Supporting Information

Transition-Metal-Free four-component reaction of nitriles and disulfides/diselenides

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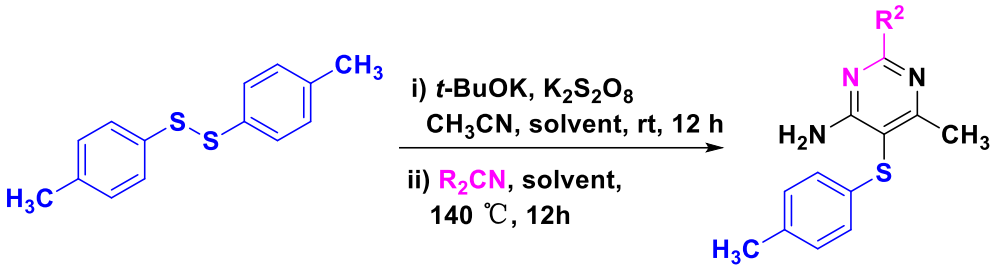
1. General Information

All reagents and solvents were purchased from Energy Chemical, Sigma-Aldrich, Bidepharm, Macklin and Meryer. All reactions were conducted using standard Schlenk techniques. Column chromatography was performed using Aluminium oxide neutral (200−300 mesh). ^{1}H NMR spectra were measured on a 400 MHz Oxford Instruments spectrometer (400 MHz for ^{1}H, 100 MHz for ^{13}C) and ^{13}C NMR spectra were measured on a 500 MHz Bruker AVANCE spectrometer (500 MHz for ^{1}H, 125 MHz for ^{13}C, 471 MHz for ^{19}F), using $CDCl_3$ as the solvent with tetramethylsilane (TMS) as the internal standard at room temperature. Chemical shifts were reported in ppm. ^{1}H NMR spectra was referenced to $CDCl_3$ (7.26 ppm), and ^{13}C-NMR spectra was referenced to $CDCl_3$ (77.0 ppm), and ^{19}F -NMR spectra was referenced to $CDCl_3$. Peak multiplicities were designated by the following abbreviations: s, singlet; d, doublet; t, triplet; m, multiplet. Chemical shifts are given in δ relative to TMS, the coupling constants J are given in Hz. Analysis of crude reaction mixture was done on the Varian 4000 GC/MS and Agilent 7890A/5975C. High-resolution mass spectra were recorded on a micrOTOF-Q II 10410 mass spectrometer. A 15 W UV light and a 500 W super high-pressure mercury lamp were used for photoirradiation. Unless otherwise noted, all reagents and solvents were obtained commercially and used without further purification. The disulfides[1]/diselenides[2] were prepared according to the corresponding literature procedures.

2. Optimization of the Reaction Conditions

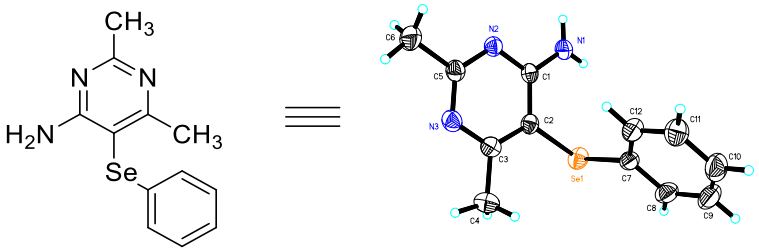
Table S1: Optimization of Reaction Conditions for the reaction of 1,2-di-*p*-tolyldisulfane with mixed nitriles.[a]



Number	Solvent	Yield (%)[b]
1	DMSO	28
2	DMF	32
3	1,4-dioxane	71
4	Toluene	65
5	cyclohexane	74
6	DME	90

[a]Reaction conditions: i) 1,2-di-*p*-tolyldisulfane (0.2 mmol), CH_3CN (0.6 mL), *t*-BuOK (0.4 mmol), $K_2S_2O_8$ (0.4 mmol), DME (1.0 mL), air, rt, 12 h; R^2CN (0.4 mmol), DME (1.0 mL), air, 140 °C, 12 h. [b] Isolated yield.

3. Crystal data and structure refinement of products



(16)

Single crystals of **16** were grown in trichloromethane and hexanes. Trichloromethane (4.0 mL) was added to **16** (20 mg in a 20 mL vial) followed by hexanes (8.0 mL). The 20 mL vial was not capped and placed at room temperature in the experimental cabinet for 3 days, whereupon crystals formed. A colorless diamond-shaped lumpy crystal of **16** was used for the X-ray crystallographic analysis. The crystal data of **16** have been deposited in CCDC with number mo_dd22001_0m and have been displayed at 50% ellipsoid contour probability level.

Table S2: Crystal data and structure refinement for mo_dd22001_0m.

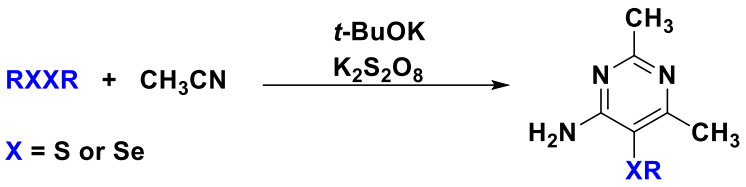
Crystal data and structure refinement for mo_dd22001_0m.	
Identification code	mo_dd22001_0m
Empirical formula	C_{12} H_{13} N_3 Se
Formula weight	278.21
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic

Space group	P -1
Unit cell dimensions	a = 10.093(3) Å a= 102.228(7)°. b = 11.029(2) Å b= 113.956(7)°. c = 12.285(3) Å g = 91.965(7)°.
Volume	1210.3(5) $Å^3$
Z	4
Density (calculated)	1.527 Mg/m^3
Absorption coefficient	3.079 mm^{-1}
F(000)	560
Crystal size	0.160 x 0.100 x 0.060 mm^3
Theta range for data collection	2.731 to 25.998°.
Index ranges	-12<=h<=12, -13<=k<=13, -15<=l<=15
Reflections collected	27602
Independent reflections	4740 [R(int) = 0.0350]
Completeness to theta = 25.242°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7456 and 0.5217
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4740 / 0 / 309
Goodness-of-fit on F^2	1.013

Final R indices [I>2sigma(I)]	R1 = 0.0267, wR2 = 0.0626
R indices (all data)	R1 = 0.0396, wR2 = 0.0693
Extinction coefficient	n/a
Largest diff. peak and hole	0.287 and -0.313 e.Å^{-3}

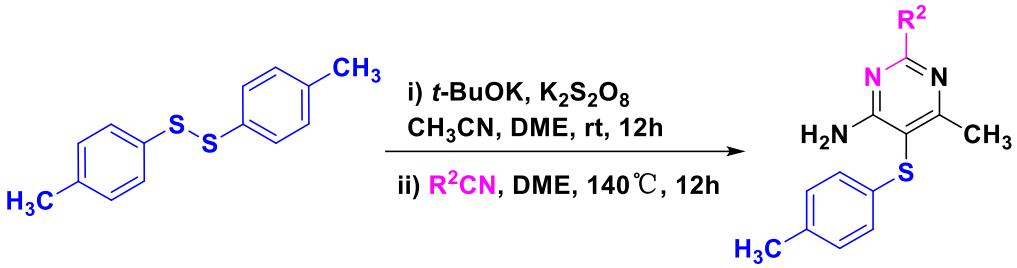
4. General Experimental Procedures and the Control Experiments

(1) General procedure for the reactions of disulfides or diselenides with CH_3CN



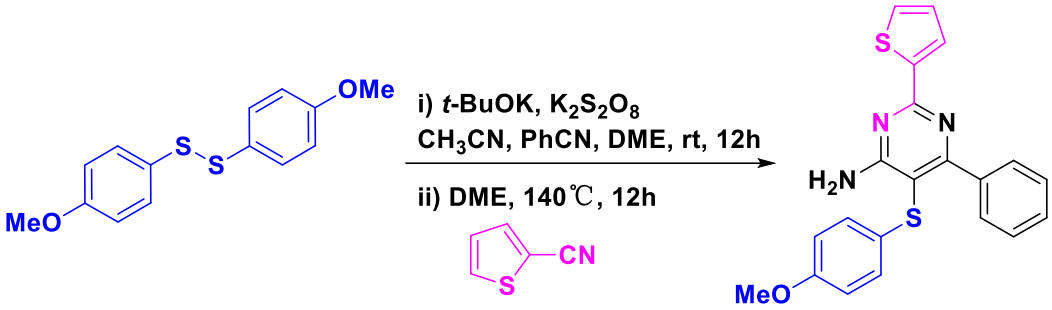
A 10 mL pressure tube equipped with a stir bar was charged with disulfides or diselenides (0.2 mmol), *t*-BuOK (2.0 equiv), $K_2S_2O_8$ (2.0 equiv), and CH_3CN (28.7 mmol, 1.5 mL). The reaction mixture was stirred at 140℃ under an air atmosphere for 24 h. After cooling the reaction to room temperature, the residue was purified by flash chromatography with neutral alumina to obtain the corresponding product.

(2) General procedure for the reactions of 1,2-di-*p*-tolyldisulfane with mixed nitriles



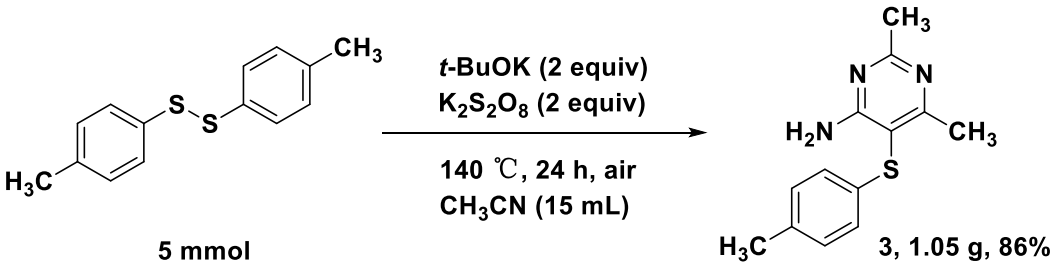
A 10 mL pressure tube equipped with a stir bar was charged with 1,2-di-*p*-tolyldisulfane (0.2 mmol), *t*-BuOK (2.0 equiv), $K_2S_2O_8$ (2.0 equiv), CH_3CN (11.5 mmol, 0.6 mL) and DME (1.0 mL). The reaction mixture was stirred at room temperature under an air atmosphere for 12 h. Next, benzonitrile (0.4 mmol) and DME (1.0 mL) were added to the mixture, and the temperature was increased to 140 ℃ under an air atmosphere for 12 h. After cooling the reaction to room temperature, the residue was purified by flash chromatography with neutral alumina to obtain the corresponding product.

(3) General procedure for the reaction of bis(4-methoxyphenyl) disulphide with three-component mixed nitriles.



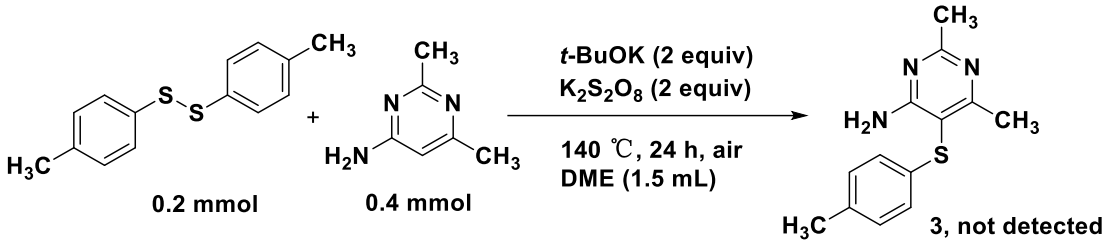
A 10 mL pressure tube equipped with a stir bar was charged with bis(4-methoxyphenyl) disulphide (0.2 mmol), *t*-BuOK (2.0 equiv), $K_2S_2O_8$ (2.0 equiv), CH_3CN (11.5 mmol, 0.6 mL), benzonitrile (1.2 mL) and DME (0.5 mL). The reaction mixture was stirred at room temperature under an air atmosphere for 12 h. Next, 2-thiophenecarbonitrile (0.4 mmol) and DME (1.0 mL) were added to the mixture, and the temperature was then increased to 140 ℃ under an air atmosphere for 12 h. After cooling the reaction to room temperature, the residue was purified by flash chromatography with neutral alumina to obtain the corresponding product.

(4) General procedure for gram-scale synthesis.



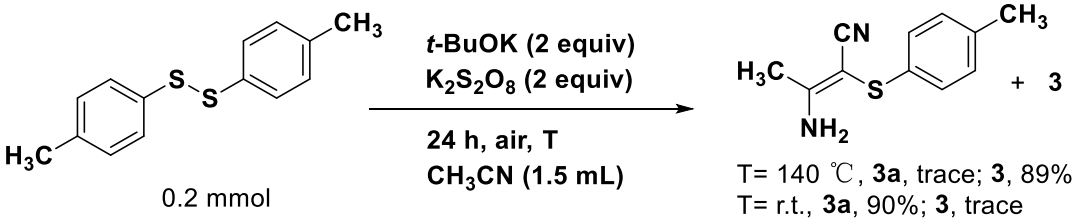
A 50 mL pressure tube equipped with a stir bar was charged with bis(4-methoxyphenyl) disulphide (5 mmol), *t*-BuOK (10 mmol, 2.0 equiv), $K_2S_2O_8$ (10 mmol, 2.0 equiv), and CH_3CN (287 mmol, 15 mL). The reaction mixture was stirred at 140 ℃ under an air atmosphere for 24 h. After cooling the reaction to room temperature, the residue was purified by flash chromatography with neutral alumina to obtain the corresponding product **3** (1.05 g, 86%).

(5) General procedure for the reaction between 1,2-di-*p*-tolyldisulfane and 2,6-dimethylpyrimidin-4-amine



A 10 mL pressure tube equipped with a stir bar was charged with bis(4-methoxyphenyl) disulphide (0.2 mmol), 2,6-dimethylpyrimidin-4-amine (0.4 mmol), *t*-BuOK (0.4 mmol, 2.0 equiv), $K_2S_2O_8$ (0.4 mmol, 2.0 equiv), and DME (1.5 mL). The reaction mixture was stirred at 140 ℃ under an air atmosphere for 24 h. After cooling the reaction to room temperature, the residue was detected by GC-MS and no formation of the product **3** was observed.

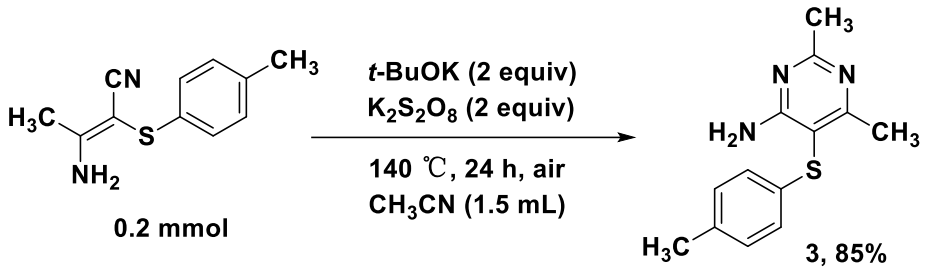
(6) General procedure for the control reaction of 1,2-di-*p*-tolyldisulfane at 140 ºC or room temperature.



A 10 mL pressure tube equipped with a stir bar was charged with bis(4-methoxyphenyl) disulfide (0.2 mmol), *t*-BuOK (0.4 mmol, 2.0 equiv), $K_2S_2O_8$ (0.4 mmol, 2.0 equiv), and CH_3CN (28.7 mmol, 1.5 mL). The reaction mixture was stirred at 140 ℃ under an air atmosphere for 24 h. After cooling the reaction to room temperature, the residue was purified by flash chromatography with neutral alumina to obtain the corresponding product **3** (43.6 mg, 89%). Meanwhile, the residue was detected by GC-MS and a trace of the product **3a** was detected. Alternatively, the reaction mixture was stirred at room temperature under an air atmosphere for 24 h. When the reaction was completed, the residue was purified by flash chromatography with neutral alumina to obtain the corresponding product

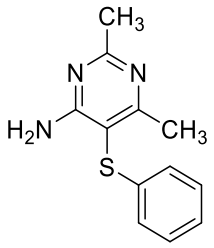
3a (36.7 mg, 90%). Meanwhile, the residue was detected by GC-MS and trace of the product **3** was detected.

(7) General procedure for the control reaction of alkenyl sulfide 3a in CH_3CN



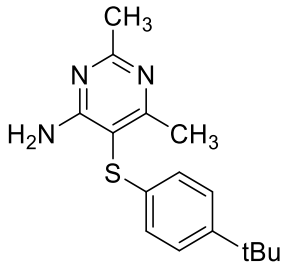
A 10 mL pressure tube equipped with a stir bar was charged with alkenyl sulfide **3a** (0.2 mmol), *t*-BuOK (0.4 mmol, 2.0 equiv), $K_2S_2O_8$ (0.4 mmol, 2.0 equiv), and CH_3CN (28.7 mmol, 1.5 mL). The reaction mixture was stirred at 140 ℃ under an air atmosphere for 24 h. After cooling the reaction to room temperature, the residue was purified by flash chromatography with neutral alumina to obtain the corresponding product **3** (41.6 mg, 85%).

5. Characterization data for the products



2,6-dimethyl-5-(phenylthio)pyrimidin-4-amine (**1)**: yellow solid (42.1 mg, 91% yield), m.p. 113.3-114.3 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.19 (d, *J*= 4.8 Hz, 2H), 7.17-7.01 (m, 1H), 6.99 (d, *J*= 5.2 Hz, 2H), 6.25 (br, 2H), 2.45 (s, 3H), 2.42 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 171.1, 167.5, 164.5, 134.6, 129.3, 125.9, 125.9, 103.0, 25.6, 23.1.

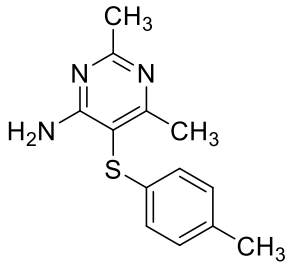
HR-MS (ESI) m/z: Calculated for $C_{12}H_{14}N_3S^+$ $[M + H]^+$: 232.0903. Found: 232.0901.



5-((4-(tert-butyl)phenyl)thio)-2,6-dimethylpyrimidin-4-amine (2): yellow solid (49.9 mg, 87% yield), m.p. 137.4-138.7 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.30 (d, *J*= 6.4 Hz, 2H), 7.03 (d, *J*= 6.4 Hz, 2H), 6.05 (br, 2H), 2.55 (s, 3H), 2.52 (s, 3H), 1.31 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 170.9, 167.4, 164.4, 149.2, 131.0, 126.4, 126.0, 103.6, 34.4, 31.3, 25.7, 23.1.

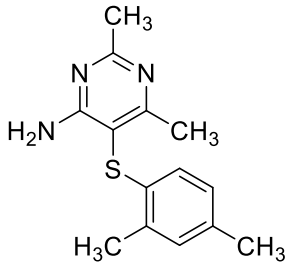
HR-MS (ESI) m/z: Calculated for $C_{16}H_{22}N_3S^+$ $[M + H]^+$: 288.1529. Found:

288.1524.



2,6-dimethyl-5-(p-tolylthio)pyrimidin-4-amine (**3)**: yellow solid (43.6 mg, 89% yield), m.p. 131.9-132.8 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.02 (d, *J*= 8.0 Hz, 2H), 6.92 (d, *J*= 8.0 Hz, 2H), 6.08 (br, 2H), 2.47 (s, 3H), 2.44 (s, 3H), 2.25 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 170.8, 167.5, 164.2, 136.0, 130.9, 130.1, 126.4, 103.7, 25.8, 23.1, 20.9.

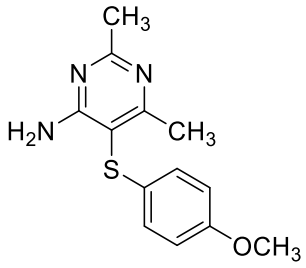
HR-MS (ESI) m/z: Calculated for $C_{13}H_{16}N_3S^+$ $[M + H]^+$: 246.1059. Found: 246.1054.



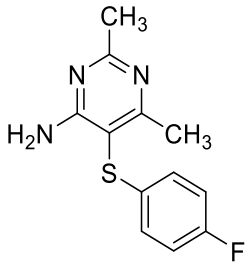
5-((2,4-dimethylphenyl)thio)-2,6-dimethylpyrimidin-4-amine (**4)**: yellow solid (45.0 mg, 87% yield), m.p. 148.4-149.3℃. **^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 6.98 (s, 1H), 6.82 (d, *J*= 6.0 Hz, 1H), 6.52 (d, *J*= 8.0 Hz, 1H), 5.86 (br, 2H), 2.48 (s, 3H), 2.45 (s, 3H), 2.37 (s, 3H), 2.24 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ (ppm) 171.0, 167.3, 164.4, 135.4, 135.2, 131.5, 129.9, 127.6, 124.3, 102.9, 25.6, 23.0, 20.7, 19.8.

HR-MS (ESI) m/z: Calculated for $C_{14}H_{18}N_3S^+$$[M + H]^+$: 260.1216. Found:

260.1210.

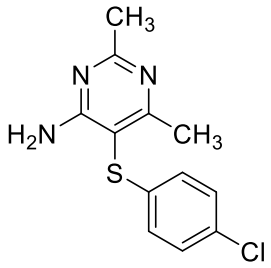


5-((4-methoxyphenyl)thio)-2,6-dimethylpyrimidin-4-amine (**5)**: yellow solid (49.1 mg, 94% yield), m.p. 125.0-125.8 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.02 (d, *J*= 8.8 Hz, 2H), 6.77 (d, *J*= 8.8 Hz, 2H), 5.99 (br, 2H), 3.72 (s, 3H), 2.48 (s, 3H), 2.44 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ 170.4, 167.2, 164.2, 158.5, 128.7, 125.1, 115.1, 104.8, 55.4, 25.7, 23.1. HRMS (ESI) m/z: $[M + H]^+$ Calculated for $C_{13}H_{16}N_3OS^+$: 262.1009; Found: 261.1013.



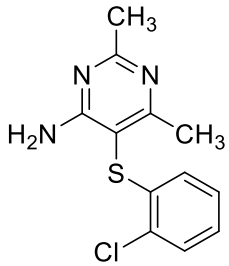
5-((4-fluorophenyl)thio)-2,6-dimethylpyrimidin-4-amine (6): yellow solid (40.8 mg, 82% yield), m.p. 114.1-116.0 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.01-6.97 (m, 2H), 6.93-6.88 (m, 2H), 6.05 (br, 2H), 2.50 (s, 3H), 2.48 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 171.0, 167.7, 164.4, 161.5 (d, J=244.6 Hz), 129.8 (d, J= 3.1 Hz), 128.2 (d, J= 7.8 Hz), 116.6 (d, J= 22.1 Hz), 103.7, 25.7, 23.1. **^{19}F NMR** (471 MHz, $CDCl_3$) δ (ppm) 116.1.

HR-MS (ESI) m/z: Calculated for $C_{12}H_{13}FN_3S^+$ $[M + H]^+$: 250.0809. Found: 250.0812.



5-((4-chlorophenyl)thio)-2,6-dimethylpyrimidin-4-amine (**7)**: yellow solid (44.5 mg, 84% yield), m.p. 156.9-157.6 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.21 (d, *J*= 6.8 Hz, 2H), 6.96 (d, *J*= 6.8 Hz, 2H), 5.66 (br, 2H), 2.50 (s, 3H), 2.48 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 174.3, 168.4, 161.7, 137.3, 131.9, 129.5, 125.1, 104.1, 26.7, 20.5.

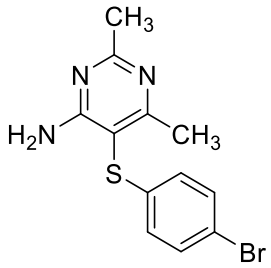
HR-MS (ESI) m/z: Calculated for $C_{12}H_{13}N_3ClS^+$[M + H]$^+$: 266.0513. Found: 266.0509.



5-((2-chlorophenyl)thio)-2,6-dimethylpyrimidin-4-amine (**8)**: yellow solid (47.7 mg, 90% yield), m.p. 169.8-170.4 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.37-7.34 (dd, *J*1= 4.0 Hz, *J*2= 6.4 Hz, 1H), 7.10 (d, *J*= 3.2 Hz, 1H), 7.08 (d, *J*= 4.0 Hz, 1H), 6.62-6.60 (dd, *J*1= 3.2 Hz, *J*2= 5.6 Hz, 1H), 5.76 (br, 2H), 2.51 (s, 3H), 2.48 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 171.7, 168.1, 164.9, 133.6, 131.6, 130.0, 127.5, 126.7,

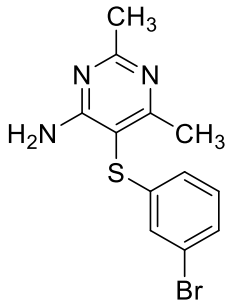
125.3, 102.2, 25.7, 23.0.

HR-MS (ESI) m/z: Calculated for $C_{12}H_{13}N_3ClS^+[M + H]^+$: 266.0513. Found: 266.0516.



5-((4-bromophenyl)thio)-2,6-dimethylpyrimidin-4-amine (**9)**: yellow solid (53.1 mg, 86% yield), m.p. 153.6-154.2 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.31 (d, *J*= 8.4 Hz, 2H), 6.56 (d, *J*= 8.4 Hz, 2H), 6.12 (br, 2H), 2.45 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 171.2, 167.8, 164.4, 133.9, 132.4, 127.4, 119.6, 102.5, 25.7, 23.1.

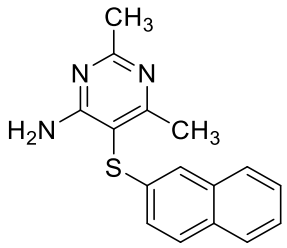
HR-MS (ESI) m/z: Calculated for $C_{12}H_{13}N_3BrS^+[M + H]^+$: 310.0008. Found: 310.0012.



5-((3-bromophenyl)thio)-2,6-dimethylpyrimidin-4-amine (**10)**: yellow solid (51.3mg, 83% yield), m.p. 146.3-147.4 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.23 (d, *J*= 8.0 Hz, 1H), 7.13 (s, 1H), 7.08-7.04 (m, 1H), 6.91 (d, *J*= 8.0 Hz, 1H), 5.98 (br, 2H), 2.46 (s, 3H), 2.45 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ (ppm) 171.3, 168.2, 164.2, 137.0, 130.6, 129.1, 128.4,

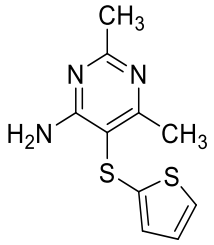
124.3, 123.4, 102.1, 25.8, 23.1.

HR-MS (ESI) m/z: Calculated for $C_{12}H_{13}N_3BrS^+[M + H]^+$: 310.0008. Found: 310.0006.



2,6-dimethyl-5-(naphthalen-2-ylthio)pyrimidin-4-amine (**11)**: yellow solid (24.7 mg, 44% yield), m.p. 160.1-161.4 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.75 (d, *J*= 8.0 Hz, 1H), 7.72 (d, *J*= 8.8 Hz, 1H), 7.64 (d, *J*= 8.0 Hz, 1H), 7.46-7.40 (m, 2H), 7.39 (s, 1H), 7.18 (d, *J*= 8.4 Hz, 1H), 5.81 (br, 2H), 2.52 (s, 6H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 172.1, 167.8, 164.4, 133.8, 131.9, 131.7, 129.2, 127.8, 127.0, 126.9, 125.8, 124.44, 123.7, 103.0, 27.1, 23.1.

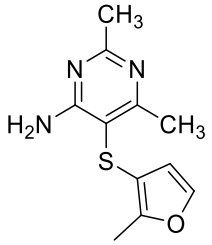
HR-MS (ESI) m/z: Calculated for $C_{16}H_{16}N_3S^+[M + H]^+$: 282.1059. Found: 282.1061.



2,6-dimethyl-5-(thiophen-2-ylthio)pyrimidin-4-amine (**12)**: yellow solid (41.8 mg, 89% yield), m.p. 143.0-144.0 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.22 (d, *J*= 5.2 Hz, 1H), 7.53 (d, *J*= 3.6 Hz, 1H), 6.91-6.88

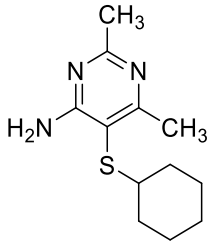
(dd, *J*1= 3.2 Hz, *J*2= 3.6 Hz, 1H), 6.08 (br, 2H), 2.60 (s, 3H), 2.42 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 169.8, 167.3, 163.7, 133.8, 130.8, 128.2, 127.5, 106.1, 25.6, 23.2.

HR-MS (ESI) m/z: Calculated for $C_{10}H_{12}N_3S_2^+[M + H]^+$: 238.0467. Found: 238.0464.



2,6-dimethyl-5-((2-methylfuran-3-yl)thio)pyrimidin-4-amine (**13)**: yellow solid (44.2 mg, 94% yield), m.p. 142.6-143.2 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.20 (d, *J*= 2.0 Hz, 1H), 6.13 (d, *J*= 2.0 Hz, 1H), 5.84 (br, 2H), 2.52 (s, 3H), 2.42 (s, 3H), 2.34 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 169.5, 166.8, 164.0, 152.5, 141.4, 113.2, 109.6, 106.1, 25.7, 23.3, 12.2.

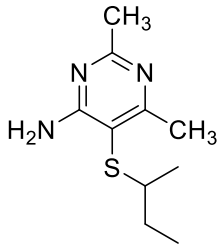
HR-MS (ESI) m/z: Calculated for $C_{11}H_{14}N_3OS^+[M + H]^+$: 236.0852. Found: 236.0858.



5-(cyclohexylselanyl)-2,6-dimethylpyrimidin-4-amine (**14)**: yellow solid (25.1mg, 53% yield), m.p. 151.5-152.4 ℃. **^{1}H NMR** (400 MHz,

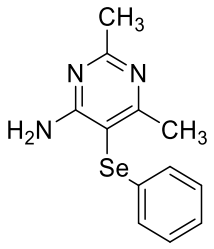
$CDCl_3$) δ (ppm) 5.79 (br, 2H), 2.86-2.81 (m, 1H), 2.55 (s, 3H), 2.44 (s, 3H), 1.87-1.85 (m, 2H), 1.75-1.71 (m, 2H), 1.39-1.32 (m, 4H), 1.29-1.17 (m, 2H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 170.2, 166.3, 164.9, 105.2, 47.1, 32.9, 26.1, 25.6, 23.3, 23.2.

HR-MS (ESI) m/z: Calculated for $C_{12}H_{20}N_3S^+[M + H]^+$: 238.1372. Found: 238.1375.



5-(*sec*-butylthio)-2,6-dimethylpyrimidin-4-amine (**15)**: yellow solid (24.9 mg, 59% yield), m.p.118.4-119.1 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 6.17 (br, 2H), 2.91-2.83 (m, 1H), 2.49 (s, 3H), 2.38 (s, 3H), 1.60-1.42 (m, 2H), 1.14 (d, *J*= 6.4 Hz, 3H), 0.93 (d, *J*= 7.6 Hz, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 170.1, 166.1, 164.9, 105.5, 45.2, 29.7, 25.4, 23.2, 20.4, 11.4.

HR-MS (ESI) m/z: Calculated for $C_{10}H_{18}N_3S^+[M + H]^+$: 212.1216. Found: 212.1211.

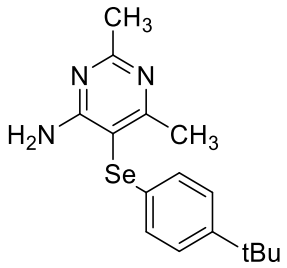


2,6-dimethyl-5-(phenylselanyl)pyrimidin-4-amine (**16)**: yellow solid

(53.0 mg, 95% yield), m.p. 128.7-129.4 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.25-7.17 (m, 5H), 5.78 (br, 2H), 2.56 (s, 3H), 2.48 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ (ppm) 170.6, 167.7, 164.2, 129.8, 129.6, 128.9, 126.7, 101.8, 25.5, 25.1.

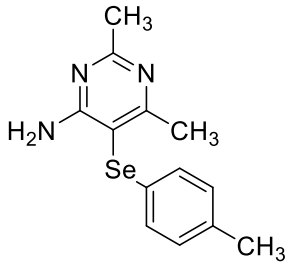
HR-MS (ESI) m/z: Calculated for $C_{12}H_{14}N_3Se^+[M + H]^+$: 280.0347. Found: 280.0345.

Structure of **16** was clearly determined by X -ray crystallographic analysis of its single crystal.

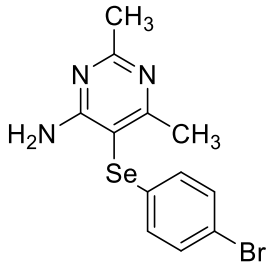


5-((4-(tert-butyl)phenyl)selanyl)-2,6-dimethylpyrimidin-4-amine (**17**): yellow solid (61.6 mg, 92% yield), m.p. 128.1-128.6 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.27 (d, *J*= 8.0 Hz, 2H), 7.15 (d, *J*= 7.6 Hz, 2H), 5.60 (br, 2H), 2.60 (s, 3H), 2.51 (s, 3H), 1.29 (s, 9H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 170.7, 167.7, 164.2, 150.1, 129.0, 126.8, 126.2, 102.2, 34.5, 31.3, 25.7, 25.3.

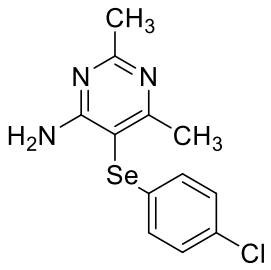
HR-MS (ESI) m/z: Calculated for $C_{16}H_{22}N_3Se^+[M + H]^+$: 336.0973. Found: 336.0975.



2,6-dimethyl-5-(p-tolylselanyl)pyrimidin-4-amine (**18)**: yellow solid (54.5mg, 93% yield), m.p. 139.5-140.3 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.08 (d, *J*= 8.0 Hz, 2H), 7.01 (d, *J*= 8.0 Hz, 2H), 5.91 (br, 2H), 2.54 (s, 3H), 2.45 (s, 3H), 2.26 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 170.5, 167.6, 164.3, 136.8, 130.4, 129.4, 126.0, 102.4, 25.6, 25.2, 21.0. HR-MS (ESI) m/z: Calculated for $C_{13}H_{16}N_3S^+[M + H]^+$: 294.0504. Found: 294.0502.

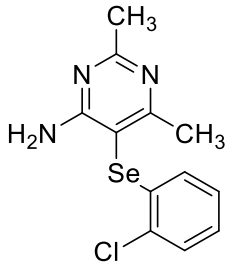


5-((4-bromophenyl)selanyl)-2,6-dimethylpyrimidin-4-amine (**19)**: yellow solid (61.4 mg, 86% yield), m.p. 156.6-157.5 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.30 (d, *J*= 8.0 Hz, 2H), 6.41 (d, *J*= 8.4 Hz, 2H), 5.63 (br, 2H), 2.55 (s, 3H), 2.49 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 170.8, 168.2, 164.1, 132.7, 130.5, 128.9, 120.8, 101.5, 25.7, 25.2. HR-MS (ESI) m/z: Calculated for $C_{12}H_{13}BrN_3Se^+[M + H]^+$: 357.9453. Found: 357.9456.



5-((4-chlorophenyl)selanyl)-2,6-dimethylpyrimidin-4-amine (**20**): yellow solid (55.1 mg, 88% yield), m.p. 157.9-158.8 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.13 (d, *J*= 8.0 Hz, 2H), 7.06 (d, *J*= 8.0 Hz, 2H), 6.06 (br, 2H), 2.50 (s, 3H), 2.42 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 170.8, 167.9, 164.3, 132.8, 130.2, 129.7, 128.2, 101.7, 25.5, 25.2.

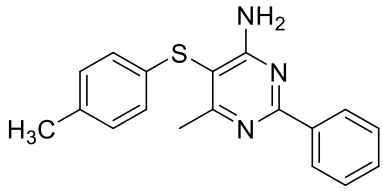
HR-MS (ESI) m/z: Calculated for $C_{12}H_{13}ClN_3Se^+[M + H]^+$: 313.9958. Found: 313.9963.



5-((2-chlorophenyl)selanyl)-2,6-dimethylpyrimidin-4-amine (**21**): yellow solid (53.8 mg, 86% yield), m.p. 167.8-168.2 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.34 (d, *J*= 8.0 Hz, 1H), 7.14-7.11 (dd, *J*1= 6.0 Hz, *J*2= 7.6 Hz, 1H), 7.07-7.04 (dd, *J*1= 6.0 Hz, *J*2= 7.6 Hz, 1H), 6.70 (d, *J*= 7.6 Hz, 1H), 5.74 (br, 2H), 2.54 (s, 3H), 2.50 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 171.7, 168.5, 164.6, 133.3, 130.2, 129.9, 127.8, 127.8, 127.5, 100.4, 25.7, 25.1.

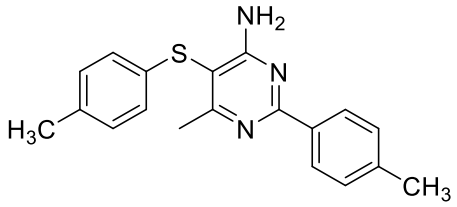
HR-MS (ESI) m/z: Calculated for $C_{12}H_{13}ClN_3Se^+[M + H]^+$: 313.9958.

Found: 313.9956.



6-methyl-2-phenyl-5-(*p*-tolylthio)pyrimidin-4-amine (**22)**: yellow solid (55.3 mg, 90% yield), m.p. 131.2-131.7 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 8.43 (d, *J*= 5.2 Hz, 2H), 7.48-7.47(m, 3H), 7.08 (d, *J*= 8.0 Hz, 2H), 7.04 (d, *J*= 8.4 Hz, 2H), 5.86 (br, 2H), 2.66 (s, 3H), 2.31 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 171.2, 164.6, 163.7, 137.7, 136.0, 131.2, 130.7, 130.2, 128.5, 128.5, 126.6, 104.7, 23.6, 21.1.

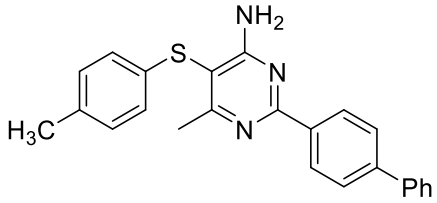
HR-MS (ESI) m/z: Calculated for $C_{18}H_{18}N_3S^+[M + H]^+$: 308.1216. Found: 308.1217.



6-methyl-2-(*p*-tolyl)-5-(*p*-tolylthio)pyrimidin-4-amine (**23)**: yellow solid (45.6 mg, 71% yield), m.p. 130.0-130.6 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 8.32 (d, *J*= 8.0 Hz, 2H), 7.29 (d, *J*= 8.0 Hz, 2H), 7.10 (d, *J*= 8.4 Hz, 2H), 7.04 (d, *J*= 8.4 Hz, 2H), 5.66 (br, 2H), 2.65 (s, 3H), 2.45 (s, 3H), 2.33 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 171.2, 164.5, 163.7, 140.9, 135.9, 134.9, 131.2, 130.2, 129.2, 128.3, 126.4, 104.2, 23.5, 21.6, 21.0.

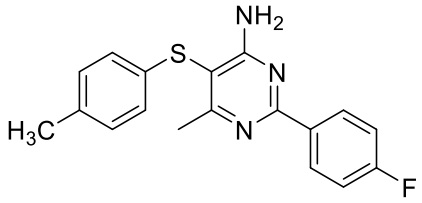
HR-MS (ESI) m/z: Calculated for $C_{19}H_{20}N_3S^+[M + H]^+$: 322.1372. Found:

322.1374.



2-([1,1'-biphenyl]-4-yl)-6-methyl-5-(*p*-tolylthio)pyrimidin-4-amine (**24)**: white solid (49.0 mg, 64% yield), m.p. 153.5-154.2 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 8.46 (d, *J*= 8.8 Hz, 2H), 7.70 (d, *J*= 8.0 Hz, 2H), 7.68 (t, *J*= 7.2 Hz, 2H), 7.47 (t, *J*= 8.0 Hz, 2H), 7.37 (t, *J*= 8.0 Hz, 1H), 7.07 (d, *J*= 8.0 Hz, 2H), 7.02 (d, *J*= 8.0 Hz, 2H), 5.59 (br, 2H), 2.64 (s, 3H), 2.30 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 171.2, 164.4, 163.4, 143.3, 140.7, 136.6, 136.0, 131.1, 130.2, 128.9, 128.8, 127.7, 127.2, 127.1, 126.5, 23.5, 21.0.

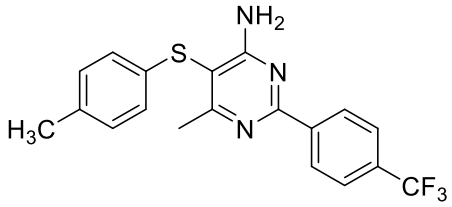
HR-MS (ESI) m/z: Calculated for $C_{24}H_{22}N_3S^+[M + H]^+$: 384.1529. Found: 384.1532.



2-(4-fluorophenyl)-6-methyl-5-(*p*-tolylthio)pyrimidin-4-amine (**25)**: yellow solid (23.4 mg, 36% yield), m.p. 146.2-147.4 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 8.41-8.38 (m, 2H), 7.14-7.10 (m, 2H), 7.06 (d, *J*= 8.4 Hz, 2H), 7.00 (d, *J*= 8.0 Hz, 2H), 5.58 (br, 2H), 2.60 (s, 3H), 2.29 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 171.2, 164.7 (d, J=248.8 Hz), 164.4, 162.7, 136.1, 133.8 (d, J=3.0Hz), 133.2, 131.0, 130.5 (d, J= 8.6 Hz),

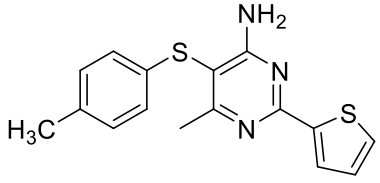
130.2, 126.5, 120.1, 115.3 (d, J= 21.4 Hz), 104.6, 23.5, 21.0. **^{19}F NMR** (471 MHz, $CDCl_3$) δ (ppm) 62.6.

HR-MS (ESI) m/z: Calculated for $C_{18}H_{17}FN_3S^+[M + H]^+$: 326.1122. Found: 326.1125.



6-methyl-5-(*p*-tolylthio)-2-(4-(trifluoromethyl)phenyl)pyrimidin-4-amine (**26)**: yellow solid (45.0 mg, 60% yield), m.p. 145.9-146.5 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 8.50 (d, *J*= 8.4 Hz, 2H), 7.70 (d, *J*= 8.4 Hz, 2H),7.08 (d, *J*= 8.4 Hz, 2H), 7.02 (d, *J*= 8.4 Hz, 2H), 5.66 (br, 2H), 2.63 (s, 3H), 2.30 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 171.3, 164.4, 162.2, 141.0, 139.7, 136.3, 132.1 (d, J= 32.0Hz) 130.7, 130.2, 127.6 (q, J= 274.5 Hz), 125.3 (q, J= 37.7 Hz), 122.9, 105.7, 23.5, 21.0. **^{19}F NMR** (471 MHz, $CDCl_3$) δ (ppm) 110.5.

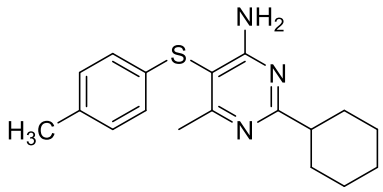
HR-MS (ESI) m/z: Calculated for $C_{19}H_{17}F_3N_3S^+[M + H]^+$: 376.1090. Found: 376.1091.



6-methyl-2-(thiophen-2-yl)-5-(*p*-tolylthio)pyrimidin-4-amine (**27)**: yellow solid (55.1 mg, 88% yield), m.p. 138.5- 138.8 ℃.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.94 (d, *J*= 0.4 Hz, 1H), 7.12-7.10 (dd, *J*1= 4.0 Hz,

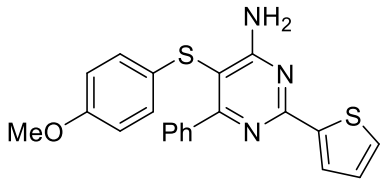
*J*2= 5.2 Hz, 1H), 7.06 (d, *J*= 8.0 Hz, 2H), 6.99 (d, *J*= 8.4 Hz, 2H), 5.66 (br, 2H), 2.57 (s, 3H), 2.29 (s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ (ppm) 171.3, 164.2, 160.2, 143.4, 136.0, 131.1, 130.1, 129.8, 129.1, 128.1, 126.4, 104.0, 23.3, 21.0.

HR-MS (ESI) m/z: Calculated for $C_{16}H_{16}N_3S_2^+[M + H]^+$: 314.0780. Found: 314.0783.



2-cyclohexyl-6-methyl-5-(*p*-tolylthio)pyrimidin-4-amine (**28)** : white solid (21.3 mg, 34% yield), m.p. 133.6-134.4 °C.**^{1}H NMR** (400 MHz, $CDCl_3$) δ (ppm) 7.06 (d, *J*= 7.6 Hz, 2H), 6.96 (d, *J*= 8.4 Hz, 2H), 5.48 (br, 2H), 2.64 (t, *J*= 12.0 Hz, 1H), 2.52 (s, 3H), 2.29 (s, 3H), 1.95 (d, *J*= 12.4 Hz, 2H), 1.83 (d, *J*= 12.0 Hz, 2H), 1.62-1.53(m, 2H), 1.42-1.25(m, 4H); **^{13}C NMR** (125 MHz, $CDCl_3$) δ (ppm) 174.0, 170.6, 164.3, 136.0, 131.1, 130.1, 126.5, 103.7, 47.3, 32.0, 26.2, 26.0, 23.1, 21.0.

HR-MS (ESI) m/z: Calculated for $C_{18}H_{24}N_3S^+[M + H]^+$: 314.1685. Found: 314.1683.



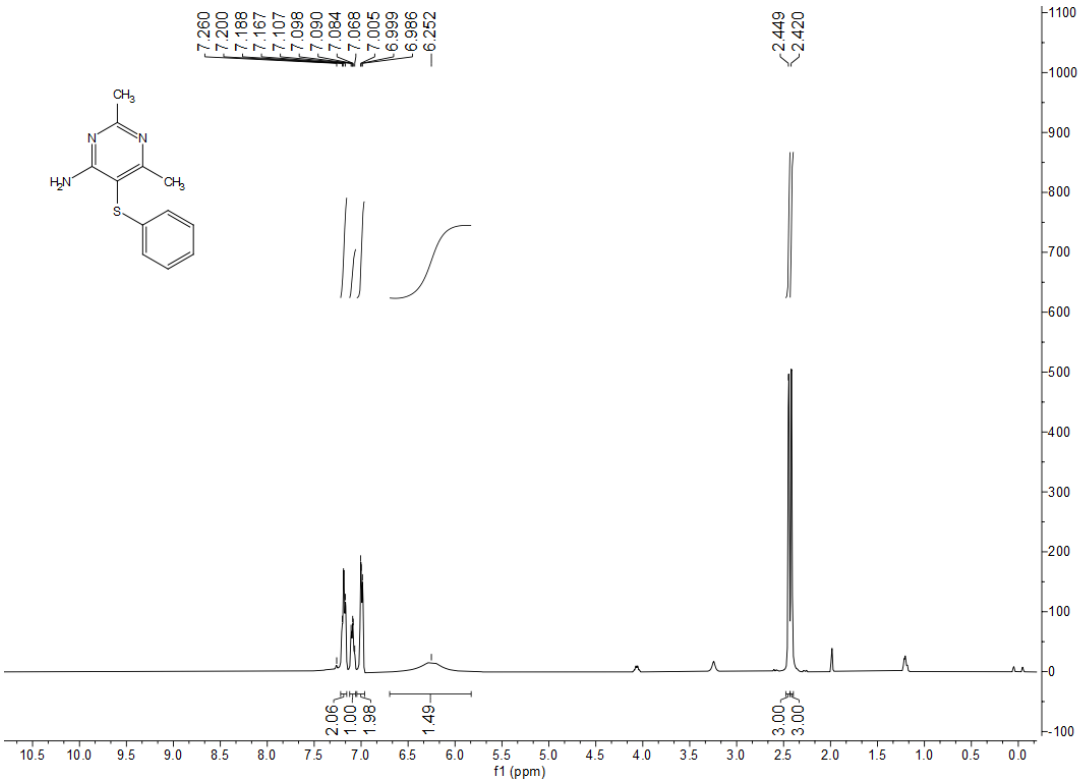
5-((4-methoxyphenyl)thio)-6-phenyl-2-(thiophen-2-yl)pyrimidin-4-amine (29) : white solid (34 mg, 43% yield), m.p. 210.0-210.2 °C.**^{1}H NMR**

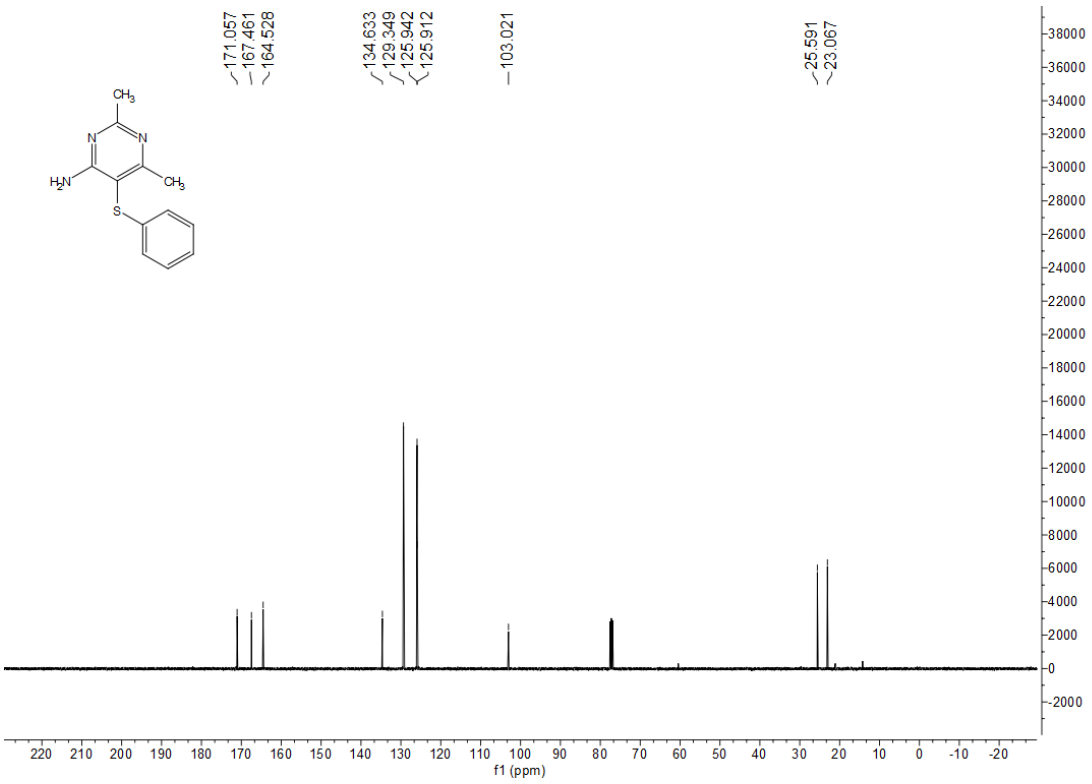
(400 MHz, $CDCl_3$) δ (ppm) 8.01 (d, *J*= 2.4 Hz, 1H), 7.71 (d, *J*= 5.6 Hz, 2H), 7.45 (d, *J*= 3.6 Hz, 1H), 7.43-7.38 (m, 3H), 7.13-7.11 (dd, *J*1= 4.0 Hz, *J*2= 5.2 Hz, 1H), 7.01 (d, *J*= 8.8 Hz, 2H), 6.77 (d, *J*= 8.8 Hz, 2H), 5.70 (br, 2H), 3.75 (s, 3H); **^{13}C NMR** (100 MHz, $CDCl_3$) δ (ppm) 169.7, 164.7, 160.2, 158.6, 143.3, 138.5, 130.0, 129.5, 129.5, 129.4, 128.7, 128.1, 127.8, 125.6, 115.1, 104.2, 55.4.

HR-MS (ESI) m/z: Calculated for $C_{16}H_{16}N_3S_2^+[M + H]^+$: 391.0813. Found: 391.0817.

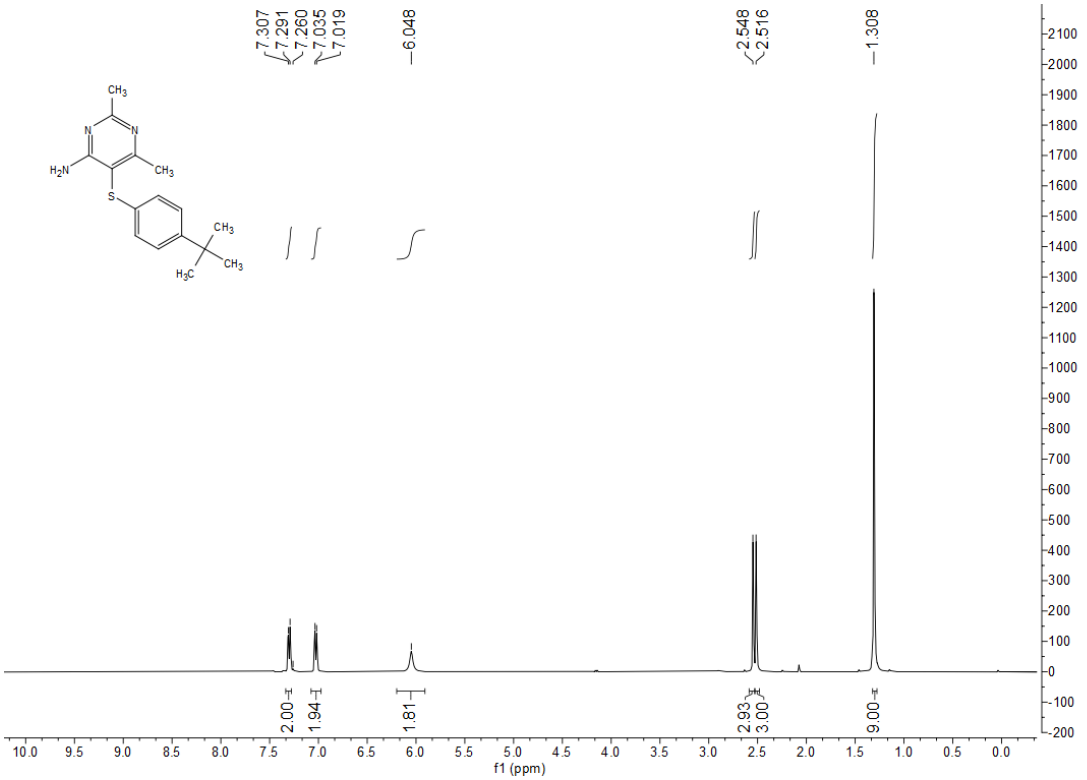
6. ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra

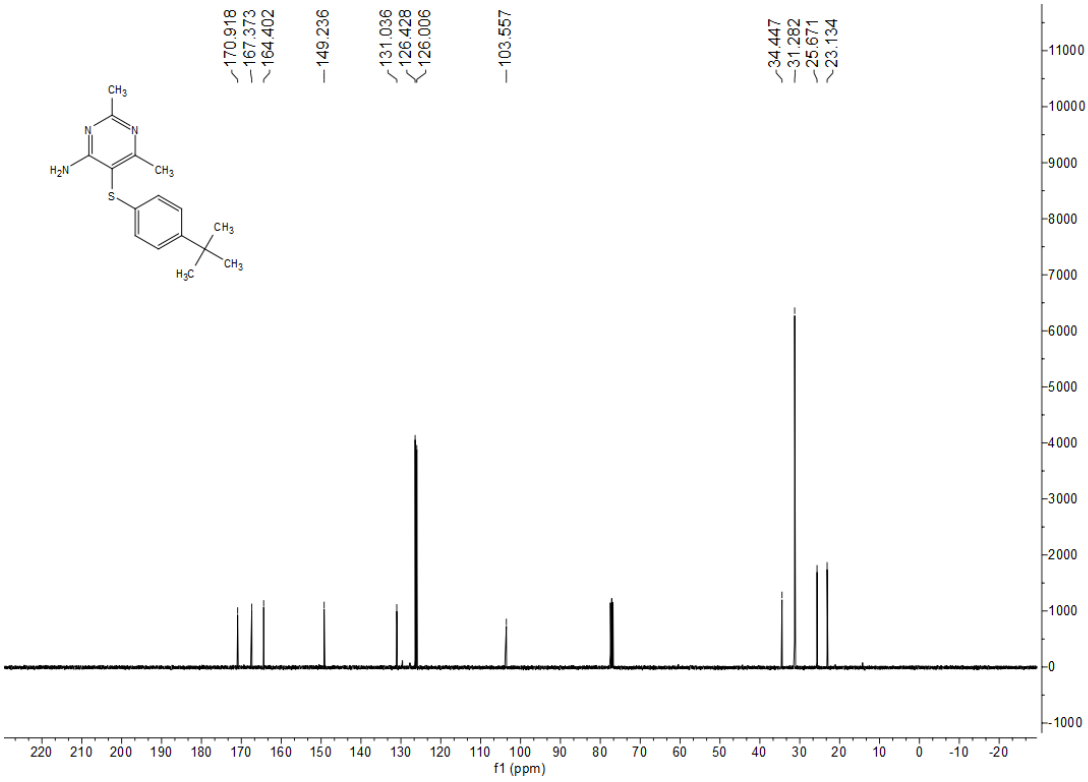
Compound (1)



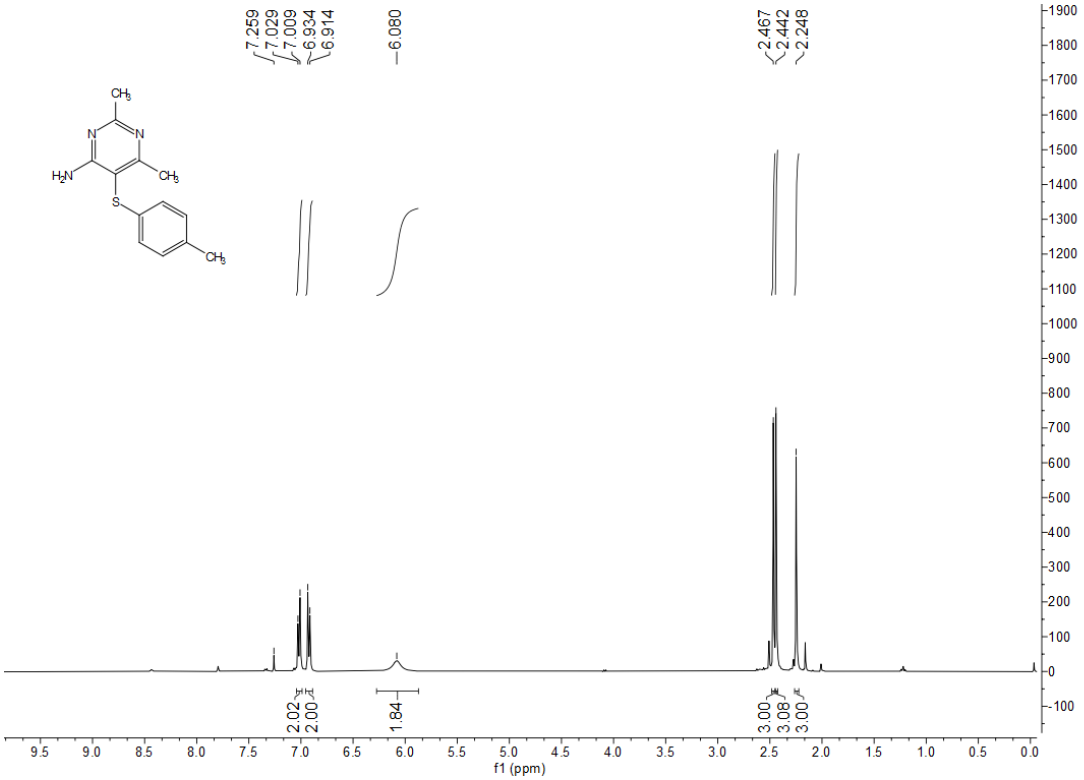


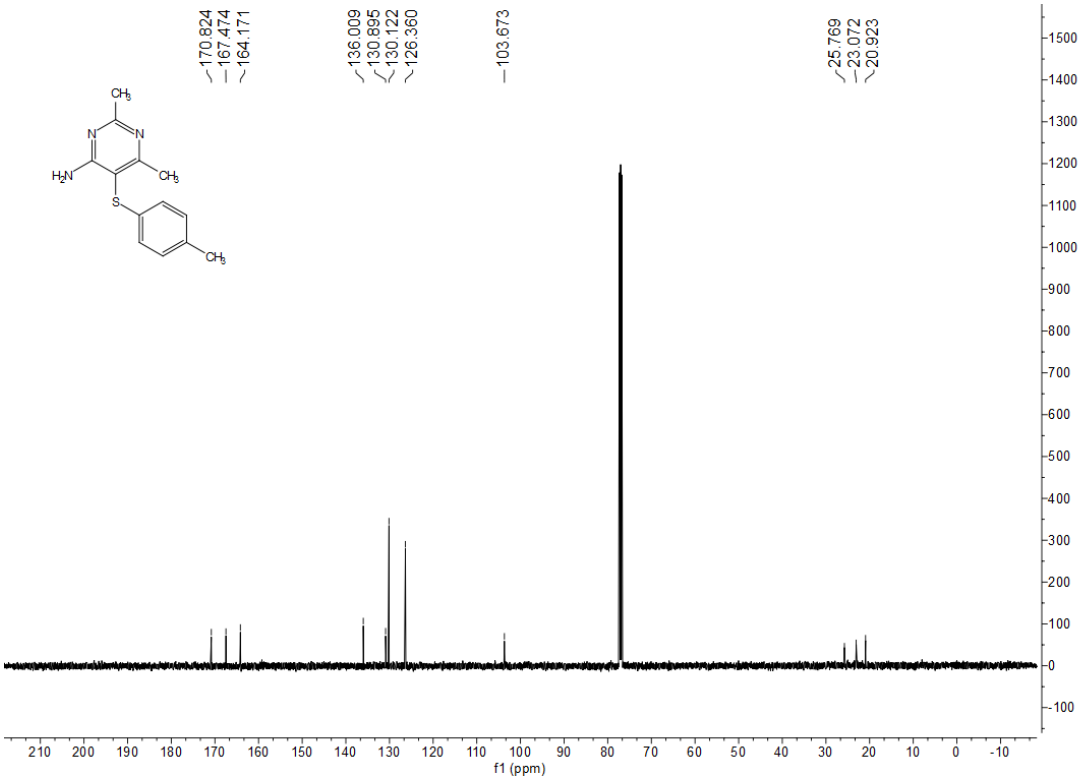
Compound (2)


7.307
7.291
7.260
7.035
7.019
6.048
2.548
2.516
1.308
2.00
1.94
1.81
2.93
3.00
9.00
f1 (ppm)

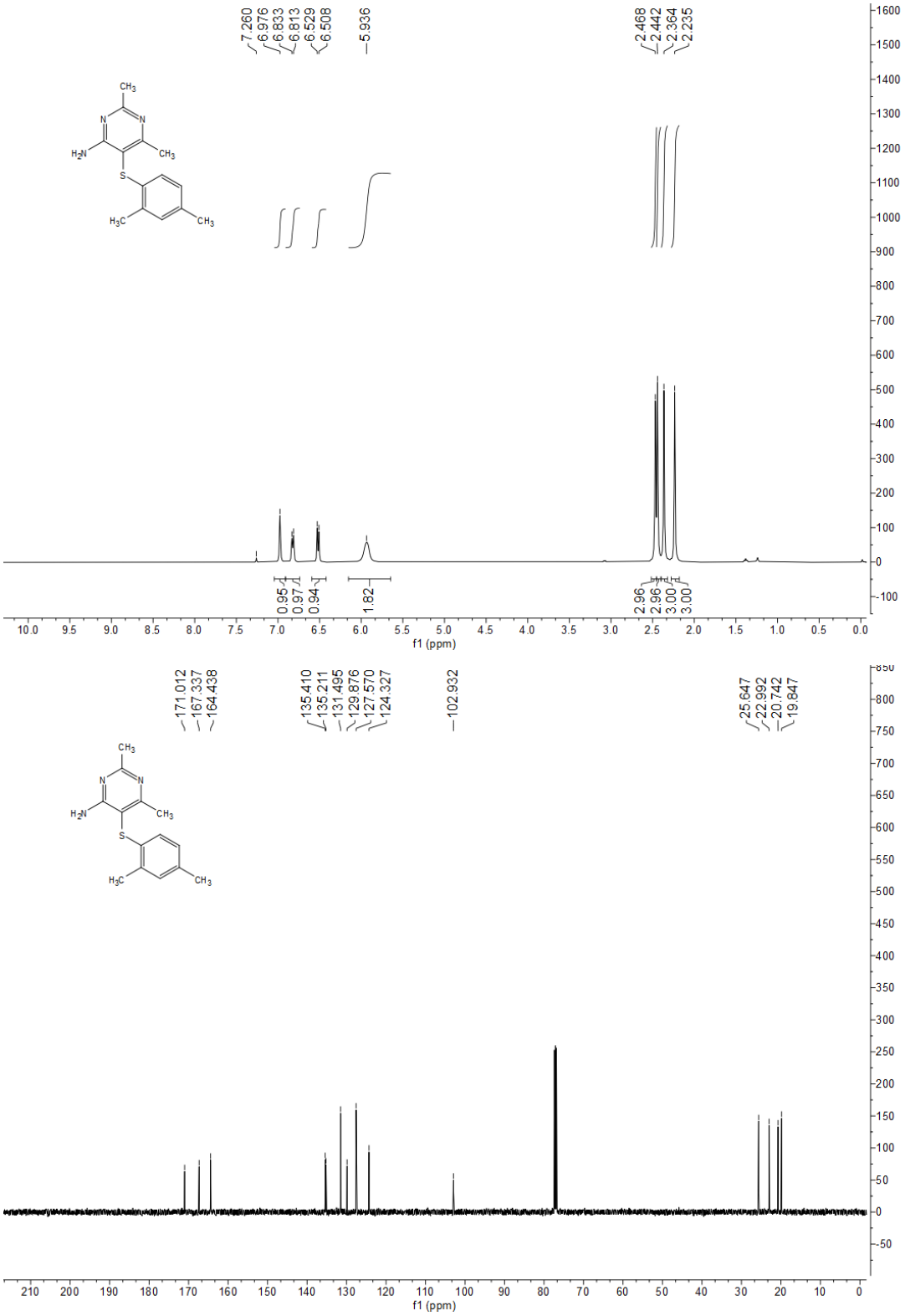

170.918
167.373
164.402
149.236
131.036
126.428
126.006
103.557
34.447
31.282
25.671
23.134
f1 (ppm)

Compound (3)

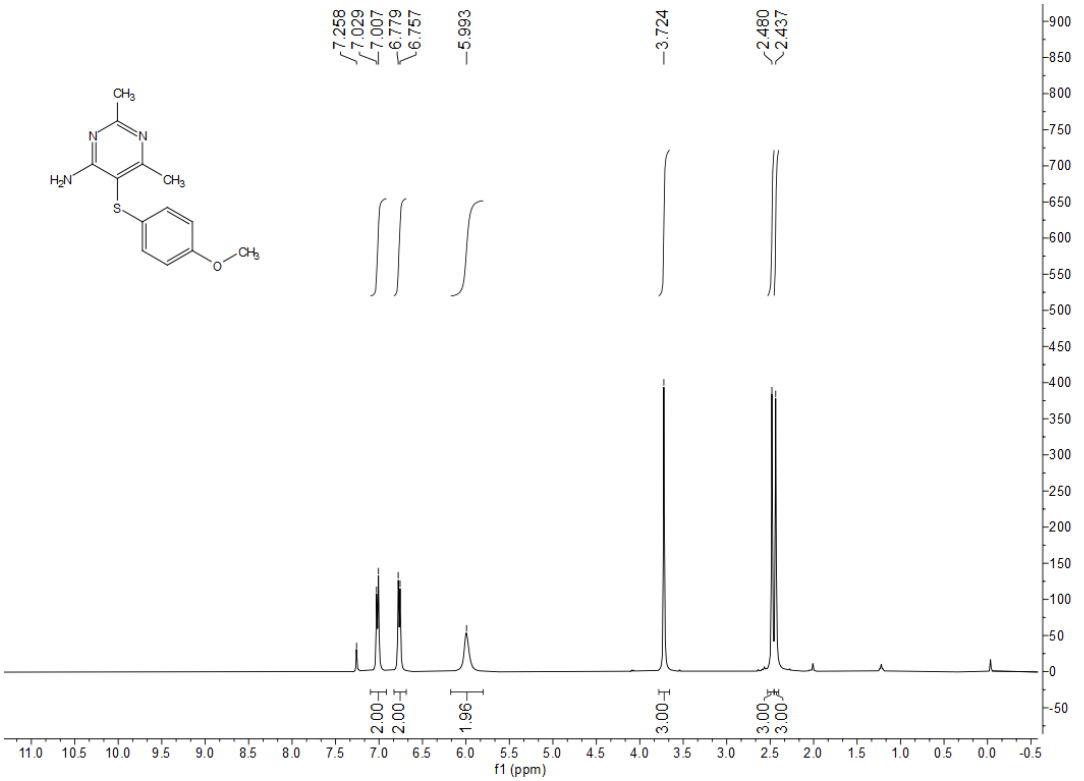

7.259
7.029
7.009
6.934
6.914
6.080
2.467
2.442
2.248
2.02
2.00
1.84
3.00
3.08
3.00
f1 (ppm)

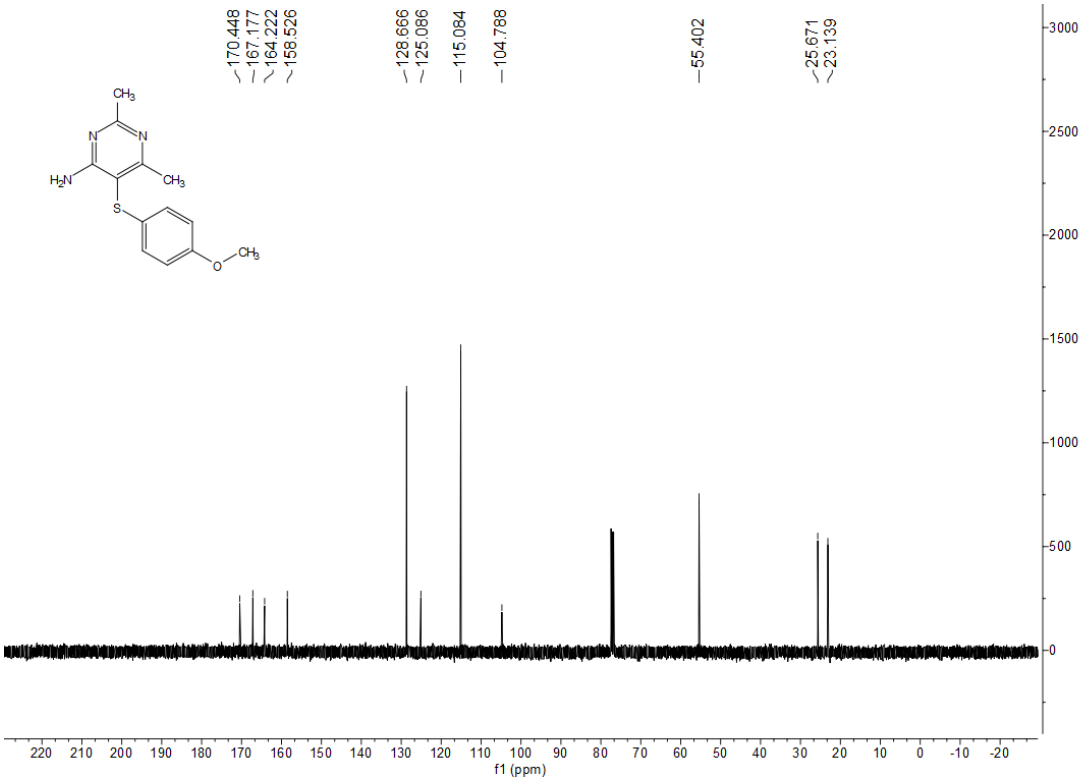

170.824
167.474
164.171
136.009
130.895
130.122
126.360
103.673
25.769
23.072
20.923
f1 (ppm)

Compound (4)

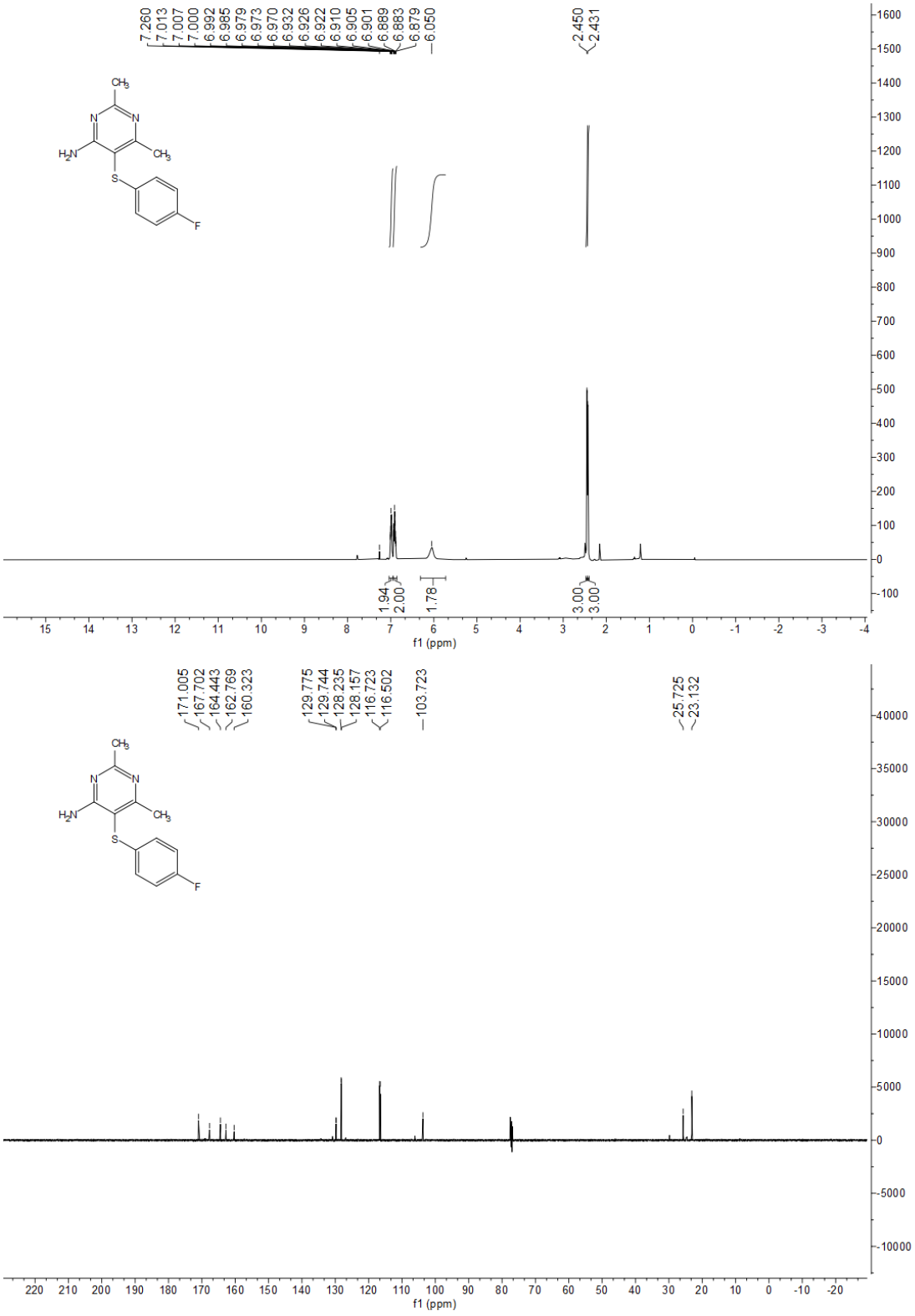

7.260
6.976
6.833
6.813
6.529
6.508
5.936
2.468
2.442
2.364
2.235
0.95
0.97
0.94
1.82
2.96
2.96
3.00
3.00
f1 (ppm)
171.012
167.337
164.438
135.410
135.211
131.495
129.876
127.570
124.327
102.932
25.647
22.992
20.742
19.847
f1 (ppm)

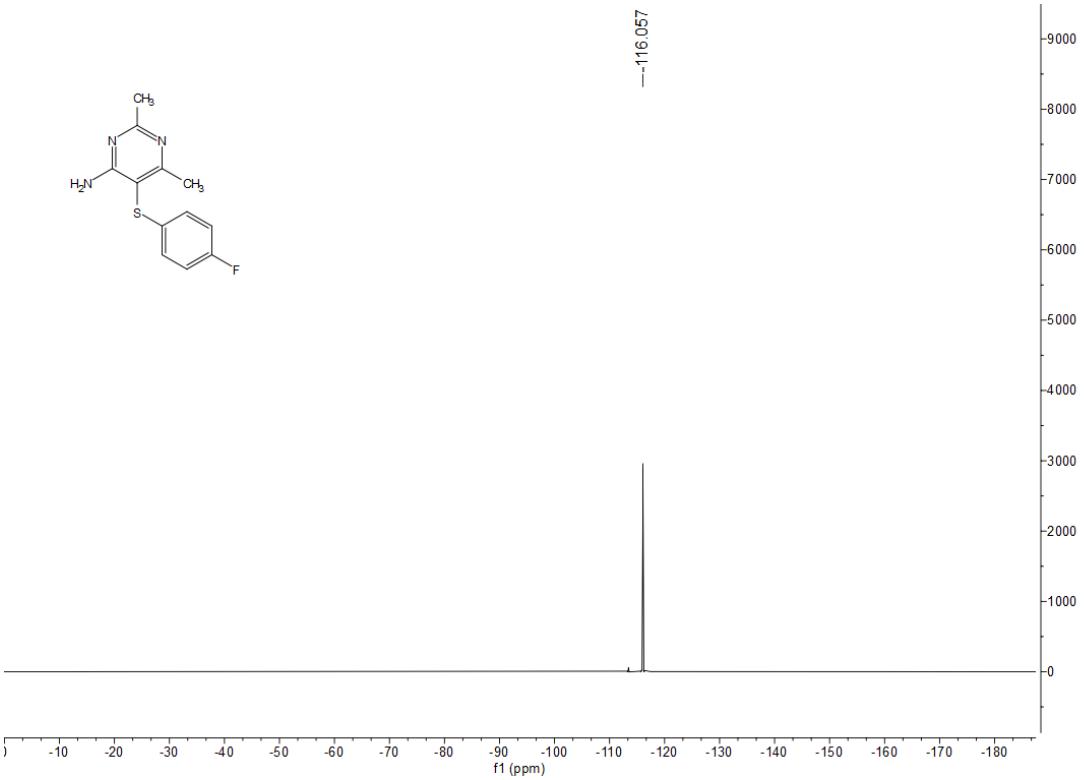
Compound (5)


7.258
7.029
7.007
6.779
6.757
5.993
3.724
2.480
2.437
2.00
2.00
1.96
3.00
3.00
3.00
f1 (ppm)

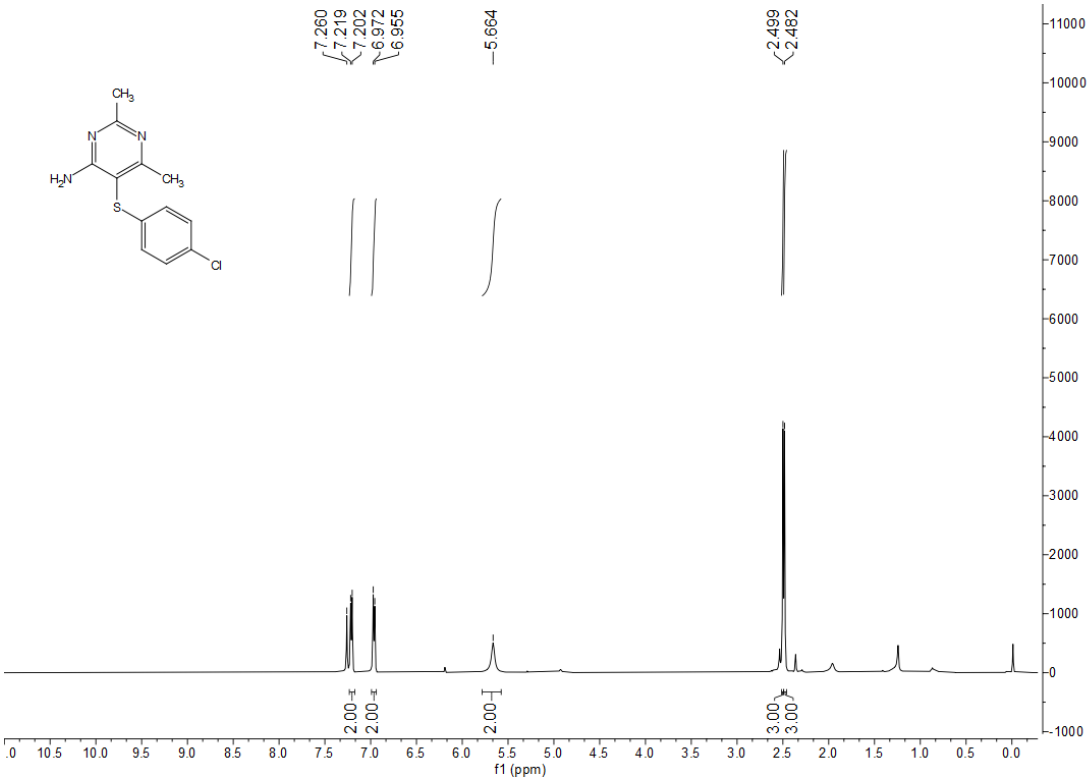

170.448
167.177
164.222
158.526
128.666
125.086
115.084
104.788
55.402
25.671
23.139
f1 (ppm)

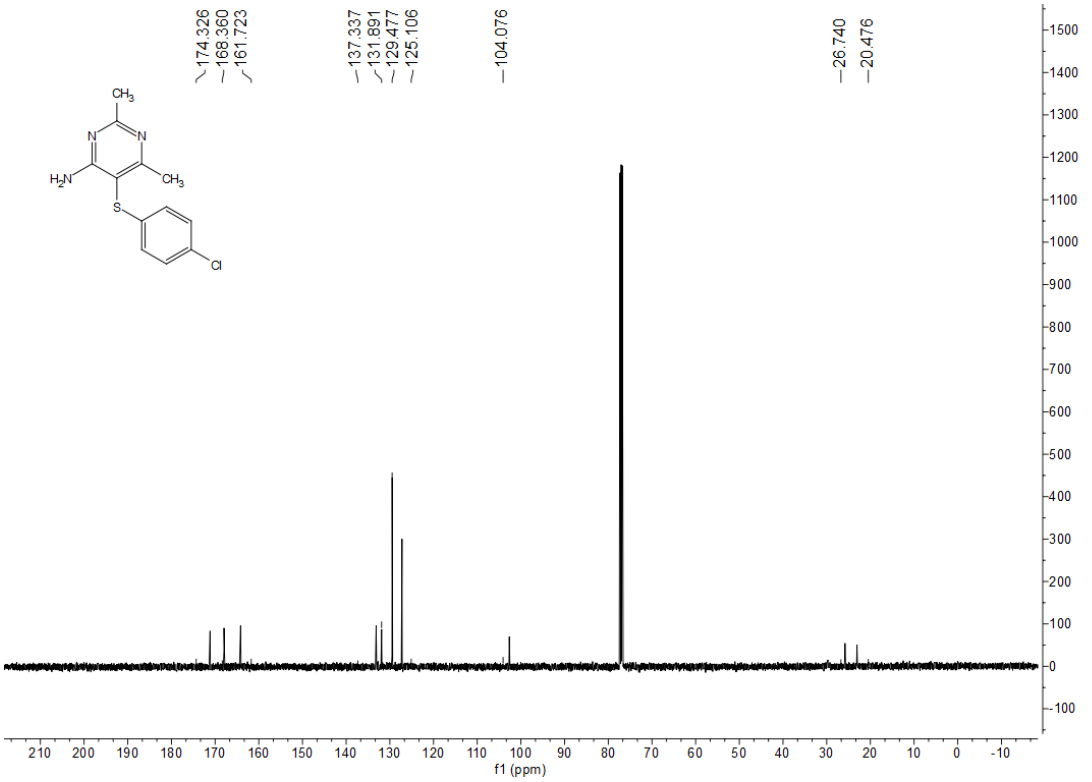
Compound (6)


7.260
7.013
7.007
7.000
6.992
6.985
6.979
6.973
6.970
6.932
6.926
6.922
6.910
6.905
6.901
6.889
6.883
6.879
6.050
2.450
2.431
1.94
2.00
1.78
3.00
3.00
f1 (ppm)
171.005
167.702
164.443
162.769
160.323
129.775
129.744
128.235
128.157
116.723
116.502
103.723
25.725
23.132
f1 (ppm)

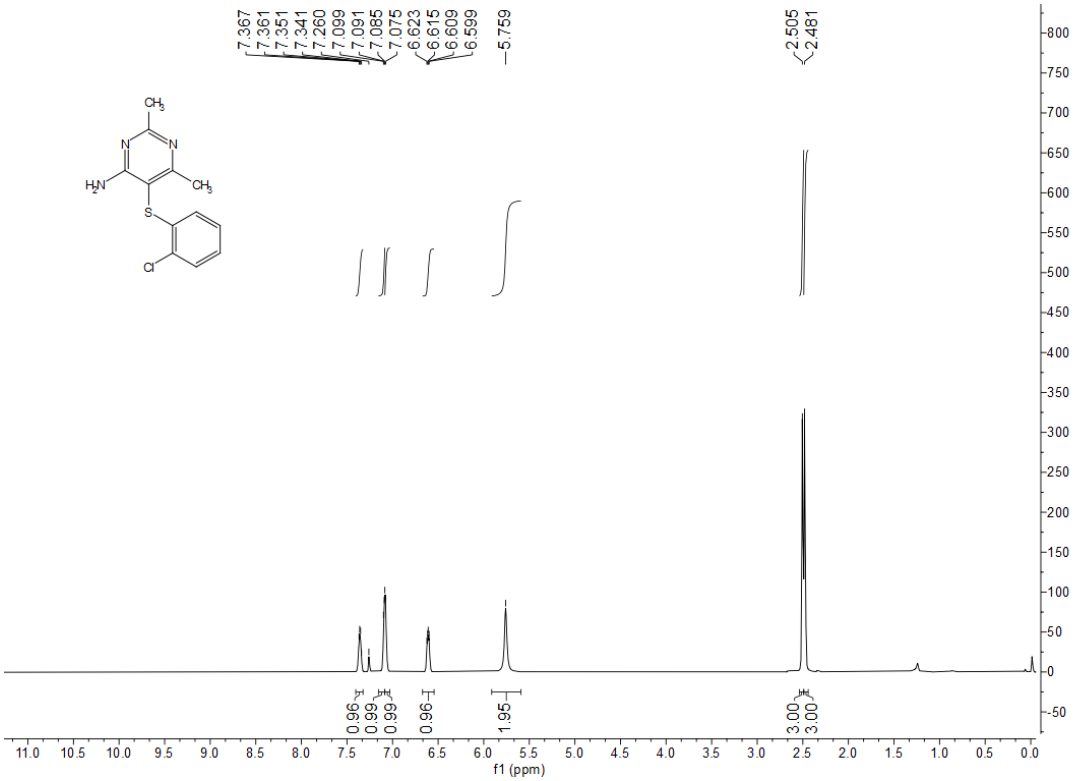

-116.057
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
f1 (ppm)
CH3
N
N
H2N
CH3
S
F

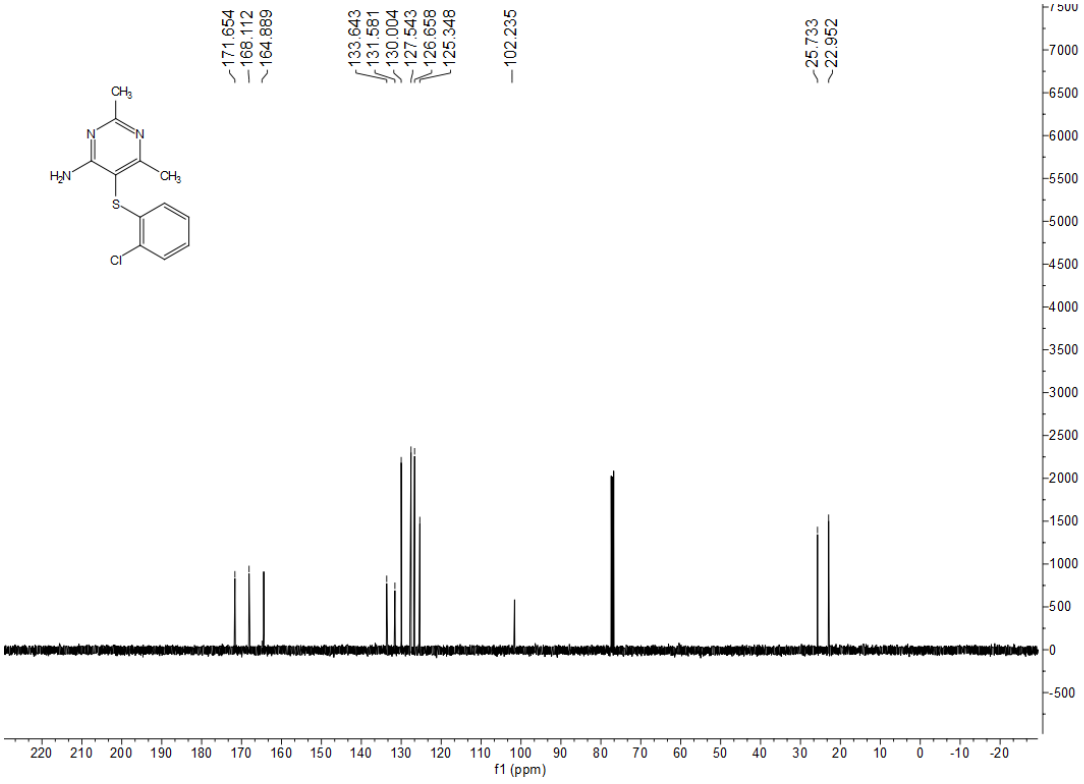
Compound (7)


7.260
7.219
7.202
6.972
6.955
5.664
2.499
2.482
2.00
2.00
2.00
3.00
3.00
f1 (ppm)

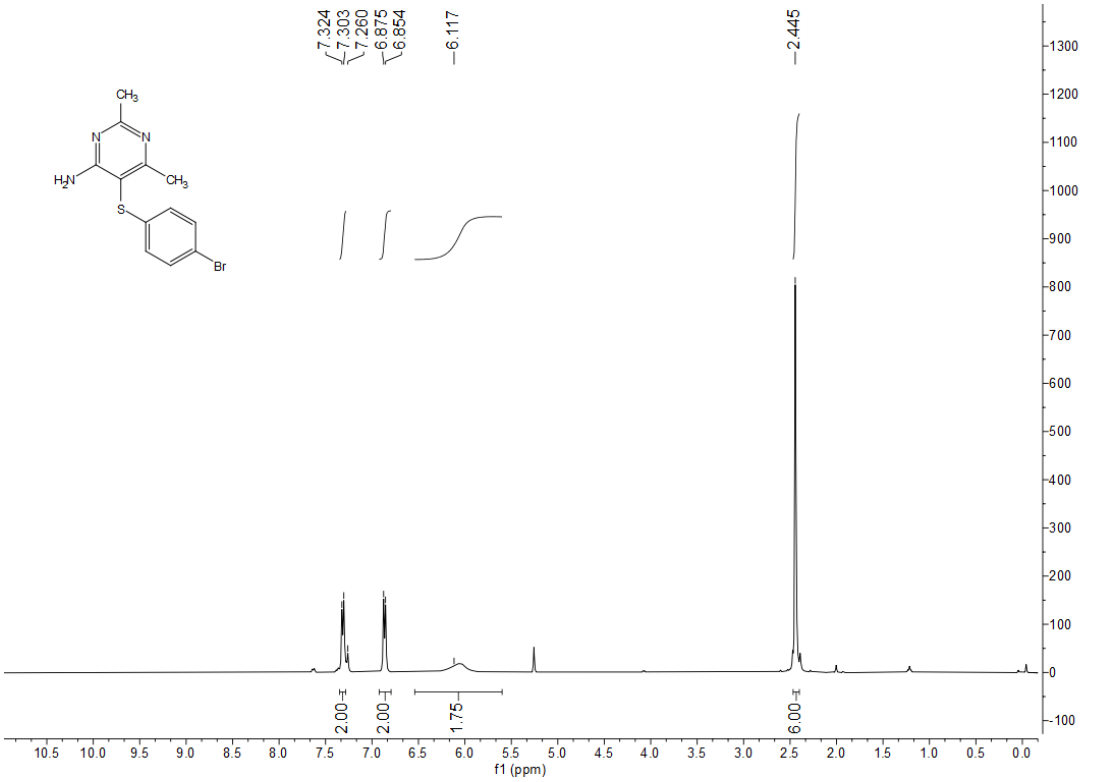

174.326
168.360
161.723
137.337
131.891
129.477
125.106
104.076
26.740
20.476
f1 (ppm)

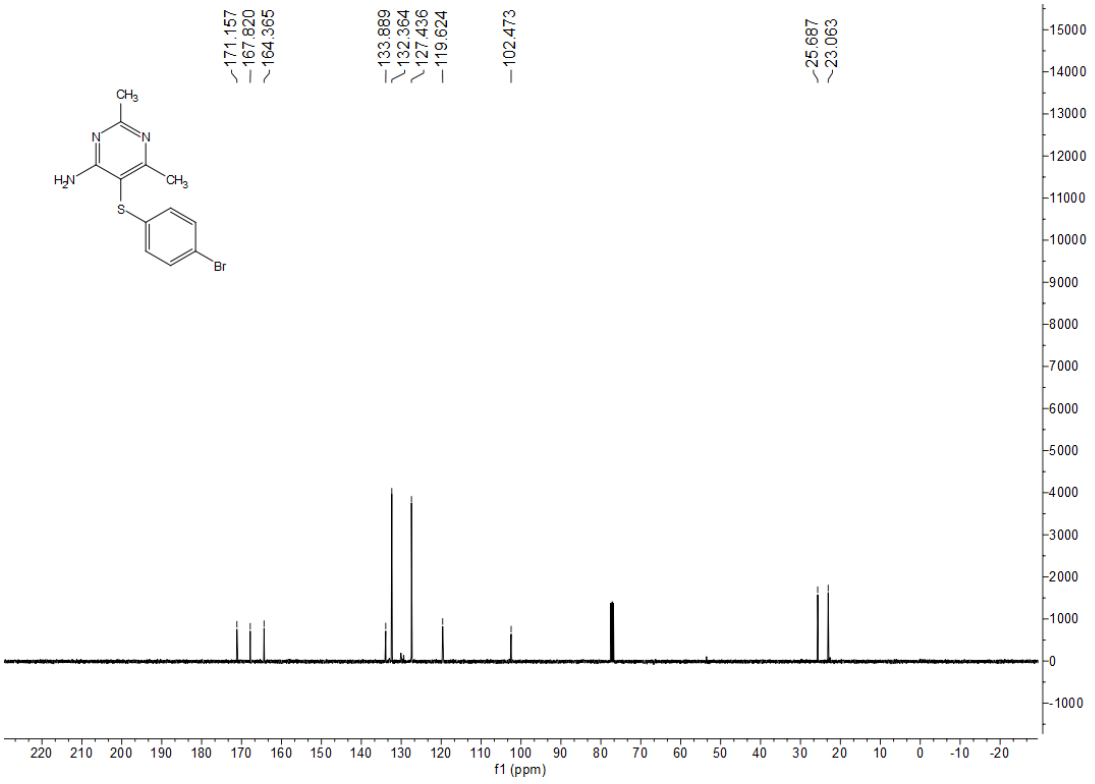
Compound (8)


7.367
7.361
7.351
7.341
7.260
7.099
7.091
7.085
7.075
6.623
6.615
6.609
6.599
5.759
2.505
2.481
0.96
0.99
0.99
0.96
1.95
3.00
3.00
f1 (ppm)

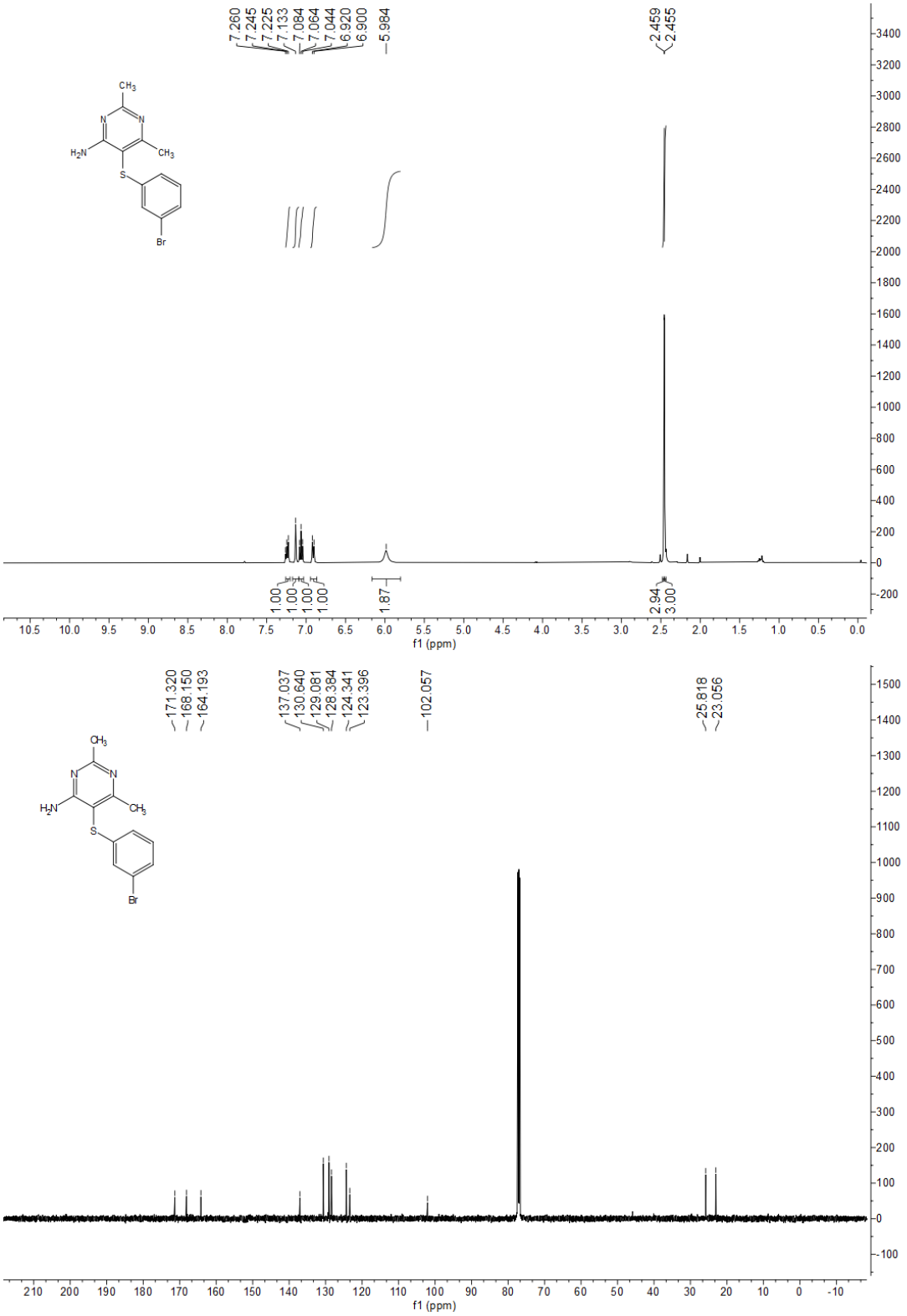

171.654
168.112
164.889
133.643
131.581
130.004
127.543
126.658
125.348
102.235
25.733
22.952
f1 (ppm)

Compound (9)

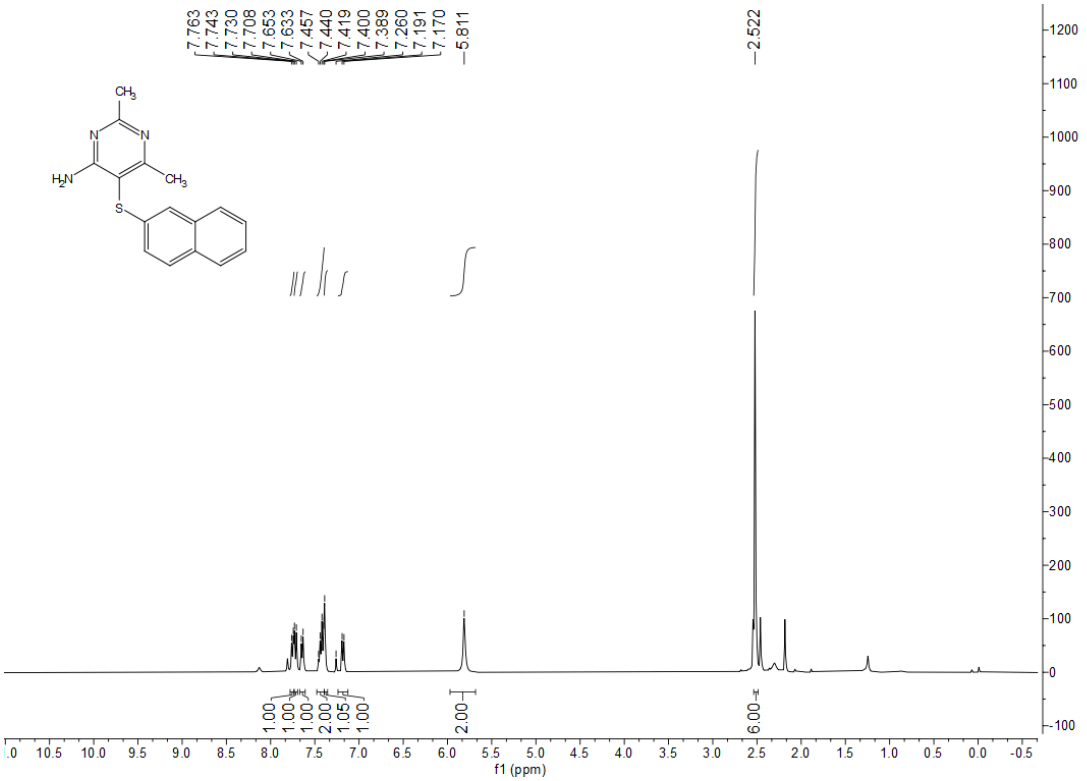

7.324
7.303
7.260
6.875
6.854
6.117
2.445
2.00
2.00
1.75
6.00
f1 (ppm)

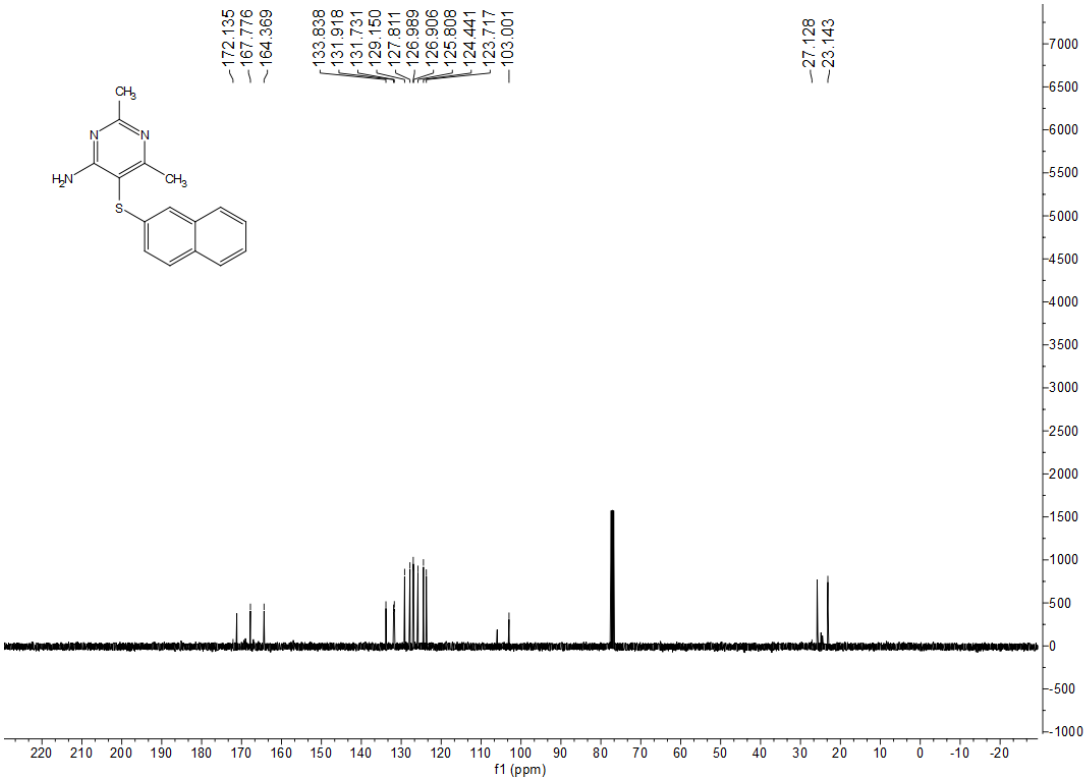

171.157
167.820
164.365
133.889
132.364
127.436
119.624
102.473
25.687
23.063
f1 (ppm)

Compound (10)

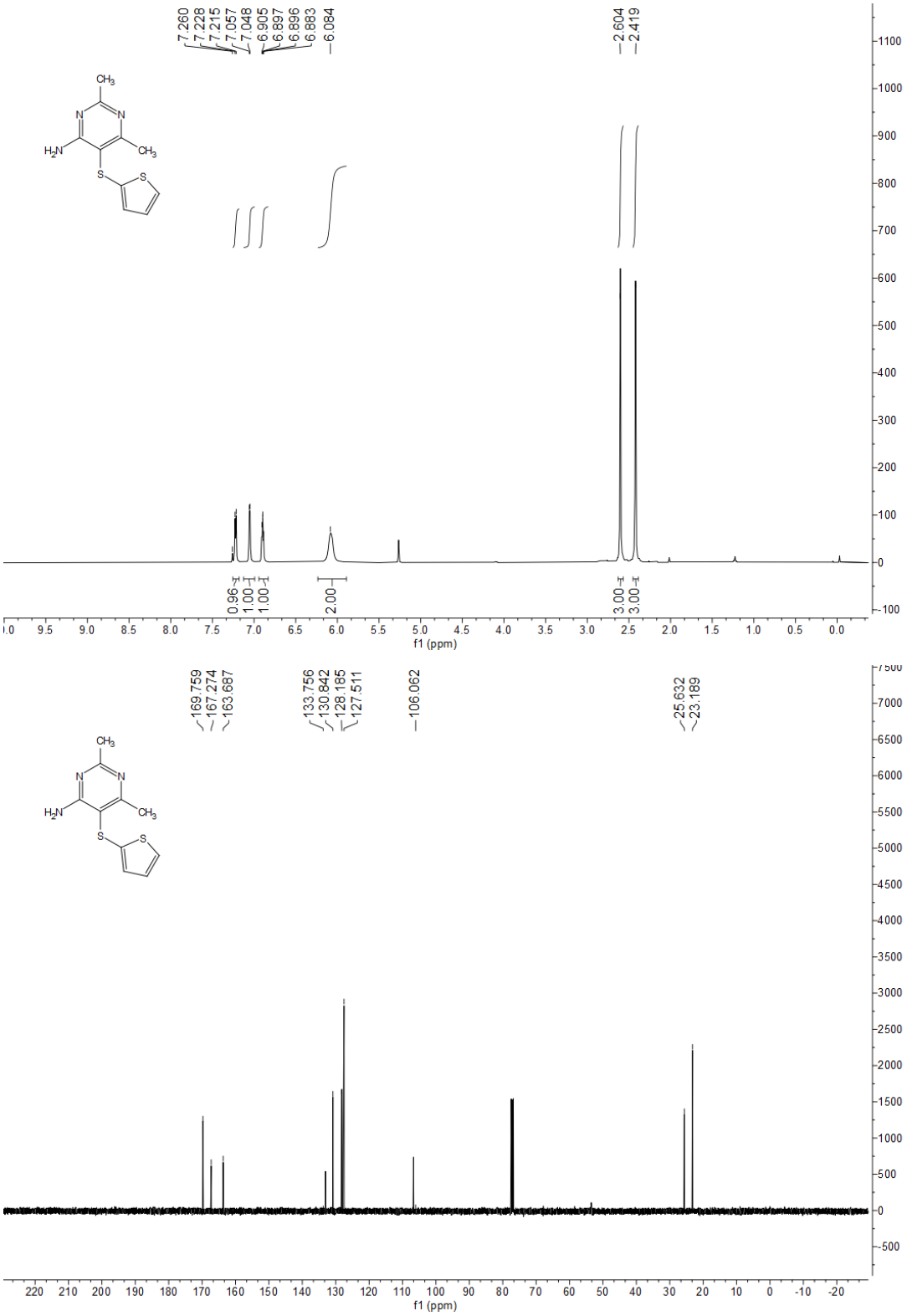

7.260
7.245
7.225
7.133
7.084
7.064
7.044
6.920
6.900
5.984
2.459
2.455
1.00
1.00
1.00
1.00
1.87
2.94
3.00
f1 (ppm)
171.320
168.150
164.193
137.037
130.640
129.081
128.384
124.341
123.396
102.057
25.818
23.056
f1 (ppm)

Compound (11)

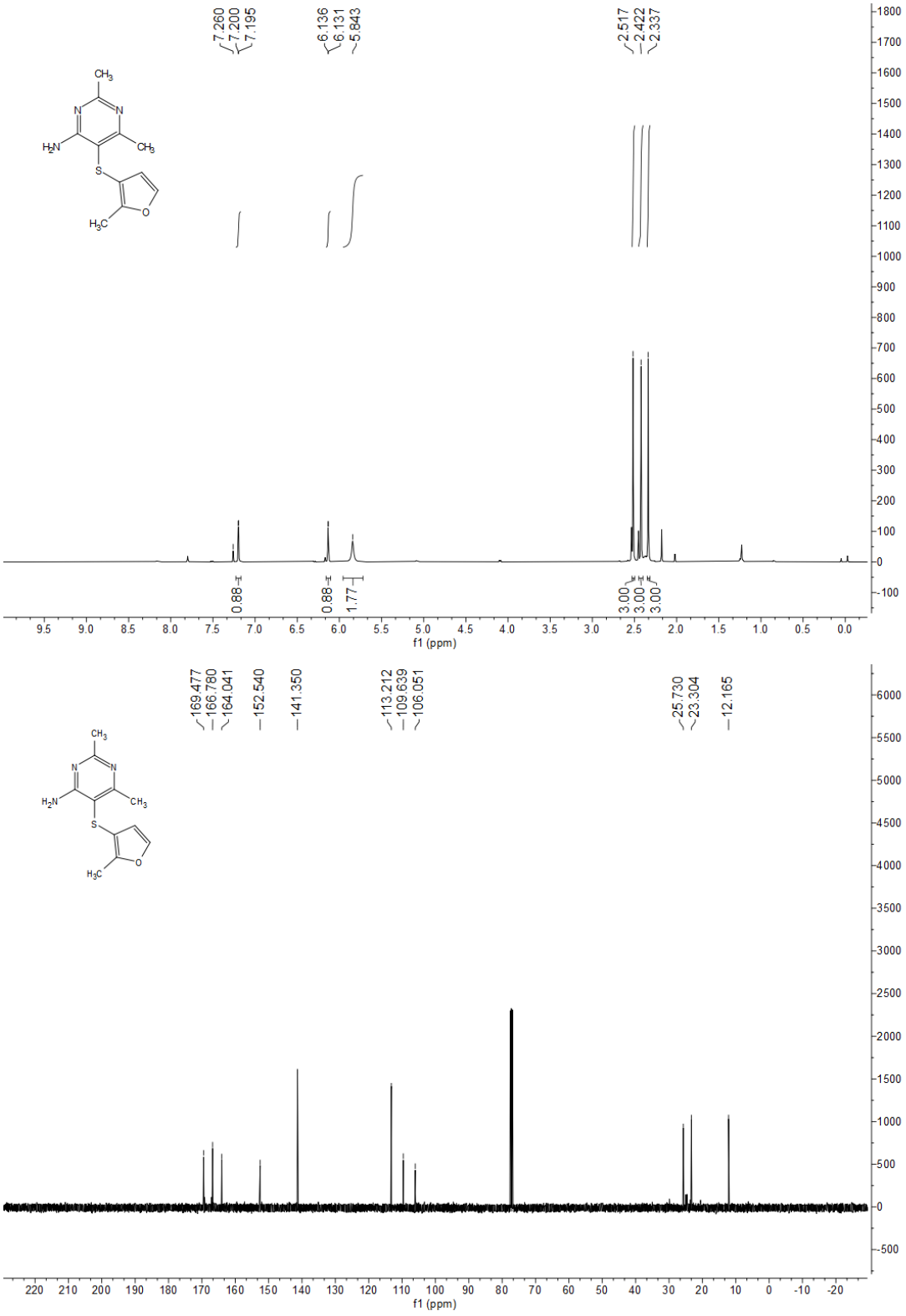

7.763
7.743
7.730
7.708
7.653
7.633
7.457
7.440
7.419
7.400
7.389
7.260
7.191
7.170
5.811
2.522
1.00
1.00
1.00
2.00
1.05
1.00
2.00
6.00
f1 (ppm)


172.135
167.776
164.369
133.838
131.918
131.731
129.150
127.811
126.989
126.906
125.808
124.441
123.717
103.001
27.128
23.143
f1 (ppm)

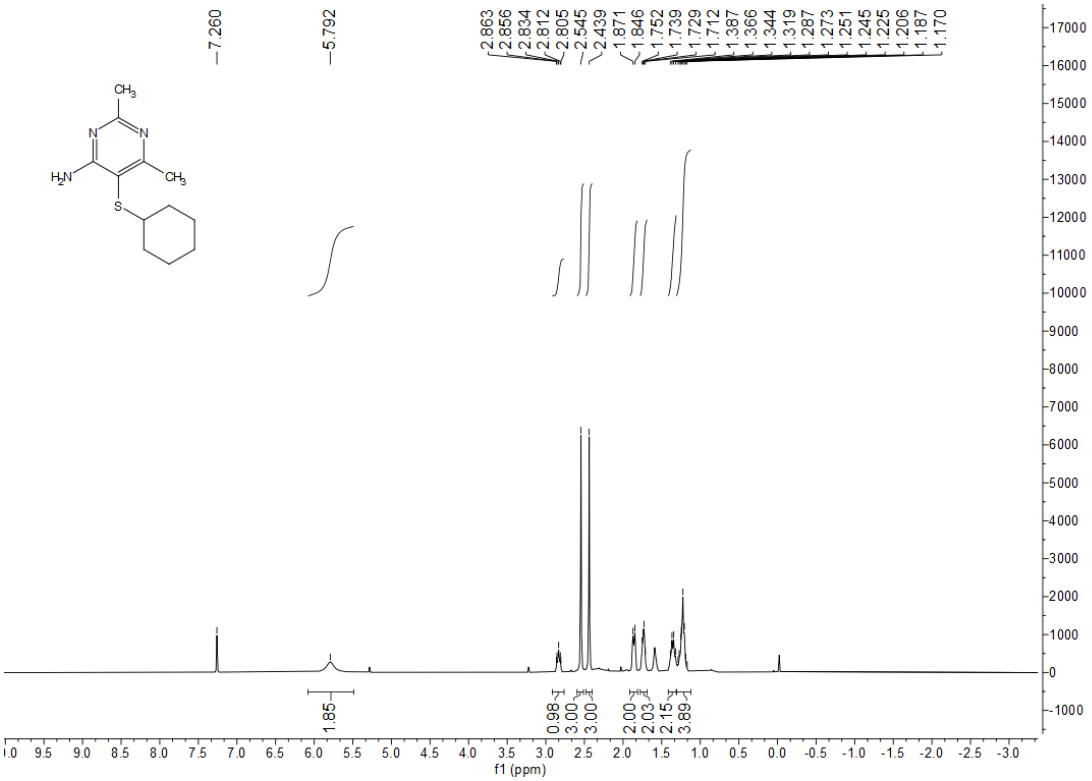
Compound (12)

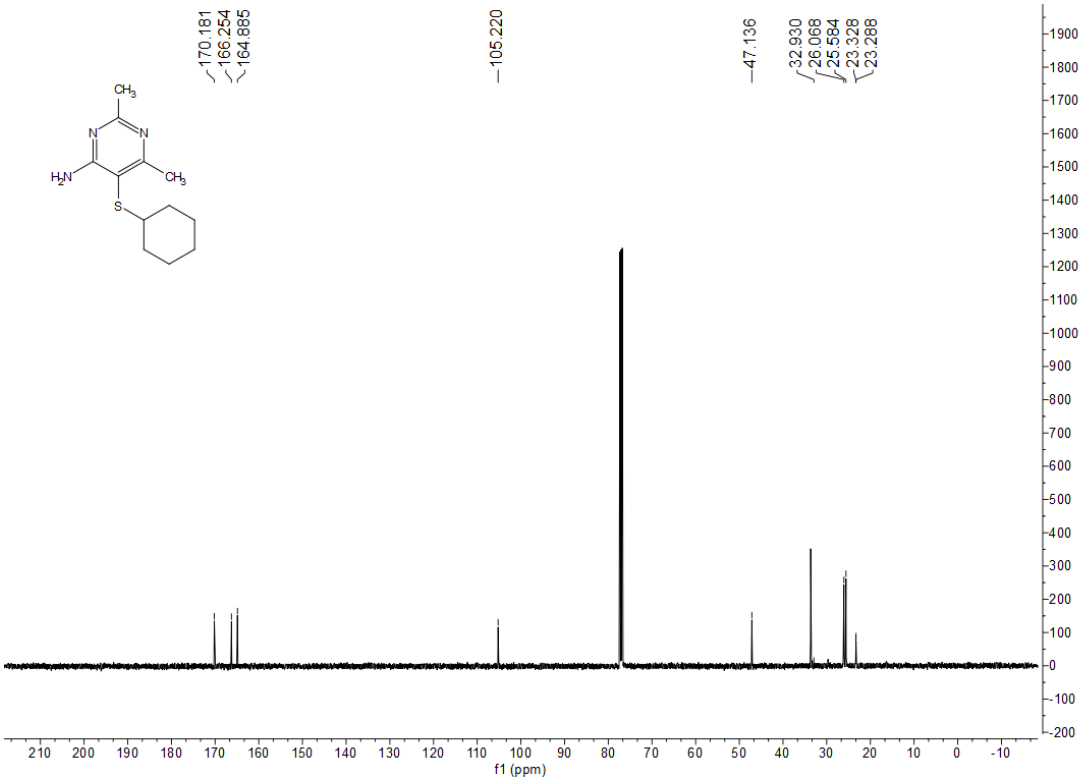

7.260
7.228
7.215
7.057
7.048
6.905
6.897
6.896
6.883
6.084
2.604
2.419
0.96
1.00
1.00
2.00
3.00
3.00
f1 (ppm)
169.759
167.274
163.687
133.756
130.842
128.185
127.511
106.062
25.632
23.189
f1 (ppm)

Compound (13)

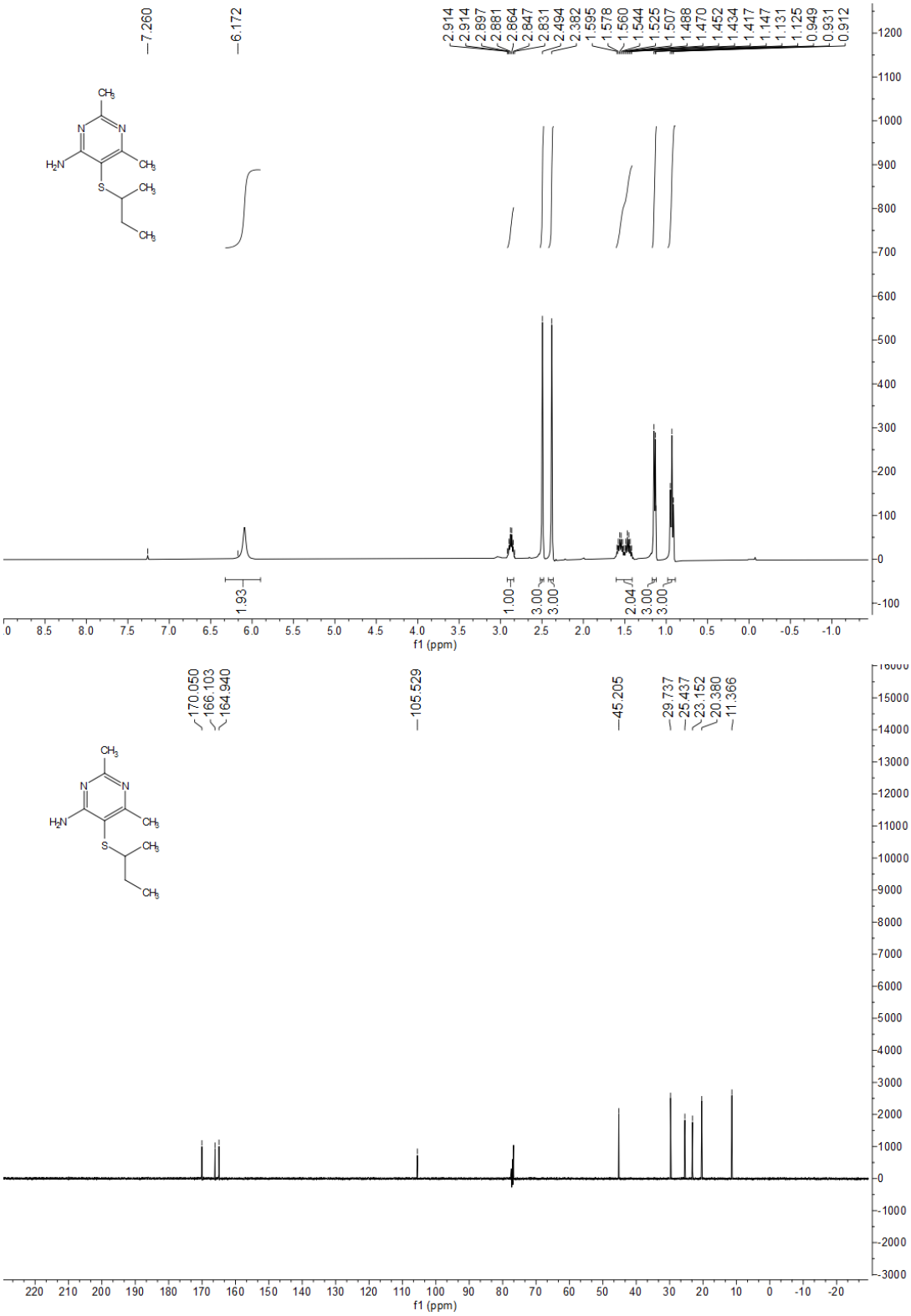

7.260
7.200
7.195
6.136
6.131
5.843
2.517
2.422
2.337
0.88
0.88
1.77
3.00
3.00
3.00
f1 (ppm)
169.477
166.780
164.041
152.540
141.350
113.212
109.639
106.051
25.730
23.304
12.165
f1 (ppm)

Compound (14)

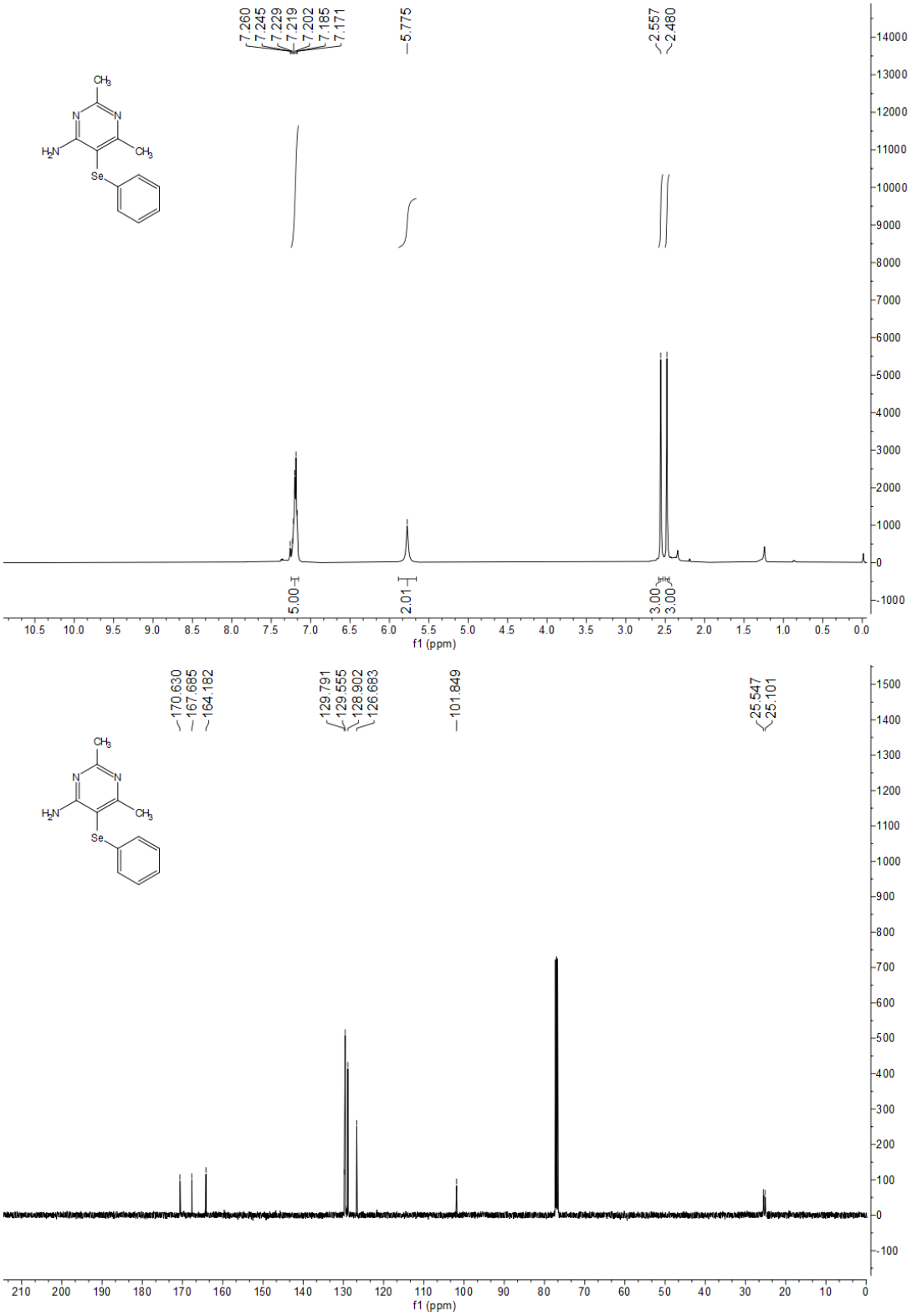

7.260
5.792
2.863
2.856
2.834
2.812
2.805
2.545
2.439
1.871
1.846
1.752
1.739
1.729
1.712
1.387
1.366
1.344
1.319
1.287
1.273
1.251
1.245
1.225
1.206
1.187
1.170
1.85
0.98
3.00
3.00
2.00
2.03
2.15
3.89
f1 (ppm)


170.181
166.254
164.885
105.220
47.136
32.930
26.068
25.584
23.328
23.288
f1 (ppm)

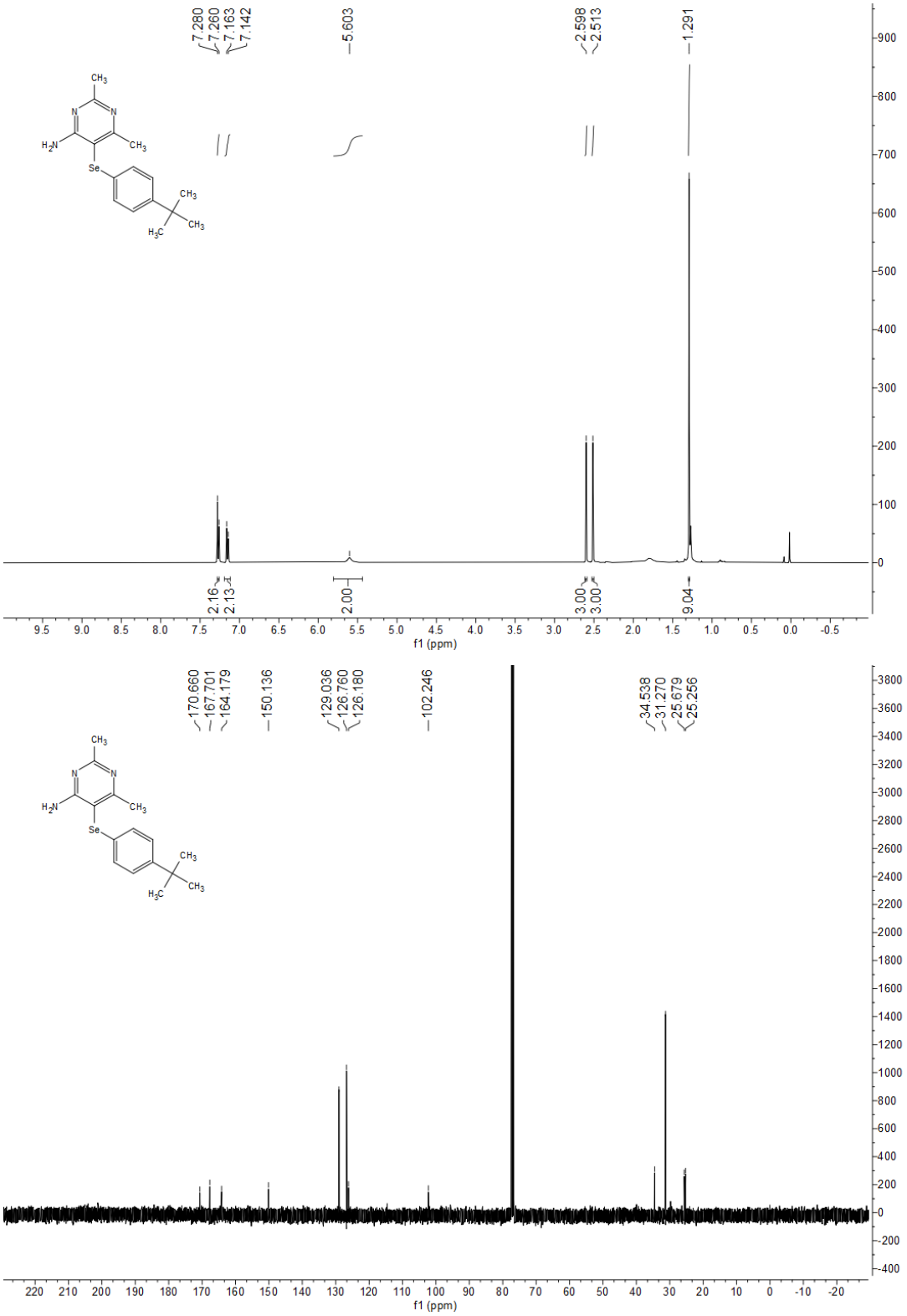
Compound (15)


7.260
6.172
2.914
2.897
2.881
2.864
2.847
2.831
2.494
2.382
1.595
1.578
1.560
1.544
1.525
1.507
1.488
1.470
1.452
1.434
1.417
1.147
1.131
1.125
0.949
0.931
0.912
1.93
1.00
3.00
3.00
2.04
3.00
3.00
f1 (ppm)
170.050
166.103
164.940
105.529
45.205
29.737
25.437
23.152
20.380
11.366
f1 (ppm)

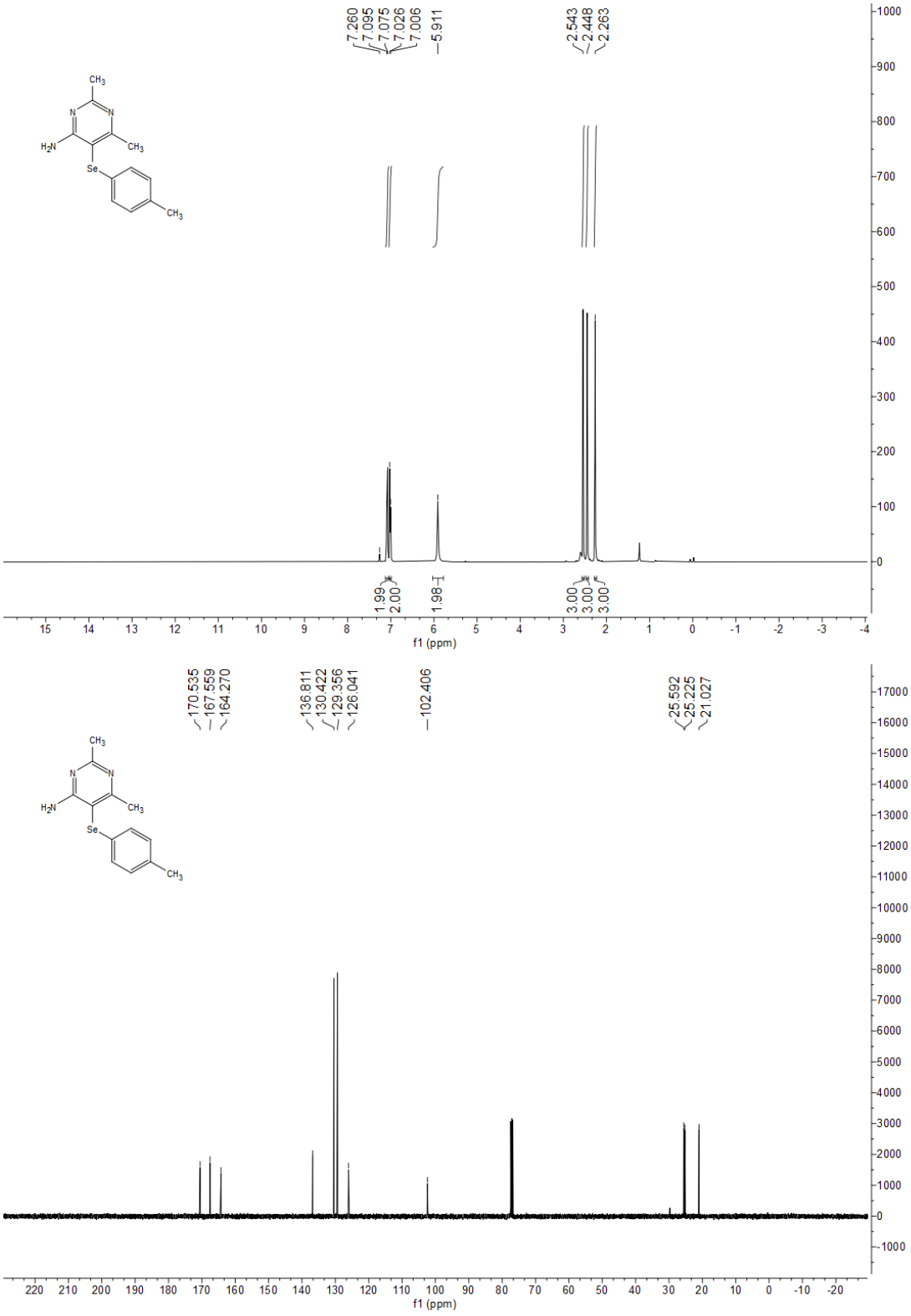
Compound (16)


7.260
7.245
7.229
7.219
7.202
7.185
7.171
5.775
2.557
2.480
5.00
2.01
3.00
3.00
f1 (ppm)
170.630
167.685
164.182
129.791
129.555
128.902
126.683
101.849
25.547
25.101
f1 (ppm)

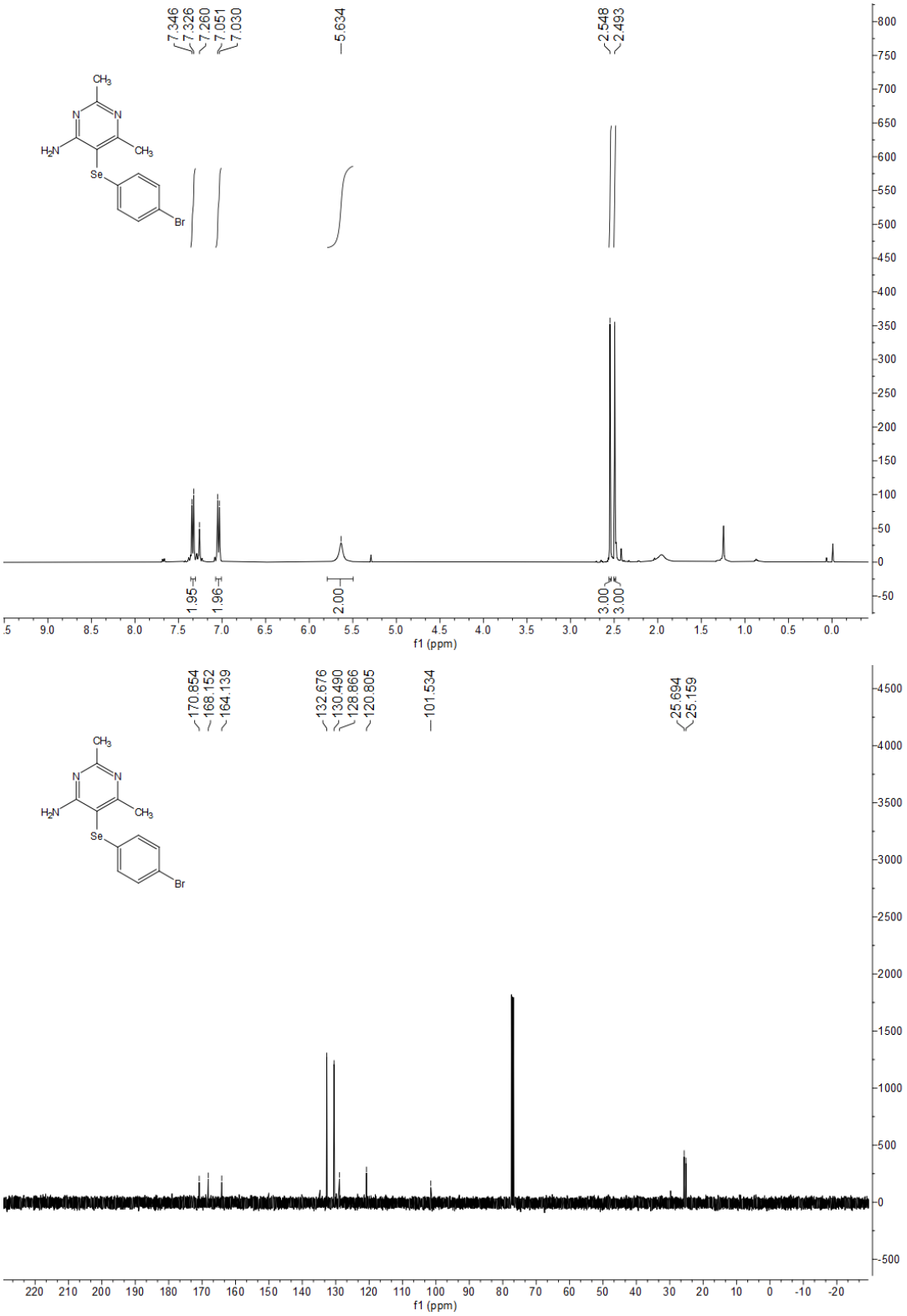
Compound (17)


7.280
7.260
7.163
7.142
5.603
2.598
2.513
1.291
2.16
2.13
2.00
3.00
3.00
9.04
f1 (ppm)
170.660
167.701
164.179
150.136
129.036
126.760
126.180
102.246
34.538
31.270
25.679
25.256
f1 (ppm)

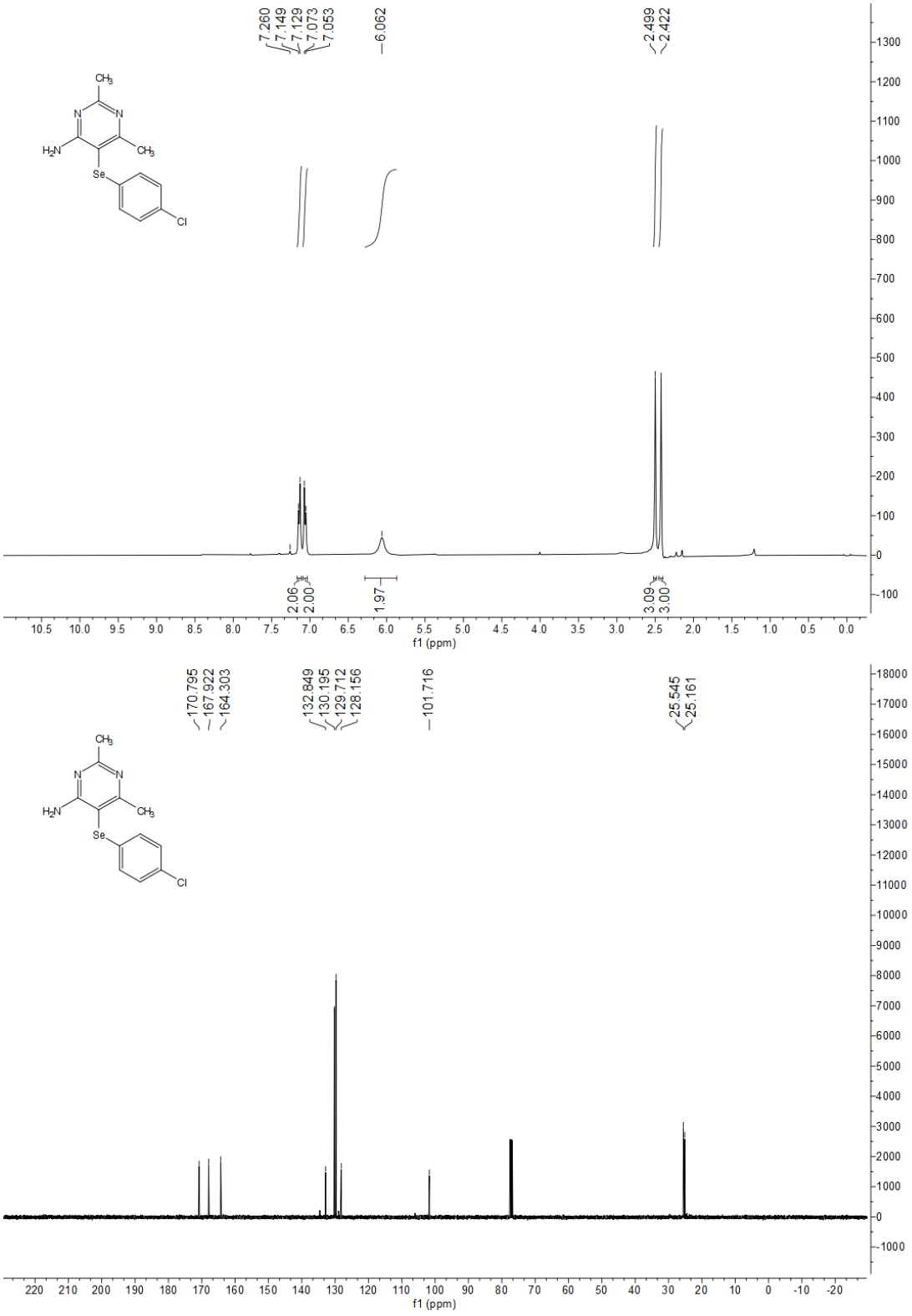
Compound (18)


7.260
7.095
7.075
7.026
7.006
5.911
2.543
2.448
2.263
1.99
2.00
1.98
3.00
3.00
3.00
f1 (ppm)
170.535
167.559
164.270
136.811
130.422
129.356
126.041
102.406
25.592
25.225
21.027
f1 (ppm)

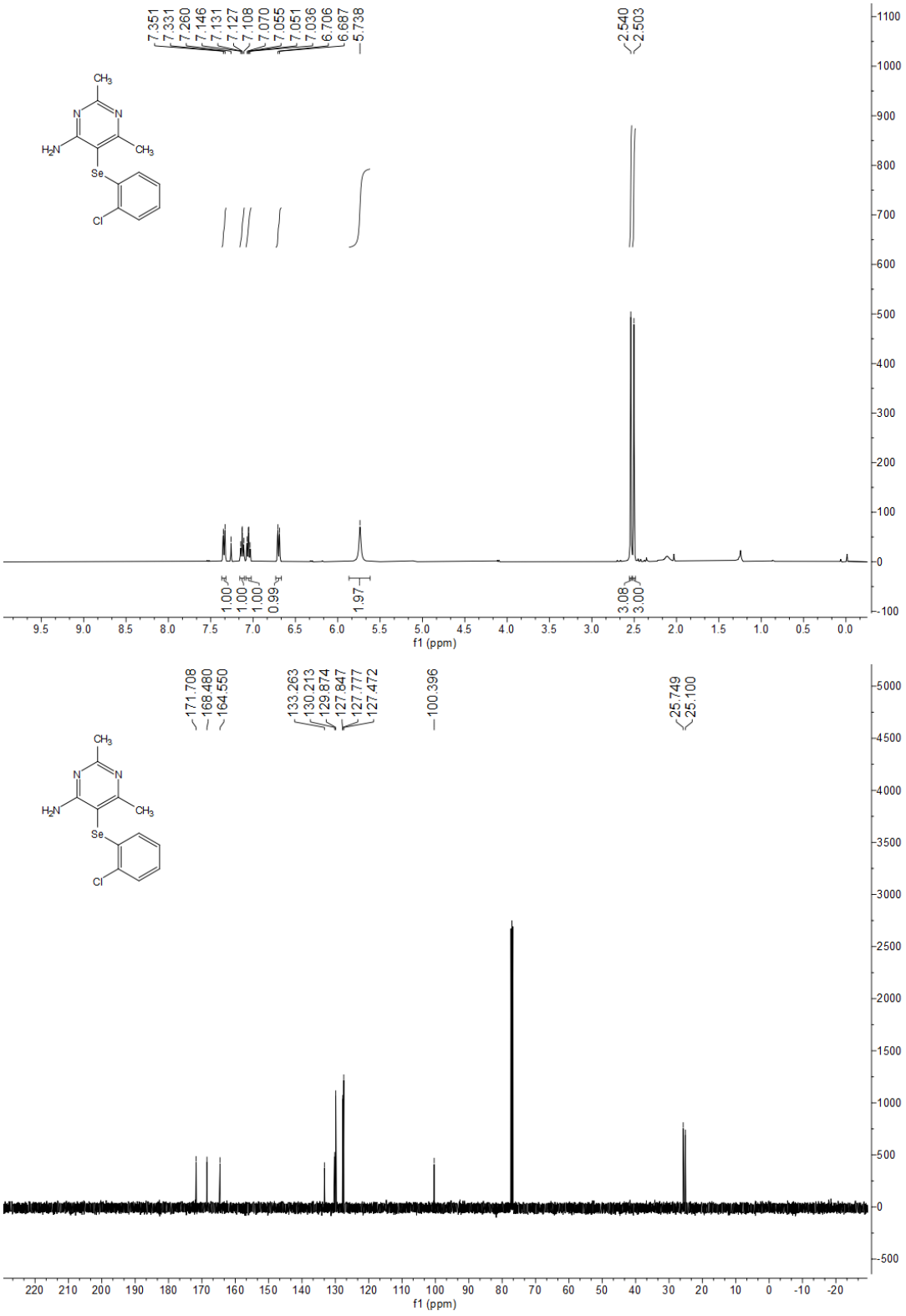
Compound (19)


7.346
7.326
7.260
7.051
7.030
5.634
2.548
2.493
1.95
1.96
2.00
3.00
3.00
f1 (ppm)
170.854
168.152
164.139
132.676
130.490
128.866
120.805
101.534
25.694
25.159
f1 (ppm)

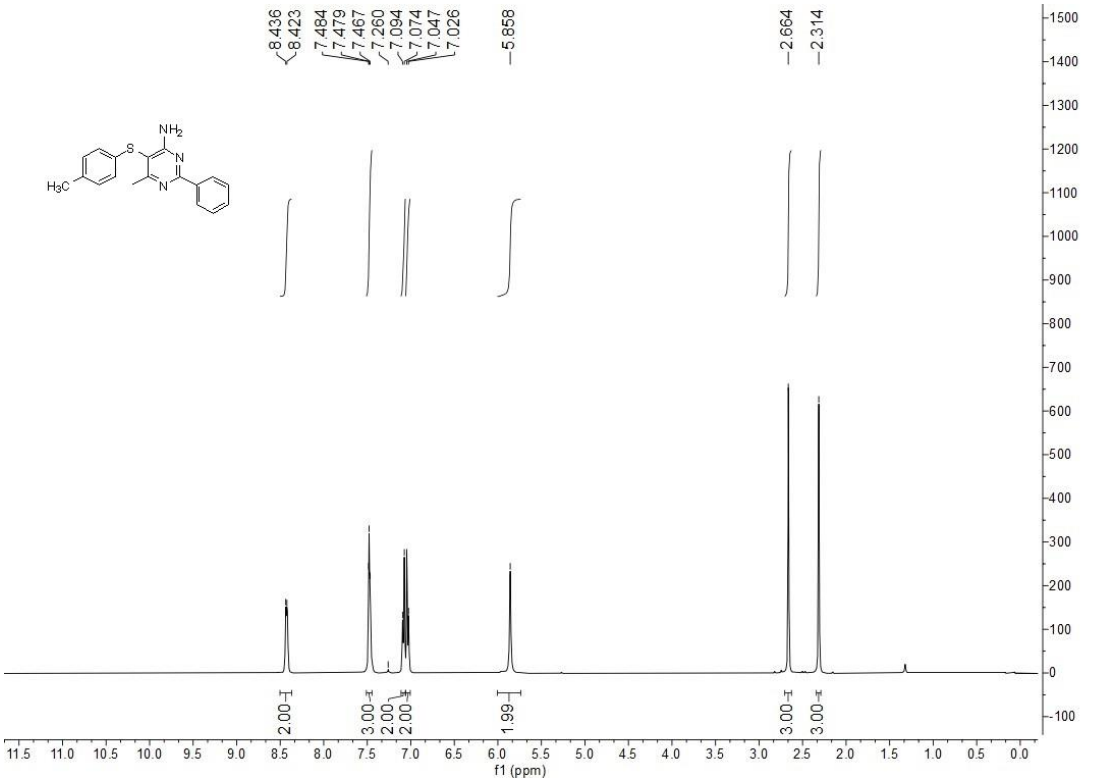
Compound (20)

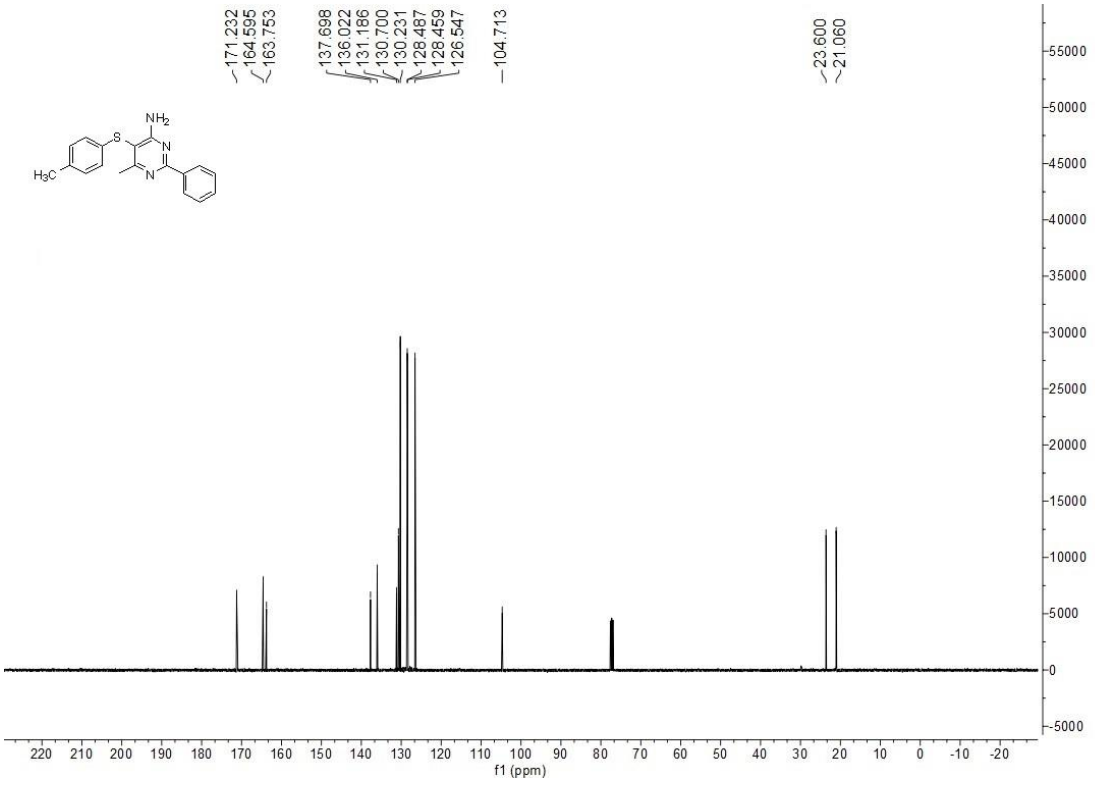

7.260
7.149
7.129
7.073
7.053
6.062
2.499
2.422
2.06
2.00
1.97
3.09
3.00
f1 (ppm)
170.795
167.922
164.303
132.849
130.195
129.712
128.156
101.716
25.545
25.161
f1 (ppm)

Compound (21)

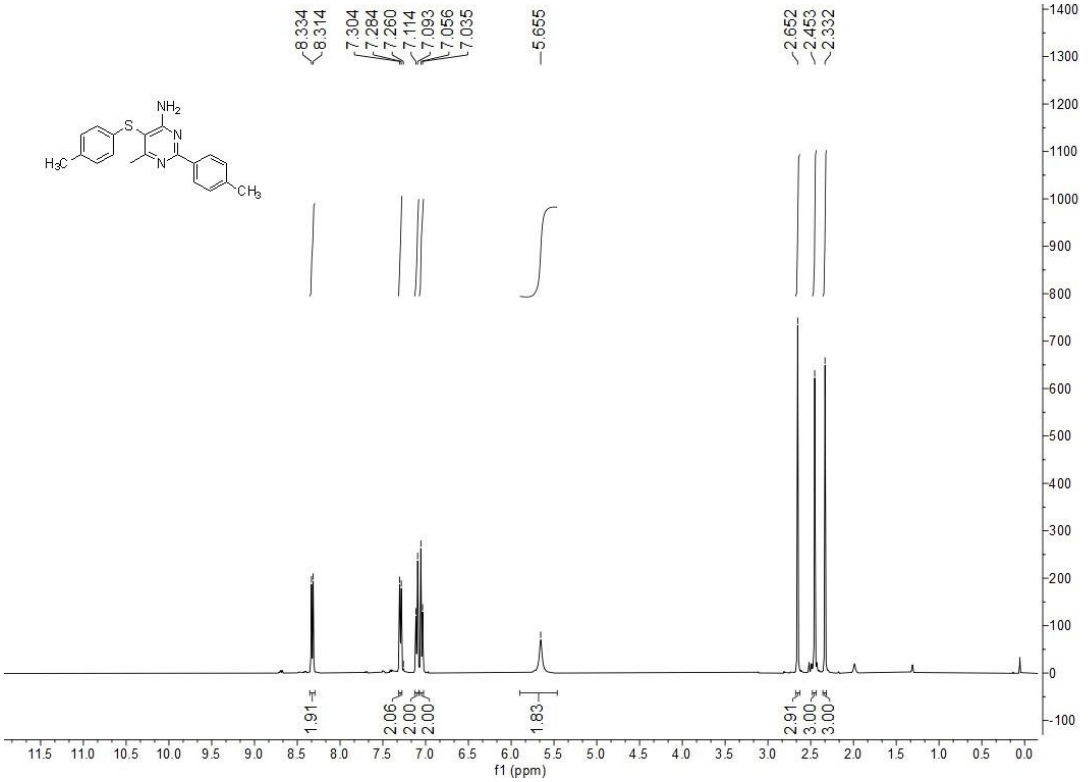

7.351
7.331
7.260
7.146
7.131
7.127
7.108
7.070
7.055
7.051
7.036
6.706
6.687
5.738
2.540
2.503
1.00
1.00
1.00
0.99
1.97
3.08
3.00
f1 (ppm)
171.708
168.480
164.550
133.263
130.213
129.874
127.847
127.777
127.472
100.396
25.749
25.100
f1 (ppm)

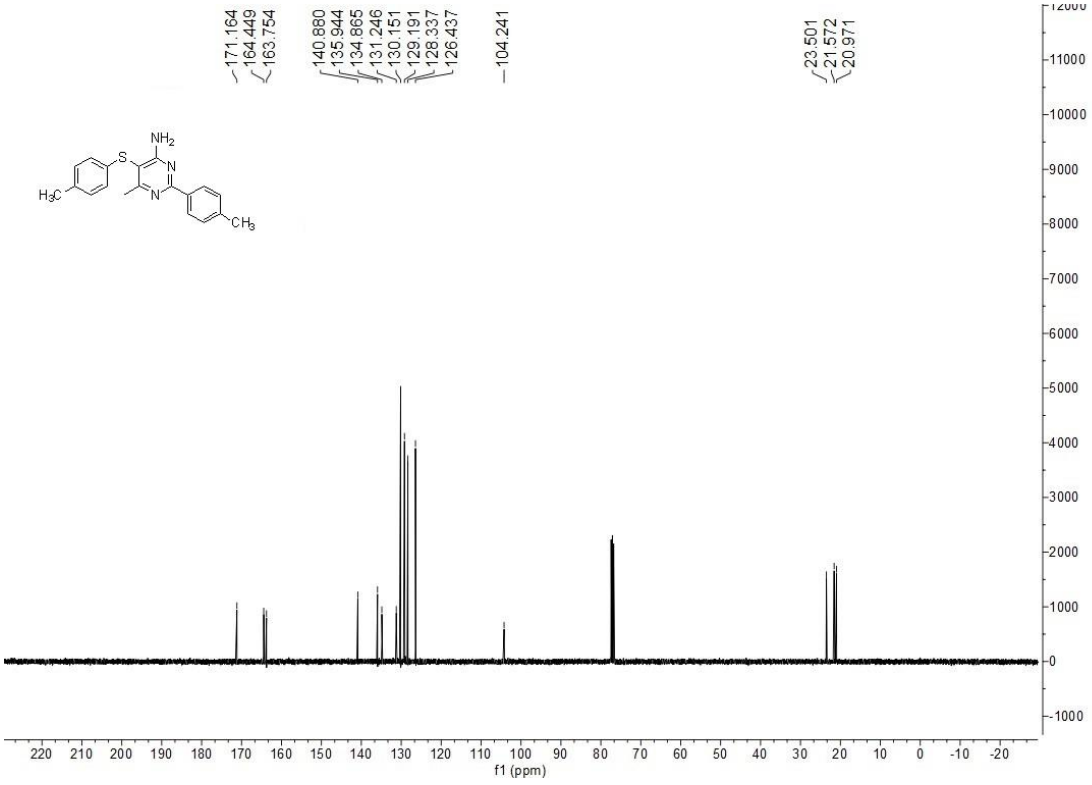
Compound (22)


8.436
8.423
7.484
7.479
7.467
7.260
7.094
7.074
7.047
7.026
5.858
2.664
2.314
NH2
S
N
N
H3C
2.00
3.00
2.00
2.00
1.99
3.00
3.00
f1 (ppm)

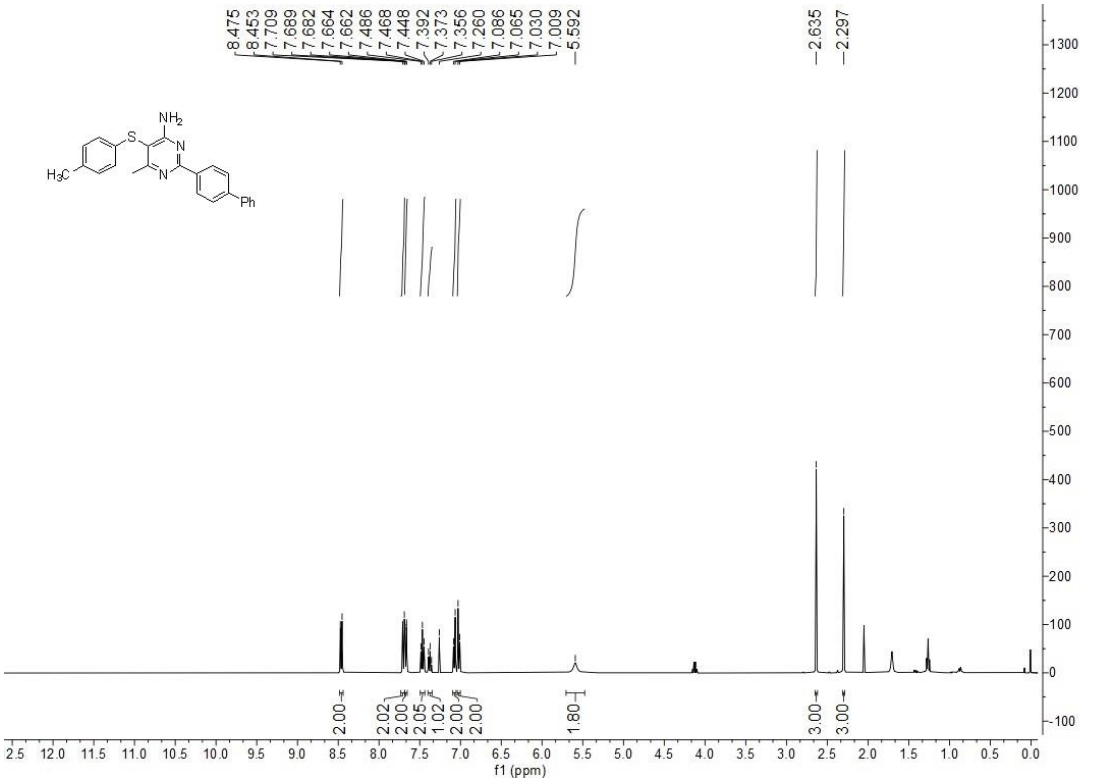

171.232
164.595
163.753
137.698
136.022
131.186
130.700
130.231
128.487
128.459
126.547
104.713
23.600
21.060
NH2
S
N
N
H3C
f1 (ppm)

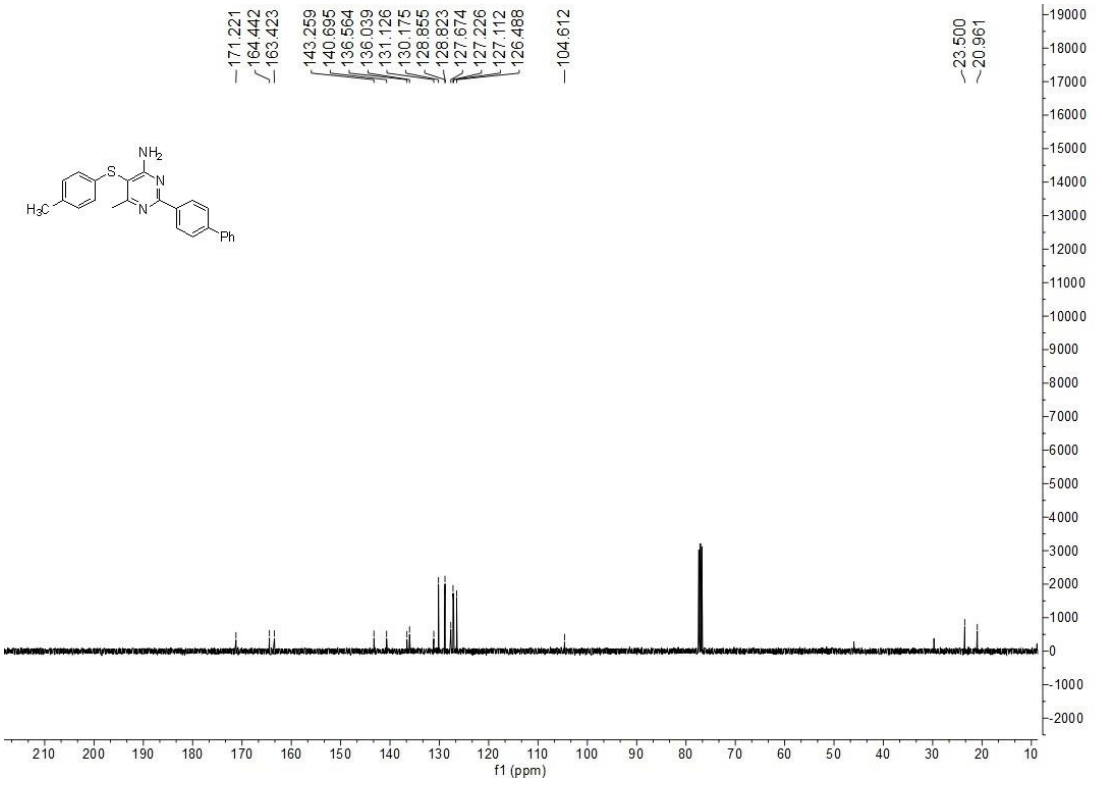
Compound (23)


8.334
8.314
7.304
7.284
7.260
7.114
7.093
7.056
7.035
5.655
2.652
2.453
2.332
NH2
S
N
N
H3C
CH3
1.91
2.06
2.00
2.00
1.83
2.91
3.00
3.00
f1 (ppm)

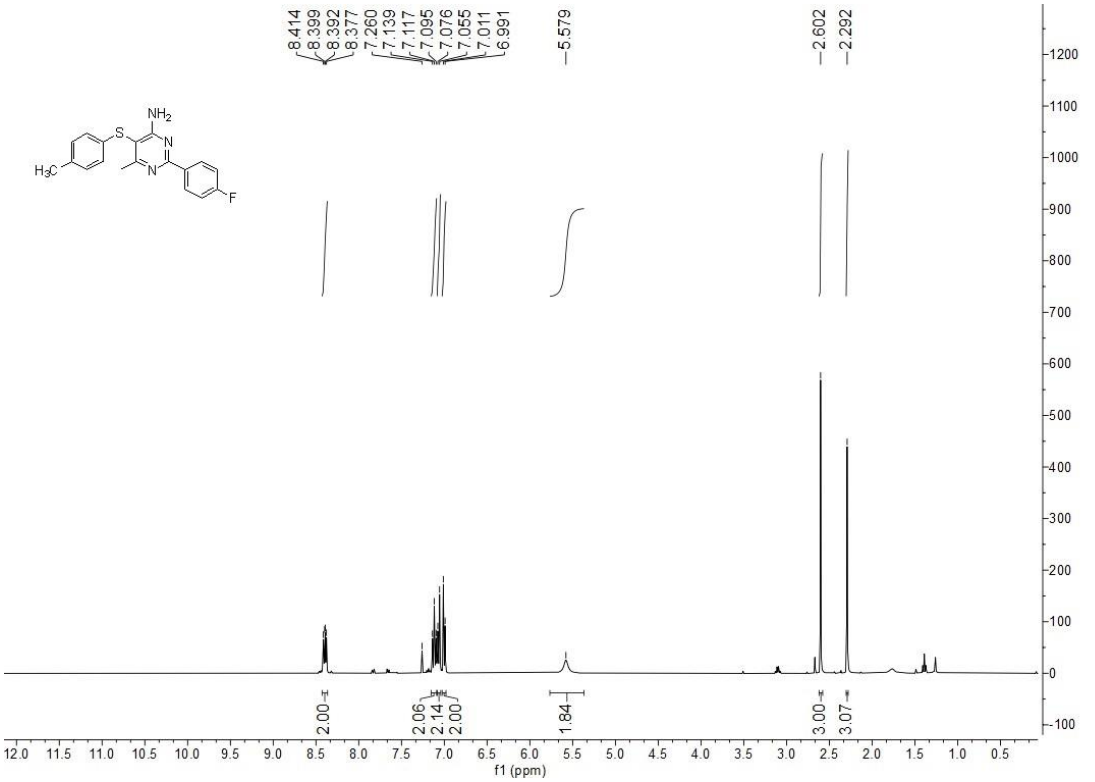

171.164
164.449
163.754
140.880
135.944
134.865
131.246
130.151
129.191
128.337
126.437
104.241
23.501
21.572
20.971
NH2
S
N
N
H3C
CH3
f1 (ppm)

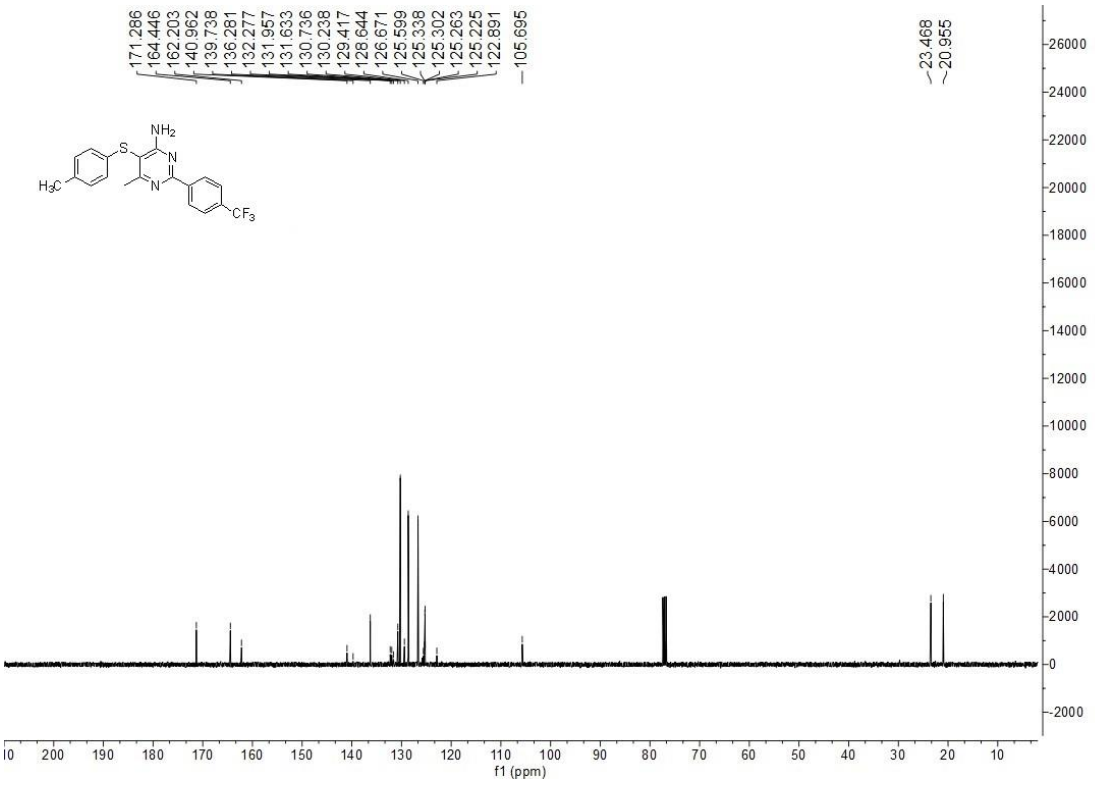
Compound (24)

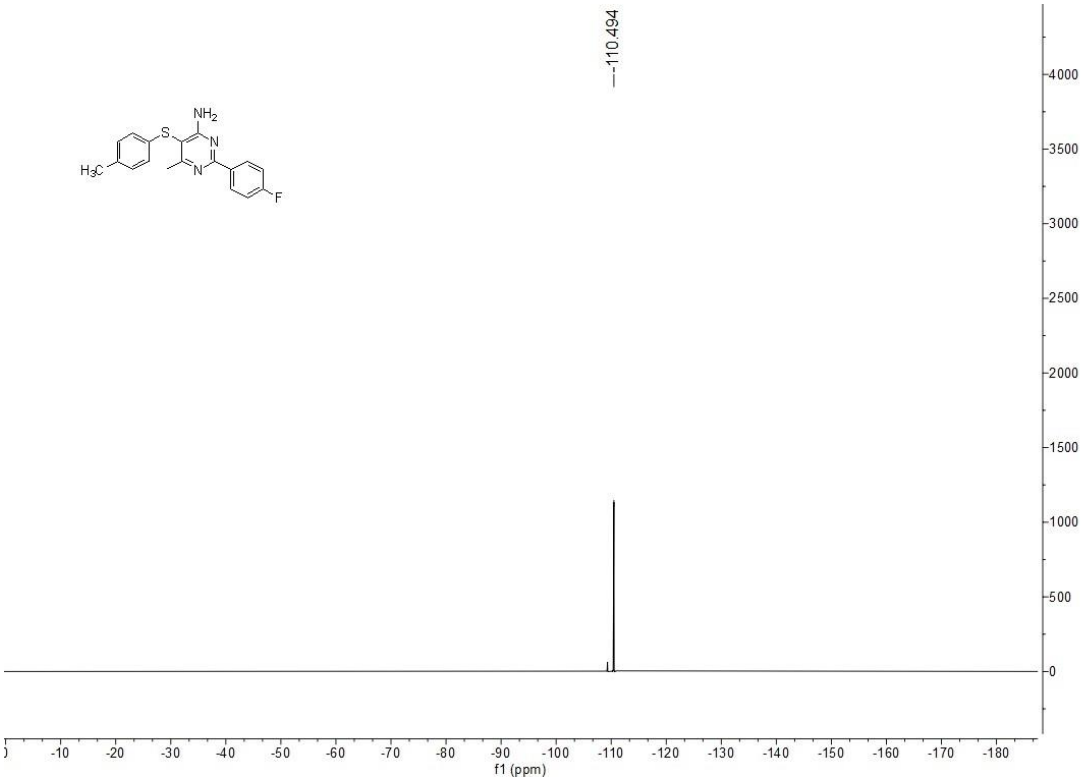

8.475
8.453
7.709
7.689
7.682
7.664
7.662
7.486
7.468
7.448
7.392
7.373
7.356
7.260
7.086
7.065
7.030
7.009
5.592
2.635
2.297
NH2
S
N
N
H3C
Ph
2.00
2.02
2.00
2.05
1.02
2.00
2.00
1.80
3.00
3.00
f1 (ppm)


171.221
164.442
163.423
143.259
140.695
136.564
136.039
131.126
130.175
128.855
128.823
127.674
127.226
127.112
126.488
104.612
23.500
20.961
NH2
S
N
N
H3C
Ph
f1 (ppm)

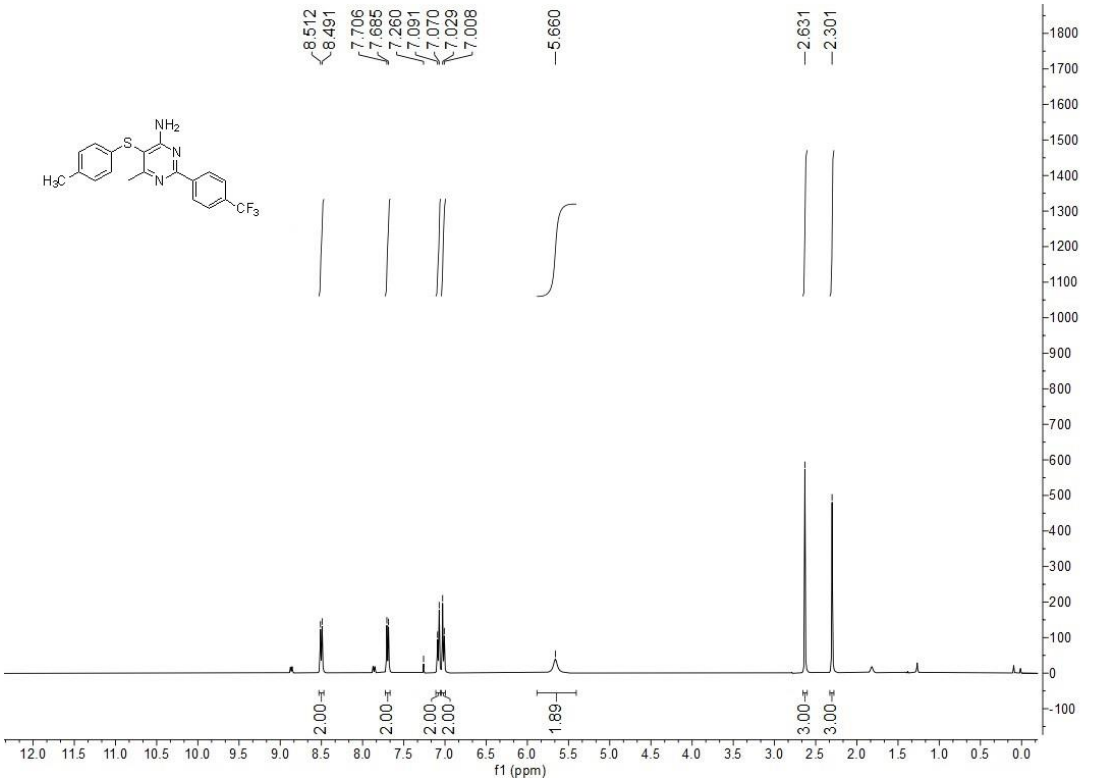
Compound (25)

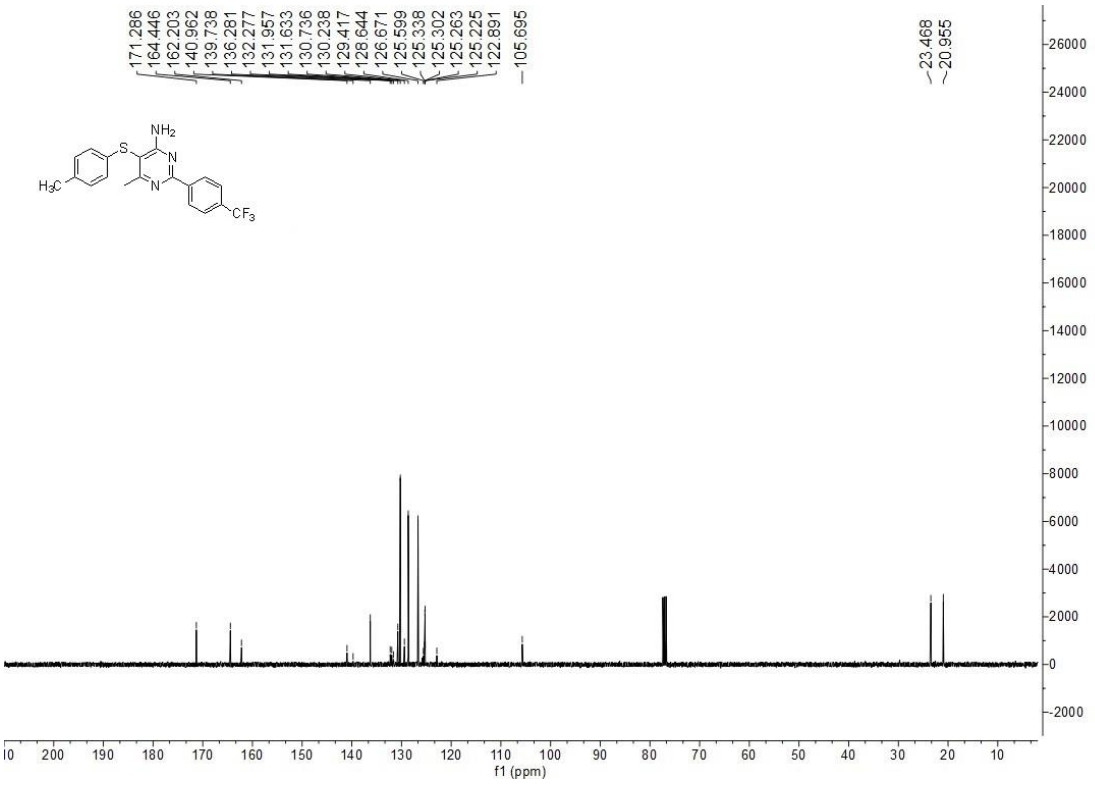

8.414
8.399
8.392
8.377
7.260
7.139
7.117
7.095
7.076
7.055
7.011
6.991
5.579
2.602
2.292
NH2
S
N
N
H3C
F
2.00
2.06
2.14
2.00
1.84
3.00
3.07
f1 (ppm)

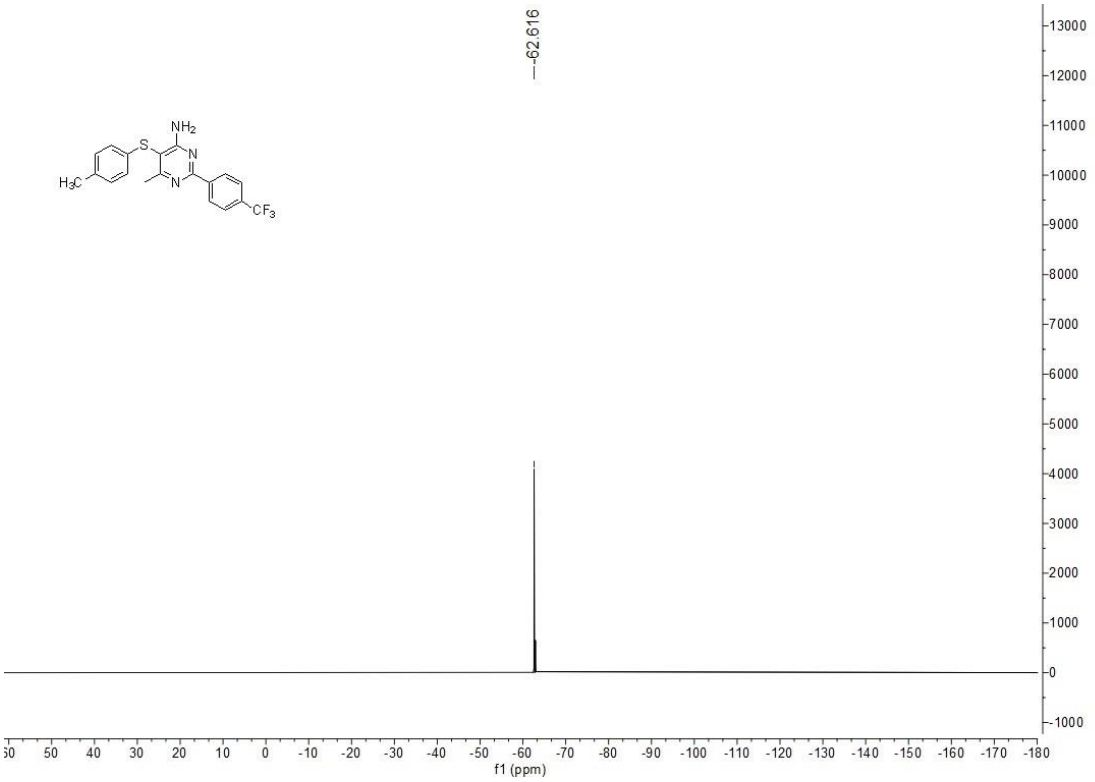

171.286
164.446
162.203
140.962
139.738
136.281
132.277
131.957
131.633
130.736
130.238
129.417
128.644
126.671
125.599
125.338
125.302
125.263
125.225
122.891
105.695
23.468
20.955
NH2
S
N
N
H3C
CF3
f1 (ppm)


-110.494
NH2
S
N
N
H3C
F
4000
3500
3000
2500
2000
1500
1000
500
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
f1 (ppm)

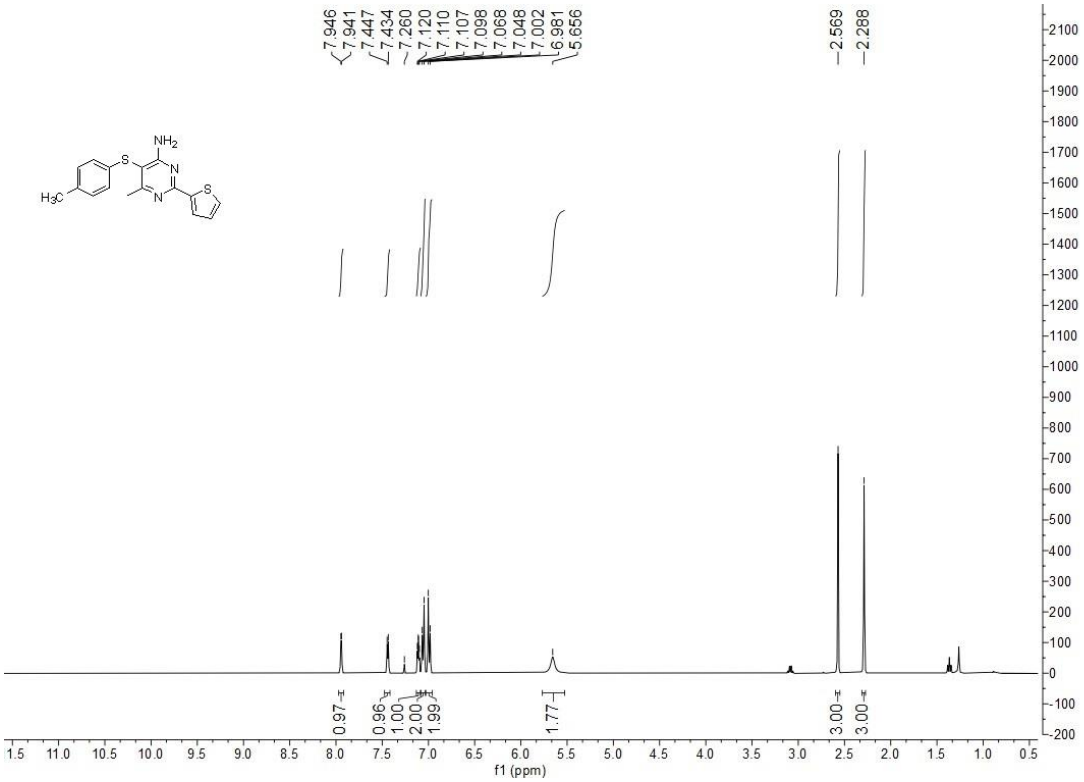
Compound (26)

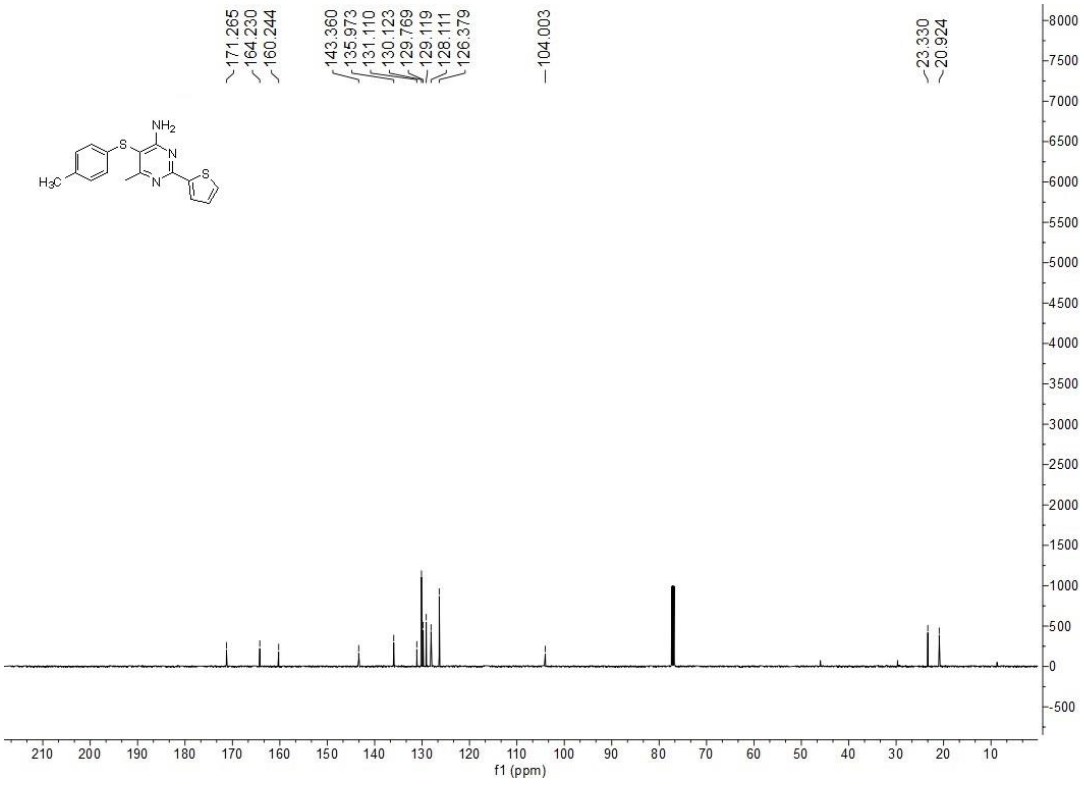

8.512
8.491
7.706
7.685
7.260
7.091
7.070
7.029
7.008
5.660
2.631
2.301
NH2
S
N
N
H3C
CF3
2.00
2.00
2.00
2.00
1.89
3.00
3.00
f1 (ppm)


171.286
164.446
162.203
140.962
139.738
136.281
132.277
131.957
131.633
130.736
130.238
129.417
128.644
126.671
125.599
125.338
125.302
125.263
125.225
122.891
105.695
23.468
20.955
NH2
S
N
N
H3C
CF3
f1 (ppm)

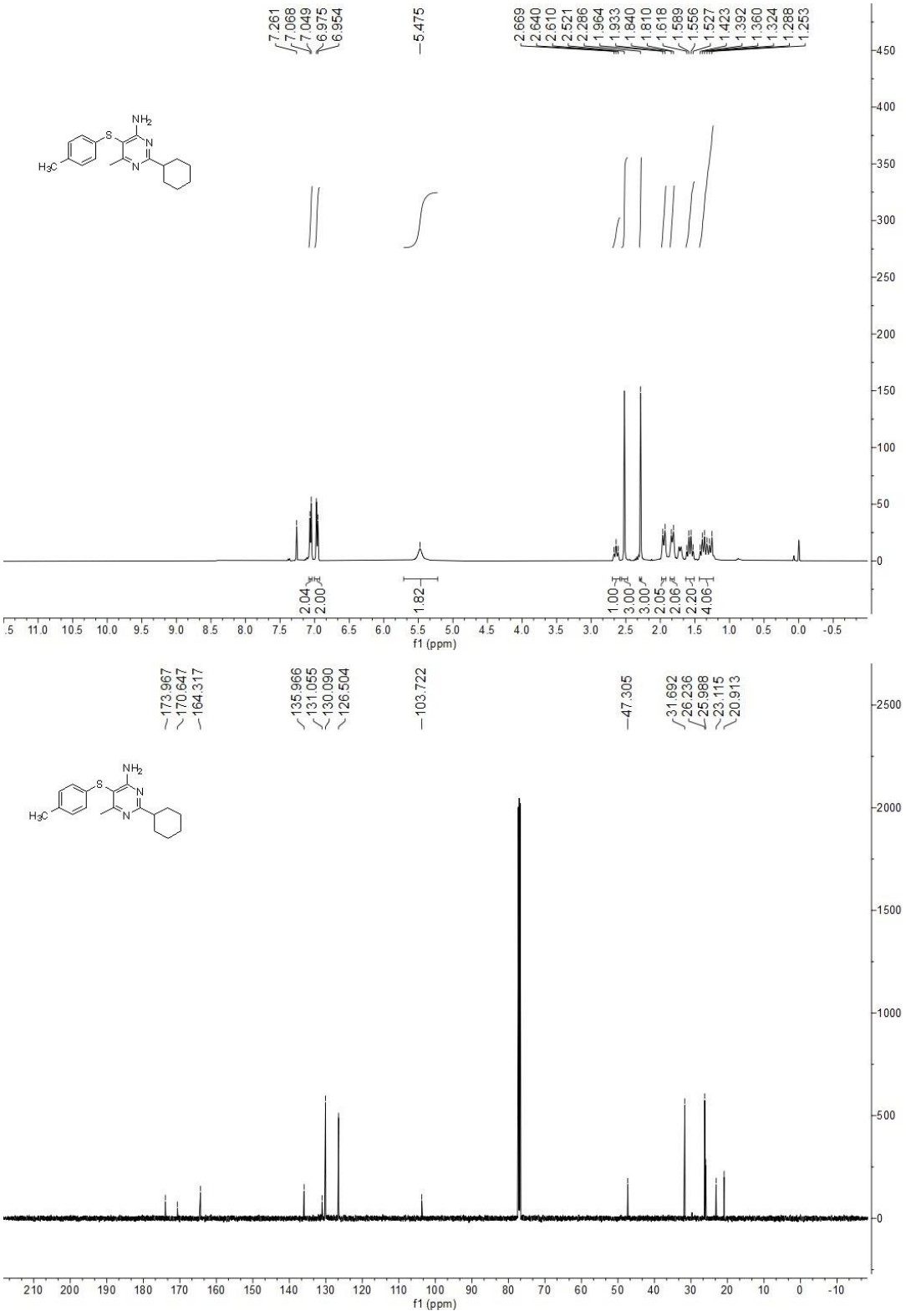

-62.616
NH2
S
N
N
H3C
CF3
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180
f1 (ppm)

Compound (27)

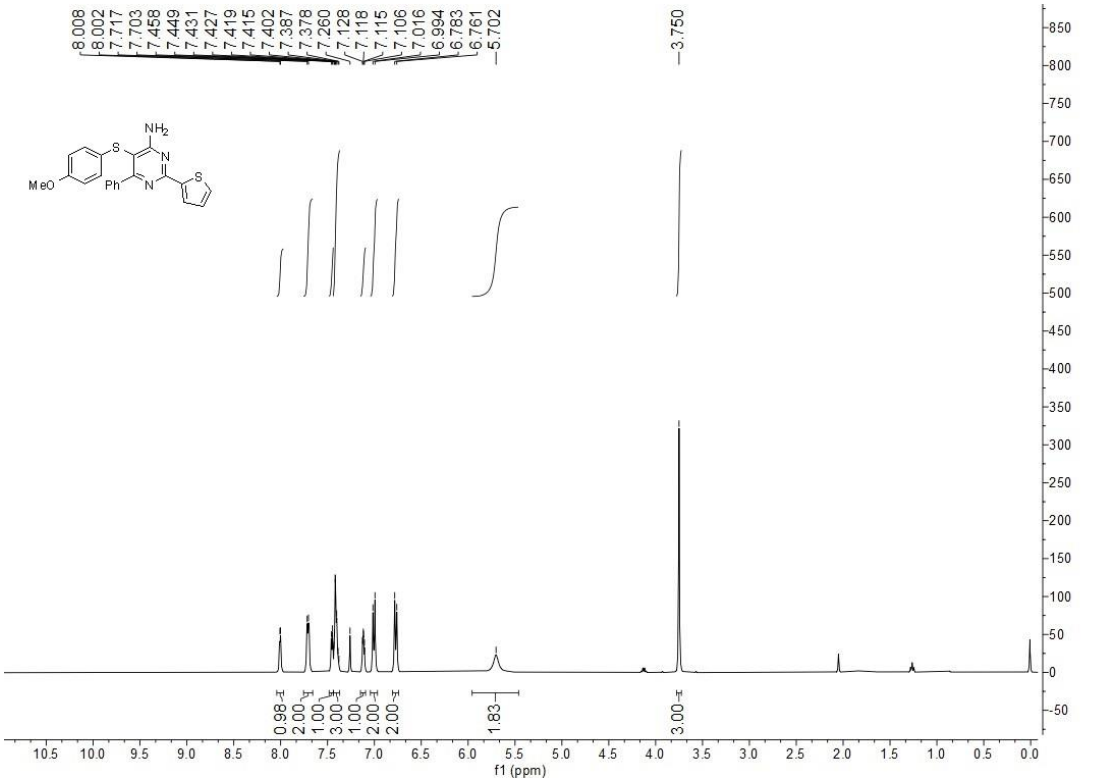

7.946
7.941
7.447
7.434
7.260
7.120
7.110
7.107
7.098
7.068
7.048
7.002
6.981
5.656
2.569
2.288
NH2
S
N
N
S
H3C
0.97
0.96
1.00
2.00
1.99
1.77
3.00
3.00
f1 (ppm)

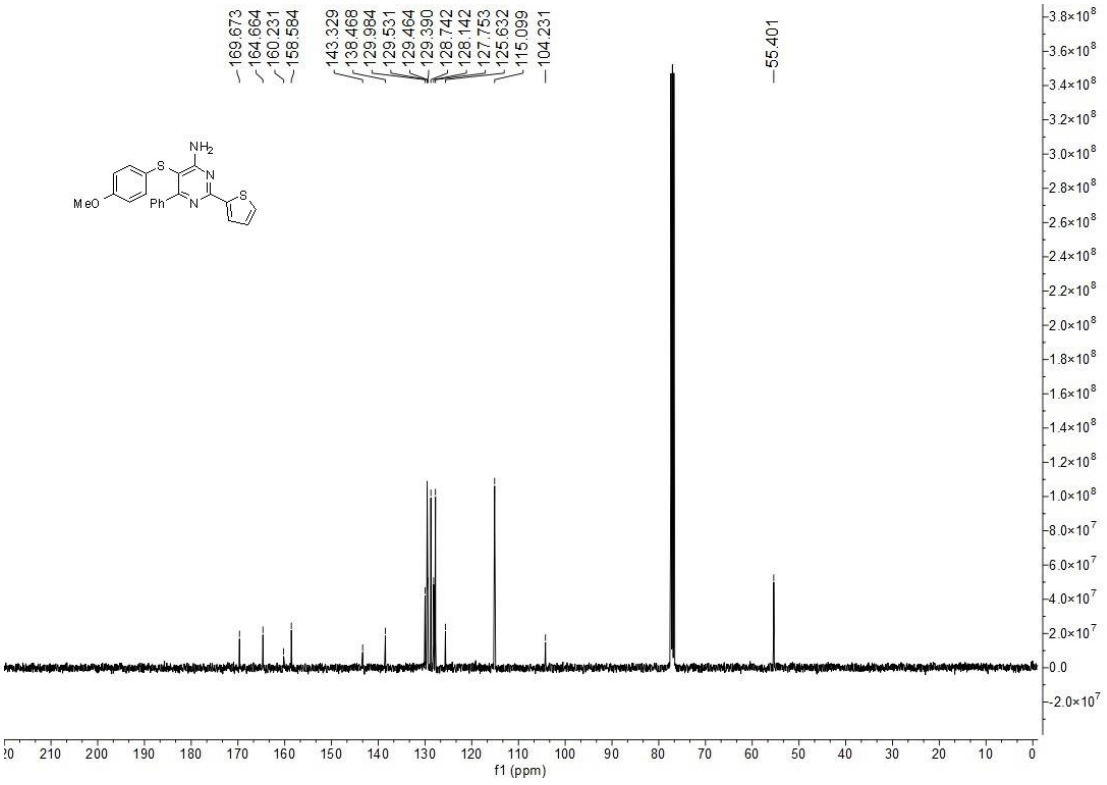

171.265
164.230
160.244
143.360
135.973
131.110
130.123
129.769
129.119
128.111
126.379
104.003
23.330
20.924
NH2
S
N
N
S
H3C
f1 (ppm)

Compound (28)


7.261
7.068
7.049
6.975
6.954
5.475
2.669
2.640
2.610
2.521
2.286
1.964
1.933
1.840
1.810
1.618
1.589
1.556
1.527
1.423
1.392
1.360
1.324
1.288
1.253
NH2
S
N
N
H3C
2.04
2.00
1.82
1.00
3.00
3.00
2.05
2.06
2.20
4.06
f1 (ppm)
173.967
170.647
164.317
135.966
131.055
130.090
126.504
103.722
47.305
31.692
26.236
25.988
23.115
20.913
NH2
S
N
N
H3C
f1 (ppm)

Compound (29)


8.008
8.002
7.717
7.703
7.458
7.449
7.431
7.427
7.419
7.415
7.402
7.387
7.378
7.260
7.128
7.118
7.115
7.106
7.016
6.994
6.783
6.761
5.702
3.750
NH2
S
N
MeO
Ph
N
S
0.98
2.00
1.00
3.00
1.00
2.00
2.00
1.83
3.00
f1 (ppm)


169.673
164.664
160.231
158.584
143.329
138.468
129.984
129.531
129.464
129.390
128.742
128.142
127.753
125.632
115.099
104.231
55.401
NH2
S
N
MeO
Ph
N
S
f1 (ppm)

7. References

1. A. Alam, Y. Takaguchi and S. Tsuboi, *Synthetic Commun.,* 2005, **35**, 1329.
2. Y.-T. Ma, C. Lin, X.-B. Huang, M.-C. Liu, Y.-B. Zhou and H.-Y. Wu, *Chem. Commun.,* 2022, **58**, 6550.