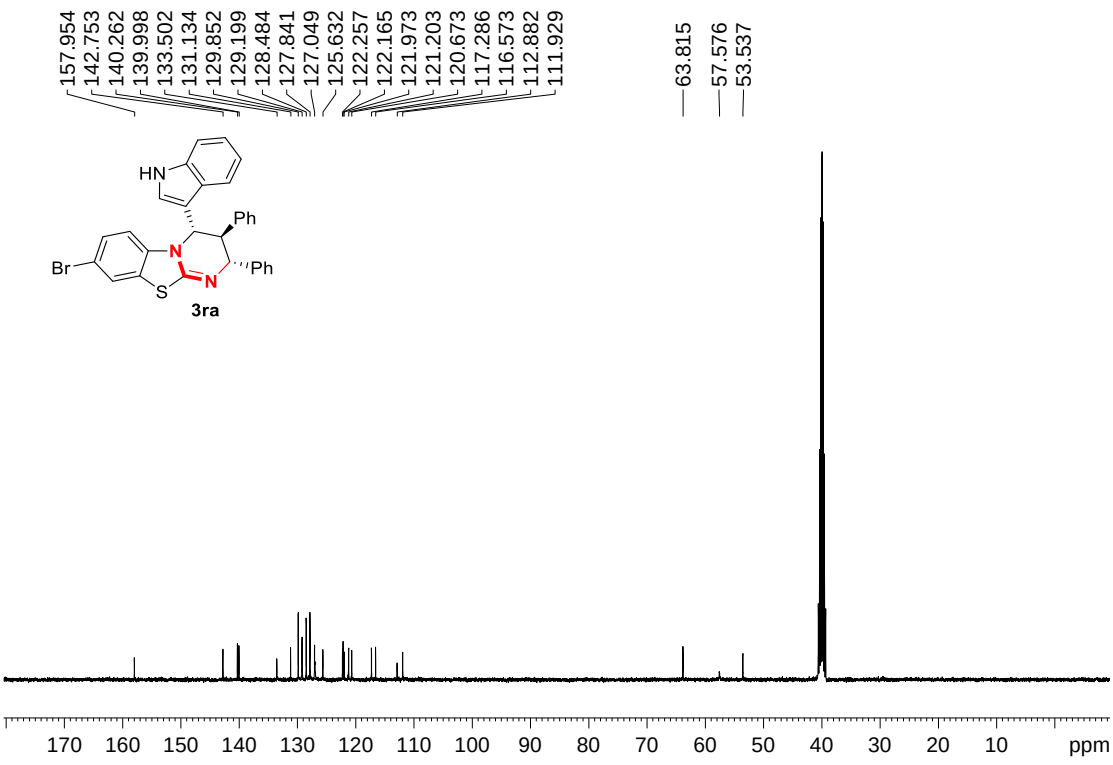
^{13}C NMR spectrum of compound **3qa** ($(CD_3)_2SO$, 100 MHz)



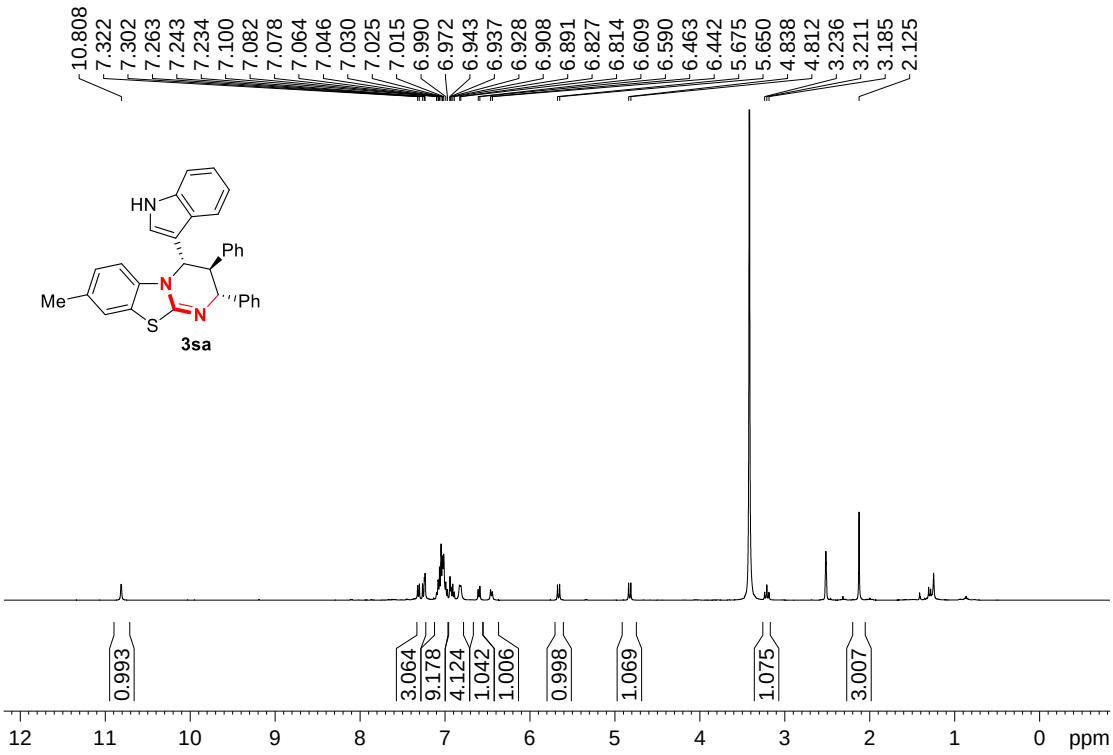
^{1}H NMR spectrum of compound **3ra** ($(CD_3)_2SO$, 400 MHz)



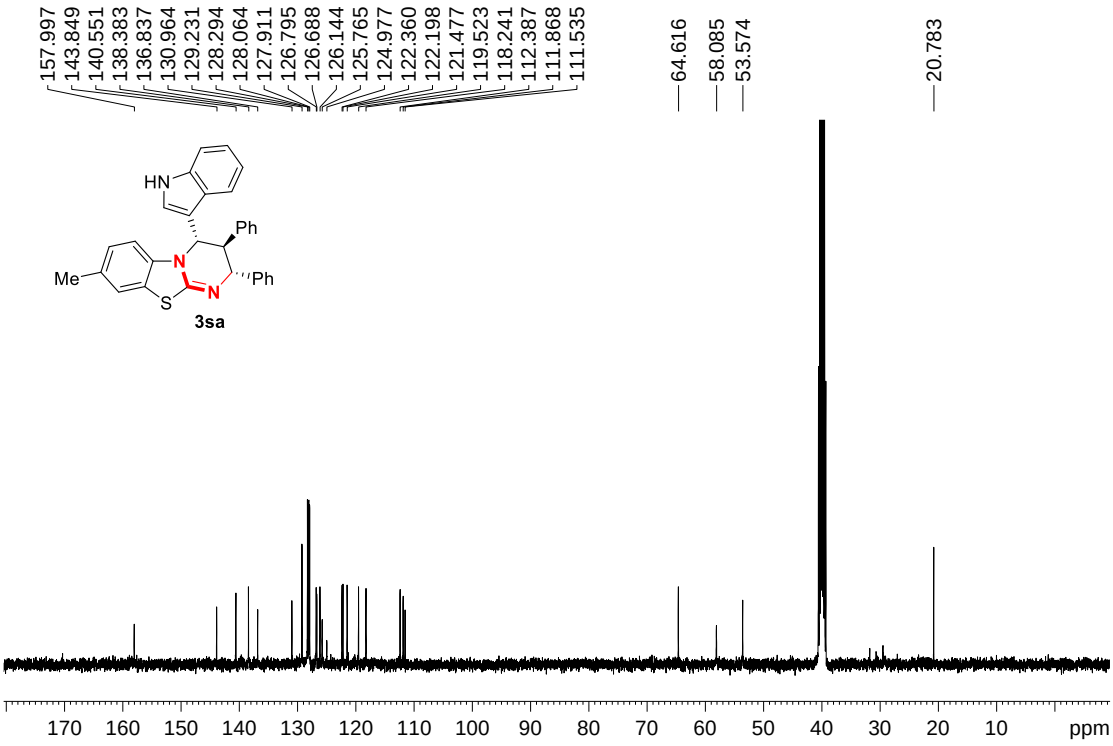
^{13}C NMR spectrum of compound **3ra** ($(CD_3)_2SO$, 100 MHz)



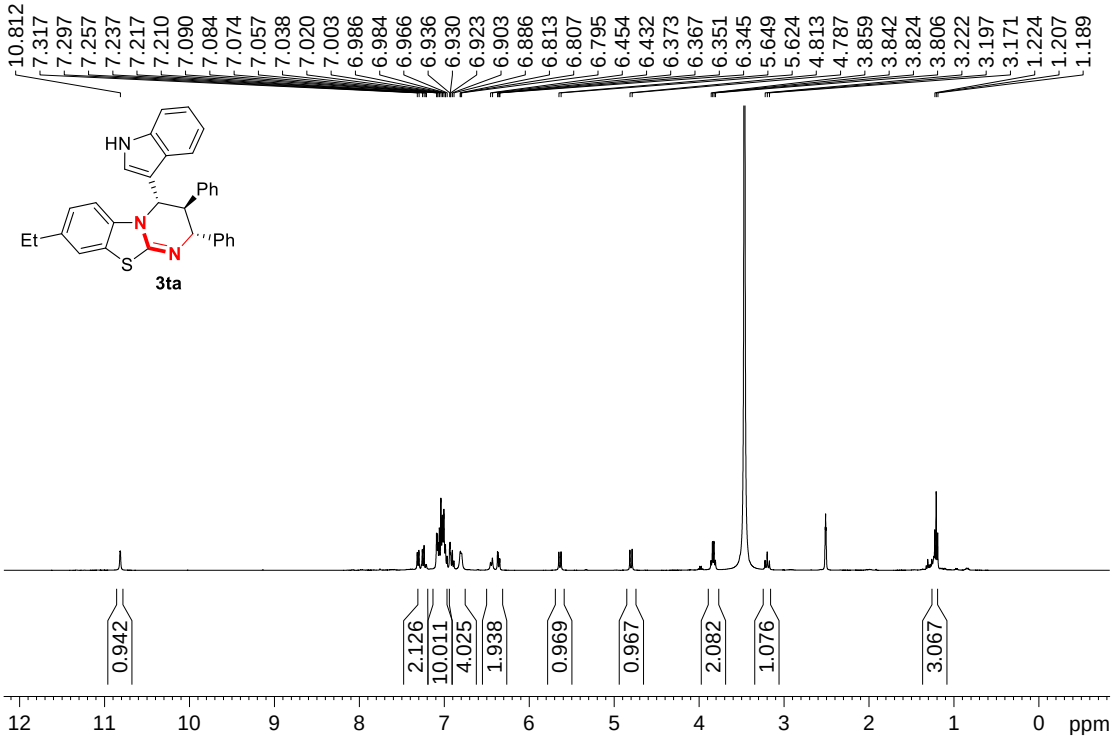
^{1}H NMR spectrum of compound **3sa** ($(CD_3)_2SO$, 400 MHz)



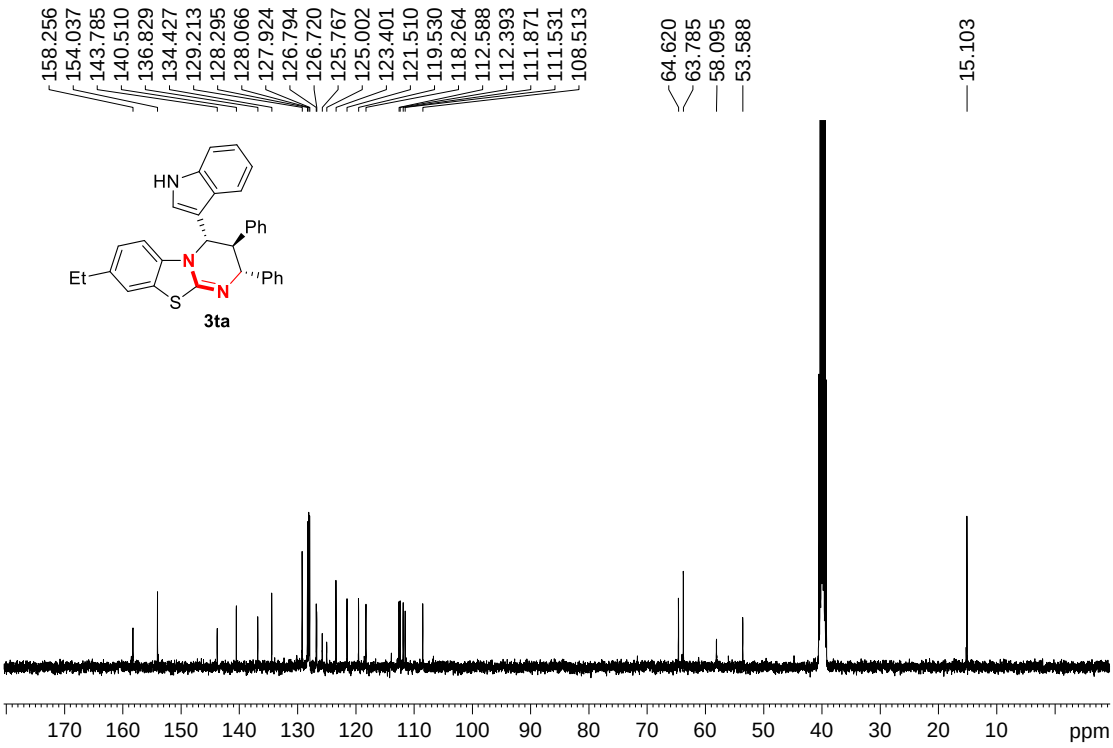
^{13}C NMR spectrum of compound **3sa** ($(CD_3)_2SO$, 100 MHz)



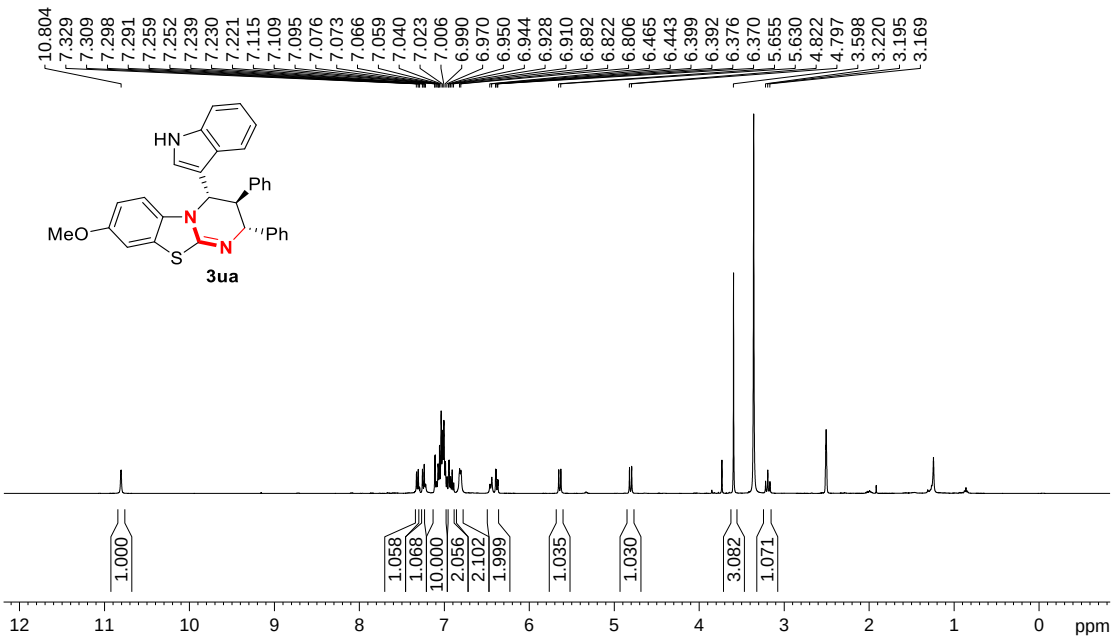
^{1}H NMR spectrum of compound **3ta** ($(CD_3)_2SO$, 400 MHz)



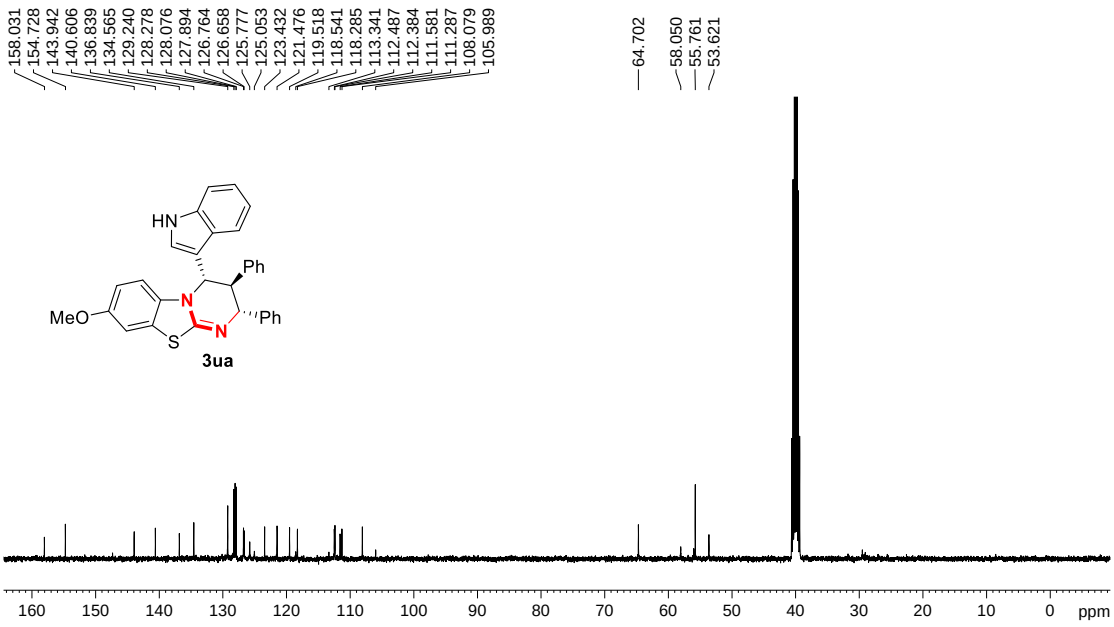
^{13}C NMR spectrum of compound **3ta** ($(CD_3)_2SO$, 100 MHz)



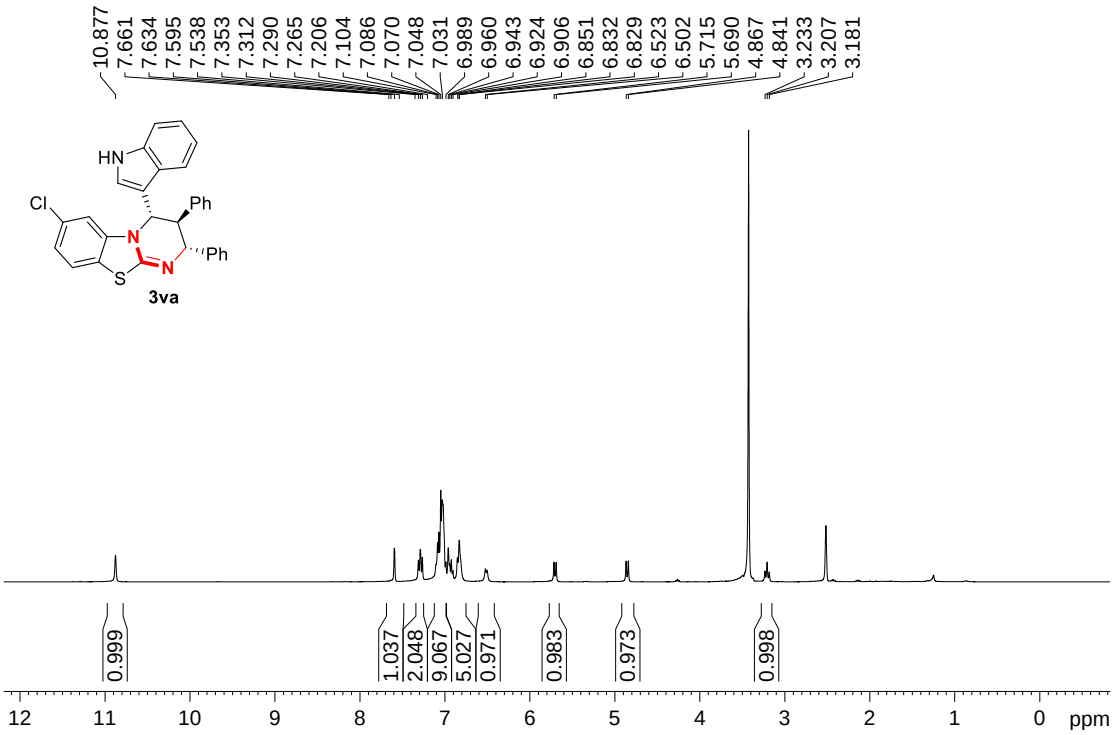
^{1}H NMR spectrum of compound **3ua** ($(CD_3)_2SO$, 400 MHz)



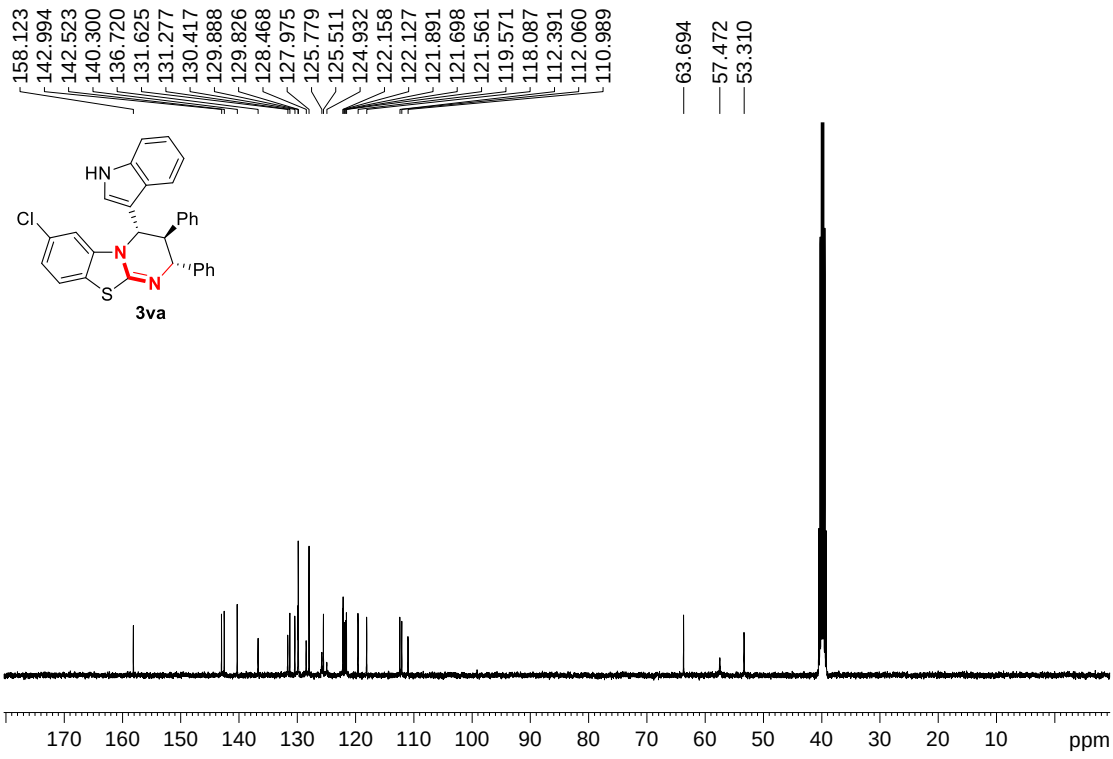
^{13}C NMR spectrum of compound **3ua** ($(CD_3)_2SO$, 100 MHz)



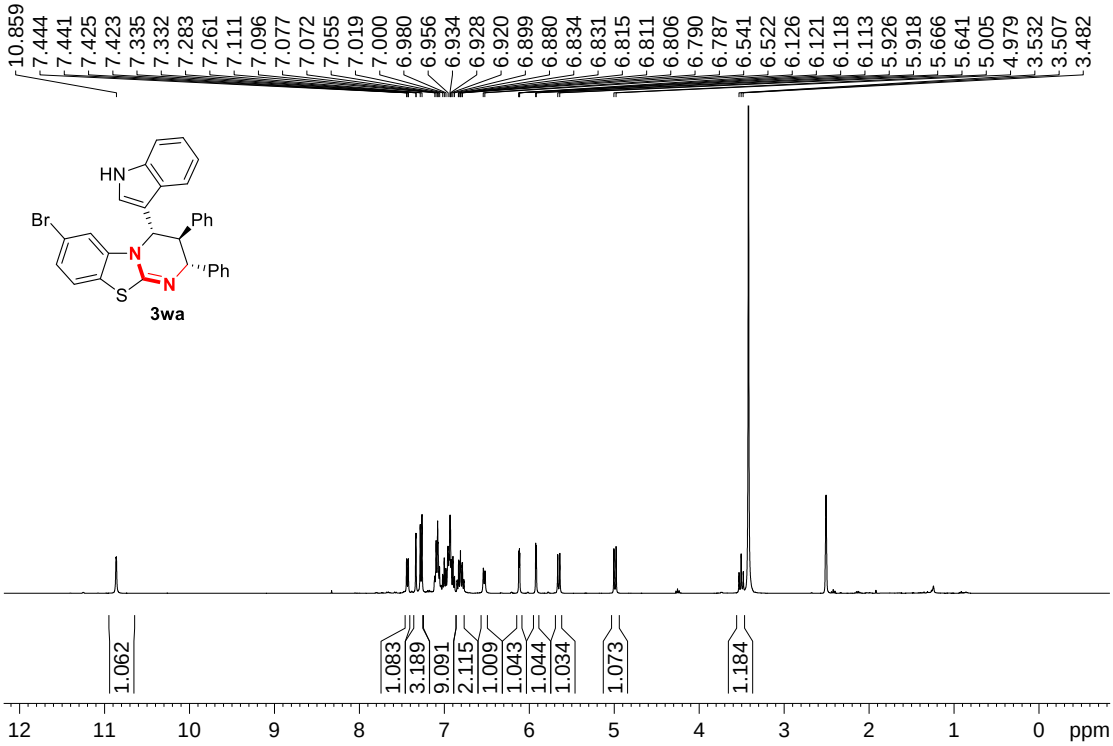
^{1}H NMR spectrum of compound **3va** ($(CD_3)_2SO$, 400 MHz)



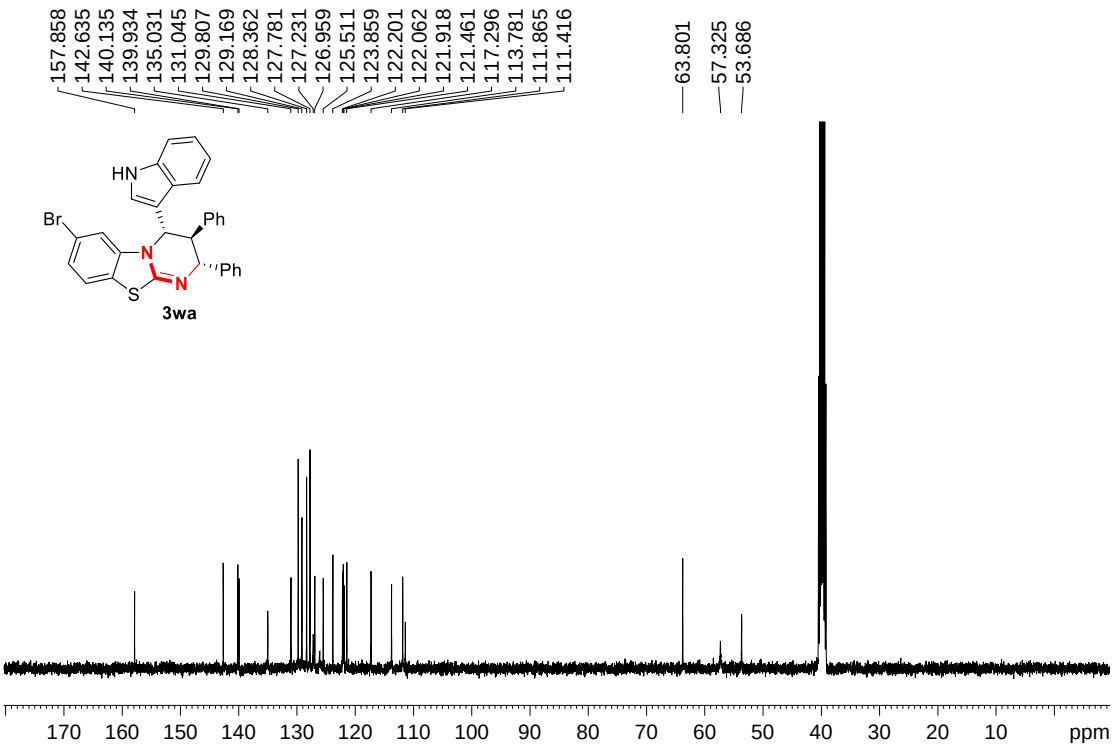
^{13}C NMR spectrum of compound **3va** ($(CD_3)_2SO$, 100 MHz)



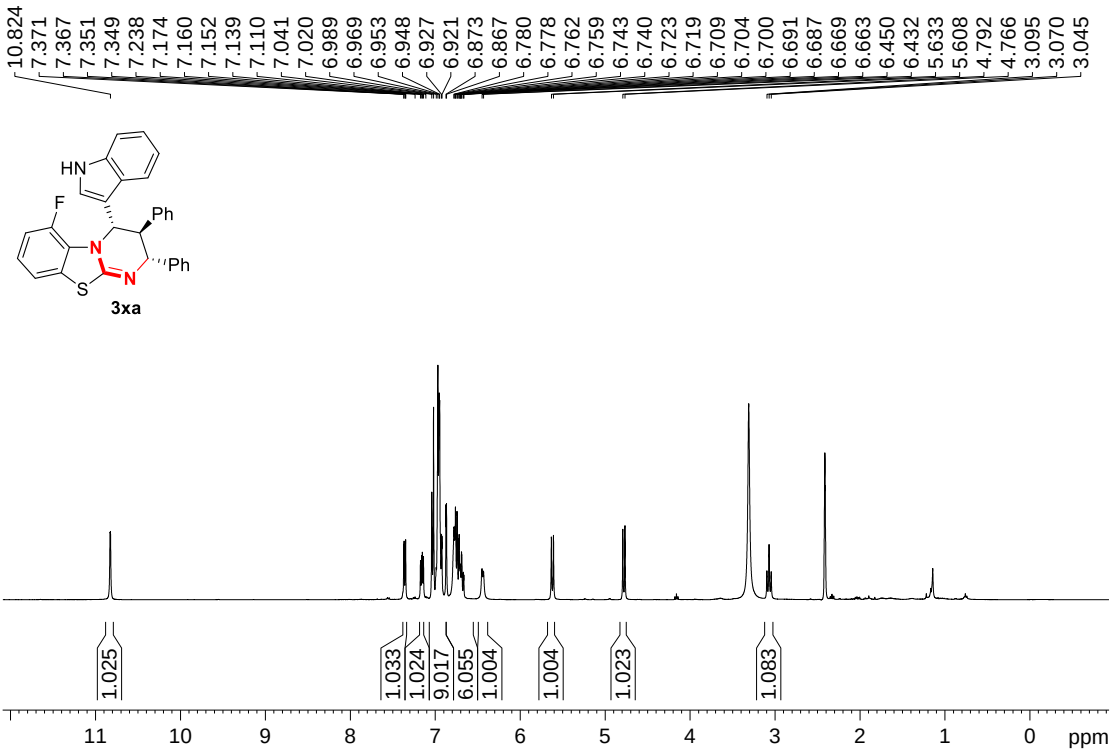
^{1}H NMR spectrum of compound **3wa** ($(CD_3)_2SO$, 400 MHz)



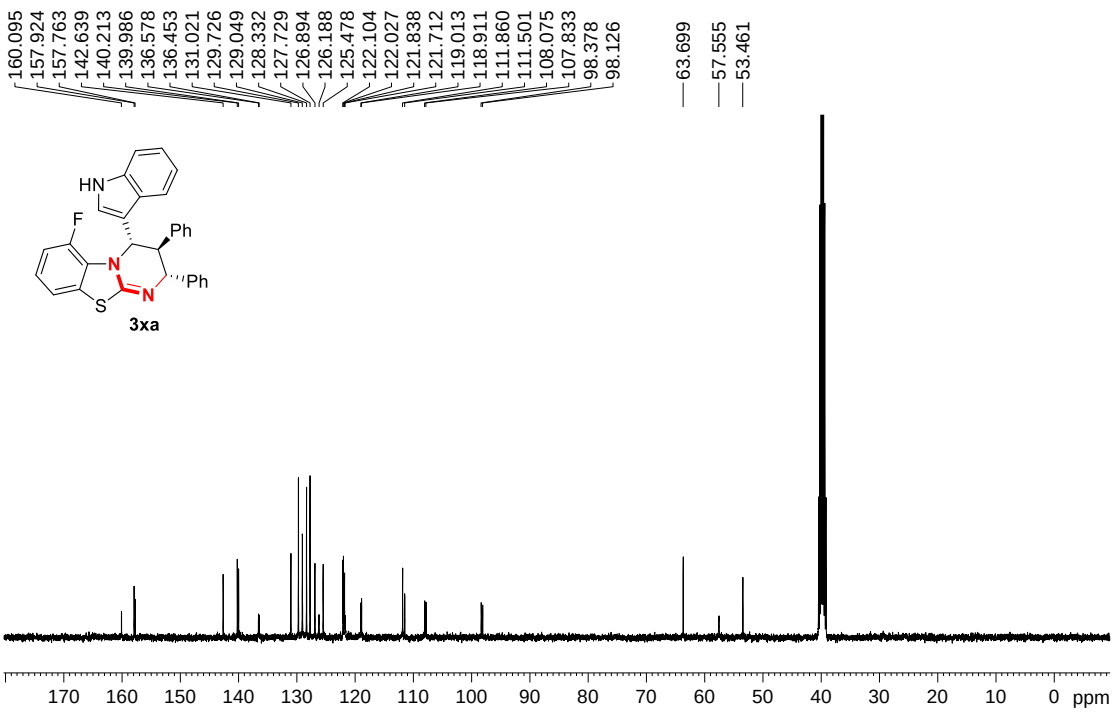
^{13}C NMR spectrum of compound **3wa** ($(CD_3)_2SO$, 100 MHz)



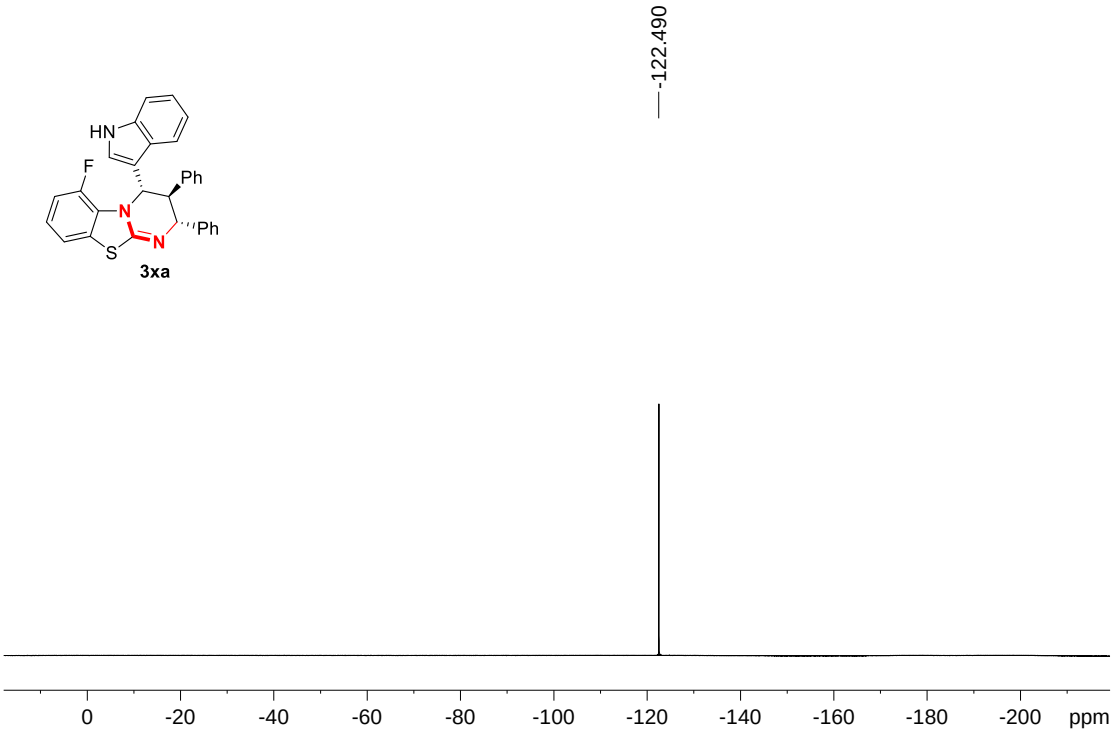
^{1}H NMR spectrum of compound **3xa** ($(CD_3)_2SO$, 400 MHz)



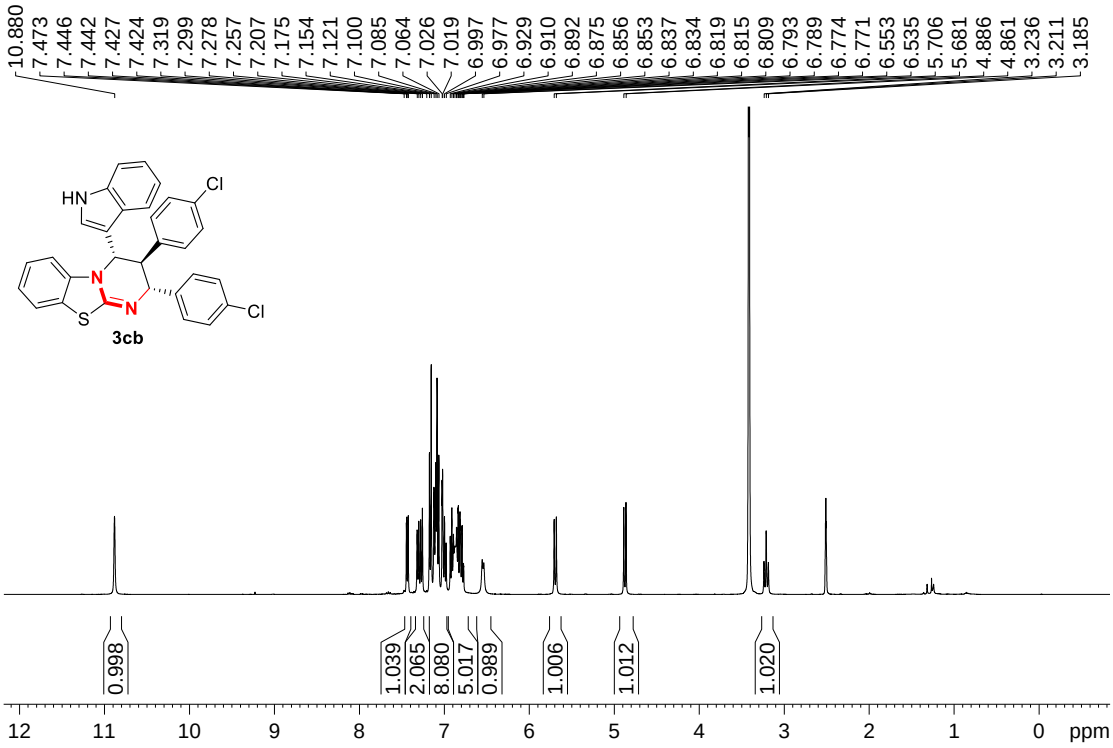
^{13}C NMR spectrum of compound **3xa** ($(CD_3)_2SO$, 100 MHz)



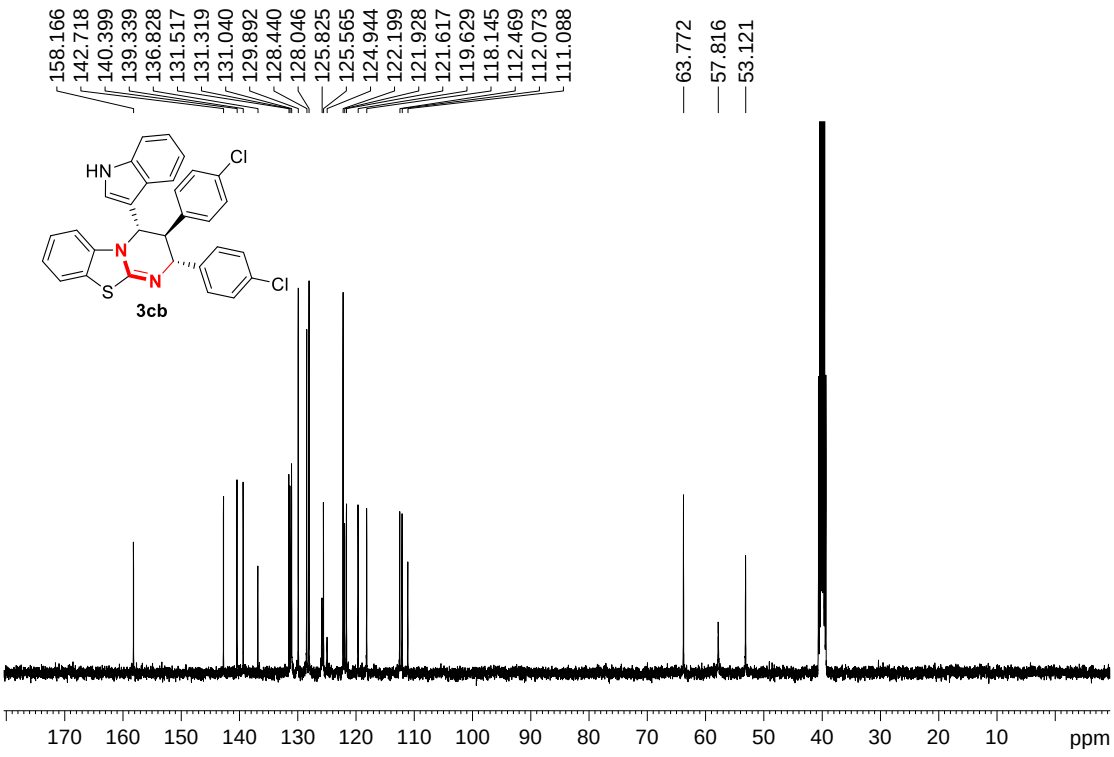
^{19}F NMR spectrum of compound **3xa** ($(CD_3)_2SO$, 376 MHz)



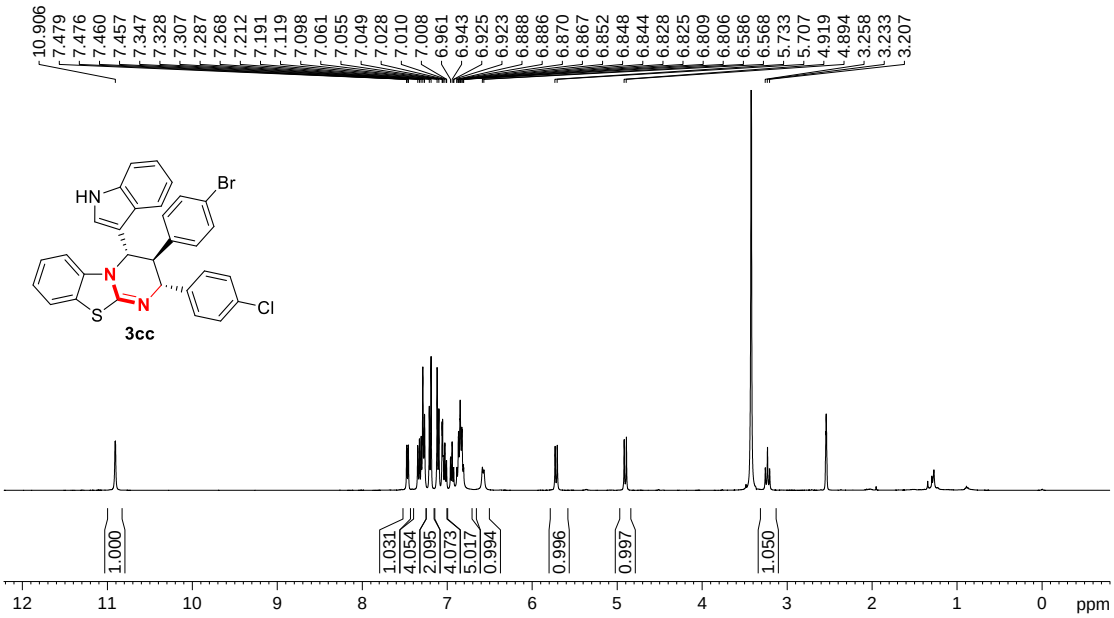
^{1}H NMR spectrum of compound **3cb** ($(CD_3)_2SO$, 400 MHz)



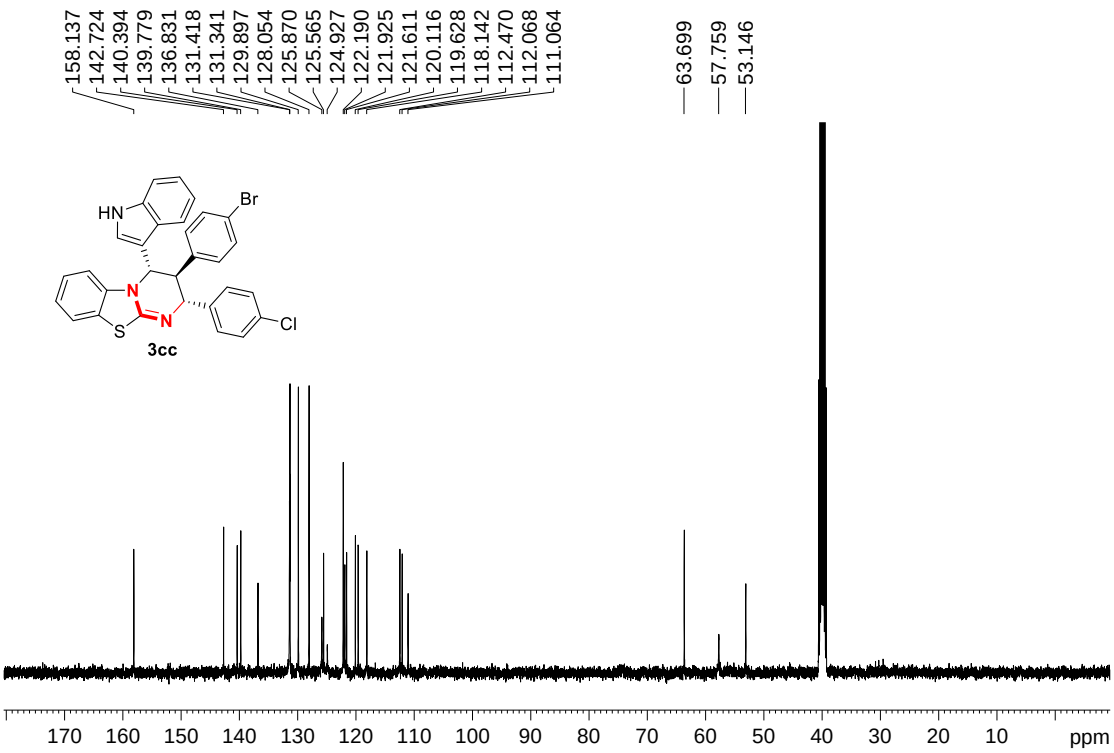
^{13}C NMR spectrum of compound **3cb** ($(CD_3)_2SO$, 100 MHz)



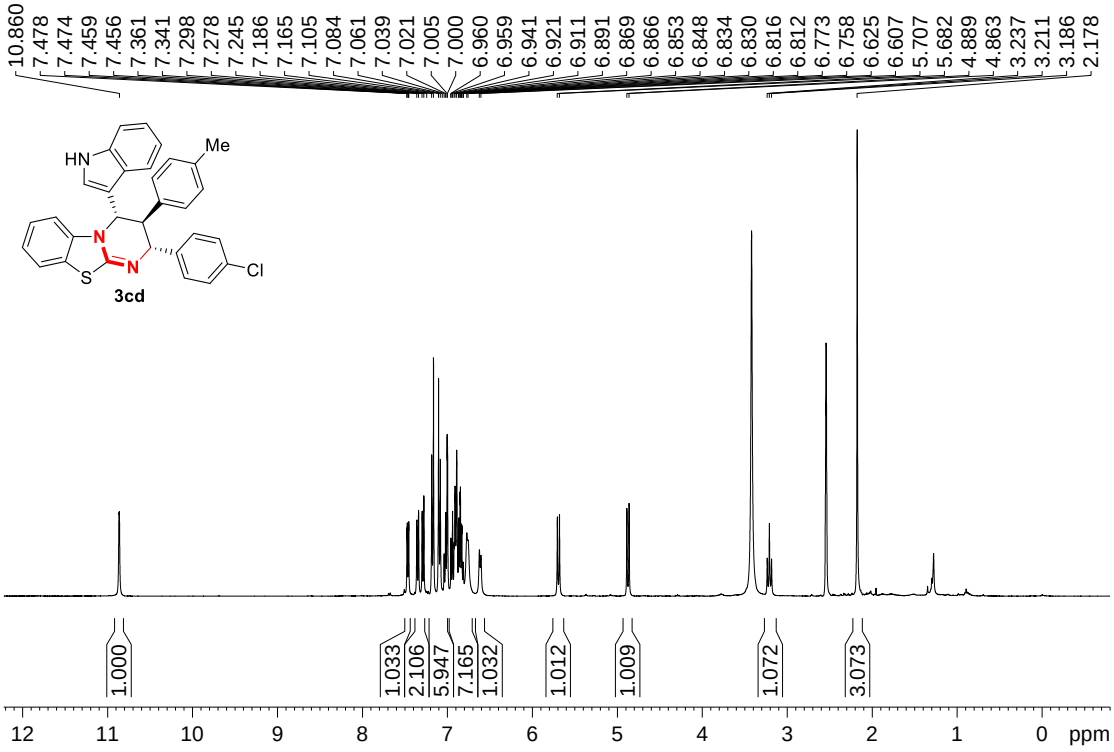
^{1}H NMR spectrum of compound **3cc** ($(CD_3)_2SO$, 400 MHz)



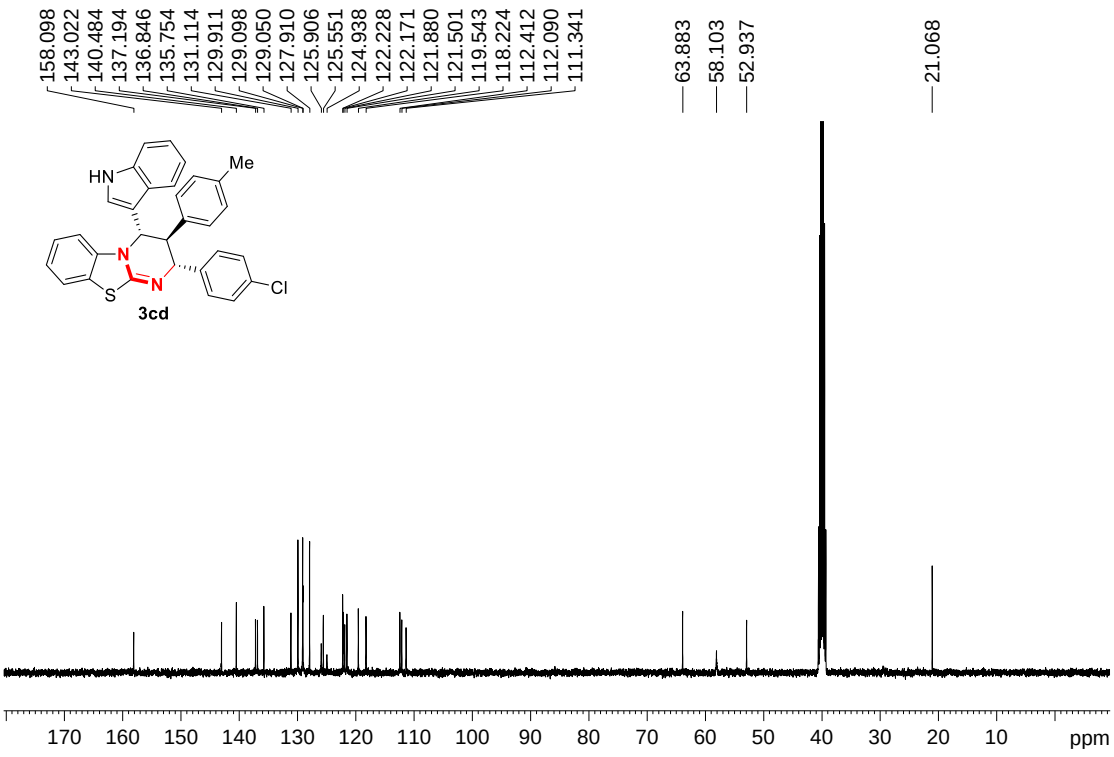
^{13}C NMR spectrum of compound **3cc** ($(CD_3)_2SO$, 100 MHz)



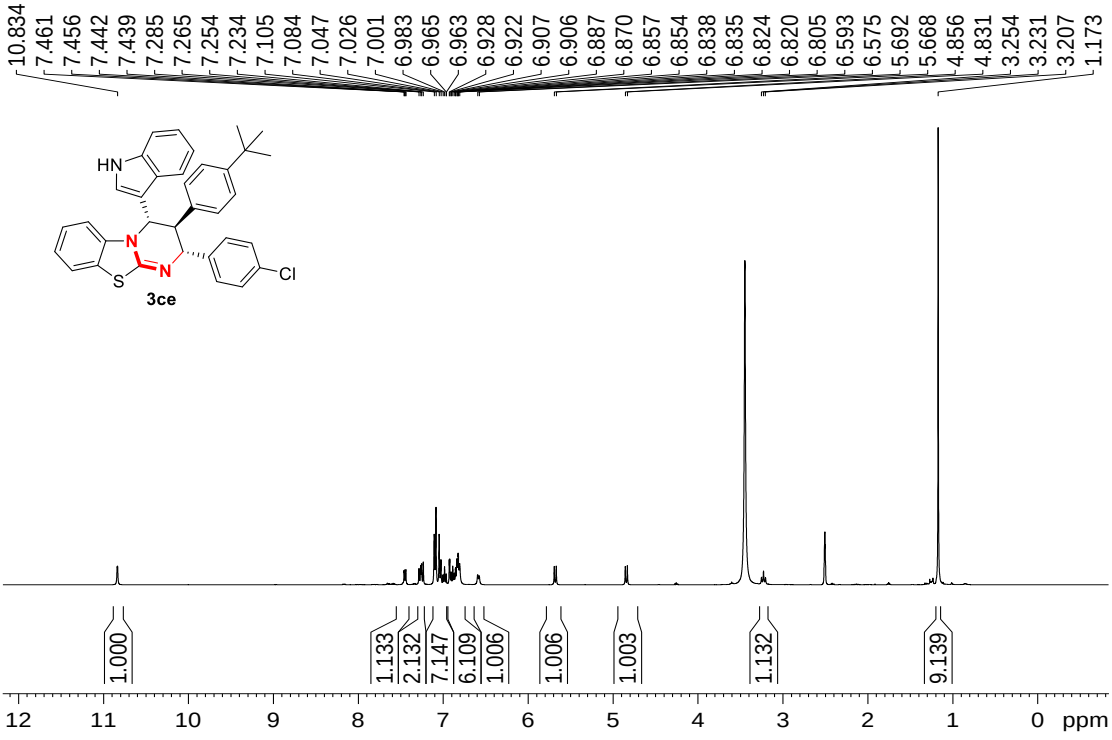
^{1}H NMR spectrum of compound **3cd** ($(CD_3)_2SO$, 400 MHz)



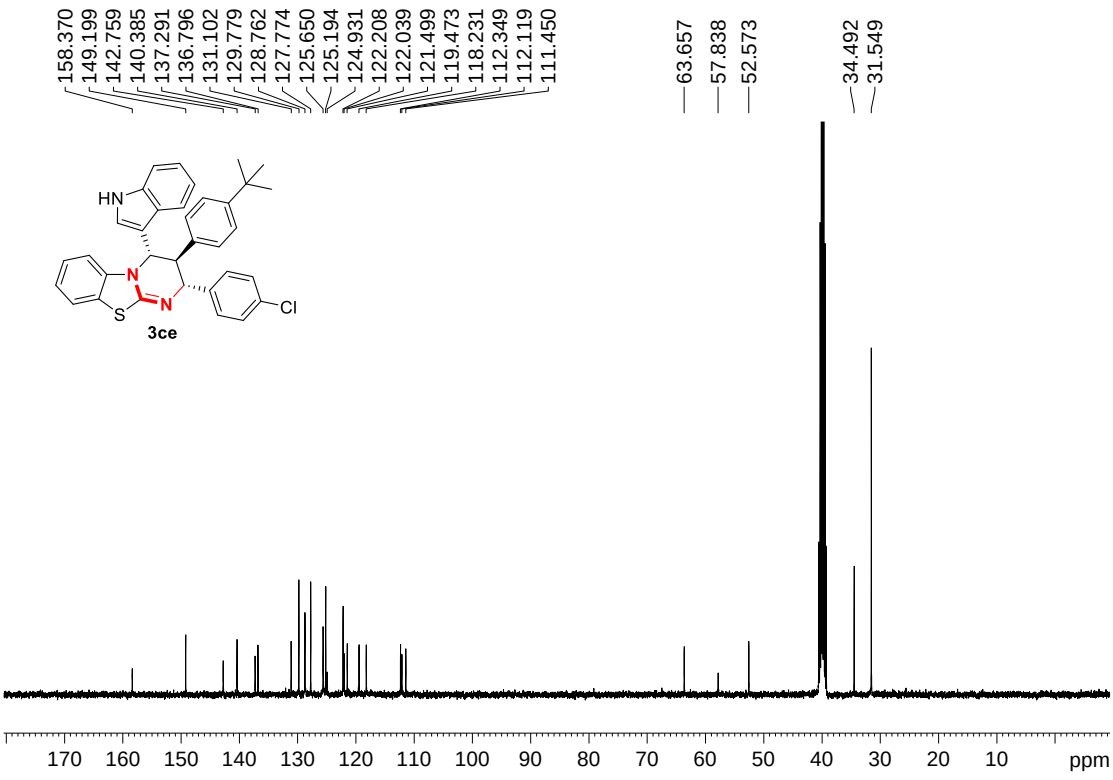
^{13}C NMR spectrum of compound **3cd** ($(CD_3)_2SO$, 100 MHz)



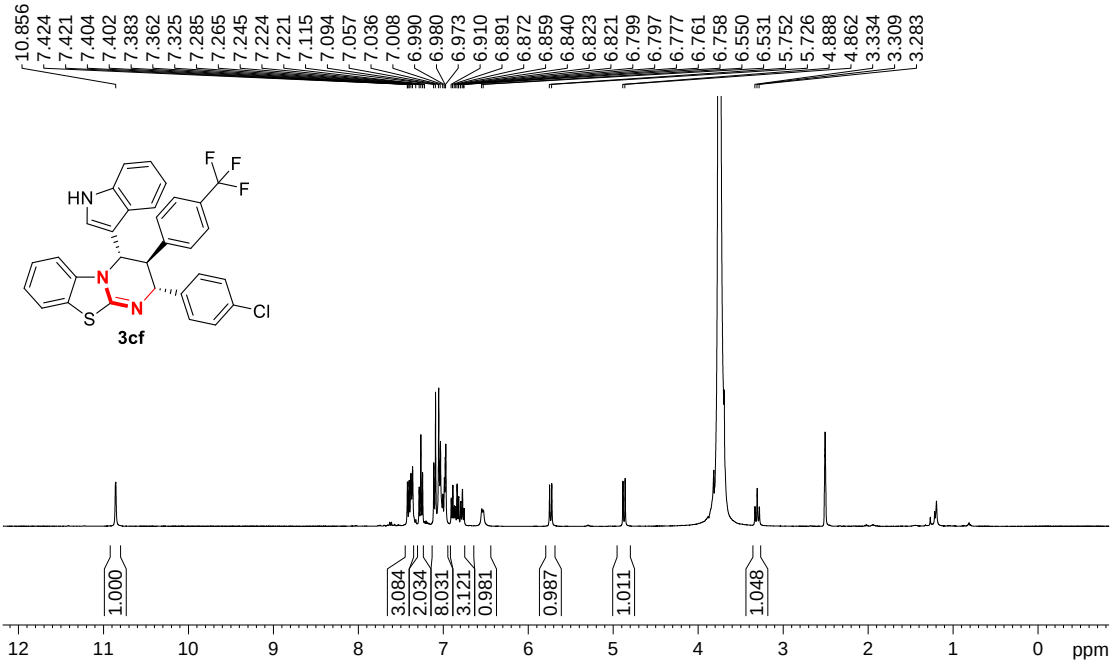
^{1}H NMR spectrum of compound **3ce** ($(CD_3)_2SO$, 400 MHz)



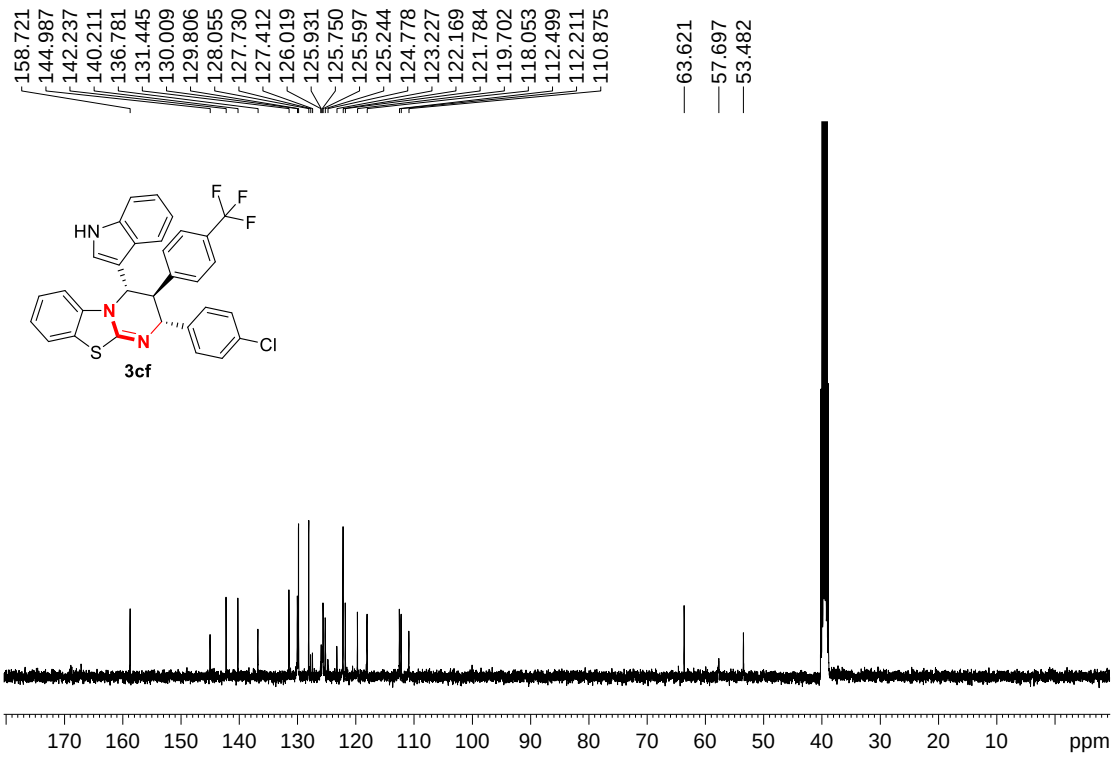
^{13}C NMR spectrum of compound **3ce** ($(CD_3)_2SO$, 100 MHz)



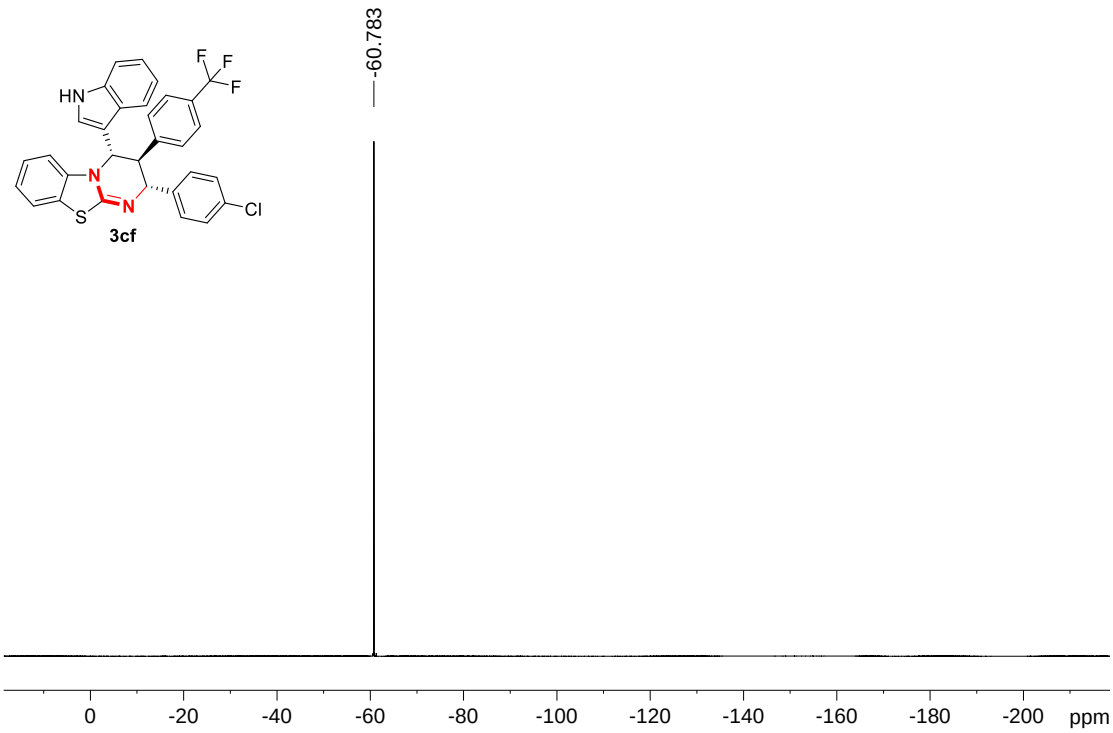
^{1}H NMR spectrum of compound **3cf** ($(CD_3)_2SO$, 400 MHz)



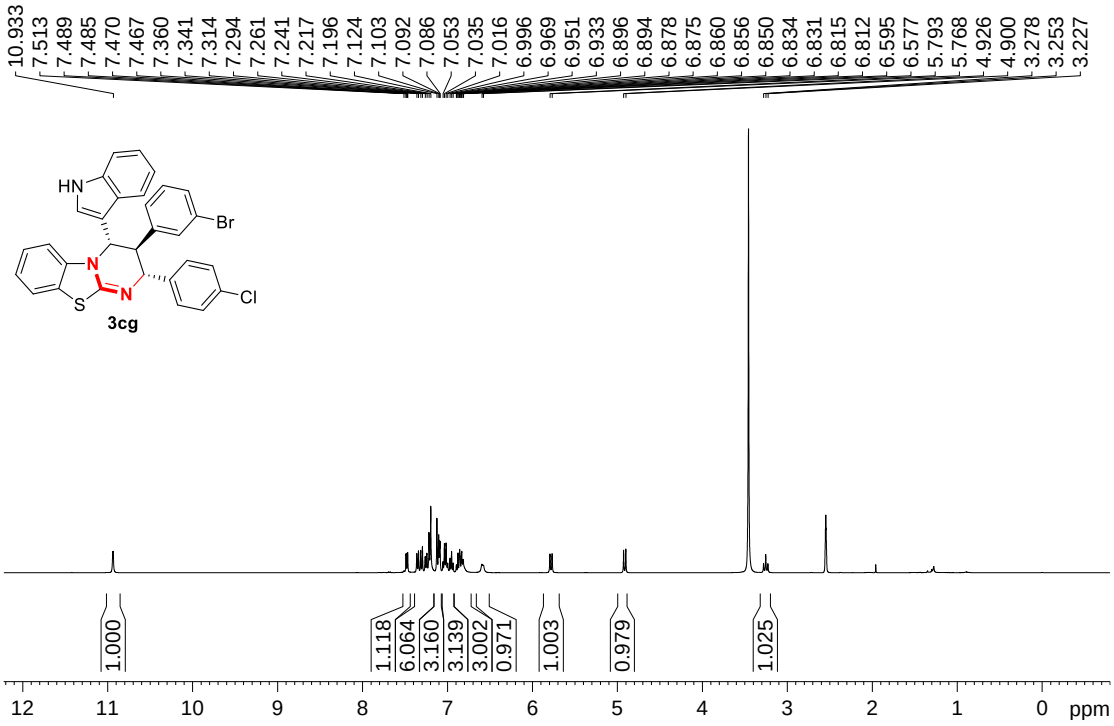
^{13}C NMR spectrum of compound **3cf** ($(CD_3)_2SO$, 100 MHz)



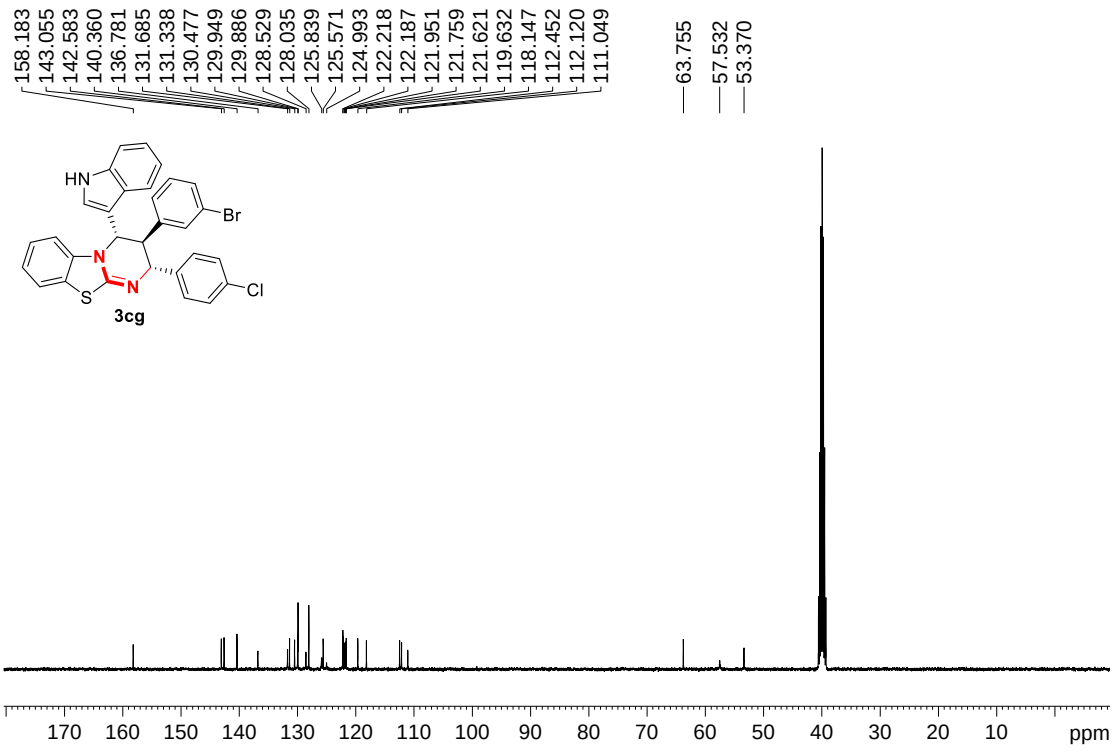
^{19}F NMR spectrum of compound **3cf** ($(CD_3)_2SO$, 376 MHz)



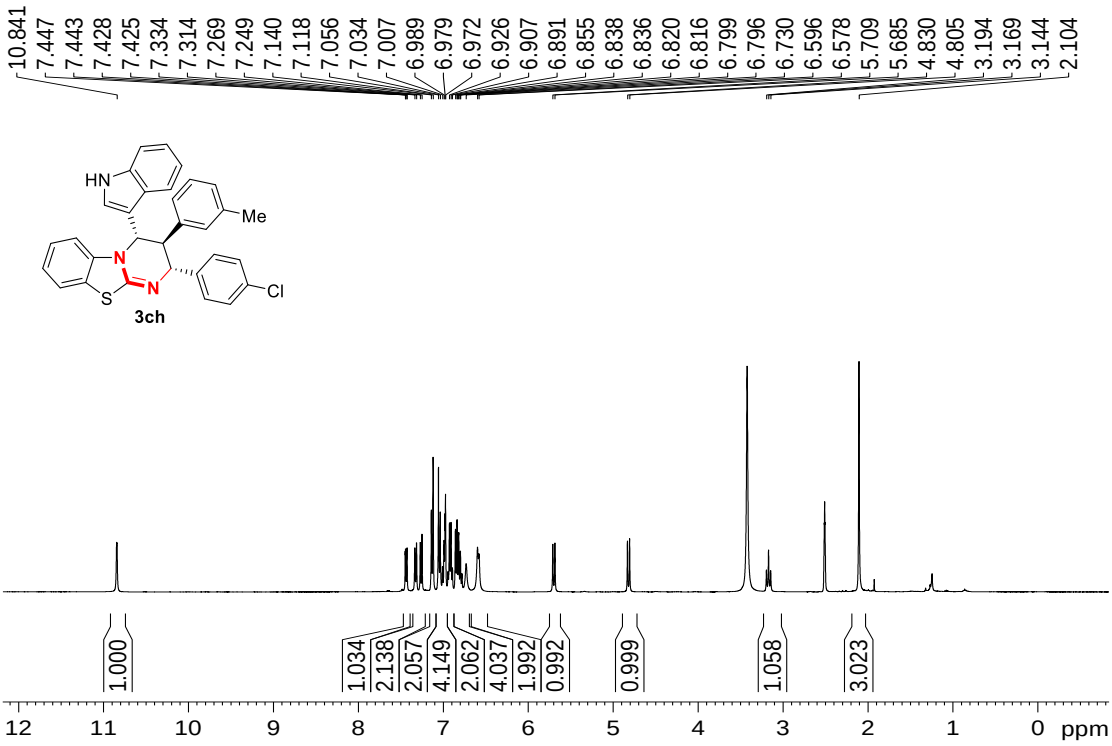
^{1}H NMR spectrum of compound **3cg** ($(CD_3)_2SO$, 400 MHz)



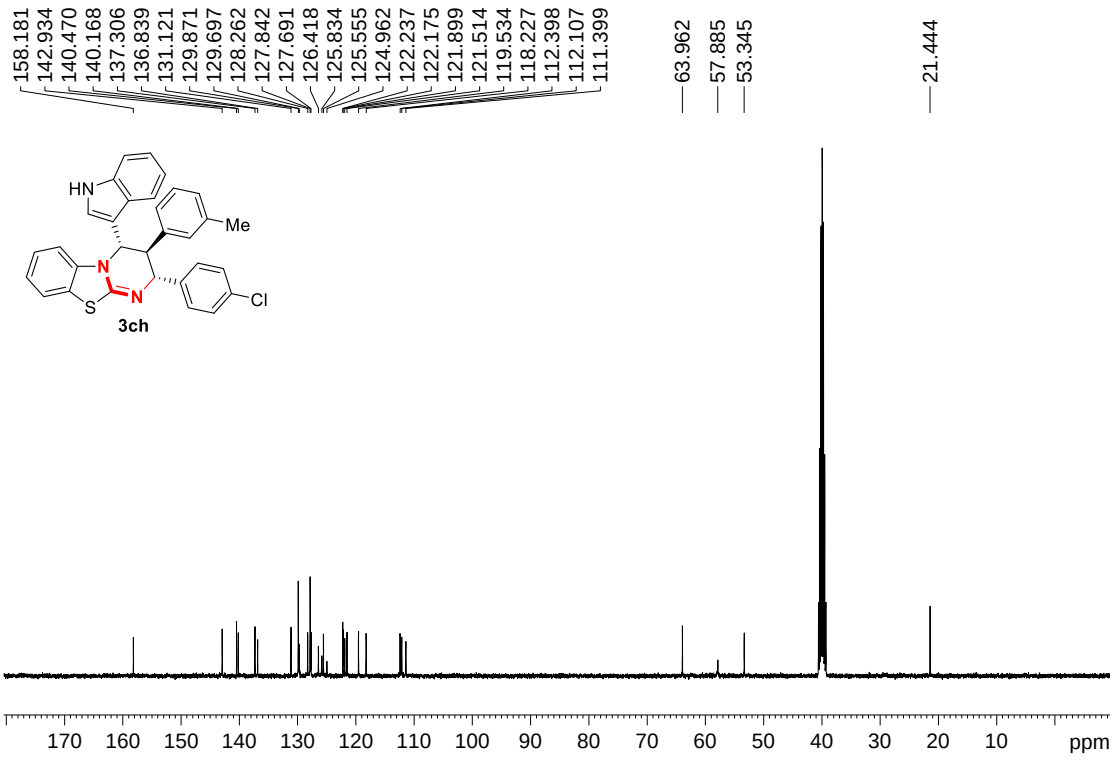
^{13}C NMR spectrum of compound **3cg** ($(CD_3)_2SO$, 100 MHz)



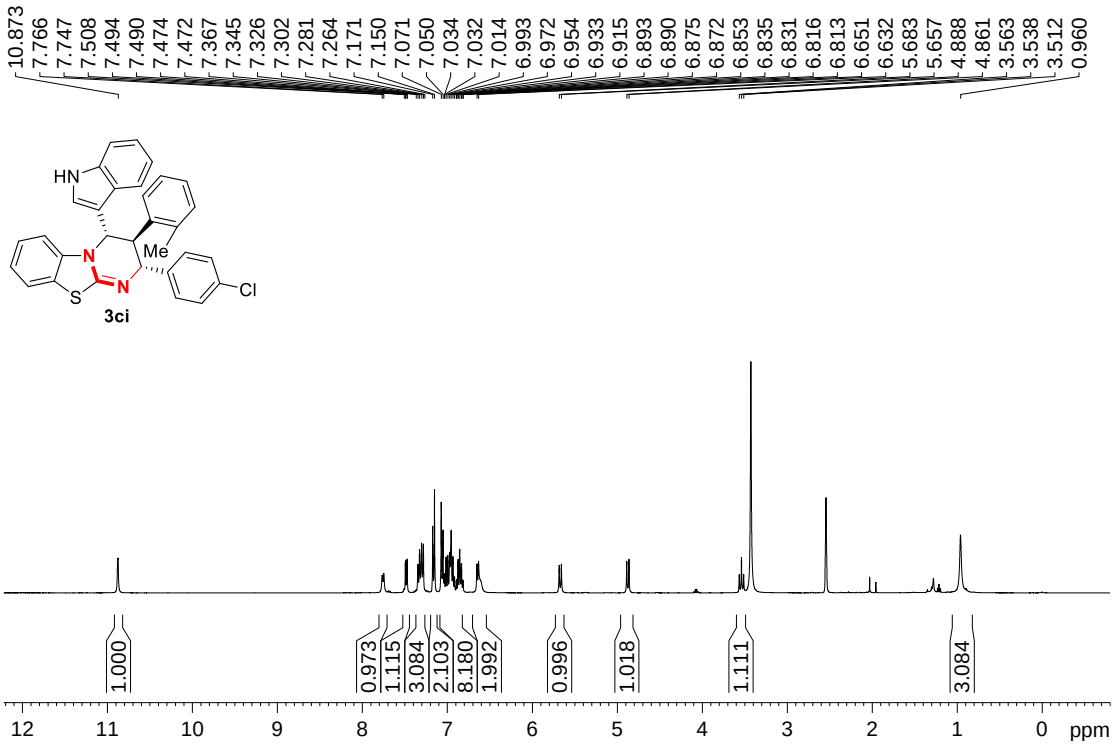
^{1}H NMR spectrum of compound **3ch** ($(CD_3)_2SO$, 400 MHz)



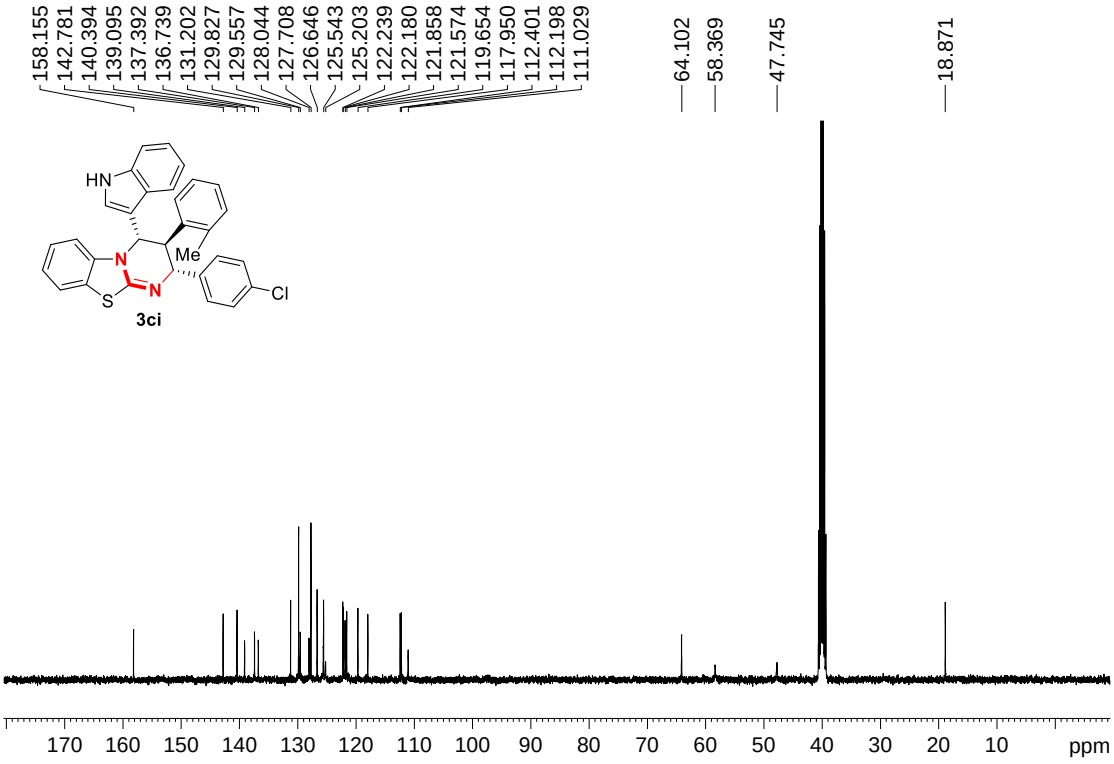
^{13}C NMR spectrum of compound **3ch** ($(CD_3)_2SO$, 100 MHz)



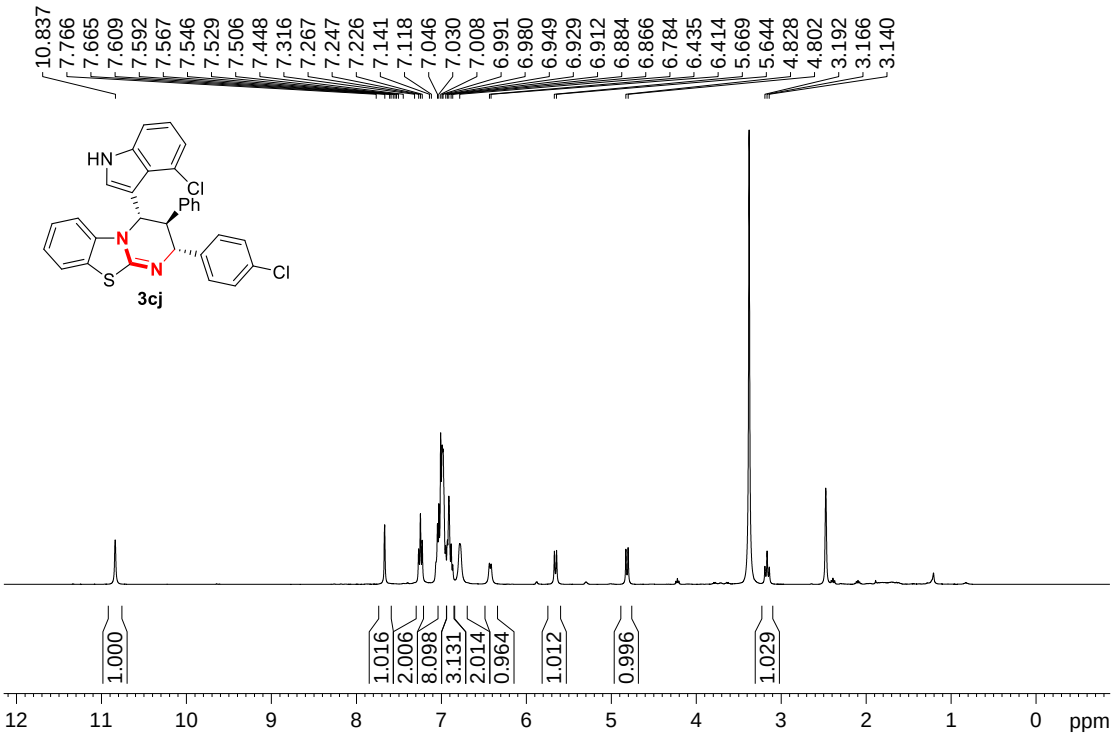
^{1}H NMR spectrum of compound **3ci** ($(CD_3)_2SO$, 400 MHz)



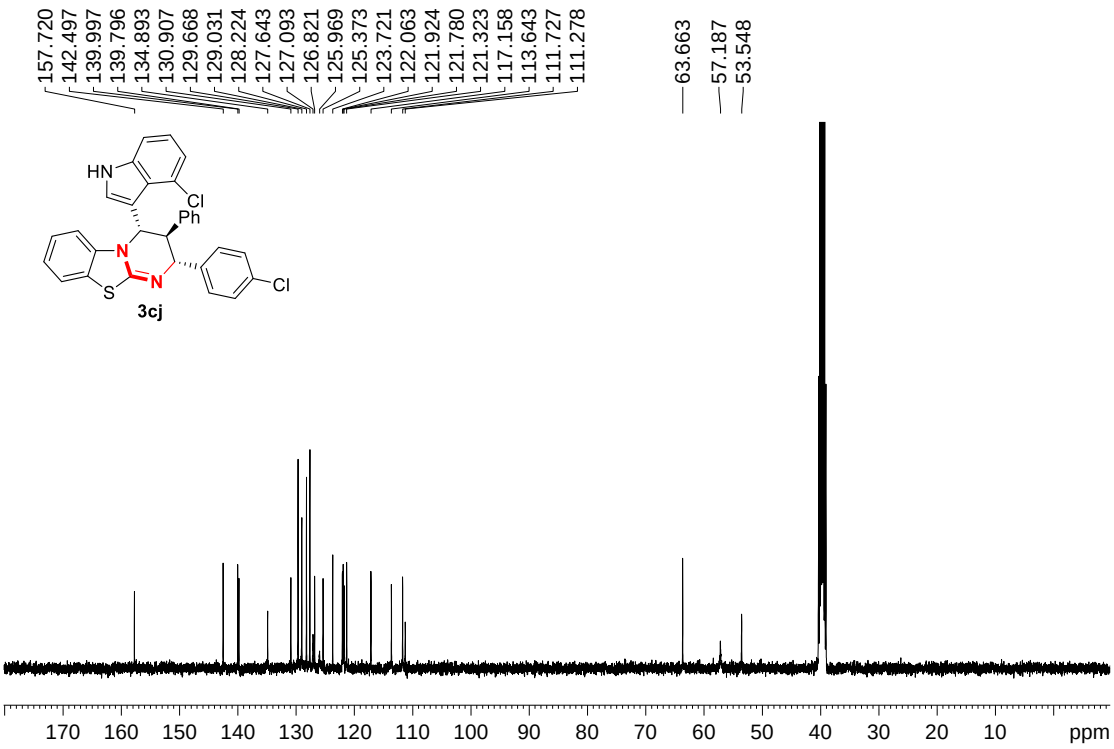
^{13}C NMR spectrum of compound **3ci** ($(CD_3)_2SO$, 100 MHz)



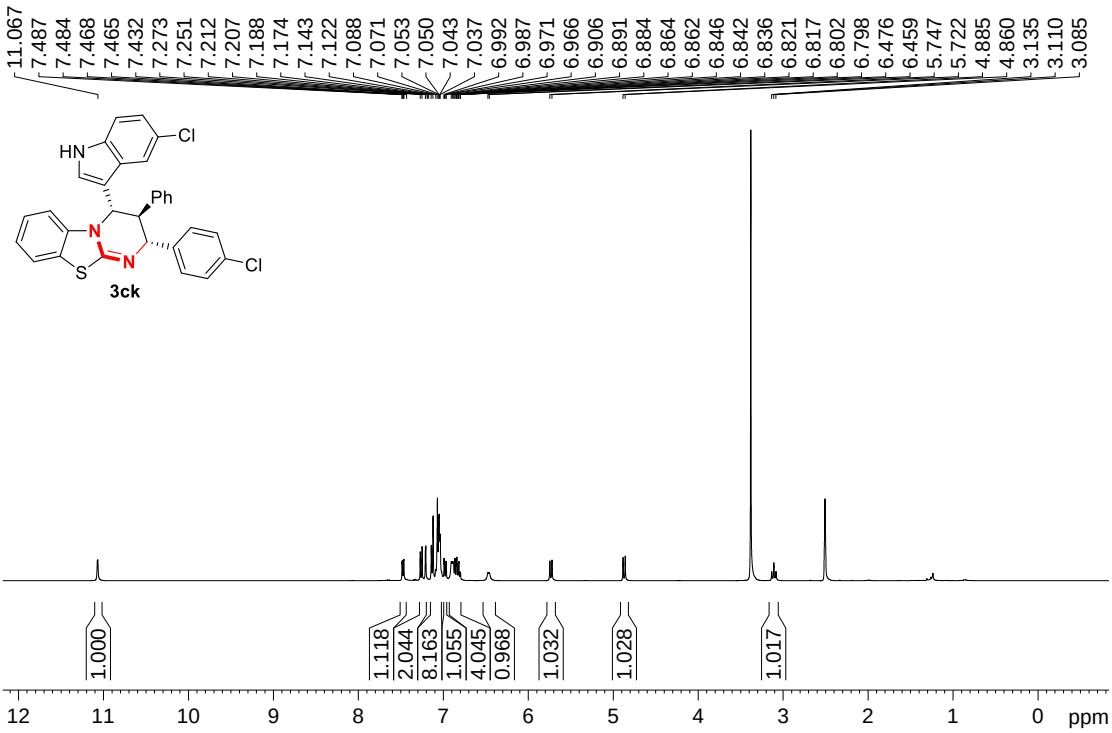
^{1}H NMR spectrum of compound **3cj** ($(CD_3)_2SO$, 400 MHz)



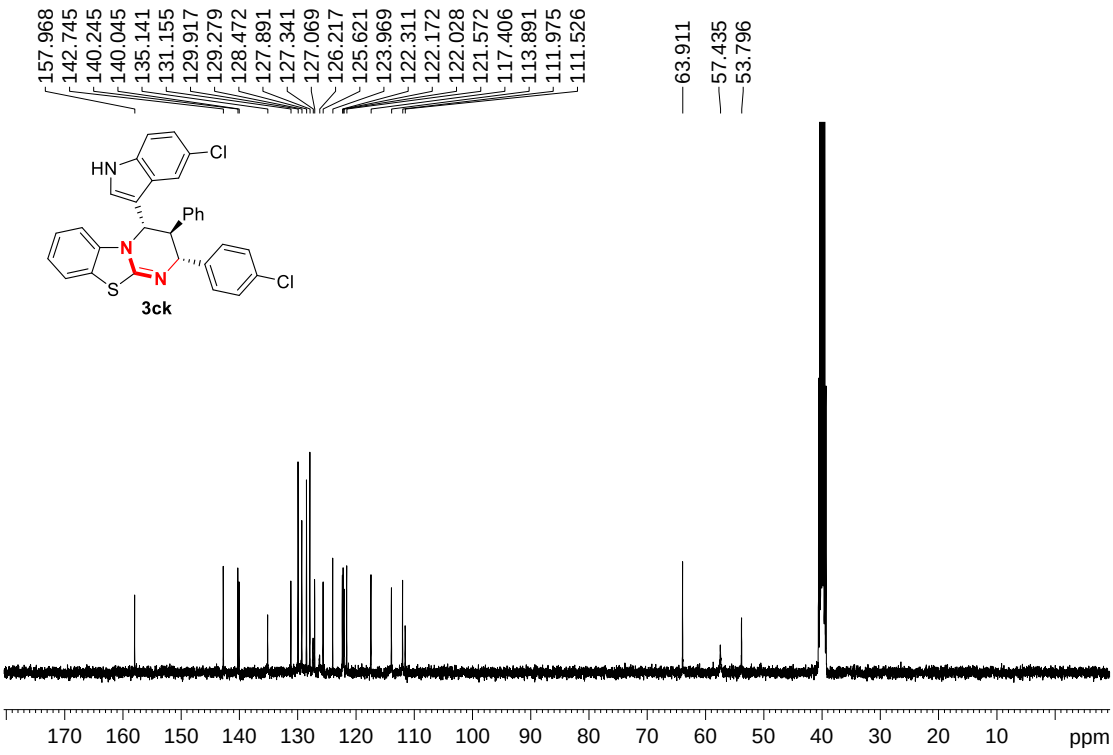
^{13}C NMR spectrum of compound **3cj** ($(CD_3)_2SO$, 100 MHz)



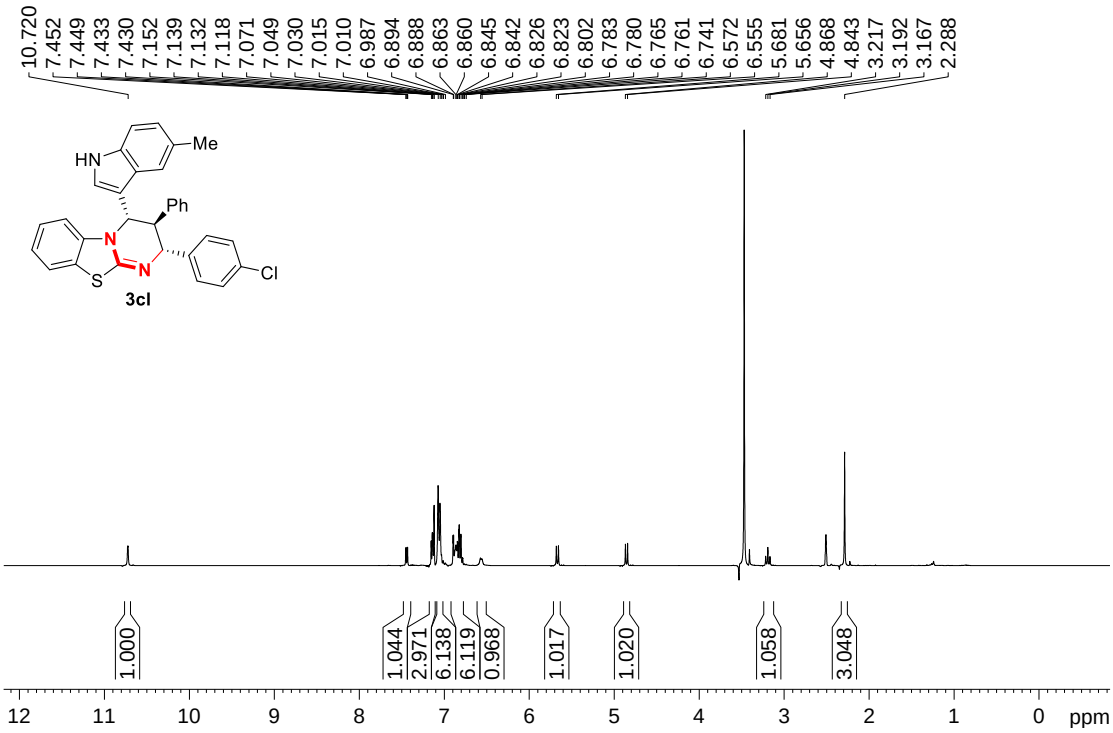
^{1}H NMR spectrum of compound **3ck** ($(CD_3)_2SO$, 400 MHz)



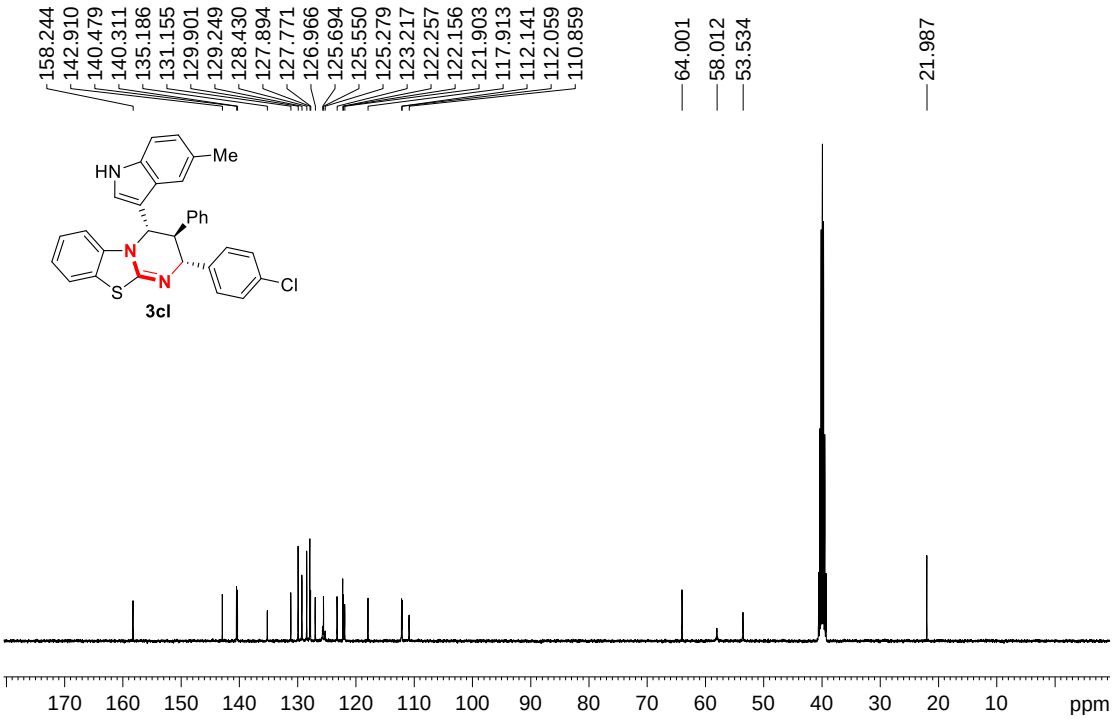
^{13}C NMR spectrum of compound **3ck** ($(CD_3)_2SO$, 100 MHz)



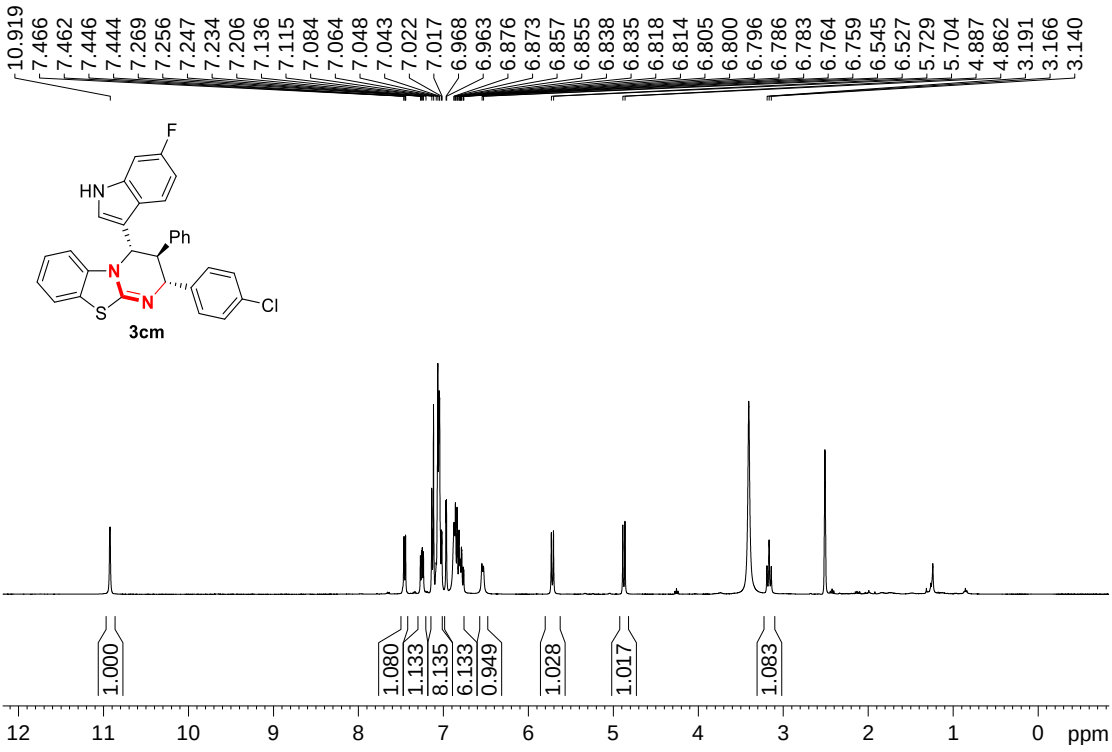
^{1}H NMR spectrum of compound **3cl** ($(CD_3)_2SO$, 400 MHz)



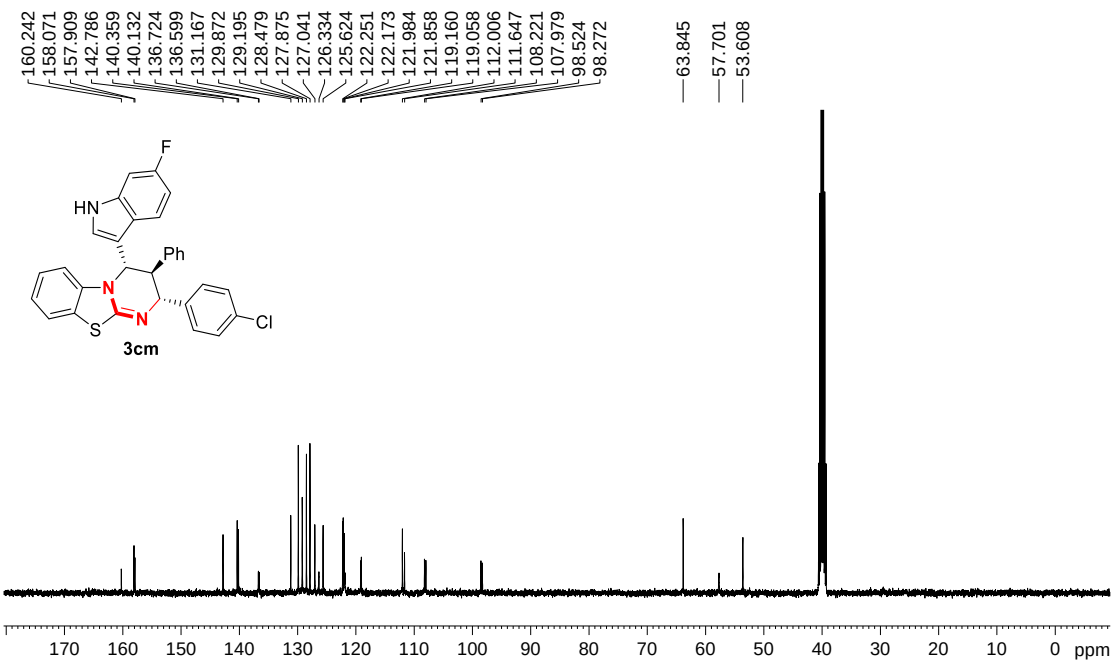
^{13}C NMR spectrum of compound **3cl** ($(CD_3)_2SO$, 100 MHz)



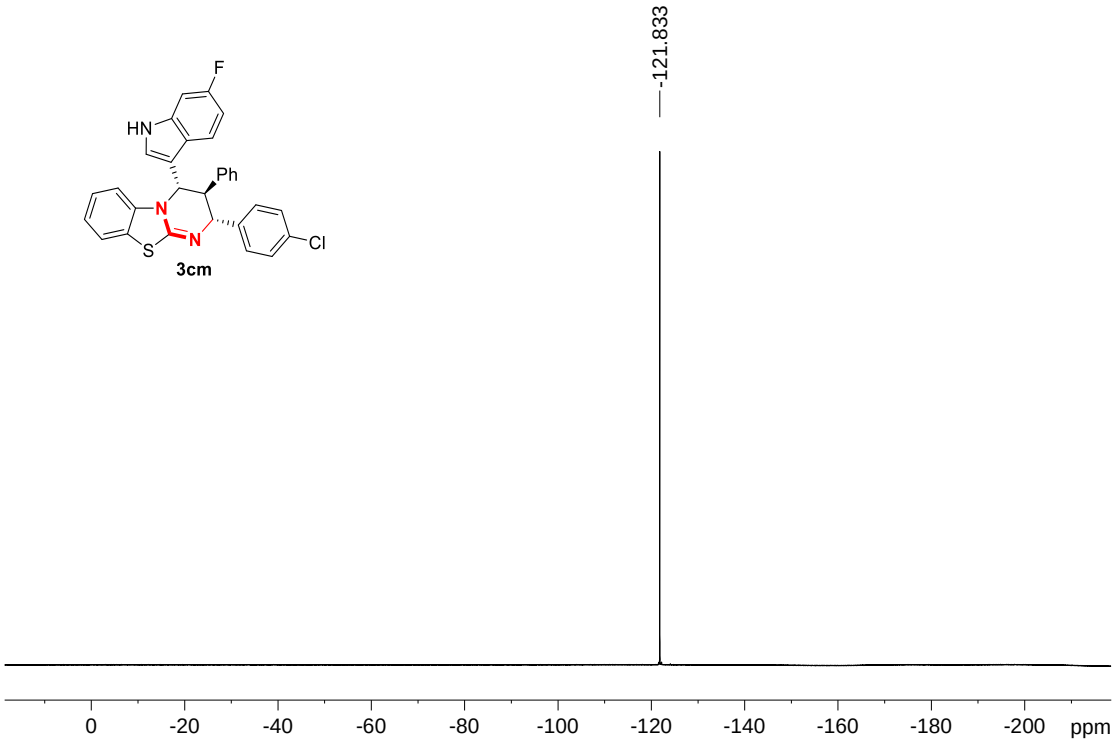
^{1}H NMR spectrum of compound **3cm** ($(CD_3)_2SO$, 400 MHz)



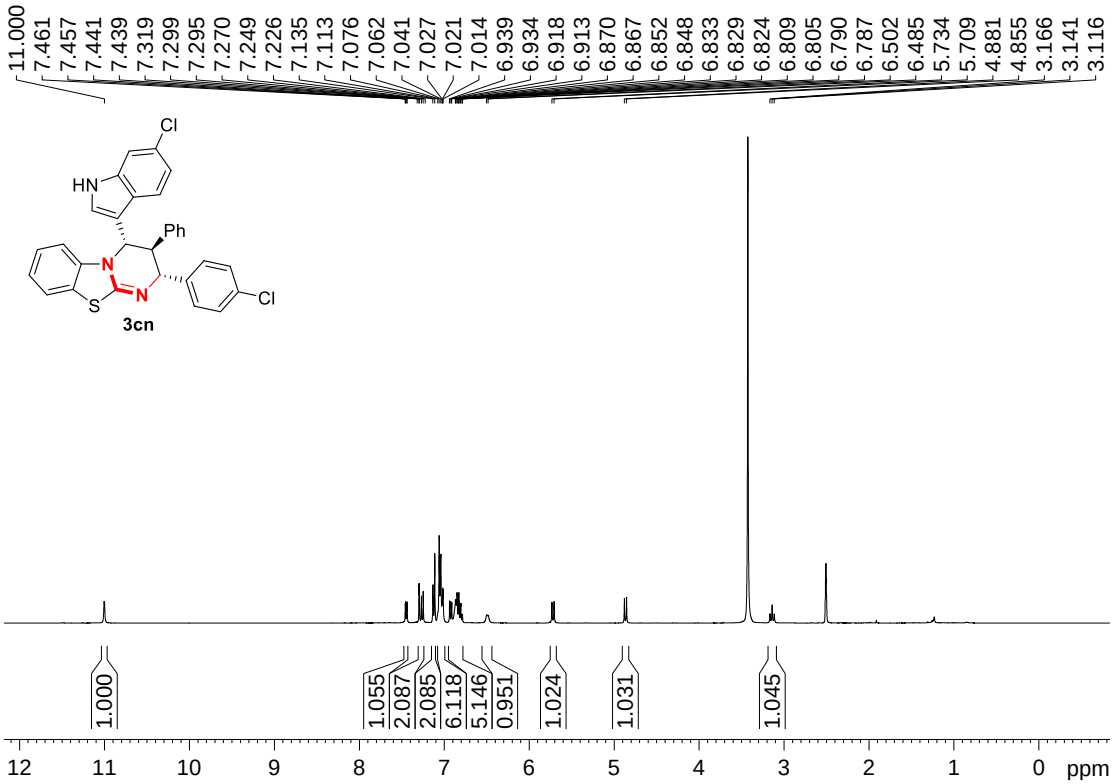
^{13}C NMR spectrum of compound **3cm** ($(CD_3)_2SO$, 100 MHz)



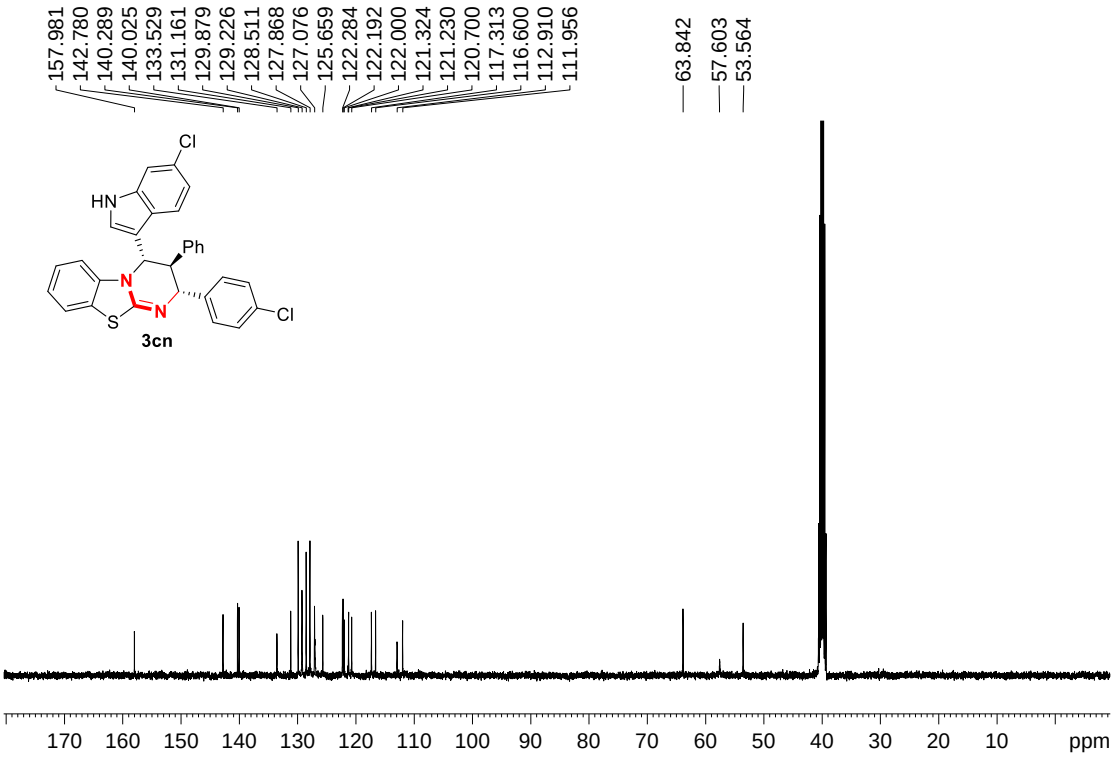
^{19}F NMR spectrum of compound **3cm** ($(CD_3)_2SO$, 376 MHz)



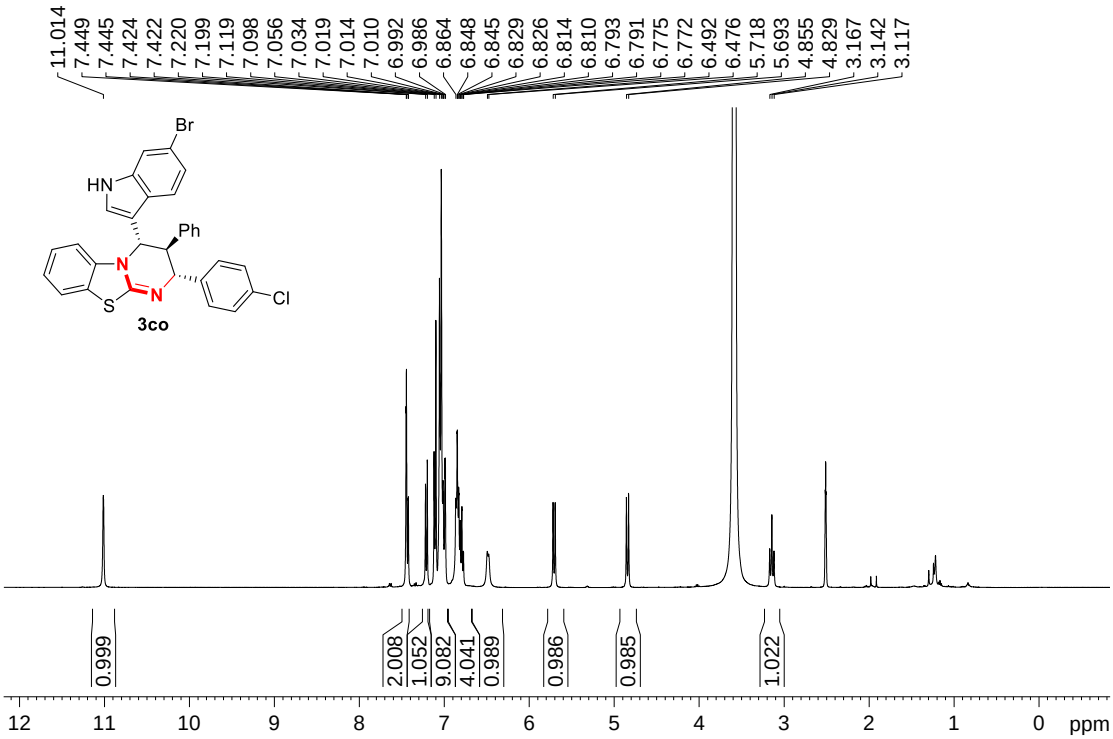
^{1}H NMR spectrum of compound **3cn** ($(CD_3)_2SO$, 400 MHz)



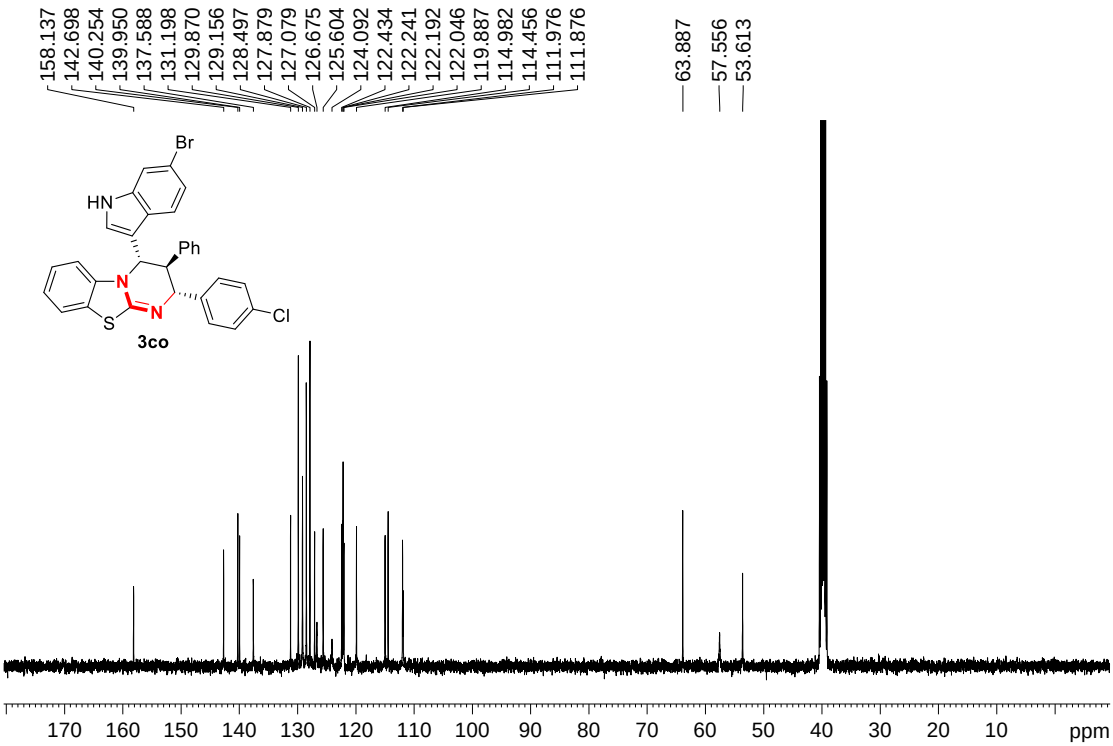
^{13}C NMR spectrum of compound **3cn** ($(CD_3)_2SO$, 100 MHz)



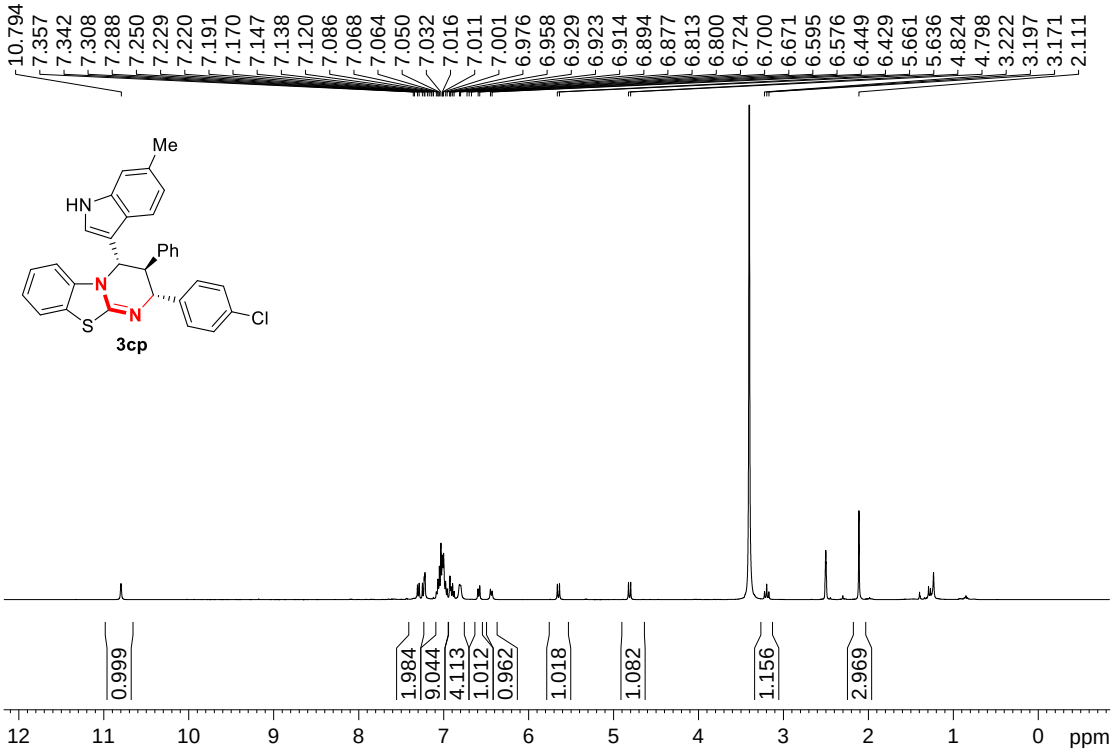
^{1}H NMR spectrum of compound **3co** ((CD$_3$)$_2$SO, 400 MHz)



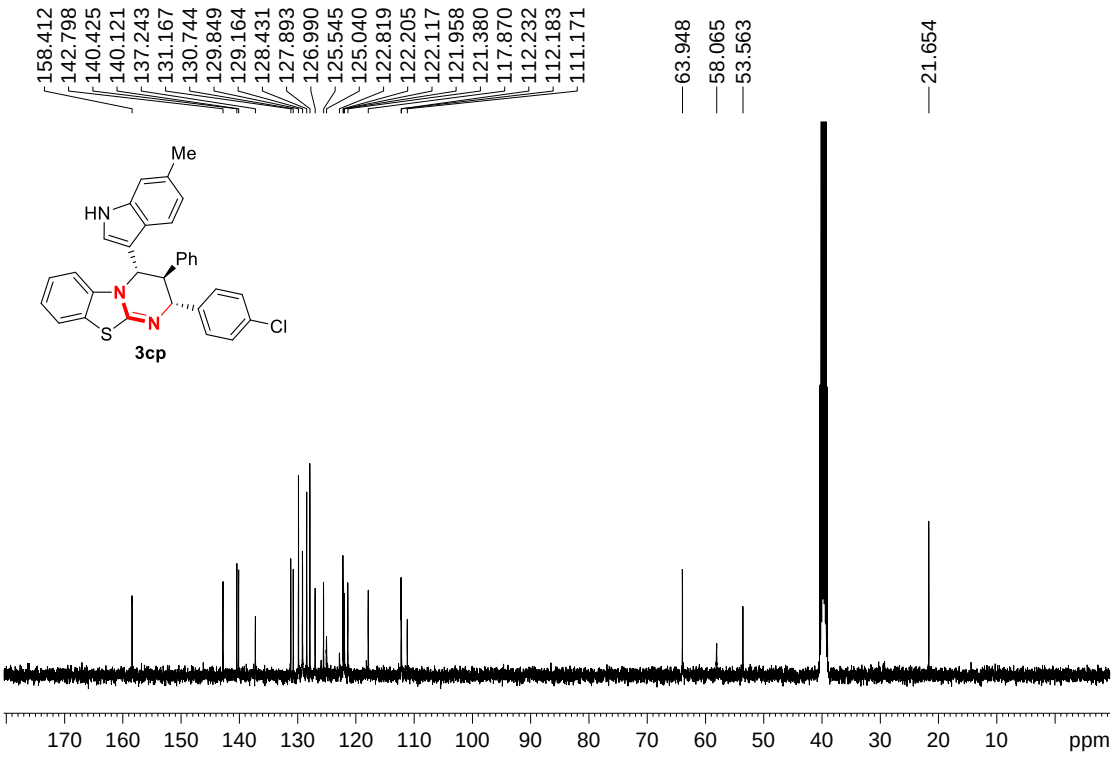
^{13}C NMR spectrum of compound **3co** ((CD$_3$)$_2$SO, 100 MHz)



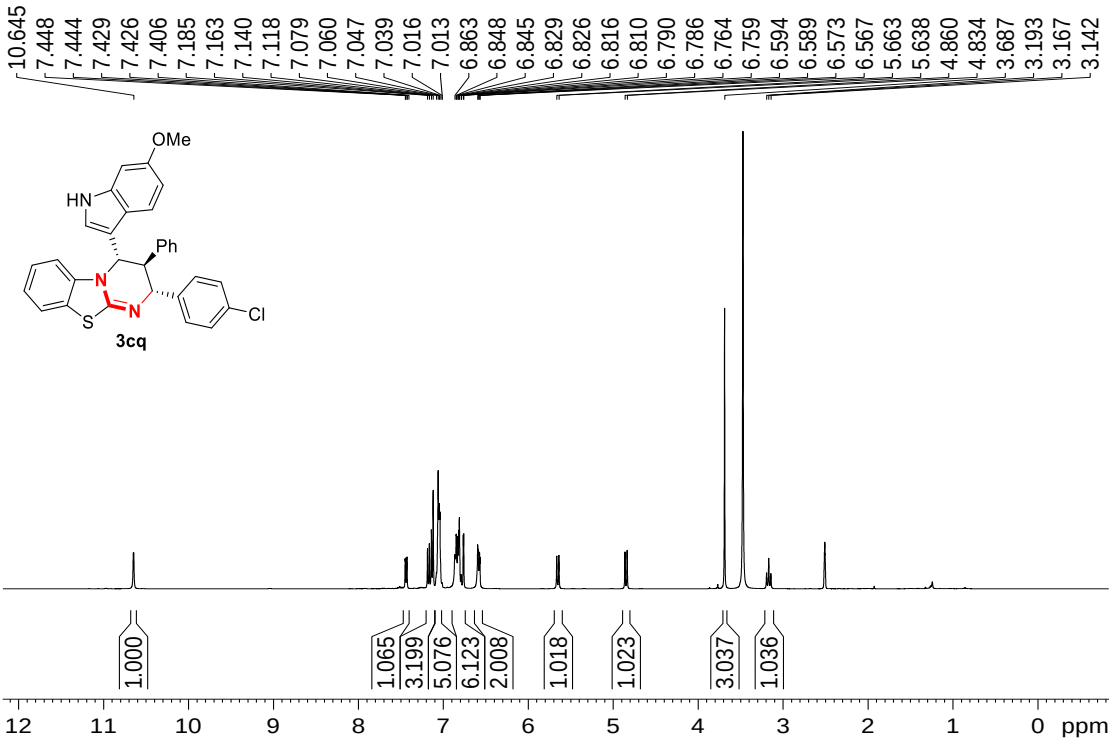
^{1}H NMR spectrum of compound **3cp** ($(CD_3)_2SO$, 400 MHz)



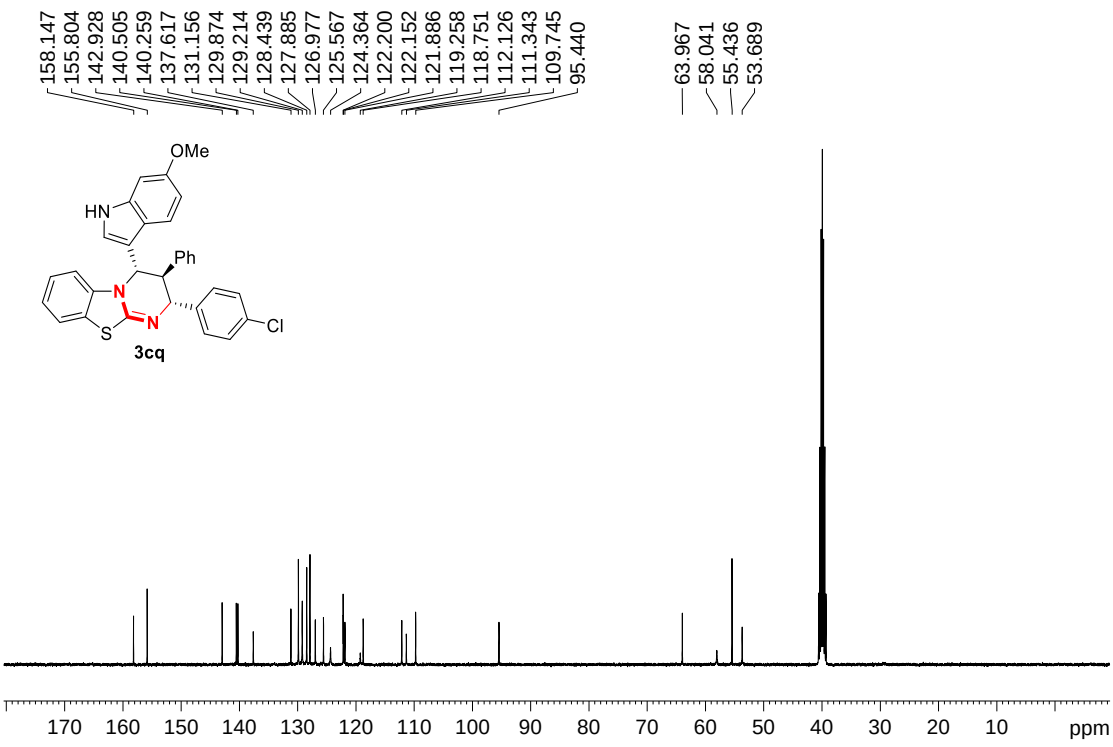
^{13}C NMR spectrum of compound **3cp** ($(CD_3)_2SO$, 100 MHz)



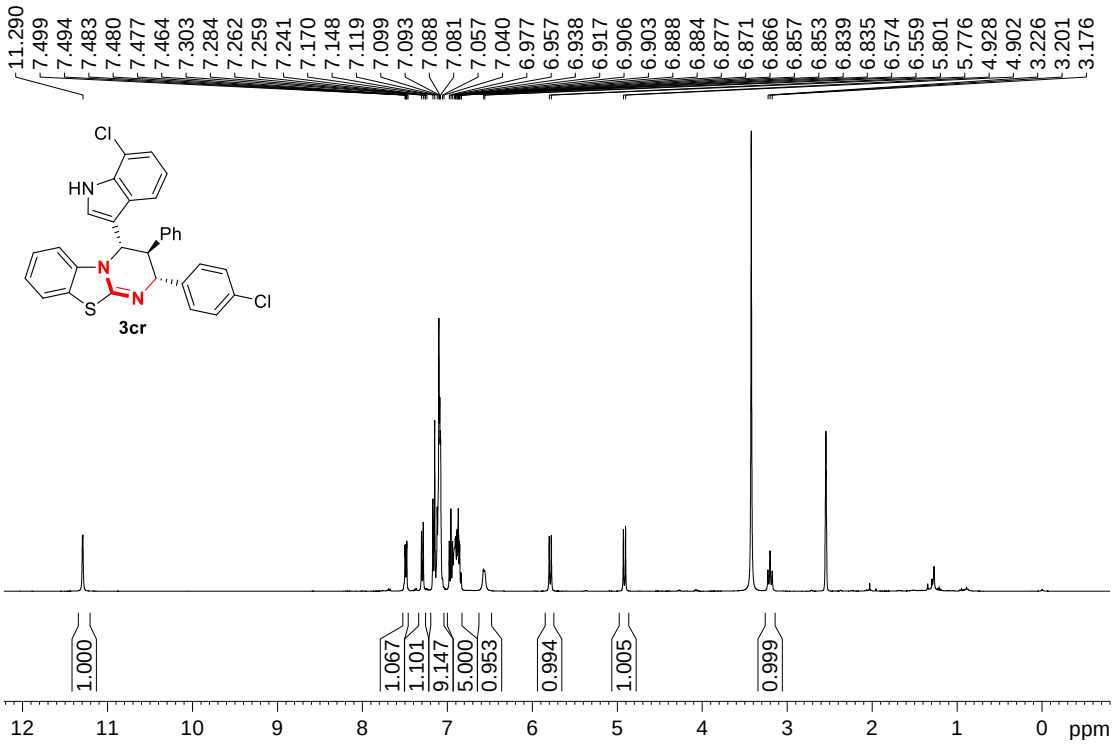
^{1}H NMR spectrum of compound **3cq** ($(CD_3)_2SO$, 400 MHz)



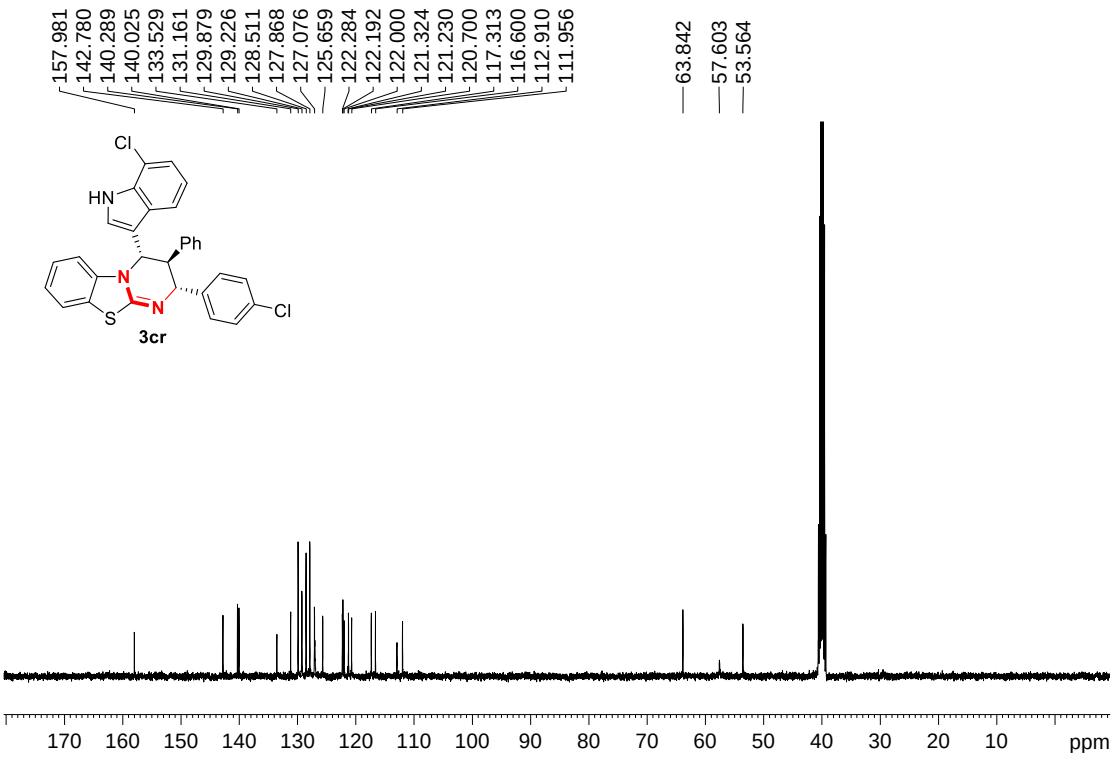
^{13}C NMR spectrum of compound **3cq** ($(CD_3)_2SO$, 100 MHz)



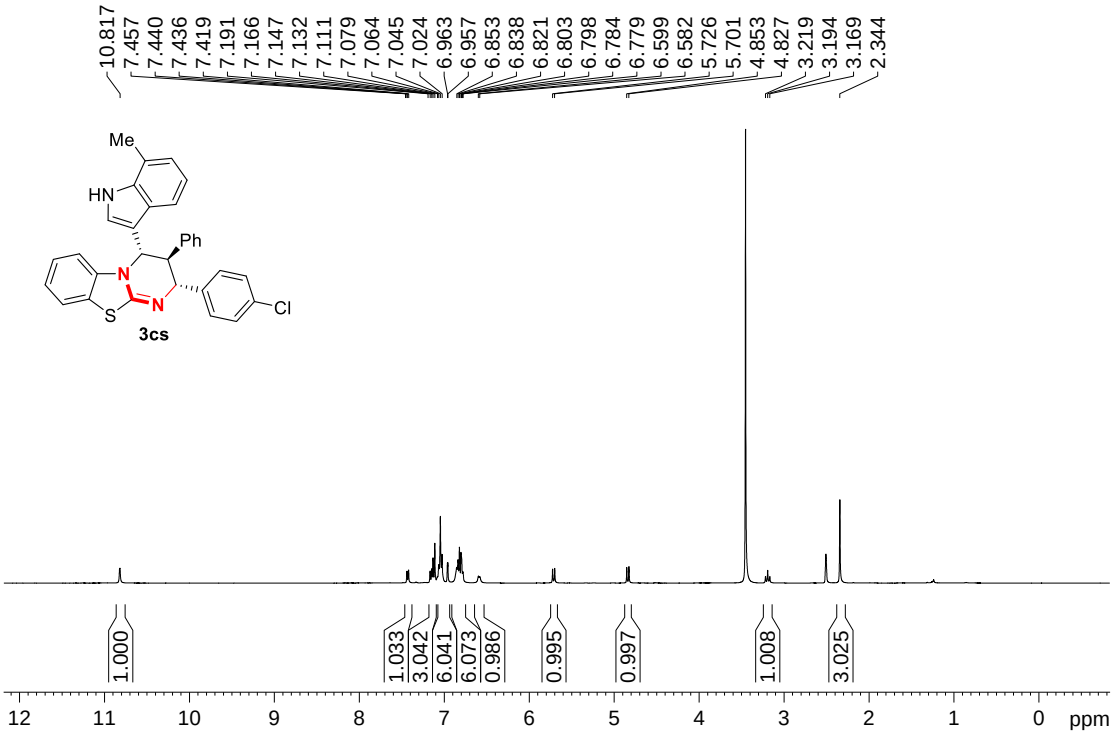
^{1}H NMR spectrum of compound **3cr** ($(CD_3)_2SO$, 400 MHz)



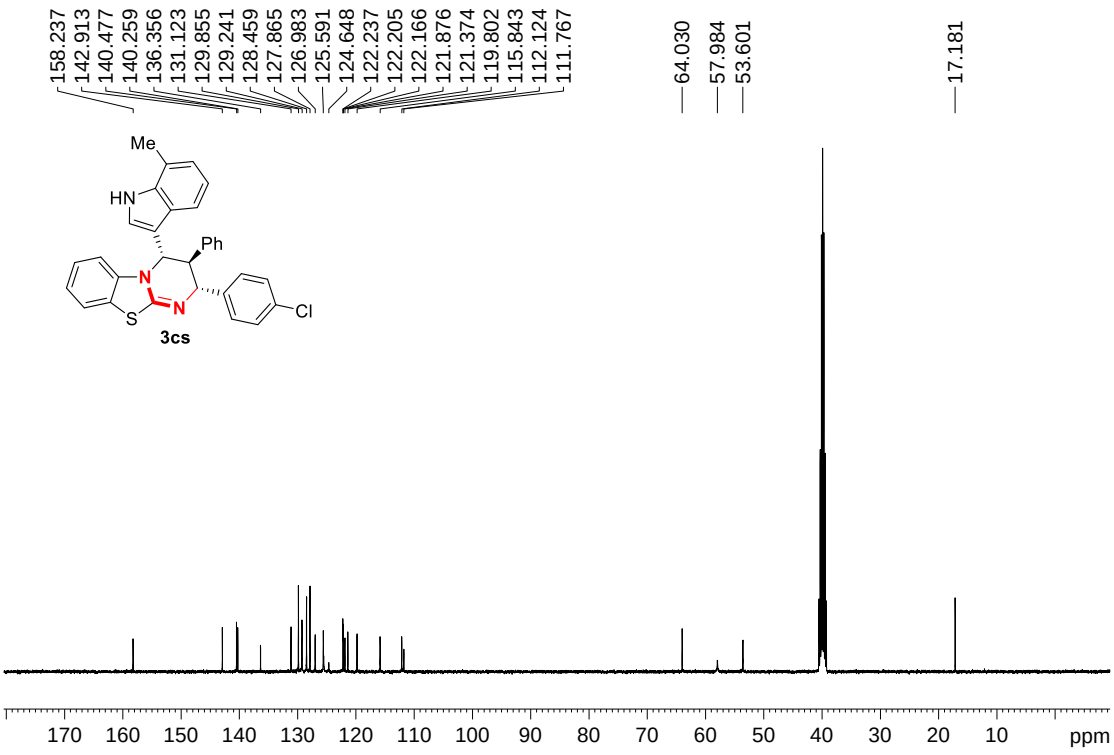
^{13}C NMR spectrum of compound **3cr** ($(CD_3)_2SO$, 100 MHz)



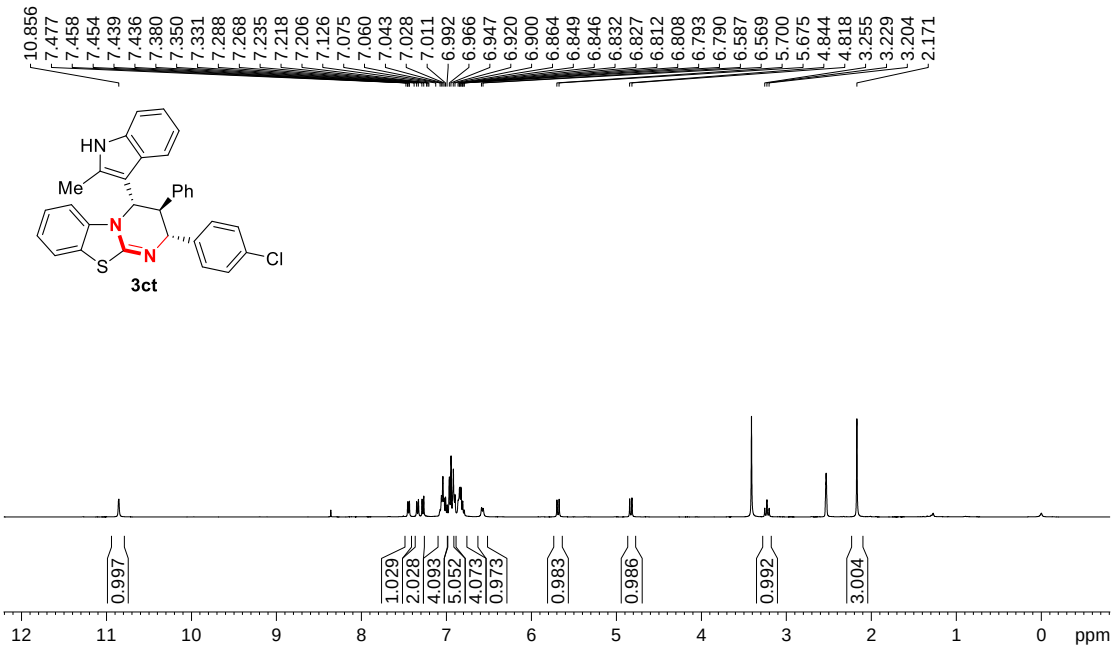
^{1}H NMR spectrum of compound **3cs** ($(CD_3)_2SO$, 400 MHz)



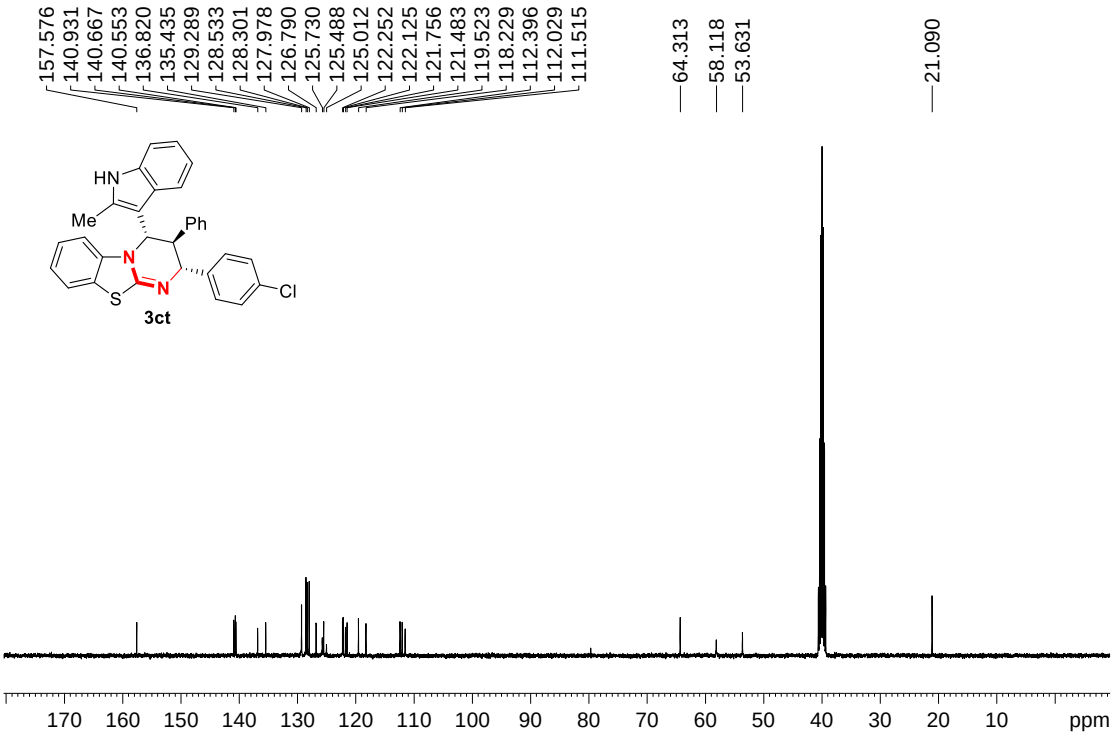
^{13}C NMR spectrum of compound **3cs** ($(CD_3)_2SO$, 100 MHz)



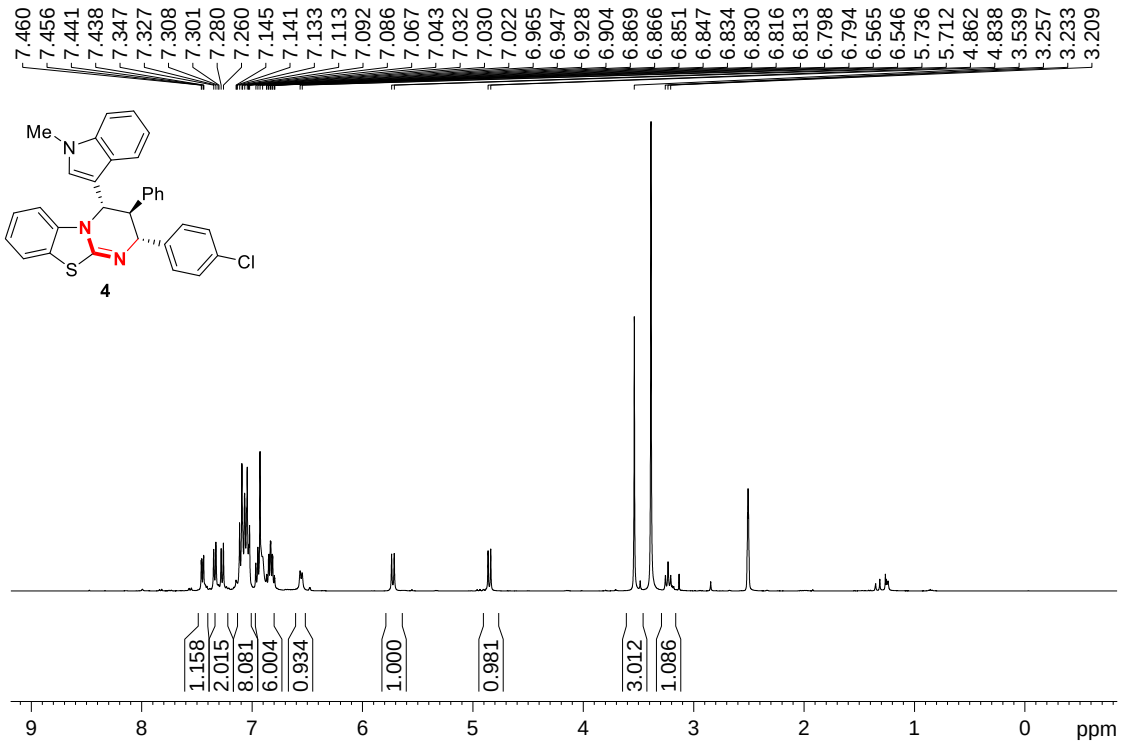
^{1}H NMR spectrum of compound **3ct** ($(CD_3)_2SO$, 400 MHz)



^{13}C NMR spectrum of compound **3ct** ($(CD_3)_2SO$, 100 MHz)



^{1}H NMR spectrum of compound **4** ($(CD_3)_2SO$, 400 MHz)



^{13}C NMR spectrum of compound **4** ($(CD_3)_2SO$, 100 MHz)