Supproting Information

Synthesis of Thiazolo[4,5-*d*]pyrimidine derivatives based on Purine via Solid-phase synthesis

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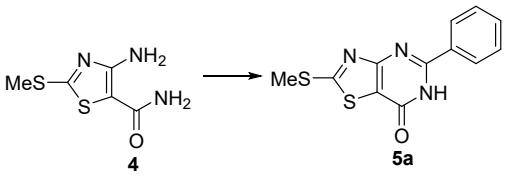
Contents

1. Experimental

1.1 General information

All the chemicals were reagent grade and used as purchased. The Merrifield resin (loading capacity 0.98 mmol/g, 100-200 mesh) was phurchased from BeadTech (Seoul, Korea). The reactions were monitored by TLC analysis using Merck silica gel 60 F-254 thin layer plates (Merck, Darmstadt, Germany). Flash column chromatography was carried out on Merck silica gel 60 (230–400 mesh). The crude products, which were derived from the solid support, were purified by parallel chromatography using CombiFlash (Isco, Lincoln, NE, USA). The ^{1}H NMR and ^{13}C NMR spectra were recorded in d units relative to the deuterated solvent ($CDCl_3$, DMSO-d_6, etc.) as an internal reference by the Bruker 500 MHz NMR instrument (Bruker, Billerca, MA, USA). High-performance liquid chromatography (HPLC) system, specifically the Ultimate 3000, coupled with the Q-Exactive Focus quadrupole-Orbitrap MS (Thermo Fisher Scientific, Mass Spectrometry Based Convergence Research Institute, Kyungpook National University, Bremen, Germany). Mass Spectrometry Based Convergence Research Institute, Kyungpook National University The solid-phase synthesis was monitored by FT-IR using JASCO FT-IR 4600

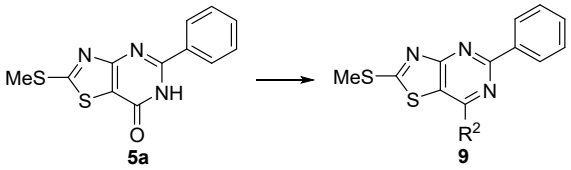
Table S1. Optimization of iodine catalyst mediated oxidative annulation reaction



Entry[a]	Solvent	I_2 (mol%)	Temp (°C)	Time (h)	Yield (%)[b]
1	DMSO	50	RT[d]	12	NR[c]
2	DMSO	10	RT	3	17
3	DMSO	10	130	1	69
4	DMSO	10	130	2	33
5	DMSO	10	40	12	NR
6	DMSO	10	60	12	Trace
7	DMSO	10	80	4	88
8	DMSO	20	80	4	90
9	DMSO	30	80	4	90
10	DMSO	120	100	0.5	95

a all reaction was performed on **4** (100 mg), benzaldehyde (1.2 eq) and DMSO (3 mL) b isolated yield c No reaction d Room temperature

Table S2. Optimization of thiazolo[4,5-*d*]pyrimidine **9** derivatives for R^2 substitution

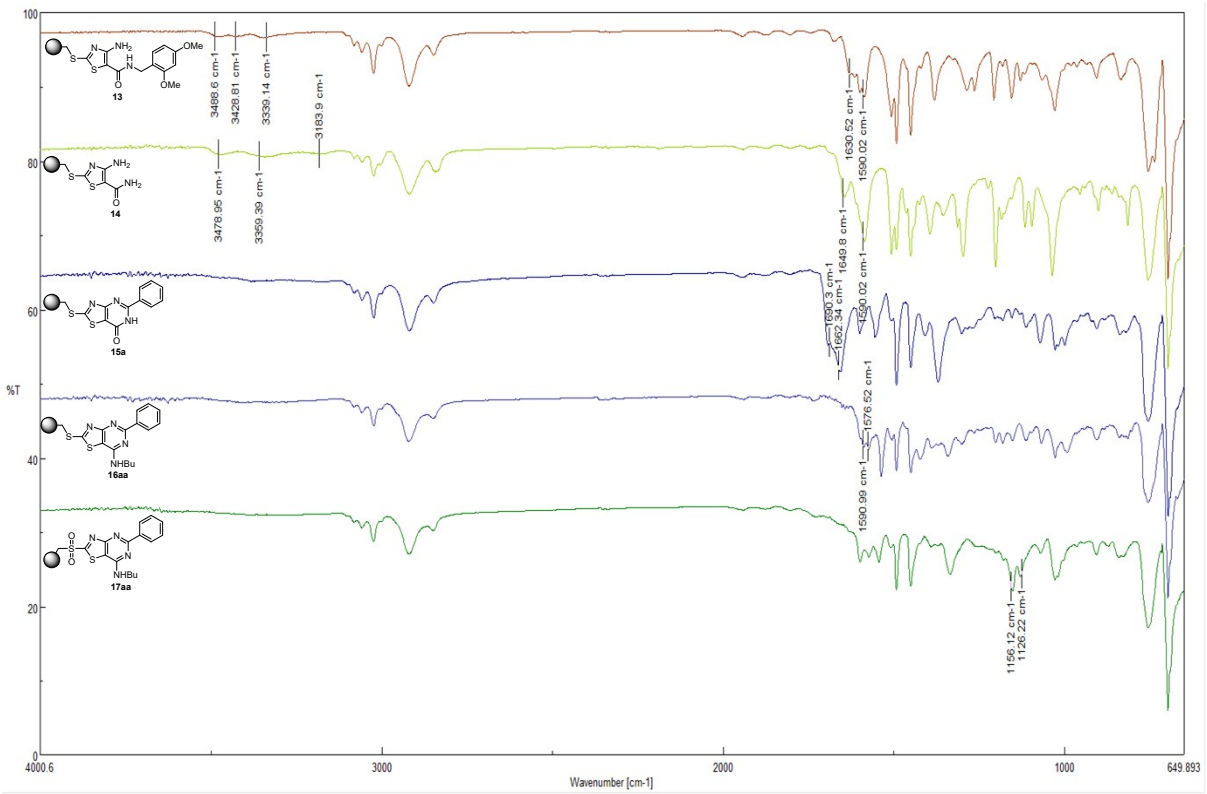


Entry[a]	Base (eq)	Reagent (eq)	Sovlent	Temp (°C)	Time (h)	Yield (%)[b]
1	DBU (1.2)	HATU (1.3)	DMF	rt[c] to 70	12	53
2	DBU (1.2)	EDC (1.3)/	DMF	rt	12	NR[d]

		HOBt (1.3)				
3	DBU (1.2)	DCC (1.3)	DMF	rt	12	NR
4	DBU (1.2)	BOP (1.3)	DMF	rt	8	90
5	Et_3N (1.2)	BOP (1.3)	DMF	rt	12	Trace

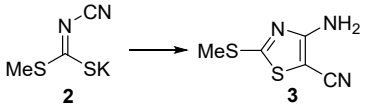
a all reaction was performed 5a (100 mg), butylamine (1.5 eq) and DMF (3 mL) under Ar b isolated yield c room temperature d No reaction

Figure S1. ATR-FTIR spectra of Solid-phase synthesis of thiazolo[4,5-*d*]pyrimidine derivatives **1**



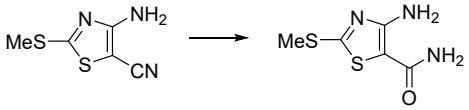
1.2 General procedure

Synthesis of 4-amino-2-(methylthio)thiazole-5-carbonitrile (**3**)[1]



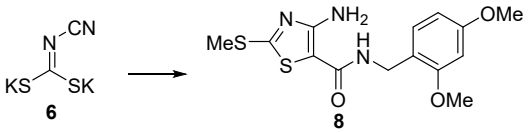
To a solution of potassium-methyl cyanocarbonimidodithioate **2** (4 g, 23.5 mmol) in acetone (50 mL) was added bromoacetonitrile (2 mL, 28.5 mmol) at 0 °C under Ar. The reaction mixture was stirred for 0 °C. The reaction mixture was stirred for 1 h at room temperature. After completion of the reaction (monitored by TLC), Et_3N (7 mL, 49.5 mmol) in acetone (20 mL) was dropwised to reaction mixture at 0 °C. The reaction mixture was stirred for 0.5 h at room temperature. After completion of the reaction (monitored by TLC), the reaction mixture was quenched with H_2O and then filtered, washed with H_2O. The solvent of residue was removed and then filtered with H_2O and dried in vacuum oven to give **3** (3.4 g, 85%) as a Ivory solid;

Synthesis of 4-amino-2-(methylthio)thiazole-5-carboxamide (**4**)



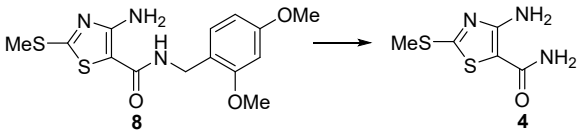
To a solution of 4-amino-2-(methylthio)thiazole-5-carbonitrile **3** (2g, 11.6 mmol) in H_2O (10 mL) was added diazobicyclo[5.4.0]undec-7ene (DBU) (2.1 mL, 14 mmol). The reaction was performed on microwave irridaiation (*MW*) at 100 °C for 0.5 h. The reaction mixture was quenched with 1N HCl for adjust pH 2~3. The solid was filtered with H_2O, and dried in vacuum oven to give **4** (2.1 g, 95%) as yellow solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 6.94 (s, 2H), 6.87 (s, 2H), 2.63 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 167.9, 164.7, 162.1, 92.4, 15.5. HRMS (ESI) m/z: $[M+H]^+$ Calcd $C_5H_8N_3OS_2^+$ 190.0103 Found 190.0103

Synthesis of 4-amino-*N*-(2,4-dimethoxybenzyl)-2-(methylthio)thiazole-5-carboxamide (**8**)



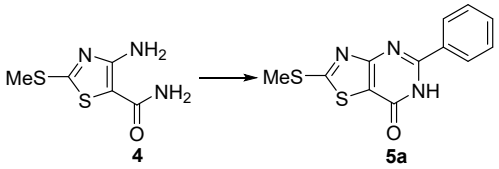
To a solution of potassium cyanocarbonimidodithioate **6** (67.0 mg, 0.34 mmol) in H_2O (0.8 mL) was added solution of 2-chloro-*N*-(2,4-dimethoxybenzyl)acetamide **7** (100.0 mg, 0.41 mmol) dissolved in acetone (4.0 mL) by dropwising at room temperature. After the addition was completed, the reaction mixture was stirred at room temperature for 1 h. The mixture was added LiOH (4.10 mg, 0.35 mmol) at room temperature and reaction mixture was heated under reflux 60 ℃ for 2 h. After cooling, CH_3I (21.16 μL, 0.34 mmol) in acetone was added dropwise. The mixture was stirred for 1 h at room temperature. The crude product was recrystallized from cold H_2O to give **8** (100.0 mg, 87%) as white solid; ; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (d, *J* = 8.2 Hz, 1H), 6.48 – 6.41 (m, 2H), 5.95 (s, 2H), 5.58 (t, *J* = 5.3 Hz, 1H), 4.45 (d, *J* = 5.7 Hz, 2H), 3.84 (s, 3H), 3.79 (s, 3H), 2.62 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 167.9, 163.4, 161.4, 160.6, 158.7, 130.5, 119.0, 104.1, 98.8, 94.3, 55.5, 55.5, 39.3, 16.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{14}H_{18}N_3O_3S_2^+$ 340.0784 Found 340.0785

Synthesis of 4-amino-2-(methylthio)thiazole-5-carboxamide (**4**)



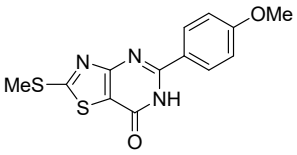
To a solution of 4-amino-*N*-(2,4-dimethoxybenzyl)-2-(methylthio)thiazole-5-carboxamide **8** (100.0 mg, 0.29 mmol) in CH_2Cl_2 (4 mL) was added trifluoroacetic acid (TFA) (0.66 mL, 8.7 mmol) at 0 °C. The reaction mixture was stirred for 5 h. After completion of the reaction (monitored by TLC), the reaction solvent was evaporated and quenched with $NaHCO_3$ solution. The mixture was extracted with CH_2Cl_2 several times. The organic layer was dried over $MgSO_4$. The solvent was removed and crude product was recrystallized from hexane:EtOAc to give 4 (43 mg, 81%) as a yellow solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 6.94 (s, 2H), 6.87 (s, 2H), 2.63 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 167.9, 164.7, 162.1, 92.4, 15.5. HRMS (ESI) m/z: $[M+H]^+$ Calcd $C_5H_8N_3OS_2^+$ 190.0103 Found 190.0103

Synthesis of 2-(methylthio)-5-phenylthiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5a**)



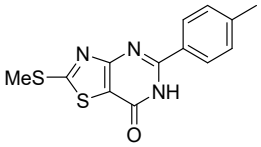
To a solution of 4-amino-2-(methylthio)thiazole-5-carboxamide **4** (100 mg, 0.53 mmol) in DMSO (3 mL) was added benzaldhyde (64 µL, 0.63 mmol) and iodine (14 mg, 0.053 mmol) at room temperature under atmosphere air. The reaction mixture was stirred at 80 °C for 8 h. After completion of the reaction (monitored by TLC), quenched with $Na_2S_2O_3$ solution and added H_2O. The solid was filter with H_2O and washed with H_2O several times. The solid dried in vacuum oven to give **5a** (131 mg, 90%) as ivory solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.55 (s, 1H), 8.28 – 8.20 (m, 2H), 7.66 – 7.53 (m, 3H), 2.86 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$+TFA) δ 182.7, 167.0, 160.2, 156.8, 133.7, 129.8, 127.8, 113.6, 16.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{10}N_3OS_2^+$ 276.0260 Found 276.0258

5-(4-Methoxyphenyl)-2-(methylthio)thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5b**)



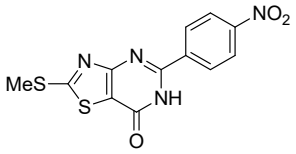
95% yield as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.83 (s, 1H), 8.20 – 8.12 (m, 2H), 7.13 – 7.07 (m, 2H), 3.85 (s, 3H), 2.82 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$+TFA) δ 183.3, 165.0, 164.7, 159.6, 156.7, 130.1, 120.5, 115.5, 112.7, 55.9, 16.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{13}H_{12}N_3O_2S_2^+$ 306.0365 Found 306.0366

2-(Methylthio)-5-(*p*-tolyl)thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5c**)



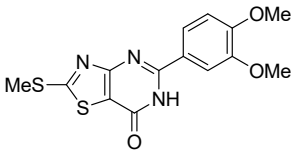
94% yield as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.92 (s, 1H), 8.06 (d, J = 8.3 Hz, 2H), 7.37 (d, J = 8.0 Hz, 2H), 2.82 (s, 3H), 2.40 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$+TFA) δ 183.9, 164.3, 159.4, 157.5, 146.2, 130.9, 128.0, 125.4, 113.4, 21.8, 16.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{13}H_{12}N_3OS_2^+$ 290.0416 Found 290.0414

2-(Methylthio)-5-(4-nitrophenyl)thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5d**)



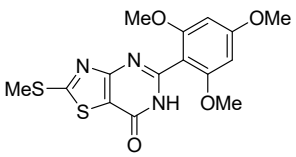
95% yield as a pale brown solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 13.33 (s, 1H), 8.39 (s, 4H), 2.83 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$+TFA) δ 183.3, 167.5, 160.3, 154.1, 150.5, 136.0, 129.0, 124.8, 114.6, 16.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_9N_4O_3S_2^+$ 321.0111 Found 321.0110

5-(3,4-Dimethoxyphenyl)-2-(methylthio)thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5e**)



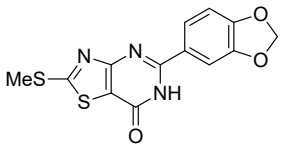
78% yield as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.86 (s, 1H), 7.85 (dd, J = 8.5, 2.2 Hz, 1H), 7.78 (d, J = 2.2 Hz, 1H), 7.13 (d, J = 8.7 Hz, 1H), 3.87 (s, 3H), 3.85 (s, 3H), 2.82 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$+TFA) δ 184.0, 164.0, 159.4, 156.6, 154.4, 149.8, 122.9, 120.1, 112.7, 111.0, 110.1, 56.4, 56.2, 16.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{14}H_{14}N_3O_3S_2^+$ 336.0471 Found 336.0470

2-(Methylthio)-5-(2,4,6-trimethoxyphenyl)thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5f**)



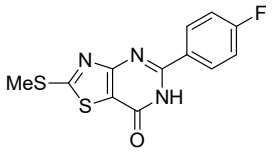
84% yield as a pale yellow solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.73 (s, 1H), 6.33 (s, 2H), 3.85 (s, 3H), 3.73 (s, 6H), 2.80 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 176.3, 167.7, 163.5, 159.6, 158.4, 152.7, 114.6, 104.4, 90.7, 56.0, 55.6, 16.3. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{15}H_{16}N_3O_4S_2^+$ 366.0577 Found 366.0576

5-(Benzo[*d*][1,3]dioxol-5-yl)-2-(methylthio)thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5g**)



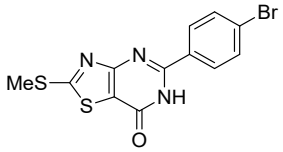
91% yield as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.80 (s, 1H), 7.78 (dd, *J* = 8.3, 1.9 Hz, 1H), 7.70 (d, *J* = 1.8 Hz, 1H), 7.09 (d, *J* = 8.3 Hz, 1H), 6.15 (s, 2H), 2.81 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$+TFA) δ 183.3, 165.6, 159.7, 156.5, 153.0, 149.3, 123.9, 122.7, 112.9, 109.5, 107.8, 102.7, 16.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{13}H_{10}N_3O_3S_2^+$ 320.0158 Found 320.0157

5-(4-Fluorophenyl)-2-(methylthio)thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5h**)



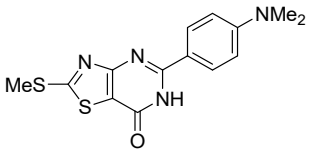
98% yield as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 13.03 (s, 1H), 8.27 – 8.18 (m, 2H), 7.41 (t, *J* = 8.9 Hz, 2H), 2.82 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$+TFA) δ 183.5, 167.3, 166.5, 165.2, 160.1, 156.0, 130.5, 130.5, 125.8, 125.8, 117.4, 117.2, 113.3, 16.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_9FN_3OS_2^+$ 294.0166 Found 294.0164

5-(4-Bromophenyl)-2-(methylthio)thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5i**)



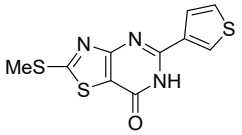
90% yield as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 13.08 (s, 1H), 8.13 – 8.06 (m, 2H), 7.82 – 7.74 (m, 2H), 2.82 (s, 3H).^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$+TFA) δ 182.2, 167.8, 160.4, 155.4, 133.0, 129.2, 129.1, 128.6, 113.5, 16.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_9BrN_3OS_2^+$ 353.9365 Found 353.9364

5-(4-(Dimethylamino)phenyl)-2-(methylthio)thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5k**)



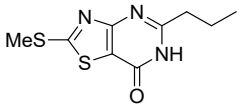
78% yield as a pale khaki solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.55 (s, 1H), 8.08 (d, J = 9.1 Hz, 2H), 6.79 (d, J = 9.2 Hz, 2H), 3.02 (s, 6H), 2.80 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$+TFA) δ 183.2, 166.7, 160.1, 153.9, 146.1, 131.5, 130.5, 121.2, 114.3, 46.9, 16.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{14}H_{15}N_4OS_2^+$ 319.0682 Found 319.0681

2-(Methylthio)-5-(thiophen-3-yl)thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5l**)



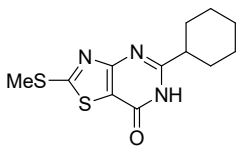
88% yield as a pale grey solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.91 (s, 1H), 8.63 (dd, J = 2.9, 1.2 Hz, 1H), 7.85 (dd, J = 5.1, 1.2 Hz, 1H), 7.73 (dd, J = 5.1, 2.9 Hz, 1H), 2.81 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 175.8, 166.8, 157.7, 151.8, 134.6, 129.6, 127.6, 126.9, 113.9, 15.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{10}H_8N_3OS_3^+$ 281.9824 Found 281.9822

2-(Methylthio)-5-propylthiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5m**)



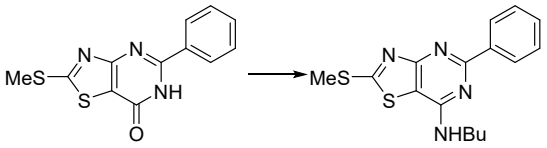
18% yield as a yellow solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.66 (s, 1H), 2.78 (s, 3H), 2.65 – 2.58 (m, 2H), 1.77 – 1.67 (m, 2H), 0.91 (t, J = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 177.5, 168.0, 161.2, 160.0, 113.7, 37.2, 21.0, 16.3, 13.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_9H_{12}N_3OS_2^+$ 242.0416 Found 242.0415

5-Cyclohexyl-2-(methylthio)thiazolo[4,5-*d*]pyrimidin-7(6*H*)-one (**5n**)



80% yield as a grey solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 11.42 (s, 1H), 2.83 (s, 3H), 2.70 (tt, *J* = 11.9, 3.4 Hz, 1H), 2.07 – 1.98 (m, 2H), 1.94 – 1.85 (m, 2H), 1.80 – 1.65 (m, 3H), 1.49 – 1.37 (m, 2H), 1.35 – 1.27 (m, 1H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 177.3, 168.0, 164.7, 159.5, 113.9, 44.3, 30.9, 25.9, 25.6, 16.3. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{12}H_{16}N_3OS_2^+$ 282.0729 Found 282.0728

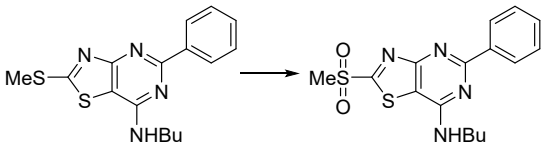
Synthesis of *N*-butyl-2-(methylthio)-5-phenylthiazolo[4,5-*d*]pyrimidin-7-amine (**9aa**)



5a **9aa**

To a solution of 2-(methylthio)-5-phenylthiazolo[4,5-*d*]pyrimidin-7(6*H*)-one **5a** (100 mg, 0.36 mmol) in DMF (5 mL) was added DBU (68 µL, 0.43 mmol) and BOP (206 mg, 0.46 mmol) at room temperature. The reaction mixture was stirred for 15 min and added butylamine (54 µL,0.54 mmol) at room temperature. The reaction mixture was stirred for 6 h. After completion of the reaction (monitored by TLC), the reaction mixture was extracted with EtOAc, washed with $NaHCO_3$ solution. The combined organic layer was washed with brine. The organic layer was dried over $MgSO_4$ and filtered. The solvent was removed and the residue purified by silica gel column chromatography (Hx:EtOAc, 2:1) to give **9aa** (107 mg, 90%) as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 – 8.51 (m, 2H), 7.49 – 7.41 (m, 3H), 4.88 (s, 1H), 3.68 (dt, *J* = 7.1, 6.0 Hz, 2H), 2.84 (s, 3H), 1.74 – 1.63 (m, 2H), 1.45 (dq, *J* = 14.7, 7.4 Hz, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 174.0, 169.9, 162.6, 157.2, 138.0, 130.3, 128.5, 128.3, 106.4, 41.6, 32.0, 20.2, 16.3, 13.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd $C_{16}H_{19}N_4S_2^+$ 331.1046 Found 331.1045

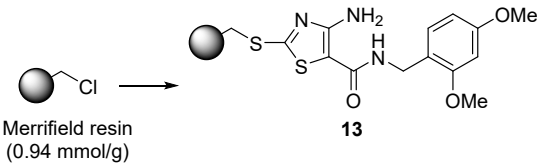
Synthesis of *N*-butyl-2-(methylsulfonyl)-5-phenylthiazolo[4,5-*d*]pyrimidin-7-amine (**10aa**)



9aa **10aa**

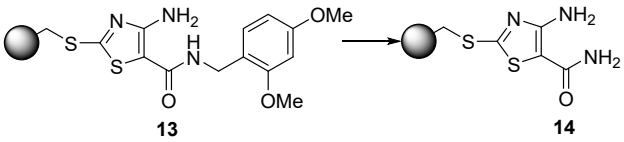
To a solution of *N*-butyl-2-(methylthio)-5-phenylthiazolo[4,5-*d*]pyrimidin-7-amine **9aa** (50 mg, 0.15 mmol) in CH_2Cl_2 (4 mL) was added *m*CPBA (87 mg, 0.37m, 77%) at room temperature. The reaction mixture was stirred at 12 h. After completion of the reaction (monitored by TLC), the reaction mixture was extracted with CH_2Cl_2, washed with $NaHCO_3$ solution. The combined organic layer was washed with brine. The organic layer was dried over $MgSO_4$ and filtered. The solvent was removed and the residue purified by silica gel column chromatography (Hx:EtOAc, 2:1) to give **9aa** (45 mg, 82%) as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.66 (t, *J* = 5.4 Hz, 1H), 8.50 – 8.41 (m, 2H), 7.57 – 7.49 (m, 3H), 3.68 (dd, *J* = 12.6, 6.9 Hz, 2H), 3.63 (s, 3H), 1.73 – 1.65 (m, 2H), 1.49 – 1.38 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 171.2, 168.1, 162.3, 157.9, 137.4, 130.7, 128.5, 127.9, 110.7, 41.9, 40.3, 30.6, 19.6, 13.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{16}H_{19}N_4O_2S_2^+$ 363.0944 Found 363.0942

Preparation of 4-amino-*N*-(2,4-dimethoxybenzyl)-2-mercaptothiazole-5-carboxamide resin (**13**)



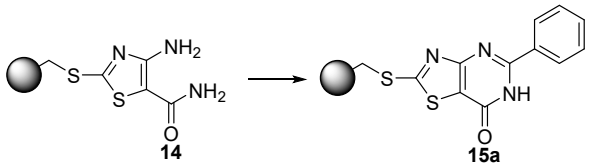
Merrifield rein (2.5 g, theoretically 2.35 mmol) in DMF (35 mL) was swollen for 0.5 h and added 4-amino-*N*-(2,4-dimethoxybenzyl)-2-mercaptothiazole-5-carboxamide **8** (1.6 g, 3.76 mmol) and Et_3N (0.6 mL, 4.35 mmol) at room temperature. The reaction mixture was shaken at 60 °C for overnight. After completion of the reaction (monitored by ATR-FTIR), the resin was filtered and washed with H_2O, DMF, MeOH and CH_2Cl_2 and dried in a vacuum oven to give **13** (3.48 g, theoretically 0.673 mmol/g) as a yellow resin.

Preparation of 4-amino-2-mercaptothiazole-5-carboxamide (**14**)



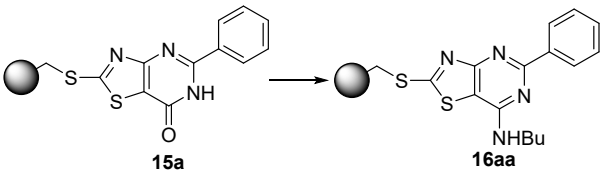
To a mixture of 4-amino-*N*-(2,4-dimethoxybenzyl)-2-mercaptothiazole-5-carboxamide resin **14** (1.0 g, theoretically 0.674 mmol) in CH_2Cl_2 (30 mL) was added TFA (2 mL, 25 mmol) under ice bath. The resin was shaken overnight at room temperature. After completion of the reaction (monitored by ATR-FTIR), the resin was filtered and washed with H_2O, DMF, MeOH and CH_2Cl_2 and dried in a vacuum oven to give **14** (0.85 g, theoretically 0.79 mmol/g) as a yellow resin.

Preparation of 2-mercapto-5-phenylthiazolo[4,5-*d*]pyrimidin-7(6*H*)-one resin (**15a**)



To a mixture of 4-amino-2-mercaptothiazole-5-carboxamide **14** (0.85 g, theoretically 0.674 mmol) in DMSO (15 mL) was added benzaldehyde (0.18 mL, 1.7 mmol) and iodine (21 mg, 0.085 mmol) at room temperature. The resin was stirred for overnight at 80 °C under open air. After completion of the reaction (monitored by ATR-FTIR), the resin was filtered and washed with H_2O, DMF, MeOH and CH_2Cl_2 and dried in a vacuum oven to give **15a** (0.88 g, theoretically 0.765 mmol/g) as a yellow resin.

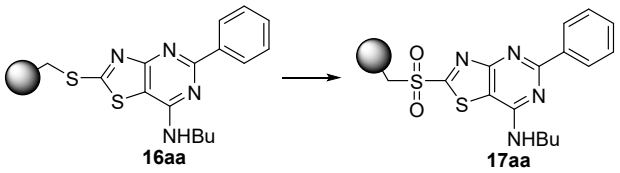
Preparation of 7-(butylamino)-5-phenylthiazolo[4,5-*d*]pyrimidine-2-thiol (**16aa**)



To a mixture of 2-mercapto-5-phenylthiazolo[4,5-*d*]pyrimidin-7(6*H*)-one resin **15a** (0.87 g, theoretically 0.674 mmol) in DMF (20 mL) was added DBU (0.25 mL, 1.7 mmol) and BOP (0.86 mg, 1.95 mmol) at room temperature under Ar. The resin was shaken for 2 h and added butylamine (0.25 mL, 2.55 mmol) at room temperature for x h. After

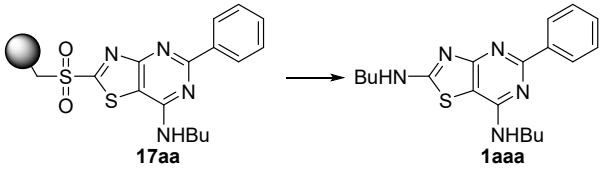
completion of the reaction (monitored by ATR-FTIR), the resin was filtered and washed with H_2O, DMF, MeOH and CH_2Cl_2 and dried in a vacuum oven to give **16aa** (0.89 g, theoretically 0.75 mmol/g) as a yellow resin.

Preparation of *N*-butyl-2-hydrosulfonyl-5-phenylthiazolo[4,5-*d*]pyrimidin-7-amine (**17aa**)



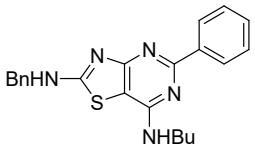
To a mixture of 7-(butylamino)-5-phenylthiazolo[4,5-*d*]pyrimidine-2-thiol **16aa** (0.87 g, theoretically 0.674 mmol) in CH_2Cl_2 (20 mL) was added *m*CPBA (0.62 g, 2.69 mmol) at room temperature under Ar. The resin was shaken for overnight and after completion of the reaction (monitored by ATR-FTIR), the resin was filtered and washed with H_2O, DMF, MeOH and CH_2Cl_2 and dried in a vacuum oven to give **17aa** (0.82 g, theoretically 0.82 mmol/g) as a yellow resin.

Synthesis of N^2-benzyl-N^7-butyl-5-phenylthiazolo[4,5-*d*]pyrimidine-2,7-diamine (**1aaa**)



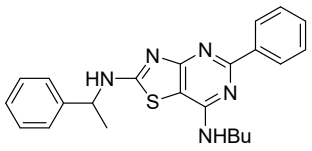
The *N*-butyl-2-hydrosulfonyl-5-phenylthiazolo[4,5-*d*]pyrimidin-7-amine resin **17aa** (0.4 g, theoretically 0.325 mmol) in CH_2Cl_2 was swollen for 0.5 h and added butylamine (0.10 mL, 0.9 mmol), Et_3N (0.14 mL, 0.9 mmol) at room temperature. The reaction mixture was shaken at room temperature for overnight and then filtered, washed several times with MeOH and CH_2Cl_2. The solvent was removed, and the residue was purified by flash silica gel column chromatography (hexane : EtOAc = 2:1) to give **1aaa** (46 mg, 36%) as a yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 – 8.46 (m, 2H), 8.05 (s, 1H), 7.48 – 7.37 (m, 3H), 4.59 (s, 1H), 3.66 (dd, *J* = 13.0, 7.0 Hz, 2H), 3.46 (t, *J* = 7.3 Hz, 2H), 1.88 – 1.79 (m, 2H), 1.72 – 1.64 (m, 2H), 1.51 – 1.40 (m, 4H), 0.96 (dt, *J* = 19.9, 7.4 Hz, 6H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.3, 170.0, 161.9, 156.7, 138.7, 129.8, 128.2, 128.1, 99.5, 45.9, 41.5, 32.3, 31.3, 20.2, 20.2, 14.0, 13.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{26}N_5S^+$ 356.1903 Found 356.1902

N^2-Benzyl-*N*^{7}-butyl-5-phenylthiazolo[4,5-*d*]pyrimidine-2,7-diamine (**1aab**)



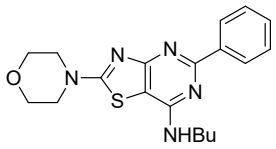
19% yield as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.34 (s, 1H), 8.37 – 8.28 (m, 2H), 7.73 (s, 1H), 7.48 (dd, *J* = 6.6, 3.6 Hz, 3H), 7.43 – 7.35 (m, 4H), 7.29 (ddd, *J* = 8.6, 3.6, 1.8 Hz, 1H), 4.66 (d, *J* = 4.7 Hz, 2H), 3.55 (dd, *J* = 12.6, 6.9 Hz, 2H), 1.66 – 1.57 (m, 2H), 1.44 – 1.33 (m, 2H), 0.93 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) 170.4, 158.8, 155.8, 138.1, 136.9, 130.3, 128.5, 128.3, 127.6, 127.4, 127.2, 99.9, 47.4, 40.1, 31.2, 19.6, 13.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{22}H_{24}N_5S^+$ 390.1747 Found 390.1746

N^7-Butyl-5-phenyl-*N*^{2}-(1-phenylethyl)thiazolo[4,5-*d*]pyrimidine-2,7-diamine (**1aac**)



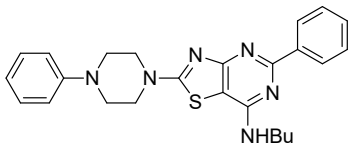
6% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 – 8.41 (m, 2H), 7.70 (s, 1H), 7.54 – 7.47 (m, 2H), 7.42 – 7.33 (m, 5H), 7.33 – 7.27 (m, 1H), 4.88 (d, *J* = 5.8 Hz, 1H), 4.46 (s, 1H), 3.63 (dd, *J* = 13.0, 7.1 Hz, 2H), 1.79 (d, *J* = 6.8 Hz, 3H), 1.65 (dt, *J* = 12.8, 7.4 Hz, 2H), 1.44 (dq, *J* = 14.7, 7.4 Hz, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 170.3, 169.7, 162.1, 156.8, 142.6, 138.7, 129.9, 129.0, 128.4, 128.2, 127.9, 126.5, 100.2, 56.1, 41.5, 32.4, 23.5, 20.2, 14.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{26}N_5S^+$ 404.1903 Found 404.1903

N-Butyl-2-morpholino-5-phenylthiazolo[4,5-*d*]pyrimidin-7-amine (**1aaf**)



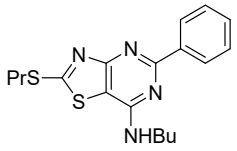
38% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.55 – 8.50 (m, 2H), 7.47 – 7.40 (m, 3H), 4.58 (s, 1H), 3.87 – 3.79 (m, 4H), 3.76 – 3.70 (m, 4H), 3.67 (td, *J* = 7.1, 5.9 Hz, 2H), 1.73 – 1.64 (m, 2H), 1.46 (dq, *J* = 14.7, 7.4 Hz, 2H), 0.98 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.2, 170.2, 162.2, 156.8, 138.4, 130.0, 128.3, 128.1, 100.3, 66.2, 48.6, 41.6, 32.3, 20.2, 13.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{24}N_5OS^+$ 370.1696 Found 370.1693

N-Butyl-5-phenyl-2-(4-phenylpiperazin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1aag**)



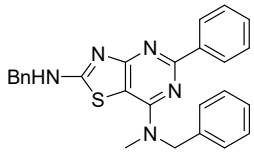
25% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.54 (ddd, *J* = 6.8, 4.6, 2.9 Hz, 2H), 7.50 – 7.40 (m, 3H), 7.37 – 7.29 (m, 2H), 7.02 – 6.87 (m, 3H), 4.87 (s, 1H), 3.97 – 3.81 (m, 4H), 3.68 (dd, *J* = 13.0, 7.1 Hz, 2H), 3.44 – 3.28 (m, 4H), 1.77 – 1.62 (m, 2H), 1.48 (dq, *J* = 14.7, 7.4 Hz, 2H), 1.00 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 170.9, 170.3, 162.2, 156.8, 150.8, 138.5, 129.9, 129.4, 128.4, 128.1, 120.9, 117.0, 100.4, 49.2, 48.4, 41.6, 32.3, 20.2, 14.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{29}N_6S^+$ 445.2169 Found 445.2169

N-Butyl-5-phenyl-2-(propylthio)thiazolo[4,5-d]pyrimidin-7-amine (**1aai**)



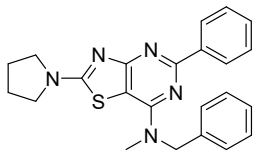
34% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 – 8.50 (m, 2H), 7.50 – 7.40 (m, 3H), 4.83 (s, 1H), 3.70 (dd, *J* = 13.0, 7.1 Hz, 2H), 3.49 – 3.41 (m, 2H), 1.90 – 1.81 (m, 2H), 1.74 – 1.66 (m, 2H), 1.46 (dq, *J* = 14.7, 7.4 Hz, 2H), 1.07 (t, *J* = 7.4 Hz, 3H), 0.98 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 173.4, 170.0, 162.5, 157.1, 138.1, 130.3, 128.5, 128.2, 106.4, 41.6, 35.7, 32.0, 22.6, 20.2, 13.9, 13.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{18}H_{23}N_4S_2^+$ 359.1359 Found 359.1358

N^2,*N*^{7}-Dibenzyl-*N*^{7}-methyl-5-phenylthiazolo[4,5-*d*]pyrimidine-2,7-diamine (**1abb**)



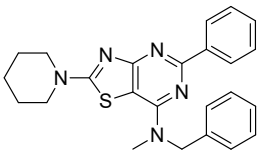
16% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 (dd, *J* = 6.7, 3.0 Hz, 2H), 7.44 – 7.27 (m, 13H), 5.95 (s, 1H), 5.03 (s, 2H), 4.72 (s, 2H), 3.32 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 170.3, 159.7, 157.3, 138.4, 138.3, 138.2, 129.8, 128.6, 128.4, 128.2, 127.5, 127.3, 127.2, 127.1, 126.9, 99.1, 52.7, 47.1, 36.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{24}N_5S^+$ 438.1747 Found 438.1746

N-Benzyl-*N*-methyl-5-phenyl-2-(pyrrolidin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1abd**)



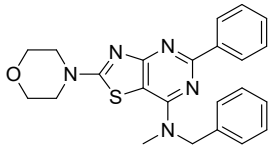
42% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 – 8.50 (m, 2H), 7.48 – 7.38 (m, 3H), 7.38 – 7.26 (m, 5H), 5.01 (s, 2H), 3.86 – 3.74 (m, 4H), 3.73 – 3.62 (m, 4H), 3.30 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.4, 168.0, 161.2, 157.9, 138.6, 138.2, 129.8, 128.8, 128.4, 128.0, 127.5, 127.4, 99.7, 53.6, 49.6, 36.4, 25.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{24}N_5S^+$ 402.1747 Found 402.1744

N-Benzyl-*N*-methyl-5-phenyl-2-(piperidin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1abe**)



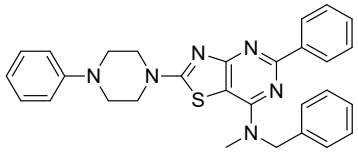
21% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.58 – 8.50 (m, 2H), 7.45 – 7.38 (m, 3H), 7.37 – 7.27 (m, 5H), 5.03 (s, 2H), 3.66 (s, 4H), 3.31 (s, 3H), 1.69 (s, 6H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.4, 171.2, 161.2, 157.8, 138.6, 138.2, 129.8, 128.8, 128.3, 128.0, 127.5, 127.4, 99.6, 53.5, 49.5, 36.3, 25.4, 24.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{26}N_5S^+$ 416.1903 Found 416.1900

N-Benzyl-*N*-methyl-2-morpholino-5-phenylthiazolo[4,5-*d*]pyrimidin-7-amine (**1abf**)



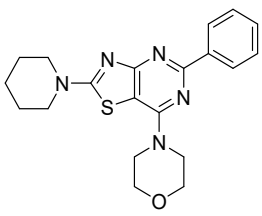
49% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 – 8.50 (m, 2H), 7.46 – 7.39 (m, 3H), 7.36 – 7.28 (m, 5H), 5.04 (s, 2H), 3.87 – 3.79 (m, 4H), 3.75 – 3.66 (m, 4H), 3.33 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.4, 168.0, 161.2, 157.9, 138.6, 138.2, 129.8, 128.8, 128.4, 128.0, 127.5, 127.4, 99.7, 53.5, 49.6, 36.4, 25.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{24}N_5OS^+$ 418.1696 Found 418.1693

N-Benzyl-*N*-methyl-5-phenyl-2-(4-phenylpiperazin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1abg**)



63% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.59 – 8.52 (m, 2H), 7.47 – 7.39 (m, 3H), 7.38 – 7.27 (m, 7H), 6.94 (ddd, *J* = 14.7, 8.0, 0.9 Hz, 3H), 5.03 (s, 2H), 3.89 – 3.83 (m, 4H), 3.33 (s, 3H), 3.32 – 3.27 (m, 4H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.3, 171.1, 161.4, 158.0, 150.9, 138.5, 138.0, 130.0, 129.4, 128.8, 128.4, 128.1, 127.5, 120.9, 117.0, 99.8, 53.6, 49.2, 48.1, 36.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{29}H_{29}N_6S^+$ 493.2169 Found 493.2167

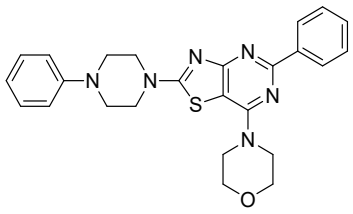
4-(5-Phenyl-2-(piperidin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-yl)morpholine (**1ace**)



33% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.53 – 8.46 (m, 2H), 7.44 – 7.35 (m, 3H), 3.89 – 3.79 (m,

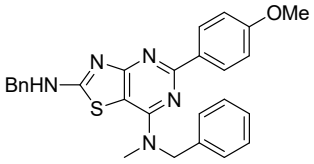
8H), 3.67 (s, 4H), 1.68 (s, 6H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 171.9, 170.8, 161.1, 157.6, 138.3, 129.9, 128.3, 128.1, 100.7, 66.8, 49.6, 46.3, 25.4, 24.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{24}N_5OS^+$ 382.1696 Found 382.1693

4-(5-Phenyl-2-(4-phenylpiperazin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-yl)morpholine (**1acg**)



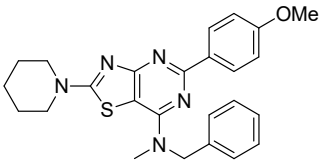
59% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.58 – 8.50 (m, 2H), 7.51 – 7.41 (m, 3H), 7.36 – 7.28 (m, 2H), 7.04 – 6.90 (m, 3H), 4.04 – 3.90 (m, 8H), 3.87 (dd, *J* = 5.5, 3.6 Hz, 4H), 3.41 – 3.30 (m, 4H). $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6) δ 170.9, 170.7, 160.0, 157.2, 150.5, 138.0, 130.0, 129.0, 128.3, 127.6, 119.6, 116.1, 100.3, 65.9, 47.9, 47.6, 45.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{27}N_6OS^+$ 459.1962 Found 459.1959

N^2,N^7-Dibenzyl-5-(4-methoxyphenyl)-N^7-methylthiazolo[4,5-*d*]pyrimidine-2,7-diamine (**1bbb**)



10% yield as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.02 (s, 1H), 8.32 – 8.24 (m, 2H), 7.39 – 7.32 (m, 6H), 7.27 (ddd, *J* = 12.2, 8.9, 4.3 Hz, 4H), 7.05 – 6.94 (m, 2H), 4.98 (s, 2H), 4.64 (d, *J* = 5.5 Hz, 2H), 3.80 (s, 3H), 3.29 (s, 3H). $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6) δ 160.8, 159.6, 157.2, 138.4, 138.2, 130.6, 129.0, 128.6, 128.4, 127.3, 127.2, 127.1, 126.9, 113.5, 98.3, 55.2, 52.7, 47.1. 36.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{27}H_{26}N_5OS^+$ 468.1853 Found 468.1852

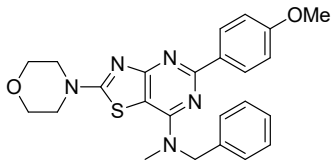
N-Benzyl-5-(4-methoxyphenyl)-*N*-methyl-2-(piperidin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1bbe**)



33% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 – 8.47 (m, 2H), 7.35 – 7.29 (m, 4H), 7.29 – 7.25 (m, 1H), 6.96 – 6.89 (m, 2H), 5.00 (s, 2H), 3.84 (s, 3H), 3.65 (s, 4H), 3.28 (s, 3H), 1.68 (s, 6H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 171.4, 171.2, 161.2, 161.0, 157.8, 138.2, 131.3, 129.9, 128.7, 127.5, 127.4, 113.3, 98.9, 55.3, 53.5, 49.4,

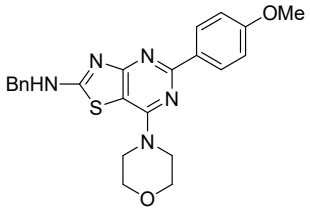
36.3, 25.4, 24.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{28}N_5OS^+$ 446.2009 Found 446.2007

N-Benzyl-5-(4-methoxyphenyl)-*N*-methyl-2-morpholinothiazolo[4,5-*d*]pyrimidin-7-amine (**1bbf**)



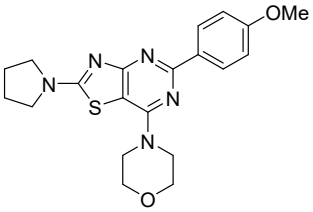
36% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 – 8.46 (m, 2H), 7.36 – 7.25 (m, 5H), 6.95 – 6.89 (m, 2H), 4.99 (s, 2H), 3.83 (s, 3H), 3.81 – 3.76 (m, 4H), 3.70 – 3.64 (m, 4H), 3.28 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.6, 170.9, 161.3, 161.2, 157.8, 138.0, 131.1, 129.9, 128.7, 127.4, 113.3, 98.9, 66.2, 55.3, 53.5, 48.2, 36.3. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{26}N_5O_2S^+$ 448.1802 Found 448.1800

N-Benzyl-5-(4-methoxyphenyl)-7-morpholinothiazolo[4,5-*d*]pyrimidin-2-amine (**1bcb**)



7% yield as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.14 (t, J = 5.2 Hz, 1H), 8.35 – 8.21 (m, 2H), 7.43 – 7.33 (m, 4H), 7.32 – 7.27 (m, 1H), 7.07 – 6.90 (m, 2H), 4.66 (d, J = 5.6 Hz, 2H), 3.81 (s, 3H), 3.75 (s, 8H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 170.9, 160.8, 159.5, 157.1, 138.3, 130.5, 129.1, 128.5, 127.3, 127.2, 113.5, 99.3, 65.9, 55.2, 45.7, 40.1. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{24}N_5O_2S^+$ 434.1646 Found 434.1648

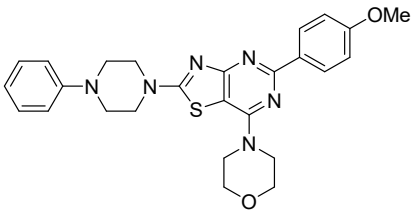
4-(5-(4-Methoxyphenyl)-2-(pyrrolidine-1-yl)thiazolo[4,5-*d*]pyrimidin-7-yl)morpholine (**1bcd**)



10% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.52 – 8.44 (m, 2H), 6.97 – 6.90 (m, 2H), 3.91 – 3.83 (m, 11H), 3.63 (s, 4H), 2.10 (t, J = 6.6 Hz, 4H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.7, 17.5, 161.2, 161.0, 157.6, 131.0, 129.8, 113.3, 100.0, 66.8, 55.3, 49.6, 46.2, 25.6. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{24}N_5O_2S^+$ 398.1646

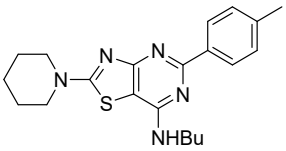
Found 398.1647

4-(5-(4-Methoxyphenyl)-2-(4-phenylpiperazin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-yl)morpholine (**1bcg**)



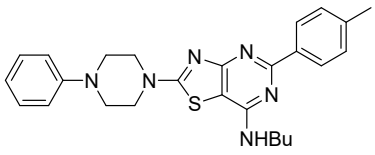
38% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.51 – 8.44 (m, 4H), 7.33 – 7.27 (m, 4H), 6.98 – 6.90 (m, 10H), 3.92 – 3.86 (m, 15H), 3.84 (dd, *J* = 7.1, 2.5 Hz, 14H), 3.34 – 3.27 (m, 8H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.5, 170.9, 161.4, 161.2, 157.6, 150.8, 130.9, 129.9, 129.3, 120.9, 117.0, 113.4, 100.1, 66.8, 55.4, 49.2, 48.2, 46.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{29}N_6O_2S^+$ 489.2067 Found 489.2066

N-Butyl-2-(piperidin-1-yl)-5-(*p*-tolyl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1cae**)



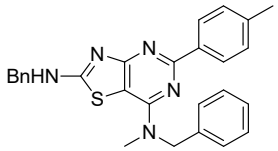
39% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.45 – 8.40 (m, 2H), 7.23 (d, *J* = 8.0 Hz, 2H), 4.51 (s, 1H), 3.74 – 3.59 (m, 6H), 2.39 (s, 3H), 1.73 – 1.63 (m, 8H), 1.45 (dq, *J* = 14.6, 7.4 Hz, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 170.8, 170.6, 162.0, 156.6, 139.8, 135.9, 128.8, 128.3, 99.9, 49.8, 41.5, 32.3, 25.4, 24.2, 21.5, 20.2, 13.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{28}N_5S^+$ 382.2060 Found 382.2057

N-Butyl-2-(4-phenylpiperazin-1-yl)-5-(*p*-tolyl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1cag**)



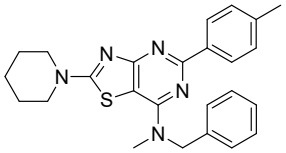
34% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.44 (d, *J* = 8.2 Hz, 2H), 7.32 – 7.27 (m, 2H), 7.25 (d, *J* = 8.0 Hz, 2H), 6.94 (dd, *J* = 15.1, 7.6 Hz, 3H), 4.62 (t, *J* = 5.2 Hz, 1H), 3.93 – 3.83 (m, 4H), 3.66 (dd, *J* = 13.0, 7.1 Hz, 2H), 3.33 – 3.27 (m, 4H), 2.40 (s, 3H), 1.72 – 1.64 (m, 2H), 1.46 (dq, *J* = 14.7, 7.4 Hz, 2H), 0.98 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 170.8, 170.3, 162.2, 156.7, 150.8, 139.9, 135.7, 129.3, 128.9, 128.3, 120.9, 117.0, 100.1, 49.1, 48.3, 41.5, 32.3, 21.5, 20.2, 13.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{31}N_6S^+$ 459.2325 Found 459.2323

N^2,*N*^{7}-Dibenzyl-*N*^{7}-methyl-5-(*p*-tolyl)thiazolo[4,5-*d*]pyrimidine-2,7-diamine (**1cbb**)



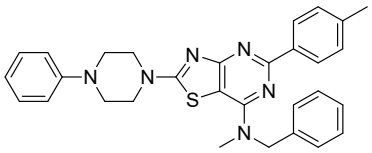
6% yield as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.03 (t, *J* = 5.2 Hz, 1H), 8.22 (d, *J* = 8.2 Hz, 2H), 7.39 – 7.22 (m, 12H), 4.99 (s, 2H), 4.64 (d, *J* = 5.5 Hz, 2H), 3.30 (s, 3H), 2.34 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 170.3, 159.7, 157.2, 139.4, 138.4, 138.2, 135.5, 128.8, 128.6, 128.4, 127.5, 127.3, 127.2, 127.1, 126.9, 98.8, 82.7, 47.1, 36.4, 20.9. HRMS (ESI) m/z: [M+H]$^+$ Calcd for $C_{27}H_{26}N_5S^+$ 452.1903 Found 452.1902

N-Benzyl-N-methyl-2-(piperidin-1-yl)-5-(*p*-tolyl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1cbe**)



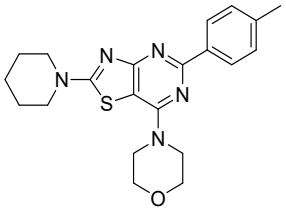
19% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 – 8.41 (m, 2H), 7.38 – 7.30 (m, 4H), 7.29 – 7.26 (m, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 5.02 (s, 2H), 3.66 (s, 4H), 3.29 (s, 3H), 2.38 (s, 3H), 1.68 (s, 6H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.4, 171.2, 161.3, 157.8, 139.8, 138.2, 135.9, 128.8, 128.7, 128.3, 127.6, 127.4, 99.3, 53.5, 49.5, 36.3, 25.4, 24.2, 21.5. HRMS (ESI) m/z: [M+H]$^+$ Calcd for $C_{25}H_{28}N_5S^+$ 430.2060 Found 430.2061

N-Benzyl-*N*-methyl-2-(4-phenylpiperazin-1-yl)-5-(*p*-tolyl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1cbg**)



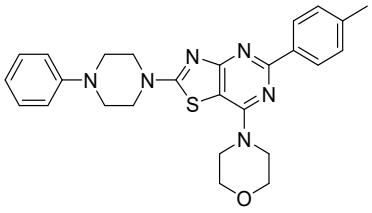
22% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.48 – 8.42 (m, 2H), 7.37 – 7.27 (m, 7H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.00 – 6.89 (m, 3H), 5.03 (s, 2H), 3.88 – 3.82 (m, 4H), 3.32 (s, 3H), 3.31 – 3.27 (m, 4H), 2.40 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.3, 171.1, 161.5, 157.9, 150.9, 140.0, 138.0, 135.7, 129.4, 128.9, 128.8, 128.3, 127.5, 127.5, 120.9, 117.0, 99.5, 53.5, 49.2, 48.1, 36.4, 21.5. HRMS (ESI) m/z: [M+H]$^+$ Calcd for $C_{30}H_{31}N_6S^+$ 507.2325 Found 507.2326

4-(2-(Piperidin-1-yl)-5-(*p*-tolyl)thiazolo[4,5-*d*]pyrimidin-7-yl)morpholine (**1cce**)



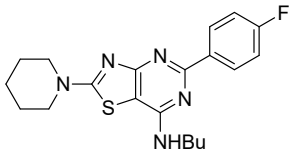
42% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (d, *J* = 8.2 Hz, 2H), 7.22 (d, *J* = 8.1 Hz, 2H), 3.85 (td, *J* = 6.7, 4.4 Hz, 8H), 3.68 (s, 4H), 2.38 (s, 3H), 1.69 (s, 6H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.8, 170.8, 161.3, 157.5, 140.0, 135.6, 128.8, 128.2, 100.4, 66.9, 49.6, 46.3, 25.4, 24.2, 21.5. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{26}N_5OS^+$ 396.1853 Found 396.1852

4-(2-(4-Phenylpiperazin-1-yl)-5-(*p*-tolyl)thiazolo[4,5-*d*]pyrimidin-7-yl)morpholine (**1ccg**)



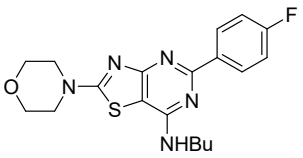
42% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.41 (d, *J* = 8.2 Hz, 2H), 7.34 – 7.27 (m, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 6.99 – 6.90 (m, 3H), 3.86 (ddd, *J* = 8.2, 5.2, 3.1 Hz, 12H), 3.34 – 3.27 (m, 4H), 2.40 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.5, 170.9, 161.4, 157.6, 150.8, 140.1, 135.5, 129.3, 128.9, 128.2, 120.9, 117.0, 100.5, 66.8, 49.1, 48.2, 46.2, 21.5. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{29}N_6OS^+$ 473.2118 Found 473.2117

N-Butyl-5-(4-fluorophenyl)-2-(piperidin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1hae**)



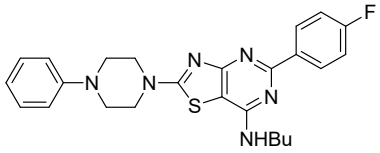
60% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 – 8.48 (m, 2H), 7.13 – 7.03 (m, 2H), 4.51 (t, *J* = 5.2 Hz, 1H), 3.74 – 3.59 (m, 6H), 1.74 – 1.61 (m, 8H), 1.45 (dq, *J* = 14.6, 7.4 Hz, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 170.8, 170.5, 165.2, 163.2, 161.1, 156.6, 134.8, 134.8, 130.4, 130.3, 114.9, 114.8, 100.1, 49.8, 41.5, 32.3, 25.4, 24.2, 20.2, 13.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{25}FN_5S^+$ 386.1809 Found 386.1807

N-Butyl-5-(4-fluorophenyl)-2-morpholinothiazolo[4,5-*d*]pyrimidin-7-amine (**1haf**)



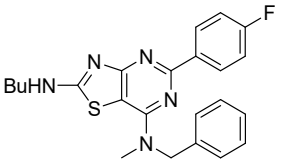
28% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 – 8.46 (m, 2H), 7.14 – 7.04 (m, 2H), 4.53 (t, *J* = 5.0 Hz, 1H), 3.82 (dd, *J* = 6.4, 3.4 Hz, 4H), 3.78 – 3.69 (m, 4H), 3.66 (dt, *J* = 13.0, 6.5 Hz, 2H), 1.75 – 1.64 (m, 2H), 1.46 (dq, *J* = 14.7, 7.4 Hz, 2H), 0.98 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.3, 170.1, 165.3, 163.3, 161.3, 156.7, 134.6, 134.6, 130.3, 130.3, 115.0, 114.9, 100.2, 66.2, 48.5, 41.5, 32.2, 20.2, 13.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{23}FN_5OS^+$ 388.1602 Found 388.1599

N-Butyl-5-(4-fluorophenyl)-2-(4-phenylpiperazin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1hag**)



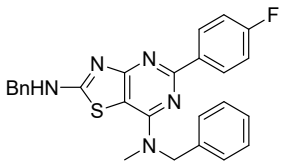
74% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.57 – 8.49 (m, 2H), 7.31 – 7.26 (m, 2H), 7.14 – 7.06 (m, 2H), 6.96 – 6.89 (m, 3H), 4.68 (t, *J* = 5.4 Hz, 1H), 3.84 (d, *J* = 4.6 Hz, 4H), 3.63 (dd, *J* = 13.0, 7.0 Hz, 2H), 3.33 – 3.24 (m, 4H), 1.72 – 1.60 (m, 2H), 1.51 – 1.38 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 170.9, 170.1, 165.2, 163.2, 161.1, 156.6, 150.7, 134.6, 134.6, 130.3, 130.2, 129.3, 120.8, 116.9, 115.0, 114.8, 100.3, 49.0, 48.3, 41.4, 32.2, 20.1, 13.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{28}FN_6S^+$ 463.2075 Found 463.2074

N^7-Benzyl-N^2-butyl-5-(4-fluorophenyl)-N^7-methylthiazolo[4,5-*d*]pyrimidine-2,7-diamine (**1hba**)



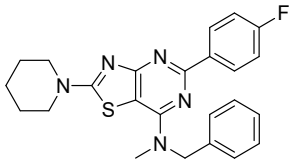
56% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.50 (dd, *J* = 8.8, 5.6 Hz, 2H), 7.52 (ddd, *J* = 41.4, 34.8, 12.3 Hz, 1H), 7.42 – 7.34 (m, 2H), 7.33 (dd, *J* = 11.7, 7.0 Hz, 3H), 7.11 (t, *J* = 8.7 Hz, 2H), 5.03 (s, 2H), 3.46 (dd, *J* = 8.4, 6.0 Hz, 2H), 3.34 (s, 3H), 1.75 (dt, *J* = 14.9, 7.5 Hz, 2H), 1.44 (dq, *J* = 14.8, 7.4 Hz, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.6, 168.4, 165.5, 163.5, 159.3, 157.6. 137.5, 133.4, 130.5, 130.5, 128.9, 127.7, 127.4, 115.2, 115.1, 98.6, 53.7, 45.7, 36.6, 36.6, 31.2, 20.1, 13.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{25}FN_5S^+$ 422.1809 Found 422.1807

N^2,N^7-Dibenzyl-5-(4-fluorophenyl)-N^7-methylthiazolo[4,5-*d*]pyrimidine-2,7-diamine (**1hbb**)



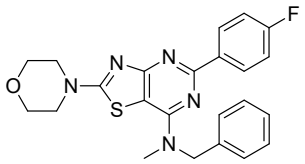
38% yield as a white solid; ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.06 (s, 1H), 8.43 – 8.34 (m, 2H), 7.43 – 7.31 (m, 6H), 7.31 – 7.22 (m, 6H), 4.98 (s, 2H), 4.64 (d, J = 5.3 Hz, 2H), 3.29 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, DMSO-d_6) δ 170.3, 164.4, 162.4, 158.8, 157.3, 138.4, 138.1, 134.7, 134.7, 129.8, 129.7, 128.6, 128.4, 127.4, 127.2, 127.1, 126.9, 115.1, 115.0, 99.0, 52.8, 47.1, 36.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{26}H_{23}FN_5S^+$ 456.1653 Found 456.1656

N-Benzyl-5-(4-fluorophenyl)-*N*-methyl-2-(piperidin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1hbe**)



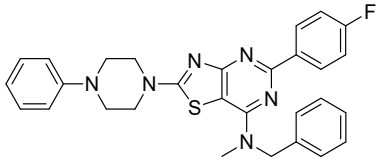
66% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.55 – 8.49 (m, 2H), 7.37 – 7.26 (m, 5H), 7.11 – 7.02 (m, 2H), 5.01 (s, 2H), 3.66 (s, 4H), 3.31 (s, 3H), 1.70 (s, 6H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.4, 171.3, 165.2, 163.3, 160.4, 157.8, 138.1, 134.8, 134.7, 130.4, 130.3, 128.8, 127.5, 115.0, 114.8, 99.5, 53.6, 49.5, 36.4, 25.4, 24.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{24}H_{25}FN_5S^+$ 434.1809 Found 434.1809

N-Benzyl-5-(4-fluorophenyl)-*N*-methyl-2-morpholinothiazolo[4,5-*d*]pyrimidin-7-amine (**1hbf**)



38% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.55 – 8.48 (m, 2H), 7.35 – 7.30 (m, 2H), 7.30 – 7.24 (m, 3H), 7.11 – 7.03 (m, 2H), 4.98 (s, 2H), 3.83 – 3.76 (m, 4H), 3.71 – 3.63 (m, 4H), 3.28 (s, 3H). ^{13}C{^{1}H} NMR (126 MHz, $CDCl_3$) δ 171.6, 170.8, 165.2, 163.2, 160.5, 157.9, 137.8, 134.5, 134.5, 130.3, 130.2, 128.8, 127.5, 127.3, 115.0, 114.8, 99.5, 66.1, 53.5, 48.2, 36.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{23}H_{23}FN_5OS^+$ 436.1602 Found 436.1601

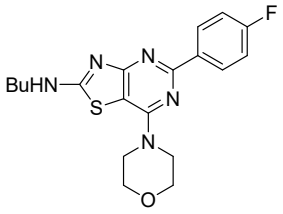
N-Benzyl-5-(4-fluorophenyl)-*N*-methyl-2-(4-phenylpiperazin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-amine (**1hbg**)



51% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 – 8.50 (m, 2H), 7.38 – 7.27 (m, 7H), 7.12 – 7.06 (m,

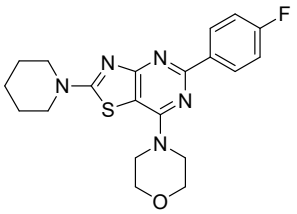
2H), 6.99 – 6.90 (m, 3H), 5.02 (s, 2H), 3.90 – 3.83 (m, 4H), 3.33 (s, 3H), 3.32 – 3.28 (m, 4H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 171.4, 171.0, 165.3, 163.3, 160.6, 158.0, 150.9, 137.9, 134.6, 134.6, 130.4, 130.3, 129.4, 128.8, 127.6, 127.4, 120.9, 117.0, 115.0, 114.9, 99.7, 53.6, 49.2, 48.1, 36.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{29}H_{28}FN_6S^+$ 511.2075 Found 511.2076

N-Butyl-5-(4-fluorophenyl)-7-morpholinothiazolo[4,5-*d*]pyrimidin-2-amine (**1hca**)



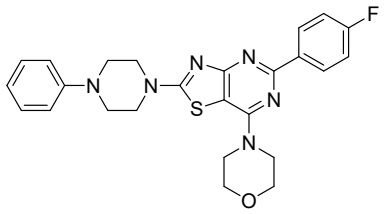
17% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.47 (dd, *J* = 8.4, 5.8 Hz, 2H), 7.09 (t, *J* = 8.6 Hz, 2H), 3.86 (s, 7H), 3.49 (t, *J* = 6.8 Hz, 2H), 1.79 (dt, *J* = 14.9, 7.4 Hz, 2H), 1.46 (dq, *J* = 14.7, 7.3 Hz, 2H), 0.96 (t, *J* = 7.4 Hz, 3H). $^{13}C\{^{1}H\}$ NMR (126 MHz, DMSO-d_6) δ 171.1, 162.4, 158.7, 157.1, 134.6, 129.8, 129.7, 115.2, 115.0, 99.7, 65.9, 45.7, 30.6, 19.5, 13.6. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{23}FN_5OS^+$ 388.1602 Found 388.1602

4-(5-(4-Fluorophenyl)-2-(piperidin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-yl)morpholine (**1hce**)



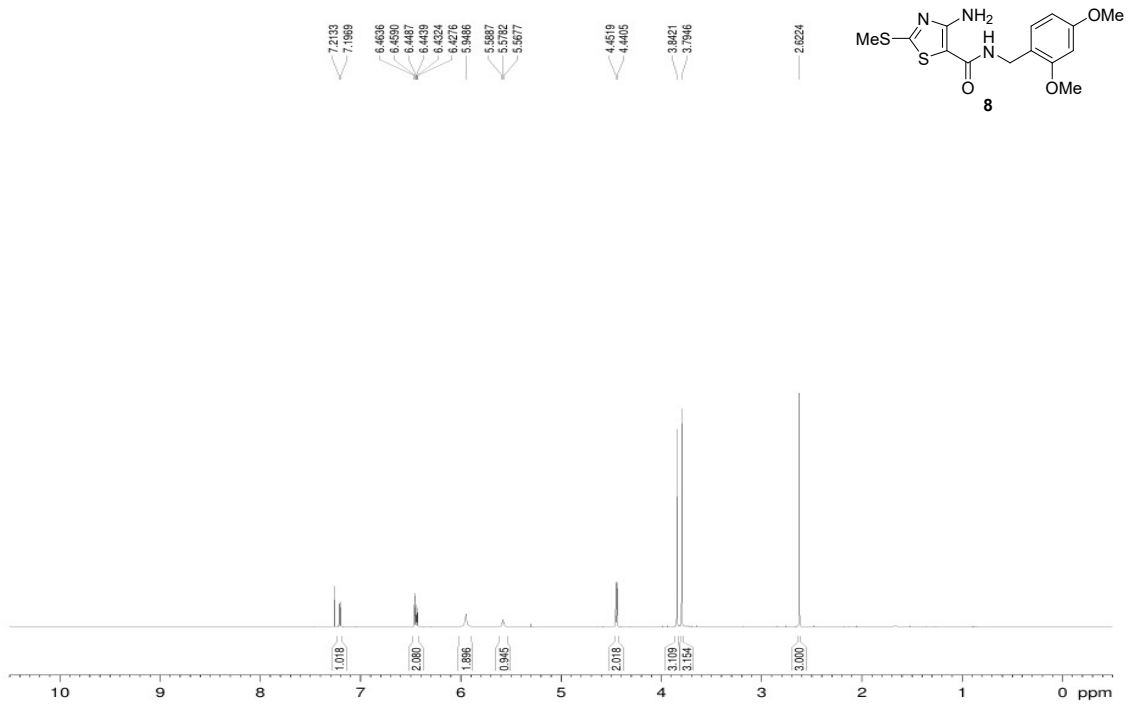
23% yield as a white solid; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.58 – 8.46 (m, 2H), 7.39 – 7.27 (m, 2H), 7.14 – 7.04 (m, 2H), 6.95 (ddd, *J* = 14.6, 8.0, 0.9 Hz, 3H), 3.87 (tdd, *J* = 8.0, 3.7, 1.8 Hz, 12H), 3.35 – 3.28 (m, 4H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 171.9, 170.9, 165.3, 160.4, 157.6, 134.6, 134.5, 130.3, 130.3, 115.0, 114.9, 100.6, 66.9, 49.7, 46.3, 25.4, 24.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{23}FN_5OS^+$ 400.1602 Found 400.1600

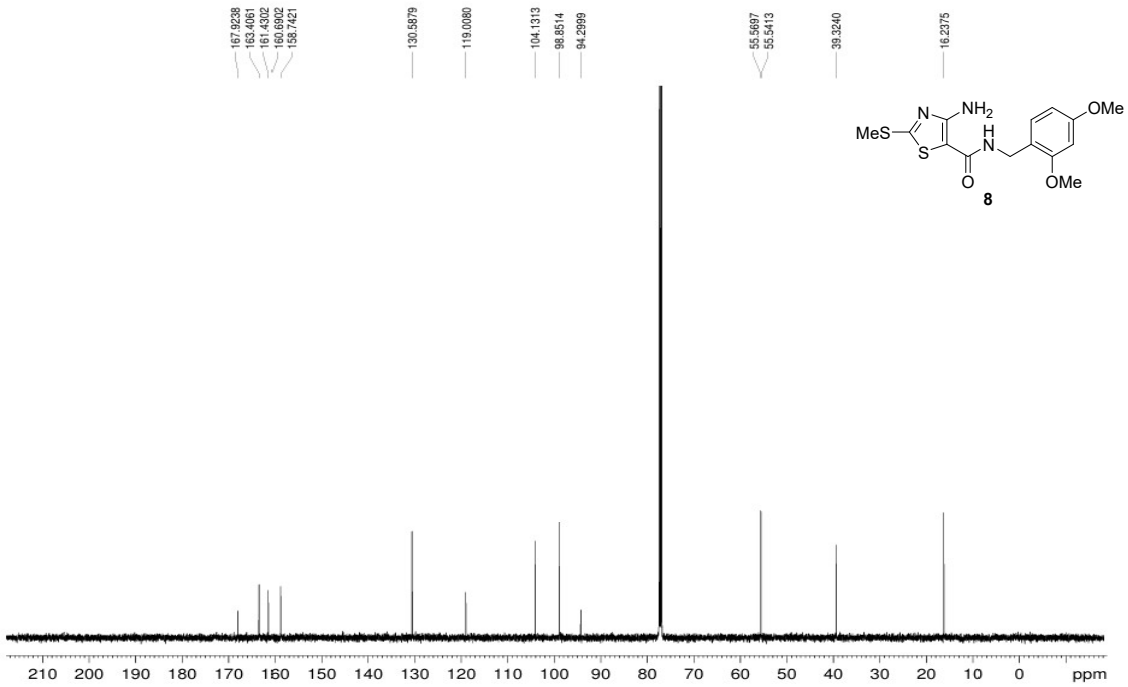
4-(5-(4-Fluorophenyl)-2-(4-phenylpiperazin-1-yl)thiazolo[4,5-*d*]pyrimidin-7-yl)morpholine (**1hcg**)

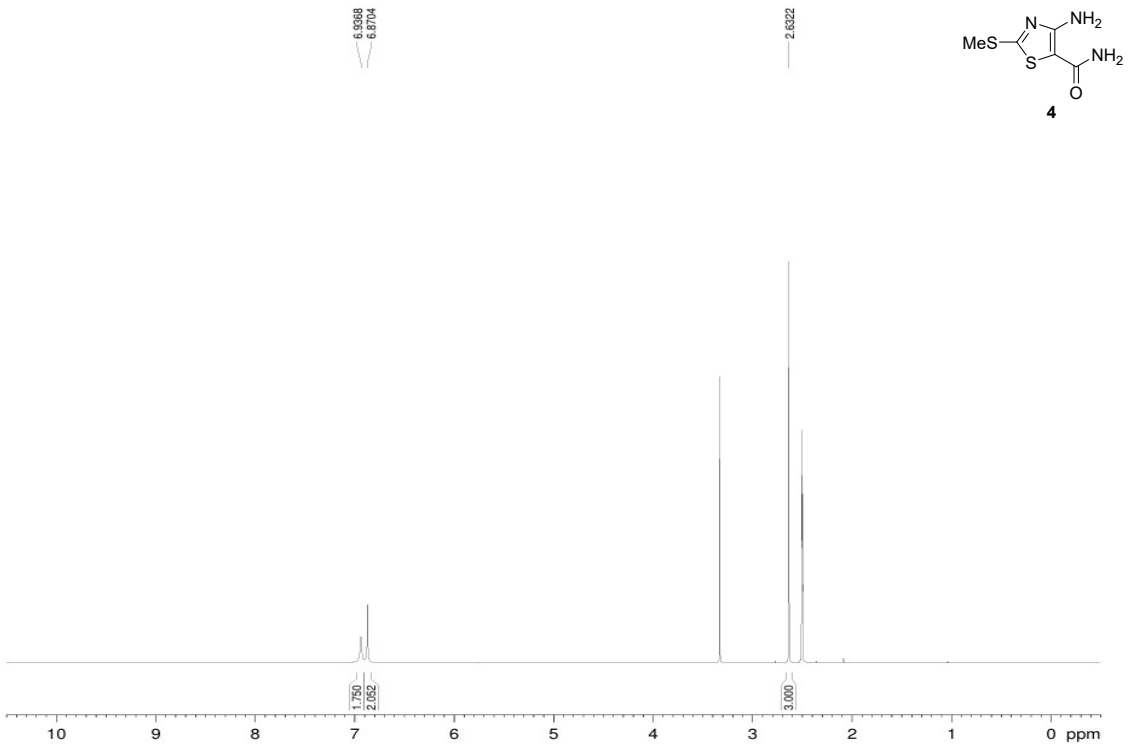


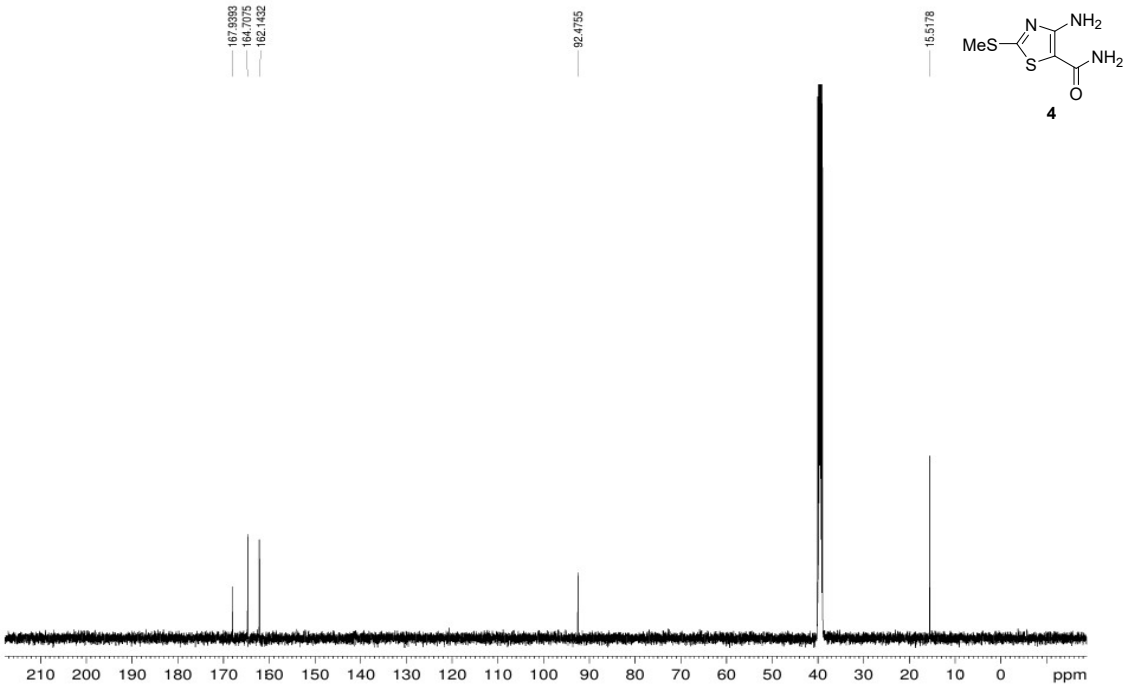
23% yield as a white soliud; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.58 – 8.46 (m, 2H), 7.39 – 7.27 (m, 2H), 7.14 – 7.04 (m, 2H), 6.95 (ddd, *J* = 14.6, 8.0, 0.9 Hz, 3H), 3.87 (tdd, *J* = 8.0, 3.7, 1.8 Hz, 12H), 3.35 – 3.28 (m, 4H). $^{13}C\{^{1}H\}$ NMR (126 MHz, $CDCl_3$) δ 171.5, 171.0, 165.3, 163.4, 160.5, 157.7, 150.8, 134.4, 134.4, 130.3, 130.3, 129.4, 121.0, 117.0, 115.1, 114.9, 100.6, 66.8, 49.2, 48.2, 46.3. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{26}FN_6OS^+$ 477.1867 Found 477.1869

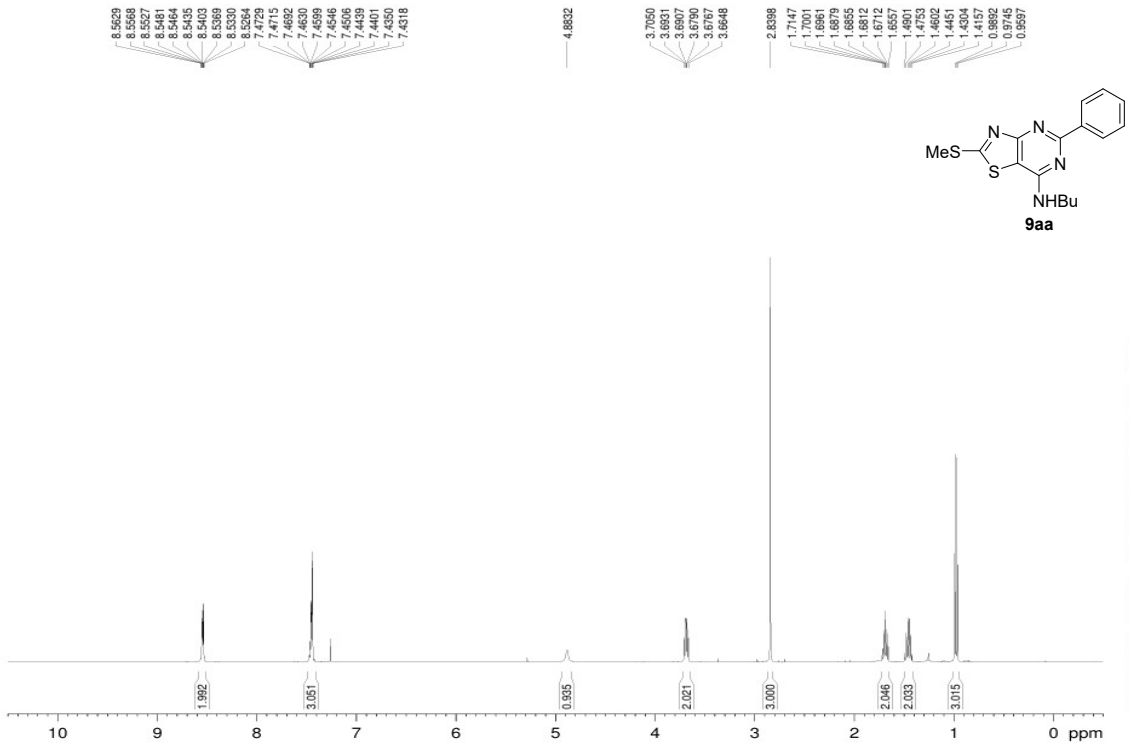
NMR spectra

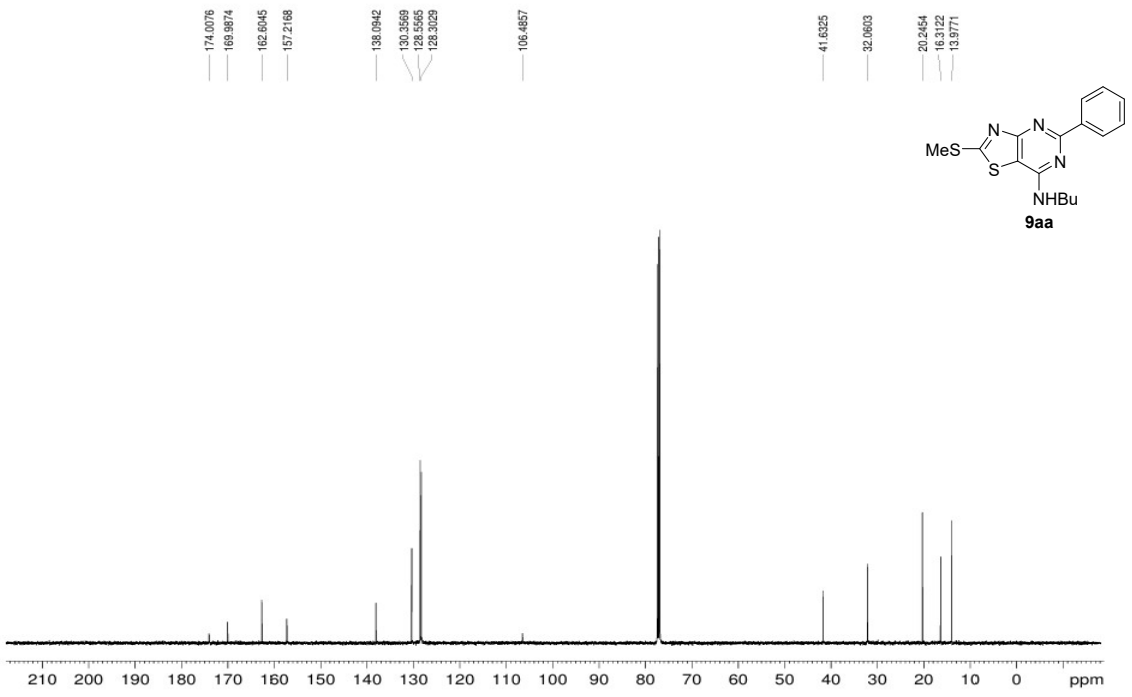

7.2133
7.1969
6.4636
6.4590
6.4487
6.4439
6.4324
6.4276
5.9486
5.5887
5.5782
5.5677
4.4519
4.4405
3.8421
3.7946
2.6224
1.018
2.060
1.896
0.945
2.018
3.109
3.154
3.000
10 9 8 7 6 5 4 3 2 1 0 ppm
NH2
MeS
N
S
H
N
O
OMe
OMe
8


167.9238
163.4061
161.4302
160.6902
158.7421
130.5879
119.0080
104.1313
98.8514
94.2999
55.5697
55.5413
39.3240
16.2375
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
NH2
MeS
N
S
H
N
O
OMe
OMe
8


6.9368
6.8704
2.6322
NH2
MeS
N
S
NH2
O
4
1.750
2.062
3.000
10
9
8
7
6
5
4
3
2
1
0 ppm


167.9393
164.7075
162.1432
92.4755
15.5178
NH2
MeS
N
S
NH2
O
4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.5629
8.5568
8.5527
8.5481
8.5464
8.5435
8.5403
8.5369
8.5330
8.5264
7.4729
7.4715
7.4692
7.4630
7.4599
7.4546
7.4506
7.4439
7.4401
7.4250
7.4318
4.8832
3.7050
3.6931
3.6907
3.6790
3.6767
3.6648
2.8398
1.7147
1.7001
1.6961
1.6879
1.6855
1.6812
1.6712
1.6557
1.4961
1.4753
1.4682
1.4451
1.4304
1.4157
0.9892
0.9745
0.9597
MeS
N
N
S
N
NHBu
9aa
1.992
3.051
0.935
2.021
3.000
2.046
2.033
3.015
10
9
8
7
6
5
4
3
2
1
0 ppm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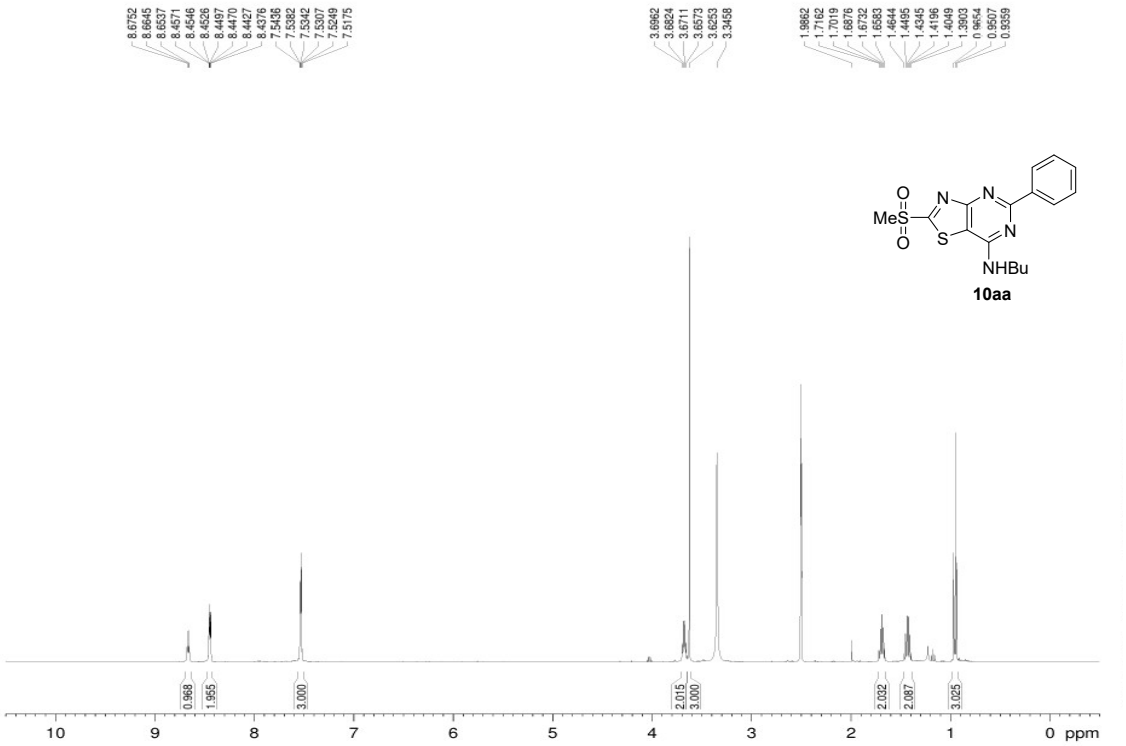
169.9874
162.6045
157.2168
138.0942
130.3569
128.5565
128.3029
106.4857
41.6325
32.0603
20.2454
16.3122
13.9771
MeS
N
N
S
N
NHBu
9aa
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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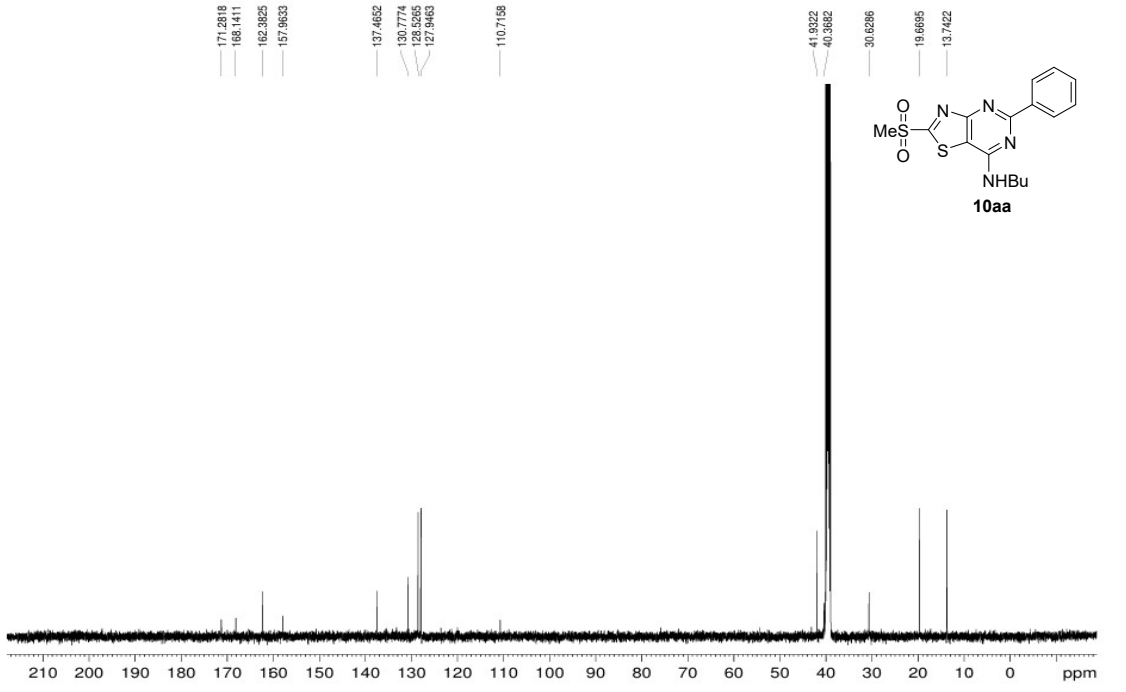
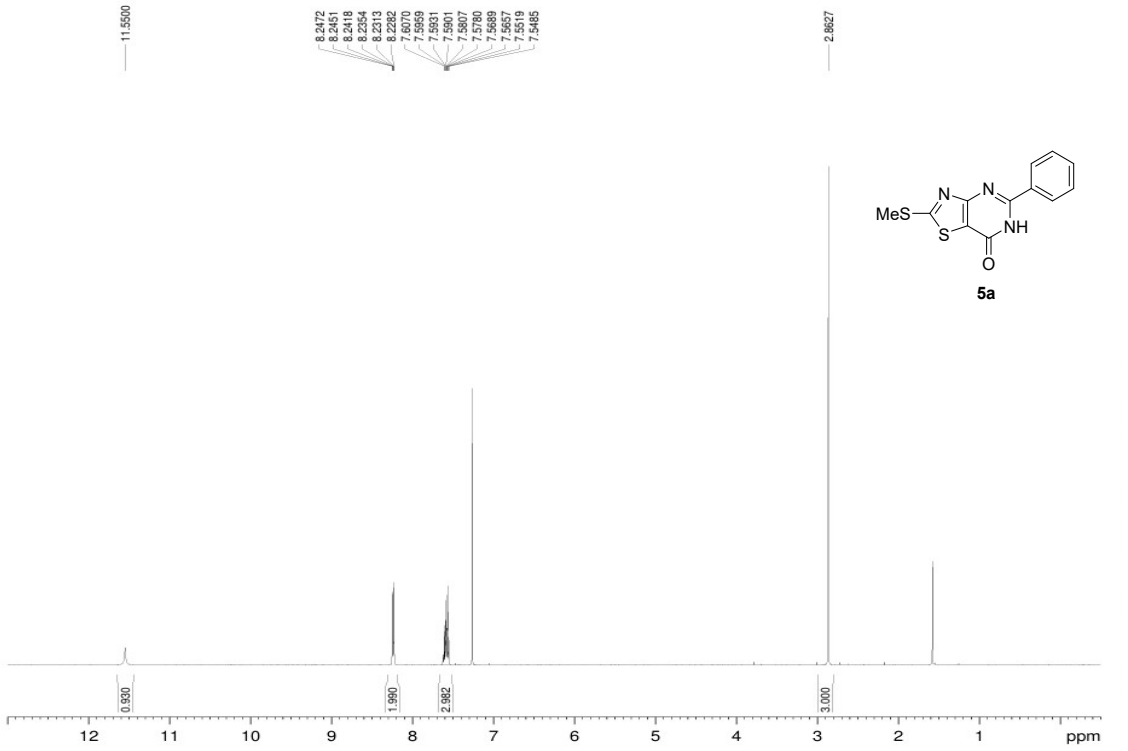
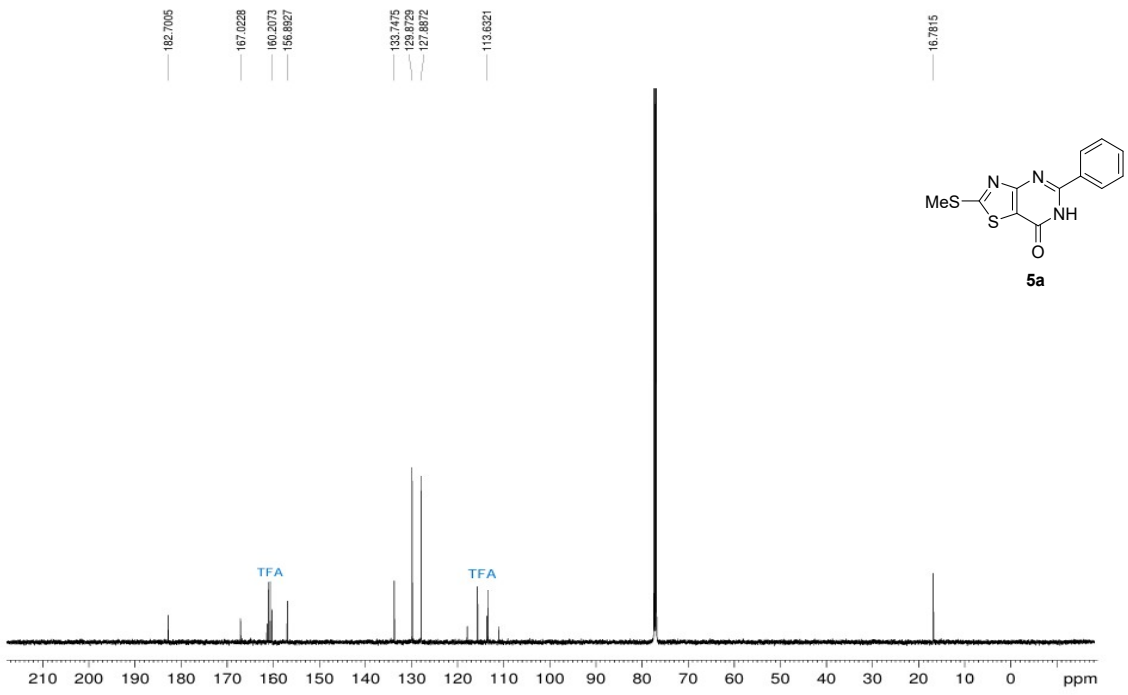
8.6645
8.6537
8.4571
8.4546
8.4526
8.4497
8.4470
8.4427
8.4376
7.5436
7.5382
7.5342
7.5307
7.5249
7.5175
3.6962
3.6824
3.6711
3.6573
3.6253
3.3458
1.9862
1.7162
1.7019
1.6876
1.6732
1.6583
1.4644
1.4495
1.4345
1.4196
1.4049
1.3903
0.9654
0.9507
0.9359
0.968
1.955
3.000
2.015
3.000
2.032
2.087
3.025
10
9
8
7
6
5
4
3
2
1
0 ppm
Me
S
O
O
N
N
S
N
NHBu
10aa

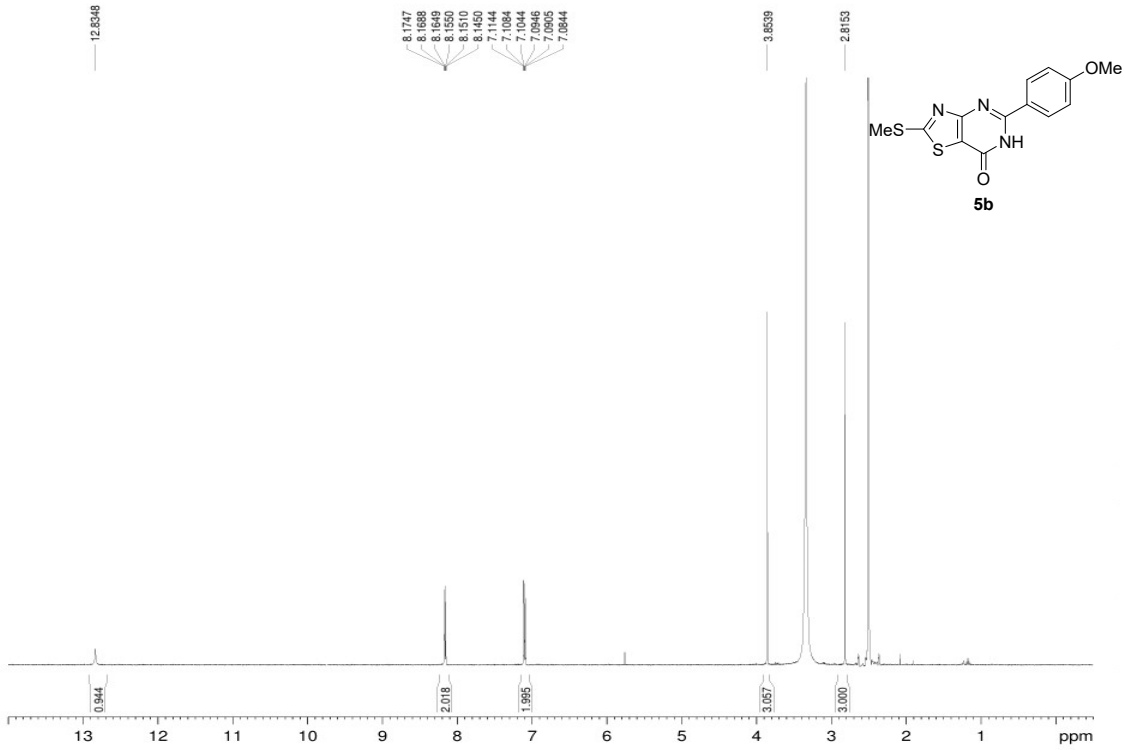

171.2818
168.1411
162.3825
157.9633
137.4652
130.7774
128.3265
127.9463
110.7158
41.9322
40.3682
30.6286
19.6695
13.7422
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
Me
S
O
O
N
N
S
N
NHBu
10aa


11.5500
8.2472
8.2451
8.2418
8.2354
8.2313
8.2282
7.6070
7.5959
7.5931
7.5901
7.5807
7.5780
7.5689
7.5657
7.5519
7.5485
2.8627
MeS
N
N
S
NH
O
0.930
1.990
2.982
3.000
12
11
10
9
8
7
6
5
4
3
2
1
ppm

5a


182.7005
167.0228
160.2073
156.8927
133.7475
129.8729
127.8872
113.6321
16.7815
MeS
N
N
S
NH
O
TFA
TFA
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

5a


12.8348
8.1747
8.1688
8.1649
8.1550
8.1510
8.1450
7.1144
7.1084
7.1044
7.0946
7.0905
7.0844
3.8539
2.8153
OMe
MeS
N
N
S
NH
O
5b
0.944
2.018
1.995
3.057
3.000
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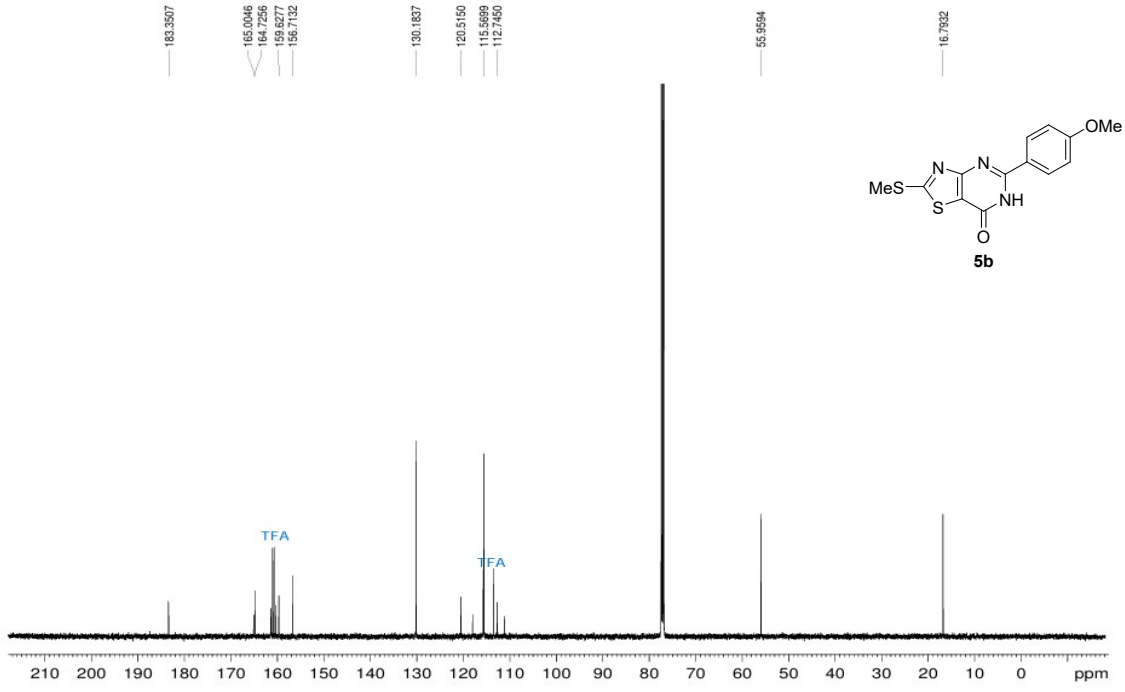
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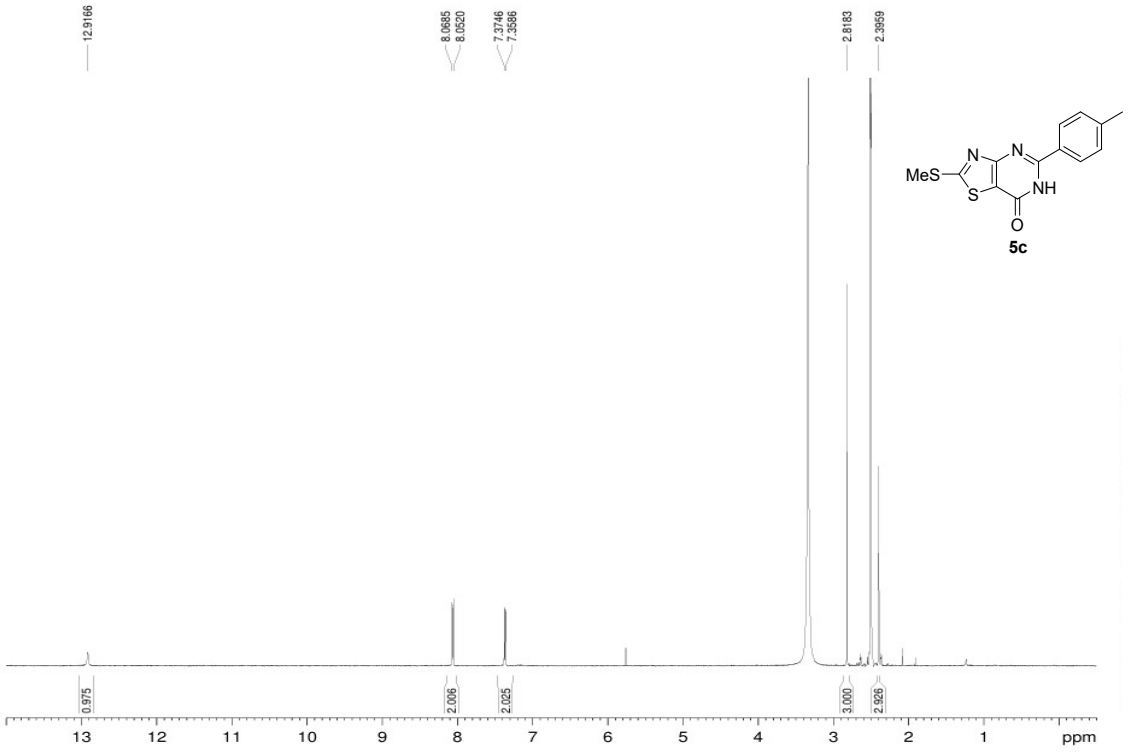
164.7256
159.6277
156.7132
130.1837
120.5150
115.5699
112.7450
55.9594
16.7932
OMe
MeS
N
N
S
NH
O
5b
TFA
TFA
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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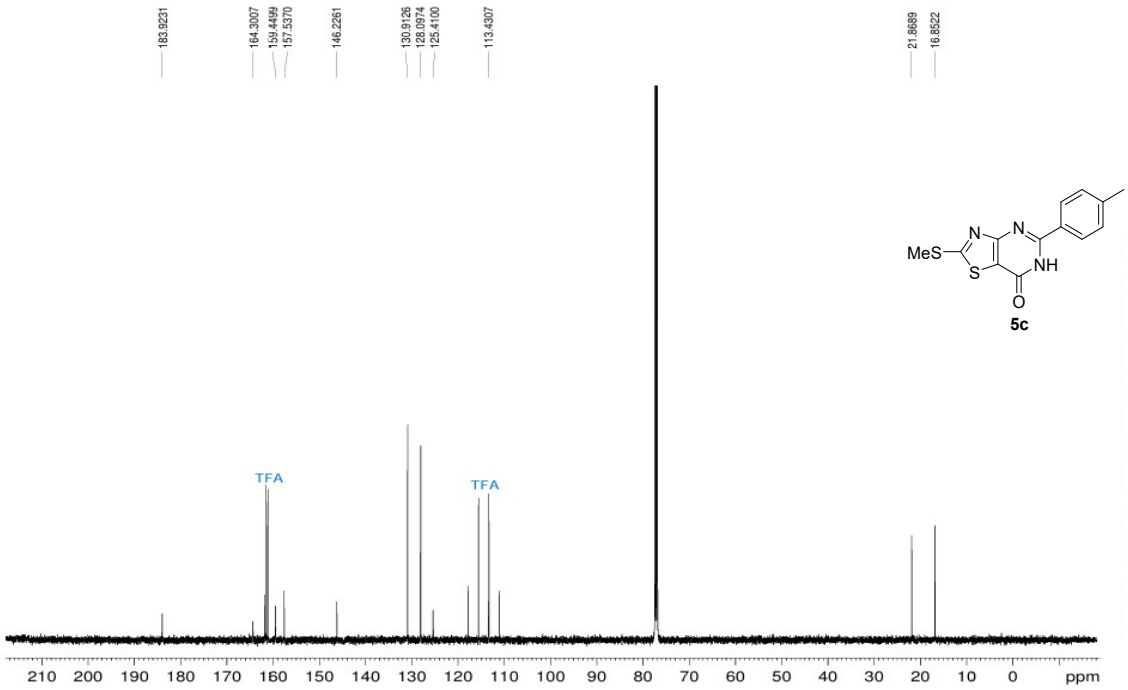
8.0685
8.0520
7.3746
7.3586
2.8183
2.3959
MeS
N
N
S
NH
O
5c
0.975
2.006
2.025
3.000
2.926
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm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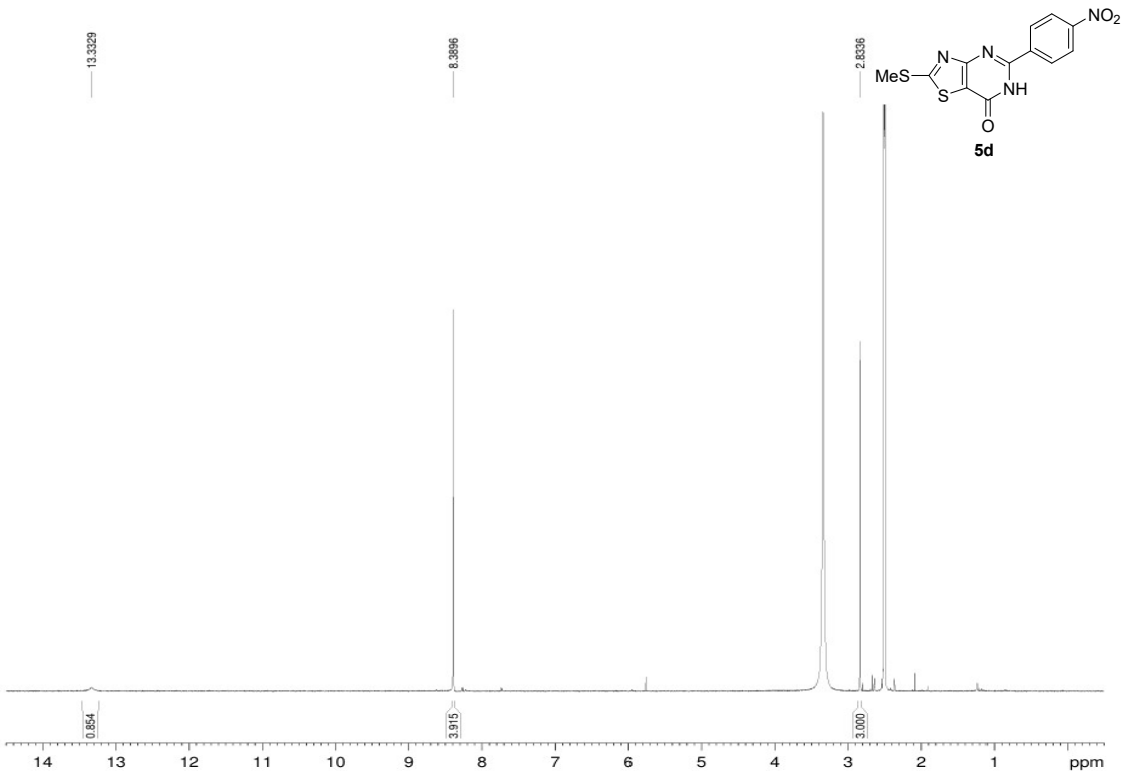
159.4499
157.5370
146.2261
130.9126
128.0974
125.4100
113.4307
21.8689
16.8522
MeS
N
N
S
NH
O
5c
TFA
TFA
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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8.3896
2.8336
MeS
N
N
S
NH
O
NO2
5d
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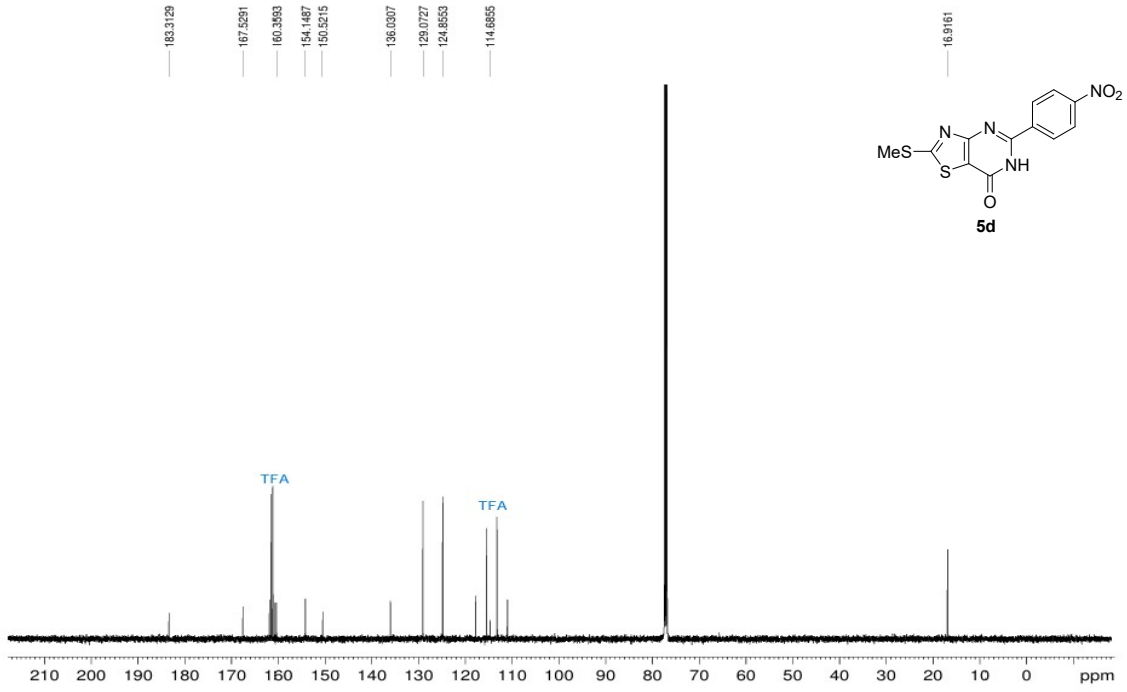
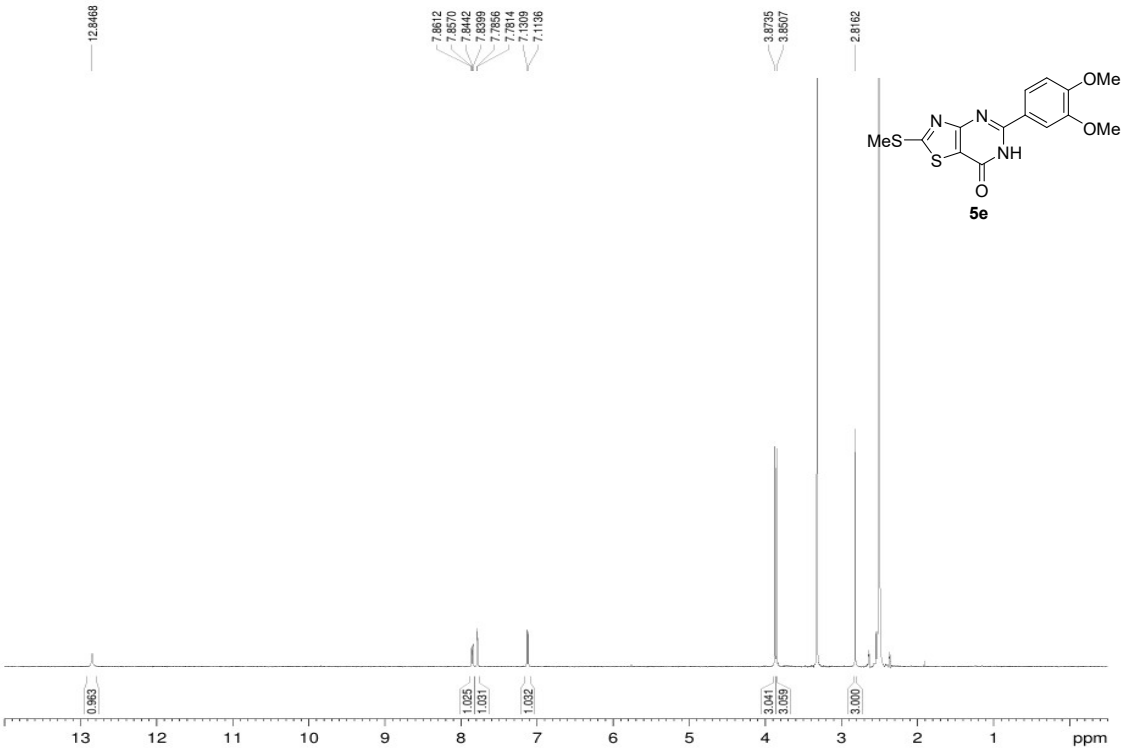
3.915
3.000
14
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm


183.3129
167.5291
160.3593
154.1487
150.5215
136.0307
129.0727
124.8553
114.6855
16.9161
TFA
TFA
NO2
MeS
N
N
S
NH
O
5d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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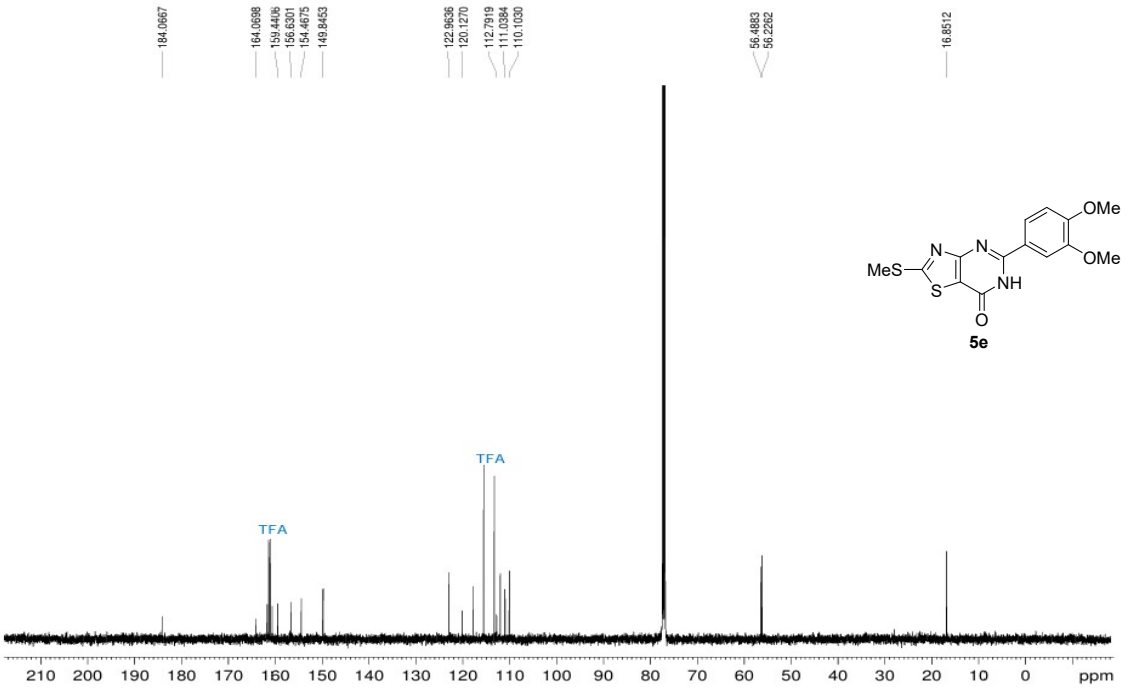
7.8612
7.8570
7.8442
7.8399
7.7856
7.7814
7.1309
7.1136
3.8735
3.8507
2.8162
OMe
OMe
MeS
N
N
S
NH
O
5e
0.963
1.025
1.031
1.032
3.041
3.059
3.000
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm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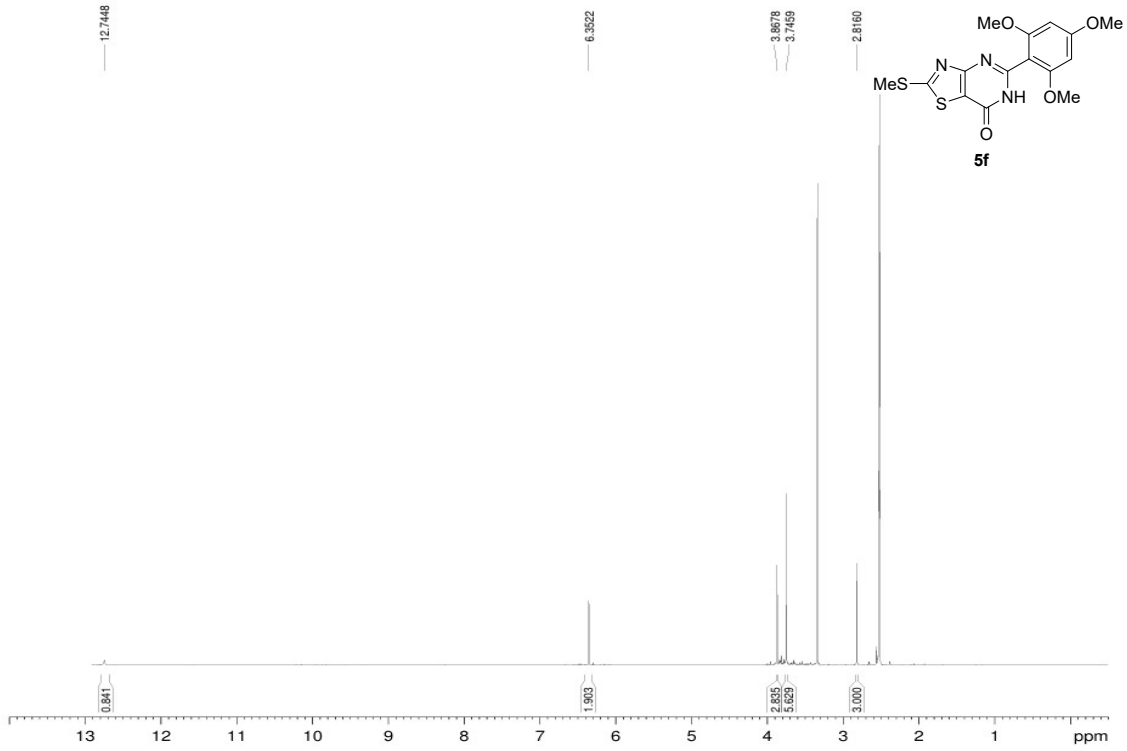
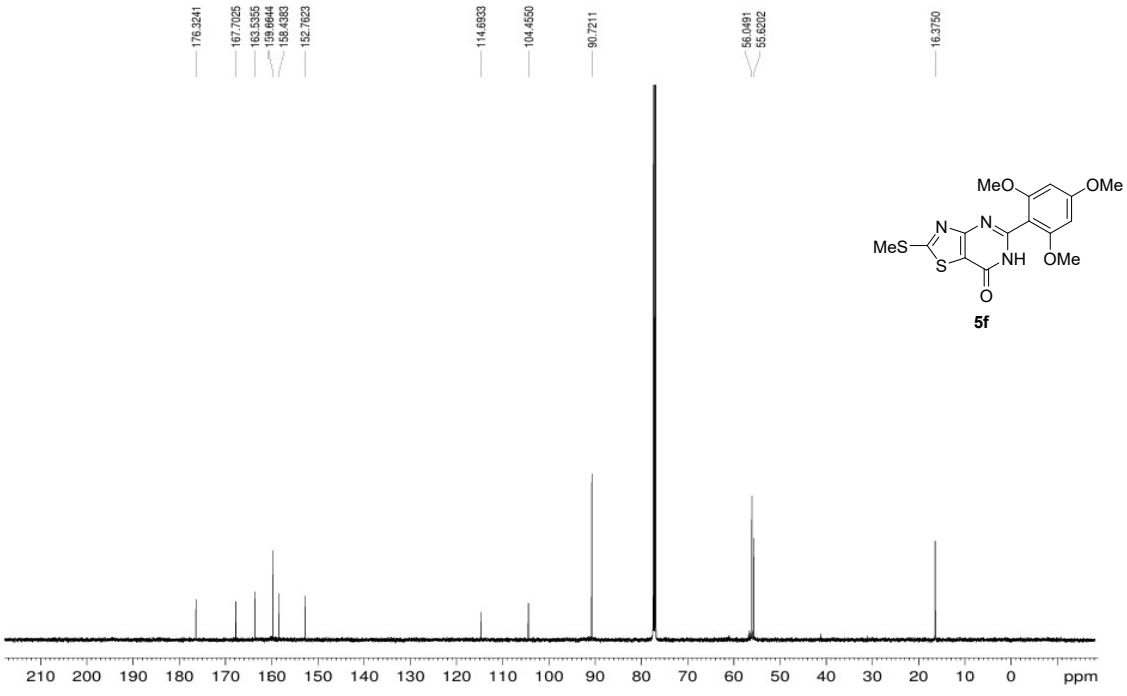
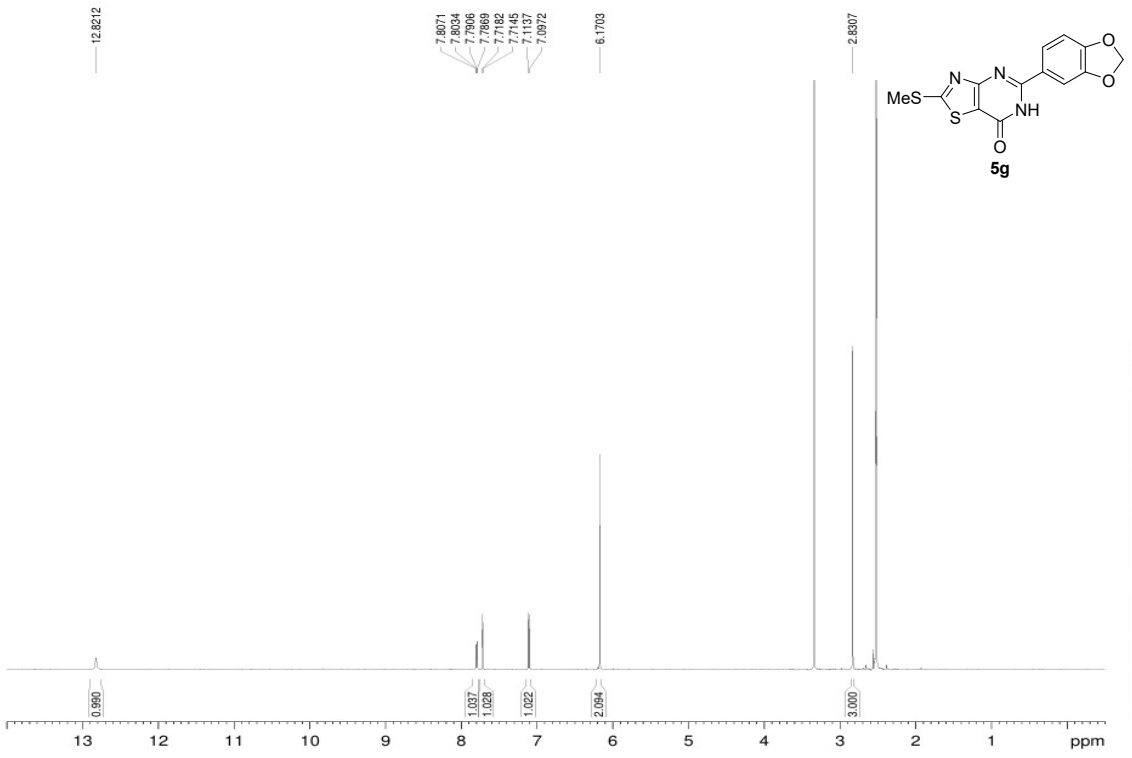
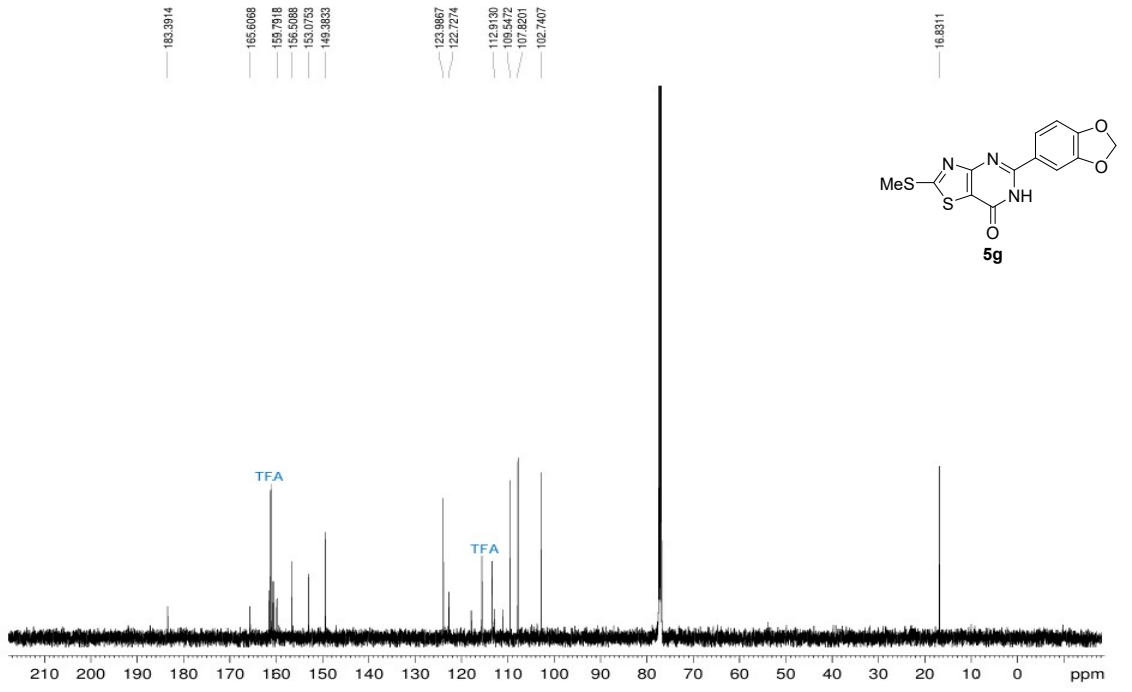
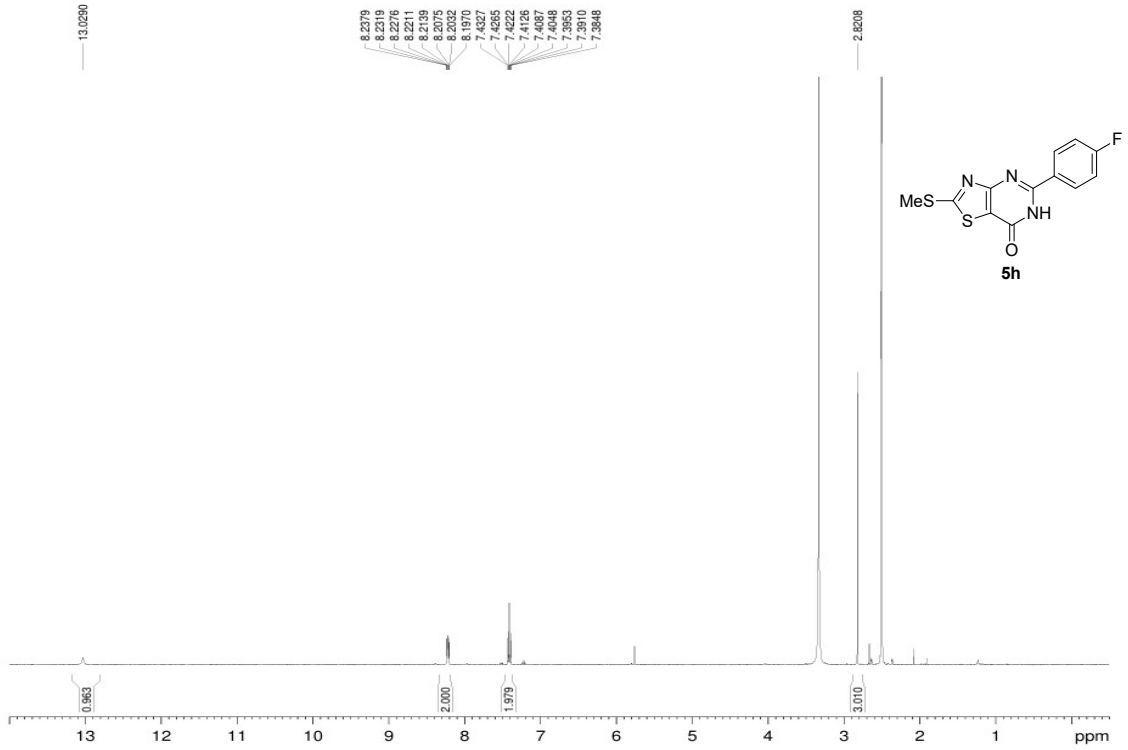
156.6301
154.4675
149.8453
122.9636
120.1270
112.7919
111.0384
110.1030
56.4883
56.2262
16.8512
OMe
OMe
MeS
N
N
S
NH
O
5e
TFA
TFA
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

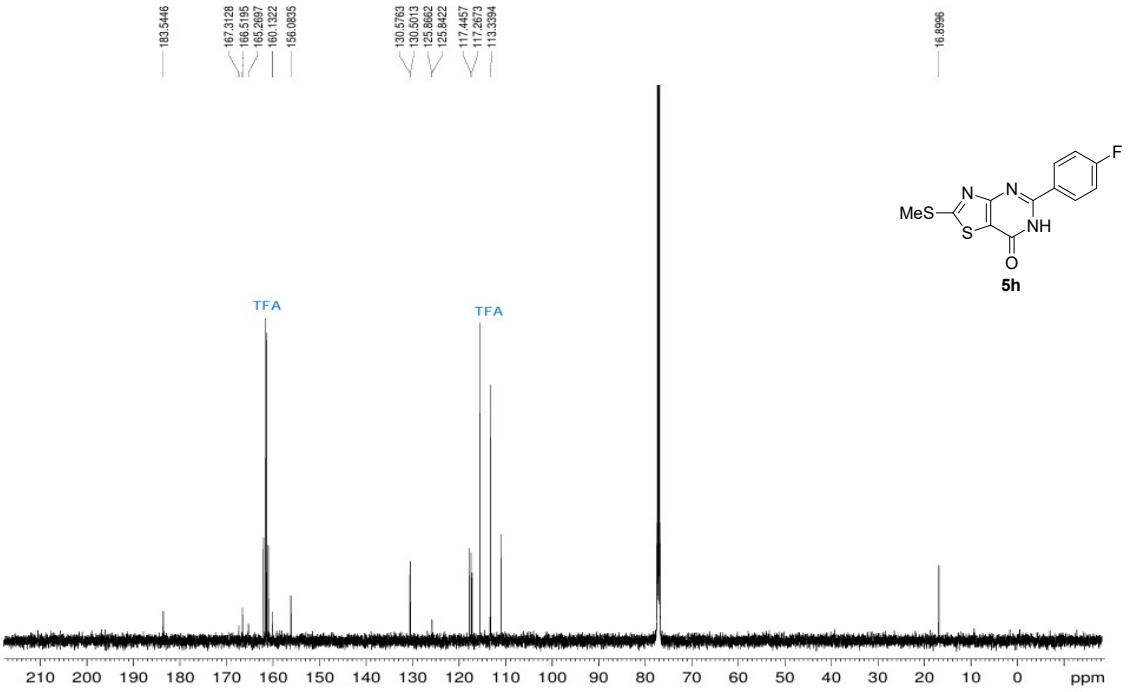

12.7448
6.3522
3.8678
3.7459
2.8160
MeO
OMe
MeS
N
N
S
NH
OMe
O
5f
0.841
1.903
2.835
5.629
3.000
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

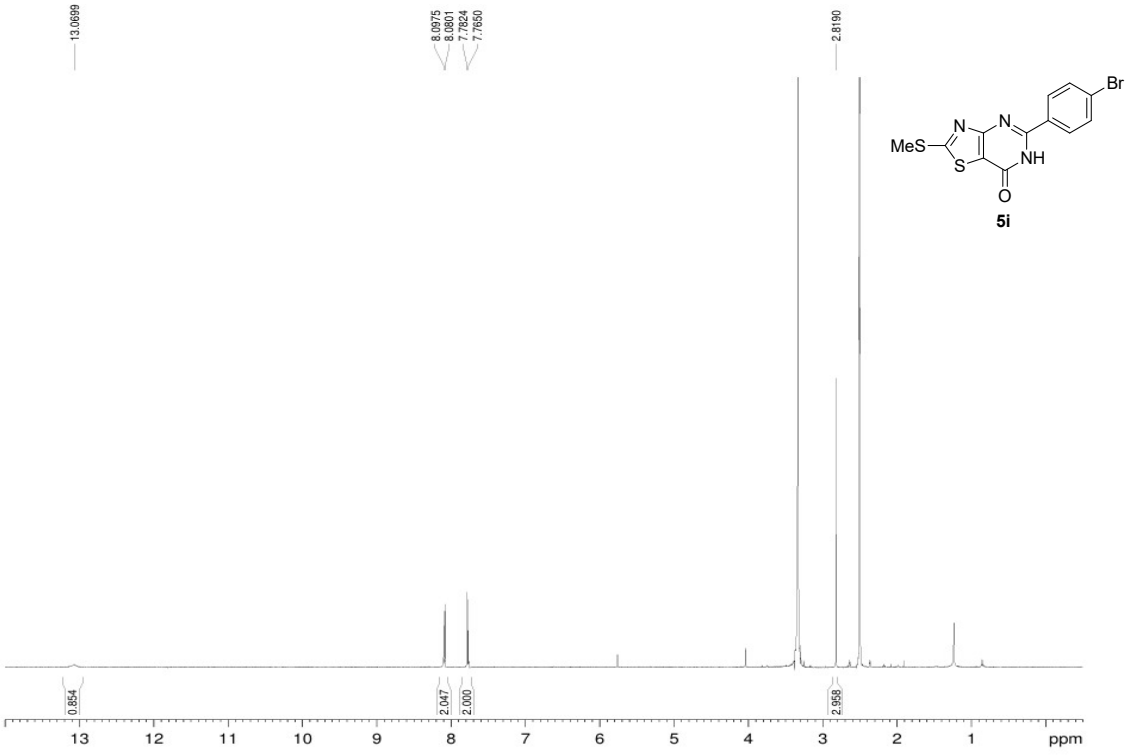

176.3241
167.7025
163.5355
159.8644
158.4383
152.7623
114.6933
104.4550
90.7211
56.0491
55.6202
16.3750
MeO
OMe
MeS
N
N
S
NH
OMe
O
5f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


12.8212
7.8071
7.8034
7.7906
7.7869
7.7182
7.7145
7.1137
7.0972
6.1703
2.8307
MeS
N
N
S
NH
O
O
O
5g
0.990
1.027
1.028
1.022
2.094
3.000
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm


183.3914
165.6068
159.7918
156.5088
153.0753
149.3833
123.9867
122.7274
112.9130
109.5472
107.8201
102.7407
16.8311
MeS
N
N
S
NH
O
O
O
5g
TFA
TFA
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


13.0290
8.2379
8.2319
8.2276
8.2211
8.2139
8.2075
8.2032
8.1970
7.4327
7.4265
7.4222
7.4126
7.4087
7.4048
7.3953
7.3910
7.3848
2.8208
MeS
N
N
S
NH
O
F
5h
0.963
2.000
1.979
3.010
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm


183.5446
167.3128
166.5195
165.2697
160.1322
156.0835
130.5763
130.5013
125.8662
125.8422
117.4457
117.2673
113.3394
16.8996
MeS
N
N
S
NH
O
F
5h
TFA
TFA
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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8.0975
8.0801
7.7824
7.7650
2.8190
Br
MeS
N
N
S
NH
O
5i
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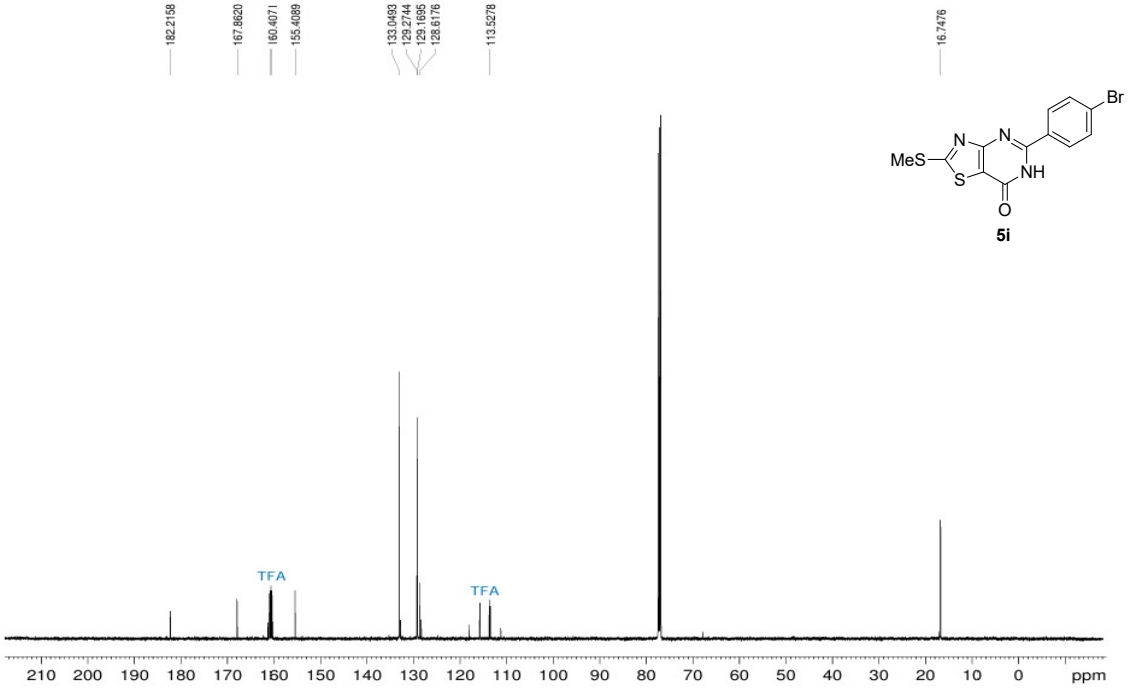
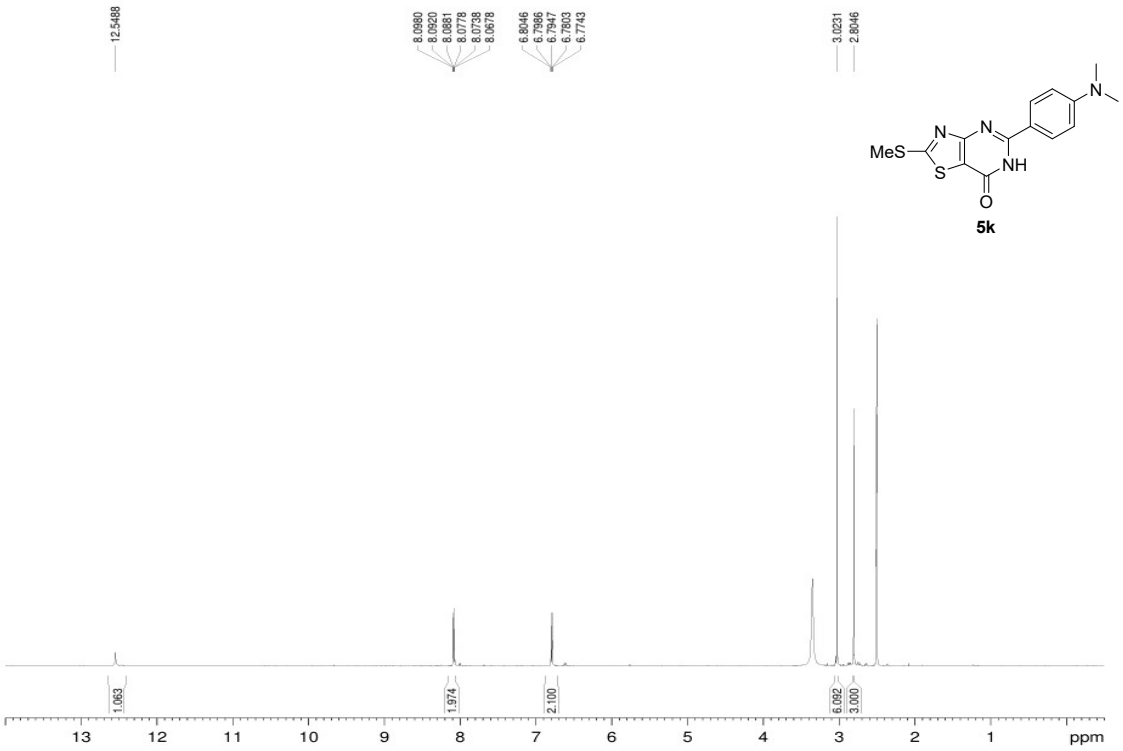
2.000
2.958
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm


182.2158
167.8620
160.4071
155.4089
133.0493
129.2744
129.1695
128.6176
113.5278
16.7476
Br
MeS
N
N
S
NH
O
5i
TFA
TFA
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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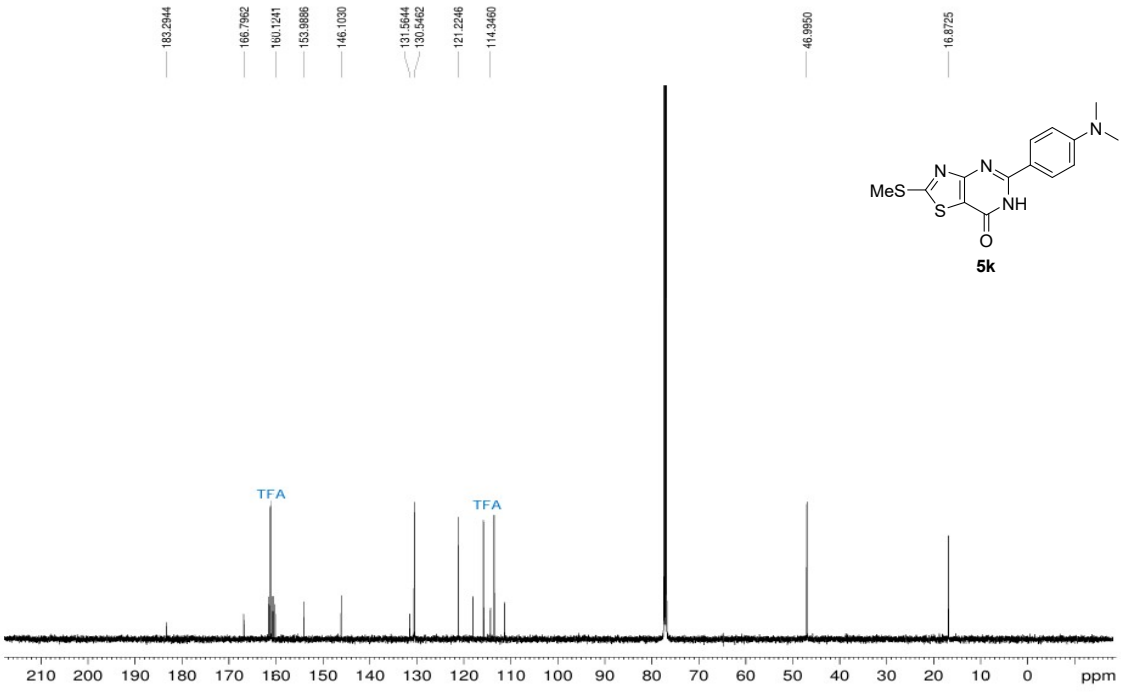
8.0920
8.0881
8.0778
8.0738
8.0678
6.8046
6.7986
6.7947
6.7803
6.7743
3.0231
2.8046
MeS
N
S
NH
O
5k
1.063
1.974
2.100
6.092
3.000
13 12 11 10 9 8 7 6 5 4 3 2 1 ppm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153.9886
146.1030
131.5644
130.5462
121.2246
114.3460
46.9950
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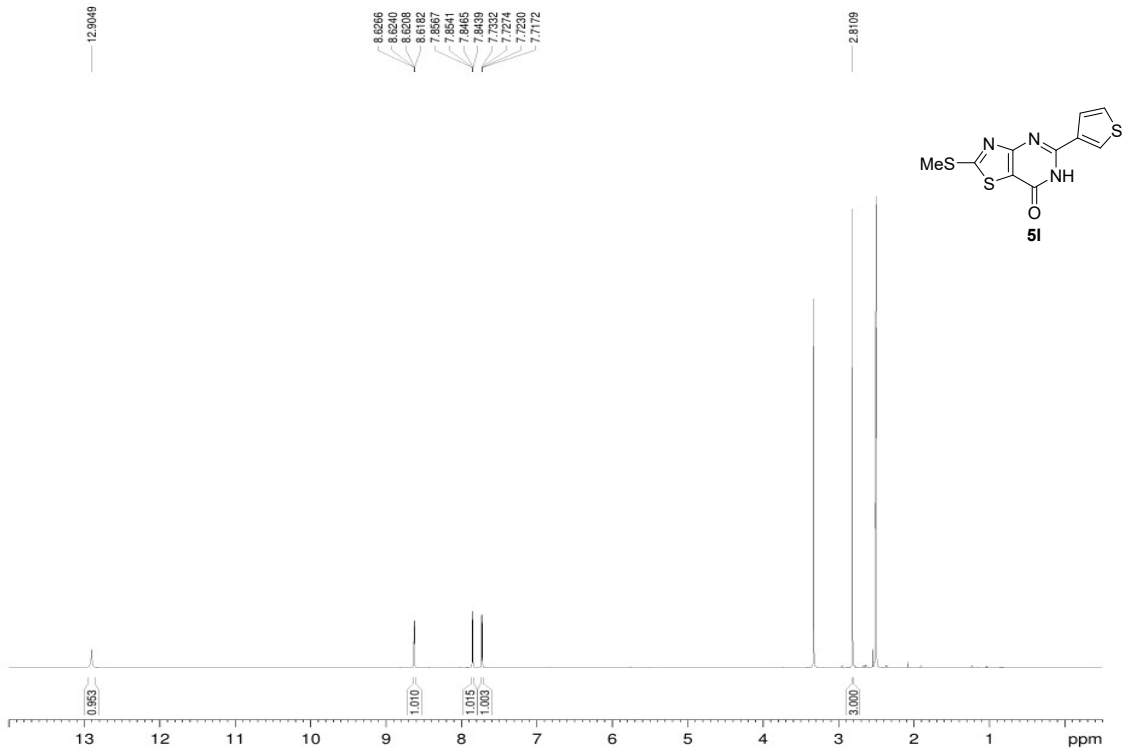
MeS
N
S
NH
O
5k
TFA
TFA
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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8.6240
8.6208
8.6182
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7.8541
7.8465
7.8439
7.7332
7.7274
7.7230
7.7172
2.8109
MeS
N
N
S
S
NH
O
5l
0.953
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1.015
1.003
3.000
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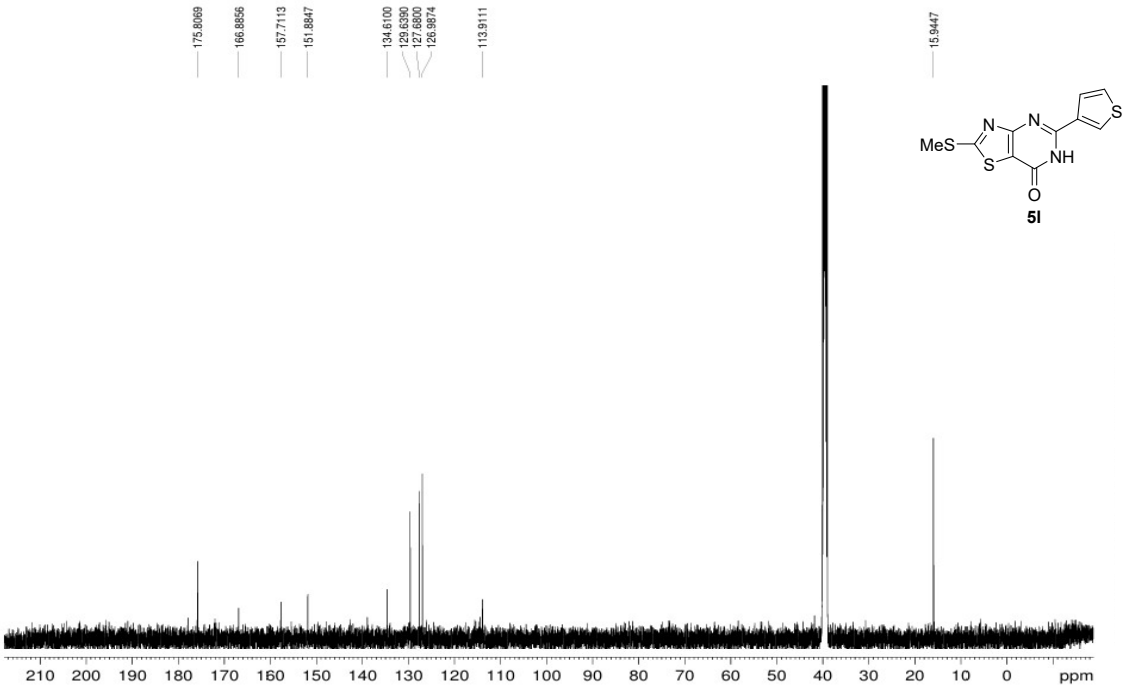
12
11
10
9
8
7
6
5
4
3
2
1
ppm


175.8069
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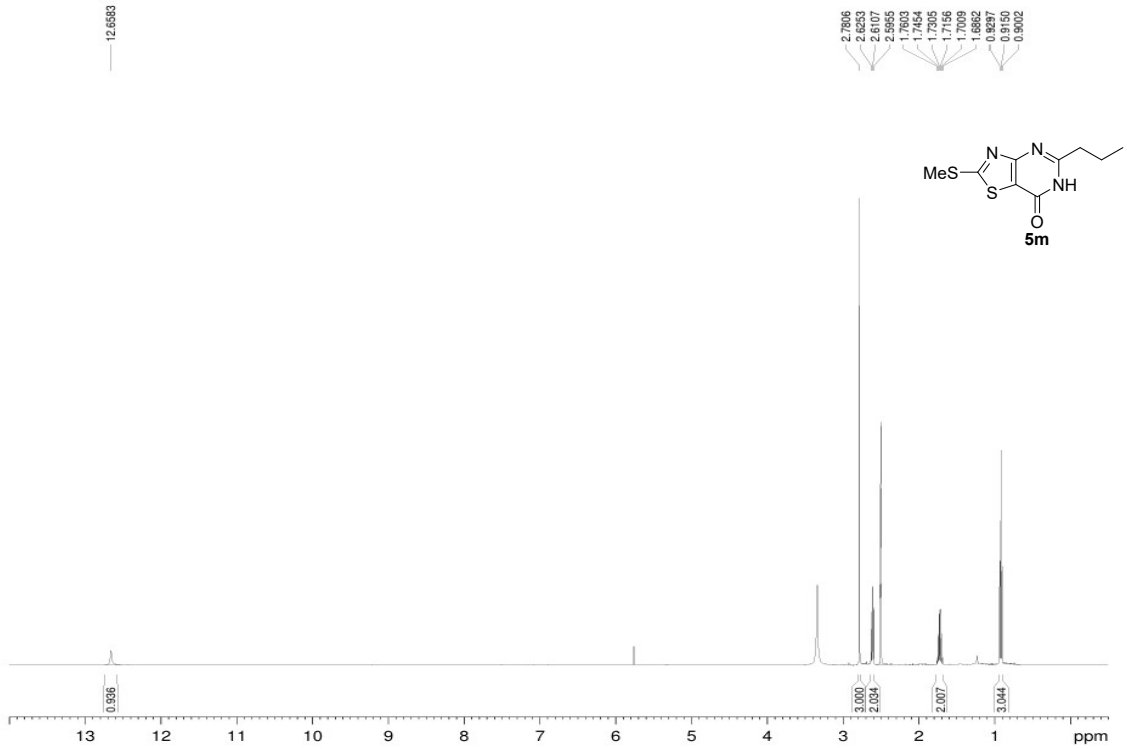
157.7113
151.8847
134.6100
129.6390
127.6800
126.9874
113.9111
15.9447
MeS
N
N
S
S
NH
O
5l
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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1.7454
1.7305
1.7156
1.7009
1.6862
0.9297
0.9150
0.9002
MeS
N
N
S
NH
O
5m
0.936
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2.007
3.044
13
12
11
10
9
8
7
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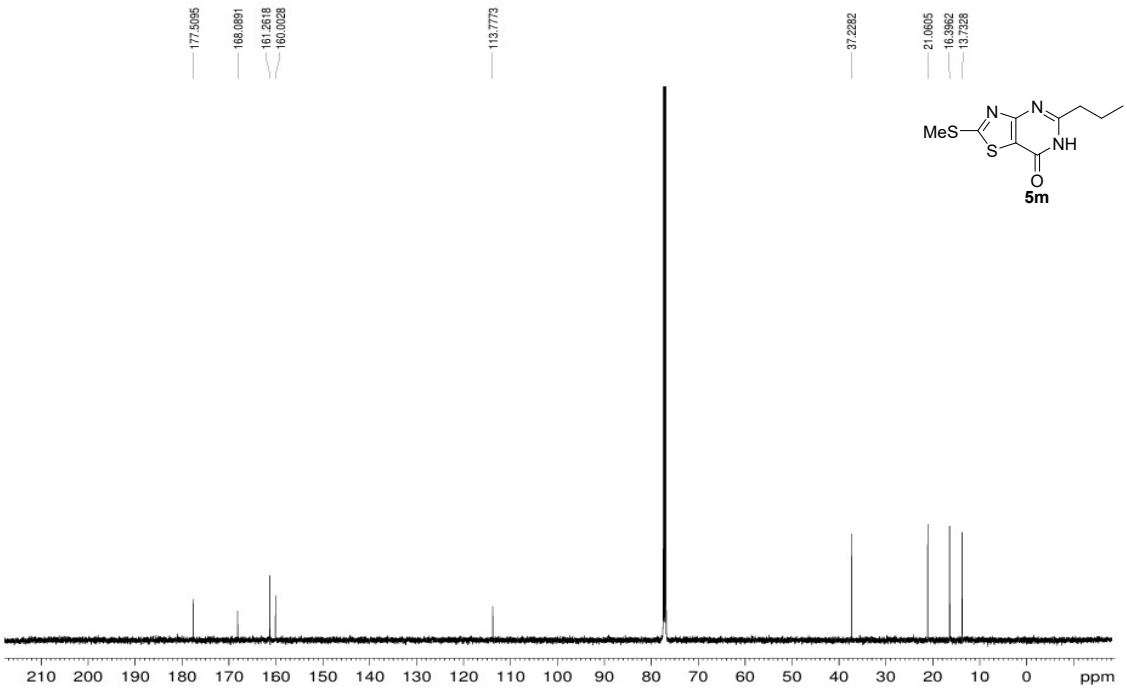
5
4
3
2
1
ppm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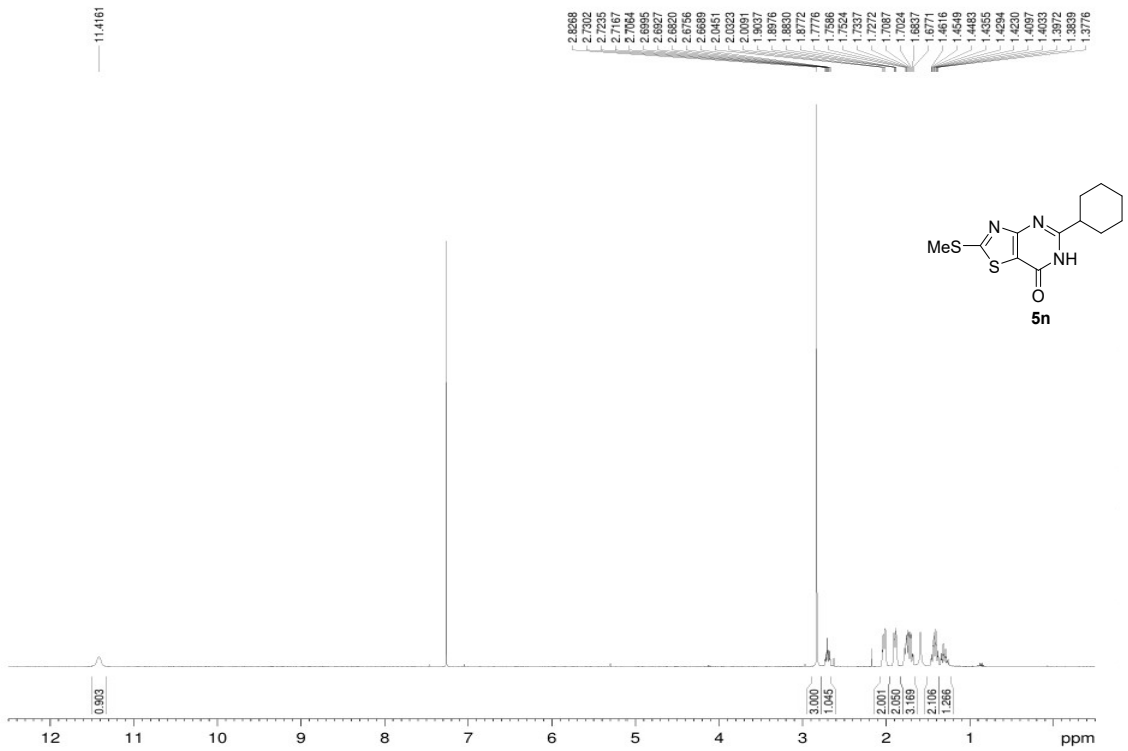
160.0028
113.7773
37.2282
21.0605
16.3962
13.7328
MeS
N
N
S
NH
O
5m
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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2.8268
2.7302
2.7235
2.7167
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2.6995
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2.6820
2.6756
2.6689
2.0451
2.0323
2.0091
1.9037
1.8976
1.8830
1.8772
1.7776
1.7586
1.7524
1.7337
1.7272
1.7087
1.7024
1.6837
1.6771
1.4616
1.4549
1.4483
1.4355
1.4294
1.4230
1.4097
1.4033
1.3972
1.3839
1.3776
MeS
N
N
S
NH
O
5n
0.903
3.000
1.045
2.001
2.050
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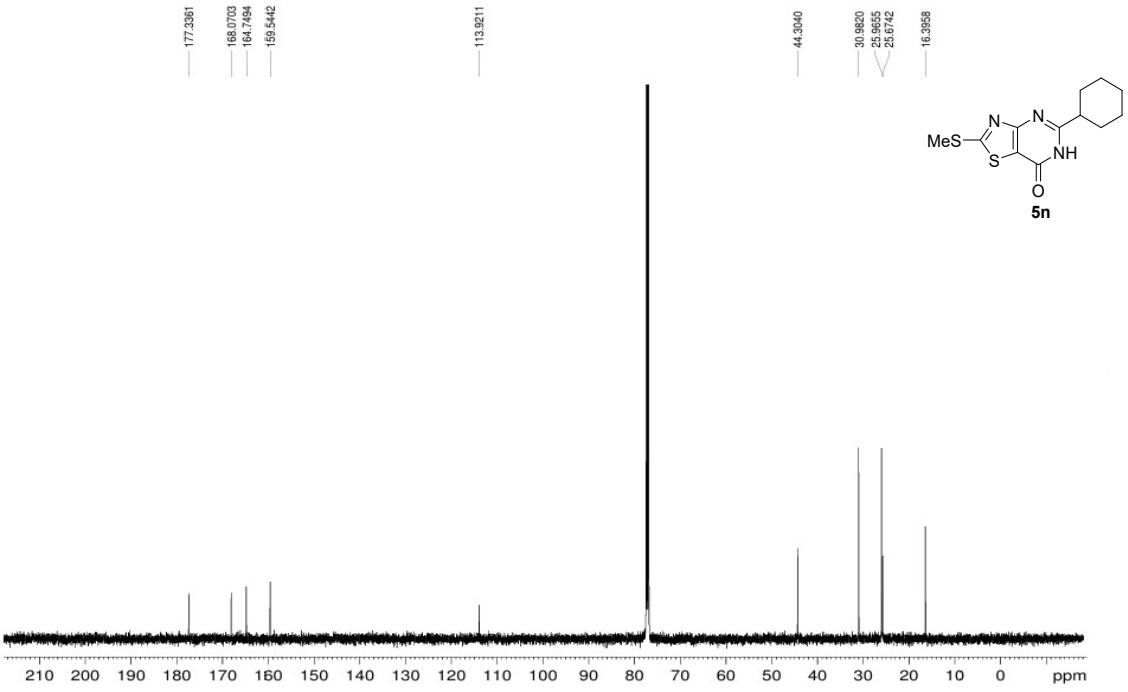
2.106
1.266
12
11
10
9
8
7
6
5
4
3
2
1
ppm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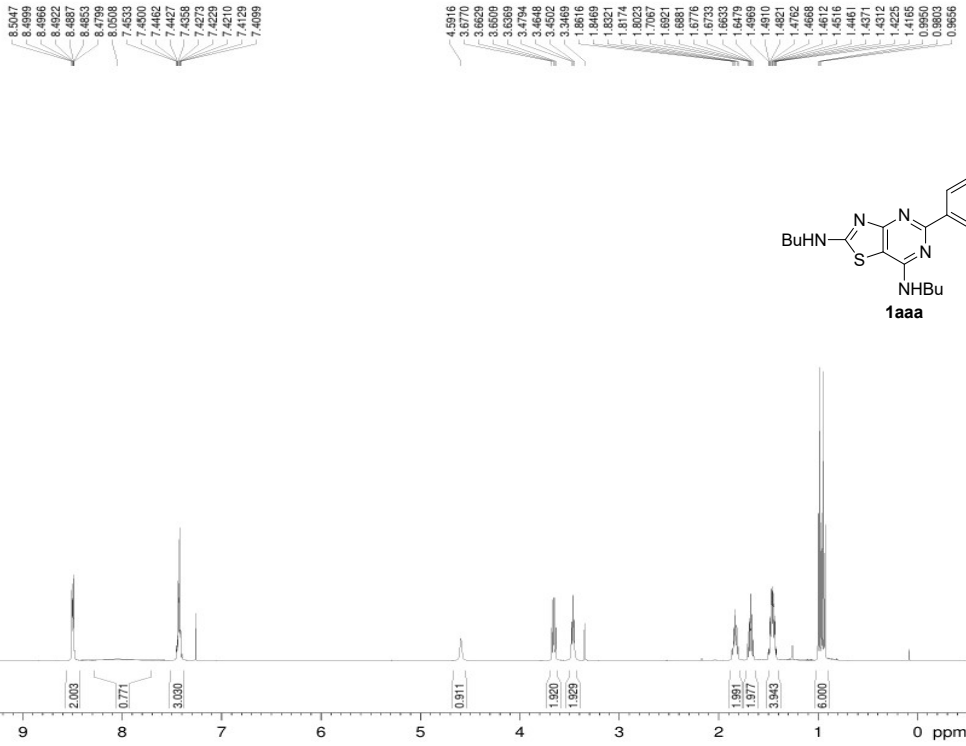
159.5442
113.9211
44.3040
30.9820
25.9655
25.6742
16.3958
MeS
N
N
S
NH
O
5n
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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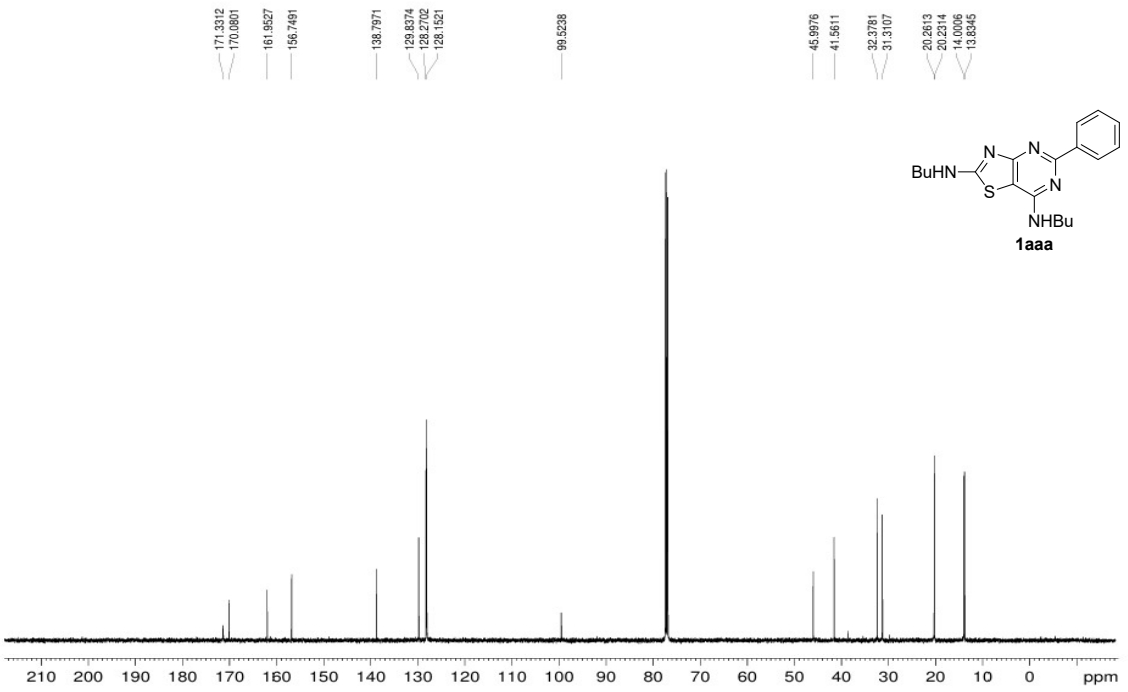
7.4533
7.4500
7.4462
7.4427
7.4358
7.4273
7.4229
7.4210
7.4129
7.4099
4.5916
3.6770
3.6629
3.6509
3.6369
3.4794
3.4648
3.4502
3.3469
1.8616
1.8469
1.8321
1.8174
1.8023
1.7067
1.6921
1.6881
1.6776
1.6733
1.6633
1.6479
1.4969
1.4910
1.4821
1.4762
1.4668
1.4612
1.4516
1.4461
1.4371
1.4312
1.4225
1.4165
0.9950
0.9803
0.9656
BuHN
N
N
S
N
NHBu
1aaa
2.003
0.771
3.030
0.911
1.920
1.929
1.991
1.977
3.943
6.000
10
9
8
7
6
5
4
3
2
1
0 ppm


171.3312
170.0801
161.9527
156.7491
138.7971
129.8374
128.2702
128.1521
99.5238
45.9976
41.5611
32.3781
31.3107
20.2613
20.2314
14.0006
13.8345
BuHN
N
N
S
N
NHBu
1aaa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


9.3430
8.3301
8.3226
8.3199
8.3156
8.3122
8.3086
8.3065
8.3032
8.2987
8.2955
7.7308
7.4871
7.4802
7.4741
7.4667
7.4078
7.4041
7.3909
7.3859
7.3809
7.3713
7.3679
7.3590
7.3555
7.3079
7.3044
7.3005
7.2951
7.2906
7.2804
7.2770
7.2734
4.6647
4.6553
3.5717
3.5580
3.5464
3.5327
1.6454
1.6312
1.6188
1.6025
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1.4026
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1.3726
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1.3435
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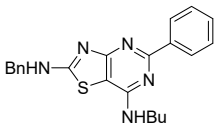
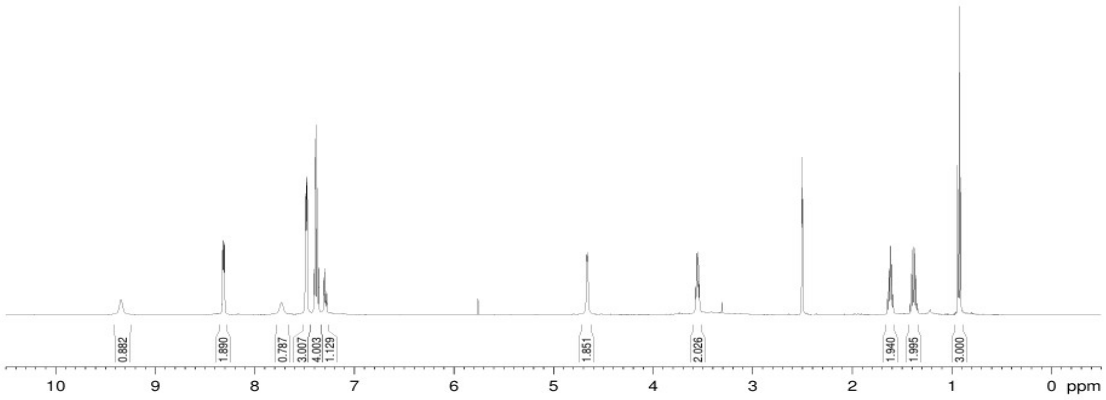
0.9250
0.9102


BnHN
N
N
S
N
NHBu

1aab


0.882
1.890
0.787
3.007
4.003
1.129
1.851
2.026
1.940
1.995
3.000
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9
8
7
6
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4
3
2
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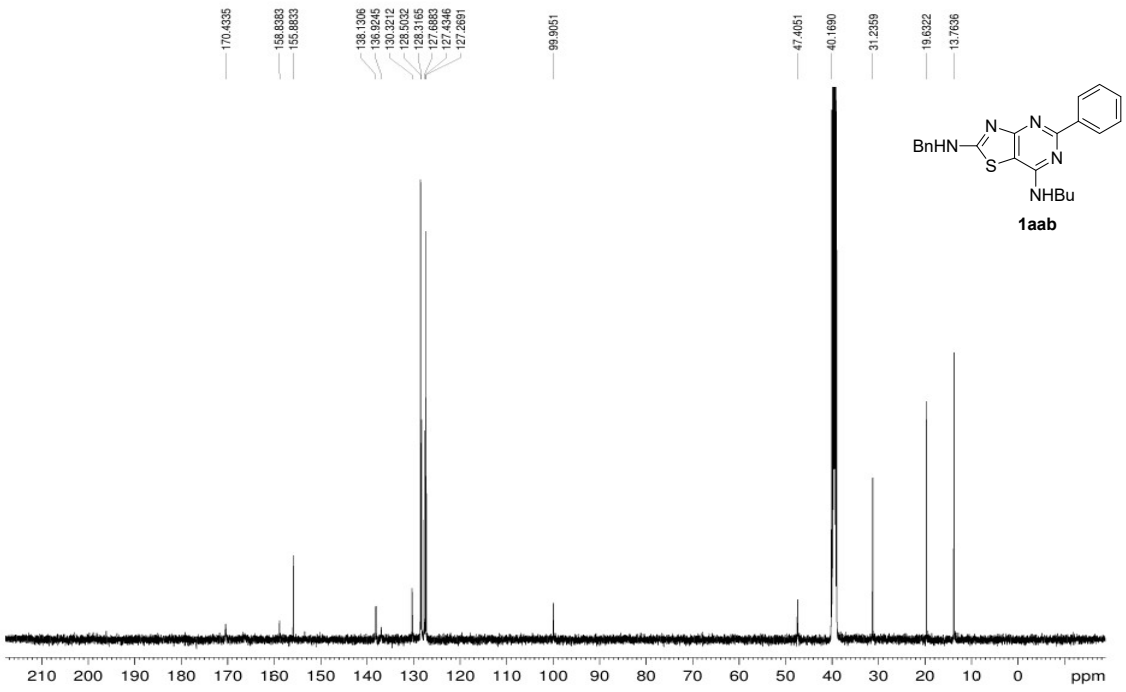
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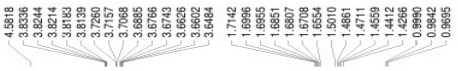
155.8833
138.1306
136.9245
130.3212
128.5032
128.3165
127.6883
127.4346
127.2691
99.9051
47.4051
40.1690
31.2359
19.6322
13.7636
BnHN
N
N
S
N
NHBu
1aab
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.5316
8.5268
8.5232
8.5210
8.5193
8.5156
8.5121
7.4502
7.4468
7.4427
7.4393
7.4324
7.4293
7.4251
7.4232
7.4176
7.4108
7.4072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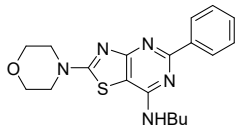
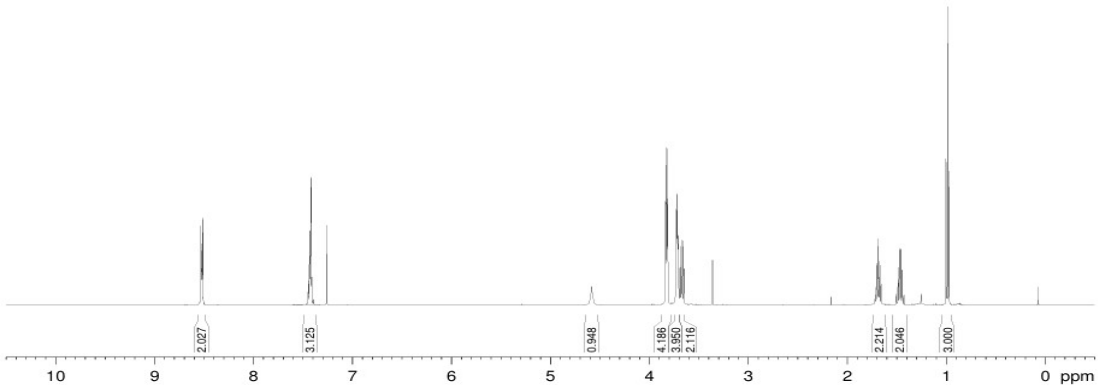
3.8214
3.8163
3.8139
3.7260
3.7157
3.7088
3.6885
3.6766
3.6743
3.6626
3.6602
3.6484
1.7142
1.6996
1.6955
1.6851
1.6807
1.6708
1.6654
1.5010
1.4861
1.4711
1.4559
1.4412
1.4266
0.9990
0.9942
0.9695


O
N
N
N
S
N
NHBu

1aaf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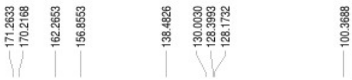
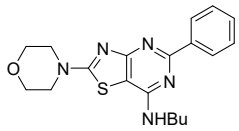
3.125
0.948
4.186
3.950
2.116
2.214
2.046
3.000
10
9
8
7
6
5
4
3
2
1
0 ppm

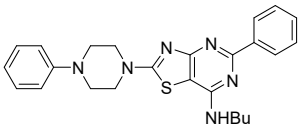

171.2633
170.2168
162.2653
156.8553
138.4826
130.0030
128.3993
128.1732
100.3688
66.2672
48.6067
41.6044
32.3478
20.2314
13.9978


O
N
N
N
S
N
NHBu

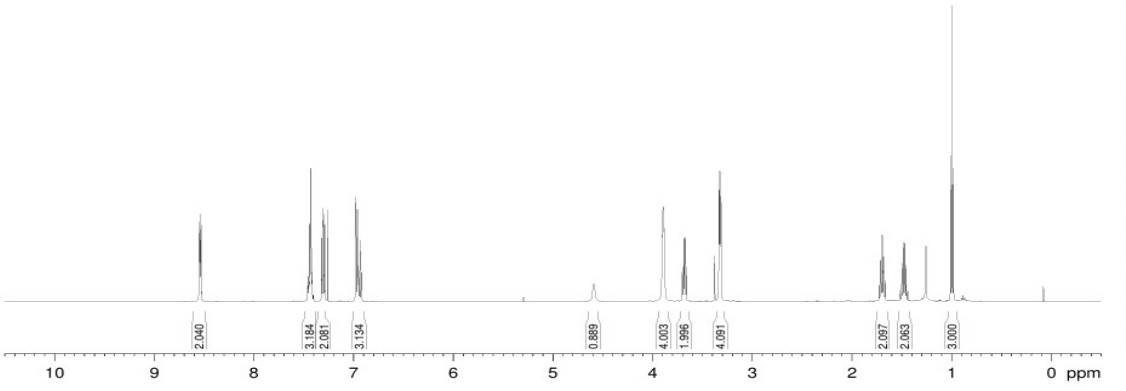
1aaf

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.5576
8.5488
8.5444
8.5407
8.5377
8.5361
8.5327
8.5294
8.5238
7.4592
7.4559
7.4523
7.4487
7.4417
7.4330
7.4281
7.4269
7.4180
7.4152
7.3242
7.3200
7.3159
7.3053
7.3026
7.2985
7.2919
7.2879
7.2834
6.9769
6.9752
6.9595
6.9578
6.9519
6.9500
6.9354
6.9226
6.9208
4.5878
3.9015
3.8920
3.8821
3.6998
3.6876
3.6856
3.6737
3.6596
3.3332
3.3227
3.3124
1.7240
1.7094
1.7054
1.6949
1.6906
1.6806
1.6652
1.5115
1.4967
1.4816
1.4665
1.4517
1.4371
1.2559
1.0081
0.9934
0.9786


N
N
N
N
S
N
NHBu

1aag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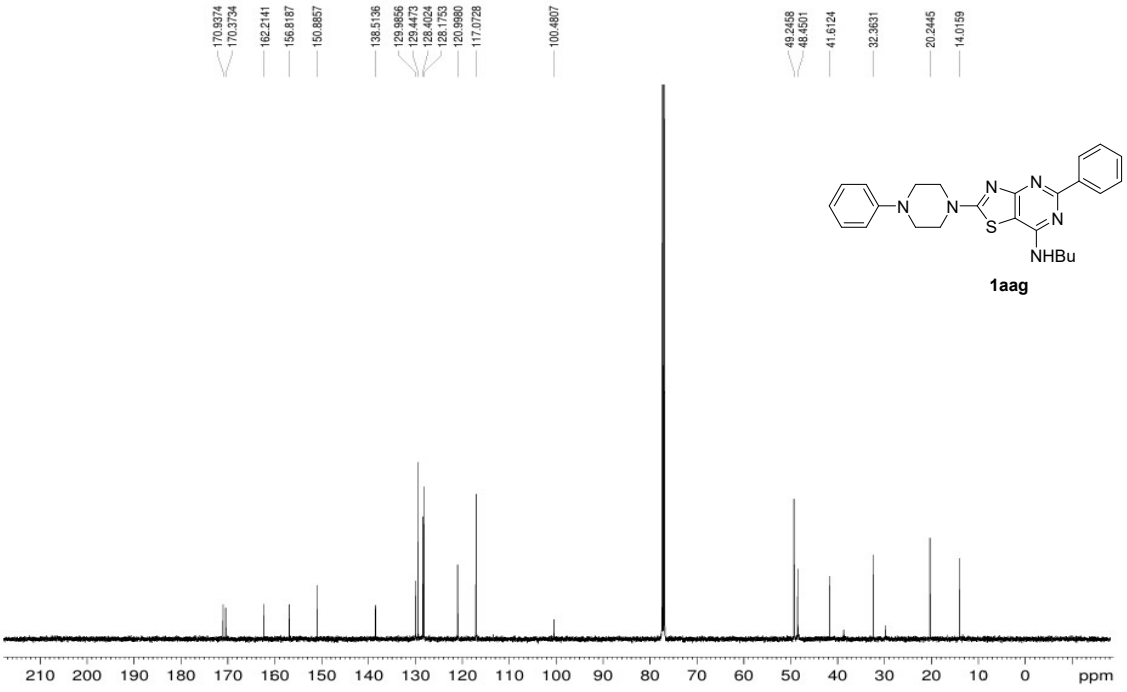
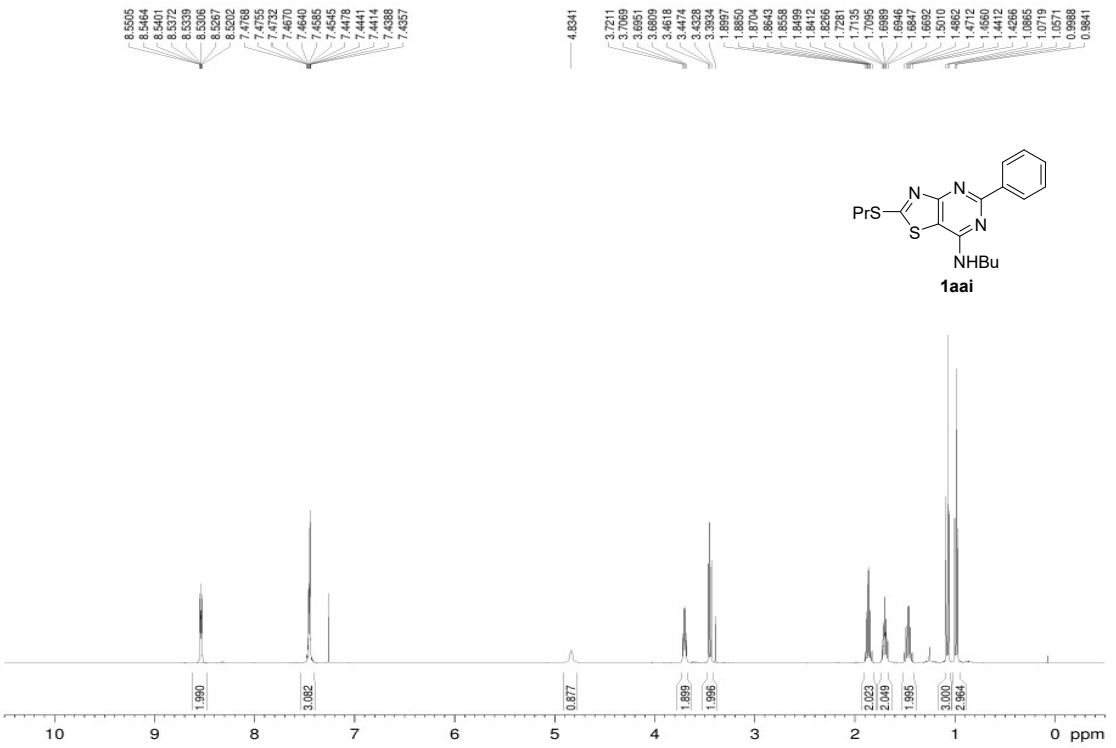
3.184
2.081
3.134
0.889
4.003
1.996
4.091
2.097
2.063
3.000
10
9
8
7
6
5
4
3
2
1
0 ppm


170.9374
170.3734
162.2141
156.8187
150.8857
138.5136
129.9856
129.4473
128.4024
128.1753
120.9980
117.0728
100.4807
49.2458
48.4501
41.6124
32.3631
20.2445
14.0159
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

N
N
N
N
S
N
NHBu

1aag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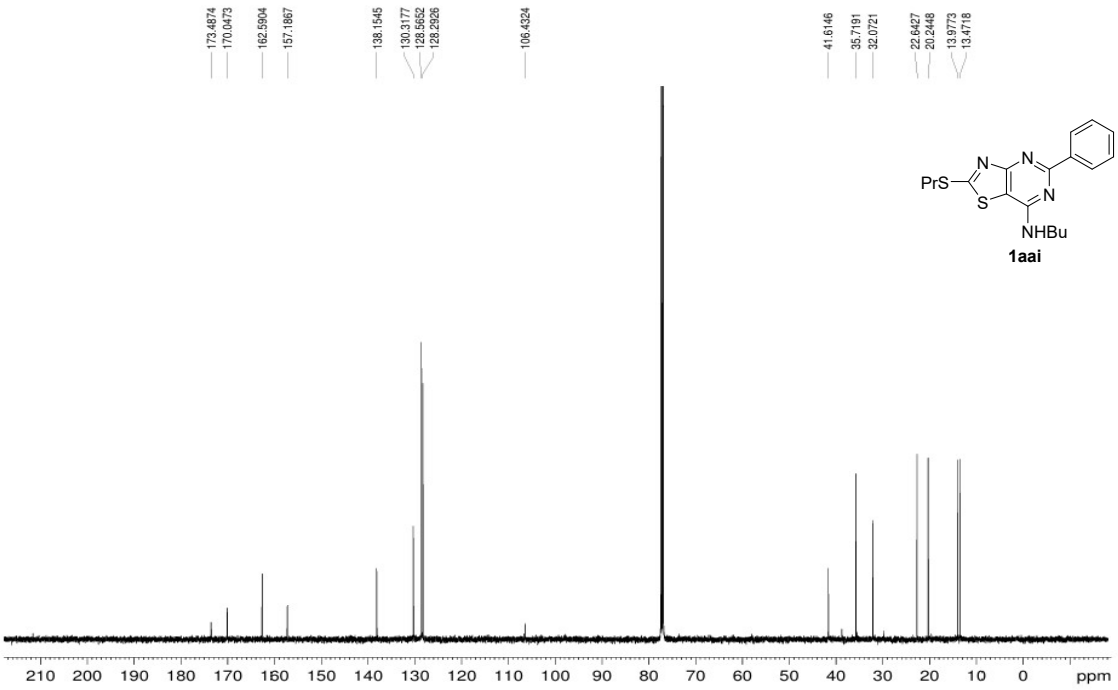
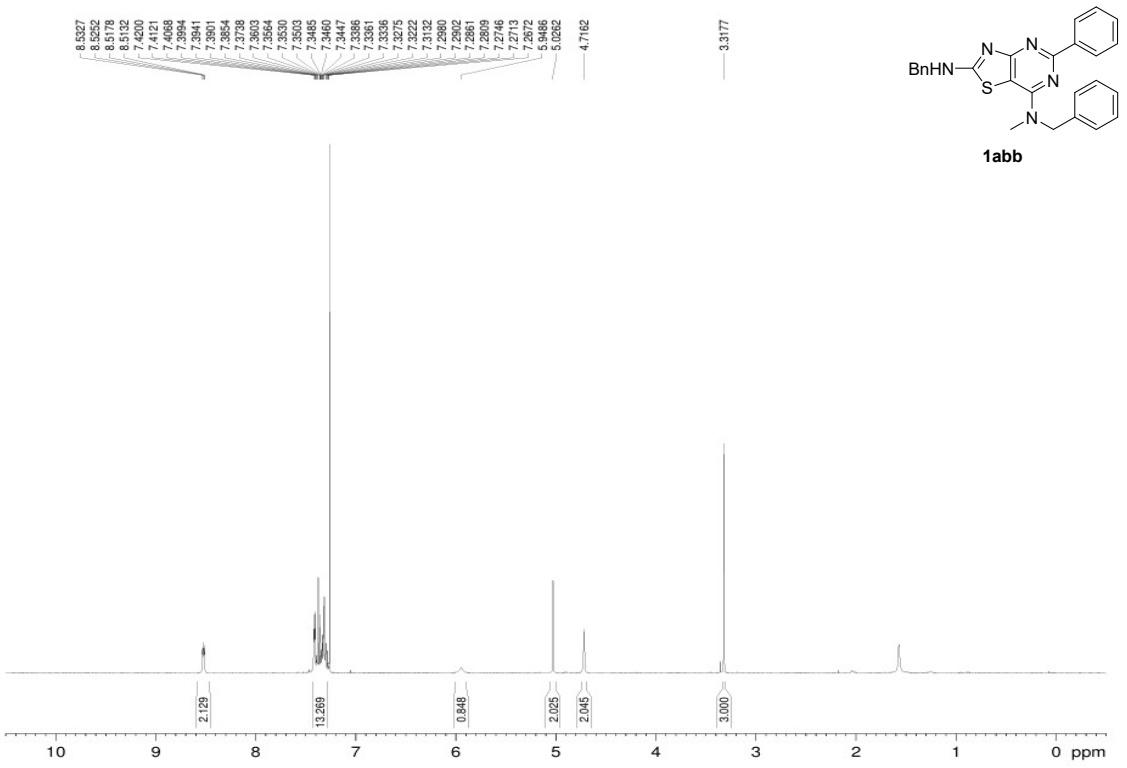
8.5464
8.5401
8.5372
8.5339
8.5306
8.5267
8.5202
7.4768
7.4755
7.4732
7.4670
7.4640
7.4585
7.4545
7.4478
7.4441
7.4414
7.4388
7.4357
4.8341
3.7211
3.7069
3.6951
3.6809
3.4618
3.4474
3.4328
3.3934
1.8997
1.8850
1.8704
1.8643
1.8558
1.8499
1.8412
1.8266
1.7281
1.7135
1.7095
1.6989
1.6946
1.6847
1.6692
1.5010
1.4862
1.4712
1.4560
1.4412
1.4266
1.0865
1.0719
1.0571
0.9988
0.9841
PrS
N
N
S
N
NHBu
1aai
1.990
3.082
0.877
1.899
1.996
2.023
2.049
1.995
3.000
2.964
10
9
8
7
6
5
4
3
2
1
0 ppm


173.4874
170.0473
162.5904
157.1867
138.1545
130.3177
128.5652
128.2926
106.4324
41.8146
35.7191
32.0721
22.6427
20.2448
13.9773
13.4718
PrS
N
N
S
N
NHBu
1aai
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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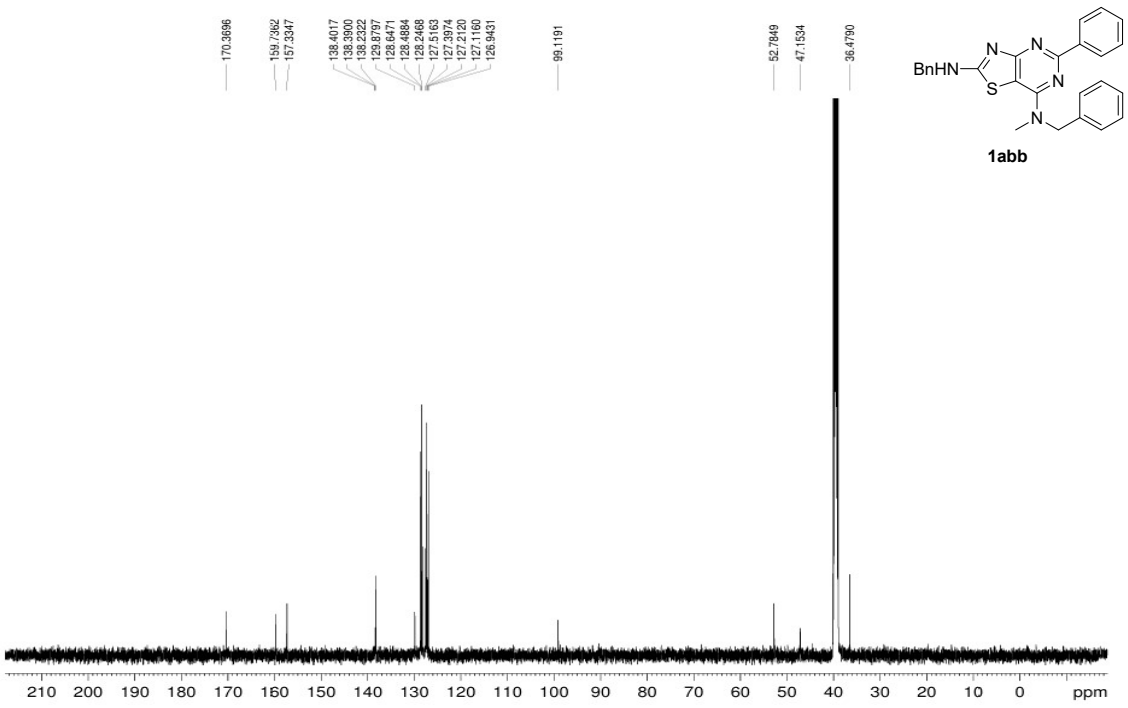
8.5252
8.5178
8.5132
7.4200
7.4121
7.4068
7.3994
7.3941
7.3901
7.3854
7.3738
7.3603
7.3564
7.3530
7.3503
7.3485
7.3460
7.3447
7.3386
7.3361
7.3336
7.3275
7.3222
7.3132
7.2980
7.2902
7.2861
7.2809
7.2746
7.2713
7.2672
5.9486
5.0262
4.7162
3.3177
BnHN
N
N
S
N
N
2.129
13.269
0.848
2.025
2.045
3.000
10
9
8
7
6
5
4
3
2
1
0 ppm

1abb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129.8797
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128.4884
128.2468
127.5163
127.3974
127.2120
127.1160
126.9431
99.1191
52.7849
47.1534
36.4790
BnHN
N
N
S
N
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

1abb


8.5614
8.5518
8.5472
8.5449
8.5430
8.5393
8.5363
8.5321
8.5252
7.4392
7.4376
7.4357
7.4284
7.4207
7.4172
7.4108
7.4066
7.3996
7.3914
7.3873
7.3728
7.3673
7.3588
7.3467
7.3442
7.3412
7.3320
7.3298
7.3274
7.3204
7.3158
7.3026
7.2893
7.2804
7.2753
7.2693
7.2652
5.0090
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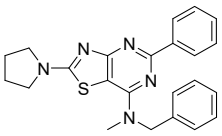
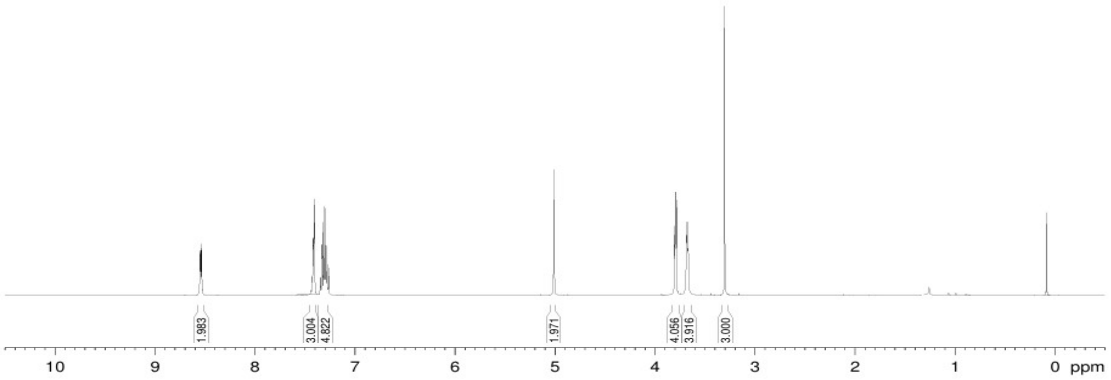
3.7939
3.7834
3.6852
3.6753
3.6666
3.3007



1abd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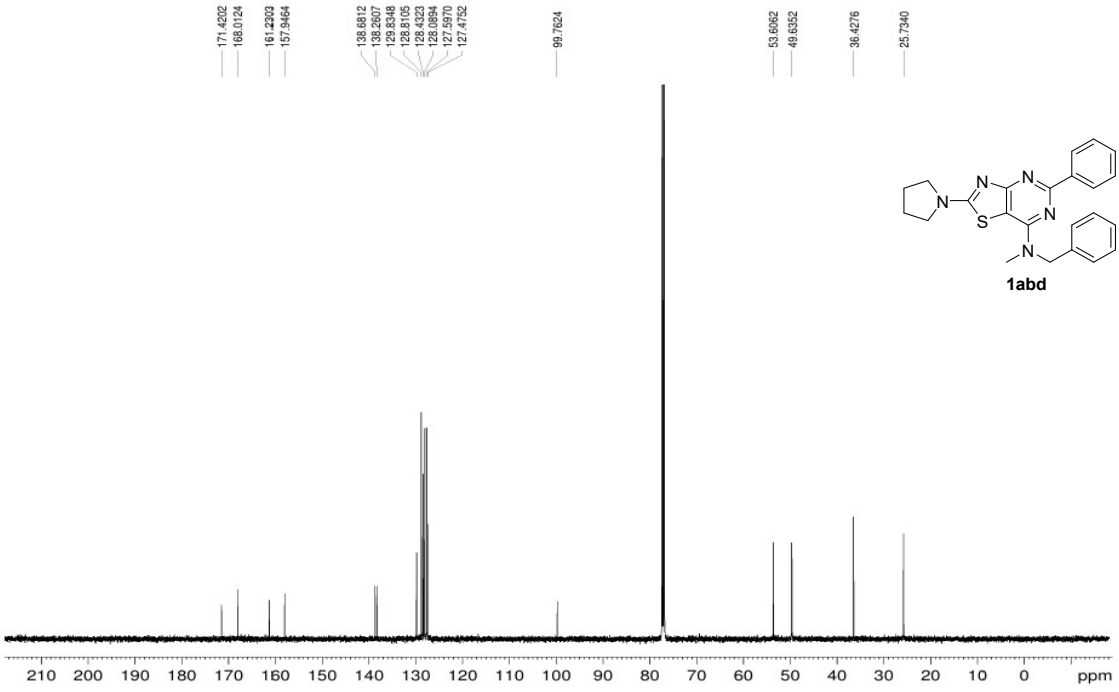
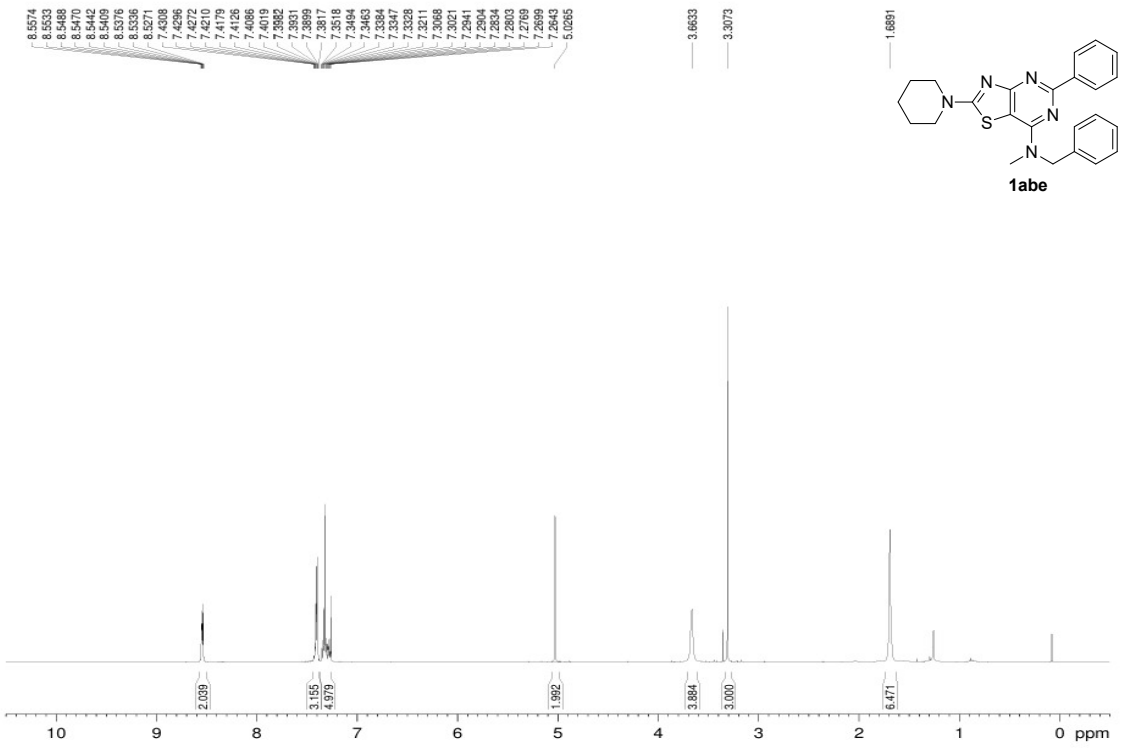
3.004
4.822
1.971
4.056
3.916
3.000
10
9
8
7
6
5
4
3
2
1
0 ppm


171.4202
168.0124
161.4293
157.9464
138.6812
138.2607
129.8348
128.8105
128.4323
128.0894
127.5970
127.4752
99.7624
53.6062
49.6352
36.4276
25.7340
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

1abd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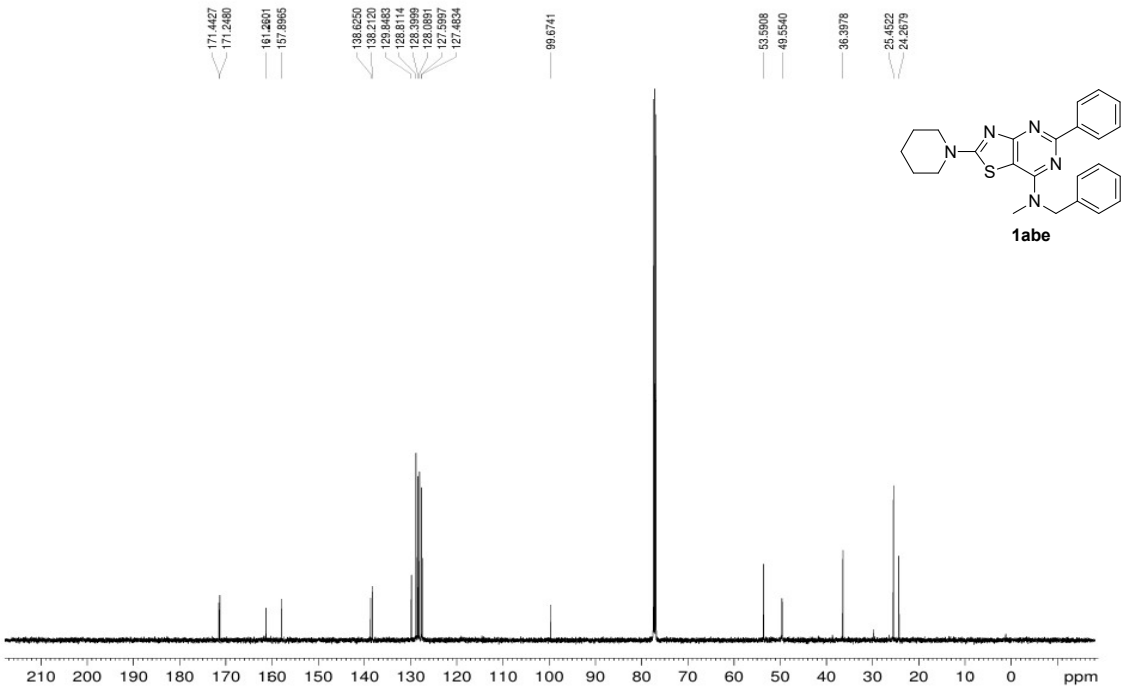
8.5488
8.5470
8.5442
8.5409
8.5376
8.5336
8.5271
7.4308
7.4296
7.4272
7.4210
7.4179
7.4126
7.4086
7.4019
7.3982
7.3931
7.3899
7.3817
7.3518
7.3494
7.3463
7.3384
7.3347
7.3328
7.3211
7.3068
7.3021
7.2941
7.2904
7.2834
7.2803
7.2769
7.2699
7.2643
5.0265
3.6633
3.3073
1.6891
2.039
3.155
4.979
1.992
3.884
3.000
6.471
10
9
8
7
6
5
4
3
2
1
0 ppm
1abe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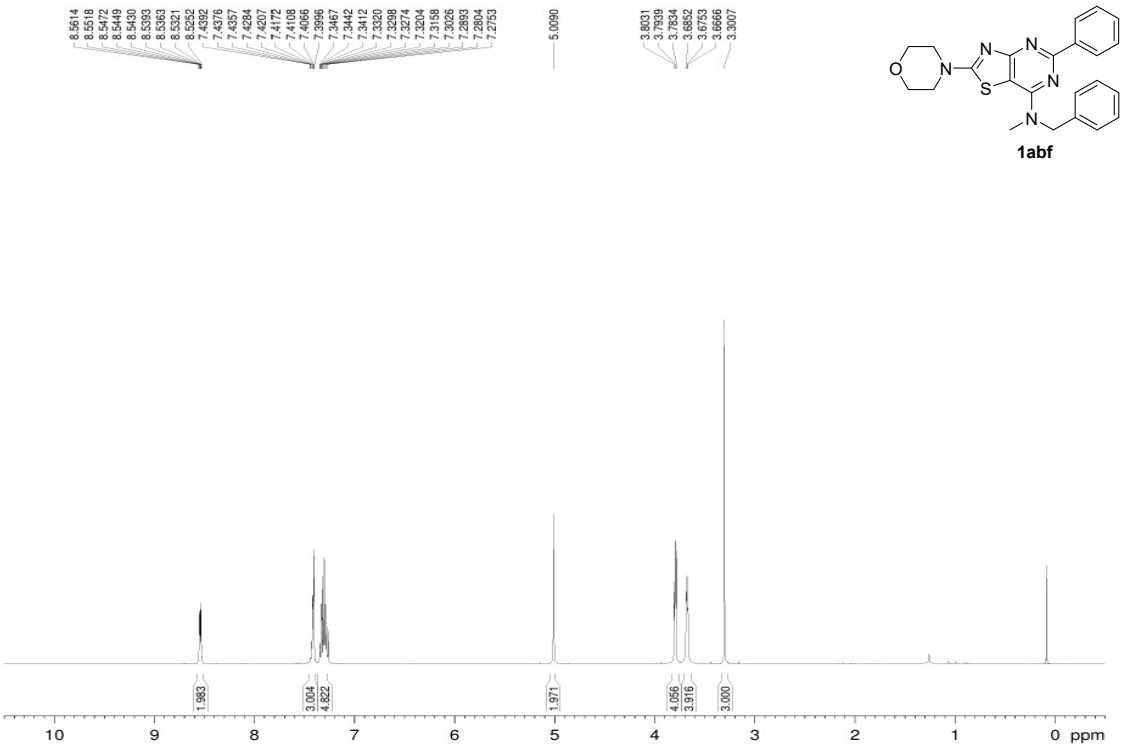
161.2601
157.8965
138.6250
138.2120
129.8483
128.8114
128.3999
128.0891
127.5997
127.4634
99.6741
53.5908
49.5540
36.3978
25.4522
24.2679
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
1abe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8.5518
8.5472
8.5449
8.5430
8.5393
8.5363
8.5321
8.5232
7.4392
7.4376
7.4357
7.4284
7.4207
7.4172
7.4108
7.4066
7.3996
7.3467
7.3442
7.3412
7.3320
7.3298
7.3274
7.3204
7.3158
7.3026
7.2893
7.2804
7.2753
5.0090
3.8031
3.7939
3.7834
3.6852
3.6753
3.6666
3.3007
1abf
1.983
3.004
4.822
1.971
4.056
3.916
3.000
10
9
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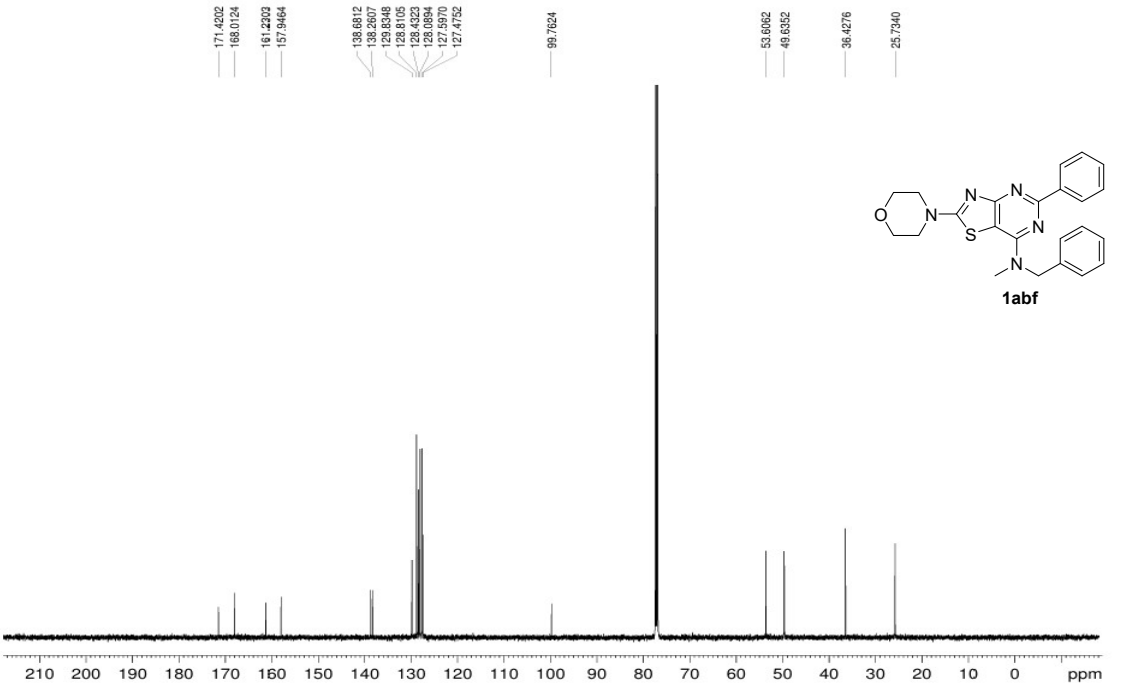
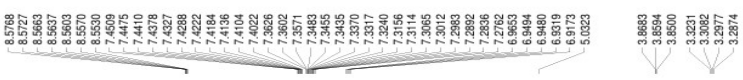
7
6
5
4
3
2
1
0 ppm


171.4202
168.0124
161.2303
157.9464
138.6812
138.2607
129.8348
128.8105
128.4323
128.0894
127.5970
127.4752
99.7624
53.6062
49.6352
36.4276
25.7340
1abf
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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8.5727
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8.5637
8.5603
8.5570
8.5530
7.4509
7.4475
7.4410
7.4378
7.4327
7.4288
7.4222
7.4184
7.4136
7.4104
7.4022
7.3626
7.3602
7.3571
7.3483
7.3455
7.3435
7.3370
7.3317
7.3240
7.3156
7.3114
7.3065
7.3012
7.2983
7.2892
7.2836
7.2762
6.9653
6.9494
6.9480
6.9319
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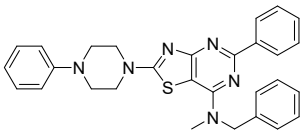
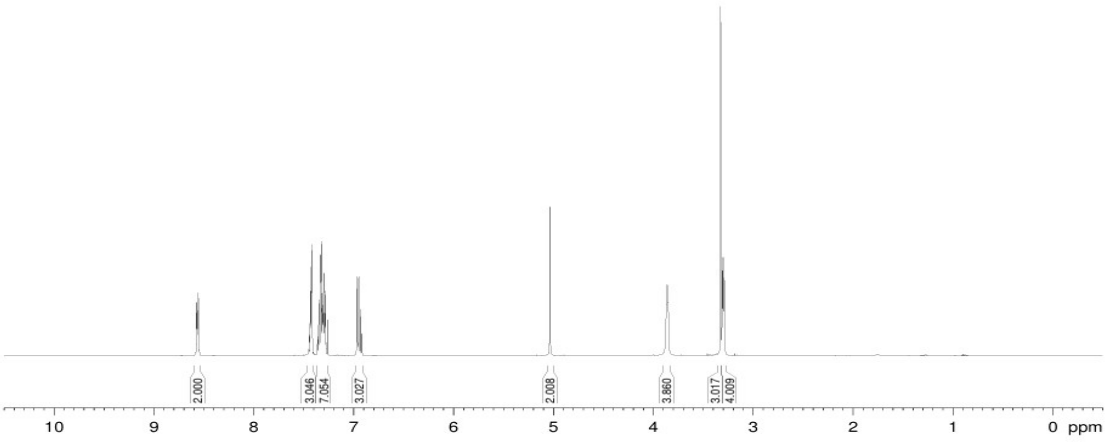
5.0323
3.8683
3.8594
3.8500
3.3231
3.3082
3.2977
3.2874



1abg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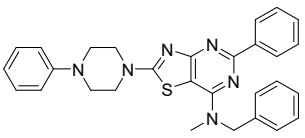
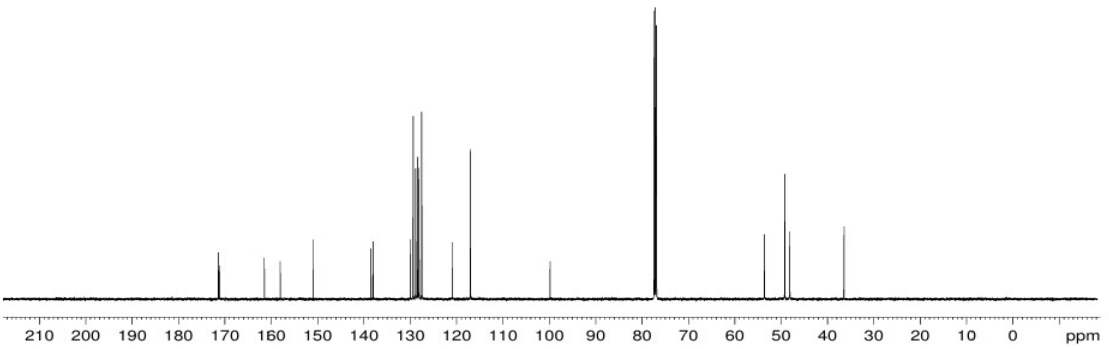
3.046
7.054
3.027
2.008
3.860
3.017
4.009
10
9
8
7
6
5
4
3
2
1
0 ppm


171.3419
171.1091
161.4128
157.9773
150.8849
138.4649
138.0172
129.9717
129.4023
128.8365
128.3990
128.1305
127.5259
120.9227
117.0210
99.8485
53.5910
49.2029
48.1115
36.4181



1abg


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


8.5200
8.5167
8.5109
8.5072
8.5056
8.5007
8.4971
7.4395
7.4360
7.4308
7.4277
7.4215
7.4181
7.4160
7.4102
7.4068
7.4021
7.4008
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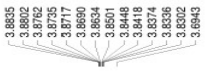
7.3891
7.3854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3.8762
3.8735
3.8717
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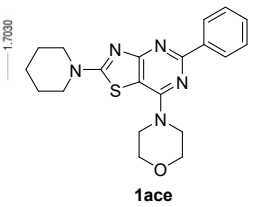
3.8634
3.8501
3.8448
3.8418
3.8374
3.8336
3.8302
3.6943


1.7030
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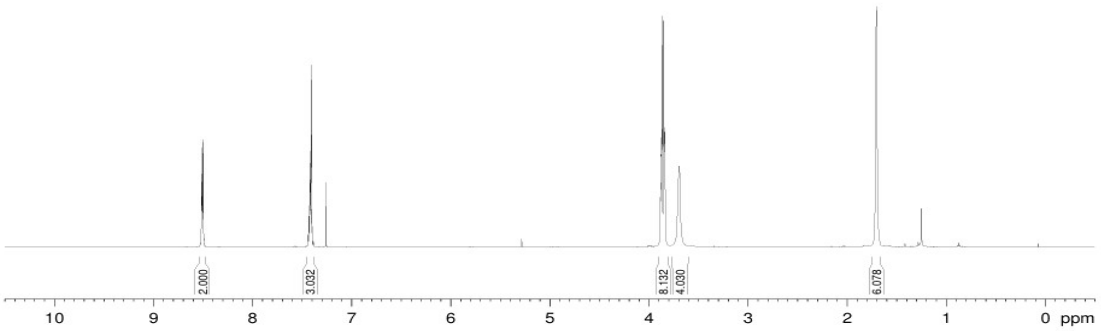
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4.030
6.078
10
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8
7
6
5
4
3
2
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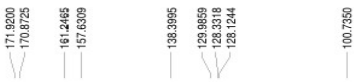
0 ppm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161.2465
157.6309
138.3995
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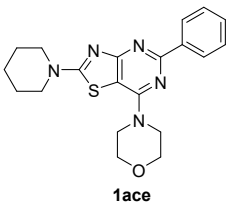
128.3318
128.1244
100.7350
66.9153
49.6922
46.3471
25.4621
24.2357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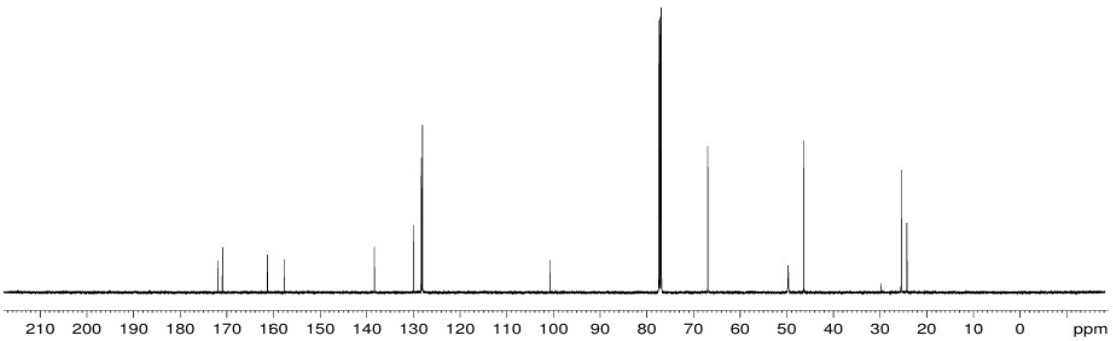
210
200
190
180
170
160
150
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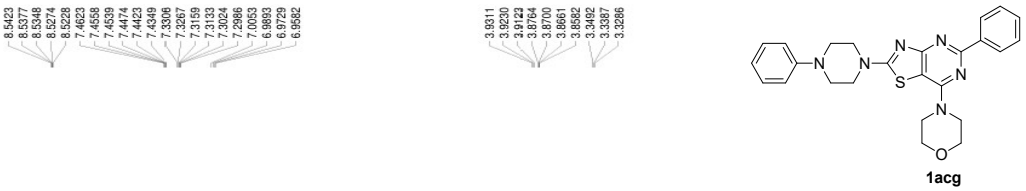
0
ppm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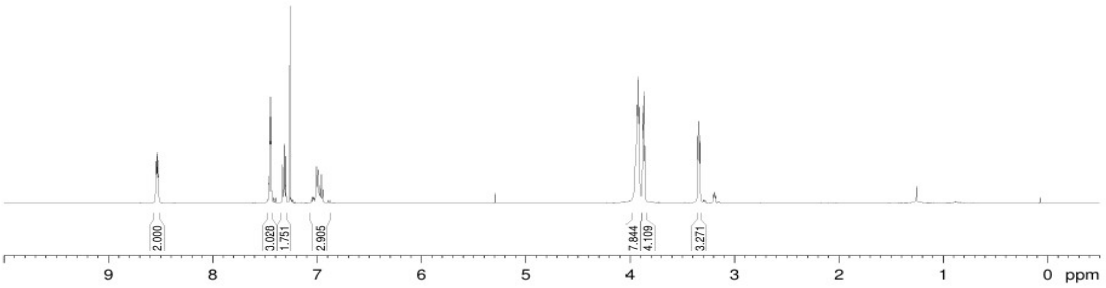
8.5348
8.5274
8.5228
7.4623
7.4558
7.4539
7.4474
7.4423
7.4349
7.3306
7.3267
7.3159
7.3133
7.3024
7.2986
7.0053
6.9893
6.9729
6.9582
3.9311
3.9230
3.9122
3.8764
3.8700
3.8661
3.8582
3.3492
3.3387
3.3286
1acg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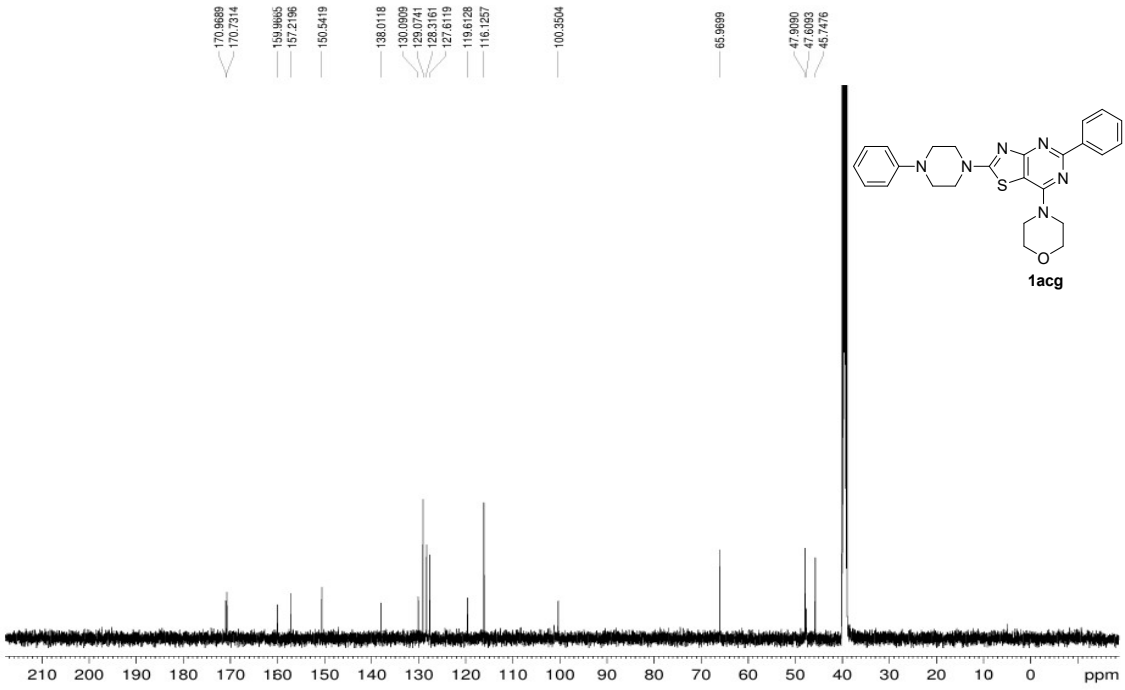
3.020
1.751
2.905
7.844
4.109
3.271
9
8
7
6
5
4
3
2
1
0 ppm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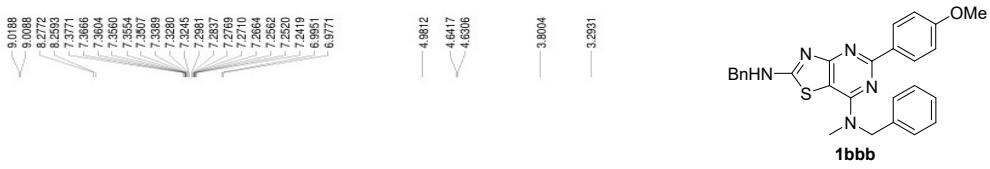
159.9665
157.2196
150.5419
138.0118
130.0909
129.0741
128.3161
127.6119
119.6128
116.1257
100.3504
65.9699
47.9090
47.6093
45.7476
1acg
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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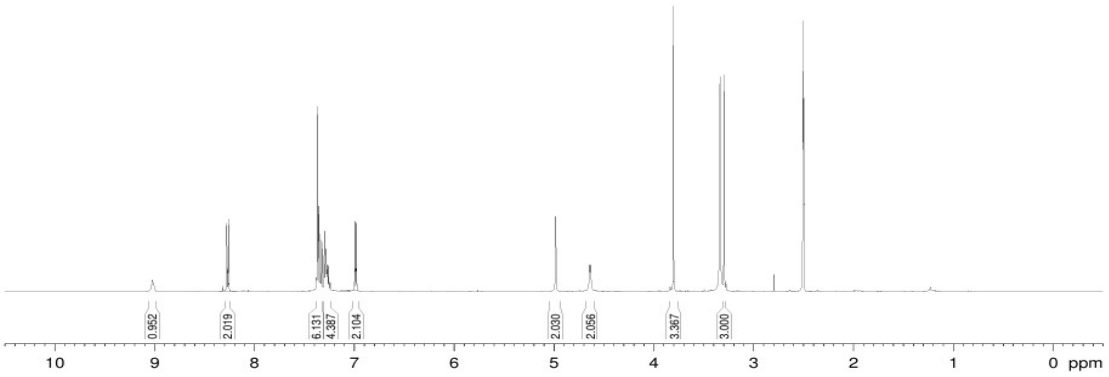
9.0088
8.2772
8.2593
7.3771
7.3666
7.3604
7.3560
7.3554
7.3507
7.3389
7.3280
7.3245
7.2861
7.2837
7.2789
7.2710
7.2664
7.2562
7.2520
7.2419
6.9951
6.9771
4.9812
4.6417
4.6306
3.8004
3.2931
OMe
BnHN
N
S
N
N
N
1bbb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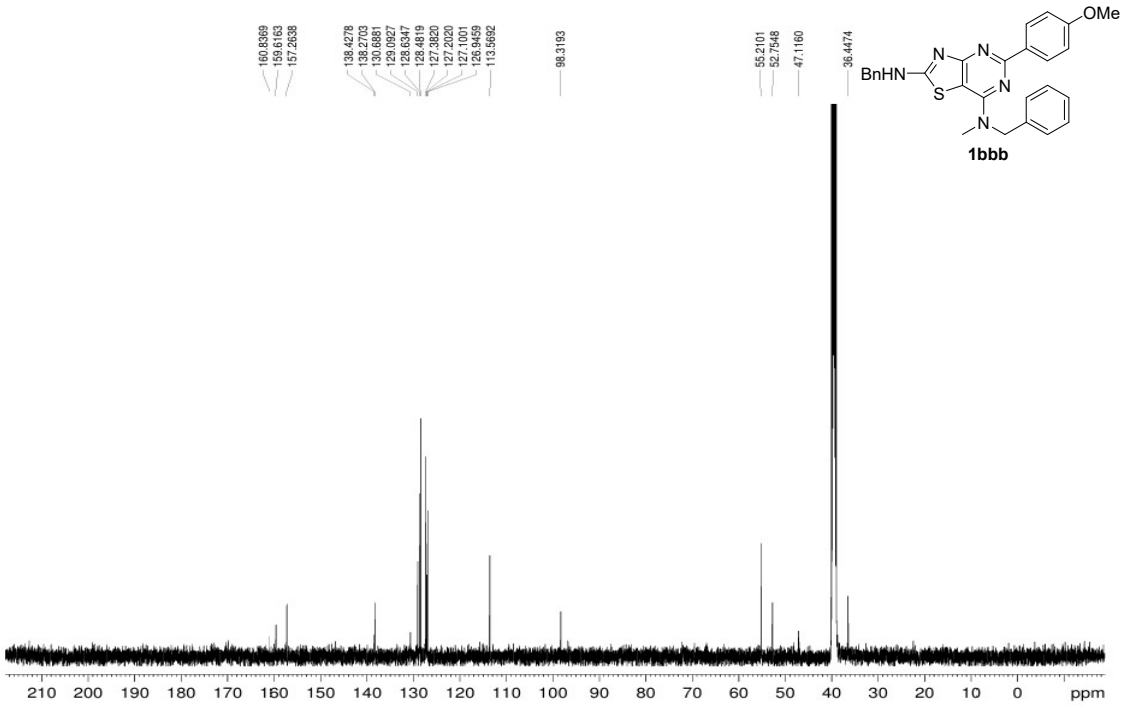
2.019
6.131
4.387
2.104
2.030
2.056
3.367
3.000
10
9
8
7
6
5
4
3
2
1
0 ppm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157.2638
138.4278
138.2703
130.6881
129.0927
128.6347
128.4819
127.3820
127.2020
127.1001
126.9459
113.5692
98.3193
55.2101
52.7548
47.1160
36.4474
OMe
BnHN
N
S
N
N
N
1bbb
210
200
190
180
170
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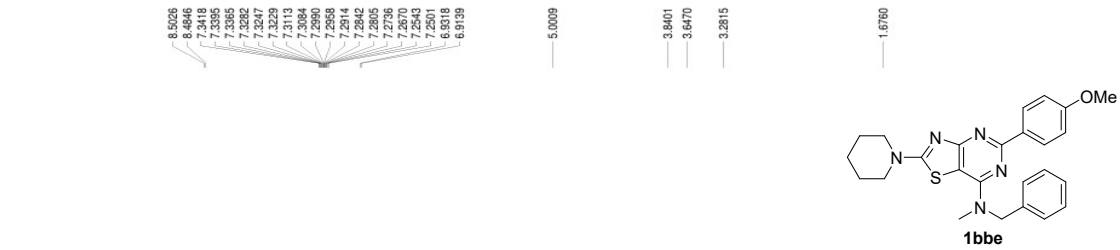
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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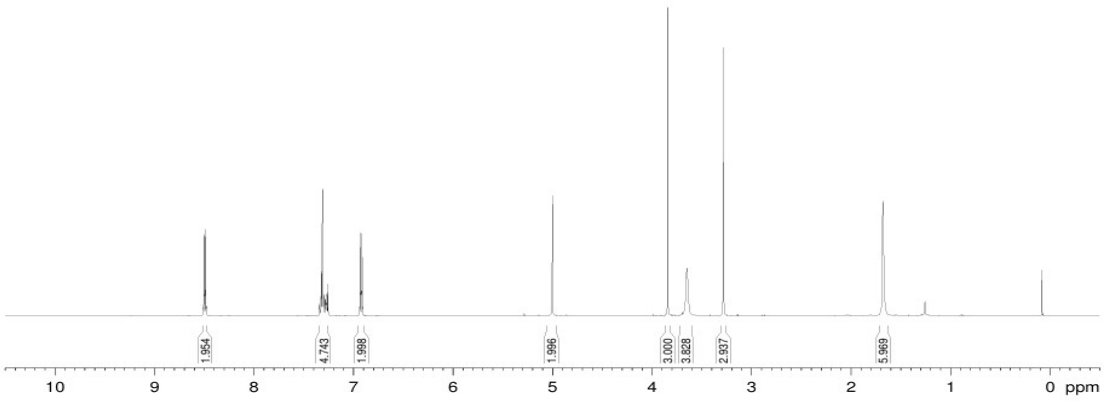
8.4846
7.3418
7.3395
7.3365
7.3282
7.3247
7.3229
7.3113
7.3084
7.2990
7.2958
7.2914
7.2842
7.2805
7.2736
7.2670
7.2543
7.2501
6.9318
6.9139
5.0009
3.8401
3.6470
3.2815
1.6760
OMe
N
N
N
S
N
N

1bbe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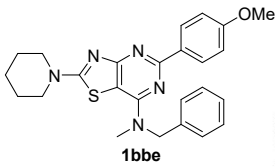
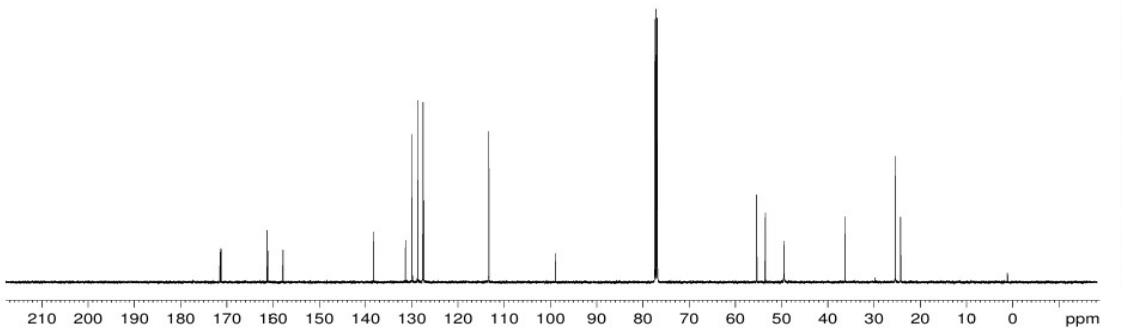
4.743
1.998
1.996
3.000
3.828
2.937
5.969
10
9
8
7
6
5
4
3
2
1
0 ppm


171.4049
171.1940
161.2106
161.0542
157.8049
138.2549
131.3584
129.9083
128.7604
127.5688
127.4178
113.3513
98.9356
55.3811
53.5193
49.4888
36.3294
25.4203
24.2432


OMe
N
N
N
S
N
N

1bbe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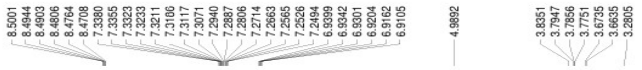
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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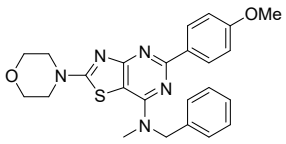
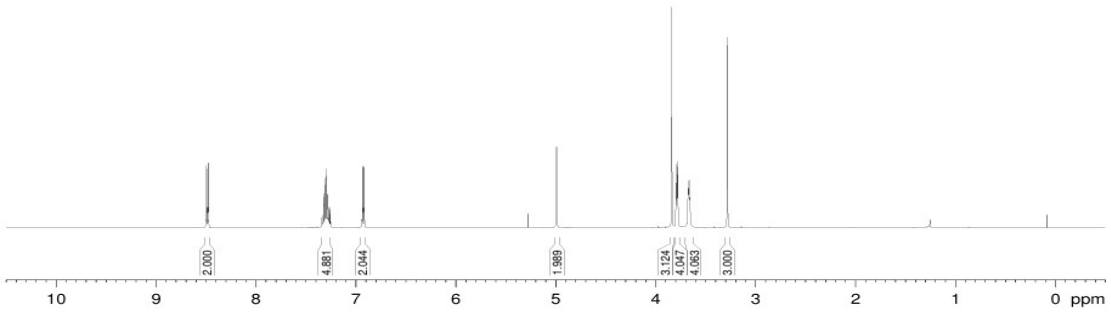
8.4708
7.3380
7.3355
7.3323
7.3233
7.3211
7.3186
7.3117
7.3071
7.2940
7.2887
7.2856
7.2714
7.2663
7.2565
7.2526
7.2494
6.9399
6.9342
6.9301
6.9204
6.9162
6.9105
4.9892
3.8351
3.7947
3.7856
3.7751
3.6735
3.6635
3.2805


OMe
N
O
N
S
N
N

1bbf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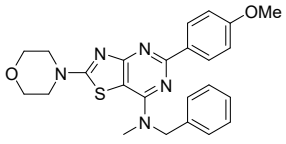
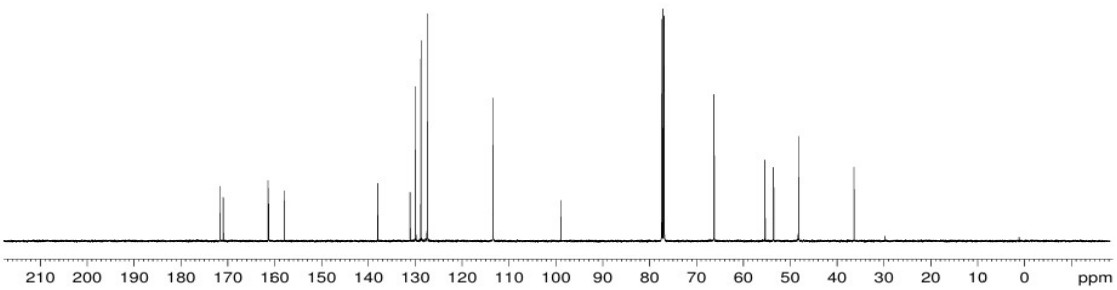
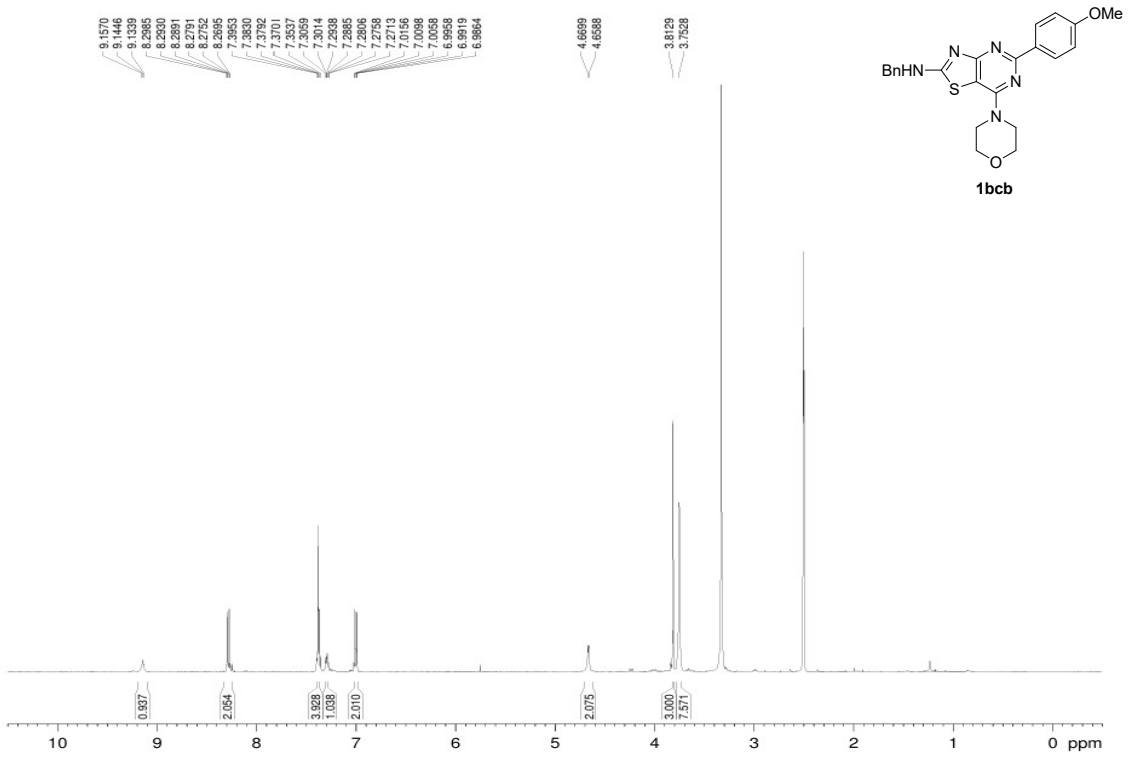
3.124
4.047
4.063
3.000
10
9
8
7
6
5
4
3
2
1
0 ppm


171.6087
170.9014
161.3116
161.2261
157.8967
138.0094
131.1130
129.9095
128.7823
127.4676
113.3892
98.9733
66.2052
55.3650
53.5122
48.2170
36.3513


OMe
N
O
N
S
N
N

1bbf


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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9.1446
9.1339
8.2985
8.2930
8.2891
8.2791
8.2752
8.2695
7.3953
7.3830
7.3792
7.3701
7.3537
7.3059
7.3014
7.2838
7.2805
7.2806
7.2758
7.2713
7.0156
7.0098
7.0058
6.9958
6.9919
6.9864
4.6699
4.6588
3.8129
3.7928
OMe
BnHN
N
S
O
1bcb
0.937
2.054
3.928
1.038
2.010
2.075
3.000
7.571
10
9
8
7
6
5
4
3
2
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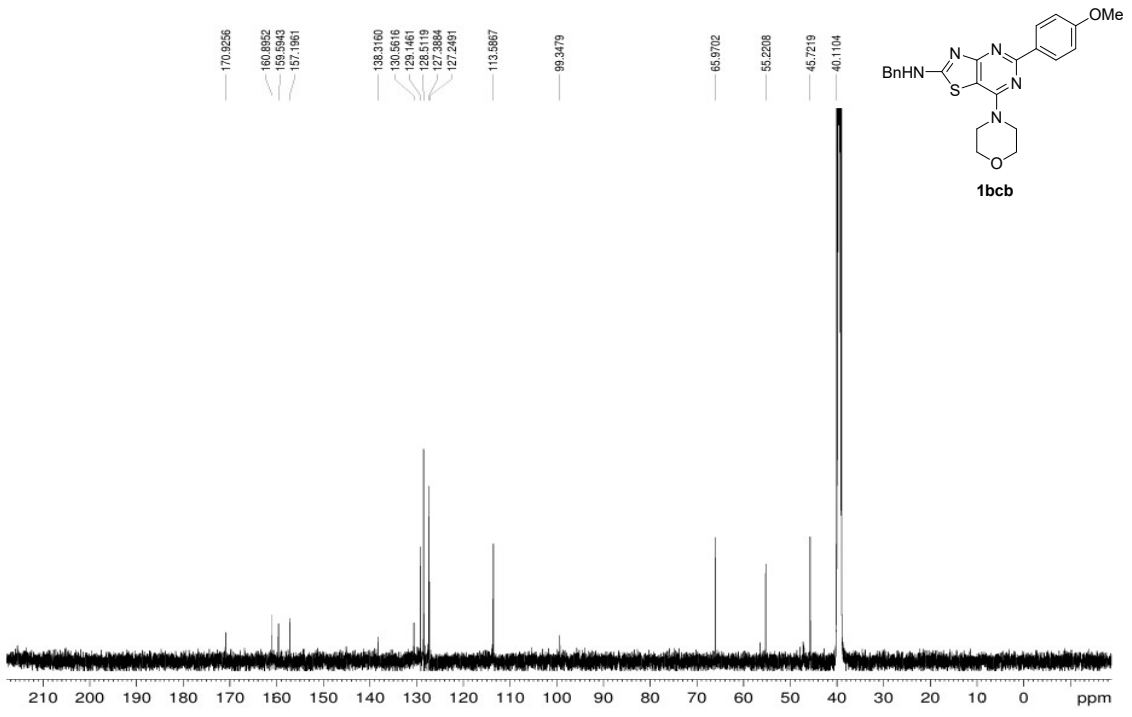
0 ppm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129.1461
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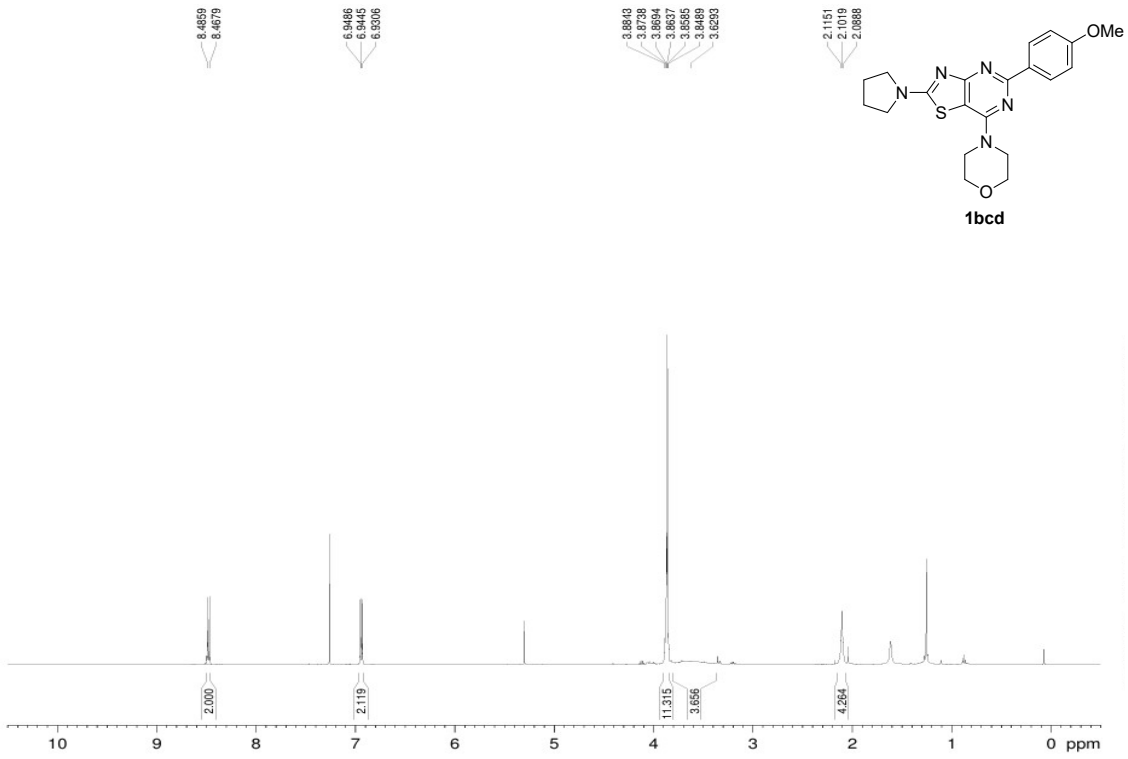
127.3884
127.2491
113.5867
99.3479
65.9702
55.2208
45.7219
40.1104
OMe
BnHN
N
S
O
1bcb
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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6.9306
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3.8738
3.8694
3.8637
3.8585
3.8489
3.8293
2.1151
2.1019
2.0888
OMe
N
N
N
S
N
O
2.000
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11.315
3.656
4.264
10
9
8
7
6
5
4
3
2
1
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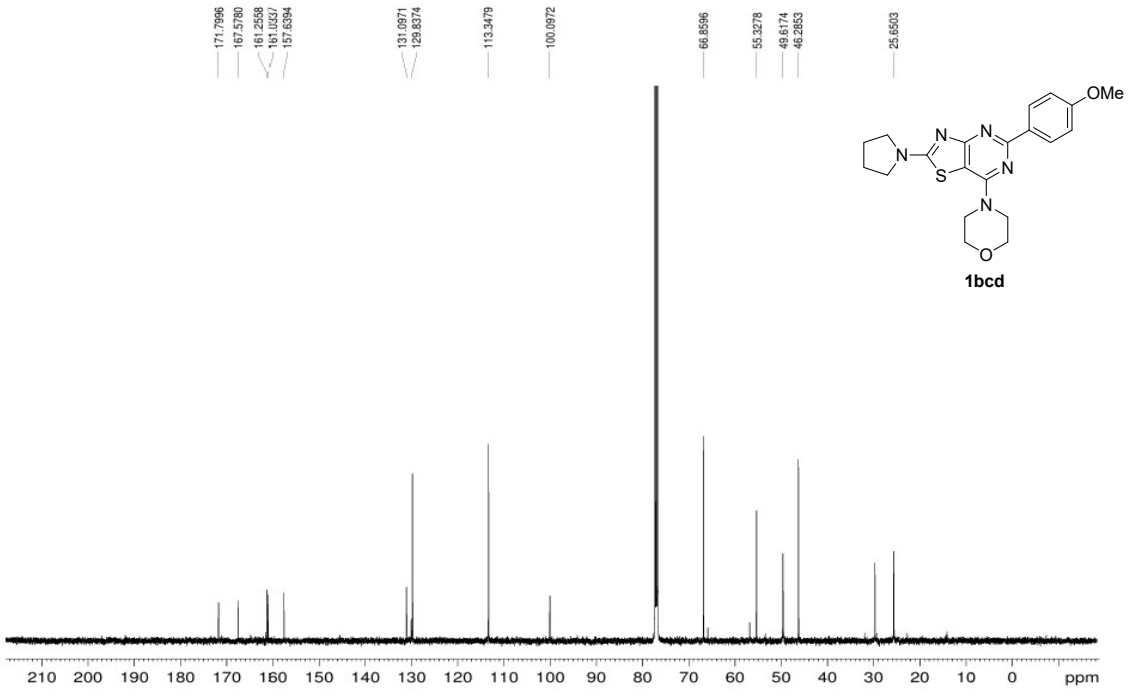
1bcd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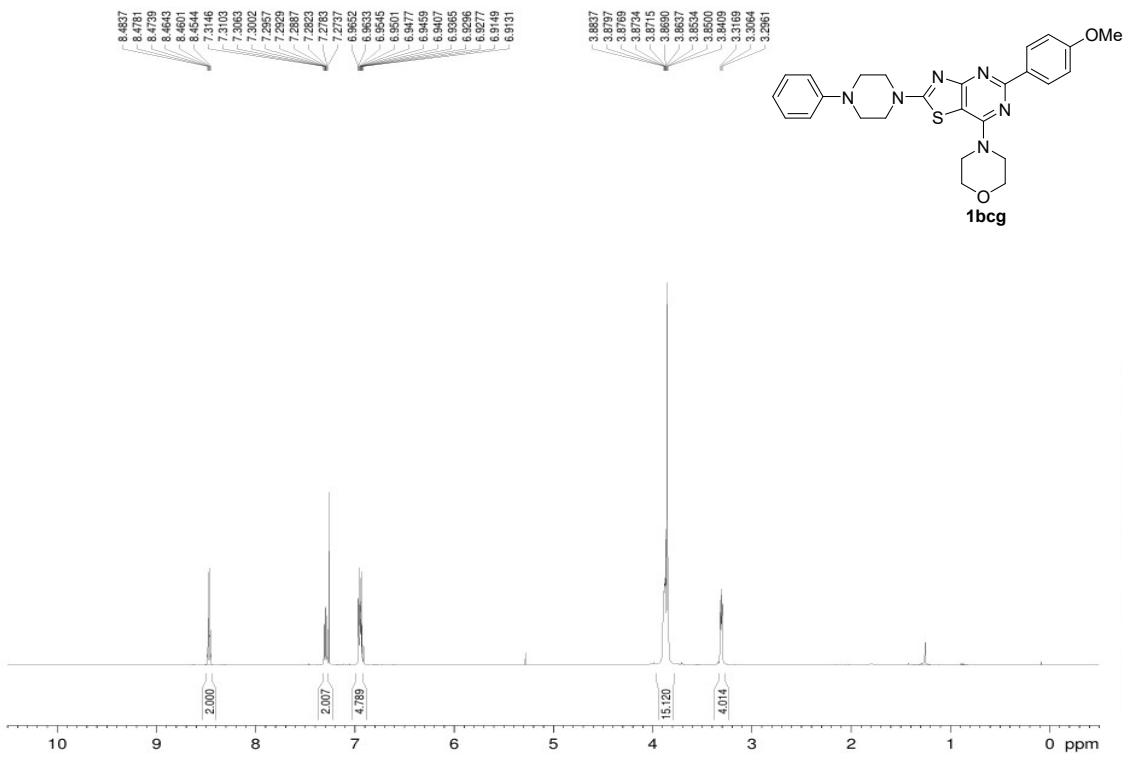
157.6394
131.0971
129.8374
113.3479
100.0972
66.8596
55.3278
49.6174
46.2853
25.6503
OMe
N
N
N
S
N
O
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

1bcd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8.4781
8.4739
8.4643
8.4601
8.4544
7.3146
7.3103
7.3063
7.3002
7.2957
7.2929
7.2887
7.2823
7.2783
7.2737
6.9652
6.9633
6.9545
6.9501
6.9477
6.9459
6.9407
6.9365
6.9296
6.9277
6.9149
6.9131
3.8837
3.8797
3.8769
3.8734
3.8715
3.8690
3.8637
3.8534
3.8500
3.8409
3.3169
3.3064
3.2961
OMe
1bcg
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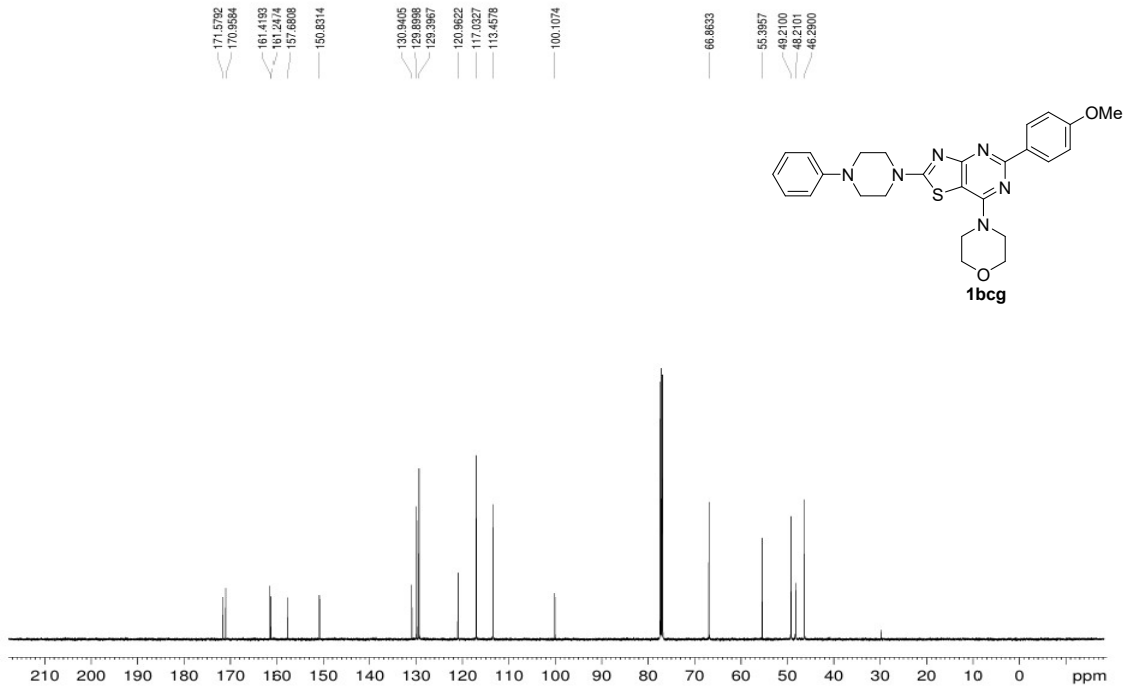
2.007
4.789
15.120
4.014
10
9
8
7
6
5
4
3
2
1
0 ppm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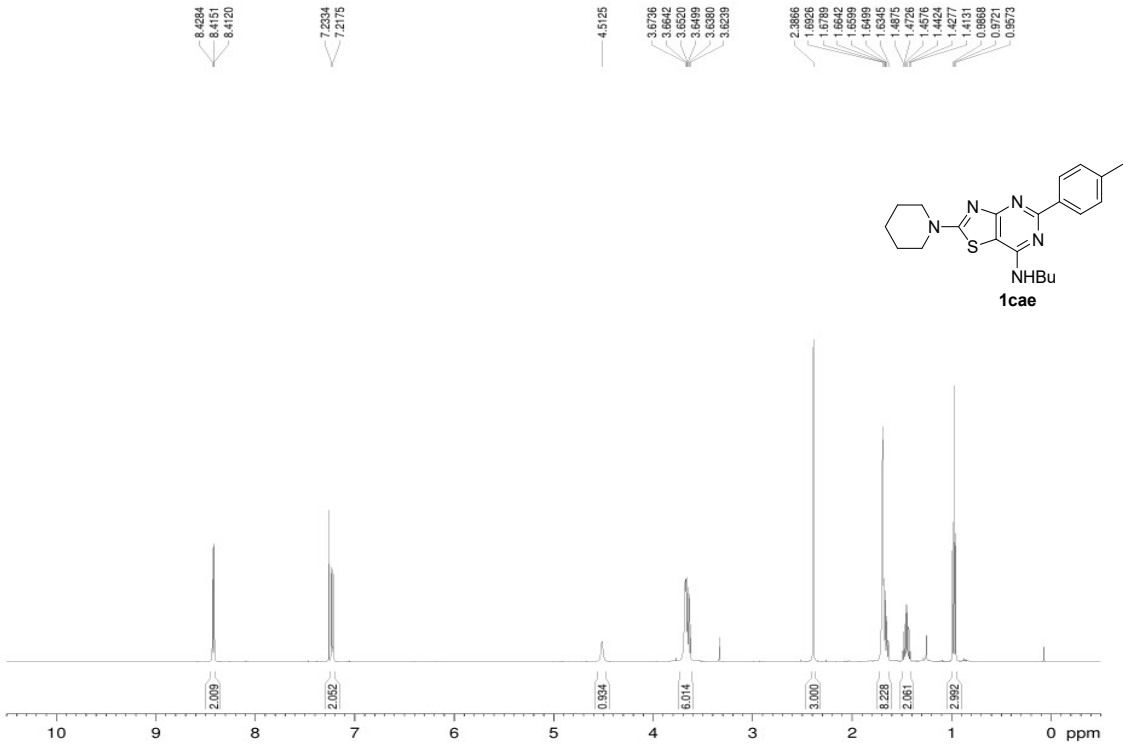
129.3967
120.9622
117.0327
113.4578
100.1074
66.8633
55.3957
49.2100
48.2101
46.2900
OMe
1bcg
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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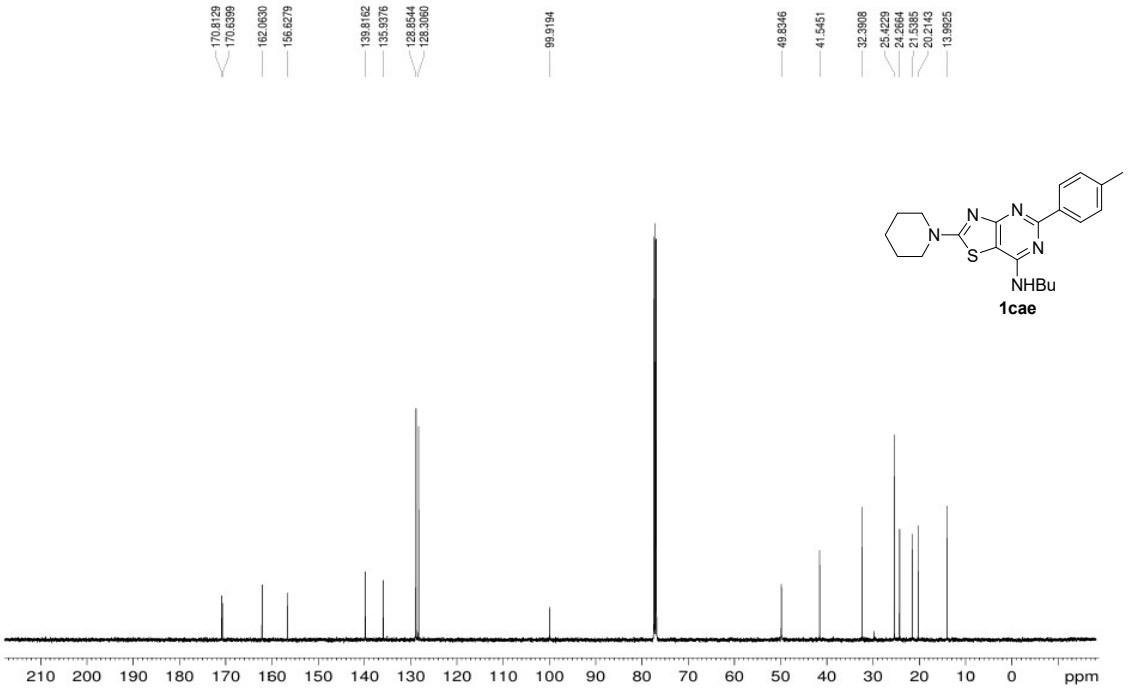
8.4151
8.4120
7.2334
7.2175
4.5125
3.6736
3.6642
3.6520
3.6499
3.6380
3.6239
2.3866
1.6926
1.6789
1.6642
1.6599
1.6499
1.6345
1.4875
1.4726
1.4576
1.4424
1.4277
1.4131
0.9868
0.9721
0.9573
N
N
N
N
S
NHBu
1cae
2.009
2.052
0.934
6.014
3.000
8.228
2.061
2.992
10
9
8
7
6
5
4
3
2
1
0 ppm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156.6279
139.8162
135.5376
128.8544
128.3060
99.9194
49.8346
41.5451
32.3908
25.4229
24.2664
21.5385
20.2143
13.9925
N
N
N
N
S
NHBu
1cae
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.4477
8.4313
7.3110
7.3070
7.2964
7.2936
7.2829
7.2790
7.2599
7.2545
7.2385
6.9586
6.9428
6.9279
6.9133
4.6340
4.6238
4.6134
3.8730
3.8644
3.8547
3.6775
3.6633
3.6514
3.6373
3.3098
3.2993
3.2890
2.4002
1.7054
1.6909
1.6869
1.6763
1.6720
1.6620
1.6466
1.4972
1.4823
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1.4521
1.4374
1.4228
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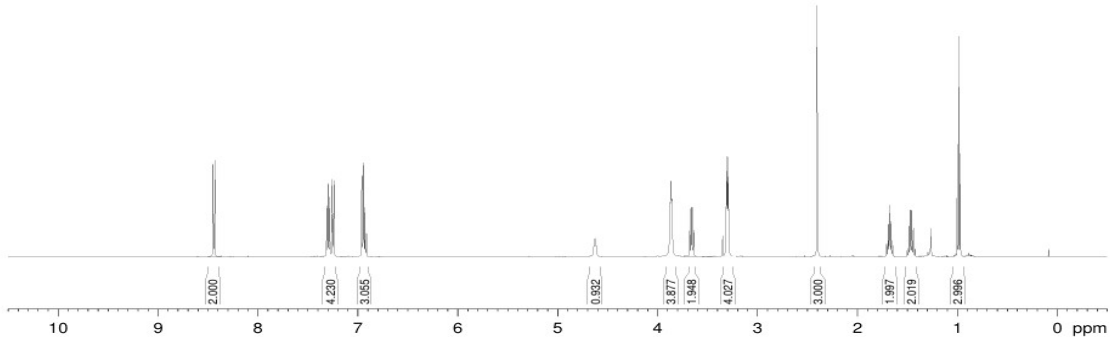
0.9826
0.9678
NHBu

1cag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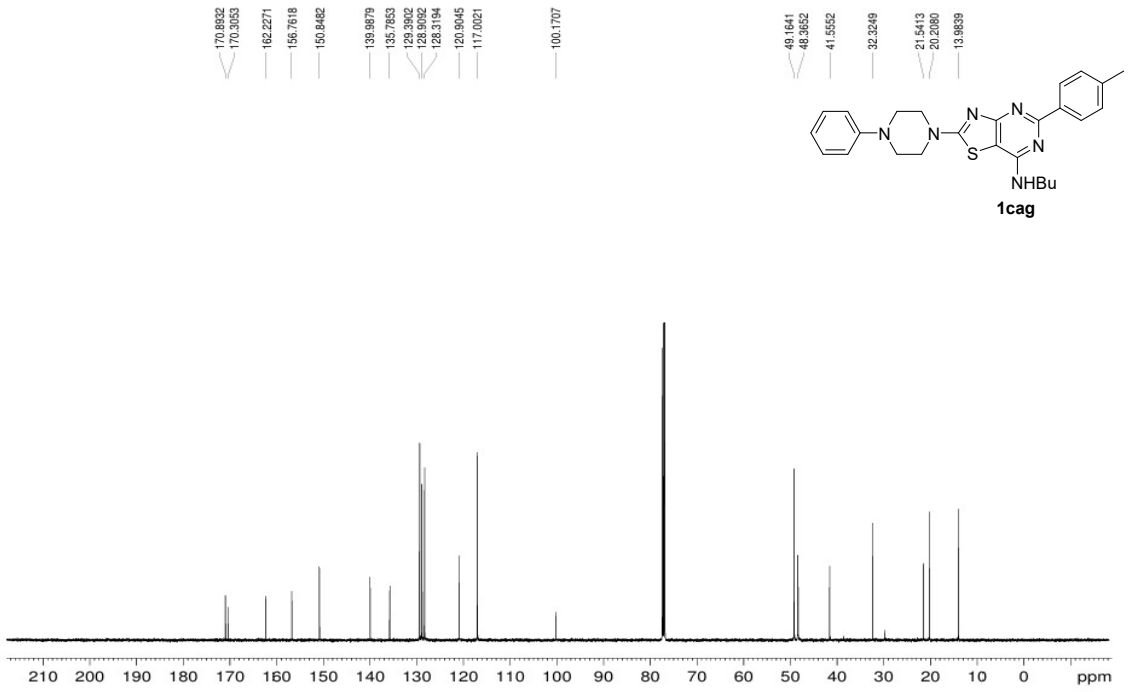
0.932
3.877
1.948
4.027
3.000
1.997
2.019
2.996
10
9
8
7
6
5
4
3
2
1
0 ppm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156.7618
150.8482
139.9879
135.7853
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128.9092
128.3194
120.9045
117.0021
100.1707
49.1641
48.3652
41.5552
32.3249
21.5413
20.2080
13.9839
NHBu
210
200
190
180
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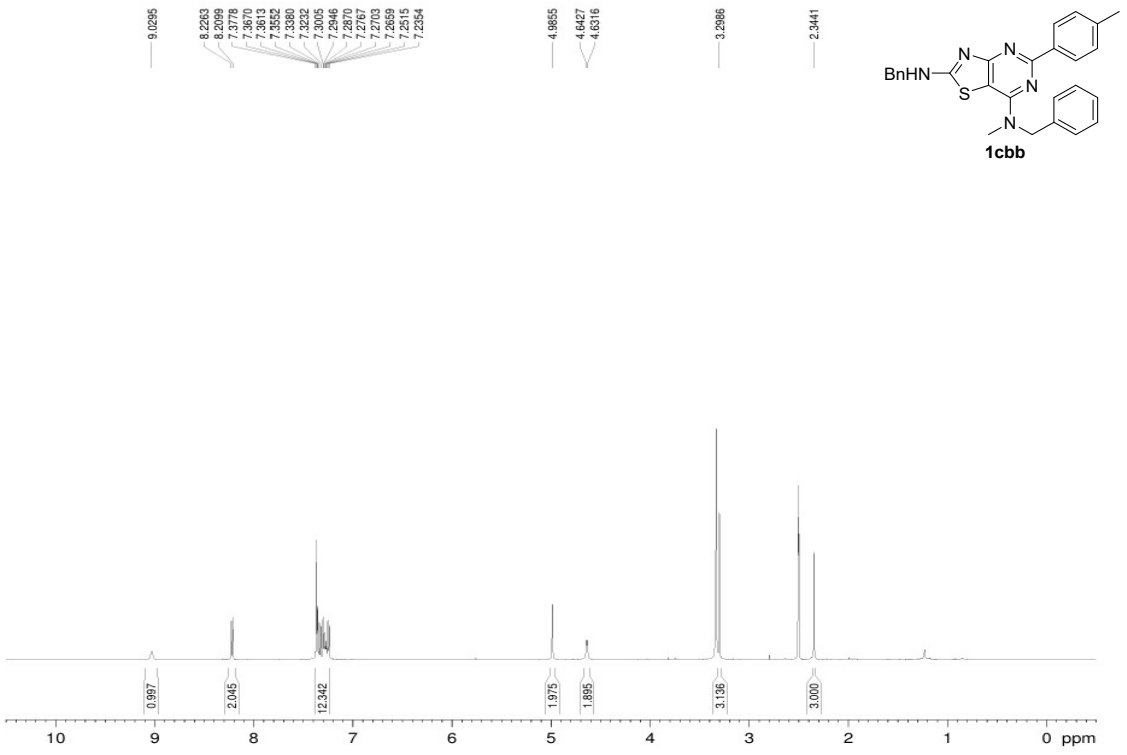
1cag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7.3232
7.3005
7.2946
7.2870
7.2767
7.2703
7.2659
7.2515
7.2354
4.9655
4.6427
4.6316
3.2986
2.3441
BnHN
N
N
S
N
N
1cbb
0.997
2.045
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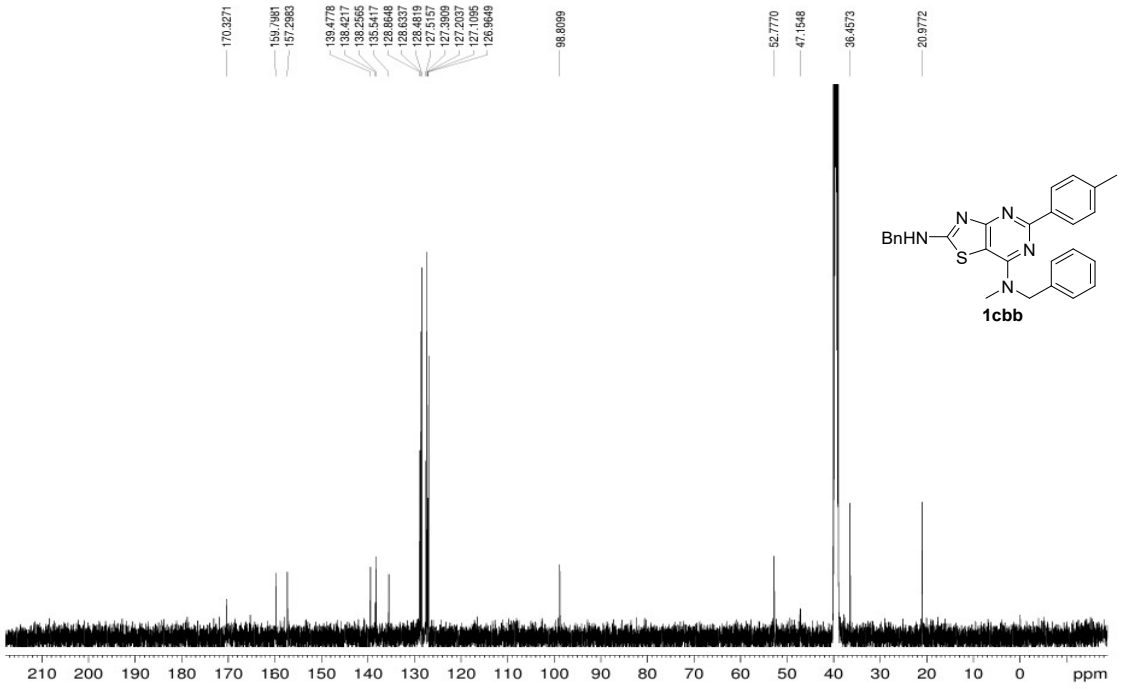
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127.5157
127.3909
127.2037
127.1095
126.9849
98.8099
52.7770
47.1548
36.4573
20.9772
BnHN
N
N
S
N
N
1cbb
210
200
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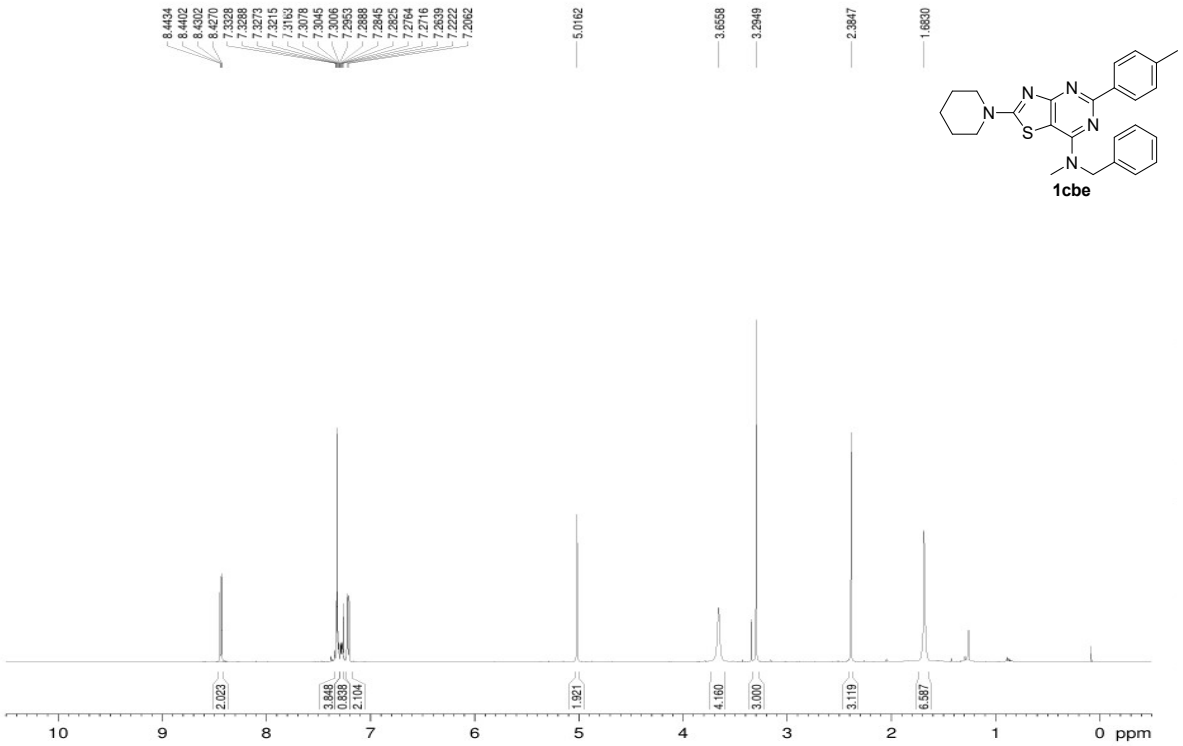
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8.4302
8.4270
7.3328
7.3288
7.3273
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7.3163
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7.3045
7.3006
7.2953
7.2888
7.2845
7.2825
7.2764
7.2716
7.2639
7.2222
7.2062
5.0162
3.6558
3.2949
2.3847
1.6830
2.023
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2.104
1.921
4.160
3.000
3.119
6.587
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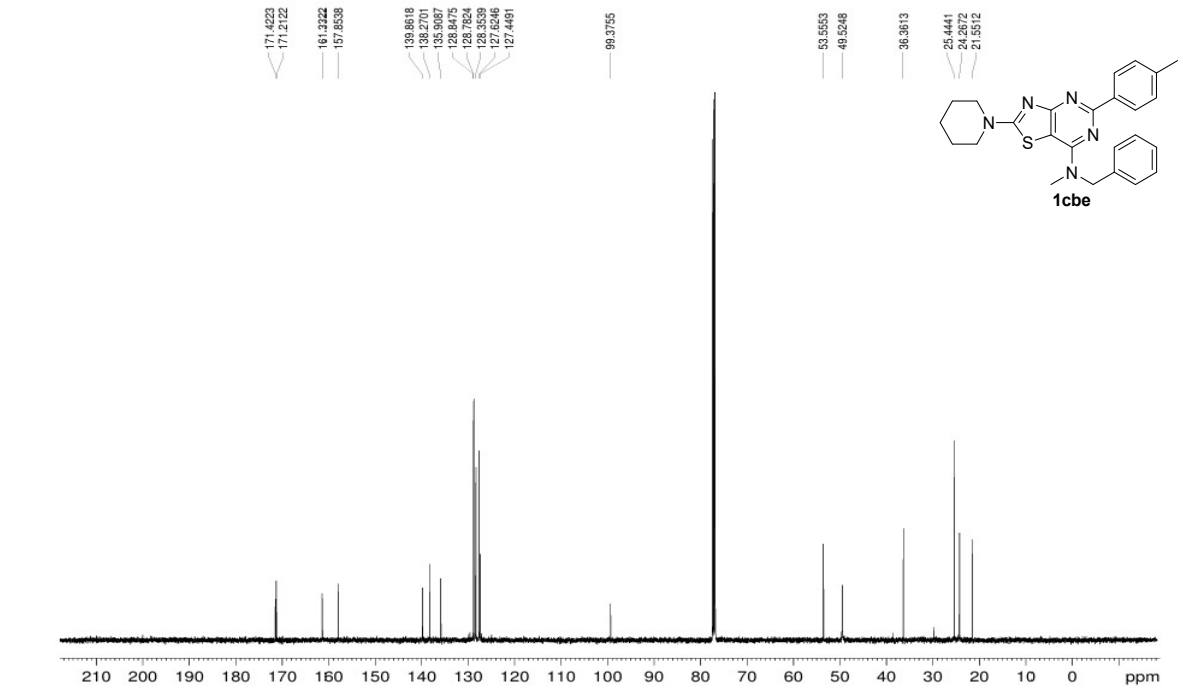
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139.8618
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135.9087
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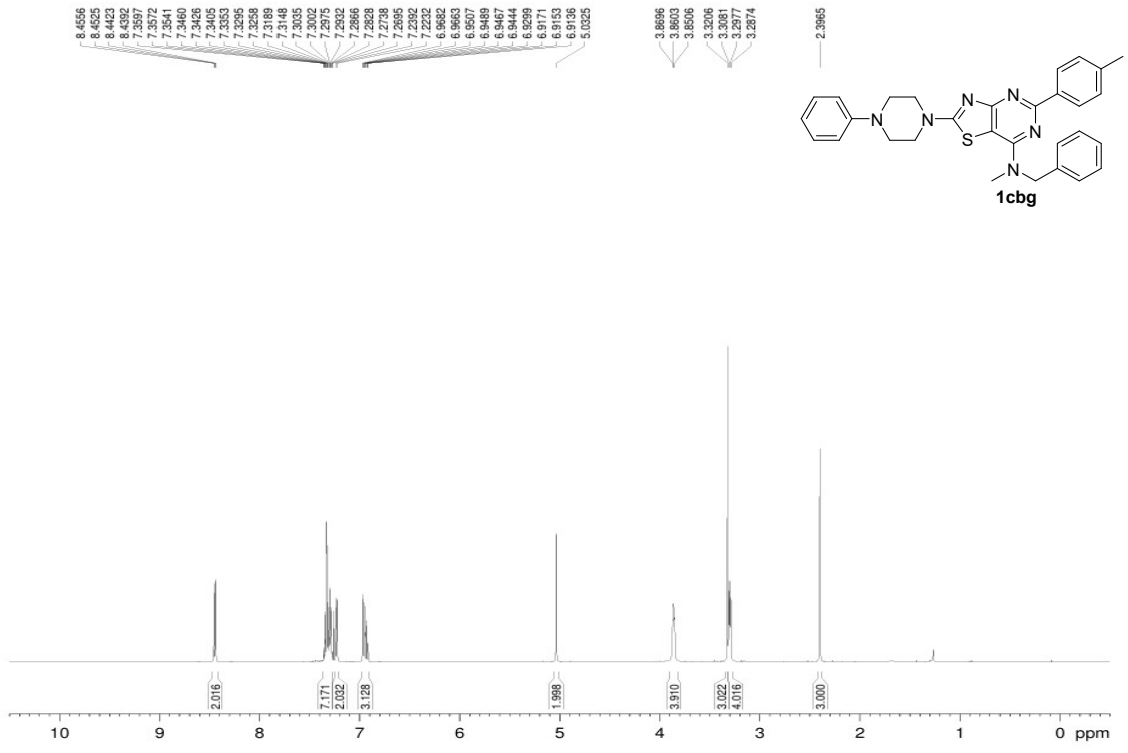
127.4491
99.3755
53.5553
49.5248
36.3613
25.4441
24.2672
21.5512
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
1cbe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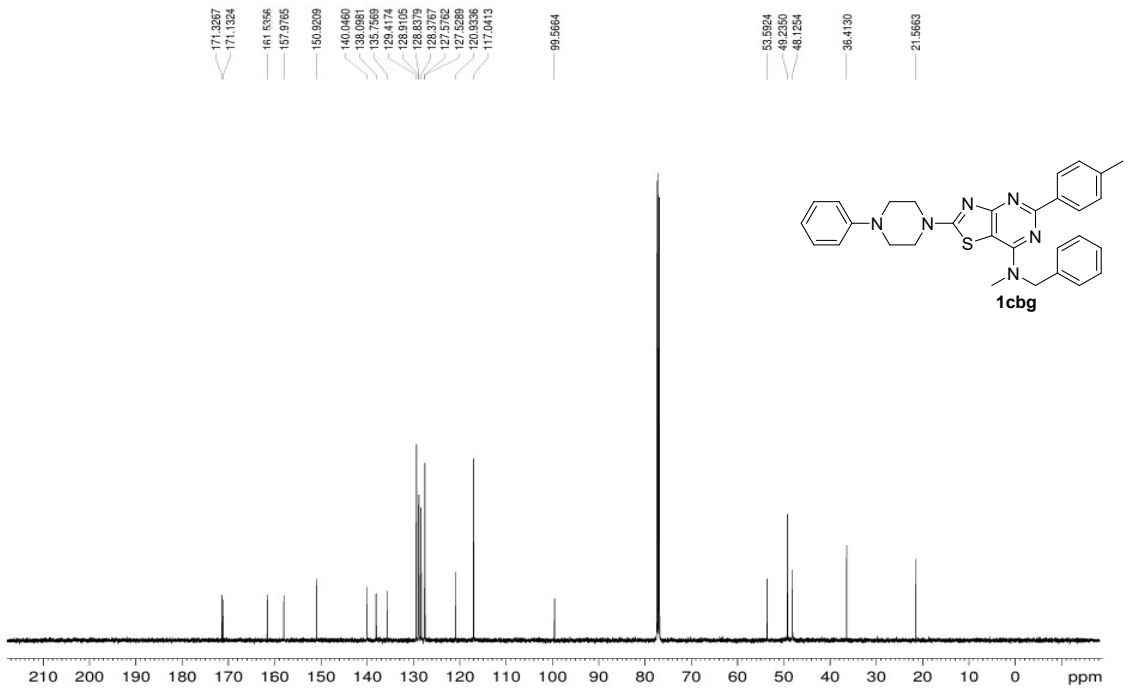
7.3572
7.3541
7.3460
7.3426
7.3405
7.3353
7.3295
7.3258
7.3189
7.3148
7.3035
7.3002
7.2975
7.2932
7.2866
7.2828
7.2738
7.2695
7.2592
7.2232
6.9682
6.9663
6.9507
6.9489
6.9467
6.9444
6.9299
6.9171
6.9153
6.9136
5.0025
3.8696
3.8603
3.8506
3.3206
3.3081
3.2977
3.2874
2.3965
2.016
7.171
2.032
3.128
1.998
3.910
3.022
4.016
3.000
10
9
8
7
6
5
4
3
2
1
0 ppm
1cbg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128.3767
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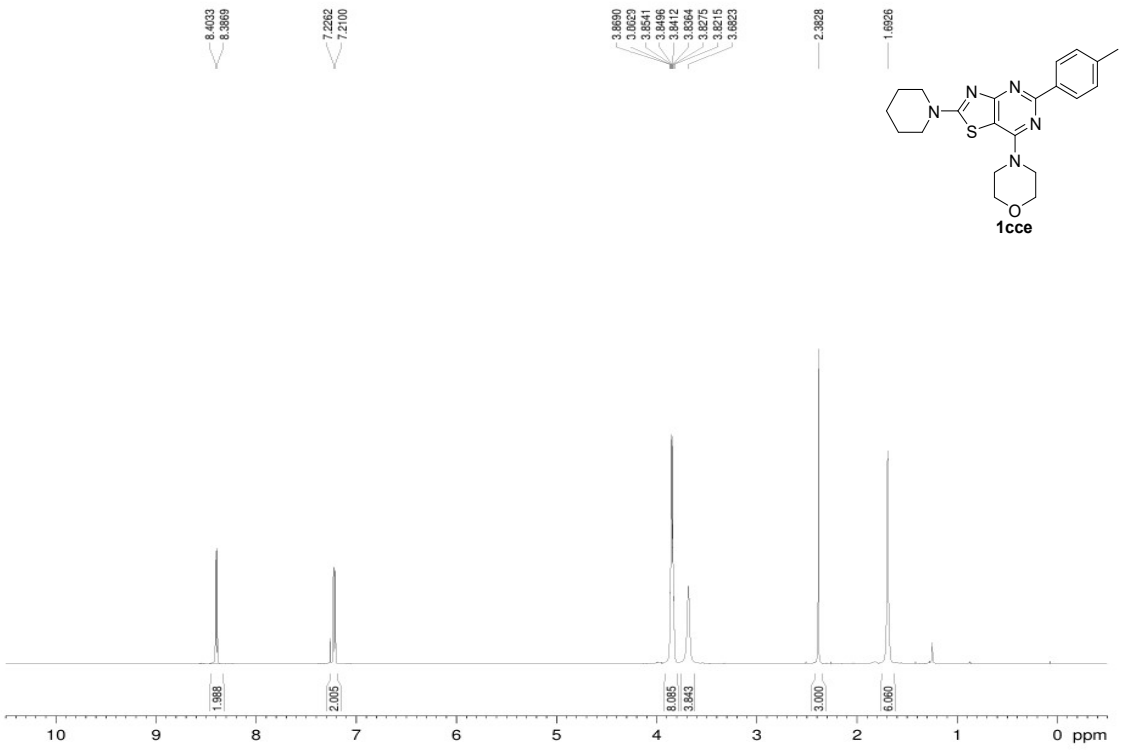
127.3289
120.9336
117.0413
99.5664
53.5924
49.2350
48.1254
36.4130
21.5663
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm
1cbg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8.3869
7.2262
7.2100
3.8690
3.8629
3.8541
3.8496
3.8412
3.8364
3.8275
3.8215
3.6823
2.3828
1.6926
1cce
1.968
2.005
8.085
3.843
3.000
6.060
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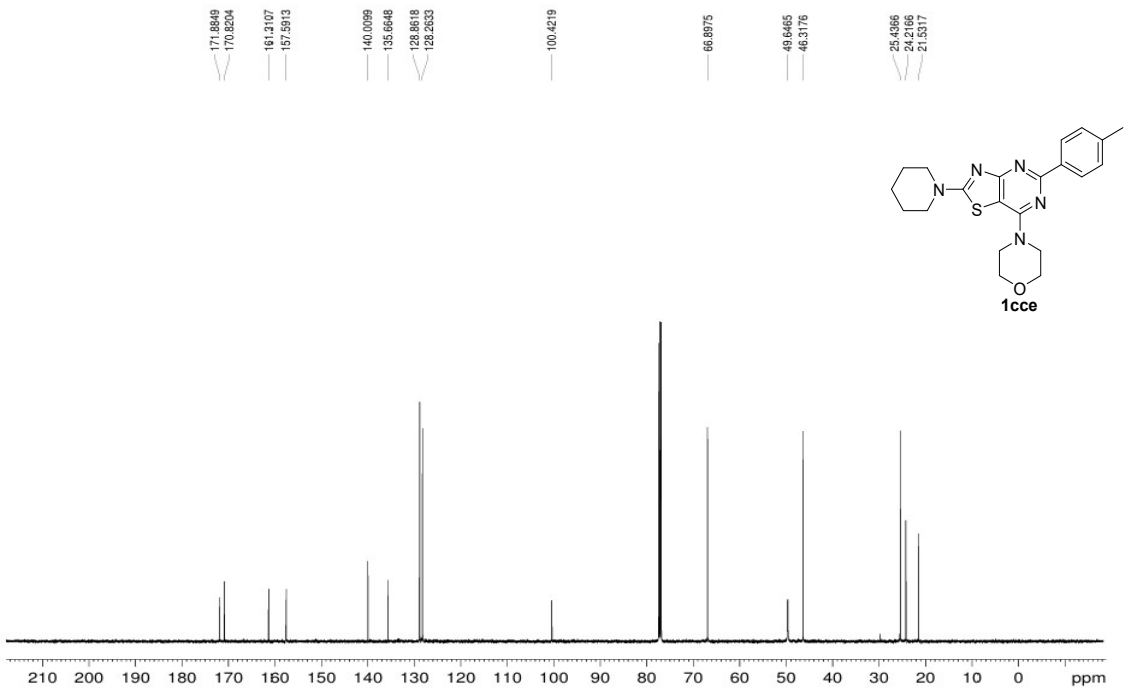
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128.2633
100.4219
66.8975
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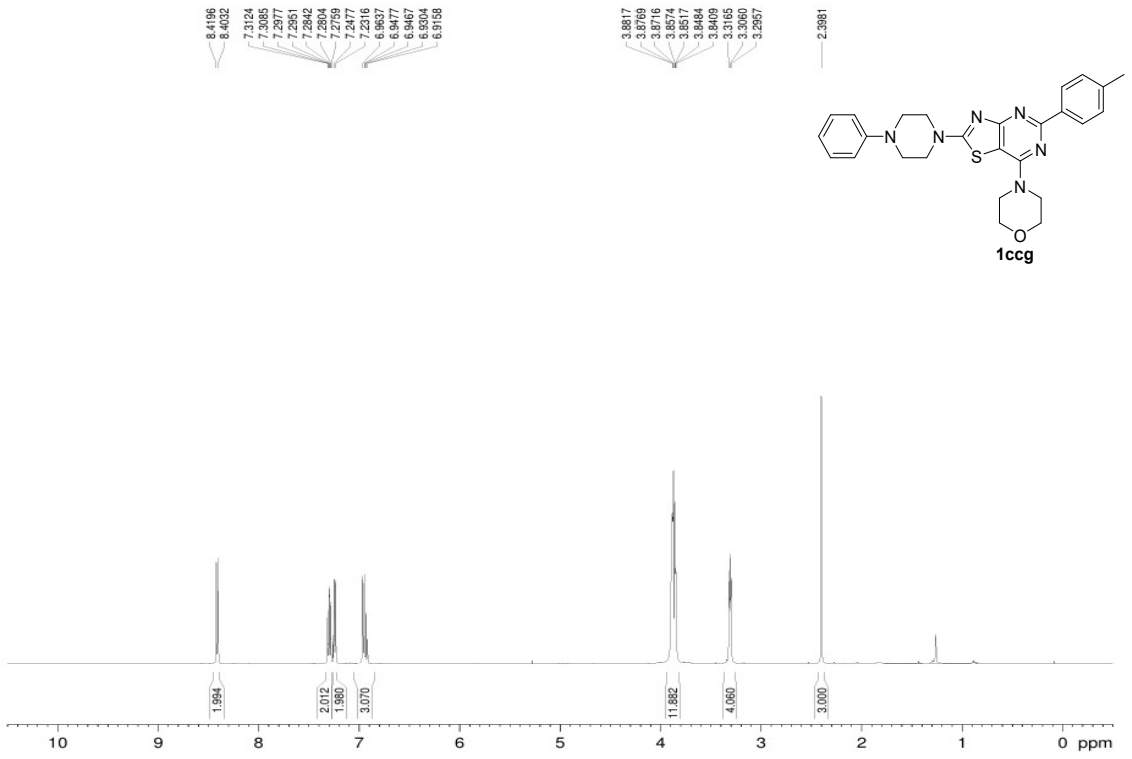
46.3176
25.4366
24.2166
21.5317
1cce
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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8.4032
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7.2977
7.2951
7.2842
7.2804
7.2759
7.2477
7.2316
6.9637
6.9477
6.9467
6.9304
6.9158
3.8817
3.8769
3.8716
3.8574
3.8517
3.8484
3.8409
3.3165
3.3060
3.2957
2.3981
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2.012
1.980
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11.882
4.060
3.000
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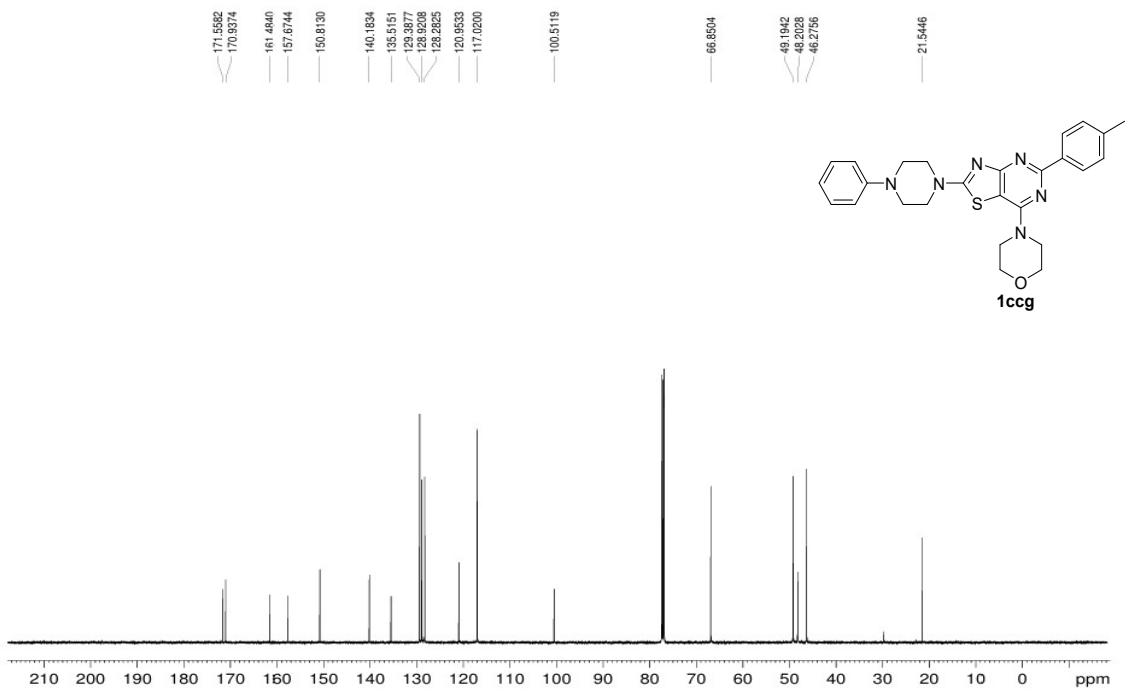
1ccg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157.6744
150.8130
140.1834
135.5151
129.3877
128.9208
128.2825
120.9533
117.0200
100.5119
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48.2028
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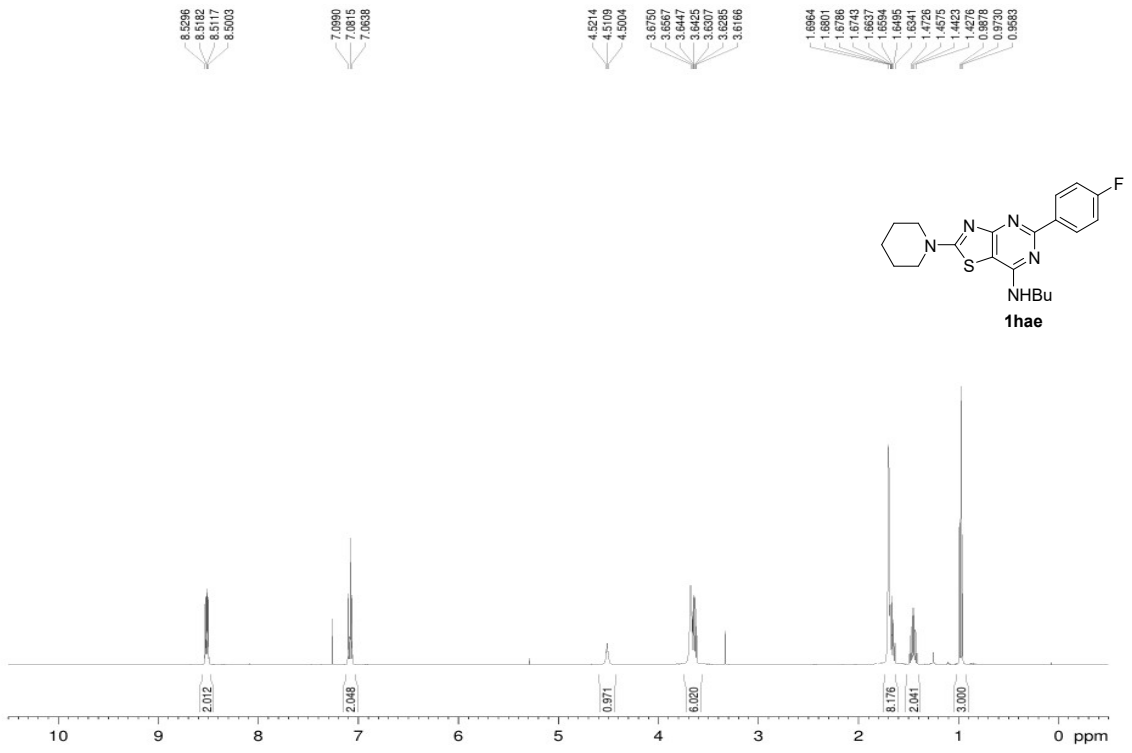
21.5446
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

1ccg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8.5117
8.5003
7.0990
7.0815
7.0638
4.5214
4.5109
4.5004
3.6750
3.6567
3.6447
3.6425
3.6307
3.6285
3.6166
1.6964
1.6801
1.6786
1.6743
1.6637
1.6594
1.6495
1.6341
1.4726
1.4575
1.4423
1.4276
0.9878
0.9730
0.9583
F
N
N
N
S
N
NHBu
1hae
2.012
2.048
0.971
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8.176
2.041
3.000
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9
8
7
6
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4
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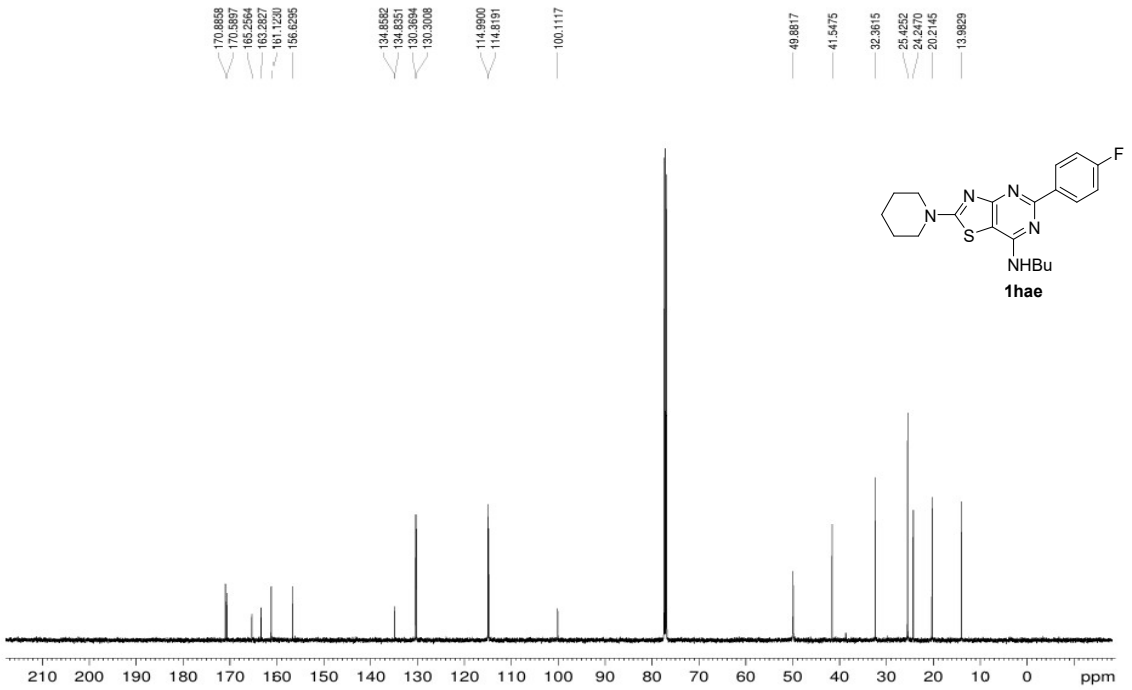
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134.8582
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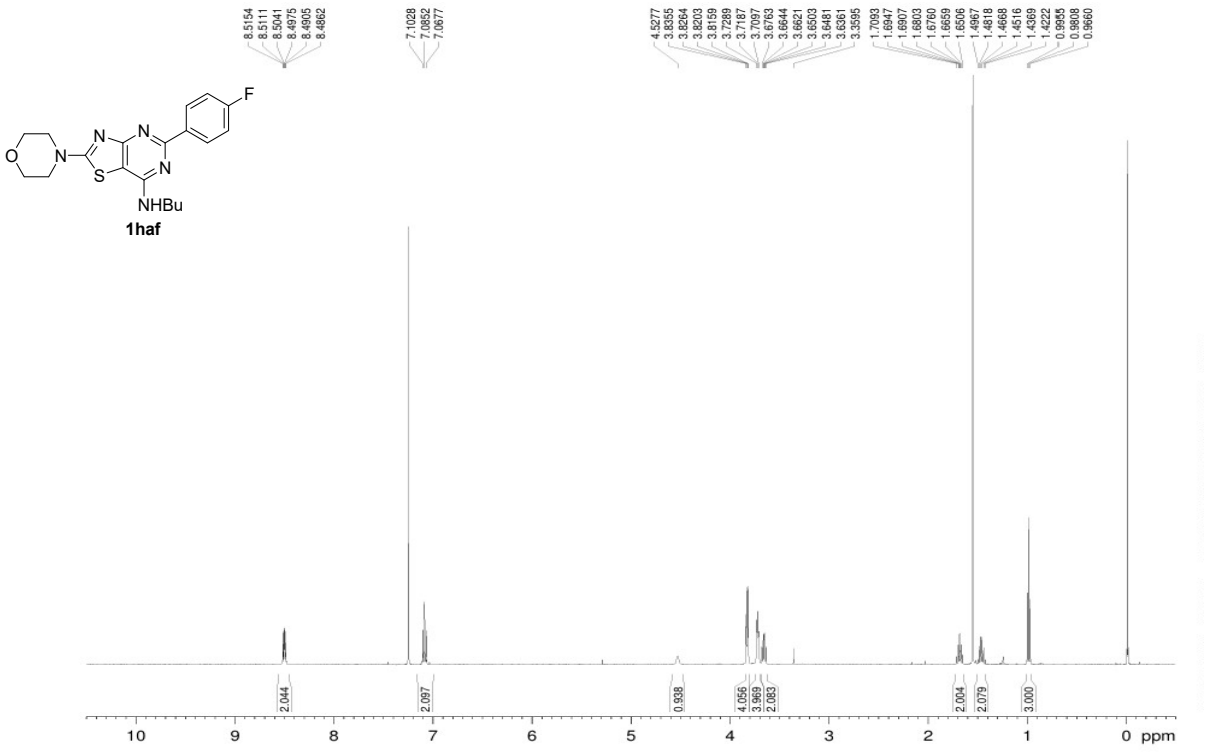
130.3694
130.3008
114.9900
114.8191
100.1117
49.8817
41.5475
32.3615
25.4252
24.2470
20.2145
13.9829
F
N
N
N
S
N
NHBu
1hae
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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8.4905
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3.8355
3.8264
3.8203
3.8159
3.7289
3.7187
3.7097
3.6763
3.6644
3.6621
3.6503
3.6481
3.6361
3.3595
1.7093
1.6947
1.6907
1.6803
1.6760
1.6659
1.6506
1.4967
1.4818
1.4668
1.4516
1.4369
1.4222
0.9935
0.9808
0.9660
F
N
O
S
NHBu
1haf
2.044
2.097
0.938
4.056
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2.004
2.079
3.000
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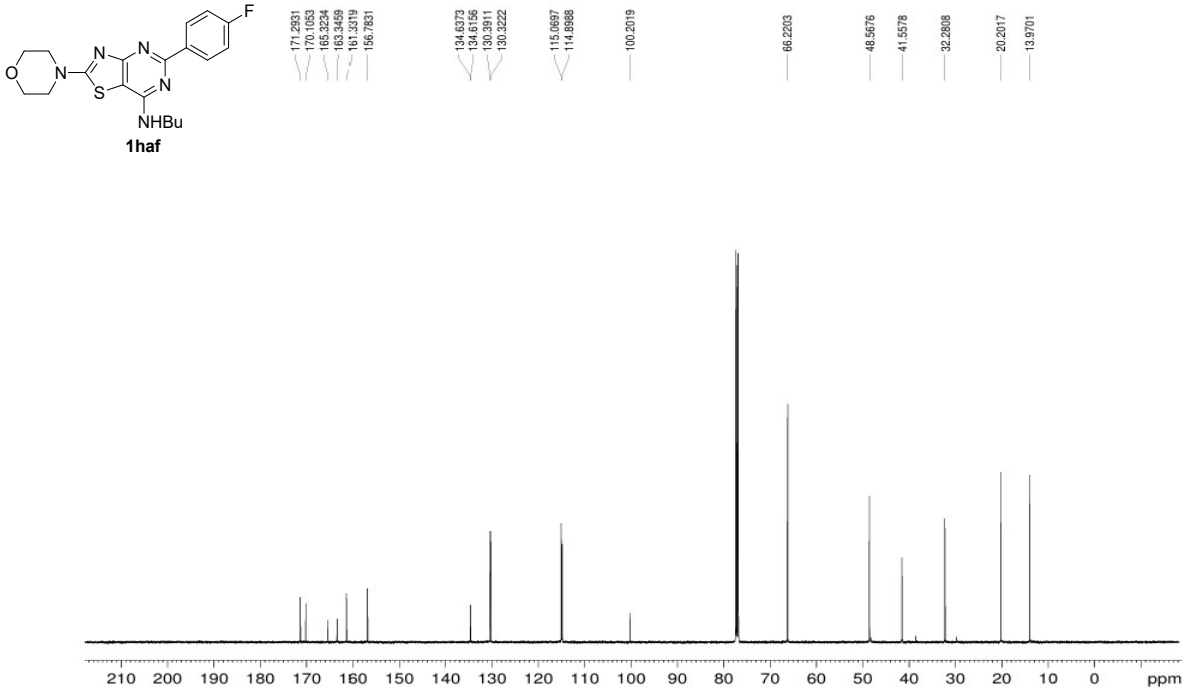
9
8
7
6
5
4
3
2
1
0 ppm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115.0697
114.8988
100.2019
66.2203
48.5676
41.5578
32.2808
20.2017
13.9701
F
N
O
S
NHBu
1haf
210
200
190
180
170
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150
140
130
120
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100
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80
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60
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20
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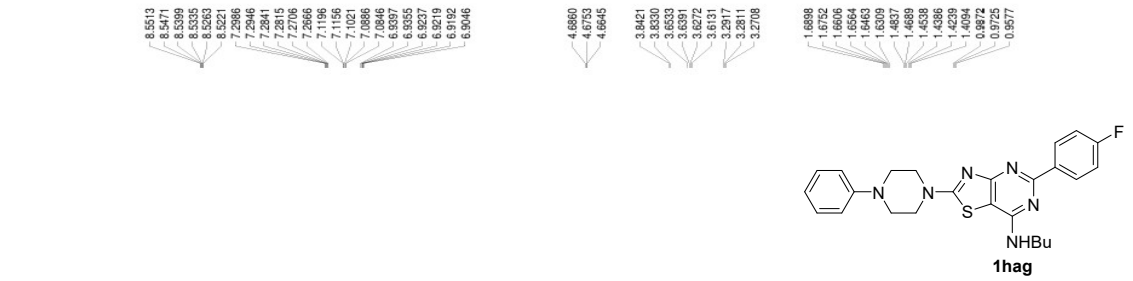
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7.2946
7.2841
7.2815
7.2706
7.2666
7.1196
7.1156
7.1021
7.0886
7.0846
6.9397
6.9355
6.9237
6.9219
6.9192
6.9046
4.6860
4.6753
4.6645
3.8421
3.8330
3.6533
3.6391
3.6272
3.5131
3.2917
3.2811
3.2708
1.6898
1.6752
1.6606
1.6564
1.6453
1.6269
1.4637
1.4689
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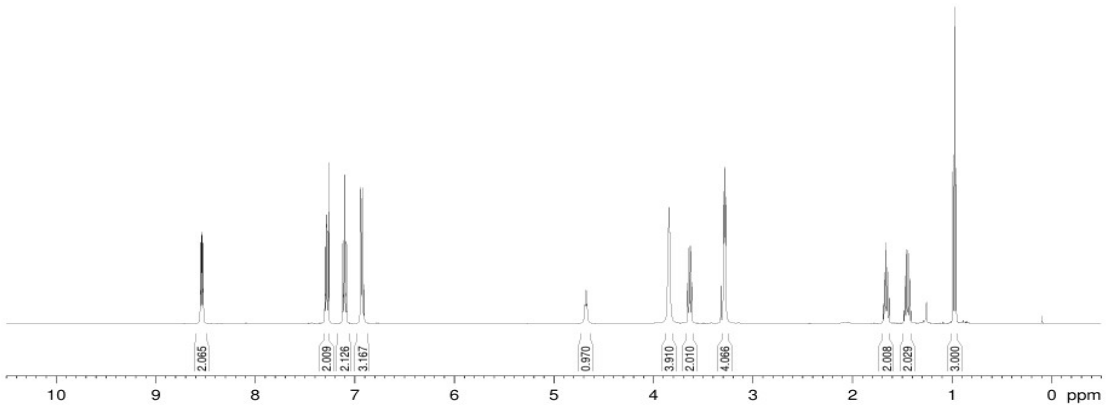
N
N
N
N
S
NHBu
1hag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3.910
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2.008
2.029
3.000
10
9
8
7
6
5
4
3
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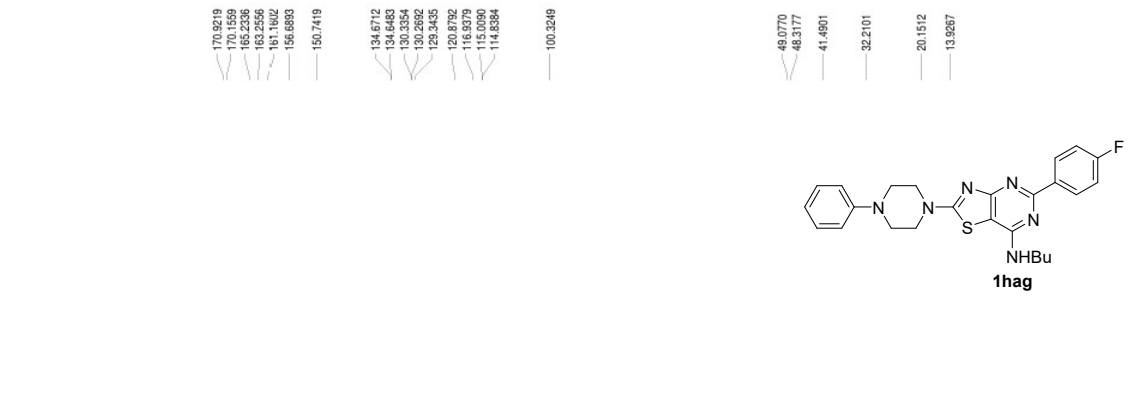
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134.6712
134.6483
130.3554
130.2692
129.3435
120.8792
116.9379
115.0090
114.8384
100.3249
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32.2101
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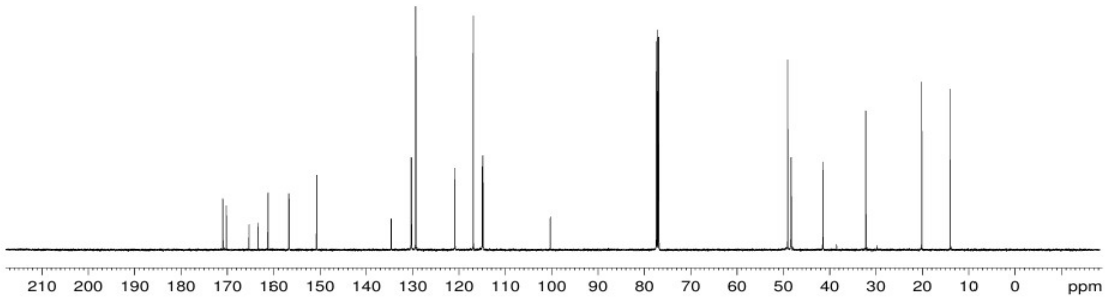
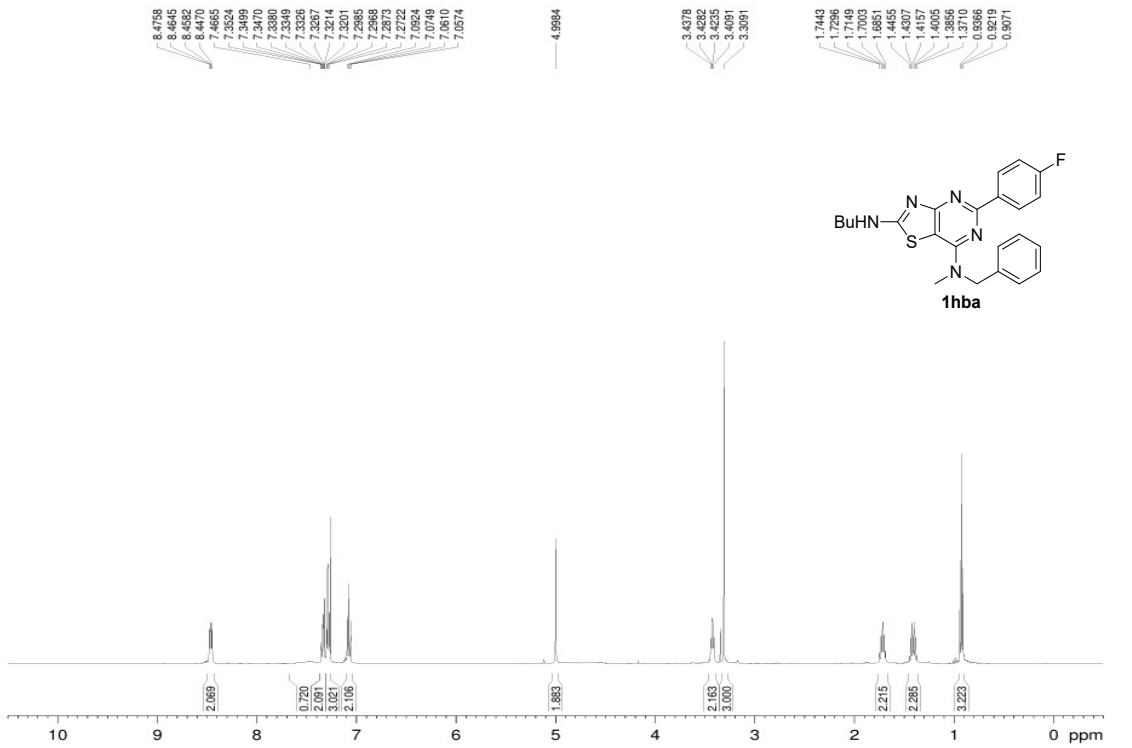
N
N
N
N
S
NHBu
1hag


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.3380
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7.3326
7.3267
7.3214
7.3201
7.2985
7.2968
7.2873
7.2722
7.0924
7.0749
7.0610
7.0574
4.9984
3.4378
3.4282
3.4235
3.4091
3.3091
1.7443
1.7296
1.7149
1.7003
1.6851
1.4455
1.4307
1.4157
1.4005
1.3856
1.3710
0.9366
0.9219
0.9071
F
BuHN
N
N
S
N
N
1hba
2.069
0.720
2.091
3.021
2.106
1.883
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2.285
3.223
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7
6
5
4
3
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1
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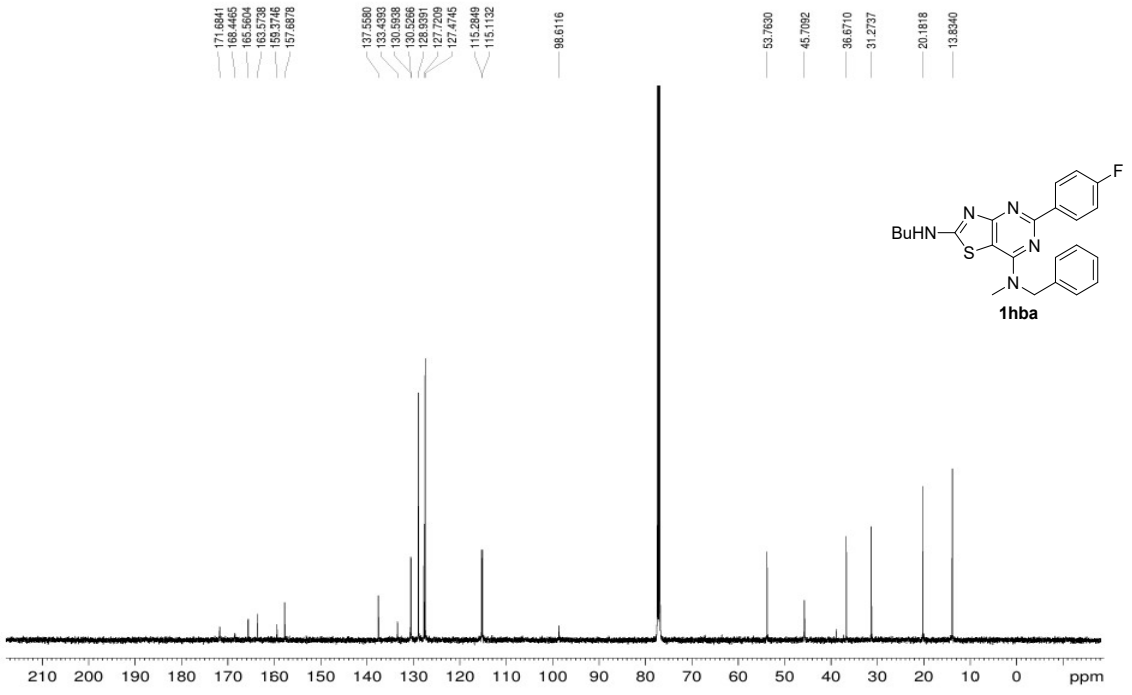
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130.5938
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128.9391
127.7209
127.4745
115.2849
115.1132
98.6116
53.7630
45.7092
36.6710
31.2737
20.1818
13.8340
F
BuHN
N
N
S
N
N
1hba
210
200
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180
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140
130
120
110
100
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80
70
60
50
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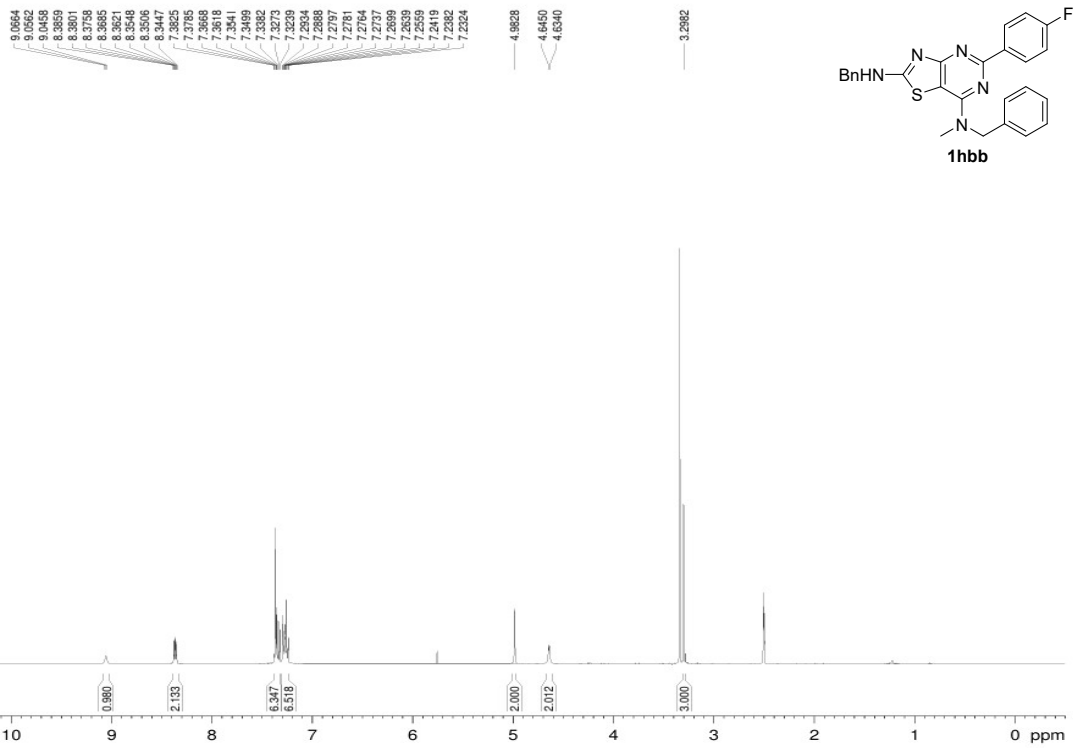
30
20
10
0
ppm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8.3685
8.3621
8.3548
8.3506
8.3447
7.3825
7.3785
7.3668
7.3618
7.3541
7.3499
7.3382
7.3273
7.3239
7.2934
7.2888
7.2797
7.2781
7.2764
7.2737
7.2699
7.2639
7.2559
7.2419
7.2382
7.2324
4.9828
4.6450
4.6340
3.2982
BnHN
N
N
S
N
N
F
1hbb
0.980
2.133
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2.000
2.012
3.000
10
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8
7
6
5
4
3
2
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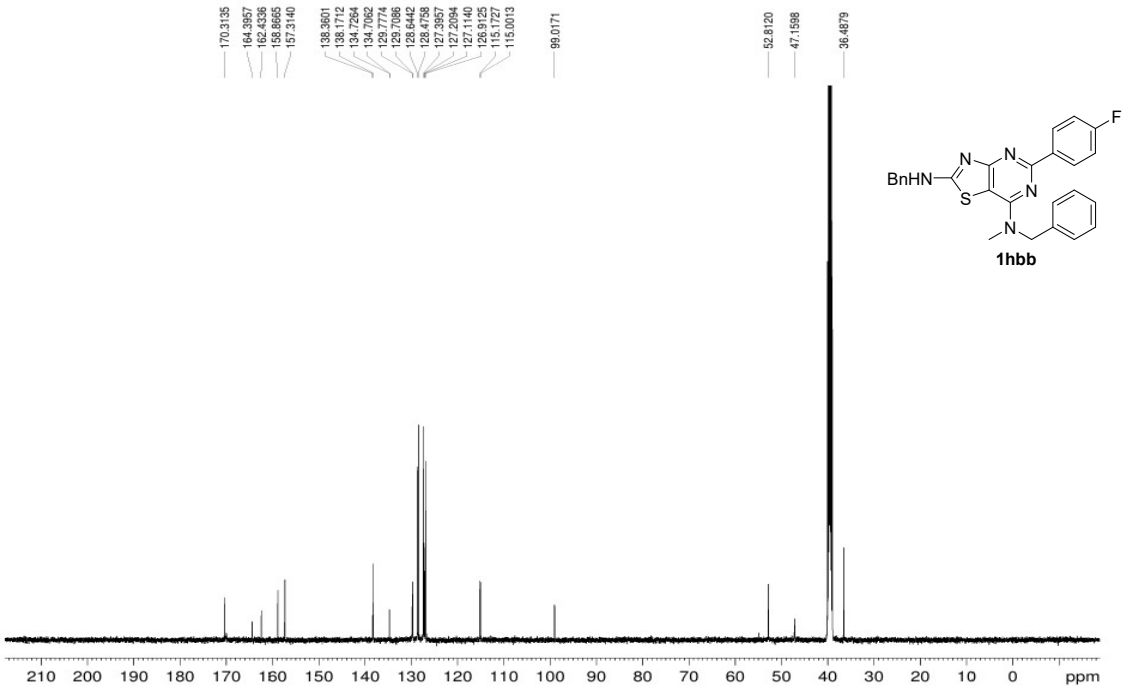
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128.6442
128.4758
127.3957
127.2094
127.1140
126.9125
115.1727
115.0013
99.0171
52.8120
47.1598
36.4879
BnHN
N
N
S
N
N
F
1hbb
210
200
190
180
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140
130
120
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100
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80
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60
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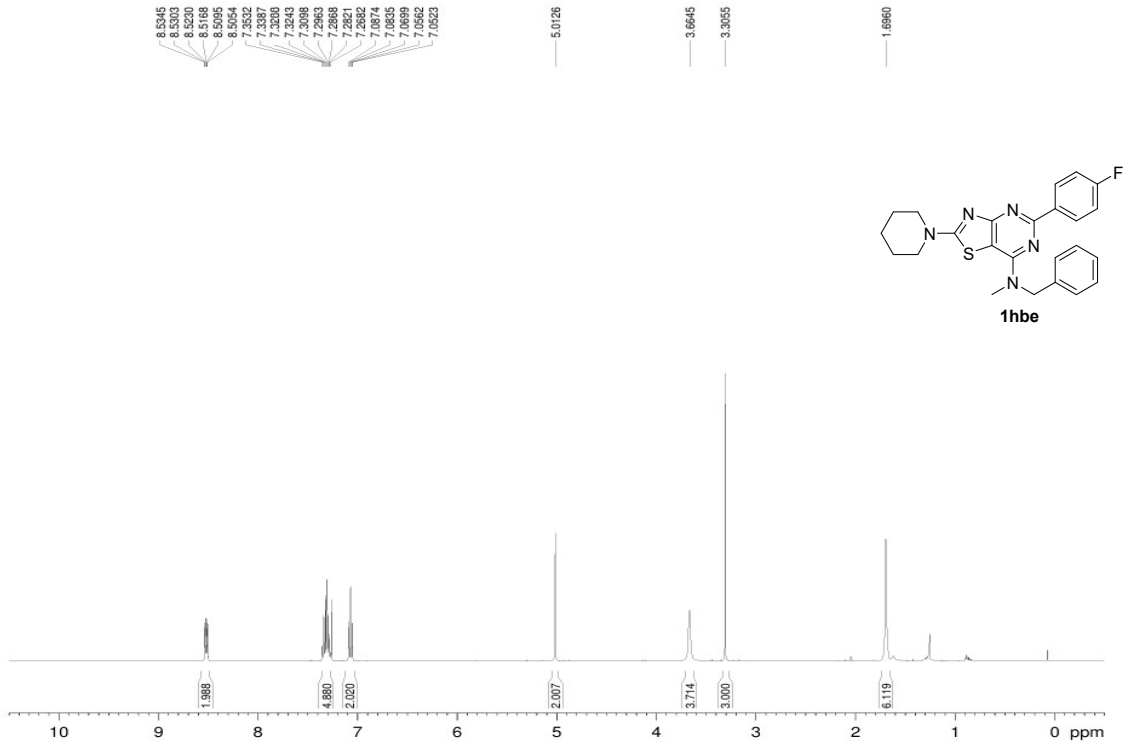
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7.2963
7.2868
7.2821
7.2692
7.0874
7.0835
7.0699
7.0562
7.0523
5.0126
3.6645
3.3055
1.6960
F
N
N
N
S
N
1hbe
1.988
4.880
2.020
2.007
3.714
3.000
6.119
10
9
8
7
6
5
4
3
2
1
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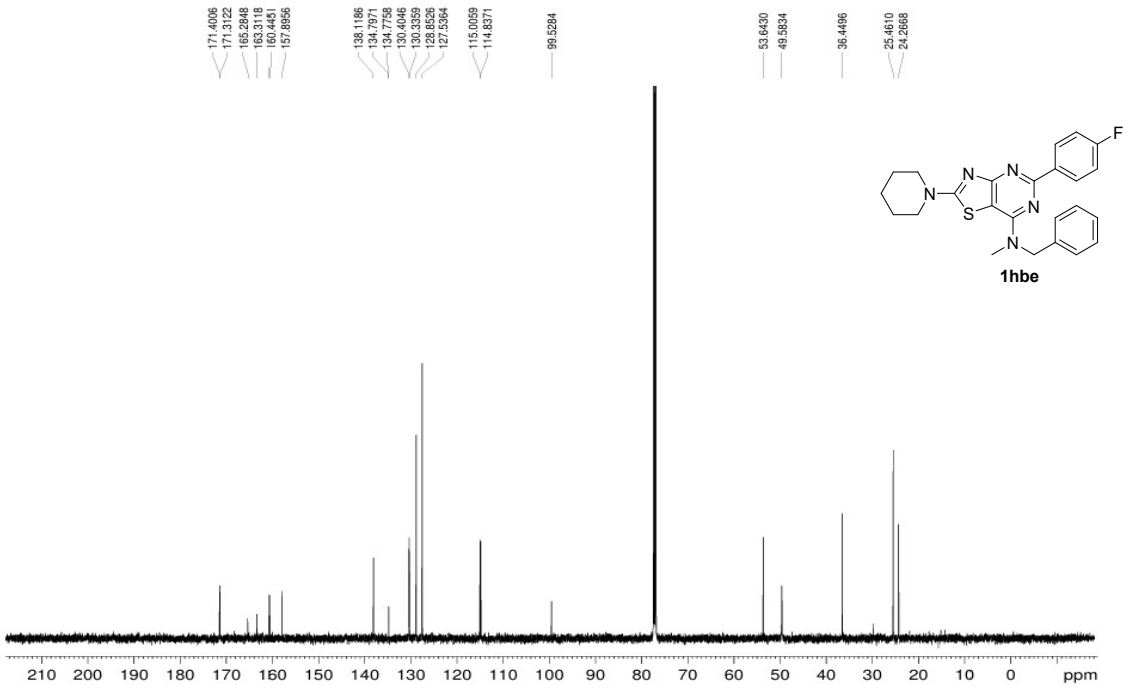
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129.8528
127.5364
115.0059
114.8371
99.5284
53.6430
49.5834
36.4496
25.4610
24.2668
F
N
N
N
S
N
1hbe
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


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8.5291
8.5249
8.5178
8.5112
8.5041
8.4998
8.4940
7.3408
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7.3353
7.3299
7.3218
7.3162
7.3096
7.2834
7.2771
7.2751
7.2698
7.2596
7.2563
7.0939
7.0881
7.0840
7.0741
7.0706
7.0671
7.0571
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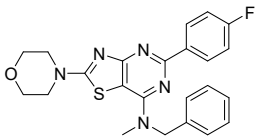
3.2846



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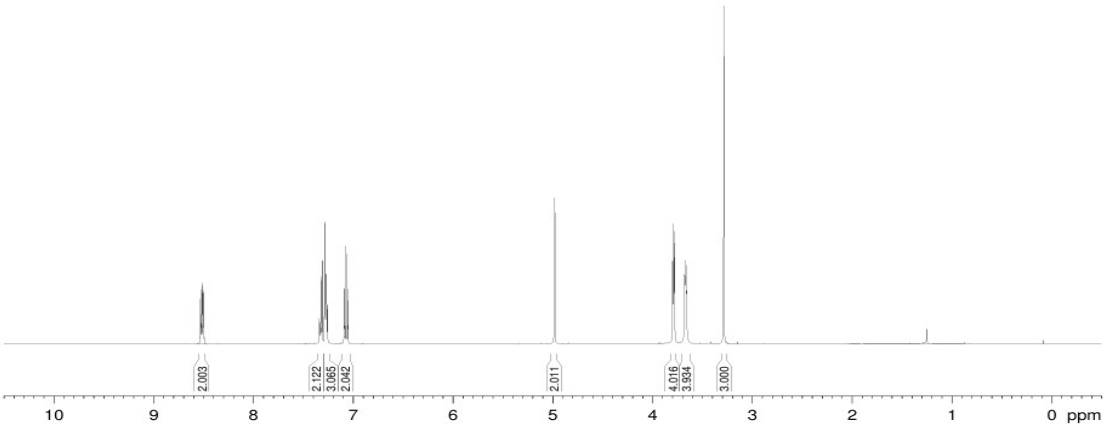
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8
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5
4
3
2
1
0 ppm


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163.2912
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157.9113
137.8160
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134.5446
130.3631
130.2964
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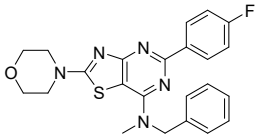

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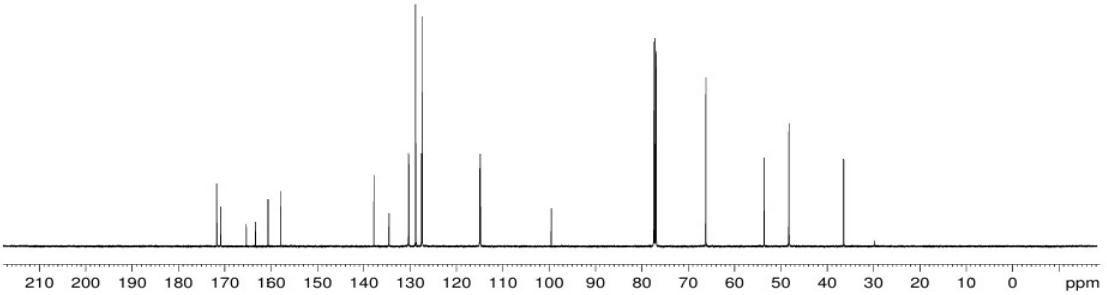
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200
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180
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160
150
140
130
120
110
100
90
80
70
60
50
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30
20
10
0
ppm


8.5513
8.5450
8.5407
8.5337
8.5271
8.5200
8.5158
8.5099
7.3654
7.3631
7.3601
7.3507
7.3465
7.3462
7.3417
7.3389
7.3345
7.3270
7.3149
7.3091
7.3004
7.2977
7.2931
7.2871
7.2830
7.2790
7.1023
7.0980
7.0883
7.0848
7.0809
7.0713
7.0672
6.9685
6.9667
6.9511
6.9491
6.9465
6.9367
6.9317
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5.0233
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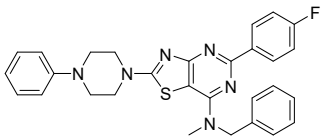
3.8635
3.8539
3.3255
3.3125
3.3021
3.2918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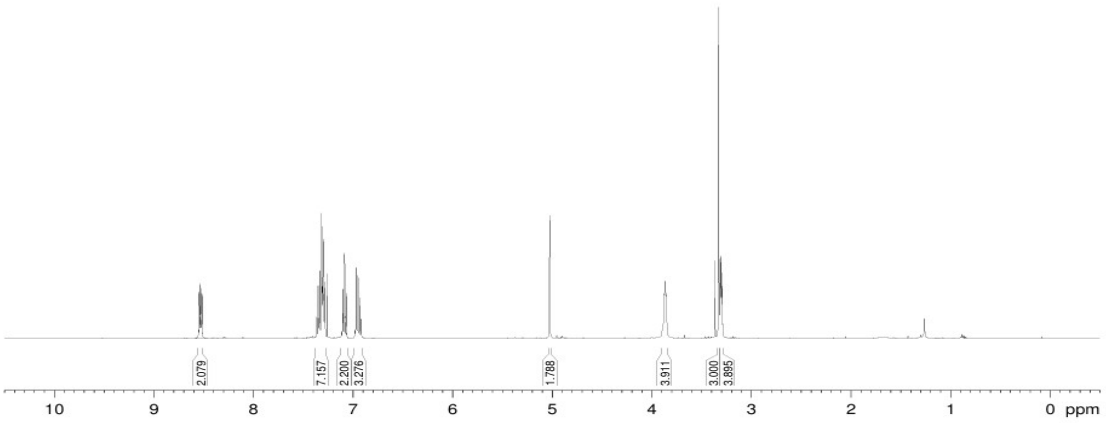
N

1hbg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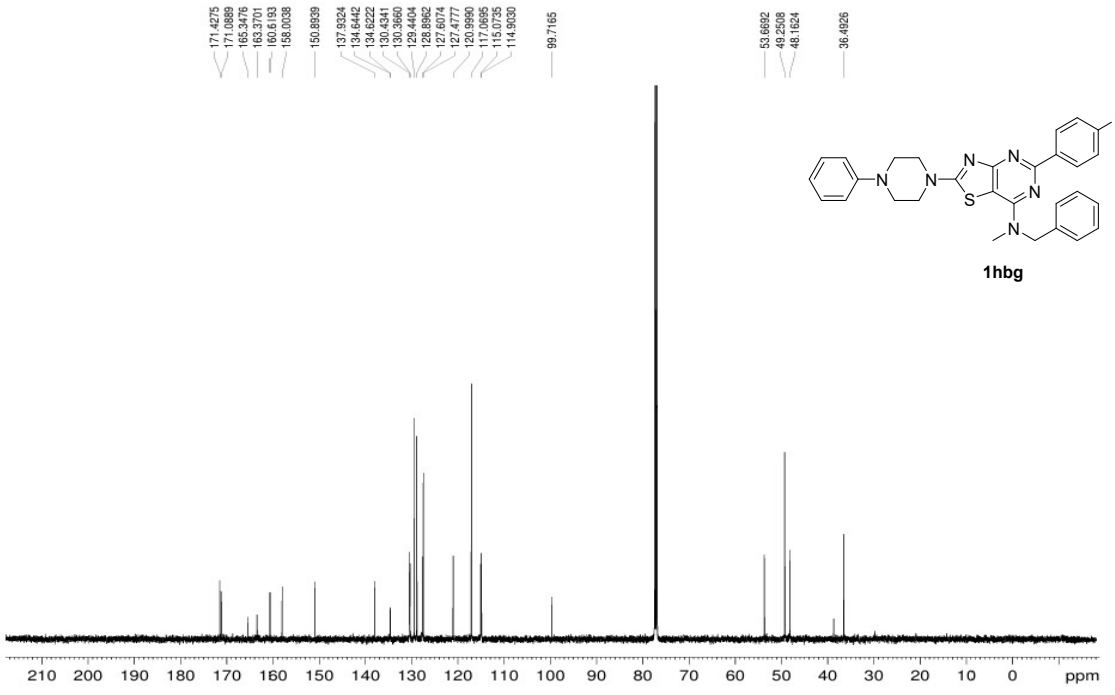
3.895
10
9
8
7
6
5
4
3
2
1
0 ppm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130.3660
129.4404
128.8962
127.6074
127.4777
120.9990
117.0695
115.0735
114.9030
99.7165
53.6692
49.2508
48.1624
36.4926
210
200
190
180
170
160
150
140
130
120
110
100
90
80
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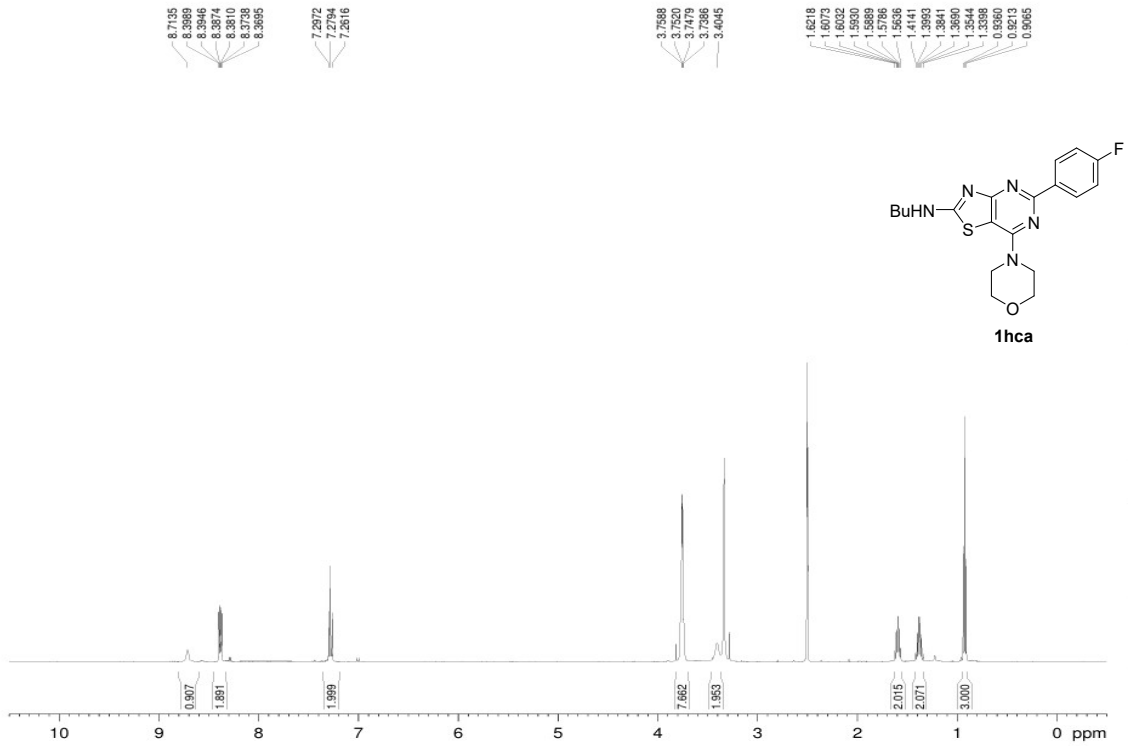
60
50
40
30
20
10
0
ppm

F
N
N
N
S
N
N

1hbg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8.3946
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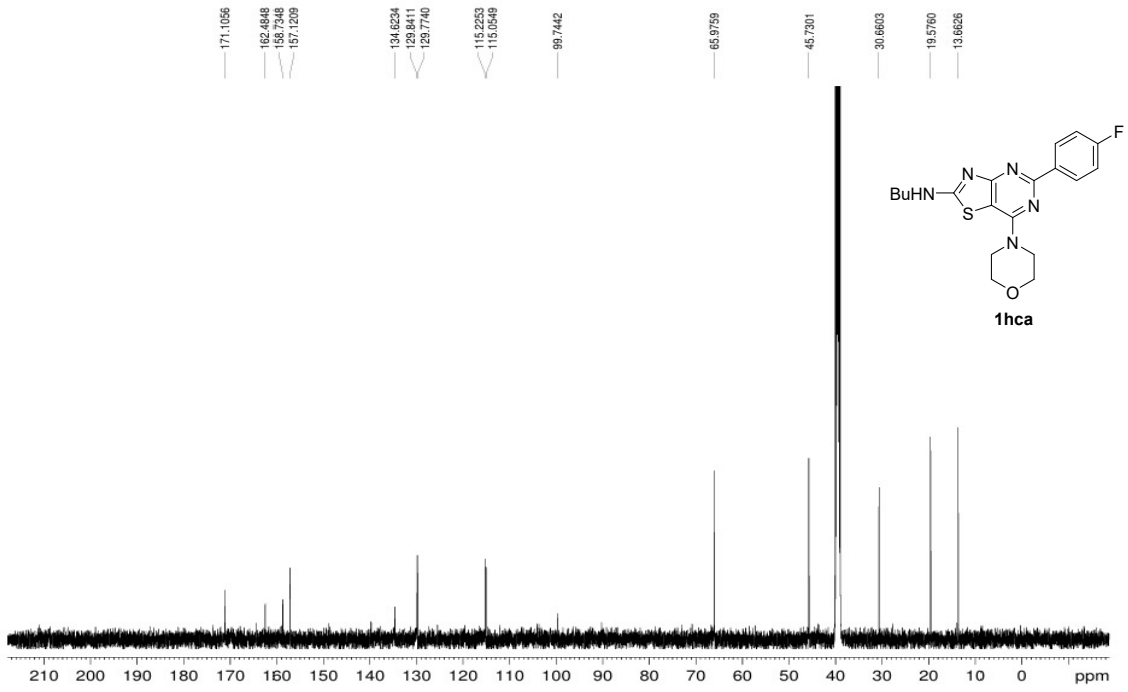
8.3810
8.3738
8.3695
7.2972
7.2794
7.2616
3.7588
3.7520
3.7479
3.7386
3.4045
1.6218
1.6073
1.6032
1.5930
1.5889
1.5786
1.5636
1.4141
1.3993
1.3841
1.3690
1.3544
1.3398
0.9360
0.9213
0.9065
BuHN
N
S
N
N
N
O
F
1hca
0.907
1.891
1.999
7.662
1.953
2.015
2.071
3.000
10
9
8
7
6
5
4
3
2
1
0 ppm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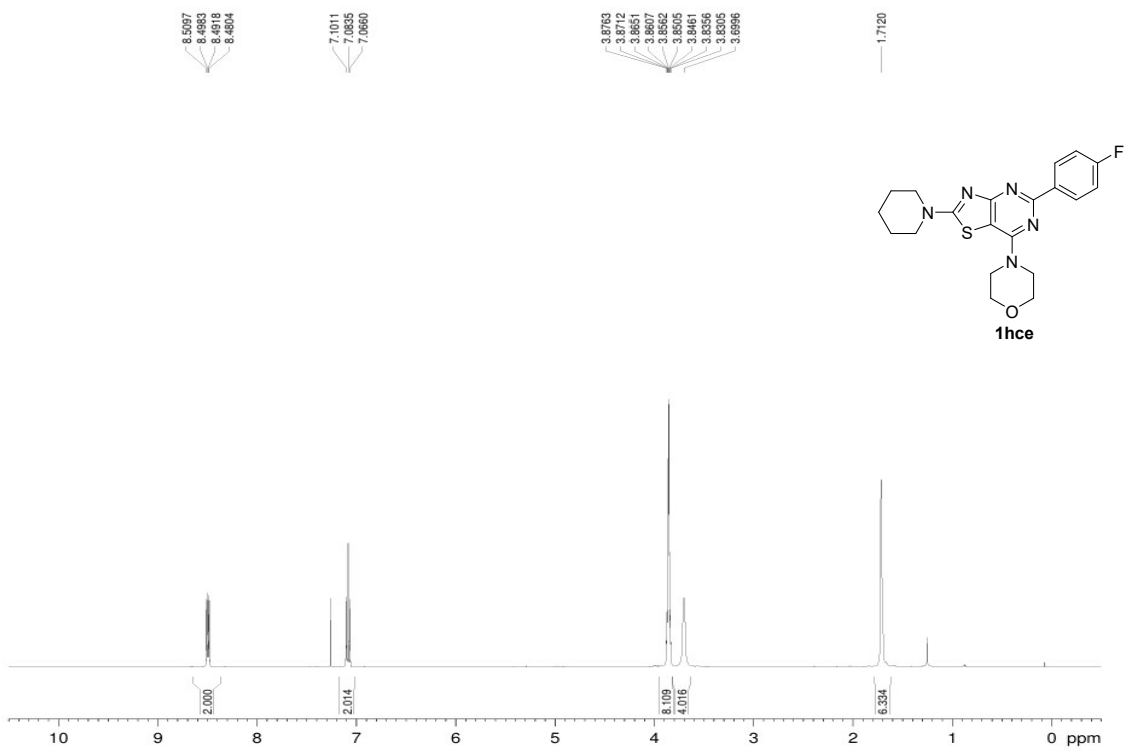
115.0549
99.7442
65.9759
45.7301
30.6603
19.5760
13.6626
BuHN
N
S
N
N
N
O
F
1hca
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.0660
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3.8712
3.8651
3.8607
3.8562
3.8505
3.8461
3.8356
3.8305
3.6996
1.7120
F
N
N
N
S
N
N
O
1hce
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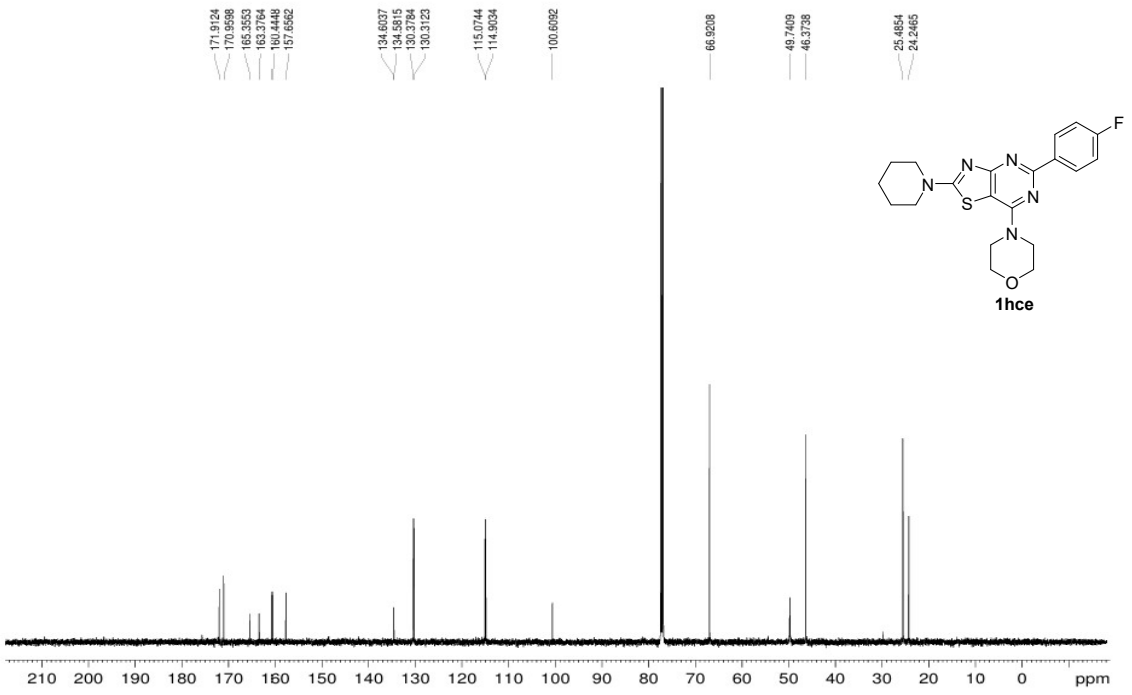
8.109
4.016
6.334
10
9
8
7
6
5
4
3
2
1
0 ppm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130.3784
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115.0744
114.9034
100.6092
66.9208
49.7409
46.3738
25.4854
24.2465
F
N
N
N
S
N
N
O
1hce
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm


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8.5063
8.4997
8.4926
8.4884
8.4827
7.3182
7.3141
7.3035
7.3008
7.2901
7.2861
7.2817
7.1220
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7.0988
7.0853
7.0813
7.0755
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6.9730
6.9573
6.9556
6.9516
6.9370
6.9241
6.9223
3.8963
3.8922
3.8893
3.8864
3.8842
3.8814
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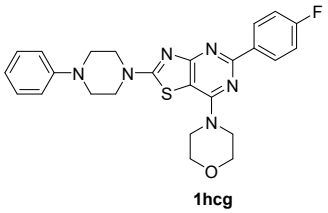
F
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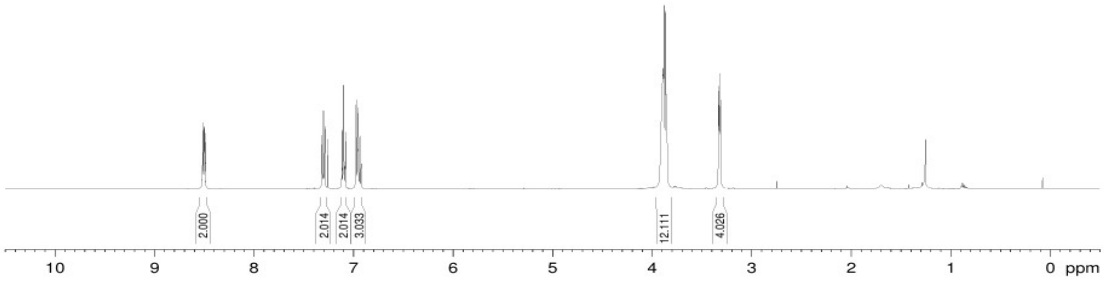
N
N
S
N
N
N
O

1hcg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2.014
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4.026
10
9
8
7
6
5
4
3
2
1
0 ppm


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171.0666
165.3984
163.4172
160.5916
157.7239
150.8245
134.4272
134.4056
130.3930
130.3267
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115.1346
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100.6716
66.8687
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48.2877
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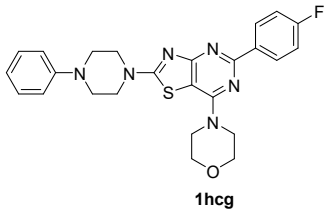
F
N
N
N
S
N
N
N
O

1hcg

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

References

1. 4-Bromo-2-(piperidin-1-yl)thiazol-5-yl-phenyl methanone (12b) inhibits Na+/K+-ATPase and Ras oncogene activity in cancer cells. Eur. J. Med. Chem., 63 (2013), 213-223