Supplementary Information

Reversal of Enantioselectivity by Tuning the Ring Size of ProPhenol

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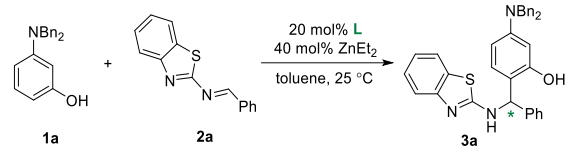
Contents

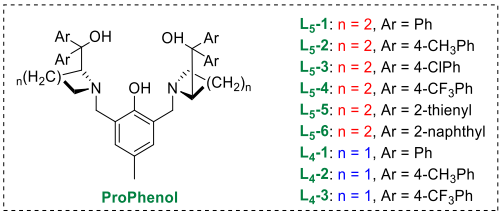
1. General information

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 $CDCl_3$ and DMSO as the solvent and TMS as an internal standard (400 MHz for ^1H 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). 3-(dibenzylamino)phenols **1**[1] and *N*-(benzo[*d*]thiazol-2-yl)-1-phenylmeth-animines **2**[2] were either employed directly from commercial sources or prepared according to the literature.

2. Representative procedures

1) Effect of ligands (Table S1)

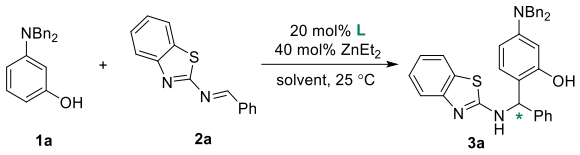




Entry[a]	Ligand	Time (h)	Yield (%)[b]	*ee* (%)[c]
1	**L_5-1**	24	60	30 (*R*)
2	**L_5-2**	24	56	18 (*R*)
3	**L_5-3**	24	65	59 (*R*)
4	**L_5-4**	24	87	60 (*R*)
5	**L_5-5**	24	55	14 (*R*)
6	**L_5-6**	24	55	17 (*R*)
7	**L_4-1**	24	42	12 (*S*)
8	**L_4-2**	24	43	10 (*S*)
9	**L_4-3**	24	93	84 (*S*)

[a]Reaction conditions: **1a** (0.05 mmol), **2a** (0.075 mmol), ligands (20 mol%), $ZnEt_2$ (40 mol%) in a specified solvent (1 mL) under N_2 at 25 °C for 24 h. [b]Isolated yields. [c]Determined by chiral HPLC analysis.

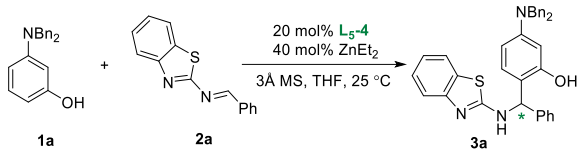
2) Effect of solvents (Table S2)



Entry[a]	Solvent	Time (h)	Yield (%)[b]	*ee* (%)[c]
1	CH_2Cl_2	24	82/95	40 (*R*)/96 (*S*)
2	CH_3CN	24	72/70	79 (*R*)/89 (*S*)
3	THF	24	86/85	85 (*R*)/80 (*S*)
4	Toluene	24	87/93	60 (*R*)/84 (*S*)
5	$CHCl_3$	24	68/65	37 (*R*)/87 (*S*)
6	1,4-dioxane	24	77/69	35 (*R*)/85 (*S*)

[a]Reaction conditions: **1a** (0.05 mmol), **2a** (0.075 mmol), ligand (20 mol%), $ZnEt_2$ (40 mol%) in a specified solvent (1 mL) under N_2 at 25 °C for 24 h. [b]Isolated yields. [c]Determined by chiral HPLC analysis.

3) Effect of additives (Table S3)

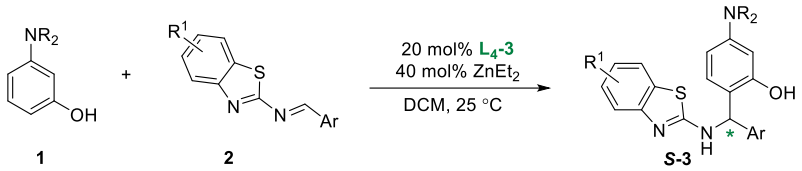


Entry[a]	Additive (20mg)	Time (h)	Yield (%)[b]	*ee* (%)[c]
1	None	24	86	85 (*R*)
2	3Å MS	24	92	92 (*R*)
3	4Å MS	24	56	46 (*R*)
4	5Å MS	24	48	37 (*R*)

[a]Reaction conditions: **1a** (0.05 mmol), **2a** (0.075 mmol), ligand (20 mol%), $ZnEt_2$ (40 mol%) in a specified solvent (1 mL) under N_2 at 25 °C for 24 h. [b]Isolated yields. [c]Determined by chiral HPLC analysis.

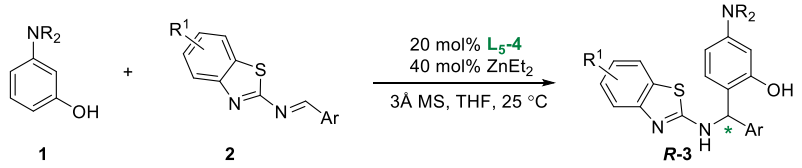
3. General procedures

1)Synthesis of ***S*-3**



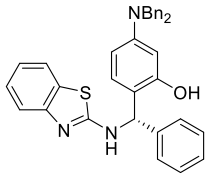
In a flame-dried Schlenk tube, a solution of diethylzinc (0.04 mL, 1.0 mol/L in hexane, 0.02 mmol) was added to a solution of the chiral ligand **L4-3** (0.02 mmol) in dry DCM (2.0 mL) under nitrogen at 25 °C. The mixture was stirred at 25 °C for 30 min. Then, 3-(dibenzylamino)phenol **1** (0.1 mmol) and *N*-(benzo[*d*]thiazol-2-yl)-1-phenylmeth-animine **2** (0.15 mmol) were added under an argon atmosphere. The solution was stirred at 25 °C for 24 h, and then quenched with aqueous NH_4Cl (5 mL), and extracted three times with EA (3 × 10 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 8:1).

2)Synthesis of ***R*-3**



In a flame-dried Schlenk tube, a solution of diethylzinc (0.04 mL, 1.0 mol/L in hexane, 0.02 mmol) was added to a solution of the chiral ligand **L5-4** (0.02 mmol) and 3Å MS (40 mg) in dry THF (2.0 mL) under nitrogen at 25 °C. The mixture was stirred at 25 °C for 30 min. Then, 3-(dibenzylamino)phenol **1** (0.1 mmol) and *N*-(benzo[*d*]thiazol-2-yl)-1-phenylmethanimine **2** (0.15 mmol) were added under an argon atmosphere. The solution was stirred at 25 °C for 24 h, and then quenched with aqueous NH_4Cl (5 mL), and extracted three times with EA (3 × 10 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 8:1).

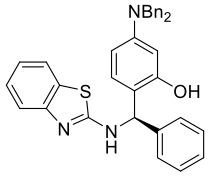
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(dibenzylamino)phenol 3a:



(*S*)-3a

White solid, M.p.: 156 – 157 °C; yield: 95%; $[\alpha]^{20}_D$ = -150 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.39 min (minor), t_2 = 8.12 min (major), *ee* = 96%; ^{1}H NMR (400 MHz, DMSO) δ 9.36 (s, 1H), 8.63 (d, *J* = 8.3 Hz, 1H), 7.65 – 7.63 (m, 1H), 7.37 – 7.16 (m, 17H), 7.01 – 6.99 (m, 1H), 6.86 (d, *J* = 8.6 Hz, 1H), 6.42 (d, *J* = 8.2 Hz, 1H), 6.23 (d, *J* = 2.4 Hz, 1H), 6.16 – 6.13 (m, 1H), 4.62 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 165.7, 155.6, 152.8, 149.2, 143.8, 139.5, 130.9, 129.0, 128.6, 127.3, 127.2, 127.0, 126.9, 125.9, 121.3, 118.5, 117.2, 103.9, 99.6, 55.3, 54.5. HRMS (ESI) calcd for $C_{34}H_{30}N_3OS^+$ $[M+H]^+$ 528.2104, found 528.2102.

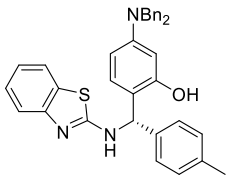
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(dibenzylamino)phenol 3a:



(*R*)-3a

White solid, yield: 92%; $[\alpha]^{20}_D$ = +146 (*c* 0.42, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.39 min (major), t_2 = 8.14 min (minor), *ee* = 92%.

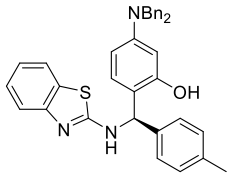
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(*p*-tolyl)methyl)-5-(dibenzylamino)phenol 3b:



(*S*)-3b

White solid, M.p.: 109 – 110 °C; yield: 94%; $[\alpha]^{20}_D$ = -281 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.03 min (minor), t_2 = 8.74 min (major), *ee* = 95%; ^{1}H NMR (400 MHz, DMSO) δ 9.29 (s, 1H), 8.56 (d, *J* = 8.3 Hz, 1H), 7.64 – 7.62 (m, 1H), 7.35 - 7.31 (m, 5H), 7.27 – 7.16 (m, 9H), 7.08 (d, *J* = 8.0 Hz, 2H), 7.00 – 6.96 (m, 1H), 6.84 (d, *J* = 8.6 Hz, 1H), 6.35 (d, *J* = 8.2 Hz, 1H), 6.21 (d, *J* = 2.4 Hz, 1H), 6.15 – 6.12 (m, 1H), 4.62 (s, 4H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 165.8, 155.6, 152.9, 1491, 140.8, 139.5, 135.9, 131.0, 129.1, 129.0, 127.2, 127.2, 127.0, 125.9, 121.3, 121.3, 118.4, 117.4, 104.8, 99.6, 55.1, 54.5, 21.1. HRMS (ESI) calcd for $C_{35}H_{32}N_3OS^+$ $[M+H]^+$ 542.2261, found 542.2268.

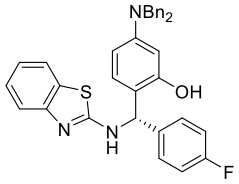
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(*p*-tolyl)methyl)-5-(dibenzylamino)phenol 3b:



(*R*)-3b

White solid, yield: 89%; $[\alpha]^{20}_D$ = +268 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.27 min (major), t_2 = 9.14 min (minor), *ee* = 92%.

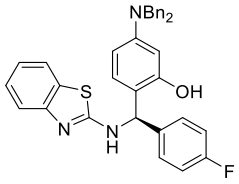
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(4-fluorophenyl)methyl)-5-(dibenzylamino)phenol 3c:



(*S*)-3c

White solid, M.p.: 100 – 111 °C; yield: 91%; $[\alpha]^{20}_D$ = -111 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 5.71 min (minor), t_2 = 7.70 min (major), *ee* = 92%; ^{1}H NMR (400 MHz, DMSO) δ 9.37 (s, 1H), 8.64 (d, *J* = 8.2 Hz, 1H), 7.66 – 7.63 (m, 1H), 7.40 – 7.31 (m, 7H), 7.28 – 7.09 (m, 9H), 7.02 – 6.98 (m, 1H), 6.88 (d, *J* = 8.6 Hz, 1H), 6.41 (d, *J* = 8.2 Hz, 1H), 6.27 – 6.12 (m, 2H), 4.63 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 165.8, 162.6, 160.2 (*J* = 241 Hz), 155.6, 152.8, 149.2, 140.0, 139.9, 139.5, 139.4, 130.9, 129.2, 129.1, 129.0, 128.8, 127.2, 127.0, 126.0, 121.4, 121.3, 118.5, 117.0, 115.4, 115.2, 104.0, 99.6, 54.9, 54.6; ^{19}F NMR (376 MHz, DMSO) δ -116.59; HRMS (ESI) calcd for $C_{34}H_{29}FN_3OS^+$ $[M+H]^+$ 546.2010, found 546.2008.

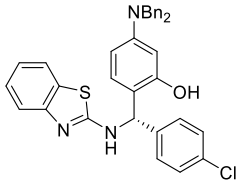
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(4-fluorophenyl)methyl)-5-(dibenzylamino)phenol 3c:



(*R*)-3c

White solid, yield: 90%; $[\alpha]^{20}_D$ = +136 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 5.79 min (major), t_2 = 7.51 min (minor), *ee* = 98%.

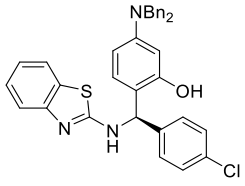
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(4-chlorophenyl)methyl)-5-(dibenzylamino)phenol 3d:



(*S*)-3d

White solid, M.p.: 127 – 128 °C; yield: 96%; $[\alpha]^{20}_D$ = -106 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 5.91 min (minor), t_2 = 8.30 min (major), *ee* = 91%; ^{1}H NMR (400 MHz, DMSO) δ 9.42 (s, 1H), 8.63 (d, *J* = 8.1 Hz, 1H), 7.67 – 7.58 (m, 1H), 7.39 – 7.28 (m, 9H), 7.27 – 7.14 (m, 7H), 7.02 – 7.00 (m, 1H), 6.85 (d, *J* = 8.6 Hz, 1H), 6.40 (d, *J* = 8.0 Hz, 1H), 6.24 (d, *J* = 2.1 Hz, 1H), 6.16 – 6.14 (m, 1H), 4.62 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 165.8, 155.6, 152.7, 149.3, 142.8, 139.4, 131.4, 130.9, 129.1, 129.0, 128.5, 127.2, 127.0, 126.0, 121.5, 121.3, 118.6, 116.7, 104.1, 99.6, 55.0, 54.5; HRMS (ESI) calcd for $C_{34}H_{29}ClN_3OS^+$ $[M+H]^+$ 562.1714, found 562.1716.

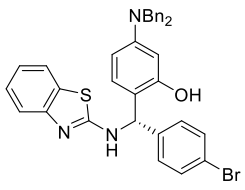
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(4-chlorophenyl)methyl)-5-(dibenzylamino)phenol 3d:



(*R*)-3d

White solid; yield: 93%; $[\alpha]^{20}_D$ = +137 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 5.82 min (major), t_2 = 7.79 min (minor), *ee* = 97%.

(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(4-bromophenyl)methyl)-5-(dibenzylamino)phenol 3e:

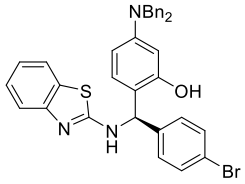


(*S*)-3e

White solid, M.p.: 116 – 117 °C; yield: 90%; $[\alpha]^{20}_D$ = -144 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.13 min (major), t_2 = 8.05 min (minor), *ee* = 95%; ^{1}H NMR (400 MHz, DMSO) δ 9.40 (s, 1H), 8.63 (d, *J* = 8.1 Hz, 1H), 7.66 – 7.64 (m, 1H), 7.48 (d, *J* = 8.5 Hz, 2H), 7.35 – 7.17 (m , 14H), 7.02 – 6.98 (m, 2H), 6.39 (d, *J* = 8.0 Hz, 1H), 6.24 (d, *J* = 2.4 Hz, 1H), 6.17

– 6.14 (m, 1H), 4.63 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 165.8, 155.6, 152.8, 149.3, 143.3, 139.4, 131.5, 131.0, 129.5, 129.0, 127.2, 127.0, 126.0, 121.4, 121.3, 119.9, 118.7, 116.6, 104.0, 99.6, 55.0, 54.5; HRMS (ESI) calcd for $C_{34}H_{29}BrN_3OS^+$ $[M+H]^+$ 606.1209, found 606.1210.

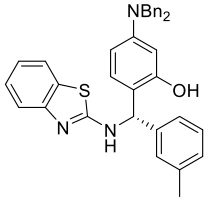
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(4-bromophenyl)methyl)-5-(dibenzylamino)phenol 3e:



(*R*)-3e

White solid; yield: 85%; $[\alpha]^{20}_D$ = +120 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.46 min (major), t_2 = 8.42 min (minor), *ee* = 91%.

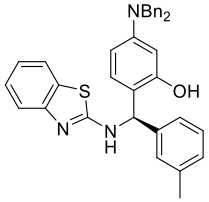
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(*m*-tolyl)methyl)-5-(dibenzylamino)phenol 3f:



(*S*)-3f

White solid, M.p.: 100 – 101 °C; yield: 92%; $[\alpha]^{20}_D$ = -171 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.17 min (minor), t_2 = 8.33 min (major), *ee* = 80%; ^{1}H NMR (400 MHz, DMSO) δ 9.32 (s, 1H), 8.58 (d, *J* = 8.3 Hz, 1H), 7.64 – 7.62 (m, 1H), 7.37 – 7.29 (m, 5H), 7.27 – 7.09 (m, 10H), 7.02 – 6.95 (m, 2H), 6.85 (d, *J* = 8.6 Hz, 1H), 6.38 (d, *J* = 8.2 Hz, 1H), 6.25 – 6.10 (m, 2H), 4.61 (d, *J* = 6.5 Hz, 4H), 2.25 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 165.9, 155.6, 152.9, 149.1, 143.8, 139.6, 139.5, 137.5, 131.0, 129.0, 128.5, 128.1, 127.9, 127.6, 127.2, 127.1, 127.0, 125.9, 124.4, 121.3, 118.4, 117.3, 104.0, 99.6, 55.3, 54.5, 21.6; HRMS (ESI) calcd for $C_{35}H_{32}N_3OS^+$ $[M+H]^+$ 542.2261, found 542.2266.

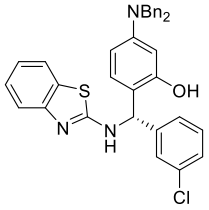
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(*m*-tolyl)methyl)-5-(dibenzylamino)phenol 3f:



(*R*)-3f

White solid; yield: 91%; $[\alpha]^{20}_D$ = +190 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.62 min (major), t_2 = 8.31 min (minor), *ee* = 90%.

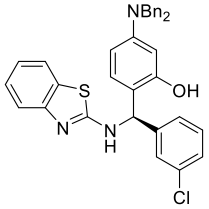
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(3-chlorophenyl)methyl)-5-(dibenzylamino)phenol 3g:



(*S*)-3g

White solid, M.p.: 135 – 136 °C; yield: 90%; $[\alpha]^{20}_D$ = -367 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 5.58 min (minor), t_2 = 6.99 min (major), *ee* = 90%; ^{1}H NMR (400 MHz, DMSO) δ 9.44 (s, 1H), 8.66 (d, *J* = 8.2 Hz, 1H), 7.64 (d, *J* = 7.3 Hz, 1H), 7.40 – 7.28 (m, 8H), 7.26 – 7.15 (m, 8H), 7.04 – 6.96 (m, 1H), 6.88 (d, *J* = 8.6 Hz, 1H), 6.43 (d, *J* = 8.1 Hz, 1H), 6.24 (d, *J* = 2.2 Hz, 1H), 6.17 – 6.15 (m, 1H), 4.62 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 165.8, 155.6, 152.7, 149.4, 146.6, 139.4, 133.3, 131.0, 130.6, 129.0, 128.9, 127.2, 127.0, 126.9, 126.8, 126.0, 126.0, 121.5, 121.4, 118.6, 116.5, 104.1, 99.6, 55.1, 54.5; HRMS (ESI) calcd for $C_{34}H_{29}ClN_3OS^+$ $[M+H]^+$ 562.1714, found 562.1718.

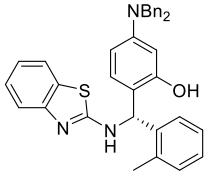
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(3-chlorophenyl)methyl)-5-(dibenzylamino)phenol 3g:



(*R*)-3g

White solid; yield: 83%; $[\alpha]^{20}_D$ = +391 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 5.52 min (major), t_2 = 6.90 min (minor), *ee* = 96%.

(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(*o*-tolyl)methyl)-5-(dibenzylamino)phenol 3h:

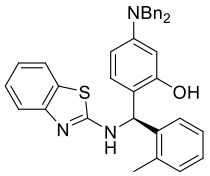


(*S*)-3h

White solid, M.p.: 105 – 106 °C; yield: 85%; $[\alpha]^{20}_D$ = -127 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.62

min (minor), t_2 = 7.81 min (major), *ee* = 90%; ^{1}H NMR (400 MHz, DMSO) δ 9.32 (s, 1H), 8.49 (d, *J* = 7.9 Hz, 1H), 7.65 – 7.58 (m, 1H), 7.40 – 7.09 (m, 16H), 6.99 (d, *J* = 7.7 Hz, 1H), 6.69 (d, *J* = 8.6 Hz, 1H), 6.45 (d, *J* = 7.8 Hz, 1H), 6.23 (d, *J* = 2.4 Hz, 1H), 6.17 – 6.09 (m, 1H), 4.62 (d, *J* = 7.6 Hz, 4H), 2.22 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 165.6, 155.9, 152.9, 149.3, 141.6, 139.6, 139.5, 136.0, 130.9, 130.6, 129.1, 129.0, 127.2, 127.1, 127.1, 127.0, 127.0, 126.4, 126.0, 125.9, 121.3, 118.4, 115.9, 103.9, 99.6, 54.5, 52.6, 19.3; HRMS (ESI) calcd for $C_{35}H_{32}N_3OS^+$ $[M+H]^+$ 542.2261, found 542.2267.

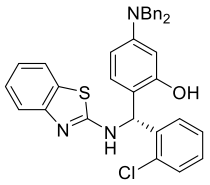
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(*o*-tolyl)methyl)-5-(dibenzylamino)phenol 3h:



(*R*)-3h

White solid; yield: 79%; $[\alpha]^{20}_D$ = +111 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.80 min (major), t_2 = 7.81 min (minor), *ee* = 78%.

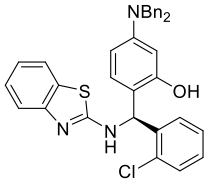
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(2-chlorophenyl)methyl)-5-(dibenzylamino)phenol 3i:



(*R*)-3i

White solid, M.p.: 110 – 111 °C; yield: 97%; $[\alpha]^{20}_D$ = -151 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 10.12 min (minor), t_2 = 13.76 min (major), *ee* = 96%; ^{1}H NMR (400 MHz, DMSO) δ 9.36 (s, 1H), 8.55 (d, *J* = 7.6 Hz, 1H), 7.64 – 7.62 (m, 0.7 Hz, 1H), 7.46 – 7.39 (m, 2H), 7.35 – 7.16 (m, 14H), 7.03 – 6.95 (m, 1H), 6.59 (t, *J* = 8.1 Hz, 2H), 6.26 (d, *J* = 2.4 Hz, 1H), 6.13 – 6.10 (m, 1H), 4.63 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 165.6, 156.3, 152.9, 149.5, 140.7, 139.4, 133.1, 131.0, 130.0, 129.1, 129.0, 128.9, 128.7, 127.4, 127.2, 127.0, 125.9, 121.4, 121.3, 118.6, 115.0 103.6, 99.6, 54.5, 53.3; HRMS (ESI) calcd for $C_{34}H_{29}ClN_3OS^+$ $[M+H]^+$ 562.1714, found 562.1715.

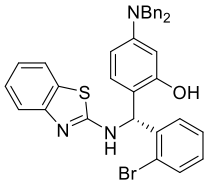
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(2-chlorophenyl)methyl)-5-(dibenzylamino)phenol 3i:



(*S*)-3i

White solid; yield: 75%; $[\alpha]^{20}_D$ = +166 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 5/95, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 10.18 min (major), t_2 = 14.45 min (minor), *ee* = 98%.

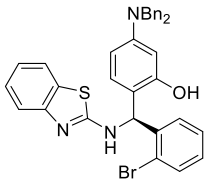
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(2-bromophenyl)methyl)-5-(dibenzylamino)phenol 3j:



(*R*)-3j

White solid, M.p.: 149 – 150 °C; yield: 93%; $[\alpha]^{20}_D$ = -170 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.21 min (minor), t_2 =7.63 min (major), *ee* = 97%; ^{1}H NMR (400 MHz, DMSO) δ 9.33 (s, 1H), 8.54 (d, *J* = 7.6 Hz, 1H), 7.64 – 7.57 (m,, 2H), 7.42 – 7.16 (m, 15H), 7.05 – 6.91 (m, 1H), 6.56 – 6.50 (m, 2H), 6.26 (d, *J* = 2.3 Hz, 1H), 6.12 – 6.10 (m, 1H), 4.63 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 165.4, 156.5, 152.3, 149.5, 142.1, 139.5, 133.2, 131.0, 129.2, 129.1, 129.0, 129.0, 127.9, 127.2, 127.1, 125.9, 124.0, 121.3, 118.6, 115.0, 103.6, 99.6, 55.8, 54.5; HRMS (ESI) calcd for $C_{34}H_{29}BrN_3OS^+$ $[M+H]^+$ 606.1209, found 606.1212.

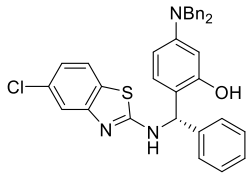
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(2-bromophenyl)methyl)-5-(dibenzylamino)phenol 3j:



(*S*)-3j

White solid; yield: 88%; $[\alpha]^{20}_D$ = +175 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.12 min (major), t_2 =7.97 min (minor), *ee* = 98%.

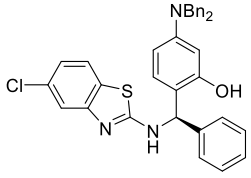
(*S*)-2-(((5-chlorobenzo[*d*]thiazol-2-yl)amino)(phenyl)methyl)-5-(dibenzylamino)phenol 3k:



(*S*)-3k

White solid, M.p.: 108 – 109 °C; yield: 90%; $[\alpha]^{20}_D$ = -73 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 8.56 min (major), t_2 = 13.69 min (minor), *ee* = 90%; ^{1}H NMR (400 MHz, DMSO) δ 9.31 (s, 1H), 8.81 (d, *J* = 8.2 Hz, 1H), 7.65 (d, *J* = 8.3 Hz, 1H), 7.39 – 7.12 (m, 16H), 7.01 – 6.99 (m, 1H), 6.81 (d, *J* = 8.6 Hz, 1H), 6.38 (d, *J* = 8.0 Hz, 1H), 6.20 (d, *J* = 2.4 Hz, 1H), 6.14 – 6.12 (m, 1H), 4.61 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 167.4, 155.6, 154.2, 149.2, 143.5, 139.4, 130.6, 129.7, 129.0, 128.6, 127.2, 127.2, 127.0, 122.5, 121.0, 117.9, 116.9, 103.9, 99.5, 88.1, 55.5, 54.5; HRMS (ESI) calcd for $C_{34}H_{29}ClN_3OS^+$ $[M+H]^+$ 562.1714, found 562.1713.

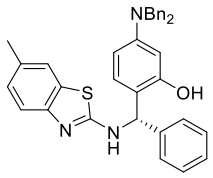
(*R*)-2-(((5-chlorobenzo[*d*]thiazol-2-yl)amino)(phenyl)methyl)-5-(dibenzylamino)phenol 3k:



(*R*)-3k

White solid; yield: 82%; $[\alpha]^{20}_D$ = +100 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 8.61 min (major), t_2 = 13.59 min (minor), *ee* = 98%.

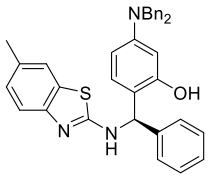
(*S*)-5-(dibenzylamino)-2-(((6-methylbenzo[*d*]thiazol-2-yl)amino)(phenyl)methyl)phenol 3l:



(*S*)-3l

White solid, M.p.: 151 – 152 °C; yield: 91%; $[\alpha]^{20}_D$ = -85 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.76 min (minor), t_2 = 8.98 min (major), *ee* = 60%; ^{1}H NMR (400 MHz, DMSO) δ 9.35 (s, 1H), 8.52 (d, *J* = 8.4 Hz, 1H), 7.44 (s, 1H), 7.36 – 7.17 (m, 16H), 7.01 – 6.99 (m, 1H), 6.88 (d, *J* = 8.6 Hz, 1H), 6.41 (d, *J* = 8.3 Hz, 1H), 6.23 (d, *J* = 2.2 Hz, 1H), 6.16 – 6.14 (m, 1H), 4.62 (s, 4H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 165.2, 155.6, 150.7, 149.2, 143.9, 139.5, 131.0, 130.4, 129.0, 128.5, 127.3, 127.2, 127.0, 126.9, 126.8, 121.3, 118.1, 117.4, 104.0, 99.6, 55.3, 54.5, 21.2; HRMS (ESI) calcd for $C_{35}H_{32}N_3OS^+$ $[M+H]^+$ 542.2261, found 542.2261.

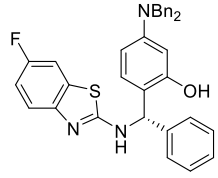
(*R*)-5-(dibenzylamino)-2-(((6-methylbenzo[*d*]thiazol-2-yl)amino)(phenyl)methyl)phenol 3l:



(*R*)-3l

White solid; yield: 85%; $[\alpha]^{20}_D$ = +123 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.69 min (major), t_2 = 8.92 min (minor), *ee* = 96%.

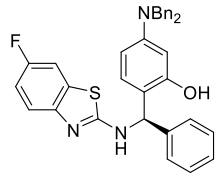
(*S*)-5-(dibenzylamino)-2-(((6-fluorobenzo[*d*]thiazol-2-yl)amino)(phenyl)methyl)phenol 3m:



(*S*)-3m

White solid, M.p.: 131 – 132 °C; yield: 93%; $[\alpha]^{20}_D$ = -156 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.54 min (minor), t_2 = 8.71 min (major), *ee* = 94%; ^{1}H NMR (400 MHz, DMSO) δ 9.33 (s, 1H), 8.61 (d, *J* = 8.2 Hz, 1H), 7.59 – 7.56 (m, 1H), 7.33 – 7.23 (m, 16H), 7.04 – 7.01 (m, 1H), 6.84 (d, *J* = 8.6 Hz, 1H), 6.39 (d, *J* = 8.2 Hz, 1H), 6.22 (d, *J* = 2.1 Hz, 1H), 6.16 – 6.13 (m, 1H), 4.62 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 165.7, 158.8, 156.4 (*J* = 235 Hz), 155.6, 149.6, 149.2, 143.7, 139.5, 132.0, 132.0, 129.0, 128.6, 127.3, 127.2, 127.0, 126.9, 126.5, 118.9, 118.8, 117.1, 113.3, 113.0, 108.4, 108.1, 103.9, 99.6, 55.4, 54.5; ^{19}F NMR (376 MHz, DMSO) δ -122.25; HRMS (ESI) calcd for $C_{34}H_{29}FN_3OS^+$ $[M+H]^+$ 546.2010, found 546.2012.

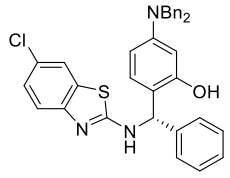
(*R*)-5-(dibenzylamino)-2-(((6-fluorobenzo[*d*]thiazol-2-yl)amino)(phenyl)methyl)phenol 3m:



(*R*)-3m

White solid; yield: 84%; $[\alpha]^{20}_D$ = +158 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.61 min (major), t_2 = 8.80 min (minor), *ee* = 95%.

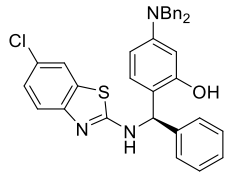
(*S*)-2-(((6-chlorobenzo[*d*]thiazol-2-yl)amino)(phenyl)methyl)-5-(dibenzylamino)phenol 3n:



(*S*)-3n

White solid, M.p.: 139 – 140 °C; yield: 90%; $[\alpha]^{20}_D$ = -458 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.87 min (minor), t_2 = 10.60 min (major), *ee* = 92%; ^{1}H NMR (400 MHz, DMSO) δ 9.35 (s, 1H), 8.76 (d, *J* = 8.2 Hz, 1H), 7.77 (d, *J* = 2.2 Hz, 1H), 7.40 – 7.16 (m, 17H), 6.84 (d, *J* = 8.6 Hz, 1H), 6.42 (d, *J* = 7.9 Hz, 1H), 6.24 (d, *J* = 1.6 Hz, 1H), 6.16 – 6.14 (m, 1H), 4.62 (d, *J* = 7.1 Hz, 4H); ^{13}C NMR (100 MHz, DMSO) δ 166.4, 155.5, 151.9, 149.2, 143.6, 139.4, 132.7, 129.0, 128.6, 128.2, 127.3, 127.2, 127.0, 127.0, 126.6, 126.0, 125.0, 121.0, 119.3, 117.0, 104.0, 99.6, 55.5, 54.5.; HRMS (ESI) calcd for $C_{34}H_{29}ClN_3OS^+$ $[M+H]^+$ 562.1714, found 562.1722.

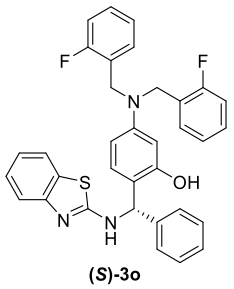
(*R*)-2-(((6-chlorobenzo[*d*]thiazol-2-yl)amino)(phenyl)methyl)-5-(dibenzylamino)phenol 3n:



(*R*)-3n

White solid; yield: 88%; $[\alpha]^{20}_D$ = +478 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.87 min (major), t_2 = 10.82 min (minor), *ee* = 96%.

(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(bis(2-fluorobenzyl)amino)phenol 3o:

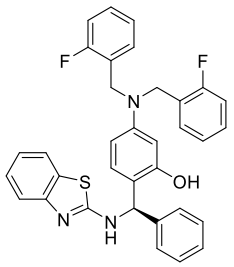


(*S*)-3o

White solid, M.p.: 143 – -144 °C; yield: 89%; $[\alpha]^{20}_D$ = -137 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 5.53 min (minor), t_2 = 6.76 min (major), *ee* = 64%; ^{1}H NMR (400 MHz, DMSO) δ 9.40 (s, 1H), 8.64 (d, *J* = 8.3 Hz, 1H), 7.72 – 7.59 (m, 1H), 7.39 – 7.10 (m, 15H), 7.03 – 6.97 (m, 1H), 6.91 (d, *J* = 8.5 Hz, 1H), 6.43 (d, *J* = 8.2 Hz, 1H), 6.27 – 6.10 (m, 2H), 4.69 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 165.9, 162.0, 159.6 (*J* = 242 Hz), 155.7, 152.8,

148.5, 143.70 130.9, 129.2, 129.2, 129.1, 128.9, 128.8, 128.6, 127.3, 126.9, 125.9, 125.9, 125.7, 124.9, 124.9, 121.3, 121.3, 118.5, 117.8, 115.9, 115.7, 103.8, 99.6, 55.4, 48.8, 48.7; ^{19}F NMR (376 MHz, DMSO) δ -118.11.; HRMS (ESI) calcd for $C_{34}H_{28}F_2N_3OS^+$ $[M+H]^+$ 564.1916, found 564.1926.

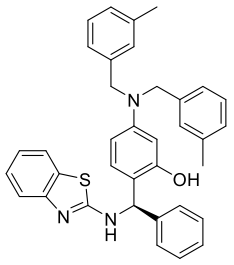
((*R*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(bis(2-fluorobenzyl)amino) phenol 3o:



(*R*)-3o

White solid; yield: 69%; $[\alpha]^{20}_D$ = +157 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 5.49 min (major), t_2 = 6.50 min (minor), *ee* = 70%.

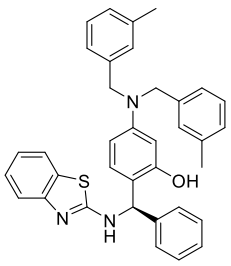
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(bis(3-methylbenzyl)amino) phenol 3p:



(*S*)-3p

White solid, M.p.: 140 – 141 °C; yield: 93%; $[\alpha]^{20}_D$ = -123 (*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 = 11.70 min (minor), t_2 = 13.58 min (major), *ee* = 92%; ^{1}H NMR (400 MHz, DMSO) δ 9.35 (s, 1H), 8.61 (d, *J* = 8.3 Hz, 1H), 7.68 – 7.57 (m, 1H), 7.37 – 7.13 (m, 9H), 7.09 – 6.95 (m, 7H), 6.85 (d, *J* = 8.6 Hz, 1H), 6.40 (d, *J* = 8.3 Hz, 1H), 6.20 (d, *J* = 2.3 Hz, 1H), 6.14 – 6.11 (m, 1H), 4.56 (s, 4H), 2.26 (s, 6H); ^{13}C NMR (100 MHz, DMSO) δ 165.9, 155.5, 152.8, 149.2, 143.8, 139.5, 138.04, 130.9, 128.9, 128.6, 127.9, 127.6, 127.3, 126.9, 125.9, 124.1, 121.3, 118.4, 117.1, 103.9, 99.5, 55.6, 54.5, 21.6; HRMS (ESI) calcd for $C_{36}H_{34}N_3OS^+$ $[M+H]^+$ 556.2417, found 556.2424.

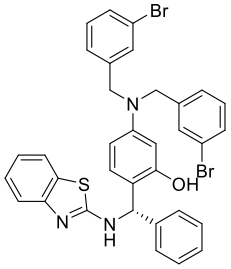
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(bis(3-methylbenzyl)amino) phenol 3p:



(*R*)-3p

White solid; yield: 83%; $[\alpha]^{20}_D$ = +141 (*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 = 11.62 min (major), t_2 = 13.68 min (minor), *ee* = 92%.

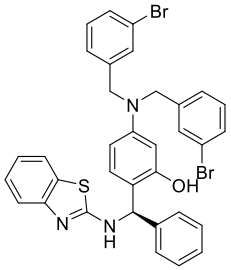
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(bis(3-bromobenzyl)amino) phenol 3q:



(*S*)-3q

White solid, M.p.: 144 – 145 °C; yield: 88%; $[\alpha]^{20}_D$ = -76 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.42 min (minor), t_2 = 7.60 min (major), *ee* = 92%; ^{1}H NMR (400 MHz, DMSO) δ 9.39 (s, 1H), 8.63 (d, *J* = 8.3 Hz, 1H), 7.64 (d, *J* = 7.7 Hz, 1H), 7.53 – 7.12 (m, 15H), 6.99 (t, *J* = 7.6 Hz, 1H), 6.88 (d, *J* = 8.5 Hz, 1H), 6.43 (d, *J* = 8.2 Hz, 1H), 6.24 – 6.12 (m, 2H), 4.65 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 165.8, 155.7, 152.8, 148.5, 143.7, 142.6, 131.2, 130.9, 130.1, 129.7, 129.1, 128.6, 127.3, 126.9, 126.1, 125.9, 122.4, 121.3, 118.5, 117.7, 103.9, 99.6, 55.3, 54.1; HRMS (ESI) calcd for $C_{34}H_{28}Br_2N_3OS^+$ $[M+H]^+$ 684.0314, found 684.0308.

(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(bis(3-bromobenzyl)amino) phenol 3q:

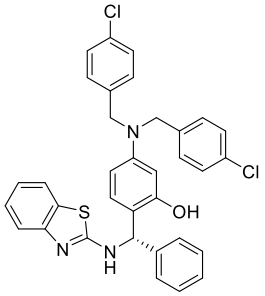


(*R*)-3q

White solid; yield: 84%; $[\alpha]^{20}_D$ = +87 (c 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.65 min (major), t_2

= 7.86 min (minor), *ee* = 96%.

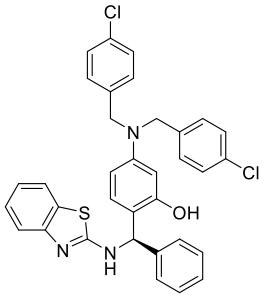
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(bis(4-chlorobenzyl)amino) phenol 3r:



(*S*)-3r

White solid, M.p.: 145 – 146 °C; yield: 93%; $[\alpha]^{20}_{D}$ = -45 (*c* 0.1, CH_2Cl_2); HPLC (ChiralpakIC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.19 min (minor), t_2 = 7.19 min (major), *ee* =70%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.35 (s, 1H), 8.63 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 7.2 Hz, 1H), 7.46 – 7.12 (m, 15H), 7.03 – 6.93 (m, 1H), 6.88 (d, *J* = 8.5 Hz, 1H), 6.42 (d, *J* = 8.3 Hz, 1H), 6.22 – 6.06 (m, 2H), 4.60 (s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.6, 160.3, 157.6, 153.4, 148.4, 143.2, 136.4, 135.7, 133.7, 133.3, 132.0, 131.7, 130.6, 126.1, 123.2, 122.3, 108.7, 104.4, 60.1, 58.7; HRMS (ESI) calcd for $C_{34}H_{28}Cl_2N_3OS^+$ $[M+H]^+$ 596.1325, found 596.1329.

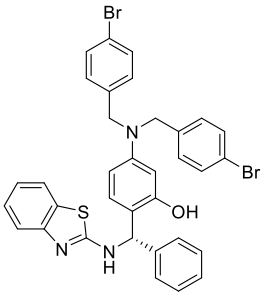
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(bis(4-chlorobenzyl)amino) phenol 3r:



(*R*)-3r

White solid; yield: 87%; $[\alpha]^{20}_{D}$ = +55 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.59 min (mor), t_2 = 7.65 min (minor), *ee* = 96%.

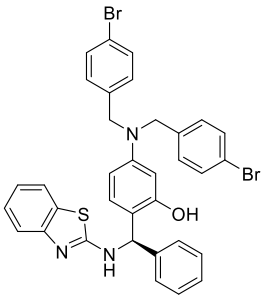
(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(bis(4-bromobenzyl)amino) phenol 3s:



(*S*)-3s

White solid, M.p.: 154 – 155 °C; yield: 90%; $[\alpha]^{20}_D$ = -95 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.04 min (minor), t_2 = 8.10 min (major), *ee* = 80%; ^{1}H NMR (400 MHz, DMSO) δ 9.36 (s, 1H), 8.62 (d, *J* = 8.4 Hz, 1H), 7.63 (d, *J* = 7.2 Hz, 1H), 7.51 (d, *J* = 8.4 Hz, 4H), 7.36 – 7.16 (m, 11H), 7.01 – 6.90 (m, 1H), 6.86 (d, *J* = 8.5 Hz, 1H), 6.39 (d, *J* = 8.2 Hz, 1H), 6.18 – 6.04 (m, 2H), 4.57 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 165.8, 155.6, 152.8, 148.6, 143.7, 138.9, 131.8, 130.9, 129.3, 129.0, 128.6, 127.3, 126.9, 125.9, 121.3, 120.1, 118.5, 117.6, 104.0, 99.7, 55.3, 54.0; HRMS (ESI) calcd for $C_{34}H_{28}Br_2N_3OS^+$ $[M+H]^+$ 684.0314, found 684.0310.

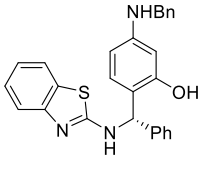
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(bis(4-bromobenzyl)amino) phenol 3s:



(*R*)-3s

White solid; yield: 85%; $[\alpha]^{20}_D$ = +127 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 6.87 min (major), t_2 = 7.90 min (minor), *ee* = 98%.

(*S*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(benzylamino)phenol 3t:

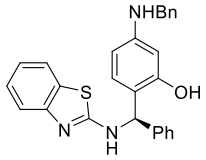


(*S*)-3t

White solid, M.p.: 134 – 135 °C; yield: 88%; $[\alpha]^{20}_D$ = -83 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 4.83 min (minor), t_2 = 5.42 min (major), *ee* = 60%; ^{1}H NMR (400 MHz, DMSO) δ 9.27 (s, 1H), 8.58 (d, *J* = 8.3 Hz, 1H), 7.64 (d, *J* = 7.3 Hz, 1H), 7.37 – 7.15 (m, 12H), 7.05 – 6.95 (m, 1H), 6.80 (d, *J* = 8.4 Hz, 1H), 6.38 (d, *J* = 8.3 Hz, 1H), 6.20 – 6.17 (m, 1H), 6.09 (d, *J* = 2.1 Hz, 1H), 6.05 – 6.02 (m, 1H), 4.20 (d, *J* = 6.0 Hz, 2H); ^{13}C NMR (100

MHz, DMSO) δ 165.9, 155.5, 152.8, 149.4, 144.0, 140.9, 130.9, 128.8, 128.7, 128.5, 127.5, 127.3, 127.0, 126.8, 125.9, 121.3, 118.4, 116.8, 104.2, 99.5, 55.4, 46.9; HRMS (ESI) calcd for $C_{27}H_{24}N_3OS^+$ $[M+H]^+$ 438.1635, found 438.1636.

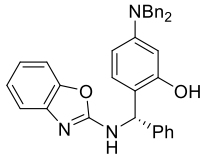
(*R*)-2-((benzo[*d*]thiazol-2-ylamino)(phenyl)methyl)-5-(benzylamino)phenol 3t:



(*R*)-3t

White solid; yield: 86%; $[\alpha]^{20}_D$ = +117 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1= 4.88 min (major), t_2 = 5.50 min (minor), *ee* = 96%.

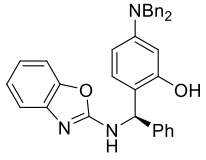
(*S*)-2-((benzo[*d*]oxazol-2-ylamino)(phenyl)methyl)-5-(dibenzylamino)phenol 3u:



(*S*)-3u

White solid, M.p.: 185 – 186 °C; yield: 90%; $[\alpha]^{20}_D$ = -110 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 8.37 min (minor), t_2 = 11.93 min (major), *ee* = 86%; ^{1}H NMR (400 MHz, DMSO) δ 9.33 (s, 1H), 8.62 (d, *J* = 9.0 Hz, 1H), 7.37 – 7.15 (m, 17H), 7.11 – 7.05 (m, 1H), 6.98 – 6.89 (m 2H), 6.28 (d, *J* = 8.9 Hz, 1H), 6.20 (d, *J* = 2.3 Hz, 1H), 6.14 – 6.11 (m, 1H), 4.62 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 162.3, 155.5, 149.2, 148.4, 143.6, 139.5, 129.0, 128.8, 128.6, 127.3, 127.1, 127.0, 127.0, 124.0, 120.6, 117.0, 115.9, 109.0, 103.91 99.5, 54.5, 54.3; HRMS (ESI) calcd for $C_{34}H_{30}N_3O_2^+$ $[M+H]^+$ 512.2333, found 512.2336.

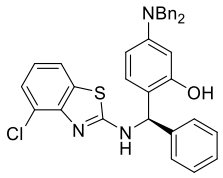
(*R*)-2-((benzo[*d*]oxazol-2-ylamino)(phenyl)methyl)-5-(dibenzylamino)phenol 3u:



(*R*)-3u

White solid; yield: 79%; $[\alpha]^{20}_D$ = +98 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 8.51 min (major), t_2 = 11.89 min (minor), *ee* = 71%;

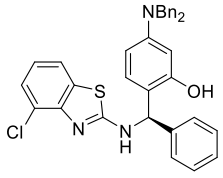
(*R*)-2-(((4-chlorobenzo[*d*]thiazol-2-yl)amino)(phenyl)methyl)-5-(dibenzylamino)phenol 3v:



(*R*)-3v

White solid, M.p.: 170 – 171 °C; yield: 82%; $[\alpha]^{20}_{D}$ = +168 (*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 = 15.27 min (minor), t_2 = 19.05 min (major), *ee* = 92%; ^{1}H NMR (400 MHz, DMSO) δ 9.37 (s, 1H), 8.96 (d, *J* = 8.4 Hz, 1H), 7.63 – 7.61 (m, 1H), 7.44 – 7.12 (m, 17H), 7.03-6.98 (m, 1H), 6.88 (d, *J* = 8.6 Hz, 1H), 6.22 (d, *J* = 2.4 Hz, 1H), 6.16 – 6.14 (m, 1H), 4.62 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 155.6, 149.6, 149.3, 143.4, 139.4, 132.2, 129.0, 128.9, 128.6, 127.3, 127.2, 127.0, 126.1, 122.0, 121.9, 120.3, 116.8, 104.0, 99.5, 55.8, 54.5; HRMS (ESI) calcd for $C_{34}H_{29}ClN_3OS^+$ $[M+H]^+$ 562.1714, found 562.1717.

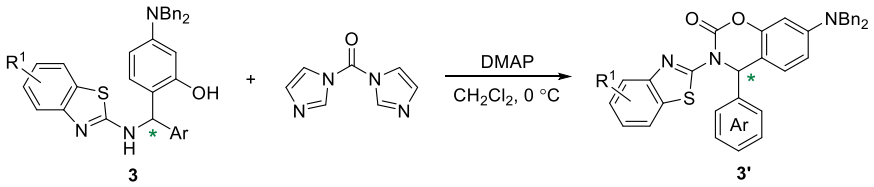
(*R*)-2-(((4-chlorobenzo[*d*]thiazol-2-yl)amino)(phenyl)methyl)-5-(dibenzylamino)phenol 3v:



(*R*)-3v

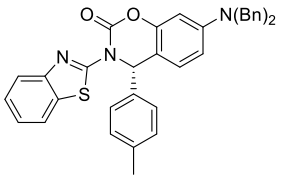
White solid; yield: 90%; $[\alpha]^{20}_{D}$ = +124 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 15.25min (minor), t_2 = 19.11 min (major), *ee* = 59%.

4. Derivatization of 3 into compounds 3′



To the solution of 1,1'-carbonyldiimidazole (0.3 mmol, 1.1 eq.), DMAP (0.04 mmol, 0.2 eq) in dry dichloromethane (2 mL), then, compounds **3** (0.2 mmol) were added to the reaction mixture, which were stirred at 0 ºC. After the completion of the reaction, which were indicated by TLC, the reaction mixture were purified through preparative thin layer chromatography on silica gel (p etroleum ether/ethyl acetate = 8:1) to afford pure products **3′**.

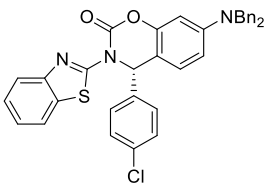
(*S*)-3-(benzo[*d*]thiazol-2-yl)-7-(dibenzylamino)-4-(*p*-tolyl)-3,4-dihydro-2*H*-benzo [*e*][1,3]oxazin-2-one 3b′:



(*S*)-3b'

White solid, M.p.: 138 – 139 °C; yield: 94%; $[\alpha]^{20}_D$ = -66 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 10.74 min (major), t_2 = 11.53 min (minor), *ee* = 90%;^{1}H NMR (400 MHz, DMSO) δ 7.98 (d, *J* = 7.8 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.47 – 7.37 (m, 1H), 7.36 – 7.19 (m, 14H), 7.13 – 7.04 (m, 3H), 6.57 – 6.54 (m, 1H), 6.46 (d, *J* = 2.4 Hz, 1H), 4.74 (s, 4H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 159.4, 149.7, 149.6, 148.7, 148.6, 138.9, 137.7, 133.4, 130.0, 129.1, 127.8, 127.4, 127.0, 126.8, 126.1, 124.8, 122.1, 121.7, 110.2, 110.0, 99.2, 60.2, 54.8, 21.0; HRMS (ESI) calcd for $C_{36}H_{30}N_3O_2S^+$ $[M+H]^+$ 567.1980, found 567.1988.

(*S*)-3-(benzo[*d*]thiazol-2-yl)-4-(4-chlorophenyl)-7-(dibenzylamino)-3,4-dihydro-2*H*-benzo[*e*][1,3]oxazin-2-one 3d′:

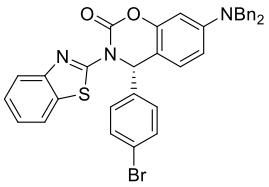


(*S*)-3d'

White solid, M.p.: 174 – 175 °C; yield: 95%; $[\alpha]^{20}_D$ = -110 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 11.58 min (major), t_2 = 12.48 min (minor), *ee* = 91%; ^{1}H NMR (400 MHz, DMSO) δ 7.97 (d,

J = 7.8 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.44 – 7.19 (m, 17H), 7.12 (s, 1H), 6.58 – 6.55 (m, 1H), 6.47 (d, *J* = 2.3 Hz, 1H), 4.73 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 159.3, 149.7, 149.4, 148.8, 148.5, 140.7, 138.8, 133.4, 133.0, 129.5, 129.1, 128.2, 127.80 127.4, 127.0, 126.8, 124.8, 122.1, 121.7, 110.3, 109.2, 99.2, 59.8, 54; HRMS (ESI) calcd for $C_{35}H_{27}ClN_3O_2S^+$ $[M+H]^+$ 588.1507, found 588.1509.

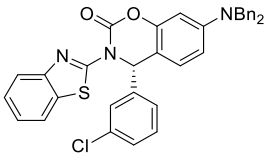
(*S*)-3-(benzo[*d*]thiazol-2-yl)-4-(4-bromophenyl)-7-(dibenzylamino)-3,4-dihydro-2*H*-benzo[*e*][1,3]oxazin-2-one 3e′:



(*S*)-3e'

White solid, M.p.: 189 – 190 °C; yield: 91%; $[\alpha]^{20}_D$ = -152 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak ID, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 11.23 min (minor), t_2 = 13.48 min (major), *ee* = 94%; ^{1}H NMR (400 MHz, DMSO) δ 7.98 (d, *J* = 7.8 Hz, 1H), 7.76 (d, *J* = 8.1 Hz, 1H), 7.51 – 7.21 (m, 17H), 7.11 (s, 1H), 6.59 – 6.56 (m, 1H), 6.48 (d, *J* = 2.1 Hz, 1H), 4.75 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 159.4, 149.7, 149.4, 148.7, 148.5, 141.2, 138.8, 133.4, 132.4, 129.1, 128.5, 127.8, 127.4, 127.0, 126.8, 124.8, 122.1, 121.7, 121.5, 110.3, 109.2, 99.2, 59.9, 54.8; HRMS (ESI) calcd for $C_{35}H_{27}BrN_3O_2S^+$ $[M+H]^+$ 632.1002, found 632.1004.

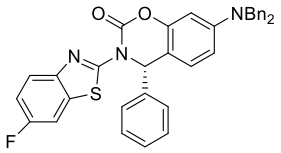
(*S*)-3-(benzo[*d*]thiazol-2-yl)-4-(3-chlorophenyl)-7-(dibenzylamino)-3,4-dihydro-2*H*-benzo[*e*][1,3]oxazin-2-one 3g′:



(*S*)-3g'

White solid, M.p.: 185 – 186 °C; yield: 94%; $[\alpha]^{20}_D$ = -80 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 10/90, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 10.74 min (major), t_2 = 11.53 min (minor), *ee* = 92%; ^{1}H NMR (400 MHz, DMSO) δ 7.96 (d, *J* = 7.9 Hz, 1H), 7.75 (d, *J* = 8.1 Hz, 1H), 7.49 (s, 1H), 7.40 (t, *J* = 8.8 Hz, 2H), 7.33 – 7.20 (m, 14H), 7.13 (s, 1H), 6.59 – 6.56 (m, 1H), 6.47 (d, *J* = 2.1 Hz, 1H), 4.72 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 159.3, 149.8, 149.4, 148.7, 148.5, 144.2, 138.7, 133.9, 133.4, 131.5, 129.1, 128.4, 127.8, 127.4, 127.0, 126.8, 126.4, 124.8, 124.5, 122.1, 121.7, 110.3, 109.0, 99.2, 59.8, 54.8; HRMS (ESI) calcd for $C_{35}H_{27}ClN_3O_2S^+$ $[M+H]^+$ 588.1507, found 588.1513.

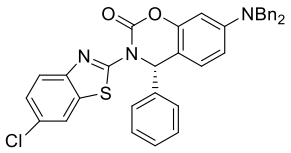
(*S*)-7-(dibenzylamino)-3-(6-fluorobenzo[*d*]thiazol-2-yl)-4-phenyl-3,4-dihydro-2*H*-benzo[*e*][1,3]oxazin-2-one 3m′:



(*S*)-3m'

White solid, M.p.: 147 – 148 °C; yield: 96%; $[\alpha]^{20}_D$ = -90 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.80 min (minor), t_2 = 9.11 min (major), *ee* = 94%;^{1}H NMR (400 MHz, DMSO) δ 7.91 – 7.88 (m, 1H), 7.79 – 7.75 (m, 1H), 7.42 – 7.15 (m, 17H), 7.09 (s, 1H), 6.58 – 6.55 (m, 1H), 6.47 (d, *J* = 2.4 Hz, 1H), 4.74 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 160.6, 159.5, 159.4 (*J* = 244 Hz), 158.2, 149.7, 149.7, 148.7, 145.3, 141.7, 138.8, 134.8, 134.6, 129.5, 129.1, 128.4, 127.8, 127.4, 127.0, 126.1, 123.0, 122.9, 115.1, 114.9, 110.3, 109.8, 108.7, 108.5, 99.2, 60.4, 54.8; ^{19}F NMR (376 MHz, DMSO) δ -117.11; HRMS (ESI) calcd for $C_{35}H_{27}FN_3O_2S^+$ $[M+H]^+$ 572.1803, found 572.1805.

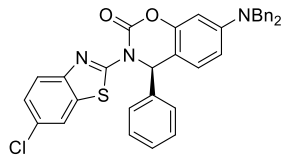
(*S*)-3-(6-chlorobenzo[*d*]thiazol-2-yl)-7-(dibenzylamino)-4-phenyl-3,4-dihydro-2*H*-benzo[*e*][1,3]oxazin-2-one 3n′:



(*S*)-3n'

White solid, M.p.: 178 – 179 °C; yield: 94%; $[\alpha]^{20}_D$ = -126 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.96 min (major), t_2 = 8.89 min (minor), *ee* = 92%; ^{1}H NMR (400 MHz, DMSO) δ 8.13 (d, *J* = 2.1 Hz, 1H), 7.75 (d, *J* = 8.7 Hz, 1H), 7.47 – 7.19 (m, 17H), 7.09 (s, 1H), 6.58 - 6.55 (m, 1H), 6.46 (d, *J* = 2.2 Hz, 1H), 4.74 (s, 4H); ^{13}C NMR (100 MHz, DMSO) δ 160.3, 149.7, 148.7, 147.4, 141.6, 138.8, 135.1, 129.5, 129.1, 128.9, 128.4, 127.8, 127.4, 127.2, 127.0, 126.1, 123.0, 121.9, 110.3, 109.7, 99.2, 60.4, 54.8; HRMS (ESI) calcd for $C_{35}H_{27}ClN_3O_2S^+$ $[M+H]^+$ 588.1507, found 588.1514.

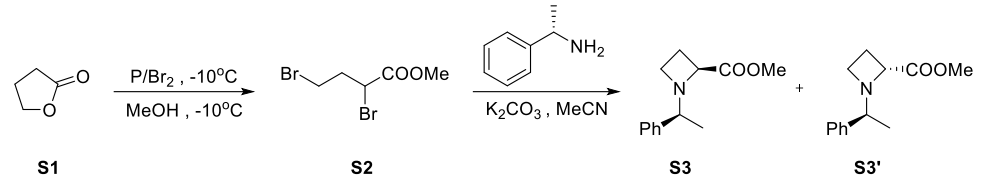
(*R*)-3-(6-chlorobenzo[*d*]thiazol-2-yl)-7-(dibenzylamino)-4-phenyl-3,4-dihydro-2*H*-benzo[*e*][1,3]oxazin-2-one 3n′:



(*R*)-3n'

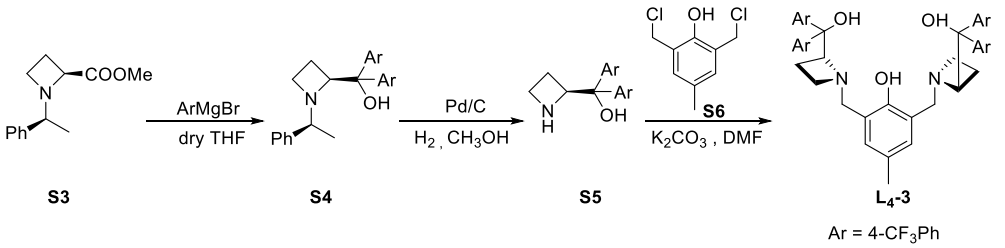
White solid, yield: 95%; $[\alpha]^{20}_D$ = +151 (*c* 0.1, CH_2Cl_2); HPLC (Chiralpak IC, *i*-propanol/hexane = 30/70, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 7.93 min (major), t_2 = 8.85 min (minor), *ee* = 96%.

5. Synthesis of L_4-3.



γ-Butyrolactone **S1** (5 g, 58.1 mmol) and P (0.5 g, 0.2 mmol) were stirred at -20 °C. Br_2 (6.3 mL) was added dropwise for 1 h to the mixture with stirring. After stirring for 3 h at 80 °C, the resulting mixture was cooled to room temperature. The residue was dissolved in MeOH (5 mL) and stirred at 25 °C for 24 h. Adding appropriate amount of EA to the above solution, then aqueous $Na_2S_2O_3$ was added to the mixture with stirring, until the red of the solution disappears. The resulting mixture was treated with saturated aqueous Na_2CO_3 and extracted with EA. The combined organics was dried by $MgSO_4$, filtered and concentrated in vacuo. The residue was purified by chromatography on silica gel (petroleum ether/ethyl acetate 10:1).to afford **S2** (75% yield) as yellow oil.

A mixture of K_2CO_3 (1.66 g, 13.2 mmol), H_2O (4.8 mL) MeCN (48 mL), compound **S2 (**1.72 g, 6.6mmol) and (*S*)-1-phenylethylamine (0.73 g, 6.62 mmol) was refluxed for 48 h. The resulting mixture was cooled to 25 °C and extracted three times with EA (3 × 10 mL). The combined organics was dried by $MgSO_4$, filtered and concentrated in vacuo. The residue was purified by chromatography on silica gel (petroleum ether/ethyl acetate 10:1) to afford **S3** (44% yield) and **S3′** (39% yield) as yellow oil.



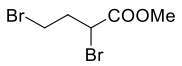
Magnesium strips (0.96 g, 40.13 mmol), dry THF (9 mL) and iodine was stirred at 25 °C , then ArBr (40.13 mmol) and THF (9 mL) was added dropwise for 1 h to the mixture with stirring. The reaction mixture was stirred for 24 h. The resulting mixture was cooled to 0 °C. Compound **S3** and dry THF (4 mL) was added dropwise for 1 h to the mixture with stirring. Then reaction mixture stirred at 25 °C for 48 h. After completion (monitored by TLC), the resulting mixture was treated with saturated aqueous NH_4Cl and extracted with EA. The combined organics was dried by $MgSO_4$, filtered and concentrated in vacuo. The residue was purified by chromatography on silica gel (petroleum ether/ethyl acetate 20:1).to afford **S4** (47% yield) as yellow oil.

A mixture of compound **S4** (1.5 mmol), CH_3OH (25 mL) HCOOH (0.31 mL) was stirred for 10 min. Then the resulting mixture was cooled to 0 °C and Pd/C was added, which was subjected to hydrogen (1 atm) and stirred for 48 h. After the completion of the reaction which was indicated by TLC. The resulting mixture was treated with saturated aqueous $NaHCO_3$ and extracted with EA. The combined organics was dried

by $MgSO_4$, filtered and concentrated in vacuo. The residue was purified by chromatography on silica gel (petroleum ether/ethyl acetate 6:1) to afford **S5** (55% yield) as yellow oil.

A mixture of compound **S5** (1.76 mmol), DMF (2.5 mL) K_2CO_3 (0.88 g, 6.98 mmol) and 2,6-bis(chloromethyl)-4-methylphenol **S6** (0.26 g, 0.88 mmol) was stirred at 25 ºC for 48 h. After the completion of the reaction which was indicated by TLC. The resulting mixture was treated with saturated aqueous NaCl and extracted with EA. The combined organics was dried by $MgSO_4$, filtered and concentrated in vacuo. The residue was purified by chromatography on silica gel (petroleum ether/ethyl acetate 6:1) to afford **L4-3** (61% yield) as white solid.

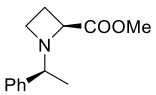
methyl 2,4-dibromobutanoate S2:



S2

Yellow oil, yield: 75%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 4.66 – 4.18 (m, 1H), 3.94 – 3.67 (m, 3H), 3.56 – 3.47 (m, 2H), 2.74 – 2.10 (m, 2H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.5, 53.2, 43.4, 36.9, 29.8.; HRMS (ESI) calcd for $C_5H_8Br_2O_2Na^+$ $[M+Na]^+$ 280.8783, found 280.8787.

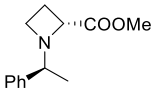
methyl (*S*)-1-((*S*)-1-phenylethyl)azetidine-2-carboxylate S3:



S3

Yellow oil, yield: 44%; $[\alpha]^{20}_D$ = -98 (c 0.1, EtOH); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.14 (m, 5H), 3.87 – 3.60 (m, 4H), 3.4 – 3.42 (m, 1H), 3.20 – 2.98 (m, 1H), 2.91 – 2.65 (m, 1H), 2.40 – 1.98 (m, 2H), 1.22 (d, *J* = 6.6 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.7, 142.5, 128.3, 127.5, 127.2, 67.3, 64.0, 51.9, 49.7, 21.0, 20.8. calcd for $C_{13}H_{18}NO_2^+$ $[M+H]^+$ 220.1332, found 220.1338.

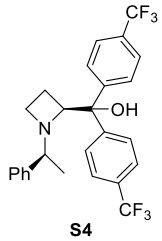
methyl (*R*)-1-((*S*)-1-phenylethyl)azetidine-2-carboxylate S3′:



S3'

Yellow oil, yield: 39%; $[\alpha]^{20}_D$ = +55 (c 0.1, EtOH).

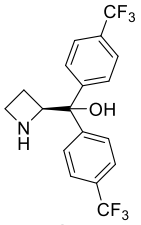
(((*R*)-1-((*S*)-1-phenylethyl)azetidin-2-yl)bis(4-(trifluoromethyl)phenyl)methanol S4:



S4

Yellow oil; yield: 47%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.3 Hz, 2H), 7.84 – 7.76 (m, 6H), 7.60 – 7.34 (m, 3H), 7.13 (d, *J* = 7.1 Hz, 2H), 6.26 (s, 1H), 4.59 (t, *J* = 7.8 Hz, 1H), 3.53 – 3.48 (m, 1H), 3.29 – 3.18 (m, 2H), 2.02 – 1.98 (m, 2H), 1.03 (d, *J* = 6.9 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 149.0(*J* = 277), 140.9, 129.9, 129.7(*J* = 18), 129.5, 129.4, 129.2, 129.0, 128.9, 128.7, 128.6, 128.6, 128.5, 128.0, 127.6, 126.5, 126.2, 125.9, 125.9, 125.5, 125.4, 125.34, 125.4, 123.2, 123.2, 120.5, 69.7, 62.0, 45.6, 27.1, 19.8, 19.5, ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.13, -62.22; HRMS (ESI) calcd for $C_{26}H_{24}F_6NO^+$ $[M+H]^+$ 480.1757, found 480.1764.

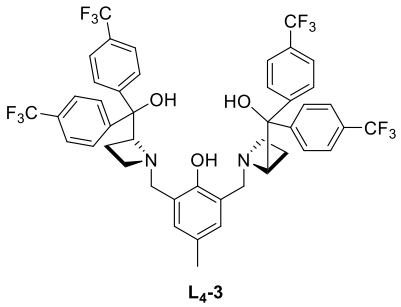
(*S*)-azetidin-2-ylbis(4-(trifluoromethyl)phenyl)methanol S5:



S5

Yellow oil; yield: 55%; ^{1}H NMR (400 MHz, DMSO) δ 7.91 – 7.47 (m, 8H), 4.95 (t, *J* = 7.6 Hz, 1H), 3.49 (s, 1H), 3.11 – 2.98 (m, 1H), 2.22 – 1.74 (m, 2H); ^{13}C NMR (100 MHz, DMSO) δ 150.9, 149.0, 128.1, 128.0, 127.8(*J* = 19 Hz), 127.7, 127.7, 127.6, 127.4, 127.4, 127.1, 126.1, 126.0, 125.6, 125.4 (*J* = 248 Hz), 125.3, 125.3, 125.3, 123.4, 123.3, 77.4, 63.4, 42.0, 21.4; HRMS (ESI) calcd for $C_{18}H_{16}F_6NO^+$ $[M+H]^+$ 376.1131, found 376.1137.

(*S*,*S*)-L_4-3:



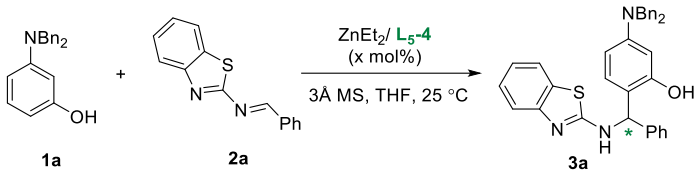
L_4-3

White solid, M.p.: 96 – 97 °C; yield: 61%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.39 (m, 16H), 6.49 (s, 2H), 4.45 (t, *J* = 7.9 Hz, 2H), 3.40 – 3.23 (m, 4H), 3.16 (d, *J* = 13.5 Hz, 2H), 2.98 – 2.91 (m, 1H), 2.25 – 1.82 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 149.4 (*J* = 276 Hz), 147.3, 129.6, 129.5(*J* = 15 Hz), 129.3, 129.2, 128.7, 128.0, 126.2, 126.1, 125.5, 125.4, 125.4, 125.3, 125.2, 122.7, 122.7, 121.9, 72.5, 58.3, 50.4,

20.3, 19.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.51, -62.56.; HRMS (ESI) calcd for $C_{45}H_{39}F_{12}N_2O_3^+$ $[M+H]^+$ 883.2764, found 883.2772.

6. Control experiments

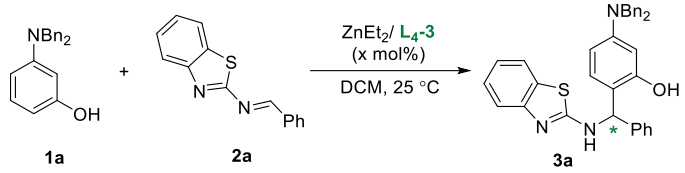
Table S4. Screening of **L$_5$-4** loading.



Entry[a]	1a	2a	3Å MS	Time (h)	Yield (%)[b]	*ee* (%)[c]
x = 20	0.05 mmol	0.075 mmol	20 mg	24	92	92 (*R*)
x = 10	0.1 mmol	0.15 mmol	40 mg	24	66	92 (*R*)
x = 5	0.2 mmol	0.30 mmol	80 mg	24	52	63 (*R*)
x = 0	0.1 mmol	0.15 mmol	-	24	31	-

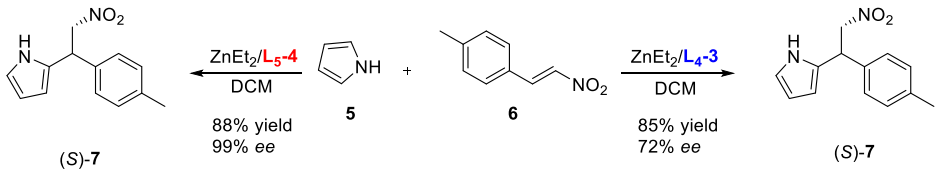
[a]Reaction conditions: **1a** (1 eq.), **2a** (1.5 eq.), ligand /$ZnEt_2$ (x mol%) in a specified solvent (2 mL) under N_2 at 25 °C for 24 h. [b]Isolated yields. [c]Determined by chiral HPLC analysis.

Table S5. Screening of **L$_4$-3** loading.



Entry[a]	1a	2a	Time (h)	Yield (%)[b]	*ee* (%)[c]
x = 20	0.05 mmol	0.075 mmol	24	95	96 (*S*)
x = 10	0.1 mmol	0.15 mmol	24	80	92 (*S*)
x = 5	0.2 mmol	0.30 mmol	24	75	71 (*S*)
x = 0	0.1 mmol	0.15 mmol	24	64	-

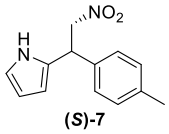
[a]Reaction conditions: **1a** (1 eq.), **2a** (1.5 eq.), ligand/$ZnEt_2$ (x mol%) in a specified solvent (2 mL) under N_2 at 25 °C for 24 h. [b]Isolated yields. [c]Determined by chiral HPLC analysis.



In a flame-dried Schlenk tube, a solution of diethylzinc (0.04 mL, 1.0 mol L^{-1} in hexane, 0.02 mmol) was added to a solution of the chiral ligand **L$_5$-4**/**L$_4$-3** (0.02 mmol) in dry DCM (2.0 mL) under nitrogen at 25 °C. The mixture was stirred at 25 °C for 30 min. Then, 1*H*-pyrrole **5** and 1-methyl-4-(2-nitrovinyl)benzene **6** were added under an argon atmosphere. The solution was stirred at 25 °C for 24 h, and then quenched with aqueous NH_4Cl (5 mL), and extracted three times with EA (3 × 10 mL). The combined organics was washed with brine before being dried by $MgSO_4$, filtered and concentrated in vacuo. The reaction mixture was purified through preparative thin layer

chromatography on silica gel (petroleum ether/ethyl acetate = 5:1) to afford the product (***S*)-7**.

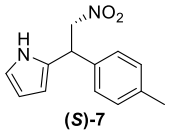
(*S*)-2-(2-nitro-1-(*p*-tolyl)ethyl)-1*H*-pyrrole 7:



(*S*)-7

Yellow oil, yield: 85%; $[\alpha]^{20}_D$ = -54 (*c* 0.1, $CHCl_3$); HPLC (Chiralpak OD-H, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 12.77 min (minor), t_2 = 14.67 min (major), *ee* = 70%; ^{1}H NMR (400 M, DMSO) δ 10.63 (s, 1H), 7.17 – 7.05 (m, 4H), 6.62 – 6.60 (m, 1H), 5.94 – 5.92 (m, 2H), 5.05 (t, *J* = 7.7 Hz, 2H), 4.72 (t, *J* = 8.3 Hz, 1H), 2.21 (s, 3H).; ^{13}C NMR (100 MHz, DMSO) δ 137.0, 136.9, 130.0, 129.6, 127.9, 118.1, 108.0, 105.3, 79.0, 42.6, 20.9.; HRMS (ESI) calcd for $C_{12}H_{13}N_2O_2^+$ $[M+H]^+$ 217.0972, found 217.0975.

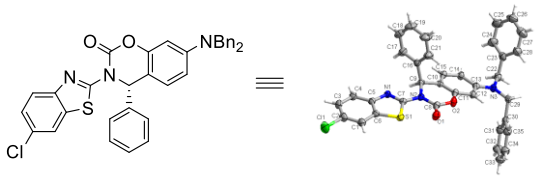
(*S*)-2-(2-nitro-1-(*p*-tolyl)ethyl)-1*H*-pyrrole 7:



(*S*)-7

Yellow oil, yield: 88%; $[\alpha]^{20}_D$ = -60 (c 0.1, $CHCl_3$); HPLC (Chiralpak OD-H, *i*-propanol/hexane = 20/80, flow rate 1.0 mL/min, λ = 254 nm), t_1 = 12.46 min (minor), t_2 = 14.69 min (major), *ee* = 99%.

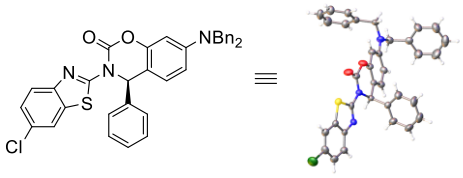
7. X-ray single crystal data for compound (*S*)-3n′ and (*R*)-3n′



CCDC: 2287151 for (*S*)-3n'

Table S6 Crystal data and structure refinement for (*S*)-3n′

Identification code	202304101_auto
Empirical formula	$C_{35}H_{26}ClN_3O_2S$
Formula weight	588.10
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.4206(2)
b/Å	17.8290(5)
c/Å	29.7449(8)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3405.00(17)
Z	4
ρ_{calc}g/cm^3	1.147
μ/mm^{-1}	1.821
F(000)	1224.0
Crystal size/mm^3	0.16 × 0.11 × 0.1
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.208 to 140.68
Index ranges	$-7 \le h \le 6$, $-20 \le k \le 21$, $-27 \le l \le 36$
Reflections collected	12228
Independent reflections	6339 [R_{int} = 0.0319, R_{sigma} = 0.0487]
Data/restraints/parameters	6339/0/379
Goodness-of-fit on F^2	1.002
Final R indexes [I>=2σ (I)]	R_1 = 0.0447, wR_2 = 0.1108
Final R indexes [all data]	R_1 = 0.0542, wR_2 = 0.1175
Largest diff. peak/hole / e Å^{-3}	0.15/-0.17
Flack parameter	0.004(13)



CCDC: 2287152 for (*R*)-3n'

Table S7 Crystal data and structure refinement for (*R*)-3n'

Identification code	230508_WQANGZ_047965_0m_a
Empirical formula	$C_{35}H_{26}ClN_3O_2S$
Formula weight	588.10
Temperature/K	193.0
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	6.3743(3)
b/Å	17.8083(8)
c/Å	29.5159(14)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3350.5(3)
Z	4
ρ_{calc}g/cm^3	1.166
μ/mm^{-1}	0.209
F(000)	1224.0
Crystal size/mm^3	? × ? × ?
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.584 to 52.76
Index ranges	-7 ≤ h ≤ 7, -21 ≤ k ≤ 22, -35 ≤ l ≤ 36
Reflections collected	28414
Independent reflections	6840 [R_{int} = 0.0597, R_{sigma} = 0.0591]
Data/restraints/parameters	6840/0/379
Goodness-of-fit on F^2	0.976
Final R indexes [I>=2σ (I)]	R_1 = 0.0448, wR_2 = 0.0992
Final R indexes [all data]	R_1 = 0.0702, wR_2 = 0.1115
Largest diff. peak/hole / e Å^{-3}	0.15/-0.21
Flack parameter	0.05(3)

8. Density functional theory studies

1）Computational method

All calculations were performed using Gaussian16 software.[1] Here, we used the B3LYP density functional[4-6] with Grimme's empirical dispersion correction and BJ-damping (D3(BJ)).[7-10] All geometric configurations were used 6-31+G (d,p) basis sets[11-14] for C, H, N, O, S, Cl atoms and the LAN2DZ basis sets[15] for Zn. Frequency calculations at the same level with the optimization were performed to determine whether the calculated structure was intermediate (no virtual frequency) or transition state (only one virtual frequency). Higher level single point energy calculations were performed using 6-311++G(d,p) basis sets[16-23] and the scalar-relativistic Stuttgart−Dresden (SDD) pseudopotential[24] on the optimized structures at M062X[25]. The solvent effect of geometric optimization and single point energy calculation was described by the SMD model (solvent= toluene)[26].

All geometries were prepared using CYLView software,[27] VMD programs[28], and Pymol.[29] Analyses of independent gradient model (IGM),[30-32] were performed with the aid of Multiwfn 3.8[32] and VMD programs.

2）Energetics and Cartesian Coordinates for All Calculated Species

Species	Electronic Energy (EE)	High-Level Single Point Energies	△△E	△△H	△△G	Imaginary Frequency (cm-1*i)
L_4	-3722.082489	-3721.646002	0.718584	0.719528	0.592677	
$ZnEt_2$	-224.034461	-385.594982	0.136113	0.137057	0.095732	
EtH	-79.842619	-79.799162	0.078442	0.079386	0.051856	
Zn-L_4	-3930.824884	-4253.573924	0.756026	0.756971	0.622092	
1	-520.126353	-519.991276	0.2478	0.248744	0.19687	
4C	-4371.135194	-4693.786959	0.925497	0.926441	0.771175	
4	-4371.188347	-4693.819647	0.926118	0.927063	0.773441	
2	-1047.270325	-1047.115165	0.218677	0.219621	0.162727	
5a	-5418.529519	-5740.979438	1.149194	1.150139	0.964031	
TS-6a	-5418.500504	-5740.952626	1.149377	1.150321	0.968755	-422.33
5b	-5418.505222	-5740.961257	1.149292	1.150236	0.96265	
TS-6b	-5418.487966	-5740.94555	1.148475	1.149419	0.964214	-394.13
5c	-5418.512124	-5740.959813	1.148951	1.149895	0.964906	
TS-6c	-5418.495059	-5740.943913	1.148227	1.149171	0.967351	-398.69
5d	-5418.520905	-5740.967589	1.148861	1.149805	0.965917	
TS-6d	-5418.498808	-5740.944848	1.148103	1.149047	0.96921	-446.86
7	-5418.505317	-5740.963261	1.151299	1.152243	0.969866	
8	-5418.50187	-5740.964019	1.149804	1.150748	0.967988	
3-S	-1567.427649	-1567.138932	0.471603	0.472547	0.384158	

L_5	-3800.782463	-3800.309518	0.78134	0.782284	0.657523	
Zn-L_5	-4009.481014	-4332.203016	0.818293	0.819237	0.677446	
4C'	-4449.824204	-4772.43282	0.988947	0.989891	0.83143	
4'	**-4449.86746**	-4772.46945	0.988847	0.989792	0.830615	
5a'	-5497.186204	-5819.602276	1.211521	1.212465	1.020286	
TS-6a'	-5497.165998	-5819.586326	1.210239	1.211183	1.024428	-451.17
5b'	-5497.193207	-5819.610983	1.2108	1.211744	1.018737	
TS-6b'	-5497.170269	-5819.593838	1.210532	1.211476	1.022881	-313.09
5c'	-5497.195559	-5819.612803	1.211423	1.212367	1.023329	
TS-6c'	-5497.170876	-5819.589066	1.210552	1.211496	1.0229	-370.40
5d'	-5497.186109	-5819.604742	1.211607	1.212551	1.022532	
TS-6d'	-5497.168612	-5819.587637	1.210923	1.211867	1.026717	-428.77
7'	-5497.176717	-5819.605108	1.21222	1.213164	1.026906	
8'	-5497.174088	-5819.603536	1.212787	1.213731	1.025855	
3-R	-1567.427618	-1567.138871	0.471601	0.472545	0.384069	

L_4

C	0.52937900	6.07496300	-0.19037900
C	1.64628200	5.33258200	-0.58160500
C	1.57196700	3.94940400	-0.73433500
C	0.35239200	3.30068300	-0.47209100
C	-0.77588300	4.02972400	-0.05373200
C	-0.67230000	5.41792400	0.06806400
H	2.59092000	5.83237700	-0.78068200
H	-1.54655900	5.98404600	0.38003400
O	0.30819100	1.95048800	-0.63253500
C	2.75337800	3.09585600	-1.12072400
H	3.58127000	3.72813900	-1.48710300
H	2.45966900	2.41861100	-1.92731600
C	-2.04690600	3.28924500	0.29130600
H	-1.93122700	2.76809000	1.24805600
H	-2.88710500	3.99611900	0.39932800
C	3.94300500	1.03935000	-0.11542800
C	4.06082200	2.81175400	1.04200500
C	4.63028400	1.38563100	1.22835700
H	4.66037400	1.03232700	-0.94808400
H	4.80504200	3.51523200	0.63331600
H	3.56055900	3.28462000	1.89368700
H	5.71466500	1.28103800	1.26202100
H	4.17746700	0.85214700	2.06407500
C	-3.44538200	1.32225900	-0.54459000
C	-2.85813600	2.71654200	-2.03242000
C	-3.80201800	1.49345500	-2.04331200
H	-4.22647200	1.72853100	0.11209700

H	-3.39950600	3.67027600	-1.96242600
H	-2.10451000	2.79101900	-2.82114100
H	-4.85064700	1.68000600	-2.27493700
H	-3.44442700	0.67898600	-2.67787700
N	-2.32836300	2.27256600	-0.72229400
N	3.15850400	2.27761100	0.01135300
C	-3.00542800	-0.06882400	-0.02995500
C	3.04727500	-0.22925500	-0.13155600
O	-1.92566200	-0.55220300	-0.82909600
O	2.03666600	-0.03426100	0.84580300
H	0.59680400	7.15289500	-0.08537400
C	-4.14916100	-1.08315800	-0.05337800
C	-3.82193900	-2.44171600	0.05900200
C	-5.49671100	-0.72744700	-0.16251100
C	-4.80762800	-3.42245000	0.06068600
H	-2.77793700	-2.72288000	0.14354600
C	-6.49957900	-1.69924700	-0.16160700
H	-5.78945100	0.31213400	-0.25339600
C	-6.14541500	-3.04005200	-0.05013900
H	-4.54834800	-4.47129400	0.14886600
H	-7.54262800	-1.41784900	-0.24974800
C	-2.44837600	0.09365400	1.38307000
C	-3.30735000	0.38672200	2.44868100
C	-1.07376100	0.02290100	1.62023900
C	-2.80494500	0.62694400	3.72522000
H	-4.38082000	0.41927000	2.28835900
C	-0.55517500	0.25856500	2.89334800
H	-0.39122800	-0.20193300	0.81530000
C	-1.42645900	0.56549200	3.93440400
H	-3.47039000	0.85384400	4.55021600
H	0.51502400	0.20617700	3.05633700
C	3.88805400	-1.43227600	0.27976500
C	3.72459900	-2.02141100	1.53632100
C	4.86867300	-1.93904100	-0.58102300
C	4.52375900	-3.09390200	1.93266900
H	2.96039800	-1.63711300	2.19981600
C	5.67985900	-3.00411800	-0.19765000
H	4.99340100	-1.51235800	-1.57094700
C	5.49860000	-3.57329400	1.06193700
H	4.39206700	-3.55262000	2.90615700
H	6.43776700	-3.39461700	-0.86708300
C	2.38479700	-0.49458900	-1.49293600
C	2.91455500	-0.07288400	-2.71580700
C	1.19196100	-1.22760200	-1.50577400

C	2.26210300	-0.34490900	-3.92128000
H	3.84089700	0.48920400	-2.75241500
C	0.53169400	-1.51461300	-2.69480900
H	0.77029400	-1.56207600	-0.56697900
C	1.06988000	-1.06018500	-3.89791900
H	2.67336200	-0.00053700	-4.86327300
H	-0.38827600	-2.08834200	-2.68917000
Cl	-0.78605100	0.87420000	5.54114900
Cl	-7.39803400	-4.26859900	-0.05022800
Cl	6.51314200	-4.92284600	1.55344000
Cl	0.22335500	-1.39316500	-5.40426000
H	1.71625200	0.87482200	0.67097500
H	-0.64998100	1.69907700	-0.73133600
H	-2.25685100	-0.70990100	-1.72210800

$ZnEt_2$

Zn	0.00002000	0.00028400	0.00017700
C	1.91708100	-0.69561900	-0.00001100
H	2.04968500	-1.34486900	0.87526000
H	2.04941700	-1.34503000	-0.87520500
C	2.98657800	0.41026100	-0.00027300
H	2.90577400	1.05829900	0.88049700
H	4.00599900	0.00072800	-0.00038700
H	2.90551500	1.05814100	-0.88113500
C	-1.91733800	0.69537100	-0.00001500
H	-2.04996900	1.34476300	-0.87517600
H	-2.05016100	1.34453600	0.87528700
C	-2.98639900	-0.41093600	-0.00027300
H	-2.90529900	-1.05898200	0.88046400
H	-4.00598800	-0.00181900	-0.00032500
H	-2.90511100	-1.05874500	-0.88116600

EtH

C	0.76487100	0.00000000	0.00000000
H	1.16407000	0.82905300	-0.59374700
H	1.16406300	-0.92872900	-0.42110700
H	1.16406800	0.09967300	1.01485500
C	-0.76487100	0.00000000	0.00000000
H	-1.16406800	-0.09943400	-1.01487800
H	-1.16407000	-0.82919200	0.59355200
H	-1.16406300	0.92863000	0.42132600

Zn-L_4

C	-0.35073200	-5.58436800	-1.50188600

C	-1.51428000	-4.83076300	-1.66435900
C	-1.51932900	-3.45971200	-1.40898600
C	-0.33296900	-2.83323300	-0.97660200
C	0.84040500	-3.58863600	-0.78169600
C	0.81486900	-4.95808000	-1.06252000
H	-2.43191400	-5.30992700	-1.99596700
H	1.71898200	-5.54193100	-0.90969300
O	-0.39107600	-1.50631000	-0.69931400
C	-2.74108500	-2.59883800	-1.59878200
H	-3.54799500	-3.17936200	-2.06914200
H	-2.48041600	-1.78092300	-2.27349700
C	2.06139700	-2.93927700	-0.18342300
H	1.80746800	-2.52245900	0.79599500
H	2.85295100	-3.68746400	-0.03131500
C	-4.00925000	-0.70239800	-0.45339300
C	-4.35361700	-2.61712400	0.38369300
C	-4.92651800	-1.21404000	0.67715300
H	-4.55479200	-0.64187500	-1.40356300
H	-4.99351900	-3.20342800	-0.29007100
H	-4.04527100	-3.24408200	1.22392800
H	-5.99865900	-1.07190500	0.54513600
H	-4.61276400	-0.82031800	1.64523100
C	3.73841100	-1.01692900	-0.49104200
C	3.34154800	-2.15797600	-2.24091200
C	4.33733100	-1.02538000	-1.91221800
H	4.33893300	-1.59397500	0.21945000
H	3.78629000	-3.15793500	-2.16870600
H	2.76176200	-2.09267800	-3.16591300
H	5.39789900	-1.26015600	-1.99557500
H	4.11494400	-0.09557800	-2.43685000
N	2.57492800	-1.82551700	-1.00282700
N	-3.22789200	-1.97563700	-0.35307000
C	3.30843400	0.37099100	0.08231500
C	-3.18212700	0.58935000	-0.16665100
O	2.44575600	0.98002900	-0.83110000
O	-2.40988200	0.41908500	0.96353300
Zn	1.03547200	-0.28372600	-1.11472100
Zn	-1.60661800	-1.36397500	1.13483900
C	-0.88864000	-2.69998600	2.50735500
H	-0.35496000	-6.65006700	-1.70501900
C	4.57944200	1.21273900	0.24432600
C	4.78953300	2.29911400	-0.60885600
C	5.56237300	0.90152300	1.19099900
C	5.95445400	3.06131800	-0.52762200

H	4.02000700	2.53871200	-1.33176100
C	6.73340700	1.65072200	1.28472800
H	5.41783600	0.07783900	1.88146100
C	6.91954400	2.72699600	0.41890300
H	6.11254600	3.90558400	-1.18929500
H	7.49020900	1.40881400	2.02220000
C	2.57300700	0.18790900	1.43229900
C	2.92196900	-0.76011200	2.40463900
C	1.45993700	1.00198900	1.68402600
C	2.18316900	-0.89794600	3.57940400
H	3.76797300	-1.42216700	2.25528500
C	0.69624000	0.86680300	2.84268400
H	1.20514000	1.75765500	0.95173300
C	1.07051400	-0.08444800	3.78816100
H	2.45475400	-1.64232500	4.31888000
H	-0.17854100	1.48612000	3.00302200
C	-4.20917800	1.71985500	0.04355200
C	-4.36001600	2.25893600	1.32307000
C	-5.02664700	2.19626100	-0.98793700
C	-5.30699800	3.25042100	1.57778600
H	-3.71366700	1.88368300	2.10718400
C	-5.98021300	3.18508900	-0.75225700
H	-4.91848800	1.81014300	-1.99650700
C	-6.11173200	3.70303900	0.53501100
H	-5.42099100	3.66865700	2.57176000
H	-6.60978000	3.55441500	-1.55390900
C	-2.27362500	0.95015500	-1.36718300
C	-2.54995300	0.66370600	-2.70790600
C	-1.06278800	1.59425000	-1.07671000
C	-1.62587400	0.93113800	-3.72306700
H	-3.48619600	0.19481300	-2.98899400
C	-0.12843500	1.89544000	-2.07535800
H	-0.86478800	1.83339700	-0.03818200
C	-0.41190700	1.52819200	-3.39886500
H	-1.84561800	0.67172000	-4.75264800
H	0.80173700	2.39788800	-1.83179300
Cl	0.13222400	-0.26373300	5.25604000
Cl	8.39380300	3.67827500	0.52929200
Cl	-7.31104800	4.95330300	0.84294800
Cl	0.77263800	1.84136600	-4.65677400
H	0.20787300	-2.64955600	2.47774700
H	-1.16285600	-2.37007500	3.51619800
C	-1.33586300	-4.15535300	2.29694200
H	-0.88396200	-4.84645400	3.02434500

H	-2.42262900	-4.26559300	2.40302200
H	-1.07750600	-4.52716400	1.30012400

1

C	0.40189000	-1.54682000	-0.36162500
C	-0.00076600	-0.22628700	-0.05816800
C	1.01262000	0.72442000	0.19684700
C	2.35974600	0.36415300	0.15425700
C	2.75193600	-0.94166200	-0.14893000
C	1.75384900	-1.87710500	-0.40463900
H	-0.33234200	-2.31947700	-0.54552600
H	0.76043700	1.75754700	0.40919100
H	3.80513900	-1.19389600	-0.17765600
H	2.03301700	-2.90102900	-0.63711600
O	3.35051500	1.27655900	0.39759400
H	2.94552200	2.12947200	0.60002600
N	-1.34023500	0.12879600	-0.01234500
C	-1.76754500	1.44409600	0.43795200
H	-2.76752500	1.33913900	0.87316400
H	-1.12089900	1.77577900	1.25736900
C	-2.38797200	-0.80539700	-0.39723000
H	-2.04557700	-1.40271100	-1.24814400
H	-3.23668300	-0.21887800	-0.76636200
C	-1.80020900	2.49299400	-0.67987400
H	-2.12861900	3.46457100	-0.29497600
H	-0.81150100	2.61444800	-1.13078100
H	-2.49146600	2.18912500	-1.47233900
C	-2.84712400	-1.71505400	0.74784100
H	-3.63671600	-2.39618100	0.41261200
H	-2.01358300	-2.31121300	1.12860400
H	-3.24023000	-1.12076800	1.57901300

4C

C	0.20762300	-0.43879300	5.72024200
C	1.29421000	0.24320500	5.17143800
C	1.27296900	0.67105000	3.84352700
C	0.14027900	0.39264700	3.05092200
C	-0.96025100	-0.30305000	3.58841000
C	-0.90986800	-0.69974200	4.92872900
H	2.16776600	0.45741800	5.78163000
H	-1.75670500	-1.23663300	5.34811600
O	0.17859300	0.78547200	1.74906700
C	2.38998000	1.48516200	3.23739200
H	3.13624200	1.73426300	4.00495100

H	1.96499300	2.42103600	2.86869500
C	-2.13833500	-0.66525800	2.71706100
H	-1.81754200	-1.32072100	1.89947700
H	-2.88426600	-1.21764700	3.30636400
C	3.76116000	1.71070200	1.08174400
C	4.30472500	0.06290000	2.31069900
C	4.87659700	0.64518800	1.00064400
H	4.12060500	2.63735200	1.54551800
H	4.83590000	0.41503700	3.20456100
H	4.15480900	-1.01802100	2.37421900
H	5.90388600	1.00705100	1.02182300
H	4.72945600	-0.01865900	0.14756900
C	-3.94560500	0.34966900	1.18242400
C	-3.55919900	1.44977600	2.95377000
C	-4.54323100	1.64000800	1.77920400
H	-4.53267600	-0.53006000	1.46369000
H	-4.00619900	0.91732300	3.80257000
H	-3.00426400	2.31552800	3.32600800
H	-5.60752000	1.63012900	2.01021600
H	-4.30283200	2.50866000	1.16342700
N	-2.76420500	0.51950200	2.10013000
N	3.04998600	0.84246600	2.08370600
C	-3.56816300	0.33763000	-0.33301800
C	2.96007200	1.97542600	-0.23357900
O	-2.68445600	1.38735500	-0.59639600
O	2.44053400	0.78367200	-0.70297600
Zn	-1.34070300	1.40403400	0.73995800
Zn	1.68970500	-0.30694300	0.78402000
C	1.56630400	-2.25734000	0.37443000
C	2.29058100	-2.71380700	-0.74522100
C	0.87617800	-3.24481200	1.09100400
C	2.32560300	-4.05863300	-1.11714200
C	0.88577400	-4.59447600	0.74522600
H	0.30199500	-2.95879400	1.97257600
C	1.61529100	-5.02993800	-0.38446900
H	2.90548800	-4.31683300	-1.99307000
H	0.32669000	-5.29635200	1.35016200
O	3.01641200	-1.86393200	-1.54454400
H	2.86173900	-0.93168300	-1.28985400
N	1.59862500	-6.36173000	-0.78982300
C	2.43311700	-6.81213600	-1.89269500
H	2.03308400	-7.77230000	-2.23428300
C	0.90138600	-7.36511000	-0.00313200
H	0.72020200	-8.22596600	-0.65510700

H	0.23159400	-0.76473700	6.75467500
H	2.31755000	-6.11986600	-2.73452000
H	-0.08807100	-6.97886800	0.26710600
C	3.92041000	-6.96915800	-1.54769300
H	4.32890000	-6.03143100	-1.16248700
H	4.06576700	-7.73960200	-0.78467800
H	4.49437100	-7.25531400	-2.43610900
C	1.64778500	-7.82576400	1.25676300
H	2.58797700	-8.32009900	0.99523300
H	1.88388900	-6.97351200	1.89925900
H	1.03878100	-8.53343600	1.83076400
C	-4.87595300	0.56948200	-1.10762000
C	-5.12185200	1.83192800	-1.65626100
C	-5.86028700	-0.41734700	-1.23317100
C	-6.32016900	2.11206800	-2.31125800
H	-4.35232400	2.58824800	-1.56937700
C	-7.06500100	-0.15455300	-1.88303600
H	-5.68879600	-1.41394200	-0.84349200
C	-7.28558600	1.11386900	-2.41549000
H	-6.50328300	3.09160300	-2.73859400
H	-7.82090700	-0.92521800	-1.98245600
C	-2.91917700	-1.01167100	-0.71141200
C	-3.34966700	-2.24870300	-0.20897900
C	-1.85910600	-1.01152600	-1.62759000
C	-2.78192700	-3.44468600	-0.64397300
H	-4.14468000	-2.30415000	0.52684700
C	-1.26850800	-2.19777900	-2.06263100
H	-1.51612700	-0.05974900	-2.01620800
C	-1.75951100	-3.41262300	-1.58995000
H	-3.13373500	-4.39553900	-0.26040100
H	-0.44423500	-2.18279900	-2.76588800
C	3.95086000	2.58886800	-1.23719900
C	4.32700100	1.84941300	-2.36074300
C	4.52007300	3.85279000	-1.04118600
C	5.25598600	2.35225200	-3.27145200
H	3.87691200	0.87663500	-2.51378900
C	5.45069900	4.37057600	-1.93953100
H	4.23191100	4.45764300	-0.18712600
C	5.81203500	3.60968600	-3.05027900
H	5.54545700	1.77558300	-4.14271700
H	5.88755800	5.35085200	-1.78630000
C	1.78242800	2.95270300	0.00245100
C	1.75871400	3.97649400	0.95421900
C	0.62902100	2.75679000	-0.77325600

C	0.60252600	4.72444900	1.20158000
H	2.63750700	4.19074600	1.55228000
C	-0.53353200	3.51021700	-0.56659400
H	0.65693000	1.98156400	-1.53141200
C	-0.54444000	4.47104200	0.45608900
H	0.59231900	5.48764700	1.97161000
H	-1.41190000	3.35325400	-1.18438800
Cl	-1.12267400	-4.91800300	-2.21178900
Cl	-8.80248600	1.45519700	-3.23643000
Cl	6.98503800	4.25396100	-4.19089500
Cl	-2.02069300	5.36266500	0.78663400

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C	1.19010800	-5.50974000	-3.10340500
C	2.31397100	-5.04813800	-2.41673200
C	2.21752000	-3.95351100	-1.56097200
C	0.97829600	-3.29142200	-1.38434000
C	-0.15851600	-3.73579200	-2.10046500
C	-0.02666900	-4.85142400	-2.93587400
H	3.27243200	-5.54735500	-2.53593400
H	-0.90340400	-5.20085300	-3.47556800
O	0.97549300	-2.24142100	-0.54015700
C	3.38300300	-3.41819200	-0.77628800
H	4.24255400	-4.10025200	-0.83424100
H	3.08804000	-3.31908100	0.27016900
C	-1.48664800	-3.00536700	-2.04668600
H	-1.40272800	-2.06688000	-2.60608000
H	-2.25965200	-3.61787200	-2.53559300
C	4.70106600	-1.27770600	-0.30574100
C	4.82189800	-1.99572400	-2.31169800
C	5.61341800	-0.94620800	-1.50530000
H	5.17716700	-1.93251500	0.43094400
H	5.34488900	-2.95302800	-2.41875400
H	4.42589500	-1.69895900	-3.28696000
H	6.67779600	-1.13894500	-1.37178100
H	5.45291900	0.07467800	-1.85052300
C	-3.23356700	-2.21099400	-0.23175800
C	-1.94819000	-3.85221000	0.26488300
C	-3.16846000	-3.21267400	0.94538800
H	-4.00677300	-2.45234900	-0.96985800
H	-2.17880300	-4.77616700	-0.27846500
H	-1.04647000	-4.00477800	0.86410700
H	-4.04264000	-3.84730200	1.08821400
H	-2.91642900	-2.71581900	1.88159900

N	-1.86470800	-2.68947900	-0.66173200
N	3.79208100	-2.06464800	-1.22506600
C	-3.30031800	-0.70368100	0.22052200
C	3.98751300	-0.04216700	0.33802700
O	-2.11162400	-0.35250200	0.87133500
O	3.33970000	0.65209900	-0.67470700
Zn	-0.61015800	-1.03686900	-0.13091200
Zn	2.08847100	-0.66909500	-1.35447500
C	0.32338400	1.91654600	-3.13503800
C	0.00830100	1.34874300	-1.89638900
C	0.05565200	3.27143200	-3.32326900
C	-0.54760300	2.12043200	-0.87866400
C	-0.50810100	4.05612600	-2.32131300
H	0.27560200	3.73047100	-4.28291600
C	-0.82498100	3.48889400	-1.06647000
H	-0.81837800	1.62531200	0.04273200
H	-0.72929500	5.09351700	-2.53249000
O	0.24268100	0.01751300	-1.67122900
N	-1.40829300	4.23525500	-0.05304300
C	-1.67737400	3.64824800	1.25358900
H	-2.47236300	4.23860400	1.72226900
C	-1.52292800	5.68315600	-0.16270900
H	-0.65514100	6.08204800	-0.69970000
H	1.26056500	-6.36958900	-3.76108200
H	-2.08608400	2.64341900	1.12546600
H	-1.46785600	6.10125100	0.84812500
C	-0.45005000	3.60527800	2.17180600
H	0.35902400	3.03310200	1.71025300
H	-0.07212200	4.61327400	2.37072700
H	-0.69824300	3.13981900	3.13187300
C	-2.82123000	6.13824300	-0.83715200
H	-2.90824600	5.71835900	-1.84282700
H	-3.68993900	5.80862600	-0.25755400
H	-2.85954900	7.23047100	-0.91288300
C	-4.48064000	-0.63361500	1.19723100
C	-4.24886700	-0.42778100	2.55803700
C	-5.79645500	-0.80341000	0.75133100
C	-5.30719700	-0.39560800	3.46691100
H	-3.22528700	-0.29298000	2.88674300
C	-6.86510000	-0.77980900	1.64472600
H	-5.99385900	-0.93459800	-0.30877700
C	-6.60675700	-0.57601700	3.00008100
H	-5.12801100	-0.23321700	4.52396700
H	-7.88453800	-0.90836400	1.29898700

C	-3.53487100	0.29072100	-0.92844900
C	-3.91308900	1.59950400	-0.59361500
C	-3.27292200	0.01180300	-2.27016400
C	-3.99122600	2.60331100	-1.54940900
H	-4.14542400	1.83154900	0.43954600
C	-3.32302100	1.01087000	-3.24637400
H	-3.02547800	-0.99270600	-2.58580600
C	-3.67290300	2.30240600	-2.87344400
H	-4.27296800	3.61122400	-1.27344700
H	-3.09128300	0.78623500	-4.28091200
C	5.06345400	0.82807400	0.99484700
C	5.28676900	2.11535800	0.50198400
C	5.84400300	0.36629400	2.06087600
C	6.27423500	2.93101600	1.05412700
H	4.66546400	2.46068000	-0.31551500
C	6.83657200	1.16645100	2.62284500
H	5.67602100	-0.62265600	2.47597500
C	7.04317300	2.44601200	2.10919800
H	6.44594100	3.93137100	0.67271100
H	7.43939400	0.80857900	3.44973600
C	2.92999100	-0.48791400	1.38592500
C	3.03171400	-1.62559000	2.19279300
C	1.74489400	0.26499000	1.45928800
C	1.96355300	-2.05573700	2.98361700
H	3.93826900	-2.22132800	2.19277300
C	0.66537800	-0.14208200	2.24816900
H	1.66989700	1.16313900	0.85511000
C	0.77899700	-1.32465000	2.98564700
H	2.04389400	-2.95976700	3.57660500
H	-0.25109700	0.43679700	2.29035900
Cl	-3.73851600	3.57159800	-4.08667900
Cl	-7.94951100	-0.53907800	4.13704600
Cl	8.29360400	3.46418400	2.81188900
Cl	-0.58981600	-1.89611500	3.92313400
H	0.74030100	1.29988300	-3.92514300

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C	-4.85134400	1.44644700	-0.00002100
C	-5.29386200	0.11167500	0.00001900
C	-4.38714100	-0.94439300	0.00003300
C	-3.02389700	-0.64359200	0.00000100
C	-2.56312500	0.70150800	-0.00004100
C	-3.49640600	1.74947600	-0.00005200
H	-5.58114000	2.25001600	-0.00002700

H	-6.35850100	-0.10020700	0.00004000
H	-4.73223800	-1.97298400	0.00006100
H	-3.14026400	2.77394700	-0.00008000
S	-1.64847900	-1.72336500	-0.00000900
N	-1.19217800	0.85807500	-0.00004800
C	-0.58744800	-0.29526400	-0.00003100
N	0.76934100	-0.55130800	-0.00003700
C	1.57837800	0.45447800	0.00017200
H	1.19947100	1.48252900	0.00035000
C	3.02477200	0.27951600	0.00008800
C	3.60927500	-1.00041500	0.00004100
C	3.85161900	1.41463000	0.00005100
C	4.99163600	-1.13364800	-0.00004000
H	2.95636600	-1.86616500	0.00007100
C	5.23758400	1.27718400	-0.00004400
H	3.39900700	2.40259100	0.00009600
C	5.80871400	0.00344500	-0.00008800
H	5.44029000	-2.12232600	-0.00006200
H	5.87092400	2.15876300	-0.00008100
H	6.88906900	-0.10597000	-0.00015300

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C	0.23530700	-5.14913100	-4.26482900
C	1.41756800	-4.72334200	-3.65985900
C	1.42520100	-3.65061300	-2.76758700
C	0.21693500	-2.97531600	-2.47652400
C	-0.97909100	-3.38105800	-3.11016900
C	-0.94989900	-4.47001900	-3.98583700
H	2.35302900	-5.23387000	-3.87551400
H	-1.87483800	-4.77654500	-4.46829700
O	0.21914700	-1.96388100	-1.60328400
C	2.69700400	-3.18226500	-2.11270100
H	3.52918600	-3.84927700	-2.38275000
H	2.59937600	-3.19375100	-1.02192200
C	-2.25413300	-2.60884900	-2.89298300
H	-2.13759600	-1.56539400	-3.21345300
H	-3.04806900	-3.04120200	-3.52170300
C	4.31449300	-1.18717000	-2.04078000
C	3.40306400	-1.52639700	-3.91951600
C	4.42421100	-0.48657200	-3.41046500
H	5.09080200	-1.95356500	-1.93902700
H	3.88225900	-2.40315400	-4.37379500
H	2.57998600	-1.19735500	-4.55942000
H	5.40627300	-0.47133700	-3.88143000

H	4.01446500	0.52463300	-3.37396600
C	-4.08905300	-2.04562500	-1.29777200
C	-3.13689200	-3.93270700	-0.98335700
C	-4.56900000	-3.40666400	-0.73644900
H	-4.52596600	-1.81733800	-2.27457400
H	-3.05651600	-4.69979500	-1.75857300
H	-2.57645000	-4.27203000	-0.10801200
H	-5.34009800	-3.89313800	-1.33575600
H	-4.88891300	-3.39328100	0.30488900
N	-2.69321500	-2.58433200	-1.47648900
N	3.02231100	-1.79665100	-2.50274500
C	-4.14385700	-0.70873500	-0.48627400
C	4.18842400	-0.30636600	-0.76302300
O	-3.07489700	0.07208100	-0.91785800
O	3.04897800	0.48086300	-0.84650400
Zn	-1.33525600	-0.81985800	-0.82214400
Zn	1.55035200	-0.42393800	-1.63871300
C	-1.16283600	2.68162900	-2.35624300
C	-0.21354100	1.94981200	-1.63303400
C	-1.18990000	4.06526700	-2.19024400
C	0.66470300	2.59562000	-0.75893800
C	-0.31011700	4.72725100	-1.33697100
H	-1.91893800	4.65352300	-2.74117400
C	0.64179900	3.99443800	-0.59302100
H	1.36407000	1.98303800	-0.20722700
H	-0.37626300	5.80315600	-1.24760700
O	-0.14077900	0.59645800	-1.77133200
N	1.51340600	4.60556700	0.29625400
C	2.63246600	3.87572100	0.88346600
H	2.97020200	3.09995900	0.19257400
H	3.47096400	4.57394200	0.98960400
C	1.46820100	6.03859400	0.53235500
H	0.42346100	6.35989700	0.58072100
H	1.88569600	6.22327000	1.52873300
N	-0.76663800	1.36596300	2.05401600
C	-1.66735500	1.80061300	1.22756300
H	-2.22524200	1.13759500	0.56007300
C	-2.06974000	3.19173500	1.19591800
C	-1.46320300	4.17027500	2.00319900
C	-3.13304400	3.54269100	0.34786600
C	-1.91735400	5.48084500	1.95497800
H	-0.64577100	3.87965000	2.65179200
C	-3.58935400	4.85729300	0.31015600
H	-3.57986400	2.77510900	-0.27455800

C	-2.98042800	5.82551600	1.10915700
H	-1.45230000	6.23960400	2.57688800
H	-4.41191600	5.12770600	-0.34437600
H	-3.33394500	6.85212600	1.07920900
C	0.40811400	-4.49619600	1.72614300
C	0.74552900	-4.44584100	3.08696400
C	0.67941300	-3.24547200	3.78698800
C	0.28227700	-2.10003500	3.09790900
C	-0.05331700	-2.13438000	1.72436600
C	0.00760300	-3.35540700	1.03830700
H	0.46086700	-5.44087100	1.19414800
H	1.06680500	-5.34582100	3.60035300
H	0.94534600	-3.19806100	4.83639300
H	-0.24127300	-3.39481400	-0.01054800
S	0.11064300	-0.47417600	3.70533400
N	-0.45621500	-0.90287500	1.19424000
C	-0.44093600	0.04807000	2.11723400
H	0.23910700	-5.98992200	-4.95025500
C	2.23659800	6.85814600	-0.51142600
H	1.83102200	6.68677000	-1.51219500
H	2.17605400	7.92952200	-0.29092800
H	3.29375900	6.57355300	-0.52476900
C	2.30654300	3.24934300	2.24311700
H	2.03060300	4.01931200	2.97215900
H	1.46814700	2.55217100	2.16289800
H	3.17659200	2.71089000	2.63559000
C	-4.04909100	-0.83680700	1.04989700
C	-4.52009600	0.22481800	1.83957900
C	-3.35175000	-1.86062700	1.70076700
C	-4.30932700	0.26717100	3.21475500
H	-5.04604300	1.04587800	1.36570700
C	-3.14636200	-1.85061900	3.08085100
H	-2.91542200	-2.67585600	1.14287800
C	-3.62360300	-0.78013000	3.82859000
H	-4.66584200	1.10429800	3.80400400
H	-2.59668400	-2.65228000	3.55961400
C	-5.47562700	-0.05325700	-0.86981800
C	-6.69799100	-0.57204100	-0.42736700
C	-5.47867900	1.05575100	-1.71776900
C	-7.90489100	0.00407200	-0.81901700
H	-6.71064700	-1.42246000	0.24799900
C	-6.67736300	1.64936000	-2.11552600
H	-4.52305200	1.44112300	-2.05447900
C	-7.88088200	1.11512200	-1.66175300

H	-8.85170400	-0.39417000	-0.47211400
H	-6.68031900	2.51458900	-2.76924800
C	5.43992600	0.58916000	-0.73864500
C	5.32201400	1.92326900	-1.13911200
C	6.70084300	0.10450900	-0.37512200
C	6.43373200	2.76373600	-1.17511600
H	4.34044500	2.28954600	-1.41312200
C	7.82432100	0.92943500	-0.40810500
H	6.81291500	-0.92125200	-0.03909700
C	7.67828700	2.25605000	-0.80932900
H	6.33760900	3.79955400	-1.48119300
H	8.79906500	0.55341800	-0.11852400
C	4.14146100	-1.15707300	0.52281700
C	4.70583000	-2.43037700	0.65823600
C	3.53226200	-0.58252700	1.64690700
C	4.67534000	-3.11383700	1.87650800
H	5.18505000	-2.91811500	-0.18324200
C	3.51527000	-1.23629100	2.87467200
H	3.07570400	0.39413600	1.54069800
C	4.08994500	-2.50221300	2.97886500
H	5.11010500	-4.10267800	1.96812800
H	3.06229200	-0.76980700	3.74063500
Cl	9.08879700	3.30724800	-0.84704400
Cl	4.08631300	-3.33376800	4.52879400
Cl	-9.39895100	1.85652600	-2.15421800
Cl	-3.34356300	-0.74002700	5.56185800
H	-1.84783700	2.16425600	-3.01790900

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C	0.31840400	-6.41981100	-1.56489500
C	1.47154700	-5.70405000	-1.25496300
C	1.45077700	-4.31531200	-1.09867800
C	0.23741400	-3.61086200	-1.27685300
C	-0.93365400	-4.33565300	-1.58630400
C	-0.87809800	-5.72389400	-1.72284200
H	2.41482000	-6.22752700	-1.12118100
H	-1.79172000	-6.26072600	-1.96517400
O	0.17460500	-2.27339600	-1.15511100
C	2.71662200	-3.58959600	-0.73606300
H	3.54646700	-4.30717500	-0.65717700
H	2.62225100	-3.09636500	0.23916100
C	-2.23432300	-3.60562300	-1.74161100
H	-2.16173600	-2.80273200	-2.48423200
H	-3.00504200	-4.30515800	-2.10055400

C	4.38015400	-1.89119800	-1.67686000
C	3.28259600	-2.93521600	-3.14455100
C	4.35698900	-1.82601700	-3.21692200
H	5.14723000	-2.59581200	-1.33593200
H	3.71077000	-3.94303300	-3.21845700
H	2.40224200	-2.87225000	-3.78987700
H	5.28590200	-2.05500500	-3.73779700
H	3.95677900	-0.87405100	-3.57183400
C	-4.09767600	-2.50956500	-0.53448400
C	-3.04106700	-3.98588100	0.58838800
C	-4.49282600	-3.45887800	0.62265900
H	-4.54295900	-2.81229000	-1.48711800
H	-2.93681500	-5.01609900	0.23692600
H	-2.45235600	-3.87184900	1.50231700
H	-5.25488000	-4.19610400	0.36506200
H	-4.77859200	-2.95925900	1.54752000
N	-2.67266000	-2.98440300	-0.47105700
N	3.04146200	-2.55091100	-1.72529000
C	-4.23177500	-0.95397700	-0.46078100
C	4.38212300	-0.58261900	-0.84212400
O	-3.16157100	-0.42132400	-1.18829800
O	3.22967800	0.13448100	-1.12485100
Zn	-1.39050000	-1.00466700	-0.57474500
Zn	1.62001700	-0.89903500	-1.39026800
C	-1.16766200	2.38649500	-1.61225900
C	0.06506600	1.63581500	-1.47269000
C	-1.03009200	3.81974600	-1.70300800
C	1.20943200	2.28771700	-1.03853400
C	0.09909900	4.46267100	-1.30993700
H	-1.89963900	4.39762000	-1.99527000
C	1.24467000	3.69438700	-0.88794900
H	2.08948000	1.69563700	-0.83931000
H	0.13113200	5.54269400	-1.32209200
O	0.02743400	0.32319100	-1.67068600
N	2.34152200	4.32111500	-0.39228800
C	3.49095000	3.58800600	0.15295400
H	3.62500800	2.64867000	-0.38099900
H	4.38506300	4.18565700	-0.05164300
C	2.40086800	5.77710500	-0.23751700
H	1.43175200	6.15238500	0.10055300
H	3.10500500	5.98601500	0.57193900
N	-1.18365900	2.17660800	1.15867800
C	-2.04619600	2.12462400	0.09065600
H	-2.45637100	1.15960300	-0.20423100

C	-3.11563500	3.16814500	0.10140900
C	-3.09219800	4.22128200	1.01983800
C	-4.18826300	3.06163300	-0.79452100
C	-4.12951900	5.15354500	1.04272400
H	-2.26729000	4.27103800	1.72067200
C	-5.22359200	3.99259300	-0.77195200
H	-4.22174700	2.22447700	-1.48348200
C	-5.19716500	5.04435700	0.14873300
H	-4.10962400	5.96349900	1.76650300
H	-6.05670500	3.88847800	-1.46116300
H	-6.00649700	5.76819600	0.17323400
C	0.76808800	-3.16617000	3.01699600
C	1.19310500	-2.54349100	4.19491500
C	1.03418800	-1.16604600	4.35579300
C	0.45992300	-0.42961500	3.32352400
C	0.02427200	-1.04602300	2.12643100
C	0.17937700	-2.43275300	1.98613900
H	0.88967100	-4.23840400	2.89667700
H	1.65436900	-3.12427600	4.98610200
H	1.36601200	-0.67774800	5.26595700
H	-0.15383000	-2.92972700	1.08626500
S	0.16071100	1.29475500	3.23824800
N	-0.54811200	-0.18930800	1.19085700
C	-0.61895900	1.09201800	1.62979200
H	0.35122800	-7.49799600	-1.67937400
C	2.85189200	6.48425800	-1.51703200
H	2.15342900	6.29474400	-2.33664700
H	2.91288900	7.56535500	-1.35722900
H	3.83888200	6.12734600	-1.82672000
C	3.33945100	3.34119700	1.65586300
H	3.27009300	4.28429200	2.20730300
H	2.43279400	2.76592900	1.86233900
H	4.19961200	2.78443600	2.03790000
C	-4.22237000	-0.38253900	0.97782400
C	-4.96396100	0.76280000	1.29581900
C	-3.35518800	-0.87777000	1.96216700
C	-4.82570300	1.41269200	2.52040500
H	-5.64055100	1.18501800	0.56533900
C	-3.20928500	-0.25462900	3.19937500
H	-2.74166400	-1.74741400	1.77203500
C	-3.93895600	0.90092300	3.46250700
H	-5.37773800	2.32266700	2.72355500
H	-2.51328000	-0.64526400	3.93245300
C	-5.56083400	-0.62685600	-1.15007900

C	-6.78386100	-1.00384900	-0.58120600
C	-5.56564500	0.00774900	-2.39260100
C	-7.98921900	-0.74183400	-1.22899000
H	-6.79987700	-1.48661100	0.39137300
C	-6.76293000	0.28455000	-3.05439700
H	-4.61114600	0.27822900	-2.82800700
C	-7.96563600	-0.09323900	-2.46341300
H	-8.93526500	-1.02741600	-0.78308000
H	-6.76457500	0.78457500	-4.01666400
C	5.60927000	0.24114500	-1.27516000
C	5.41771000	1.31483100	-2.15197500
C	6.91228800	-0.05887000	-0.86354700
C	6.49260400	2.07706400	-2.60670000
H	4.40622200	1.54869600	-2.46030900
C	8.00007300	0.69065000	-1.31004600
H	7.09231300	-0.86929200	-0.16669800
C	7.77911800	1.75577500	-2.18044500
H	6.33616400	2.91044500	-3.28268100
H	9.00632300	0.45792700	-0.98045000
C	4.44869200	-0.90623600	0.66558800
C	5.22039700	-1.93740300	1.21815200
C	3.71397700	-0.09763100	1.53879400
C	5.27186200	-2.14540300	2.59719100
H	5.79427300	-2.60461300	0.58403800
C	3.77474600	-0.26977800	2.91808400
H	3.08425400	0.67390300	1.11929200
C	4.55422200	-1.29925700	3.43782800
H	5.86416200	-2.95225700	3.01367900
H	3.21363500	0.38143900	3.57478100
Cl	9.14357900	2.71278900	-2.74181300
Cl	4.62353700	-1.54364300	5.17650900
Cl	-9.48318000	0.25399800	-3.28502300
Cl	-3.72628400	1.72830300	4.99765300
H	-1.92640200	1.91518300	-2.23038800

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C	-1.02218300	-4.36496200	-4.73883900
C	-2.04702900	-3.47346800	-4.41507200
C	-1.90044500	-2.54598600	-3.38254900
C	-0.69791800	-2.52547300	-2.64585200
C	0.34642200	-3.41558700	-2.97134000
C	0.17119100	-4.32404600	-4.01775000
H	-2.97624500	-3.48808500	-4.97912200
H	0.97612800	-5.01454100	-4.25790800

O	-0.55594400	-1.67904400	-1.62427100
C	-2.96724000	-1.53852100	-3.04701800
H	-3.78496700	-1.60271300	-3.78286600
H	-2.54649400	-0.53007700	-3.10264800
C	1.60777600	-3.35868600	-2.15934300
H	1.38689900	-3.46285400	-1.09014400
H	2.27406700	-4.18870400	-2.43619000
C	-4.69316200	-0.92273300	-1.25827000
C	-4.27256900	-2.98223100	-1.46309400
C	-5.27874600	-2.19118000	-0.61174700
H	-5.28559300	-0.60844900	-2.12612200
H	-4.70687700	-3.34163700	-2.40589300
H	-3.71754300	-3.79271400	-0.99245400
H	-6.33874000	-2.38507000	-0.77363500
H	-5.04599200	-2.22642800	0.45318900
C	3.68445900	-2.06754700	-1.67746000
C	2.96361900	-1.94101600	-3.68896200
C	4.37306400	-1.95305400	-3.06020500
H	3.85602700	-3.02711200	-1.18279200
H	2.72545700	-2.79113800	-4.33256900
H	2.67885500	-1.02422800	-4.20979200
H	4.98201000	-2.81699800	-3.33179700
H	4.95449600	-1.04395000	-3.21211600
N	2.32496000	-2.06413200	-2.33155600
N	-3.49166700	-1.72676700	-1.68519800
C	3.85946600	-0.95607600	-0.57491800
C	-4.37507300	0.25196000	-0.29627800
O	2.65556800	-0.82018800	0.10853300
O	-3.45425100	-0.18163700	0.65083800
Zn	1.07729300	-0.71853800	-0.98850200
Zn	-1.87398400	-0.97226900	-0.15716000
C	-1.08629900	1.66688800	1.69989400
C	-0.24626600	1.53172100	0.58624400
C	-0.95876100	2.79735900	2.49848000
C	0.69937700	2.51771700	0.29633000
C	-0.01310900	3.78053800	2.23461500
H	-1.61047100	2.91400200	3.36009000
C	0.85827300	3.64838800	1.12828400
H	1.32629800	2.37229700	-0.57380600
H	0.05816700	4.63106700	2.89763600
O	-0.34496400	0.43729100	-0.21016400
N	1.86332100	4.57638700	0.89315900
C	2.61304000	4.53963800	-0.35464500
H	3.49849300	5.16919700	-0.22547900

H	2.98771400	3.52444400	-0.50852500
C	1.99248400	5.75784200	1.73260800
H	1.91393500	5.45182500	2.78139800
H	3.01204500	6.13637800	1.60440700
N	-0.16459600	-1.00282200	3.26249400
C	0.85464300	-0.42665500	2.70591400
H	1.30023700	-0.82934400	1.79284600
C	1.54236400	0.71090200	3.29143600
C	1.18554800	1.23369800	4.54720700
C	2.60505300	1.28389400	2.57117900
C	1.88967400	2.30768500	5.07306800
H	0.35944200	0.78201500	5.08531000
C	3.30301700	2.36599100	3.10256000
H	2.85550900	0.87254100	1.59927300
C	2.94862900	2.87548600	4.35124600
H	1.61815100	2.71134500	6.04367000
H	4.11217400	2.81459400	2.53567300
H	3.49400600	3.71757100	4.76788400
C	-1.92037600	-5.71040300	0.04142400
C	-2.08836800	-6.41563000	1.24162300
C	-1.86929600	-5.79058300	2.46704400
C	-1.49189000	-4.44777900	2.46661900
C	-1.35435200	-3.71604000	1.26413000
C	-1.55709400	-4.36703200	0.04211200
H	-2.06915600	-6.21518900	-0.90777100
H	-2.37778600	-7.46124500	1.21872500
H	-1.97707600	-6.33675700	3.39806900
H	-1.41302800	-3.83577700	-0.88620500
S	-1.06783300	-3.42703100	3.82281600
N	-0.95655100	-2.38169300	1.42081000
C	-0.69607400	-2.11575500	2.69030300
H	-1.15158000	-5.07927800	-5.54502800
C	0.98869700	6.87941800	1.43240200
H	-0.03837900	6.51097700	1.49769700
H	1.10544900	7.70202900	2.14660200
H	1.13757900	7.28000200	0.42597000
C	1.82550000	5.00134300	-1.58691000
H	0.91852700	4.40773400	-1.72209800
H	1.52208300	6.04714100	-1.48873500
H	2.43907600	4.91220300	-2.48822700
C	4.25681800	0.41681300	-1.17056000
C	5.32499400	1.17013300	-0.67060000
C	3.50118500	0.98789100	-2.20723800
C	5.66128900	2.41395600	-1.20868600

H	5.91897300	0.78149600	0.14709400
C	3.82570500	2.21829400	-2.77147100
H	2.64866600	0.45900500	-2.62125000
C	4.92104400	2.92104300	-2.27087200
H	6.49537600	2.97948400	-0.80883500
H	3.23615000	2.62962900	-3.58248700
C	4.95314300	-1.47491400	0.36548500
C	6.22081800	-1.82412600	-0.12052500
C	4.68845300	-1.64056200	1.72521800
C	7.20553900	-2.32343000	0.72873300
H	6.45487100	-1.69137200	-1.17267200
C	5.66383000	-2.13517100	2.59213500
H	3.70858000	-1.37458700	2.09795000
C	6.91513700	-2.47367900	2.08467400
H	8.18563300	-2.58983900	0.34963100
H	5.45498900	-2.25652300	3.64907400
C	-5.70380100	0.62217000	0.37833400
C	-5.90020700	0.32463700	1.72781100
C	-6.74292100	1.22447800	-0.34044600
C	-7.11246700	0.61290100	2.35546000
H	-5.07976300	-0.12740400	2.27221200
C	-7.96222900	1.51500900	0.26780500
H	-6.59498800	1.49101900	-1.38296100
C	-8.13455500	1.20192700	1.61557100
H	-7.26421300	0.38574200	3.40492900
H	-8.76567100	1.98472600	-0.28835000
C	-3.83082200	1.49379600	-1.03433100
C	-3.80216900	1.66489900	-2.42165900
C	-3.29900900	2.51574300	-0.23736800
C	-3.19952300	2.78576400	-3.00300600
H	-4.24962900	0.93120600	-3.08128200
C	-2.68417100	3.63234600	-0.79015100
H	-3.33931100	2.40837200	0.83654900
C	-2.62850600	3.74887800	-2.17864700
H	-3.17182100	2.90338900	-4.08052100
H	-2.23259800	4.38381600	-0.15299900
Cl	-9.67063800	1.56785100	2.39603700
Cl	-1.82799200	5.14197600	-2.90094900
Cl	8.15186900	-3.09871500	3.16656700
Cl	5.35070500	4.47268700	-2.96858600
H	-1.85236500	0.92781500	1.89177100

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C	-1.03027400	-4.64227000	-4.54434200

C	-2.04463700	-3.72713400	-4.25357600
C	-1.87879000	-2.75359000	-3.26814900
C	-0.67066100	-2.71659500	-2.54219600
C	0.37067400	-3.61950400	-2.84270300
C	0.17432200	-4.57348600	-3.84503700
H	-2.97800900	-3.75833000	-4.81003900
H	0.97316400	-5.27661000	-4.06801100
O	-0.51865400	-1.82033000	-1.56395600
C	-2.91523800	-1.69232300	-3.00249700
H	-3.73809300	-1.78953000	-3.72847200
H	-2.46366400	-0.70480300	-3.14135000
C	1.65541200	-3.53078100	-2.06473200
H	1.46721400	-3.61148200	-0.98691800
H	2.32076100	-4.36191700	-2.33894600
C	-4.59503100	-0.82694800	-1.27986900
C	-4.30047200	-2.92293600	-1.29792700
C	-5.25015200	-1.99628400	-0.51908400
H	-5.17160000	-0.56104200	-2.17429200
H	-4.76218500	-3.33318300	-2.20608800
H	-3.78534900	-3.71831900	-0.76096100
H	-6.32131600	-2.13865300	-0.65917600
H	-5.01100900	-1.95279200	0.54420800
C	3.72678200	-2.17619700	-1.64992700
C	2.97511500	-2.13383700	-3.65600200
C	4.39245300	-2.09316300	-3.04625800
H	3.93049400	-3.10947300	-1.11895300
H	2.74870400	-3.00781200	-4.27143900
H	2.66096000	-1.23879800	-4.19758400
H	5.01715600	-2.95178400	-3.29819900
H	4.95137200	-1.17685400	-3.23602600
N	2.35828700	-2.23378100	-2.28793500
N	-3.44674800	-1.73956900	-1.63088800
C	3.88994400	-1.00975700	-0.59677800
C	-4.20423000	0.41352200	-0.42943000
O	2.69716500	-0.85932700	0.09952500
O	-3.31702600	0.01346100	0.55701100
Zn	1.13456000	-0.89864400	-0.99757200
Zn	-1.85454900	-1.08569600	-0.13485100
C	-0.81638800	1.34235200	1.75759100
C	-0.08854700	1.40560300	0.50761800
C	-0.77897200	2.52456900	2.57665600
C	0.82374300	2.42579400	0.27221400
C	0.10635400	3.52924200	2.34573200
H	-1.43380800	2.57175800	3.44084000

C	0.98679000	3.47720100	1.20241000
H	1.41377500	2.37678800	-0.63150400
H	0.14115300	4.37548900	3.01672600
O	-0.24823000	0.40834900	-0.33910300
N	1.93685800	4.43295900	1.02755800
C	2.69778900	4.50614100	-0.22363100
H	3.56191900	5.14881200	-0.04075600
H	3.09667600	3.51531000	-0.45427100
C	2.20141600	5.45304000	2.04376500
H	2.07709700	5.00214800	3.03100000
H	3.25992000	5.71727700	1.96329500
N	-0.72151000	-0.77810900	3.39899400
C	0.18383500	-0.05069100	2.66479800
H	0.58228500	-0.54261600	1.77423700
C	1.23937900	0.67163800	3.42239800
C	1.05443900	1.04029900	4.76125000
C	2.42225800	1.03251000	2.76359700
C	2.02791100	1.78342000	5.42253700
H	0.14414800	0.72963600	5.26242100
C	3.39627800	1.77841800	3.43063300
H	2.58032200	0.71007900	1.73946300
C	3.19851700	2.16438500	4.75635900
H	1.87947400	2.06548600	6.46107100
H	4.31244300	2.04696900	2.91206200
H	3.95708000	2.74242600	5.27668700
C	-2.19515500	-5.66179400	0.33377000
C	-2.83942800	-6.14054700	1.47962600
C	-2.90973800	-5.35062500	2.62970900
C	-2.34080300	-4.08024000	2.60696500
C	-1.72138800	-3.56888500	1.44105600
C	-1.63562900	-4.38383400	0.30586600
H	-2.12371100	-6.28836100	-0.55013800
H	-3.27357000	-7.13524500	1.48461200
H	-3.38789900	-5.72479400	3.52923600
H	-1.13246800	-4.02453800	-0.58094800
S	-2.20374400	-2.91309400	3.91021600
N	-1.22008600	-2.26846400	1.54571700
C	-1.27852900	-1.81866500	2.82614800
H	-1.17490400	-5.39374100	-5.31325500
C	1.33997700	6.71024800	1.89740900
H	0.27530900	6.46542900	1.94744600
H	1.56764100	7.42272200	2.69674300
H	1.52627200	7.20373700	0.93945400
C	1.88225200	5.04956400	-1.39955300

H	1.00589400	4.43043700	-1.60126900
H	1.53180200	6.06496700	-1.19516900
H	2.49846100	5.07648500	-2.30163600
C	4.24588300	0.34710600	-1.25852900
C	5.32773200	1.12846600	-0.83679200
C	3.42529600	0.88461500	-2.26409100
C	5.60903400	2.36856100	-1.41400600
H	5.97459100	0.76603400	-0.04790300
C	3.68767900	2.11478300	-2.86168400
H	2.56482200	0.33132400	-2.62789000
C	4.79526500	2.84709100	-2.43484200
H	6.45632900	2.95388100	-1.07476700
H	3.04565600	2.49971100	-3.64582500
C	5.00548300	-1.45943100	0.35325300
C	6.27363200	-1.81506500	-0.12606600
C	4.75515000	-1.54676500	1.72340200
C	7.27709500	-2.24059000	0.74184000
H	6.49434400	-1.74583900	-1.18742700
C	5.74986700	-1.96632300	2.60765800
H	3.77118100	-1.28222800	2.08742200
C	7.00324100	-2.30930100	2.10774200
H	8.25825600	-2.51235100	0.36930200
H	5.55268500	-2.02645400	3.67203300
C	-5.50883400	0.93067000	0.19572500
C	-5.73208900	0.74775000	1.56175500
C	-6.49824200	1.55010900	-0.57607700
C	-6.92277100	1.16865400	2.15434400
H	-4.95094800	0.27521500	2.14551700
C	-7.69530700	1.97362300	-0.00219700
H	-6.32932200	1.72429900	-1.63478900
C	-7.89527100	1.77551500	1.36335700
H	-7.09598600	1.02881300	3.21564400
H	-8.46039700	2.45700400	-0.59922700
C	-3.57089200	1.54539200	-1.26601800
C	-3.59538800	1.63243700	-2.66045200
C	-2.90321200	2.55423700	-0.55734500
C	-2.92774600	2.65930800	-3.33730100
H	-4.13263600	0.89976300	-3.25126300
C	-2.23697800	3.58594300	-1.20657600
H	-2.89711600	2.50795100	0.52371500
C	-2.24302100	3.61905300	-2.60166600
H	-2.94036300	2.70840300	-4.42038100
H	-1.70871800	4.34533900	-0.64183500
Cl	-9.40250000	2.31119100	2.09997100

Cl	-1.37238700	4.89967700	-3.44243200
Cl	8.26552600	-2.83730000	3.21245600
Cl	5.15574100	4.39609300	-3.18048200
H	-1.77197300	0.82864300	1.69803900

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C	-1.08873600	-5.31229300	-3.25759000
C	-2.00609700	-4.26208000	-3.27969600
C	-1.81689900	-3.12025100	-2.49928100
C	-0.70909900	-3.04674500	-1.62495500
C	0.29118400	-4.04172300	-1.70799200
C	0.07550100	-5.16928700	-2.50328400
H	-2.87382900	-4.31204300	-3.93289200
H	0.85008000	-5.93105300	-2.55077600
O	-0.57845800	-2.01136400	-0.79069100
C	-2.72167100	-1.92498100	-2.62431200
H	-3.39835100	-2.05801800	-3.48381300
H	-2.12488500	-1.02491700	-2.80567300
C	1.65050900	-3.74108200	-1.13766900
H	1.64648100	-3.61902600	-0.04804300
H	2.34229400	-4.56797100	-1.36119400
C	-4.61742300	-0.71706500	-1.38422300
C	-4.46503500	-2.81445300	-1.09504500
C	-5.52961800	-1.76765000	-0.72077800
H	-4.94649500	-0.47167700	-2.40015800
H	-4.72007000	-3.36620800	-2.00848200
H	-4.13214700	-3.52063300	-0.33570800
H	-6.52029000	-1.89667200	-1.15686300
H	-5.61599500	-1.59872100	0.35123200
C	3.59221700	-2.19018800	-1.61440200
C	2.26237600	-2.54688900	-3.24246800
C	3.77417900	-2.25485100	-3.14891000
H	4.09968800	-2.99025000	-1.06662200
H	2.00366400	-3.53078600	-3.63979100
H	1.65679300	-1.79597100	-3.75592200
H	4.41335200	-3.06795000	-3.49748600
H	4.09530000	-1.32137800	-3.61185600
N	2.12908300	-2.47408000	-1.74762100
N	-3.49348000	-1.71943100	-1.39358900
C	3.87388300	-0.85129400	-0.84575900
C	-4.29907000	0.54089300	-0.52787200
O	2.98182300	-0.77869200	0.21342200
O	-3.68523700	0.12830600	0.64962800
Zn	1.10631500	-1.04593600	-0.15056600

Zn	-2.06036600	-0.85980600	0.17771600
C	-1.12488800	1.49507400	2.18274100
C	-0.20385400	1.32640100	1.13124500
C	-0.93712400	2.55391300	3.07078100
C	0.88918700	2.18905000	1.00909800
C	0.16221000	3.39397500	2.98362000
H	-1.66246300	2.71796900	3.86335000
C	1.12475100	3.20914800	1.95431200
H	1.56550900	2.02031200	0.18244900
H	0.27502900	4.18741700	3.70862300
O	-0.35512900	0.31531100	0.25049400
N	2.26856200	3.98412400	1.90220400
C	3.15886100	3.91925300	0.74770000
H	4.11534300	4.35317400	1.05577000
H	3.36462900	2.87019900	0.50871300
C	2.49645400	5.04093400	2.87776200
H	2.25130300	4.65610900	3.87293900
H	3.57224800	5.24317200	2.89066900
N	0.62865200	-1.55850600	2.27946900
C	0.56554000	-0.68440500	3.25541000
H	-0.30059900	-0.72295900	3.92095700
C	1.59424300	0.25739900	3.64171200
C	2.77107000	0.46163500	2.89880900
C	1.39406800	0.98522300	4.82793900
C	3.73122900	1.35440300	3.35582200
H	2.91210900	-0.05769900	1.95693800
C	2.36355500	1.87422800	5.28426200
H	0.47308700	0.85043900	5.38733800
C	3.53583800	2.05716600	4.54925300
H	4.63442400	1.50724900	2.77304200
H	2.20165500	2.42658300	6.20441800
H	4.29200300	2.75303600	4.90083600
C	-4.68536300	-4.24944200	2.24602800
C	-4.03998300	-5.49652700	2.27510400
C	-2.64867800	-5.59096200	2.25956700
C	-1.91358500	-4.40686000	2.20708500
C	-2.55960000	-3.15221600	2.14462100
C	-3.95400100	-3.06828500	2.17533100
H	-5.76945700	-4.20698200	2.27069500
H	-4.63165500	-6.40518900	2.32014800
H	-2.15630400	-6.55652200	2.29780700
H	-4.41691600	-2.08868700	2.13070600
S	-0.17292100	-4.16198700	2.26642300
N	-1.70334900	-2.05387500	2.09095100

C	-0.44908200	-2.41605100	2.20611400
H	-1.24942300	-6.19884600	-3.86183800
C	1.73272500	6.34486600	2.61107500
H	0.65805900	6.15984900	2.53345000
H	1.90070100	7.06009900	3.42379600
H	2.06074000	6.80973300	1.67761000
C	2.63126300	4.65117900	-0.49035000
H	1.69811600	4.20900300	-0.84610100
H	2.44306700	5.70544900	-0.27014200
H	3.35638200	4.59696100	-1.30498400
C	3.70127800	0.40247600	-1.74190100
C	4.70528400	1.36405800	-1.90461900
C	2.46988400	0.65438700	-2.37198700
C	4.51518700	2.49890600	-2.69520500
H	5.66249100	1.23211300	-1.41678700
C	2.25323800	1.78264400	-3.15833200
H	1.65132100	-0.05194100	-2.28758000
C	3.29287800	2.69539900	-3.32810700
H	5.31179500	3.22472500	-2.81541300
H	1.29193500	1.95545600	-3.62665000
C	5.31522300	-0.97919800	-0.33677700
C	6.38517300	-1.16516500	-1.22476000
C	5.58173000	-0.98798600	1.03320200
C	7.68906400	-1.33085300	-0.76266300
H	6.20724900	-1.16618100	-2.29550100
C	6.88154200	-1.14977500	1.51553100
H	4.75686500	-0.88350100	1.72354100
C	7.92619100	-1.31647500	0.61123700
H	8.51163400	-1.46778800	-1.45551000
H	7.07961100	-1.15194400	2.58165800
C	-5.63870500	1.22617200	-0.23496500
C	-6.14621100	1.22027800	1.06523100
C	-6.38728400	1.83204900	-1.25062900
C	-7.38250000	1.79841800	1.35465300
H	-5.54406200	0.76351600	1.84158400
C	-7.62575100	2.41081200	-0.98188200
H	-5.99336700	1.87260800	-2.26201500
C	-8.11321800	2.38454300	0.32428700
H	-7.77548400	1.79763600	2.36541200
H	-8.20372200	2.88287500	-1.76835300
C	-3.37203600	1.52981500	-1.26746400
C	-3.08215100	1.49799900	-2.63503700
C	-2.74368300	2.50639500	-0.48203800
C	-2.15749700	2.38287100	-3.19995300

H	-3.56576600	0.78175400	-3.28915200
C	-1.82333700	3.39563000	-1.02167700
H	-2.95437500	2.53009100	0.57871300
C	-1.52938600	3.31693100	-2.38313400
H	-1.93094000	2.34550800	-4.25983800
H	-1.31996600	4.11954800	-0.39190400
Cl	-9.67666000	3.11447600	0.67617100
Cl	-0.33895200	4.40854200	-3.07729300
Cl	9.56941500	-1.51748500	1.20664400
Cl	3.06051200	4.11311900	-4.33563900
H	-2.00948800	0.87283000	2.23377100

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C	-1.10312600	-5.11288700	-3.62567100
C	-2.04486200	-4.09030900	-3.51447300
C	-1.85964200	-3.02942300	-2.62646500
C	-0.72984500	-3.02040000	-1.77385900
C	0.29356200	-3.97319100	-1.98951300
C	0.08013700	-5.01575700	-2.89407800
H	-2.92801200	-4.09404600	-4.14880100
H	0.87062600	-5.74763800	-3.04267700
O	-0.60230100	-2.07808100	-0.83942300
C	-2.77332000	-1.83227800	-2.64712300
H	-3.47334200	-1.91709000	-3.49343800
H	-2.18277500	-0.92122000	-2.79546300
C	1.66155300	-3.72149200	-1.41051300
H	1.67912200	-3.77452700	-0.31550700
H	2.36317200	-4.48733100	-1.77529500
C	-4.61115400	-0.64472200	-1.30398000
C	-4.51459400	-2.75571500	-1.10916200
C	-5.50924700	-1.69016800	-0.61280800
H	-4.98823600	-0.38197500	-2.29890900
H	-4.83991500	-3.23362300	-2.04201500
H	-4.17144000	-3.52072600	-0.41363800
H	-6.53750800	-1.76484100	-0.96615900
H	-5.49413400	-1.56385500	0.46924900
C	3.56927900	-2.08033000	-1.67220400
C	2.21405100	-2.21018300	-3.31192600
C	3.74355700	-2.04171300	-3.20862300
H	4.08328000	-2.90180400	-1.16475000
H	1.86603300	-3.09213000	-3.85293900
H	1.66962300	-1.33697400	-3.67689200
H	4.30840500	-2.88354100	-3.61422000
H	4.14523700	-1.11127200	-3.61142200

N	2.10408700	-2.36123500	-1.81880300
N	-3.51897800	-1.67873600	-1.39146600
C	3.84180700	-0.77137300	-0.83798200
C	-4.22829800	0.60165200	-0.45229900
O	2.95142300	-0.73276600	0.21689600
O	-3.56033400	0.17902600	0.68717600
Zn	1.10472300	-1.21270200	-0.06531200
Zn	-2.08520200	-1.00097000	0.17294000
C	-0.79733800	1.02698000	2.29398800
C	-0.13783400	1.19206700	1.01243800
C	-0.70476600	2.15059700	3.19545000
C	0.82159300	2.18548900	0.83670400
C	0.22272400	3.12585000	3.02111000
H	-1.34849100	2.17401400	4.06953800
C	1.09760700	3.10697700	1.86613300
H	1.36279400	2.19415800	-0.09694800
H	0.30716400	3.91935000	3.74967500
O	-0.36190700	0.28907900	0.09010500
N	2.14664300	3.96434300	1.79016700
C	2.98512400	4.02157300	0.58625800
H	3.94619900	4.44595000	0.88725300
H	3.18978000	3.00257200	0.24451400
C	2.49153300	4.85452000	2.90133600
H	2.31733600	4.32395100	3.84053300
H	3.56998300	5.02646400	2.84901700
N	0.50704100	-1.46747400	2.13182700
C	0.26859500	-0.42883700	3.03694200
H	-0.48022400	-0.69219300	3.78610700
C	1.44923500	0.23998500	3.65162200
C	2.61384900	0.53834400	2.93517200
C	1.35588900	0.64092200	4.99204200
C	3.65069600	1.24331000	3.54904200
H	2.71917900	0.21839500	1.90443000
C	2.39470100	1.33668800	5.60614900
H	0.45453200	0.41258900	5.55562000
C	3.54632900	1.64992500	4.87984900
H	4.54680900	1.46896700	2.97768100
H	2.30618000	1.63278300	6.64725400
H	4.35865300	2.19454900	5.35278200
C	-4.49115400	-4.71378200	2.07537300
C	-3.71609800	-5.87283600	1.92809900
C	-2.32382600	-5.79973200	1.86020800
C	-1.72400400	-4.54428300	1.93303600
C	-2.50125000	-3.36807800	2.04557300

C	-3.89274000	-3.45684800	2.13382300
H	-5.57150600	-4.79515200	2.14172200
H	-4.20103600	-6.84241100	1.87741300
H	-1.72537400	-6.69921600	1.76260600
H	-4.47275600	-2.54749600	2.24450100
S	-0.01680200	-4.12400400	1.96734300
N	-1.77303300	-2.17846700	2.05646500
C	-0.46460100	-2.39737000	2.07370100
H	-1.26063600	-5.93670300	-4.31366600
C	1.75112500	6.19450400	2.87776400
H	0.66749200	6.04791400	2.89842200
H	2.03254200	6.79820300	3.74664800
H	1.99448900	6.76257300	1.97596400
C	2.37287100	4.85730900	-0.53880900
H	1.43319000	4.42778700	-0.89206400
H	2.17519300	5.87938900	-0.20389200
H	3.05525700	4.90115200	-1.38992100
C	3.67299600	0.51247800	-1.69646500
C	4.72392900	1.39229900	-1.98205600
C	2.40021400	0.86332000	-2.18064000
C	4.53421700	2.54276100	-2.75201700
H	5.71746200	1.18654100	-1.60506000
C	2.18674600	2.00088700	-2.95500600
H	1.53484000	0.24871300	-1.96677600
C	3.26845500	2.83025900	-3.24921300
H	5.36609900	3.20478400	-2.96574400
H	1.19501700	2.24649700	-3.31539600
C	5.27890500	-0.90796200	-0.31416300
C	6.36074100	-1.15201000	-1.17251300
C	5.52133200	-0.84886800	1.05957200
C	7.65541800	-1.30551000	-0.67903700
H	6.20234900	-1.21500400	-2.24464200
C	6.81031600	-0.99809100	1.57242500
H	4.68084400	-0.70642500	1.72456400
C	7.86874300	-1.22019700	0.69582400
H	8.48801100	-1.48940800	-1.34869400
H	6.98938300	-0.95023000	2.64090200
C	-5.54952300	1.29294700	-0.08545900
C	-5.99745700	1.25613900	1.23608700
C	-6.33818700	1.93092800	-1.04968000
C	-7.21343600	1.83682900	1.59698700
H	-5.36580700	0.77038900	1.97036900
C	-7.55733400	2.51328600	-0.70901500
H	-5.99212100	1.99407500	-2.07721000

C	-7.98437900	2.45732500	0.61710400
H	-7.56061100	1.81105800	2.62407500
H	-8.16633000	3.01037200	-1.45565600
C	-3.34104400	1.60036700	-1.22550600
C	-3.16658900	1.62328400	-2.61176900
C	-2.64653800	2.54507300	-0.45664300
C	-2.30135600	2.54001300	-3.21913500
H	-3.69702100	0.92502600	-3.24914900
C	-1.79318300	3.47269000	-1.03934300
H	-2.76853800	2.51794700	0.61951400
C	-1.62094100	3.45511800	-2.42418500
H	-2.16288800	2.54307400	-4.29459300
H	-1.25300600	4.18824100	-0.43072900
Cl	-9.52189100	3.19259700	1.05975900
Cl	-0.51805900	4.60284000	-3.17373500
Cl	9.50011500	-1.40545300	1.32966000
Cl	3.03347600	4.25833000	-4.24547000
H	-1.75958000	0.52507500	2.25569900

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C	-0.27894400	2.13136600	-4.83194400
C	0.97107700	1.56630700	-4.56829700
C	1.13754200	0.68111900	-3.50832800
C	0.04503300	0.36681500	-2.66207500
C	-1.24694000	0.84925100	-2.98805600
C	-1.37339500	1.73645400	-4.06426100
H	1.82487200	1.80848300	-5.19635300
H	-2.36316400	2.11476400	-4.30863100
O	0.30698000	-0.38850000	-1.58867300
C	2.42879600	-0.04918600	-3.26397000
H	3.13026900	0.13466100	-4.09058500
H	2.20313800	-1.11800700	-3.24804600
C	-2.49935300	0.41495400	-2.24780700
H	-2.66209900	0.99567600	-1.33487400
H	-3.37078900	0.59874600	-2.89633100
C	4.08451400	-0.81503700	-1.52618900
C	4.20066300	1.25119700	-1.96917700
C	5.05123200	0.30701100	-1.09821500
H	4.47194300	-1.37274800	-2.38742600
H	4.61442000	1.39169700	-2.97603500
H	3.91901000	2.22445300	-1.56334500
H	6.10041900	0.18577200	-1.36651700
H	4.95568300	0.51418900	-0.03158200
C	-3.63279600	-1.72603500	-1.34350400

C	-2.26576500	-1.99829600	-2.95590100
C	-3.26238000	-2.92771600	-2.23568200
H	-4.56875800	-1.24797500	-1.65019400
H	-2.63833300	-1.60991700	-3.91146200
H	-1.23732700	-2.34566900	-3.08417800
H	-4.06426100	-3.34916800	-2.84125700
H	-2.77462000	-3.71629300	-1.66685600
N	-2.43122400	-0.99551800	-1.86370500
N	3.10153500	0.23664900	-1.97699000
C	-3.55598900	-1.97852500	0.19473600
C	3.55552000	-1.75195300	-0.39804300
O	-2.27376600	-2.41646200	0.52123500
O	2.98276100	-0.97325100	0.58394300
Zn	-0.99395300	-1.16885200	-0.22718400
Zn	1.71105600	0.29883600	-0.16538200
C	-0.47197400	1.48995100	2.90584900
C	-0.52849200	1.20509600	1.53562600
C	-0.93576000	2.72701900	3.34693700
C	-1.07712600	2.14126900	0.64901300
C	-1.45568000	3.67498300	2.47182600
H	-0.90531700	2.96098200	4.40762400
C	-1.53158000	3.40426800	1.08633000
H	-1.05945200	1.90020700	-0.40385600
H	-1.81466500	4.61130600	2.87357100
O	0.01131500	0.04584900	1.06125300
N	-1.97440800	4.37037300	0.18840900
C	-2.31966300	4.04624400	-1.18769600
H	-2.15244600	4.94678700	-1.78672100
H	-1.61976500	3.30605200	-1.57735500
C	-2.29813700	5.71251200	0.65402500
H	-1.53058700	6.02034100	1.37130900
H	-2.18917700	6.38496100	-0.20242400
N	2.21672900	2.31296000	0.66089600
C	3.00195700	2.50730300	1.68411700
H	3.35296400	3.52803100	1.85212600
C	3.44691200	1.52154200	2.64537900
C	2.73371700	0.34516400	2.94081100
C	4.62824100	1.81287800	3.35991900
C	3.20786500	-0.52012700	3.92090800
H	1.80982600	0.11850700	2.42952900
C	5.11295100	0.92747500	4.31342900
H	5.16472600	2.73361400	3.14753400
C	4.39656500	-0.24056700	4.59774100
H	2.65317900	-1.42509900	4.14427400

H	6.03261500	1.14869800	4.84507300
H	4.76342400	-0.92864400	5.35341700
C	0.43408000	7.76123200	-0.98061100
C	0.14553000	7.26289800	-2.26293600
C	0.37597400	5.92613400	-2.58246300
C	0.89951400	5.09997100	-1.58913000
C	1.18885800	5.58635800	-0.28828000
C	0.95179600	6.93471600	0.01009600
H	0.24538100	8.80718900	-0.76085200
H	-0.26295300	7.92812200	-3.01707600
H	0.14939400	5.53556900	-3.56888600
H	1.17224900	7.30449200	1.00541000
S	1.28081700	3.39512700	-1.67200000
N	1.67926300	4.64268900	0.59561400
C	1.77335000	3.47978000	0.02581300
H	-0.41023100	2.82226800	-5.65834500
C	-3.69275500	5.88004700	1.27265900
H	-3.86166700	5.15928100	2.07563000
H	-3.80498600	6.88941200	1.68431700
H	-4.47855600	5.73452100	0.52657700
C	-3.75643400	3.54860400	-1.38595300
H	-3.96385000	2.70469300	-0.72523800
H	-4.48573700	4.33278500	-1.16673500
H	-3.91002700	3.22705800	-2.42235700
C	-4.58508400	-3.07718700	0.50333500
C	-5.96320000	-2.84291200	0.43182300
C	-4.13964700	-4.36545300	0.80918700
C	-6.88044200	-3.86869100	0.65206400
H	-6.33559500	-1.84584100	0.22113700
C	-5.04226300	-5.40427400	1.03484100
H	-3.07225300	-4.53468700	0.87265800
C	-6.40776100	-5.14529100	0.95038400
H	-7.94714400	-3.68194000	0.60031500
H	-4.69235400	-6.40248000	1.27342800
C	-3.90260300	-0.70007600	0.98844200
C	-4.77735700	0.29818100	0.53931200
C	-3.32701200	-0.54813300	2.25574000
C	-5.07584600	1.41019000	1.32925200
H	-5.24482900	0.22949300	-0.43685500
C	-3.61524900	0.55085500	3.05910500
H	-2.63299600	-1.30777300	2.59451400
C	-4.49021200	1.52476000	2.58609300
H	-5.75271600	2.17798900	0.97248600
H	-3.15397400	0.66170000	4.03197600

C	4.78875300	-2.48425700	0.16260700
C	5.31792300	-2.04540200	1.38017300
C	5.43792600	-3.52225700	-0.51429700
C	6.46821600	-2.62134000	1.91548900
H	4.80257500	-1.25139200	1.90223000
C	6.59039900	-4.11102900	0.00579500
H	5.04032400	-3.89992200	-1.44991400
C	7.09715900	-3.65076000	1.21932700
H	6.87041400	-2.27746600	2.86215200
H	7.08647200	-4.91983700	-0.51876400
C	2.50829800	-2.75726800	-0.93150100
C	2.56725000	-3.37787700	-2.18262500
C	1.40640100	-3.04190400	-0.10903500
C	1.55653000	-4.24013700	-2.61612400
H	3.39871800	-3.18979500	-2.85381800
C	0.38312000	-3.89765600	-0.52031100
H	1.37260900	-2.56939300	0.86757400
C	0.47186600	-4.49027700	-1.78206100
H	1.61154300	-4.71100300	-3.59126900
H	-0.47306700	-4.08857700	0.11753700
Cl	8.55113200	-4.38748600	1.88461000
Cl	-0.79046800	-5.58870200	-2.31986300
Cl	-4.87632200	2.91036700	3.59712900
Cl	-7.55801500	-6.44812900	1.23123100
H	-0.08189600	0.74984200	3.59403200

TS-6d

C	0.42619100	1.95964900	4.98709700
C	-0.88009700	1.61648100	4.63177800
C	-1.13169300	0.83259100	3.51011500
C	-0.06041500	0.41588100	2.68178400
C	1.27208700	0.66493800	3.09522200
C	1.48226300	1.44428800	4.24088600
H	-1.71609800	1.94524700	5.24407800
H	2.50542600	1.63666800	4.55567300
O	-0.37274700	-0.20874300	1.53913500
C	-2.50585000	0.27795600	3.23664700
H	-3.19319900	0.58493800	4.03784300
H	-2.41967000	-0.81073000	3.28101300
C	2.48386300	0.09264200	2.38190500
H	2.77787500	0.68287100	1.50980500
H	3.34060300	0.12210100	3.07443000
C	-4.15221700	-0.42938000	1.47152100
C	-4.15331200	1.65646000	1.84046000

C	-5.01967200	0.73733300	0.95698200
H	-4.61713800	-0.92039000	2.33552200
H	-4.60125000	1.85316400	2.82314400
H	-3.78856900	2.59330600	1.41564400
H	-6.08694200	0.69187600	1.17156500
H	-4.85597300	0.90639900	-0.10820000
C	3.37912600	-2.08434900	1.34095600
C	2.01605400	-2.30958100	2.96737100
C	2.93149900	-3.28472200	2.20114300
H	4.35864600	-1.69368800	1.63632700
H	2.42323600	-1.99088200	3.93422500
H	0.96527800	-2.58062300	3.09275100
H	3.70803900	-3.78167200	2.78185300
H	2.38153200	-4.01880900	1.61621800
N	2.25382200	-1.27477800	1.91672200
N	-3.12302100	0.57355900	1.92626300
C	3.24283800	-2.28425900	-0.20063500
C	-3.64178900	-1.45547400	0.41277900
O	1.92453700	-2.62147000	-0.49851300
O	-2.96157000	-0.78059700	-0.57732000
Zn	0.78422600	-1.26673400	0.28897100
Zn	-1.76342000	0.56963500	0.14132400
C	0.19882200	1.81414800	-2.71335700
C	0.62762000	1.20820900	-1.46993400
C	0.90503300	3.00447600	-3.12263000
C	1.41362000	1.94937800	-0.59341800
C	1.71143300	3.69972300	-2.27886400
H	0.73480100	3.38278300	-4.12660100
C	1.90574000	3.23176800	-0.92800400
H	1.56533800	1.54749300	0.39267700
H	2.17198000	4.61665900	-2.61270500
O	0.08077100	0.06107500	-1.12345800
N	2.50291800	4.03553100	-0.01174800
C	2.62705200	3.66821500	1.40147600
H	2.35259400	4.55022600	1.98754300
H	1.88172700	2.91540600	1.64584900
C	2.99753800	5.37197300	-0.36776800
H	2.24723500	5.87390600	-0.98337800
H	3.04373900	5.94489800	0.56067000
N	-1.75115800	2.44438100	-0.79352600
C	-1.63312000	2.47628000	-2.17487100
H	-1.52154800	3.48651400	-2.55960500
C	-2.57546200	1.65514700	-3.00112300
C	-2.48026100	0.27072000	-3.17883300

C	-3.61160200	2.35347500	-3.63993200
C	-3.40045700	-0.39759500	-3.98490700
H	-1.69415200	-0.28374300	-2.68353800
C	-4.54272300	1.68071000	-4.43003000
H	-3.68684000	3.42986200	-3.51094500
C	-4.43427200	0.30082800	-4.61010800
H	-3.31533100	-1.47234300	-4.10983200
H	-5.34102300	2.23544600	-4.91383000
H	-5.14821400	-0.22600600	-5.23637400
C	0.31737700	7.76928300	0.90331900
C	0.41969700	7.29546500	2.21885000
C	0.00309500	6.00109100	2.54296600
C	-0.50264800	5.19735500	1.52538700
C	-0.60546800	5.65857300	0.18472400
C	-0.19286800	6.96449100	-0.11404200
H	0.64015200	8.78012600	0.67299500
H	0.81970000	7.93902400	2.99603200
H	0.07691900	5.62926400	3.56005800
H	-0.27777200	7.32400900	-1.13418800
S	-1.05559000	3.53482800	1.60541700
N	-1.08878600	4.74417400	-0.72604200
C	-1.33698600	3.58797200	-0.16873900
H	0.61873700	2.56981400	5.86332400
C	4.36405300	5.36596600	-1.05590100
H	4.34940800	4.77643700	-1.97492100
H	4.65877500	6.39002400	-1.30705400
H	5.13249200	4.94194500	-0.40402700
C	4.02885400	3.19030200	1.78209800
H	4.33555200	2.35148000	1.15267300
H	4.76894000	3.98760900	1.67050000
H	4.04043000	2.86616400	2.82731400
C	4.18744000	-3.43652400	-0.57360600
C	5.57855400	-3.30433300	-0.49190600
C	3.65097500	-4.66675900	-0.95899000
C	6.42086500	-4.37650000	-0.77837600
H	6.02005800	-2.35088100	-0.21956500
C	4.47835000	-5.75059600	-1.25244500
H	2.57416800	-4.75410500	-1.03106000
C	5.85867900	-5.59519000	-1.15527100
H	7.49806100	-4.27031700	-0.71753700
H	4.05914800	-6.70435200	-1.55295500
C	3.65049300	-1.01772400	-0.98731200
C	4.56283700	-0.05620800	-0.53733000
C	3.08726000	-0.84625100	-2.25951200

C	4.91700000	1.03795900	-1.33231000
H	5.02456600	-0.14593800	0.44013500
C	3.42888500	0.23364900	-3.06693000
H	2.36082500	-1.57598200	-2.59587500
C	4.35115700	1.16658300	-2.59591900
H	5.62957900	1.77382300	-0.97739100
H	2.98795100	0.35429800	-4.04961200
C	-4.90656900	-2.11588100	-0.17131300
C	-5.36902400	-1.65956900	-1.40935600
C	-5.64370800	-3.09725000	0.49954400
C	-6.53904000	-2.16513200	-1.97196800
H	-4.78644300	-0.90894000	-1.92563400
C	-6.81733300	-3.61554500	-0.04825700
H	-5.30104100	-3.48680000	1.45188000
C	-7.25548200	-3.14064800	-1.28247000
H	-6.88912500	-1.80773500	-2.93421400
H	-7.38194700	-4.38163600	0.47115300
C	-2.71229700	-2.52228100	1.03493300
C	-2.87281500	-3.08043700	2.30625200
C	-1.62255500	-2.95577800	0.26209600
C	-1.97310000	-4.02649900	2.80607200
H	-3.70116100	-2.78094400	2.93962900
C	-0.71306500	-3.90256700	0.73707500
H	-1.52207300	-2.53813300	-0.73566300
C	-0.90044900	-4.42876400	2.01745800
H	-2.10613500	-4.44647400	3.79686400
H	0.13251400	-4.20858700	0.13154000
Cl	-8.73472500	-3.79041600	-1.98278800
Cl	0.22280700	-5.63021300	2.63933200
Cl	4.82035400	2.51367700	-3.62445600
Cl	6.91358200	-6.95523600	-1.52047900
H	-0.10778900	1.12966900	-3.49468300

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C	0.20436400	-6.36239600	-1.61324600
C	1.35901500	-5.65864200	-1.28408900
C	1.35412700	-4.26851000	-1.13757100
C	0.15521500	-3.54761500	-1.34786100
C	-1.01916800	-4.26237400	-1.67012900
C	-0.97937700	-5.65201100	-1.79704400
H	2.29245000	-6.19279100	-1.12624800
H	-1.89620600	-6.17803200	-2.05045500
O	0.10076600	-2.20598400	-1.24083800
C	2.62548900	-3.56641000	-0.74827800

H	3.44498700	-4.29631500	-0.67576300
H	2.52746500	-3.09289800	0.23682700
C	-2.31364000	-3.52346500	-1.83132400
H	-2.22778400	-2.70346800	-2.55286400
H	-3.08335900	-4.21111000	-2.21404400
C	4.31953200	-1.89141200	-1.69251200
C	3.15950100	-2.88038500	-3.15123900
C	4.26321600	-1.80150000	-3.23083600
H	5.07882600	-2.61640500	-1.37818700
H	3.55476500	-3.89873500	-3.25595500
H	2.26493200	-2.77805000	-3.77142800
H	5.17331200	-2.04848300	-3.77621700
H	3.88145800	-0.83453900	-3.56389300
C	-4.17977300	-2.42982600	-0.62276700
C	-3.16024300	-3.94448800	0.48397500
C	-4.59822500	-3.38232100	0.52330900
H	-4.62195000	-2.71797800	-1.58140600
H	-3.08058600	-4.96873700	0.10920400
H	-2.57323700	-3.86408600	1.40220900
H	-5.38013100	-4.09666000	0.26062100
H	-4.86733700	-2.88289400	1.45329100
N	-2.76344400	-2.92937700	-0.55188700
N	2.96560900	-2.51737400	-1.71988200
C	-4.28421000	-0.87147500	-0.53148100
C	4.36483900	-0.59609000	-0.83794700
O	-3.18582600	-0.35031000	-1.22473900
O	3.21909000	0.14571100	-1.09042400
Zn	-1.46024000	-0.99095100	-0.55195100
Zn	1.57781600	-0.85504700	-1.30807400
C	-1.13215000	2.53134300	-1.31956000
C	0.14308300	1.75611800	-1.37808100
C	-0.93893600	4.00120300	-1.37113700
C	1.34425300	2.38154100	-1.08008500
C	0.24144600	4.59094900	-1.12478000
H	-1.82295300	4.60751600	-1.53354200
C	1.41561800	3.77049200	-0.84947600
H	2.22667200	1.76493600	-0.99647500
H	0.31441800	5.66933800	-1.11887400
O	0.05110100	0.47661700	-1.61675700
N	2.54552000	4.35274600	-0.40304500
C	3.70576200	3.57084800	0.05728100
H	3.76648100	2.63151400	-0.48713000
H	4.60443800	4.13945900	-0.20097000
C	2.66264700	5.80436100	-0.20654900

H	1.73434900	6.19868500	0.21174700
H	3.42855600	5.96007400	0.55637500
N	-0.99727200	2.12192300	1.18208500
C	-1.88604500	2.13572000	0.05706400
H	-2.33497800	1.16747600	-0.17152300
C	-3.04681600	3.08967800	0.27560400
C	-3.09041600	3.94367800	1.37819600
C	-4.11384600	3.08771000	-0.63114500
C	-4.19137400	4.77876500	1.57678100
H	-2.26679000	3.91380200	2.08144200
C	-5.21218300	3.92307800	-0.43624900
H	-4.10437900	2.39242800	-1.46399700
C	-5.25527200	4.77247400	0.67269500
H	-4.22214500	5.42927100	2.44642600
H	-6.04088100	3.89526000	-1.13820200
H	-6.11356600	5.41866600	0.83252800
C	0.65586400	-3.36273700	2.91161300
C	1.16165900	-2.79001600	4.08024600
C	1.09459100	-1.40537800	4.26352200
C	0.53420200	-0.61605800	3.26587800
C	0.01888600	-1.18111900	2.07448800
C	0.07826600	-2.57274500	1.91362500
H	0.70257200	-4.43827900	2.76852100
H	1.61109400	-3.41069400	4.84789100
H	1.48770200	-0.95430700	5.16859700
H	-0.31720900	-3.03623700	1.02050200
S	0.36210400	1.13187700	3.21713100
N	-0.51096800	-0.27754200	1.15991100
C	-0.50595100	1.01761400	1.62359900
H	0.22597800	-7.44159600	-1.72052200
C	3.04893500	6.53368000	-1.49382800
H	2.28486500	6.40301200	-2.26520300
H	3.16842200	7.60469900	-1.30409700
H	3.99413600	6.14766700	-1.88708200
C	3.63363000	3.31324000	1.56364500
H	3.65361900	4.24866300	2.13167500
H	2.71228400	2.78233700	1.81899900
H	4.48336400	2.70249500	1.87991100
C	-4.29698200	-0.33275500	0.92034600
C	-5.09050400	0.76303800	1.28146400
C	-3.40061700	-0.81978200	1.88358500
C	-4.97549400	1.37472100	2.52830500
H	-5.79291700	1.17730400	0.57168900
C	-3.26112500	-0.22187400	3.13362700

H	-2.76367500	-1.66752600	1.67067800
C	-4.04653800	0.88558500	3.44028600
H	-5.57247700	2.24629500	2.76687700
H	-2.53469600	-0.59833900	3.84446600
C	-5.58789400	-0.50342600	-1.24654700
C	-6.82990400	-0.91005400	-0.74246000
C	-5.55108000	0.20573300	-2.44717400
C	-8.01294500	-0.60518500	-1.41212900
H	-6.87901000	-1.45120900	0.19782200
C	-6.72542300	0.52581700	-3.13029700
H	-4.58198300	0.49673200	-2.83396500
C	-7.94752100	0.11702000	-2.60341000
H	-8.97355600	-0.91455200	-1.01598300
H	-6.69467000	1.08270100	-4.06033400
C	5.59587100	0.21493600	-1.28369100
C	5.41463700	1.24350700	-2.21636500
C	6.89246000	-0.04872400	-0.82969200
C	6.49085000	1.99509200	-2.68425500
H	4.40858300	1.45521300	-2.55685700
C	7.98217800	0.69194900	-1.28742300
H	7.06470300	-0.82179200	-0.09010100
C	7.77079600	1.71065300	-2.21339300
H	6.34105600	2.79236300	-3.40392000
H	8.98263000	0.48774600	-0.92309000
C	4.44960200	-0.94895600	0.66073200
C	5.21987400	-1.99945800	1.17860600
C	3.73375800	-0.15381400	1.56095400
C	5.28639800	-2.24028800	2.55135100
H	5.78097600	-2.65490300	0.52110200
C	3.81004000	-0.35969100	2.93499700
H	3.10177700	0.63044100	1.16836200
C	4.58592900	-1.40811900	3.42035900
H	5.87545100	-3.06250800	2.94151400
H	3.26040400	0.28056300	3.61194400
Cl	9.13646600	2.65727000	-2.78847200
Cl	4.66817600	-1.69879500	5.15085100
Cl	-9.43679800	0.51785800	-3.45274200
Cl	-3.85106000	1.68448800	4.99357100
H	-1.80697800	2.19283400	-2.11148900

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C	0.35916300	-4.17616900	4.99777700
C	-0.82346500	-3.86983700	4.33045900
C	-0.89049000	-2.85632700	3.36814000

C	0.27275500	-2.09497100	3.09399900
C	1.48494700	-2.42448100	3.74955500
C	1.51129800	-3.45555000	4.68879600
H	-1.72404000	-4.43992800	4.54481000
H	2.44912100	-3.68741200	5.18733300
O	0.27058400	-1.08260400	2.21121000
C	-2.18161200	-2.69563200	2.59179000
H	-2.99035500	-3.20396500	3.13996000
H	-2.09932600	-3.19235200	1.61611600
C	2.74080500	-1.67147800	3.40221700
H	2.59187900	-0.58884900	3.46894400
H	3.54180500	-1.93673400	4.10742900
C	-3.88753200	-0.90373500	1.82719500
C	-2.71633700	-0.40768600	3.52467700
C	-3.84852300	0.31650400	2.76922700
H	-4.65876500	-1.61989400	2.13082600
H	-3.07324700	-0.96575000	4.39953400
H	-1.81637800	0.14859800	3.80736800
H	-4.75698200	0.54735800	3.32403700
H	-3.50202500	1.19737400	2.22874300
C	4.51457700	-1.29520900	1.66392200
C	3.79721700	-3.30729200	1.81077400
C	5.12466900	-2.67851600	1.32678000
H	4.95556400	-0.85287500	2.56215200
H	3.87381200	-3.86044400	2.75113600
H	3.24025200	-3.91771000	1.09502100
H	6.00178500	-2.94454200	1.91814700
H	5.34809700	-2.83353000	0.27192800
N	3.19598700	-1.94649800	2.01361500
N	-2.53510400	-1.29522300	2.34769500
C	4.35591700	-0.12498100	0.63472800
C	-3.90231700	-0.60247200	0.29763100
O	3.20847100	0.58272500	1.02620600
O	-2.77007800	0.11884900	-0.04350200
Zn	1.77070100	-0.70384200	0.87061000
Zn	-1.17608600	-0.49357300	0.82698100
C	-0.22607400	2.70781200	-0.62389200
C	-0.79630400	2.52679500	0.63000100
C	-0.81844800	3.69375100	-1.42129500
C	-1.85747600	3.28001800	1.11544900
C	-1.88996900	4.45895600	-0.98631800
H	-0.40356200	3.87653400	-2.40695400
C	-2.43822300	4.28118100	0.30793300
H	-2.27345600	3.03464600	2.08473000

H	-2.28529500	5.21911800	-1.64672200
O	-0.30488400	1.45325900	1.39780800
N	-3.50681400	5.03643900	0.75305600
C	-3.91611800	5.04697000	2.15100300
H	-3.04003000	4.85735100	2.77910900
H	-4.24161900	6.06501100	2.39588500
C	-4.23342700	5.92770400	-0.14156000
H	-4.29722200	5.46655000	-1.13210500
H	-5.26372200	5.99417400	0.22495100
N	0.47557900	0.90417800	-2.10590200
C	0.93982500	1.86026000	-1.11331900
H	1.39232300	1.38205000	-0.24063800
C	2.04733000	2.71840800	-1.70895300
C	2.18241500	2.89410700	-3.08765300
C	2.97235500	3.31696800	-0.84800900
C	3.23245400	3.66042400	-3.59821900
H	1.48422700	2.39110100	-3.74674900
C	4.02733200	4.07257500	-1.35596900
H	2.88727800	3.14246800	0.21878800
C	4.16101300	4.24662200	-2.73622000
H	3.33279600	3.78752400	-4.67264600
H	4.75700200	4.50505000	-0.67772900
H	4.98636300	4.82889500	-3.13544300
C	0.07375800	-4.80118800	-0.32003200
C	-0.27917200	-5.12207300	-1.63064400
C	-0.38899000	-4.11315300	-2.59106500
C	-0.15791900	-2.79268000	-2.21840900
C	0.17936000	-2.45360700	-0.89247600
C	0.31038900	-3.47380000	0.05480800
H	0.16760300	-5.58252600	0.42772500
H	-0.47449900	-6.15141600	-1.91117700
H	-0.66380500	-4.35524700	-3.61193000
H	0.58752400	-3.25472800	1.07691700
S	-0.23123000	-1.36476800	-3.23187600
N	0.35264700	-1.06377100	-0.64509800
C	0.27203800	-0.32097900	-1.84849900
H	0.38382200	-4.96773500	5.73902200
C	-3.62693200	7.33160900	-0.23926700
H	-2.60146800	7.29096400	-0.61608800
H	-4.21807600	7.96282900	-0.91076900
H	-3.60285900	7.81231400	0.74391300
C	-5.03962000	4.05785400	2.47612100
H	-5.94077000	4.28480200	1.89921000
H	-4.75126900	3.03519200	2.22773500

H	-5.29654800	4.10473800	3.53997200
C	4.16761500	-0.55215500	-0.83916200
C	4.46366600	0.37546100	-1.84925100
C	3.52930300	-1.74253300	-1.22288000
C	4.15393800	0.12737200	-3.18215700
H	4.92213500	1.32119800	-1.59009700
C	3.20809200	-2.00927200	-2.55545500
H	3.25362800	-2.49792200	-0.49813900
C	3.52657700	-1.06797100	-3.52746400
H	4.37426700	0.86884300	-3.93985700
H	2.70462100	-2.93001100	-2.82375200
C	5.60956600	0.73745500	0.77777800
C	6.85483100	0.28010000	0.33138000
C	5.53072900	1.98375400	1.39958900
C	8.00344800	1.05131300	0.49704500
H	6.92799200	-0.67839500	-0.17386000
C	6.66909000	2.77202000	1.57035600
H	4.56034800	2.32431700	1.73822000
C	7.89680800	2.29613200	1.11631500
H	8.96664500	0.70002100	0.14480300
H	6.60704500	3.74381700	2.04755100
C	-5.14766100	0.25840400	0.03685800
C	-4.97346500	1.59262700	-0.34087100
C	-6.44504800	-0.23439100	0.21286500
C	-6.07236300	2.43015500	-0.52728400
H	-3.96294300	1.95508600	-0.48295600
C	-7.55442900	0.59233900	0.03962500
H	-6.59930400	-1.27757500	0.47387600
C	-7.35318900	1.92340300	-0.32404100
H	-5.93622500	3.46465900	-0.82144800
H	-8.56046000	0.21280600	0.17839000
C	-3.95869600	-1.89551600	-0.53907000
C	-4.37436300	-3.14405000	-0.06531700
C	-3.53040300	-1.80115900	-1.87015100
C	-4.33282800	-4.27945600	-0.88027800
H	-4.72624100	-3.26472900	0.95327400
C	-3.49976200	-2.91453200	-2.70069600
H	-3.18421300	-0.84172400	-2.23426800
C	-3.88958800	-4.15234000	-2.19122000
H	-4.63318300	-5.24818900	-0.49732200
H	-3.15248400	-2.82878000	-3.72368700
Cl	-8.74476400	2.98406900	-0.52961200
Cl	-3.79081700	-5.57912800	-3.21585000
Cl	9.33864000	3.28342700	1.32213000

Cl	3.12680600	-1.38298700	-5.20604100
H	-0.35805100	1.63798100	2.34485700

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C	-1.18591500	0.22496900	0.20259900
C	-1.66967800	-0.95575100	0.78981100
C	-2.11422700	1.01588800	-0.47667500
C	-3.01179300	-1.31963200	0.70952000
C	-3.45881900	0.67837000	-0.56919300
H	-1.77255800	1.94037500	-0.93014000
C	-3.94607000	-0.50657900	0.02928200
H	-3.31865800	-2.25579500	1.16235400
H	-4.12910100	1.35155100	-1.08609200
O	-0.75512300	-1.74636900	1.43203300
N	-5.28042200	-0.86130400	-0.04670600
C	-5.81315900	-1.99828100	0.68965700
H	-5.31718800	-2.06507100	1.66375300
H	-6.86641200	-1.79000200	0.90659500
C	-6.22734300	-0.09382600	-0.84481200
H	-5.73661400	0.24204800	-1.76349600
H	-7.02172200	-0.77770400	-1.16307000
N	1.02358000	-0.26202100	-0.67212700
C	0.28845800	0.56274000	0.30260600
H	0.64495600	0.27594700	1.29824200
C	0.56965200	2.04530100	0.12157900
C	1.03709500	2.56886400	-1.08463300
C	0.31102400	2.91550500	1.18596500
C	1.24265300	3.94274500	-1.22644300
H	1.24956000	1.89213500	-1.90520600
C	0.51363600	4.28658100	1.04721100
H	-0.05319000	2.51082500	2.12671300
C	0.98061400	4.80572900	-0.16290000
H	1.61212700	4.33696000	-2.16877700
H	0.31284300	4.95010100	1.88339700
H	1.14370800	5.87383300	-0.27210200
C	6.63981400	-0.79897200	1.15601100
C	6.86492500	-1.76637900	0.16737600
C	5.83956600	-2.14972000	-0.69908400
C	4.59462200	-1.54539200	-0.55282400
C	4.34924400	-0.56613200	0.44344000
C	5.39210900	-0.19685200	1.30048700
H	7.45055400	-0.51359100	1.81953800
H	7.84456800	-2.22383200	0.07063400
H	6.01204200	-2.89820300	-1.46564600

H	5.20708800	0.55362100	2.06147300
S	3.12121800	-1.81068500	-1.48471800
N	3.06245800	-0.05186100	0.48157700
C	2.32144500	-0.58976700	-0.43792300
C	-6.83607500	1.09480800	-0.09337200
H	-6.05785800	1.79157700	0.22920800
H	-7.54411900	1.63602300	-0.72980400
H	-7.37146500	0.75457100	0.79882300
C	-5.69530100	-3.32550200	-0.06805500
H	-6.23894900	-3.27648900	-1.01674300
H	-4.65073200	-3.55530300	-0.29574800
H	-6.11148000	-4.14950600	0.52126900
H	-1.21141100	-2.49324600	1.83952800
H	0.46732200	-0.91493100	-1.20247300

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C	0.41704700	-3.50599000	0.44574100
C	-0.78414900	-4.23463700	0.40853400
C	-0.72200000	-5.62698000	0.31682400
C	0.50304000	-6.28582900	0.23497200
C	1.68238000	-5.53924100	0.23949400
C	1.66308300	-4.14783700	0.34753200
H	-1.64927300	-6.19416100	0.30171600
H	2.64349100	-6.04147200	0.16413000
O	0.37730500	-2.15212700	0.59239700
C	-2.10752100	-3.50385800	0.38805500
H	-2.92441600	-4.20910300	0.61558200
H	-2.28398700	-3.09804100	-0.61240700
C	-3.34944300	-1.50597500	1.13929500
C	-2.02078800	-2.73438100	2.73535600
C	-3.89448900	-1.28544000	2.56592900
H	-4.06987500	-2.06103900	0.52876700
C	-2.69444700	-1.58388500	3.47490800
H	-0.96992000	-2.87619700	3.00128900
H	-2.54908900	-3.68188200	2.92919700
H	-4.30927000	-0.28921800	2.71708600
H	-4.69513400	-2.00692800	2.76199800
H	-2.02654600	-0.71952600	3.52269000
H	-2.98493700	-1.85169300	4.49364000
N	-2.13888900	-2.35378200	1.31106300
C	-3.03008200	-0.20567900	0.33747200
O	-2.30953100	-0.69724200	-0.79638100
H	0.53937300	-7.36784900	0.16214600
C	2.93064500	-3.32732200	0.30853400

H	3.80061100	-4.00273400	0.39828600
H	2.96608700	-2.64645100	1.16144300
C	3.82181000	-1.29886900	-0.84389900
C	3.32425700	-3.27964800	-2.12969400
C	4.46688700	-1.18881600	-2.23703600
H	4.61854900	-1.42467400	-0.09316200
C	4.61658200	-2.65223300	-2.66362500
H	2.51656300	-3.19168500	-2.87127300
H	3.42776800	-4.34501400	-1.90142800
H	3.79567200	-0.66407800	-2.92549700
H	5.41173500	-0.64425700	-2.20848300
H	4.74528800	-2.77976600	-3.74211900
H	5.48469800	-3.09923700	-2.16524000
N	2.99700400	-2.51852600	-0.90948700
C	3.03497500	-0.03344200	-0.35885700
O	2.43585200	-0.33399200	0.90437800
C	-4.30141600	0.50016600	-0.15561800
C	-4.13955100	1.66963100	-0.91395900
C	-5.60077500	0.03810500	0.06889500
C	-5.22775200	2.34897800	-1.44860500
H	-3.14411800	2.06598100	-1.08643600
C	-6.70882800	0.71254300	-0.45001200
H	-5.78052300	-0.85354900	0.65695000
C	-6.51266000	1.86096200	-1.20915500
H	-5.08532200	3.24671300	-2.03895800
H	-7.71265100	0.34696600	-0.26642800
C	-2.17428800	0.76676800	1.15198400
C	-2.75688400	1.69314500	2.02995200
C	-0.78162400	0.72386000	1.06428700
C	-1.97090000	2.51617700	2.83209600
H	-3.83586200	1.79030400	2.07780300
C	0.02457200	1.53714600	1.86060600
H	-0.31127200	0.06485700	0.35045600
C	-0.58121500	2.42063800	2.74708200
H	-2.42725600	3.22944600	3.50893800
H	1.10199200	1.45561100	1.78539300
C	1.91460800	0.45866800	-1.29169700
C	1.53208500	1.80840700	-1.27043900
C	1.14157200	-0.42940200	-2.05202300
C	0.43812900	2.27062600	-1.99789700
H	2.08771900	2.51407300	-0.66468600
C	0.05214100	0.01653900	-2.80120300
H	1.37207000	-1.48460000	-2.01868100
C	-0.29067200	1.36659300	-2.76774500

H	0.15275700	3.31578400	-1.96468100
H	-0.53333000	-0.68131900	-3.38930700
C	4.07576300	1.05428100	-0.09692800
C	4.63630900	1.79633000	-1.14488800
C	4.53582500	1.28338400	1.20305300
C	5.63027000	2.74263700	-0.90811600
H	4.28220100	1.65101600	-2.15946800
C	5.52905000	2.22933800	1.45881500
H	4.10301300	0.71785800	2.01832200
C	6.07012700	2.95027100	0.39836900
H	6.05504800	3.31701500	-1.72339700
H	5.87698200	2.40648000	2.47015800
Cl	-7.89875500	2.71264400	-1.86879700
Cl	0.41692800	3.45145500	3.76186600
Cl	7.32123500	4.14540100	0.70829800
Cl	-1.67795100	1.93413900	-3.69476800
H	1.72428300	-0.98958600	0.75569200
H	-0.57139700	-1.91082900	0.83497300
H	-1.97234400	0.04958900	-1.30970900

Zn-L_5

C	-0.23665700	2.13311700	-2.13492700
C	0.90431800	2.32466000	-2.95225500
C	0.78845100	3.12438100	-4.09510900
C	-0.42238800	3.69718800	-4.47412300
C	-1.55453900	3.44837500	-3.69990000
C	-1.47963300	2.67277400	-2.54243100
H	1.67308800	3.28580400	-4.70639400
H	-2.51611400	3.86354400	-3.99167500
O	-0.18636100	1.44928300	-0.98072000
C	2.22240700	1.61389100	-2.72173200
H	3.00067200	2.12732500	-3.30474100
H	2.16340700	0.59309000	-3.12694000
C	3.94152600	0.79961400	-1.15384900
C	2.77143400	2.80668100	-0.63969700
C	4.96783600	1.93946000	-1.31716700
H	4.01462000	0.06570000	-1.96113000
C	4.26100300	3.20259500	-0.77301800
H	2.49300800	2.70863800	0.40925400
H	2.08454900	3.51473400	-1.10409000
H	5.90770200	1.74532000	-0.80387100
H	5.20369300	2.05928800	-2.37967100
H	4.66362100	3.48970500	0.20014900
H	4.39292500	4.05113400	-1.44908000

N	2.62435800	1.47851200	-1.30028300
C	3.98225800	-0.06080100	0.18291500
O	2.75952700	-0.69235700	0.36960400
Zn	1.20858200	0.06821800	-0.43510500
H	-0.48448800	4.31585200	-5.36284100
C	-2.71254100	2.37686600	-1.73358700
H	-3.54463900	2.99603100	-2.09376500
H	-2.55780000	2.61557100	-0.67782900
C	-4.38185700	0.74751200	-0.94643400
C	-3.44480700	0.50044100	-3.16077700
C	-5.50552100	0.34515400	-1.92679500
H	-4.61693400	1.73082200	-0.53237400
C	-4.95427600	0.71905600	-3.31298300
H	-3.18556500	-0.55415300	-3.28742100
H	-2.83881500	1.06511800	-3.86988000
H	-5.72409800	-0.72278200	-1.87120000
H	-6.43378800	0.86760000	-1.68766700
H	-5.38508200	0.12615300	-4.12457000
H	-5.15789100	1.77276000	-3.53311900
N	-3.11843800	0.92465900	-1.77062900
C	-4.11819200	-0.11099200	0.33922600
O	-2.95007000	0.39063500	0.92753000
Zn	-1.58116000	0.05329100	-0.40856000
C	-0.24050200	-1.68161600	-0.58710000
C	5.06204600	-1.15414400	0.05796900
C	4.98693800	-2.21888900	0.96697900
C	6.10386600	-1.15356400	-0.87333100
C	5.91837200	-3.25044400	0.95401800
H	4.17163900	-2.22939700	1.68074900
C	7.05020000	-2.18287500	-0.90321600
H	6.20437700	-0.35566000	-1.59964800
C	6.94929400	-3.22220700	0.01336900
H	5.85037300	-4.07036800	1.66012900
H	7.85286800	-2.17480600	-1.63193100
C	4.33088200	0.80682400	1.41682800
C	5.64166600	1.21059600	1.70475800
C	3.31961400	1.19235500	2.30138400
C	5.92712500	2.03058400	2.79497500
H	6.46219900	0.86020600	1.08838000
C	3.58082800	2.01233500	3.39836400
H	2.31536500	0.82159600	2.13496000
C	4.88662500	2.43871200	3.62752400
H	6.94493400	2.33872200	3.00585900
H	2.78541100	2.30779400	4.07338600

C	-3.89525800	-1.62499600	0.13402600
C	-3.63665200	-2.36345000	1.30437700
C	-3.76735400	-2.28830400	-1.08904900
C	-3.26217500	-3.69909400	1.25830700
H	-3.71225500	-1.85954900	2.26125000
C	-3.38460900	-3.63357000	-1.15881100
H	-3.95824100	-1.77877400	-2.02072700
C	-3.13111600	-4.32758500	0.01548400
H	-3.06320300	-4.25247400	2.16907900
H	-3.28148200	-4.12709500	-2.11835000
C	-5.32770100	0.11304300	1.25429900
C	-6.51898800	-0.60347800	1.09578700
C	-5.25666800	1.09423200	2.24575400
C	-7.62690900	-0.34121700	1.89999900
H	-6.58185500	-1.38938600	0.34965100
C	-6.35393600	1.36872100	3.06136200
H	-4.32012900	1.62432500	2.37363100
C	-7.53255500	0.64893900	2.87646300
H	-8.54791400	-0.90024900	1.77947100
H	-6.29724100	2.12663000	3.83474400
Cl	8.13420000	-4.52143200	-0.01366800
Cl	5.23276400	3.47883700	5.00123300
Cl	-8.92344000	0.98627000	3.89959900
Cl	-2.63654700	-6.00993400	-0.05651800
H	-1.06613900	-2.19407800	-0.07640800
H	0.62336800	-2.09708800	-0.04960900
C	-0.19442100	-2.13764600	-2.06206300
H	-1.06934700	-1.79284300	-2.62579500
H	0.68443300	-1.74643000	-2.59247700
H	-0.16130300	-3.22932800	-2.15834800

4C'

C	0.67897000	3.42150100	1.16817000
C	-0.42761700	4.28392700	1.32388100
C	-0.21035400	5.65759500	1.45234700
C	1.07790500	6.18947300	1.43519100
C	2.16099000	5.33397300	1.23622100
C	1.98634500	3.95591200	1.07698300
H	-1.06765700	6.31575400	1.57076300
H	3.16631200	5.74348600	1.17342600
O	0.48887700	2.10229300	1.09255200
C	-1.82558500	3.72212100	1.36424900
H	-2.54081400	4.55508000	1.41033800
H	-1.97208100	3.13161000	2.27812300

C	-3.60479900	2.43402300	0.27762900
C	-1.95626600	3.45650700	-1.09914900
C	-4.33621200	3.53828500	-0.52319000
H	-3.90066700	2.44670700	1.32903300
C	-3.27055000	4.18816400	-1.43847200
H	-1.75418100	2.67527700	-1.83255200
H	-1.08664600	4.11310500	-1.05437200
H	-5.18546700	3.14681500	-1.08080700
H	-4.74256500	4.27912900	0.17241500
H	-3.51238200	4.07106800	-2.49718400
H	-3.18720200	5.25996700	-1.23779000
N	-2.15967200	2.81193500	0.22589900
C	-3.76475100	0.92013700	-0.12333300
O	-2.92402900	0.19337400	0.71214400
Zn	-1.11350100	0.88730600	0.66481400
H	1.23448700	7.25674900	1.54939300
C	3.16053200	3.10977500	0.64252500
H	4.04853000	3.75433200	0.58210300
H	2.98272400	2.71906800	-0.36483500
C	4.68381600	1.19892600	0.82935200
C	3.89438600	2.27638800	2.85362500
C	5.78488100	1.13984100	1.90318100
H	5.03215300	1.85060200	0.02278200
C	5.42752000	2.29726600	2.84964300
H	3.51800000	1.52674600	3.55789100
H	3.43290400	3.22967200	3.11922500
H	5.78038200	0.18686300	2.43698500
H	6.77320400	1.24880400	1.45243600
H	5.85329500	2.18752400	3.85066700
H	5.78810800	3.24689000	2.43877800
N	3.49526800	1.90064200	1.46852000
C	4.24092900	-0.10187400	0.07571000
O	3.07766300	0.25335700	-0.63484700
Zn	1.82265400	0.58339600	0.91052400
C	0.33399700	-0.85547600	0.84762900
C	-0.37791500	-1.42139800	1.94096000
C	0.33855000	-1.65918500	-0.33021200
C	-1.14313300	-2.56887000	1.85511800
H	-0.36437000	-0.90453900	2.90092200
C	-0.44056200	-2.80846300	-0.44850700
C	-1.24200400	-3.26312500	0.62080700
H	-1.69640700	-2.89699000	2.72327300
H	-0.40852200	-3.33015500	-1.39548600
O	1.06359800	-1.32078300	-1.42754900

H	1.85899700	-0.76653200	-1.18306300
N	-2.07268300	-4.35451600	0.47595400
C	-2.99174700	-4.72600200	1.54994800
H	-3.31250200	-5.75464100	1.35931600
H	-2.43567100	-4.75628100	2.49196100
C	-2.31714600	-4.92298100	-0.84695800
H	-1.35585900	-5.12632900	-1.33073400
H	-2.78964900	-5.89780000	-0.69564300
C	-3.19271900	-4.05860600	-1.76501700
H	-3.27606900	-4.51913900	-2.75502700
H	-4.20096500	-3.95048800	-1.35629500
H	-2.76968200	-3.05885200	-1.89005500
C	-4.21531700	-3.80964400	1.68167500
H	-4.87727200	-3.91377300	0.81813800
H	-4.79179900	-4.06570800	2.57697000
H	-3.91912400	-2.75959200	1.74708800
C	-5.19747000	0.41859300	0.11109100
C	-5.45814200	-0.91990200	-0.21777100
C	-6.22785700	1.16877400	0.68075900
C	-6.70377900	-1.49367400	0.00317600
H	-4.66063700	-1.51736300	-0.64446700
C	-7.48973800	0.61089500	0.91070400
H	-6.07298400	2.20291300	0.96488600
C	-7.71648300	-0.71614000	0.56766000
H	-6.89460800	-2.52917900	-0.25543200
H	-8.28352400	1.20234800	1.35282800
C	-3.40298900	0.68300700	-1.61156300
C	-4.15554400	1.19340200	-2.67929300
C	-2.27145800	-0.07796100	-1.92111100
C	-3.73827900	1.03253300	-3.99872100
H	-5.09082300	1.70717800	-2.49070600
C	-1.82853200	-0.24866900	-3.23424800
H	-1.76273200	-0.60955100	-1.12860100
C	-2.56040500	0.33123300	-4.26499700
H	-4.32170000	1.43978500	-4.81699000
H	-0.93164300	-0.82462800	-3.43267700
C	3.85840100	-1.30976500	0.96153100
C	3.51770700	-2.49314000	0.28430500
C	3.58200100	-1.24528800	2.33379200
C	2.88466700	-3.54631300	0.93007700
H	3.70757800	-2.56215600	-0.78067600
C	2.95543100	-2.30162100	3.00431300
H	3.83632700	-0.36904400	2.91359600
C	2.59348800	-3.43627400	2.29148600

H	2.59389200	-4.43579200	0.38403500
H	2.73736500	-2.22950700	4.06368600
C	5.38113300	-0.47471600	-0.87202600
C	6.52012100	-1.14933600	-0.41869900
C	5.30740800	-0.09617000	-2.21383500
C	7.57613100	-1.43304400	-1.28251200
H	6.57842200	-1.47496300	0.61535600
C	6.35305200	-0.37512600	-3.09373800
H	4.41022300	0.40671500	-2.55536100
C	7.48136500	-1.03838600	-2.61646000
H	8.45677700	-1.95955500	-0.93252100
H	6.29379800	-0.08737600	-4.13741900
Cl	-9.30026600	-1.42924200	0.84876500
Cl	-2.02279400	0.14966400	-5.92872600
Cl	8.80671100	-1.39518400	-3.71636300
Cl	1.75426900	-4.74431300	3.10323900

4’

C	0.05873800	3.66111800	0.39700400
C	1.25405400	4.37598100	0.64450400
C	1.18541400	5.67964500	1.14276400
C	-0.03646500	6.30282800	1.37994000
C	-1.20961000	5.59205600	1.13858800
C	-1.18956300	4.27488000	0.66961800
H	2.11232700	6.21410300	1.33524400
H	-2.17153600	6.05831100	1.33623800
O	0.11160700	2.41304500	-0.08540300
C	2.60613800	3.79268900	0.31775600
H	3.38037300	4.46403200	0.71428900
H	2.74953600	3.76777500	-0.77113100
C	4.25157600	1.99238600	0.51246700
C	2.64542200	2.23730600	2.25710900
C	5.04076400	2.42300600	1.77266000
H	4.57714900	2.55751700	-0.36334700
C	4.00594900	2.53758900	2.91817300
H	2.34967200	1.20439200	2.44938700
H	1.83813700	2.89139700	2.58963800
H	5.85549600	1.73976000	2.00589800
H	5.50517300	3.39633000	1.58578600
H	4.20489700	1.82604800	3.72265500
H	4.01973600	3.53929900	3.35615900
N	2.84033800	2.39830800	0.79237300
C	4.27579300	0.50362000	0.00073300
O	3.39132400	0.43797800	-1.07691000

Zn	1.67107200	1.12753500	-0.53592000
H	-0.07472100	7.31989200	1.75481100
C	-2.50146800	3.52807400	0.58909500
H	-3.31545800	4.23588500	0.79998800
H	-2.55250300	2.75673700	1.36600300
C	-4.14198800	2.12217000	-0.57262800
C	-2.86803300	3.74343700	-1.85059400
C	-4.98950400	2.62786000	-1.75230000
H	-4.59689000	2.48404100	0.35480700
C	-4.36268600	3.99043700	-2.08537400
H	-2.40922000	3.27418700	-2.72774100
H	-2.29350800	4.64534100	-1.63058700
H	-4.92466900	1.95335500	-2.60945600
H	-6.04292300	2.69844600	-1.47452800
H	-4.57866800	4.33233500	-3.10116700
H	-4.72957900	4.75590900	-1.39224100
N	-2.79515200	2.81026800	-0.69200300
C	-3.97468400	0.57908800	-0.32781600
O	-2.92721600	0.42050000	0.59685000
Zn	-1.41292600	1.12578700	-0.40554700
C	0.58725800	-2.05073100	-2.18006200
C	0.49633300	-3.44141400	-2.14902900
C	0.02302100	-1.33499600	-1.12225300
C	-0.12038700	-4.11624800	-1.09927800
H	0.91840800	-4.01981500	-2.96514900
C	-0.60114600	-1.99167300	-0.06023900
C	-0.67903000	-3.39770900	-0.01544800
H	-0.14402100	-5.19753200	-1.11771800
H	-1.05867800	-1.38732400	0.71078100
O	0.08674600	0.03225100	-1.10637500
N	-1.28061500	-4.03599300	1.06124300
C	-1.22889400	-5.48751600	1.18382000
H	-2.02606600	-5.78573300	1.87233500
H	-1.48356000	-5.94029500	0.22074800
C	-1.60610200	-3.29689600	2.28103100
H	-1.54519400	-4.00388200	3.11404700
H	-0.83631700	-2.53982400	2.47663400
C	-2.99106900	-2.64458800	2.25825800
H	-3.22243400	-2.21708400	3.24054400
H	-3.04496200	-1.83562000	1.52705900
H	-3.76014900	-3.38738900	2.02215700
C	0.12225500	-6.01167300	1.68559600
H	0.36101600	-5.59114900	2.66773700
H	0.11072500	-7.10318500	1.77467500

H	0.92566700	-5.73062600	0.99920300
C	5.67060600	0.11095700	-0.51149300
C	5.81953200	-1.18830000	-1.01863600
C	6.77559100	0.96396500	-0.55374200
C	7.02920100	-1.63109100	-1.53936500
H	4.96528200	-1.85614000	-1.00689800
C	8.00253800	0.53755000	-1.07144900
H	6.70941300	1.98287800	-0.19179800
C	8.11885100	-0.75885500	-1.55687300
H	7.13241800	-2.63770500	-1.92846100
H	8.85432200	1.20772300	-1.09758400
C	3.86758000	-0.50838600	1.10454700
C	4.58597000	-0.68683200	2.29730800
C	2.74858900	-1.32164100	0.89518700
C	4.15071300	-1.57197800	3.28119000
H	5.51184700	-0.15025100	2.46341200
C	2.29978800	-2.22356500	1.86246000
H	2.25449800	-1.30468200	-0.06695600
C	2.99399300	-2.32223100	3.06146700
H	4.70805500	-1.69127800	4.20363500
H	1.43521000	-2.84436100	1.66454400
C	-3.59560200	-0.26575000	-1.56448200
C	-3.68696700	-1.66328600	-1.45141500
C	-2.95436300	0.24958900	-2.70025100
C	-3.18090700	-2.51222000	-2.42735400
H	-4.14789900	-2.09090500	-0.56905000
C	-2.43154800	-0.58907000	-3.68988700
H	-2.85654900	1.31674000	-2.85046300
C	-2.55270400	-1.96511000	-3.54667600
H	-3.24365500	-3.58745200	-2.31212100
H	-1.93775000	-0.17233500	-4.56004300
C	-5.30149800	0.10033300	0.26506400
C	-6.42013700	-0.14897100	-0.53778200
C	-5.41854500	-0.04287100	1.64910100
C	-7.63625400	-0.53240200	0.02511700
H	-6.33944400	-0.06414900	-1.61696400
C	-6.62604500	-0.42929100	2.23001100
H	-4.54030500	0.13750300	2.25697200
C	-7.72632100	-0.66833700	1.40965100
H	-8.50050900	-0.73171100	-0.59825000
H	-6.71394300	-0.54872200	3.30408800
Cl	9.65908900	-1.30919000	-2.20431500
Cl	2.42987300	-3.43556100	4.30166100
Cl	-9.25420800	-1.15884700	2.13035800

Cl	-1.91468400	-3.02538200	-4.78832600
H	1.06964100	-1.52365800	-2.99460000

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C	-0.64334600	-1.93197400	2.98689500
C	0.48606700	-2.16297400	3.81405000
C	0.31087100	-2.77307200	5.06116700
C	-0.94289900	-3.15854600	5.52364500
C	-2.04501500	-2.96440000	4.69461300
C	-1.91721200	-2.37671200	3.43484200
H	1.18841000	-2.94686500	5.67921400
H	-3.03026900	-3.29262900	5.01656800
O	-0.52830300	-1.35047000	1.78401500
C	1.89312900	-1.78149600	3.41286900
H	2.58719300	-2.25159900	4.12320600
H	2.05235800	-0.70162000	3.50598200
C	3.68580100	-1.85314800	1.74745600
C	2.10705200	-3.61424800	1.79301000
C	4.45012100	-3.07672500	2.29520600
H	3.92563300	-0.94267100	2.30173900
C	3.44803000	-4.25478200	2.22140700
H	1.92160100	-3.78879000	0.73482400
H	1.24933900	-3.98305900	2.35634900
H	5.36850900	-3.27219300	1.74339200
H	4.74473200	-2.88840500	3.33225300
H	3.76027800	-5.00506400	1.49246000
H	3.35800900	-4.75283500	3.19042800
N	2.24948400	-2.14861200	2.01430800
C	3.89100300	-1.45488100	0.23802500
O	2.94402700	-0.49121200	-0.07375500
Zn	1.18084600	-0.59410200	0.79935400
H	-1.05517000	-3.62263300	6.49754700
C	-3.12468200	-2.29537900	2.53565900
H	-3.93423400	-2.90199800	2.96497800
H	-2.88482300	-2.71874600	1.55515000
C	-4.76322900	-0.93044200	1.30431000
C	-4.08208300	-0.21378100	3.49185900
C	-6.04758700	-0.67183100	2.13191900
H	-4.79744900	-1.93929600	0.88984200
C	-5.57580100	-0.55427700	3.59949100
H	-3.92299800	0.85862700	3.36140600
H	-3.48937400	-0.53352700	4.35068400
H	-6.56734600	0.22548800	1.79599800
H	-6.75538300	-1.49404100	2.00427700

H	-6.13053900	0.19676700	4.16939500
H	-5.70595900	-1.51074300	4.11658500
N	-3.60650100	-0.90587500	2.26985800
C	-4.43925300	-0.07171800	0.02396200
O	-3.19136200	-0.51892600	-0.41525000
Zn	-1.99938000	-0.11075300	1.07118600
C	0.92929400	1.41010000	2.01773300
C	2.19254500	2.06089100	2.02100600
C	-0.20935500	2.14445500	1.53853700
C	2.36047900	3.33921300	1.54668200
H	3.06042500	1.52817900	2.40202000
C	-0.02094400	3.44994800	1.04659800
C	1.22242700	4.09505600	1.11042400
H	3.35102100	3.77231100	1.51441200
H	-0.91478200	3.95869100	0.71653200
O	-1.42231400	1.66037300	1.59283300
N	1.34872400	5.42861300	0.78878400
C	2.51255100	6.20242700	1.21568700
H	2.15383600	7.18330700	1.54777700
H	2.94956700	5.72727300	2.09831300
C	0.20173600	6.17371300	0.26752100
H	-0.67669200	6.00113700	0.90082900
H	0.44247400	7.23624300	0.35532700
N	0.31699200	1.42232300	-2.09042300
C	1.57461300	1.48249200	-1.77658400
H	2.10692800	0.61464200	-1.37431900
C	2.41940600	2.63022600	-2.05136600
C	2.00354000	3.70249600	-2.85713800
C	3.75164300	2.56340500	-1.60474500
C	2.91728200	4.68312300	-3.22542700
H	0.97815000	3.72678200	-3.20783400
C	4.66327000	3.54489500	-1.98046800
H	4.04893700	1.72871900	-0.97994100
C	4.24740400	4.60034800	-2.79693400
H	2.60344900	5.50559300	-3.86088900
H	5.69470100	3.48066800	-1.64769100
H	4.95912500	5.36270100	-3.09972100
C	-1.51128400	-4.18386200	-1.09720400
C	-2.22504600	-4.11132300	-2.30368300
C	-2.24438300	-2.93402700	-3.04653800
C	-1.53906300	-1.83560700	-2.55684300
C	-0.82099800	-1.89598700	-1.34332700
C	-0.80911800	-3.08741400	-0.60915900
H	-1.49923900	-5.11307800	-0.53671400

H	-2.76404300	-4.98108100	-2.66498700
H	-2.79563300	-2.86982600	-3.97834200
H	-0.27639300	-3.13592500	0.32873700
S	-1.37341000	-0.24813500	-3.26337800
N	-0.14196200	-0.71289200	-1.01291900
C	-0.29696500	0.20592000	-1.95485400
C	-0.13451900	5.85400400	-1.19013900
H	-1.02266900	6.41355000	-1.49933900
H	0.69936100	6.12004800	-1.84455500
H	-0.33861900	4.78889000	-1.32159900
C	3.57334800	6.38181400	0.13089800
H	3.14817500	6.86445900	-0.75433600
H	4.39848100	7.00226300	0.49809700
H	3.97434900	5.41719200	-0.18378200
C	5.27353100	-0.80684800	0.02826100
C	5.57804600	-0.38436200	-1.27492000
C	6.19273300	-0.52155400	1.04027800
C	6.74099700	0.32011800	-1.56170100
H	4.87362700	-0.59790500	-2.07143300
C	7.37168800	0.18261800	0.77362700
H	6.01288300	-0.83441700	2.06210500
C	7.63100800	0.60502600	-0.52447200
H	6.95643100	0.65117200	-2.57130500
H	8.07495900	0.40327700	1.56866100
C	3.76914100	-2.66843000	-0.71204900
C	4.76738200	-3.64448400	-0.83245000
C	2.62396000	-2.80325900	-1.50173900
C	4.59564500	-4.75844000	-1.65280200
H	5.70607200	-3.52871600	-0.30184300
C	2.42580200	-3.91167000	-2.32379000
H	1.88007800	-2.02105100	-1.46958500
C	3.41278800	-4.89194200	-2.37954600
H	5.37176900	-5.51087500	-1.73627400
H	1.51800000	-4.01002300	-2.90847600
C	-4.36084400	1.46535300	0.18754900
C	-3.66320700	2.13100600	-0.83530100
C	-4.85348800	2.23714500	1.24264200
C	-3.44393600	3.50142700	-0.80395100
H	-3.26152200	1.53825100	-1.64779400
C	-4.63341600	3.61742600	1.30182600
H	-5.40951100	1.78934000	2.05307000
C	-3.92646500	4.23487000	0.27996700
H	-2.89409700	3.99469400	-1.59738000
H	-5.00471200	4.19881600	2.13809700

C	-5.51366000	-0.42688600	-1.01171200
C	-6.71409000	0.27819700	-1.13571200
C	-5.29205800	-1.53227200	-1.83934300
C	-7.68370600	-0.11206800	-2.06053800
H	-6.89074300	1.15629700	-0.52288300
C	-6.24769200	-1.93616400	-2.76861400
H	-4.34869600	-2.05579300	-1.74805100
C	-7.43973900	-1.21999800	-2.86833900
H	-8.61164200	0.43970800	-2.16019400
H	-6.07327000	-2.79177100	-3.41212900
Cl	9.09759900	1.51302900	-0.86868900
Cl	3.17887100	-6.30464700	-3.39971100
Cl	-8.65348600	-1.71873800	-4.04319000
Cl	-3.63412300	5.97172400	0.35276000
H	0.71783900	0.65729400	2.77369300

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C	-0.23380400	-1.79813300	2.94431500
C	0.91433300	-1.64128700	3.75142900
C	0.87389600	-2.04121600	5.09058900
C	-0.28346000	-2.57312300	5.65366500
C	-1.41835900	-2.70906900	4.85572700
C	-1.41161000	-2.33672700	3.50976500
H	1.76627700	-1.91787500	5.69933800
H	-2.33147500	-3.12199600	5.27700200
O	-0.21455600	-1.44658900	1.64702100
C	2.15384900	-0.99260500	3.20027500
H	2.90339100	-0.91931800	3.99876400
H	1.92803100	0.03076200	2.88144500
C	3.96187000	-0.98229700	1.55351500
C	3.17347900	-3.07443700	2.35407900
C	5.07282400	-1.51951100	2.47683800
H	3.77805600	0.08179500	1.71685900
C	4.64361400	-2.96394900	2.82696000
H	3.11029100	-3.69242000	1.45811200
H	2.49763000	-3.48914300	3.10313000
H	6.05771200	-1.48465200	2.01463500
H	5.12348600	-0.90348700	3.38012200
H	5.26328400	-3.69601800	2.30567200
H	4.73635600	-3.15474800	3.89900900
N	2.73066200	-1.69286500	2.01147300
C	4.16751000	-1.12222600	-0.00978900
O	2.93963200	-1.01906900	-0.64618700
Zn	1.33915300	-1.38277700	0.34120300

H	-0.30187100	-2.87411100	6.69561800
C	-2.63423500	-2.53375700	2.65619100
H	-3.39016300	-3.09039400	3.22736200
H	-2.38225200	-3.13648700	1.77718600
C	-4.43088200	-1.56181100	1.31400700
C	-3.65796800	-0.34693700	3.20738700
C	-5.62455800	-1.48619600	2.29913900
H	-4.31682300	-2.58198300	0.94510300
C	-5.08132400	-0.80137500	3.58026700
H	-3.66168700	0.66734300	2.80523000
H	-2.95102800	-0.37851600	4.03825200
H	-6.47563400	-0.96498300	1.86049300
H	-5.97969000	-2.49469600	2.52656000
H	-5.69560000	0.04261100	3.90694200
H	-5.05360100	-1.51261600	4.41132100
N	-3.20748200	-1.26104400	2.12920700
C	-4.41885100	-0.74793800	-0.03957800
O	-3.18568300	-1.02083200	-0.61406600
Zn	-1.78067900	-0.51771900	0.62812500
C	0.84763100	1.75458300	0.76260200
C	1.88638900	2.61553000	1.27291700
C	-0.52096500	2.24985400	0.88135200
C	1.66569100	3.93475500	1.49767400
H	2.89385700	2.22026100	1.36749100
C	-0.72286000	3.63651400	1.02266900
C	0.33965400	4.50058100	1.31906000
H	2.49387800	4.56948700	1.77705700
H	-1.74586000	3.98128200	0.96730000
O	-1.51331700	1.44513200	0.80584300
N	0.14711900	5.84274200	1.48124800
C	1.24364900	6.74425600	1.84173200
H	0.79165400	7.62309400	2.31015700
H	1.85152700	6.27251000	2.61853000
C	-1.13332900	6.45937500	1.11424700
H	-1.95133800	5.89652800	1.57316500
H	-1.15062900	7.45308200	1.56886500
N	0.05913000	1.17905200	-1.88390800
C	1.16610000	1.60273400	-1.18325700
H	1.97601200	0.87510500	-1.07648400
C	1.65072600	2.94755300	-1.60128500
C	0.77350600	3.90882500	-2.11589700
C	3.01590100	3.24652400	-1.51483800
C	1.25655800	5.14543700	-2.53948600
H	-0.27672100	3.65564500	-2.20308400

C	3.50335000	4.47804600	-1.94815400
H	3.69936400	2.50342600	-1.12112700
C	2.62183400	5.43226300	-2.46191100
H	0.56902300	5.88232400	-2.94365600
H	4.56802700	4.68423200	-1.89721000
H	2.99752500	6.39148300	-2.80616500
C	-1.36732800	-4.61675100	-1.50445800
C	-2.03474900	-4.48336300	-2.72654500
C	-2.07008400	-3.25129900	-3.38557000
C	-1.42324900	-2.16413000	-2.80741900
C	-0.73782200	-2.29294200	-1.58263600
C	-0.71647400	-3.52591400	-0.92522300
H	-1.35552900	-5.57639100	-0.99736800
H	-2.53531700	-5.34003500	-3.16606900
H	-2.60321000	-3.14151800	-4.32397800
H	-0.24133100	-3.62192000	0.04796200
S	-1.33270800	-0.50694200	-3.37092300
N	-0.15838300	-1.11028900	-1.10082800
C	-0.33833400	-0.05798500	-1.95385200
C	-1.35516500	6.56875600	-0.39630700
H	-2.33091700	7.01790200	-0.59786100
H	-0.58078600	7.18266400	-0.86286000
H	-1.33268300	5.58272100	-0.86367900
C	2.12071500	7.17368900	0.66227100
H	1.53920100	7.73455900	-0.07396300
H	2.93552100	7.81585500	1.01342700
H	2.55005700	6.30942100	0.15125700
C	5.04231500	0.04126900	-0.52046100
C	5.08740600	0.22378100	-1.91099800
C	5.74808100	0.93799300	0.28585600
C	5.79972200	1.27059200	-2.48313200
H	4.52642900	-0.45724300	-2.54037500
C	6.46603200	2.00266000	-0.27080300
H	5.75518100	0.83482300	1.36486800
C	6.48232500	2.16020100	-1.65105900
H	5.81352600	1.41213600	-3.55759200
H	7.00112600	2.69994200	0.36380300
C	4.85392200	-2.45245200	-0.39217500
C	6.23528900	-2.64784200	-0.26403700
C	4.08728100	-3.50138800	-0.90881200
C	6.82706500	-3.87191100	-0.57089200
H	6.86984700	-1.82708200	0.05291900
C	4.65790100	-4.73425600	-1.22263800
H	3.03230600	-3.33447800	-1.09124700

C	6.02633800	-4.91412200	-1.03486400
H	7.89674800	-4.01345100	-0.46578400
H	4.05259500	-5.54108100	-1.62048400
C	-4.60859800	0.78521500	0.05393800
C	-3.96851400	1.54338800	-0.93776000
C	-5.34556500	1.47389300	1.02359700
C	-4.02138000	2.93295800	-0.94591700
H	-3.39143900	1.01696700	-1.68762900
C	-5.40028300	2.87015800	1.04458100
H	-5.88669300	0.94352000	1.79417200
C	-4.72630000	3.58572800	0.06267100
H	-3.50599400	3.50198100	-1.71154200
H	-5.95775800	3.39022100	1.81550000
C	-5.53098500	-1.35695500	-0.91097700
C	-6.85176100	-0.89938200	-0.91008400
C	-5.19845600	-2.45038000	-1.71854800
C	-7.83035500	-1.52540100	-1.68426100
H	-7.12502400	-0.02905700	-0.32268700
C	-6.16106600	-3.08697200	-2.49784000
H	-4.16597800	-2.77576900	-1.73617100
C	-7.47376400	-2.61856700	-2.46921700
H	-8.85278400	-1.16459000	-1.68622400
H	-5.89816200	-3.93163400	-3.12542000
Cl	7.35842000	3.51032400	-2.35831800
Cl	6.75925300	-6.46442900	-1.41775100
Cl	-8.70010600	-3.41485600	-3.45264700
Cl	-4.76572700	5.35030000	0.10296600
H	0.92601000	0.70984400	1.04369000

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C	0.56244300	-3.75642000	0.46540700
C	-0.56706400	-4.55963800	0.75514300
C	-0.41808300	-5.94759100	0.81127900
C	0.81153700	-6.56063900	0.58532700
C	1.93006600	-5.76021300	0.35957000
C	1.83332100	-4.36664200	0.32388800
H	-1.29187000	-6.55612000	1.03131500
H	2.90721900	-6.21937300	0.23201200
O	0.43558000	-2.43499200	0.30892100
C	-1.94898400	-3.97744800	0.97132800
H	-2.52560200	-4.68986000	1.58123300
H	-2.47643400	-3.90062300	0.01048000
C	-3.33247700	-2.16755800	1.90291400
C	-1.20292100	-2.56665700	2.85902100

C	-3.60811000	-2.71860500	3.31786100
H	-4.00494800	-2.60034100	1.15756000
C	-2.22147500	-2.82870500	3.99189700
H	-0.76388500	-1.57473400	2.95779300
H	-0.39005800	-3.29114000	2.83974800
H	-4.29699500	-2.09461200	3.88588900
H	-4.07387100	-3.70617400	3.23619600
H	-2.10342100	-2.08960600	4.78691300
H	-2.07839800	-3.81702500	4.43695600
N	-1.95706200	-2.62280200	1.57571300
C	-3.44210800	-0.61314200	1.66631900
O	-2.89088000	-0.34718700	0.42776700
Zn	-1.28715700	-1.28801300	-0.14961600
H	0.90360800	-7.64100800	0.61726000
C	3.10465800	-3.55349400	0.28904500
H	3.95399000	-4.24421000	0.19291800
H	3.23498600	-3.03336300	1.24498600
C	4.57348300	-1.81120900	-0.57535400
C	3.17910400	-3.04251000	-2.13154100
C	5.32256400	-1.99230400	-1.90997700
H	5.10254500	-2.38900400	0.18725300
C	4.64283400	-3.21287800	-2.55106900
H	2.66402500	-2.33823200	-2.79387000
H	2.59941100	-3.96805600	-2.13029400
H	5.21466000	-1.11416900	-2.55016000
H	6.39049100	-2.14345200	-1.74079300
H	4.76818800	-3.25779200	-3.63632500
H	5.04827300	-4.14056800	-2.13163000
N	3.22586500	-2.48306400	-0.75327200
C	4.44473100	-0.37057900	0.07300300
O	3.40286500	-0.39327500	1.00742300
Zn	1.83471100	-1.00718900	0.07258600
C	-0.11146200	1.36822800	-2.42841600
C	-0.11180000	2.64139800	-3.00059600
C	0.22263900	1.24876600	-1.07296400
C	0.21021700	3.77276400	-2.26537500
H	-0.38834600	2.75675600	-4.04445300
C	0.55290000	2.37496800	-0.32027700
C	0.56810500	3.66036700	-0.90019600
H	0.17305000	4.74094400	-2.74456300
H	0.85184100	2.21503100	0.70632500
O	0.25254200	0.02648000	-0.47930700
N	0.91323900	4.76998600	-0.15190500
C	1.22318700	6.04838900	-0.77789300

H	1.99823500	6.53462900	-0.17393500
H	1.67497600	5.86618000	-1.75658300
C	1.06714000	4.68900100	1.29379900
H	0.83835500	5.67803500	1.70639100
H	0.30396400	4.01345800	1.69456900
N	-3.27938000	0.44739900	-2.90062300
C	-2.99379200	1.23507200	-1.90821500
H	-2.70438400	0.84368700	-0.93535300
C	-3.17491300	2.67310300	-1.97957700
C	-2.83717700	3.42547000	-0.84215800
C	-3.64369700	3.32529400	-3.13239600
C	-2.97513700	4.81049000	-0.85155200
H	-2.44408200	2.91495100	0.03115100
C	-3.77550900	4.70769100	-3.13947200
H	-3.89624100	2.72717400	-4.00131100
C	-3.44446100	5.45162900	-1.99893900
H	-2.70484000	5.38857000	0.02576200
H	-4.13867600	5.21439000	-4.02843800
H	-3.55199500	6.53232900	-2.00923700
C	-0.99382900	-5.06901900	-2.89561800
C	-2.03675900	-5.45795100	-3.74985800
C	-3.01502900	-4.54575600	-4.14375300
C	-2.94697400	-3.24409300	-3.64645800
C	-1.92851300	-2.85658300	-2.74464000
C	-0.92571600	-3.77073900	-2.40250600
H	-0.23047800	-5.78437800	-2.60749000
H	-2.07593600	-6.47577700	-4.12459200
H	-3.80481100	-4.83884000	-4.82733800
H	-0.11027400	-3.45530400	-1.76837200
S	-3.95383000	-1.85927700	-4.00440700
N	-2.00498400	-1.54188600	-2.28619800
C	-2.98398200	-0.87519700	-2.88799300
C	2.46310000	4.25088500	1.75269900
H	2.51662000	4.22181000	2.84631700
H	2.71726200	3.26152300	1.36546100
H	3.22370500	4.95289300	1.39511700
C	0.01423600	6.98075100	-0.90860500
H	-0.42725500	7.18342700	0.07306300
H	0.30993400	7.93817000	-1.35120700
H	-0.75902600	6.53056000	-1.53560800
C	-4.91773100	-0.16993400	1.61880500
C	-5.16309500	1.14957200	1.21006200
C	-6.01626900	-0.98178100	1.90771400
C	-6.45359200	1.64831600	1.08971200

H	-4.32154400	1.78834300	0.97112900
C	-7.32480800	-0.49882000	1.79655700
H	-5.88338000	-2.01095600	2.21875300
C	-7.53144900	0.81278200	1.38884000
H	-6.62718000	2.66824700	0.76560100
H	-8.17047500	-1.13896200	2.02126100
C	-2.73030200	0.22188300	2.75916000
C	-3.27175600	0.41188300	4.03724100
C	-1.51932100	0.85763000	2.45998700
C	-2.60321300	1.15774100	5.00744600
H	-4.24613400	0.00040000	4.27716500
C	-0.83186300	1.60438900	3.41654100
H	-1.10937400	0.78030700	1.46194400
C	-1.37705800	1.73998300	4.69047200
H	-3.03294400	1.29824600	5.99288000
H	0.11396000	2.07695100	3.17473400
C	4.16852000	0.77732800	-0.91784300
C	4.54396400	2.08325200	-0.56664200
C	3.43351200	0.61387500	-2.09826300
C	4.25927300	3.17088100	-1.38539300
H	5.08065400	2.24823500	0.36028000
C	3.14332000	1.69016000	-2.93910400
H	3.08153800	-0.36533400	-2.40134500
C	3.57986500	2.96013200	-2.58387100
H	4.56938900	4.17092600	-1.10475400
H	2.58171100	1.54083400	-3.85190900
C	5.78912900	-0.14439100	0.77935800
C	6.96243700	0.12359800	0.06333200
C	5.86140000	-0.26545100	2.16786700
C	8.18656800	0.26144400	0.71468300
H	6.92154800	0.25004300	-1.01382200
C	7.07768300	-0.12812000	2.83777400
H	4.94353400	-0.45860400	2.71008900
C	8.23135400	0.13089500	2.10208900
H	9.09266000	0.47434500	0.15875900
H	7.13125800	-0.21704900	3.91715200
Cl	-9.17251200	1.43030800	1.24405500
Cl	-0.52302000	2.68347900	5.90414100
Cl	9.77156200	0.30577700	2.93535200
Cl	3.30752700	4.31441500	-3.67119600
H	-0.34631600	0.47883000	-2.99977800

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C	0.41783100	-3.75662900	0.66554700

C	-0.73923500	-4.54984200	0.86382100
C	-0.60378600	-5.93642000	0.96410200
C	0.63631900	-6.56177900	0.86648700
C	1.77395000	-5.77384900	0.71392200
C	1.68889700	-4.38083400	0.63554600
H	-1.49848500	-6.53507500	1.11538500
H	2.75485800	-6.24047100	0.67142200
O	0.31448600	-2.43046100	0.49287300
C	-2.13652500	-3.96695000	0.93319200
H	-2.77067800	-4.67283800	1.49103100
H	-2.56234700	-3.90478000	-0.07815300
C	-3.59866900	-2.14115000	1.71784300
C	-1.56041500	-2.52899500	2.85889300
C	-3.99489800	-2.68604400	3.10628200
H	-4.20612400	-2.57302700	0.91800800
C	-2.67379600	-2.76989000	3.90345000
H	-1.12932300	-1.53578700	2.97756300
H	-0.75123100	-3.25488000	2.92395000
H	-4.73736500	-2.06632700	3.60700900
H	-4.43832800	-3.68071600	2.99216500
H	-2.63172900	-2.00953600	4.68609600
H	-2.56565500	-3.74535900	4.38532500
N	-2.20014800	-2.60563600	1.51631600
C	-3.67943400	-0.58204300	1.47594400
O	-2.96481500	-0.29339400	0.33470700
Zn	-1.39006600	-1.32323700	-0.16461700
H	0.71665800	-7.64149300	0.93167500
C	2.96837700	-3.58199500	0.62942200
H	3.81484500	-4.28136900	0.59611000
H	3.07154300	-3.02281900	1.56759600
C	4.48469300	-1.91011600	-0.31080600
C	3.07721000	-3.19734500	-1.81021900
C	5.24767500	-2.20324800	-1.61850800
H	4.98841700	-2.43566500	0.50474500
C	4.53901900	-3.43848900	-2.19537000
H	2.59331600	-2.51674700	-2.51806700
H	2.46570200	-4.09992100	-1.76808200
H	5.17342000	-1.36408400	-2.31431300
H	6.30802300	-2.37561900	-1.42470400
H	4.67759100	-3.55155600	-3.27384100
H	4.90860200	-4.35191100	-1.71590400
N	3.12792700	-2.56484000	-0.46195300
C	4.38584600	-0.41405300	0.20916200
O	3.32443200	-0.30822700	1.11378500

Zn	1.74854000	-1.06380100	0.31796100
C	-0.28918100	1.38841200	-2.11368300
C	0.01520600	2.60640000	-2.82771700
C	0.27980800	1.28431000	-0.78133300
C	0.55184700	3.69039100	-2.21203100
H	-0.29775800	2.67881500	-3.86424400
C	0.82590300	2.38460700	-0.14863600
C	0.95503800	3.61887600	-0.82977000
H	0.67285700	4.60936500	-2.76472800
H	1.20690600	2.24772000	0.85299400
O	0.21012700	0.11324400	-0.16716600
N	1.45511200	4.70781500	-0.19910500
C	1.67880400	5.97882700	-0.89433600
H	2.47865700	6.49816500	-0.35807900
H	2.06759900	5.77691200	-1.89460500
C	1.70296000	4.70638800	1.24626300
H	1.58636400	5.73791700	1.59091600
H	0.91598000	4.12731900	1.73786700
N	-2.68518200	0.64880300	-2.92100400
C	-2.13522900	1.35937700	-1.86878200
H	-2.18322900	0.87686500	-0.89643500
C	-2.58450800	2.77589300	-1.73773900
C	-2.44784800	3.41502400	-0.49870300
C	-3.10116200	3.49015800	-2.82419300
C	-2.79592500	4.75869600	-0.35467900
H	-2.07439400	2.85434200	0.35196500
C	-3.44892000	4.83108600	-2.68045900
H	-3.23127400	2.96916700	-3.76656700
C	-3.28934900	5.47288300	-1.44777700
H	-2.69063600	5.24326000	0.61171900
H	-3.85193700	5.37883800	-3.52758500
H	-3.56540100	6.51754500	-1.33727600
C	-0.80266600	-5.01516600	-3.05975700
C	-1.64516700	-5.22530800	-4.15691500
C	-2.44560500	-4.18636900	-4.63960300
C	-2.40400400	-2.95066500	-3.99922100
C	-1.58372500	-2.73680100	-2.86570200
C	-0.75951500	-3.77648600	-2.42127800
H	-0.17221100	-5.81974400	-2.69329400
H	-1.67200100	-6.19409600	-4.64562400
H	-3.08662700	-4.33800200	-5.50220300
H	-0.08748600	-3.60862400	-1.59342500
S	-3.24702800	-1.46723700	-4.40487000
N	-1.66139900	-1.46930000	-2.29222000

C	-2.46135500	-0.63405200	-3.01629000
C	3.08750800	4.17752600	1.62620000
H	3.23186200	4.24933100	2.70860700
H	3.21314200	3.13397700	1.32977700
H	3.87234000	4.76381400	1.13793000
C	0.42102100	6.84930500	-0.94956300
H	0.07273200	7.09100000	0.05951000
H	0.63063300	7.78842700	-1.47110400
H	-0.39354600	6.33416300	-1.46483100
C	-5.13901600	-0.14413500	1.23917500
C	-5.32370900	1.13348600	0.68994500
C	-6.27119900	-0.91483100	1.51133800
C	-6.59236100	1.63388600	0.42622900
H	-4.45207200	1.73070000	0.45172600
C	-7.55779800	-0.42934300	1.25259700
H	-6.18193200	-1.91395100	1.92085800
C	-7.70567300	0.84297500	0.71541600
H	-6.72025100	2.62059500	-0.00441500
H	-8.43059400	-1.03711200	1.46315000
C	-3.13153100	0.24919100	2.66512200
C	-3.85915300	0.46494600	3.84213200
C	-1.87997900	0.86590700	2.54713400
C	-3.33947400	1.22368700	4.89110900
H	-4.86360700	0.06651500	3.93560100
C	-1.34187200	1.62935900	3.58211400
H	-1.32310100	0.75125700	1.62657900
C	-2.07572700	1.79424200	4.75415400
H	-3.91342600	1.38498700	5.79670700
H	-0.36743600	2.09512200	3.47849100
C	4.16972700	0.63933600	-0.89754400
C	4.68341200	1.93362400	-0.74236200
C	3.35749300	0.40005900	-2.01498300
C	4.44462800	2.93514300	-1.68049700
H	5.29412200	2.16240500	0.12255400
C	3.11247000	1.38388600	-2.97278500
H	2.91229900	-0.57527200	-2.17377800
C	3.67596300	2.64494300	-2.80367900
H	4.86270900	3.92676900	-1.54856500
H	2.49725200	1.17158800	-3.83866200
C	5.71954400	-0.16579700	0.92977200
C	6.92725400	-0.03971100	0.23099900
C	5.74364400	-0.11727900	2.32443900
C	8.13519800	0.12567500	0.90557600
H	6.92924900	-0.04608400	-0.85414000

C	6.94343000	0.04891100	3.01726000
H	4.80208100	-0.20485500	2.85279600
C	8.13080300	0.16624800	2.29933200
H	9.06720100	0.22828500	0.36135000
H	6.95847800	0.08967400	4.10073700
Cl	-9.32009600	1.46557900	0.38913400
Cl	-1.40980100	2.75963900	6.06678800
Cl	9.64953600	0.37786300	3.16073500
Cl	3.42715500	3.88688800	-4.02260800
H	-0.21894500	0.45486600	-2.66630400

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C	-0.86696800	3.31474200	-0.34537400
C	0.14184000	4.21465400	-0.77384800
C	-0.19879300	5.53716600	-1.06563800
C	-1.50610800	6.00169800	-0.93893900
C	-2.47799700	5.13315100	-0.44731700
C	-2.17494700	3.80803100	-0.12532200
H	0.58485400	6.21446600	-1.39644000
H	-3.49226500	5.48968300	-0.28509300
O	-0.59660900	2.02679500	-0.12493600
C	1.58315900	3.78590900	-0.91050200
H	2.20625900	4.68577300	-1.01483500
H	1.73699700	3.19858200	-1.82701400
C	3.50074400	2.66945900	0.17241600
C	1.81815400	3.60936200	1.53683100
C	4.15902800	3.89068500	0.84530000
H	3.77043700	2.58895400	-0.88417900
C	3.09424100	4.43334100	1.82919700
H	1.66741000	2.84385800	2.29478800
H	0.91561000	4.21649300	1.48775900
H	5.09895600	3.63736100	1.33499400
H	4.39683600	4.64137000	0.08495400
H	3.40113800	4.30362600	2.86877900
H	2.92127200	5.50072000	1.66698500
N	2.04244800	2.94027200	0.22449800
C	3.79729800	1.23893600	0.76765000
O	2.95797200	0.32782800	0.14750500
Zn	1.19240600	0.95778700	-0.36487700
H	-1.75307300	7.02991500	-1.18054800
C	-3.21042100	2.95099100	0.55060200
H	-4.08523600	3.57286200	0.78338800
H	-2.82662500	2.58004300	1.50729300
C	-4.73366900	1.04117400	0.59875700

C	-4.28116500	2.13637000	-1.50168500
C	-6.04815700	1.16476000	-0.20350600
H	-4.84113000	1.61902100	1.52006000
C	-5.77376700	2.29929500	-1.20440100
H	-4.12088700	1.35139500	-2.23785000
H	-3.79627500	3.03429200	-1.88222000
H	-6.28626900	0.23818200	-0.72882200
H	-6.88820200	1.37726000	0.46068000
H	-6.38261000	2.23480200	-2.11040300
H	-5.96952500	3.27425800	-0.74406800
N	-3.65605400	1.73681400	-0.21153100
C	-4.25768300	-0.35471400	1.12881600
O	-2.96618400	-0.18664800	1.63287700
Zn	-1.86578600	0.45560600	0.17994000
C	-0.74783600	-2.59299500	-1.18071700
C	-0.44343200	-3.93972200	-1.38017600
C	0.10402600	-1.82975200	-0.36964300
C	0.69249700	-4.52140000	-0.82540400
H	-1.10111600	-4.54766700	-1.99382700
C	1.25709300	-2.39463200	0.18125500
C	1.58081000	-3.74488800	-0.04107500
H	0.90739300	-5.56278300	-1.03056200
H	1.91158200	-1.74439600	0.74303300
O	-0.16908600	-0.52457500	-0.12776200
N	2.74608900	-4.28855100	0.47520900
C	2.92692800	-5.72585100	0.60202100
H	3.48741000	-5.91500000	1.52552800
H	1.95032300	-6.20086500	0.74056700
C	3.76549300	-3.44039500	1.07627500
H	4.73618100	-3.92724600	0.92192300
H	3.80911700	-2.49921000	0.52354100
N	0.96244600	0.35757600	-2.68189900
C	1.28849500	-0.86780400	-3.01404700
H	0.56013700	-1.45737700	-3.57292100
C	2.56395100	-1.49634300	-2.76992300
C	2.66183300	-2.88193800	-3.00754500
C	3.70994200	-0.77548500	-2.38726600
C	3.87367700	-3.53714900	-2.83172600
H	1.77402600	-3.43393000	-3.29533100
C	4.92192400	-1.43378600	-2.22920800
H	3.63859000	0.28793100	-2.21531600
C	5.00292200	-2.81345200	-2.44047600
H	3.94161700	-4.60565400	-3.00001500
H	5.80301100	-0.87521900	-1.93951700

H	5.95388300	-3.32165000	-2.30955800
C	-4.48850500	1.10680300	-5.00687800
C	-4.23799100	2.48723900	-5.09481200
C	-3.02089400	3.02318300	-4.67948300
C	-2.06114600	2.15304600	-4.16097100
C	-2.31222500	0.76135900	-4.03869000
C	-3.53456900	0.24031700	-4.48518800
H	-5.43880900	0.71287200	-5.35281500
H	-4.99918500	3.14593600	-5.50044000
H	-2.82714400	4.08790900	-4.75394000
H	-3.70702600	-0.82681600	-4.41658800
S	-0.45544900	2.50249000	-3.56422400
N	-1.29001200	0.02406900	-3.46997700
C	-0.26838500	0.77829400	-3.18491300
C	3.54733000	-3.18251700	2.57279000
H	4.35920300	-2.57936300	2.99327500
H	2.60856100	-2.65131400	2.74607700
H	3.51045500	-4.12425200	3.13017200
C	3.66532200	-6.36881700	-0.57698400
H	4.64252700	-5.89820200	-0.72366200
H	3.82329700	-7.43826400	-0.39969800
H	3.09603700	-6.25376700	-1.50308900
C	5.24982400	0.82141000	0.45301200
C	5.69980900	-0.38539000	1.00782000
C	6.11445000	1.50537500	-0.40485000
C	6.95334700	-0.90666000	0.71451300
H	5.04419900	-0.92359300	1.67984200
C	7.38351300	1.00220000	-0.71298700
H	5.82502700	2.44674000	-0.85667700
C	7.79080000	-0.20351400	-0.15325500
H	7.28094700	-1.84521200	1.14726700
H	8.04444500	1.54279300	-1.38102600
C	3.60373200	1.17928800	2.30181600
C	4.52233500	1.73391300	3.20262700
C	2.49348200	0.50920200	2.82720700
C	4.31573200	1.67623700	4.57979700
H	5.43158500	2.19489300	2.83291700
C	2.26703500	0.43842400	4.20154400
H	1.80382100	0.02337800	2.14859900
C	3.17838000	1.03547700	5.06875100
H	5.03304300	2.10979300	5.26752600
H	1.39982300	-0.08140300	4.59305000
C	-4.22118200	-1.51612400	0.11493100
C	-3.91016900	-2.78249300	0.64223400

C	-4.37917600	-1.41190500	-1.27014300
C	-3.80341800	-3.90655000	-0.16423400
H	-3.74644900	-2.87340100	1.70991400
C	-4.28488300	-2.53598000	-2.09952000
H	-4.58991900	-0.46303600	-1.74074800
C	-4.00851600	-3.77405800	-1.53858400
H	-3.55818100	-4.87352500	0.25907100
H	-4.43486300	-2.44774100	-3.16869200
C	-5.23343500	-0.71175300	2.26135600
C	-6.50101000	-1.24727200	2.00643500
C	-4.86671300	-0.44742500	3.58248200
C	-7.39432600	-1.50469600	3.04486100
H	-6.79199700	-1.48555500	0.98833200
C	-5.74587100	-0.70145800	4.63515600
H	-3.87383700	-0.05420400	3.76653600
C	-7.00576100	-1.22483300	4.35394000
H	-8.37428400	-1.92368700	2.84606600
H	-5.45823100	-0.50165500	5.66141100
Cl	9.37640400	-0.85402600	-0.54494100
Cl	2.90836900	0.95727700	6.80372900
Cl	-8.12462800	-1.54917300	5.67369000
Cl	-3.89240200	-5.19017500	-2.57540900
H	-1.61927500	-2.13407900	-1.62943600

TS-6c'

C	-1.00875100	3.16544700	1.22759500
C	-0.05008000	4.11542100	1.65660500
C	-0.46528100	5.42188200	1.92521200
C	-1.79609400	5.80864000	1.78624300
C	-2.74518500	4.84401900	1.45240800
C	-2.38133900	3.51776700	1.20887200
H	0.27796600	6.14988100	2.24195300
H	-3.79712100	5.11404400	1.40602400
O	-0.62996500	1.93833200	0.85538100
C	1.42754300	3.79459200	1.78902700
H	1.85463700	4.46996100	2.54705200
H	1.94918600	4.02299600	0.84909800
C	3.15461400	2.09905100	2.30757100
C	1.05070100	1.96046100	3.37499600
C	3.42315200	2.44530400	3.78649200
H	3.71017700	2.74584800	1.62275500
C	2.07712400	2.19922200	4.50794500
H	0.78861400	0.90671600	3.30458400
H	0.12932900	2.52572300	3.50846100

H	4.23854700	1.86291800	4.21461400
H	3.71371700	3.49800800	3.86467500
H	2.12790900	1.32841100	5.16449500
H	1.79904300	3.05935700	5.12292000
N	1.71156000	2.37592500	2.10628600
C	3.47960800	0.63133200	1.82128800
O	2.90449000	0.44694700	0.57985700
Zn	1.24346900	1.32947900	0.12628000
H	-2.09580000	6.83330200	1.97913700
C	-3.47420200	2.47507900	1.13682600
H	-4.44401600	2.98833500	1.19181800
H	-3.41012100	1.83269900	2.02238700
C	-4.62285200	0.53714000	0.19489500
C	-3.76194100	2.23203600	-1.30682600
C	-5.60175400	0.71777200	-0.98444000
H	-5.13599600	0.85749200	1.10547900
C	-5.27342100	2.12094300	-1.52454900
H	-3.20716800	1.74134700	-2.11055800
H	-3.39084600	3.25480900	-1.24613400
H	-5.45320100	-0.03868300	-1.75707200
H	-6.63560400	0.62569200	-0.64528200
H	-5.55468700	2.26207400	-2.57136900
H	-5.79494500	2.88595500	-0.93864200
N	-3.49604200	1.52642700	-0.02567300
C	-4.07744700	-0.89041500	0.58424300
O	-2.99369800	-0.71292800	1.45450200
Zn	-1.74157200	0.35200700	0.43184800
C	-0.00300600	-0.47135800	-2.76985700
C	0.14389300	-1.37665800	-3.87955800
C	0.25003500	-1.03383000	-1.46011900
C	0.77205600	-2.57471100	-3.75558500
H	-0.17495500	-1.04162700	-4.86252500
C	0.90118200	-2.24884100	-1.32951300
C	1.20980200	-3.03540200	-2.46101500
H	0.93994500	-3.18290500	-4.63189000
H	1.12813900	-2.57912900	-0.32712100
O	-0.04843100	-0.32180700	-0.38834500
N	1.87799600	-4.20802800	-2.33358800
C	2.15741800	-5.08034400	-3.47603500
H	2.26167200	-6.09633100	-3.08459100
H	1.28689500	-5.10202200	-4.13540100
C	2.39282900	-4.64726800	-1.03456200
H	3.25555000	-5.29085000	-1.22880400
H	2.77301500	-3.77881600	-0.49006500

N	1.24655200	1.80703700	-2.00150900
C	1.37727800	0.84543900	-3.00215500
H	0.97106500	1.20017500	-3.94940700
C	2.66108900	0.12407400	-3.22767900
C	2.96814700	-0.20664600	-4.55852300
C	3.55669900	-0.25163900	-2.21929500
C	4.13470000	-0.89414800	-4.88146700
H	2.28334200	0.08556100	-5.35033600
C	4.72585300	-0.94232700	-2.54504600
H	3.37251500	0.00119900	-1.18061700
C	5.01982000	-1.27003000	-3.86815500
H	4.35610700	-1.12723800	-5.91895700
H	5.41674400	-1.20584900	-1.75038700
H	5.93486500	-1.80219800	-4.11216700
C	-3.41796300	5.05398000	-3.80577500
C	-3.02904500	6.06736300	-2.91624200
C	-1.86246100	5.94322600	-2.16082900
C	-1.10125200	4.78601700	-2.30809900
C	-1.49997500	3.73664700	-3.17612200
C	-2.66277000	3.89226300	-3.94227200
H	-4.32400900	5.17533000	-4.39171200
H	-3.63905100	6.95937200	-2.81455400
H	-1.56368500	6.71904600	-1.46436000
H	-2.96396900	3.09587800	-4.61514900
S	0.39940500	4.33839700	-1.52205500
N	-0.71586000	2.59752500	-3.13500200
C	0.29032300	2.73324800	-2.29985700
C	1.34487400	-5.39916100	-0.20993100
H	1.76126300	-5.69698400	0.75712400
H	0.46636100	-4.77378700	-0.03035400
H	1.01330700	-6.30026000	-0.73497900
C	3.42144800	-4.66616900	-4.23231600
H	4.29269800	-4.69103800	-3.57082400
H	3.60629600	-5.34578600	-5.07034400
H	3.33327200	-3.64675900	-4.61563100
C	5.00030100	0.43505600	1.65791400
C	5.41442000	-0.78465100	1.10077100
C	5.98082800	1.37354700	1.98255700
C	6.75562800	-1.06447300	0.87248100
H	4.65763300	-1.51545200	0.83721000
C	7.33787700	1.11332700	1.75918600
H	5.71443100	2.33159700	2.41286400
C	7.71309900	-0.10384100	1.20609700
H	7.06389500	-2.01186100	0.44404600

H	8.09046800	1.85155900	2.01213300
C	2.97433100	-0.46034700	2.79879800
C	3.63103300	-0.76993700	3.99631900
C	1.84673500	-1.21537300	2.45401900
C	3.15231800	-1.76108600	4.85287400
H	4.54958600	-0.25566000	4.25756900
C	1.34943000	-2.20936100	3.29634600
H	1.35614200	-1.02344800	1.50838800
C	2.00505100	-2.46798800	4.49784500
H	3.66906400	-1.99262100	5.77749700
H	0.46676500	-2.77695500	3.02174600
C	-3.57679200	-1.79726100	-0.55780900
C	-3.26178300	-3.12071100	-0.19542400
C	-3.28173000	-1.39559900	-1.86337200
C	-2.71603100	-4.01776200	-1.10170400
H	-3.45373600	-3.43989600	0.82255000
C	-2.75028500	-2.29278400	-2.80021500
H	-3.46730200	-0.38064000	-2.19054600
C	-2.47766600	-3.59613400	-2.41210200
H	-2.48764200	-5.03624500	-0.80818100
H	-2.55444200	-1.97352600	-3.81563200
C	-5.24241300	-1.58297100	1.30352100
C	-6.31634200	-2.13708000	0.59774400
C	-5.26040800	-1.61825200	2.69887800
C	-7.39626000	-2.70921400	1.26754600
H	-6.30533400	-2.14005700	-0.48781900
C	-6.33134200	-2.18968200	3.38637000
H	-4.41338000	-1.20143900	3.23100000
C	-7.39253000	-2.72728200	2.66158700
H	-8.22592400	-3.14215900	0.72022700
H	-6.34295500	-2.22260700	4.47013900
Cl	9.41538900	-0.44510600	0.92213800
Cl	1.39438000	-3.72317500	5.56878100
Cl	-8.74887900	-3.45113900	3.51769600
Cl	-1.83881000	-4.74927400	-3.57741400
H	-0.80264800	0.26248300	-2.83040000

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C	1.23412700	1.56107200	2.97668700
C	0.17017500	1.89342900	3.85801200
C	0.46539100	2.19382500	5.19104400
C	1.77289300	2.19680500	5.67344400
C	2.81726600	1.96505600	4.77866900
C	2.57033700	1.67504000	3.43639100

H	-0.35455000	2.44247500	5.86070500
H	3.84793600	2.03324400	5.11819700
O	1.00304700	1.17790300	1.72194100
C	-1.27863300	1.96854100	3.40460000
H	-1.82635700	2.60240900	4.11818000
H	-1.76591000	0.98299200	3.43955100
C	-2.82446100	2.64424600	1.57487800
C	-0.78378100	3.80282000	1.84409900
C	-3.21733600	4.05336200	2.06330000
H	-3.41927300	1.86076000	2.05269000
C	-1.88958200	4.84615200	2.12663000
H	-0.41851000	3.88754100	0.82327900
H	0.06985200	3.89267700	2.51410400
H	-3.96024900	4.52574400	1.42102400
H	-3.66742200	3.97873700	3.05845700
H	-1.85872000	5.64358700	1.38182400
H	-1.75740000	5.30763200	3.10907000
N	-1.41699800	2.46487400	2.01358600
C	-2.93028500	2.33043000	0.02958300
O	-2.34780600	1.09030300	-0.19380500
Zn	-0.83042700	0.60145300	0.90349500
H	1.97590800	2.42628100	6.71395100
C	3.71308100	1.61437600	2.45610400
H	4.63799800	1.91048600	2.96913400
H	3.54453100	2.34764700	1.65975200
C	5.09616500	0.41969500	0.82349800
C	4.26322200	-0.76360200	2.73883600
C	6.30836100	-0.24536000	1.52343600
H	5.28899100	1.48688600	0.70394000
C	5.78860600	-0.70870300	2.90250100
H	3.93493100	-1.72280700	2.33850700
H	3.71284300	-0.59566500	3.66236100
H	6.70364000	-1.07388900	0.93638800
H	7.12846900	0.46877500	1.62390300
H	6.20230200	-1.67238300	3.21408700
H	6.05798600	0.01843500	3.67518600
N	3.92190900	0.30080800	1.76500600
C	4.69101900	0.00700400	-0.63574600
O	3.55171900	0.75664600	-0.94432900
Zn	2.22705500	0.24448300	0.37109600
C	0.68260300	-2.80085200	-0.64699100
C	0.11010700	-3.95112300	-1.19810100
C	0.03329700	-1.57750600	-0.84772900
C	-1.08090400	-3.90607600	-1.91177000

H	0.60352900	-4.90880200	-1.06108600
C	-1.14381800	-1.50546700	-1.59284000
C	-1.73886600	-2.66717600	-2.12884900
H	-1.50331800	-4.82946700	-2.28430900
H	-1.60799600	-0.53382700	-1.69307100
O	0.48403000	-0.44778300	-0.24369800
N	-2.92646100	-2.59228400	-2.82914300
C	-3.51403100	-3.76497700	-3.46256100
H	-4.10038700	-3.41745400	-4.31999500
H	-2.72048300	-4.39431000	-3.87925900
C	-3.61595600	-1.32329000	-3.03484000
H	-4.68600400	-1.53969600	-3.12514700
H	-3.51524600	-0.70386900	-2.14407200
N	-1.78109800	-1.50867900	1.70087900
C	-0.92505100	-2.47310600	1.90173400
H	-1.15297200	-3.46226700	1.50731200
C	0.23832500	-2.37996700	2.77056400
C	1.19477600	-3.41309700	2.74212800
C	0.31560300	-1.40684600	3.77869600
C	2.19454000	-3.46991200	3.70621600
H	1.13025900	-4.16970900	1.96698000
C	1.31987300	-1.45958400	4.73975600
H	-0.44948300	-0.64613000	3.83639200
C	2.25150300	-2.49962200	4.71284700
H	2.92149900	-4.27584100	3.68478600
H	1.36554000	-0.69550000	5.50825400
H	3.02458600	-2.55434700	5.47358700
C	-6.73050100	-4.57043000	0.40125600
C	-7.30731800	-3.40107700	-0.12921100
C	-6.60950400	-2.19614500	-0.13833700
C	-5.31967000	-2.18485100	0.39844900
C	-4.72228400	-3.35789300	0.92245600
C	-5.44567400	-4.55981900	0.92912300
H	-7.29916300	-5.49507500	0.39321000
H	-8.31258700	-3.43726000	-0.53736200
H	-7.05332400	-1.29439400	-0.54724500
H	-4.98714900	-5.45561000	1.33397000
S	-4.19298600	-0.85354600	0.49246800
N	-3.43965100	-3.18773900	1.40037500
C	-3.02723300	-1.96022200	1.22924800
C	-3.11981900	-0.56530200	-4.26967800
H	-3.68024000	0.36591200	-4.40767300
H	-2.06027100	-0.31478800	-4.16584700
H	-3.23798000	-1.16738800	-5.17654200

C	-4.40597500	-4.57138700	-2.51523800
H	-5.22967600	-3.95744000	-2.14167600
H	-4.82977800	-5.44358600	-3.02520800
H	-3.83805800	-4.91818800	-1.64865200
C	-4.40531400	2.21298600	-0.40611500
C	-4.62996200	1.85953000	-1.74463300
C	-5.50644100	2.28148400	0.44856900
C	-5.89725900	1.53355600	-2.21017800
H	-3.78207900	1.80438500	-2.41763000
C	-6.79281300	1.96192900	0.00142800
H	-5.38734300	2.54847600	1.49168800
C	-6.97322100	1.57425500	-1.32085300
H	-6.05374600	1.23936700	-3.24194100
H	-7.63828300	1.99771400	0.67897200
C	-2.24601200	3.39448600	-0.85626000
C	-2.79428200	4.66601000	-1.06641100
C	-1.05135200	3.07528500	-1.51194800
C	-2.13848100	5.61909400	-1.84364100
H	-3.75985100	4.91589500	-0.64047900
C	-0.37880400	4.01371900	-2.29453000
H	-0.65496200	2.07135100	-1.41865100
C	-0.92288600	5.28750100	-2.44022300
H	-2.56825800	6.60266000	-1.99653700
H	0.54975400	3.75581300	-2.79156200
C	4.37551500	-1.48628300	-0.88833600
C	3.69971000	-1.75772800	-2.09146200
C	4.70206800	-2.57403200	-0.07042700
C	3.37094200	-3.05199900	-2.47290600
H	3.41964400	-0.91896300	-2.71741600
C	4.36574900	-3.88438700	-0.42915900
H	5.23880800	-2.43718400	0.85596900
C	3.71097600	-4.11233400	-1.63240800
H	2.83851700	-3.24001600	-3.39760200
H	4.62252100	-4.71520000	0.21852900
C	5.86244700	0.42837200	-1.53658300
C	6.94801800	-0.41254800	-1.80339000
C	5.86509500	1.71979500	-2.07235400
C	8.02506500	0.02544900	-2.57362500
H	6.94984400	-1.43076000	-1.42831700
C	6.93159000	2.17443300	-2.84565500
H	5.00531900	2.35273500	-1.88662700
C	8.00715300	1.32094900	-3.08485400
H	8.86239600	-0.63059900	-2.78292900
H	6.92908900	3.17459000	-3.26455100

Cl	-8.57759300	1.11671600	-1.88182200
Cl	-0.08362900	6.48568600	-3.41507900
Cl	9.35990400	1.88384700	-4.05959200
Cl	3.28650800	-5.75563100	-2.08846600
H	1.61071300	-2.83793600	-0.08930500

TS-6d'

C	1.09837000	1.00129400	3.09523700
C	-0.01700200	1.08216400	3.97181700
C	0.20374600	1.07570500	5.35195300
C	1.48563700	1.00788400	5.89304900
C	2.57761000	1.01350000	5.02742400
C	2.40625400	1.03535600	3.64247200
H	-0.65661000	1.13429400	6.01432600
H	3.58803100	1.02034300	5.42868700
O	0.93193200	0.92268000	1.77139000
C	-1.45040000	1.19694900	3.47843400
H	-2.05429800	1.63625900	4.28658200
H	-1.88254100	0.20555600	3.27895000
C	-2.96030300	2.19798000	1.77215400
C	-0.98700500	3.34562600	2.37492500
C	-3.43589200	3.44566800	2.54251800
H	-3.52891100	1.30506800	2.04111800
C	-2.15103000	4.26297900	2.81915000
H	-0.58505700	3.66145700	1.41502200
H	-0.16626600	3.32108000	3.09014800
H	-4.18896200	4.01385300	1.99685800
H	-3.90123400	3.13342000	3.48311100
H	-2.13651400	5.19646700	2.25345300
H	-2.07176100	4.51894800	3.87928500
N	-1.56329900	1.98092000	2.22367800
C	-3.00421900	2.23775400	0.18931700
O	-2.32632800	1.13023200	-0.29809700
Zn	-0.87750800	0.40668600	0.80160700
H	1.63090000	0.99569500	6.96791500
C	3.61044600	1.19644500	2.74910000
H	4.50096500	1.34469700	3.37454300
H	3.50018900	2.10155400	2.14020000
C	5.07929400	0.35264700	0.96230300
C	4.09535200	-1.20204200	2.49638500
C	6.23394500	-0.47376800	1.58414700
H	5.29502300	1.41757700	1.06366100
C	5.60529300	-1.24579200	2.76715600
H	3.78132800	-2.02336200	1.85499200

H	3.48173900	-1.24305000	3.39290700
H	6.69029900	-1.13848900	0.85071300
H	7.03416800	0.18881700	1.92126700
H	5.97288200	-2.27263900	2.85275200
H	5.83560600	-0.74595700	3.71333800
N	3.85011400	0.07528200	1.78627800
C	4.74289000	0.24422300	-0.56963000
O	3.66896000	1.11477800	-0.78027500
Zn	2.25801400	0.40790600	0.34586700
C	0.56075200	-2.49457400	-0.80715000
C	0.05539700	-3.61530600	-1.57274000
C	0.12050900	-1.18893800	-1.24768800
C	-1.03512600	-3.49891700	-2.37530900
H	0.51130300	-4.58972800	-1.43045600
C	-0.98493200	-1.06266800	-2.06614800
C	-1.66342700	-2.20710900	-2.54944400
H	-1.45427500	-4.37833400	-2.84354000
H	-1.38254800	-0.06809500	-2.20384300
O	0.60861500	-0.11311000	-0.65405600
N	-2.87166100	-2.09426600	-3.13830400
C	-3.58811500	-3.24549700	-3.69888900
H	-4.25675600	-2.85360300	-4.47071900
H	-2.87842200	-3.89640700	-4.21591900
C	-3.59665700	-0.81372000	-3.15656000
H	-4.66275100	-1.04930600	-3.09594500
H	-3.35807200	-0.25454500	-2.25137100
N	-1.38265300	-1.67979000	1.04858600
C	-0.42049800	-2.66951000	0.91118100
H	-0.86151300	-3.63792600	0.68865700
C	0.62441200	-2.82038000	1.96901600
C	1.61826200	-3.80829800	1.85340600
C	0.48177700	-2.15875100	3.19299300
C	2.42535100	-4.13470700	2.93920600
H	1.73798900	-4.34618400	0.91756600
C	1.30186500	-2.47007400	4.27803100
H	-0.31367800	-1.43678800	3.30314900
C	2.26804500	-3.46810200	4.15899300
H	3.17409200	-4.91491600	2.83774800
H	1.17395500	-1.93202000	5.21166000
H	2.89647800	-3.72619800	5.00607700
C	-6.41714400	-4.84473800	0.59216200
C	-7.12945000	-3.66462400	0.32702500
C	-6.47692100	-2.43083100	0.30465200
C	-5.10506800	-2.40708200	0.54975000

C	-4.37044800	-3.59091900	0.80842500
C	-5.04613200	-4.81861400	0.83549900
H	-6.94407700	-5.79422000	0.60639000
H	-8.19736600	-3.70948900	0.13710100
H	-7.01969500	-1.51444900	0.09304700
H	-4.48789900	-5.72727700	1.03586600
S	-4.01074000	-1.03830200	0.49961300
N	-3.01549100	-3.41447100	1.00257900
C	-2.66030500	-2.15676600	0.88235400
C	-3.29649000	0.00103200	-4.41450700
H	-3.88408800	0.92330100	-4.41571100
H	-2.23759600	0.27037100	-4.46139900
H	-3.54484600	-0.55940800	-5.32161400
C	-4.38141400	-4.01694700	-2.64439100
H	-5.11565100	-3.37482400	-2.15153200
H	-4.91389900	-4.85349300	-3.10734000
H	-3.72244100	-4.41050100	-1.86795300
C	-4.46380800	2.13676800	-0.30628600
C	-4.65865300	2.14029600	-1.69492800
C	-5.57913000	1.92941300	0.50808300
C	-5.90697700	1.90703400	-2.25974300
H	-3.80322600	2.31229500	-2.33887200
C	-6.84496700	1.69125600	-0.03703000
H	-5.48697300	1.92065800	1.58713200
C	-6.99538000	1.66974900	-1.41858000
H	-6.04219900	1.90542200	-3.33572700
H	-7.69990200	1.51912200	0.60718400
C	-2.38415900	3.52562200	-0.39905800
C	-3.03088100	4.76711900	-0.35792900
C	-1.14249700	3.45047400	-1.04056900
C	-2.43275500	5.91465700	-0.87650200
H	-4.02874800	4.84362600	0.06001800
C	-0.52605400	4.58566400	-1.56622200
H	-0.66671500	2.48162300	-1.13551900
C	-1.17349500	5.81487400	-1.46555500
H	-2.93986500	6.87215300	-0.83674100
H	0.43955400	4.51610500	-2.05487600
C	4.34383500	-1.15845900	-1.09727200
C	3.57613900	-1.16467700	-2.27583000
C	4.68781000	-2.39859400	-0.54433100
C	3.16915500	-2.34800000	-2.88254200
H	3.29134200	-0.20825400	-2.69734500
C	4.27342100	-3.59999100	-1.12892900
H	5.29276400	-2.46387000	0.34767300

C	3.52326200	-3.56416800	-2.29841100
H	2.57200100	-2.33116500	-3.78687700
H	4.54251300	-4.55038300	-0.68184300
C	5.98296100	0.73815200	-1.32822400
C	7.02266900	-0.11299200	-1.71728700
C	6.09764600	2.10538200	-1.59968900
C	8.16250600	0.38467800	-2.34874000
H	6.94152900	-1.18193600	-1.55019200
C	7.22840600	2.62048800	-2.23011400
H	5.27407500	2.75318900	-1.32367300
C	8.25562100	1.75206800	-2.59544700
H	8.96373000	-0.27907700	-2.65334100
H	7.31261800	3.68036100	-2.44302800
Cl	-8.57637300	1.34327400	-2.11775700
Cl	-0.40722700	7.25745700	-2.11766200
Cl	9.68804800	2.39079200	-3.39283500
Cl	3.00228700	-5.07160200	-3.03831300
H	1.58654900	-2.55345200	-0.46137700

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C	0.23506200	-3.78760500	-0.12671000
C	-0.95612200	-4.45881100	-0.50902900
C	-0.90068900	-5.82686300	-0.78935600
C	0.28858600	-6.54867600	-0.73852700
C	1.45857800	-5.87950100	-0.39756100
C	1.45111800	-4.51599200	-0.08868400
H	-1.82203000	-6.33145100	-1.06798300
H	2.40337700	-6.41633600	-0.36750200
O	0.23504400	-2.47574100	0.17209700
C	-2.28973700	-3.76501800	-0.70078400
H	-3.06448700	-4.54126800	-0.77077400
H	-2.29400500	-3.23345300	-1.65808300
C	-3.92813700	-2.13298900	0.17316400
C	-2.70333200	-3.43093800	1.68498300
C	-4.92187400	-3.20584100	0.65109400
H	-4.02230800	-1.92059400	-0.89302200
C	-4.17409500	-3.91276200	1.81081700
H	-2.47168000	-2.68466700	2.44309700
H	-1.97043500	-4.23523100	1.75856800
H	-5.88294100	-2.79931800	0.95980800
H	-5.11945800	-3.90736500	-0.16582700
H	-4.58634400	-3.62643600	2.78036900
H	-4.25044800	-5.00011300	1.72570000
N	-2.60066500	-2.77974400	0.35531600

C	-3.95041600	-0.72136500	0.94115400
O	-2.65979400	-0.23683400	1.09625100
Zn	-1.31323500	-1.04239100	-0.05752100
H	0.30201400	-7.60915300	-0.96584500
C	2.76053000	-3.85156800	0.25473200
H	3.56038500	-4.60274800	0.21614800
H	2.76264800	-3.46113500	1.28079000
C	4.49653500	-2.17761100	-0.30988800
C	3.12779000	-3.11227500	-2.07432100
C	5.33923200	-2.37536300	-1.58661500
H	4.88795400	-2.81924100	0.48485600
C	4.58662600	-3.45440400	-2.37354400
H	2.79121500	-2.28474600	-2.70466900
H	2.43134300	-3.93681300	-2.22379900
H	5.37346500	-1.44794500	-2.16641900
H	6.36601900	-2.65716700	-1.34767100
H	4.81040700	-3.44435500	-3.44351900
H	4.82863900	-4.45272600	-1.99151500
N	3.11141400	-2.69445600	-0.64065500
C	4.47262400	-0.73408100	0.33437800
O	3.40935000	-0.65591000	1.23838400
Zn	1.79332900	-1.26349200	0.39668700
C	-0.08501000	2.01620700	-0.99439900
C	0.42608700	3.33581800	-1.40120100
C	0.62380300	1.42993100	0.16839300
C	1.32936200	4.02966100	-0.68129000
H	-0.00671800	3.77601900	-2.29333500
C	1.52664800	2.15827200	0.91673800
C	1.88297100	3.47206700	0.53969100
H	1.62623600	5.01509600	-1.00848400
H	2.02159600	1.64936500	1.73012900
O	0.37988800	0.17334400	0.44720500
N	2.72942900	4.19722400	1.29784000
C	3.20111400	5.52695600	0.89558000
H	4.17529400	5.67549800	1.37033200
H	3.38352100	5.53207300	-0.18084300
C	3.14237600	3.74279900	2.63414000
H	3.34957100	4.64281600	3.21993500
H	2.29118000	3.24929300	3.11029500
N	-2.41955000	1.76946200	-1.93490200
C	-1.70679300	2.08083100	-0.73539100
H	-1.91493900	1.35359900	0.05723600
C	-2.06022100	3.45026900	-0.19916600
C	-1.74746200	3.76763900	1.12695500

C	-2.65717400	4.41781700	-1.01105900
C	-2.00355800	5.04386900	1.62841000
H	-1.30610000	3.00887700	1.76692600
C	-2.91882700	5.69287200	-0.50974300
H	-2.93420900	4.13845700	-2.02119300
C	-2.58649600	6.01349800	0.80861700
H	-1.76273200	5.27750800	2.66183500
H	-3.39272100	6.43463100	-1.14629900
H	-2.79541700	7.00509500	1.19964900
C	-0.32294200	-3.30964300	-4.18935200
C	-1.19071400	-3.15023100	-5.27341500
C	-2.08994700	-2.07829000	-5.30393900
C	-2.11664600	-1.18646100	-4.23638400
C	-1.27036400	-1.36229000	-3.11386200
C	-0.35087500	-2.41723200	-3.11668800
H	0.38075000	-4.13682700	-4.17387600
H	-1.16283800	-3.85058700	-6.10213300
H	-2.75050800	-1.93828500	-6.15385000
H	0.31668600	-2.53918200	-2.27500600
S	-3.08729400	0.26768700	-4.03639500
N	-1.42096500	-0.42950100	-2.09213600
C	-2.24115400	0.61284300	-2.46986200
C	4.36506600	2.82431000	2.62480900
H	4.66532000	2.59898100	3.65266600
H	4.15761700	1.88017500	2.11827800
H	5.21063300	3.30612500	2.12454500
C	2.23098800	6.63832900	1.30255000
H	2.10399900	6.66376400	2.38913300
H	2.61111600	7.61286300	0.98173500
H	1.24547200	6.48207600	0.85542400
C	-4.76573300	0.31431900	0.13170100
C	-4.71767000	1.63291400	0.60787100
C	-5.49556400	0.06376500	-1.03106100
C	-5.33178700	2.67655000	-0.06874800
H	-4.15228200	1.84009500	1.50864000
C	-6.11557500	1.10208300	-1.73485500
H	-5.59199000	-0.93880400	-1.43142100
C	-6.01567400	2.39956200	-1.25217800
H	-5.25518800	3.69420300	0.29422300
H	-6.65454000	0.89980900	-2.65318400
C	-4.61236800	-0.82291900	2.33537300
C	-6.00067100	-0.89691300	2.50506200
C	-3.80971400	-0.78448300	3.47813600
C	-6.57240100	-1.00221000	3.77174900

H	-6.65153800	-0.84411000	1.63817800
C	-4.35944500	-0.88532700	4.75579600
H	-2.74315900	-0.65243900	3.34018900
C	-5.74013300	-1.00832800	4.88961700
H	-7.64797100	-1.06350300	3.89355100
H	-3.72871900	-0.85965700	5.63767200
C	4.29945500	0.41236900	-0.69491200
C	5.00128700	1.61750500	-0.57615200
C	3.31622700	0.34679800	-1.69592100
C	4.74970500	2.70342100	-1.41500700
H	5.76272000	1.72009600	0.18547100
C	3.05059500	1.41407800	-2.55025100
H	2.73865800	-0.55762300	-1.84447000
C	3.77832800	2.59272000	-2.40366000
H	5.30968700	3.62543800	-1.30372600
H	2.29051100	1.33004600	-3.31841400
C	5.80419100	-0.60169900	1.08994000
C	7.03796800	-0.50625800	0.43180500
C	5.79401600	-0.61387600	2.48654800
C	8.23224700	-0.42413800	1.14525800
H	7.07536200	-0.46800400	-0.65136800
C	6.97918000	-0.53188200	3.21817500
H	4.83541200	-0.68044800	2.98586100
C	8.19087900	-0.43848800	2.53876200
H	9.18276200	-0.34368600	0.63012800
H	6.96428700	-0.53941200	4.30239800
Cl	-6.75485100	3.72290800	-2.14967300
Cl	-6.44880500	-1.14374900	6.49630600
Cl	9.69125200	-0.32829600	3.44819000
Cl	3.46441300	3.95144600	-3.46952000
H	-0.00305700	1.28082300	-1.80297700

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C	0.00337600	2.77911000	2.59026600
C	1.20629300	3.40884600	2.99667600
C	1.13413500	4.55769600	3.79498100
C	-0.08015600	5.12300500	4.16754700
C	-1.25902200	4.51627500	3.73895300
C	-1.23539700	3.35595800	2.96518600
H	2.06325100	5.02638400	4.10994300
H	-2.22101200	4.93903100	4.01735100
O	0.00218100	1.66822800	1.83278700
C	2.58333100	3.01680900	2.49791000
H	3.32833400	3.41738000	3.20112000

H	2.77157000	3.51889900	1.53826300
C	4.20254500	1.31729200	1.79130400
C	2.62245600	0.76537500	3.50161400
C	5.01251600	1.15699800	3.09142400
H	4.51252100	2.19731300	1.22252100
C	4.02754600	0.54171500	4.10979800
H	2.16426300	-0.18805400	3.23560800
H	1.93711800	1.29110500	4.16811800
H	5.90240000	0.54241200	2.96220200
H	5.34947800	2.14210300	3.43097900
H	4.21591300	-0.52603300	4.23610700
H	4.12299400	1.01319700	5.09111400
N	2.80676400	1.57213500	2.26095700
C	4.23070800	0.13097100	0.74424500
O	3.13507000	0.25081900	-0.09677600
Zn	1.52447900	1.03649900	0.56413700
H	-0.10767800	6.01704500	4.78100500
C	-2.52684900	2.68280700	2.59569800
H	-3.34862300	3.16111100	3.14473600
H	-2.49711200	1.63376800	2.90411000
C	-4.16924000	1.88310800	0.99472500
C	-3.09612700	3.99222800	0.55046000
C	-5.25747400	2.90237200	0.58381800
H	-4.41270300	1.51775000	1.99383800
C	-4.58739800	4.28109600	0.75916200
H	-2.84297700	3.95880000	-0.51260000
H	-2.42564400	4.71421300	1.01766900
H	-5.60124600	2.74881000	-0.43841300
H	-6.13861100	2.79264700	1.21987700
H	-4.96574700	5.03510400	0.06343200
H	-4.75885000	4.65968500	1.77262700
N	-2.86685200	2.64351400	1.13247900
C	-3.93955300	0.54797700	0.21290100
O	-2.81211700	-0.03803300	0.80529900
Zn	-1.38502000	1.21123200	0.36672200
C	-0.05358500	-2.11789400	-1.10939300
C	-0.66461700	-3.14199300	-1.84277000
C	-0.52724700	-1.92760000	0.18304400
C	-1.67980900	-3.92718100	-1.32055000
H	-0.31878900	-3.31844100	-2.85635900
C	-1.50338500	-2.72683600	0.76174900
C	-2.12664900	-3.74349000	0.01161100
H	-2.12085300	-4.69242500	-1.94499600
H	-1.84980400	-2.47996600	1.75561200

O	-0.02210200	-0.83487300	0.91000600
N	-3.13783500	-4.52705300	0.55206000
C	-4.10975300	-5.16249500	-0.33869600
H	-3.58308500	-5.74807700	-1.09763800
H	-4.66607100	-5.89007800	0.25905200
C	-3.55557700	-4.31398500	1.93520600
H	-3.66757900	-3.24409100	2.14686700
H	-4.55606600	-4.73961800	2.04453500
N	0.45019000	-0.26469100	-2.62132000
C	1.02186700	-1.24133400	-1.70849300
H	1.56752900	-0.75754400	-0.89786900
C	2.11349000	-2.04444200	-2.41021100
C	2.69892100	-3.13230200	-1.74918300
C	2.62872400	-1.64504500	-3.64448500
C	3.78830300	-3.79877100	-2.30521900
H	2.30945100	-3.44674400	-0.78701600
C	3.71669200	-2.31733200	-4.20723200
H	2.17320800	-0.80129100	-4.14931800
C	4.30355100	-3.39221700	-3.53918400
H	4.23868000	-4.63111100	-1.77251700
H	4.10811100	-1.99467600	-5.16788600
H	5.15360000	-3.91003000	-3.97380200
C	-0.00396100	5.37959600	-0.68587200
C	-0.40872500	5.72368500	-1.97524400
C	-0.54764900	4.73082300	-2.94897300
C	-0.29774000	3.40378100	-2.60830200
C	0.05906700	3.03747400	-1.29279200
C	0.23351000	4.04507800	-0.34284700
H	0.13059100	6.14650800	0.07045300
H	-0.59656000	6.76109800	-2.23269100
H	-0.82880200	4.98799200	-3.96516600
H	0.53632300	3.81429400	0.66574300
S	-0.32288100	2.00985200	-3.66410400
N	0.18942000	1.63368800	-1.06228600
C	0.17516000	0.93010800	-2.30105700
C	-2.60712100	-4.96927900	2.94236000
H	-2.93868600	-4.77508300	3.96804600
H	-2.57358500	-6.05127900	2.78692500
H	-1.58858700	-4.58653800	2.83417700
C	-5.07266000	-4.16782700	-0.99525200
H	-4.52743100	-3.44025800	-1.60264800
H	-5.78647400	-4.68844300	-1.64210200
H	-5.63496100	-3.61490400	-0.23857400
C	5.49168400	0.21523400	-0.13448500

C	5.47389300	-0.54255000	-1.31503700
C	6.63244600	0.96564500	0.15803200
C	6.56096400	-0.55524100	-2.17980200
H	4.58920700	-1.11692600	-1.55622300
C	7.73632200	0.96600400	-0.70191900
H	6.69056700	1.56915600	1.05699100
C	7.68913000	0.20277200	-1.86230000
H	6.52931600	-1.14451400	-3.08879600
H	8.61763600	1.55374100	-0.47108100
C	4.23798300	-1.25141300	1.44263500
C	5.41032300	-1.82523100	1.95259700
C	3.05250500	-1.98183200	1.55675400
C	5.39351000	-3.05814800	2.60348800
H	6.36061400	-1.32064400	1.81641400
C	3.01022700	-3.21669400	2.20247000
H	2.14810600	-1.58988100	1.11768500
C	4.18578200	-3.74177000	2.73257200
H	6.30777500	-3.49210800	2.99235600
H	2.08015400	-3.76990800	2.27666500
C	-3.68409200	0.63096700	-1.30636100
C	-3.19172000	-0.55467100	-1.88232500
C	-3.91321000	1.72256100	-2.15320500
C	-2.97389800	-0.66815300	-3.24894300
H	-2.97201600	-1.39187900	-1.23246100
C	-3.70776000	1.62218900	-3.53153600
H	-4.25360200	2.67217400	-1.76765100
C	-3.25497500	0.42343800	-4.06958500
H	-2.57616400	-1.58461500	-3.66699700
H	-3.87982900	2.47619400	-4.17619100
C	-5.18035800	-0.32002500	0.46543300
C	-6.26765600	-0.36121000	-0.41233500
C	-5.24250300	-1.06842200	1.64467000
C	-7.39225100	-1.13691700	-0.12829500
H	-6.23323600	0.19951200	-1.34037400
C	-6.35674900	-1.84774600	1.94765800
H	-4.38971800	-1.04236800	2.31271300
C	-7.42506200	-1.87584400	1.05203200
H	-8.22797300	-1.17642900	-0.81760400
H	-6.39699200	-2.43352500	2.85928100
Cl	9.07404600	0.19385100	-2.94971900
Cl	4.15153000	-5.29807500	3.55038300
Cl	-8.82614800	-2.87634900	1.41045600
Cl	-2.98438600	0.29980900	-5.79760400
H	-0.43332900	-0.80738700	1.78662800

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C	-1.18373100	0.22654300	-0.22306300
C	-2.10887500	1.05956000	0.40839400
C	-1.67304400	-0.98216100	-0.74518400
C	-3.45446800	0.73252700	0.52167900
H	-1.76053500	2.00054300	0.82108500
C	-3.01884200	-1.32980100	-0.65464200
C	-3.94841800	-0.47860500	-0.01582000
H	-4.11365000	1.41645400	1.03877500
H	-3.33992300	-2.26289000	-1.10395900
O	-0.76397300	-1.80676300	-1.35115200
N	-5.28497500	-0.82093200	0.07769500
C	-6.26947900	0.10167600	0.62761900
H	-6.02384200	1.12150600	0.31564800
H	-7.23425100	-0.12881200	0.16295800
C	-5.77574300	-2.11757700	-0.36551700
H	-5.03853600	-2.88912900	-0.11914300
H	-6.66446300	-2.35662700	0.22831800
N	1.01891500	-0.22371000	0.68721900
C	0.29314500	0.54904900	-0.33569500
H	0.65195300	0.20377000	-1.31169000
C	0.58320300	2.03784900	-0.23863200
C	0.32760200	2.84818900	-1.35003300
C	1.05708500	2.62570300	0.93497200
C	0.53964000	4.22348900	-1.28957100
H	-0.04178000	2.39338900	-2.26552700
C	1.27196500	4.00404100	0.99835700
H	1.26723400	1.99513700	1.79210000
C	1.01306000	4.80717600	-0.11178100
H	0.34106700	4.83993000	-2.16155400
H	1.64634800	4.44845600	1.91609500
H	1.18346200	5.87862700	-0.06357600
C	6.63211700	-0.92592000	-1.09328400
C	6.84596500	-1.83411100	-0.04763200
C	5.81549900	-2.15410500	0.83827000
C	4.57699600	-1.54721300	0.65322900
C	4.34302500	-0.62734000	-0.40071800
C	5.39083200	-0.32100800	-1.27634000
H	7.44665100	-0.68930800	-1.77119200
H	7.82075100	-2.29475900	0.07852500
H	5.97922500	-2.85670100	1.64891500
H	5.21457400	0.38402400	-2.08157500
S	3.09954900	-1.74117400	1.59628000

N	3.06164400	-0.10322900	-0.47233300
C	2.31380400	-0.57748000	0.47623600
C	-6.12422700	-2.16133700	-1.85756900
H	-6.48978100	-3.15324500	-2.14390300
H	-6.90398400	-1.42994000	-2.09205000
H	-5.25072100	-1.92323800	-2.47072300
C	-6.39551500	0.02026000	2.15249600
H	-5.44180900	0.25084000	2.63472500
H	-7.14871800	0.72571100	2.51900100
H	-6.69250200	-0.98685100	2.46225400
H	-1.22205200	-2.57954200	-1.70475000
H	0.45562900	-0.83578300	1.25728700

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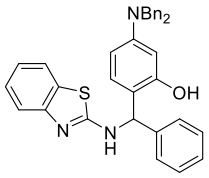

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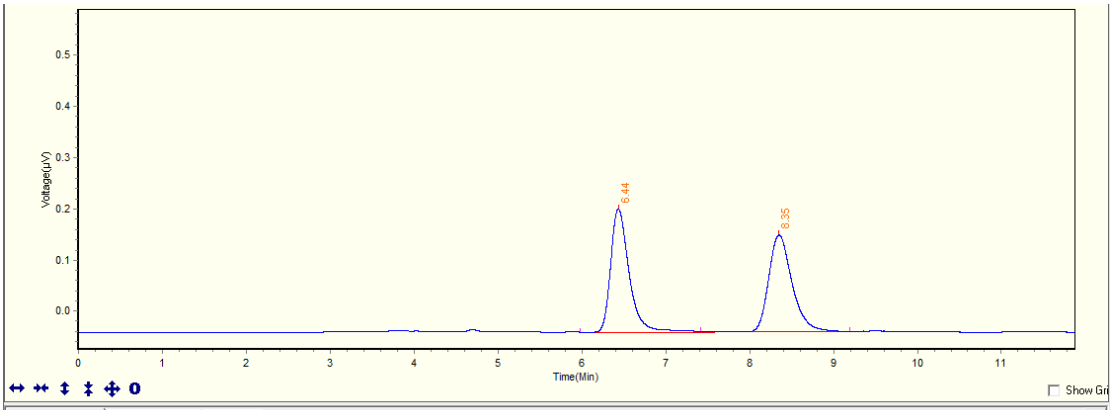
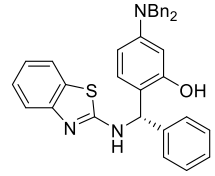


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.44	1822574	120367	50.42%	1.441	BV
2	8.35	1792220	94117	49.58%	1.779	VB
Total		3,614,794	214,484	100.00%		



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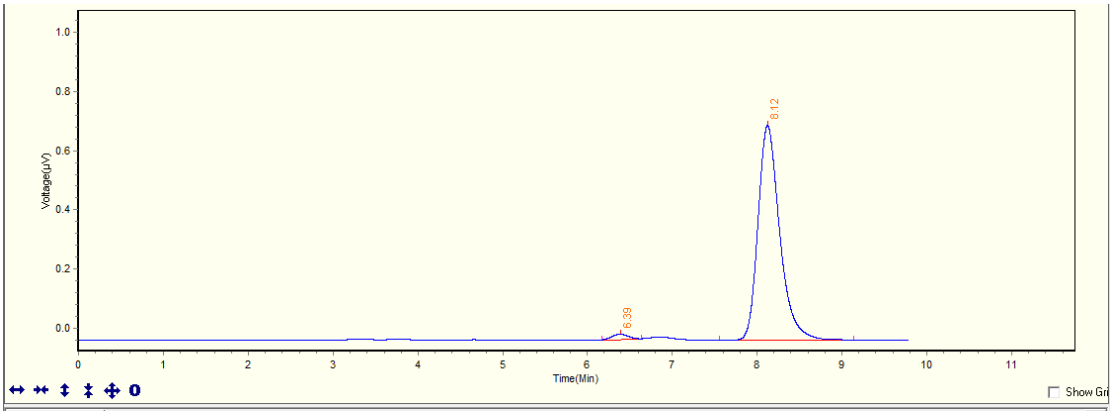
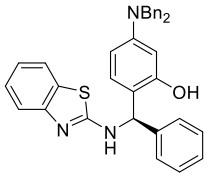


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.39	109678	8427	1.68%	0.466	BB
2	8.12	6406542	362111	98.32%	1.583	BB
Total		6,516,220	370,538	100.00%		



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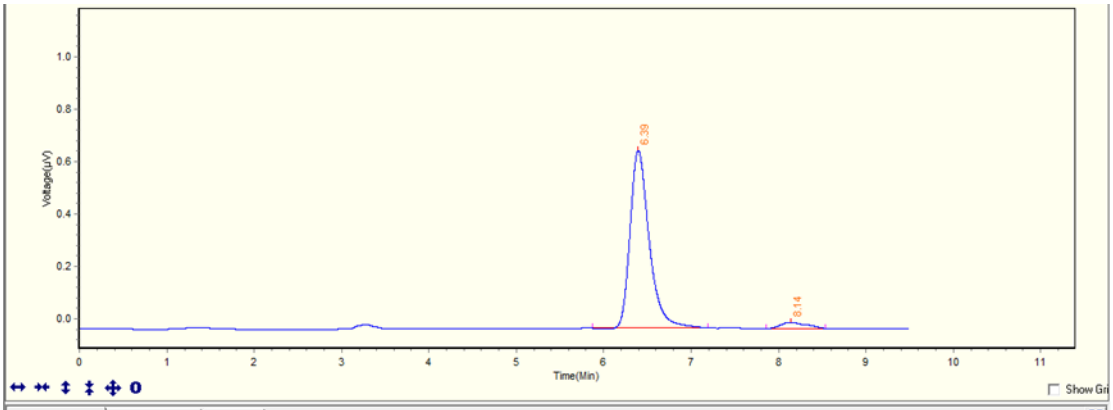
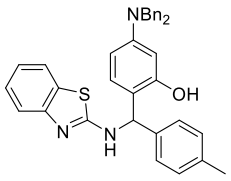


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.39	5134672	338362	95.59%	1.321	BB
2	8.14	236943	11834	4.41%	0.677	BB
Total		5,371,615	350,196	100.00%		



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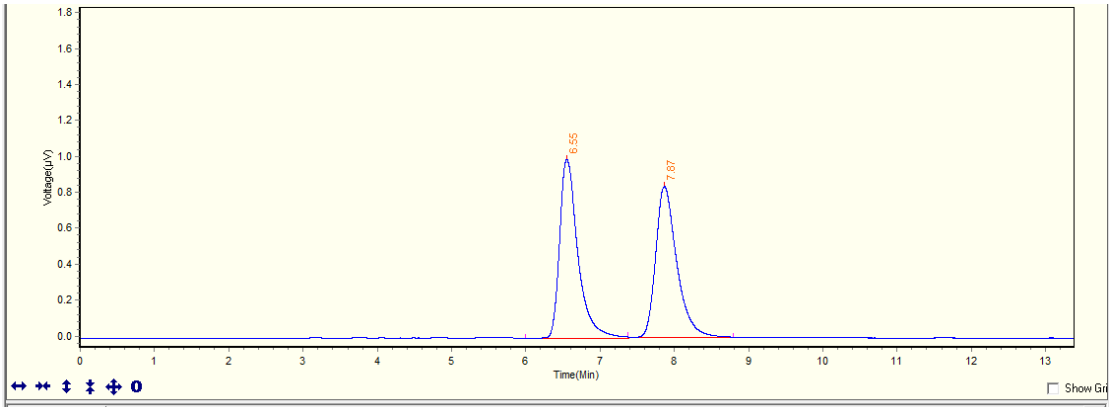
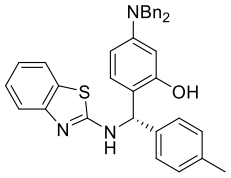


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.55	8422083	496201	50.43%	1.379	BV
2	7.87	8277169	420058	49.57%	1.418	VB
Total		16,699,252	916,259	100.00%		



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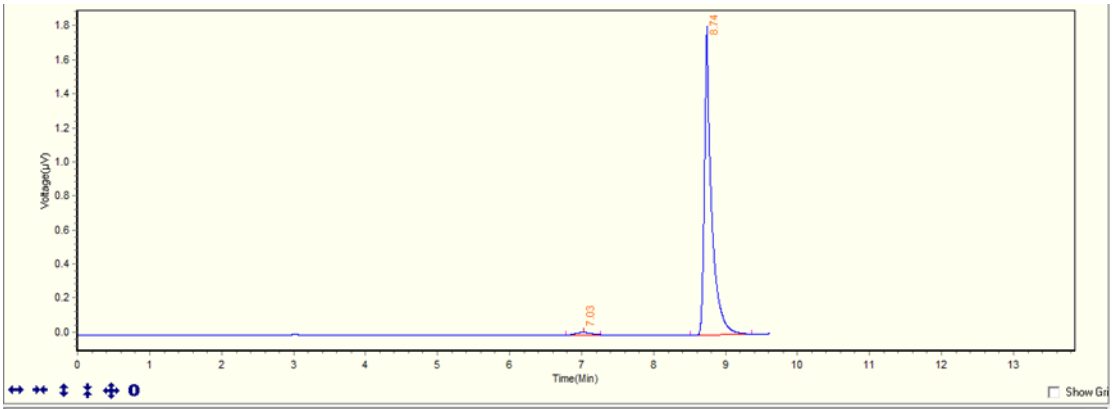
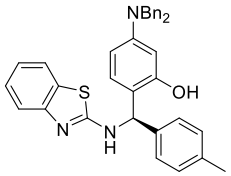


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.03	112307	7475	1.81%	0.478	BB
2	8.74	6096623	908147	98.19%	0.84	BB
Total		6,208,930	915,622	100.00%		



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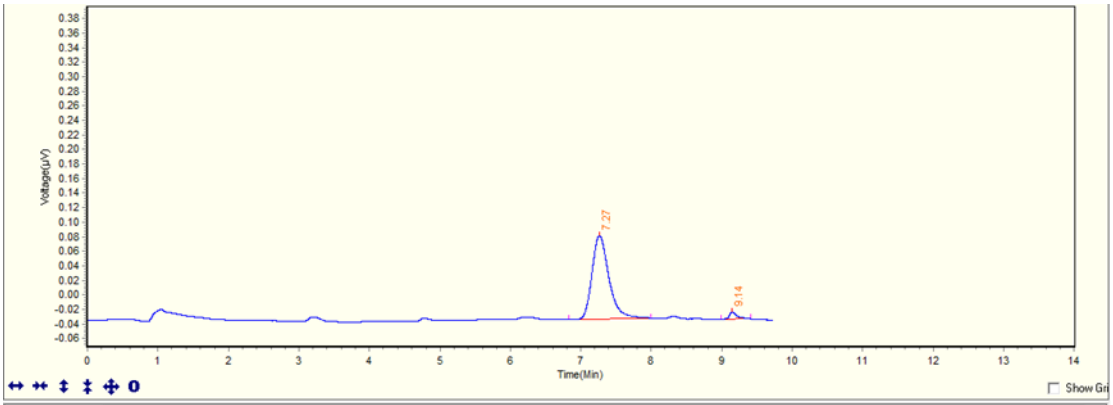
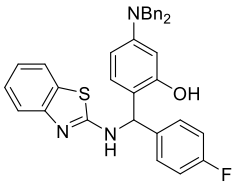


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.27	946885	57050	96.39%	1.163	BB
2	9.14	35508	4749	3.61%	0.421	BB
Total		982,393	61,799	100.00%		



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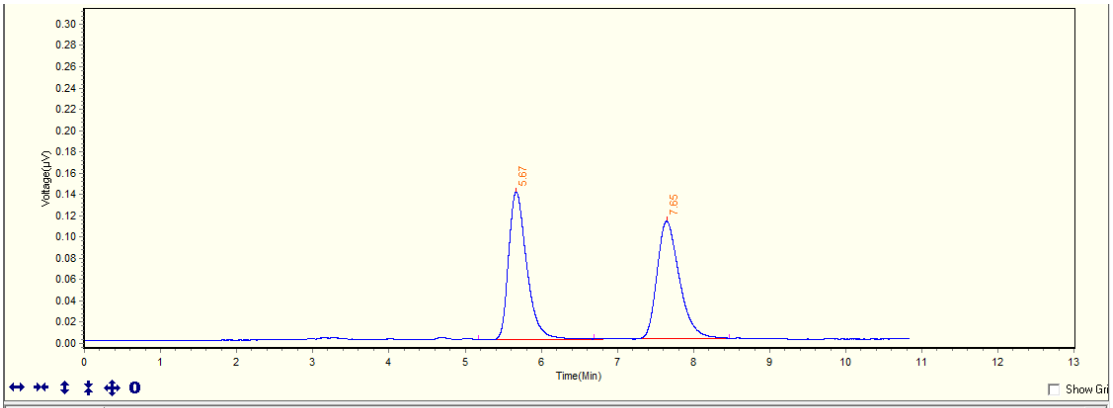
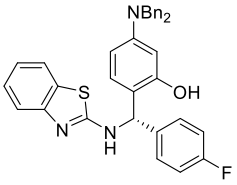


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.67	1132714	69212	50.40%	1.517	BV
2	7.65	1114809	55183	49.60%	1.777	VB
Total		2,247,523	124,395	100.00%		



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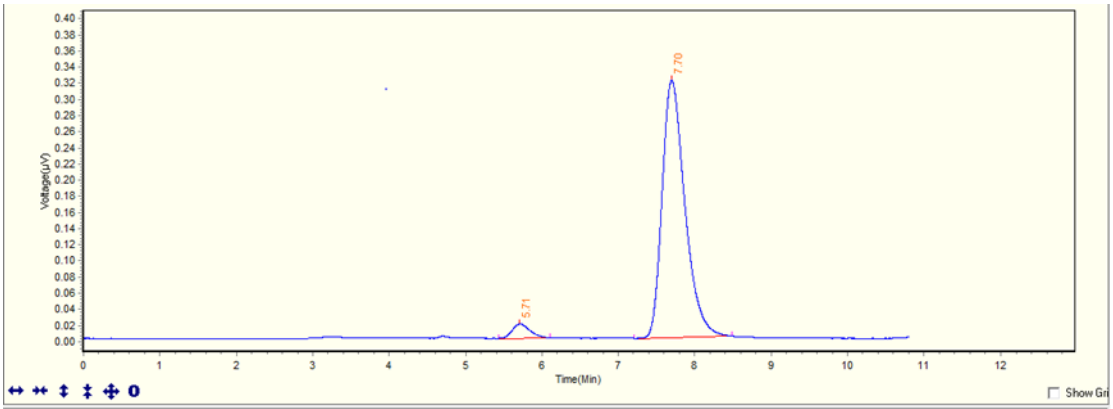
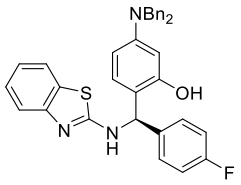


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.71	139055	8704	4.05%	0.673	BB
2	7.70	3298455	159249	95.95%	1.281	BB
Total		3,437,510	167,953	100.00%		



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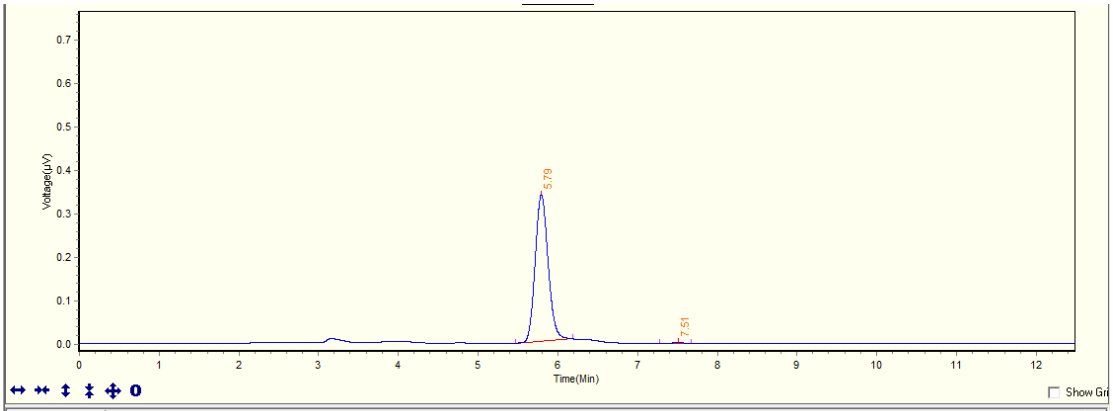
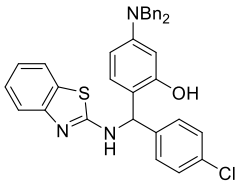


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.79	1901029	168213	99.38%	0.717	BB
2	7.51	11861	1299	0.62%	0.403	BB
Total		1,912,890	169,512	100.00%		



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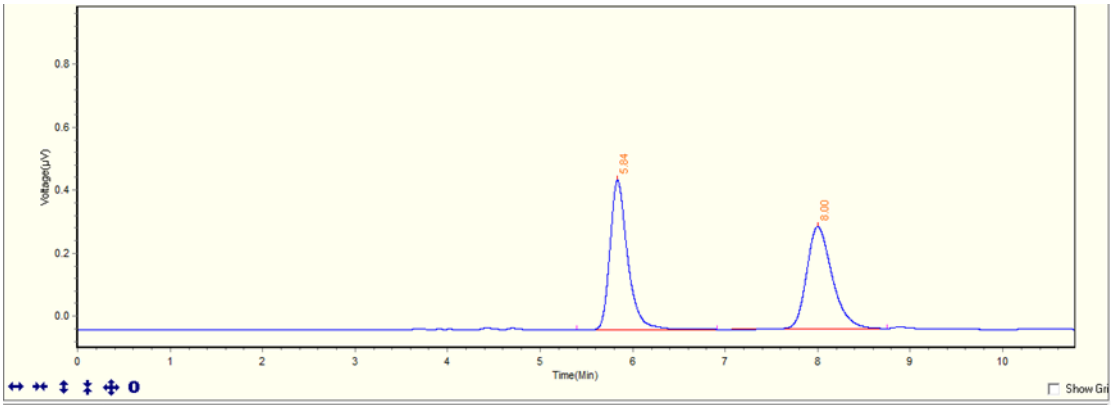
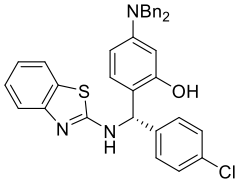


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.84	3115493	237158	50.25%	1.513	BV
2	8.00	3084999	162567	49.75%	1.842	VB
Total		6,200,492	399,725	100.00%		



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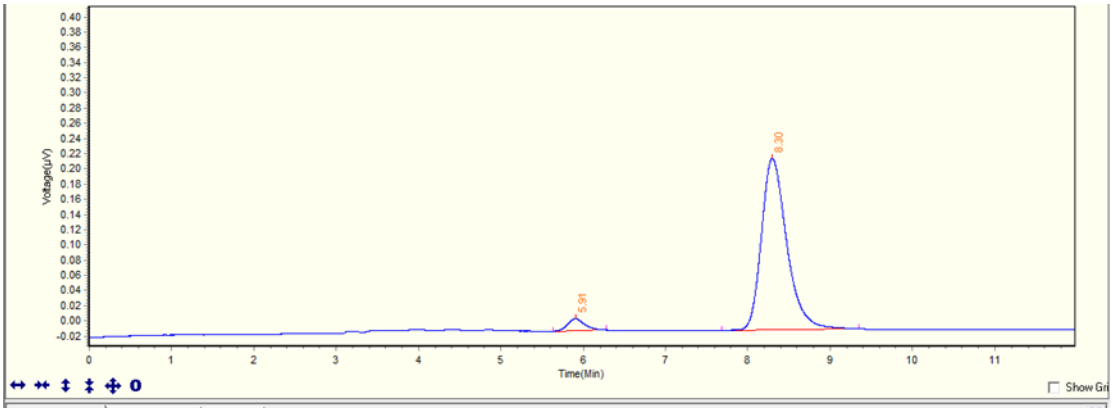
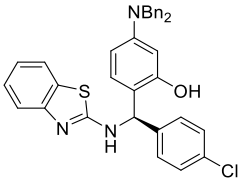


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.91	112823	7840	4.47%	0.648	BB
2	8.30	2409381	112581	95.53%	1.667	BB
Total		2,522,204	120,421	100.00%		



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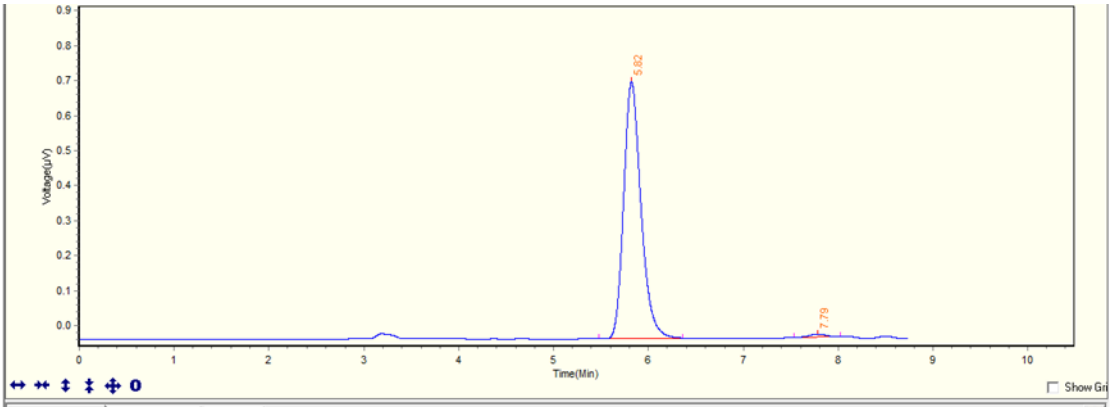
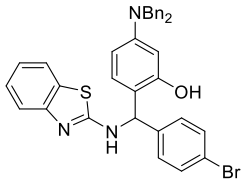


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.82	4628752	366946	98.87%	0.883	BB
2	7.79	53091	4125	1.13%	0.488	BB
Total		4,681,843	371,071	100.00%		



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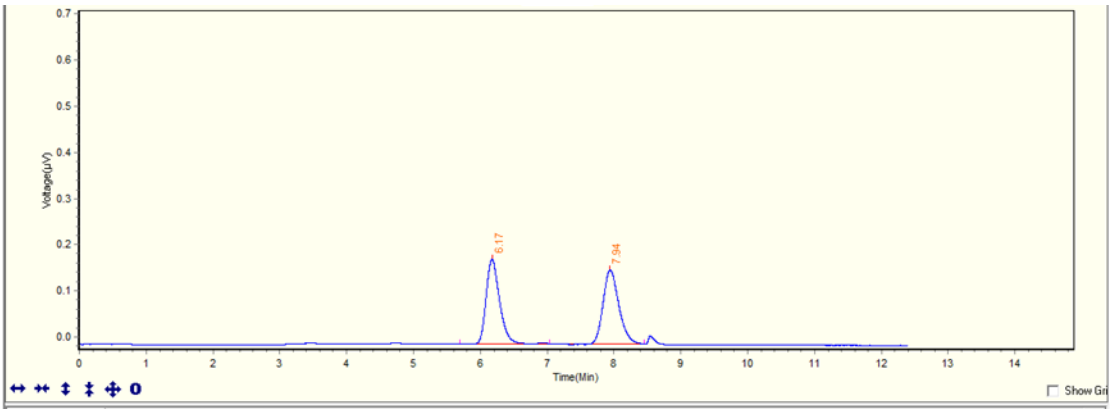
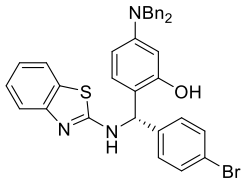


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.17	1281149	91459	49.57%	1.343	BV
2	7.94	1303311	80116	50.43%	1.415	VB
Total		2,584,460	171,575	100.00%		



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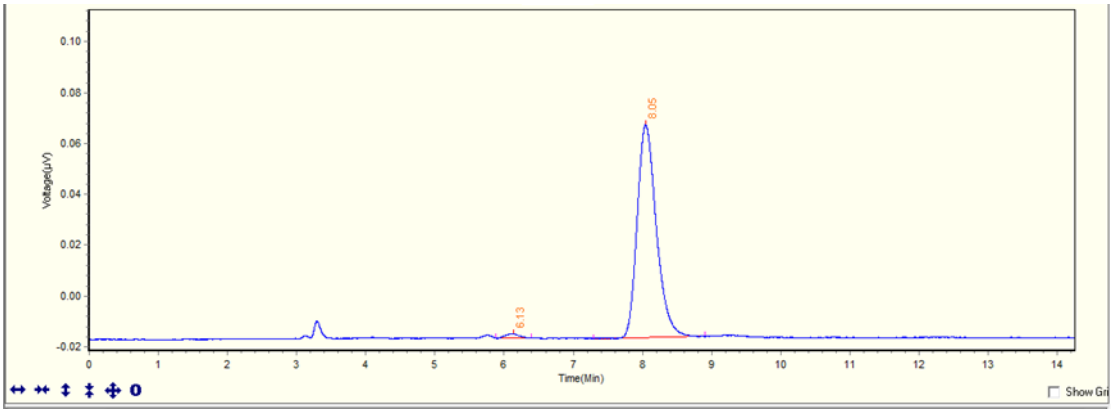
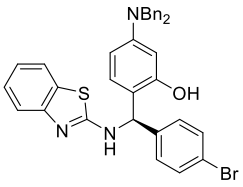


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.13	10147	829	1.25%	0.513	BB
2	8.05	804843	41845	98.75%	1.61	BB
Total		814,990	42,674	100.00%		



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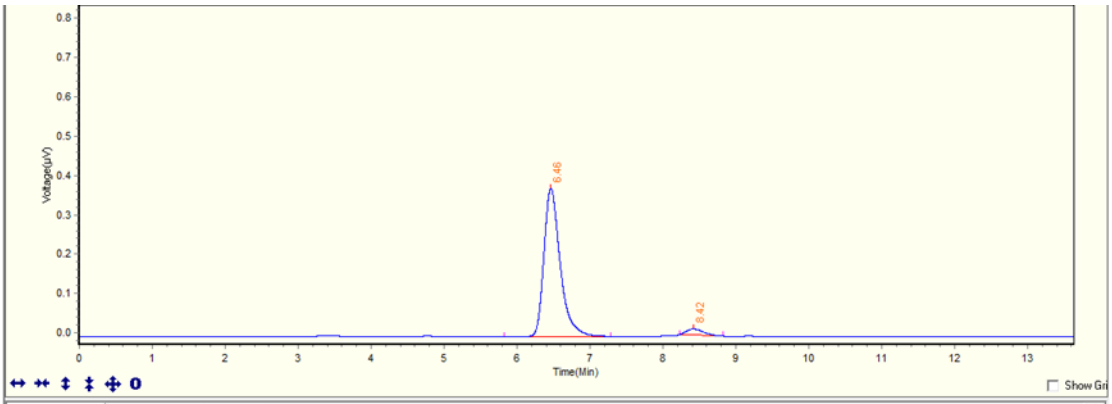
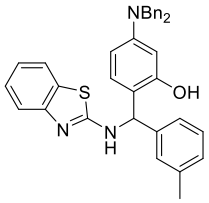


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.46	2923352	188652	95.81%	1.458	BB
2	8.42	127714	7847	4.19%	0.594	BB
Total		3,051,066	196,499	100.00%		



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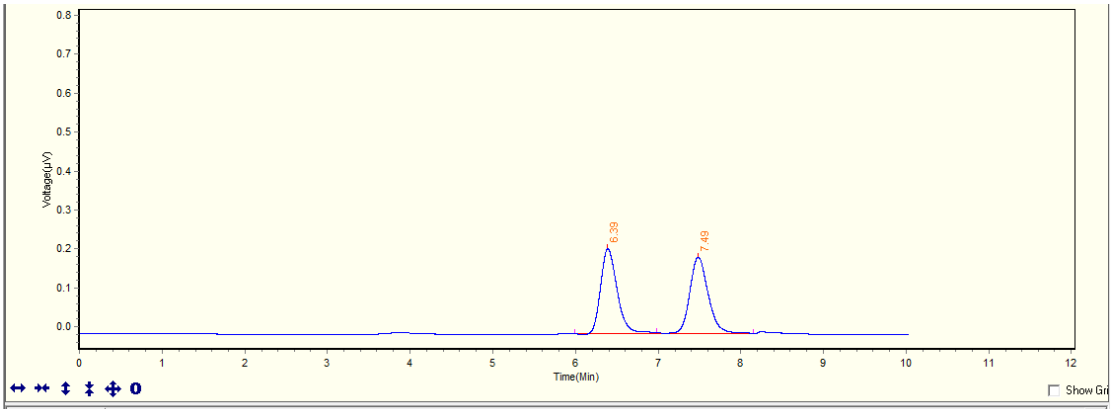
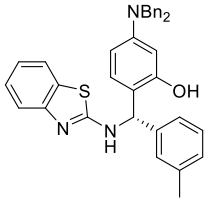


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.39	1521899	109232	50.18%	0.991	BV
2	7.49	1511134	97954	49.82%	1.169	VB
Total		3,033,033	207,186	100.00%		



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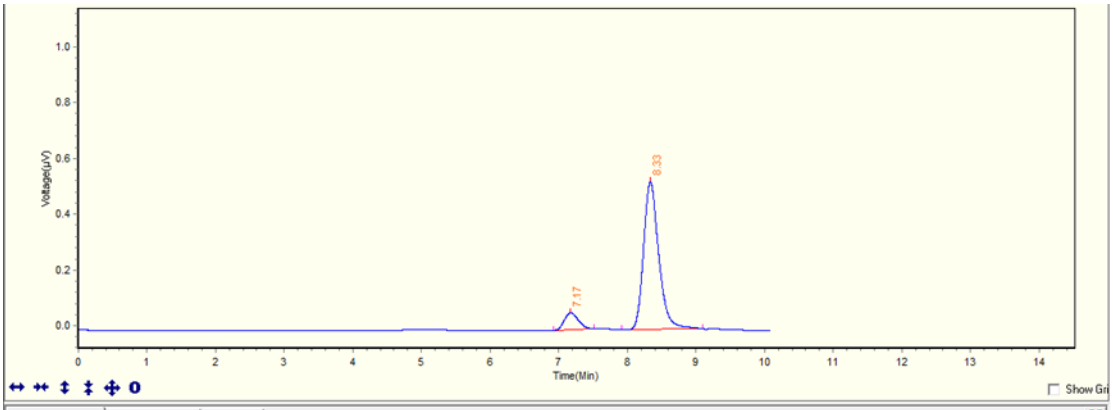
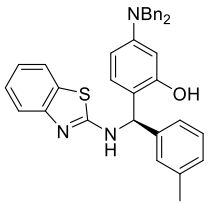


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.17	431402	30500	9.56%	0.59	BB
2	8.33	4079222	264890	90.44%	1.18	BB
Total		4,510,624	295,390	100.00%		



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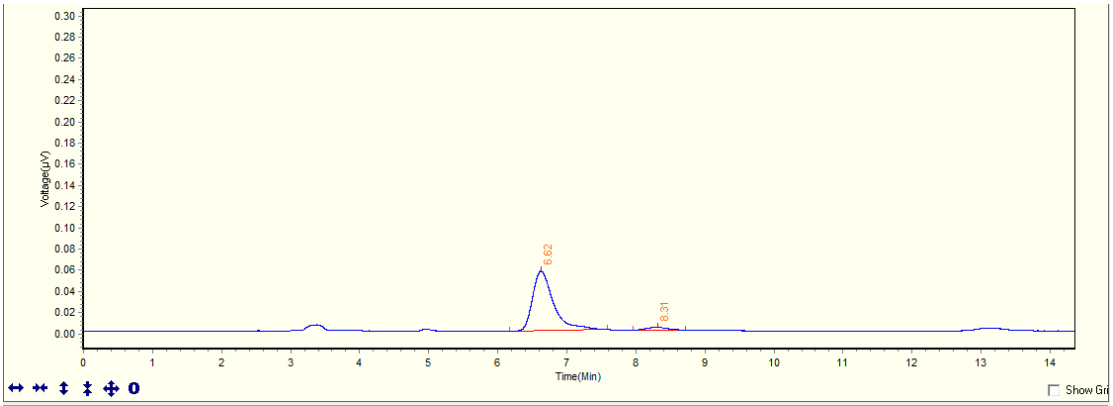
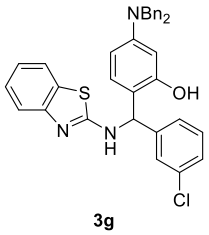


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.62	587205	27935	95.33%	1.42	BB
2	8.31	28735	1367	4.67%	0.763	BB
Total		615,940	29,302	100.00%		



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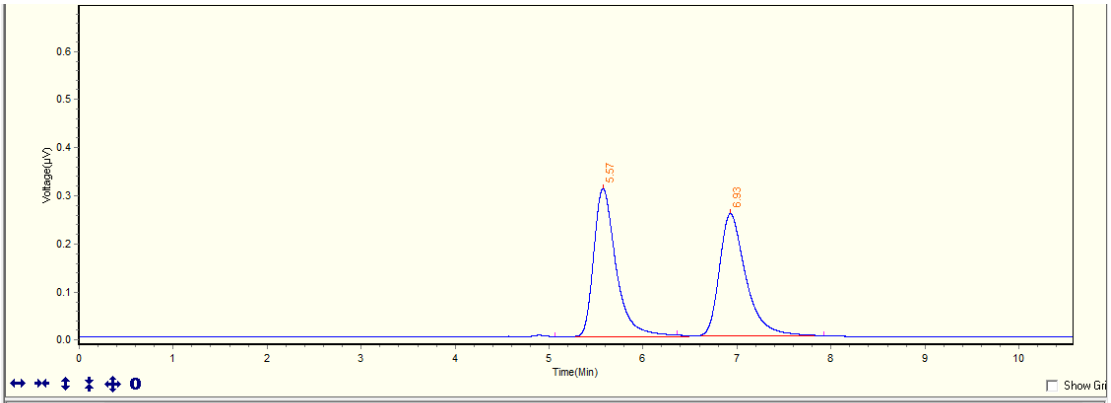
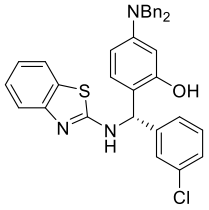


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.57	2535359	153832	50.41%	1.299	BV
2	6.93	2494554	127232	49.59%	1.561	VB
Total		5,029,913	281,064	100.00%		



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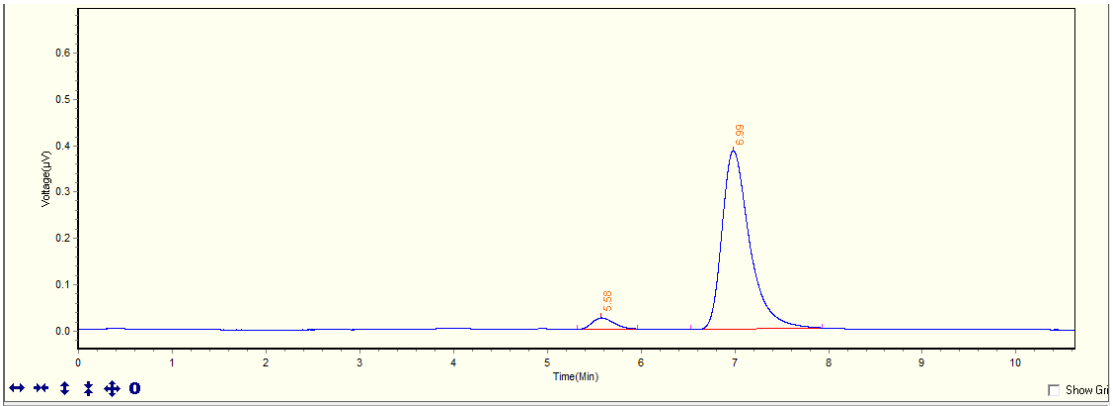
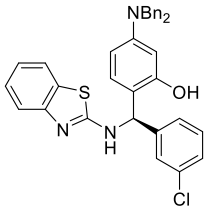


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.58	195910	12271	4.74%	0.642	BB
2	6.99	3935556	192288	95.26%	1.401	BB
Total		4,131,466	204,559	100.00%		



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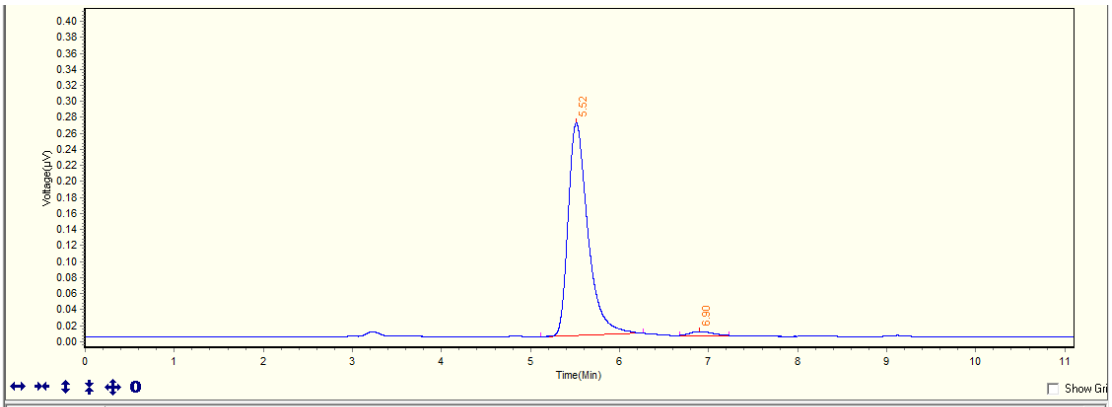
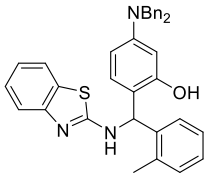


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.52	2050435	132826	98.03%	1.153	BB
2	6.90	41197	2465	1.97%	0.563	BB
Total		2,091,632	135,291	100.00%		



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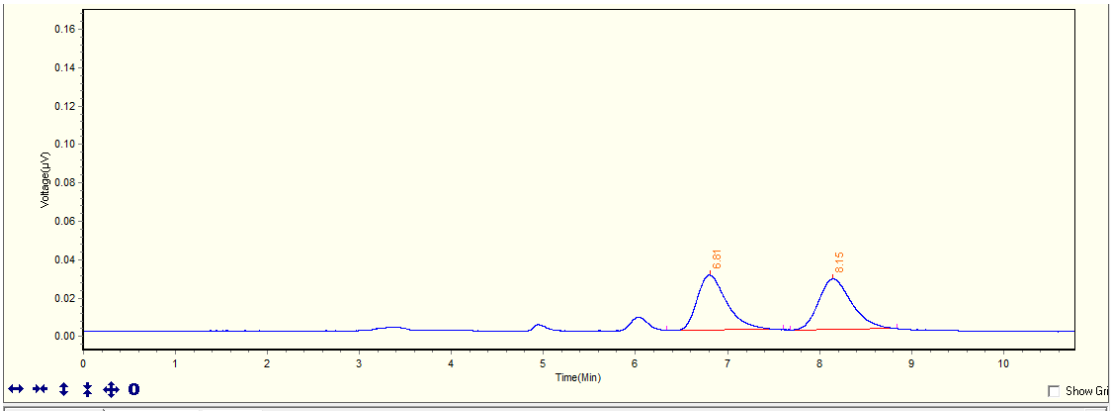
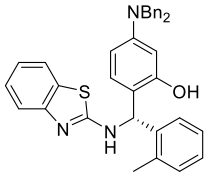


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.81	319025	14299	49.45%	1.263	BB
2	8.15	326183	13102	50.55%	1.161	BB
Total		645,208	27,401	100.00%		



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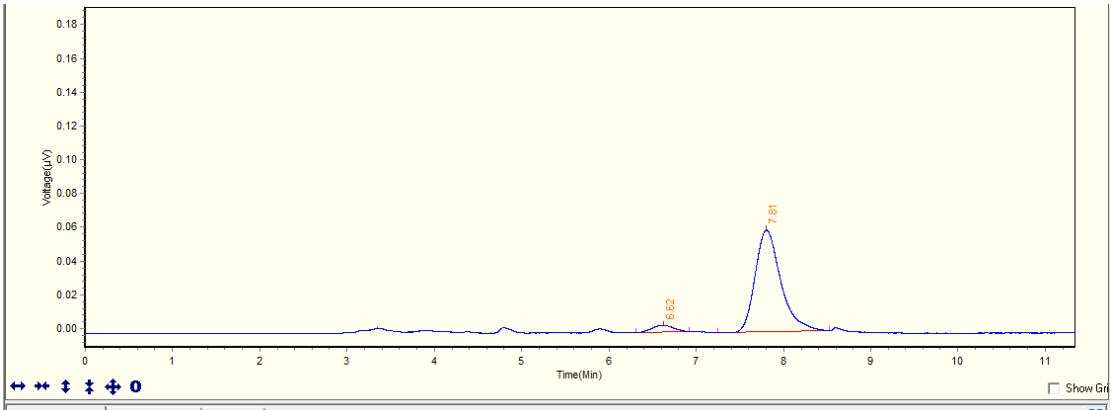
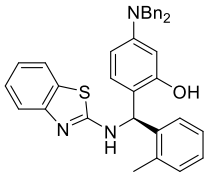


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.62	34607	2028	5.34%	0.611	BB
2	7.81	613839	30065	94.66%	1.275	BB
Total		648,446	32,093	100.00%		



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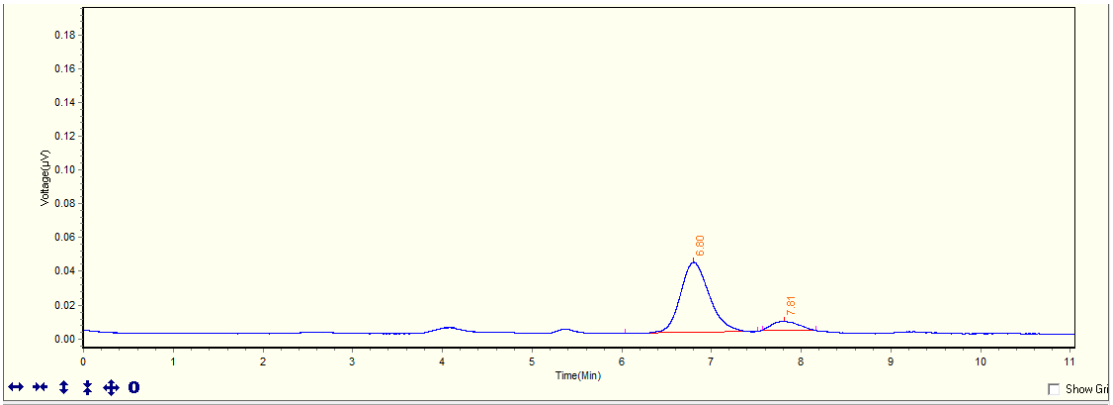
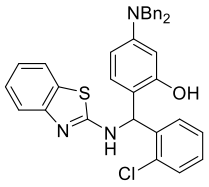


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.80	463030	20777	89.36%	1.476	BB
2	7.81	55114	2636	10.64%	0.595	BB
Total		518,144	23,413	100.00%		



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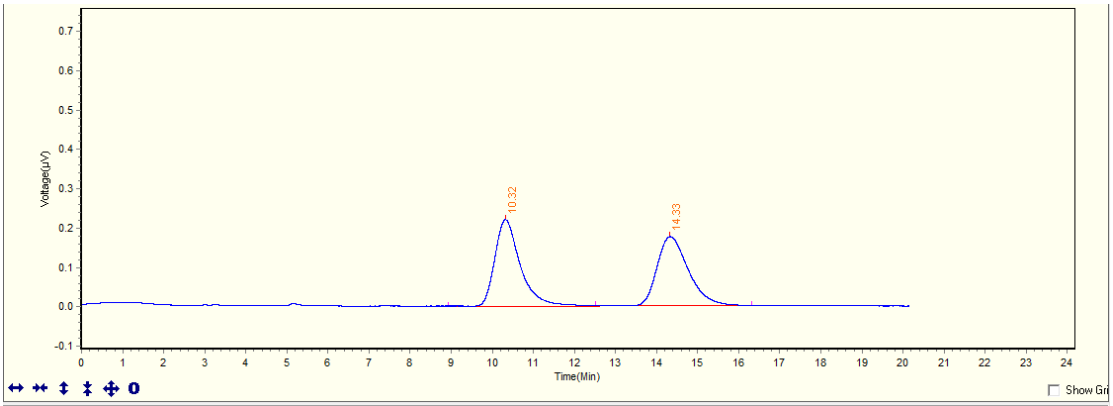
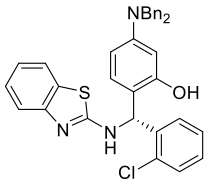


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.32	4674017	109640	50.42%	3.586	BV
2	14.33	4595524	87706	49.58%	3.802	VB
Total		9,269,541	197,346	100.00%		



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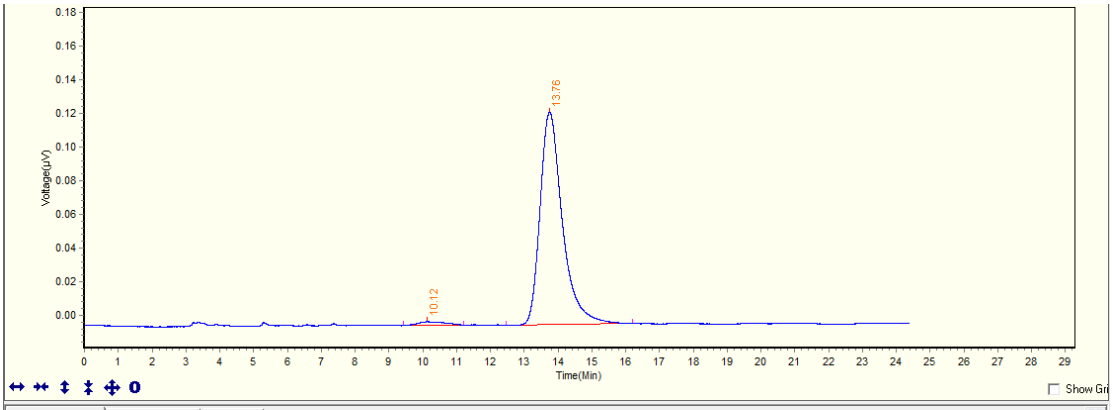
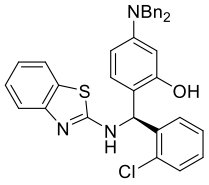


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.12	59447	1132	2.02%	1.781	BB
2	13.76	2888058	63161	97.98%	3.737	BB
Total		2,947,505	64,293	100.00%		



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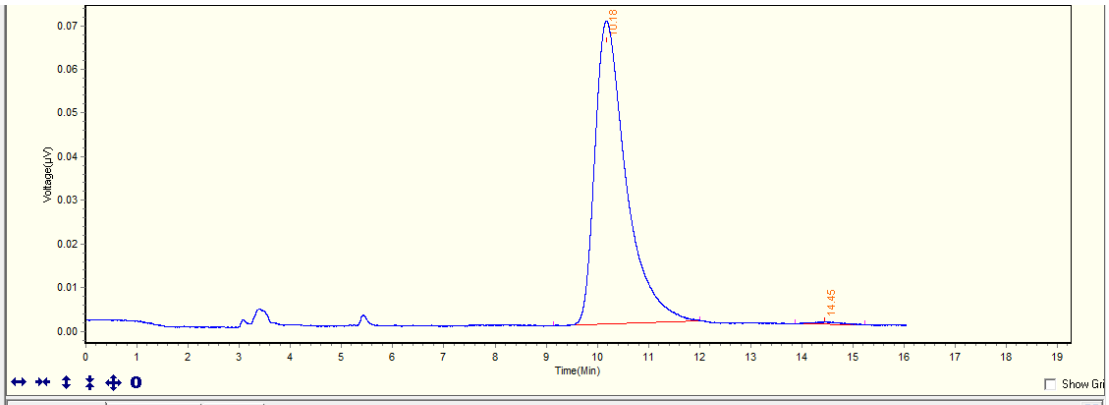
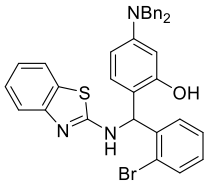


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.18	1465272	34683	99.37%	2.862	BB
2	14.45	9259	256	0.63%	1.364	BB
Total		1,474,531	34,939	100.00%		



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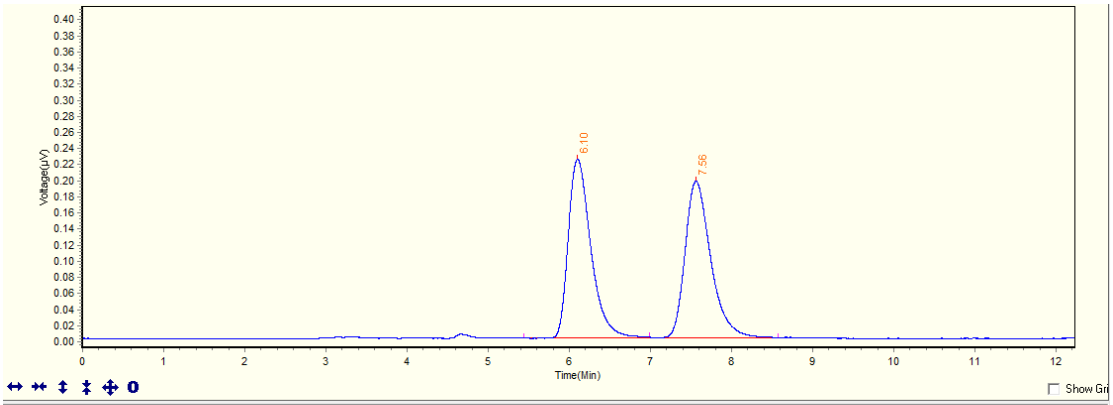
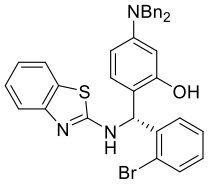


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.10	2149790	111078	50.20%	1.549	BV
2	7.56	2133010	97262	49.80%	1.585	VB
Total		4,282,800	208,340	100.00%		



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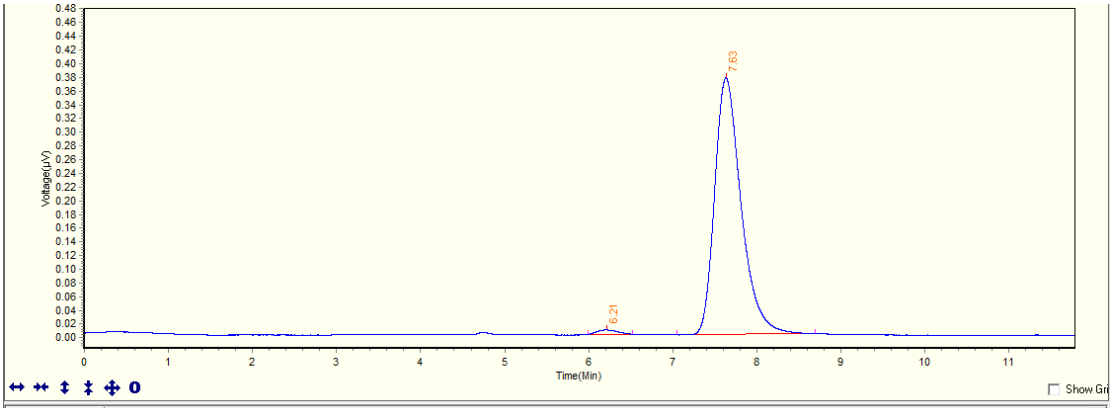
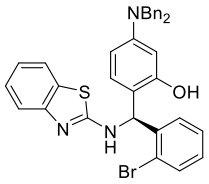


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.21	52684	3167	1.27%	0.529	BB
2	7.63	4096481	187181	98.73%	1.645	BB
Total		4,149,165	190,348	100.00%		



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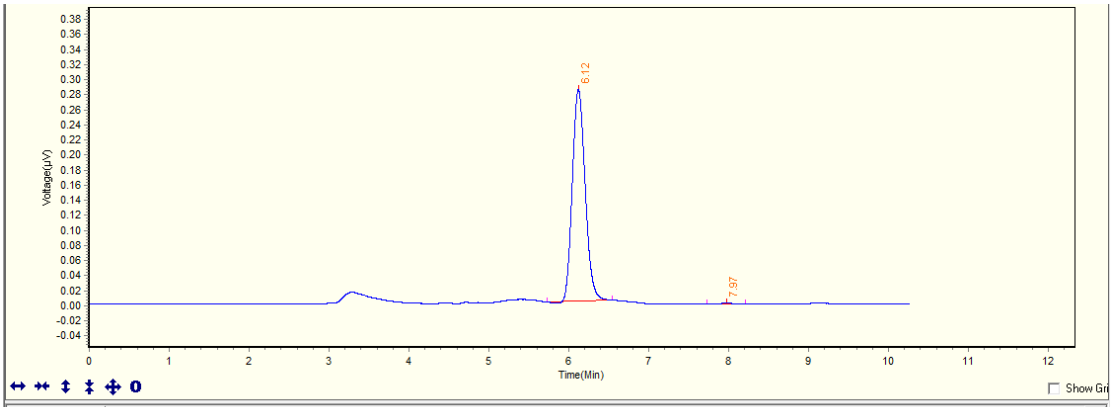
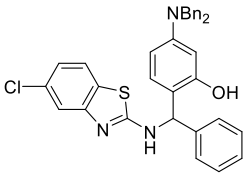


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.12	1565141	140313	99.60%	0.814	BB
2	7.97	6255	670	0.40%	0.483	BB
Total		1,571,396	140,983	100.00%		



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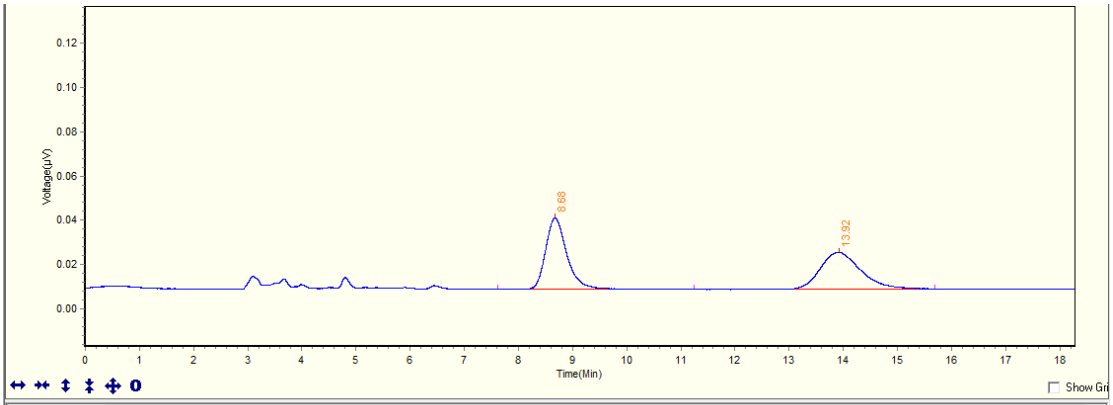
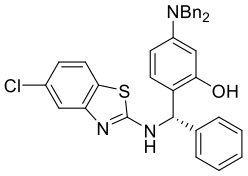


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	8.68	426784	16050	50.32%	3.622	BV
2	13.92	421427	8290	49.68%	4.44	VB
Total		848,211	24,340	100.00%		



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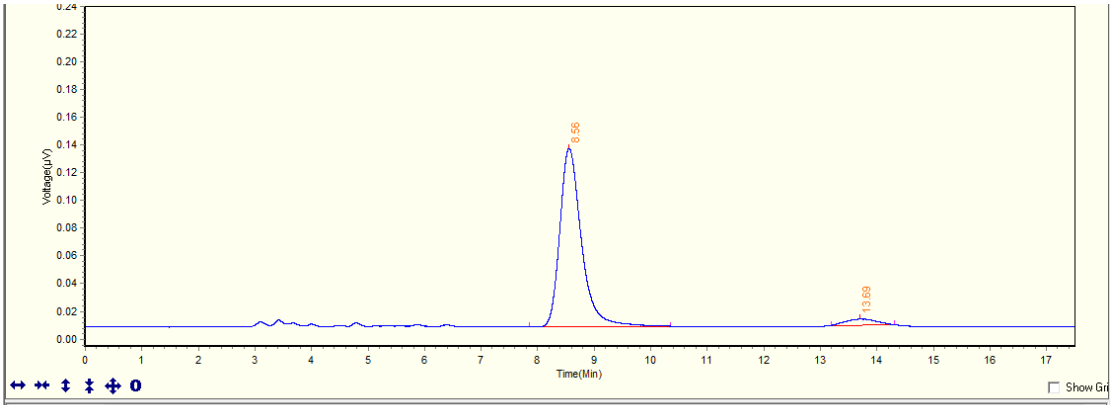
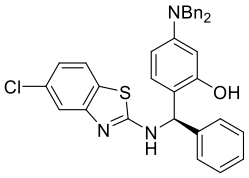


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	8.56	1705344	64356	95.45%	2.496	BB
2	13.69	81315	2194	4.55%	1.117	BB
Total		1,786,659	66,550	100.00%		



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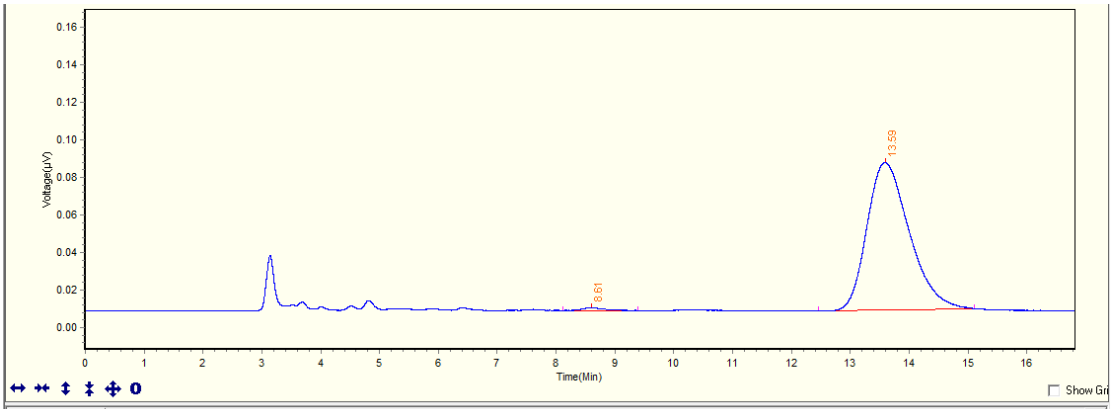
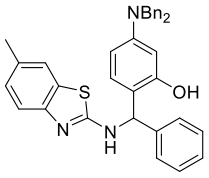


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	8.61	18646	759	0.94%	1.274	BB
2	13.59	1964150	39418	99.06%	2.65	BB
Total		1,982,796	40,177	100.00%		



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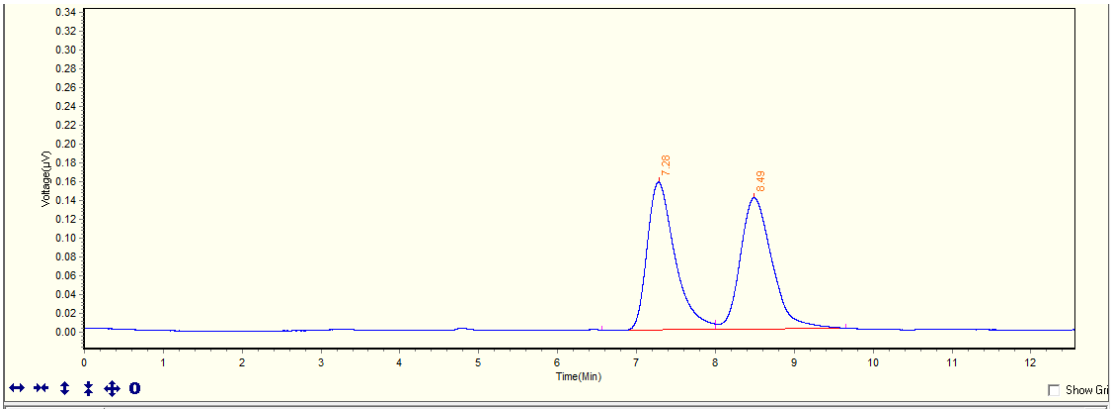
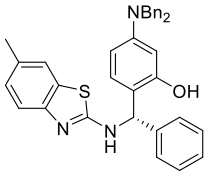


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.28	1907388	78379	49.54%	1.44	BV
2	8.49	1942431	69691	50.46%	1.652	VB
Total		3,849,819	148,070	100.00%		



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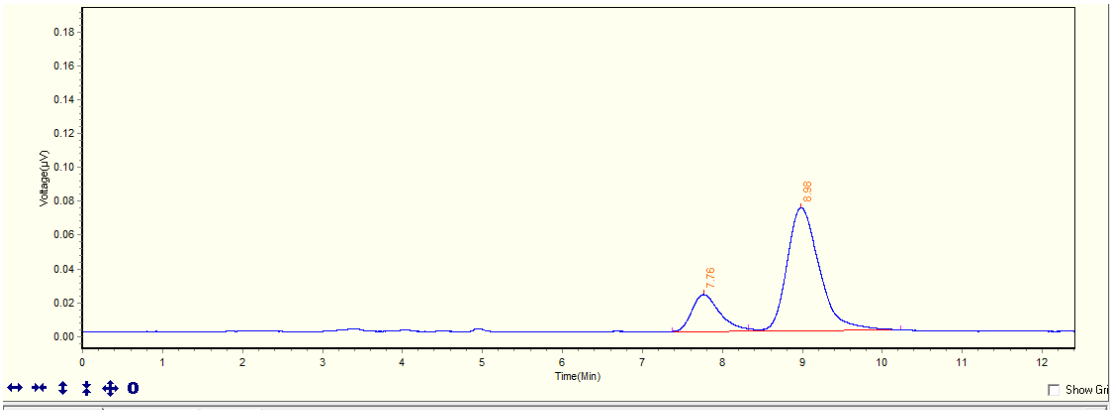
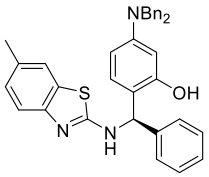


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.76	263915	10900	20.43%	0.952	BV
2	8.98	1027962	36426	79.57%	1.905	VB
Total		1,291,877	47,326	100.00%		



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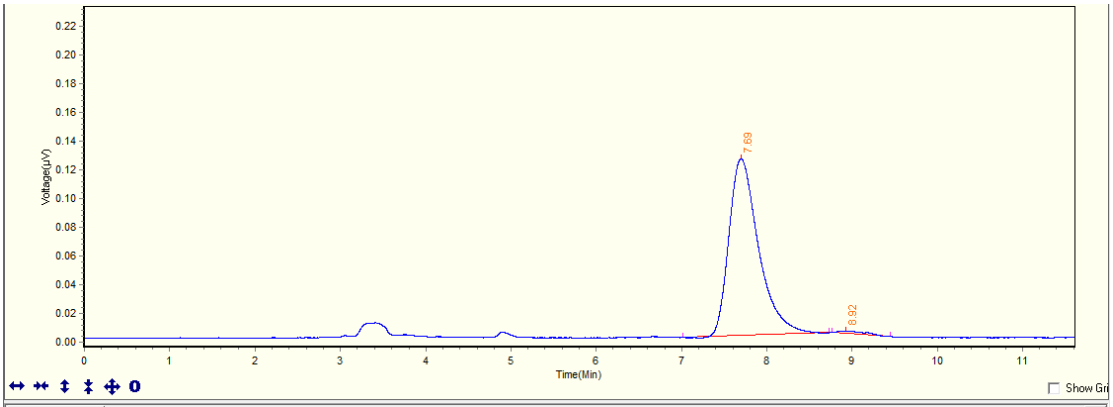
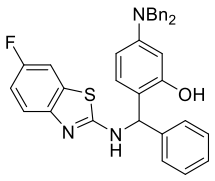


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.69	1485120	61552	98.64%	1.713	BB
2	8.92	20513	810	1.36%	0.683	BB
Total		1,505,633	62,362	100.00%		



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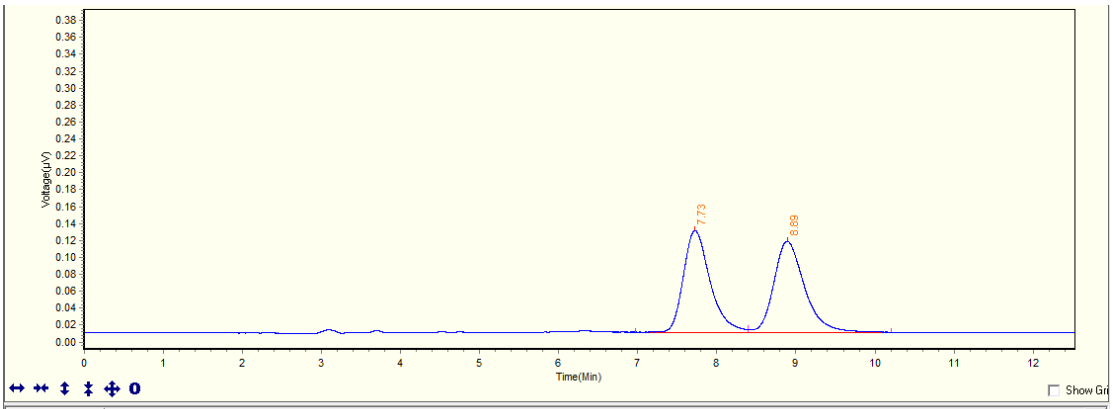
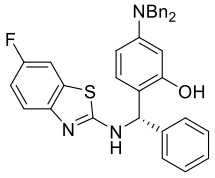


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.73	1401957	60041	49.33%	1.424	BV
2	8.89	1440314	53630	50.67%	1.811	VB
Total		2,842,271	113,671	100.00%		



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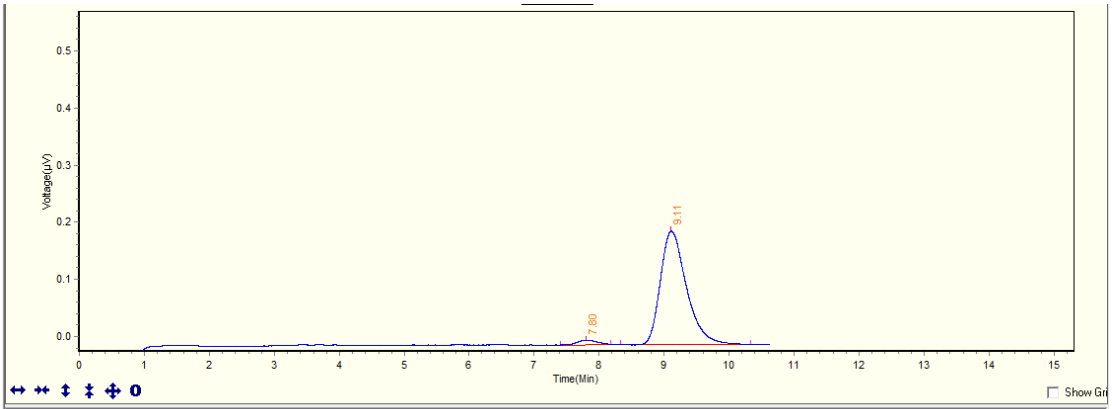
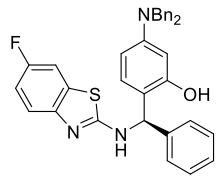


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.80	78012	3805	2.74%	0.784	BB
2	9.11	2774222	99476	97.26%	1.998	BB
Total		2,852,234	103,281	100.00%		



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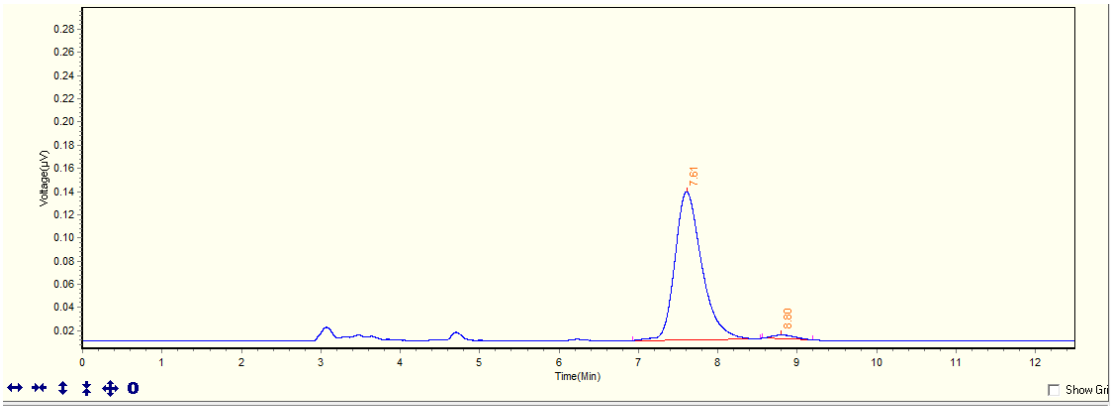
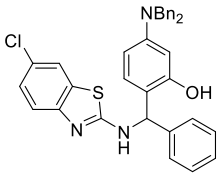


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.61	1487536	63760	97.80%	1.607	BB
2	8.80	33457	1651	2.20%	0.636	BB
Total		1,520,993	65,411	100.00%		



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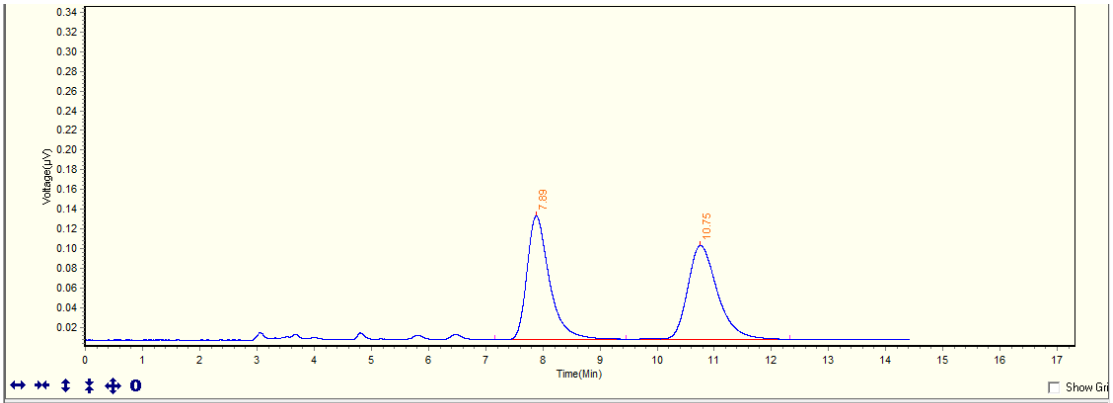
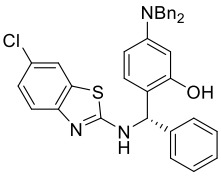


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.89	1718110	62643	49.89%	2.295	BV
2	10.75	1725526	47577	50.11%	2.863	VB
Total		3,443,636	110,220	100.00%		



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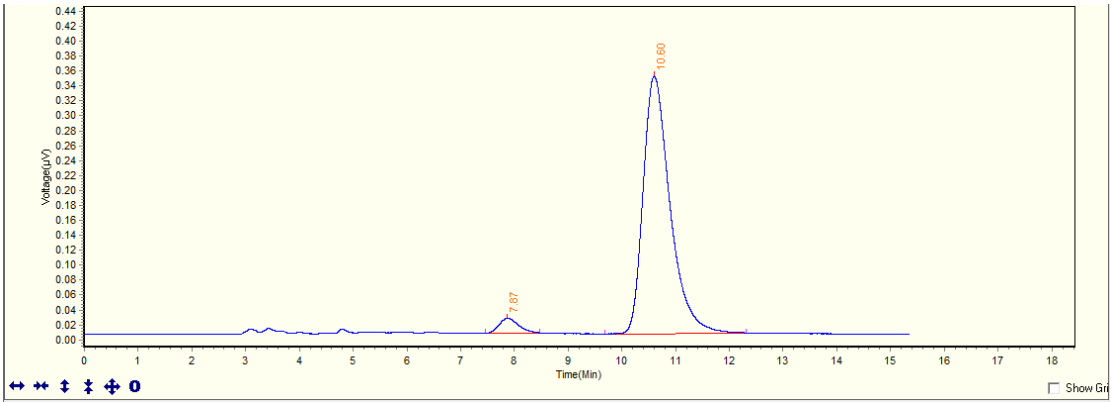
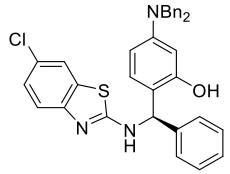


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.87	248657	10050	4.00%	1.011	BB
2	10.60	5967948	172236	96.00%	2.628	BB
Total		6,216,605	182,286	100.00%		



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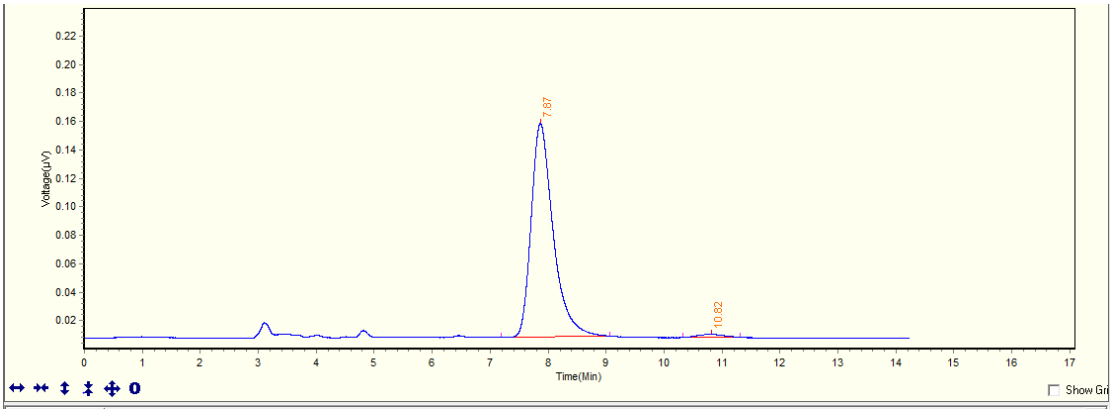
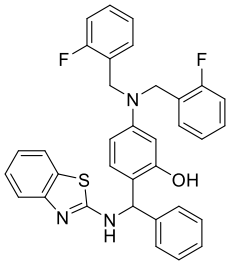


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.87	1969247	74923	98.34%	1.874	BB
2	10.82	33236	1100	1.66%	0.988	BB
Total		2,002,483	76,023	100.00%		



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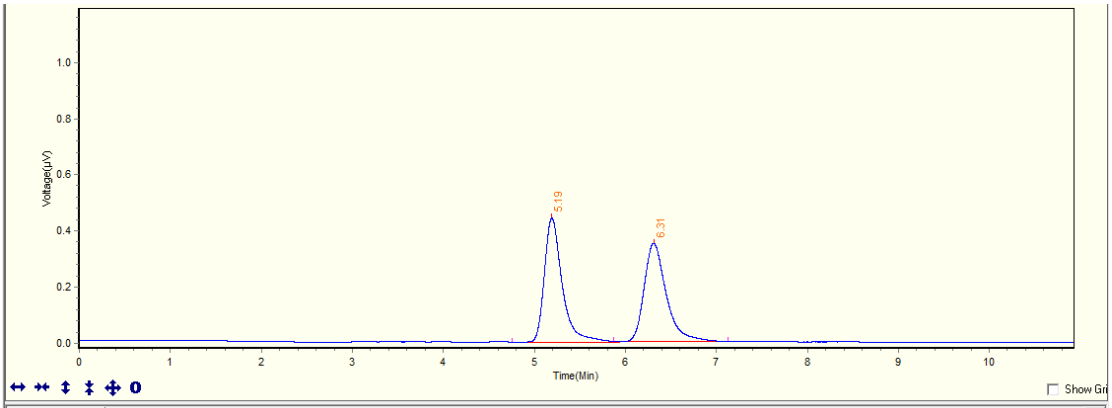
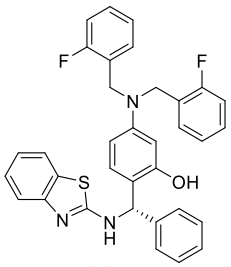


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.19	2980632	220434	50.17%	1.116	BV
2	6.31	2960674	174984	49.83%	1.256	VB
Total		5,941,306	395,418	100.00%		



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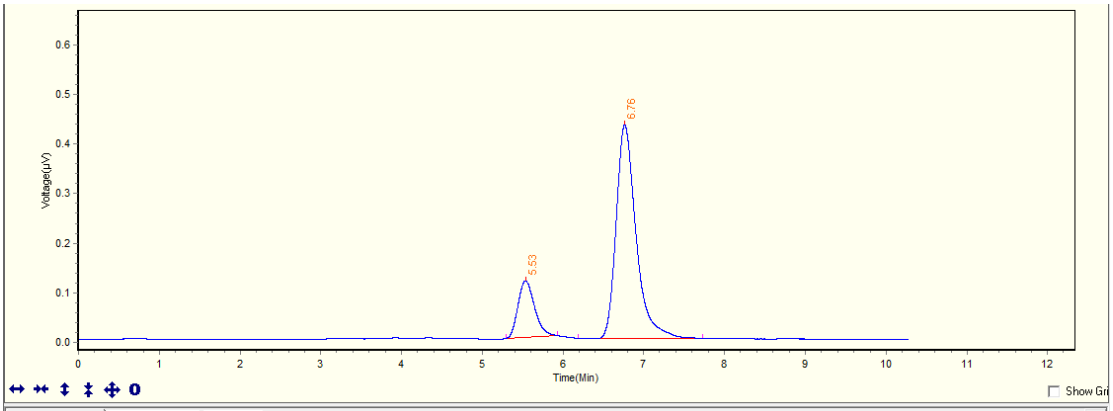
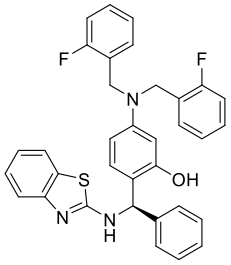


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.53	816670	57209	18.17%	0.636	BB
2	6.76	3677894	215214	81.83%	1.541	BB
Total		4,494,564	272,423	100.00%		



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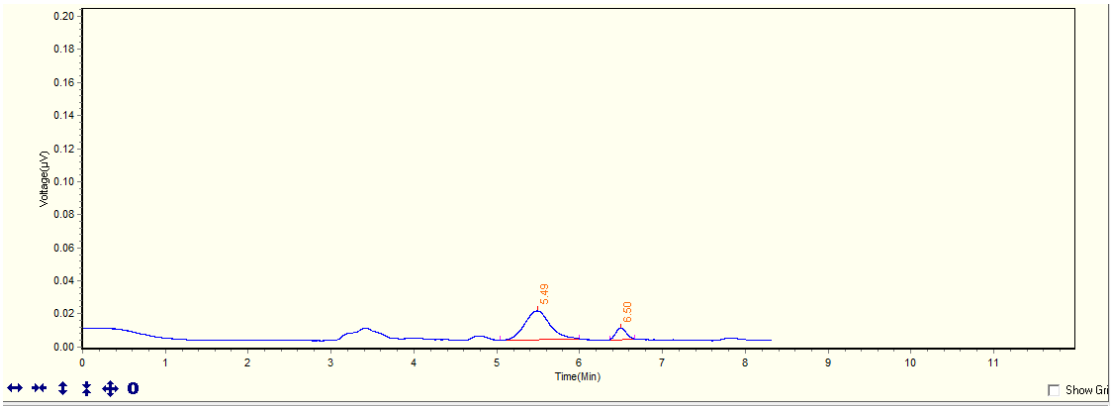
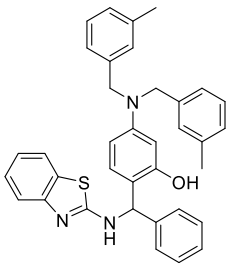


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.49	181612	8680	85.92%	0.946	BB
2	6.50	29772	3484	14.08%	0.298	BB
Total		211,384	12,164	100.00%		



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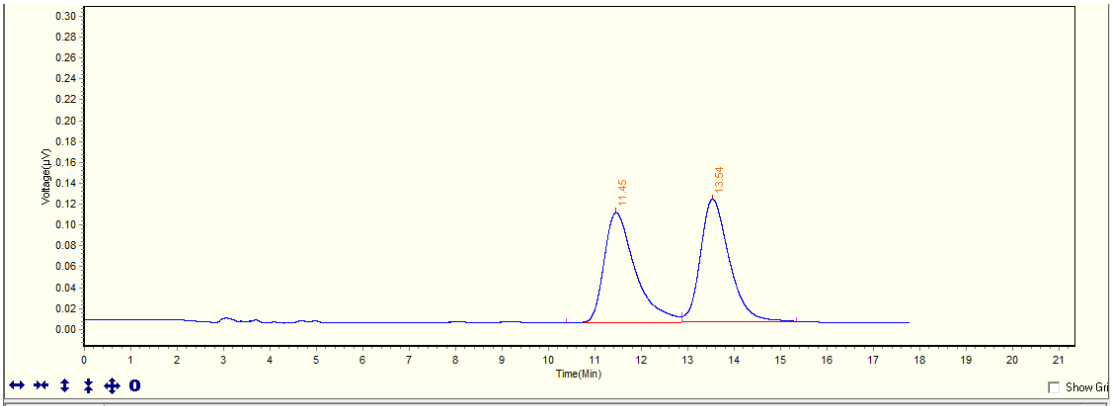
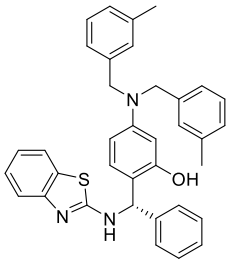


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.45	2437664	52604	49.12%	2.488	BV
2	13.54	2524510	58802	50.88%	2.468	VB
Total		4,962,174	111,406	100.00%		



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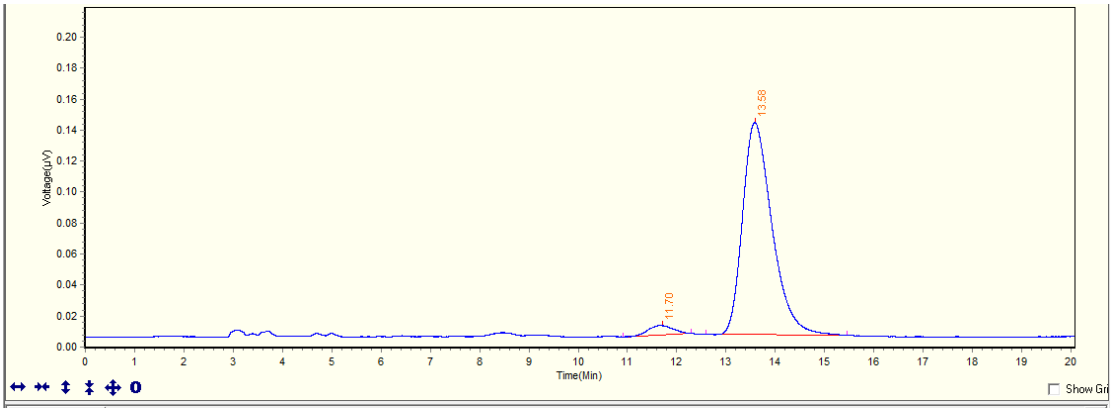
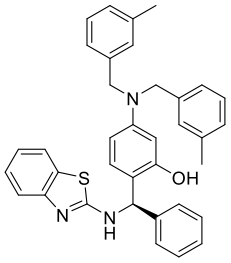


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.70	105902	3037	3.59%	1.381	BB
2	13.58	2842324	68525	96.41%	2.863	BB
Total		2,948,226	71,562	100.00%		



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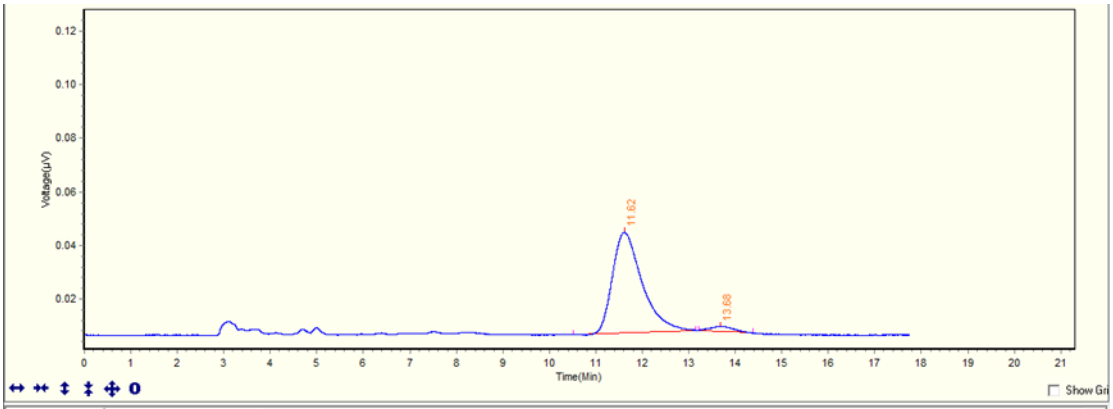
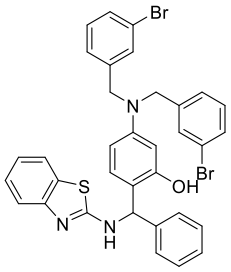


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.62	829149	18773	96.44%	2.634	BB
2	13.68	30646	918	3.56%	1.168	BB
Total		859,795	19,691	100.00%		



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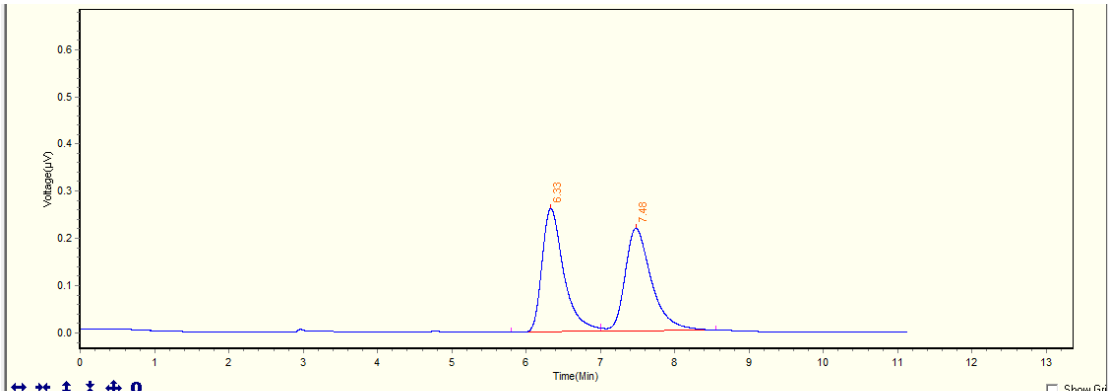
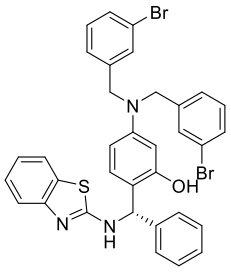


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.33	2634602	130247	49.52%	1.205	BV
2	7.48	2685904	108521	50.48%	1.548	VB
Total		5,320,506	238,768	100.00%		



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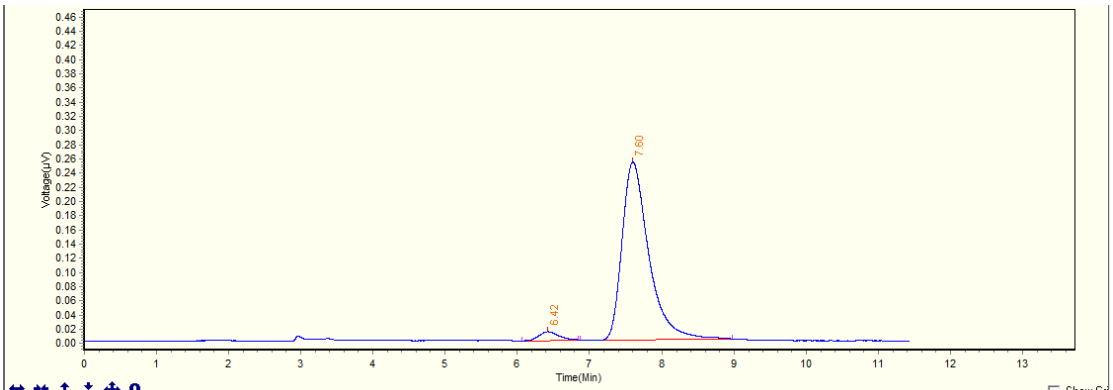
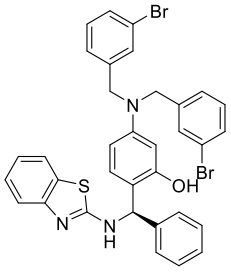


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.42	110611	6042	3.35%	0.781	BB
2	7.60	3195894	125118	96.65%	2.108	BB
Total		3,306,505	131,160	100.00%		



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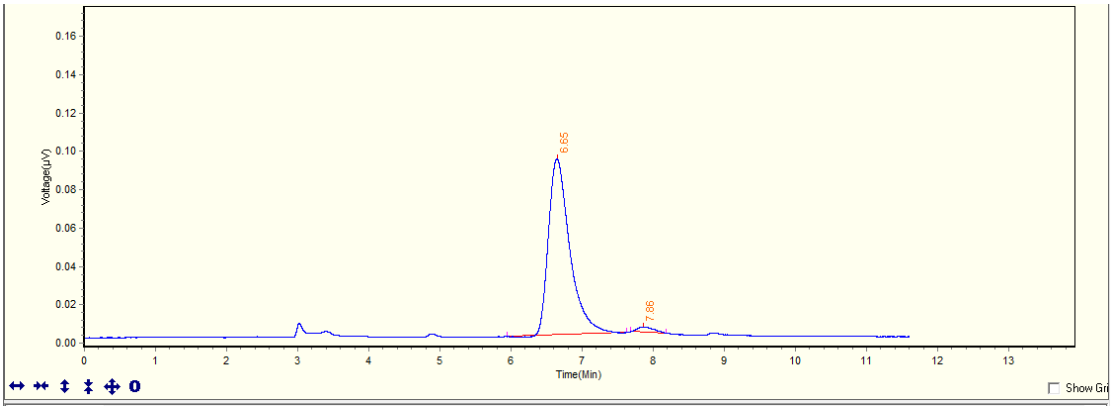
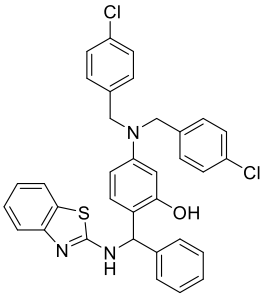


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.65	950675	45827	97.81%	1.68	BB
2	7.86	21326	1322	2.19%	0.5	BB
Total		972,001	47,149	100.00%		



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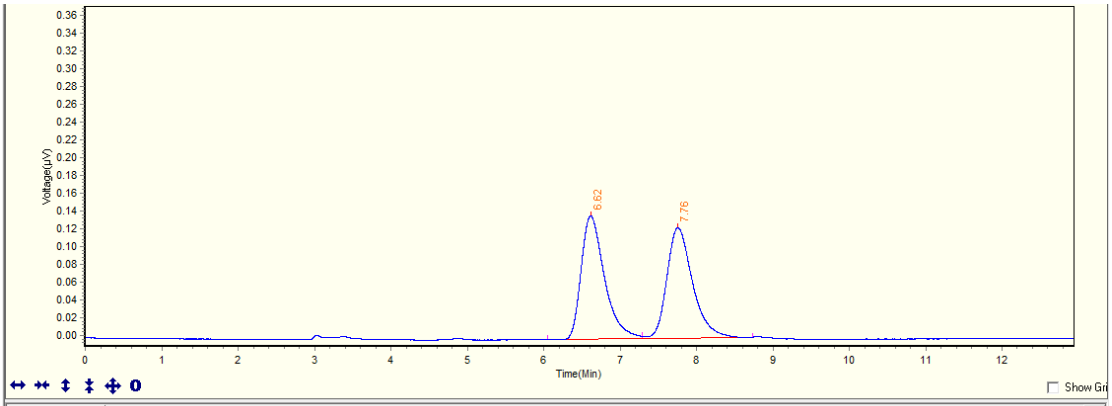
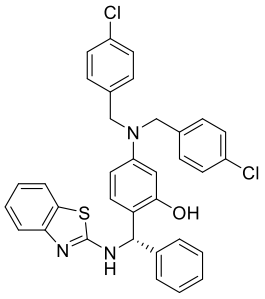


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.62	1469670	69163	50.45%	1.238	BV
2	7.76	1443394	61874	49.55%	1.444	VB
Total		2,913,064	131,037	100.00%		



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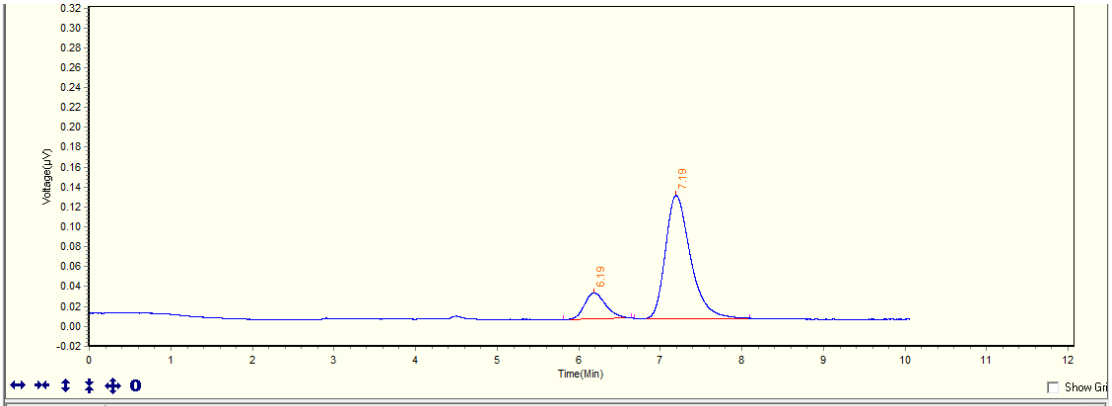
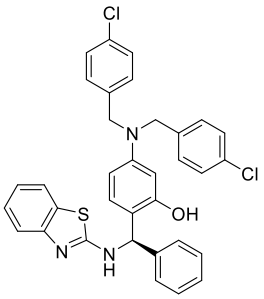


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.19	232778	13057	15.09%	0.833	BB
2	7.19	1309752	61683	84.91%	1.413	BB
Total		1,542,530	74,740	100.00%		



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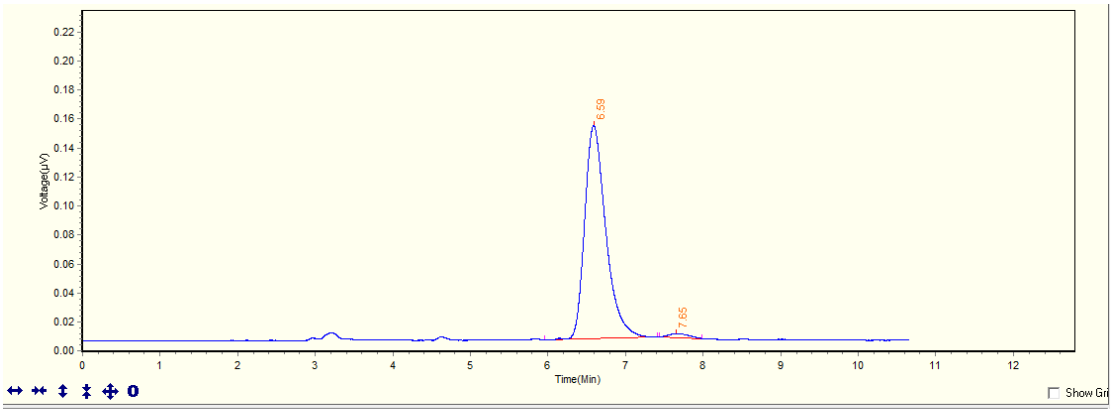
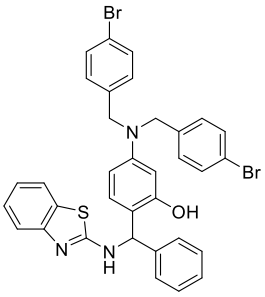


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.59	1388781	73424	98.18%	1.454	BB
2	7.65	25749	1381	1.82%	0.548	BB
Total		1,414,530	74,805	100.00%		



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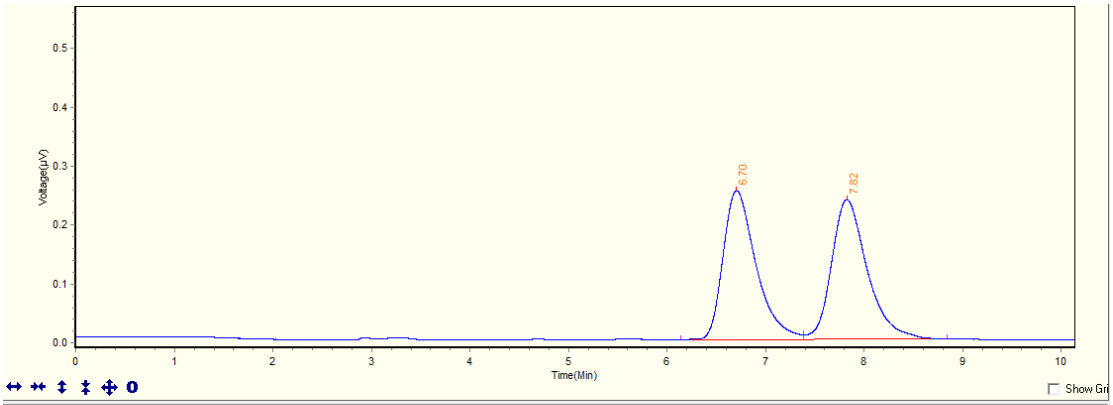
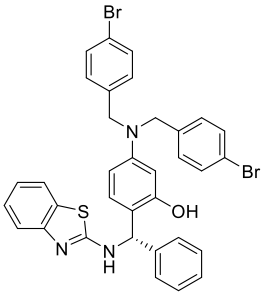


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.70	2945925	126551	49.66%	1.246	BV
2	7.82	2985672	118656	50.34%	1.456	VB
Total		5,931,597	245,207	100.00%		



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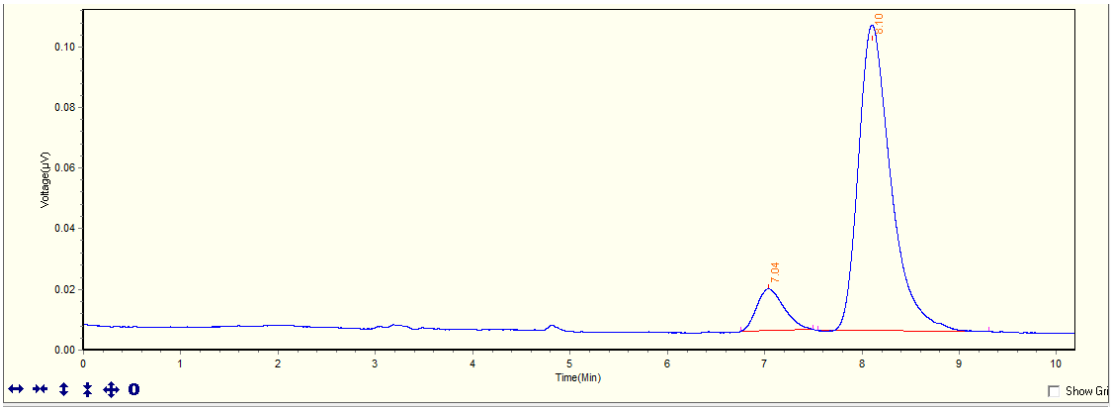
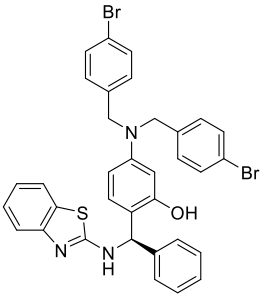


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.04	133584	6883	10.31%	0.744	BB
2	8.10	1161540	50392	89.69%	1.755	BB
Total		1,295,124	57,275	100.00%		



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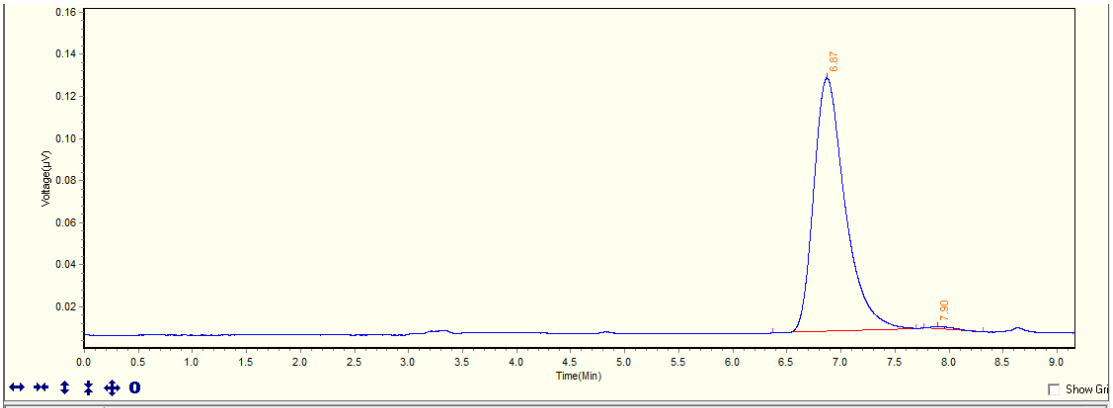
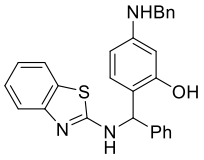


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	6.87	1210820	60197	99.27%	1.327	BB
2	7.90	8911	563	0.73%	0.547	BB
Total		1,219,731	60,760	100.00%		



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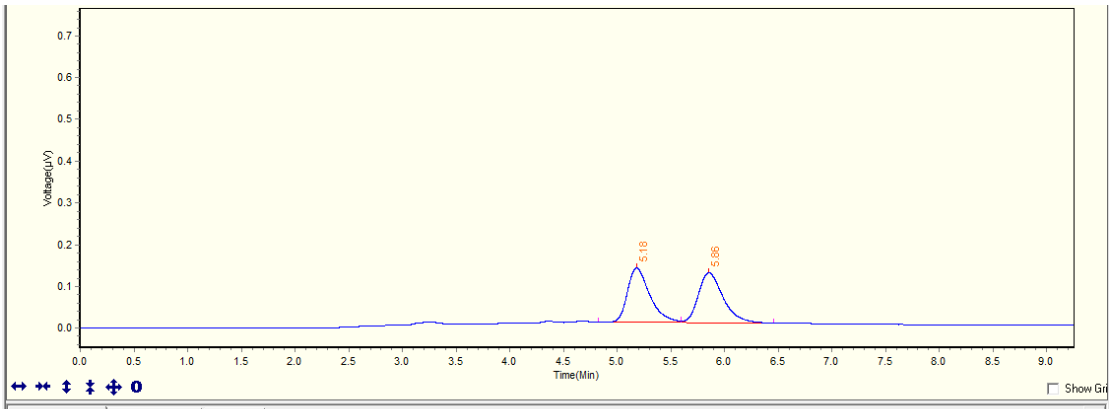
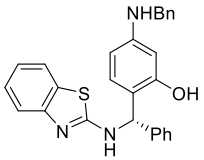


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	5.18	942687	65014	49.43%	0.771	BV
2	5.86	964464	59870	50.57%	0.862	VB
Total		1,907,151	124,884	100.00%		



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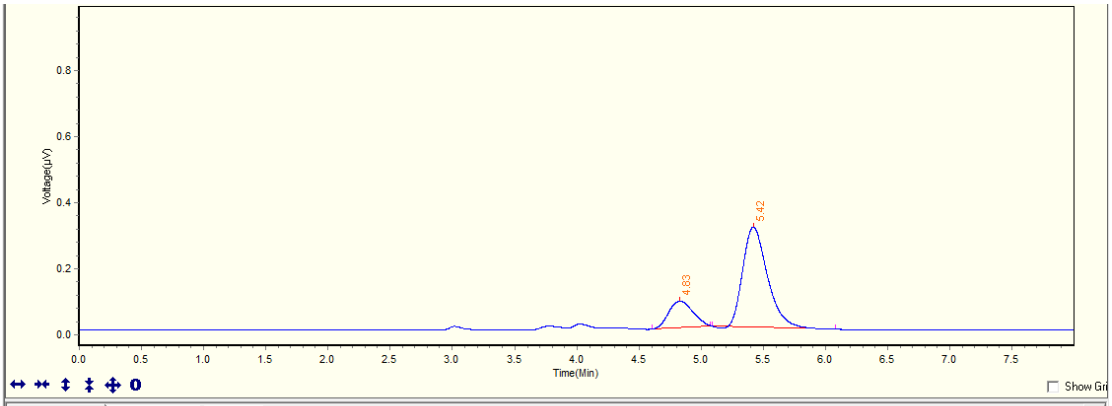
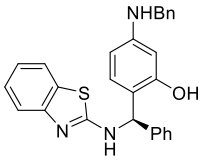


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	4.83	533209	39539	20.31%	0.468	BB
2	5.42	2092027	151667	79.69%	0.991	BB
Total		2,625,236	191,206	100.00%		



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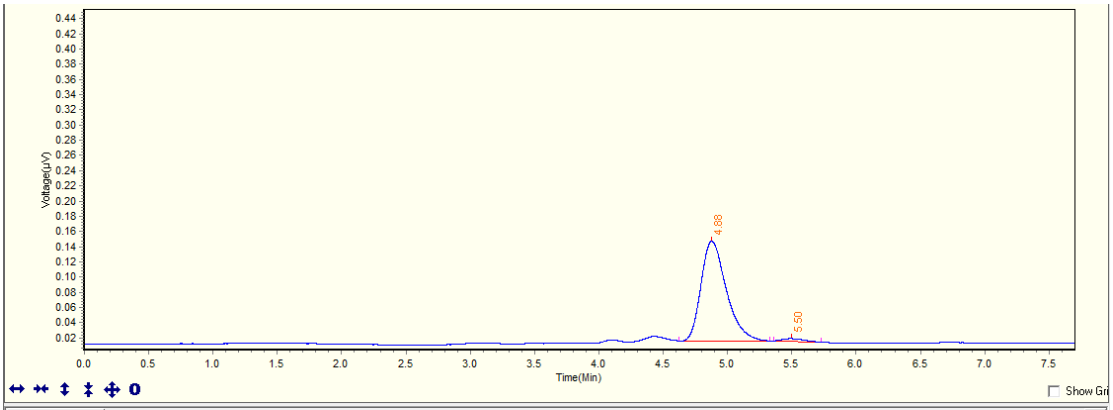
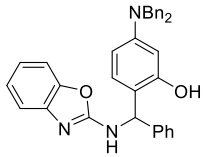


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	4.88	893905	65640	97.75%	0.707	BB
2	5.50	20586	1827	2.25%	0.369	BB
Total		914,491	67,467	100.00%		



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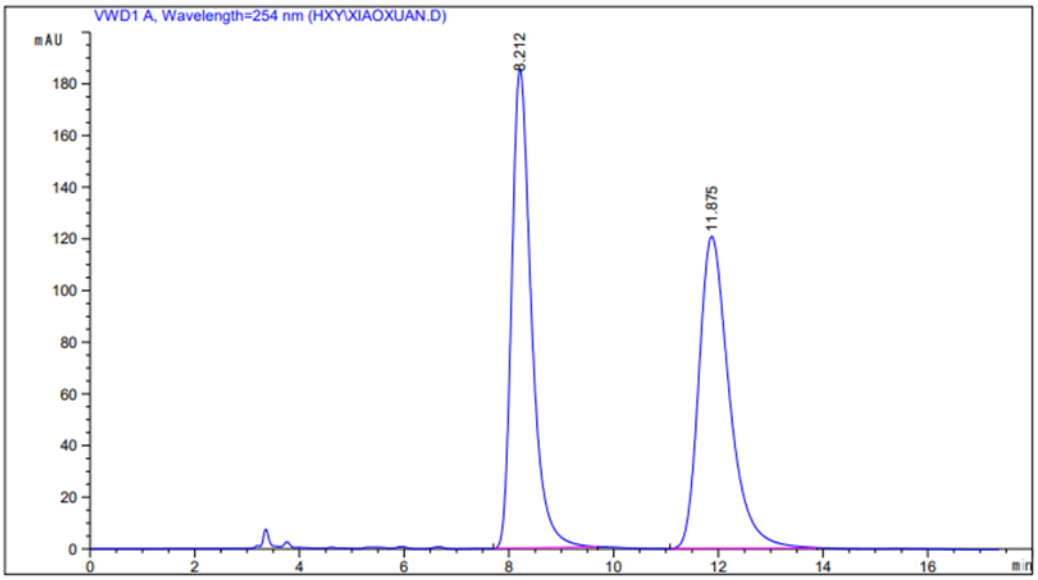
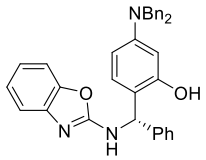


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.212	BB	0.3964	4842.37695	185.42378	49.8242
2	11.875	BB	0.6120	4876.53906	120.84646	50.1758
Totals :				9718.91602	306.27024	



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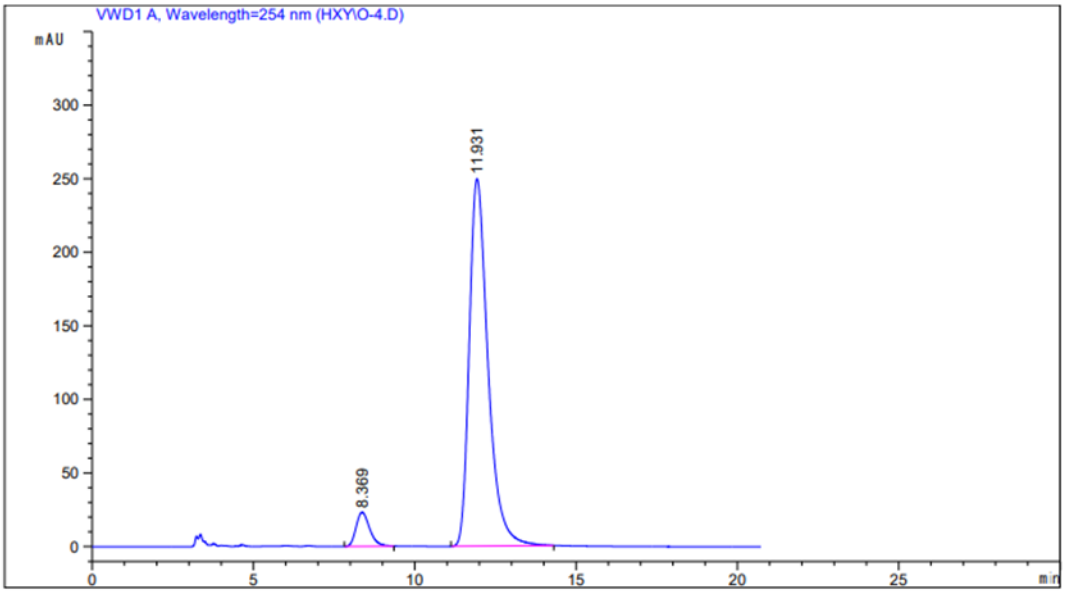
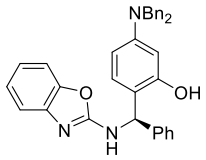


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.369	BB	0.4548	679.40326	23.13196	6.3273
2	11.931	BB	0.6128	1.00583e4	249.63490	93.6727
Totals :				1.07377e4	272.76686	



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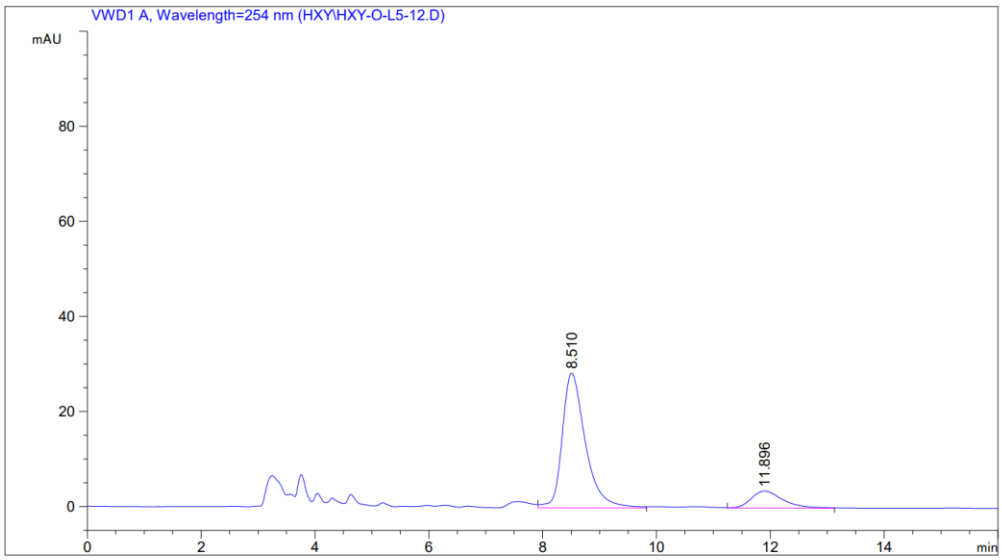
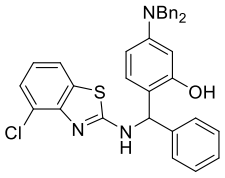


Peak #	RetTime [min]	Type	Width [min]	Area mAU *s	Height [mAU]	Area %
1	8.510	VB	0.4299	803.63519	28.33875	85.2110
2	11.896	VB	0.5937	139.47687	3.58478	14.7890
Totals :				943.11206	31.92353	



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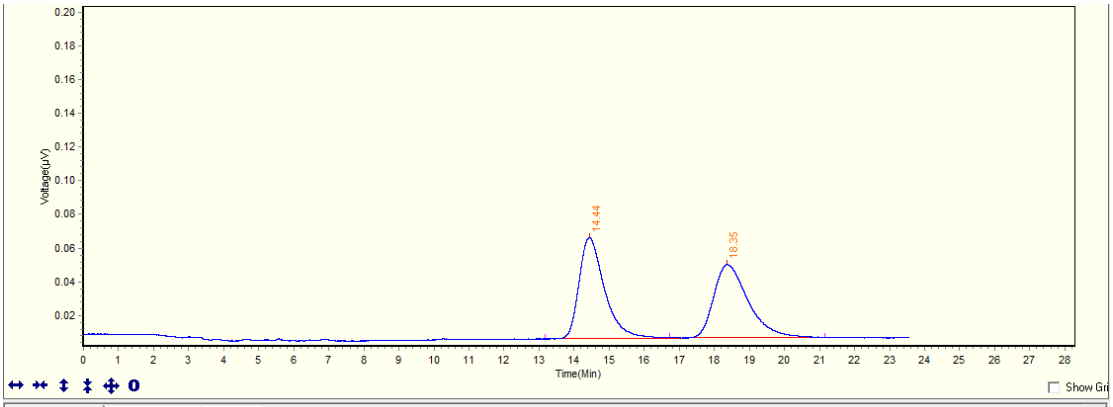
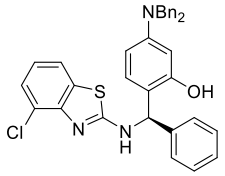


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	14.44	1515884	29973	50.52%	3.553	BV
2	18.35	1484627	21771	49.48%	4.427	VB
Total		3,000,511	51,744	100.00%		



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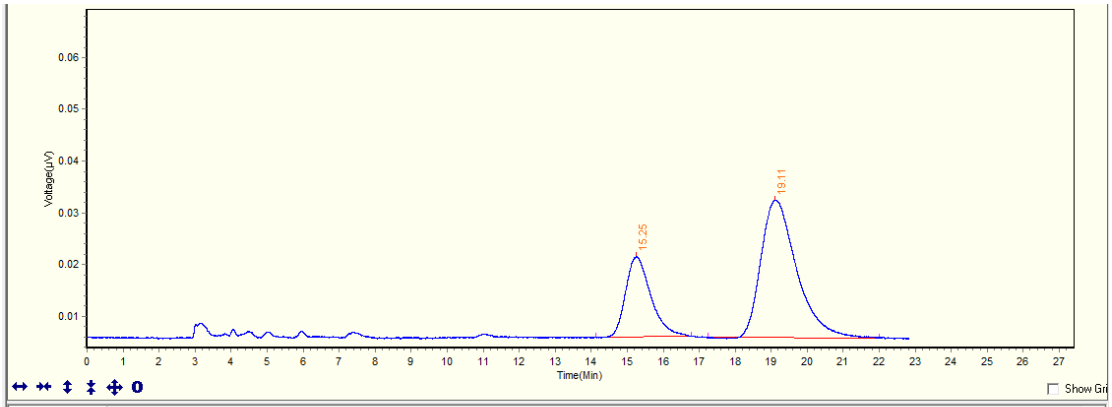
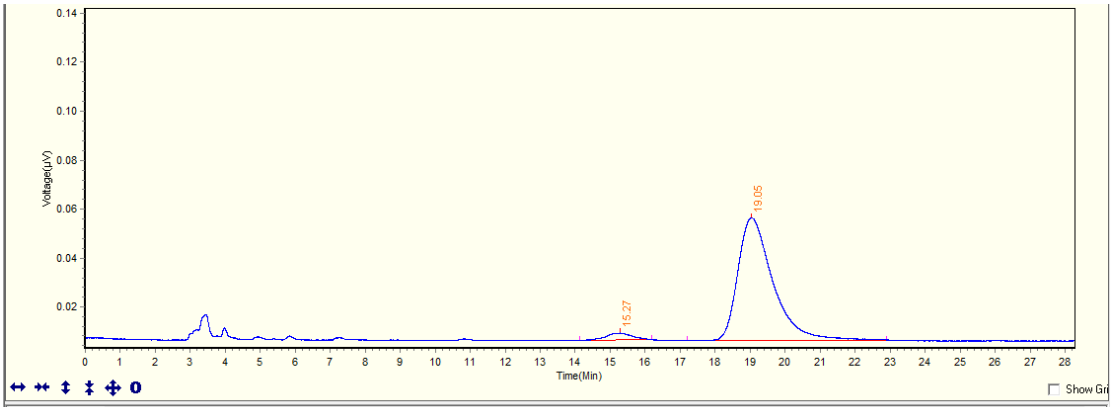


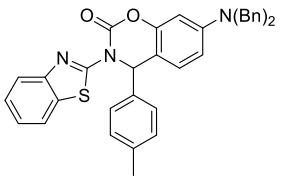
Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	15.25	373949	7718	29.14%	2.651	BB
2	19.11	909442	13249	70.86%	4.755	BB
Total		1,283,391	20,967	100.00%		



Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	15.27	71636	1397	3.97%	2.046	BB
2	19.05	1734616	25017	96.03%	5.701	BB
Total		1,806,252	26,414	100.00%		



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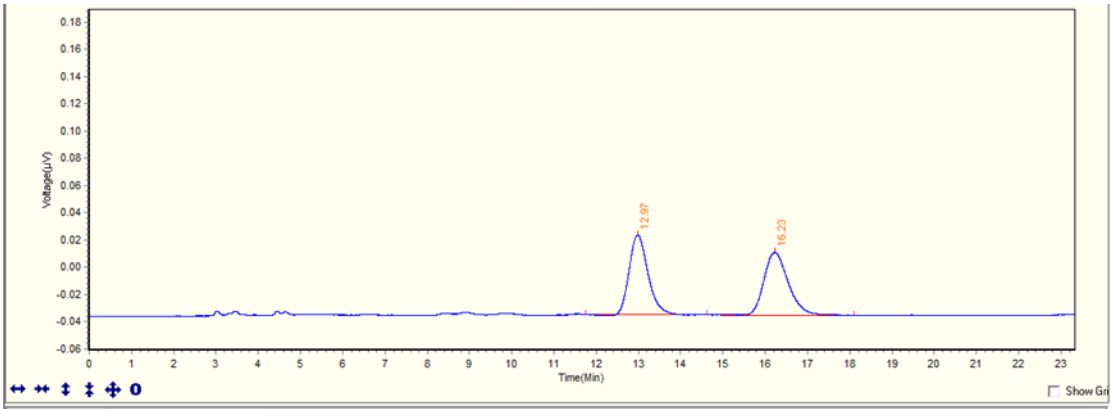
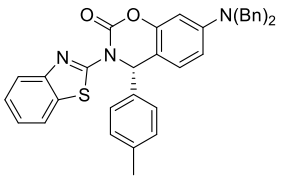


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.97	885721	29192	49.27%	2.872	BV
2	16.23	911913	22975	50.73%	3.479	VB
Total		1,797,634	52,167	100.00%		



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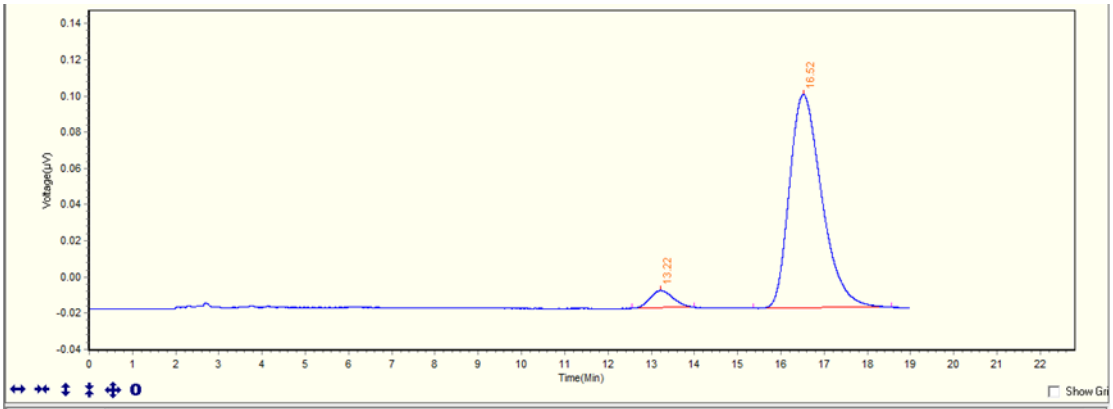
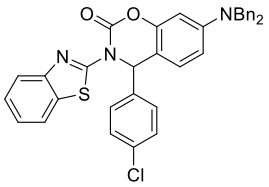


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	13.22	177271	4838	5.46%	1.438	BB
2	16.52	3067973	58924	94.54%	3.196	BB
Total		3,245,244	63,762	100.00%		



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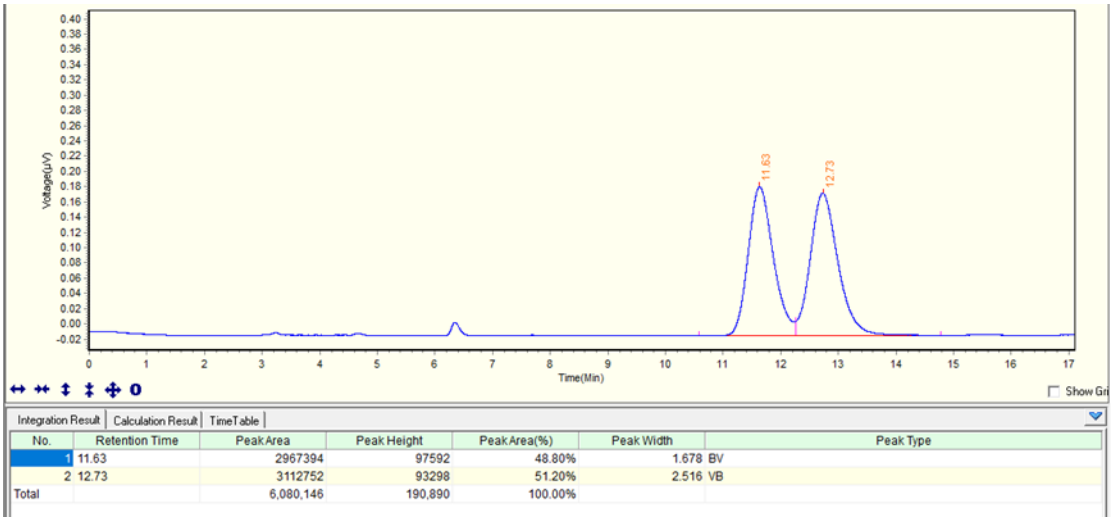
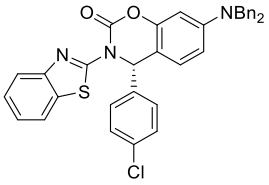


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.63	2967394	97592	48.80%	1.678	BV
2	12.73	3112752	93298	51.20%	2.516	VB
Total		6,080,146	190,890	100.00%		



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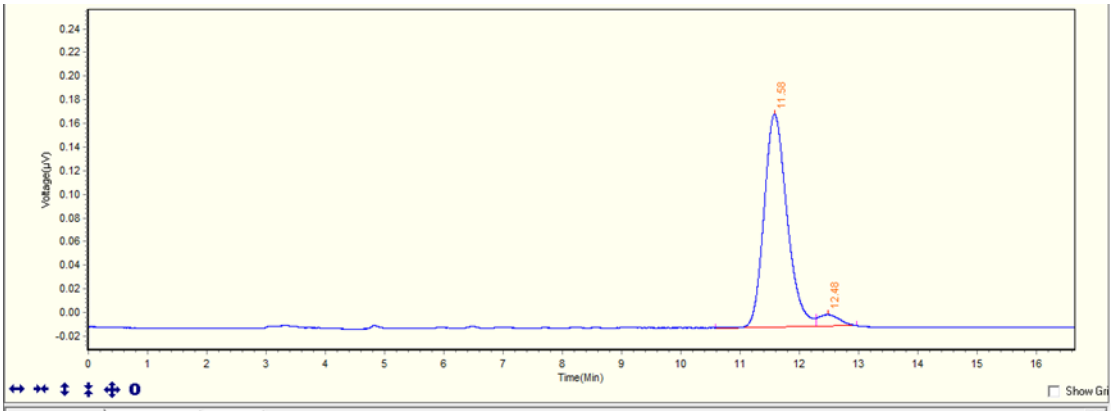
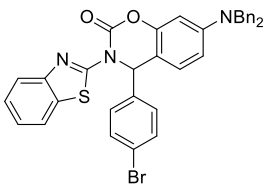


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.58	2426739	90047	95.45%	1.701	BV
2	12.48	115708	4771	4.55%	0.682	VB
Total		2,542,447	94,818	100.00%		



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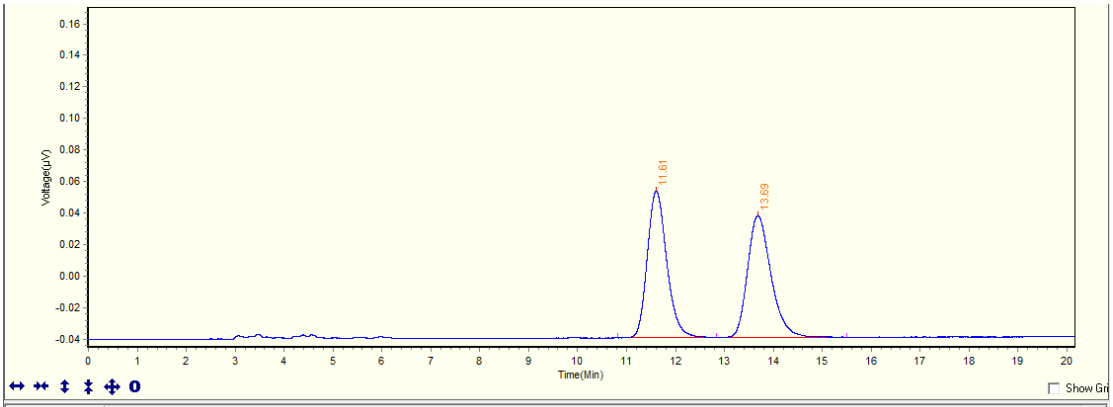
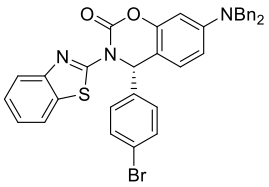


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.61	1286169	46532	50.06%	2.018	BV
2	13.69	1283280	38579	49.94%	2.663	VB
Total		2,569,449	85,111	100.00%		



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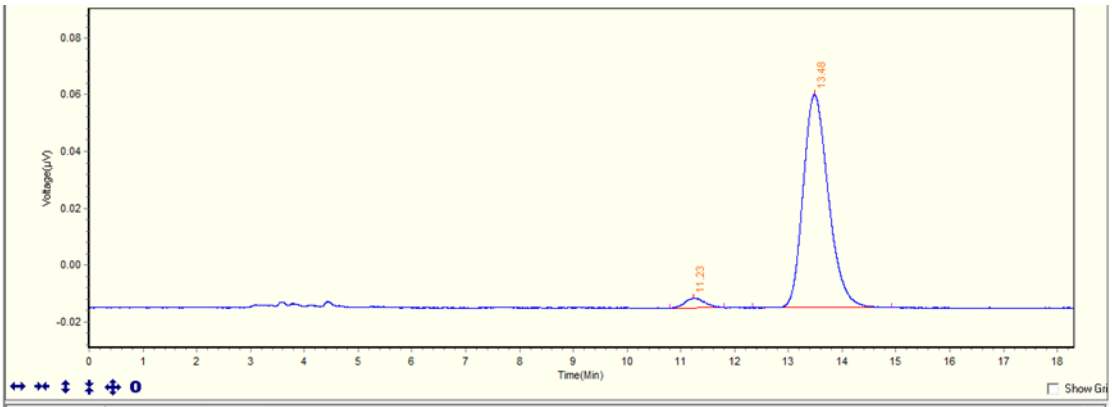
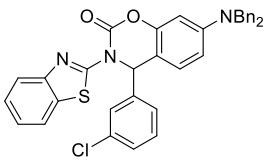


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	11.23	43320	1704	3.43%	1.008	BB
2	13.48	1220987	37431	96.57%	2.584	BB
Total		1,264,307	39,135	100.00%		



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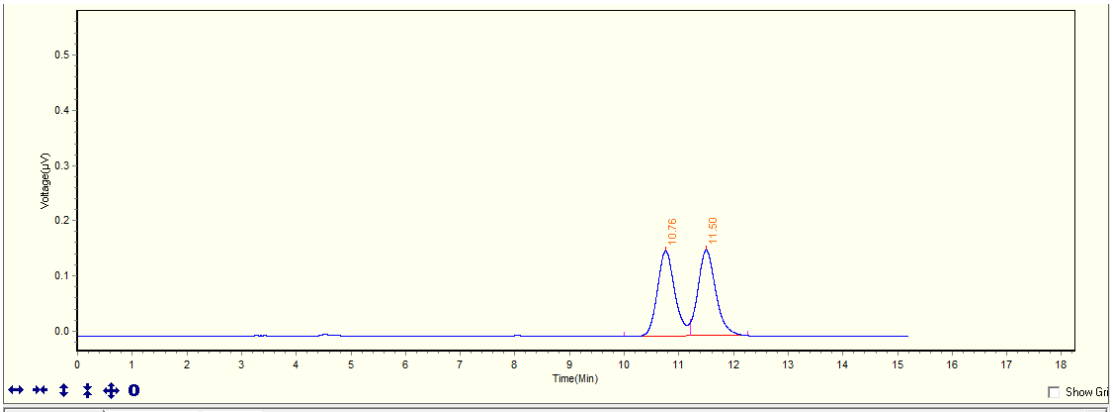
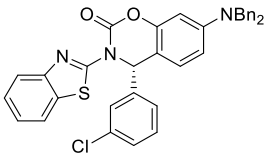


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.76	1716952	77140	49.52%	1.211	BV
2	11.50	1750051	77707	50.48%	1.049	VB
Total		3,467,003	154,847	100.00%		



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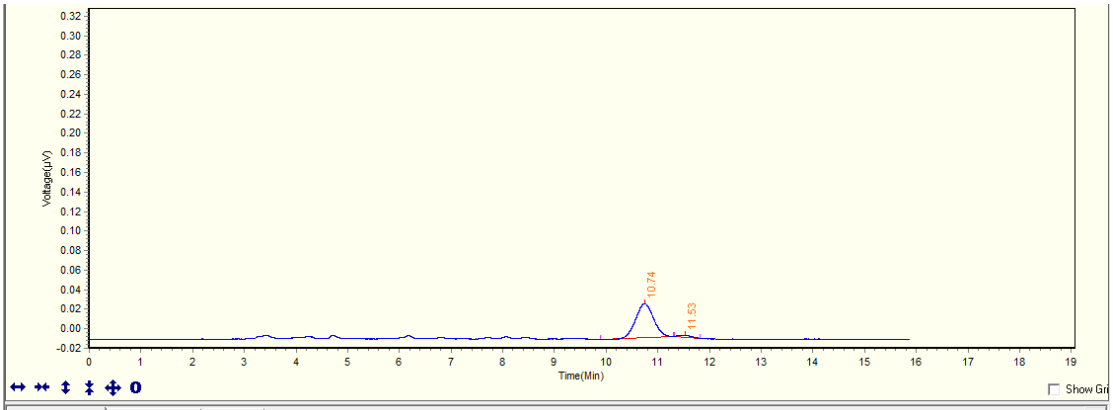
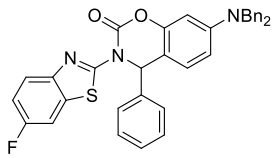


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	10.74	407657	17283	96.63%	1.413	BB
2	11.53	14234	1001	3.37%	0.496	BB
Total		421,891	18,284	100.00%		



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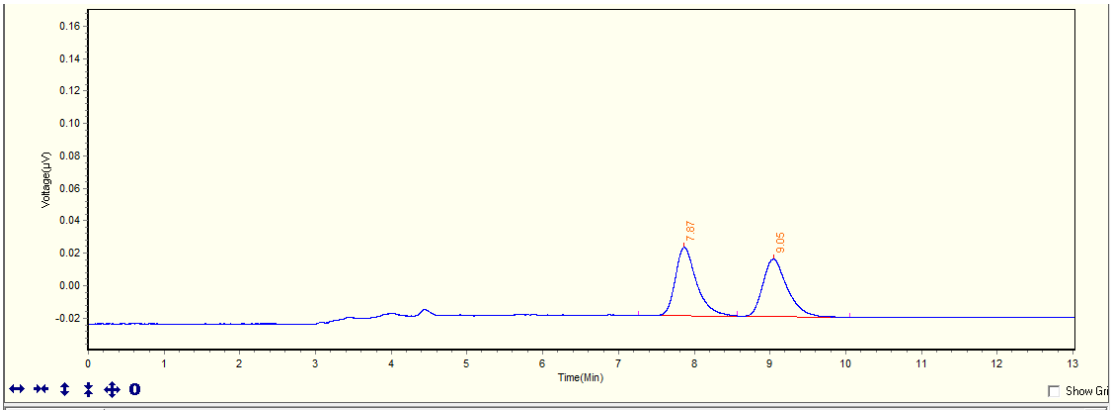
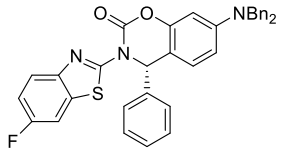


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.87	411820	21157	50.84%	1.304	BV
2	9.05	398182	17732	49.16%	1.486	VB
Total		810,002	38,889	100.00%		



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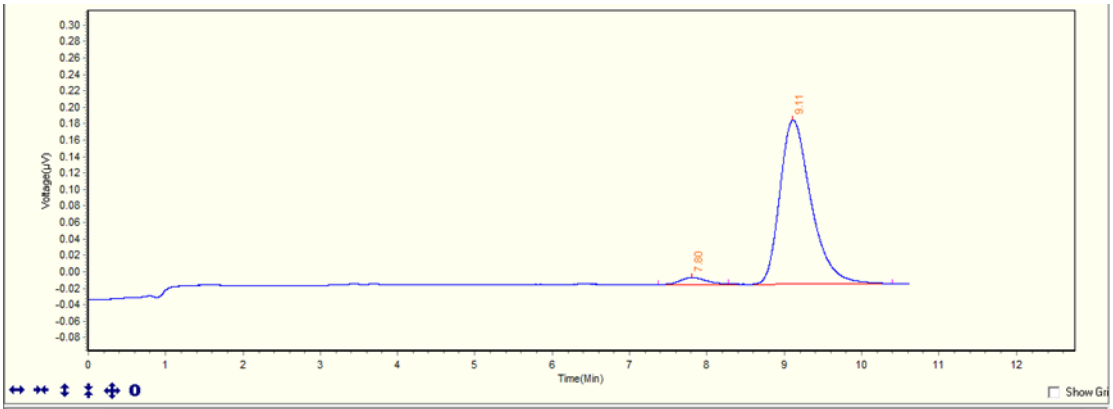
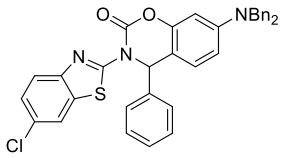


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.80	92051	4072	3.20%	0.906	BV
2	9.11	2782354	99538	96.80%	2.12	VB
Total		2,874,405	103,610	100.00%		



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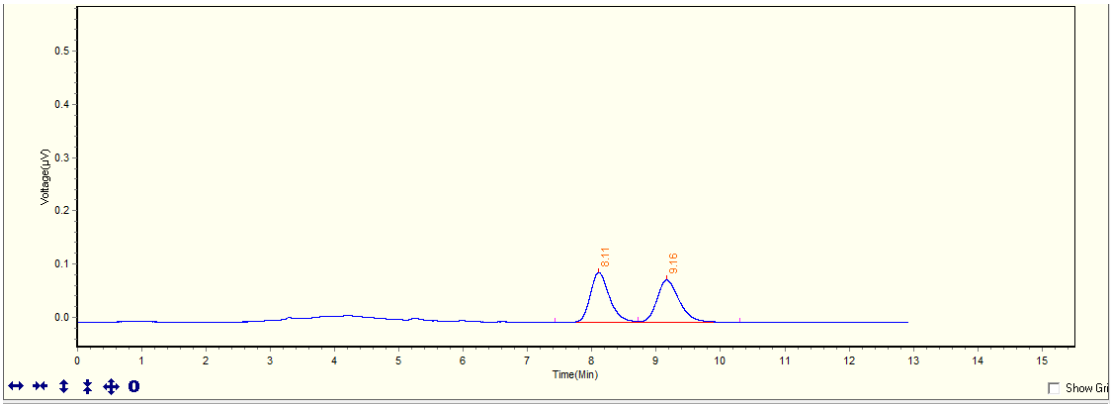
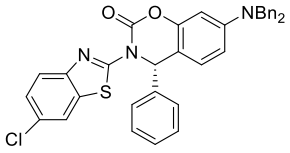


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	8.11	957053	46669	50.07%	1.291	BV
2	9.16	954479	39700	49.93%	1.583	VB
Total		1,911,532	86,369	100.00%		



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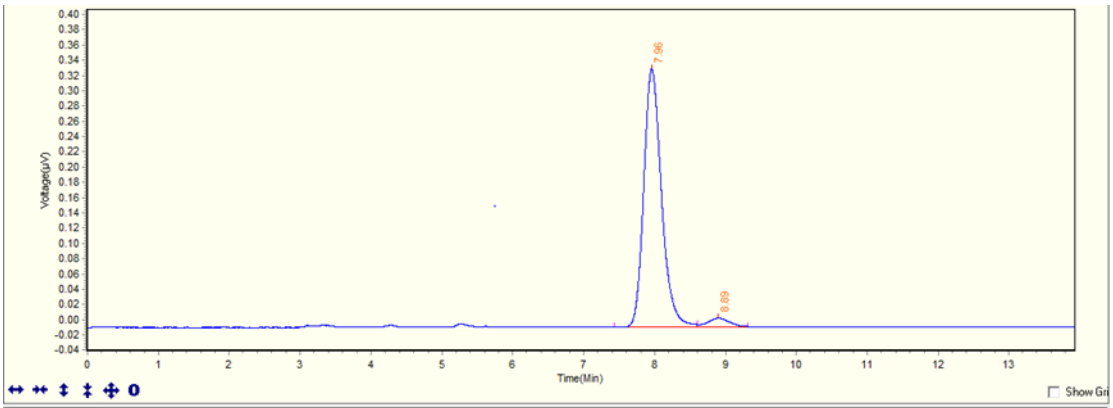
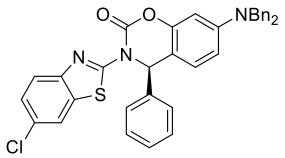


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.96	2927673	168997	96.23%	1.171	BV
2	8.89	114549	5524	3.77%	0.71	VB
Total		3,042,222	174,521	100.00%		



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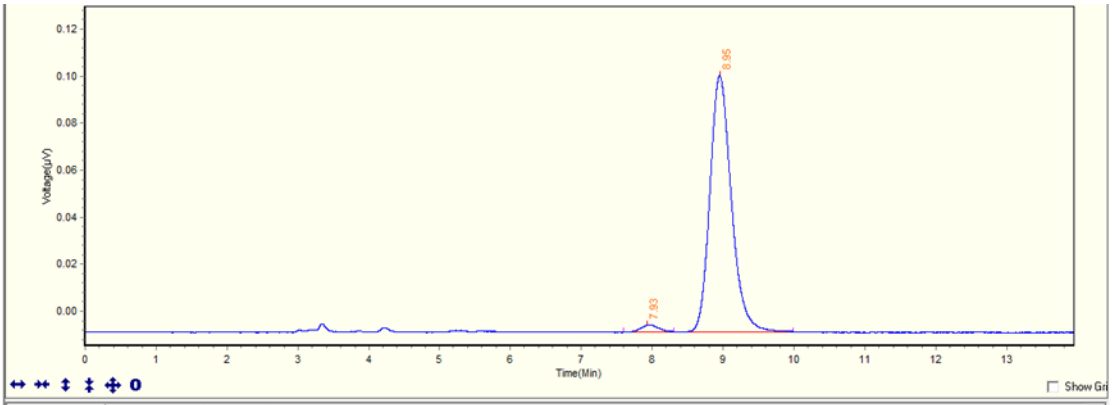
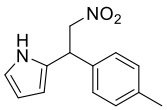


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	7.93	26687	1530	2.28%	0.708	BV
2	8.95	1144065	54439	97.72%	1.683	VB
Total		1,170,752	55,969	100.00%		



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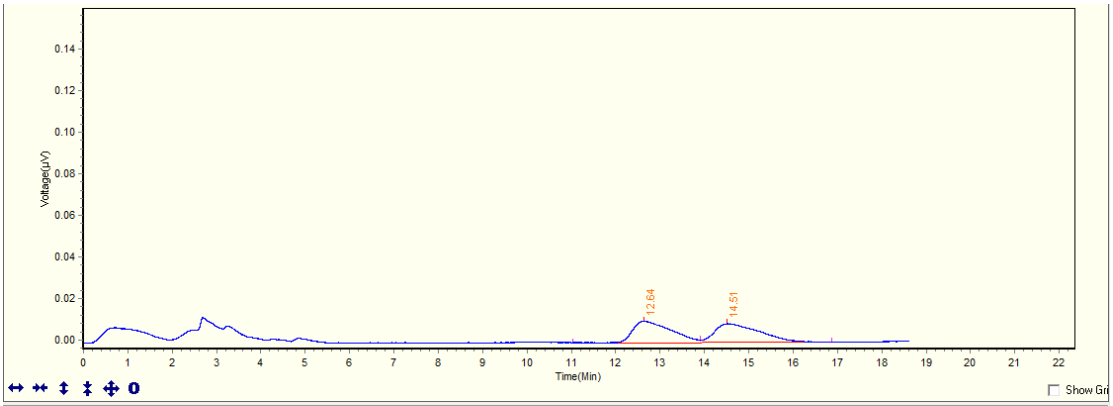
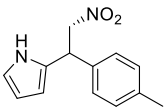
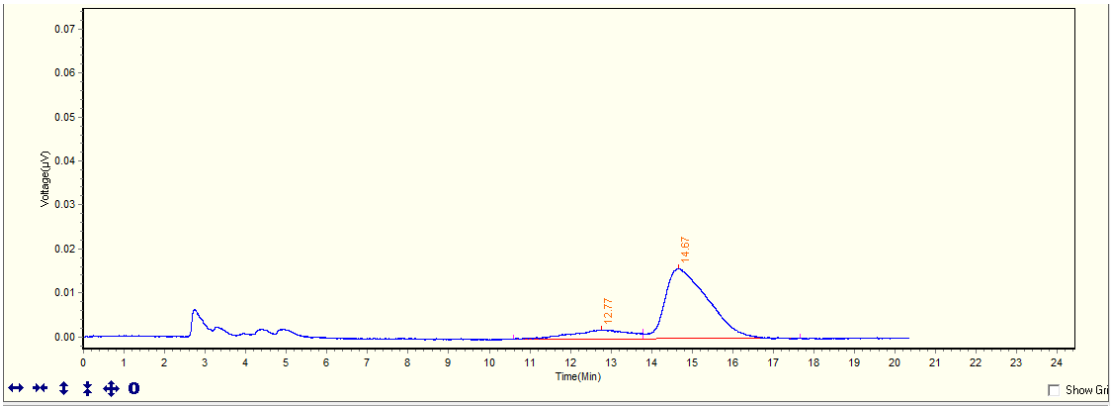


Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.64	300818	5164	49.26%	2.875	BV
2	14.51	309845	4478	50.74%	2.963	VB
Total		610,663	9,642	100.00%		

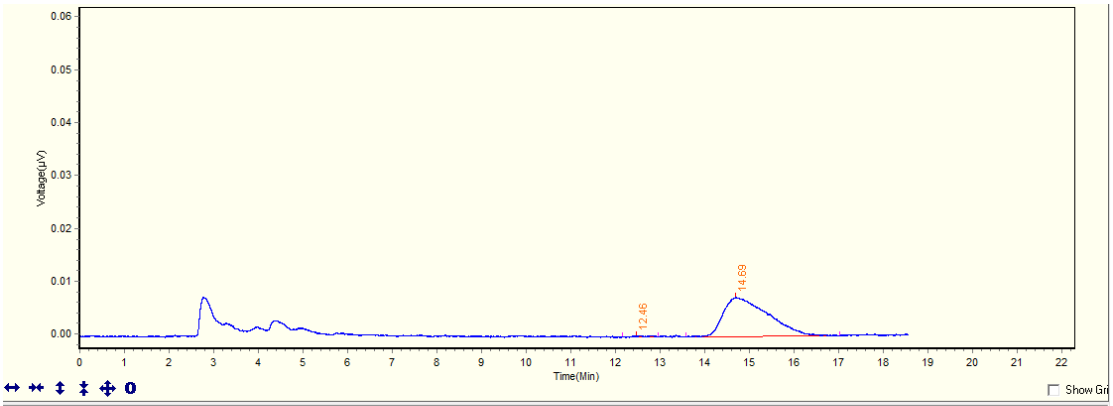


(*S*)-7



Integration Result | Calculation Result | TimeTable

No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.77	100661	1038	14.62%	3.19	BV
2	14.67	587673	7970	85.38%	3.873	VB
Total		688,334	9,008	100.00%		

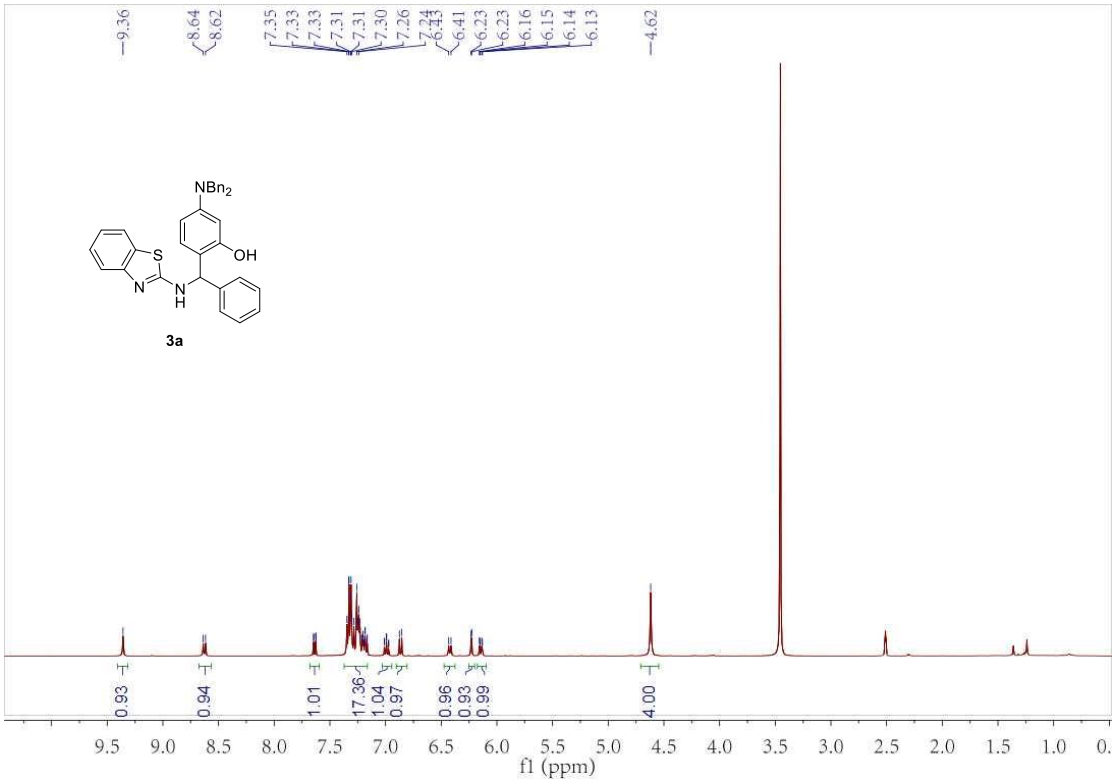


Integration Result | Calculation Result | TimeTable

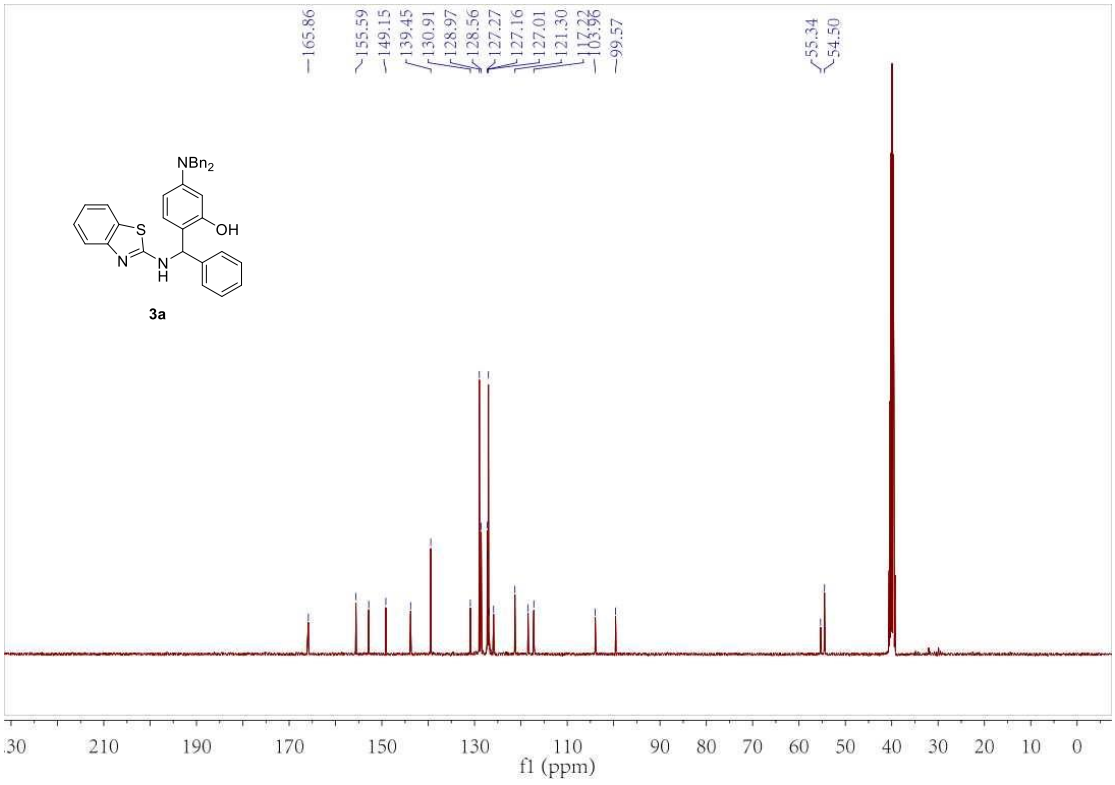
No.	Retention Time	Peak Area	Peak Height	Peak Area(%)	Peak Width	Peak Type
1	12.46	1339	105	0.52%	0.786	BB
2	14.69	255335	3681	99.48%	3.433	BB
Total		256,674	3,786	100.00%		

10. NMR Spectra

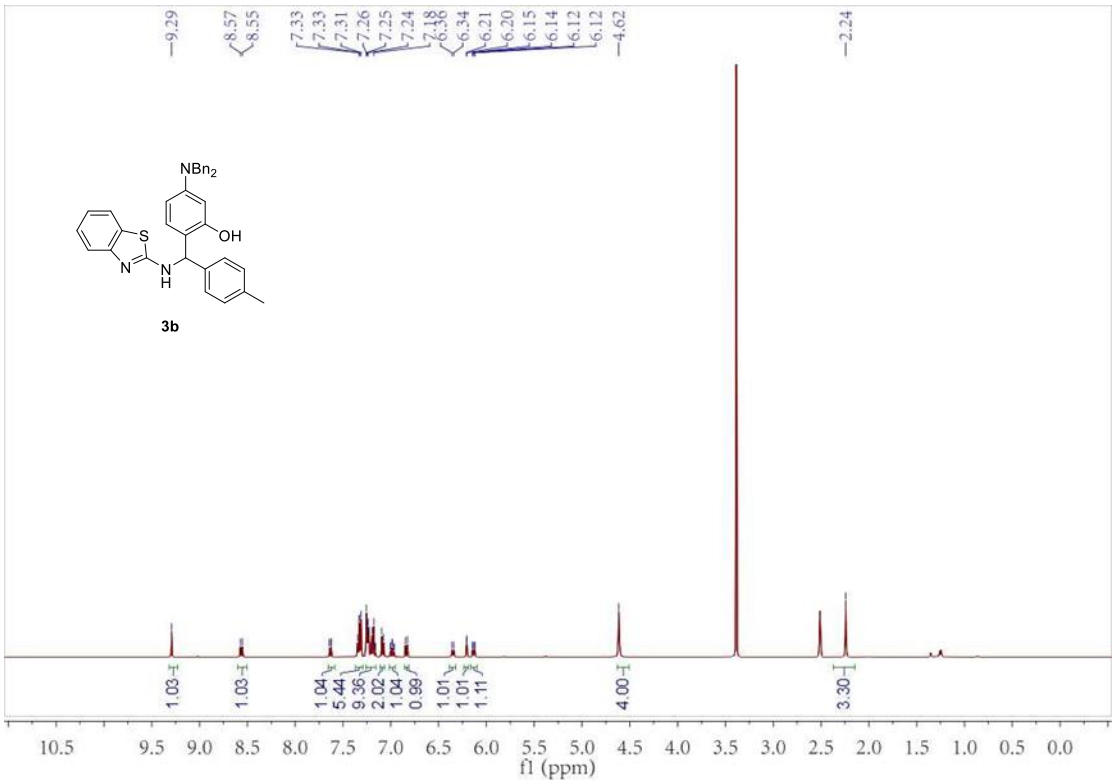
^{1}H NMR spectrum of compound **3a** (DMSO, 400 MHz)



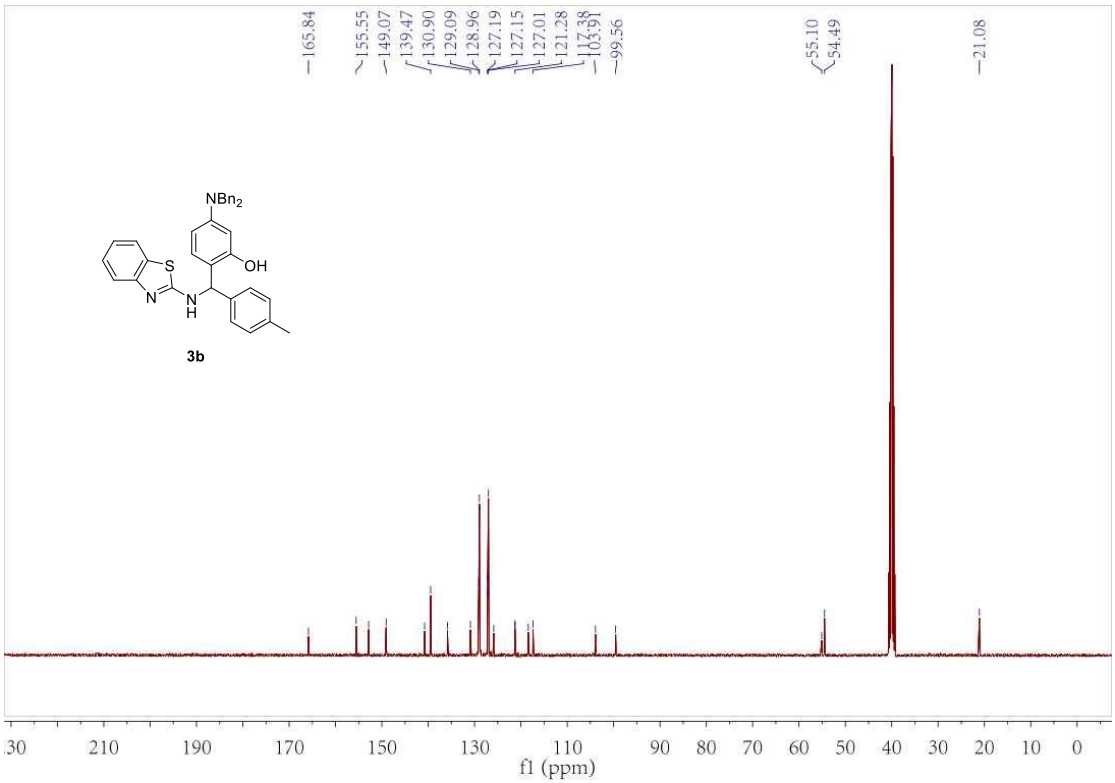
^{13}C NMR spectrum of compound **3a** (DMSO, 100 MHz)



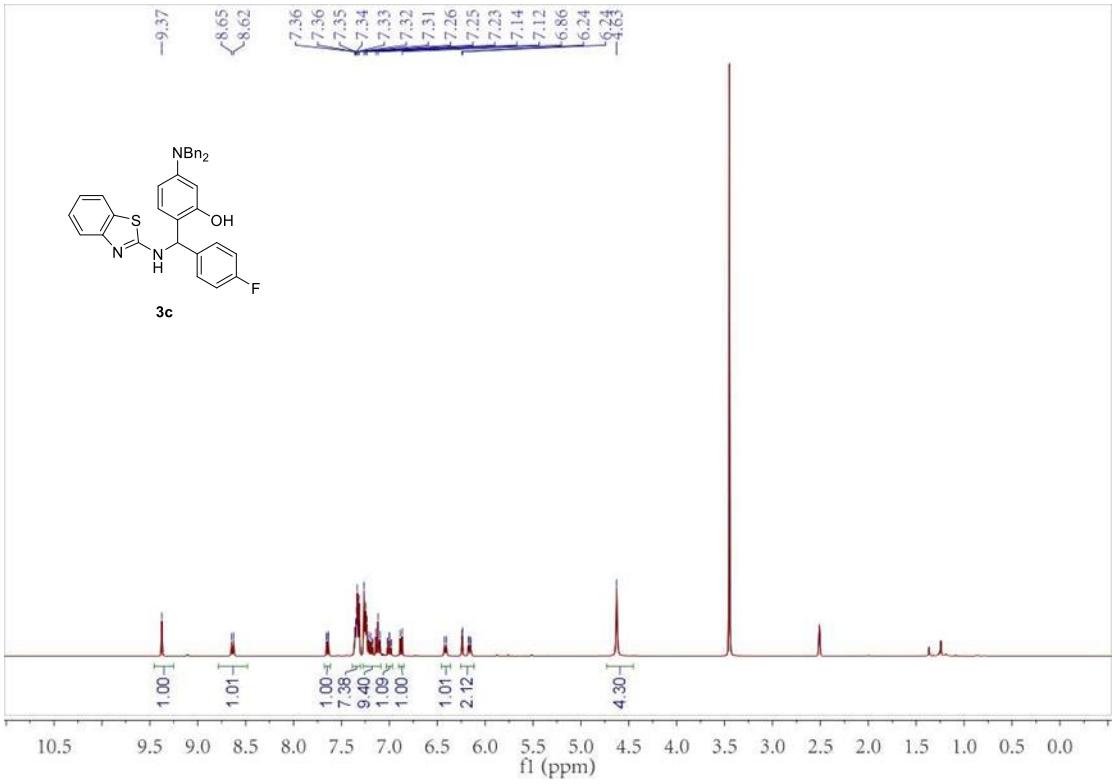
^{1}H NMR spectrum of compound **3b** (DMSO, 400 MHz)



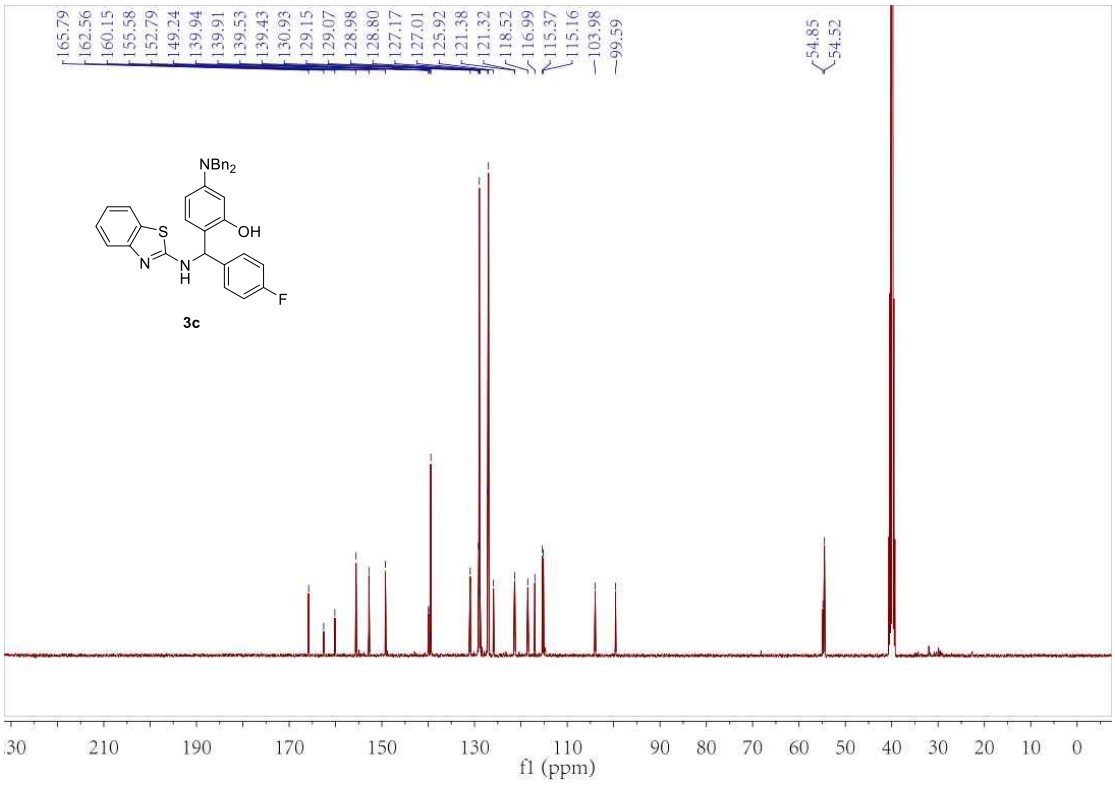
^{13}C NMR spectrum of compound **3b** (DMSO, 100 MHz)



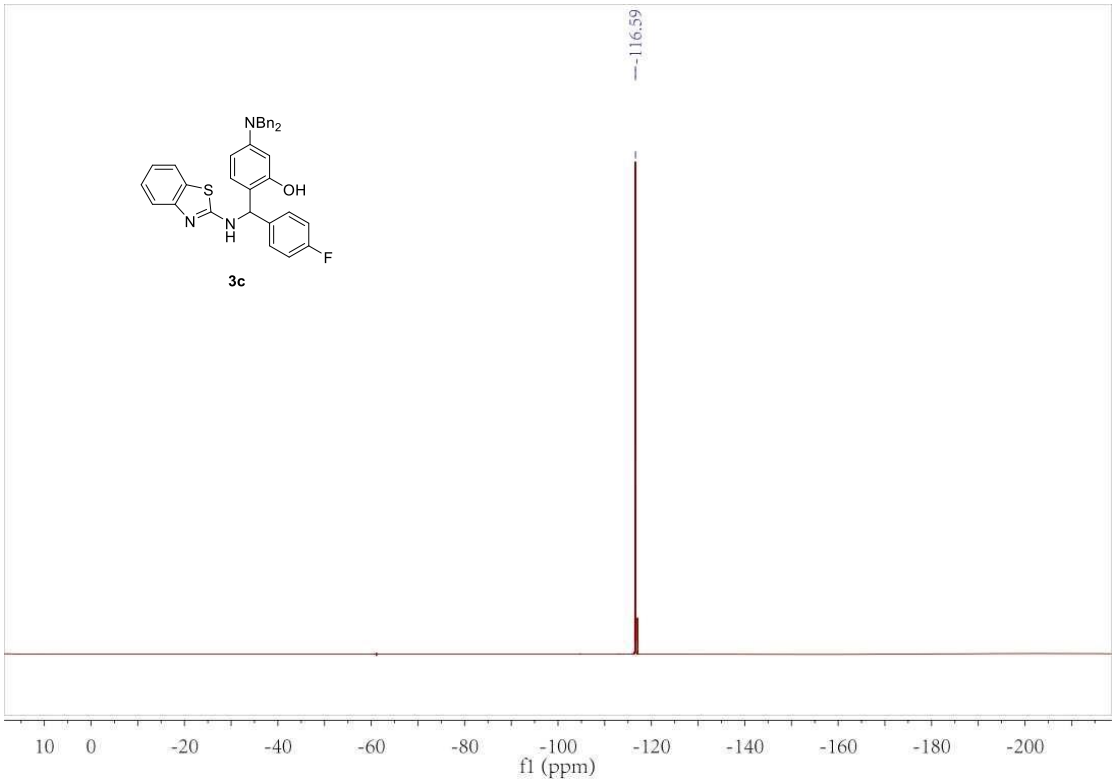
^{1}H NMR spectrum of compound **3c** (DMSO, 400 MHz)



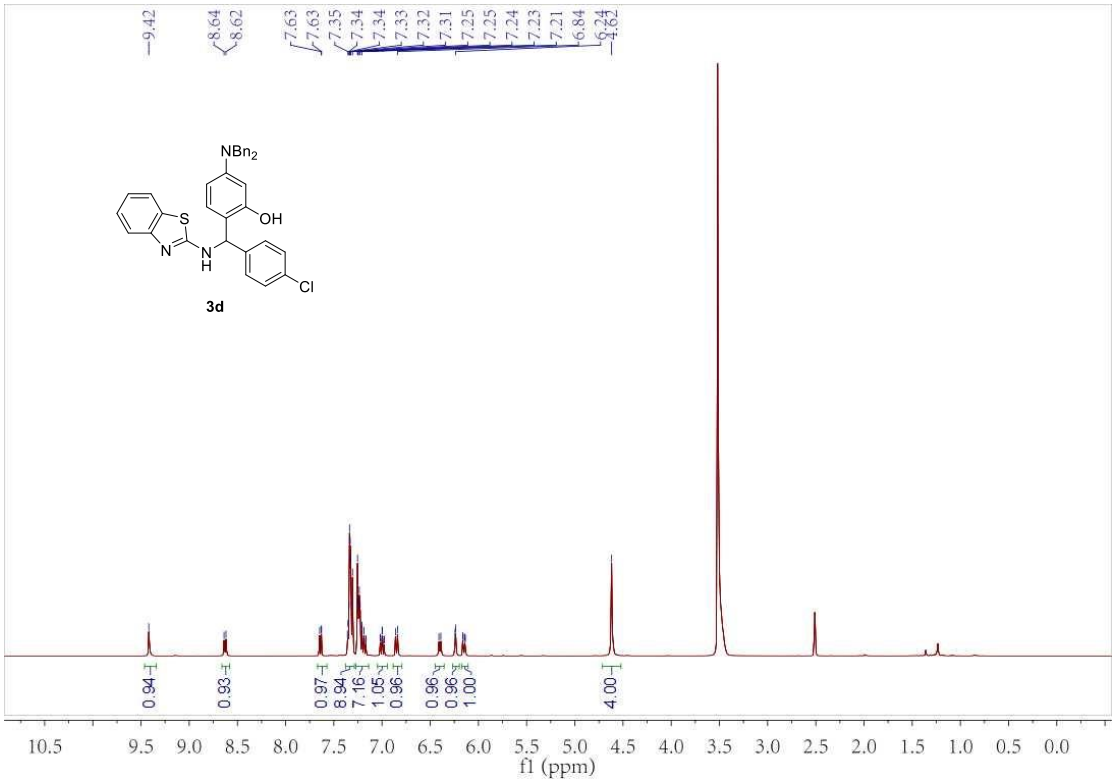
^{13}C NMR spectrum of compound **3c** (DMSO, 100 MHz)



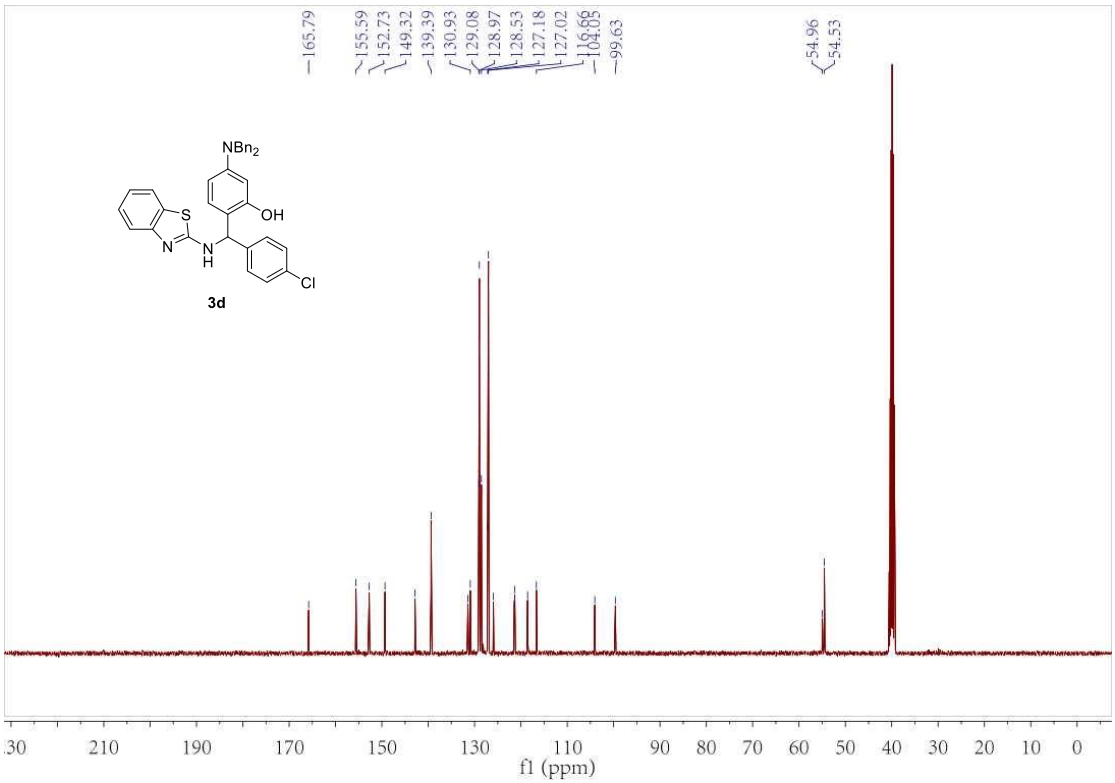
^{19}F NMR spectrum of compound **3c** (DMSO, 376 MHz)



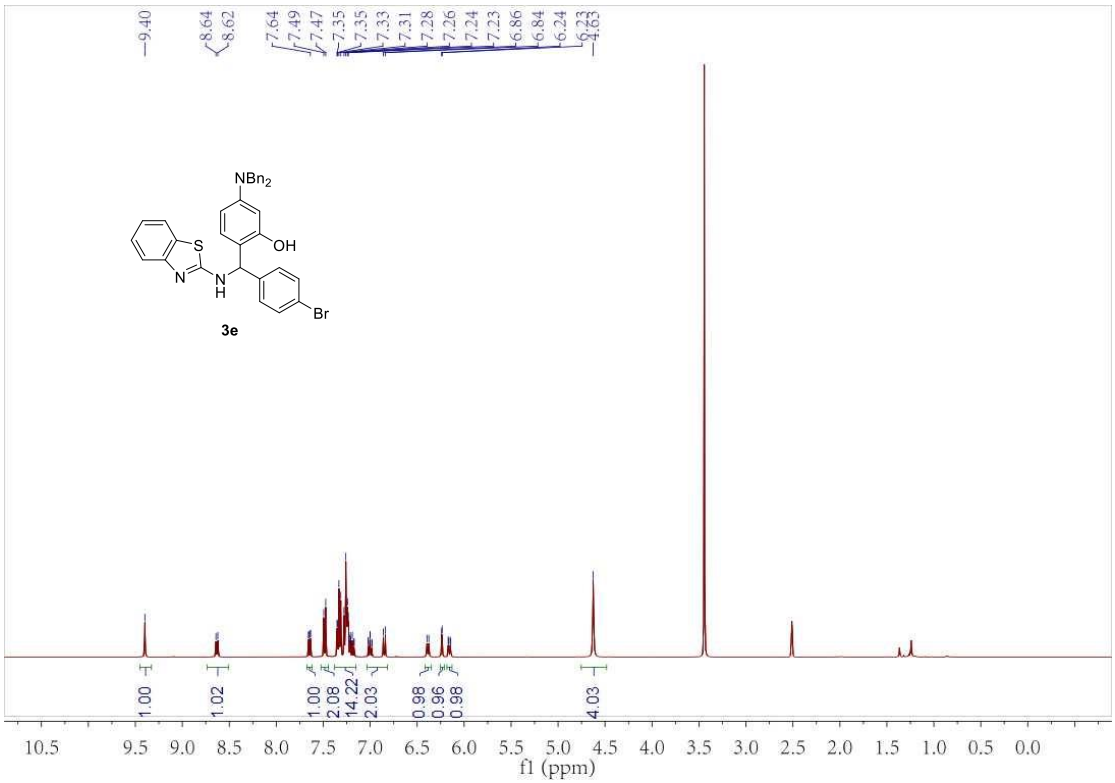
^{1}H NMR spectrum of compound **3d** (DMSO, 400 MHz)



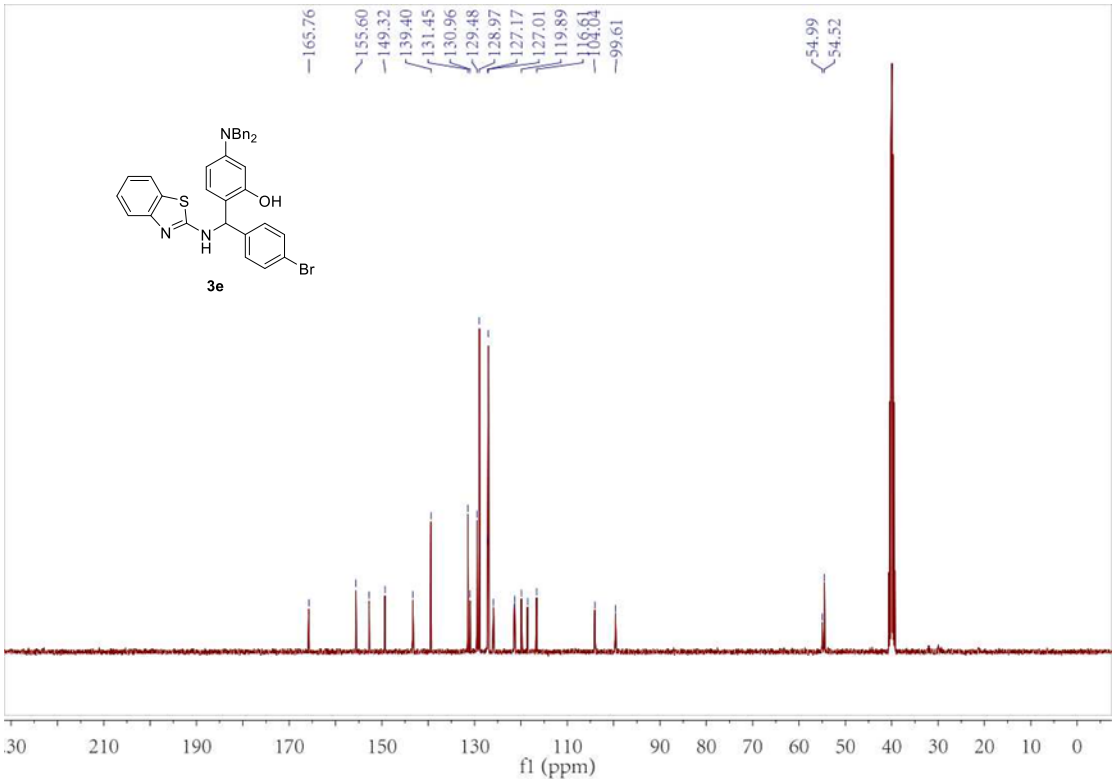
^{13}C NMR spectrum of compound **3d** (DMSO, 100 MHz)



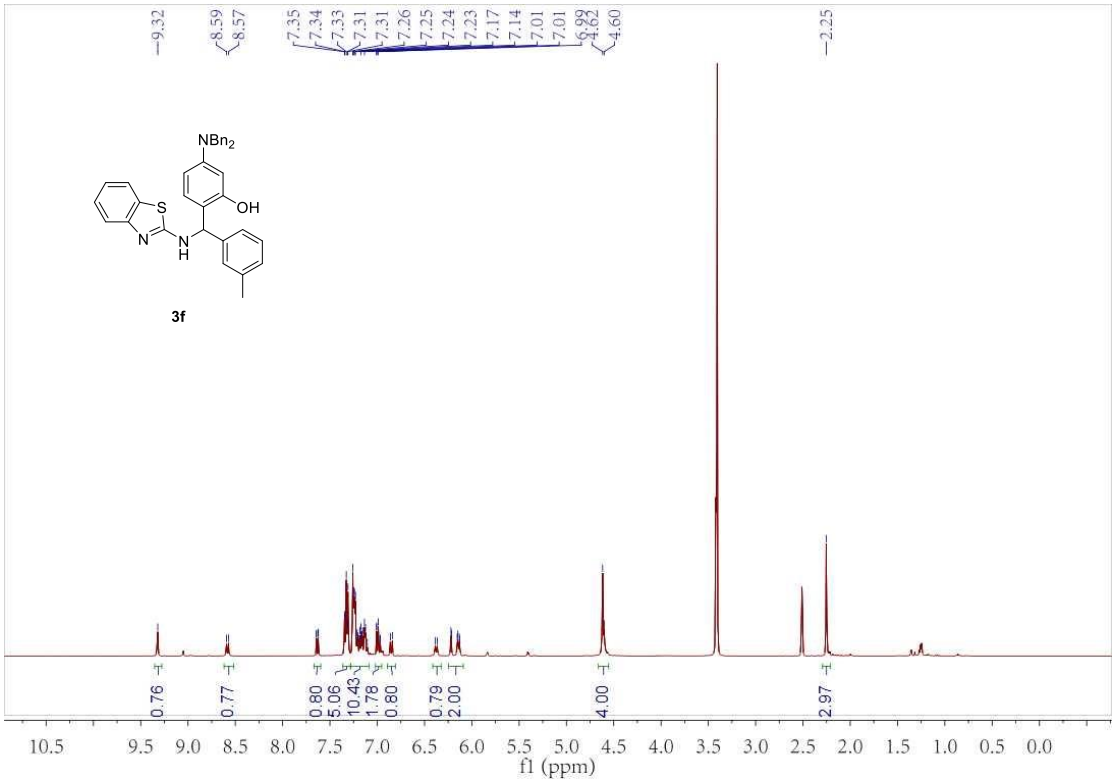
^{1}H NMR spectrum of compound **3e** (DMSO, 400 MHz)



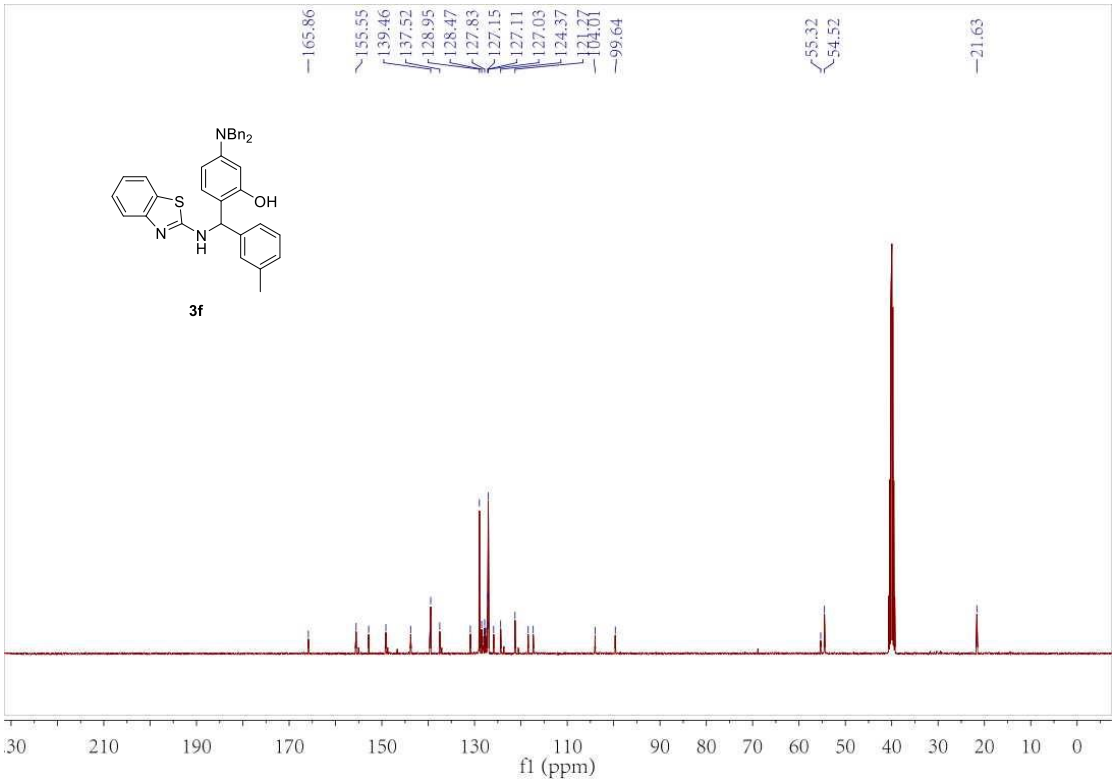
^{13}C NMR spectrum of compound **3e** (DMSO, 100 MHz)



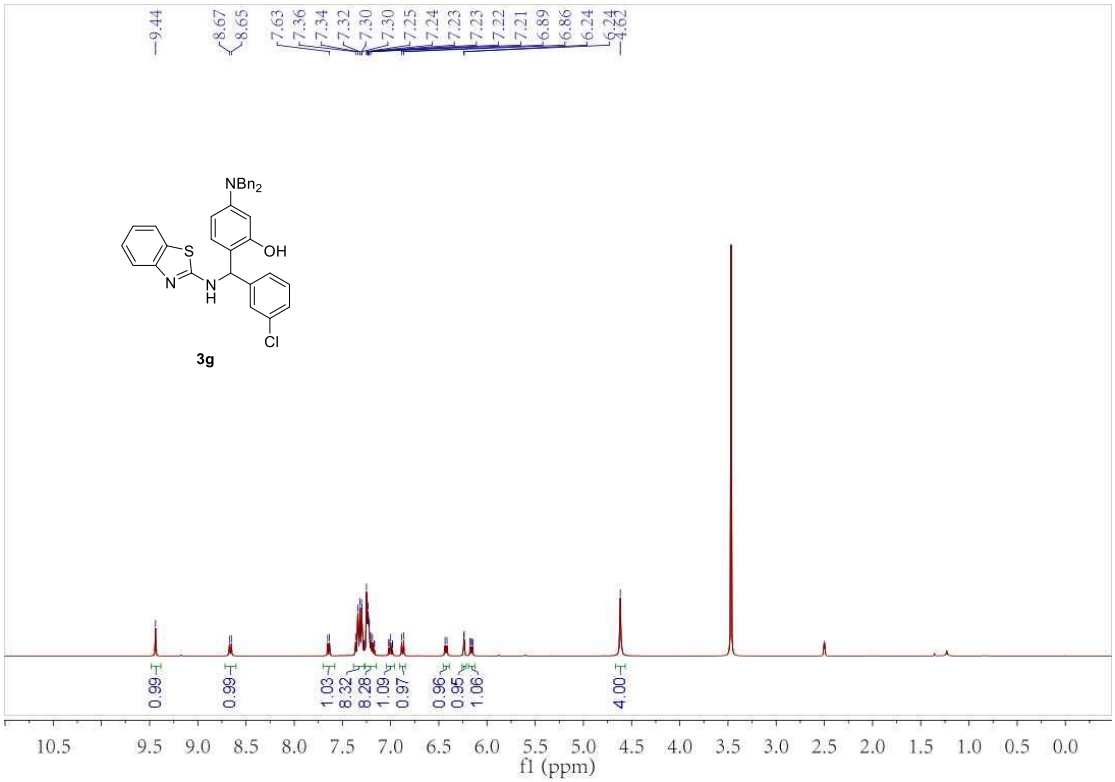
^{1}H NMR spectrum of compound **3f** (DMSO, 400 MHz)



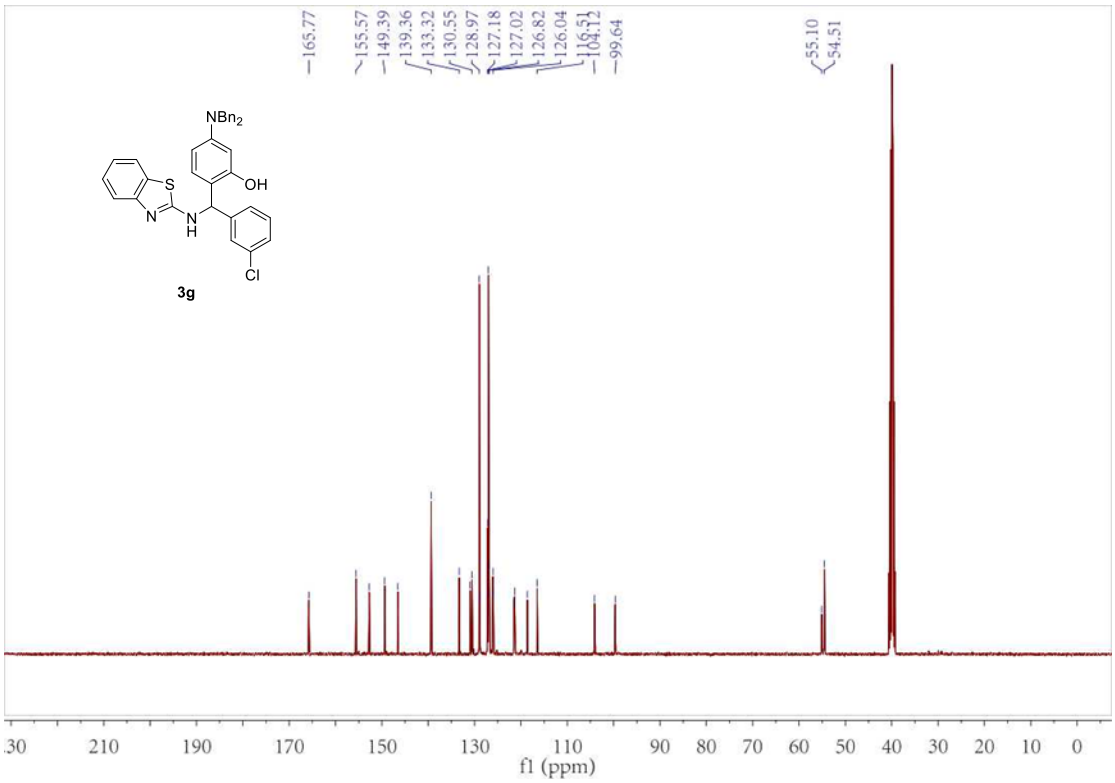
^{13}C NMR spectrum of compound **3f** (DMSO, 100 MHz)



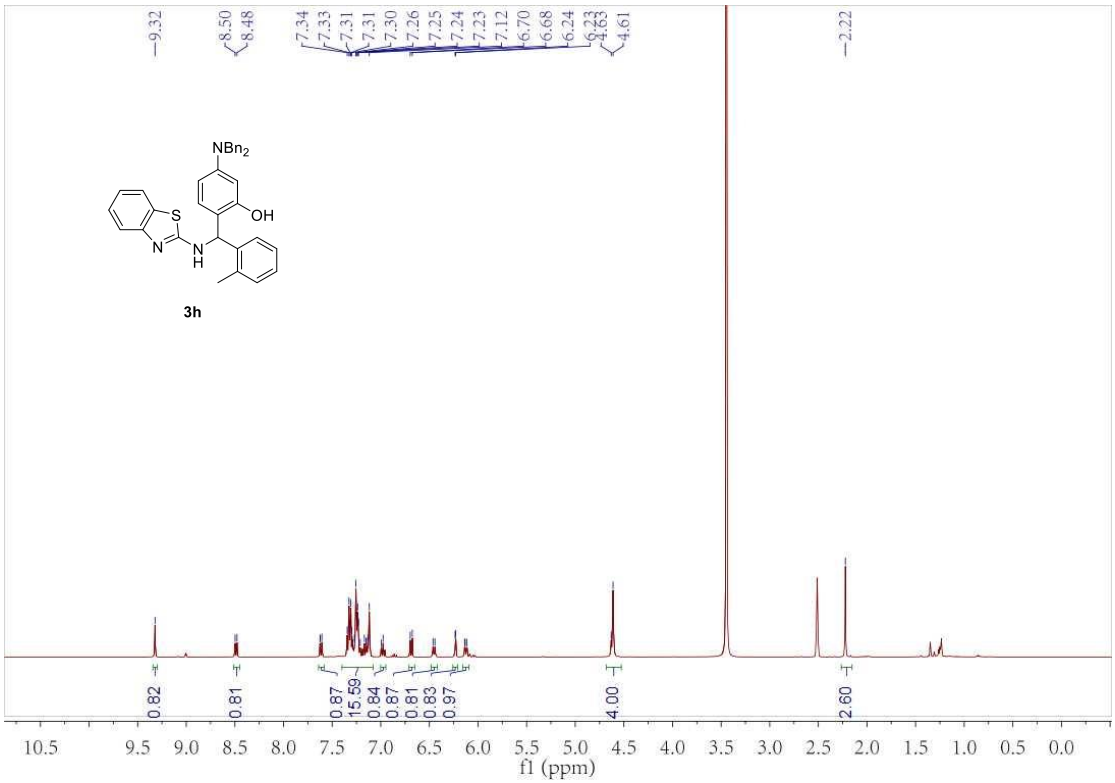
^{1}H NMR spectrum of compound **3g** (DMSO, 400 MHz)



^{13}C NMR spectrum of compound **3g** (DMSO, 100 MHz)

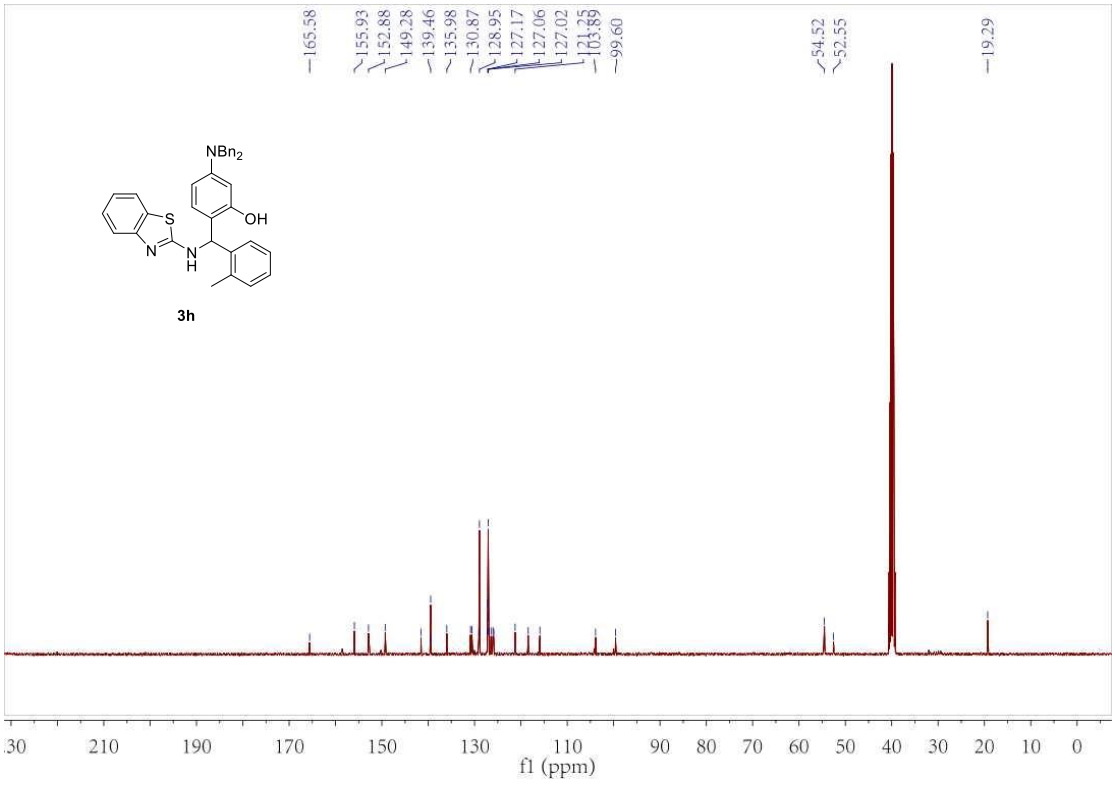


^{1}H NMR spectrum of compound **3h** (DMSO, 400 MHz)

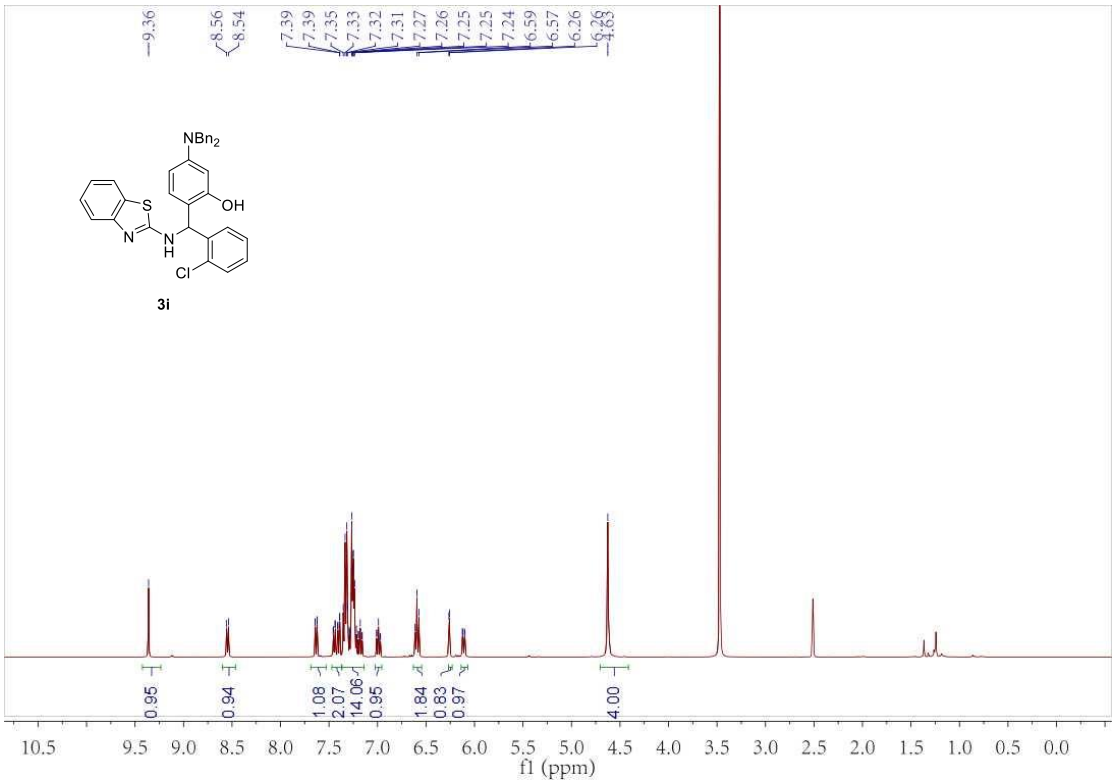


^{13}C NMR spectrum of compound **3h** (DMSO, 100 MHz)

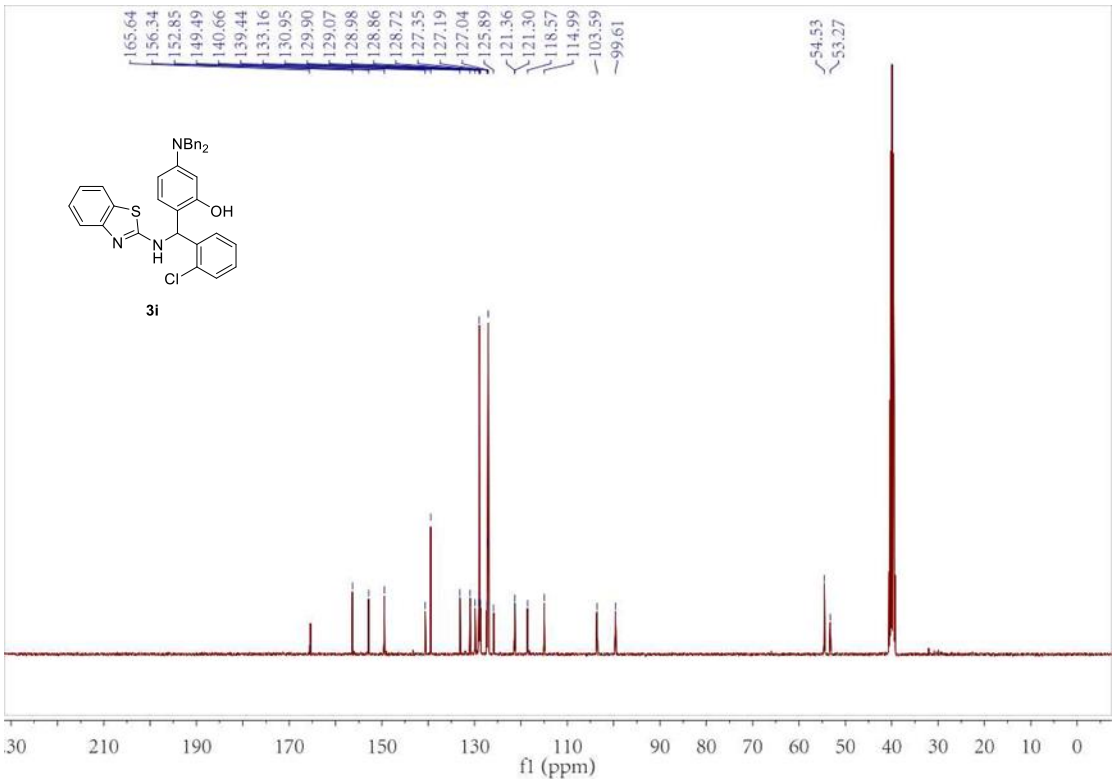
f



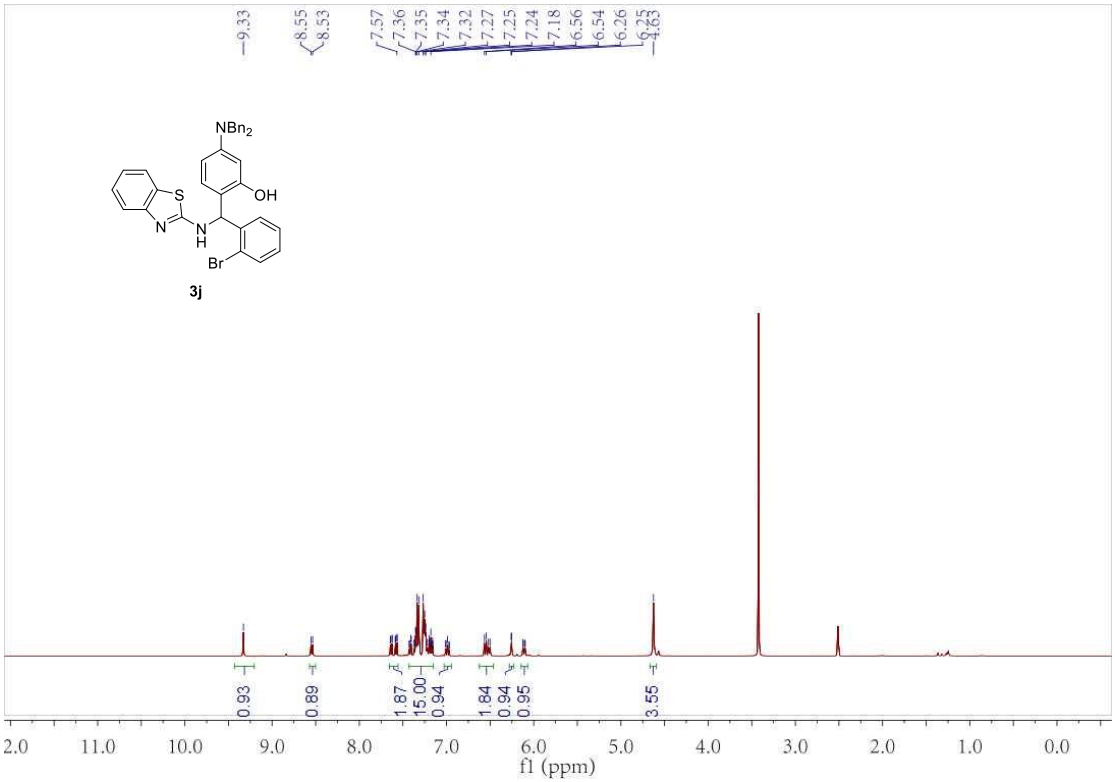
^{1}H NMR spectrum of compound **3i** (DMSO, 400 MHz)



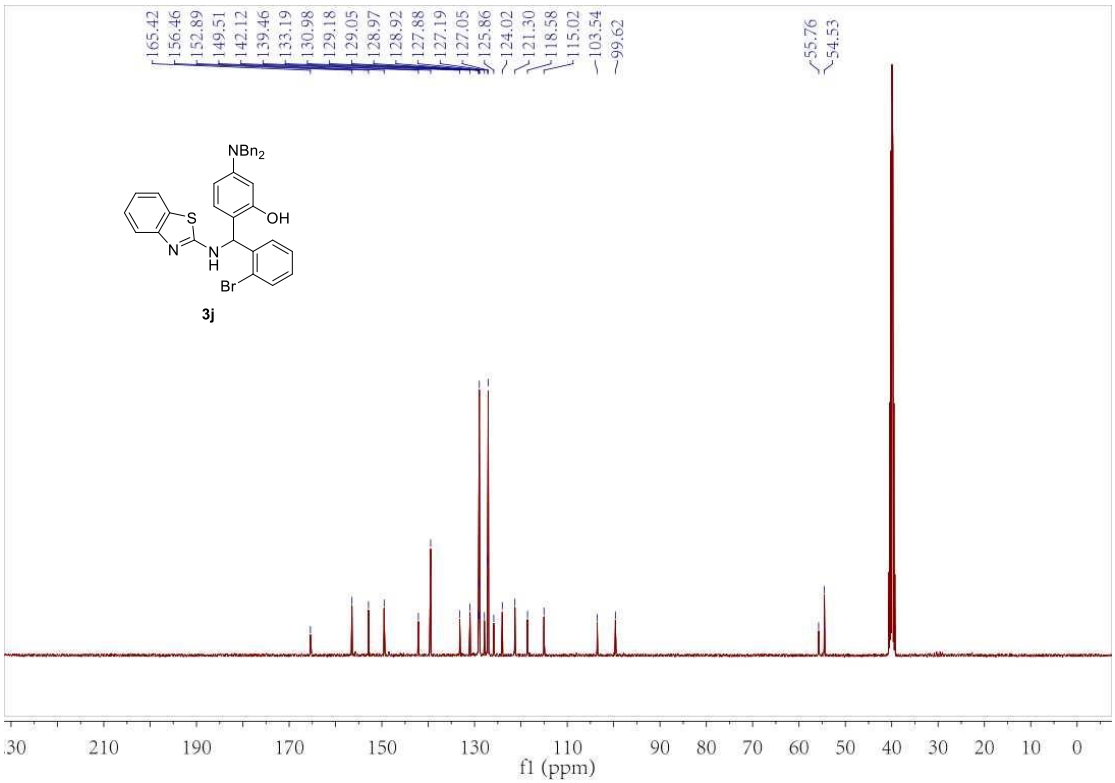
^{13}C NMR spectrum of compound **3i** (DMSO, 100 MHz)



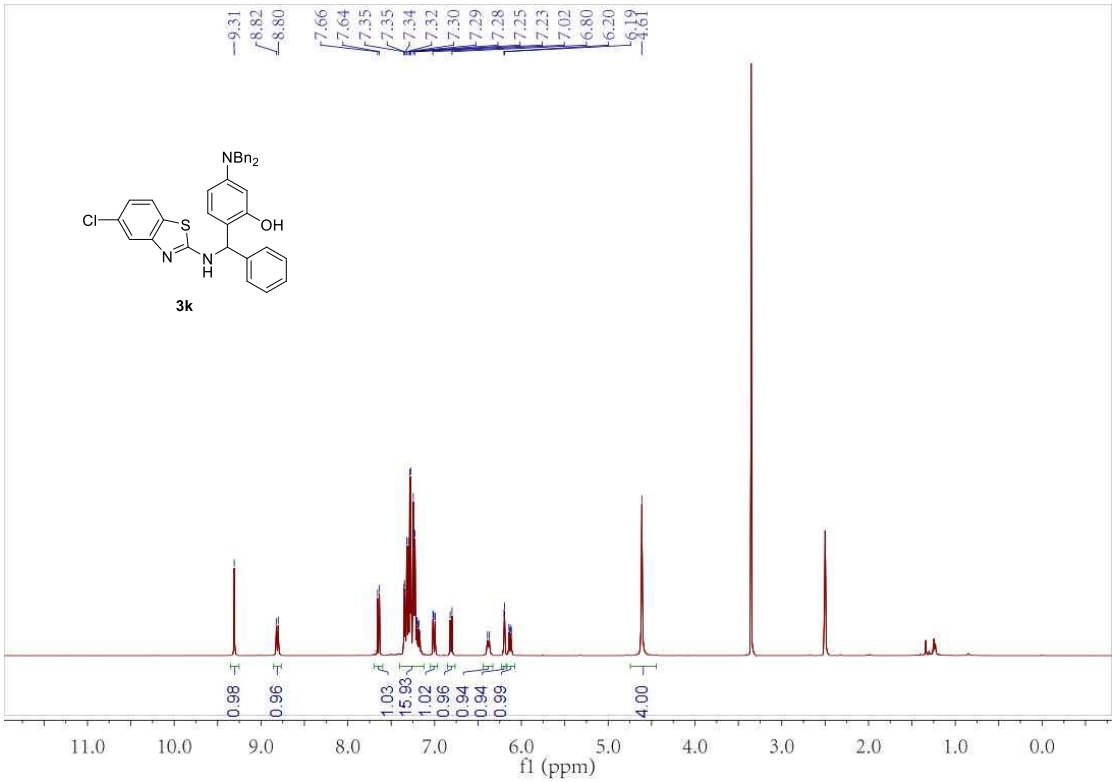
^{1}H NMR spectrum of compound **3j** (DMSO, 400 MHz)



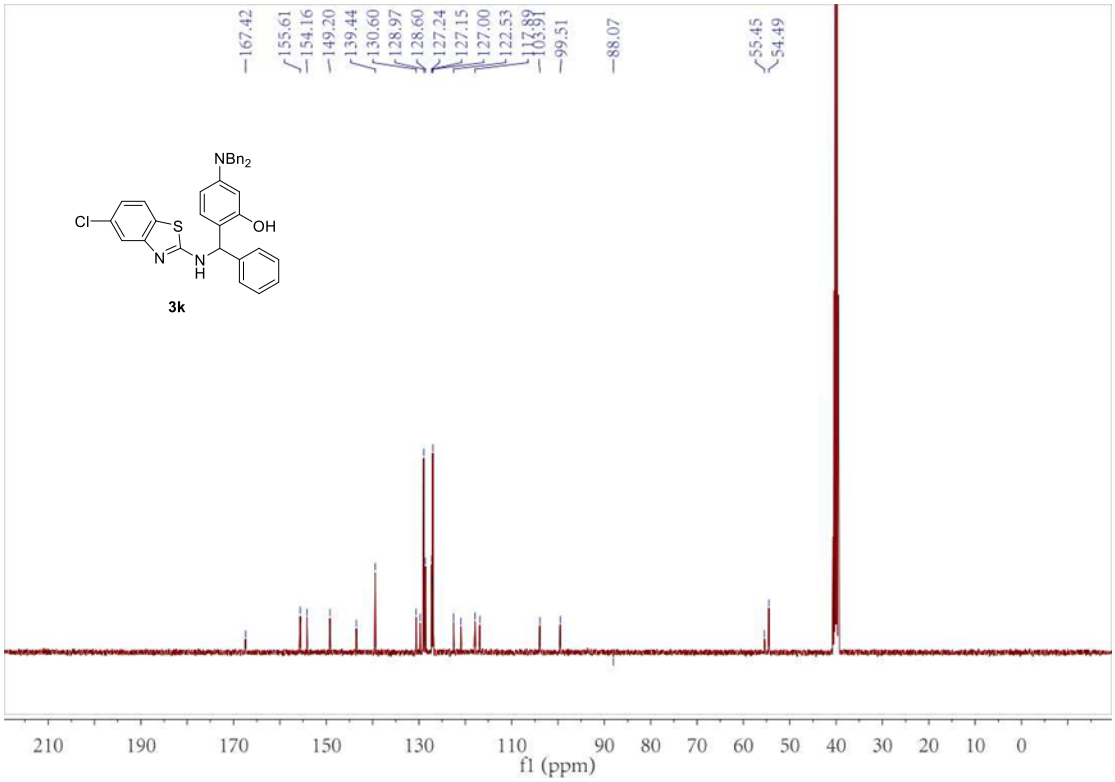
^{13}C NMR spectrum of compound **3j** (DMSO, 100 MHz)



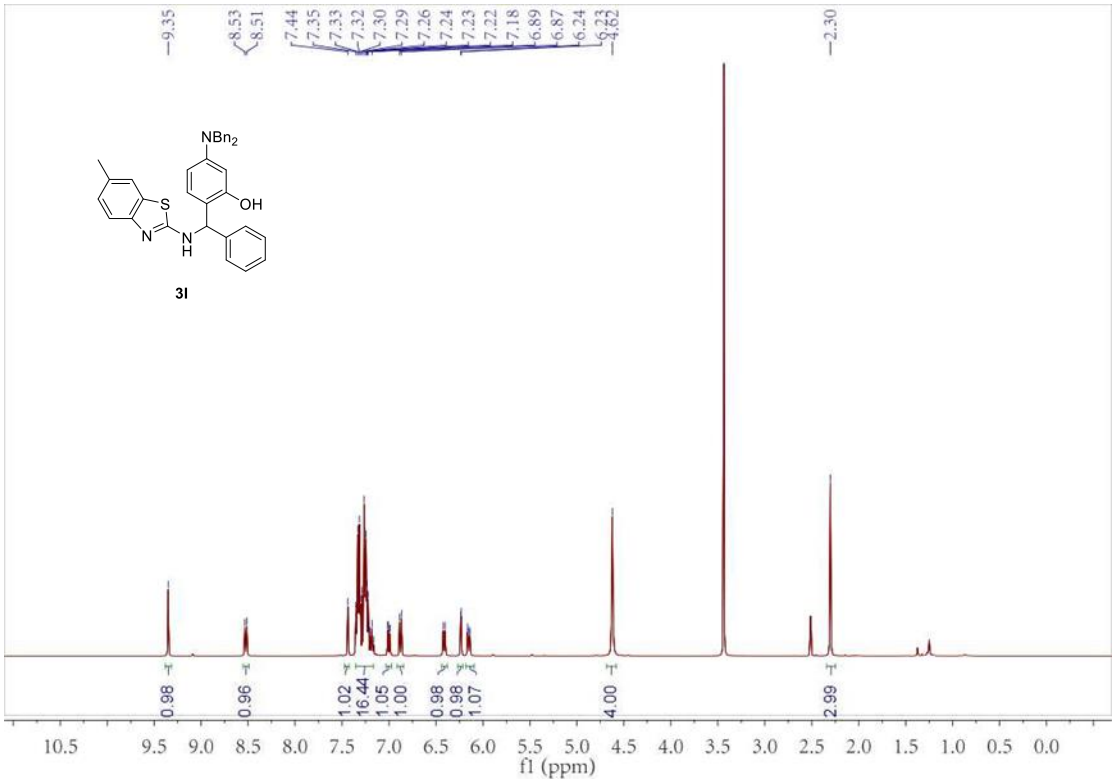
^{1}H NMR spectrum of compound **3k** (DMSO, 400 MHz)



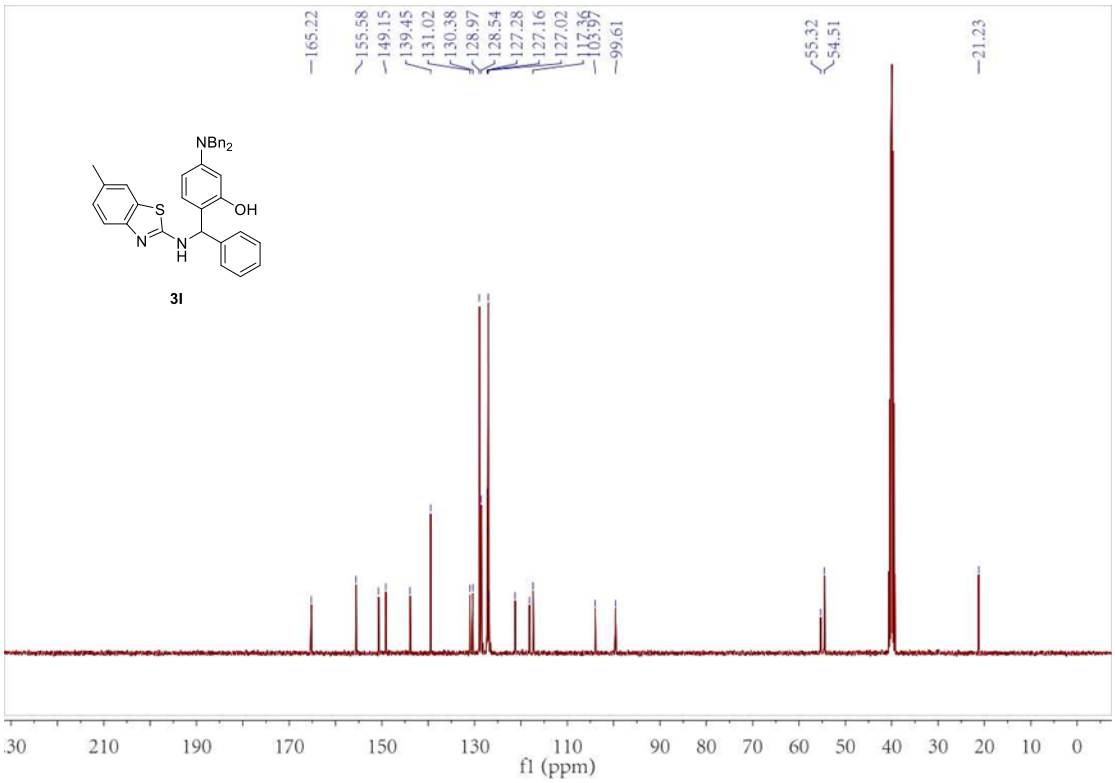
^{13}C NMR spectrum of compound **3k** (DMSO, 100 MHz)



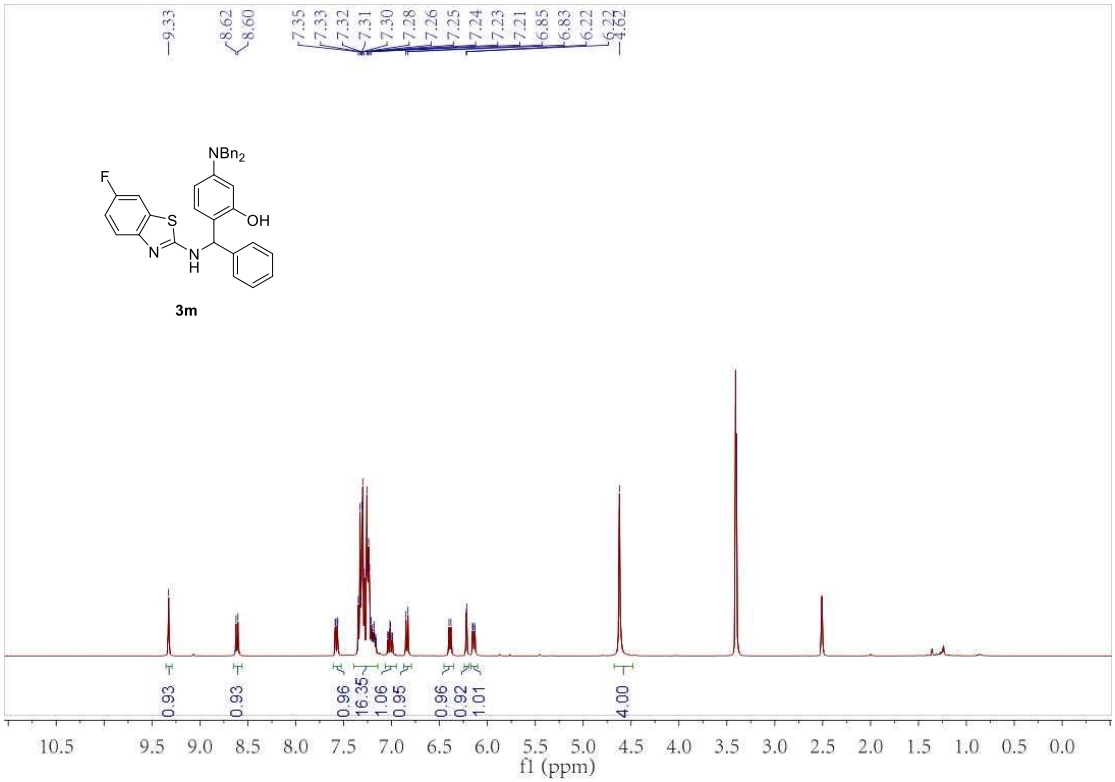
^{1}H NMR spectrum of compound **3l** (DMSO, 400 MHz)



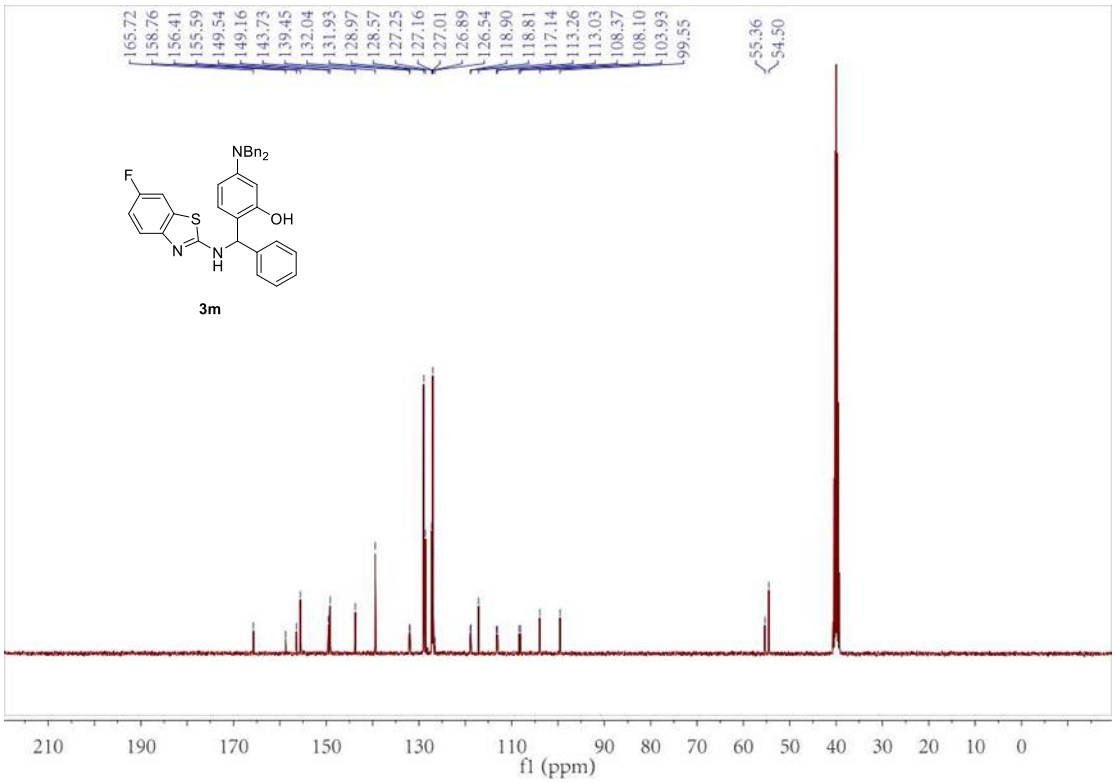
^{13}C NMR spectrum of compound **3l** (DMSO, 100 MHz)



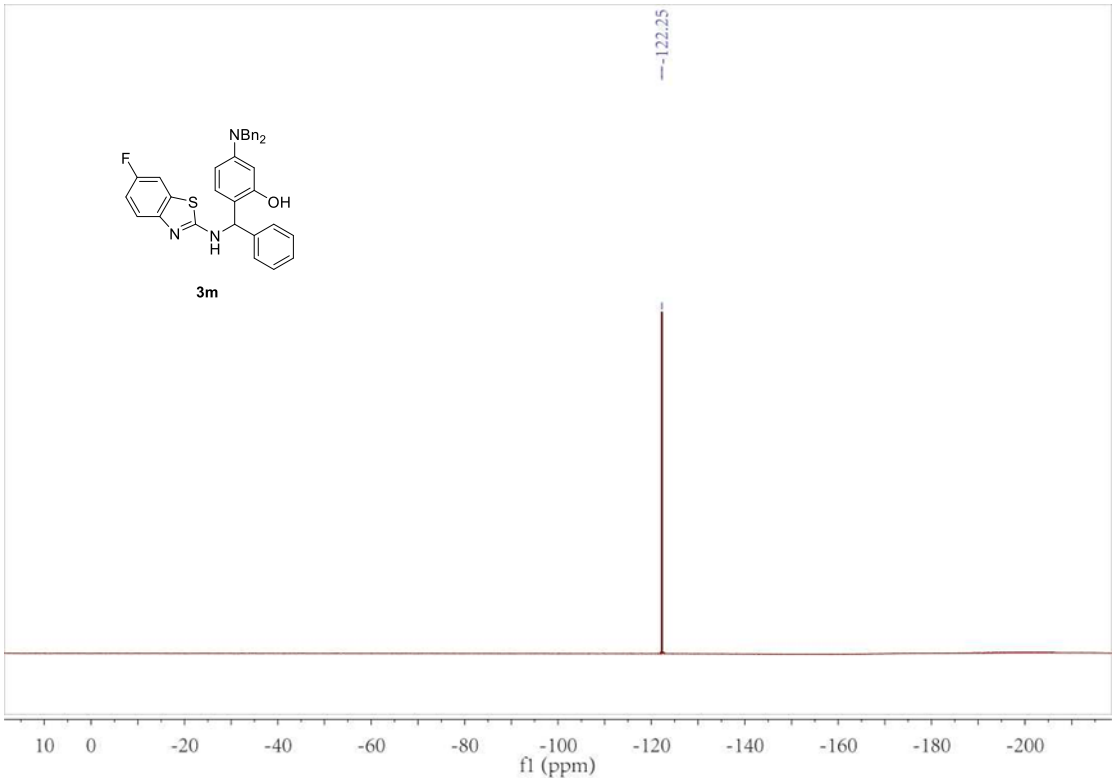
^{1}H NMR spectrum of compound **3m** (DMSO, 400 MHz)



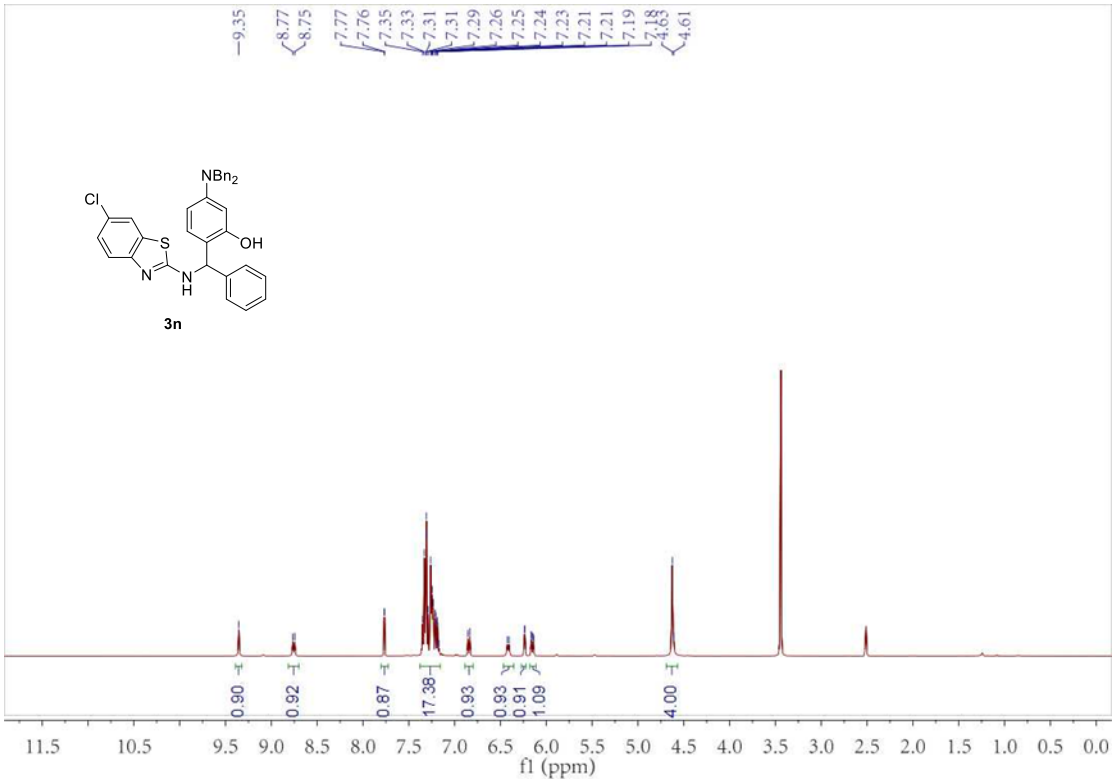
^{13}C NMR spectrum of compound **3m** (DMSO, 100 MHz)



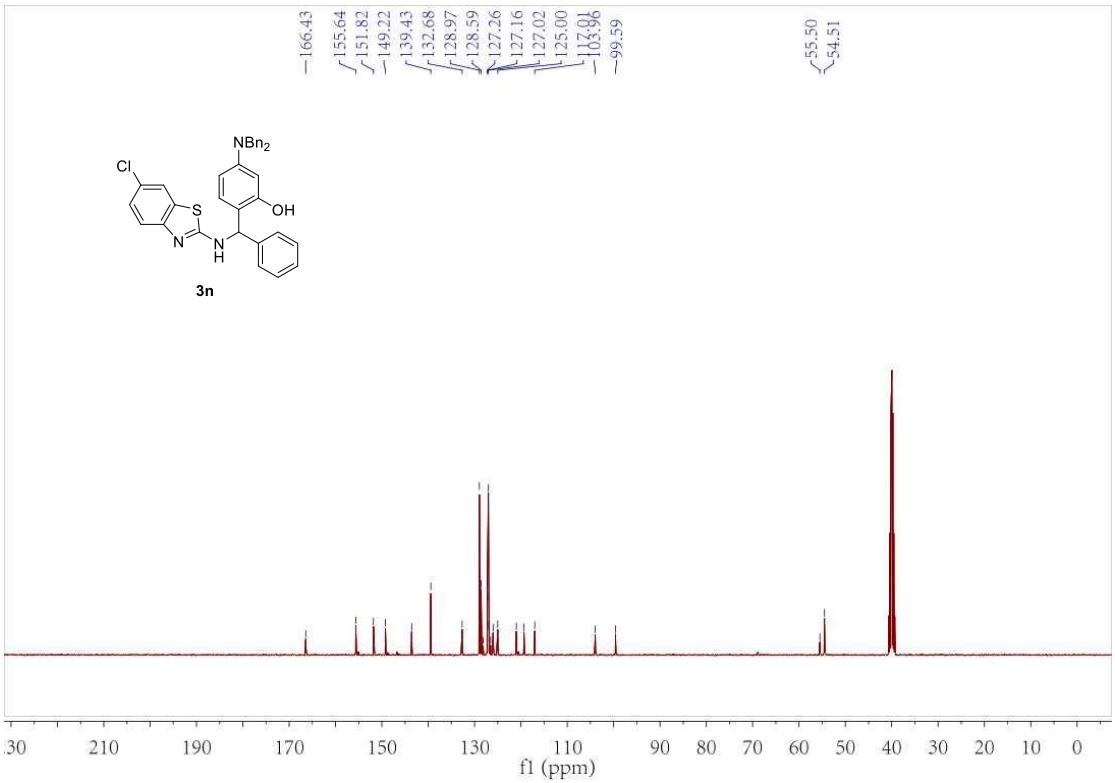
^{19}F NMR spectrum of compound **3m** (DMSO, 376 MHz)



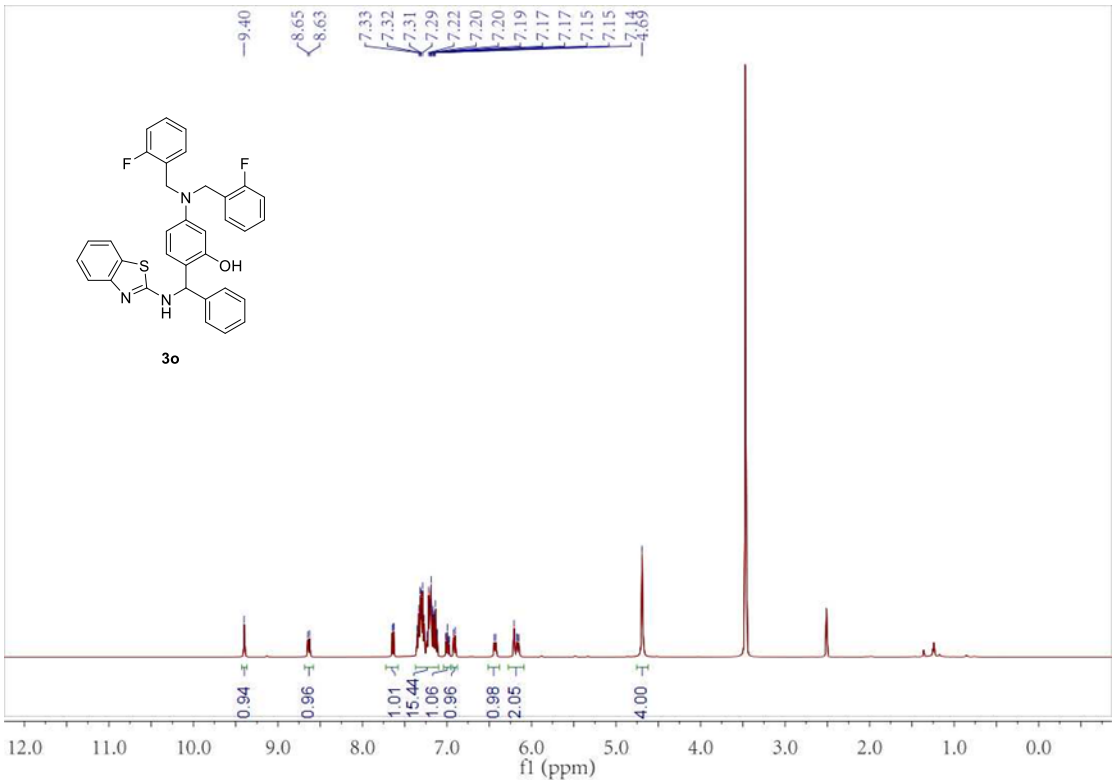
^{1}H NMR spectrum of compound **3n** (DMSO, 400 MHz)



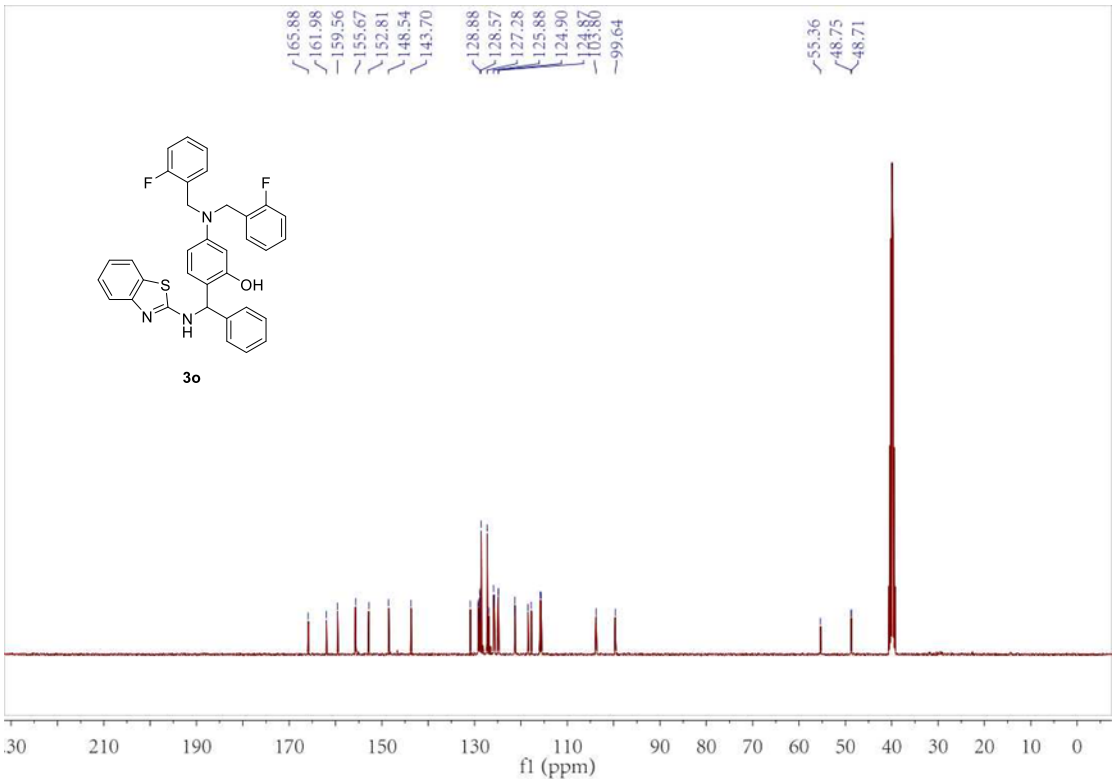
^{13}C NMR spectrum of compound **3n** (DMSO, 100 MHz)



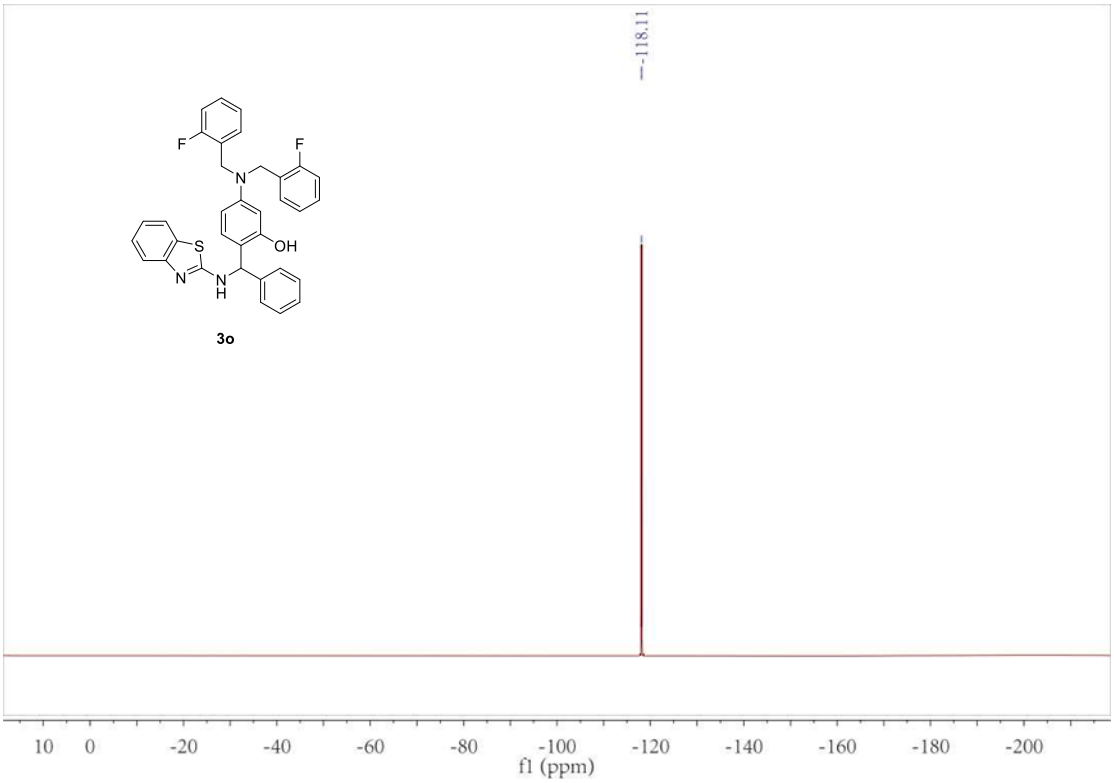
^{1}H NMR spectrum of compound **3o** (DMSO, 400 MHz)



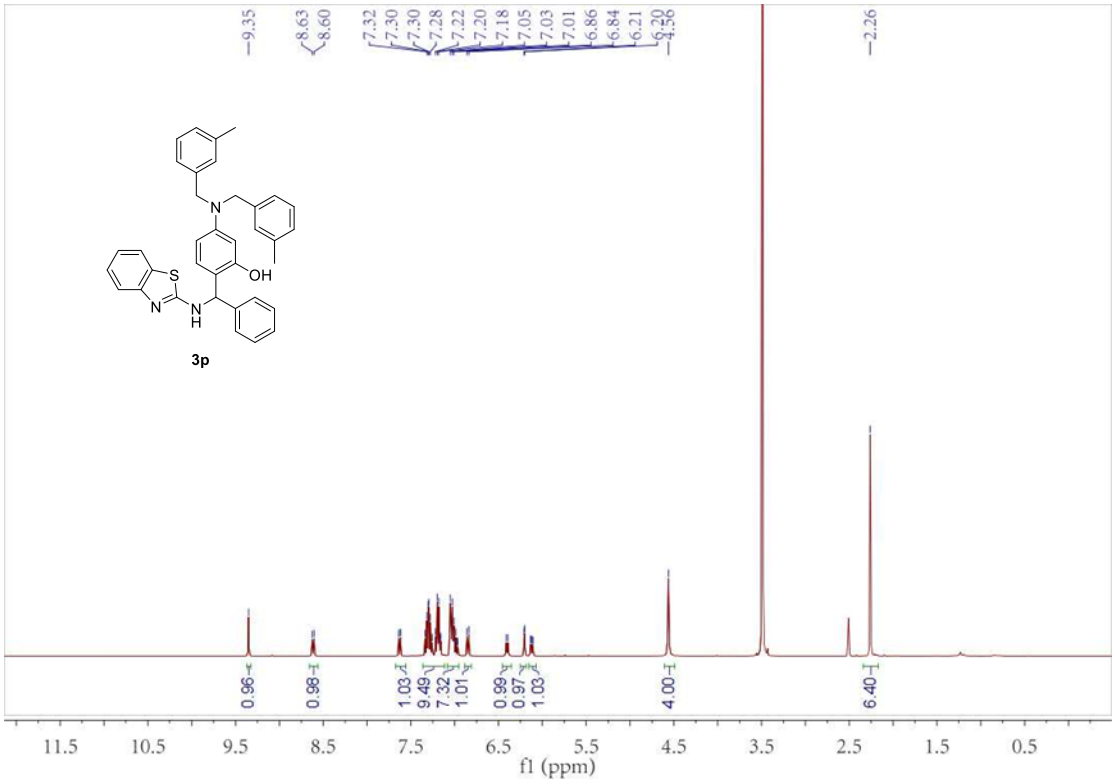
^{13}C NMR spectrum of compound **3o** (DMSO, 100 MHz)



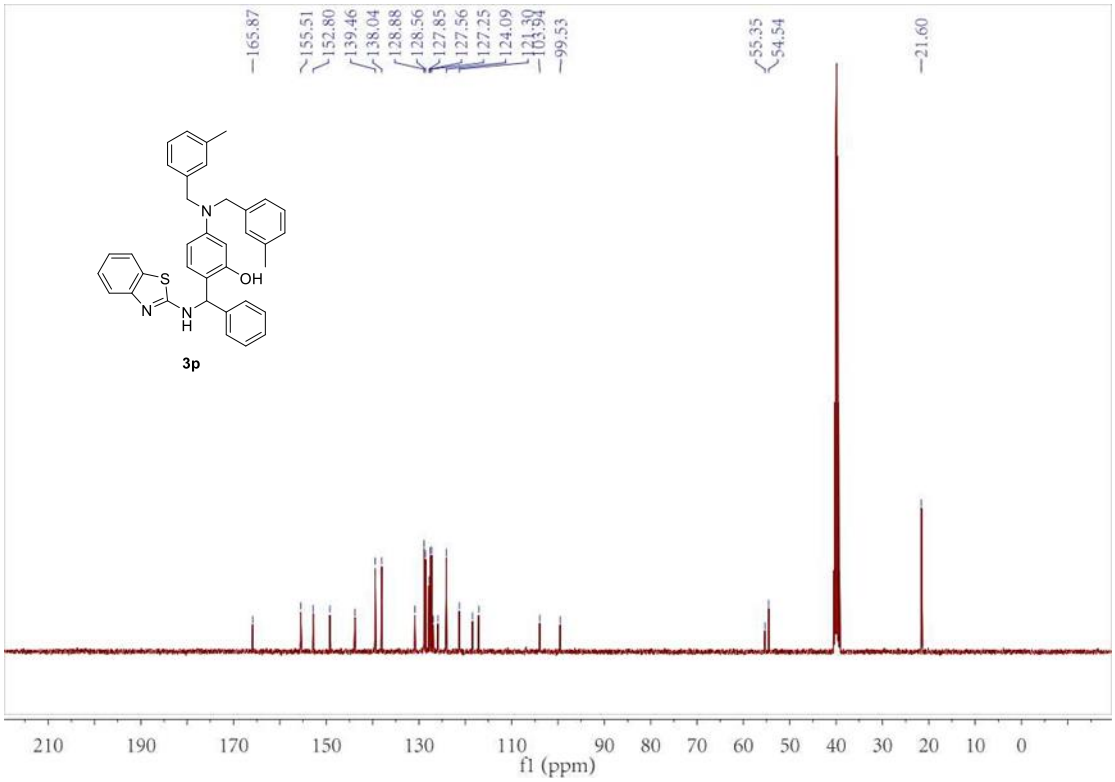
^{19}F NMR spectrum of compound **3o** (DMSO, 376 MHz)



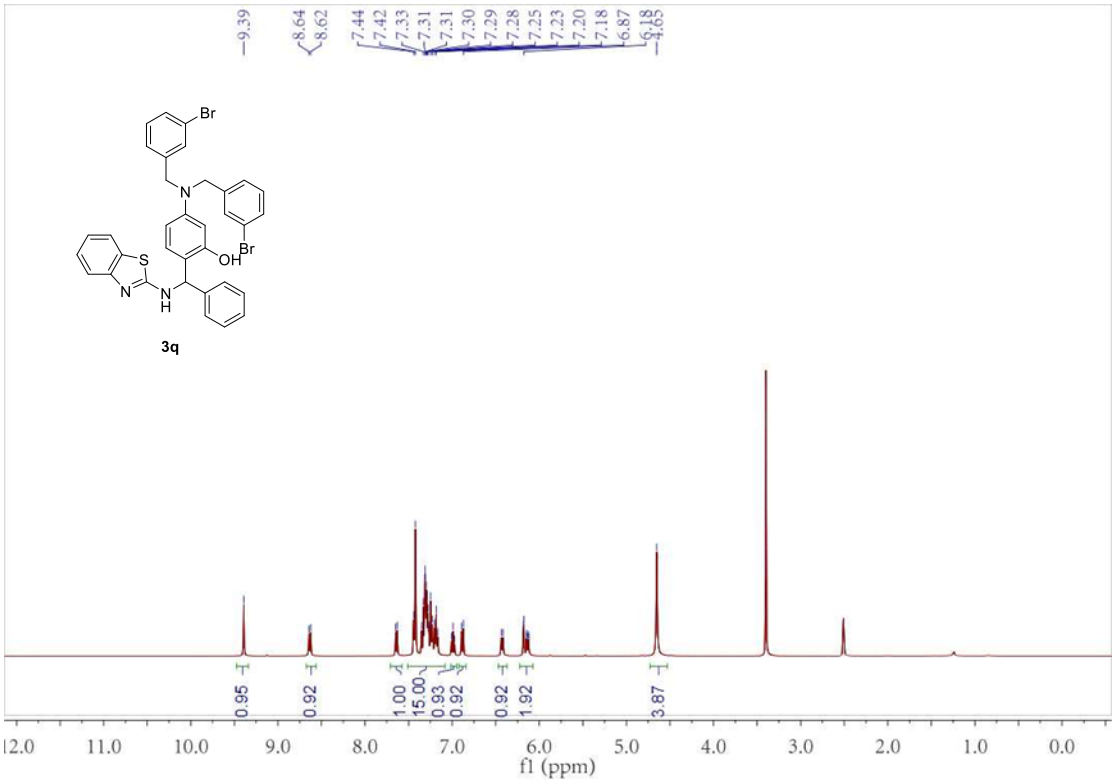
^{1}H NMR spectrum of compound **3p** (DMSO, 400 MHz)



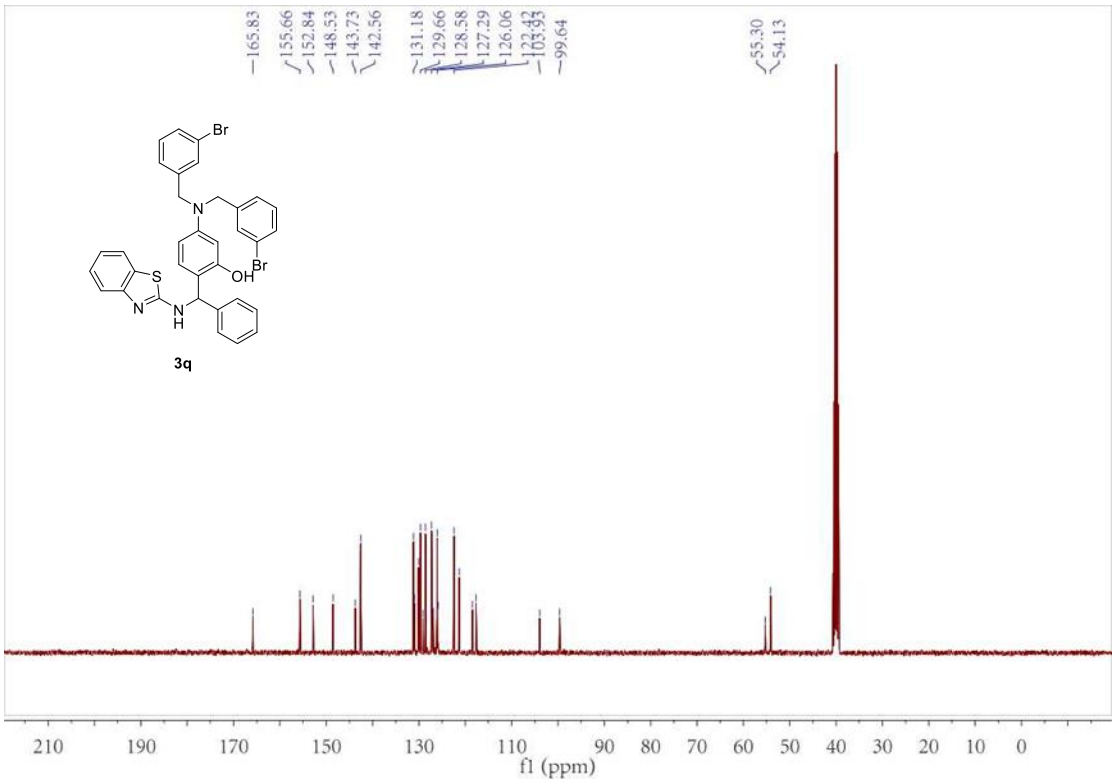
^{13}C NMR spectrum of compound **3p** (DMSO, 100 MHz)



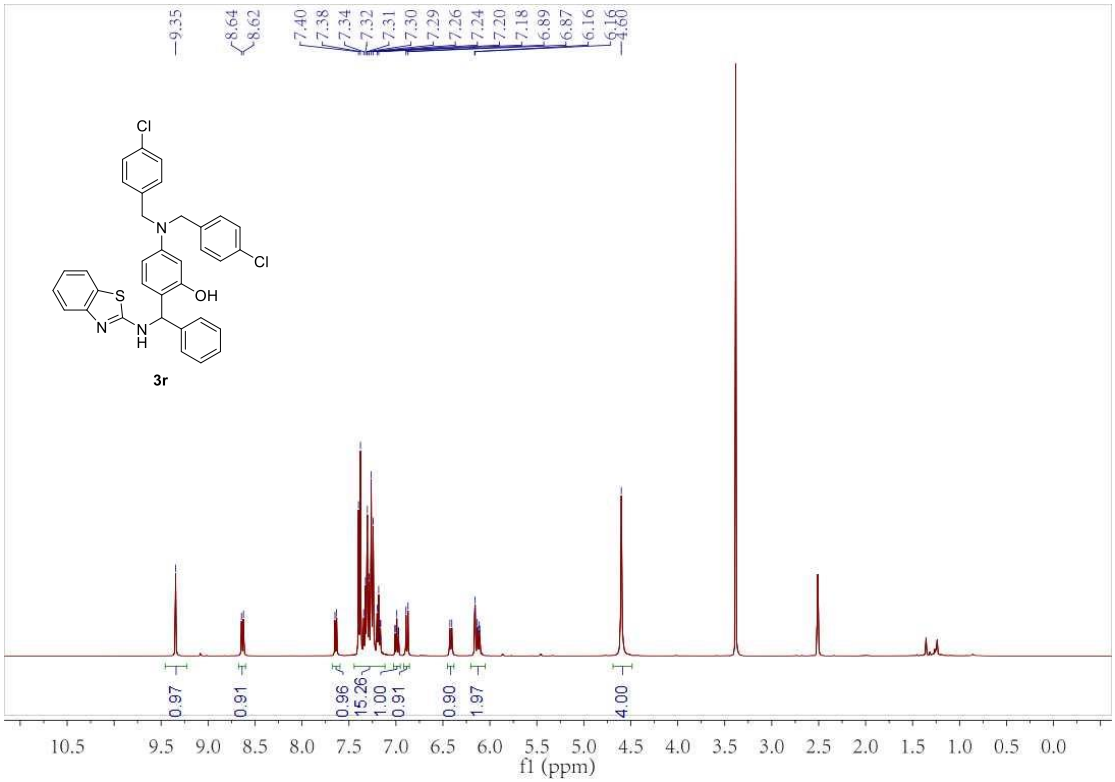
^{1}H NMR spectrum of compound **3q** (DMSO, 400 MHz)



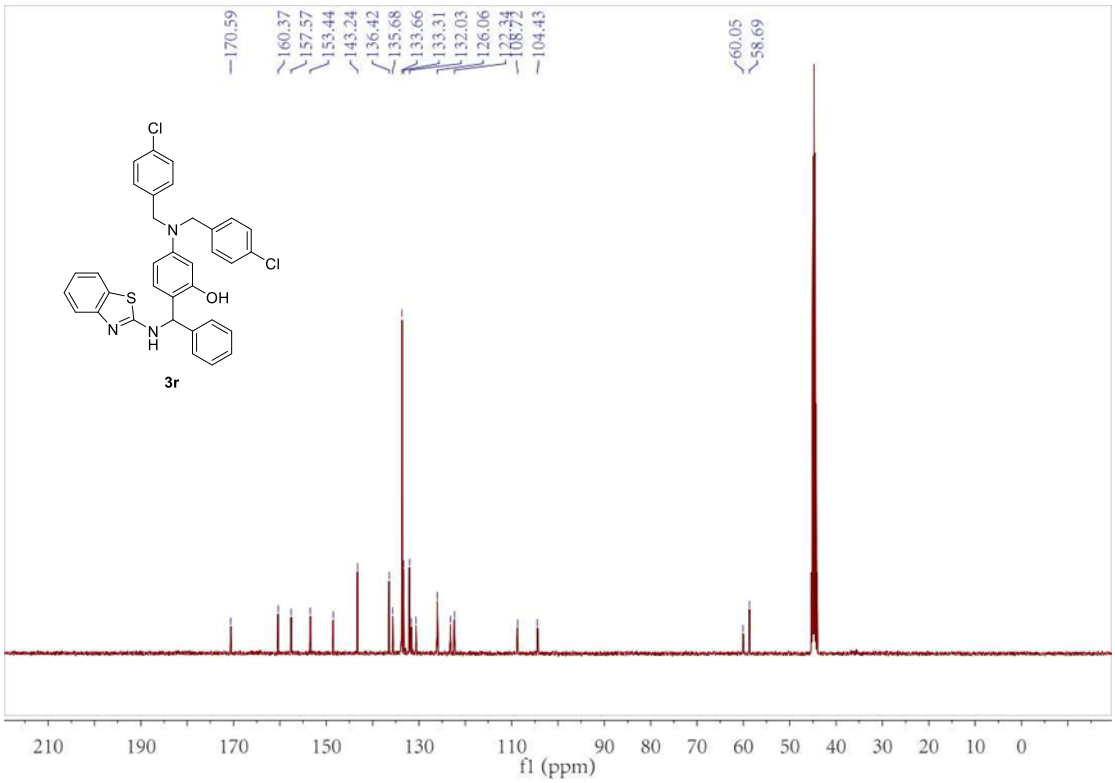
^{13}C NMR spectrum of compound **3q** (DMSO, 100 MHz)



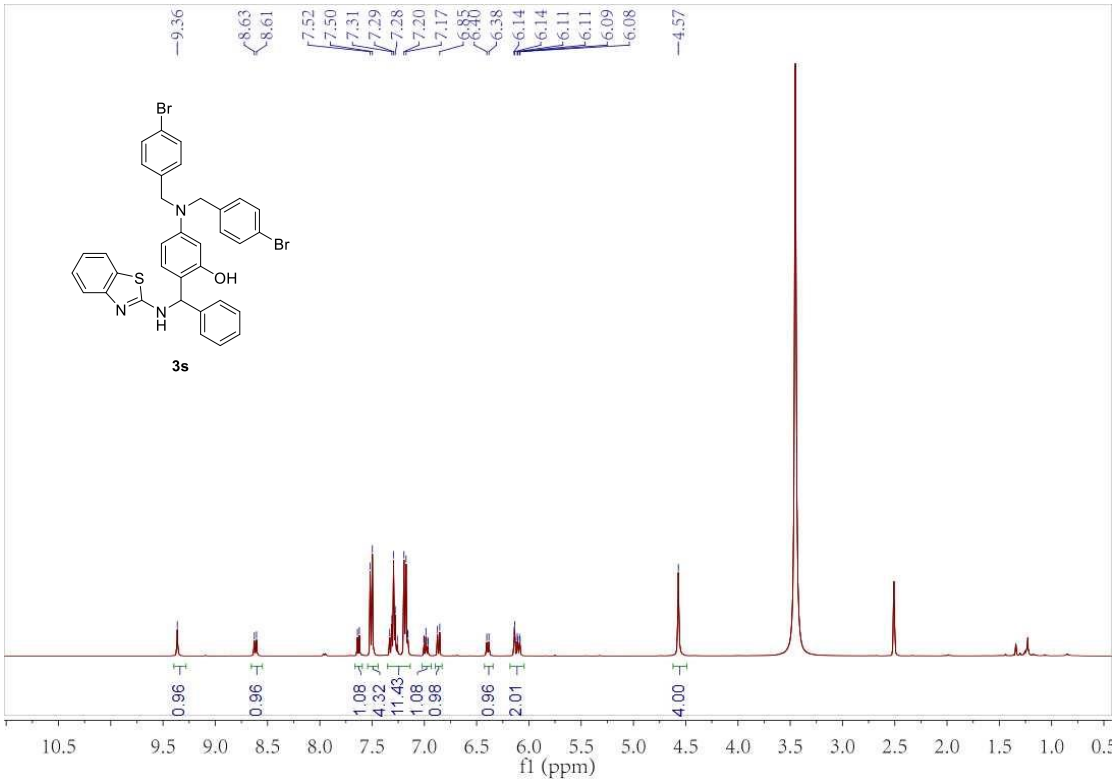
^{1}H NMR spectrum of compound **3r** (DMSO, 400 MHz)



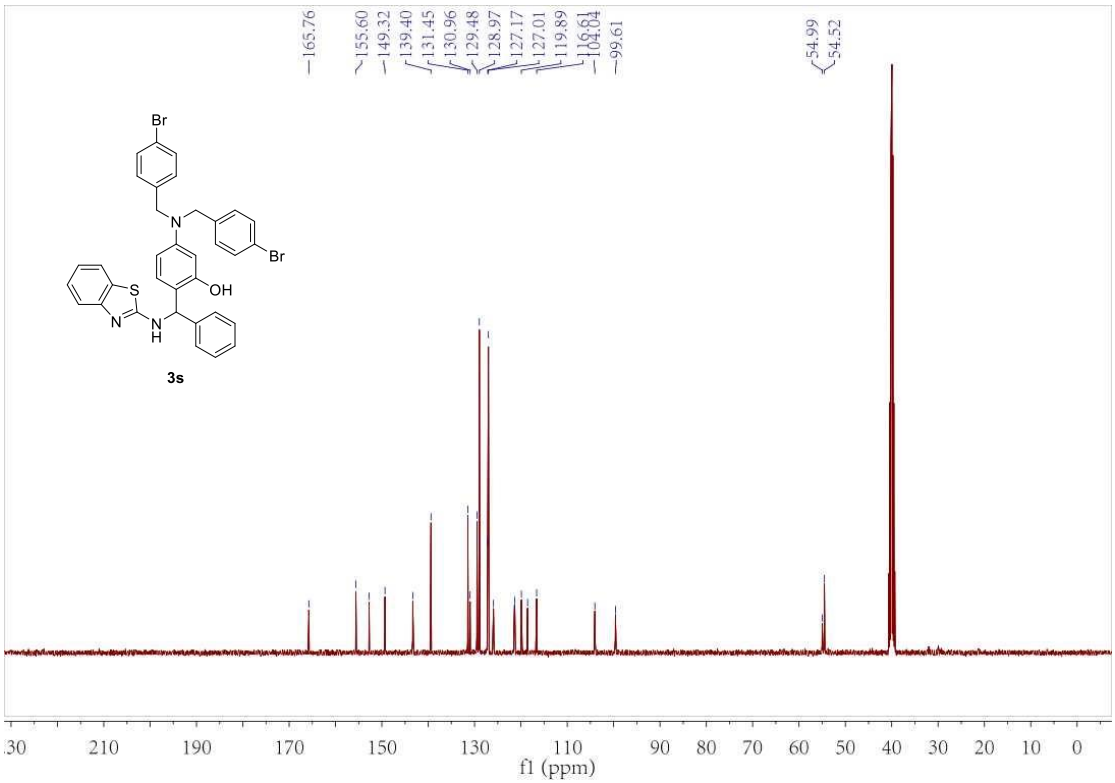
^{13}C NMR spectrum of compound **3r** (DMSO, 100 MHz)



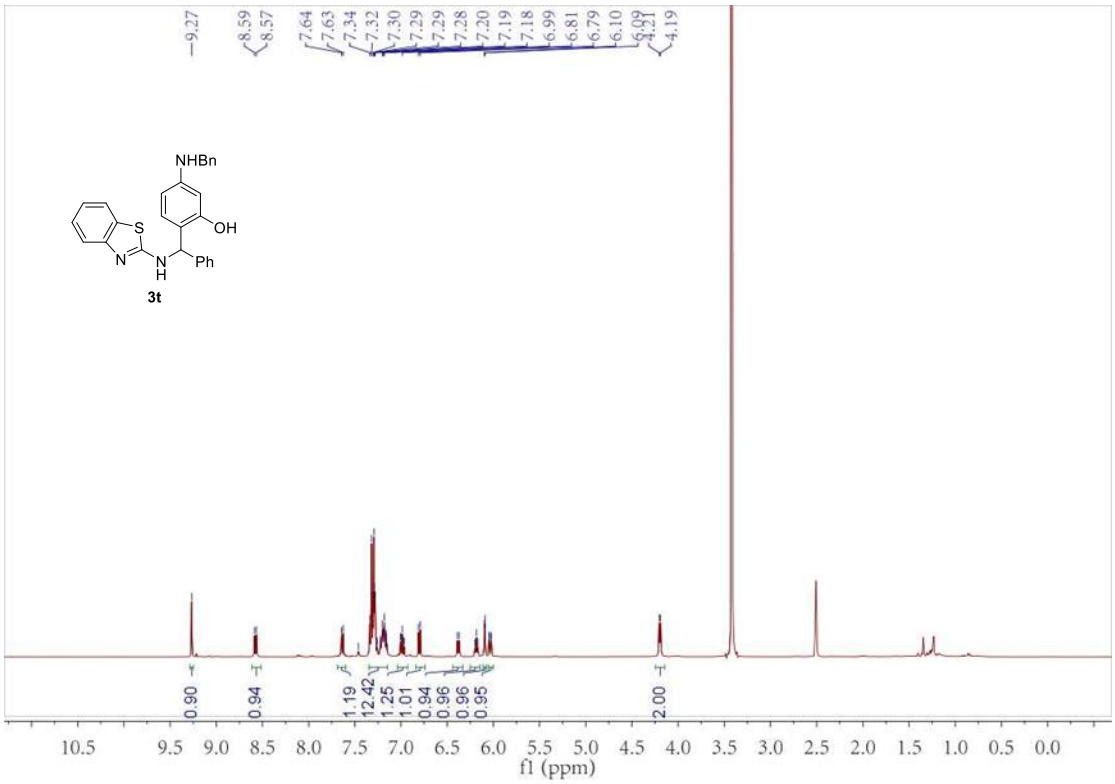
^{1}H NMR spectrum of compound **3s** (DMSO, 400 MHz)



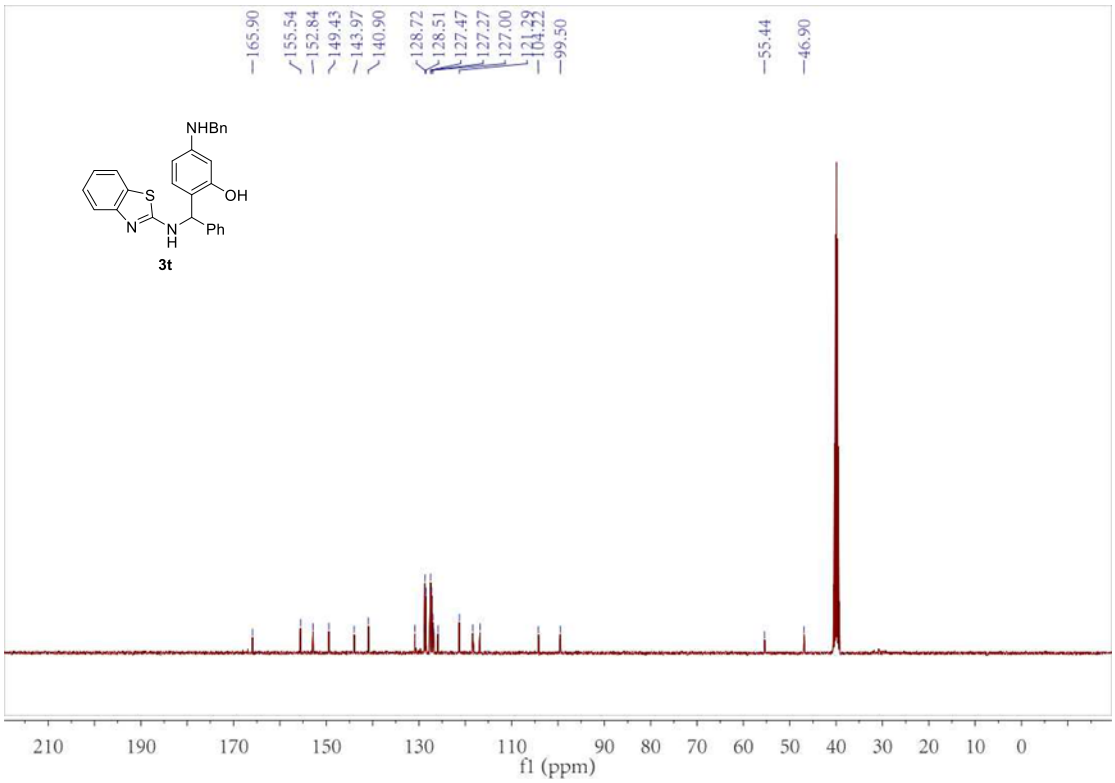
^{13}C NMR spectrum of compound **3s** (DMSO, 100 MHz)



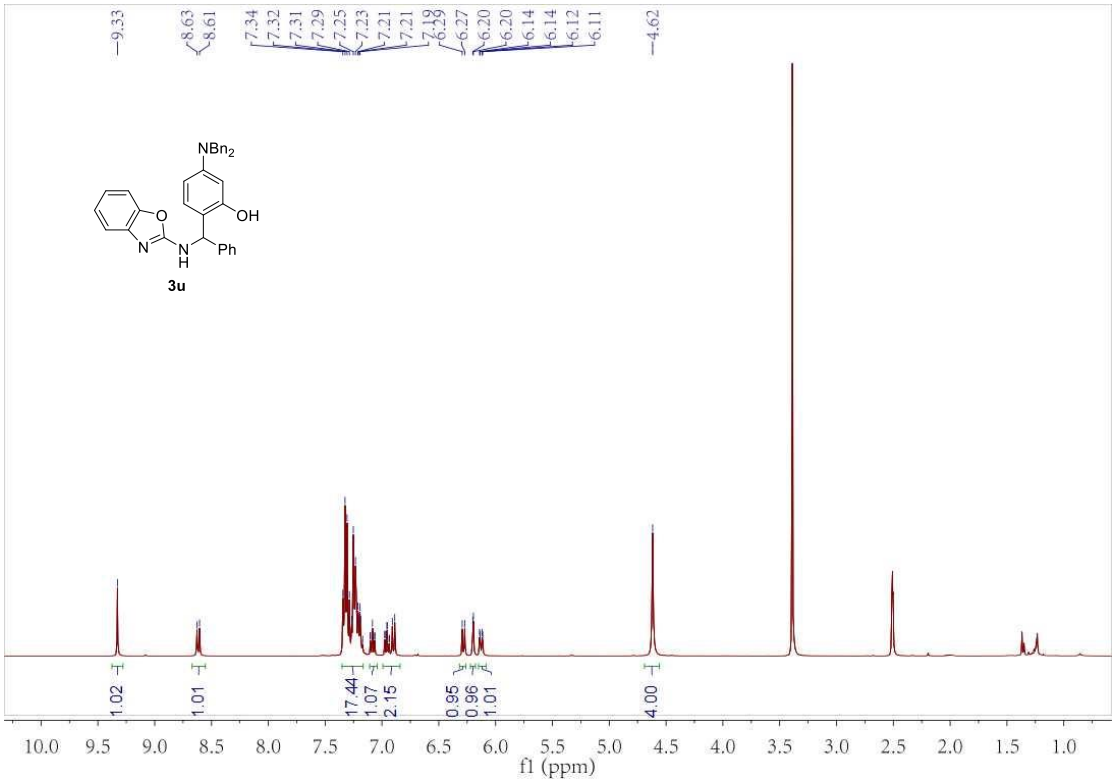
^{1}H NMR spectrum of compound **3t** (DMSO, 400 MHz)



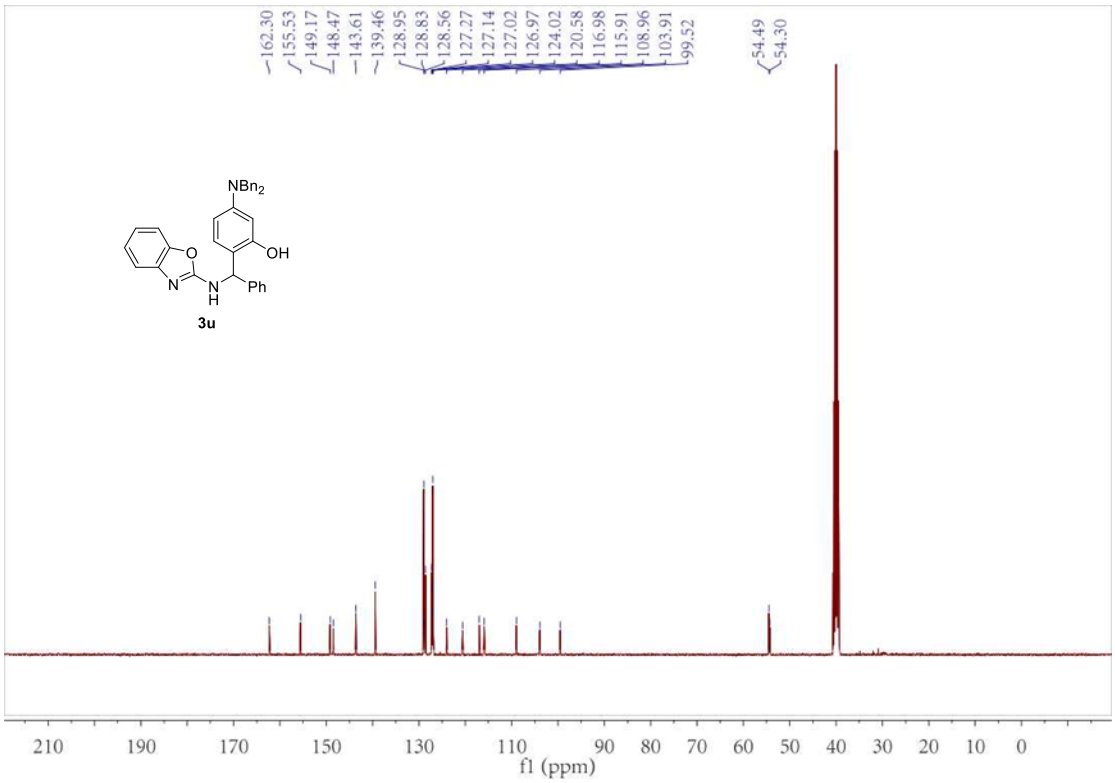
^{13}C NMR spectrum of compound **3t** (DMSO, 100 MHz)



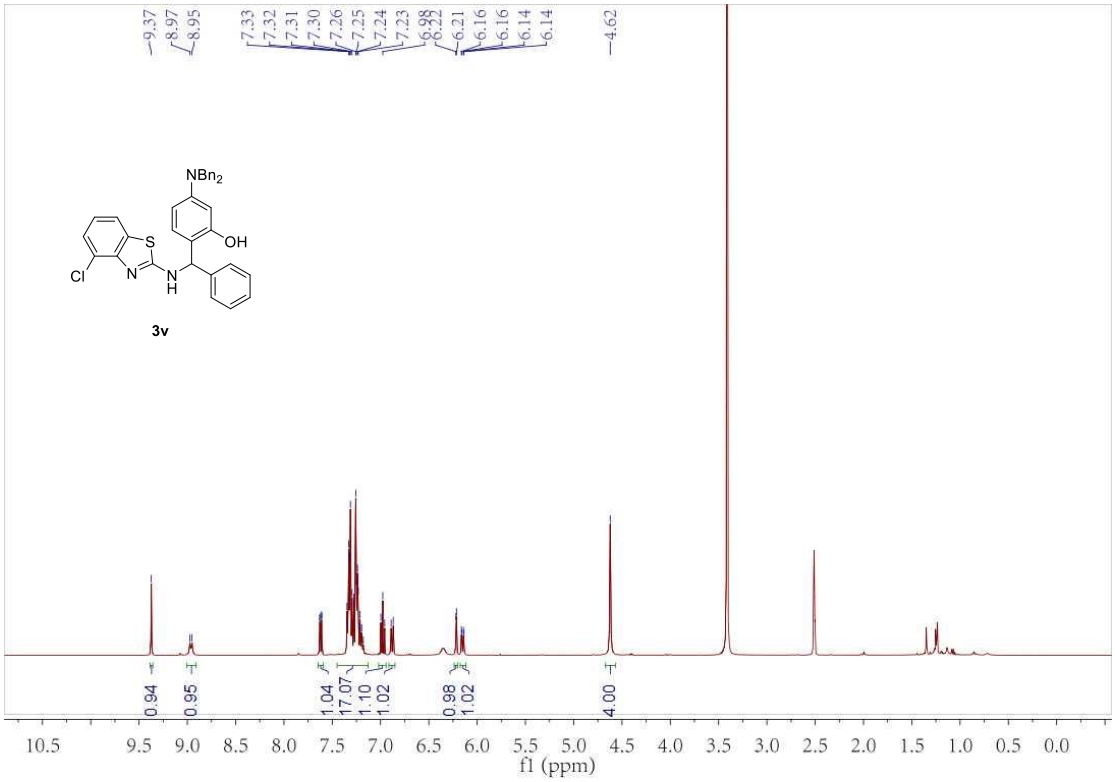
^{1}H NMR spectrum of compound **3u** (DMSO, 400 MHz)



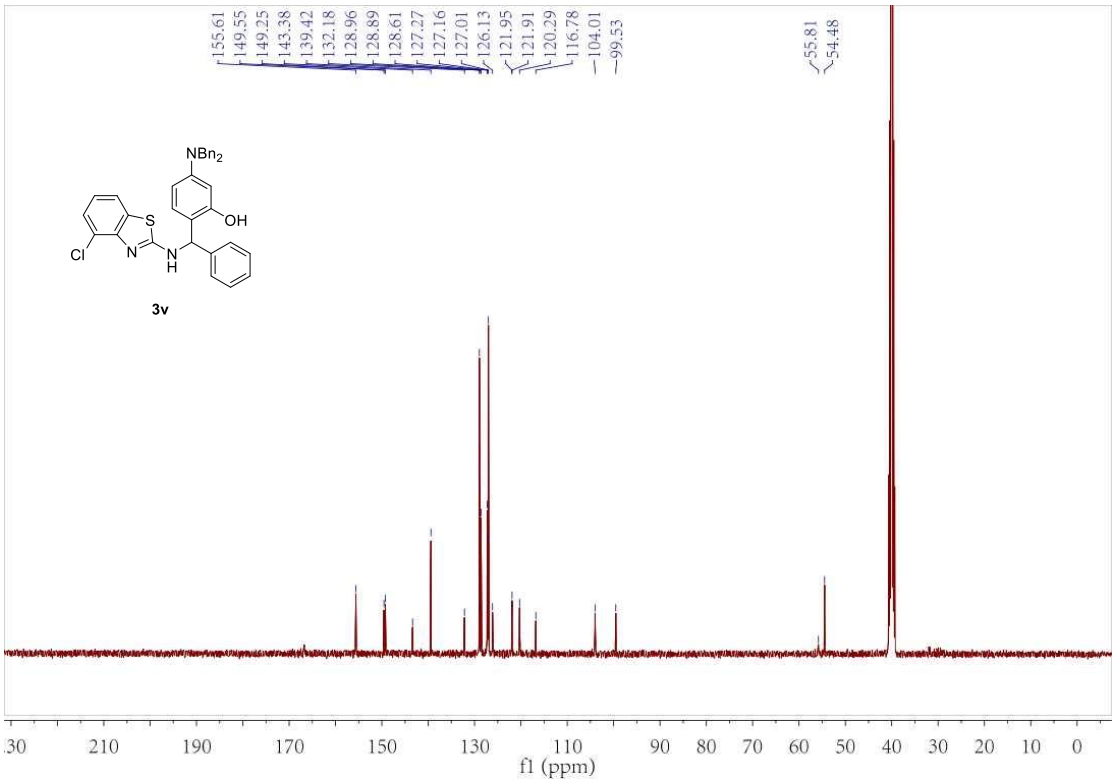
^{13}C NMR spectrum of compound **3u** (DMSO, 100 MHz)



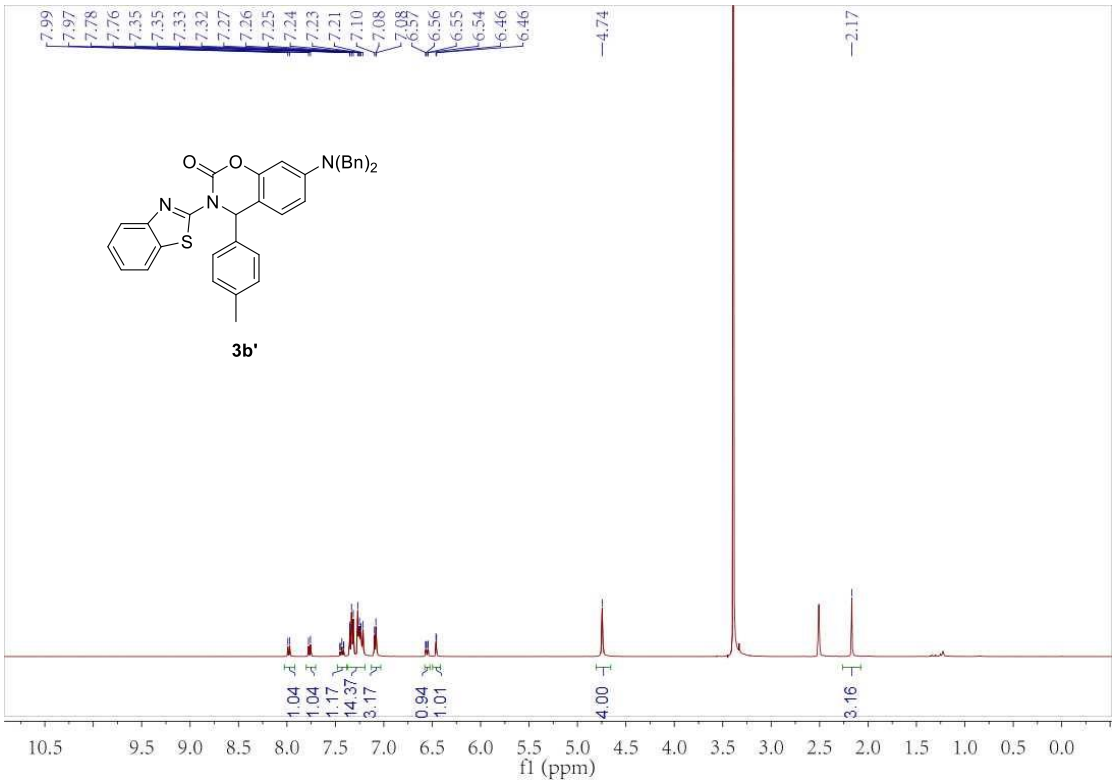
^{1}H NMR spectrum of compound **3v** (DMSO, 400 MHz)



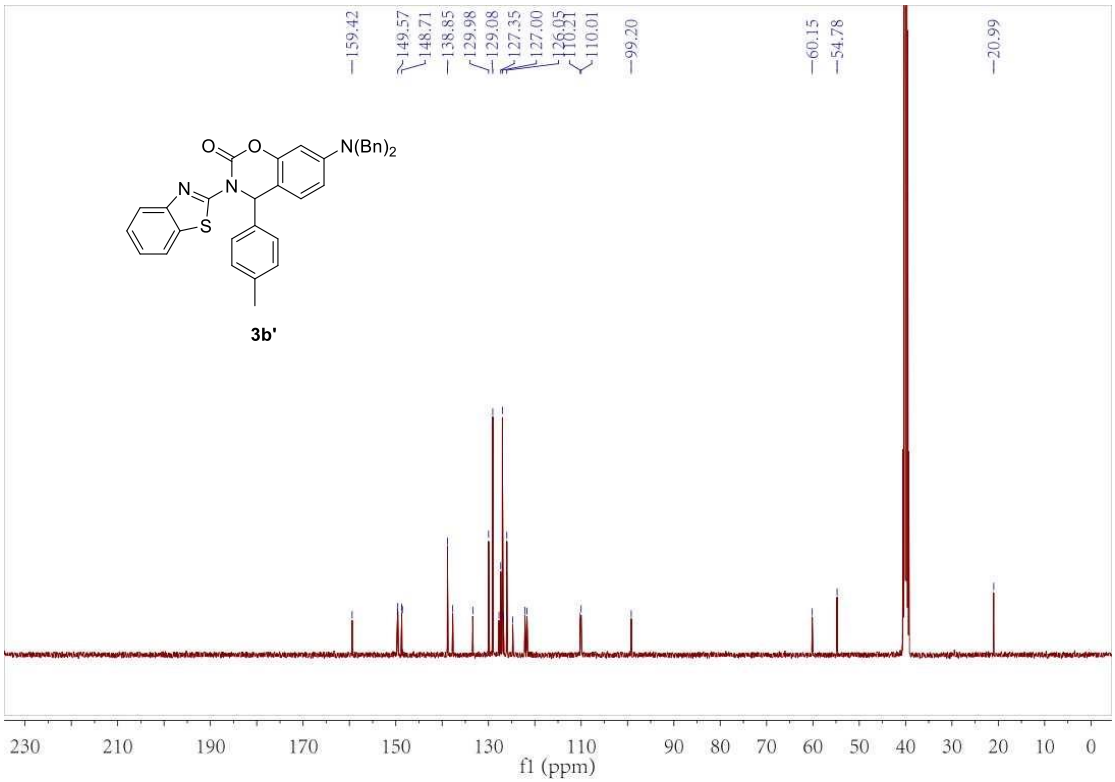
^{13}C NMR spectrum of compound **3v** (DMSO, 100 MHz)



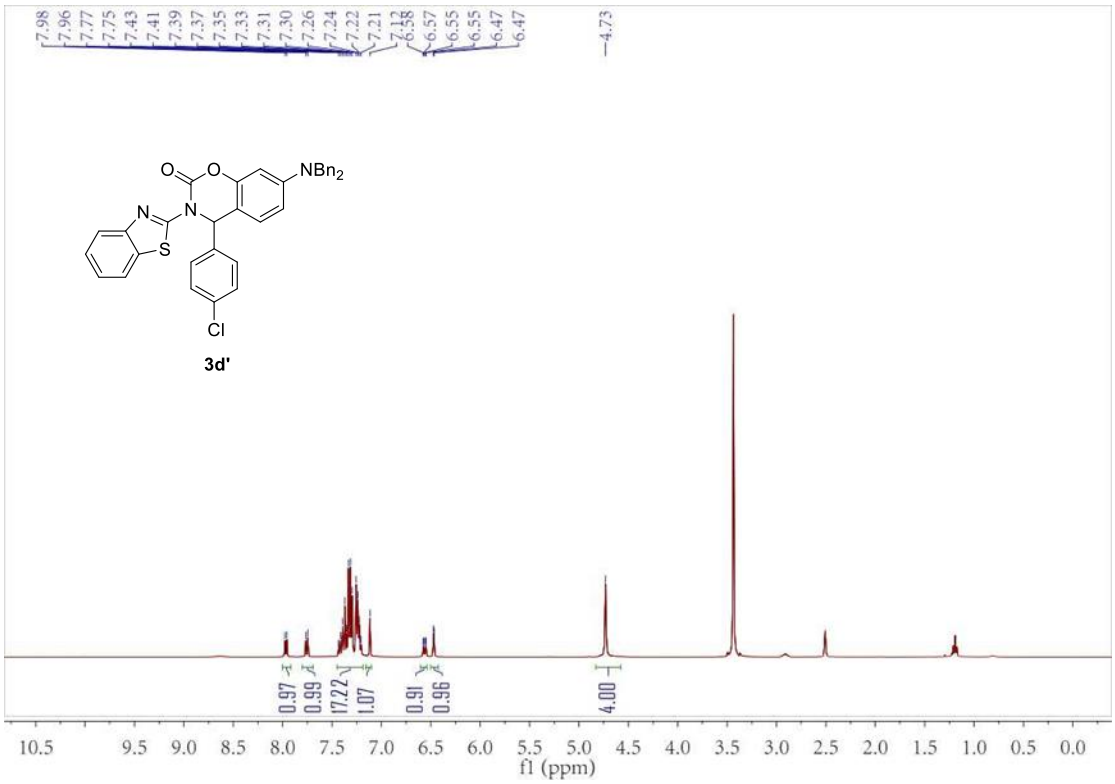
H NMR spectrum of compound **4a** (DMSO, 400 MHz)



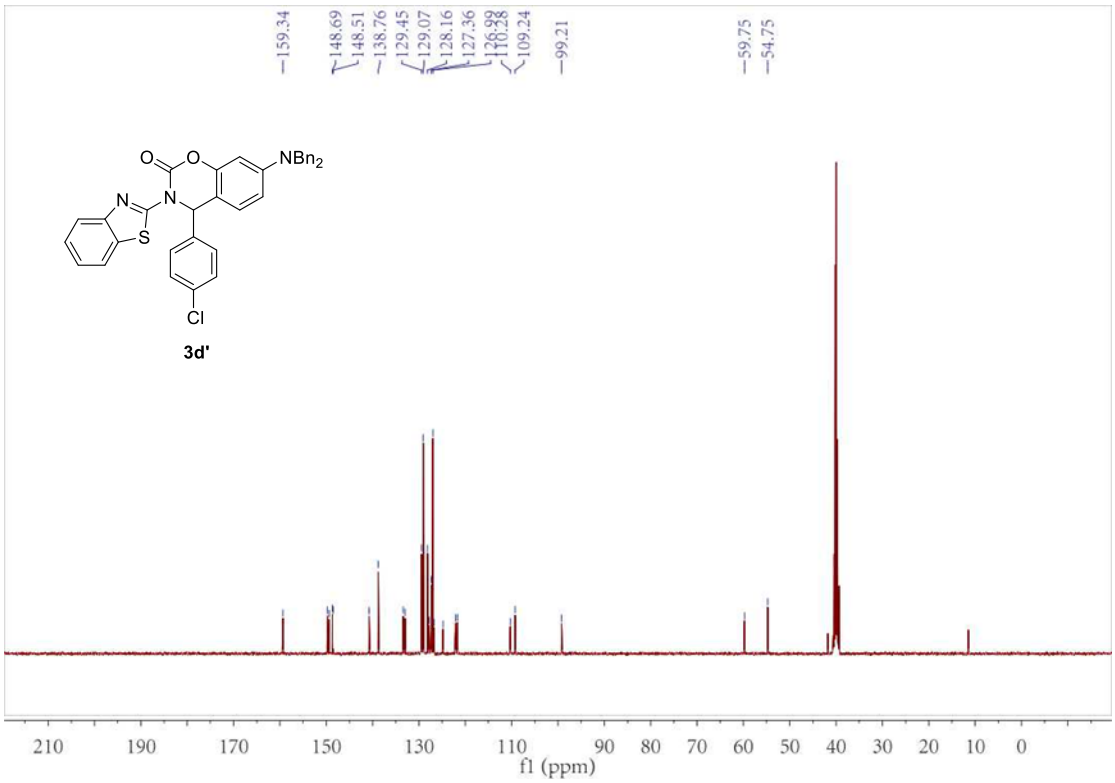
^{13}C NMR spectrum of compound **4a** (DMSO, 100 MHz)



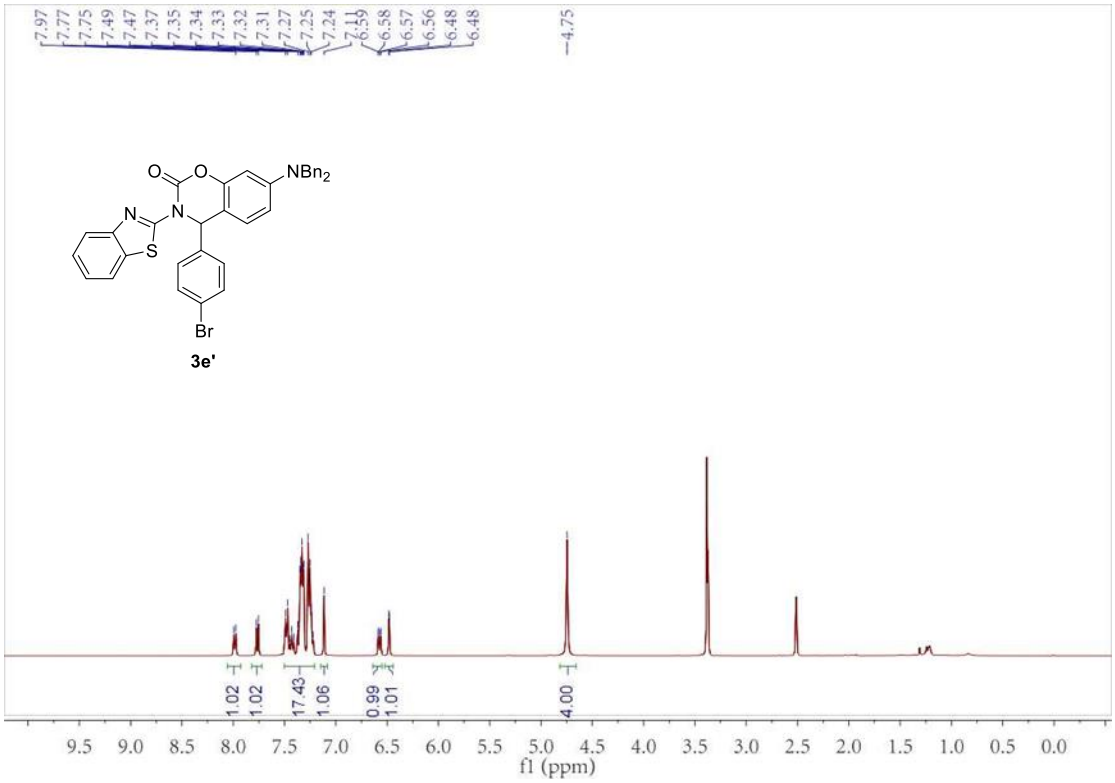
^{1}H NMR spectrum of compound **4b** (DMSO, 400 MHz)



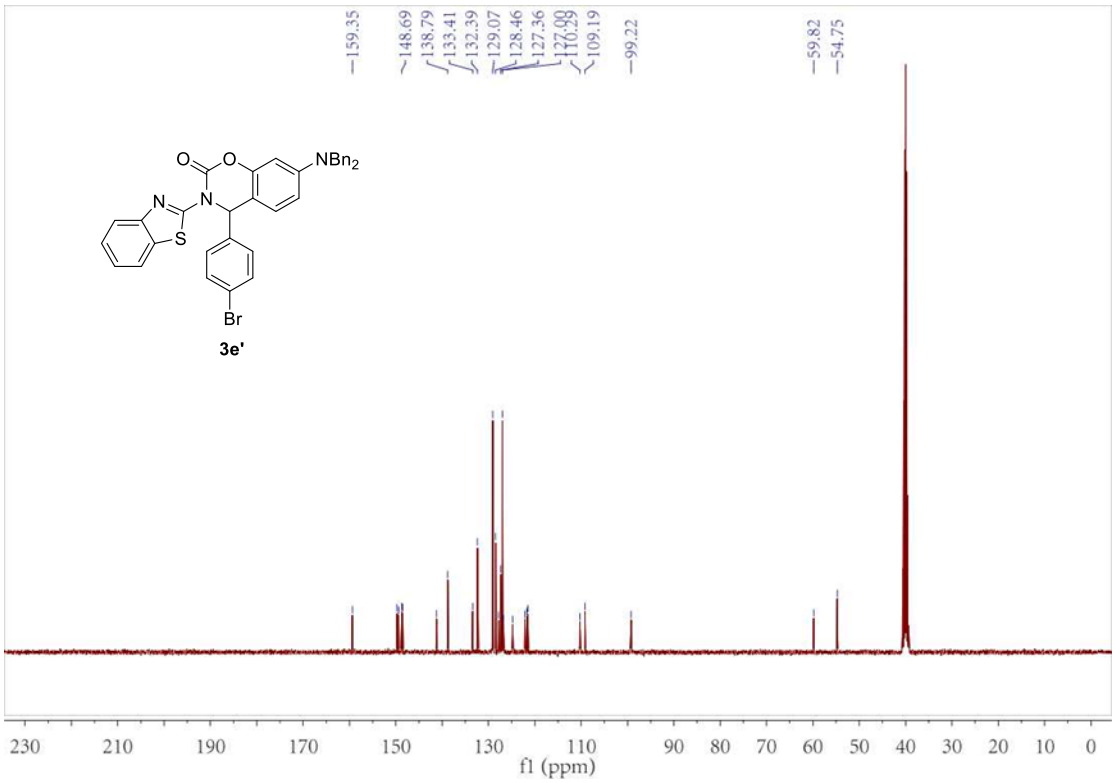
^{13}C NMR spectrum of compound **4b** (DMSO, 100 MHz)



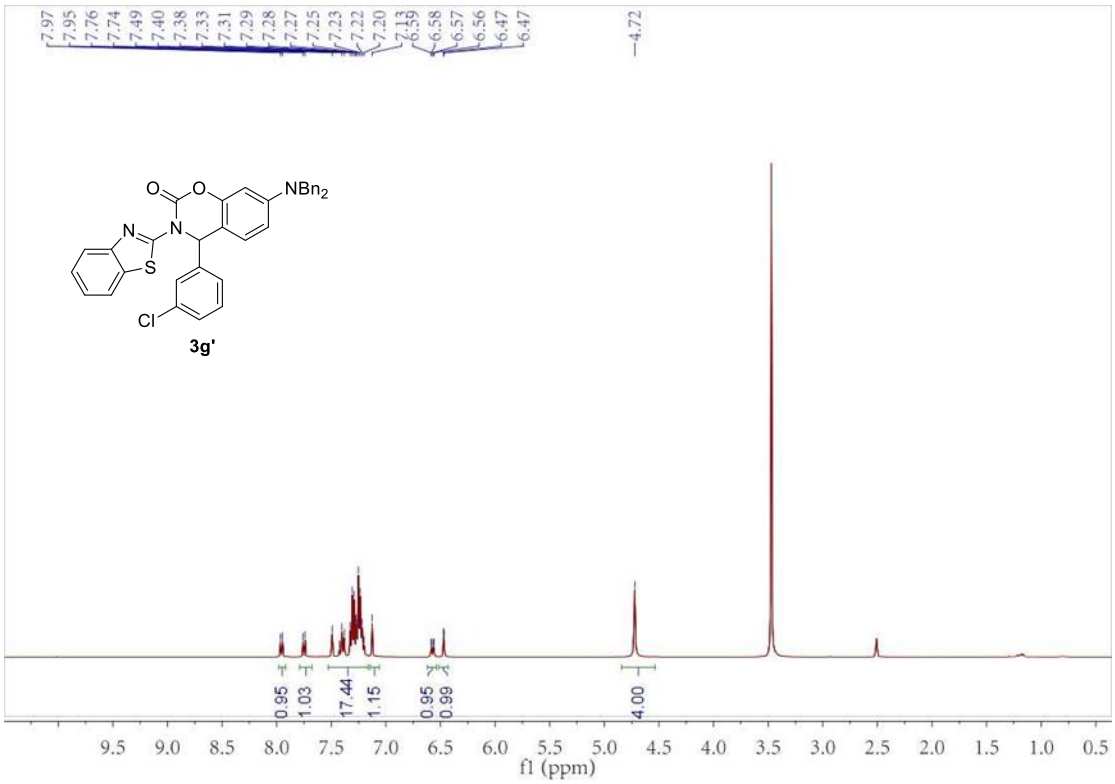
^{1}H NMR spectrum of compound **4c** ($CDCl_3$, 400 MHz)



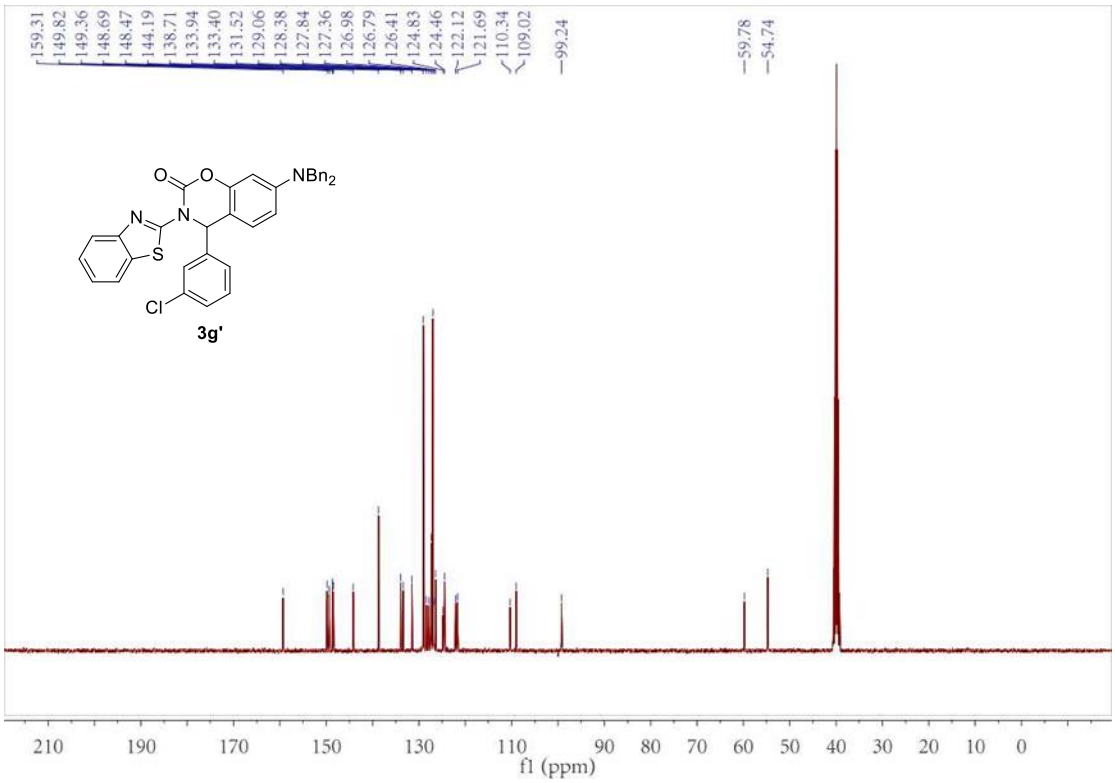
^{13}C NMR spectrum of compound **4c** (DMSO, 100 MHz)



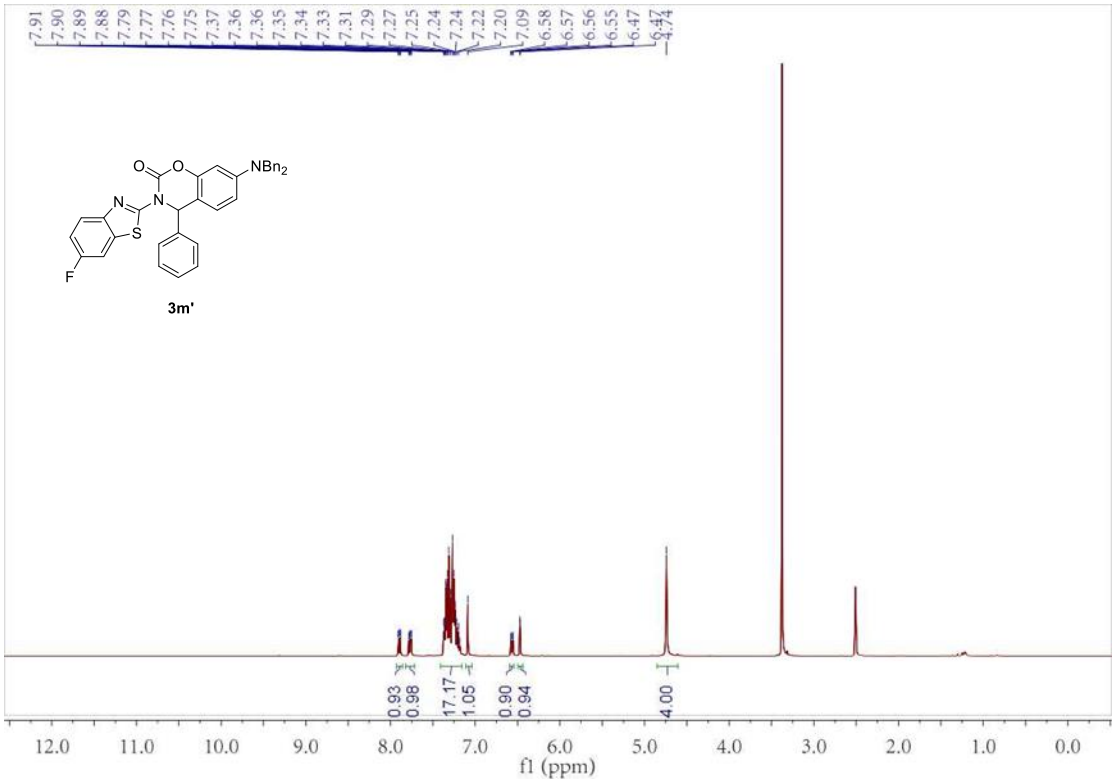
^{1}H NMR spectrum of compound **4d** ($CDCl_3$, 400 MHz)



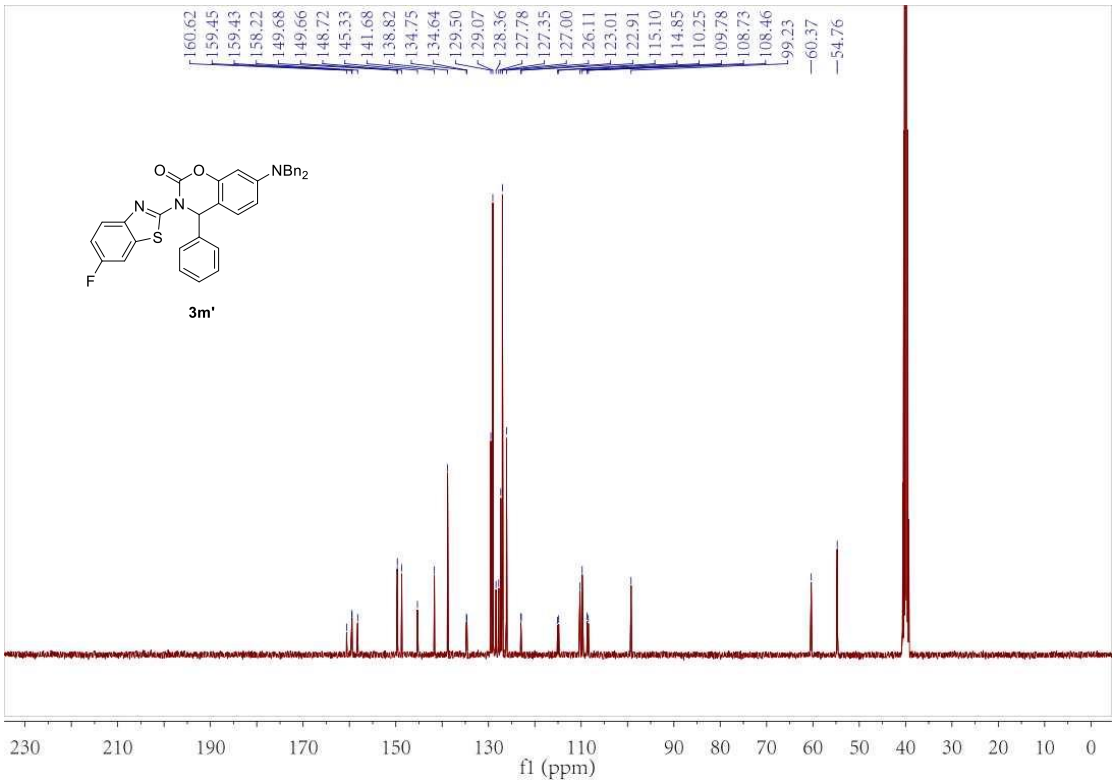
^{13}C NMR spectrum of compound **4d** ($CDCl_3$, 100 MHz)



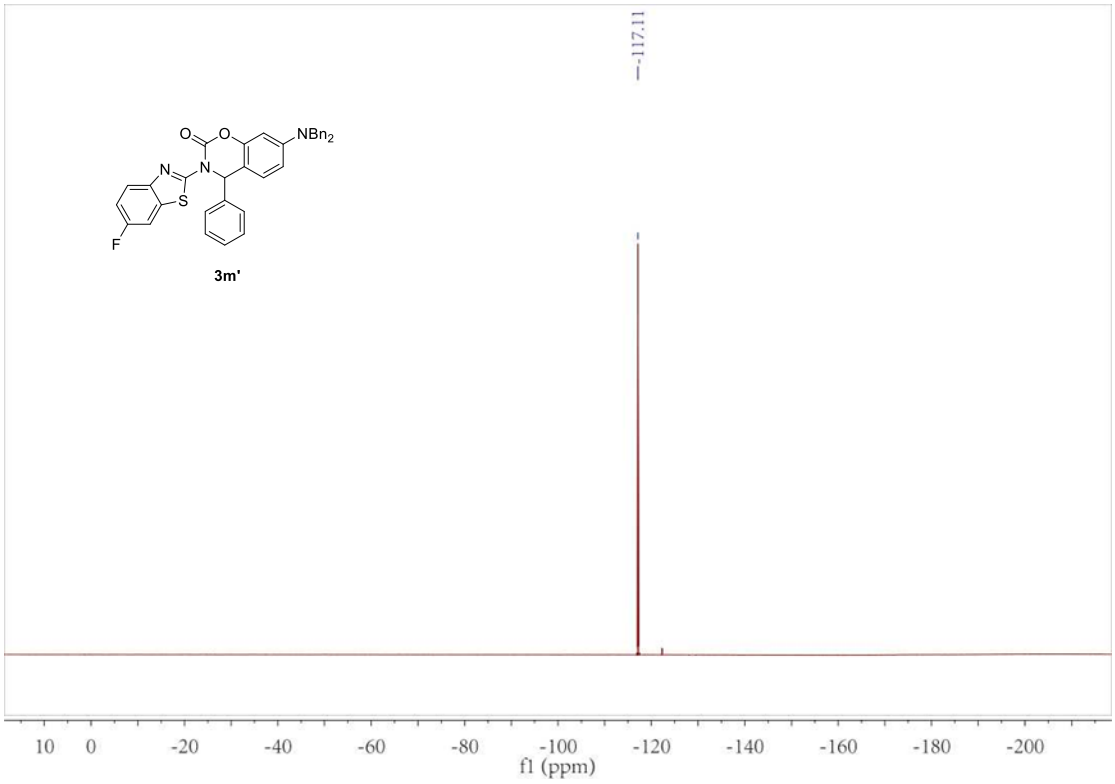
^{1}H NMR spectrum of compound **4e** (DMSO, 400 MHz)



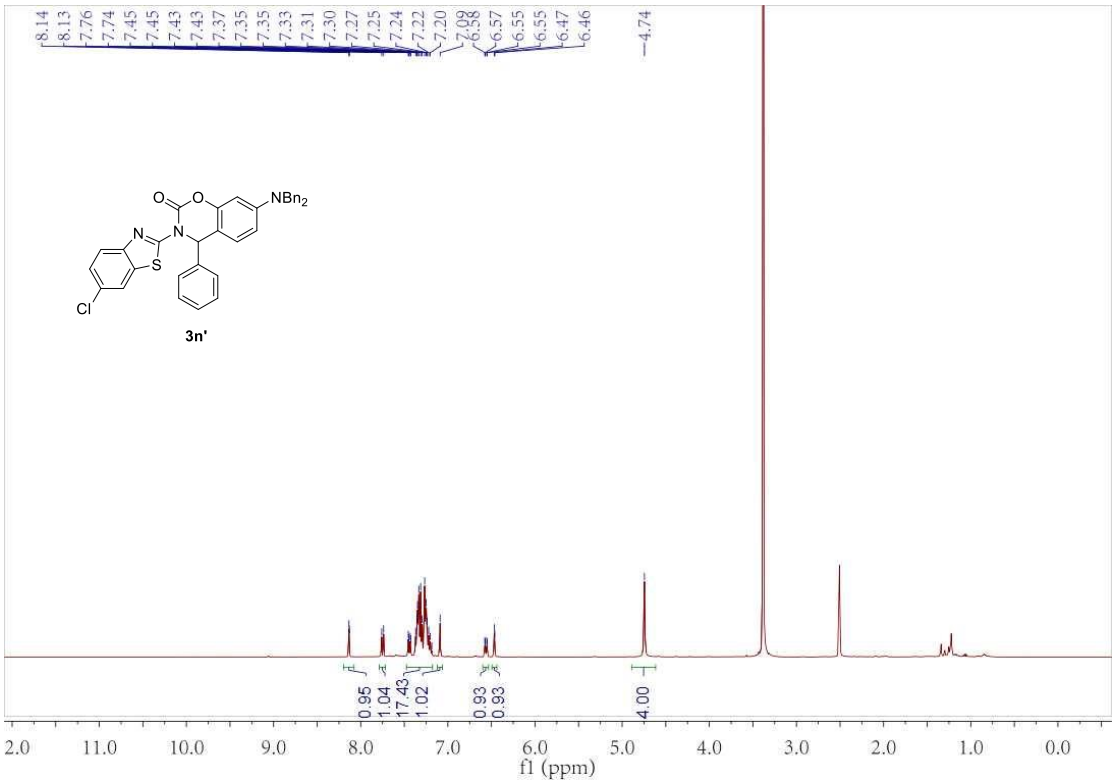
^{13}C NMR spectrum of compound **4e** (DMSO, 100 MHz)



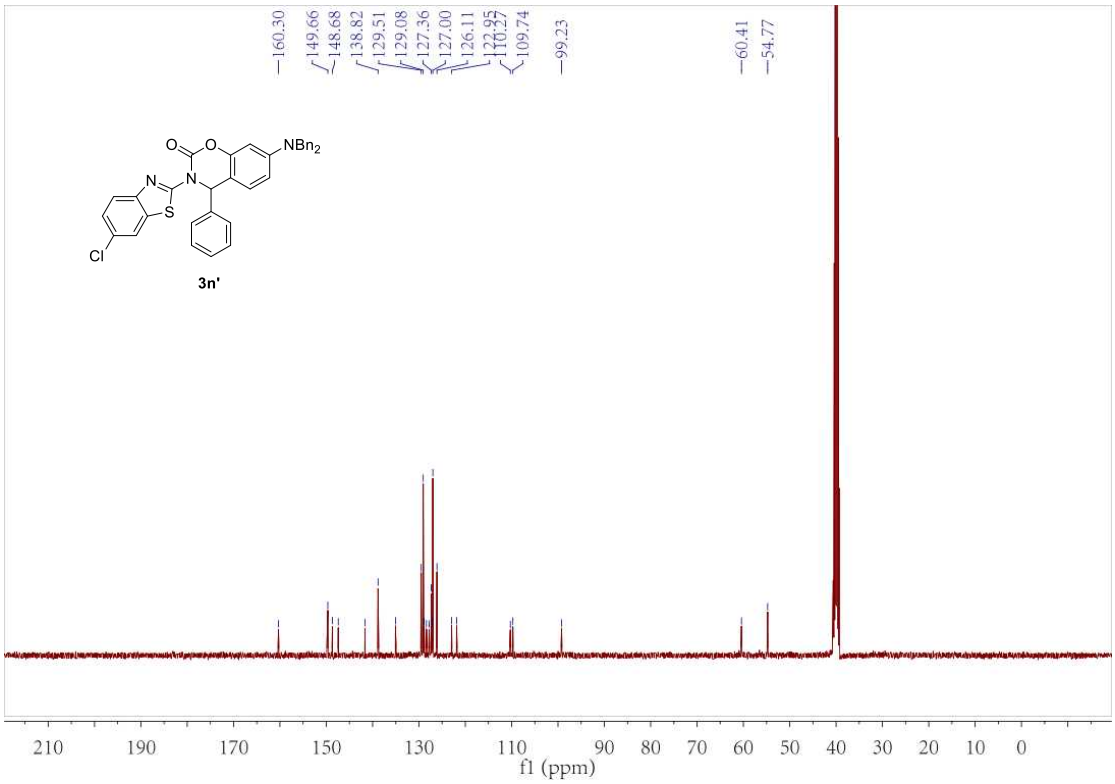
^{19}F NMR spectrum of compound **4e** (DMSO, 376 MHz)



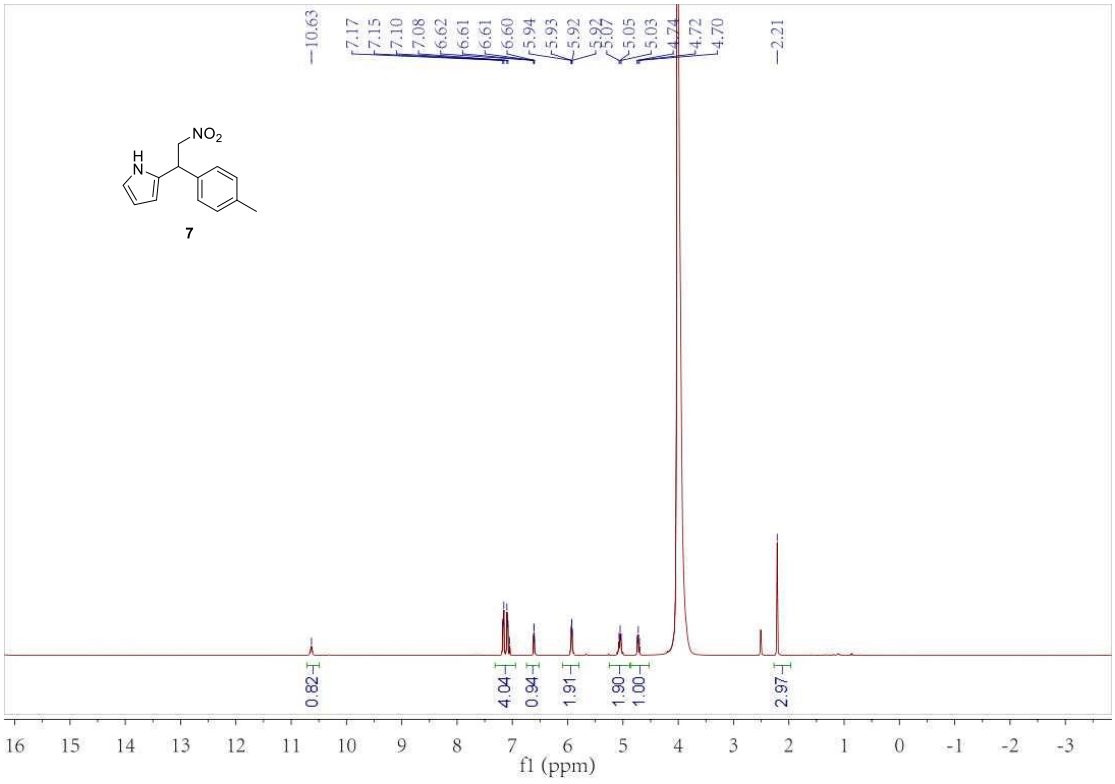
^{1}H NMR spectrum of compound **4f** (DMSO, 400 MHz)



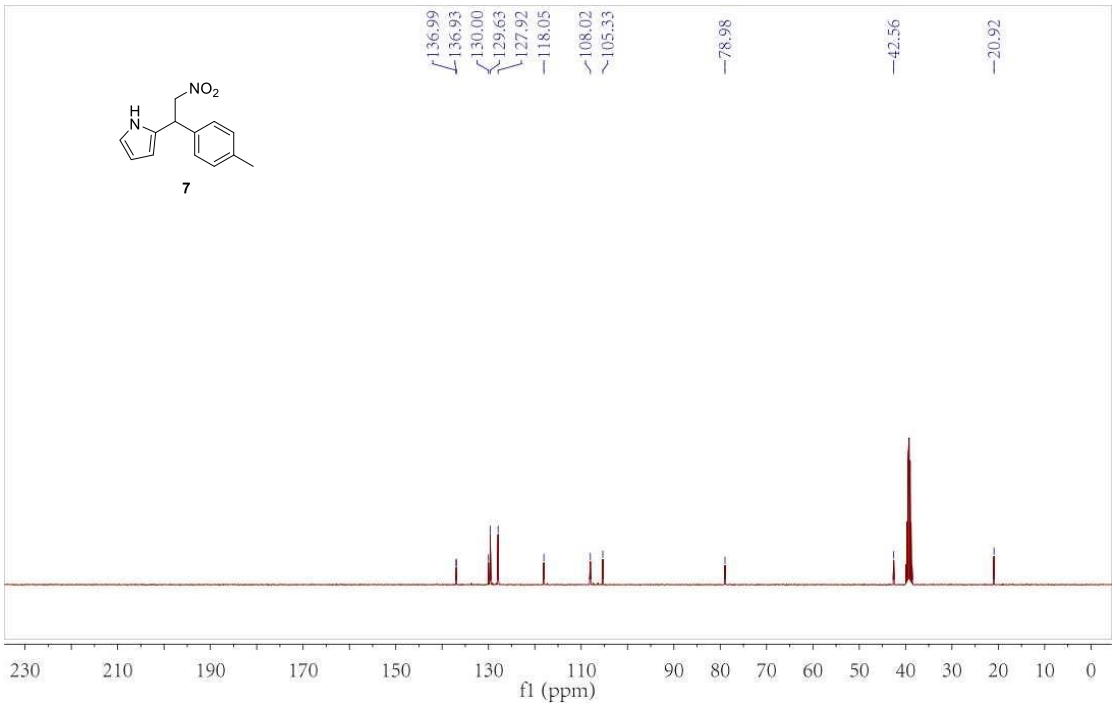
^{13}C NMR spectrum of compound **4f** (DMSO, 100 MHz)



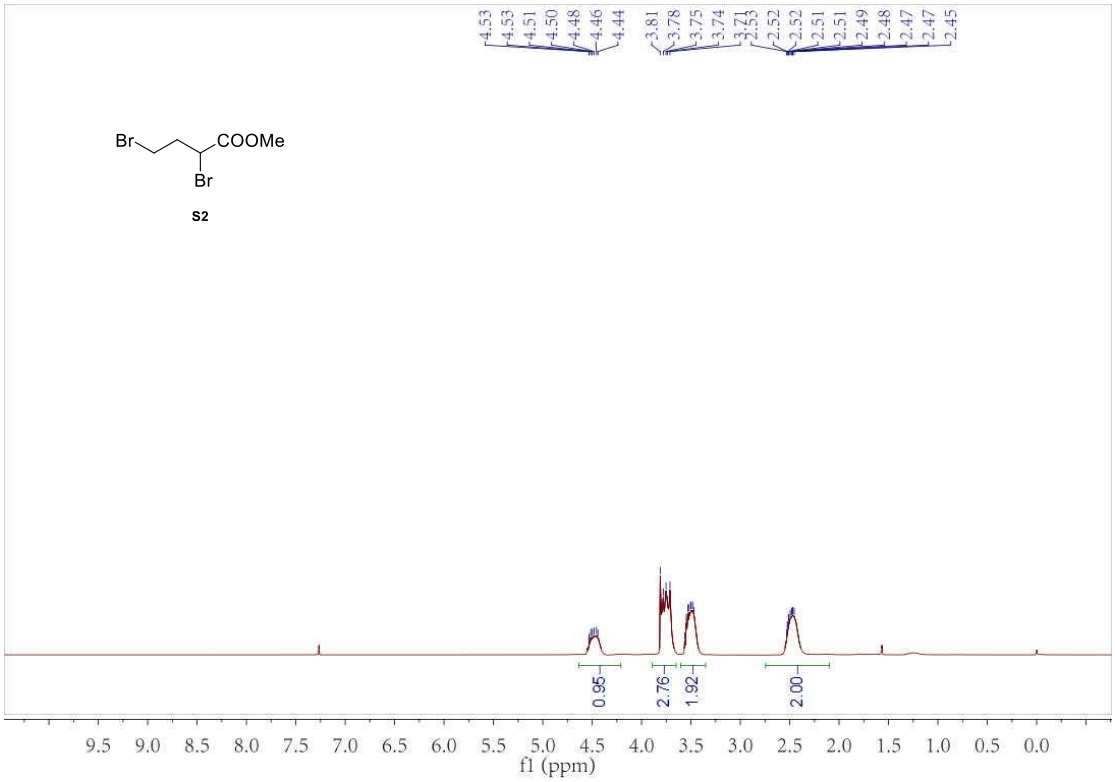
^{1}H NMR spectrum of compound **7** (DMSO, 400 MHz)



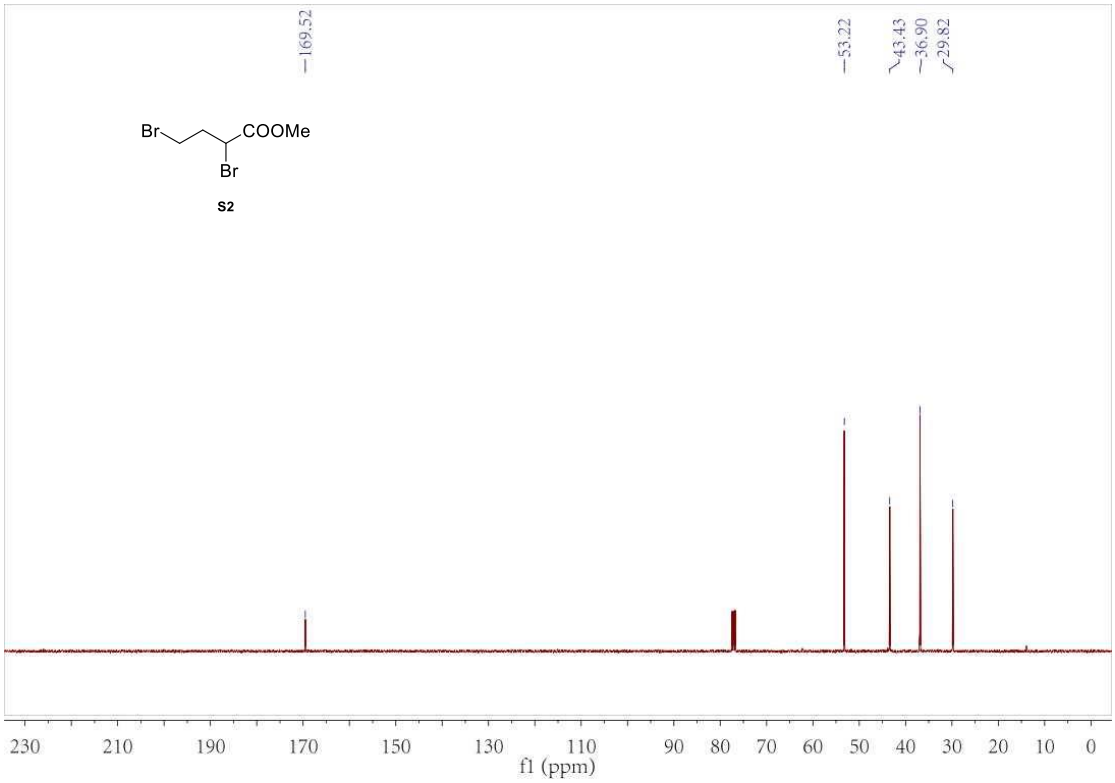
^{13}C NMR spectrum of compound **7** (DMSO, 100 MHz)



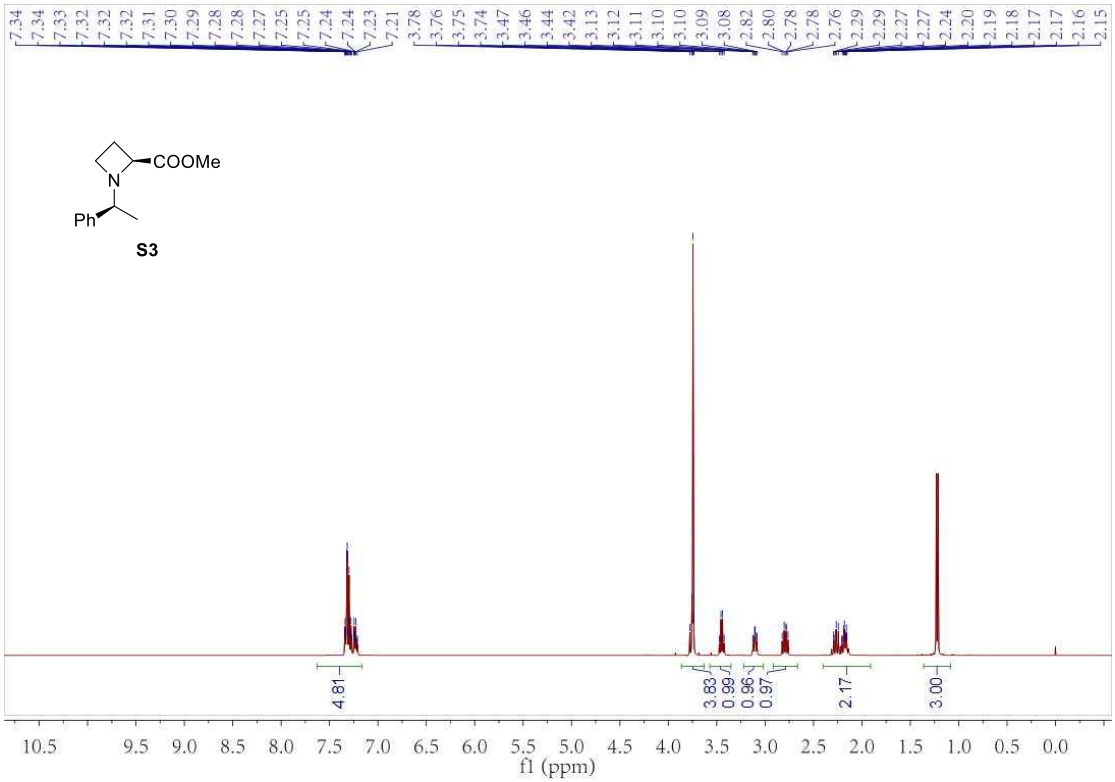
^{1}H NMR spectrum of compound **S2** ($CDCl_3$, 400 MHz)



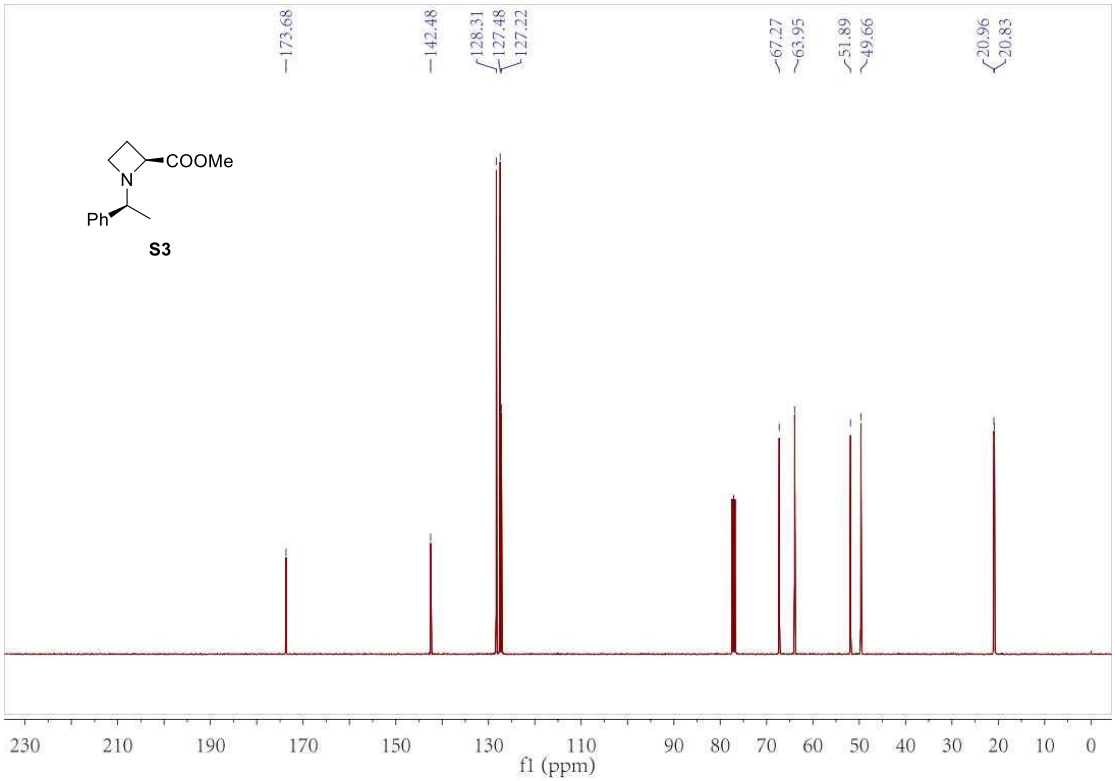
^{13}C NMR spectrum of compound **S2** ($CDCl_3$, 100 MHz)



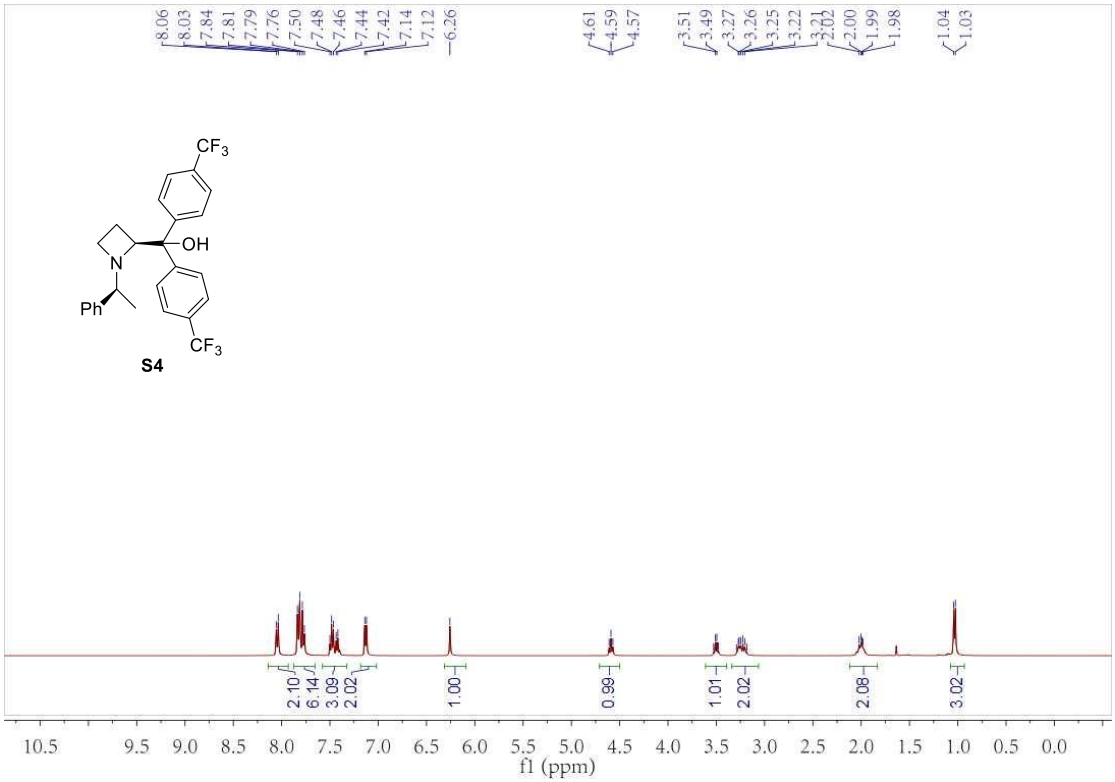
^{1}H NMR spectrum of compound **S3** ($CDCl_3$, 400 MHz)



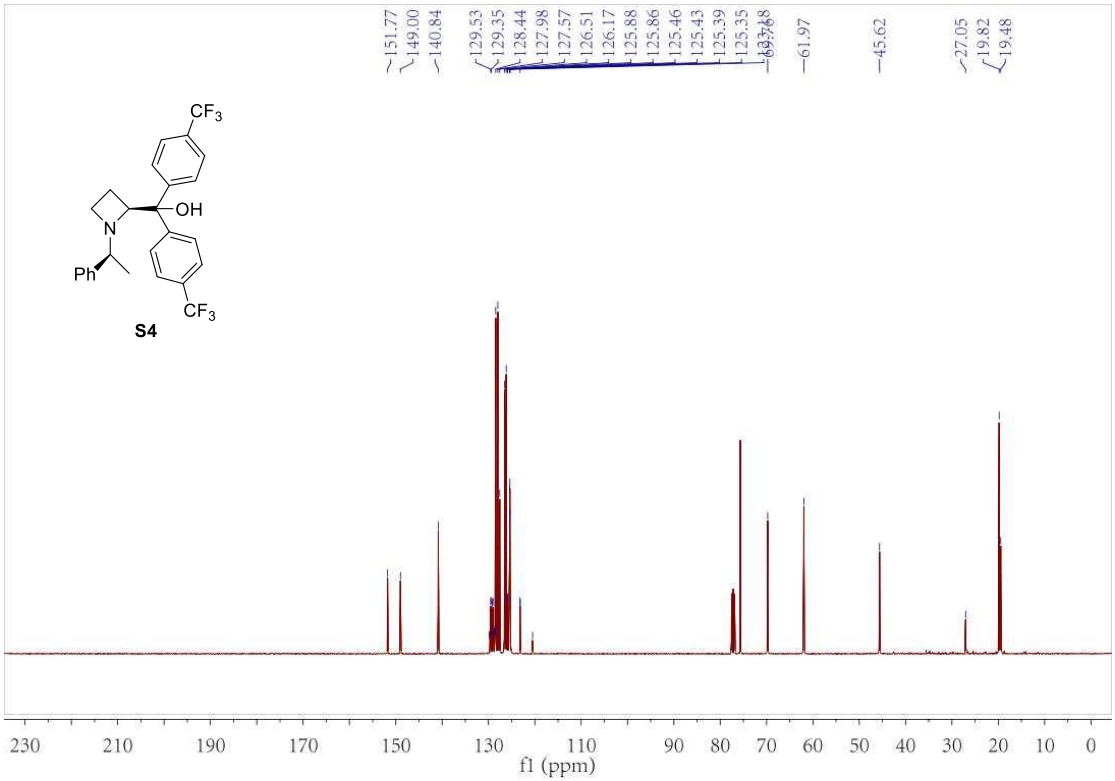
^{13}C NMR spectrum of compound **S3** ($CDCl_3$, 100 MHz)



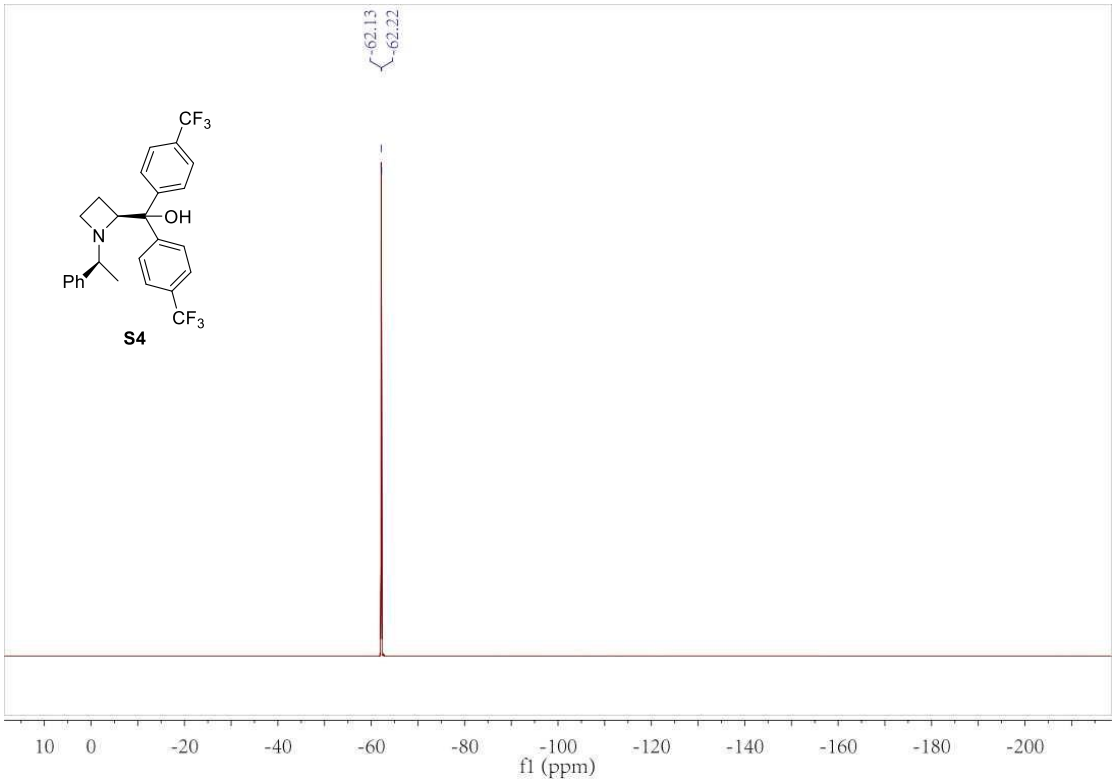
^{1}H NMR spectrum of compound **S4** ($CDCl_3$, 400 MHz)



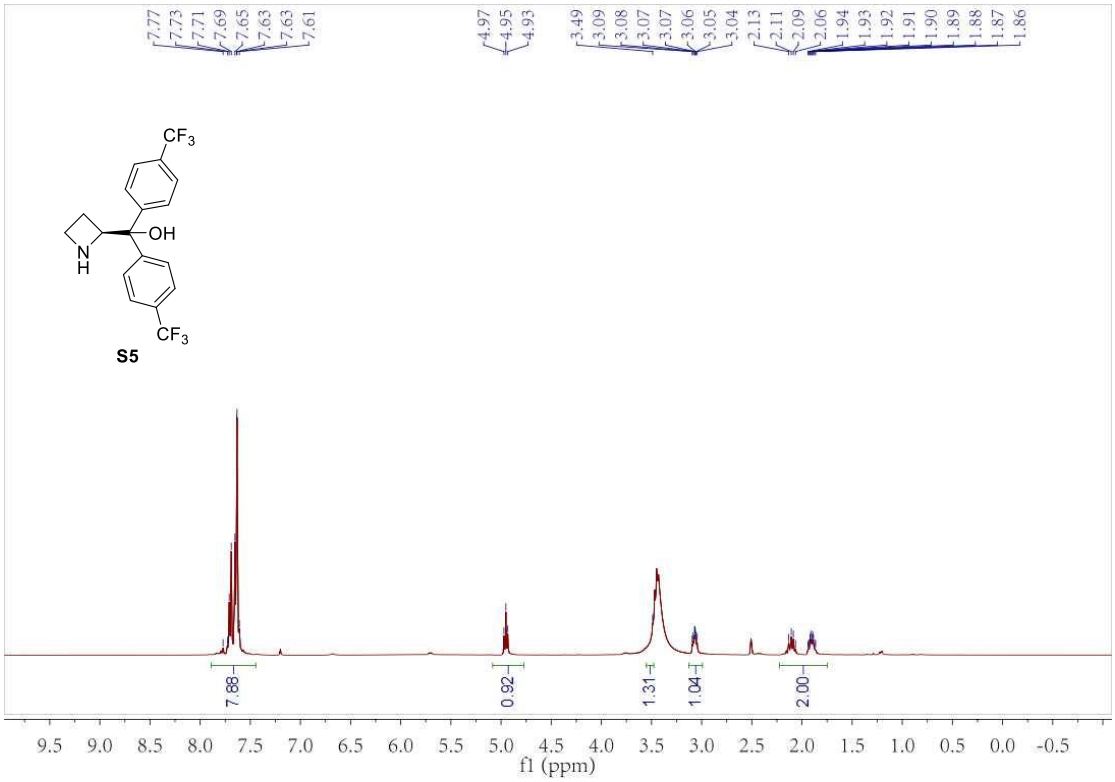
^{13}C NMR spectrum of compound **S4** ($CDCl_3$, 100 MHz)



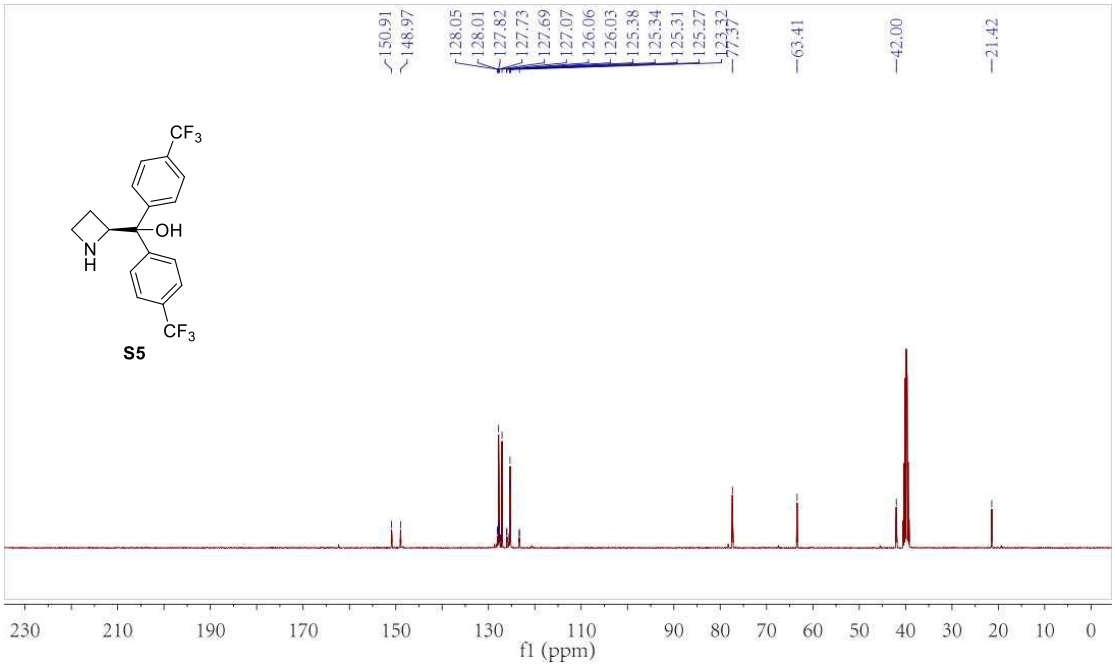
^{19}F NMR spectrum of compound **S4** ($CDCl_3$, 376 MHz)



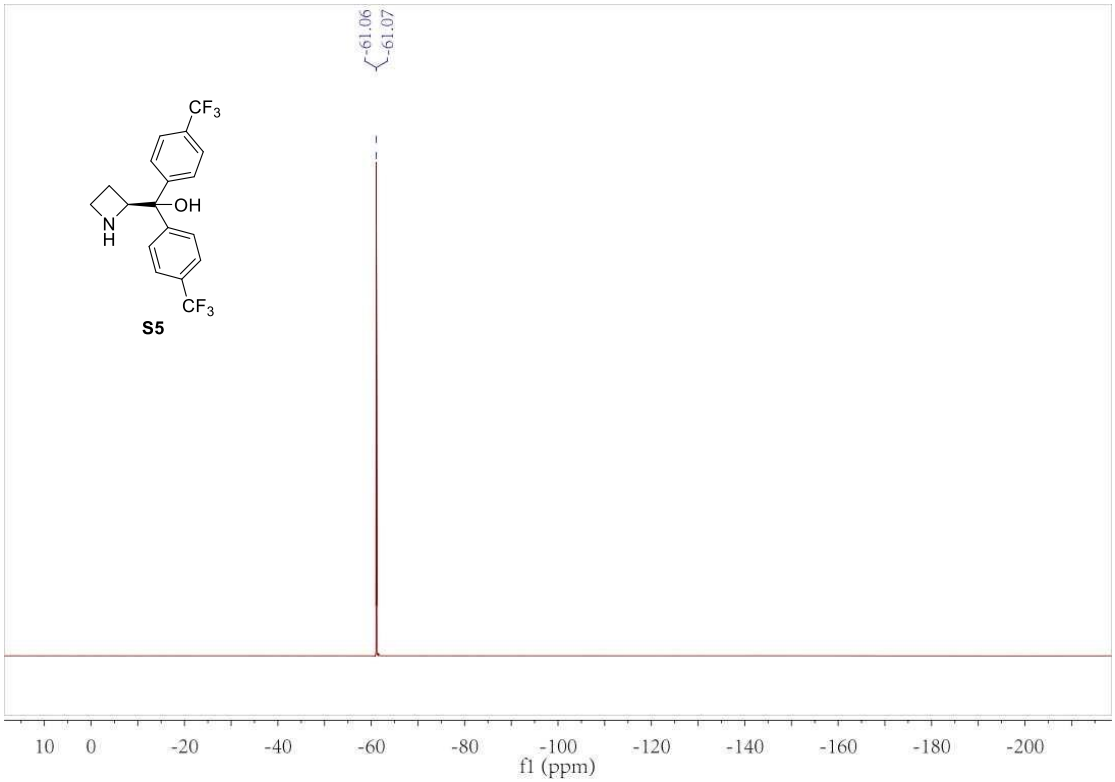
^{1}H NMR spectrum of compound **S5** (DMSO, 400 MHz)



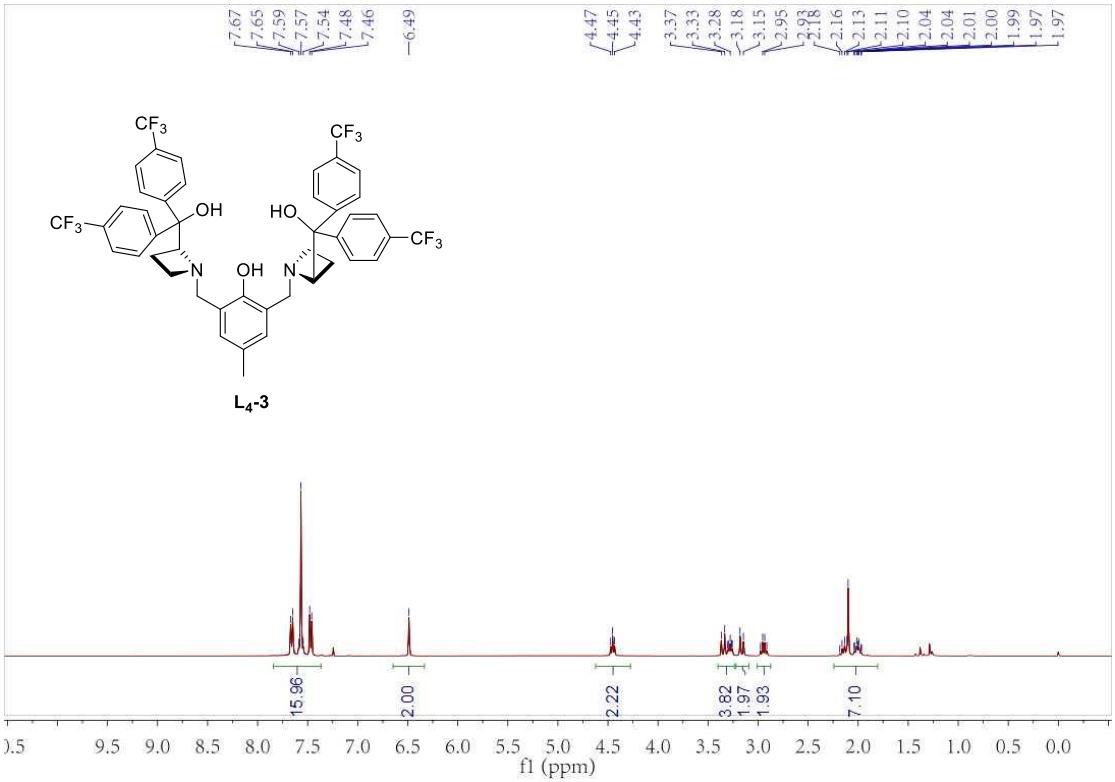
^{13}C NMR spectrum of compound **S5** (DMSO, 100 MHz)



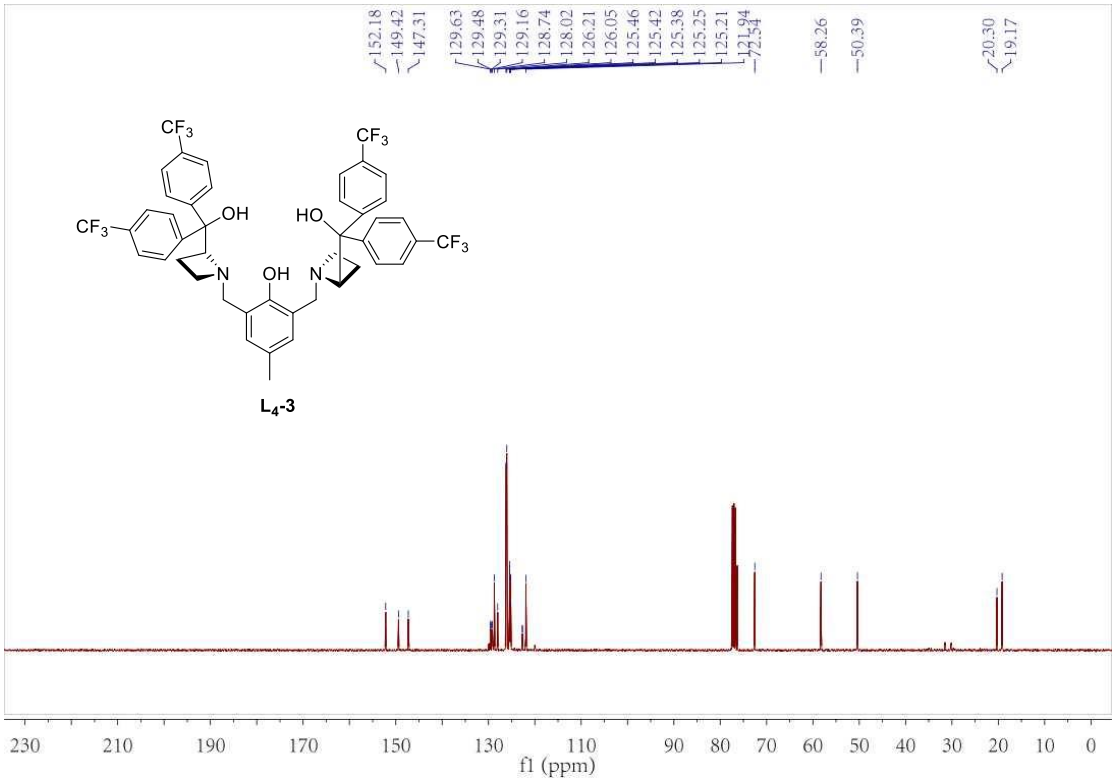
^{19}F NMR spectrum of compound **2-6** (DMSO, 376 MHz)



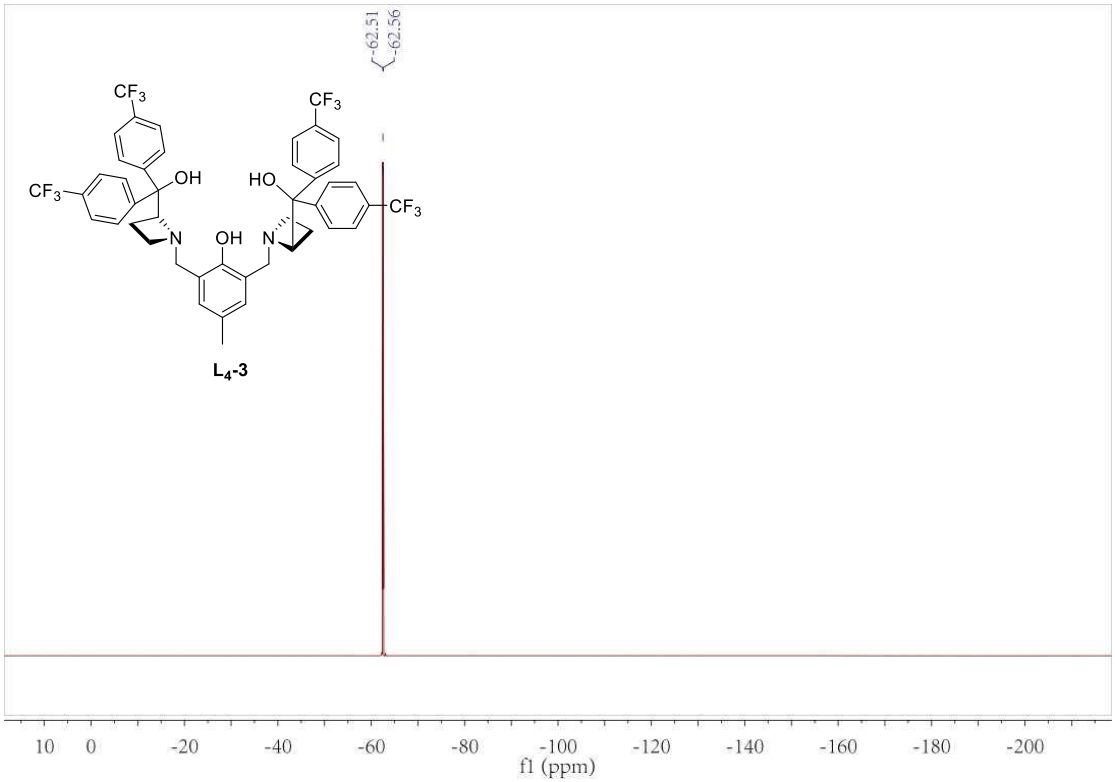
^{1}H NMR spectrum of compound **L_4-3** ($CDCl_3$, 400 MHz)



^{13}C NMR spectrum of compound **L_4-3** ($CDCl_3$, 400 MHz)



^{19}F NMR spectrum of compound **L_4-3** ($CDCl_3$, 376 MHz)



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