Supplementary Information

Sodium Pyruvate as a Peroxide Scavenger in Aerobic Oxidation under Carbene Catalysis

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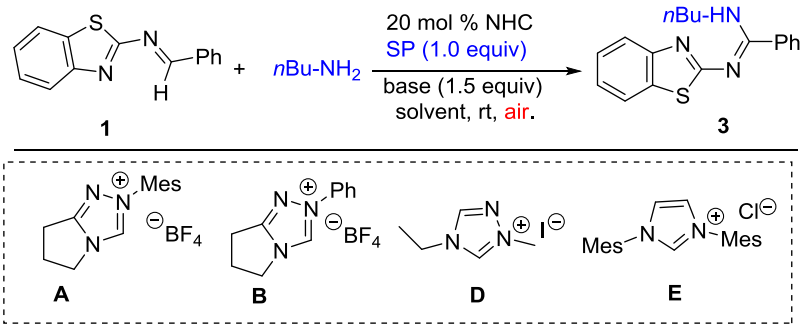
I: General Information

Chemicals were purchased as reagent grade and used without further purification. Solvents (THF, toluene) were distilled from appropriate drying agents prior to use. In addition, more solvents were purchased from commercial suppliers and dried over molecular sieves. Proton nuclear magnetic resonance (1H NMR) spectra were recorded on a Bruker (400 MHz) spectrometer. Chemical shifts were recorded in parts per million (ppm, δ) relative to tetramethylsilane (δ 0.00) or chloroform (δ = 7.26, singlet). 1H NMR splitting patterns are designated as singlet (s), doublet (d), triplet (t), quartet (q), dd (doublet of doublets); m (multiplets), and etc. All first-order splitting patterns were assigned on the basis of the appearance of the multiplet. Splitting patterns that could not be easily interpreted are designated as multiplet (m) or broad (br). Carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on a Bruker (400 MHz) (100 MHz) spectrometer. Fourier transform infrared spectroscopy (FT-IR, a Bruker model VECTOR-22 Fourier transform spectrometer). High resolution mass spectral analysis (HRMS) was performed on a Waters Q–TOF Permier Spectrometer. X-ray crystallography analysis was performed on Bruker X8 APEX X-ray diffractionmeter. Analytical thin-layer chromatography (TLC) was carried out on Merck 60 F254 precoated silica gel plate (0.2 mm thickness). Aldimines **1** was prepared as as a single isomer according to the literature. [1]

II.

a) Condition Optimization.

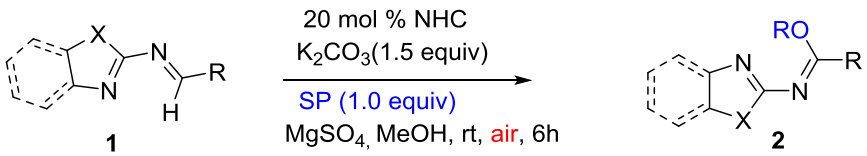
Table S1. Screening of modified reaction conditions for nitrogen nucleophiles**.**



entry[a]	NHC	solvent	base(equiv)	yield (%)[b]
1	**A**	THF	K_2CO_3	55
2	**A**	1,4-dioxane	K_2CO_3	49
3	**A**	DCM	K_2CO_3	31
4	**A**	DMF	K_2CO_3	26
5	**A**	CH_3CN	K_2CO_3	<10
6	**B**	THF	K_2CO_3	48
7	**C**	THF	K_2CO_3	42
8	**D**	THF	K_2CO_3	30
9	**A**	THF	Cs_2CO_3	50
10	**A**	THF	DBU	20
11	**A**	THF	KO^{t}Bu	<10
12	**A**	THF	NaOAc	66
13[c]	**A**	THF	NaOAc	70
14[d]	**A**	THF	NaOAc	77
15[e]	**A**	THF	NaOAc	69
16[d]	**A**	2-MeTHF	NaOAc	68

[a] Standard condition: aldimine (0.1 mmol) **NHC** precursor (20 mol %), base (1.5 equiv), *n*-Butylamine (3.0 equiv), solvent (0.1 M), **SP** (1.0 equiv), $MgSO_4$ (50 mg), rt, 6 h. [b] Isolated yields after column chromatography. [c] 2.0 equiv *n*-Butylamine was used. [d] Replace 50mg $MgSO_4$ with 100mg 4Å MS. [e] Without addition of **SP**. "**SP**" = Sodium pyruvate.

b) General procedure for the synthesis of imidate product 2.

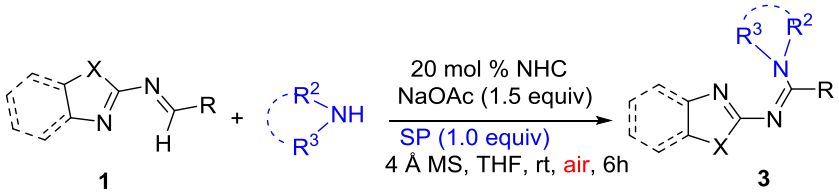


To an oven-dried screw-capped test tube equipped with a magnetic stir bar the triazolium salt NHC **A** (6.3 mg, 20 mol %), K_2CO_3 (21.0 mg, 0.15 mmol), Sodium pyruvate (11.0 mg, 0.10 mmol), anhydrous $MgSO_4$ (50 mg) and aldimine **1** (0.10 mmol, 1.0 equiv) were added. To this mixture was added anhydrous methanol (1.0 mL, 0.1M). The resultant reaction mixture was kept stirring at room temperature for 6 h. When the reaction is complete, the crude residue was purified by flash column

chromatography on silica gel using Petroleum ether/EtOAc (10:1) as eluent to afford the desired product **2**.

2ab-2ad was synthesized based on the modified reaction conditions (Table S1, entry 14).

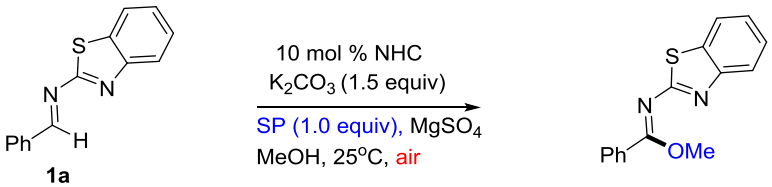
c) General procedure for the synthesis of aldimine product 3.



1 **3**

To an oven-dried screw-capped test tube equipped with a magnetic stir bar the triazolium salt NHC **A** (6.3 mg, 20 mol %), anhydrous NaOAc (12.3 mg, 0.15 mmol), Sodium pyruvate (11.0 mg, 0.10 mmol), anhydrous 4Å MS (100 mg) and aldimine **1** (0.10 mmol, 1.0 equiv) were added. To this mixture was added anhydrous THF (1.0 mL, 0.1M) and then amine (0.20 mmol, 2.0 equiv). The resultant reaction mixture was kept stirring at room temperature for 6 h. When the reaction is complete, the crude residue was purified by flash column chromatography on silica gel using Petroleum ether/EtOAc (10:1) as eluent to afford the desired product **3**.

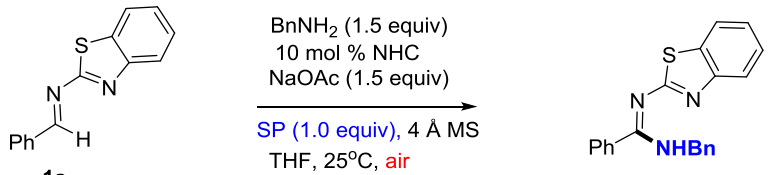
d) Experimental procedure for the scale-up reaction.



1a
2 mmol

2a, 68% yield

A dry 25 mL Schlenk tube equipped with a magnetic stirring bar was successively charged with aldimine **1a** (476 mg, 2.0 mmol), NHC pre-catalyst **A** (63.0 mg, 0.20 mmol), K_2CO_3 (414 mg, 3.0 mmol), Sodium pyruvate (220 mg, 2.0 mmol), anhydrous $MgSO_4$ (500 mg). To this reaction mixture was added anhydrous methanol (8.0 mL). Upon completion of the reaction, which was monitored by TLC, the crude residue was purified by flash column chromatography on silica gel using eluent Petroleum ether/EtOAc (10:1) to afford **2a** as yellow oil (365 mg, 68% yield).



1a
2 mmol

3d, 61% yield

To a 25 mL oven-dried Schlenk tube equipped with a magnetic stir bar the triazolium salt NHC **A** (63.0 mg, 10 mol %), anhydrous NaOAc (246 mg, 1.5 equiv), sodium pyruvate (220 mg, 2.0 mmol), anhydrous 4Å MS (500 mg) and aldimine **1a**

(476 mg, 1.0 equiv) were added. To this mixture was added anhydrous THF (8.0 mL) and then amine (3.0 mmol, 1.5 equiv). The resultant reaction mixture was kept stirring at room temperature. After completition, the resulting mixture was filtrated, concentrated in vacuo and purified by column chromatography on silica gel using Petroleum ether/EtOAc (8:1) as eluent to afford the desired product as a white solid (418 mg, 61% yield).

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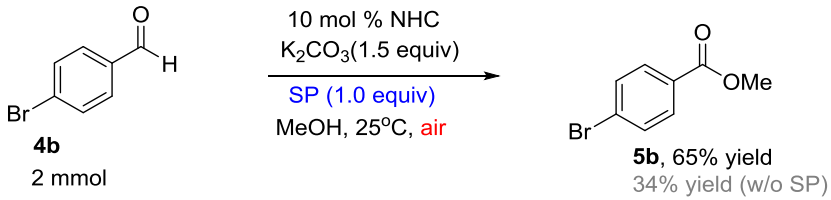
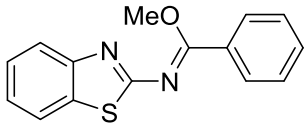


4b
2 mmol

5b, 65% yield
34% yield (w/o SP)

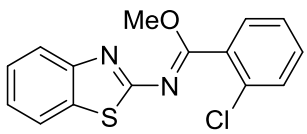
To a 25 mL oven-dried Schlenk tube equipped with a magnetic stir bar the triazolium salt NHC **A** (63.0 mg, 10 mol %), anhydrous K_2CO_3 (414 mg, 3.0 mmol), sodium pyruvate (220 mg, 2.0 mmol) and 4-Bromobenzaldehyde **4b** (370 mg, 1.0 equiv) were added. To this mixture was added anhydrous methanol (8.0 mL). The resultant reaction mixture was kept stirring at room temperature. After completition, the resulting mixture was filtrated, concentrated in vacuo and purified by column chromatography on silica gel using Petroleum ether/EtOAc (8:1) as eluent to afford the desired ester product **5b** as a white solid (280 mg, 65% yield). The yield for the reaction without the presence of the sodium pyruvate under otherwise identical conditions is 34%.

e) Characterizations of products



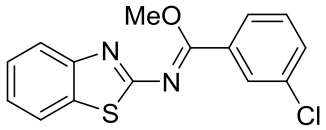
2a

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)benzimidate (2a): colorless oil, 24.7mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.79 (d, J = 8.0 Hz, 1H), 7.64 (d, J = 8.0 Hz, 1H), 7.53–7.56 (m, 2H), 7.35–7.43 (m, 2H), 7.27–7.32 (m, 2H), 7.20–7.25 (m, 1H), 4.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 164.6, 151.8, 134.4, 131.5, 130.0, 129.3, 128.4, 125.8, 123.7, 121.8, 121.2, 55.5; HRMS (ESI) Calcd for $C_{15}H_{13}N_2OS^+$ $[M+H]^+$ 269.0743; Found: 269.0741.



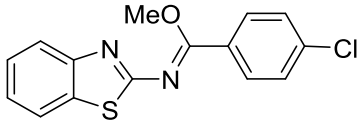
2b

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-2-chlorobenzimidate (2b): colorless oil, 25.7mg, 85% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.79 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.32–7.40 (m, 4H), 7.23–7.28 (m, 1H), 7.18–7.22 (m, 1H), 4.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 165.0, 151.2, 134.4, 132.2, 131.7, 131.2, 129.9, 129.8, 126.9, 125.8, 124.0, 122.1, 121.1, 55.8; HRMS (ESI) Calcd for $C_{15}H_{12}ClN_2OS^+$ $[M+H]^+$ 303.0353; Found: 303.0348.



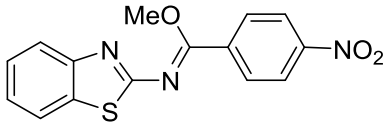
2c

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-3-chlorobenzimidate (2c): colorless oil, 22.1mg, 73% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.78 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.62 (t, *J* = 1.6 Hz, 1H), 7.33–7.40 (m, 3H), 7.22–7.26 (m, 1H), 7.17 (t, *J* = 8.0 Hz, 1H), 4.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 163.0, 151.7, 134.6, 134.4, 131.7, 131.6, 129.6, 129.3, 127.3, 125.9, 123.9, 121.9, 121.2, 55.7; HRMS (ESI) Calcd for $C_{15}H_{12}ClN_2OS^+$ $[M+H]^+$ 303.0353; Found: 303.0351.



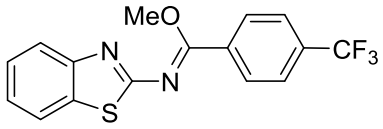
2d

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-4-chlorobenzimidate (2d): colorless oil, 23.0mg, 76% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.78 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.47–7.50 (m, 2H), 7.36–7.40 (m, 1H), 7.22–7.28 (m, 3H), 4.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 163.3, 151.7, 137.8, 134.3, 130.7, 128.8, 128.4, 125.9, 123.8, 121.8, 121.2, 55.6; HRMS (ESI) Calcd for $C_{15}H_{12}ClN_2OS^+$ $[M+H]^+$ 303.0353; Found: 303.0349.



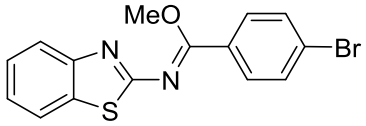
2e

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-4-nitrobenzimidate (2e): colorless oil, 13.2mg, 42% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.13 (d, *J* = 8.8 Hz, 2H), 7.66–7.75 (m, 4H), 7.38 (t, *J* = 8.4 Hz, 1H), 7.23–7.27 (m, 1H), 4.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 162.3, 151.5, 149.1, 136.1, 134.3, 130.3, 126.2, 124.2, 123.6, 122.0, 121.3, 56.0; HRMS (ESI) Calcd for $C_{15}H_{12}N_3O_3S^+$ $[M+H]^+$ 314.0594; Found: 314.0599.



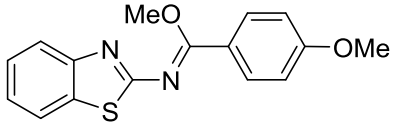
2f

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-4-(trifluoromethyl)benzimidate (2f): colorless oil, 18.8mg, 56% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.78 (d, *J* = 8.0 Hz, 1H), 7.66–7.68 (m, 3H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.37–7.41 (m, 1H), 7.23–7.27 (m, 1H), 4.11 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 163.0, 151.7, 134.4, 129.6, 126.0, 125.5, 125.5, 125.4, 125.4, 124.0, 121.9, 121.3, 55.8; HRMS (ESI) Calcd for $C_{16}H_{12}F_3N_2OS^+$ $[M+H]^+$ 337.0617; Found: 337.0620.



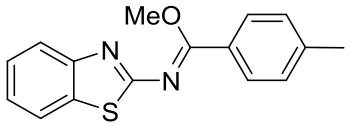
2g

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-4-bromobenzimidate (2g): colorless oil, 28.1mg, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.78 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.35–7.41 (m, 5H), 7.21–7.26 (m, 1H), 4.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 163.4, 151.7, 134.3, 131.8, 130.8, 128.9, 126.4, 125.9, 123.9, 121.8, 121.2, 55.6; HRMS (ESI) Calcd for $C_{15}H_{12}BrN_2OS^+$ $[M+H]^+$ 346.9848; Found: 346.9849.



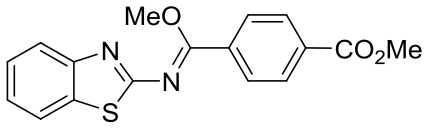
2h

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-4-methoxybenzimidate (2h): colorless oil, 27.4mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.80 (d, *J* = 8.4 Hz, 1H), 7.64 (d, *J* = 8.8 Hz, 1H), 7.49–7.53 (m, 2H), 7.37 (t, *J* = 7.2 Hz, 1H), 7.22 (t, *J* = 7.2 Hz, 1H), 6.75–6.79 (m, 2H), 4.05 (s, 3H), 3.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 164.0, 162.1, 151.9, 134.4, 131.4, 125.7, 123.6, 121.8, 121.7, 121.2, 113.7, 55.3, 55.3; HRMS (ESI) Calcd for $C_{16}H_{15}N_2O_2S^+$ $[M+H]^+$ 299.0849; Found: 299.0851.



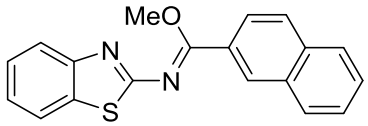
2i

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-4-methylbenzimidate (2i): colorless oil, 26.3mg, 93% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.80 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.0 Hz, 1H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.35–7.39 (m, 1H), 7.20–7.24 (m, 1H), 7.09 (d, *J* = 7.6 Hz, 2H), 4.07 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 164.6, 151.9, 142.1, 134.4, 129.3, 129.1, 127.0, 125.7, 123.6, 121.7, 121.2, 55.4, 21.5; HRMS (ESI) Calcd for $C_{16}H_{15}N_2OS^+$ $[M+H]^+$ 283.0900; Found: 283.0905.



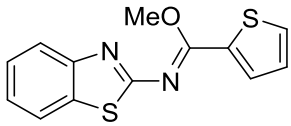
2j

Methyl (*Z*)-4-((benzo[*d*]thiazol-2-ylimino)(methoxy)methyl)benzoate (2j): colorless oil, 23.2mg, 71% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.94 (d, J = 8.4 Hz, 2H), 7.66 (d, J = 8.0 Hz, 1H), 7.58–7.64 (m, 3H), 7.36 (t, J = 8.4 Hz, 1H), 7.22 (t, J = 8.4 Hz, 1H), 4.09 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 166.1, 163.7, 151.7, 134.3, 134.2, 132.5, 129.6, 129.2, 125.9, 123.9, 121.9, 121.2, 55.7, 52.4; HRMS (ESI) Calcd for $C_{17}H_{15}N_2O_3S^+$ $[M+H]^+$ 327.0798; Found: 327.0799.



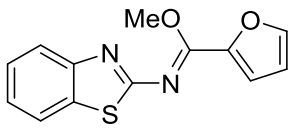
2k

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-2-naphthimidate (2k): colorless oil, 28.0mg, 88% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.19 (s, 1H), 7.75–7.83 (m, 3H), 7.69 (d, J = 8.8 Hz, 1H), 7.60 (d, J = 8.0 Hz, 1H), 7.44–7.53 (m, 3H), 7.37 (t, J = 8.0 Hz, 1H), 7.21 (t, J = 7.6 Hz, 1H), 4.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 164.8, 151.8, 134.4, 134.4, 132.5, 130.5, 129.1, 128.1, 128.1, 127.7, 127.4, 126.7, 125.8, 125.1, 123.7, 121.7, 121.2, 55.7; HRMS (ESI) Calcd for $C_{19}H_{15}N_2OS^+$ $[M+H]^+$ 319.0900; Found: 319.0904.



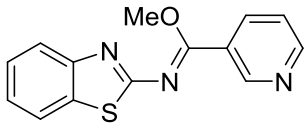
2l

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)thiophene-2-carbimidate (2l): colorless oil, 18.4mg, 67% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.85 (d, J = 8.0 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.40–7.44 (m, 2H), 7.27–7.31 (m, 2H), δ = 6.90 (dd, J = 5.2, 4.0 Hz, 1H), 4.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.0, 157.1, 151.9, 134.7, 133.2, 131.5, 130.5, 127.6, 125.9, 123.9, 121.9, 121.4, 55.3; HRMS (ESI) Calcd for $C_{13}H_{11}N_2OS_2^+$ $[M+H]^+$ 275.0307; Found: 275.0309.



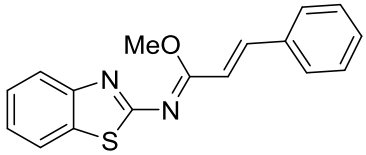
2m

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)furan-2-carbimidate (2m): colorless oil, 10.9mg, 42% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.83 (d, J = 8.0 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.38–7.43 (m, 2H), 7.26–7.30 (m, 1H), 6.73–6.74 (m, 1H), δ = 6.36 (dd, J = 3.6, 1.6 Hz, 1H), 4.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 153.5, 151.8, 145.85, 142.7, 134.6, 125.8, 123.7, 121.8, 121.3, 118.1, 111.8, 55.0; HRMS (ESI) Calcd for $C_{13}H_{11}N_2O_2S^+$ $[M+H]^+$ 259.0536; Found: 259.0538.



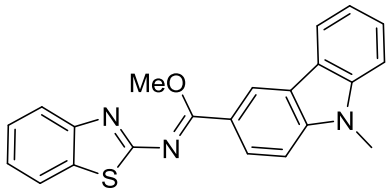
2n

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)nicotinimidate (2n): colorless oil, 15.1mg, 56% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 8.79 (s, 1H), 8.61 (d, *J* = 5.2 Hz, 1H), 7.75 (dt, J = 8.0 Hz, 2.0 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.20–7.26 (m, 2H), 4.10 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 162.1, 152.0, 151.6, 150.0, 136.6, 134.4, 126.4, 126.0, 124.0, 123.1, 121.9, 121.3, 55.8; HRMS (ESI) Calcd for $C_{14}H_{12}N_3OS^+$ $[M+H]^+$ 270.0696; Found: 270.0699.



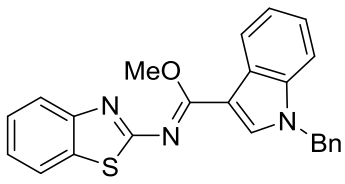
2o

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)cinnamimidate (2o): colorless oil, 18.0mg, 61% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.88 (d, *J* = 8.0 Hz,1H), 7.77 (d, *J* = 8.4 Hz, 1H), 7.60 (d, *J* = 15.6 Hz, 1H), 7.41–7.46 (m, 3H), 7.28–7.35 (m, 4H), 6.89 (d, *J* = 16 Hz, 1H), 4.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.5, 162.6, 152.1, 142.4, 134.9, 130.2, 128.8, 128.2, 126.0, 123.8, 121.9, 121.2, 114.5, 54.7; HRMS (ESI) Calcd for $C_{17}H_{15}N_2OS^+$ $[M+H]^+$ 295.0900; Found: 295.0903.



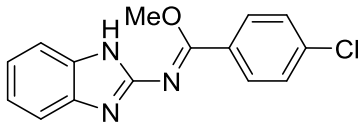
2p

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-9-methyl-9H-carbazole-3-carbimidate (2p): colorless oil, 35.7mg, 96% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 8.43 (s, 1H), 7.96 (d, *J* = 7.6 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.60 (t, *J* = 8.8 Hz, 2H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.38 (t, *J* = 8.0 Hz, 1H), 7.32 (d, *J* = 8.4 Hz, 1H), 7.18-7.25 (m, 2H), 7.16 (d, *J* = 8.8 Hz, 1H), 4.17 (s, 3H), 4.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.9, 165.6, 152.0, 142.5, 141.5, 134.4, 127.1, 126.5, 125.7, 123.5, 122.6, 122.5, 121.6, 121.2, 120.5, 120.0, 119.9, 108.9, 108.2, 55.5, 29.1; HRMS (ESI) Calcd for $C_{22}H_{18}N_3OS^+$ $[M+H]^+$ 372.1165; Found: 372.1167.



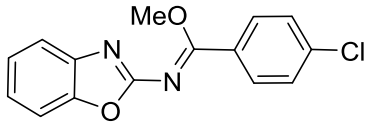
2q

Methyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-1-benzyl-1H-indole-3-carbimidate (2q): colorless oil, 36.2mg, 91% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.98–8.02 (m, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.38 (d, *J* = 8.8 Hz, 1H), 7.20–7.26 (m, *J* = 8.0 Hz, 4H), 7.16 (s, 1H), 7.07–7.14 (m, 3H), 6.89 (d, *J* = 8.8 Hz, 2H), 5.04 (s, 2H), 4.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 169.4, 161.5, 152.0, 135.9, 135.0, 134.4, 133.7, 128.8, 128.1, 127.3, 126.7, 125.7, 123.5, 123.1, 122.1, 122.0, 121.6, 121.3, 110.3, 105.2, 54.7, 50.6; HRMS (ESI) Calcd for $C_{24}H_{20}N_3OS^+$ $[M+H]^+$ 398.1322; Found: 398.1321.



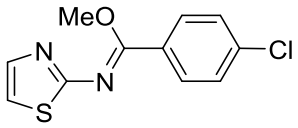
2r

Methyl (*Z*)-*N*-(1H-benzo[*d*]imidazol-2-yl)-4-chlorobenzimidate (2r): colorless oil, 18.0mg, 63% yield. ^{1}H NMR (400 MHz, DMSO) δ = 11.90 (s, 1H), 7.27–7.39 (m, 6H), 6.98–7.01 (m, 2H), 3.96 (s, 3H); ^{13}C NMR (100 MHz, DMSO) δ 163.6, 153.8, 136.5, 130.7, 130.2, 129.0, 121.2, 55.6; HRMS (ESI) Calcd for $C_{15}H_{13}ClN_3O^+$ $[M+H]^+$ 286.0742; Found: 286.0749.



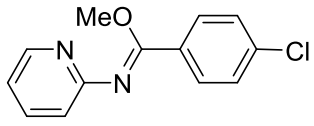
2s

Methyl (*Z*)-*N*-(benzo[*d*]oxazol-2-yl)-4-chlorobenzimidate (2s): colorless oil, 18.6mg, 65% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.50–7.53 (m, 1H), 7.41–7.45 (m, 2H), 7.35–7.37 (m, 1H), 7.18–7.30 (m, 4H), 4.12 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 161.7, 149.5, 142.1, 138.3, 130.0, 128.9, 128.8, 124.1, 123.4, 118.8, 109.9, 56.0; HRMS (ESI) Calcd for $C_{15}H_{12}ClN_2O_2^+$ $[M+H]^+$ 287.0582; Found: 287.0587.



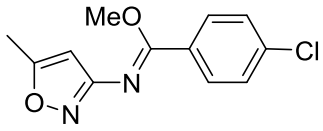
2t

Methyl (*Z*)-4-chloro-*N*-(thiazol-2-yl)benzimidate (2t): colorless oil, 23.2mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.36–7.40 (m, 3H), 7.27–7.30 (m, 2H), 6.92 (d, *J* = 3.6 Hz, 1H), 4.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.1, 163.3, 140.2, 137.4, 130.5, 128.8, 128.6, 115.4, 55.4; HRMS (ESI) Calcd for $C_{11}H_{10}ClN_2OS^+$ $[M+H]^+$ 253.0197; Found: 253.0190.



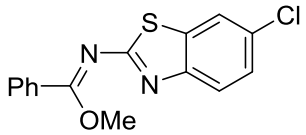
2u

Methyl (*Z*)-4-chloro-*N*-(pyridin-2-yl)benzimidate (2u): colorless oil, 9.70mg, 40% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.32 (d, *J* = 6.0 Hz, 1H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.18–7.26 (m, 4H), 6.91 (t, *J* = 5.6 Hz, 1H), 8.59 (d, *J* = 8.0 Hz, 1H), 4.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 160.1, 148.9, 137.9, 136.5, 130.5, 129.6, 128.4, 118.5, 116.3, 54.6; HRMS (ESI) Calcd for $C_{13}H_{12}ClN_2O^+$ $[M+H]^+$ 247.0633; Found: 247.0634.



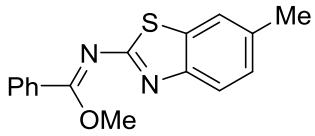
2v

Methyl (*Z*)-4-chloro-*N*-(5-methylisoxazol-3-yl)benzimidate (2v): colorless oil, 20.3mg, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 7.29–7.46 (m, 5H), 5.37 (s, 1H), 4.00 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.6, 166.4, 164.1, 131.1, 130.9, 128.8, 128.2, 97.7, 54.8, 12.7; HRMS (ESI) Calcd for $C_{12}H_{12}ClN_2O_2^+$ $[M+H]^+$ 251.0582; Found: 251.0584.



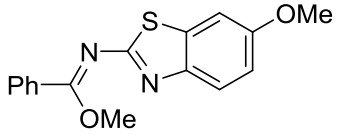
2w

Methyl (*Z*)-*N*-(6-chlorobenzo[*d*]thiazol-2-yl)benzimidate (2w): colorless oil, 25.1mg, 83% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.68 (d, *J* = 8.4 Hz, 1H), 7.60 (s, 1H), 7.53 (s, 1H), 7.51 (s, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 7.26–7.33(m, 3H), 4.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 165.0, 150.3, 135.5, 131.7, 129.8, 129.3, 129.2, 128.5, 126.5, 122.5, 120.8, 55.2; HRMS (ESI) Calcd for $C_{15}H_{12}ClN_2OS^+$ $[M+H]^+$ 303.0353; Found: 303.0353.



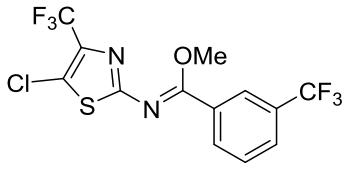
2x

Methyl (*Z*)-*N*-(6-methylbenzo[*d*]thiazol-2-yl)benzimidate (2x): colorless oil, 23.2mg, 82% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.68 (d, *J* = 8.0 Hz, 1H), 7.52-7.55 (m, 2H), 7.38-7.43 (m, 2H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.18 (d, *J* = 9.2 Hz, 1H), 4.08 (s, 3H), 2.42 (s, 3H); ^{13}CNMR (100 MHz, $CDCl_3$) δ 167.2, 164.6, 149.8, 134.5, 133.6, 131.4, 130.1, 129.3, 128.4, 127.2, 121.3, 121.2, 55.4, 21.4; HRMS (ESI) Calcd for $C_{16}H_{15}N_2OS^+$ $[M+H]^+$ 283.0900; Found: 283.0903.



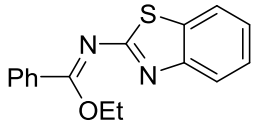
2y

Methyl (*Z*)-*N*-(6-methoxybenzo[*d*]thiazol-2-yl)benzimidate (2y): colorless oil, 25.4mg, 85% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.67 (d, *J* = 8.8 Hz, 1H), 7.52–7.55 (m, 2 H), 7.41 (d, *J* = 7.6 Hz, 1H), 7.29 (t, *J* = 7.6 Hz, 2H), 7.12 (d, *J* = 2.4 Hz, 1H), 7.00 (dd, *J* = 8.8, 2.4 Hz, 1H), 4.07 (s, 3H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 164.7, 156.6, 146.0, 135.5, 131.4, 130.2, 129.2, 128.4, 122.2, 114.3, 104.6, 55.8, 55.4; HRMS (ESI) Calcd for $C_{16}H_{15}N_2O_2S^+$ $[M+H]^+$ 299.0849; Found: 299.0850.



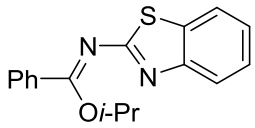
2z

Methyl (Z)-N-(5-chloro-4-(trifluoromethyl)thiazol-2-yl)-3-(trifluoromethyl)benzimidate (2z): colorless oil, 26.4mg, 68% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.82 (s, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 8.0 Hz, 2H), 7.52 (t, *J* = 8.0 Hz, 1H), 4.06 (s, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.0, -63.0; ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 164.6, 136.9 (q, 36.4 Hz), 132.3, 131.4 (q, 33.0 Hz), 130.5, 129.2, 128.5, 126.3, 123.5 (q, 271.0 Hz), 122.5 (q, 214.4 Hz), 118.7, 56.2; HRMS (ESI) Calcd for $C_{13}H_8ClF_6N_2OS^+$ $[M+H]^+$ 388.9945; Found: 388.9951.



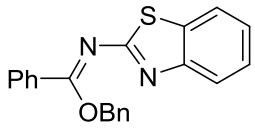
2aa

Ethyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)benzimidate (2aa): colorless oil, 22.9mg, 81% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.77–7.80 (m, 1H), 7.62–7.64 (m, 1H), 7.54–7.56 (m, 2H), 7.34–7.43 (m, 2H), 7.20–7.32 (m, 3H), 4.50–4.56 (q, *J* = 7.2 Hz, 2H), 1.48 (t, *J* = 16.0 Hz, 3H); ^{13}CNMR (100 MHz, $CDCl_3$) δ 168.2, 164.2, 151.8, 134.4, 131.4, 130.3, 129.3, 128.4, 125.7, 123.6, 121.7, 121.2, 100.0, 64.4, 14.2; HRMS (ESI) Calcd for $C_{16}H_{15}N_2OS^+$ $[M+H]^+$ 283.0900; Found: 283.0905.



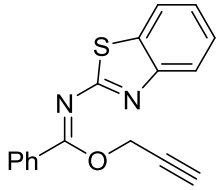
2ab

Isopropyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)benzimidate (2ab): colorless oil, 13.3mg, 45% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.78 (d, *J* = 8.4 Hz, 1H), 7.62 (d, *J* = 4.0 Hz, 1H), 7.53–7.55 (m, 2H), 7.34–7.41 (m, 2H), 7.19–7.30 (m, 3H), 5.44–5.50 (m, 1H), 1.46–1.48 (d, *J* = 6.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 163.7, 151.8, 134.4, 131.3, 130.7, 129.3, 128.4, 125.7, 123.5, 121.6, 121.1, 71.5, 21.8; HRMS (ESI) Calcd for $C_{17}H_{17}N_2OS^+$ $[M+H]^+$ 297.1056; Found: 297.1060.



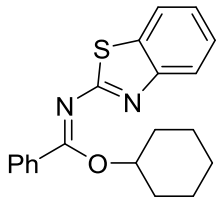
2ac

Benzyl (*Z*)-*N*-(benzo[d]thiazol-2-yl)benzimidate (2ac): colorless oil, 22.7mg, 66% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.81 (d, *J* = 10.4 Hz, 1H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.58 (d, *J* = 7.2 Hz, 2H), 7.51 (d, *J* = 9.6 Hz, 2H), 7.35–7.44 (m, 5H), 7.22–7.31 (m, 3H), 5.51 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.9, 163.8, 151.8, 135.7, 134.4, 131.6, 129.9, 129.4, 128.7, 128.5, 128.4, 128.4, 125.8, 123.7, 121.8, 121.2, 70.1; HRMS (ESI) Calcd for $C_{21}H_{17}N_2OS^+$ $[M+H]^+$ 345.1056; Found: 345.1058.



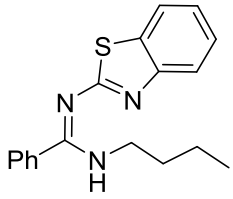
2ad

Prop-2-yn-1-yl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)benzimidate (2ad): colorless oil, 20.5mg, 70% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.80 (d, *J* = 8.0 Hz, 1H), 7.65 (d, *J* = 7.2 Hz, 1H), 7.58 (d, *J* = 7.2 Hz, 2H), 7.36–7.45 (m, 2H), 7.22–7.32 (m, 3H), 5.09 (d, *J* = 2.4Hz, 2H), 2.59(t, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 162.8, 151.7, 134.4, 131.8, 129.4, 129.2, 128.5, 125.9, 123.8, 121.9, 121.2, 77.5, 75.6, 55.7; HRMS (ESI) Calcd for $C_{17}H_{13}N_2OS^+$ $[M+H]^+$ 293.0743; Found: 293.0740.



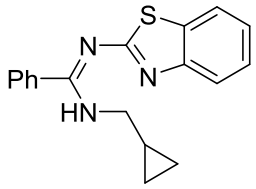
2ae

Cyclohexyl (*Z*)-*N*-(benzo[*d*]thiazol-2-yl)benzimidate (2ae): colorless oil, 22.9mg, 68% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.78 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.55 (d, *J* = 7.2 Hz, 2H), 7.33–7.41 (m, 2H), 7.18–7.30 (m, 3H), 5.22–5.28 (m, 1H), 2.08–2.13 (m, 2H), 1.79–1.86 (m, 2H), 1.59–1.74 (m, 3H), 1.31–1.52 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 163.6, 151.9, 134.4, 131.3, 130.8, 129.3, 128.3, 125.7, 123.5, 121.6, 121.1, 76.2, 31.4, 25.5, 23.8; HRMS (ESI) Calcd for $C_{20}H_{21}N_2OS^+$ $[M+H]^+$ 337.1369; Found: 337.1367.



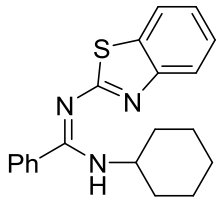
3a

(*Z*)-*N*'-(benzo[d]thiazol-2-yl)-*N*-butylbenzimidamide (3a): colorless oil, 23.8mg, 77% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 11.25 (s, 1H), 7.74 (t, *J* = 8.4 Hz, 2H), 7.58 (s, 2H), 7.47 (s, 3H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.24 (t, *J* = 7.6 Hz, 1H), 3.38 (q, *J* = 6.0 Hz, 2H), 1.62 (m, 2H), 1.44 (m, 2H), 0.94 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.9, 164.0, 151.2, 135.0, 132.5, 130.0, 128.6, 128.2, 125.6, 123.4, 121.1, 120.5, 45.2, 32.8, 19.9, 13.7; HRMS (ESI) Calcd for $C_{18}H_{20}N_3S^+$ $[M+H]^+$ 310.1372; Found: 310.1375.



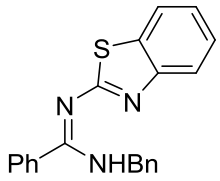
3b

(*Z*)-*N*'-(benzo[*d*]thiazol-2-yl)-*N*-(cyclopropylmethyl)benzimidamide (3b): colorless oil, 24.0mg, 78% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 11.30 (s, 1H), 7.70–7.76 (m, 2H), 7.57 (s, 2H), 7.46 (s, 3H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.23 (t, *J* = 6.4 Hz, 1H), 3.28 (s, 2H), 1.08 (s, 1H), 0.60 (q, *J* = 5.6Hz, 2H), 0.27 (q, *J* = 5.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.7, 151.3, 135.0, 130.1, 128.6, 128.2, 125.6, 123.4, 121.1, 120.5, 50.3, 11.7, 3.5; HRMS (ESI) Calcd for $C_{18}H_{18}N_3S^+$ $[M+H]^+$ 308.1216; Found: 308.1218.



3c

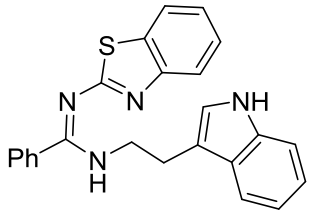
(*Z*)-*N*'-(benzo[*d*]thiazol-2-yl)-*N*-cyclohexylbenzimidamide (3c): colorless oil, 24.2mg, 72% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 11.39 (s, 1H), 7.71–7.76 (m, 2H), 7.57 (s, 2H), 7.47 (s, 3H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.23 (t, *J* = 7.6 Hz, 1H), 3.53 (s, 1H), 1.85–1.89 (m, 2H), 1.76–1.79 (m, 2H), 1.48–1.54 (m, 3H), 1.27–1.39 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.8, 163.2, 151.3, 135.4, 132.4, 129.9, 128.6, 127.8, 125.6, 123.4, 121.1, 120.5, 53.3, 34.1, 25.3, 24.0; HRMS (ESI) Calcd for $C_{20}H_{22}N_3S^+$ $[M+H]^+$ 336.1529; Found: 336.1533.



3d

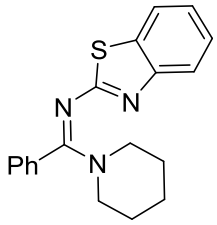
(*Z*)-*N*'-(benzo[*d*]thiazol-2-yl)-*N*-benzylbenzimidamide (3d): colorless oil, 31.6mg, 92% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 11.63 (s, 1H), 7.69–7.74 (m, 2H), 7.58 (s, 2H), 7.46 (s, 3H), 7.38 (t, *J* = 7.6 Hz, 3H), 7.32 (d, *J* = 6.4 Hz, 3H), 7.24 (t, *J* = 6.8 Hz, 1H), 4.63 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2 151.1, 138.0, 134.7, 132.6,

130.2, 128.9, 128.7, 128.2, 127.7, 126.7, 125.6, 123.5, 121.1, 120.7, 49.1; HRMS (ESI) Calcd for $C_{21}H_{18}N_3S^+$ $[M+H]^+$ 344.1216; Found: 344.1213.



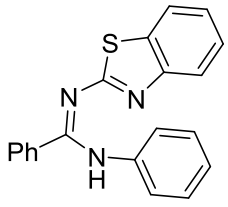
3e

(*Z*)-*N*-(2-(1H-indol-3-yl)ethyl)-*N'*-(benzo[*d*]thiazol-2-yl)benzimidamide (3e): colorless oil, 23.8mg, 60% yield. ^{1}H NMR (400 MHz, $CDCl_3$)δ = 11.19 (s, 1H), 8.23 (s, 1H), 7.71 (s, 1H), 7.55 (s, 1H), 7.34–7.45 (m, 8H), 7.18–7.26 (m, 2H), 7.08 (t, *J* = 7.2 Hz, 1H), 7.00 (s, 1H), 3.71 (s, 2H), 3.06 (s, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.0, 164.0, 151.2, 136.4, 135.0, 132.6, 130.0, 128.6, 128.1, 127.1, 125.6, 123.4, 122.8, 122.2, 121.1, 120.5, 119.5, 118.4, 111.9, 111.4, 46.0, 26.9; HRMS (ESI) Calcd for $C_{24}H_{21}N_4S^+$ $[M+H]^+$ 397.1481; Found: 397.1480.



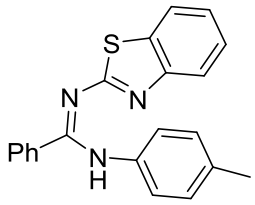
3f

(*Z*)-*N*-(benzo[*d*]thiazol-2-yl)-1-phenyl-1-(piperidin-1-yl)methanimine (3f): colorless oil, 26.4mg, 82% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 7.65 (d, *J* = 8.0 Hz, 1H), 7.36–7.45 (m, 4H), 7.30–7.33 (m, 2H), 7.20-7.24 (m, 1H), 7.02-7.07 (m, 1H), 3.97 (s, 2H), 3.20 (s, 2H), 1.70-1.76 (m, 4H), 1.51 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 163.4, 151.3, 134.3, 132.2, 130.1, 129.0, 128.6, 125.1, 122.4, 120.7, 120.6, 49.2, 45.8, 26.7, 25.5, 24.6; HRMS (ESI) Calcd for $C_{19}H_{20}N_3S^+$ $[M+H]^+$ 322.1372; Found: 322.1370.



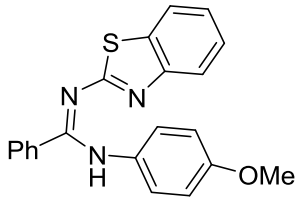
3g

(*Z*)-*N*'-(benzo[*d*]thiazol-2-yl)-*N*-phenylbenzimidamide (3g): colorless oil, 22.4mg, 68% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 12.92 (s, 1H), 7.77–7.84 (dd, *J* = 8.0, 21.2 Hz, 2H), 7.61 (d, *J* = 7.2 Hz, 2H), 7.38–7.45 (m, 2H), 7.23–7.35 (m, 5H), 7.13 (t, *J* = 7.6 Hz 1H), 7.00 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 150.8, 137.6, 134.3, 130.6, 129.5, 129.2, 128.5, 126.0, 124.0, 121.3, 121.0; HRMS (ESI) Calcd for $C_{20}H_{16}N_3S^+$ $[M+H]^+$ 330.1059; Found: 330.1063.



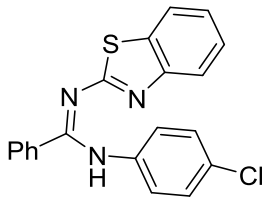
3h

(*Z*)-*N*'-(benzo[*d*]thiazol-2-yl)-*N*-(*p*-tolyl)benzimidamide (3h): colorless oil, 26.1mg, 76% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 12.83 (s, 1H), 7.80 (t, *J* = 9.2 Hz, 2H), 7.58 (d, *J* = 6.8 Hz, 2H), 7.38–7.42 (m, 2H), 7.25–7.31 (m, 3H), 7.03 (d, *J* = 8.0 Hz, 2H), 6.88 (s, 2H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 151.0, 136.3, 135.1, 130.3, 129.6, 129.5, 128.3, 125.8, 124.3, 123.8, 121.2, 120.9, 20.9; HRMS (ESI) Calcd for $C_{21}H_{18}N_3S^+$ $[M+H]^+$ 344.1216; Found: 344.1210.



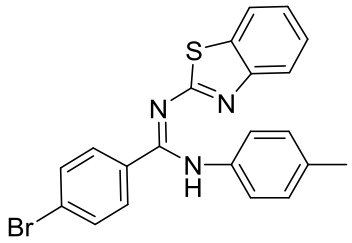
3i

(*Z*)-*N*'-(benzo[*d*]thiazol-2-yl)-*N*-(4-methoxyphenyl)benzimidamide (3i): colorless oil, 28.0mg, 78% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 12.78 (s, 1H), 7.77 (t, *J* = 8.0 Hz, 2H), 7.56 (d, *J* = 6.8 Hz, 2H), 7.34–7.42 (m, 2H), 7.25–7.32 (m, 3H), 6.93 (d, *J* = 8.4 Hz, 2H), 6.76 (d, *J* = 8.8 Hz, 2H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 157.3, 151.0, 134.7, 131.9, 130.2, 129.5, 128.2, 126.0, 125.8, 123.7, 121.2, 120.8, 114.2, 55.4; HRMS (ESI) Calcd for $C_{21}H_{18}N_3OS^+$ $[M+H]^+$ 360.1165; Found: 360.1168.



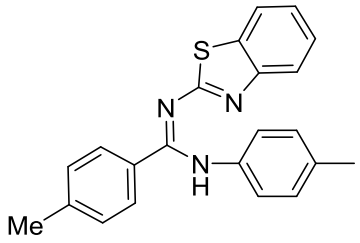
3j

(*Z*)-*N*'-(benzo[*d*]thiazol-2-yl)-*N*-(4-chlorophenyl)benzimidamide (3j): colorless oil, 20.7mg, 57% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 12.87 (s, 1H), 7.76–7.82 (m, 2H), 7.56 (d, *J* = 7.2 Hz, 2H), 7.29–7.43 (m, 5H), 7.19 (d, *J* = 8.8 Hz, 2H), 6.89 (d, *J* = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 150.8, 137.6, 134.3, 130.6, 129.5, 129.2, 128.5, 126.0, 124.0, 121.3, 121.0; HRMS (ESI) Calcd for $C_{20}H_{15}ClN_3S^+$ $[M+H]^+$ 364.0670; Found: 364.0675.



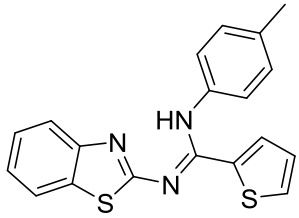
3k

(*Z*)-*N*'-(benzo[*d*]thiazol-2-yl)-4-bromo-*N*-(*p*-tolyl)benzimidamide (3k): colorless oil, 34.6mg, 82% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 12.80 (s, 1H), 7.78 (t, *J* = 8.8 Hz, 2H), 7.39–7.47 (m, 5H), 7.27–7.30 (m, 1H), 7.06 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 150.9, 136.1, 135.5, 133.7, 131.5, 131.2, 129.8, 125.9, 124.9, 124.4, 123.9, 121.3, 121.0, 21.0; HRMS (ESI) Calcd for $C_{21}H_{17}BrN_3S^+$ $[M+H]^+$ 422.0321; Found: 422.0323.



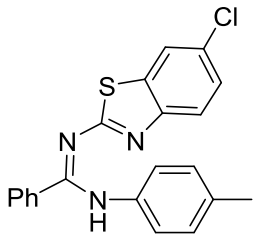
3l

(*Z*)-*N*'-(benzo[*d*]thiazol-2-yl)-4-methyl-N-(*p*-tolyl)benzimidamide (3l): colorless oil, 19.3mg, 54% yield. ^{1}HNMR (400 MHz, $CDCl_3$) δ = 12.79 (s, 1H), 7.76–7.80 (q, *J* = 8.0 Hz, 2H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.27 (t, *J* = 7.6 Hz, 1H), 7.03–7.13 (dd, *J* = 8.0, 30.4 Hz, 4H), 6.91 (s, 2H), 2.33 (d, *J* = 18.4 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.3, 160.3, 151.1, 140.6, 136.6, 135.0, 132.8, 131.8, 129.6, 129.6, 129.0, 125.8, 124.2, 123.7, 121.2, 120.8, 21.5, 20.9; HRMS (ESI) Calcd for $C_{22}H_{20}N_3S^+$ $[M+H]^+$ 358.1372; Found: 358.1370.



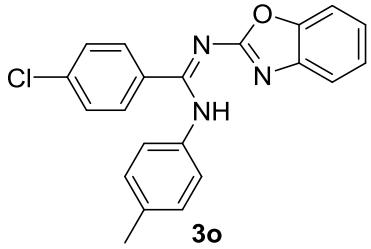
3m

(*Z*)-*N*'-(benzo[*d*]thiazol-2-yl)-*N*-(*p*-tolyl)thiophene-2-carboximidamide (3m): colorless oil, 23.1mg, 66% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 12.70 (s, 1H), 7.76 (q, *J* = 4.4 Hz, 2H), 7.36–7.41 (m, 2H), 7.26 (t, *J* = 7.6 Hz, 1H), 7.17 (q, *J* = 8.4 Hz, 4H), 6.97 (d, *J* = 3.6 Hz, 1H), 6.88 (t, J = 4.4 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 154.4, 151.1, 137.8, 136.9, 136.1, 132.6, 131.9, 130.5, 130.0, 127.4, 126.2, 125.8, 123.6, 121.2, 120.7, 21.2; HRMS (ESI) Calcd for $C_{19}H_{16}N_3S_2^+$ $[M+H]^+$ 350.0780; Found: 350.0781.



3n

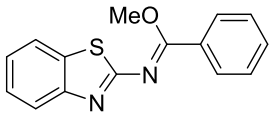
(*Z*)-*N*'-(6-chlorobenzo[*d*]thiazol-2-yl)-*N*-(*p*-tolyl)benzimidamide (3n): colorless oil, 24.9mg, 66% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 12.67 (s, 1H), 7.71 (d, *J* = 2.0 Hz, 1H), 7.68 (d, *J* = 8.8 Hz, 1H), 7.57 (d, *J* = 7.2 Hz, 2H), 7.29–7.40 (m, 4H), 7.03 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 7.6 Hz, 2H), 2.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.5, 160.5, 149.6, 136.2, 135.4, 134.6, 134.0, 130.4, 129.7, 129.5, 129.2, 128.3, 126.5, 124.3, 121.6, 120.9, 21.0; HRMS (ESI) Calcd for $C_{21}H_{17}ClN_3S^+$ $[M+H]^+$ 378.0826; Found: 378.0821.



3o

(*Z*)-*N*'-(benzo[*d*]oxazol-2-yl)-4-chloro-*N*-(*p*-tolyl)benzimidamide (3o): colorless oil, 25.3mg, 70% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 12.33 (s, 1H), 7.51–7.57 (m, 3H), 7.44–7.46 (m, 1H), 7.21–7.29 (m, 4H), 7.05 (d, *J* = 8.0 Hz, 2H), 6.87 (d, *J* = 8.0 Hz, 2H), 2.30 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.4, 161.6, 147.7, 141.2, 136.8, 136.0, 135.9, 132.8, 131.1, 129.9, 128.5, 124.6, 124.0, 123.7, 117.9, 110.0, 21.0; HRMS (ESI) Calcd for $C_{21}H_{17}ClN_3O^+$ $[M+H]^+$ 362.1055; Found: 362.1056.

1. (a) M. Frıas, A. C. Carrasco, A. Fraile and J. Aleman, *Chem.–Eur. J.*, **2018**, *24*, 3117; (b) H.-X. He, W. Yang and D.-M. Du, *Adv. Synth. Catal.*, **2013**, *355*, 1137; (c) Q. Ni, X. Song, J. Xiong, G. Raabe, D. Enders, *Chem. Commun.*, **2015**, *51*, 1263. (d) L. Jarrige, D. Glavac, G. Levitre, P. Retailleau, G. Bernadat, L. Neuville, G. Masson. *Chem. Sci.*, **2019**,*10*, 3765. (e) Q. Ni, X. Wang, F. Xu, X. Chen, X. Song. *Chem. Commun.*, **2020**, *56*, 3155.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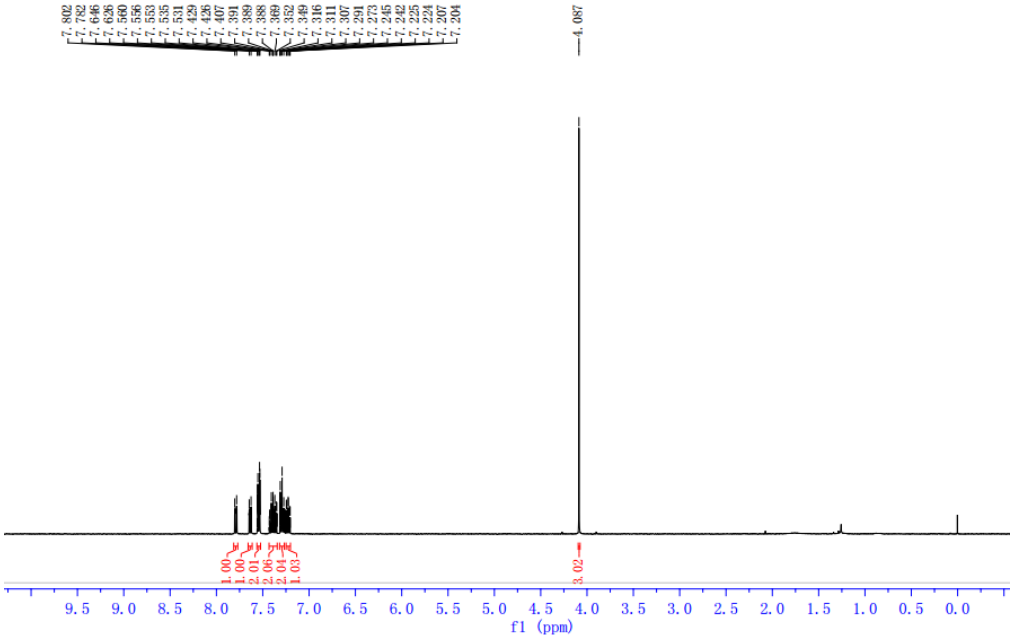
S
N
N

2a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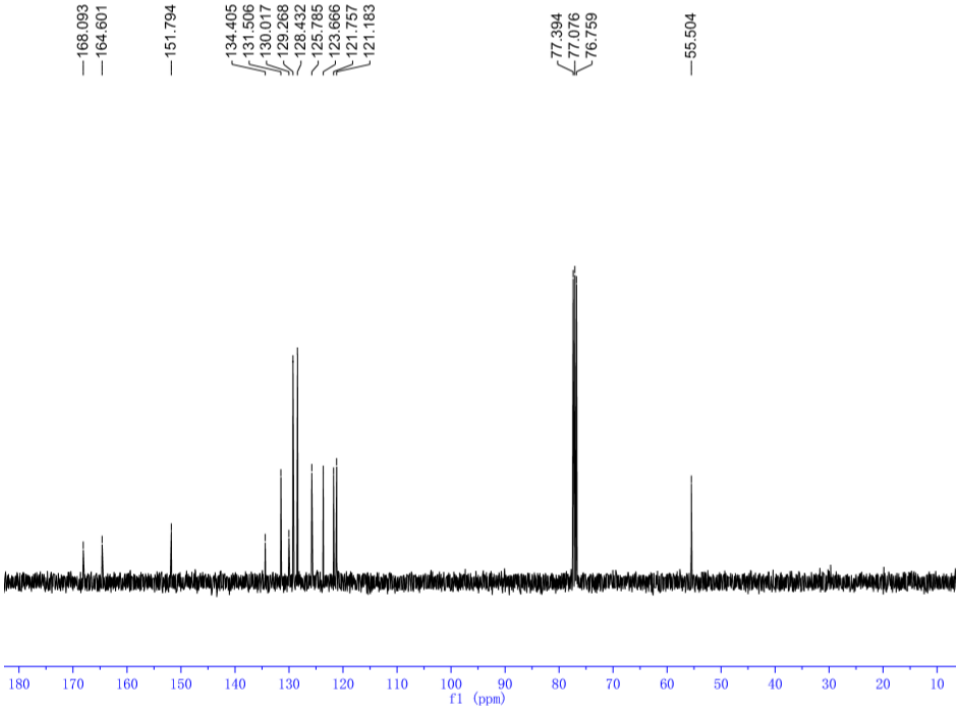
1.03
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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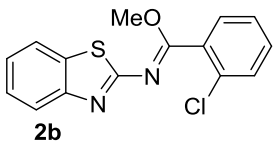
MeO
S
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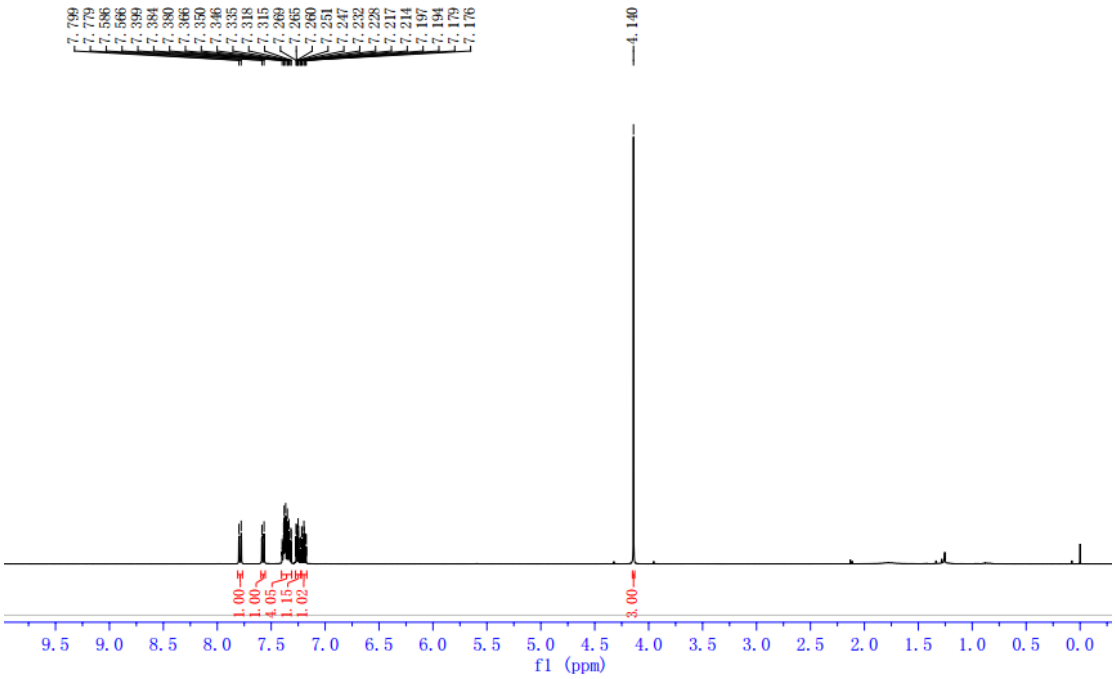
N
Cl

2b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1.02
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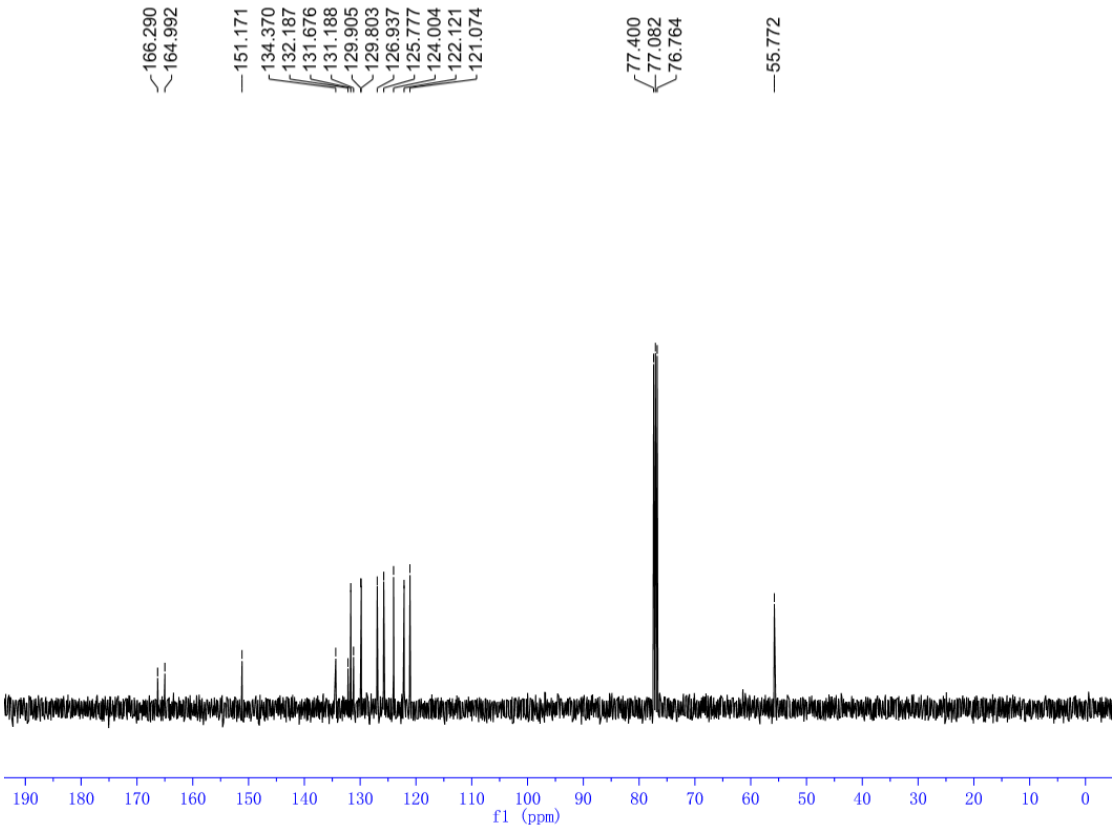
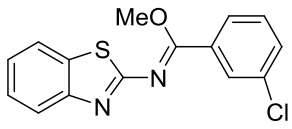
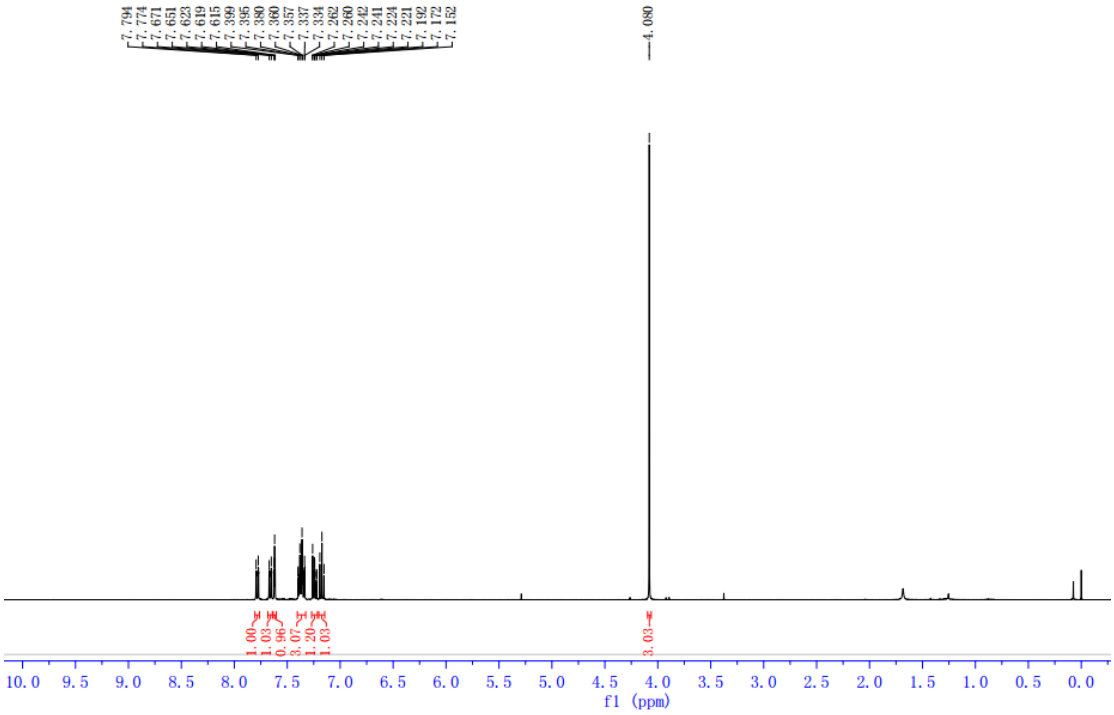
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


166.290
164.992
151.171
134.370
132.187
131.676
131.188
129.905
129.803
126.937
125.777
124.004
122.121
121.074
77.400
77.082
76.764
55.772
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


MeO
S
N
N
Cl

2c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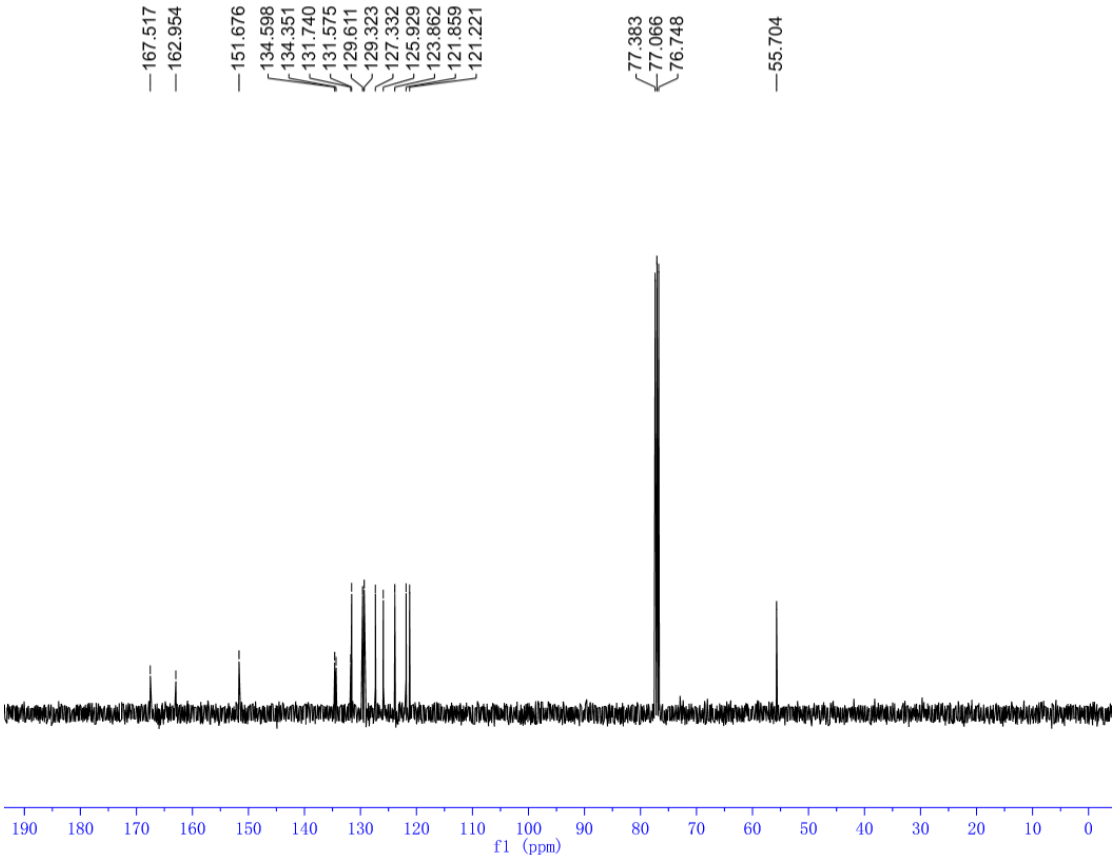
7.774
7.671
7.651
7.623
7.619
7.615
7.399
7.395
7.380
7.360
7.357
7.337
7.334
7.262
7.260
7.242
7.241
7.224
7.221
7.192
7.172
7.152
4.080
1.00
1.03
0.96
3.07
1.20
1.03
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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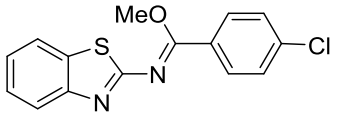
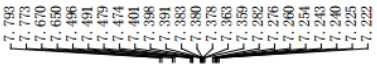
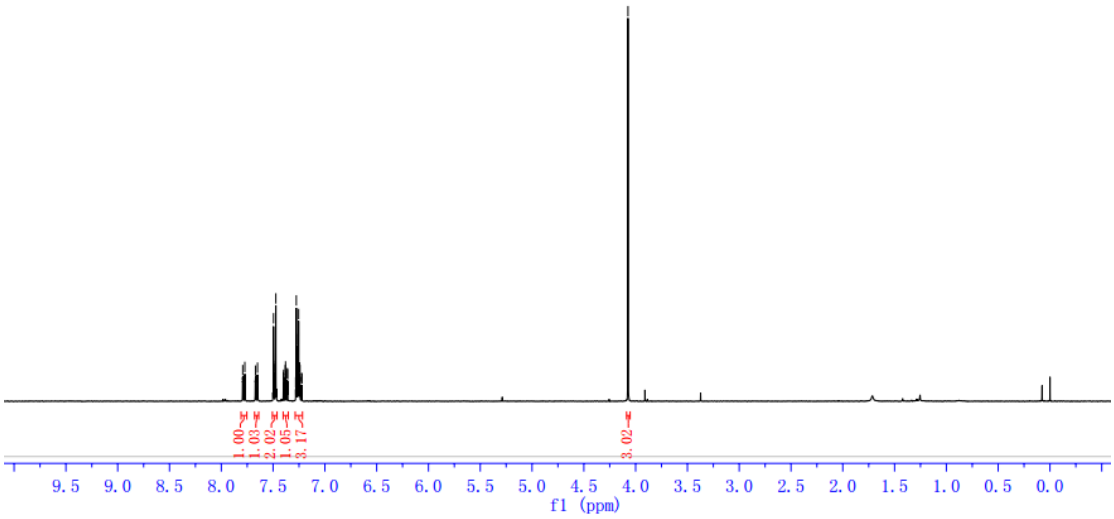
162.954
151.676
134.598
134.351
131.740
131.575
129.611
129.323
127.332
125.929
123.862
121.859
121.221
77.383
77.066
76.748
55.704
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

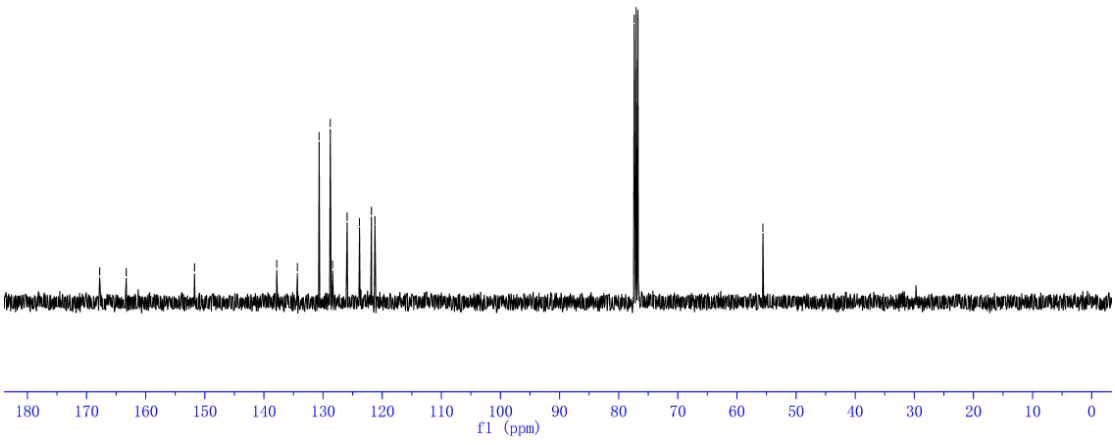

MeO
S
N
N
Cl

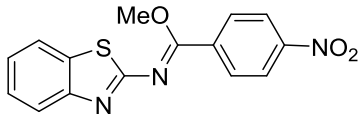
2d


7.793
7.773
7.670
7.650
7.496
7.491
7.479
7.474
7.401
7.398
7.391
7.383
7.380
7.378
7.363
7.359
7.282
7.276
7.260
7.254
7.243
7.240
7.225
7.222
4.074

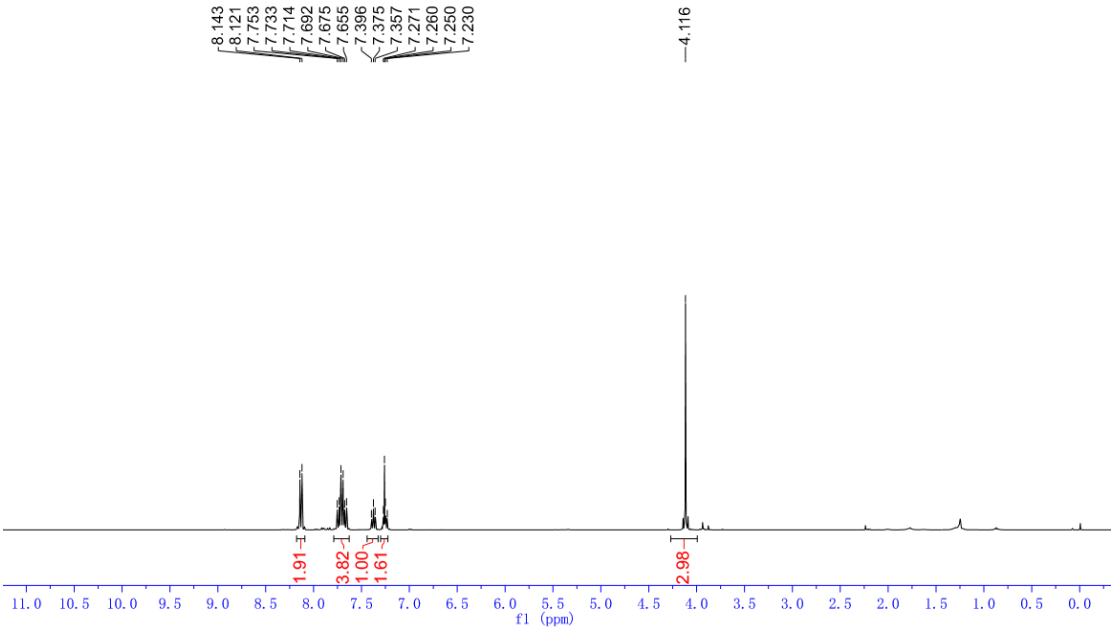

1.00
1.03
2.02
1.05
3.17
3.02
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

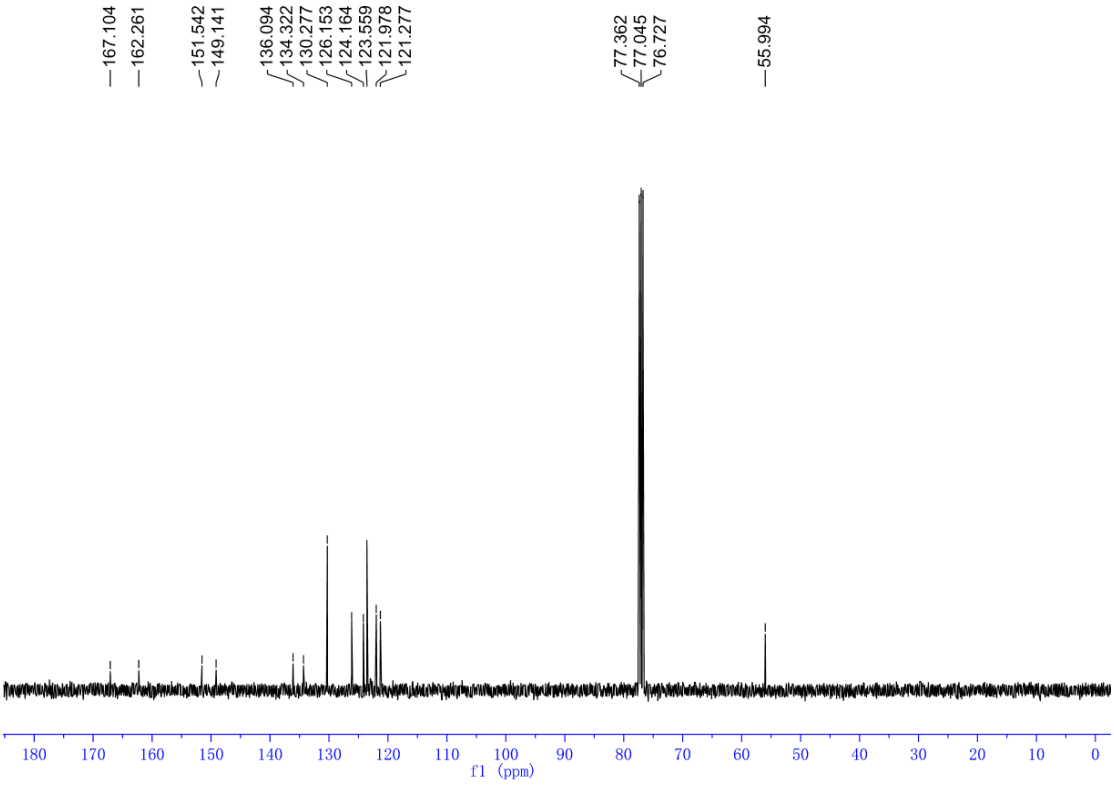

167.781
163.285
151.734
137.836
134.340
130.659
128.783
128.388
125.926
123.840
121.821
121.226
77.377
77.060
76.742
55.604

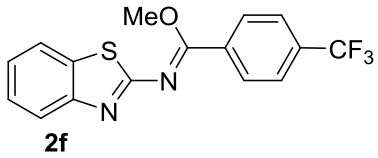

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


MeO
S
N
N
NO2

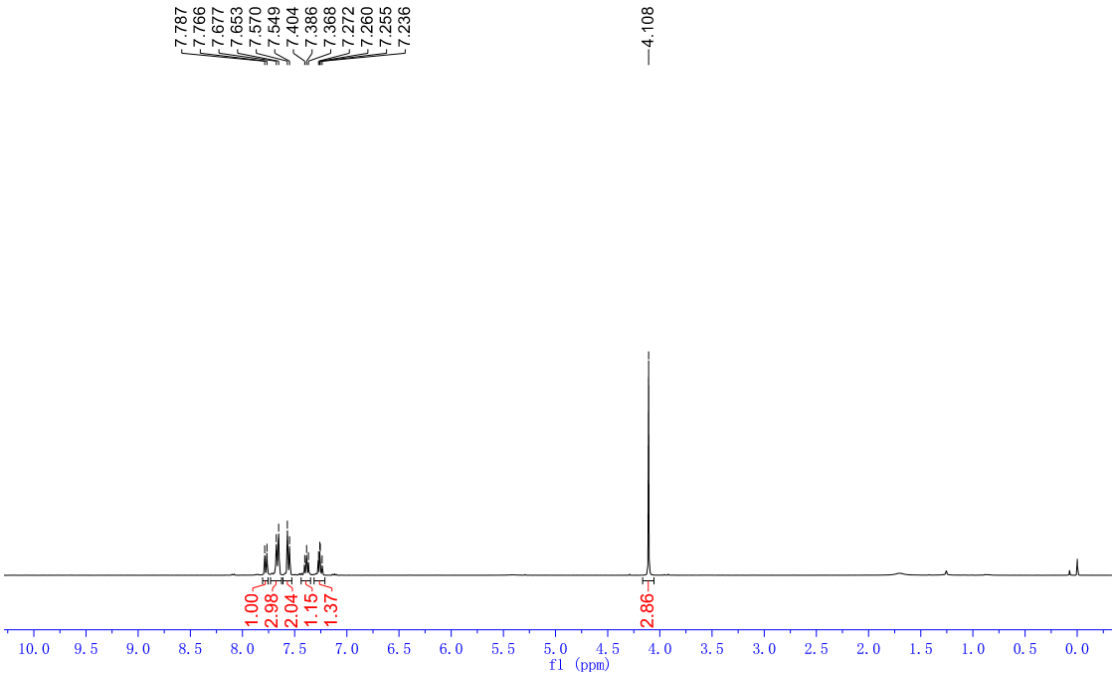
2e

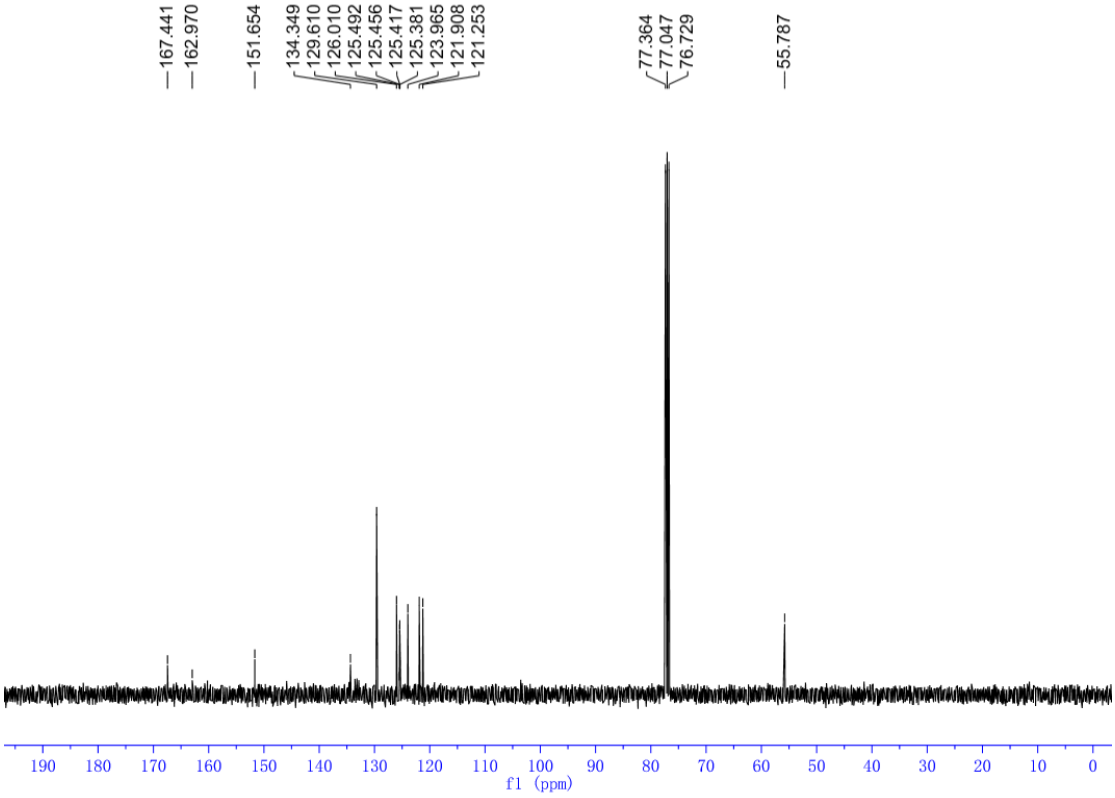

8.143
8.121
7.753
7.733
7.714
7.692
7.675
7.655
7.396
7.375
7.357
7.271
7.260
7.250
7.230
4.116
1.91
3.82
1.00
1.61
2.98
f1 (ppm)

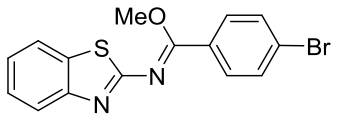

167.104
162.261
151.542
149.141
136.094
134.322
130.277
126.153
124.164
123.559
121.978
121.277
77.362
77.045
76.727
55.994
f1 (ppm)


MeO
S
N
N
CF3

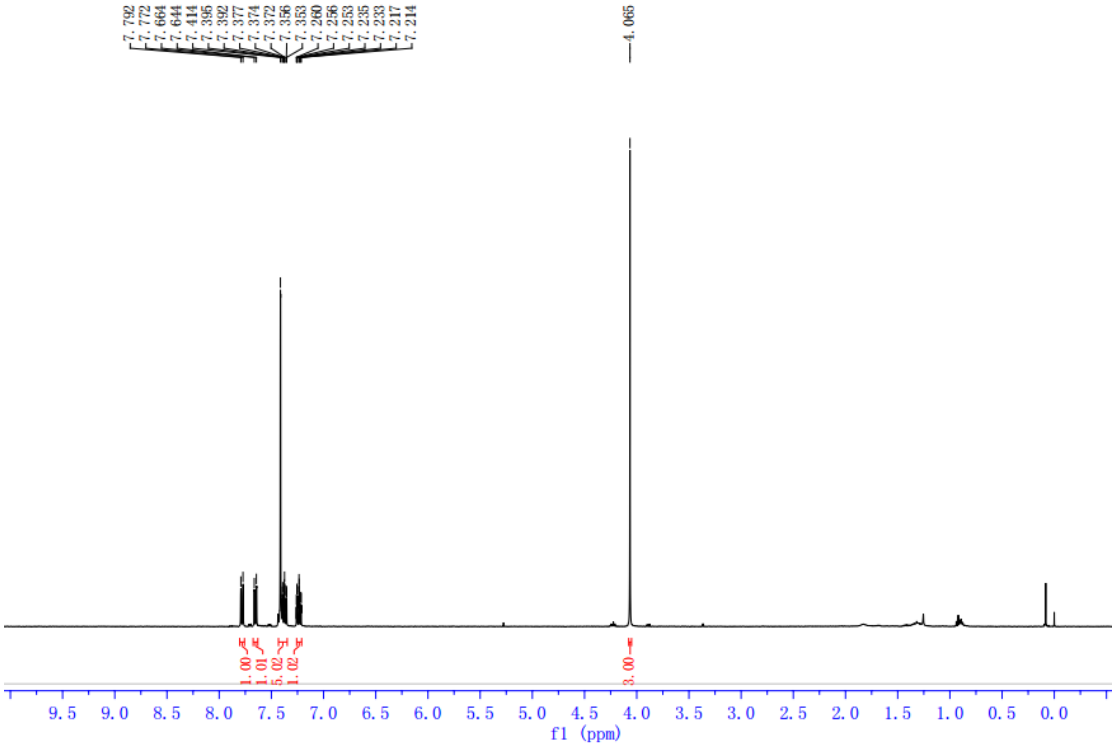
2f

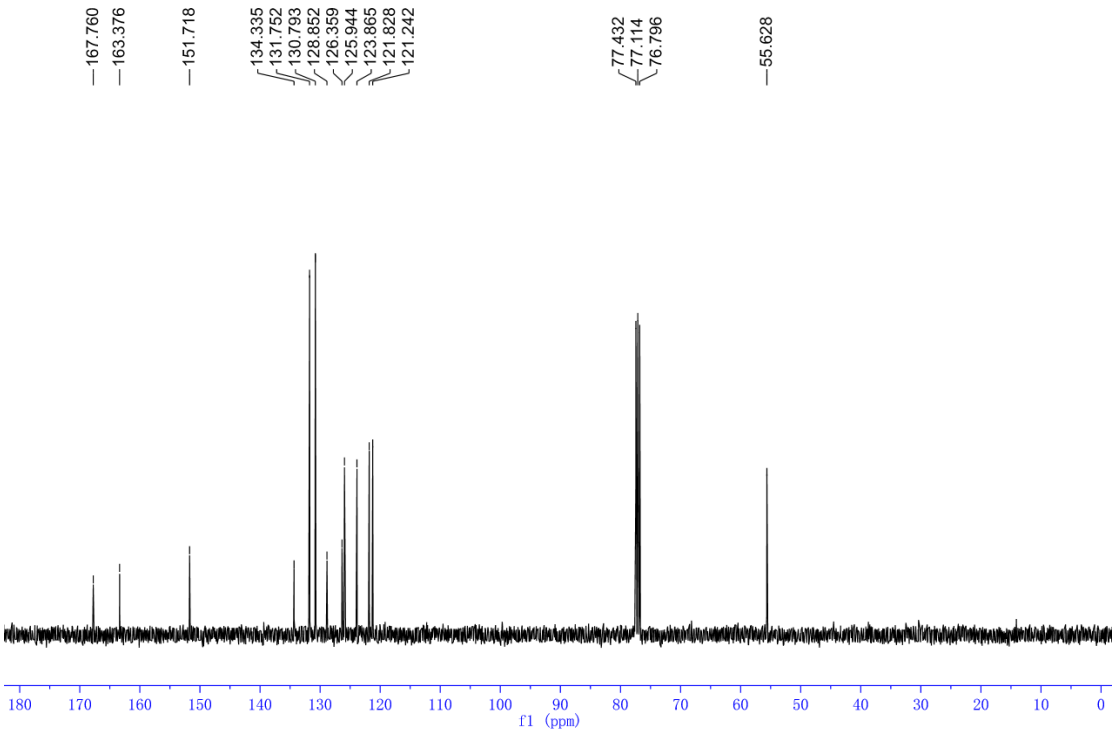

7.787
7.766
7.677
7.653
7.570
7.549
7.404
7.386
7.368
7.272
7.260
7.255
7.236
4.108
1.00
2.98
2.04
1.15
1.37
2.86
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


167.441
162.970
151.654
134.349
129.610
126.010
125.492
125.456
125.417
125.381
123.965
121.908
121.253
77.364
77.047
76.729
55.787
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


MeO
S
N
N
Br

2g


7.792
7.772
7.664
7.644
7.414
7.395
7.392
7.377
7.374
7.372
7.356
7.353
7.260
7.256
7.253
7.235
7.233
7.217
7.214
4.065
1.00
1.01
5.02
1.02
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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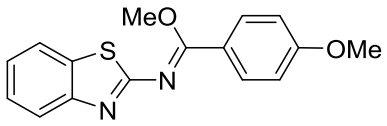
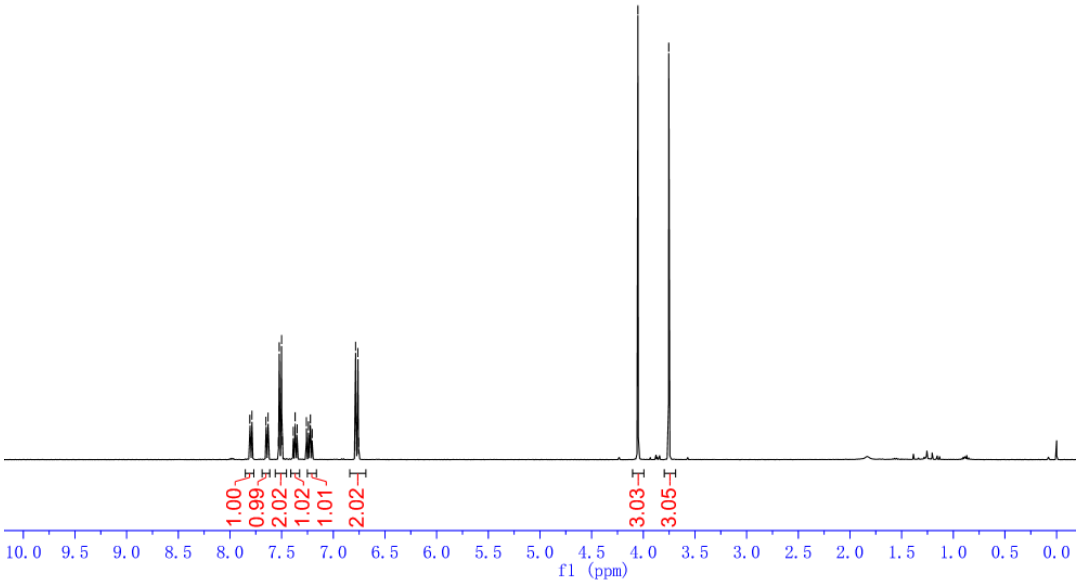
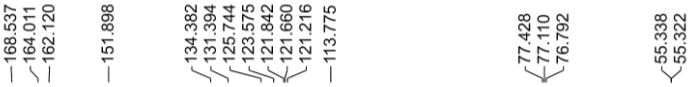
151.718
134.335
131.752
130.793
128.852
126.359
125.944
123.865
121.828
121.242
77.432
77.114
76.796
55.628
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

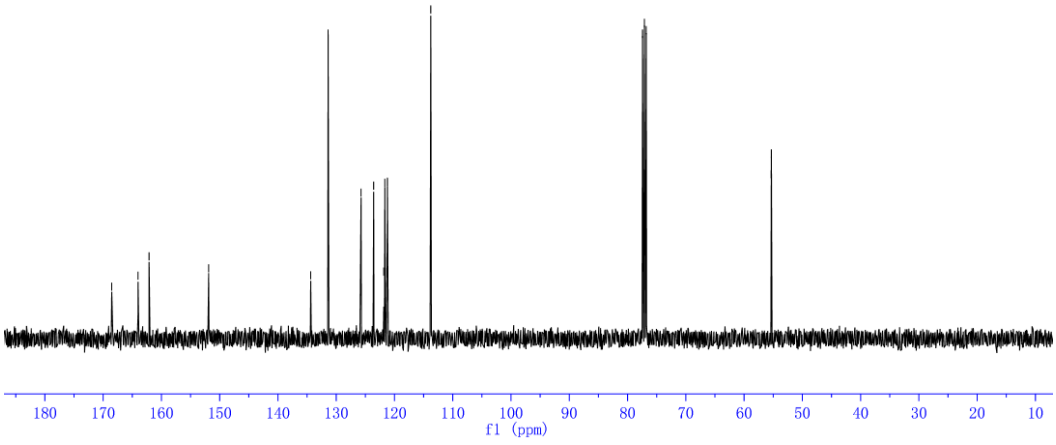

MeO
S
N
N
OMe

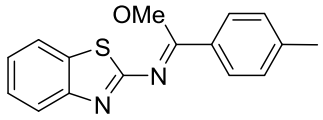
2h


7.808
7.787
7.653
7.631
7.531
7.523
7.501
7.493
7.388
7.370
7.349
7.260
7.240
7.222
7.205
6.793
6.784
6.762
6.754
4.052
3.753

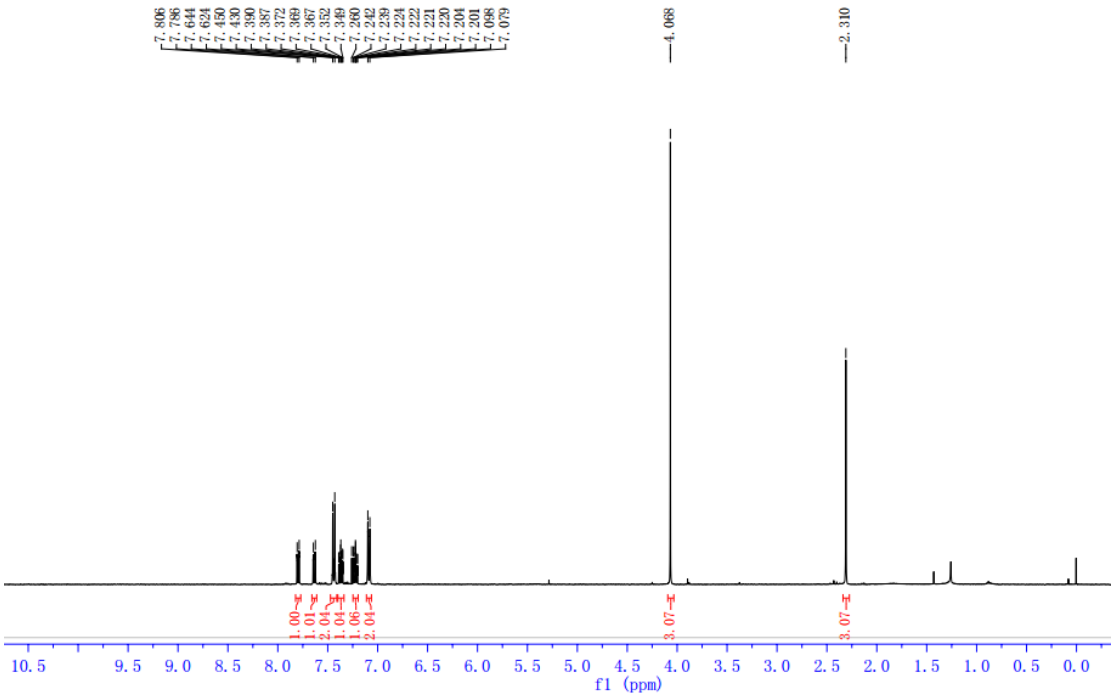

1.00
0.99
2.02
1.02
1.01
2.02
3.03
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


168.537
164.011
162.120
151.898
134.382
131.394
125.744
123.575
121.842
121.660
121.216
113.775
77.428
77.110
76.792
55.338
55.322


180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


OMe
S
N
N

2i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7.390
7.387
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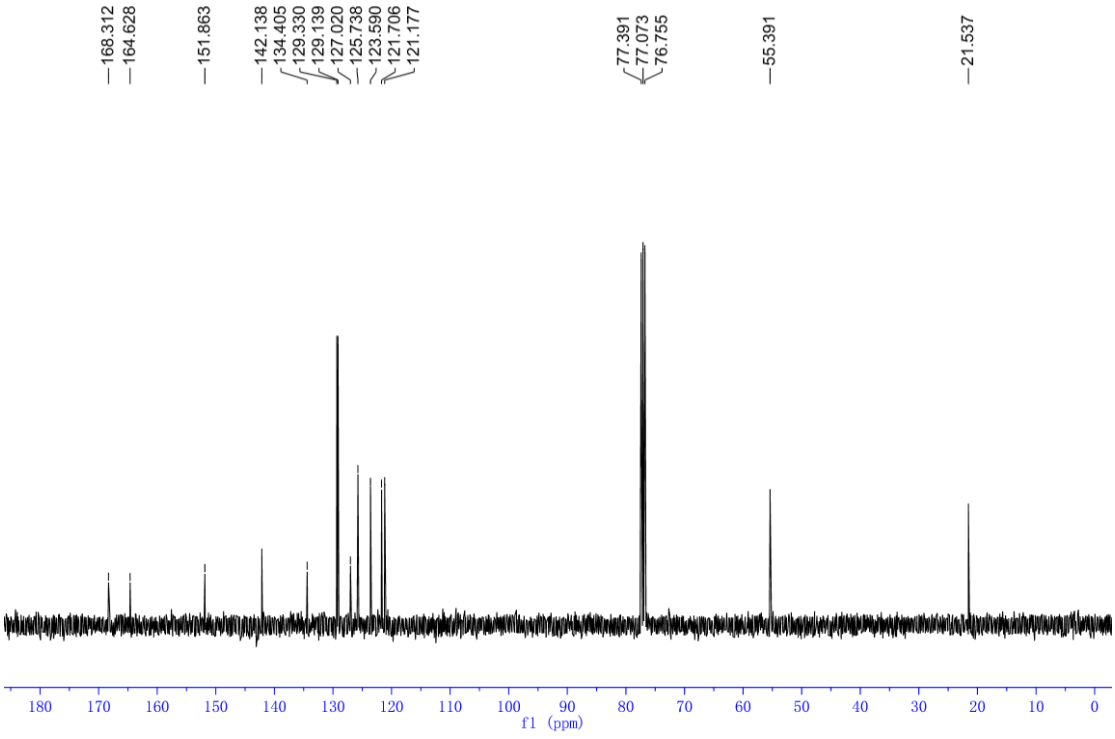
7.369
7.367
7.332
7.349
7.260
7.242
7.239
7.224
7.222
7.221
7.220
7.204
7.201
7.098
7.079
4.068
2.310
1.00
1.01
2.04
1.04
1.06
2.04
3.07
3.07
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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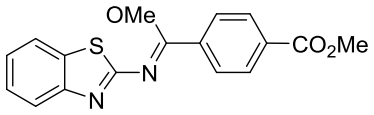
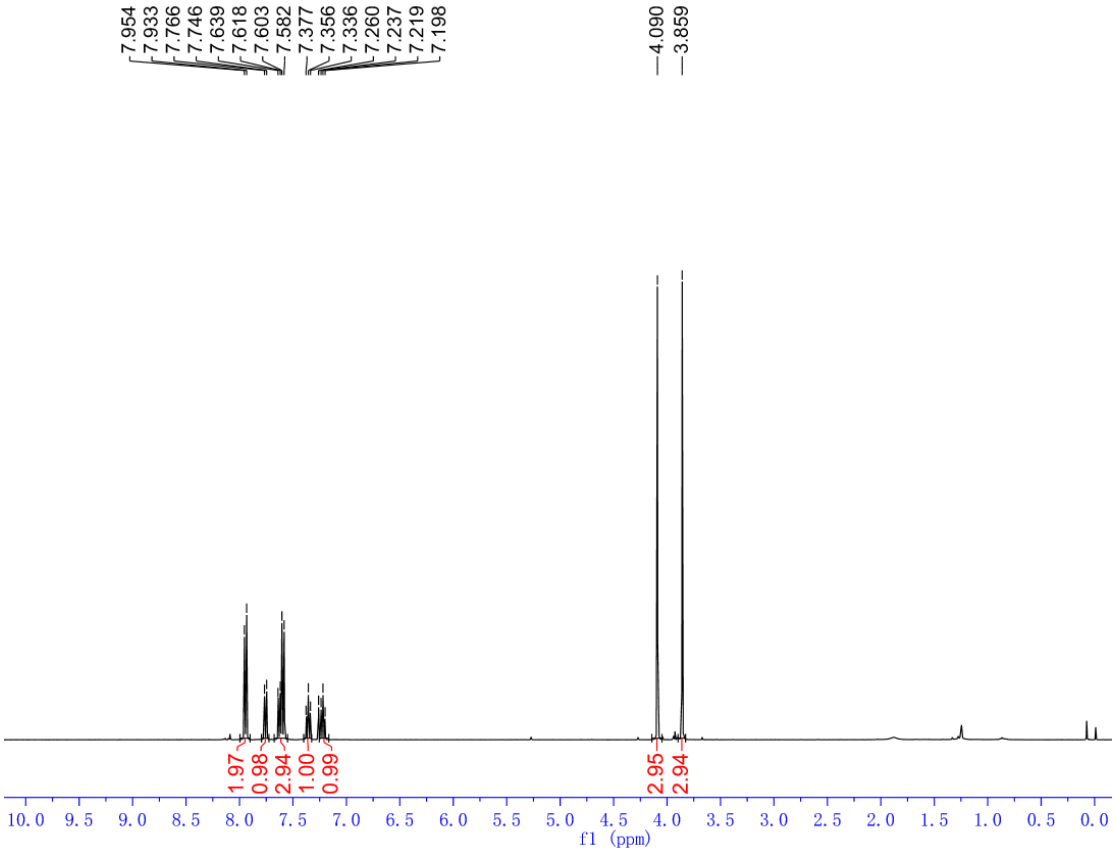
164.628
151.863
142.138
134.405
129.330
129.139
127.020
125.738
123.590
121.706
121.177
77.391
77.073
76.755
55.391
21.537
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
S
N
N
CO2Me

2j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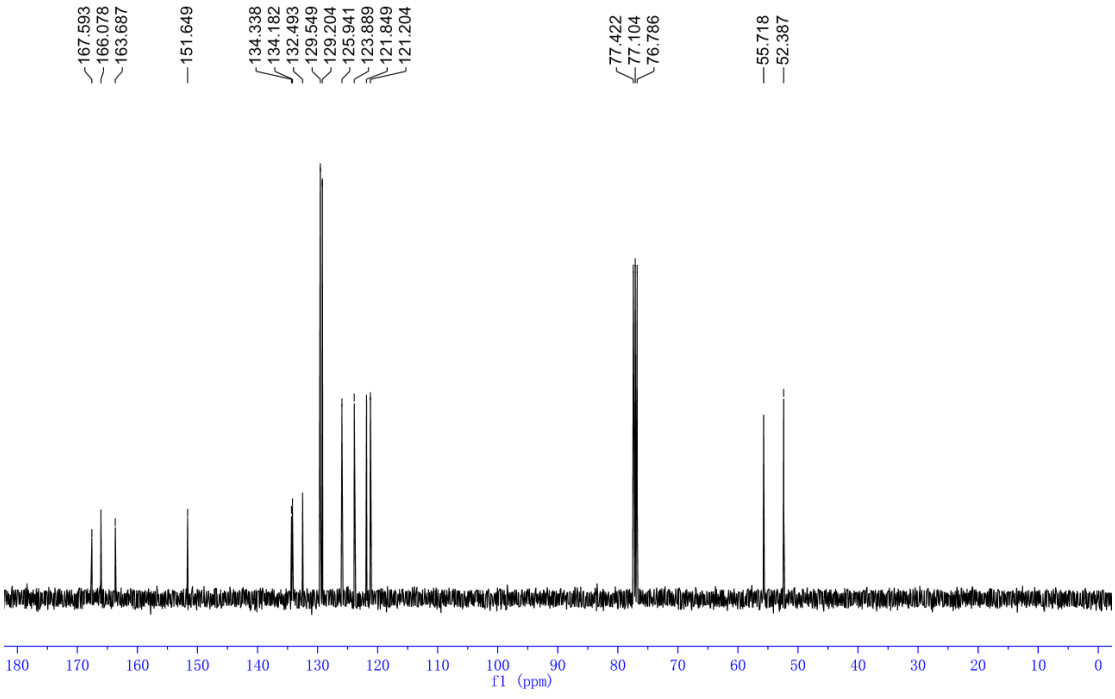
7.933
7.766
7.746
7.639
7.618
7.603
7.582
7.377
7.356
7.336
7.260
7.237
7.219
7.198
4.090
3.859
1.97
0.98
2.94
1.00
0.99
2.95
2.94
f1 (ppm)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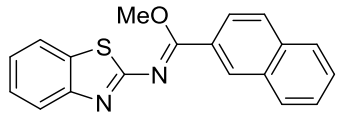
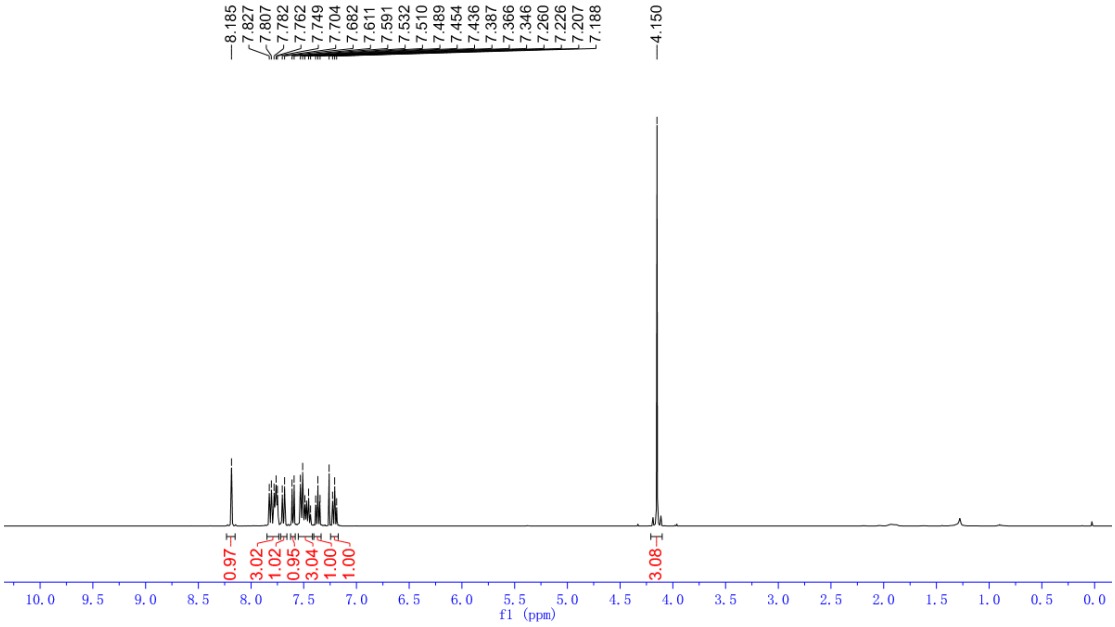
166.078
163.687
151.649
134.338
134.182
132.493
129.549
129.204
125.941
123.889
121.849
121.204
77.422
77.104
76.786
55.718
52.387
f1 (ppm)


MeO
S
N
N

2k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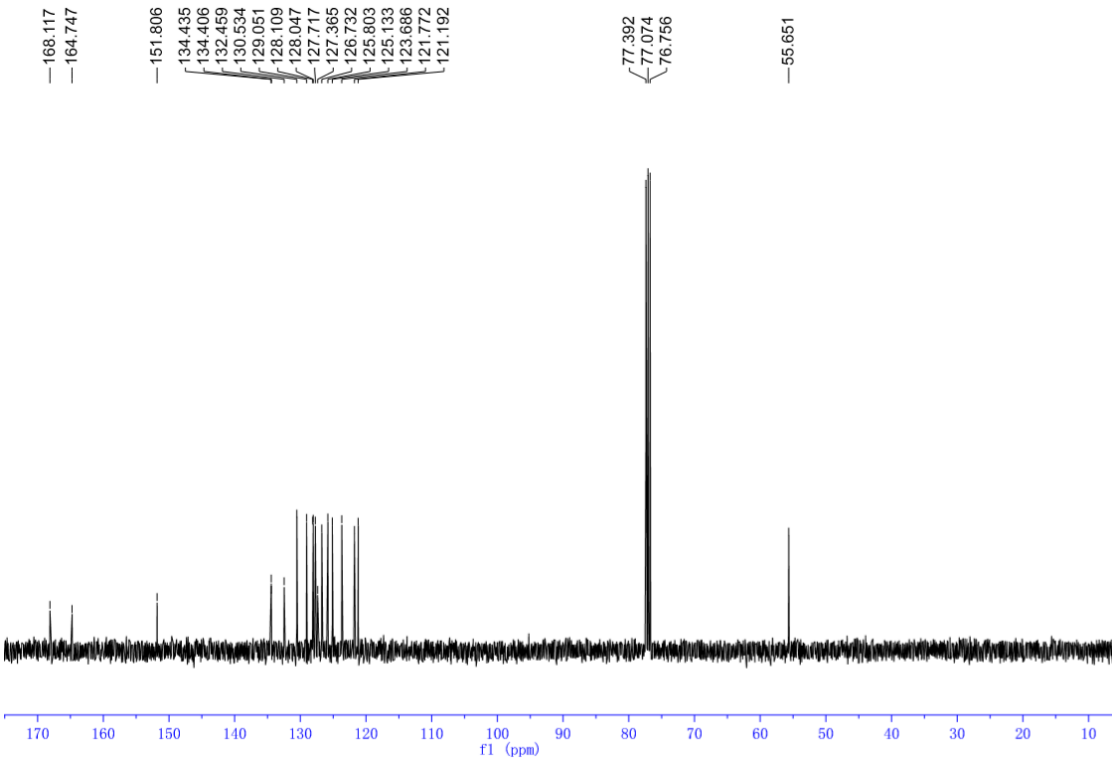
7.827
7.807
7.782
7.762
7.749
7.704
7.682
7.611
7.591
7.532
7.510
7.489
7.454
7.436
7.387
7.366
7.346
7.260
7.226
7.207
7.188
4.150
0.97
3.02
1.02
0.95
3.04
1.00
1.00
3.08
f1 (ppm)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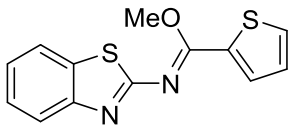
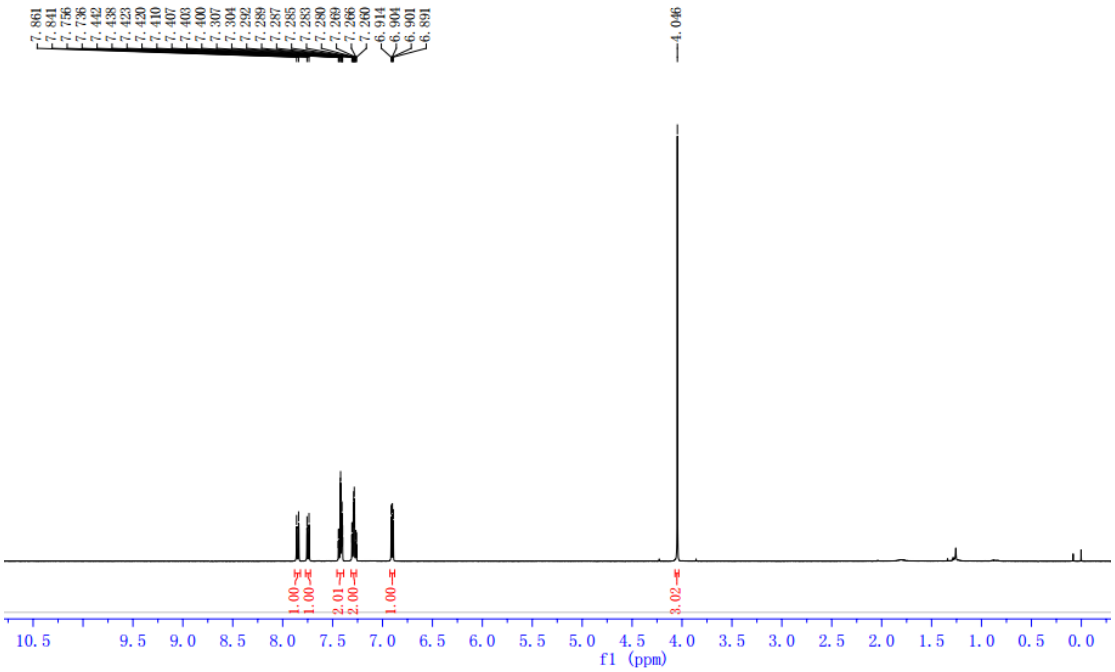
134.406
132.459
130.534
129.051
128.109
128.047
127.717
127.365
126.732
125.803
125.133
123.686
121.772
121.192
77.392
77.074
76.756
55.651
f1 (ppm)


MeO
S
S
N
N

2l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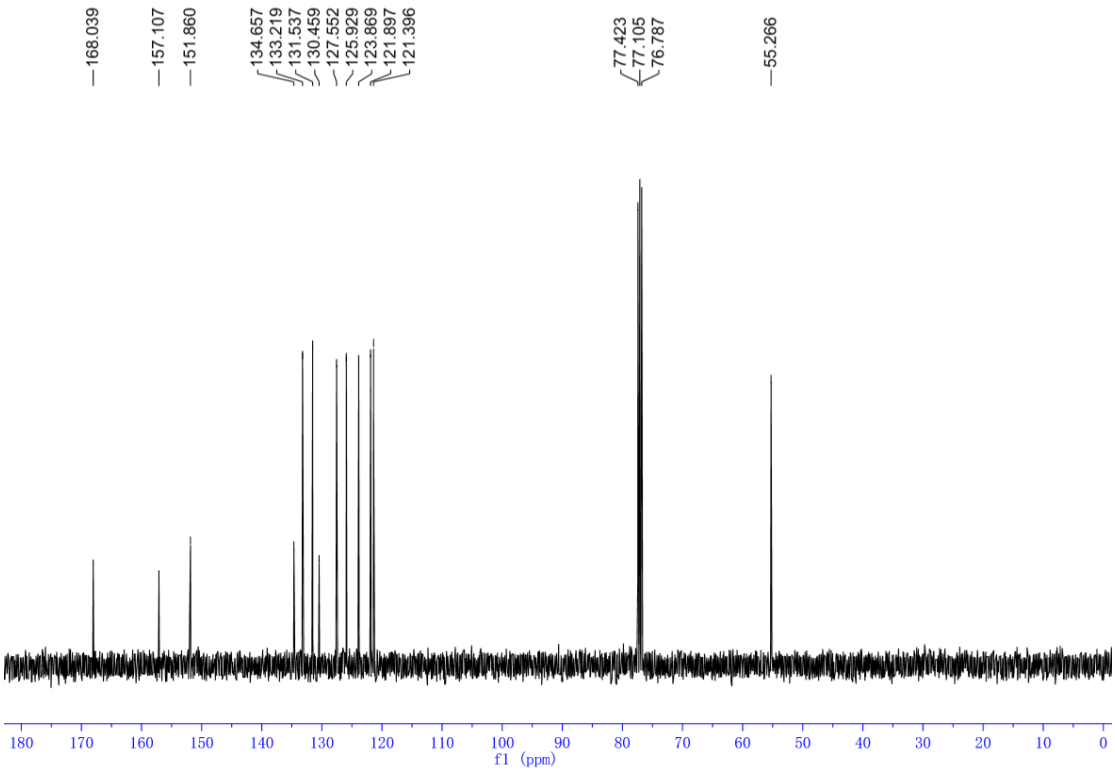
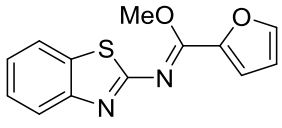
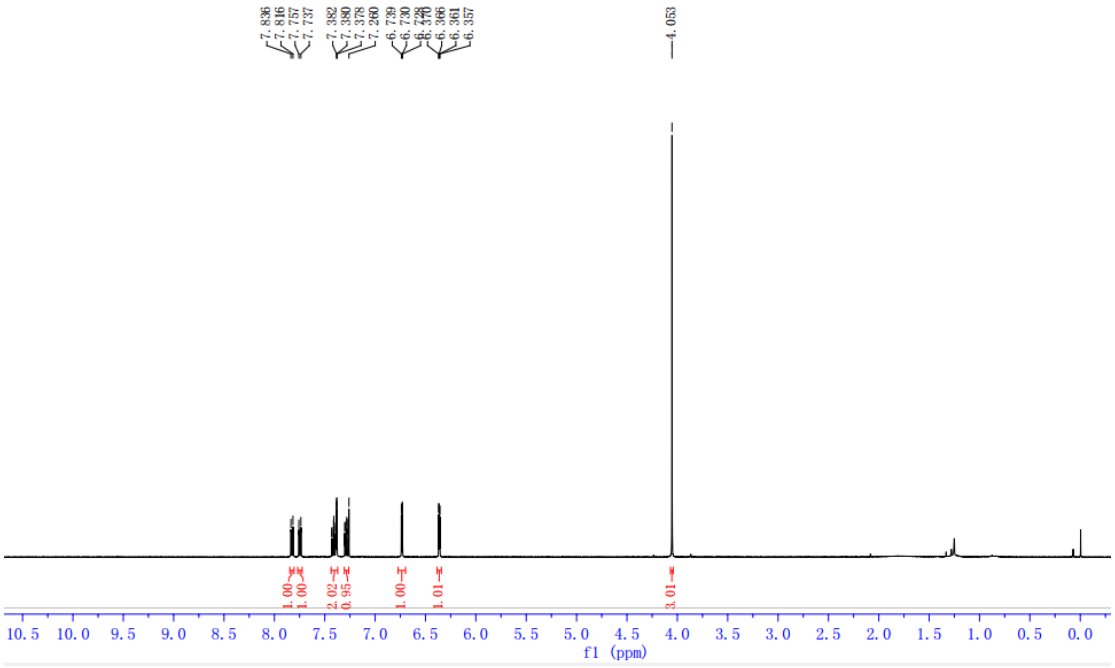
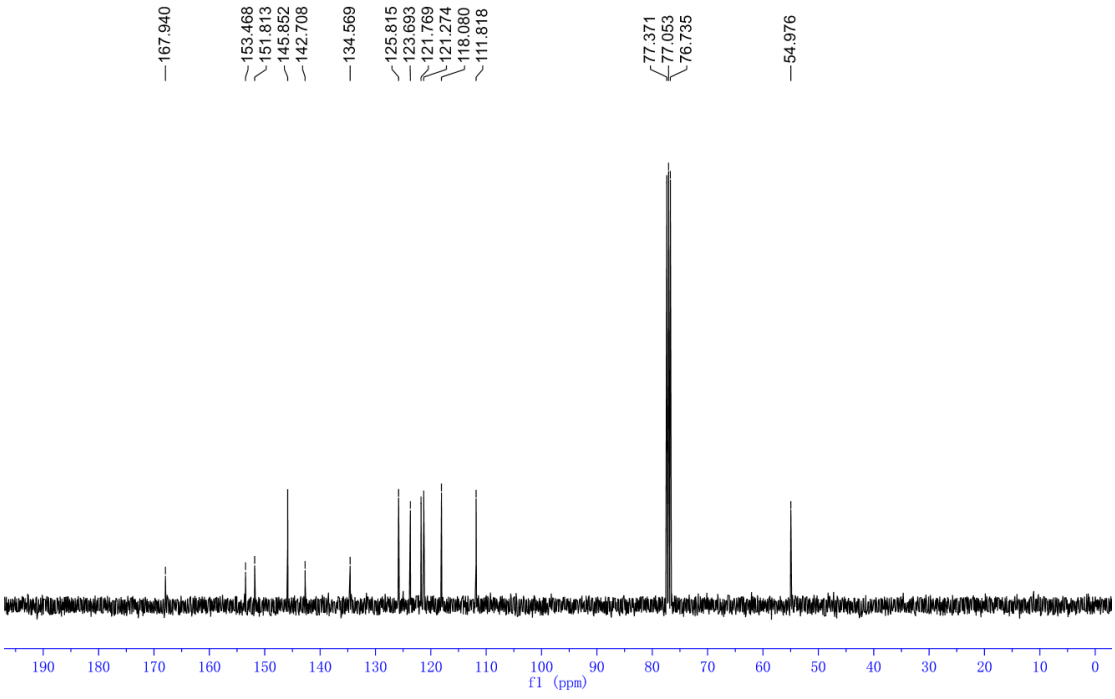
7.423
7.420
7.410
7.407
7.403
7.400
7.307
7.304
7.292
7.289
7.287
7.285
7.283
7.280
7.269
7.266
7.260
6.914
6.904
6.901
6.891
4.046
1.00
1.00
2.01
2.00
1.00
3.02
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

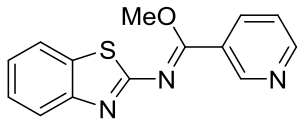

168.039
157.107
151.860
134.657
133.219
131.537
130.459
127.552
125.929
123.869
121.897
121.396
77.423
77.105
76.787
55.266
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


MeO
O
S
N
N

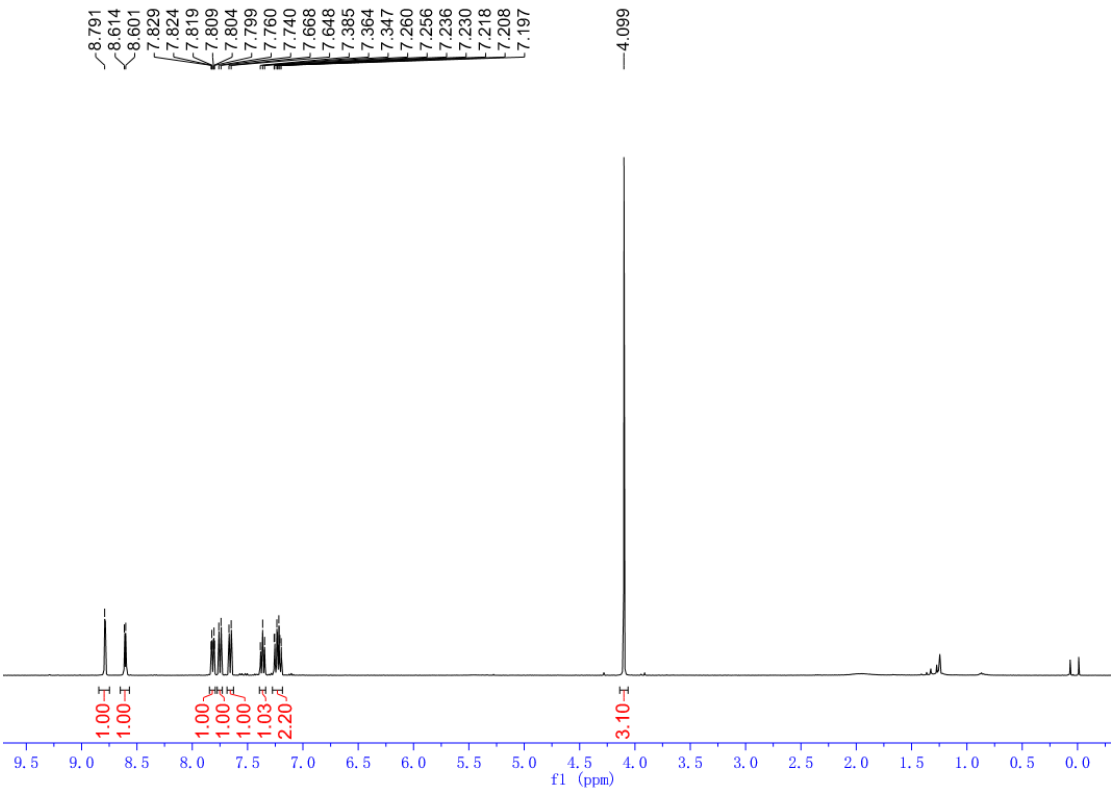
2m

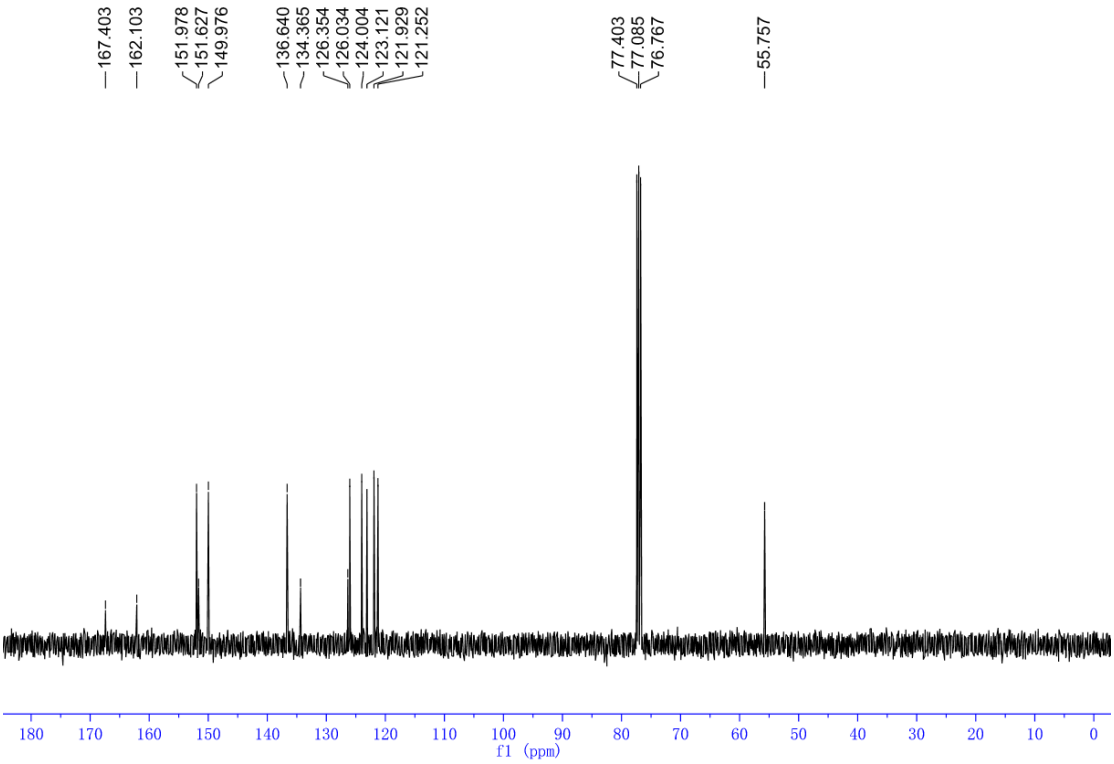

7.836
7.816
7.757
7.737
7.382
7.380
7.378
7.260
6.739
6.730
6.729
6.370
6.366
6.361
6.357
4.053
1.00
1.00
2.02
0.95
1.00
1.01
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

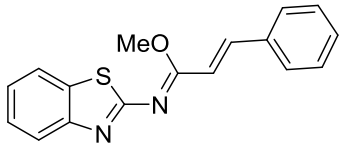

167.940
153.468
151.813
145.852
142.708
134.569
125.815
123.693
121.769
121.274
118.080
111.818
77.371
77.053
76.735
54.976
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


MeO
S
N
N
N

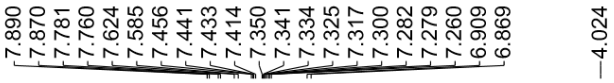
2n

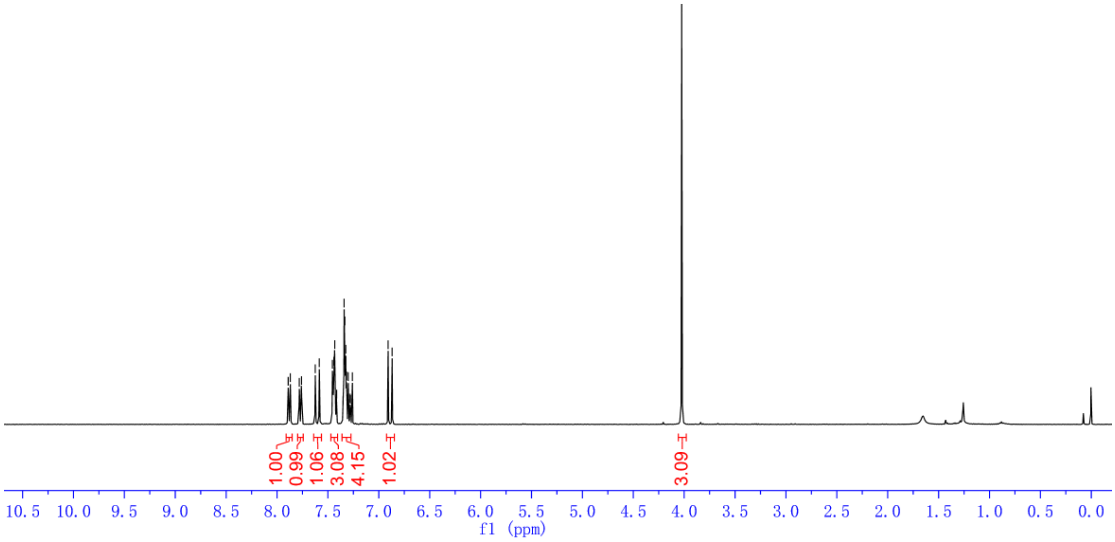

8.791
8.614
8.601
7.829
7.824
7.819
7.809
7.804
7.799
7.760
7.740
7.668
7.648
7.385
7.364
7.347
7.260
7.256
7.236
7.230
7.218
7.208
7.197
4.099
1.00
1.00
1.00
1.00
1.00
1.03
2.20
3.10
f1 (ppm)

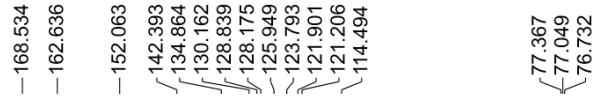

167.403
162.103
151.978
151.627
149.976
136.640
134.365
126.354
126.034
124.004
123.121
121.929
121.252
77.403
77.085
76.767
55.757
f1 (ppm)

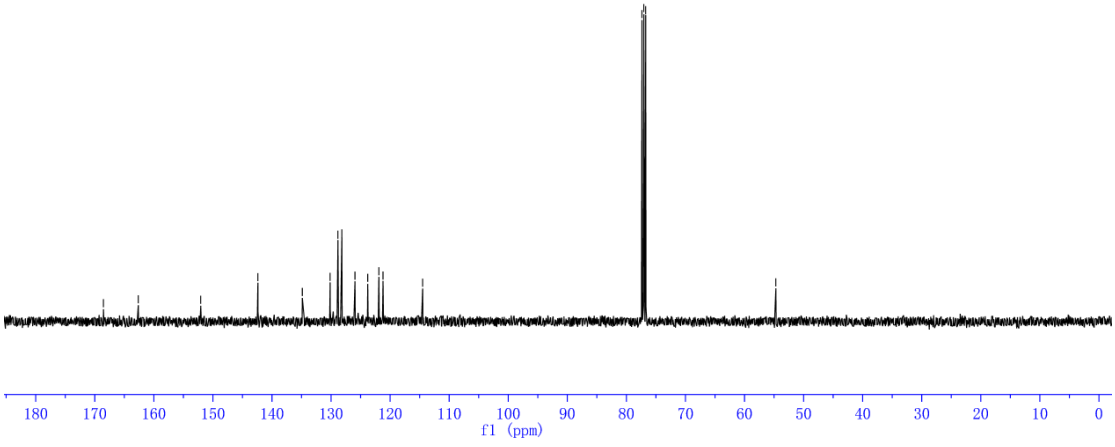

MeO
S
N
N

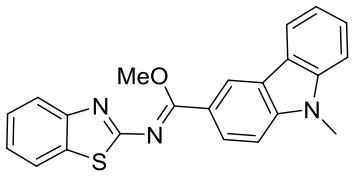
2o


7.890
7.870
7.781
7.760
7.624
7.585
7.456
7.441
7.433
7.414
7.350
7.341
7.334
7.325
7.317
7.300
7.282
7.279
7.260
6.909
6.869
4.024

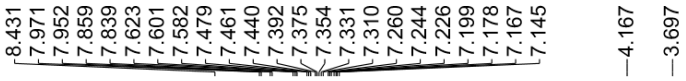

1.00
0.99
1.06
3.08
4.15
1.02
3.09
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

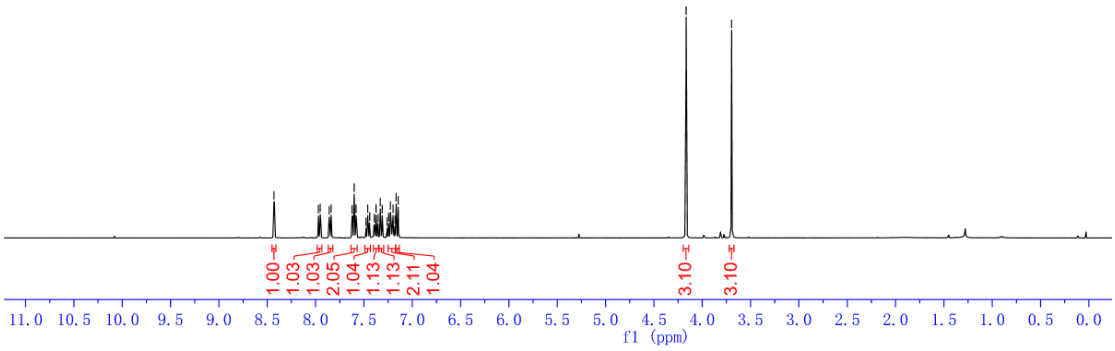

168.534
162.636
152.063
142.393
134.864
130.162
128.839
128.175
125.949
123.793
121.901
121.206
114.494
77.367
77.049
76.732
54.700


180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

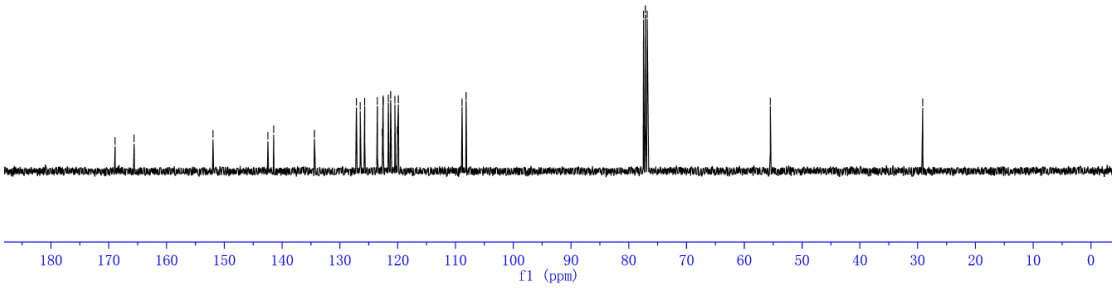

MeO
N
N
S
N

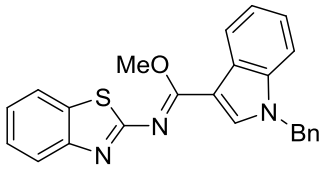
2p


8.431
7.971
7.952
7.859
7.839
7.623
7.601
7.582
7.479
7.461
7.440
7.392
7.375
7.354
7.331
7.310
7.260
7.244
7.226
7.199
7.178
7.167
7.145
4.167
3.697


1.00
1.03
1.03
2.05
1.04
1.13
1.13
2.11
1.04
3.10
3.10
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

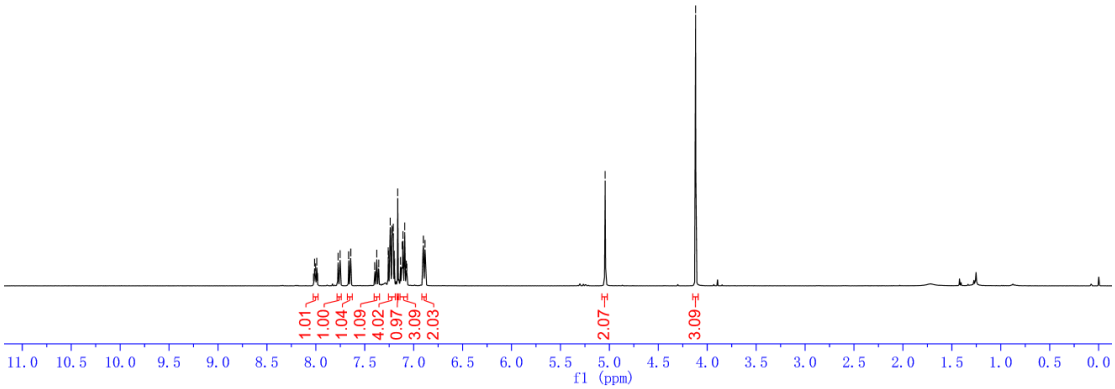

168.908
165.617
151.963
142.462
141.459
134.406
127.143
126.481
125.709
123.517
122.641
122.520
121.613
121.208
120.485
120.040
119.880
108.859
108.156
77.447
77.129
76.811
55.504
29.130


180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

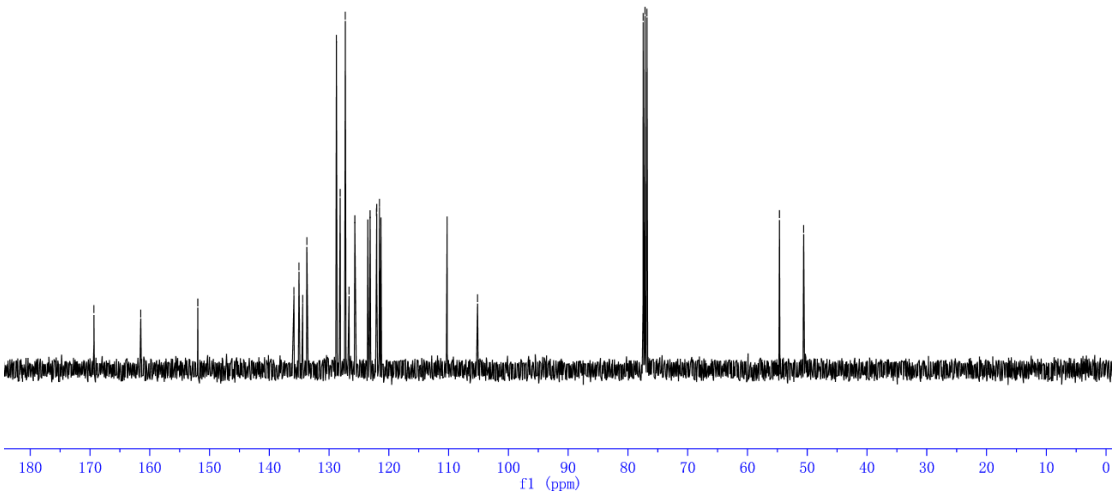

MeO
S
N
N
N
Bn

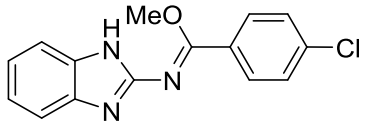
2q


8.013
8.002
7.990
7.772
7.752
7.664
7.643
7.399
7.377
7.357
7.260
7.257
7.240
7.222
7.218
7.209
7.199
7.195
7.163
7.135
7.117
7.110
7.092
7.075
7.070
6.901
6.885
6.843
4.119

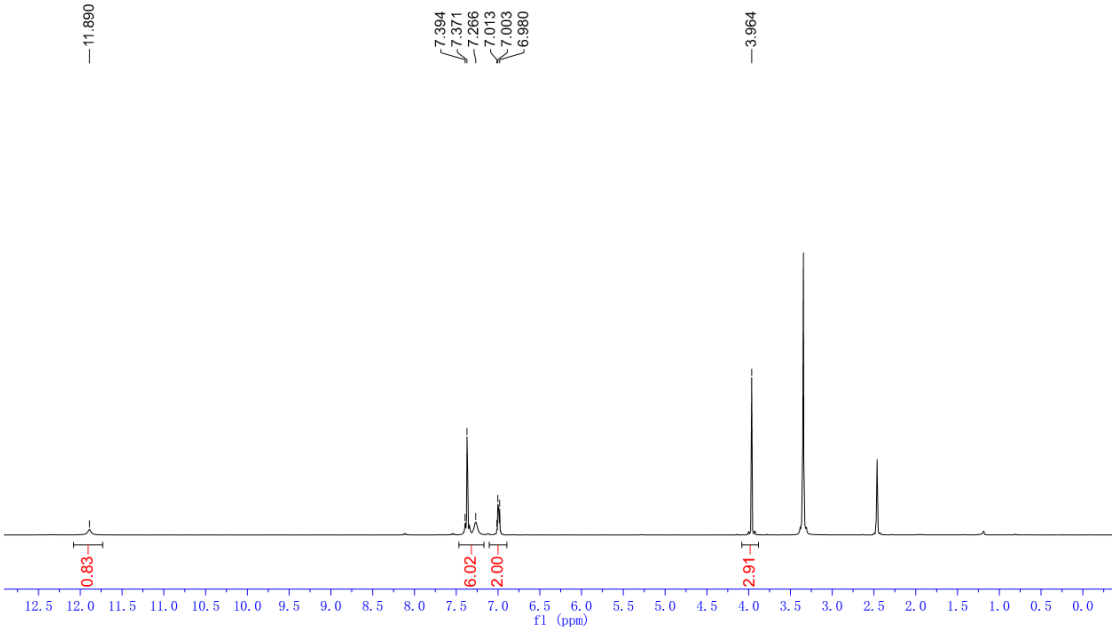

1.01
1.00
1.04
1.09
4.02
0.97
3.09
2.03
2.07
3.09
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

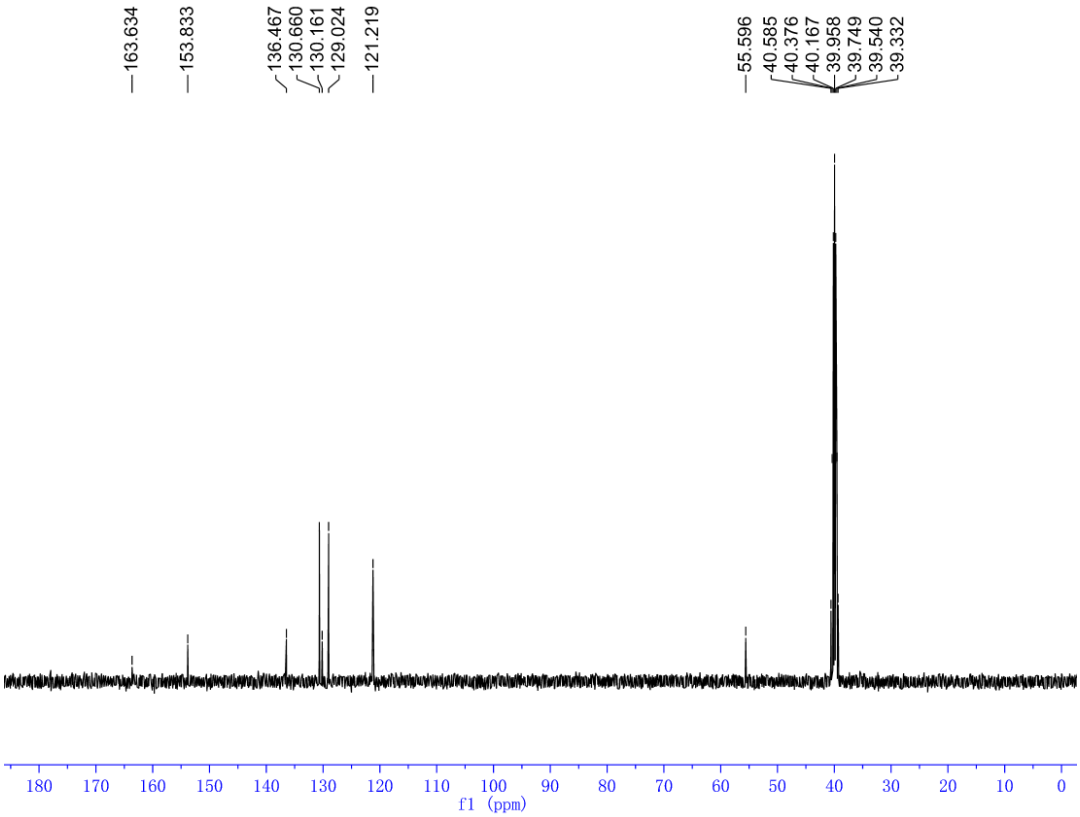

169.346
161.511
151.961
135.876
135.040
134.418
133.718
128.775
128.144
127.286
126.661
125.688
123.517
123.139
122.074
122.028
121.576
121.326
110.257
105.157
77.454
77.136
76.817
54.646
50.604

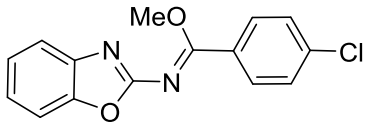

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


MeO
H
N
N
N
Cl

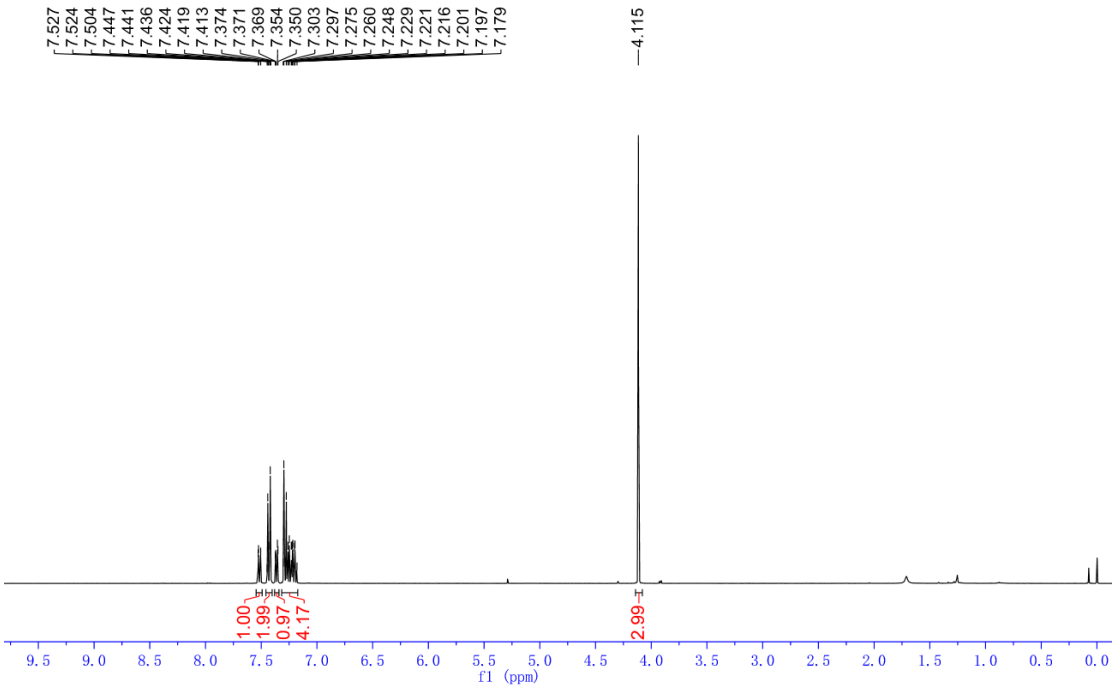
2r


11.890
7.394
7.371
7.266
7.013
7.003
6.980
3.964
0.83
6.02
2.00
2.91
f1 (ppm)


163.634
153.833
136.467
130.660
130.161
129.024
121.219
55.596
40.585
40.376
40.167
39.958
39.749
39.540
39.332
f1 (ppm)


MeO
N
N
O
Cl

2s


7.527
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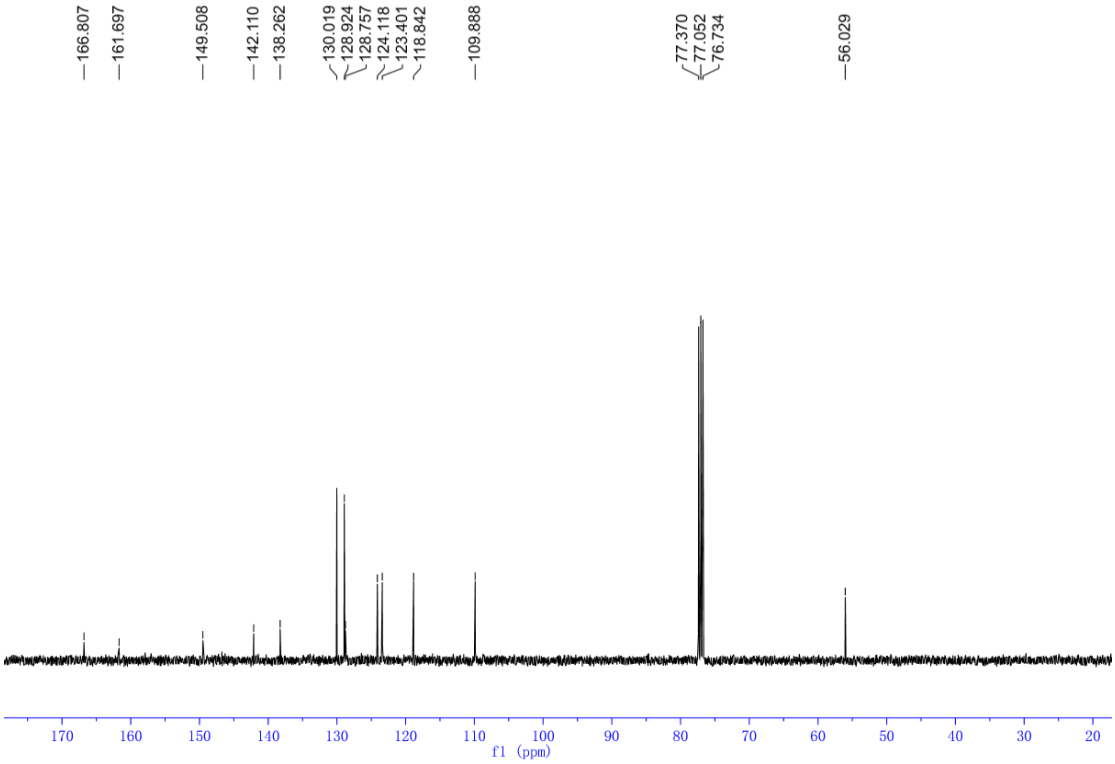
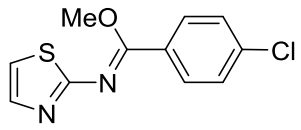
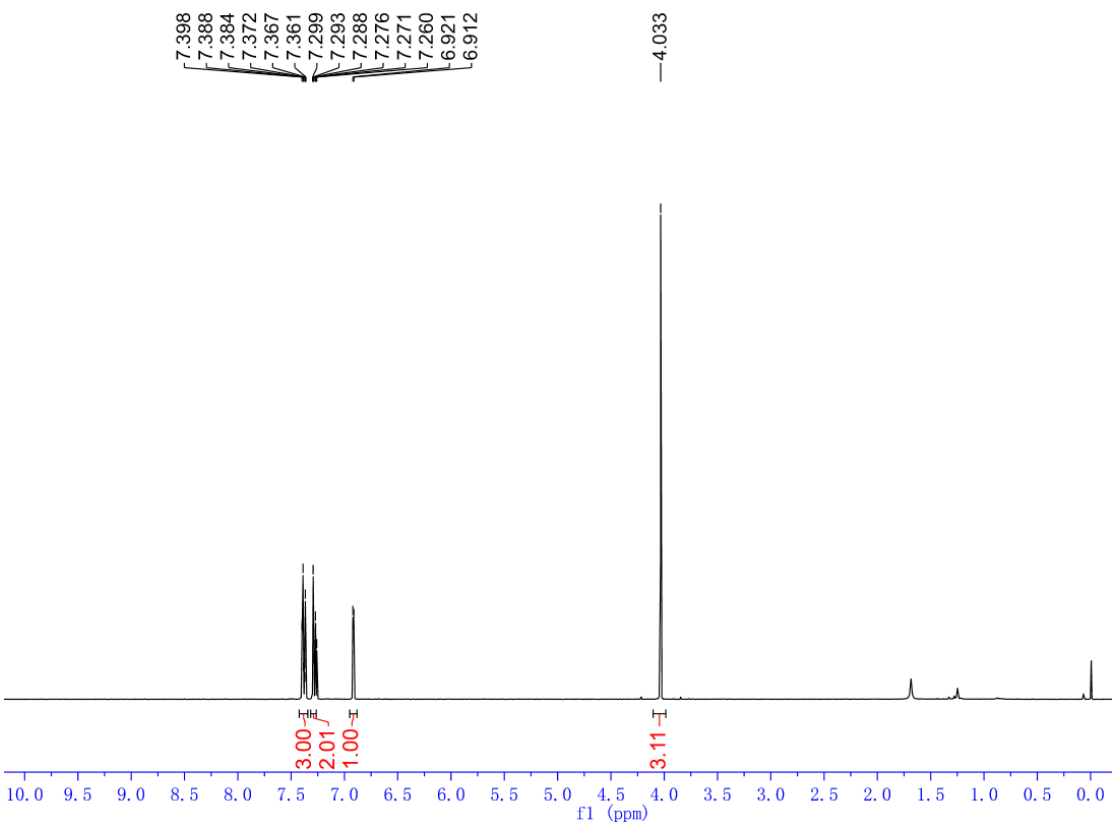
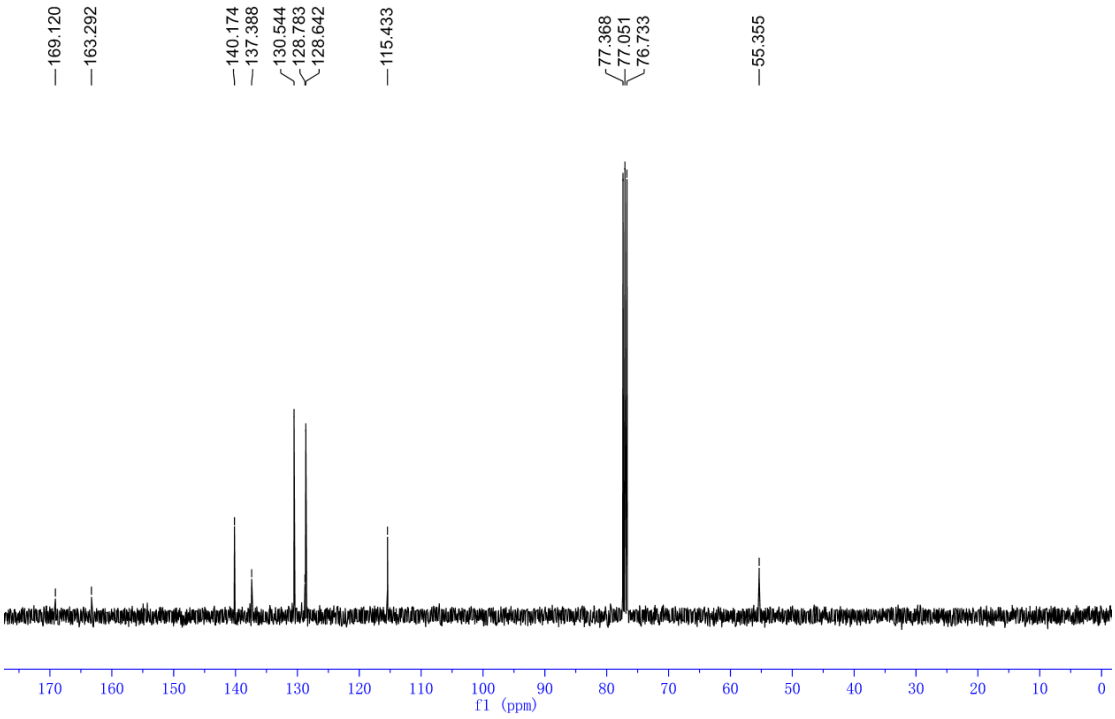
7.504
7.447
7.441
7.436
7.424
7.419
7.413
7.374
7.371
7.369
7.354
7.350
7.303
7.297
7.275
7.260
7.248
7.229
7.221
7.216
7.201
7.197
7.179
4.115
1.00
1.99
0.97
4.17
2.99
f1 (ppm)

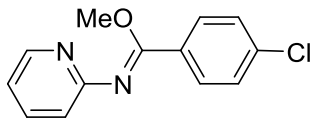

166.807
161.697
149.508
142.110
138.262
130.019
128.924
128.757
124.118
123.401
118.842
109.888
77.370
77.052
76.734
56.029
f1 (ppm)


MeO
S
N
N
Cl

2t

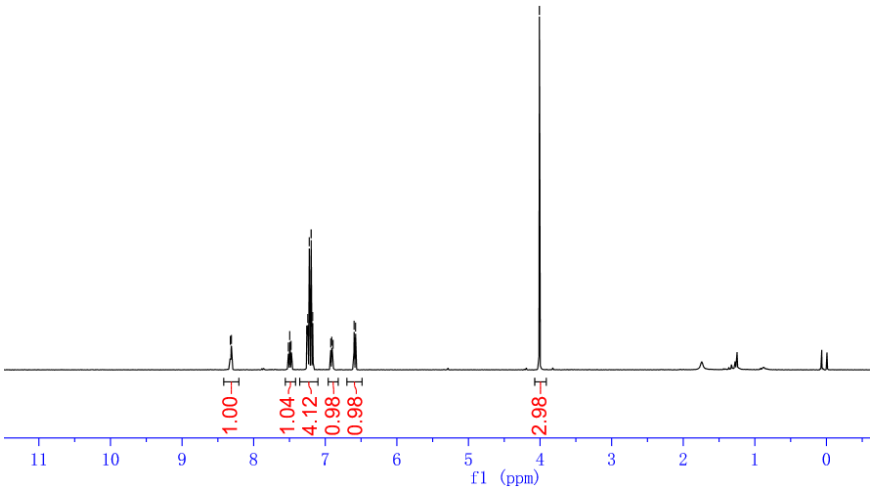

7.398
7.388
7.384
7.372
7.367
7.361
7.299
7.293
7.288
7.276
7.271
7.260
6.921
6.912
4.033
3.00
2.01
1.00
3.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

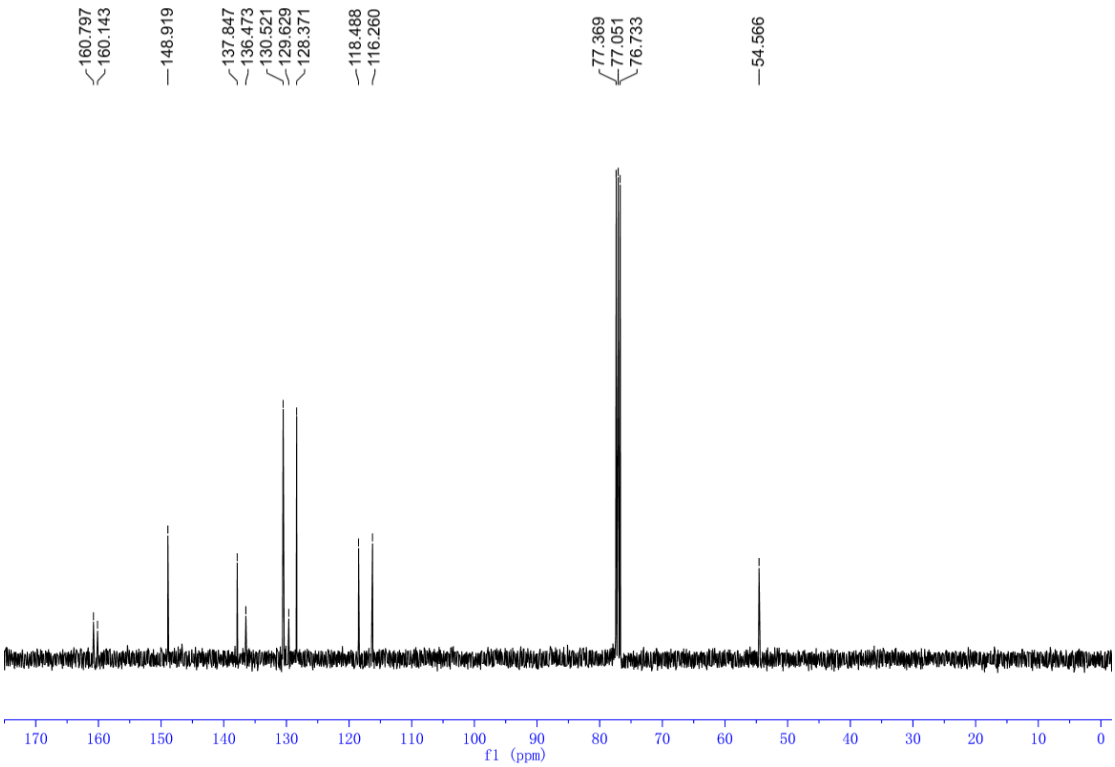

169.120
163.292
140.174
137.388
130.544
128.783
128.642
115.433
77.368
77.051
76.733
55.355
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

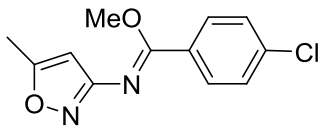

MeO
N
N
Cl

2u

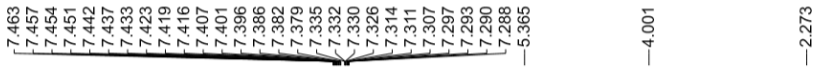

8.326
8.311
7.516
7.497
7.478
7.260
7.245
7.223
7.197
7.176
6.923
6.909
6.891
6.597
6.577
4.010

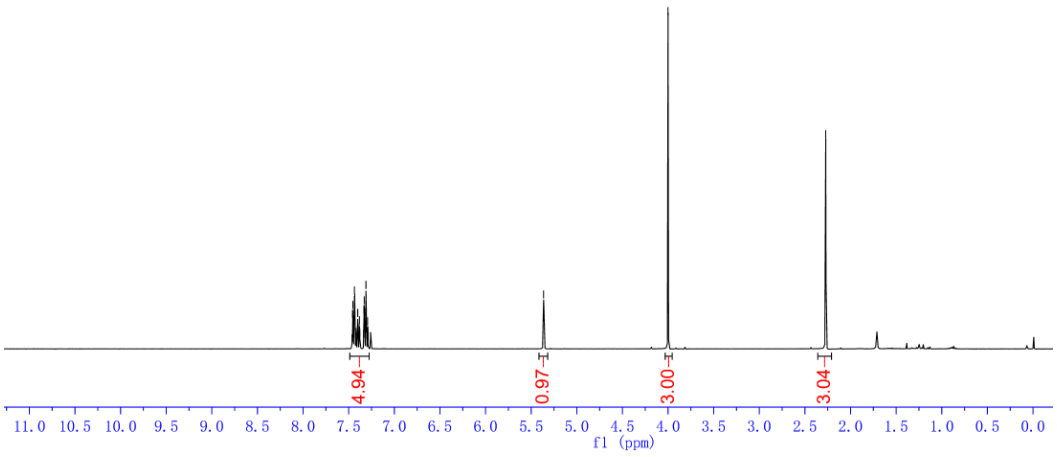

1.00
1.04
4.12
0.98
0.98
2.98
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

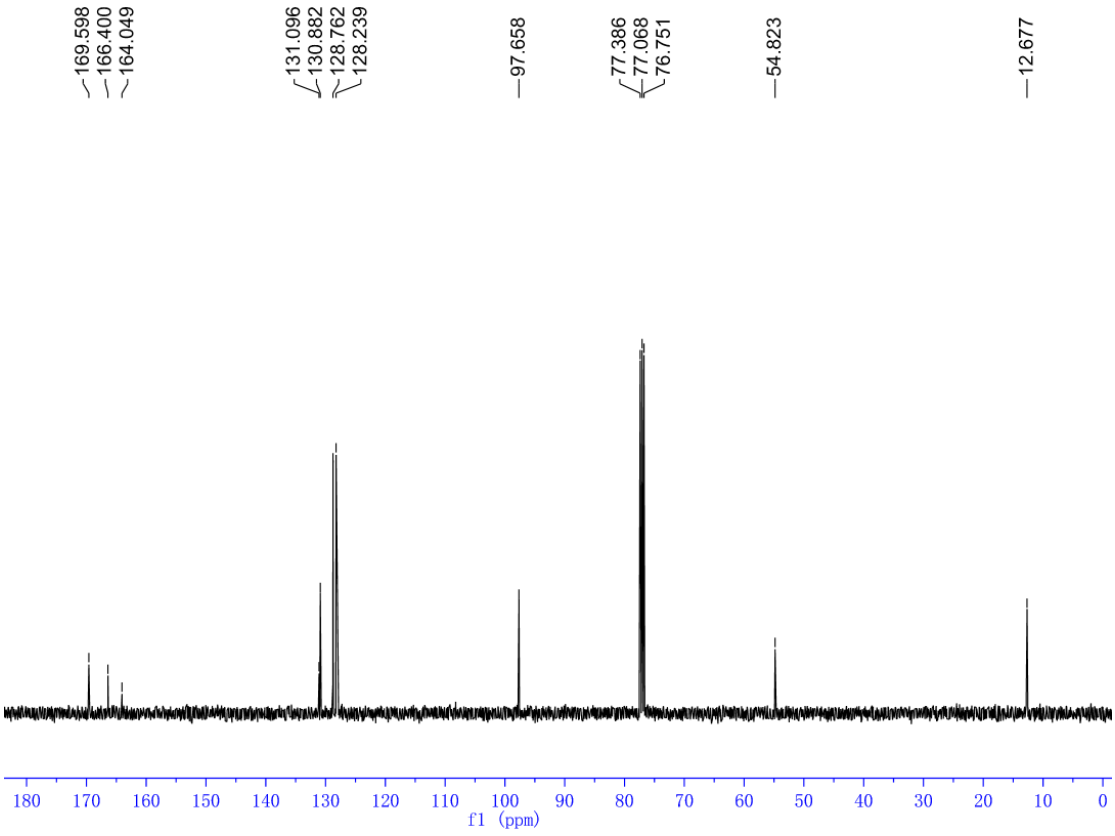

160.797
160.143
148.919
137.847
136.473
130.521
129.629
128.371
118.488
116.260
77.369
77.051
76.733
54.566
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

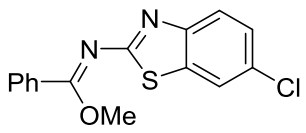

MeO
Cl
N
O
N

2v

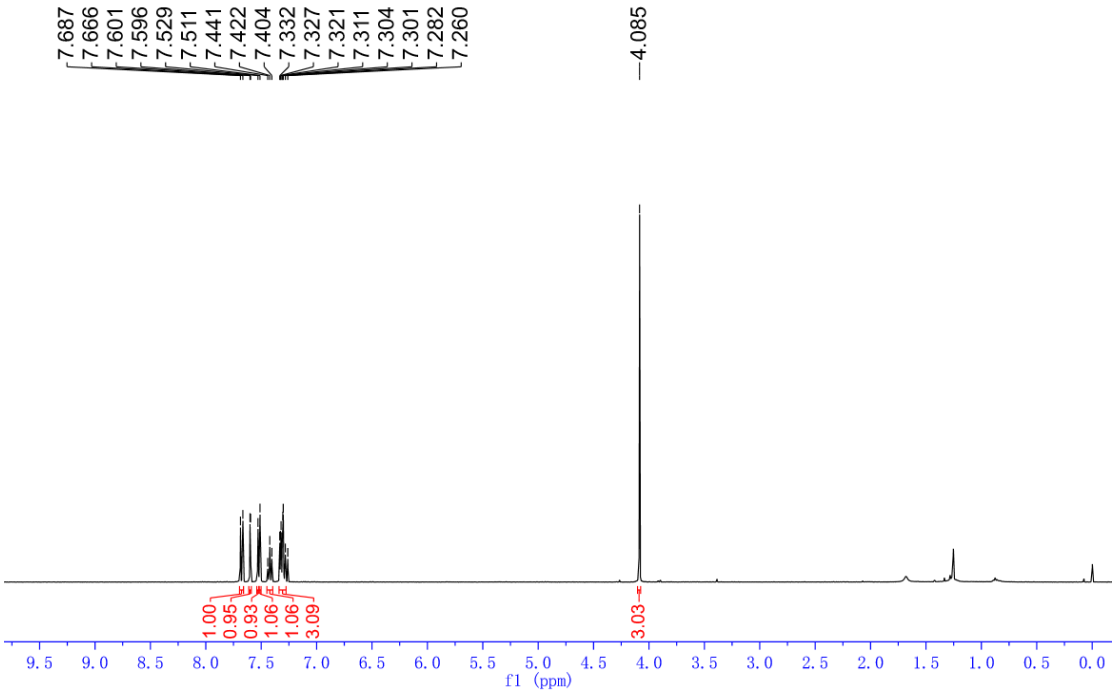

7.463
7.457
7.454
7.451
7.442
7.437
7.433
7.423
7.419
7.416
7.407
7.401
7.396
7.386
7.382
7.379
7.335
7.332
7.330
7.326
7.314
7.311
7.307
7.297
7.293
7.290
7.288
5.365
4.001
2.273

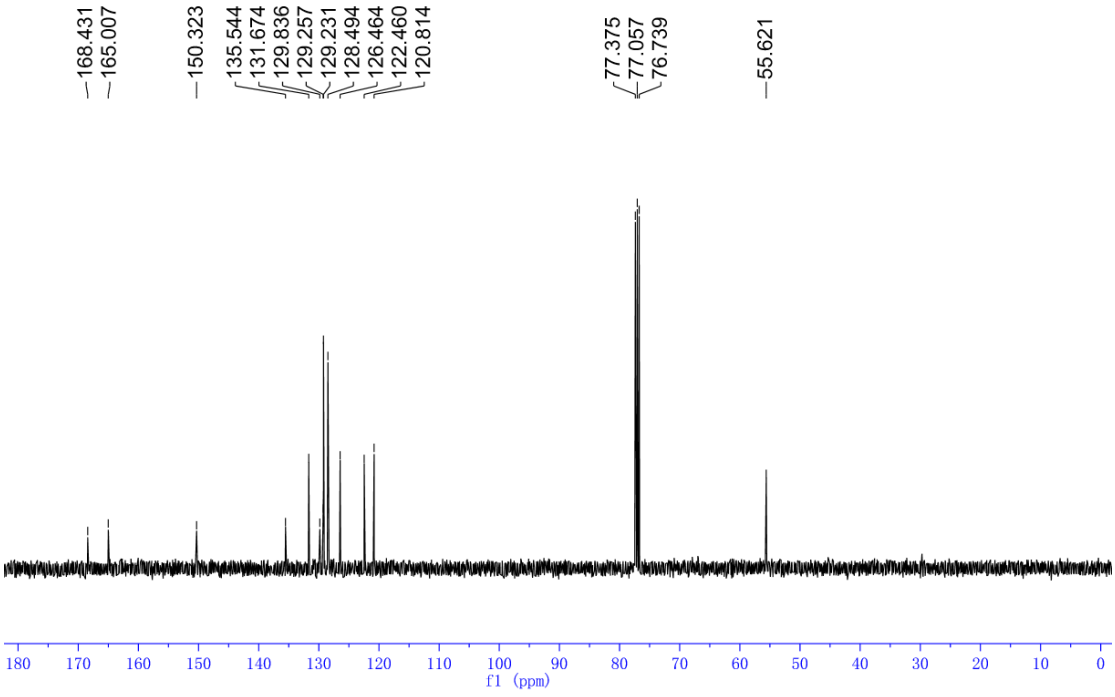

4.94
0.97
3.00
3.04
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

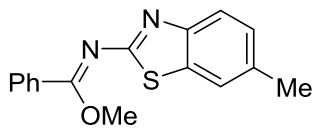

169.598
166.400
164.049
131.096
130.882
128.762
128.239
97.658
77.386
77.068
76.751
54.823
12.677
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


N
N
S
Ph
OMe
Cl

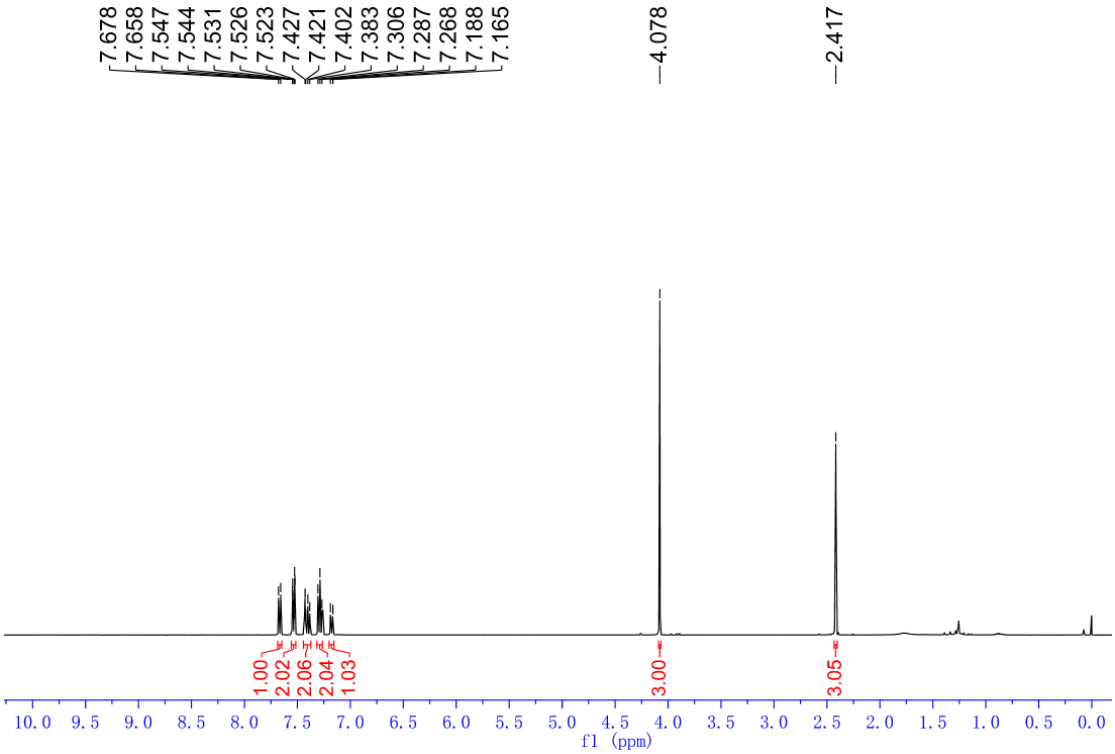
2w


7.687
7.666
7.601
7.596
7.529
7.511
7.441
7.422
7.404
7.332
7.327
7.321
7.311
7.304
7.301
7.282
7.260
4.085
1.00
0.95
0.93
1.06
1.06
3.09
3.03
f1 (ppm)


168.431
165.007
150.323
135.544
131.674
129.836
129.257
129.231
128.494
126.464
122.460
120.814
77.375
77.057
76.739
55.621
f1 (ppm)


N
N
S
Ph
OMe
Me

2x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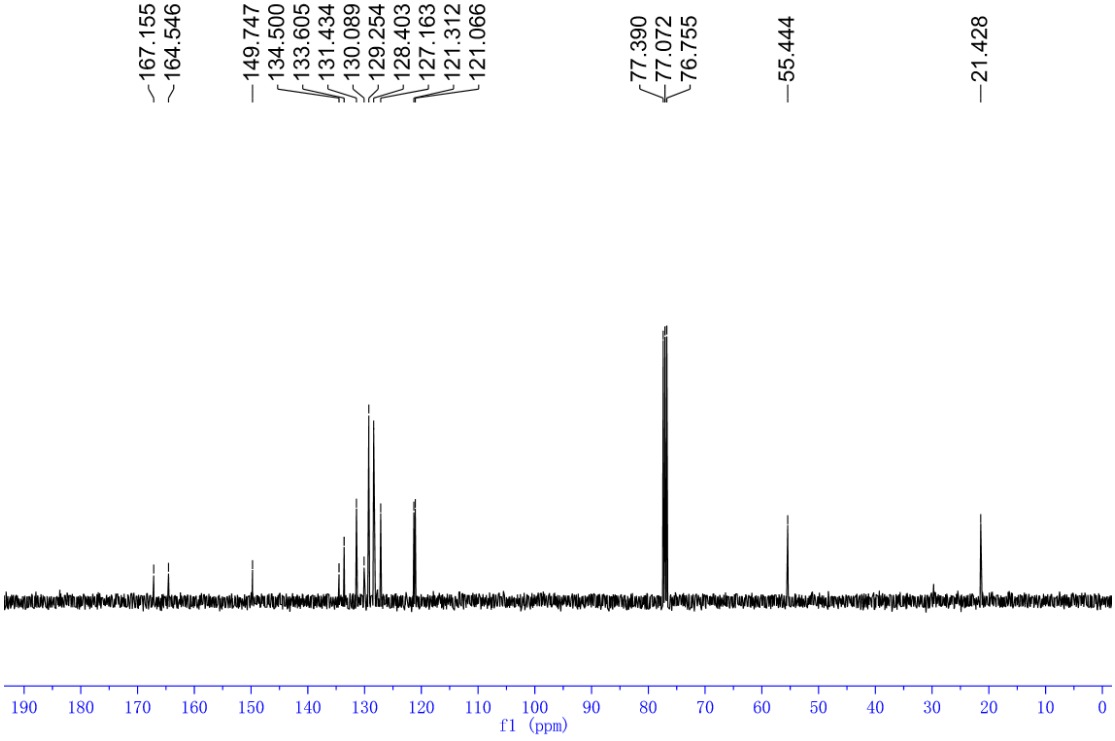
7.523
7.427
7.421
7.402
7.383
7.306
7.287
7.268
7.188
7.165
4.078
2.417
1.00
2.02
2.06
2.04
1.03
3.00
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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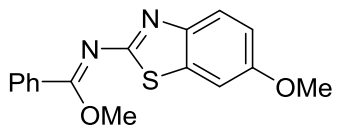
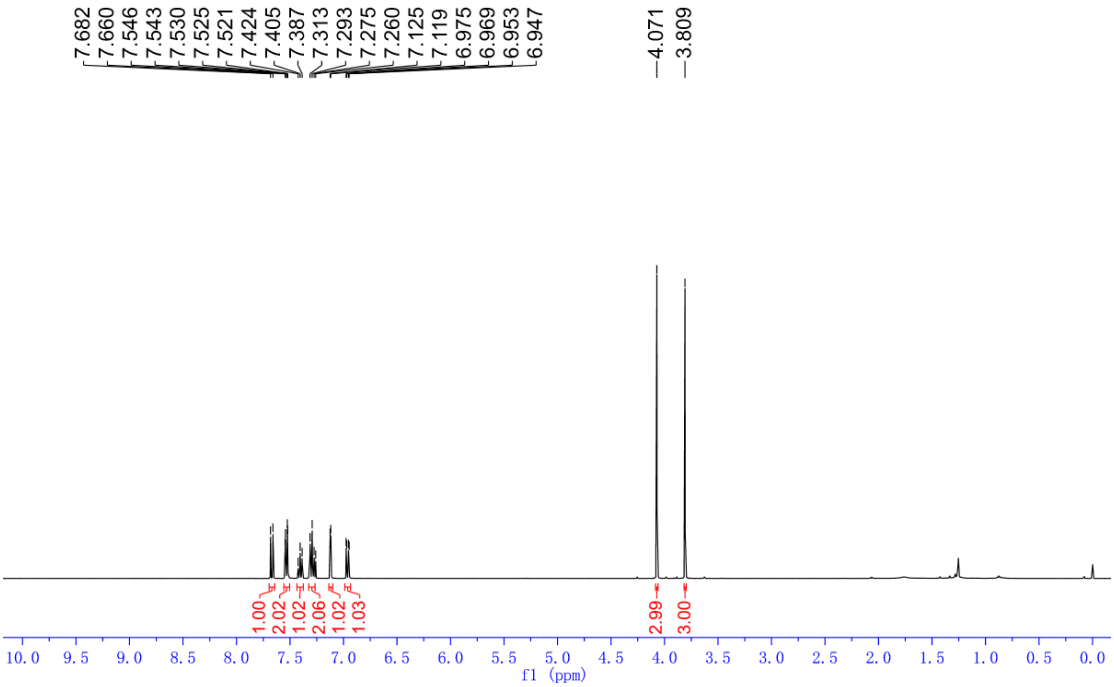
164.546
149.747
134.500
133.605
131.434
130.089
129.254
128.403
127.163
121.312
121.066
77.390
77.072
76.755
55.444
21.428
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


N
N
S
Ph
OMe
OMe

2y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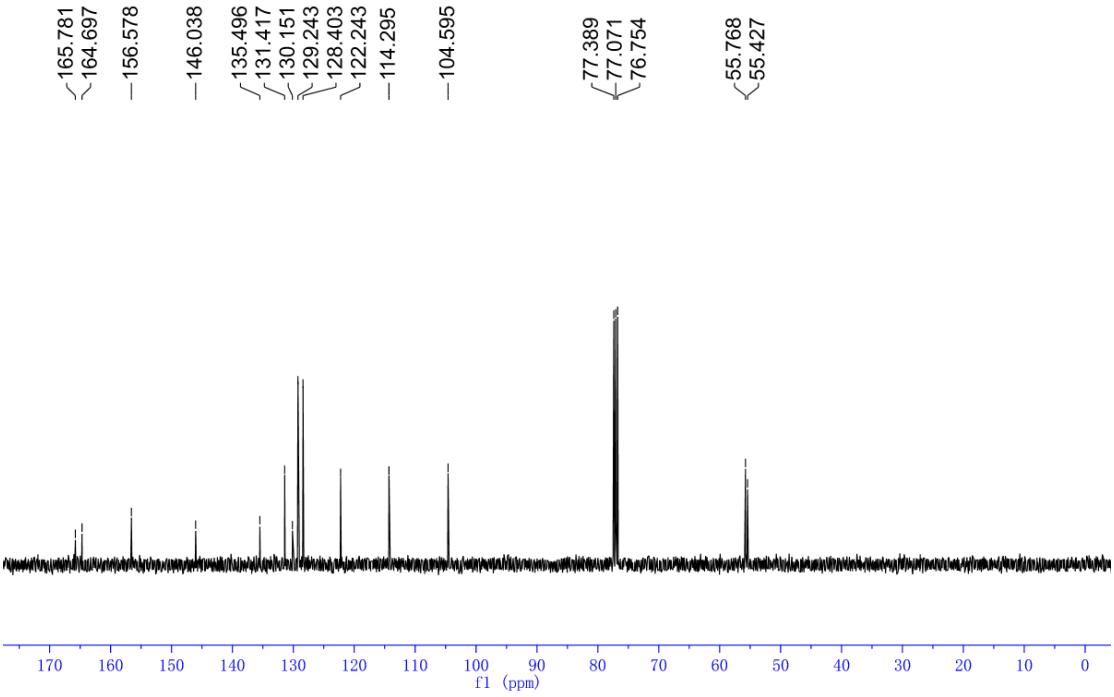
7.660
7.546
7.543
7.530
7.525
7.521
7.424
7.405
7.387
7.313
7.293
7.275
7.260
7.125
7.119
6.975
6.969
6.953
6.947
4.071
3.809
1.00
2.02
1.02
2.06
1.02
1.03
2.99
3.00
f1 (ppm)


165.781
164.697
156.578
146.038
135.496
131.417
130.151
129.243
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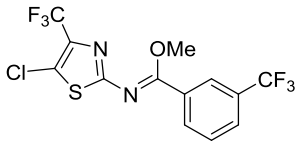
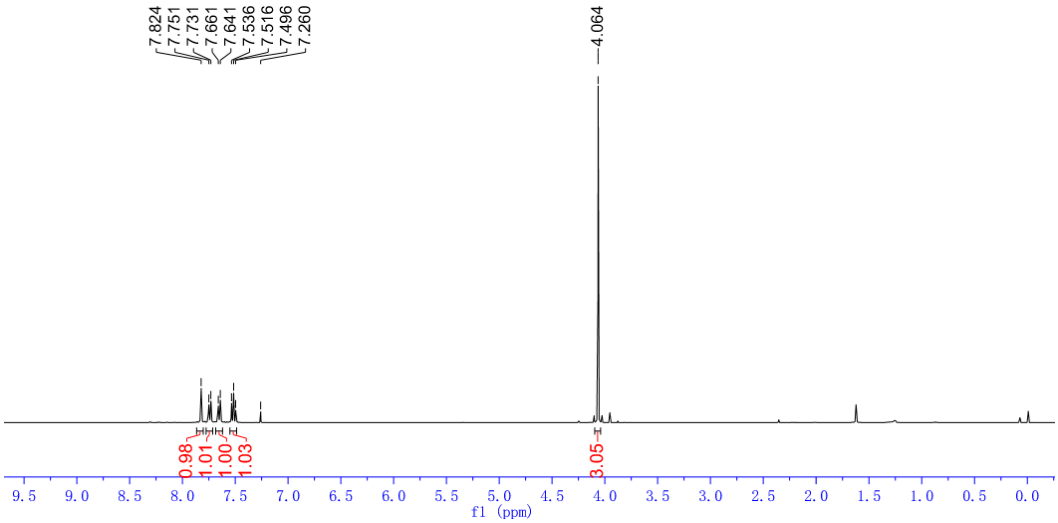
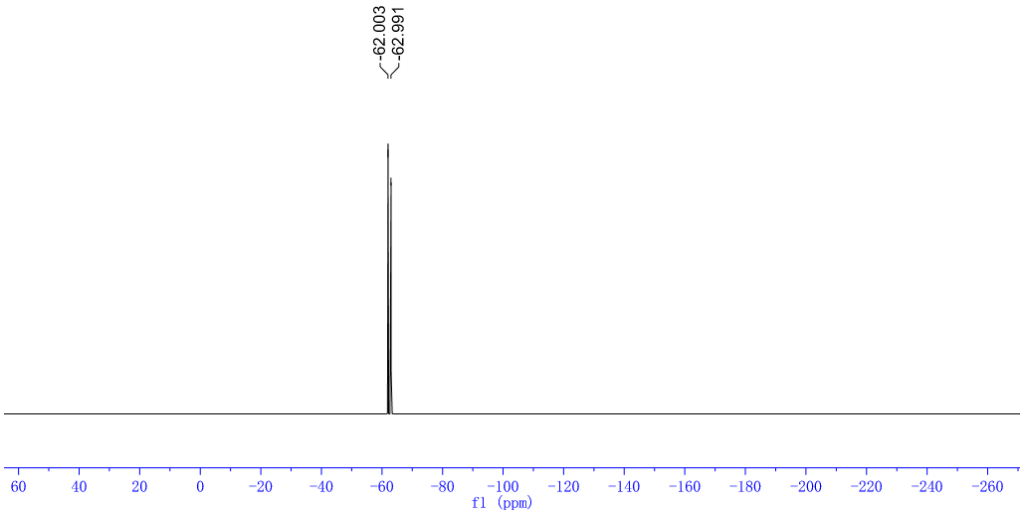
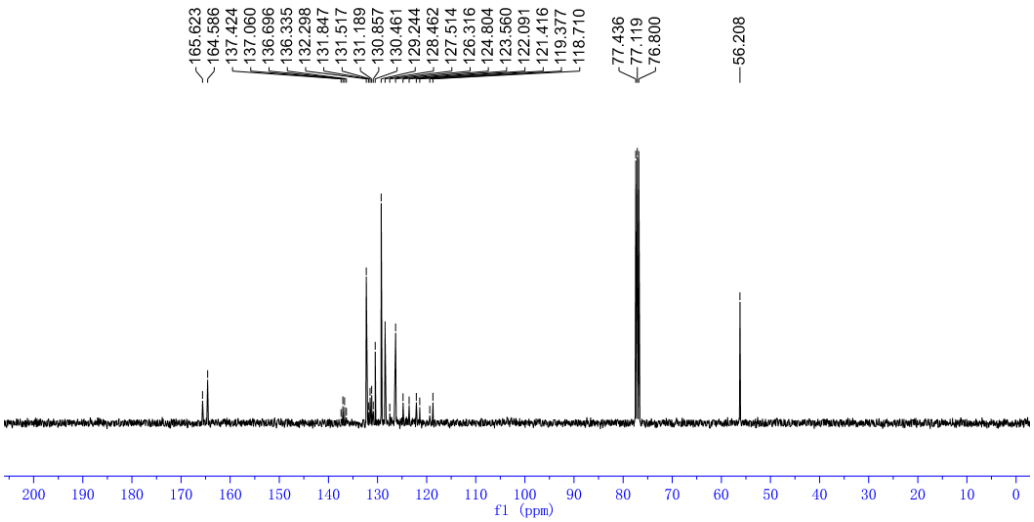
122.243
114.295
104.595
77.389
77.071
76.754
55.768
55.427
f1 (ppm)


F3C
N
OMe
Cl
S
N
CF3

2z


7.824
7.751
7.731
7.661
7.641
7.536
7.516
7.496
7.260
4.064
0.98
1.01
1.00
1.03
3.05
f1 (ppm)


-62.003
-62.991
f1 (ppm)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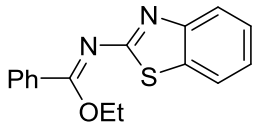
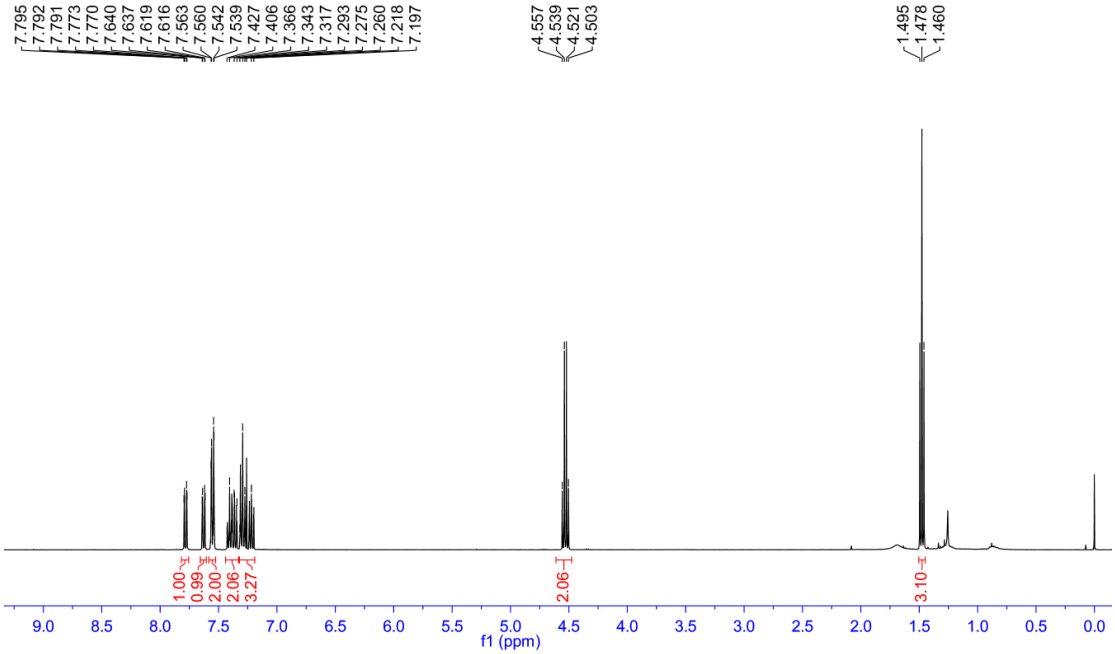
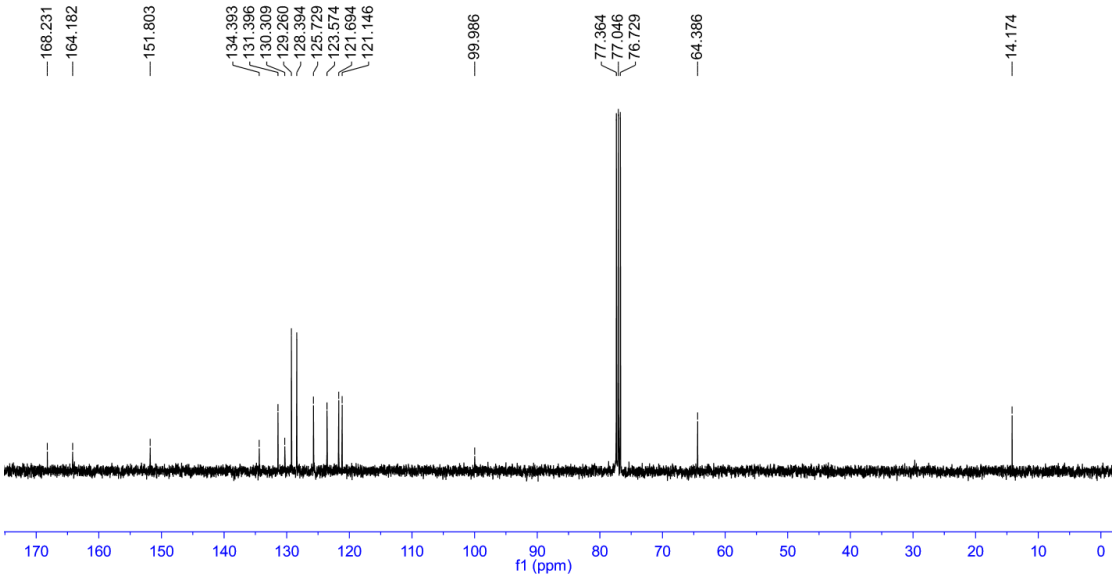
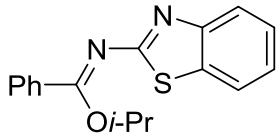
164.586
137.424
137.060
136.696
136.335
132.298
131.847
131.517
131.189
130.857
130.461
129.244
128.462
127.514
126.316
124.804
123.560
122.091
121.416
119.377
118.710
77.436
77.119
76.800
56.208
f1 (ppm)


N
N
S
Ph
OEt

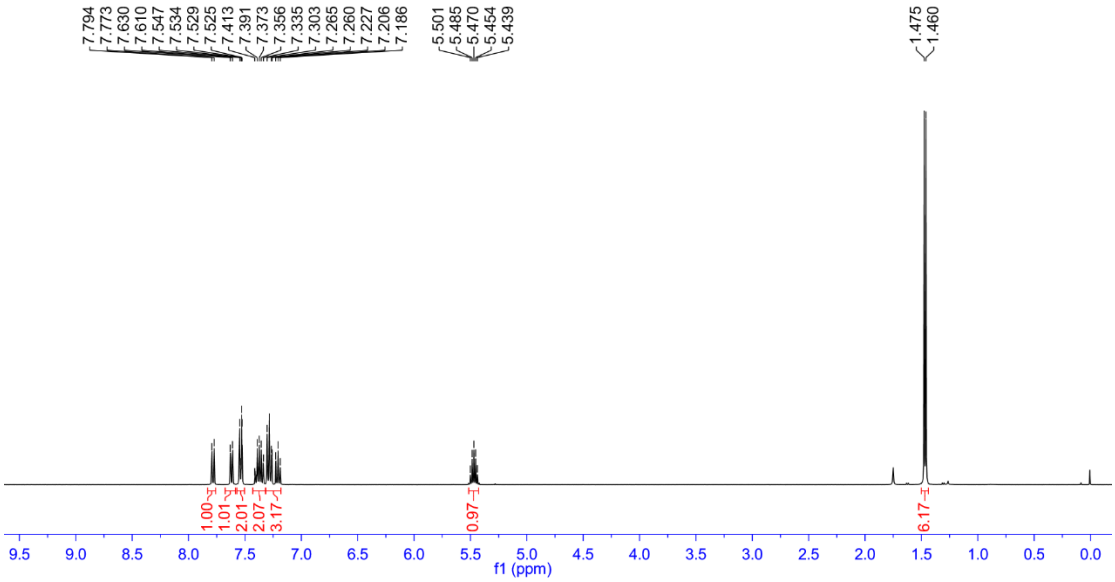
2aa


7.795
7.792
7.791
7.773
7.770
7.640
7.637
7.619
7.616
7.563
7.560
7.542
7.539
7.427
7.406
7.366
7.343
7.317
7.293
7.275
7.260
7.218
7.197
4.557
4.539
4.521
4.503
1.495
1.478
1.460
1.00
0.99
2.00
2.06
3.27
2.06
3.10
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


168.231
164.182
151.803
134.393
131.396
130.309
129.260
128.394
125.729
123.574
121.694
121.146
99.986
77.364
77.046
76.729
64.386
14.174
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


N
N
S
Ph
O*i*-Pr

2ab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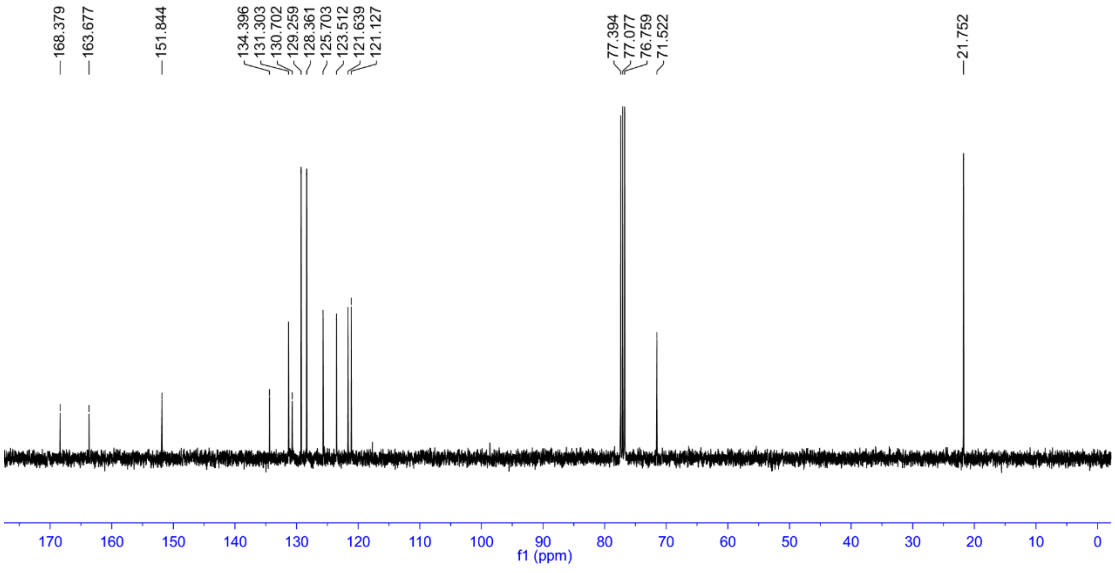
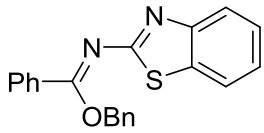
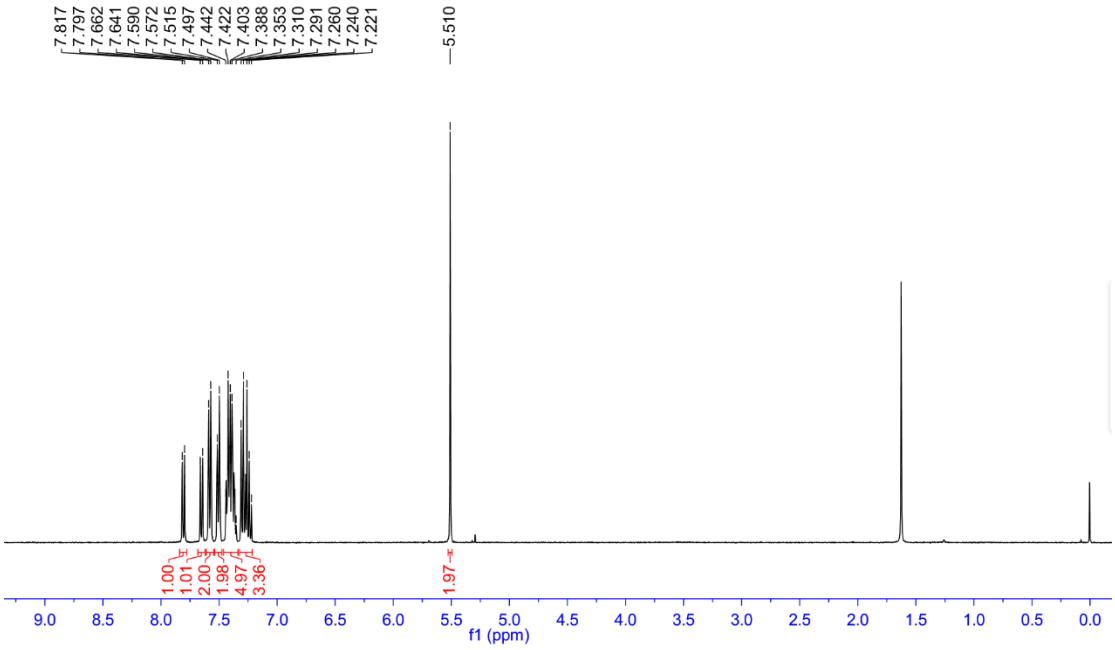
7.610
7.547
7.534
7.529
7.525
7.413
7.391
7.373
7.356
7.335
7.303
7.265
7.260
7.227
7.206
7.186
5.501
5.485
5.470
5.454
5.439
1.475
1.460
1.00
1.01
2.01
2.07
3.17
0.97
6.17
f1 (ppm)


168.379
163.677
151.844
134.396
131.303
130.702
129.259
128.361
125.703
123.512
121.639
121.127
77.394
77.077
76.759
71.522
21.752
f1 (ppm)


N
N
S
Ph
OBn

2ac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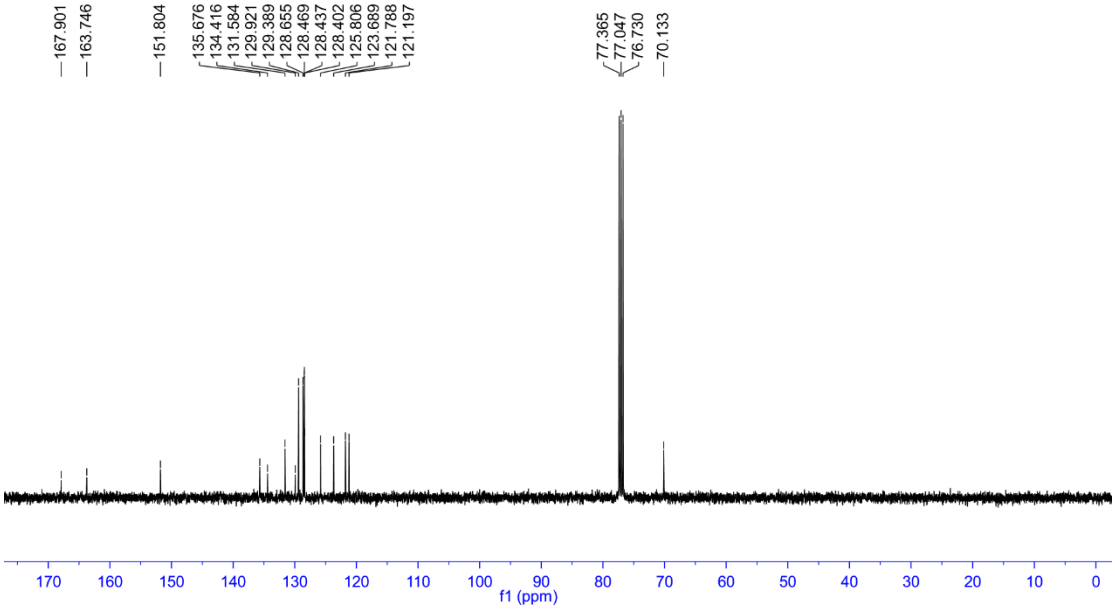
7.572
7.515
7.497
7.442
7.422
7.403
7.388
7.353
7.310
7.291
7.260
7.240
7.221
5.510
1.00
1.01
2.00
1.98
4.97
3.36
1.97
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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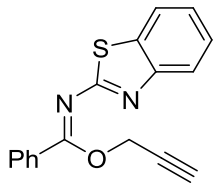
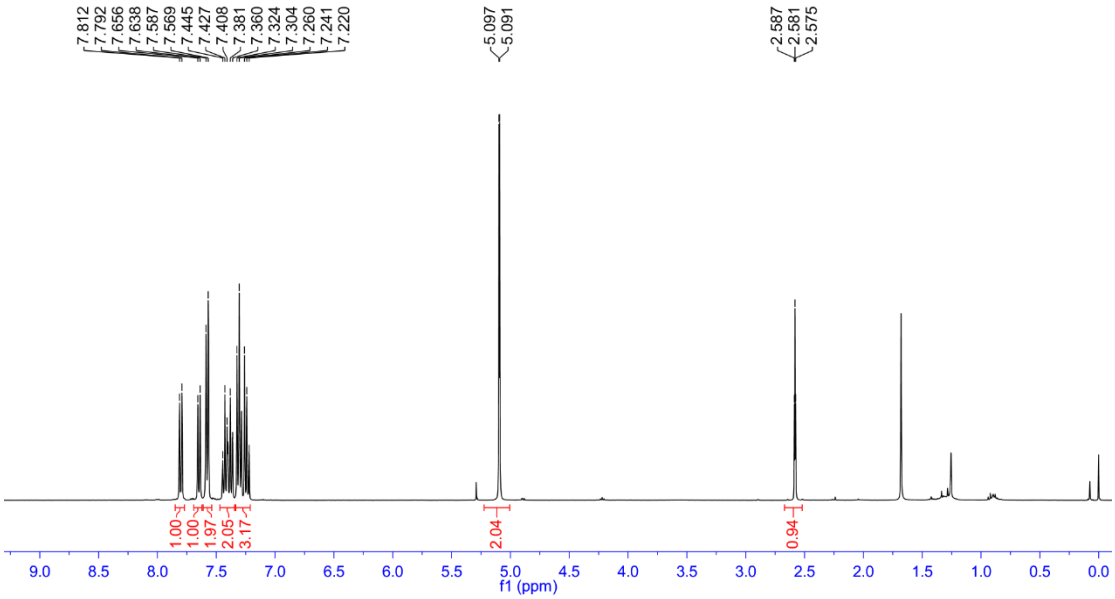
151.804
135.676
134.416
131.584
129.921
129.389
128.655
128.469
128.437
128.402
125.806
123.689
121.788
121.197
77.365
77.047
76.730
70.133
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


S
N
N
Ph
O

2ad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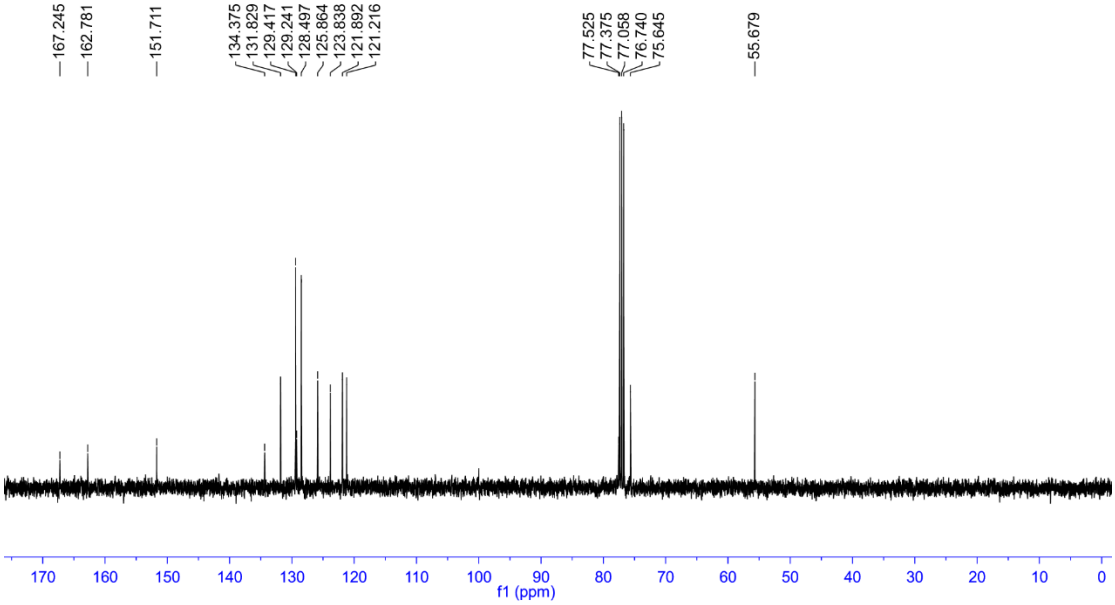
7.569
7.445
7.427
7.406
7.381
7.360
7.324
7.304
7.260
7.241
7.220
5.097
5.091
2.587
2.581
2.575
1.00
1.00
1.97
2.05
3.17
2.04
0.94
f1 (ppm)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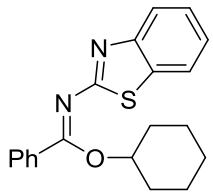
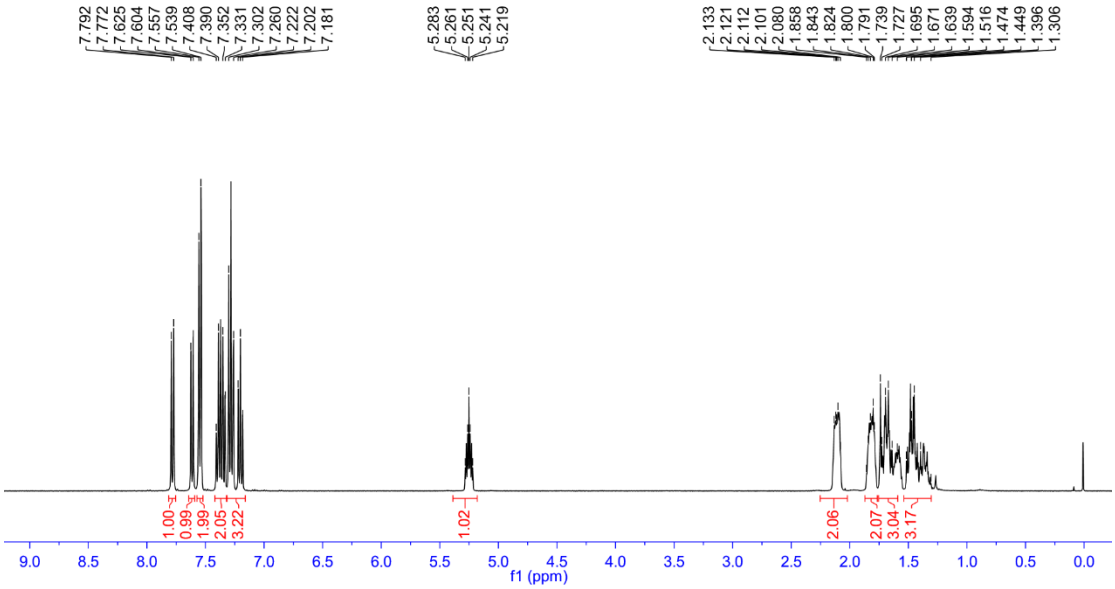
151.711
134.375
131.829
129.417
129.241
128.497
125.864
123.838
121.892
121.216
77.525
77.375
77.058
76.740
75.645
55.679
f1 (ppm)


N
N
S
Ph
O

2ae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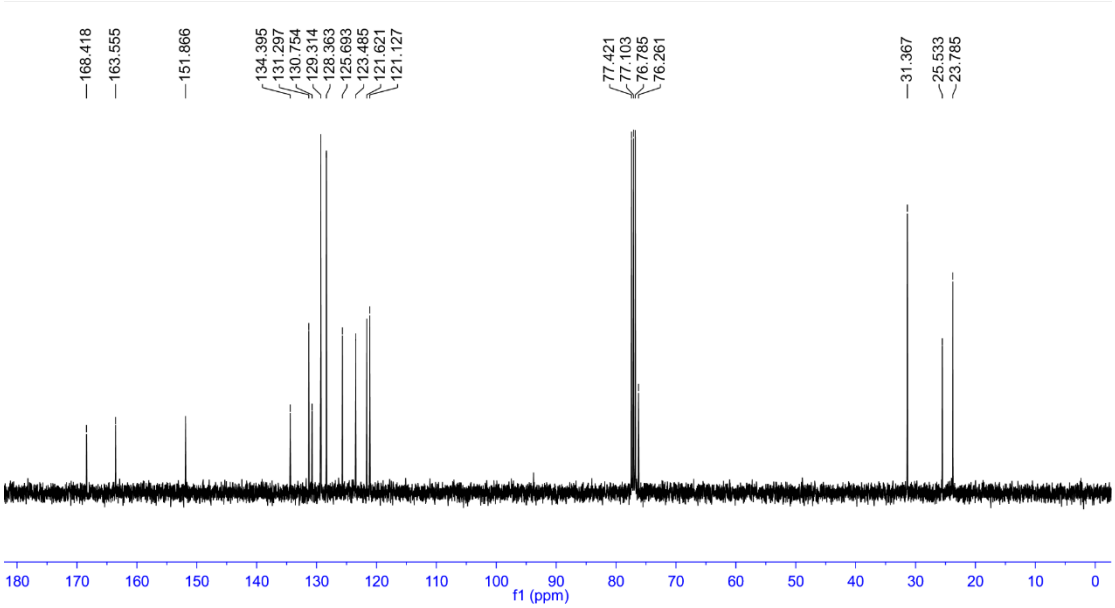
7.604
7.557
7.539
7.408
7.390
7.352
7.331
7.302
7.260
7.222
7.202
7.181
5.283
5.261
5.251
5.241
5.219
2.133
2.121
2.112
2.101
2.080
1.858
1.843
1.824
1.800
1.791
1.739
1.727
1.695
1.671
1.639
1.594
1.516
1.474
1.449
1.396
1.306
1.00
0.99
1.99
2.05
3.22
1.02
2.06
2.07
3.04
3.17
f1 (ppm)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151.866
134.395
131.297
130.754
129.314
128.363
125.693
123.485
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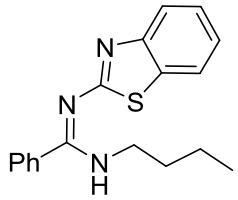
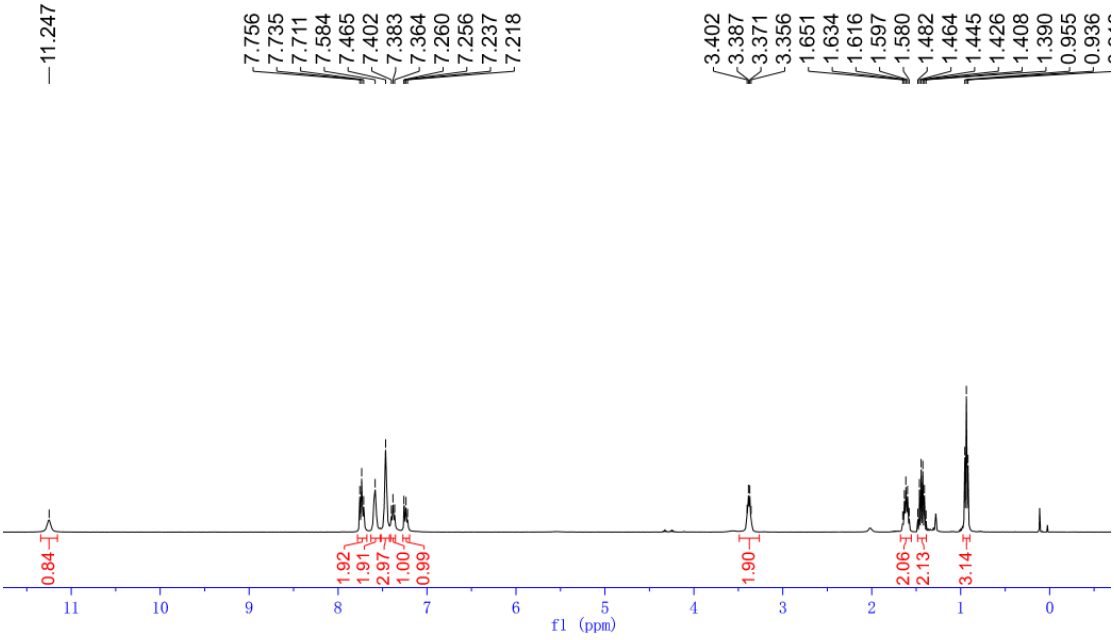
121.127
77.421
77.103
76.785
76.261
31.367
25.533
23.785
f1 (ppm)


N
S
N
Ph
N
H

3a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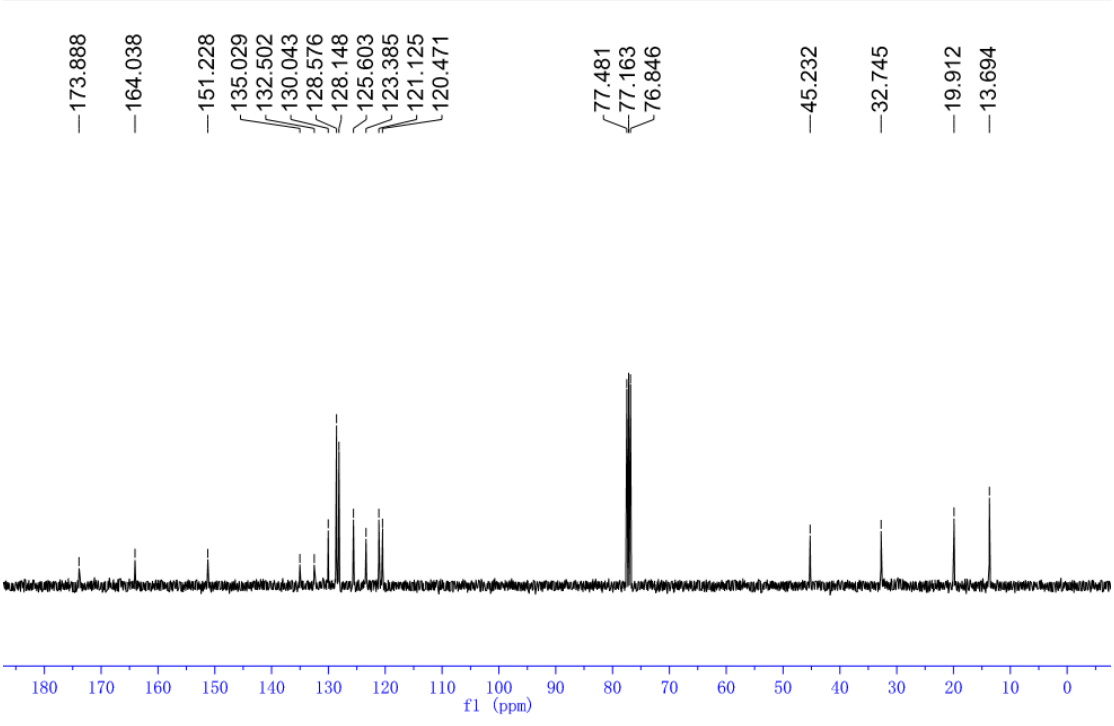
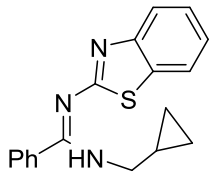
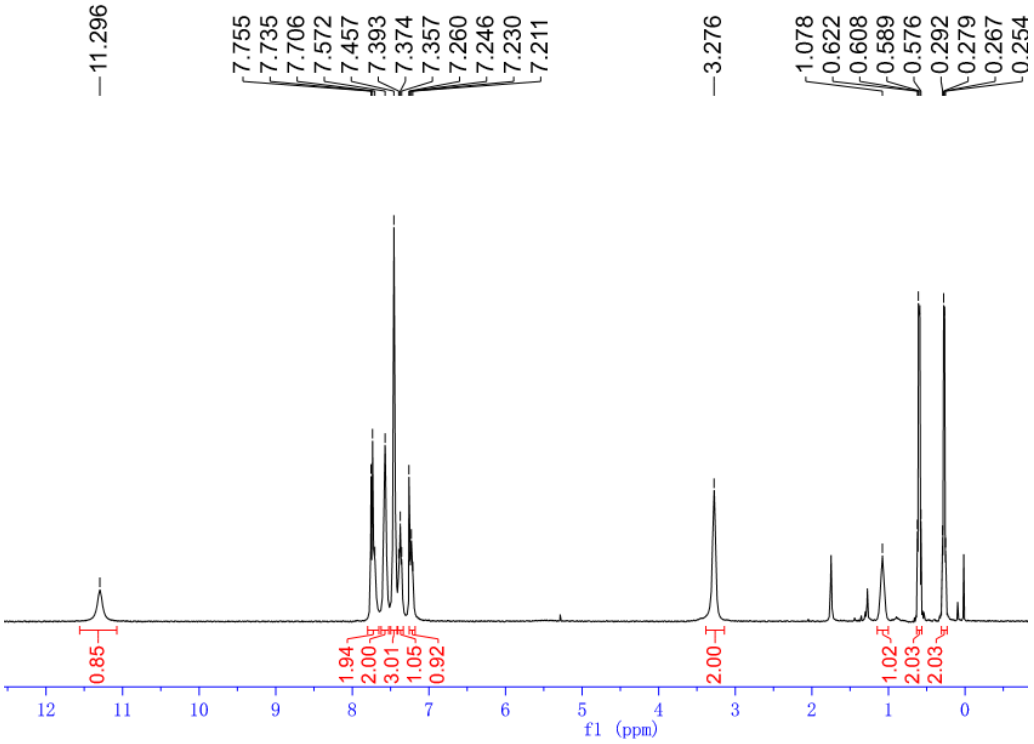
7.735
7.711
7.584
7.465
7.402
7.383
7.364
7.260
7.256
7.237
7.218
3.402
3.387
3.371
3.356
1.651
1.634
1.616
1.597
1.580
1.482
1.464
1.445
1.426
1.408
1.390
0.955
0.936
0.84
1.92
1.91
2.97
1.00
0.99
1.90
2.06
2.13
3.14
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)


173.888
164.038
151.228
135.029
132.502
130.043
128.576
128.148
125.603
123.385
121.125
120.471
77.481
77.163
76.846
45.232
32.745
19.912
13.694
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


N
N
S
Ph
HN

3b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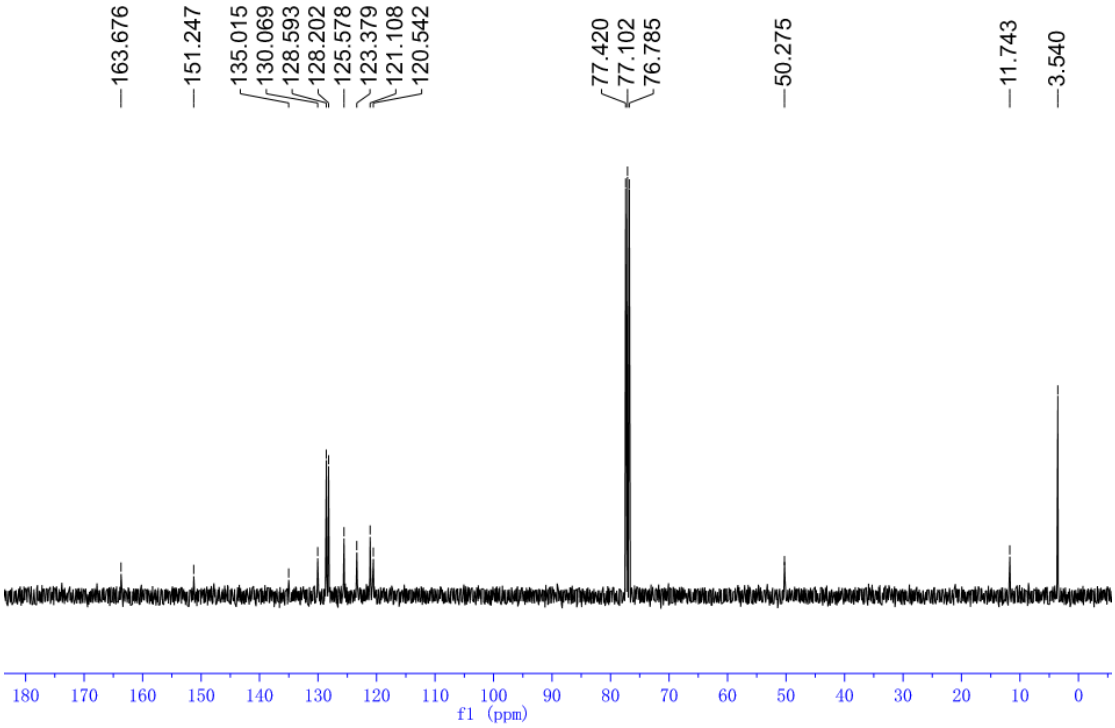
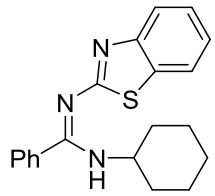
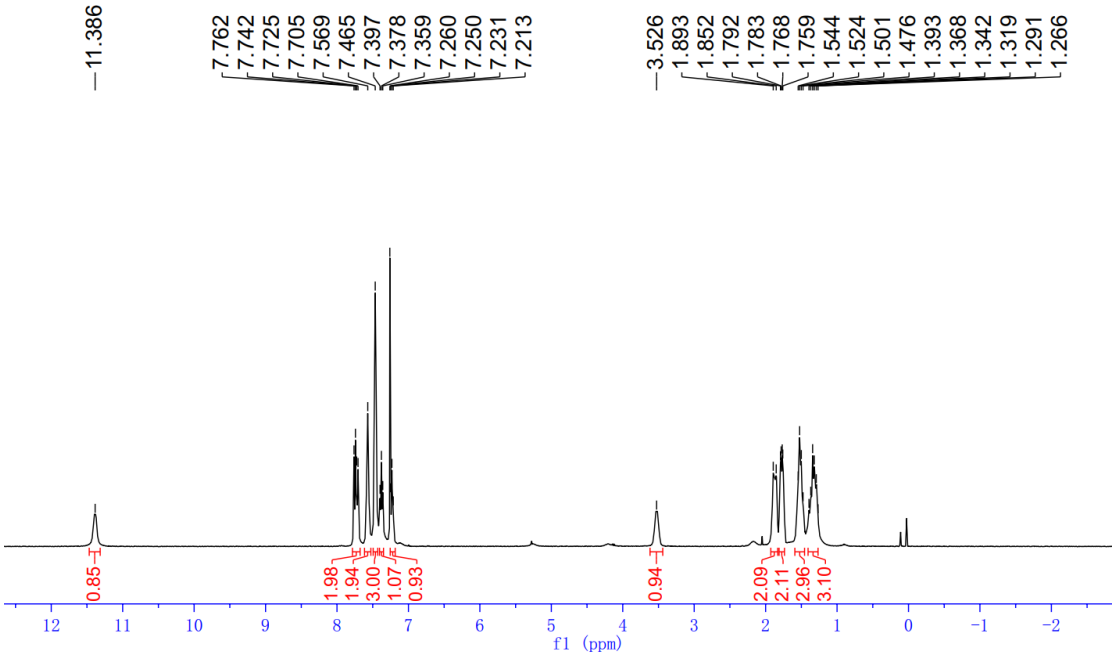
7.706
7.572
7.457
7.393
7.374
7.357
7.260
7.246
7.230
7.211
3.276
1.078
0.622
0.608
0.589
0.576
0.292
0.279
0.267
0.254
0.85
1.94
2.00
3.01
1.05
0.92
2.00
1.02
2.03
2.03
f1 (ppm)


163.676
151.247
135.015
130.069
128.593
128.202
125.578
123.379
121.108
120.542
77.420
77.102
76.785
50.275
11.743
3.540
f1 (ppm)


N
N
S
Ph
N
H

3c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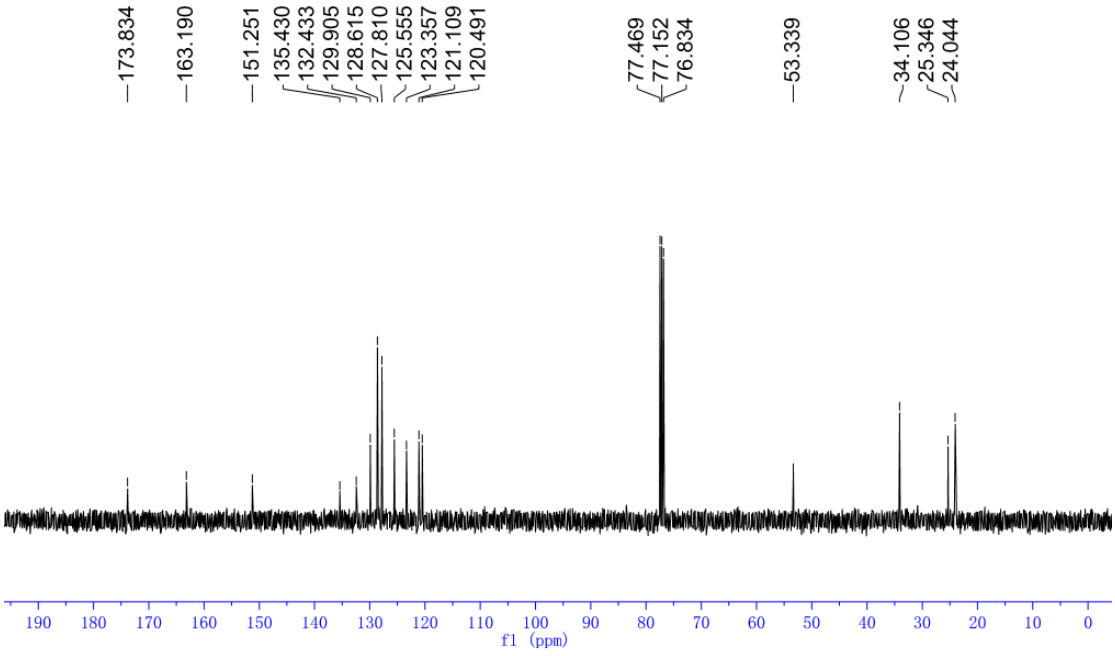
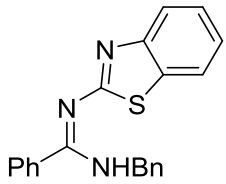
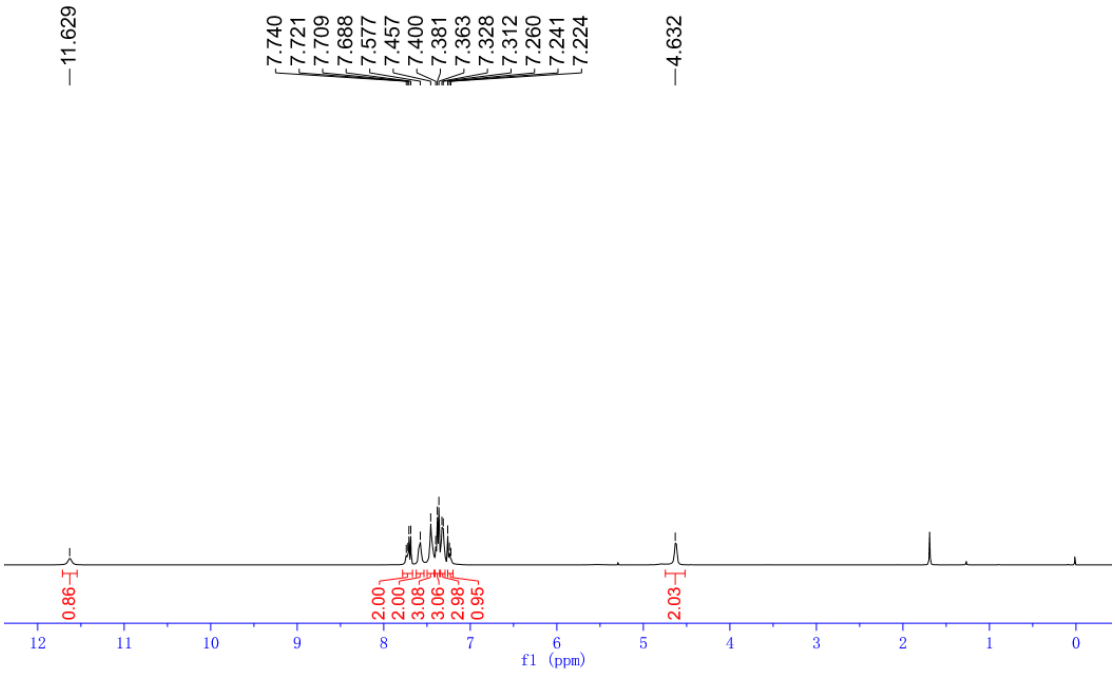
7.397
7.378
7.359
7.260
7.250
7.231
7.213
3.526
1.893
1.852
1.792
1.783
1.768
1.759
1.544
1.524
1.501
1.476
1.393
1.368
1.342
1.319
1.291
1.266
0.85
1.98
1.94
3.00
1.07
0.93
0.94
2.09
2.11
2.96
3.10
f1 (ppm)


173.834
163.190
151.251
135.430
132.433
129.905
128.615
127.810
125.555
123.357
121.109
120.491
77.469
77.152
76.834
53.339
34.106
25.346
24.044
f1 (ppm)


N
N
S
Ph
NHBn

3d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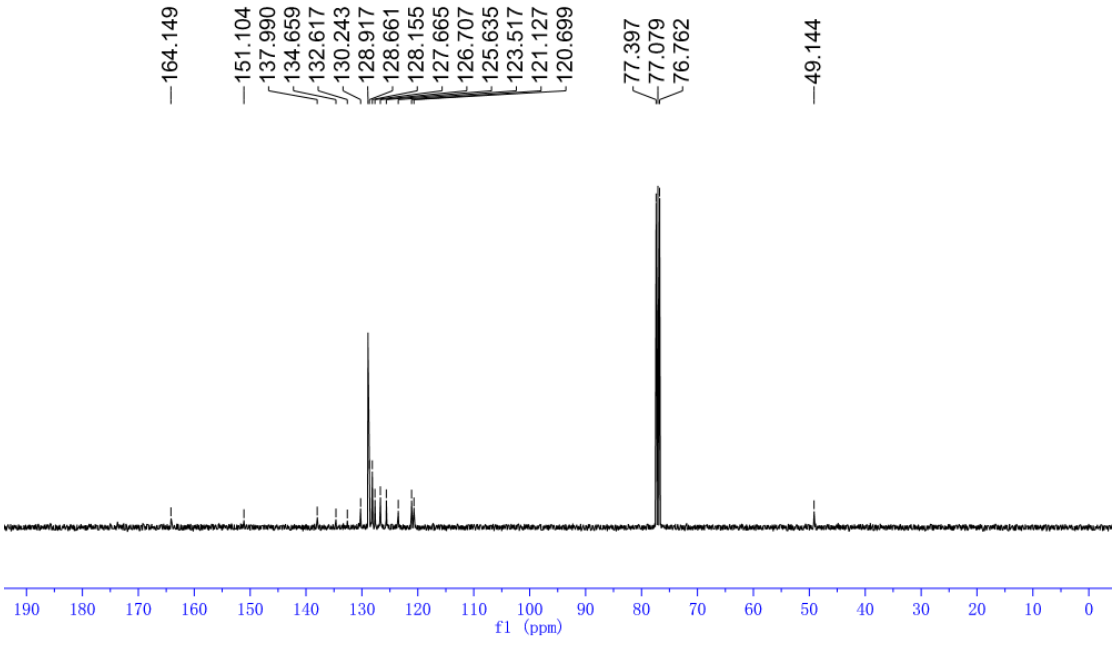
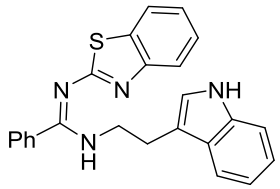
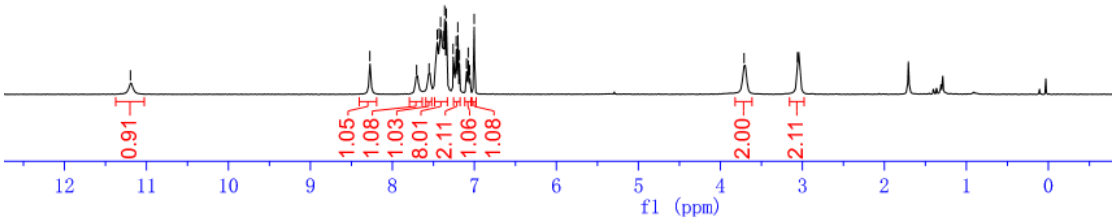
7.740
7.721
7.709
7.688
7.577
7.457
7.400
7.381
7.363
7.328
7.312
7.260
7.241
7.224
4.632
0.86
2.00
2.00
3.08
3.06
2.98
0.95
2.03
f1 (ppm)

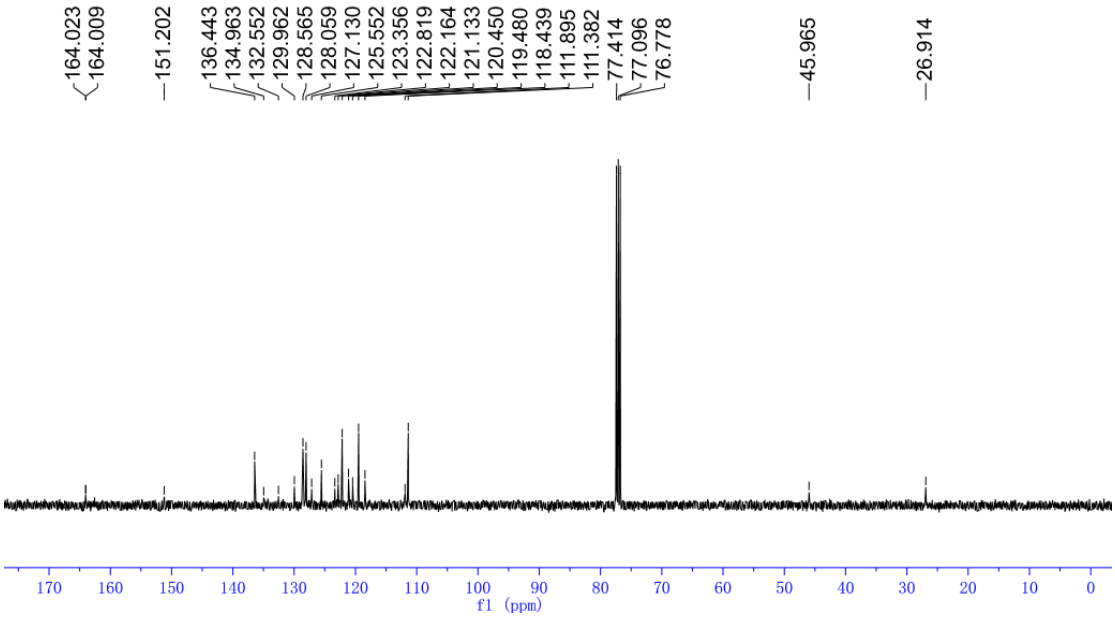

164.149
151.104
137.990
134.659
132.617
130.243
128.917
128.661
128.155
127.665
126.707
125.635
123.517
121.127
120.699
77.397
77.079
76.762
49.144
f1 (ppm)

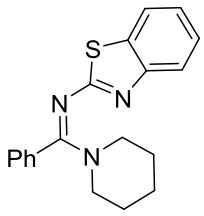

S
N
N
NH
Ph
N
H

3e

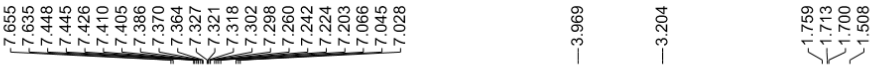

11.194
8.275
7.706
7.553
7.453
7.429
7.412
7.379
7.363
7.343
7.260
7.247
7.221
7.202
7.183
7.094
7.076
7.058
7.003
3.712
3.060

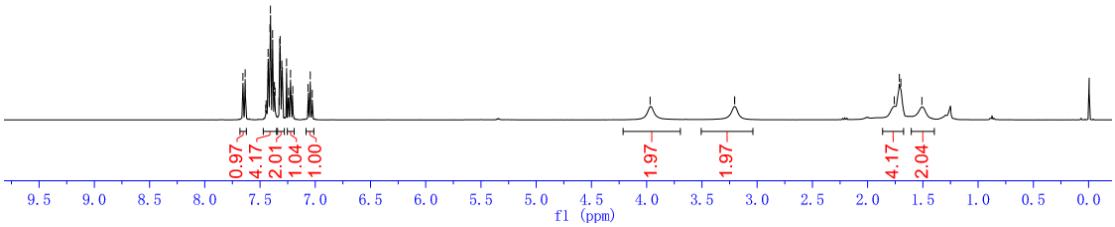

0.91
1.05
1.08
1.03
8.01
2.11
1.06
1.08
2.00
2.11
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

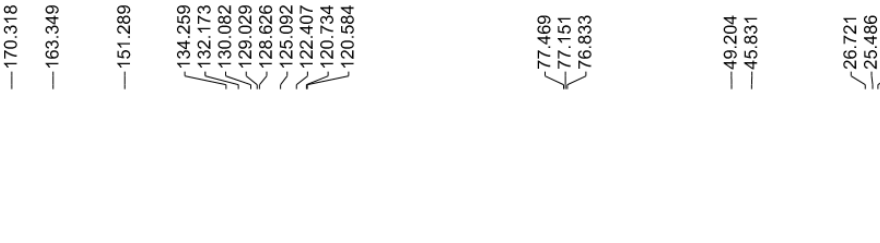

164.023
164.009
151.202
136.443
134.963
132.552
129.962
128.565
128.059
127.130
125.552
123.356
122.819
122.164
121.133
120.450
119.480
118.439
111.895
111.382
77.414
77.096
76.778
45.965
26.914
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

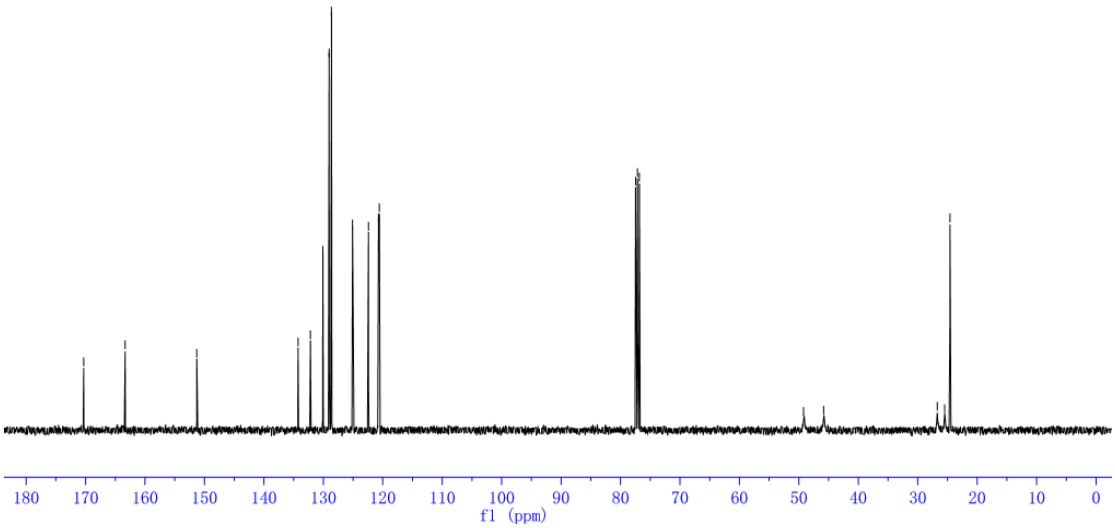

S
N
N
Ph
N

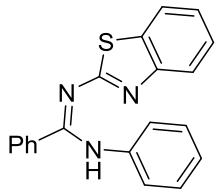
3f


7.655
7.635
7.448
7.445
7.426
7.410
7.405
7.386
7.370
7.364
7.327
7.321
7.318
7.302
7.298
7.260
7.242
7.224
7.203
7.066
7.045
7.028
3.969
3.204
1.759
1.713
1.700
1.508

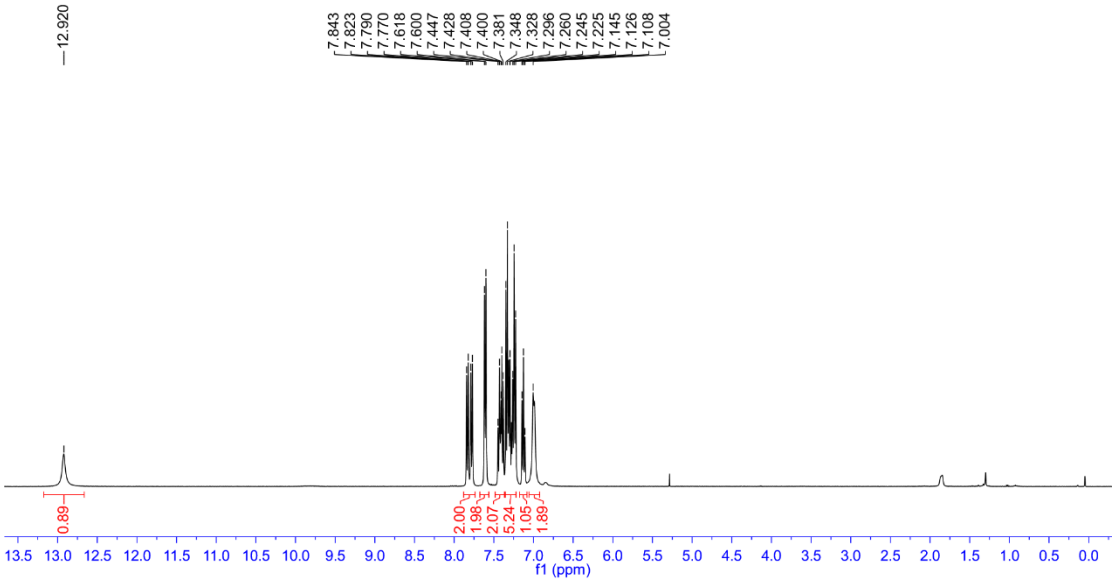

0.97
4.17
2.01
1.04
1.00
1.97
1.97
4.17
2.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


170.318
163.349
151.289
134.259
132.173
130.082
129.029
128.626
125.092
122.407
120.734
120.584
77.469
77.151
76.833
49.204
45.831
26.721
25.486
24.588


180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


S
N
N
Ph
N
H

3g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7.823
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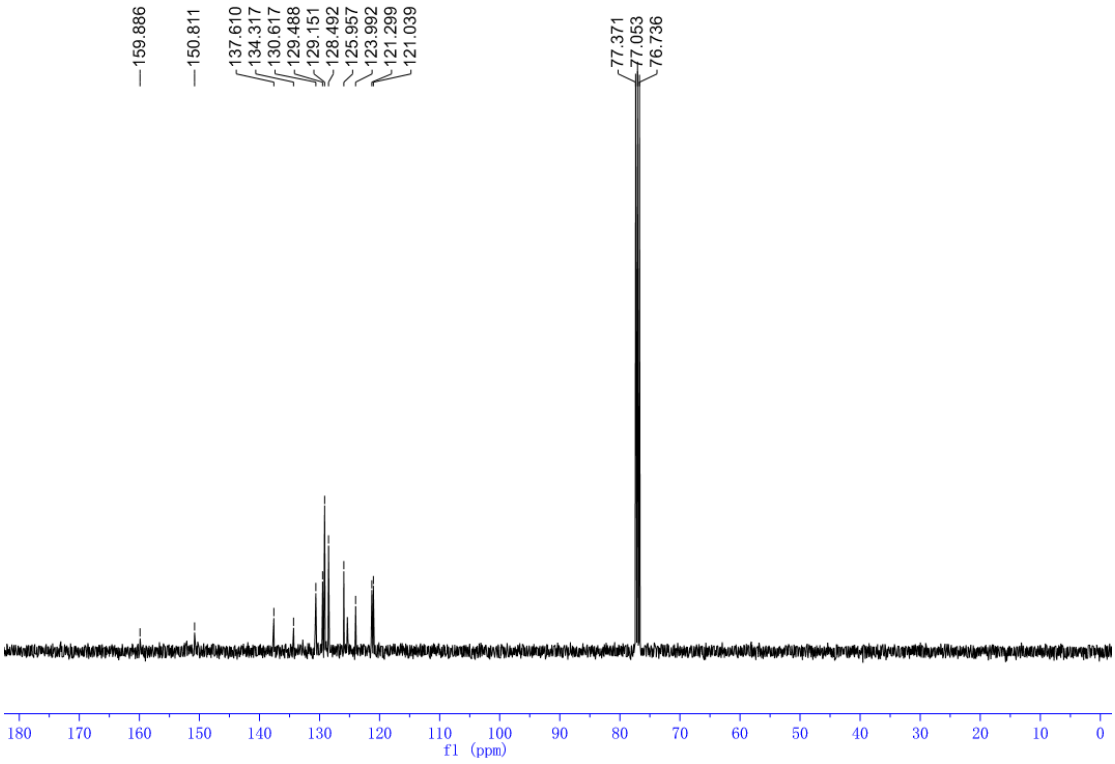
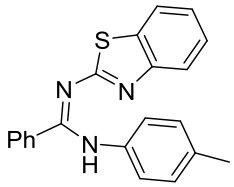
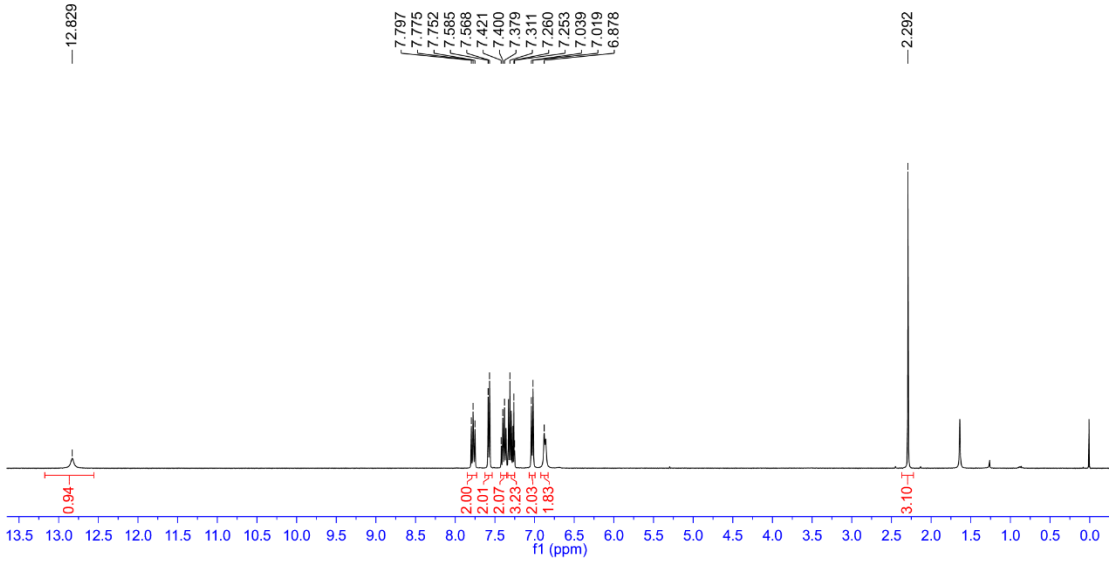
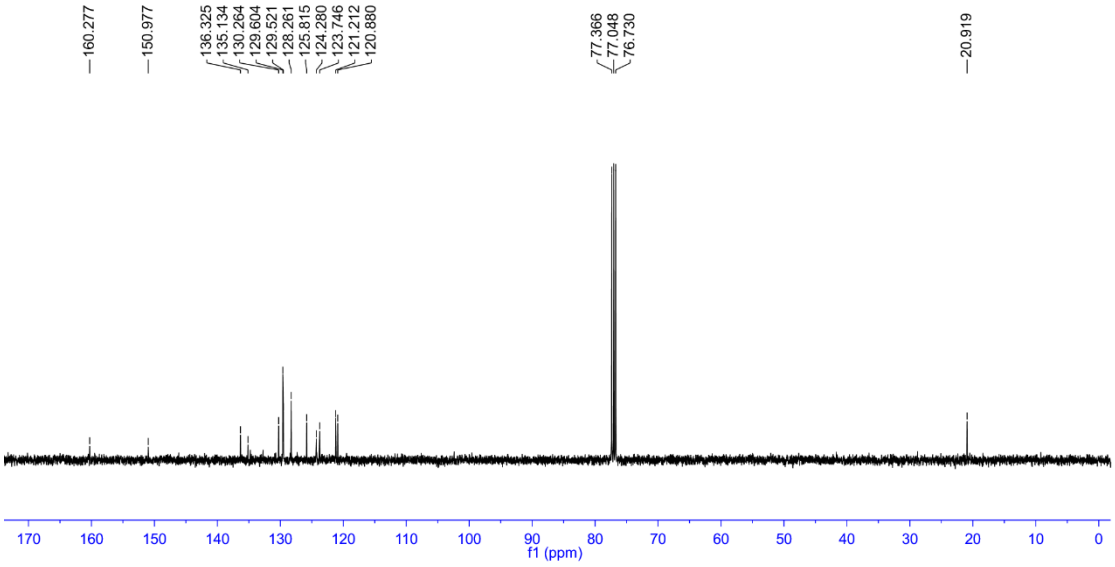
7.770
7.618
7.600
7.447
7.428
7.408
7.400
7.381
7.348
7.328
7.296
7.260
7.245
7.225
7.145
7.126
7.108
7.004
0.89
2.00
1.98
2.07
5.24
1.05
1.89
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

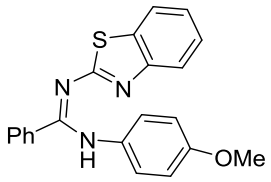

159.886
150.811
137.610
134.317
130.617
129.488
129.151
128.492
125.957
123.992
121.299
121.039
77.371
77.053
76.736
f1 (ppm)


S
N
N
Ph
N
H

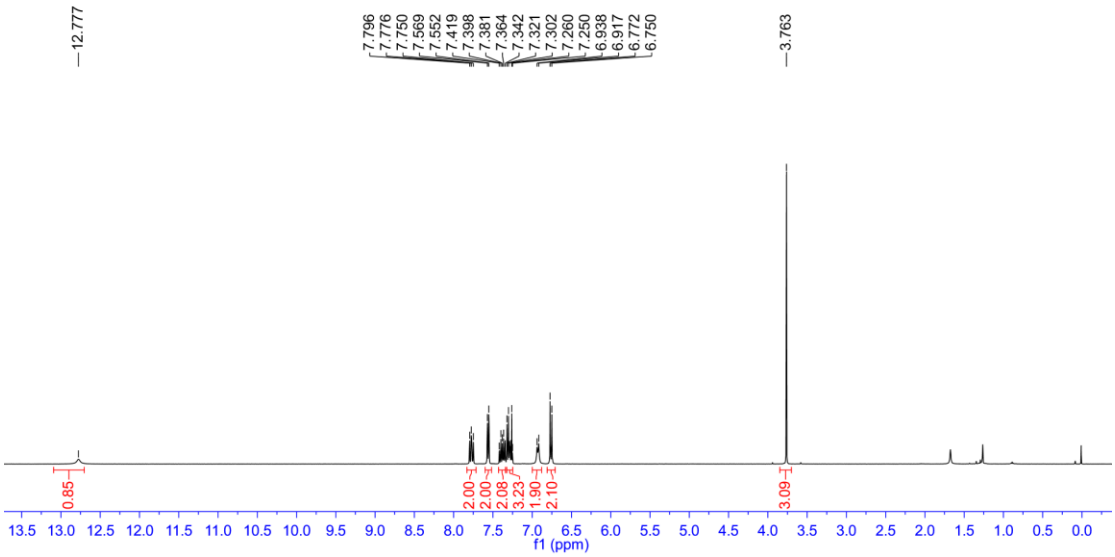
3h

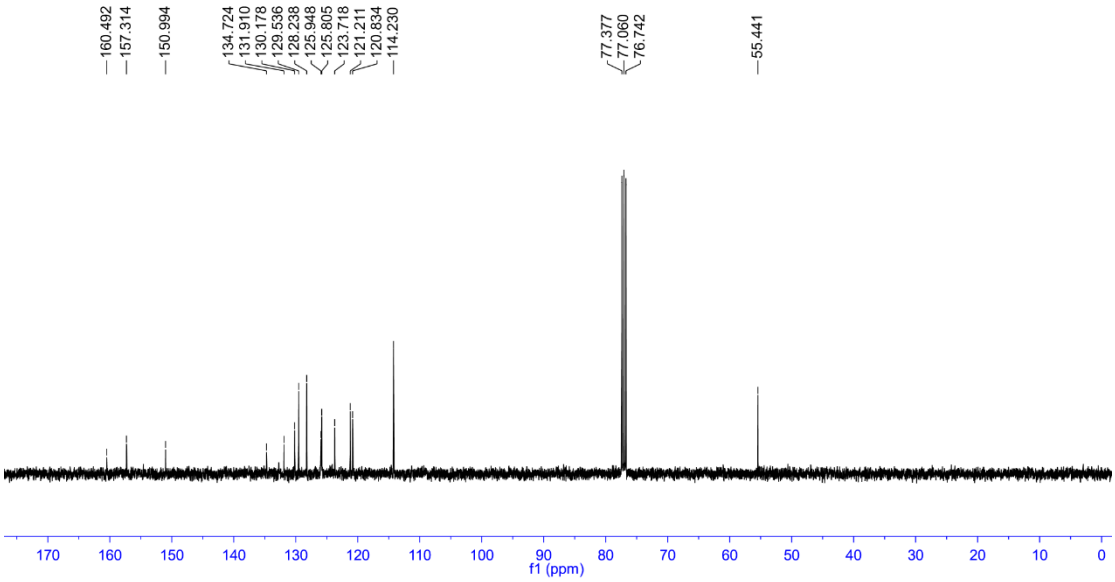

12.829
7.797
7.775
7.752
7.585
7.568
7.421
7.400
7.379
7.311
7.260
7.253
7.039
7.019
6.878
2.292
0.94
2.00
2.01
2.07
3.23
2.03
1.83
3.10
f1 (ppm)

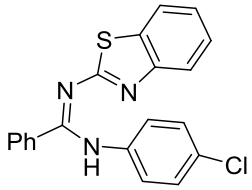

160.277
150.977
136.325
135.134
130.264
129.604
129.521
128.261
125.815
124.280
123.746
121.212
120.880
77.366
77.048
76.730
20.919
f1 (ppm)


S
N
N
Ph
N
H
OMe

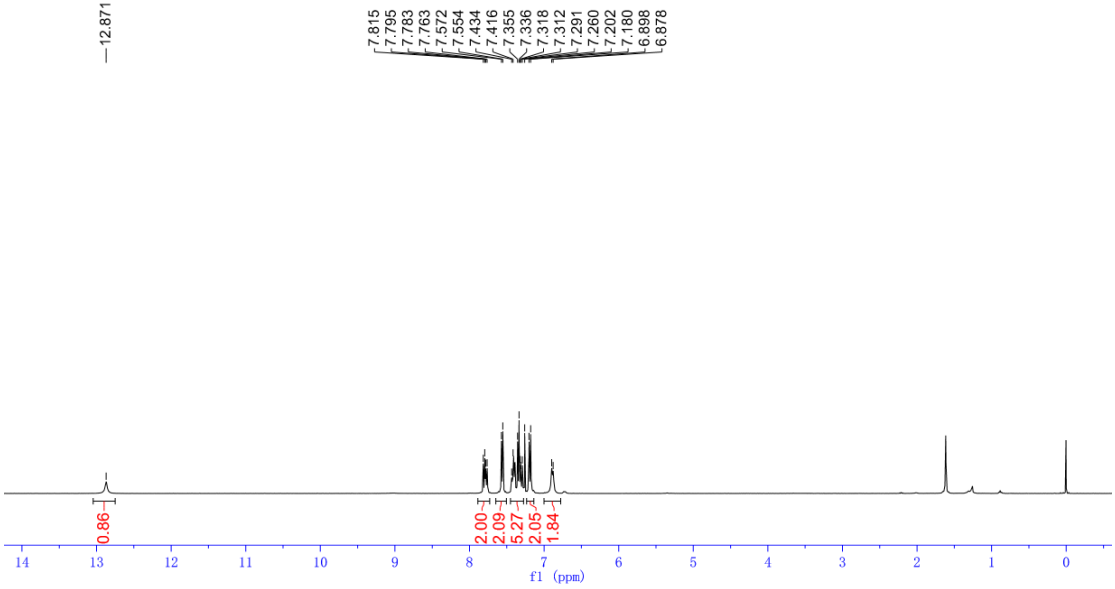
3i


12.777
7.796
7.776
7.750
7.569
7.552
7.419
7.398
7.381
7.364
7.342
7.321
7.302
7.260
7.250
6.938
6.917
6.772
6.750
3.763
0.85
2.00
2.00
2.08
3.23
1.90
2.10
3.09
f1 (ppm)


160.492
157.314
150.994
134.724
131.910
130.178
129.536
128.238
125.948
125.805
123.718
121.211
120.834
114.230
77.377
77.060
76.742
55.441
f1 (ppm)


S
N
N
Ph
N
H
Cl

3j


12.871
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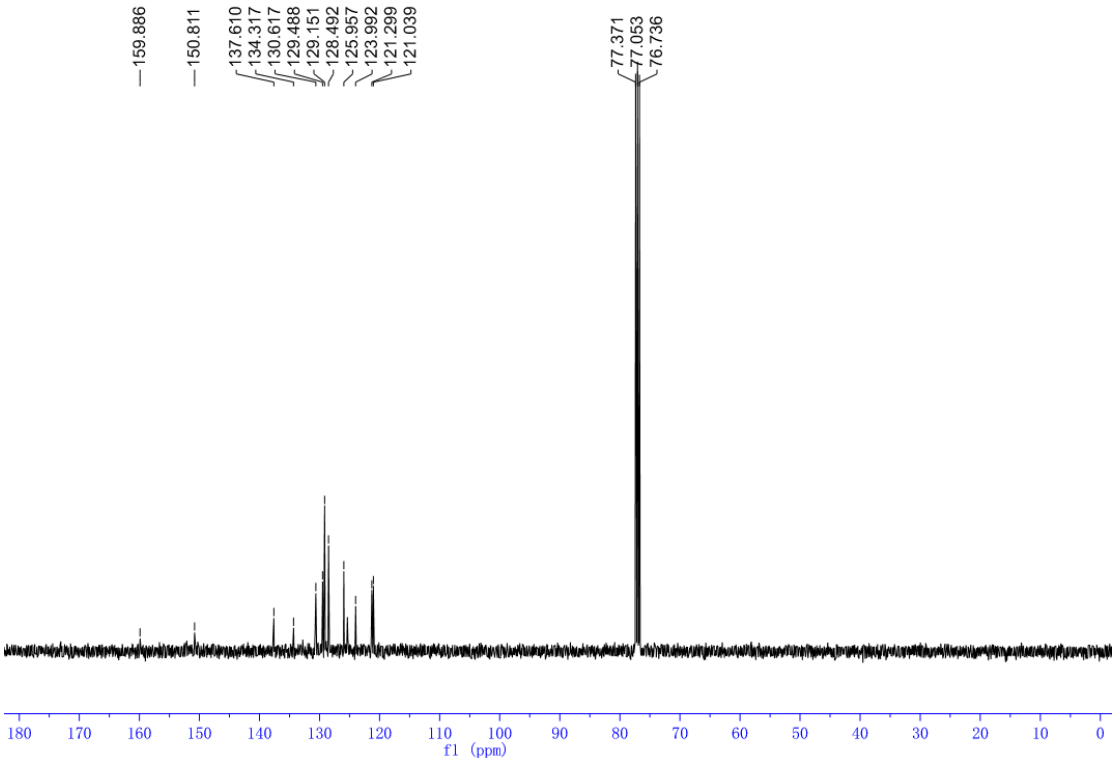
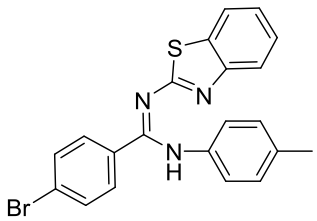
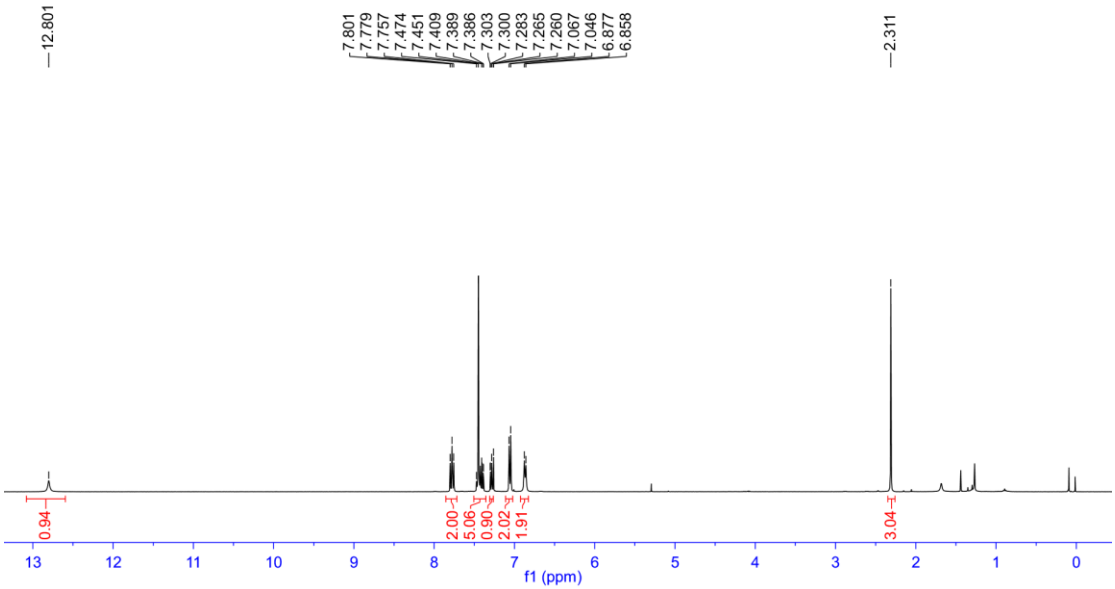
7.795
7.783
7.763
7.572
7.554
7.434
7.416
7.355
7.336
7.318
7.312
7.291
7.260
7.202
7.180
6.898
6.878
0.86
2.00
2.09
5.27
2.05
1.84
f1 (ppm)


159.886
150.811
137.610
134.317
130.617
129.488
129.151
128.492
125.957
123.992
121.299
121.039
77.371
77.053
76.736
f1 (ppm)


S
N
N
H
Br

3k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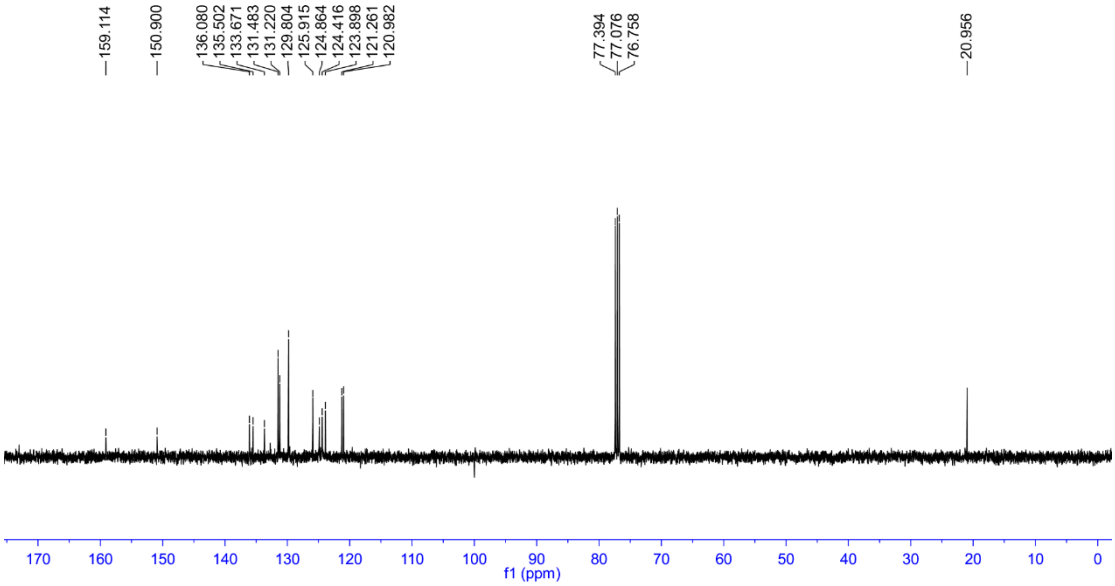
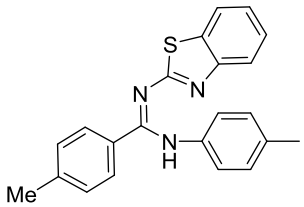
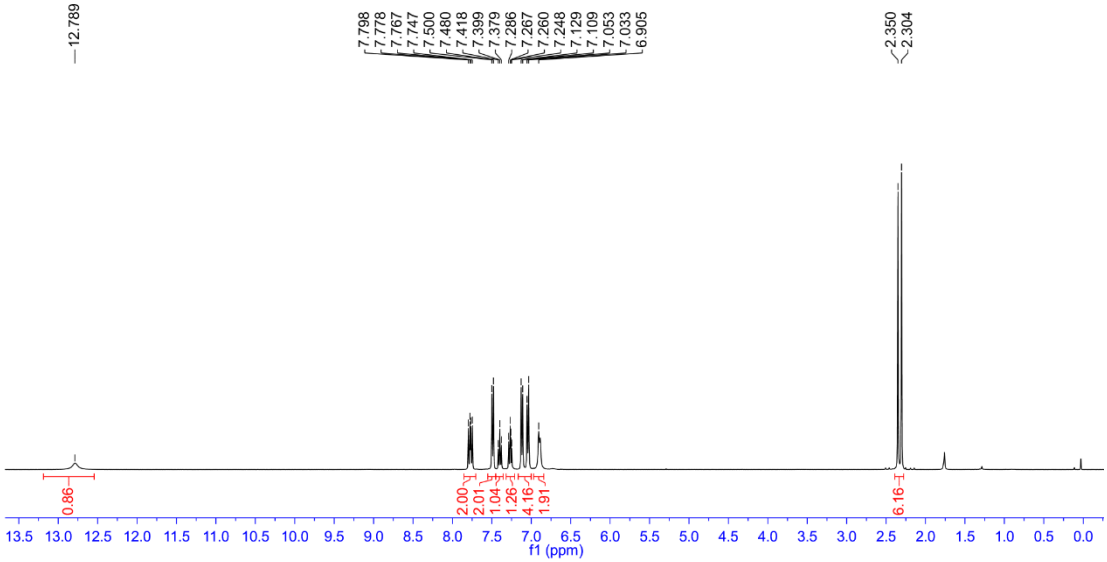
7.779
7.757
7.474
7.451
7.409
7.389
7.386
7.303
7.300
7.283
7.265
7.260
7.067
7.046
6.877
6.858
2.311
0.94
2.00
5.06
0.90
2.02
1.91
3.04
f1 (ppm)


159.114
150.900
136.080
135.502
133.671
131.483
131.220
129.804
125.915
124.864
124.416
123.898
121.261
120.982
77.394
77.076
76.758
20.956
f1 (ppm)


S
N
N
N
H
Me

3l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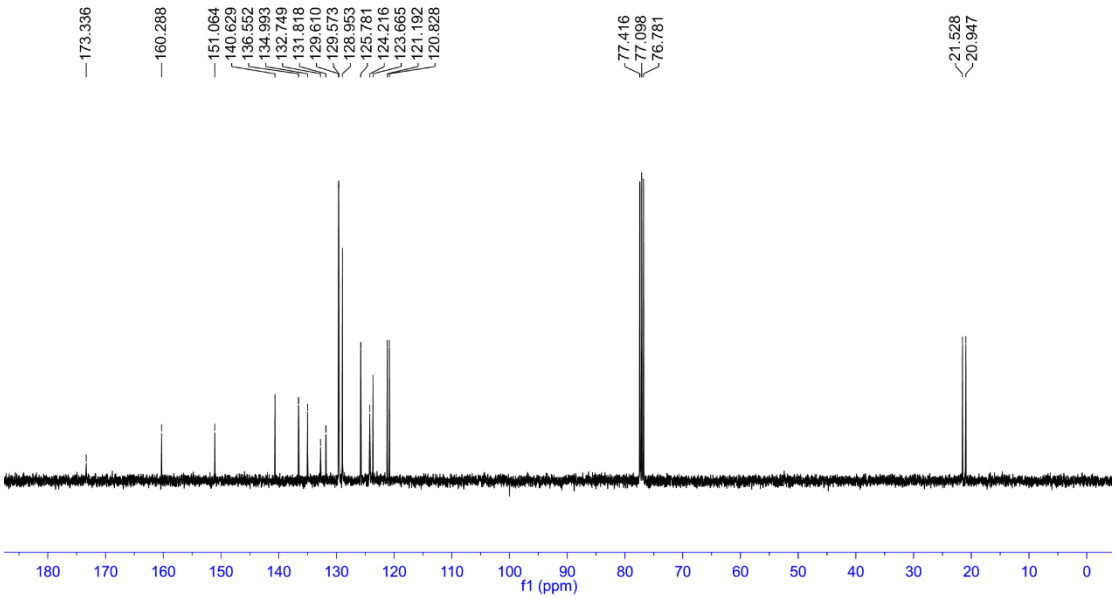
7.500
7.480
7.418
7.399
7.379
7.286
7.267
7.260
7.248
7.129
7.109
7.053
7.033
6.905
2.350
2.304
0.86
2.00
2.01
1.04
1.26
4.16
1.91
6.16
f1 (ppm)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134.993
132.749
131.818
129.610
129.573
128.953
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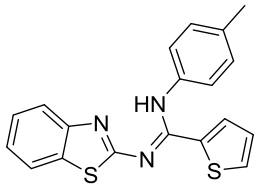
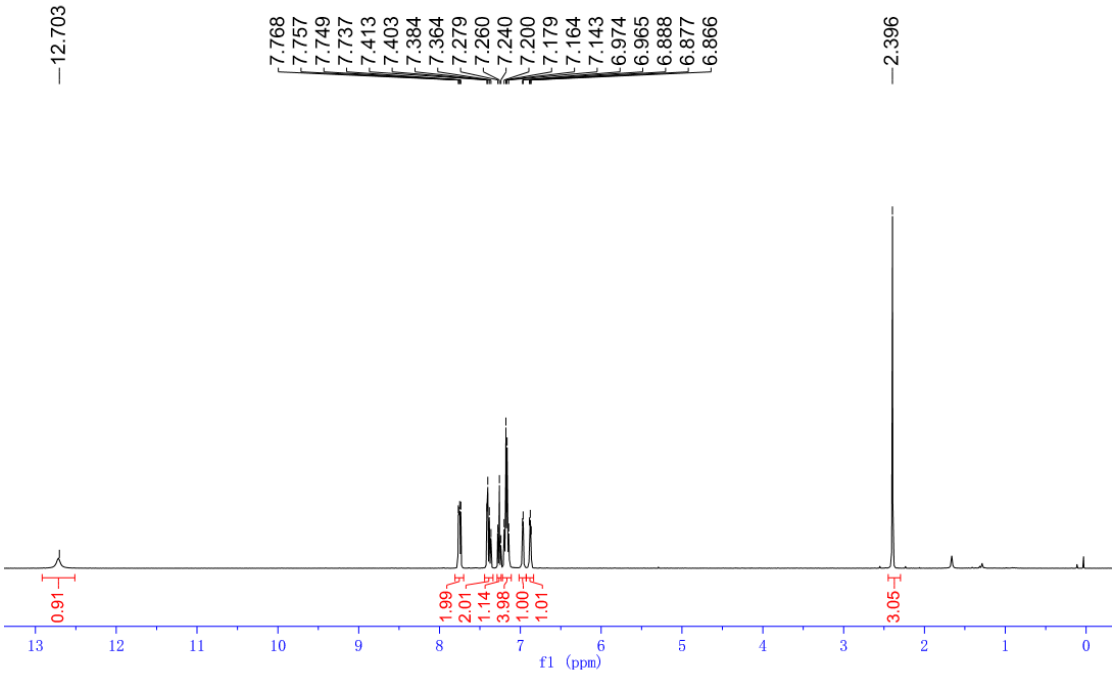
21.528
20.947
f1 (ppm)


HN
N
N
S
S

3m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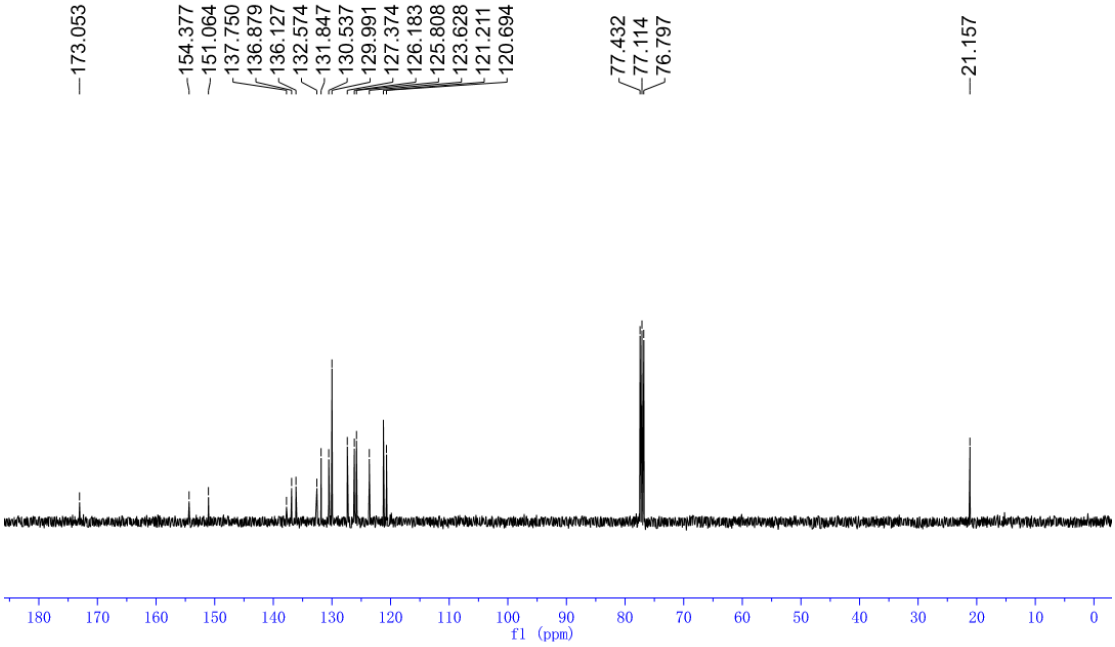
7.757
7.749
7.737
7.413
7.403
7.384
7.364
7.279
7.260
7.240
7.200
7.179
7.164
7.143
6.974
6.965
6.888
6.877
6.866
2.396
0.91
1.99
2.01
1.14
3.98
1.00
1.01
3.05
f1 (ppm)


173.053
154.377
151.064
137.750
136.879
136.127
132.574
131.847
130.537
129.991
127.374
126.183
125.808
123.628
121.211
120.694
77.432
77.114
76.797
21.157
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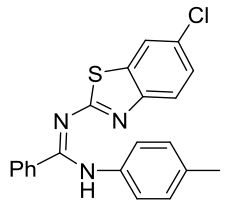
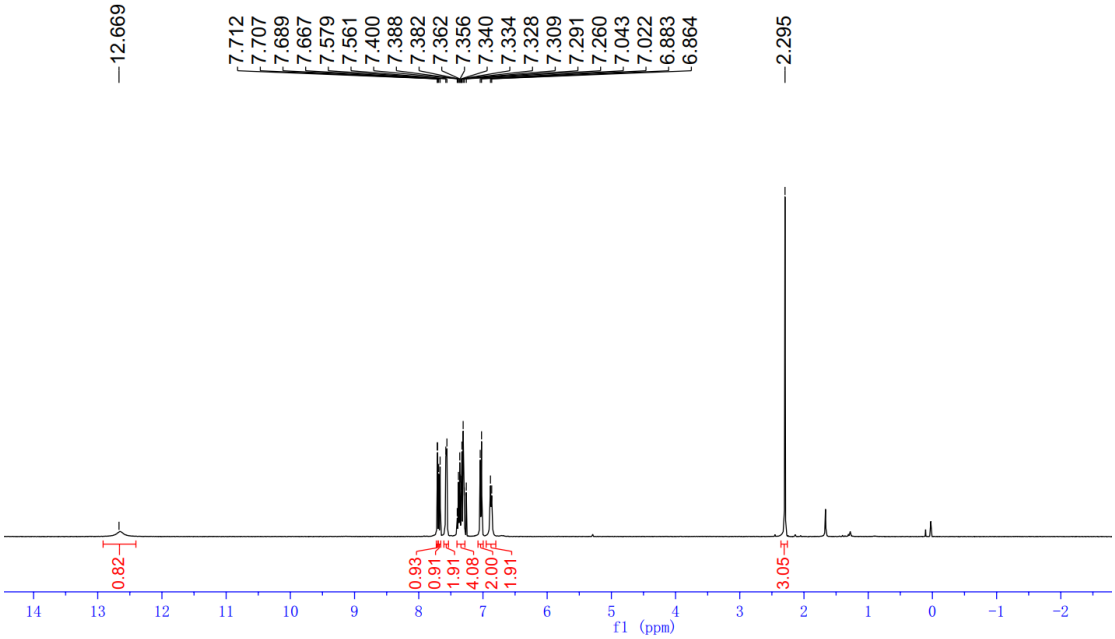
f1 (ppm)


Cl
S
N
N
Ph
N
H

3n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7.689
7.667
7.579
7.561
7.400
7.388
7.382
7.362
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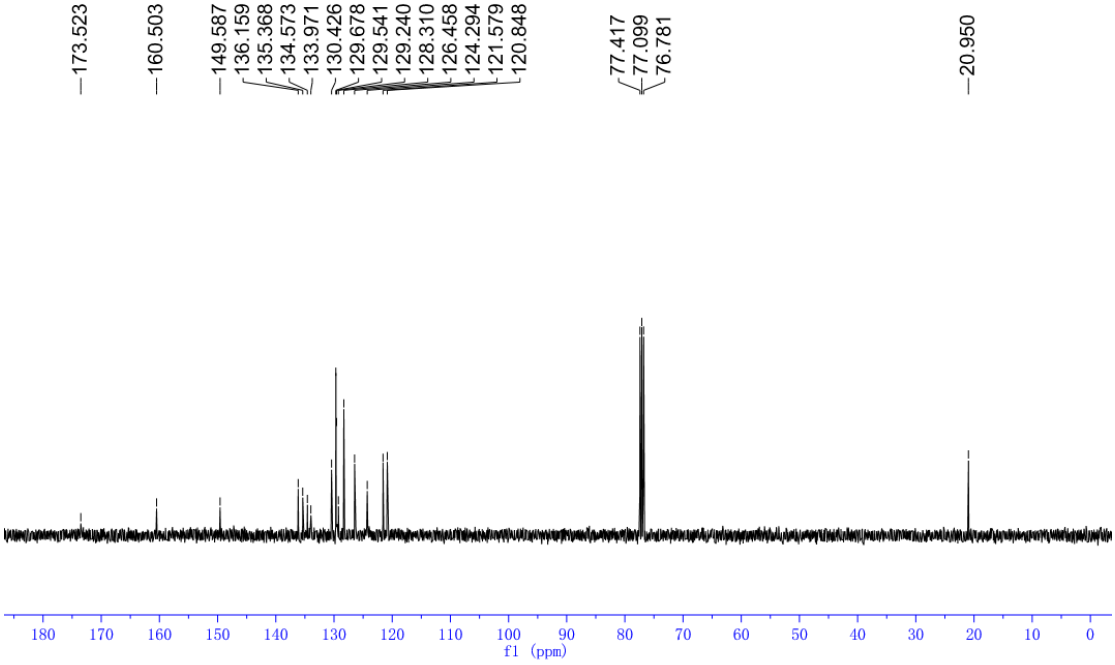
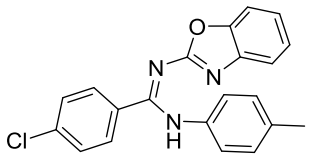
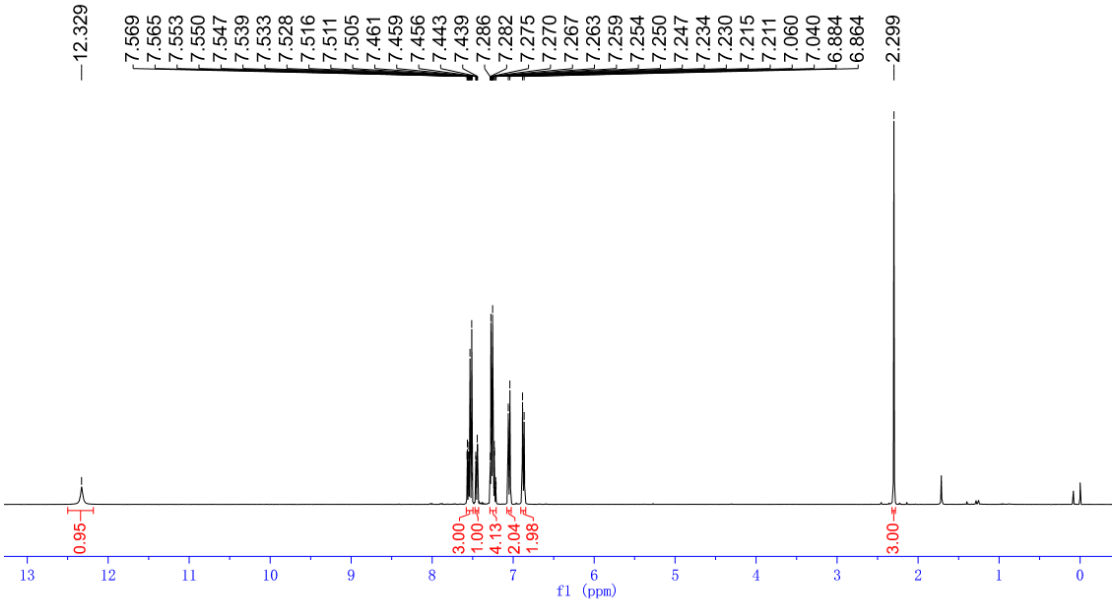
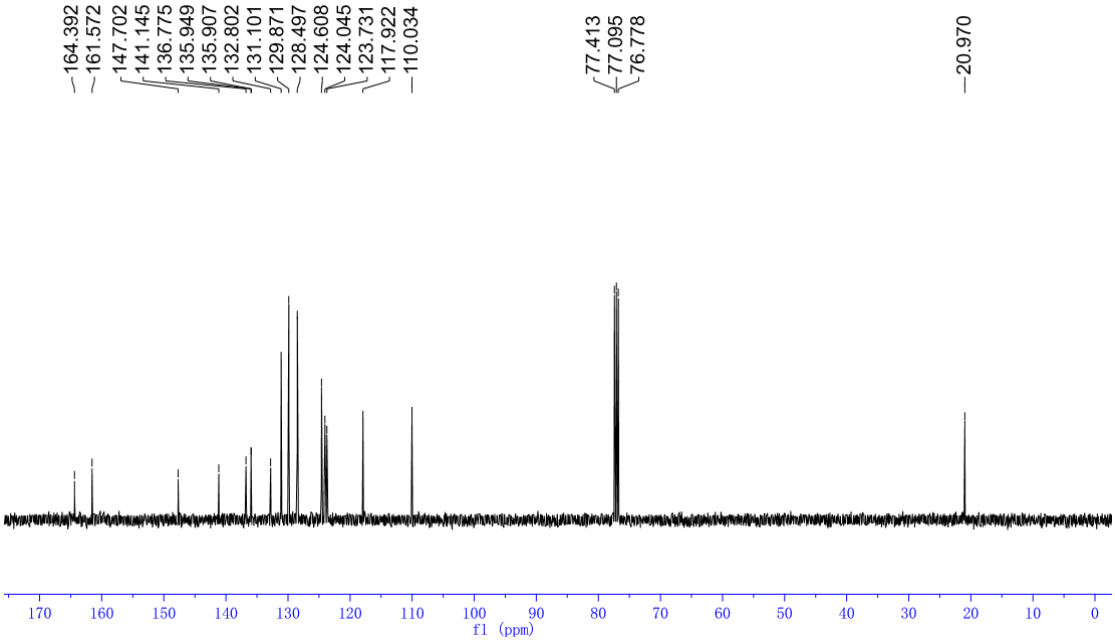
7.340
7.334
7.328
7.309
7.291
7.260
7.043
7.022
6.883
6.864
2.295
0.82
0.93
0.91
1.91
4.08
2.00
1.91
3.05
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2
f1 (ppm)

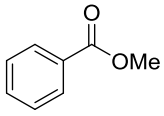

173.523
160.503
149.587
136.159
135.368
134.573
133.971
130.426
129.678
129.541
129.240
128.310
126.458
124.294
121.579
120.848
77.417
77.099
76.781
20.950
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O
N
N
N
H
Cl

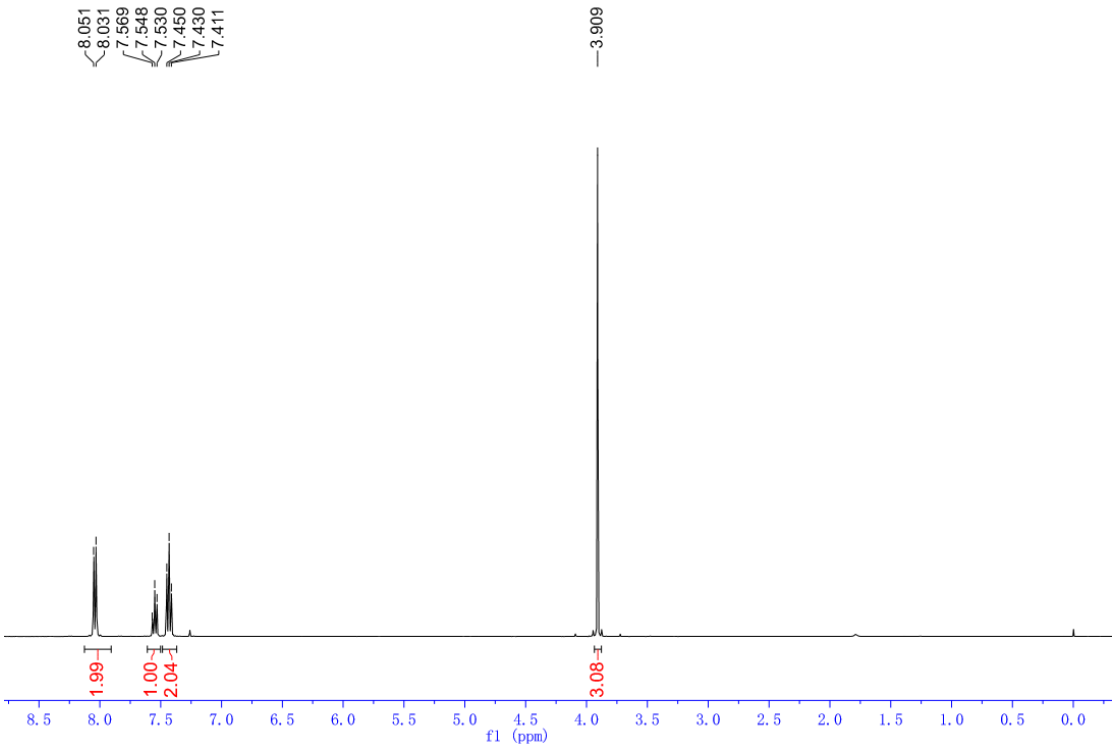
3o

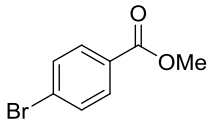

12.329
7.569
7.565
7.553
7.550
7.547
7.539
7.533
7.528
7.516
7.511
7.505
7.461
7.459
7.456
7.443
7.439
7.286
7.282
7.275
7.270
7.267
7.263
7.259
7.254
7.250
7.247
7.234
7.230
7.215
7.211
7.060
7.040
6.884
6.864
2.299
0.95
3.00
1.00
4.13
2.04
1.98
3.00
13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


164.392
161.572
147.702
141.145
136.775
135.949
135.907
132.802
131.101
129.871
128.497
124.608
124.045
123.731
117.922
110.034
77.413
77.095
76.778
20.970
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

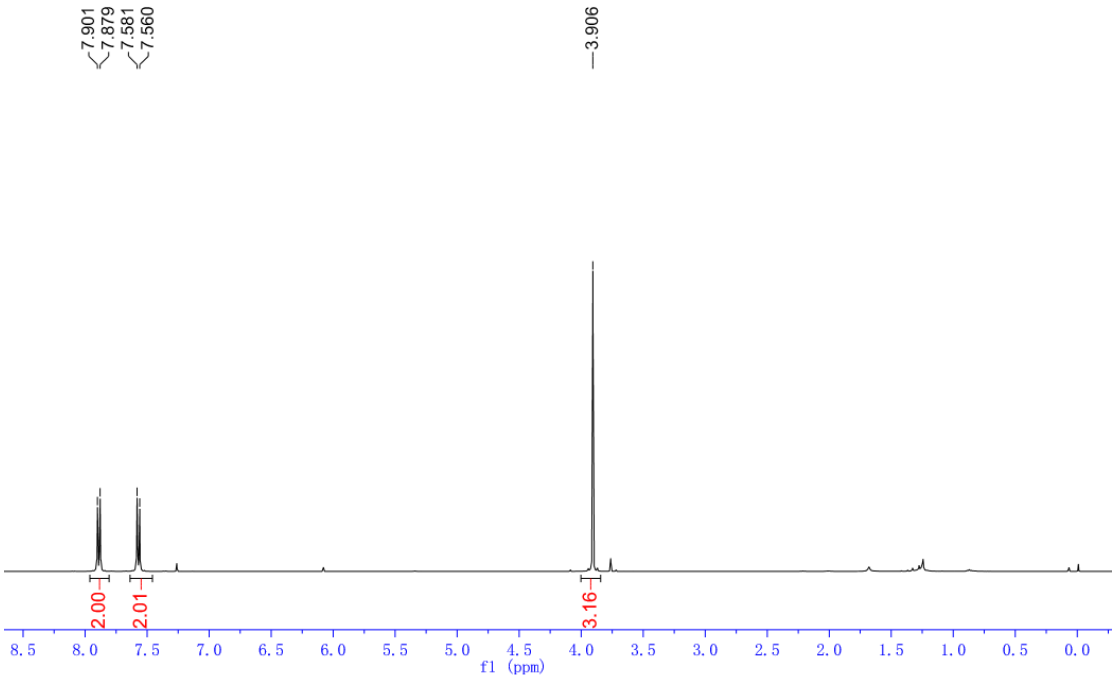

O
OMe

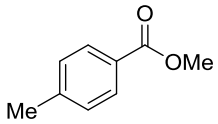
5a


8.051
8.031
7.569
7.548
7.530
7.450
7.430
7.411
3.909
1.99
1.00
2.04
3.08
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

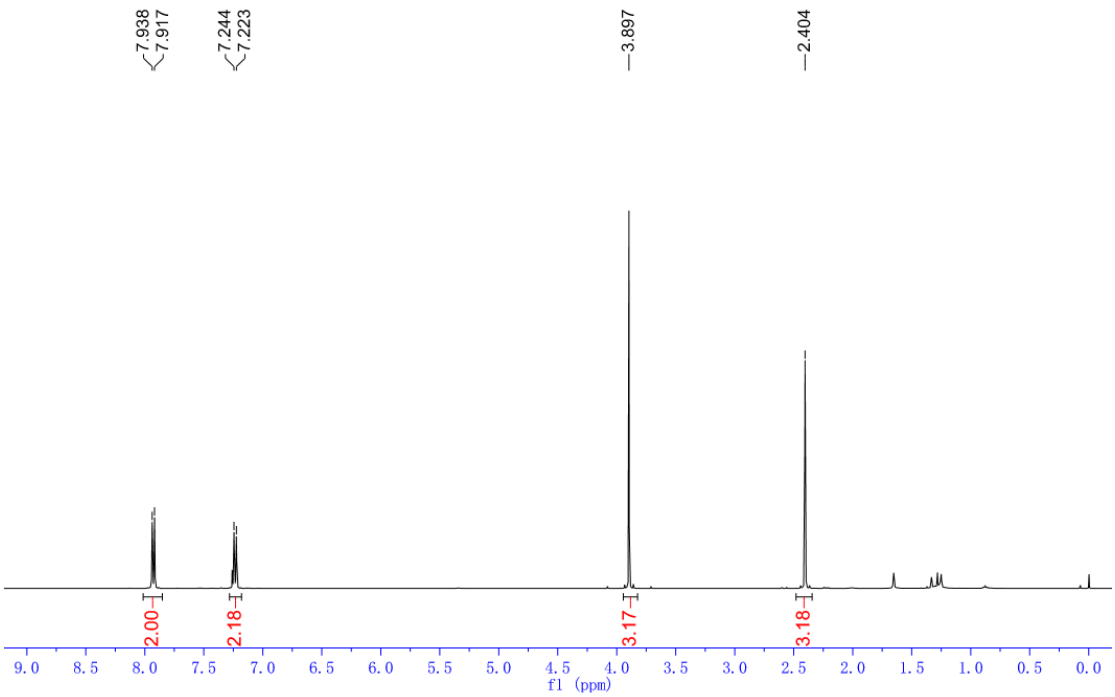

O
OMe
Br

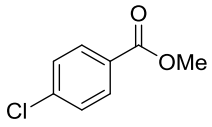
5b


7.901
7.879
7.581
7.560
3.906
2.00
2.01
3.16
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

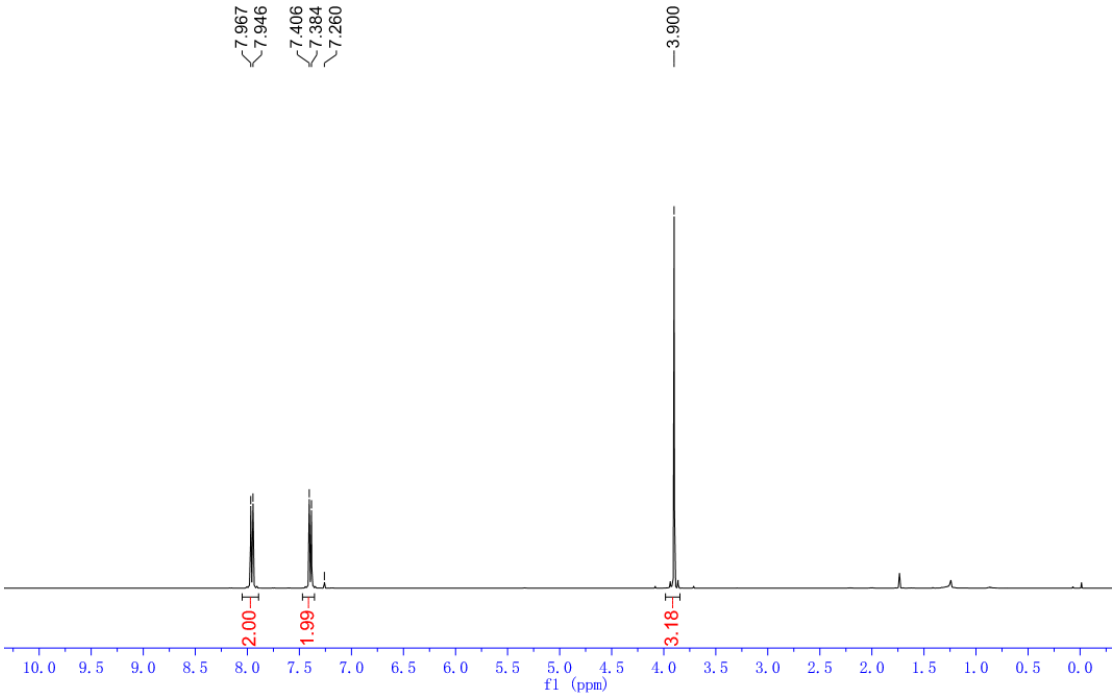

O
OMe
Me

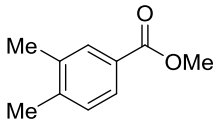
5c


7.938
7.917
7.244
7.223
3.897
2.404
2.00
2.18
3.17
3.18
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

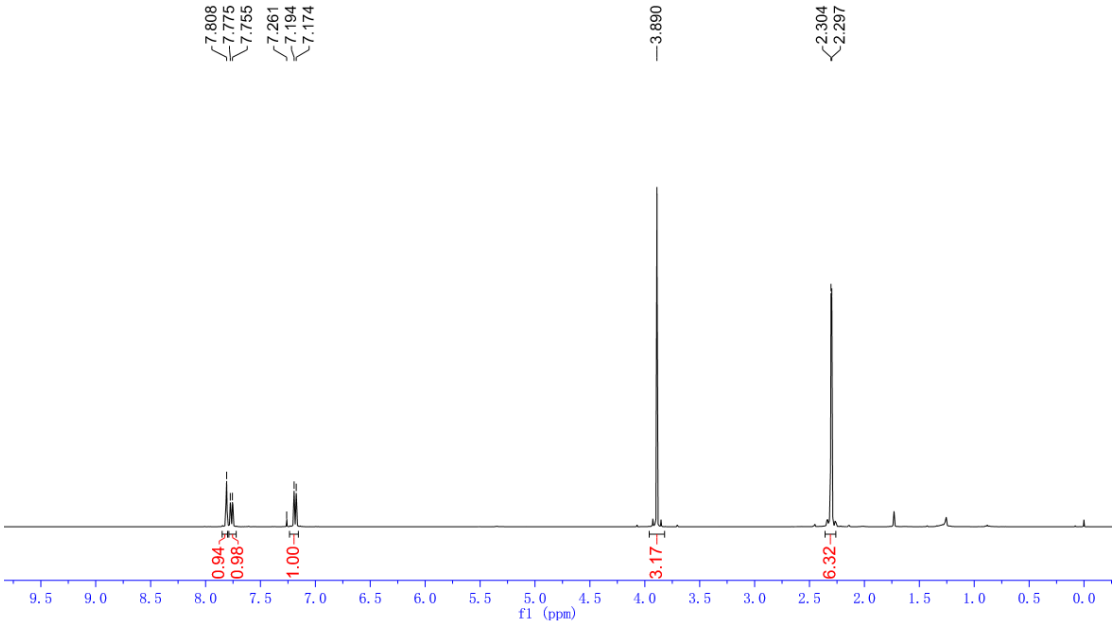

O
OMe
Cl

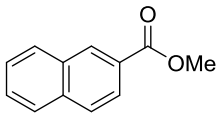
5d


7.967
7.946
7.406
7.384
7.260
3.900
2.00
1.99
3.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

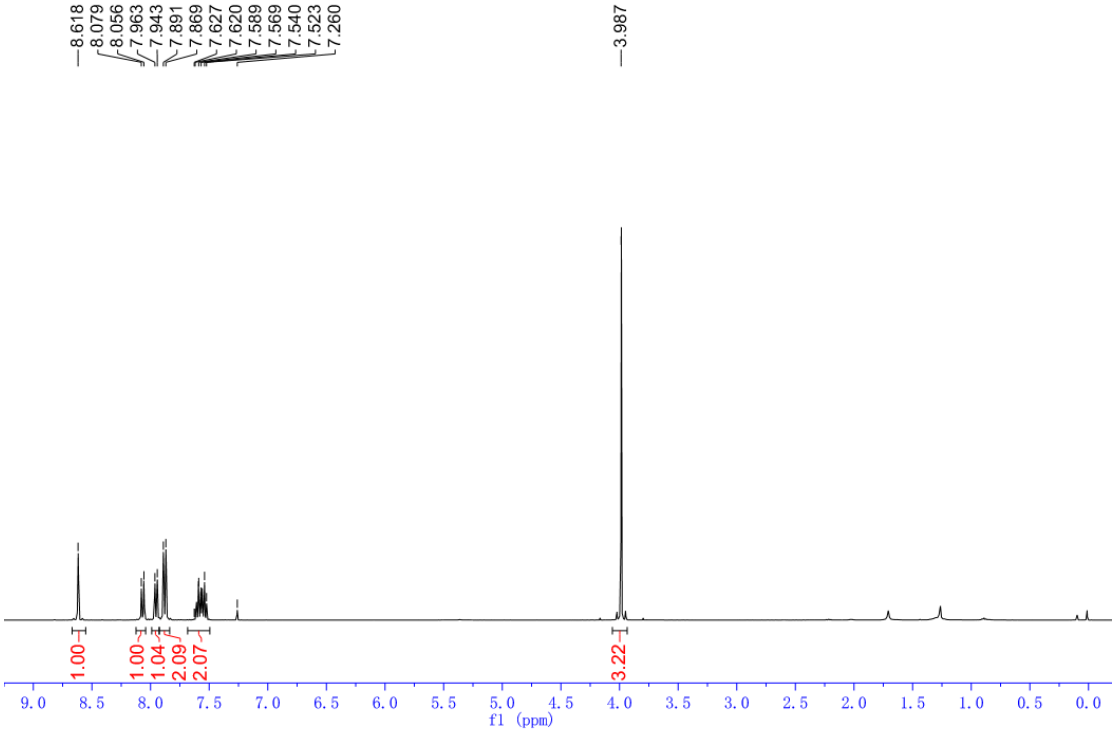

O
OMe
Me
Me

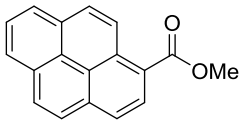
5e


7.808
7.775
7.755
7.261
7.194
7.174
3.890
2.304
2.297
0.94
0.98
1.00
3.17
6.32
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

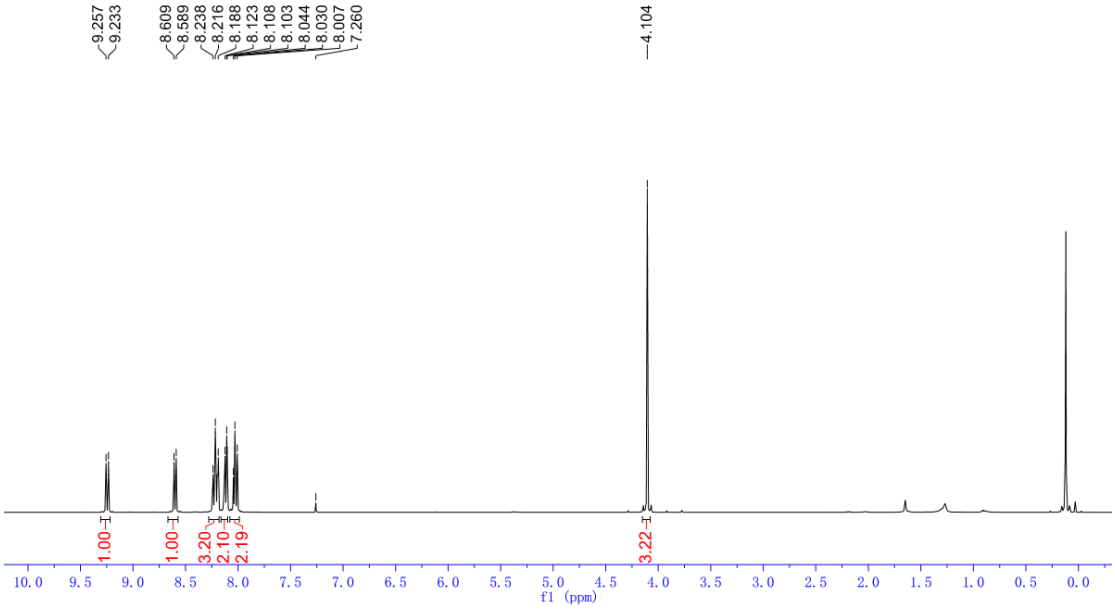

O
OMe

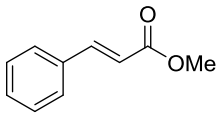
5f


8.618
8.079
8.056
7.963
7.943
7.891
7.869
7.627
7.620
7.589
7.569
7.540
7.523
7.260
3.987
1.00
1.00
1.04
2.09
2.07
3.22
f1 (ppm)

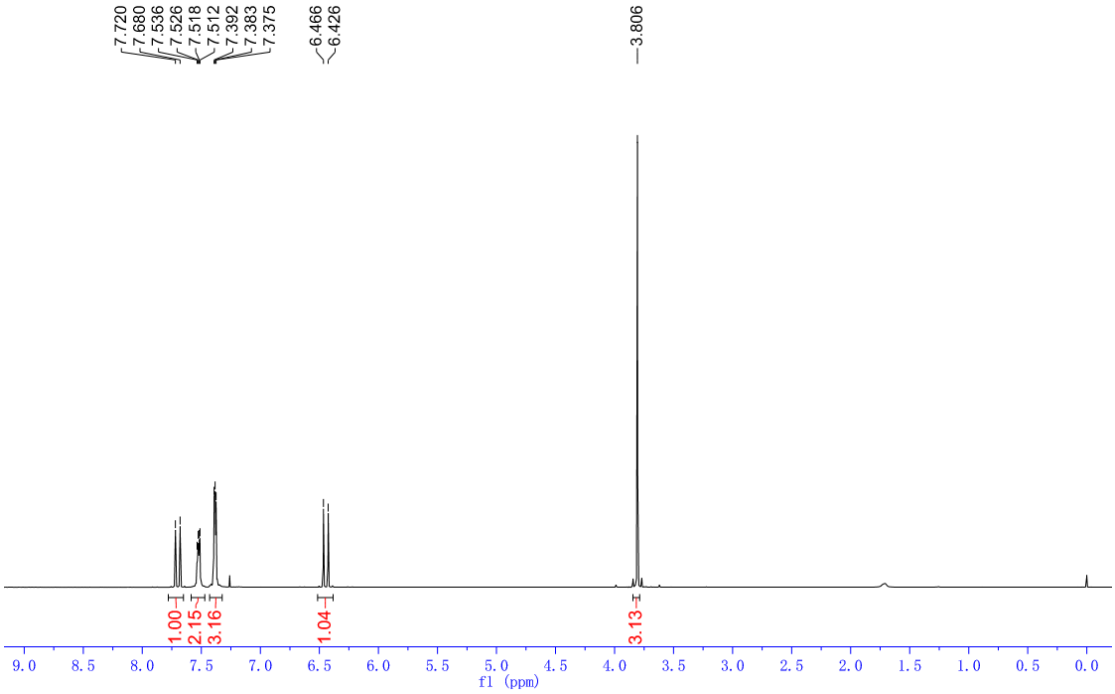

O
OMe

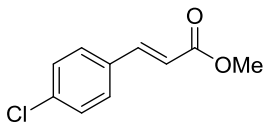
5g


9.257
9.233
8.609
8.589
8.238
8.216
8.188
8.123
8.108
8.103
8.044
8.030
8.007
7.260
4.104
1.00
1.00
3.20
2.10
2.19
3.22
f1 (ppm)

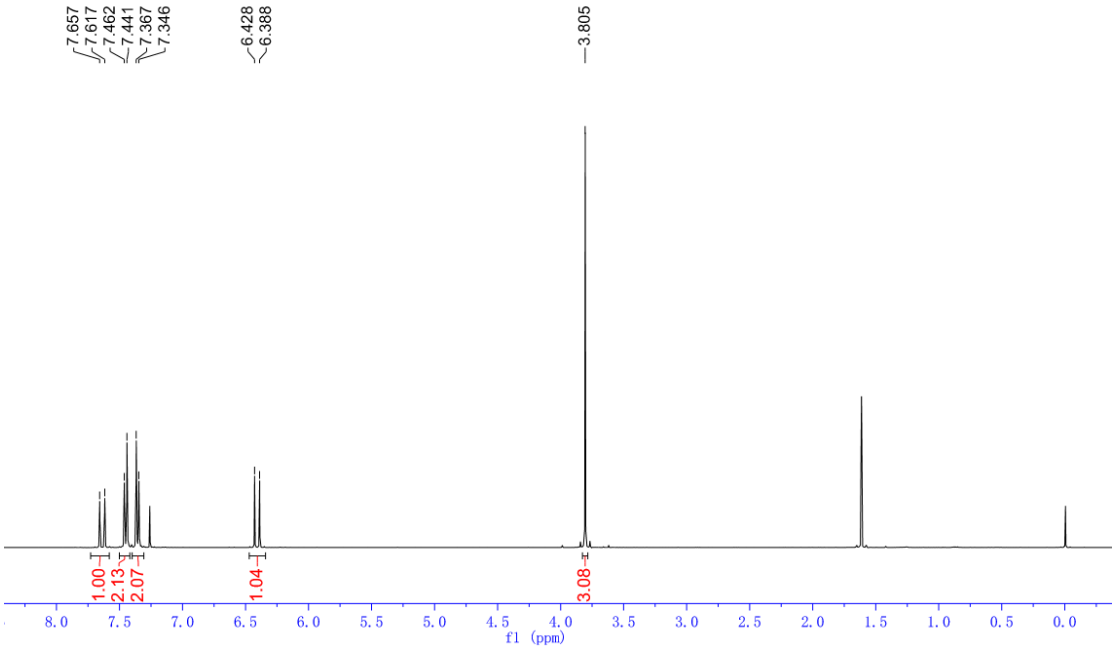

O
OMe

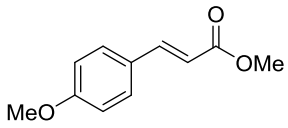
5h


7.720
7.680
7.536
7.526
7.518
7.512
7.392
7.383
7.375
6.466
6.426
3.806
1.00
2.15
3.16
1.04
3.13
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

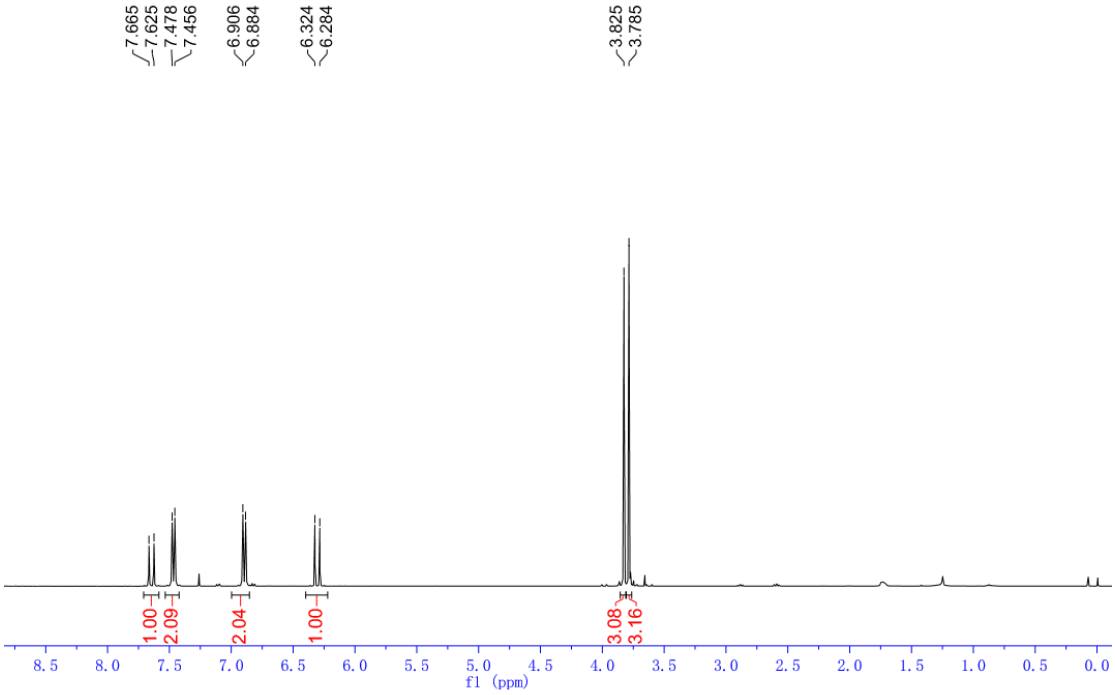

O
OMe
Cl

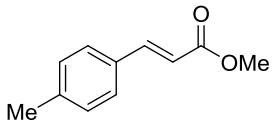
5i


7.657
7.617
7.462
7.441
7.367
7.346
6.428
6.388
3.805
1.00
2.13
2.07
1.04
3.08
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

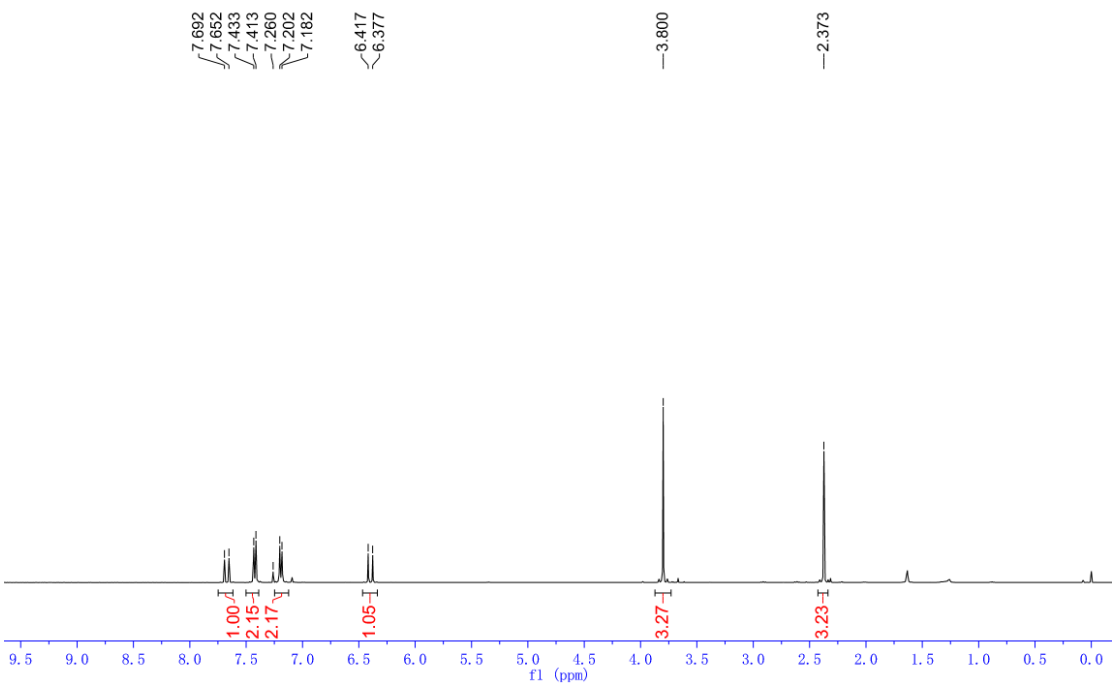

O
OMe
MeO

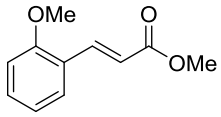
5j


7.665
7.625
7.478
7.456
6.906
6.884
6.324
6.284
3.825
3.785
1.00
2.09
2.04
1.00
3.08
3.16
f1 (ppm)

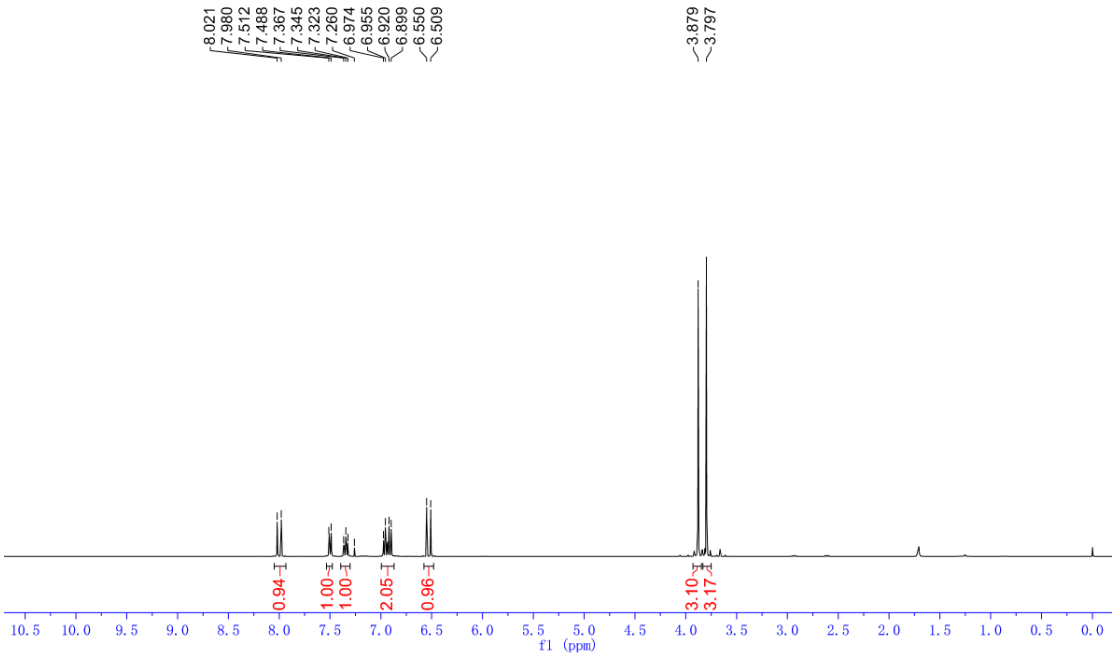

O
OMe
Me

5k


7.692
7.652
7.433
7.413
7.260
7.202
7.182
6.417
6.377
3.800
2.373
1.00
2.15
2.17
1.05
3.27
3.23
f1 (ppm)


OMe
O
OMe

5l


8.021
7.980
7.512
7.488
7.367
7.345
7.323
7.260
6.974
6.955
6.920
6.899
6.550
6.509
3.879
3.797
0.94
1.00
1.00
2.05
0.96
3.10
3.17
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)