Supporting Information

Efficient synthesis of 1,2-benzisothiazoles from *o*-haloarylamidines and elemental sulfur *via* N-S/C-S bond formation under transition-metal-free conditions

Hao Xie,[a] Guozheng Li,[a] Feng Zhang,[b,*] Fuhong Xiao,[a] and Guo-Jun Deng[a,*]

[a] Key Laboratory for Green Organic Synthesis and Application of Hunan Province，Key Laboratory of Environmentally Friendly Chemistry and Application of Ministry of Education, College of Chemistry, Xiangtan University, Xiangtan 411105, China. E-mail: zhangf@iccas.ac.cn; gjdeng@xtu.edu.cn
[b]College of Science, Hunan Agricultural University, Changsha, 410128, China.

List of Contents

1. General information:

All reactions were carried out under an atmosphere of air unless otherwise noted. Column chromatography was performed using silica gel (200-300 mesh). ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument internally referenced to tetramethylsilane (TMS) or chloroform signals. Mass spectra were measured on Agilent 5975 GC-MS instrument (EI). High-resolution mass spectra were recorded at Jiangxi University of Traditional Chinese Medicine. The structures of known compounds were further corroborated by comparing their ^{1}H NMR, ^{13}C NMR data and MS data with those of literature. Reagents were used as received or prepared by our laboratory.

2. General procedures for the synthesis of *o*-halo amidines [1]

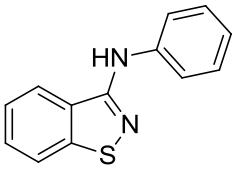
A round bottom flask (100 mL) equipped with a stir bar was charged with NaH (264 mg, 11.0 mmol, 95%, 1.10 equiv) under argon atmosphere. Under a balloon of argon, DMSO (5 mL) was added, and the resulting suspension cooled with an ice-water bath prior to the addition of aniline (12.0 mmol, 1.20 equiv) and *o*-halo carbonitrile (10.0 mmol). The mixture was kept at 0 ℃ for 30-60 min and then stirred for the indicated time at room temperature. The septum was removed, and ice-water (50 mL) was added while maintaining vigorous stirring. In the cases, when the amidine precipitated upon addition of water, the solid was filtered off and dissolved in EtOAc (20 mL). In all other cases, the aqueous layer was extracted with EtOAc (3 × 20 mL). The extracts were combined and washed with water (2 × 50 mL). In both of the aforementioned cases, the organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was either purified by silica gel chromatography or recrystallization.

3. General procedure for reaction: (2a):

A 10 mL oven-dried reaction vessel was charged with 2-chloro-*N*-phenylbenzimidamide (**1a**, 46 mg, 0.2 mmol), S (32 mg, 1.0 mmol), potassium phosphate tribasic trihydrate (107 mg, 0.4 mmol), PhMe (0.4 mL) and DMSO (0.2 mL) under air. The reaction vessel was stirred at 135 ^{o}C for 36 h. After cooling to room temperature, the volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to yield the desired product **2a** as off-white solid, 37.0 mg, yield 83%.

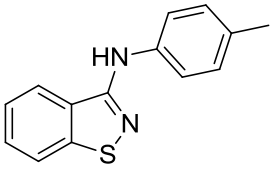
4. Characterization data of products

2-Chloro-*N*-phenylbenzimidamide (2a)



^{1}H NMR (400 MHz, DMSO-d_6, ppm) δ 9.60 (s, 1H), 8.49 (d, J = 8.1 Hz, 1H), 8.06 (d, J = 8.1 Hz, 1H), 7.96 (d, J = 7.7 Hz, 2H), 7.60 (t, J = 7.5 Hz, 1H), 7.51 (t, J = 7.5 Hz, 1H), 7.34 (t, J = 8.0 Hz, 2H), 6.97 (t, J = 7.3 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 155.3, 149.9, 141.3, 128.8, 128.5, 127.5, 124.5, 122.8, 121.4, 120.6, 117.9; HRMS calcd. for: $C_{13}H_{11}N_2S$ $[M+H]^+$ 227.0638, found 227.0636.

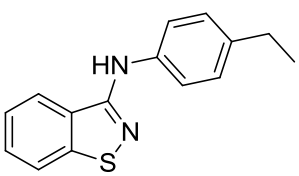
***N*-(*p*-Tolyl)benzo[d]isothiazol-3-amine (2b)**



2-Chloro-*N*-(*p*-tolyl)benzimidamide (**1b**, 48.8 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2b** as brown solid, 30.2 mg, yield 63%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.83 (d, J = 8.1 Hz, 1H), 7.77 (d, J = 8.1 Hz, 1H), 7.61 (d, J = 8.3 Hz, 2H), 7.52 (t, J = 7.3 Hz, 1H), 7.40 (t, J = 7.5 Hz, 1H), 7.17 (d, J = 8.2 Hz, 2H), 6.98 (s, 1H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.7, 151.0, 137.7, 131.9, 129.6, 128.1, 127.0, 124.1, 120.8, 120.4, 118.5, 20.8; HRMS calcd. for: $C_{14}H_{13}N_2S$ $[M+H]^+$ 241.0794, found 241.0790.

***N*-(4-Ethylphenyl)benzo[d]isothiazol-3-amine (2c)**

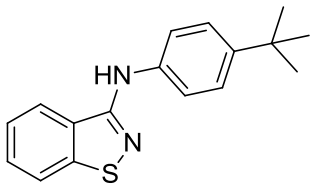


2-Chloro-*N*-(4-ethylphenyl)benzimidamide (**1c**, 51.6 mg, 0.2 mmol) was used as the substrate

under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2c** as white solid, 36.5 mg, yield 72%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.84 (d, J = 8.1 Hz, 1H), 7.77 (d, J = 8.7 Hz, 1H), 7.64 (d, J = 8.5 Hz, 2H), 7.52 (t, J = 7.6 Hz, 1H), 7.41 (t, J = 7.6 Hz, 1H), 7.20 (d, J = 8.2 Hz, 2H), 6.98 (s, 1H), 2.64 (q, J = 7.6 Hz, 2H), 1.24 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.6, 151.0, 138.4, 137.8, 128.4, 128.1, 127.0, 124.1, 120.8, 120.4, 118.5, 28.2, 15.7; HRMS calcd. for: $C_{15}H_{15}N_2S$ $[M+H]^+$ 255.0951, found 255.0949.

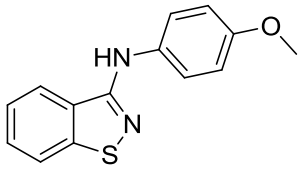
***N*-(4-(*tert*-Butyl)phenyl)benzo[d]isothiazol-3-amine (2d)**



2-Chloro-*N*-(4-ethylphenyl)benzimidamide (**1d**, 57.2 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2d** as gray solid, 53.0 mg, yield 94%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.84 (d, J = 8.1 Hz, 1H), 7.78 (d, J = 8.1 Hz, 1H), 7.65 (d, J = 8.4 Hz, 2H), 7.52 (t, J = 7.6 Hz, 1H), 7.43-7.35 (m, 3H), 6.98 (s, 1H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.6, 151.0, 145.3, 137.6, 128.1, 127.0, 125.9, 124.1, 120.8, 120.4, 118.1, 34.2, 31.4; HRMS calcd. for: $C_{17}H_{19}N_2S$ $[M+H]^+$ 283.1264, found 283.1264.

***N*-(4-Methoxyphenyl)benzo[d]isothiazol-3-amine (2e)**

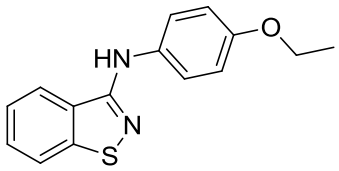


2-Chloro-*N*-(4-methoxyphenyl)benzimidamide (**1e**, 52.0 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2e** as brown solid, 47.1 mg, yield 92%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.80 (d, J = 8.1 Hz, 1H), 7.73 (d, J = 8.1 Hz, 1H), 7.64-7.57 (m, 2H), 7.49 (t, J = 7.3 Hz, 1H), 7.36 (t, J = 7.5 Hz, 1H), 6.96-6.84 (m, 3H), 3.78 (s, 3H); ^{13}C

NMR (100 MHz, $CDCl_3$, ppm) δ 155.3, 155.1, 151.0, 133.6, 128.0, 126.9, 124.0, 120.8, 120.4, 120.3, 114.3, 55.5; HRMS calcd. for: $C_{14}H_{13}N_2OS$ $[M+H]^+$ 257.0743, found 257.0743.

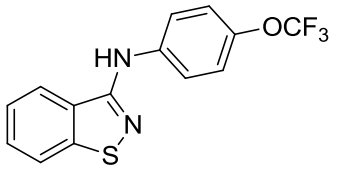
***N*-(4-Ethoxyphenyl)benzo[d]isothiazol-3-amine (2f)**



2-Chloro-*N*-(4-ethoxyphenyl)benzimidamide (**1f**, 42.8 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2f** as gray solid, 39.4 mg, yield 73%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.80 (d, J = 8.1 Hz, 1H), 7.72 (d, J = 8.1 Hz, 1H), 7.64-7.55 (m, 2H), 7.49 (t, J = 7.5 Hz, 1H), 7.35 (t, J = 7.5 Hz, 1H), 6.98-6.83 (m, 3H), 4.00 (q, J = 7.0 Hz, 2H), 1.39 (t, J = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.1, 154.6, 151.0, 133.5, 128.0, 126.9, 124.0, 120.9, 120.4, 120.3, 115.0, 63.7, 14.8; HRMS calcd. for: $C_{15}H_{15}N_2OS$ $[M+H]^+$ 271.0900, found 271.0894.

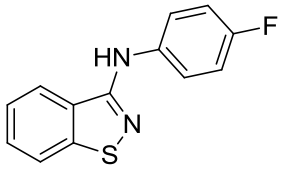
***N*-(4-(Trifluoromethoxy)phenyl)benzo[d]isothiazol-3-amine (2g)**



2-Chloro-*N*-(4-(trifluoromethoxy)phenyl)benzimidamide (**1g**, 62.8 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2g** as white solid, 37.2 mg, yield 60%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.84 (d, J = 8.1 Hz, 1H), 7.82-7.72 (m, 3H), 7.53 (t, J = 7.6 Hz, 1H), 7.41 (t, J = 7.5 Hz, 1H), 7.19 (d, J = 8.8 Hz, 2H), 7.07 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.0, 151.0, 143.7 (q, J = 1.7, 1.7 Hz), 139.0, 128.3, 126.9, 124.3, 121.9, 120.6, 120.6 (q, J = 254.7 Hz), 120.5, 118.9; HRMS calcd. for: $C_{14}H_{10}F_3N_2OS$ $[M+H]^+$ 311.0461, found 311.0458.

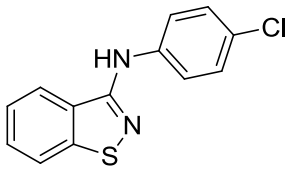
***N*-(4-Fluorophenyl)benzo[d]isothiazol-3-amine (2h)**



2-Chloro-*N*-(4-fluorophenyl)benzimidamide (**1h**, 50.0 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2h** as white solid, 31.7 mg, yield 65%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.85 (d, J = 8.1 Hz, 1H), 7.77 (d, J = 8.1 Hz, 1H), 7.73-7.66 (m, 2H), 7.56-7.52 (m, 1H), 7.44-7.40 (m, 1H), 7.10-7.03 (m, 2H), 6.98 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 158.3 (d, J = 239.6 Hz), 154.5, 151.1, 136.3 (d, J = 2.5 Hz), 128.3, 126.8, 124.3, 120.7, 120.5, 119.9 (d, J = 7.7 Hz), 115.7 (d, J = 22.3 Hz); HRMS calcd. for: $C_{13}H_{10}FN_2S$ $[M+H]^+$ 245.0543, found 245.0543.

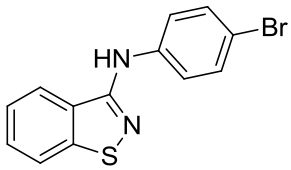
***N*-(4-Chlorophenyl)benzo[d]isothiazol-3-amine (2i)**



2-Chloro-*N*-(4-chlorophenyl)benzimidamide (**1i**, 52.8 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2i** as yellow solid, 34.8 mg, yield 67%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.86 (d, J = 8.1 Hz, 1H), 7.78 (d, J = 8.1 Hz, 1H), 7.71 (d, J = 8.8 Hz, 2H), 7.55 (t, J = 7.6 Hz, 1H), 7.43 (t, J = 7.5 Hz, 1H), 7.31 (d, J = 8.7 Hz, 2H), 7.07 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.0, 151.0, 138.8, 129.0, 128.3, 126.9, 126.9, 124.3, 120.7, 120.5, 119.2; HRMS calcd. for: $C_{13}H_{10}ClN_2S$ $[M+H]^+$ 261.0248, found 261.0244.

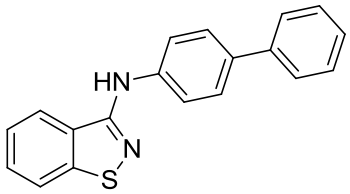
***N*-(4-Bromophenyl)benzo[d]isothiazol-3-amine (2j)**



N-(4-Bromophenyl)-2-chlorobenzimidamide (**1j**, 61.9 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2j** as white solid, 39.6 mg, yield 65%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.85 (d, J = 8.1 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.66 (d, J = 7.8 Hz, 2H), 7.54 (t, J = 7.5 Hz, 1H), 7.48-7.38 (m, 3H), 7.01 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 153.9, 151.0, 139.3, 131.9, 128.3, 126.9, 124.3, 120.6, 120.5, 119.5, 114.3; HRMS calcd. for: $C_{13}H_{10}BrN_2S$ $[M+H]^+$ 304.9743, found 304.9746.

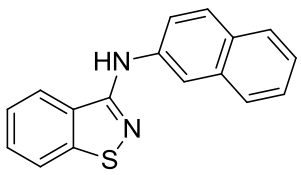
_N_-([1,1'-Biphenyl]-4-yl)benzo[d]isothiazol-3-amine (2k)



N-([1,1'-Biphenyl]-4-yl)-2-chlorobenzimidamide (**1k**, 61.2 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2k** as yellow solid, 48.3 mg, yield 80%.

^{1}H NMR (400 MHz, DMSO-d_6, ppm) δ 9.75 (s, 1H), 8.53 (d, J = 8.1 Hz, 1H), 8.08 (d, J = 8.8 Hz, 3H), 7.70-7.67 (m, 4H), 7.63 (t, J = 7.5 Hz, 1H), 7.54 (t, J = 7.5 Hz, 1H), 7.45 (t, J = 7.6 Hz, 2H), 7.32 (t, J = 7.3 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 155.29, 149.99, 140.9, 140.1, 133.0, 129.0, 128.6, 127.6, 127.0, 126.8, 126.2, 124.5, 122.8, 120.7, 118.2; HRMS calcd. for: $C_{19}H_{15}N_2S$ $[M+H]^+$ 303.0951, found 303.0946.

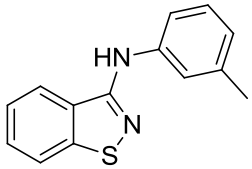
_N_-(Naphthalen-2-yl)benzo[d]isothiazol-3-amine (2l)



2-Chloro-*N*-(naphthalen-2-yl)benzimidamide (**1l**, 56.0 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2l** as yellow solid, 37.0 mg, yield 67%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.53 (d, J = 1.7 Hz, 1H), 7.89-7.77 (m, 5H), 7.61-7.53 (m, 2H), 7.45 (q, J = 7.0 Hz, 2H), 7.38-7.34 (m, 1H), 7.22 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.3, 151.0, 137.7, 134.4, 129.7, 128.8, 128.2, 127.5, 127.4, 127.2, 126.4, 124.3, 124.1, 120.7, 120.5, 119.3, 113.4; HRMS calcd. for: $C_{17}H_{13}N_2S$ $[M+H]^+$ 277.0794, found 277.0790.

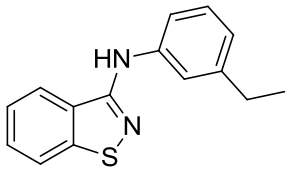
***N*-(*m*-Tolyl)benzo[d]isothiazol-3-amine (2m)**



2-Chloro-*N*-(*m*-tolyl)benzimidamide (**1m**, 48.8 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2m** as gray solid, 26.0 mg, yield 54%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.84 (d, J = 8.0 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.57-7.50 (m, 3H), 7.40 (t, J = 7.4 Hz, 1H), 7.24 (t, J = 7.7 Hz, 1H), 6.99 (s, 1H), 6.86 (d, J = 7.3 Hz, 1H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.4, 151.0, 140.2, 139.0, 128.9, 128.1, 127.1, 124.1, 123.2, 120.7, 120.4, 118.7, 115.2, 21.6; HRMS calcd. for: $C_{14}H_{13}N_2S$ $[M+H]^+$ 241.0794, found 241.0790.

***N*-(3-Ethylphenyl)benzo[d]isothiazol-3-amine (2n)**

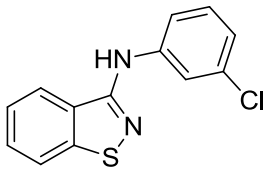


2-Chloro-*N*-(3-ethylphenyl)benzimidamide (**1n**, 51.6 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2n** as yellow solid, 41.1 mg, yield 81%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.84 (d, J = 8.1 Hz, 1H), 7.78 (d, J = 8.1 Hz, 1H), 7.61-7.49 (m, 3H), 7.41 (t, J = 7.6 Hz, 1H), 7.28 (t, J = 7.8 Hz, 1H), 7.01 (s, 1H), 6.90 (d, J = 7.6, 1H), 2.68 (q, J = 7.6 Hz, 2H), 1.27 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.4, 151.0, 145.4, 140.2, 129.0, 128.1, 127.1, 124.1, 121.9, 120.7, 120.4, 117.6, 115.5, 29.0, 15.5; HRMS

calcd. for: $C_{15}H_{15}N_2S$ $[M+H]^+$ 255.0951, found 255.0949.

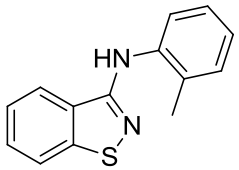
***N*-(3-Chlorophenyl)benzo[d]isothiazol-3-amine (2o)**



2-Chloro-*N*-(3-chlorophenyl)benzimidamide (**1o**, 52.8 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2o** as white solid, 23.4 mg, yield 45%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.93 (t, J = 2.0 Hz, 1H), 7.86 (d, J = 8.1 Hz, 1H), 7.78 (d, J = 8.1 Hz, 1H), 7.55 (t, J = 7.6 Hz, 2H), 7.44 (t, J = 7.4 Hz, 1H), 7.27 (t, J = 6.5 Hz, 1H), 7.09 (s, 1H), 7.01 (d, J = 7.9, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 153.7, 151.0, 141.4, 134.8, 130.1, 128.3, 126.9, 124.4, 122.2, 120.6, 120.5, 117.8, 115.9; HRMS calcd. for: $C_{13}H_{10}ClN_2S$ $[M+H]^+$ 261.0248, found 261.0244.

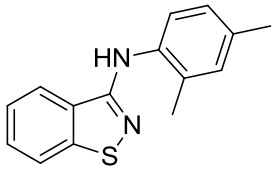
***N*-(*o*-Tolyl)benzo[d]isothiazol-3-amine (2p)**



2-Chloro-*N*-(o-tolyl)benzimidamide (**1p**, 48.8 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2p** as off white solid, 31.7 mg, yield 66%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.22 (d, J = 8.0 Hz, 1H), 7.84 (d, J = 8.1 Hz, 1H), 7.73 (d, J = 8.1 Hz, 1H), 7.54-7.50 (m , 1H), 7.40 (t, J = 7.3 Hz, 1H), 7.28-7.21 (m, 2H), 7.01 (t, J = 7.1 Hz, 1H), 6.82 (s, 1H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.9, 151.3, 138.5, 130.5, 128.1, 127.2, 127.0, 126.5, 124.2, 122.9, 120.9, 120.5, 119.7, 17.7; HRMS calcd. for: $C_{14}H_{13}N_2S$ $[M+H]^+$ 241.0794, found 241.0795.

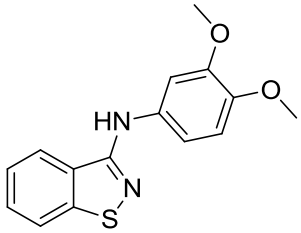
***N*-(2,4-Dimethylphenyl)benzo[d]isothiazol-3-amine (2q)**



2-Chloro-*N*-(2,4-dimethylphenyl)benzimidamide (**1q**, 51.6 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2q** as white solid, 39.1 mg, yield 77%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.95 (d, J = 8.6 Hz, 1H), 7.83 (d, J = 8.1 Hz, 1H), 7.72 (d, J = 8.1 Hz, 1H), 7.56-7.49 (m, 1H), 7.43-7.36 (m, 1H), 7.07-7.05 (m, 2H), 6.75 (s, 1H), 2.3 (s, 3H), 2.3 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.5, 151.3, 135.8, 133.0, 131.3, 128.1, 127.7, 127.5, 127.0, 124.1, 121.0, 120.8, 120.5, 20.8, 17.7; HRMS calcd. for: $C_{15}H_{15}N_2S$ $[M+H]^+$ 255.0951, found 255.0948.

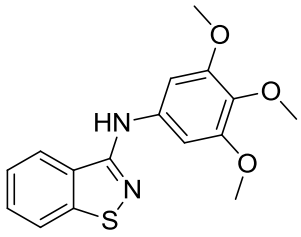
***N*-(3,4-Dimethoxyphenyl)benzo[d]isothiazol-3-amine (2r)**



2-Chloro-*N*-(3,4-dimethoxyphenyl)benzimidamide (**1r**, 58.0 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 10:1) to give **2r** as violet solid, 50.3 mg, yield 88%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.84 (d, J = 8.1 Hz, 1H), 7.78 (d, J = 8.1 Hz, 1H), 7.55-7.50 (m, 2H), 7.43-7.37 (m, 1H), 7.15 (dd, J = 8.6, 2.3 Hz, 1H), 7.00 (s, 1H), 6.87 (d, J = 8.6 Hz, 1H), 3.92 (s, 3H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.0, 150.9, 149.2, 144.6, 134.1, 128.1, 126.9, 124.1, 120.9, 120.3, 111.8, 110.5, 103.9, 56.2, 55.8; HRMS calcd. for: $C_{15}H_{15}N_2O_2S$ $[M+H]^+$ 287.0849, found 287.0848.

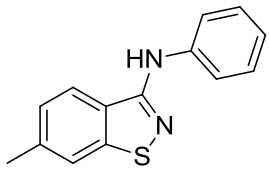
***N*-(3,4,5-Trimethoxyphenyl)benzo[d]isothiazol-3-amine (2s)**



2-Chloro-*N*-(3,4,5-trimethoxyphenyl)benzimidamide (**1s**, 64.0 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 5:1) to give **2s** as yellow solid, 32.8 mg, yield 52%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.83 (dd, J = 10.5, 8.2 Hz, 2H), 7.53 (t, J = 7.4 Hz, 1H), 7.40 (t, J = 7.7 Hz, 1H), 7.08 (s, 3H), 3.88 (s, 6H), 3.83 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.5, 153.5, 150.9, 136.6, 133.2, 128.2, 127.0, 124.2, 120.8, 120.4, 96.1, 61.0, 56.1; HRMS calcd. for: $C_{16}H_{17}N_2O_3S$ $[M+H]^+$ 317.0955, found 317.0954.

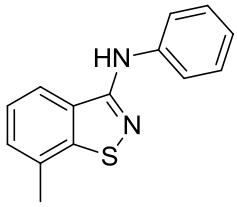
6-Methyl-*N*-phenylbenzo[d]isothiazol-3-amine (2u)



2-Chloro-4-methyl-*N*-phenylbenzimidamide (**1u**, 48.8 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2u** as yellow solid, 38.0 mg, yield 72%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.76-7.68 (m, 2H), 7.63-7.54 (m, 2H), 7.34 (t, J = 7.9 Hz, 2H), 7.18 (d, J = 8.2 Hz, 1H), 7.02 (t, J = 7.4 Hz, 1H), 6.96 (s, 1H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.2, 151.4, 140.3, 138.7, 129.1, 126.0, 125.2, 122.1, 120.3, 120.1, 117.9, 21.6; HRMS calcd. for: $C_{14}H_{13}N_2S$ $[M+H]^+$ 241.0794, found 241.0794.

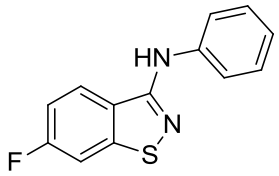
7-Methyl-*N*-phenylbenzo[d]isothiazol-3-amine (2v)



2-Chloro-3-methyl-*N*-phenylbenzimidamide (**1v**, 48.8 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2v** as violet solid, 19.7 mg, yield 41%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.77-7.72 (m, 2H), 7.61 (d, J = 7.9 Hz, 1H), 7.38-7.28 (m, 4H), 7.04 (t, J = 7.4 Hz, 1H), 7.00 (s, 1H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 155.0, 151.4, 140.3, 130.7, 129.1, 128.2, 126.9, 125.0, 122.2, 118.2, 118.0, 19.9; HRMS calcd. for: $C_{14}H_{13}N_2S$ $[M+H]^+$ 241.0794, found 241.0790.

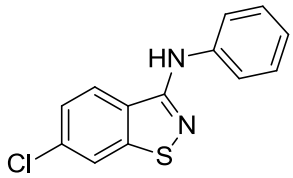
6-Fluoro-*N*-phenylbenzo[d]isothiazol-3-amine (2w)



2-Chloro-4-fluoro-N-phenylbenzimidamide (**1w**, 49.6 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2w** as yellow solid, 36.6 mg, yield 75%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.75-7.68 (m, 3H), 7.49 (dd, J = 8.2, 2.0 Hz, 1H), 7.36 (t, J = 7.9 Hz, 2H), 7.14 (td, J = 8.6, 2.1 Hz, 1H), 7.05 (t, J = 7.4 Hz, 1H), 6.96 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 162.8 (d, J = 249.7 Hz), 153.8, 152.8 (d, J = 10.2 Hz), 140.0, 129.1, 123.8, 122.5, 122.2 (d, J = 10.2 Hz), 118.2, 113.5 (d, J = 25.4 Hz), 106.4 (d, J = 25.2 Hz); HRMS calcd. for: $C_{13}H_{10}FN_2S$ $[M+H]^+$ 245.0543, found 245.0549.

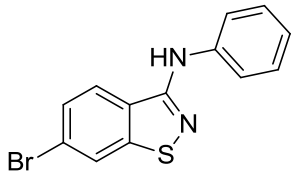
6-Chloro-*N*-phenylbenzo[d]isothiazol-3-amine (2x)



2,4-Dichloro-*N*-phenylbenzimidamide (**1x**, 52.8 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2x** as gray solid, 44.7 mg, yield 86%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.82 (d, J = 1.6 Hz, 1H), 7.72-7.67 (m, 3H), 7.39-7.34 (m, 3H), 7.08-7.04 (m, 1H), 7.00 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 153.9, 152.4, 140.0, 135.1, 129.2, 125.6, 125.1, 122.6, 121.6, 120.0, 118.1; HRMS calcd. for: $C_{13}H_{10}ClN_2S$ $[M+H]^+$ 261.0248, found 261.0245.

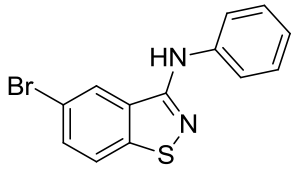
6-Bromo-*N*-phenylbenzo[d]isothiazol-3-amine (2y)



4-Bromo-2-chloro-*N*-phenylbenzimidamide (**1y**, 61.6 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2y** as off white solid, 35.9 mg, yield 59%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.96 (d, J = 1.4 Hz, 1H), 7.69 (dd, J = 8.6, 0.9 Hz, 2H), 7.59 (d, J = 8.6 Hz, 1H), 7.48 (dd, J = 8.6, 1.6 Hz, 1H), 7.38-7.33 (m, 2H), 7.05 (t, J = 7.4 Hz, 1H), 6.97 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.0, 152.7, 139.9, 129.1, 127.6, 125.9, 123.3, 123.0, 122.5, 121.7, 118.1; HRMS calcd. for: $C_{13}H_{10}BrN_2S$ $[M+H]^+$ 304.9743, found 304.9741.

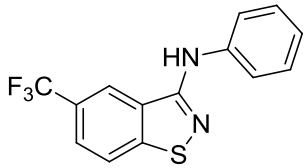
5-Bromo-*N*-phenylbenzo[d]isothiazol-3-amine (2z)



5-Bromo-2-chloro-*N*-phenylbenzimidamide (**1z**, 61.6 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2z** as white solid, 58.3 mg, yield 96%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.94 (d, J = 1.3 Hz, 1H), 7.72 (d, J = 8.5 Hz, 3H), 7.62 (dd, J = 8.6, 1.7 Hz, 1H), 7.42-7.34 (m, 2H), 7.08 (t, J = 7.4 Hz, 1H), 6.97 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 153.4, 149.9, 139.9, 131.3, 129.2, 128.7, 123.7, 122.6, 121.7, 118.2, 118.0; HRMS calcd. for: $C_{13}H_{10}BrN_2S$ $[M+H]^+$ 304.9743, found 304.9747.

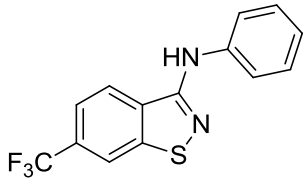
***N*-Phenyl-5-(trifluoromethyl)benzo[d]isothiazol-3-amine (2aa)**



2-Chloro-*N*-phenyl-5-(trifluoromethyl)benzimidamide (**1aa**, 59.6 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2aa** as white solid, 58.8 mg, yield 97%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.05 (s, 1H), 7.94 (d, J = 8.5 Hz, 1H), 7.74 (dd, J = 8.6, 1.0 Hz, 3H), 7.42-7.34 (m, 2H), 7.13-7.01 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.5, 154.3, 139.8, 129.2, 126.9 (q, J = 32.7 Hz), 126.8, 124.5 (q, J = 2.8 Hz), 124.1 (q, J = 270.6 Hz), 122.8, 121.1, 118.4, 118.3; HRMS calcd. for: $C_{14}H_{10}F_3N_2S$ $[M+H]^+$ 295.0512, found 295.0515.

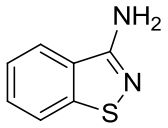
***N*-Phenyl-6-(trifluoromethyl)benzo[d]isothiazol-3-amine (2ab)**



2-Chloro-*N*-phenyl-4-(trifluoromethyl)benzimidamide (**1ab**, 59.6 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2ab** as gray solid, 48.8 mg, yield 83%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.13 (s, 1H), 7.88 (d, J = 8.4 Hz, 1H), 7.73 (d, J = 8.4 Hz, 2H), 7.63 (d, J = 8.4 Hz, 1H), 7.38 (t, J = 7.6 Hz, 2H), 7.09-7.05 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 154.1, 151.2, 139.8, 130.3 (q, J = 32.5 Hz), 129.2, 128.9, 123.9 (q, J = 271.3 Hz), 122.8, 121.6, 121.0 (q, J = 3.2 Hz), 118.2, 117.9 (q, J = 4.3 Hz); HRMS calcd. for: $C_{14}H_{10}F_3N_2S$ $[M+H]^+$ 295.0512, found 295.0515.

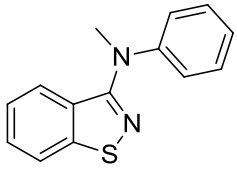
Benzo[d]isothiazol-3-amine (2ac)



2-Chloro-benzamidine hydrochloride (**1ac**, 38.0 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 5:1) to give **2ac** as faint yellow solid, 24.3 mg, yield 81%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.81 (d, J = 8.2 Hz, 1H), 7.71 (d, J = 8.1 Hz, 1H), 7.53-7.48 (m, 1H), 7.38 (t, J = 7.5 Hz, 1H), 4.69 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 158.6, 151.9, 128.0, 126.3, 124.0, 121.6, 120.4; HRMS calcd. for: $C_7H_7N_2S$ $[M+H]^+$ 151.0325, found 151.0321.

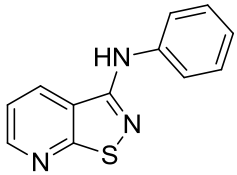
***N*-Methyl-*N*-phenylbenzo[d]isothiazol-3-amine (2ad)**



2-Chloro-*N*-methyl-*N*-phenylbenzimidamide (**1ad**, 48.8 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 20:1) to give **2ad** as yellow solid, 15.8 mg, yield 33%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.76 (d, J = 8.2 Hz, 1H), 7.38-7.31 (m, 3H), 7.22-7.14 (m, 3H), 7.04-7.00 (m, 1H), 6.91-6.88 (m, 1H), 3.60 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 160.7, 152.7, 147.9, 129.4, 127.7, 127.2, 125.2, 125.0, 124.6, 123.5, 120.1, 42.3; HRMS calcd. for: $C_{14}H_{13}N_2S$ $[M+H]^+$ 241.0794, found 241.0788.

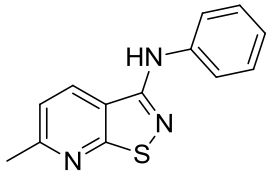
***N*-Phenylisothiazolo[5,4-*b*]pyridin-3-amine (2ae)**



2-Chloro-*N*-phenylnicotinimidamide (**1ae**, 46.2 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **2ae** as yellow solid, 43.6 mg, yield 96%.

^{1}H NMR (400 MHz, DMSO-d_6, ppm) δ 9.81 (s, 1H), 8.96-8.68 (m, 2H), 7.92 (d, J = 8.0 Hz, 2H), 7.66-7.47 (m, 1H), 7.35 (t, J = 7.5 Hz, 2H), 6.99 (t, J = 7.0 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 169.9, 153.9, 151.0, 140.8, 131.7, 128.8, 121.6, 120.6, 119.4, 117.9.

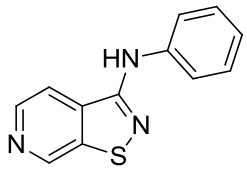
6-Methyl-*N*-phenylisothiazolo[5,4-*b*]pyridin-3-amine (2af)



2-Chloro-6-methyl-*N*-phenylnicotinimidamide (**1af**, 49.0 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 3:1) to give **2af** as yellow solid, 42.0 mg, yield 87%.

^{1}H NMR (400 MHz, DMSO-d_6, ppm) δ 9.74 (s, 1H), 8.72 (d, J = 8.4 Hz, 1H), 7.91 (d, J = 7.9 Hz, 2H), 7.48-7.32 (m, 3H), 6.98 (t, J = 7.3 Hz, 1H), 2.65 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 169.9, 160.5, 153.8, 140.8, 131.6, 128.8, 121.5, 119.6, 118.6, 117.7, 24.3.

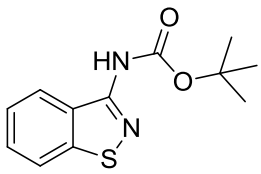
***N*-Phenylisothiazolo[5,4-*c*]pyridin-3-amine (2ag)**



3-Chloro-*N*-phenylisonicotinimidamide (**1ag**, 46.2 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 4:1) to give **2ag** as yellow solid, 42.7 mg, yield 94%.

^{1}H NMR (400 MHz, DMSO-d_6, ppm) δ 9.82 (s, 1H), 9.41 (s, 1H), 8.63 (d, J = 5.5 Hz, 1H), 8.44 (d, J = 5.2 Hz, 1H), 7.95 (d, J = 7.9 Hz, 2H), 7.35 (t, J = 7.9 Hz, 2H), 7.00 (t, J = 7.3 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6, ppm) δ 154.8, 145.7, 143.8, 143.0, 140.8, 132.5, 128.8, 121.7, 117.8, 116.5.

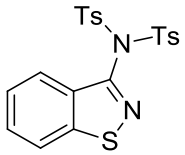
***tert*-Butyl benzo[*d*]isothiazol-3-ylcarbamate (4a)**



A 10 mL oven-dried reaction vessel was charged with benzo[*d*]isothiazol-3-amine (**2ac**, 30 mg, 0.2 mmol), Boc_2O (43 mg, 0.2 mmol, 1.0 equiv), Et_3N (84 μL, 0.6 mmol, 3.0 equiv), CH_2Cl_2 (1.0 mL) under air. The reaction vessel was stirred at room temperature for 24 h. The volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to yield the desired product **4a** as white solid, 37.0 mg, yield 82%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.05 (d, J = 8.2 Hz, 1H), 7.83 (d, J = 8.2 Hz, 1H), 7.80 (s, 1H), 7.54-7.48 (m, 1H), 7.45-7.38 (m, 1H), 1.56 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 152.4, 152.1, 152.0, 128.1, 128.0, 124.4, 123.9, 119.9, 81.7, 28.2; HRMS calcd. for: $C_{12}H_{15}N_2O_2S$ $[M+H]^+$ 251.0849, found 251.0846.

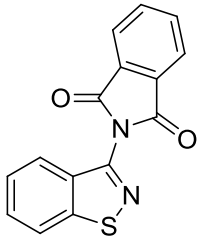
***N*-(Benzo[*d*]isothiazol-3-yl)-4-methyl-*N*-tosylbenzenesulfonamide (4b)**



A 10 mL oven-dried reaction vessel was charged with benzo[*d*]isothiazol-3-amine (**2ac**, 30 mg, 0.2 mmol), tosyl chloride (76.2 mg, 0.4 mmol, 2.0 equiv), Et_3N (84 μL, 0.6 mmol, 3.0 equiv), CH_2Cl_2 (1.0 mL) under air. The reaction vessel was stirred at room temperature for 24 h. The volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to yield the desired product **4b** as white solid, 37.0 mg, yield 73%.

^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.91 (d, J = 8.2 Hz, 1H), 7.79 (d, J = 8.4 Hz, 4H), 7.68 (d, J = 8.2 Hz, 1H), 7.59-7.53 (m, 1H), 7.42-7.37 (m, 1H), 7.30 (d, J = 8.1 Hz, 4H), 2.47 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 152.8, 148.7, 145.4, 135.9, 132.9, 129.5, 129.0, 128.5, 125.8, 123.9, 120.0, 21.7; HRMS calcd. for: $C_{21}H_{19}N_2O_4S_3$ $[M+H]^+$ 459.0502, found 459.0492.

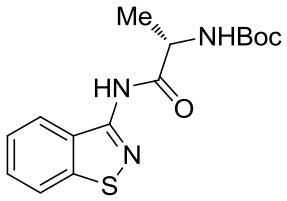
2-(Benzo[*d*]isothiazol-3-yl)isoindoline-1,3-dione (4c)



A 10 mL oven-dried reaction vessel was charged with benzo[*d*]isothiazol-3-amine (**2ac**, 30 mg, 0.2 mmol), phthalic anhydride (44.4 mg, 0.3 mmol, 1.5 equiv), 1-butyl-3-methylimidazolium hexafluorophosphate ([bmim][PF_6], 1.0 ml) under air. The reaction vessel was stirred at 135 ^oC for 24 h. The volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to yield the desired product **4c** as white solid, 37.0 mg, yield 94%.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 8.07-7.94 (m, 3H), 7.88-7.80 (m, 3H), 7.61-7.56 (m, 1H), 7.48-7.44 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 166.0, 153.1, 147.0, 134.8, 131.7, 130.4, 128.4, 125.4, 124.2, 123.5, 120.1; HRMS calcd. for: $C_{15}H_9N_2O_2S$ $[M+H]^+$ 281.0379, found 281.0374.

(S)-*tert*-Butyl (1-(benzo[*d*]isothiazol-3-ylamino)-1-oxopropan-2-yl)carbamate (4d)

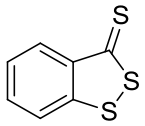


A 10 mL oven-dried reaction vessel was charged with benzo[*d*]isothiazol-3-amine (**2ac**, 30 mg, 0.2 mmol), Boc-Ala-OH (41.6 mg, 0.22 mmol, 1.1 equiv), T3P (2,4,6-tripropyl-1,3,5,2,4,6-trioxatriphosphinane 2,4,6-trioxide) in DMF (280 μl, c = 1.43 M, 0.4 mmol, 2.0 equiv), Et_3N (52 μL, 0.4 mmol, 2.0 equiv), CH_2Cl_2 (1.0 mL) under air. The reaction vessel was stirred at room temperature for 24 h. The volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 20:1) to yield the desired product **4d** as white solid, 37.0 mg, yield 70%.

^1H NMR (400 MHz, $CDCl_3$, ppm) δ 9.97 (s, 1H), 7.99 (d, J = 8.2 Hz, 1H), 7.79-7.74 (m, 1H), 7.50-7.44 (m, 1H), 7.35-7.27 (m, 1H), 5.58 (s, 1H), 4.58 (s, 1H), 1.51 (d, J = 7.0 Hz, 3H), 1.46 (s,

9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 171.4, 156.3, 151.9, 151.5, 128.1, 124.5, 124.0, 123.3, 119.7, 80.6, 50.5, 28.3, 17.5; HRMS calcd. for: $C_{15}H_{20}N_3O_3S$ $[M+H]^+$ 322.1220, found 322.1216.

3*H*-benzo[*c*][1,2]dithiole-3-thione (6a') [2]



(2-chlorophenyl)methanamine (**5a**, 28.2 mg, 0.2 mmol) was used as the substrate under the given reaction conditions. The residue was purified by column chromatography (silica gel, petroleum ether/ethyl acetate = 100:1) to give **6a'** as yellow solid, 31.5 mg, yield 86%.

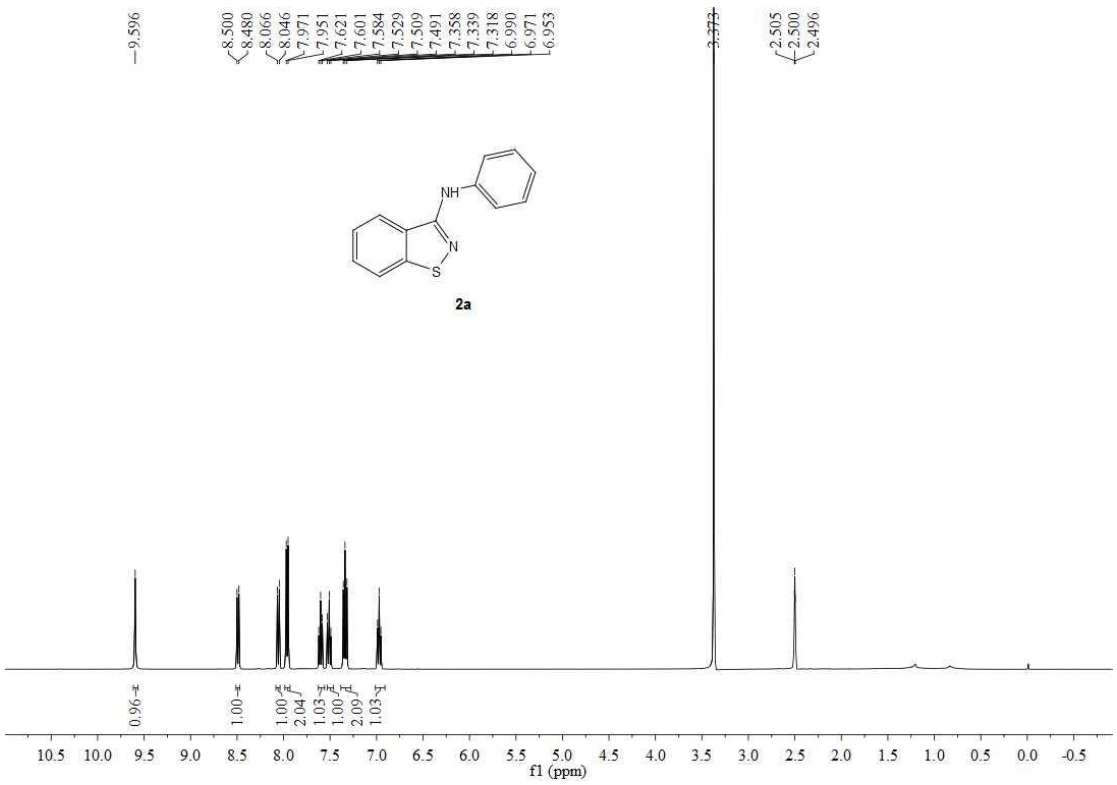
^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 8.21 (d, J = 8.2 Hz, 1H), 7.74-7.66 (m, 2H), 7.49-7.42 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 216.8, 152.7, 140.7, 132.7, 128.5, 126.0, 124.3.

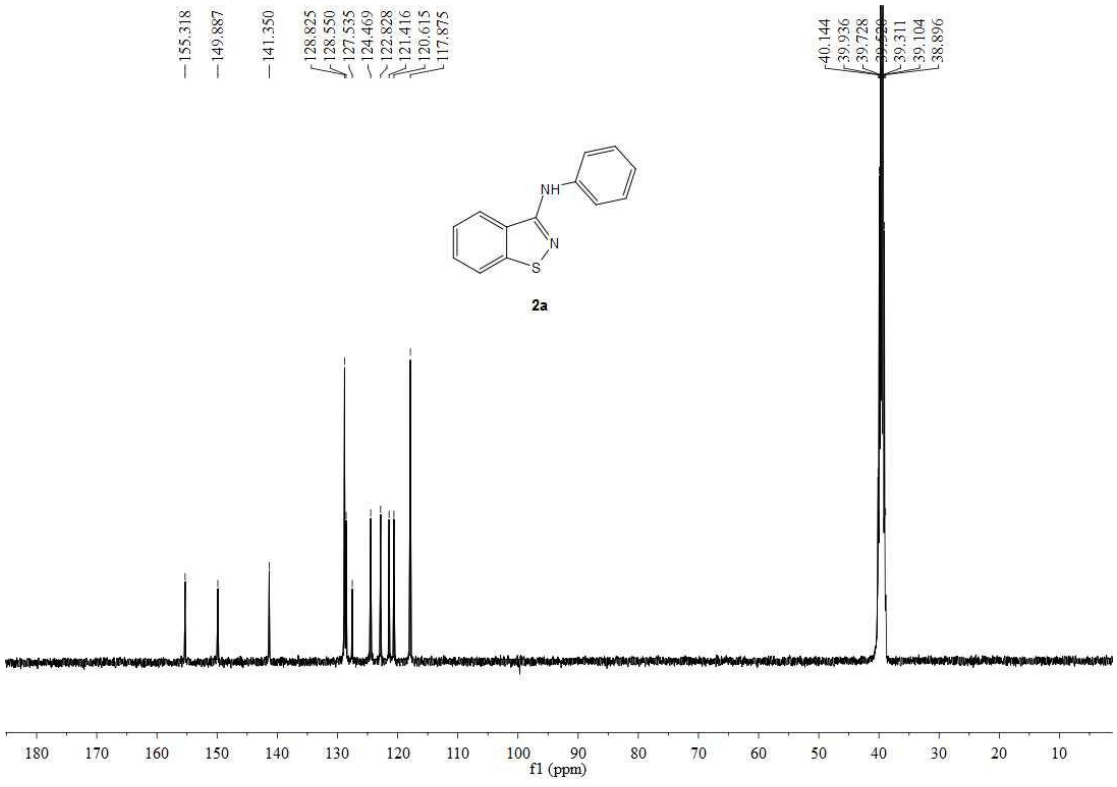
5. Reference

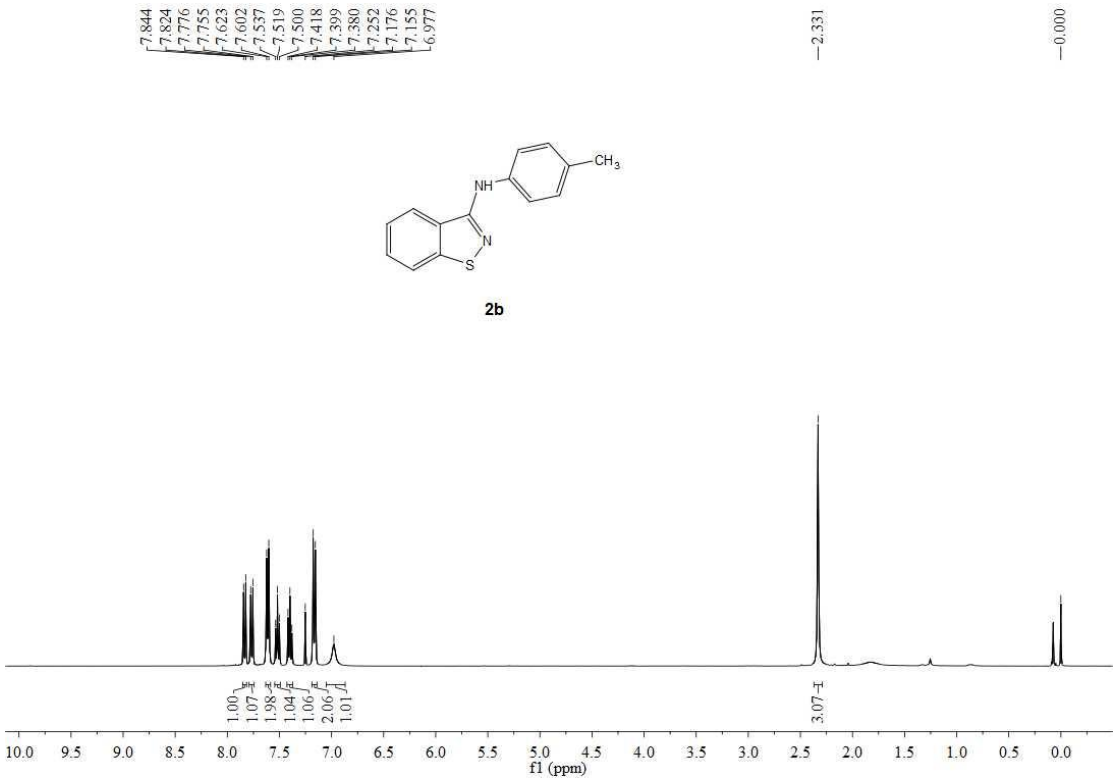
[1] G. Brasche, S. L. Buchwald, *Angew. Chem. Int. Ed.*, **2008**, *120*, 1958.

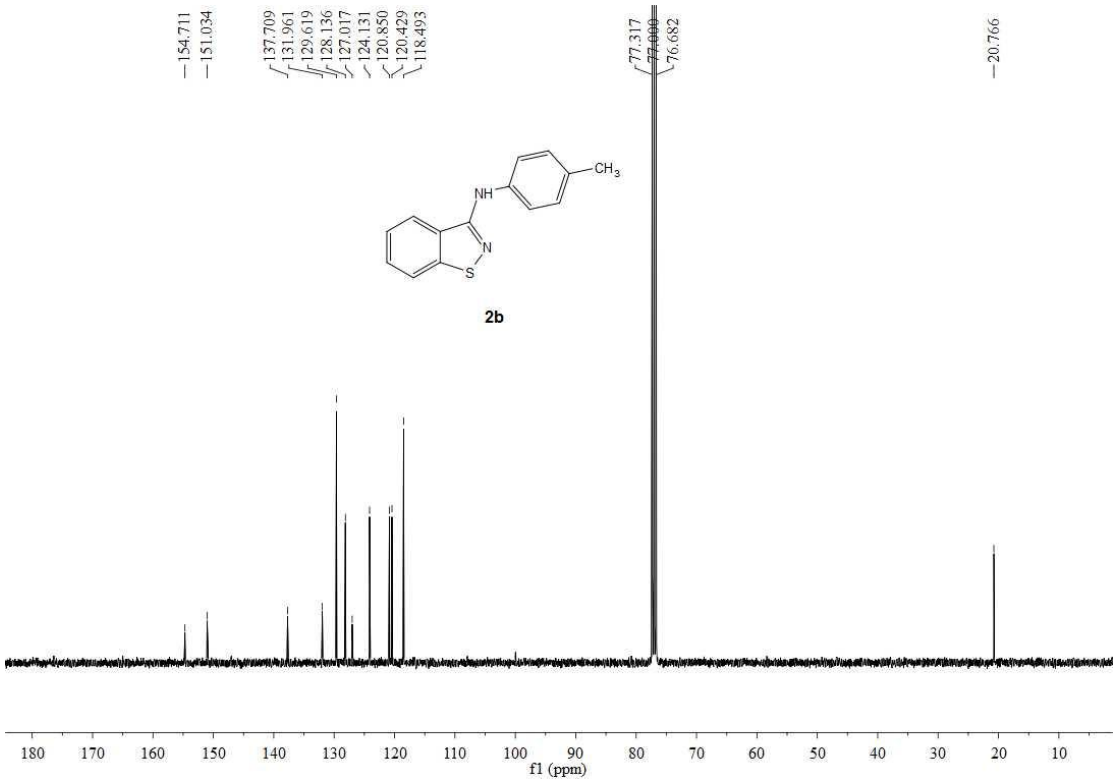
[2] H. L. Jin, D. Jiang, J. Gao, G. Qiang, Y. Gong, *Phosphorus, Sulfur, and Silicon and the Related Elements*, **2011**, *186*, 2341.

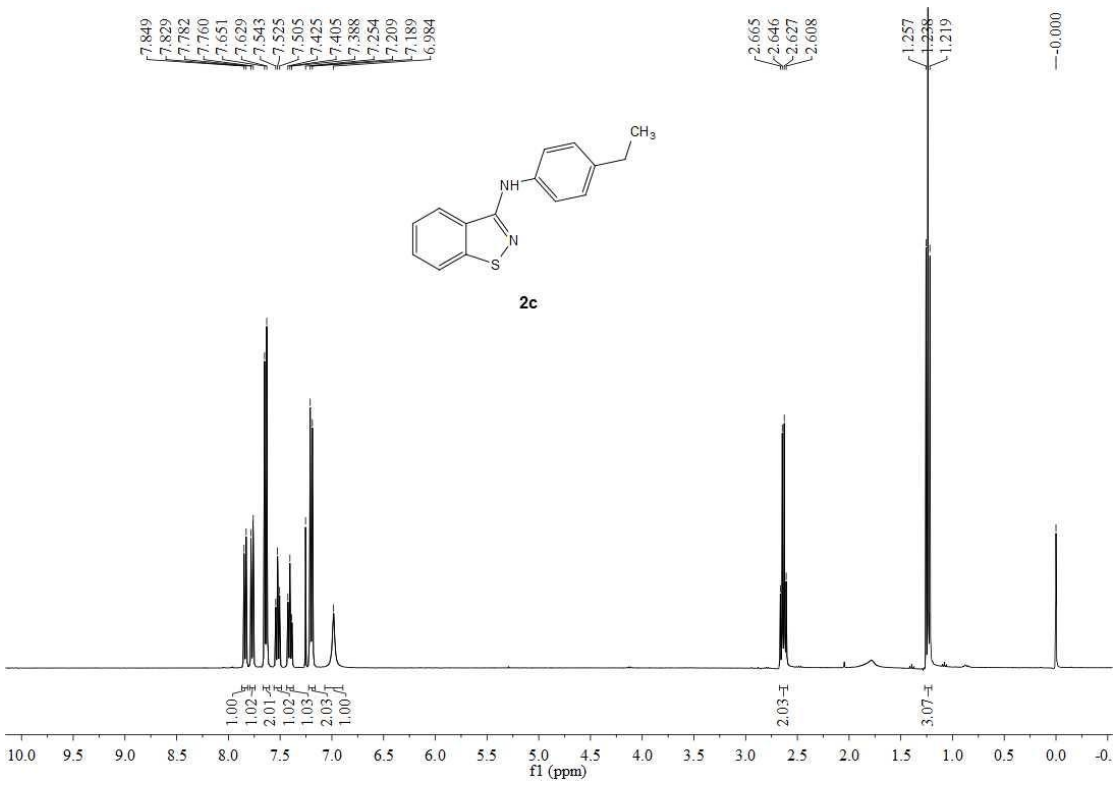
6. ^{1}H and ^{13}C NMR spectra of products

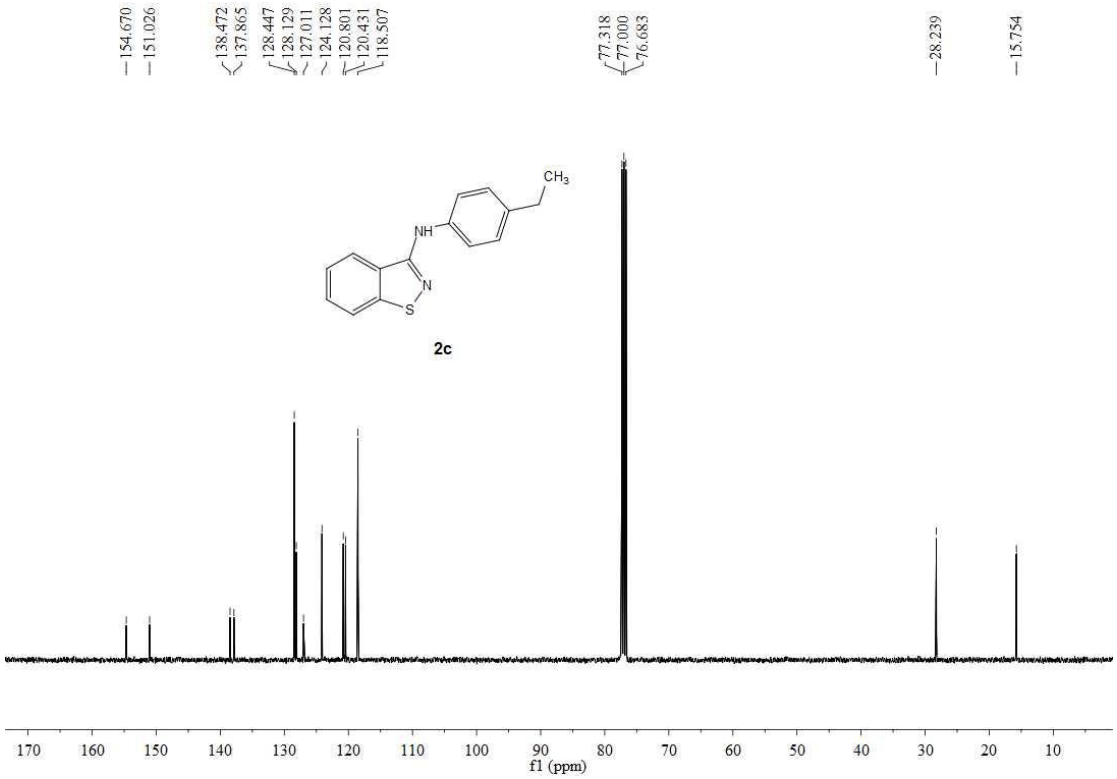


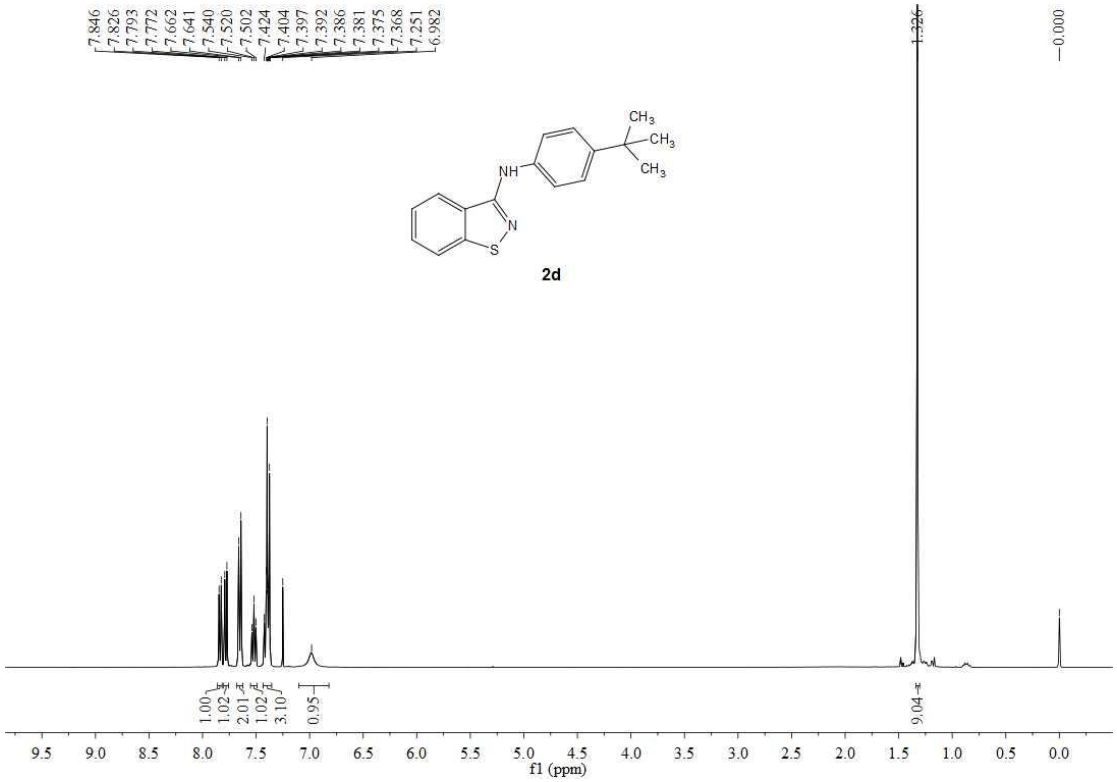


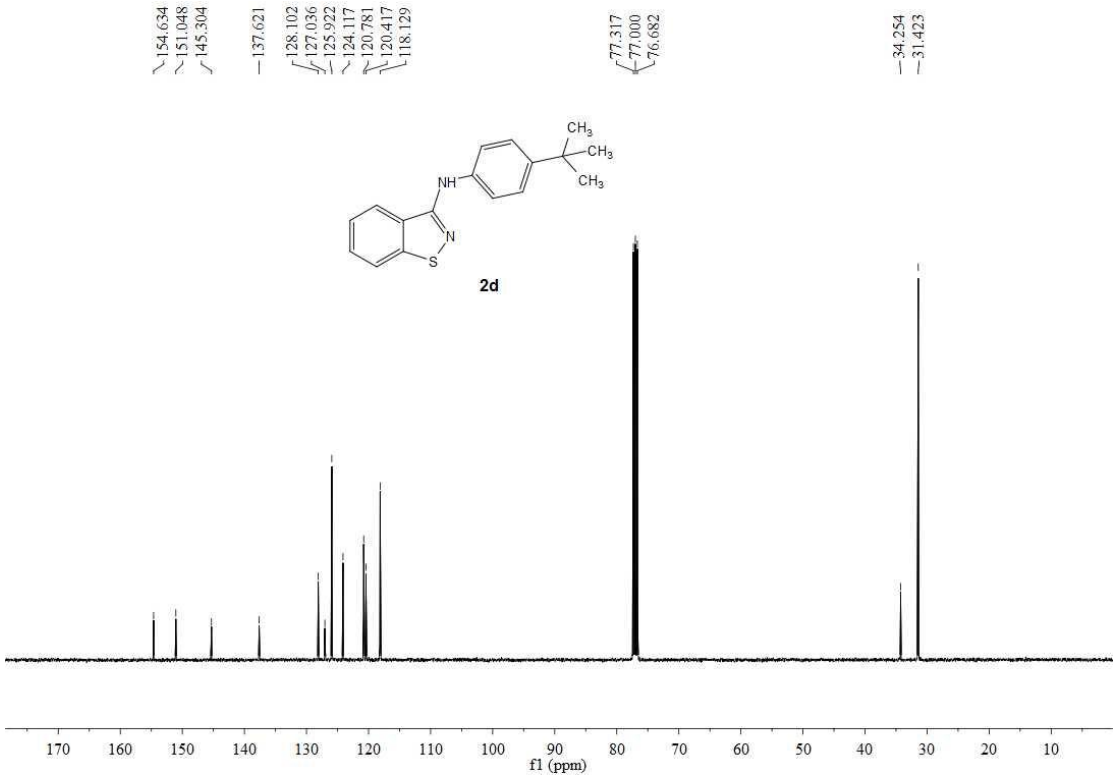

7.844
7.824
7.776
7.755
7.623
7.602
7.537
7.519
7.500
7.418
7.399
7.380
7.252
7.176
7.155
6.977
2.331
0.000
NH
N
S
CH3
2b
1.00
1.07
1.98
1.04
1.06
2.06
1.01
3.07
f1 (ppm)

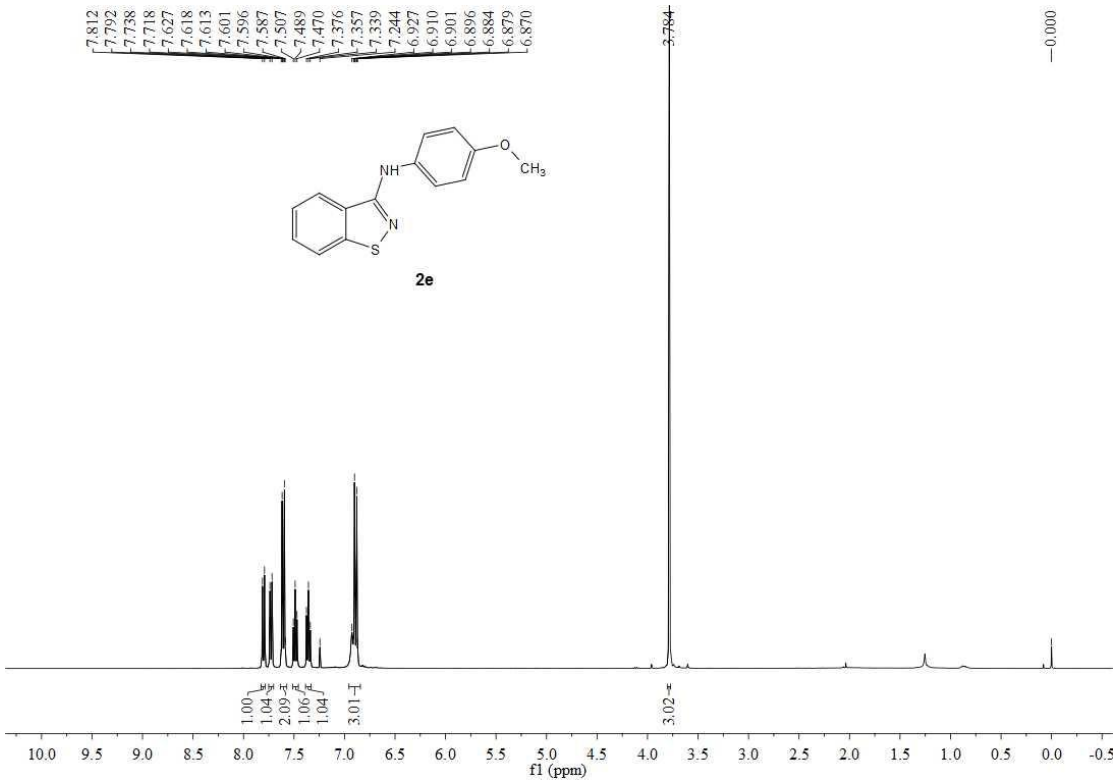

154.711
151.034
137.709
131.961
129.619
128.136
127.017
124.131
120.850
120.429
118.493
77.317
77.000
76.682
20.766
NH
N
S
CH3
2b
f1 (ppm)

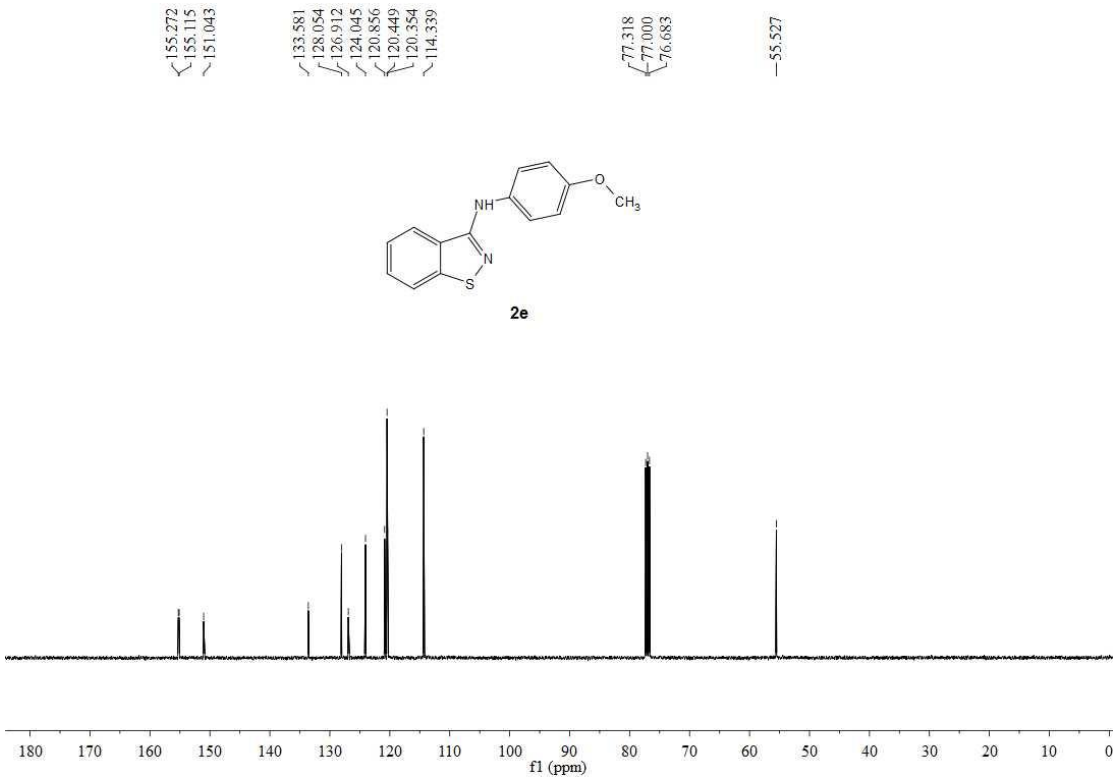

7.849
7.829
7.782
7.760
7.651
7.629
7.543
7.525
7.505
7.425
7.405
7.388
7.254
7.209
7.189
6.984
2.665
2.646
2.627
2.608
1.257
1.238
1.219
-0.000
NH
N
S
CH3
2c
1.00
1.02
2.01
1.02
1.03
2.03
1.00
2.03
3.07
f1 (ppm)

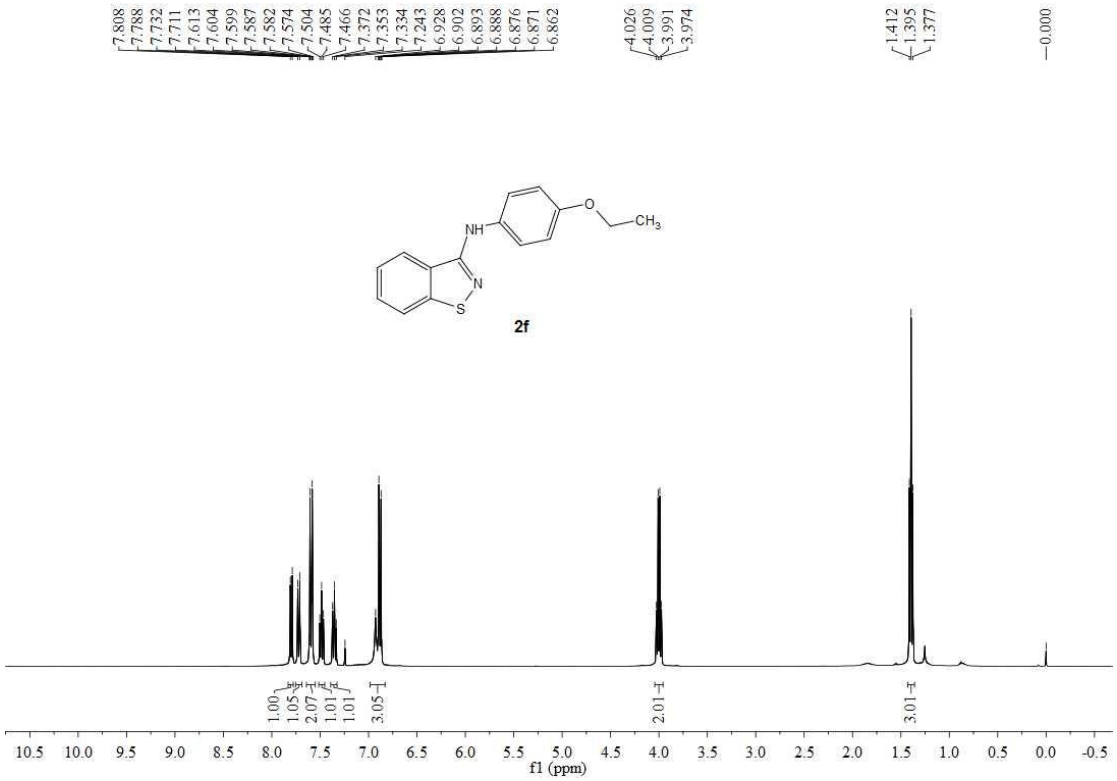

154.670
151.026
138.472
137.865
128.447
128.129
127.011
124.128
120.801
120.431
118.507
77.318
77.000
76.683
28.239
15.754
NH
N
S
CH3
2c
f1 (ppm)

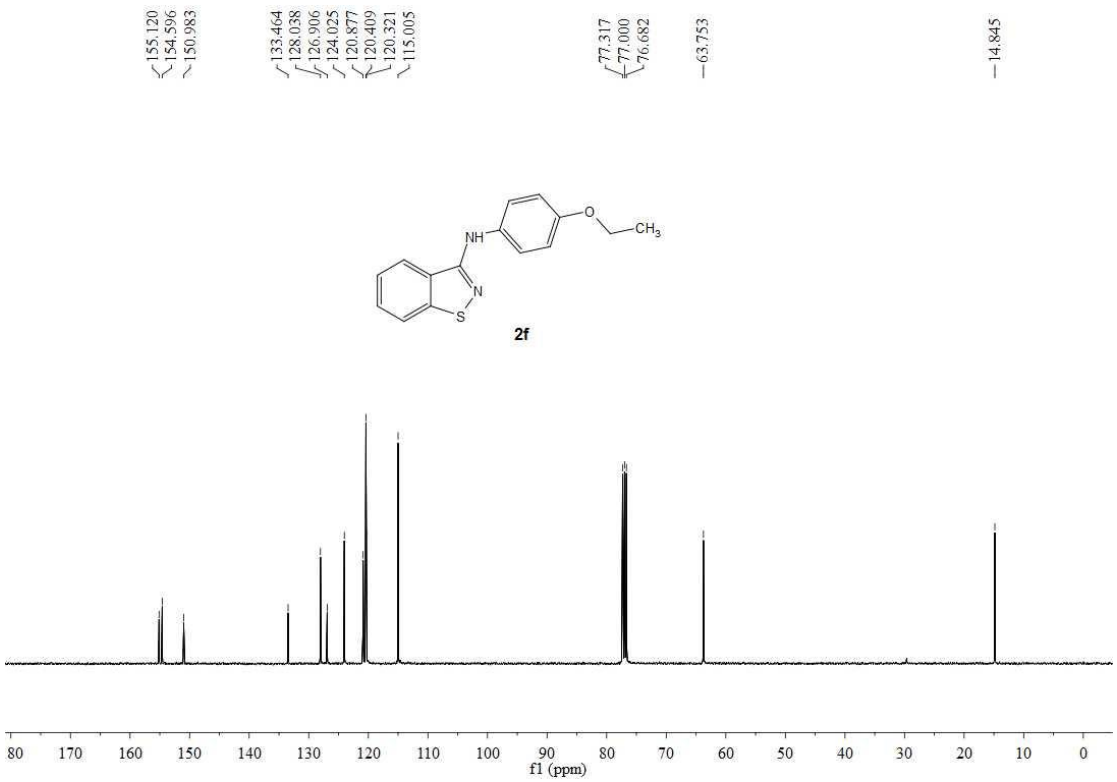

7.846
7.826
7.793
7.772
7.662
7.641
7.540
7.520
7.502
7.424
7.404
7.397
7.392
7.386
7.381
7.375
7.368
7.251
6.982
1.326
0.000
NH
N
S
CH3
CH3
CH3
2d
1.00
1.02
2.01
1.02
3.10
0.95
9.04
f1 (ppm)

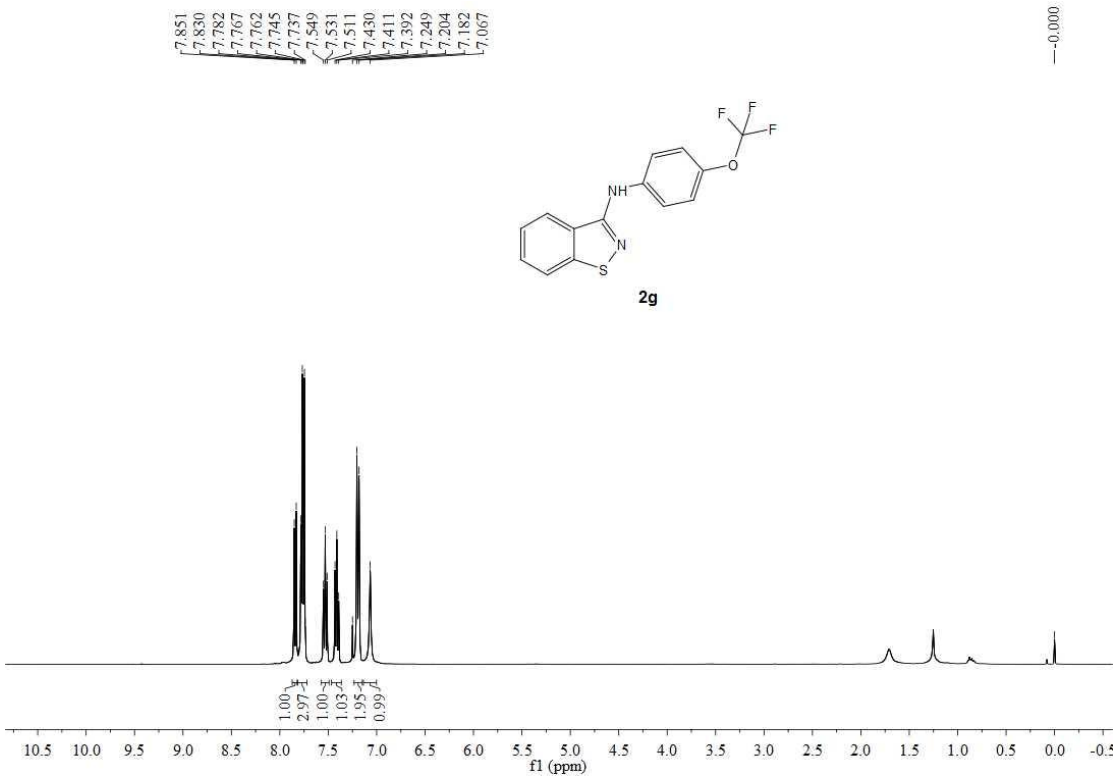

154.634
151.048
145.304
137.621
128.102
127.036
125.922
124.117
120.781
120.417
118.129
77.317
77.000
76.682
34.254
31.423
NH
N
S
CH3
CH3
CH3
2d
f1 (ppm)

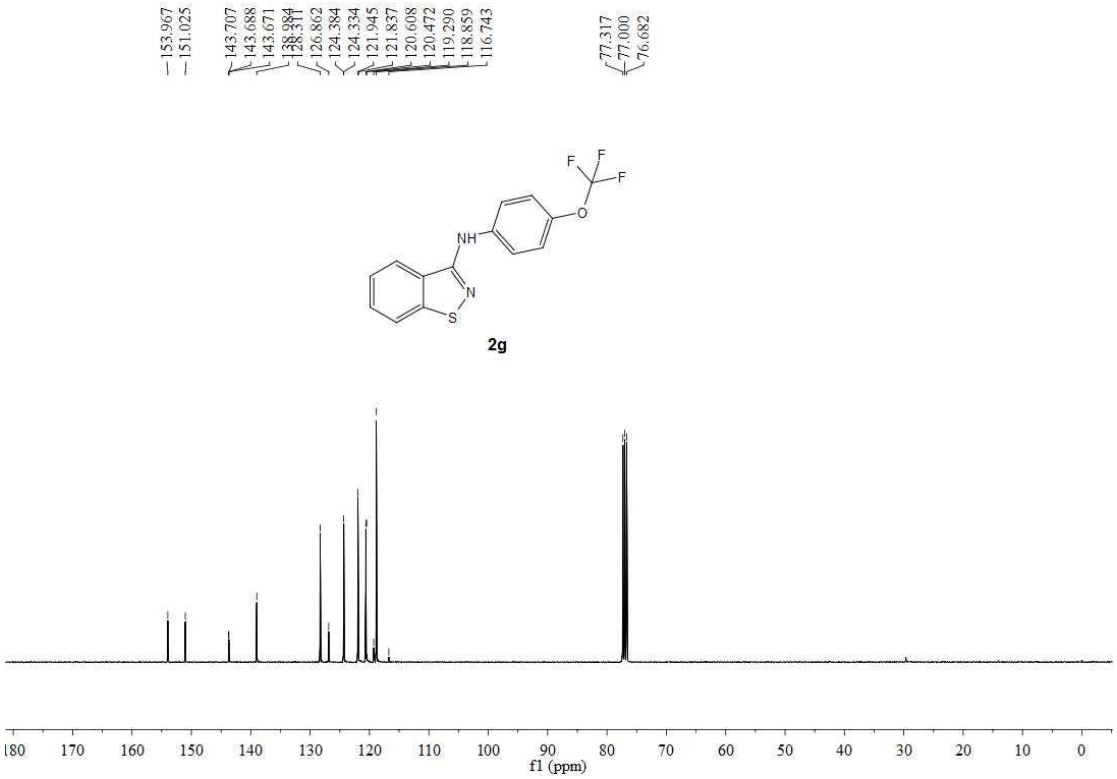

7.812
7.792
7.738
7.718
7.627
7.618
7.613
7.601
7.596
7.587
7.507
7.489
7.470
7.376
7.357
7.339
7.244
6.927
6.910
6.901
6.896
6.884
6.879
6.870
3.784
0.000
NH
O
CH3
N
S
2e
1.00
1.04
2.09
1.06
1.04
3.01
3.02
f1 (ppm)

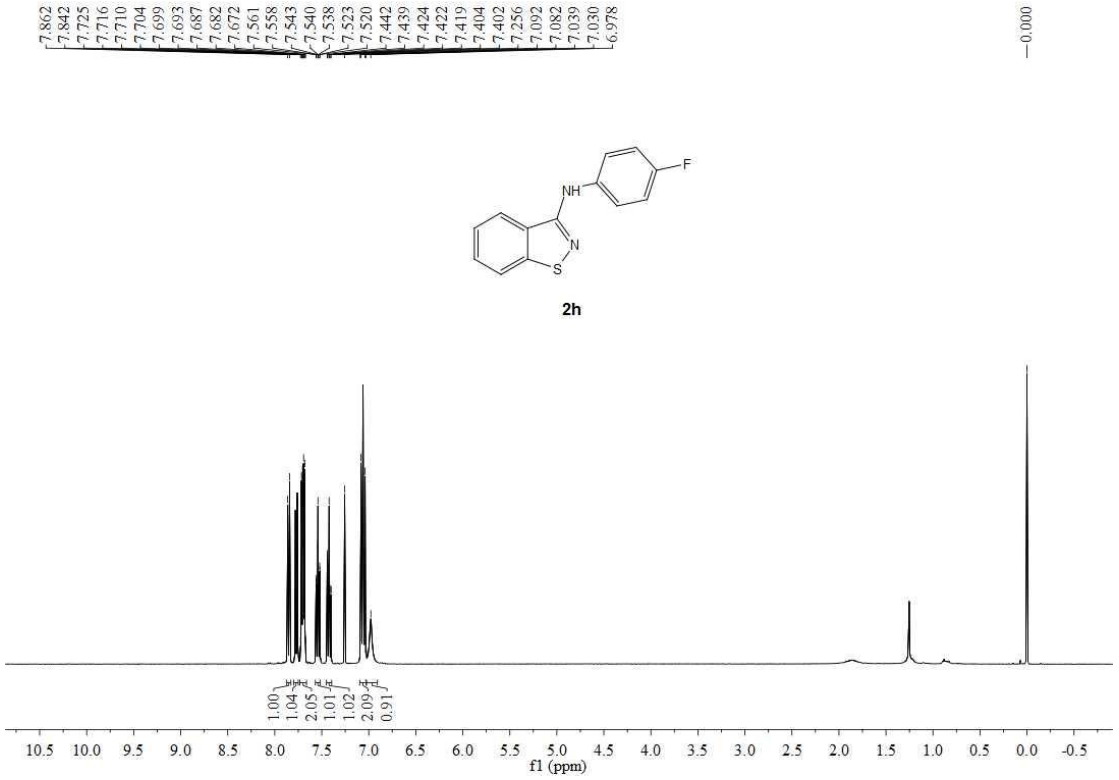

155.272
155.115
151.043
133.581
128.054
126.912
124.045
120.856
120.449
120.354
114.339
77.318
77.000
76.683
55.527
NH
O
CH3
N
S
2e
f1 (ppm)

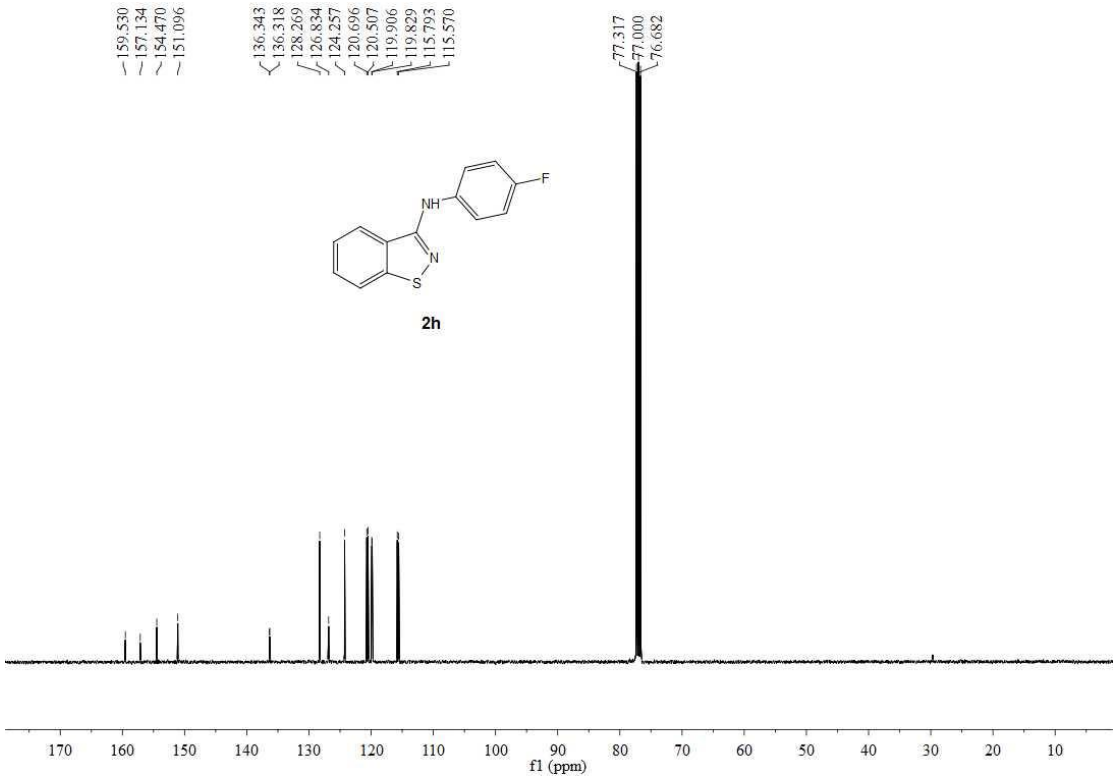

7.808
7.788
7.732
7.711
7.613
7.604
7.599
7.587
7.582
7.574
7.504
7.485
7.466
7.372
7.353
7.334
7.243
6.928
6.902
6.893
6.888
6.876
6.871
6.862
4.026
4.009
3.991
3.974
1.412
1.395
1.377
0.000
NH
O
CH3
N
S
2f
1.00
1.05
2.07
1.01
1.01
3.05
2.01
3.01
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

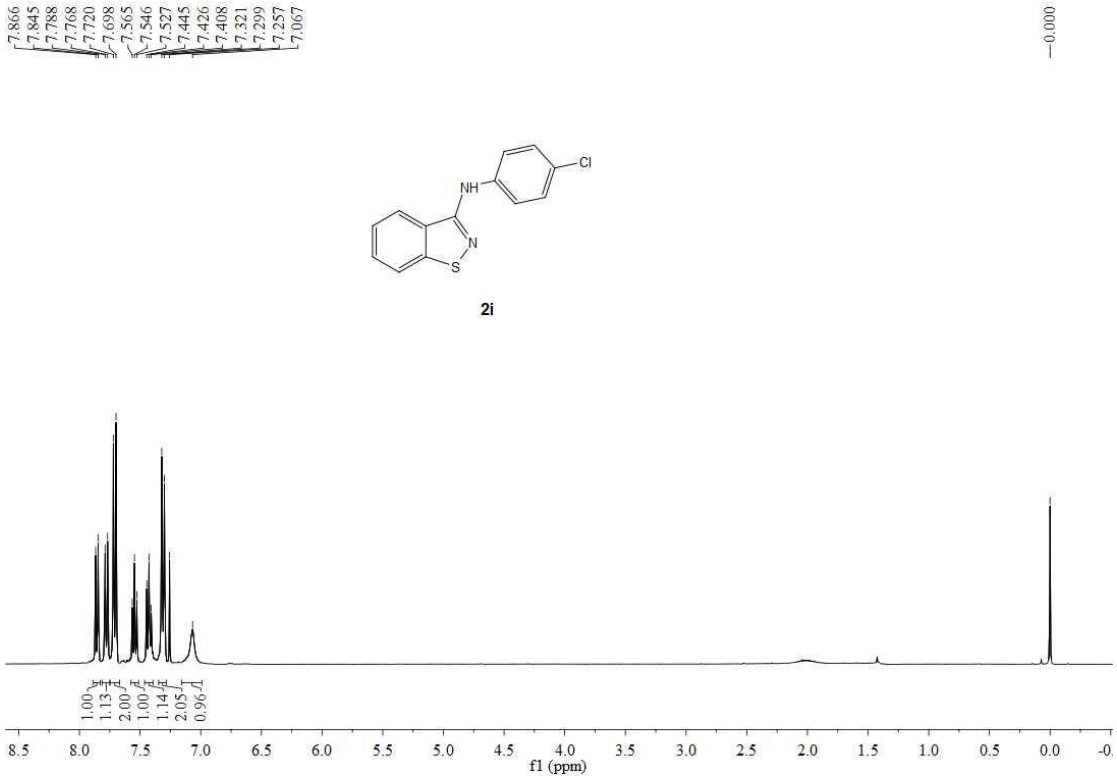

155.120
154.596
150.983
133.464
128.038
126.906
124.025
120.877
120.409
120.321
115.005
77.317
77.000
76.682
63.753
14.845
NH
O
CH3
N
S
2f
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

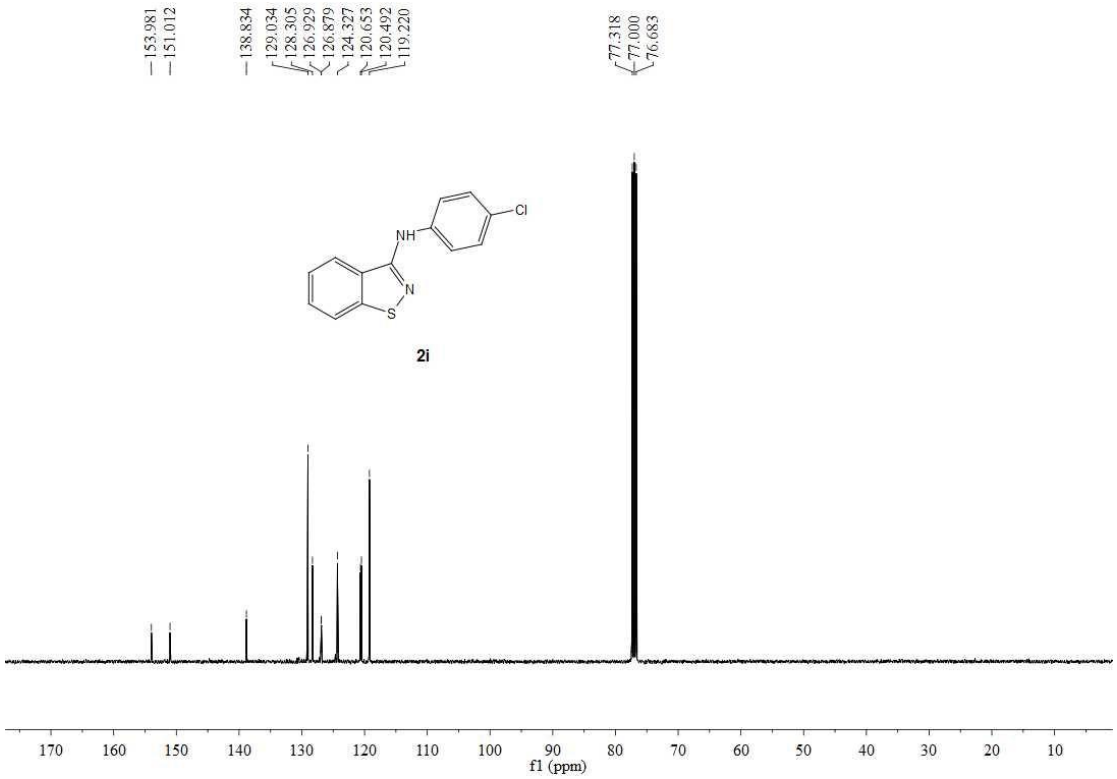

7.851
7.830
7.782
7.767
7.762
7.745
7.737
7.549
7.531
7.511
7.430
7.411
7.392
7.249
7.204
7.182
7.067
-0.000
F
F
F
O
NH
N
S
2g
1.00
2.97
1.00
1.03
1.95
0.99
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

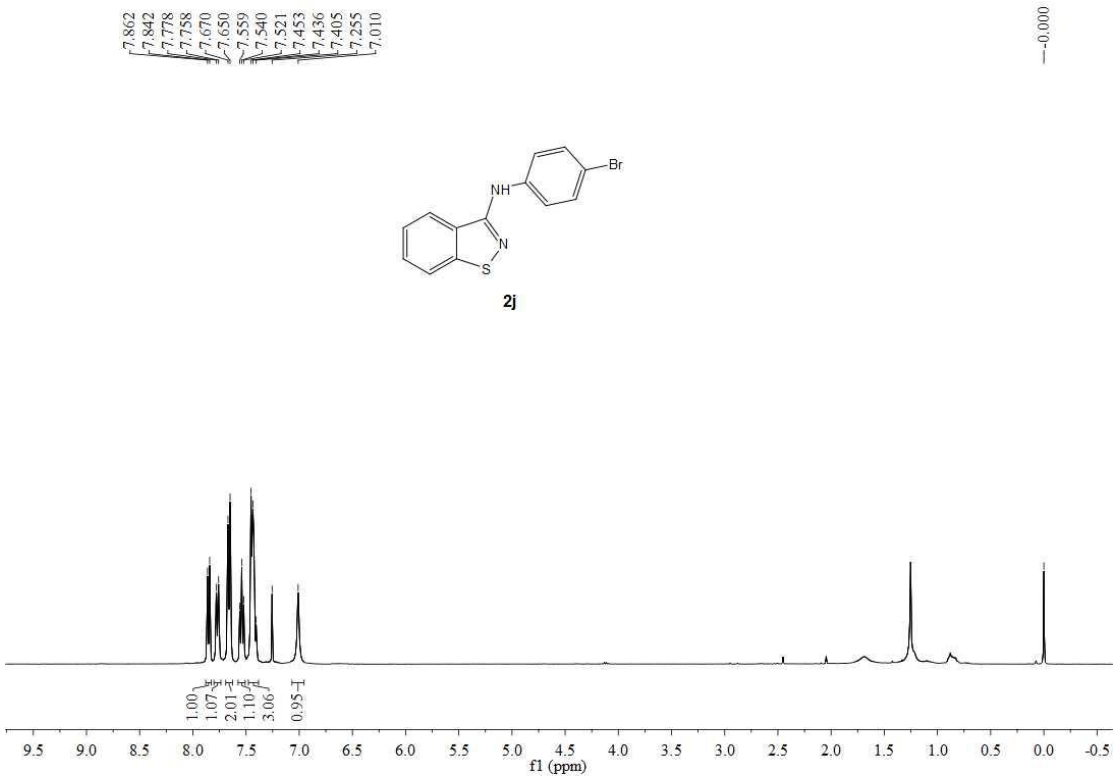

153.967
151.025
143.707
143.688
143.671
138.984
128.311
126.862
124.384
124.334
121.945
121.837
120.608
120.472
119.290
118.859
116.743
77.317
77.000
76.682
F
F
F
O
NH
N
S
2g
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

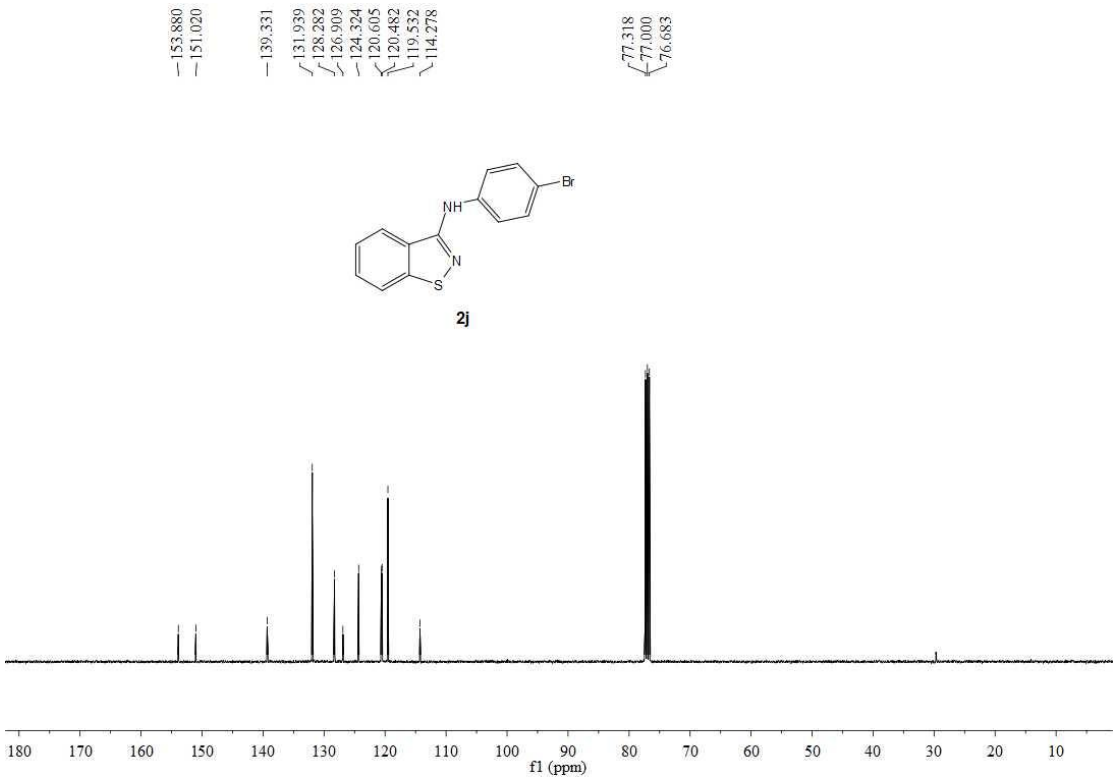

7.862
7.842
7.725
7.716
7.710
7.704
7.699
7.693
7.687
7.682
7.672
7.561
7.558
7.543
7.540
7.538
7.523
7.520
7.442
7.439
7.424
7.422
7.419
7.404
7.402
7.256
7.092
7.082
7.039
7.030
6.978
0.000
NH
F
N
S
2h
1.00
1.04
2.05
1.01
1.02
2.09
0.91
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

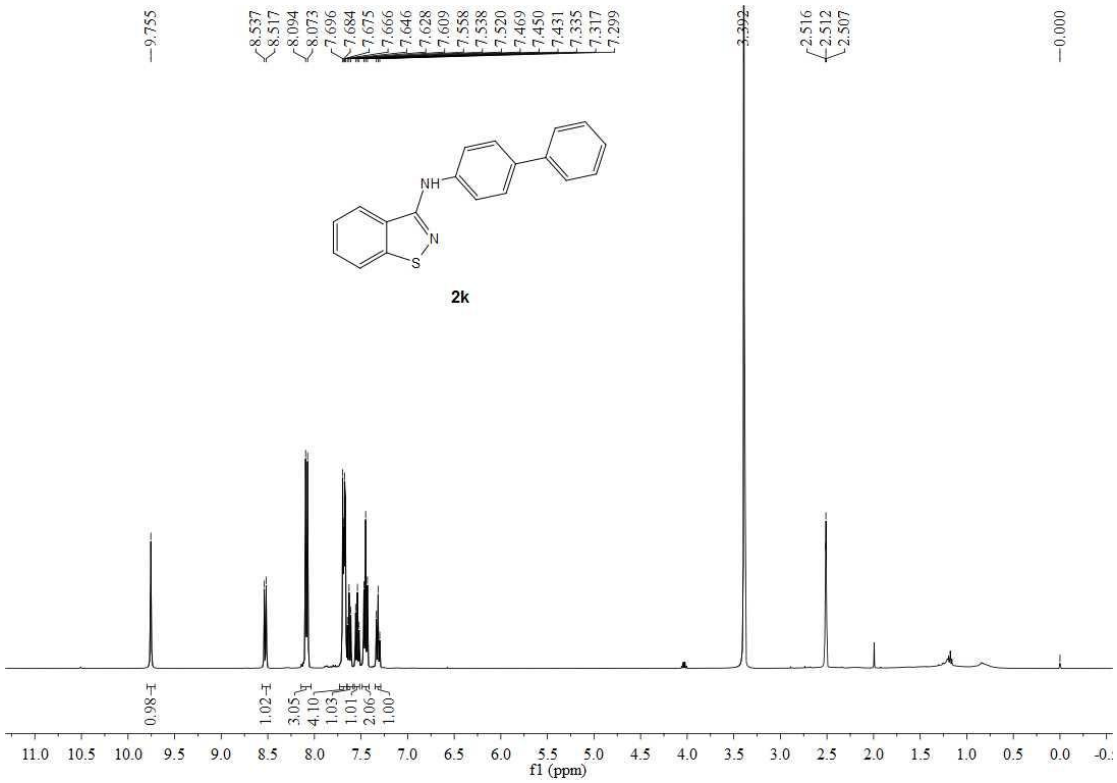

159.530
157.134
154.470
151.096
136.343
136.318
128.269
126.834
124.257
120.696
120.507
119.906
119.829
115.793
115.570
77.317
77.000
76.682
NH
F
N
S
2h
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

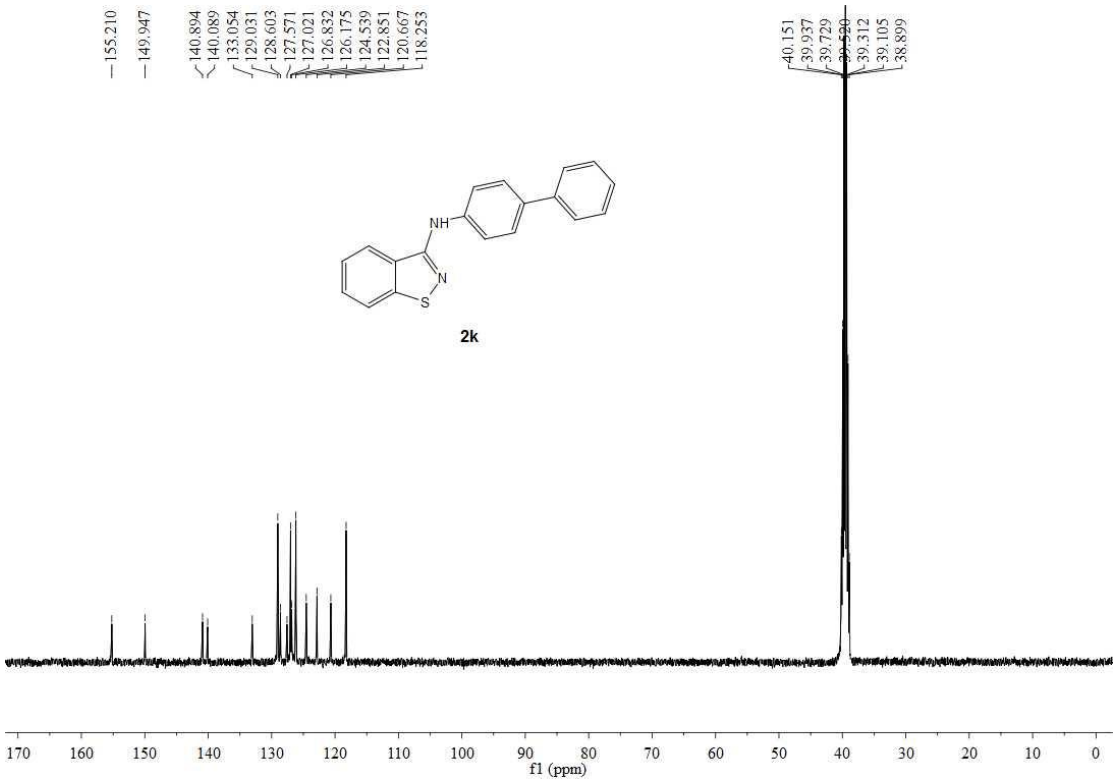

7.866
7.845
7.788
7.768
7.720
7.698
7.565
7.546
7.527
7.445
7.426
7.408
7.321
7.299
7.257
7.067
0.000
Cl
NH
N
S
2i
1.00
1.13
2.00
1.00
1.14
2.05
0.96
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

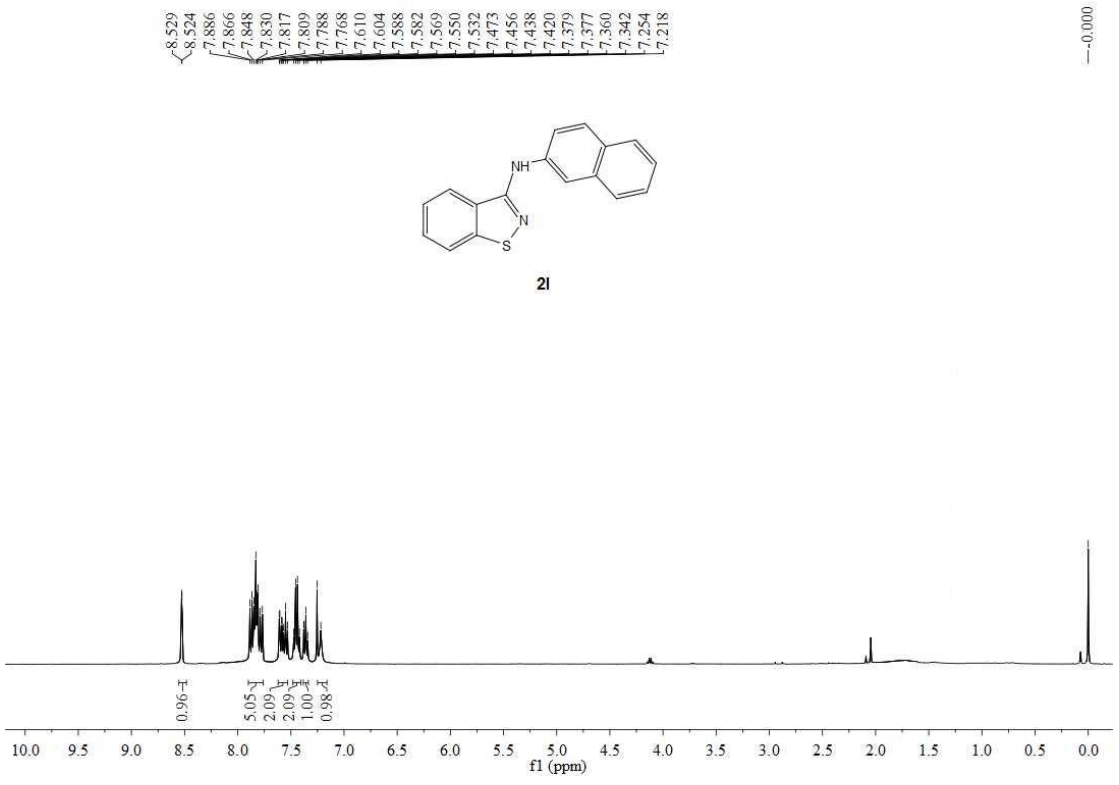

153.981
151.012
138.834
129.034
128.305
126.929
126.879
124.327
120.653
120.492
119.220
77.318
77.000
76.683
Cl
NH
N
S
2i
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

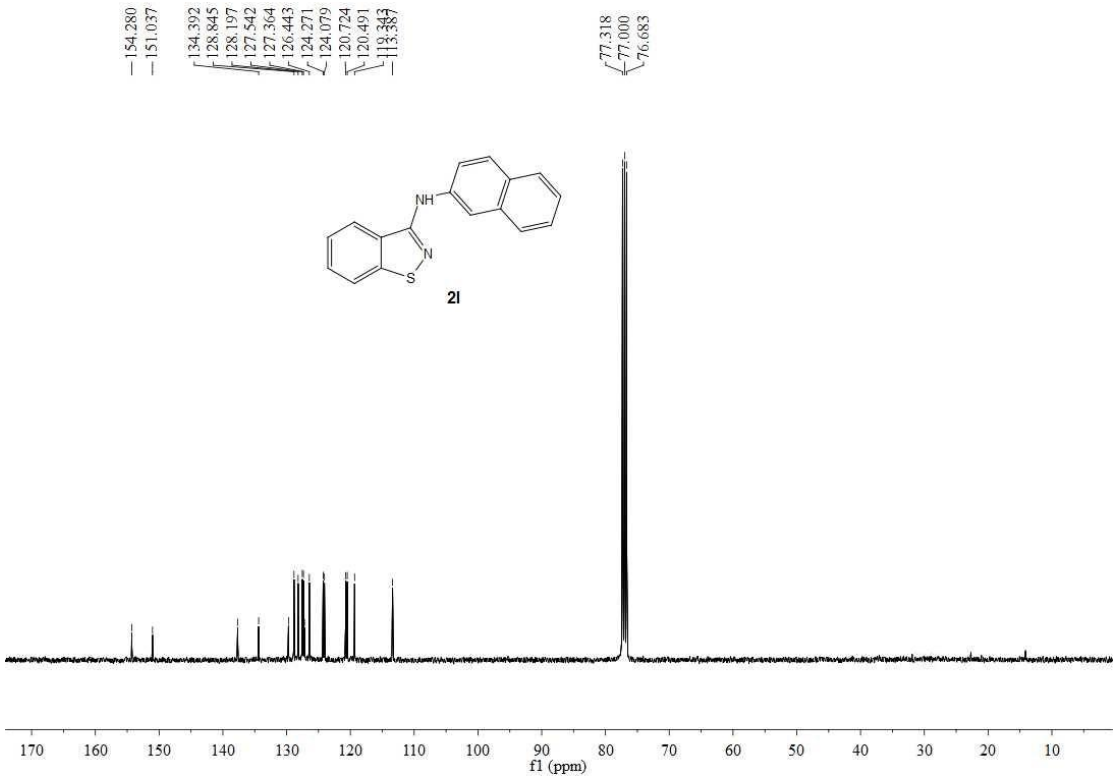

7.862
7.842
7.778
7.758
7.670
7.650
7.559
7.540
7.521
7.453
7.436
7.405
7.255
7.010
0.000
Br
NH
N
S
2j
1.00
1.07
2.01
1.10
3.06
0.95
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

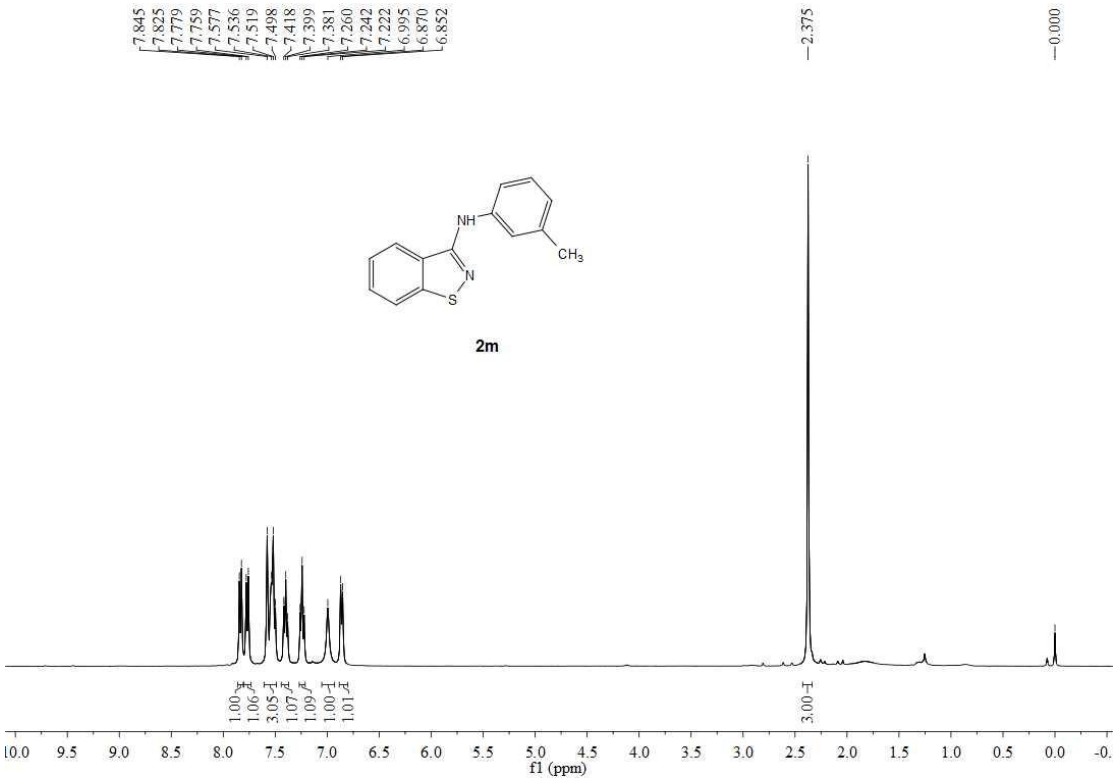

153.880
151.020
139.331
131.939
128.282
126.909
124.324
120.605
120.482
119.532
114.278
77.318
77.000
76.683
Br
NH
N
S
2j
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

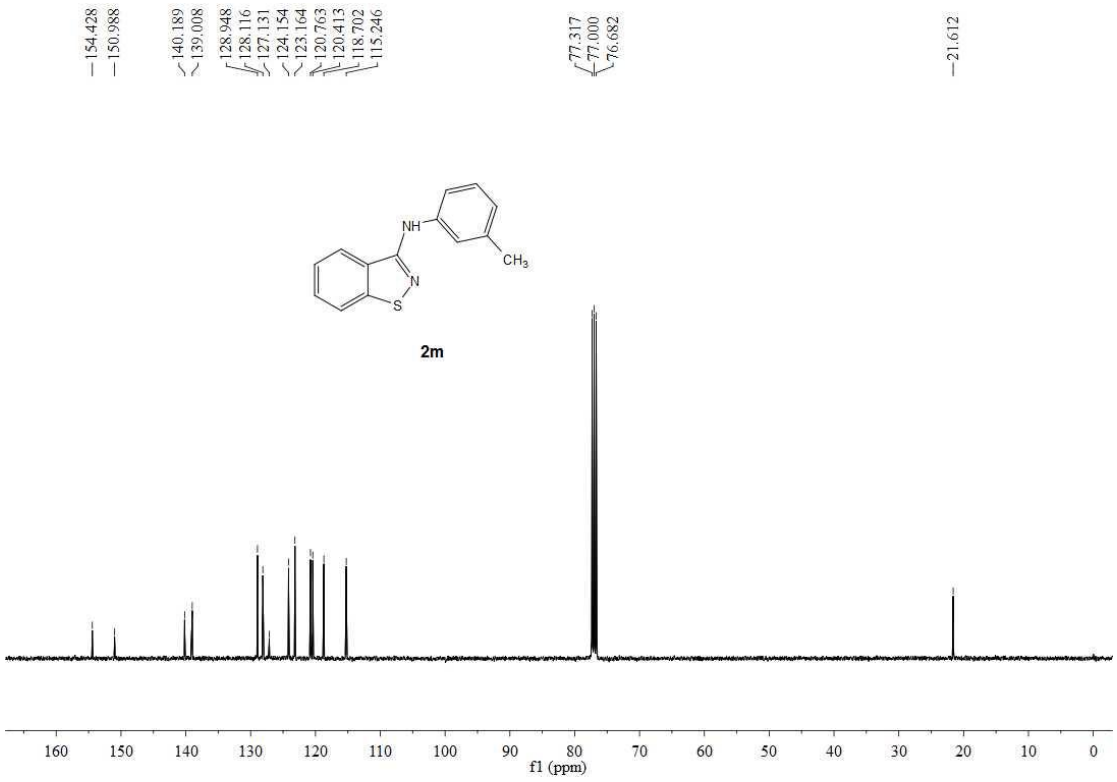

9.755
8.537
8.517
8.094
8.073
7.696
7.684
7.675
7.666
7.646
7.628
7.609
7.558
7.538
7.520
7.469
7.450
7.431
7.335
7.317
7.299
3.392
2.516
2.512
2.507
0.000
NH
N
S
2k
0.98
1.02
3.05
4.10
1.03
1.01
2.06
1.00
f1 (ppm)

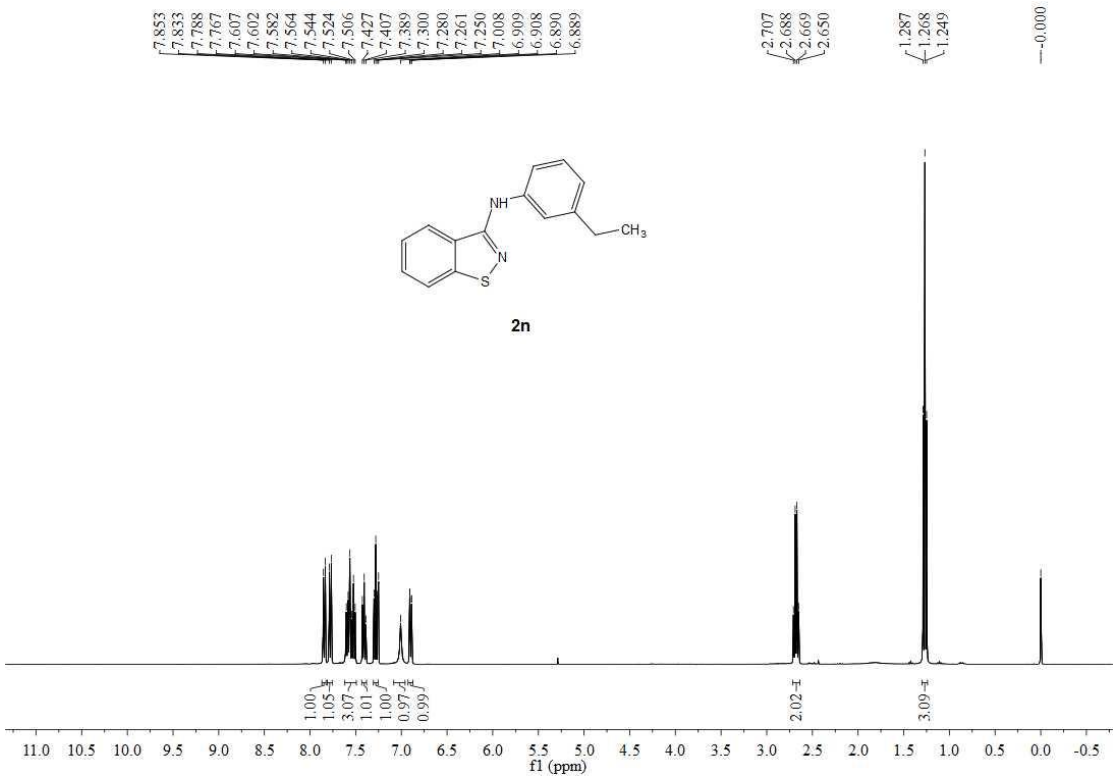

155.210
149.947
140.894
140.089
133.054
129.031
128.603
127.571
127.021
126.832
126.175
124.539
122.851
120.667
118.253
40.151
39.937
39.729
39.520
39.312
39.105
38.899
NH
N
S
2k
f1 (ppm)

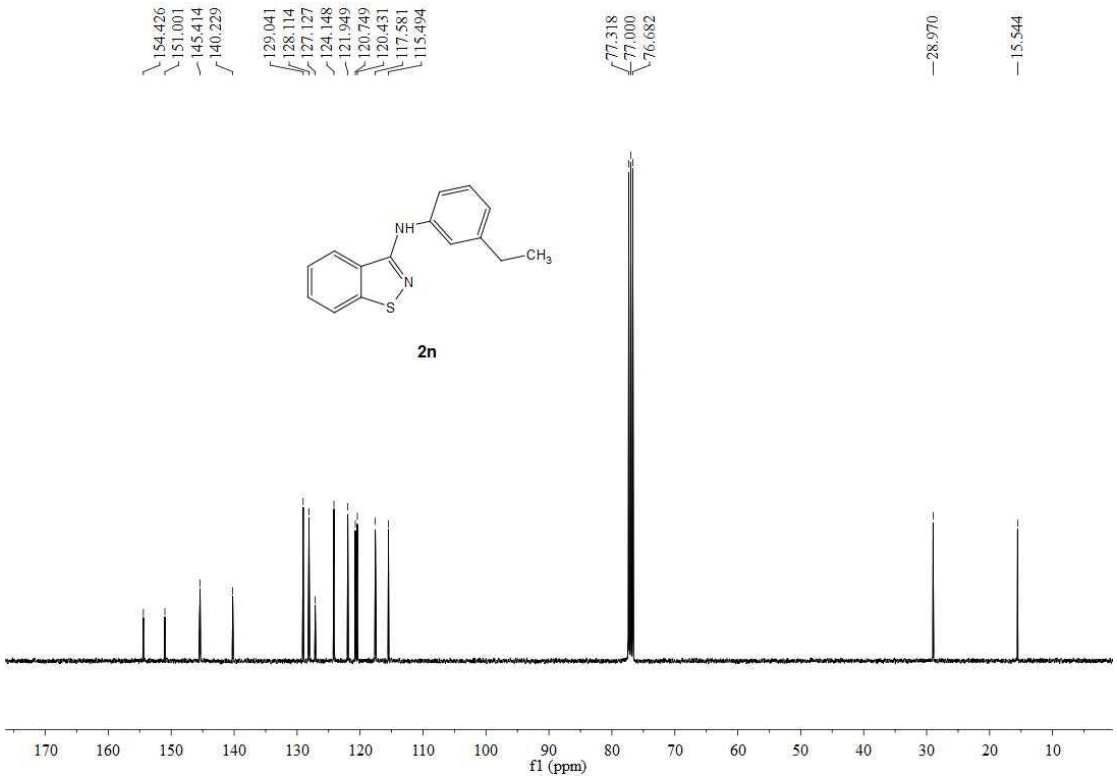

8.529
8.524
7.886
7.866
7.848
7.830
7.817
7.809
7.788
7.768
7.610
7.604
7.588
7.582
7.569
7.550
7.532
7.473
7.456
7.438
7.420
7.379
7.377
7.360
7.342
7.254
7.218
-0.000
NH
N
S
2l
0.96
5.05
2.09
2.09
1.00
0.98
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

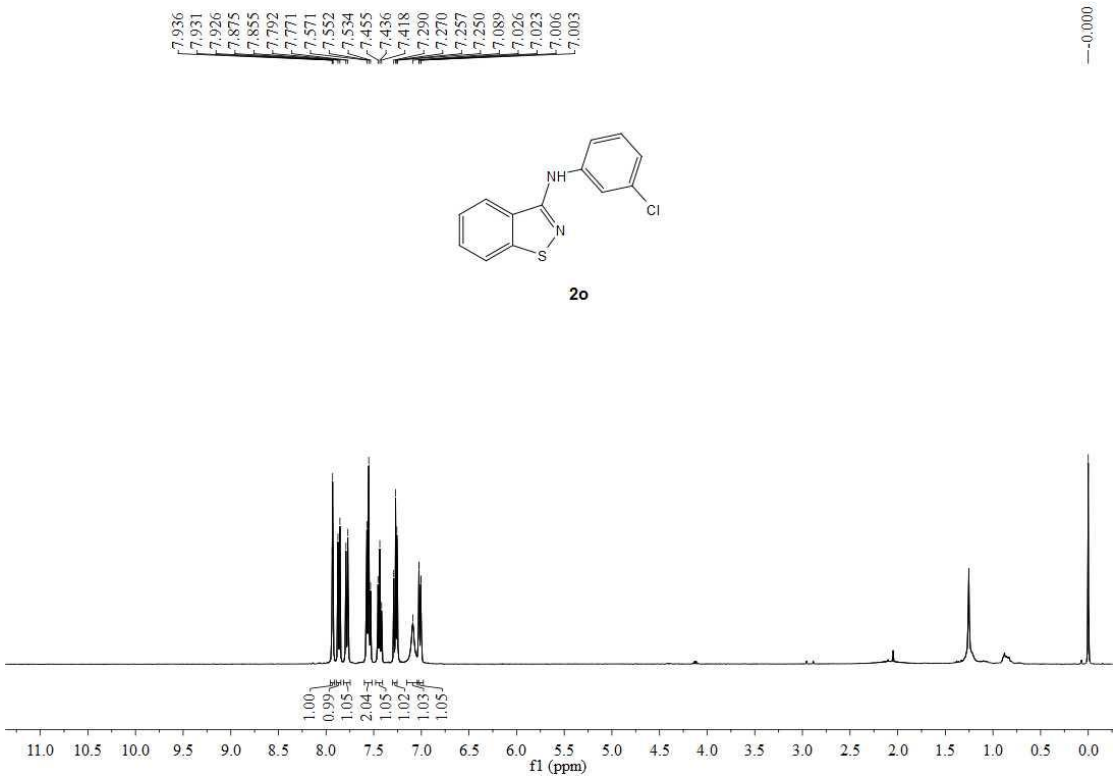

154.280
151.037
134.392
128.845
128.197
127.542
127.364
126.443
124.271
124.079
120.724
120.491
113.387
77.318
77.000
76.683
NH
N
S
2l
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

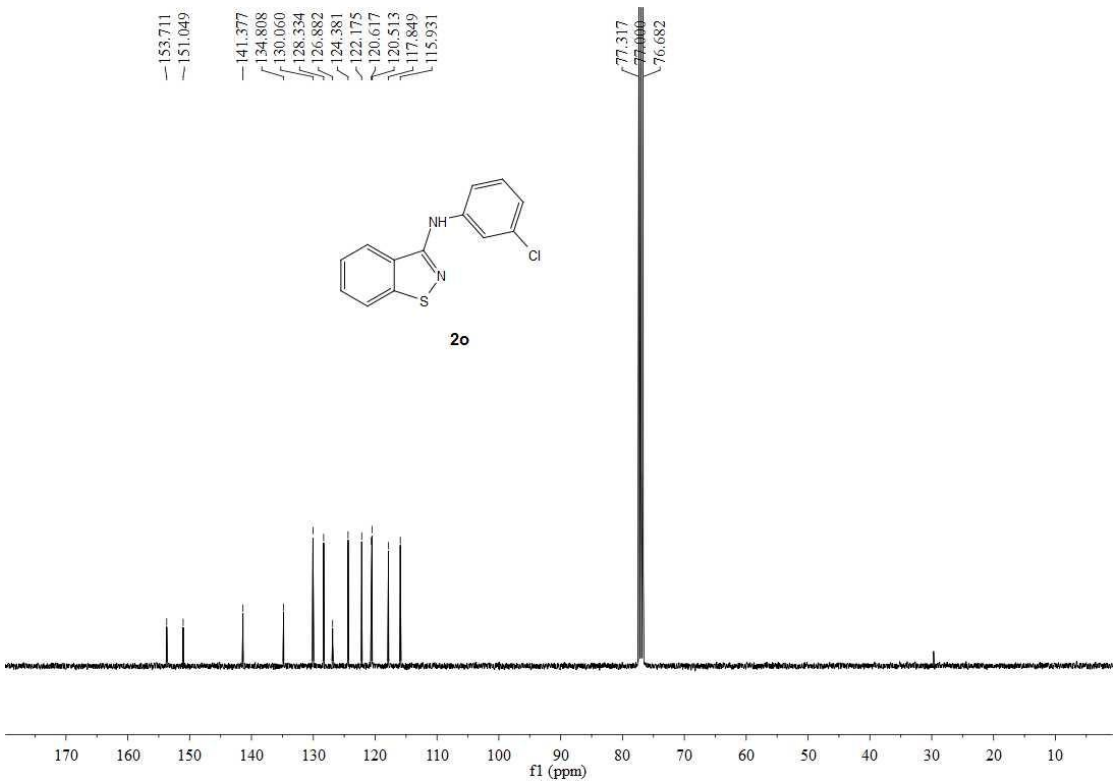

7.845
7.825
7.779
7.759
7.577
7.536
7.519
7.498
7.418
7.399
7.381
7.260
7.242
7.222
6.995
6.870
6.852
2.375
0.000
NH
CH3
N
S
2m
1.00
1.06
3.05
1.07
1.09
1.00
1.01
3.00
f1 (ppm)

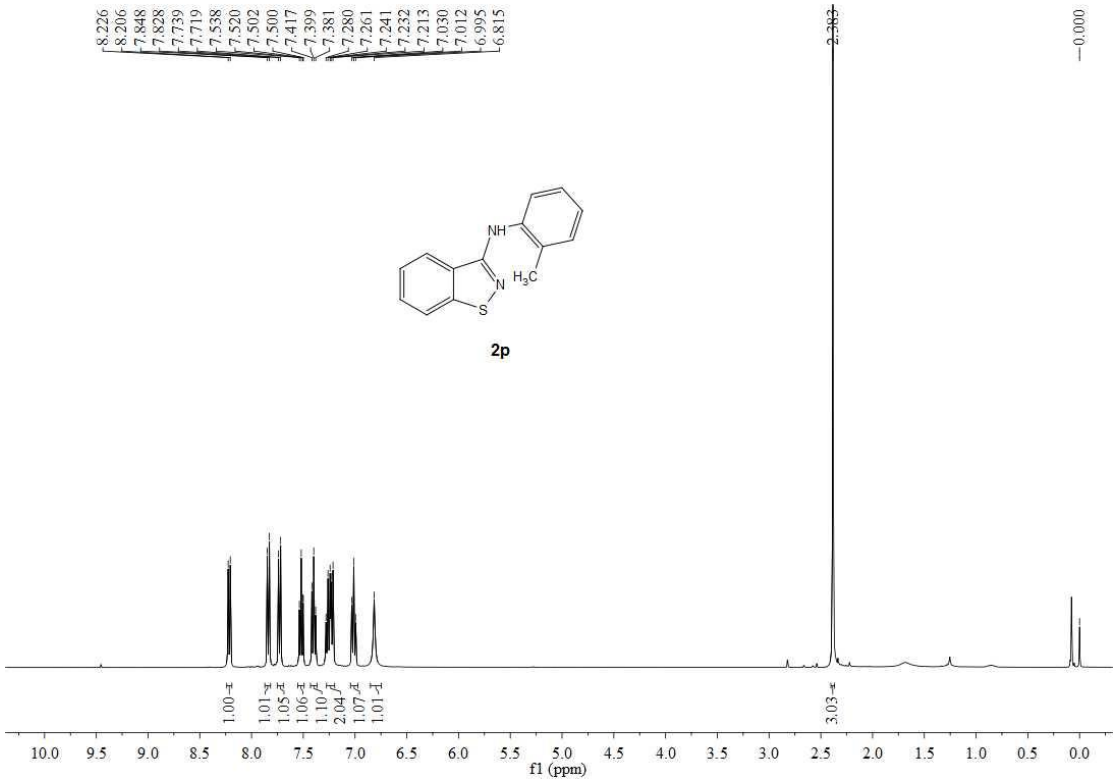

154.428
150.988
140.189
139.008
128.948
128.116
127.131
124.154
123.164
120.763
120.413
118.702
115.246
77.317
77.000
76.682
21.612
NH
CH3
N
S
2m
f1 (ppm)


7.853
7.833
7.788
7.767
7.607
7.602
7.582
7.564
7.544
7.524
7.506
7.427
7.407
7.389
7.300
7.280
7.261
7.250
7.008
6.909
6.908
6.890
6.889
2.707
2.688
2.669
2.650
1.287
1.268
1.249
0.000
NH
CH3
N
S
2n
1.00
1.05
3.07
1.01
1.00
0.97
0.99
2.02
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 -0.5
f1 (ppm)

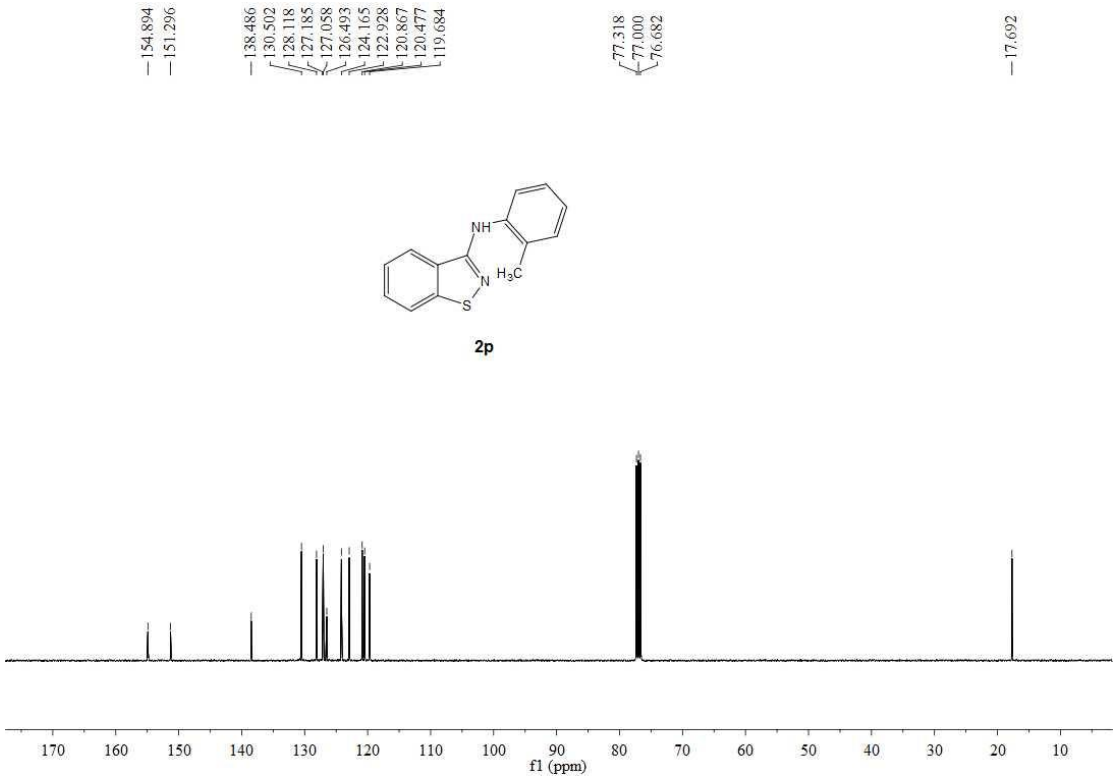

154.426
151.001
145.414
140.229
129.041
128.114
127.127
124.148
121.949
120.749
120.431
117.581
115.494
77.318
77.000
76.682
28.970
15.544
NH
CH3
N
S
2n
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)


7.936
7.931
7.926
7.875
7.855
7.792
7.771
7.571
7.552
7.534
7.455
7.436
7.418
7.290
7.270
7.257
7.250
7.089
7.026
7.023
7.006
7.003
-0.000
NH
Cl
N
S
2o
1.00
0.99
1.05
2.04
1.05
1.02
1.03
1.05
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)

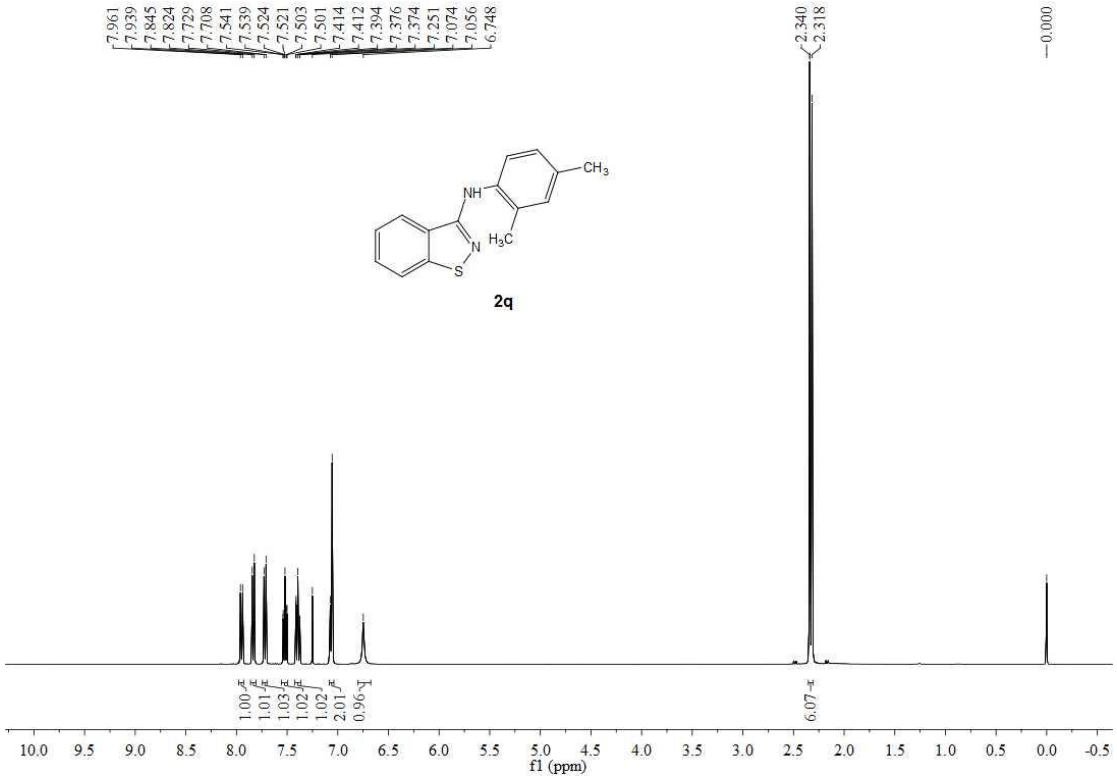

153.711
151.049
141.377
134.808
130.060
128.334
126.882
124.381
122.175
120.617
120.513
117.849
115.931
77.317
77.000
76.682
NH
Cl
N
S
2o
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

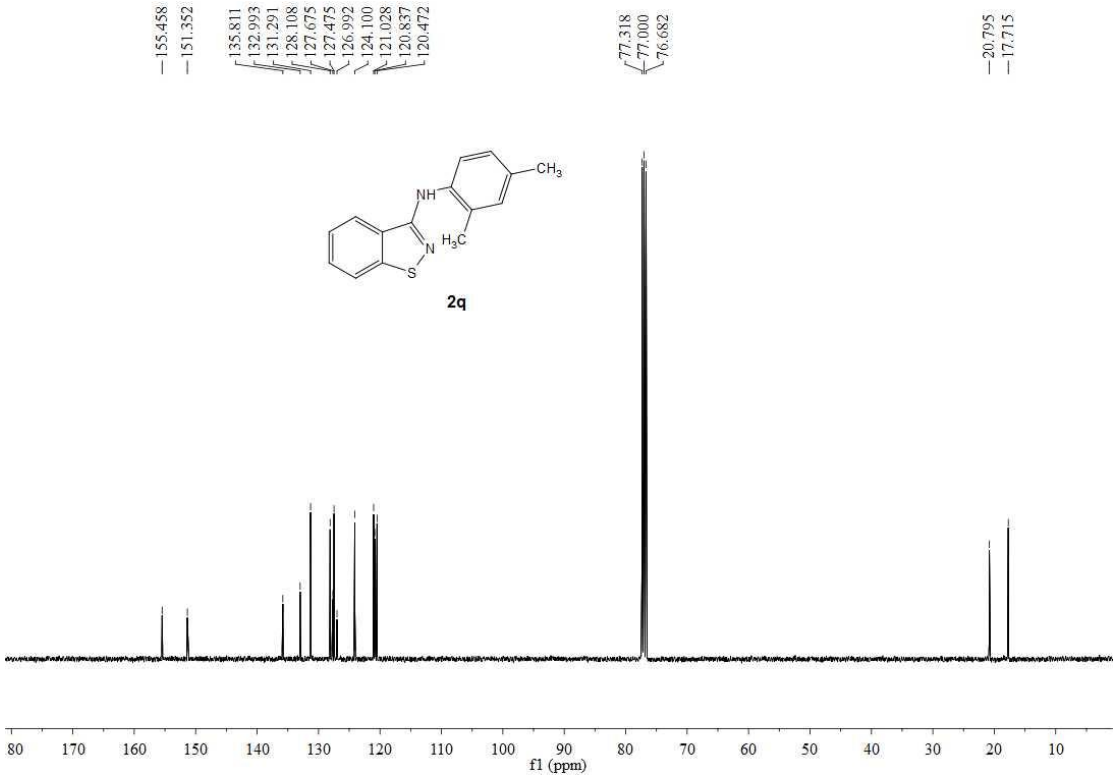

8.226
8.206
7.848
7.828
7.739
7.719
7.538
7.520
7.502
7.500
7.417
7.399
7.381
7.280
7.261
7.241
7.232
7.213
7.030
7.012
6.995
6.815
2.383
0.000
NH
N
S
H3C
1.00
1.01
1.05
1.06
1.10
2.04
1.07
1.01
3.03
f1 (ppm)

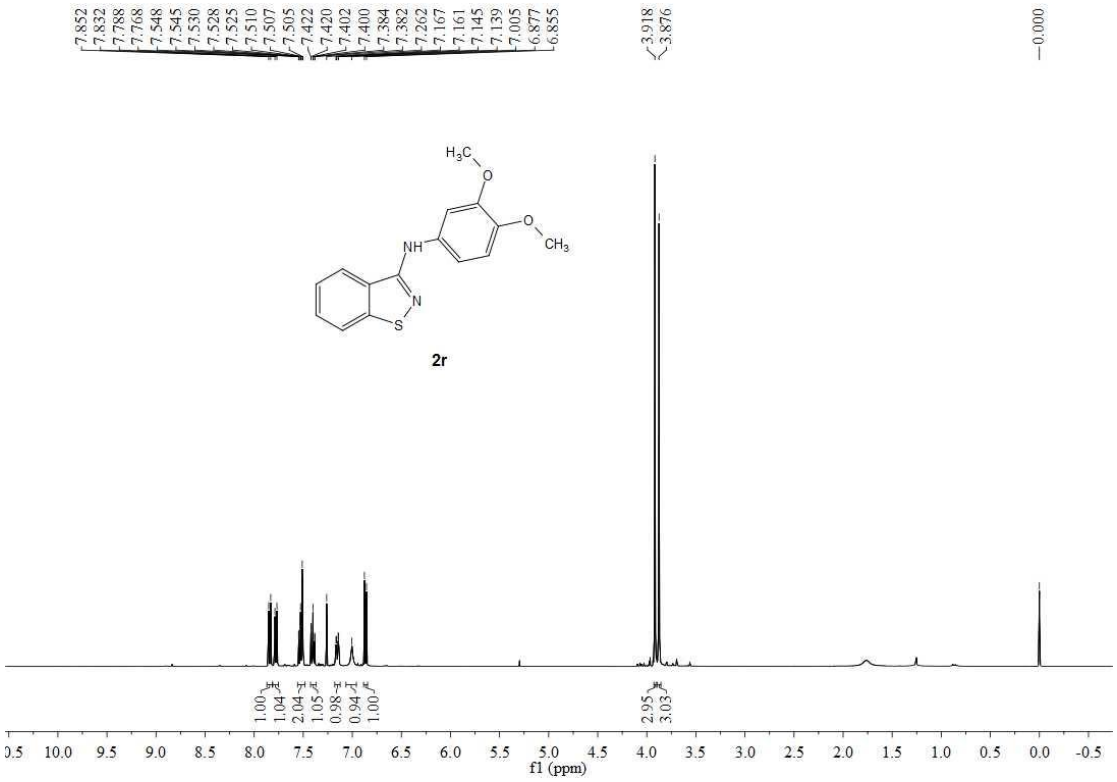
2p

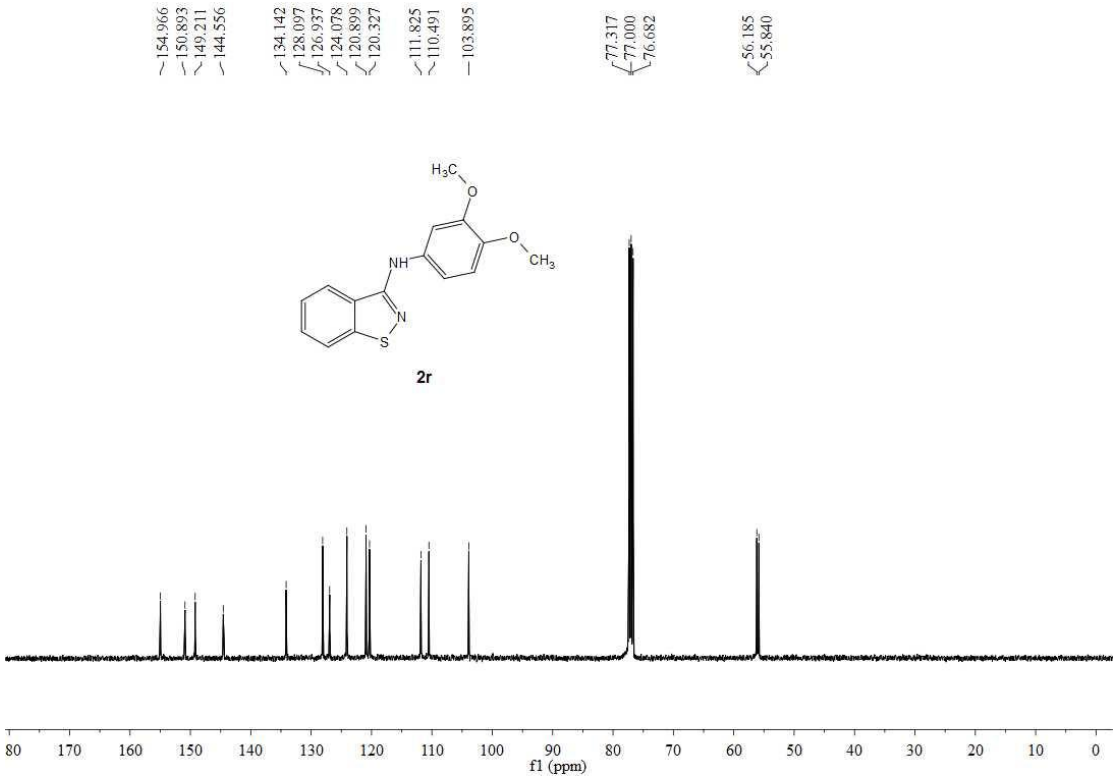

154.894
151.296
138.486
130.502
128.118
127.185
127.058
126.493
124.165
122.928
120.867
120.477
119.684
77.318
77.000
76.682
17.692
NH
N
S
H3C
f1 (ppm)

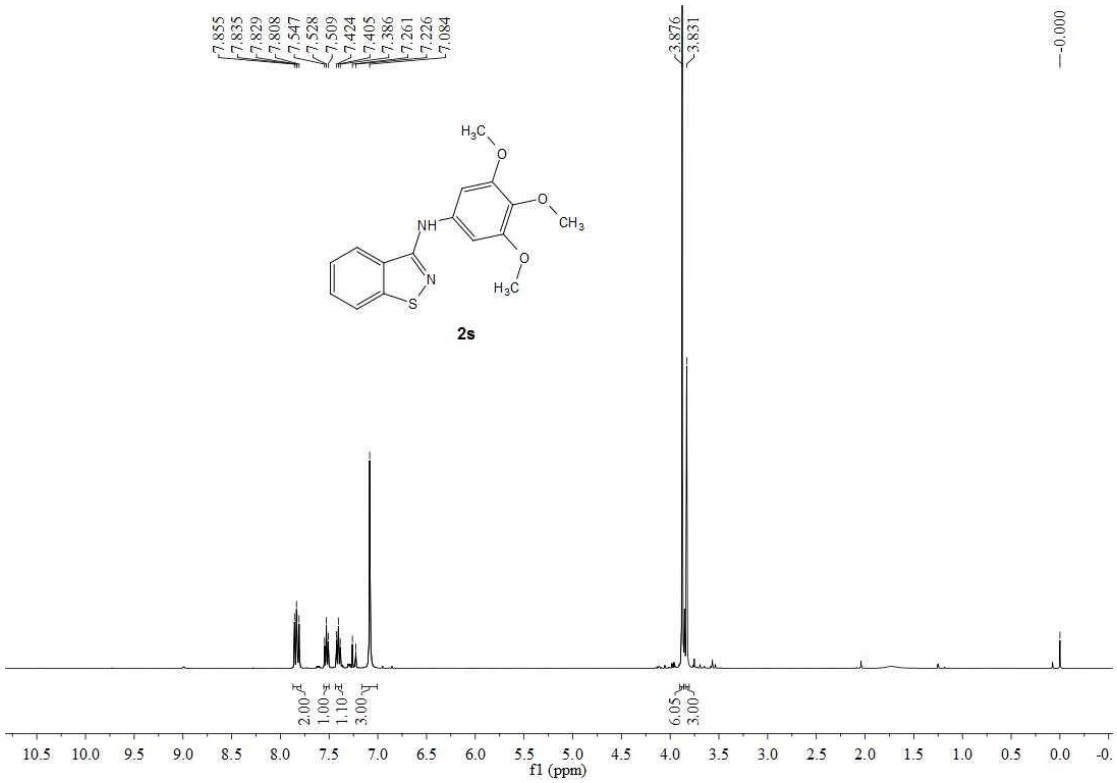
2p

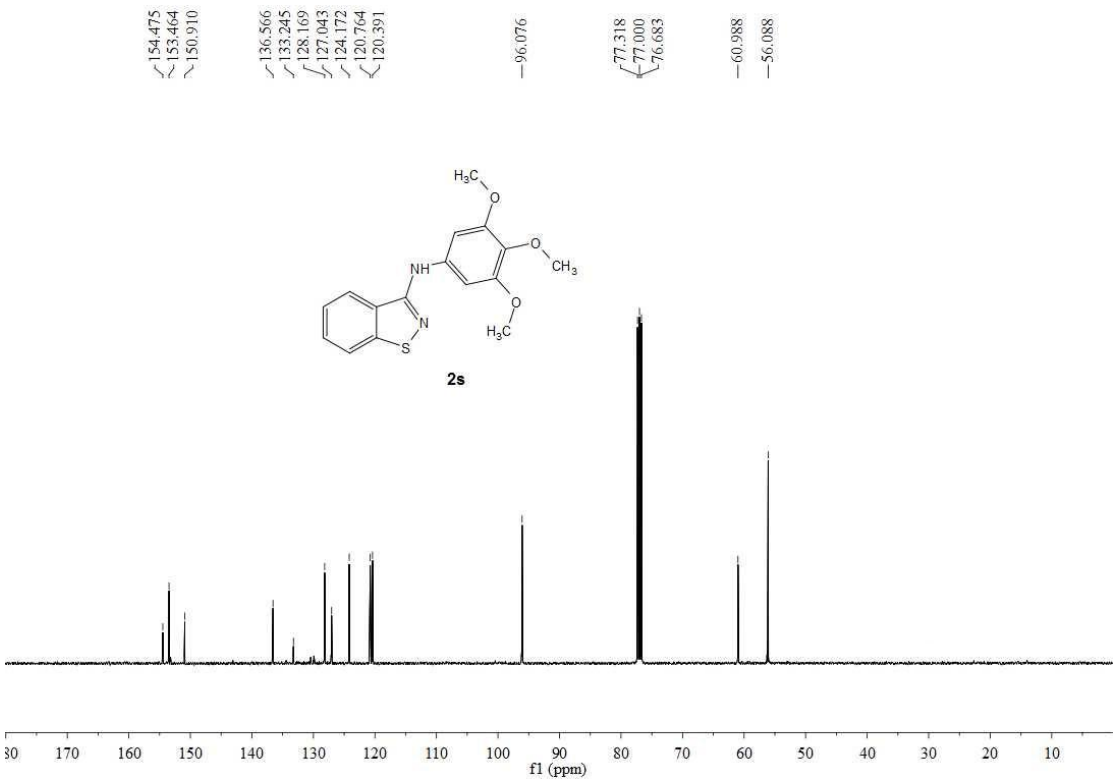

7.961
7.939
7.845
7.824
7.729
7.708
7.541
7.539
7.524
7.521
7.503
7.501
7.414
7.412
7.394
7.376
7.374
7.251
7.074
7.056
6.748
2.340
2.318
0.000
NH
CH3
H3C
N
S
2q
1.00
1.01
1.03
1.02
1.02
2.01
0.96
6.07
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

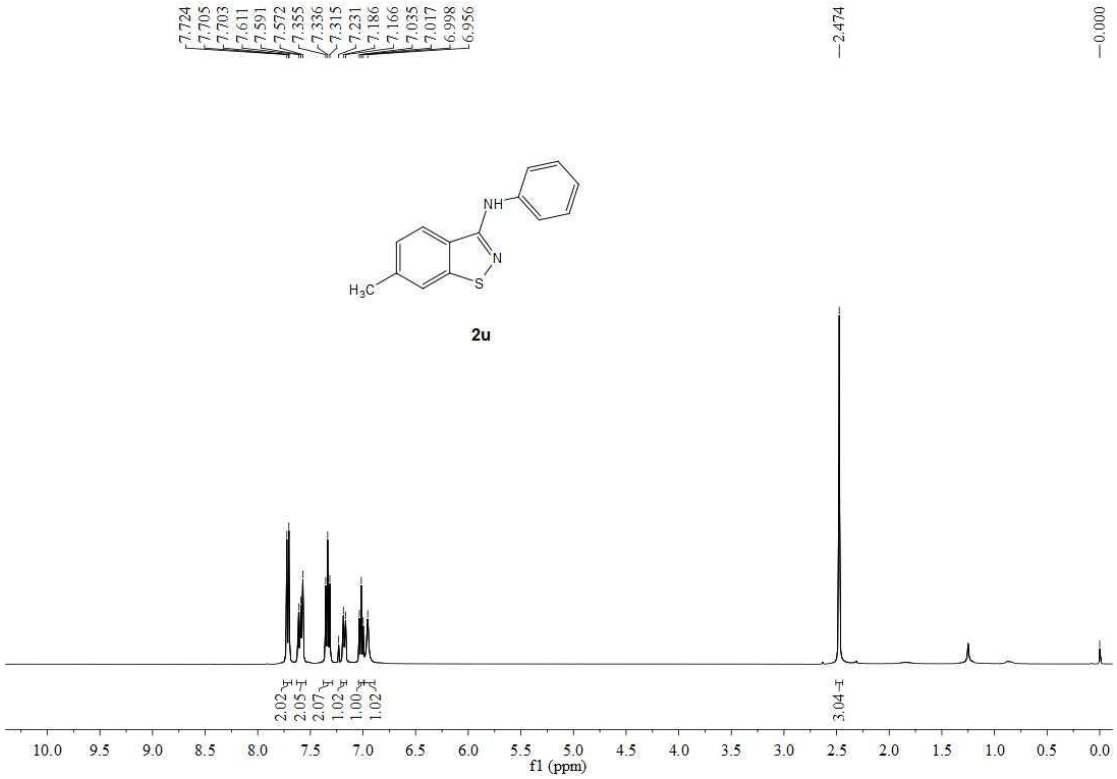

155.458
151.352
135.811
132.993
131.291
128.108
127.675
127.475
126.992
124.100
121.028
120.837
120.472
77.318
77.000
76.682
20.795
17.715
NH
CH3
H3C
N
S
2q
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

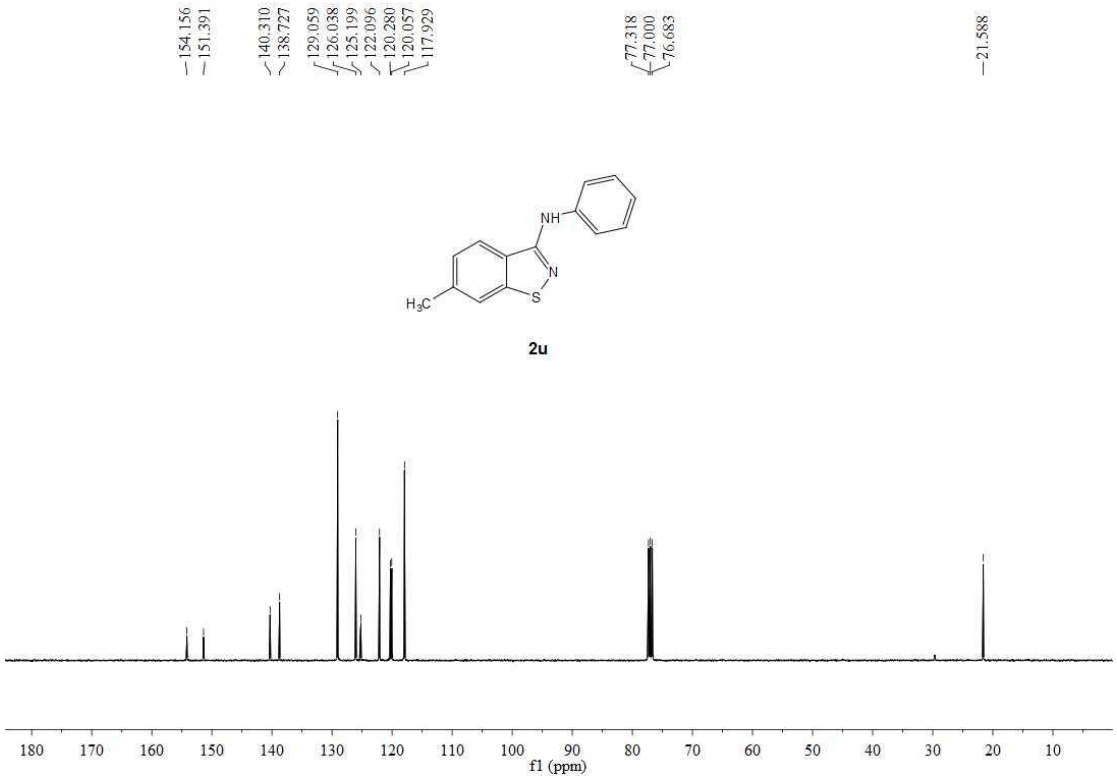

7.852
7.832
7.788
7.768
7.548
7.545
7.530
7.528
7.525
7.510
7.507
7.505
7.422
7.420
7.402
7.400
7.384
7.382
7.262
7.167
7.161
7.145
7.139
7.005
6.877
6.855
3.918
3.876
0.000
H3C
O
O
CH3
NH
N
S
2r
1.00
1.04
2.04
1.05
0.98
0.94
1.00
2.95
3.03
f1 (ppm)

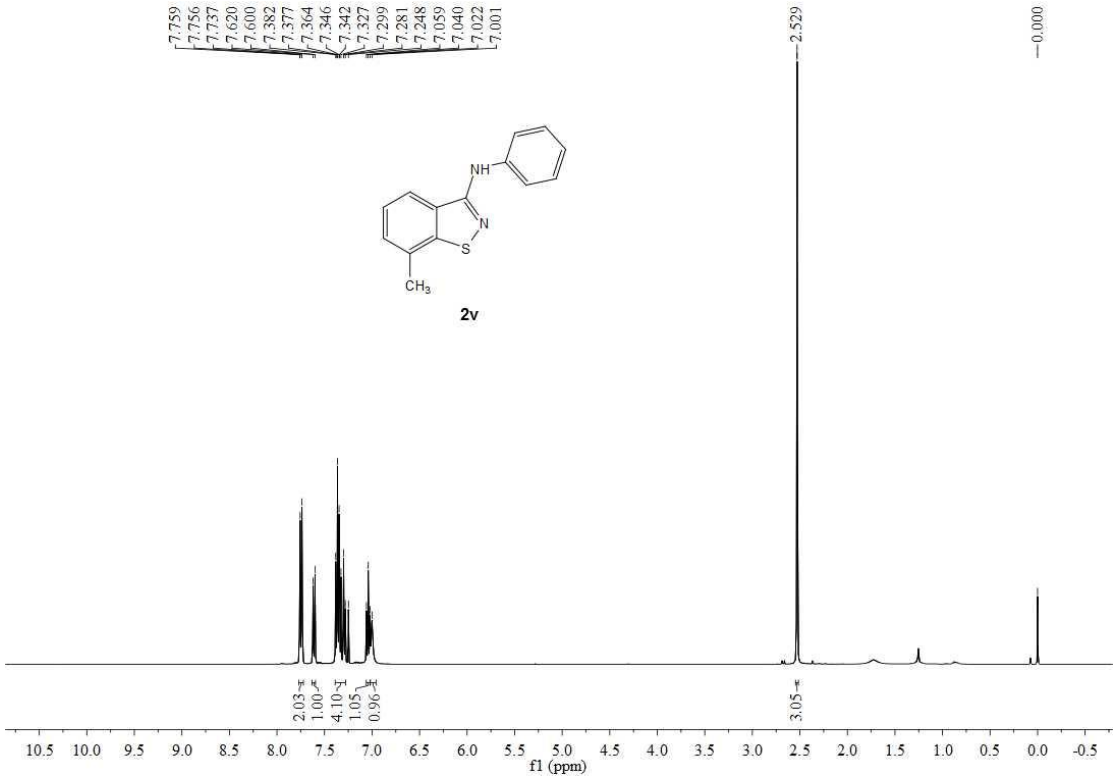

154.966
150.893
149.211
144.556
134.142
128.097
126.937
124.078
120.899
120.327
111.825
110.491
103.895
77.317
77.000
76.682
56.185
55.840
H3C
O
O
CH3
NH
N
S
2r
f1 (ppm)

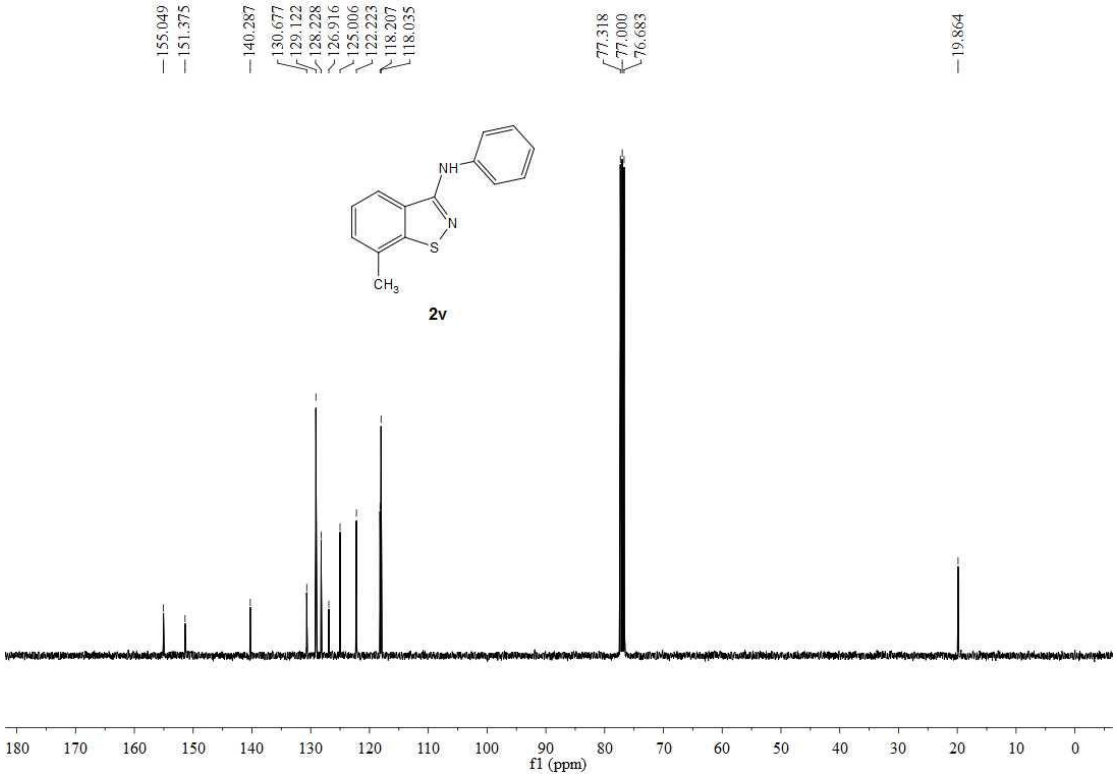

7.855
7.835
7.829
7.808
7.547
7.528
7.509
7.424
7.405
7.386
7.261
7.226
7.084
3.876
3.831
-0.000
2s
2.00
1.00
1.10
3.00
6.05
3.00
f1 (ppm)

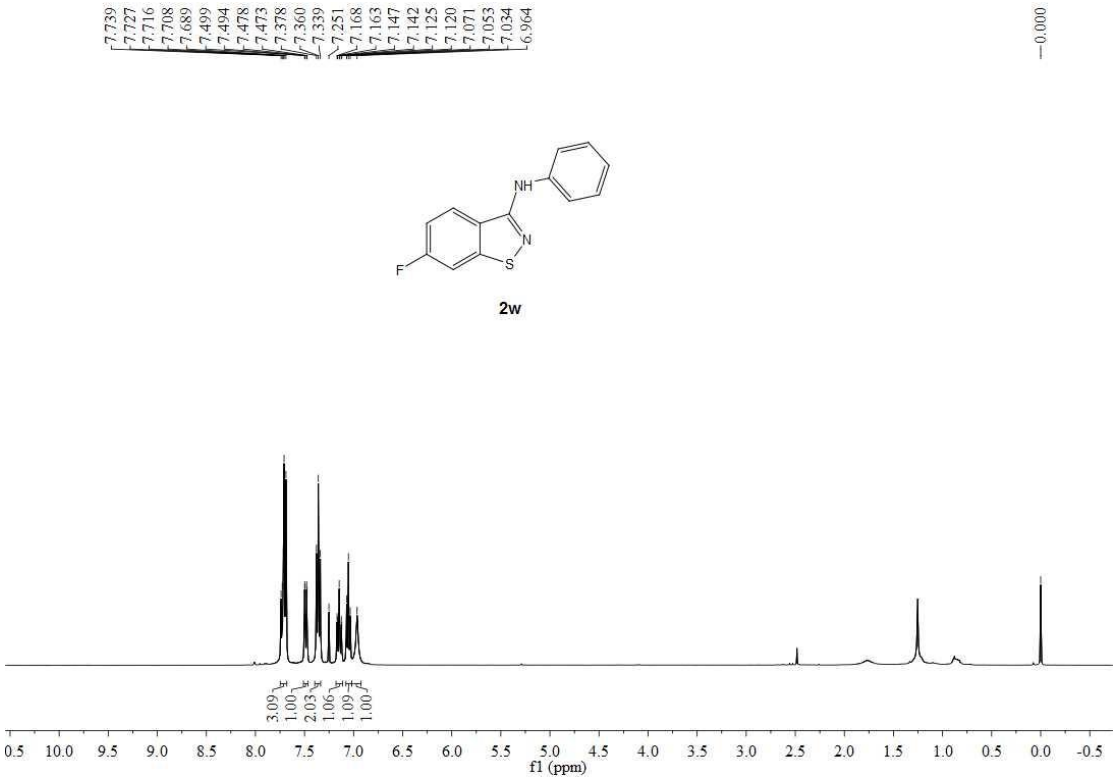

154.475
153.464
150.910
136.566
133.245
128.169
127.043
124.172
120.764
120.391
96.076
77.318
77.000
76.683
60.988
56.088
2s
f1 (ppm)

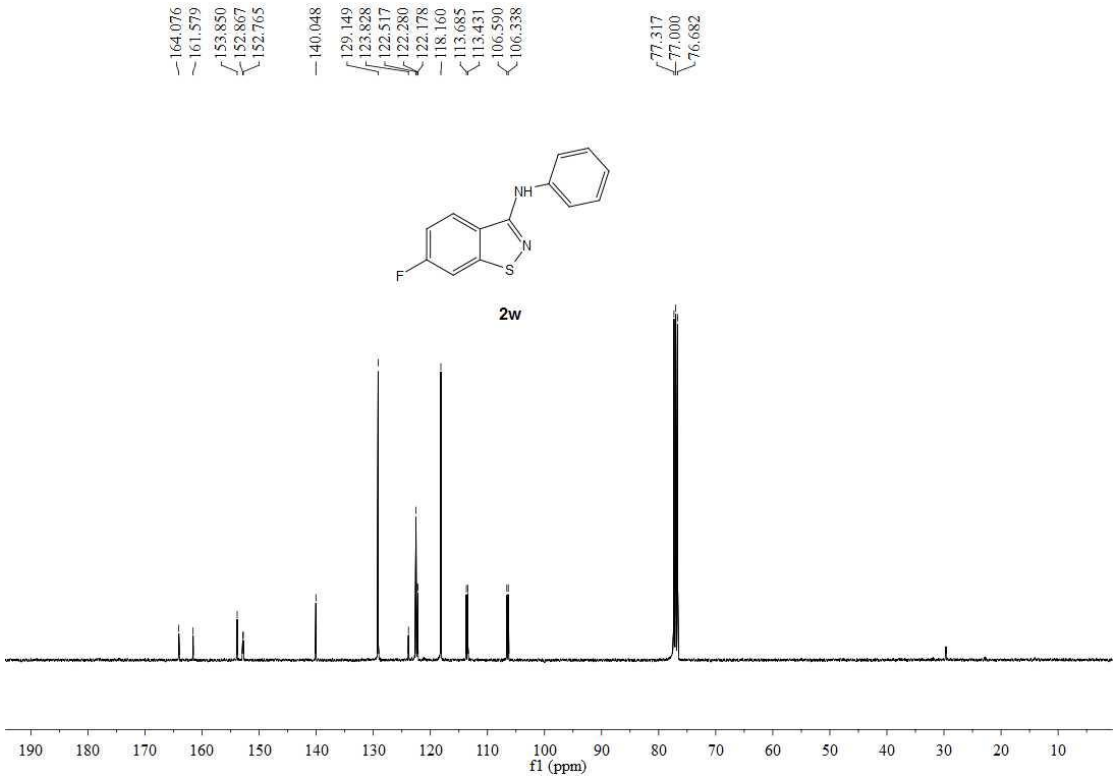

7.724
7.705
7.703
7.611
7.591
7.572
7.355
7.336
7.315
7.231
7.186
7.166
7.035
7.017
6.998
6.956
2.474
0.000
NH
N
S
H3C
2u
2.02
2.05
2.07
1.02
1.00
1.02
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

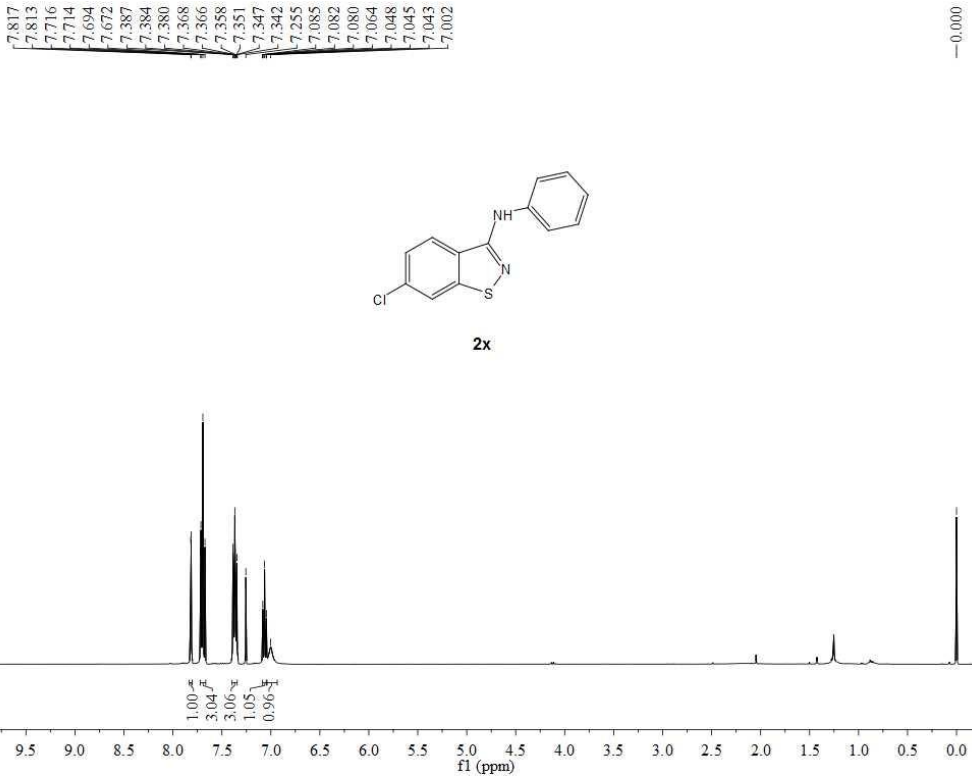

154.156
151.391
140.310
138.727
129.059
126.038
125.199
122.096
120.280
120.057
117.929
77.318
77.000
76.683
21.588
NH
N
S
H3C
2u
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

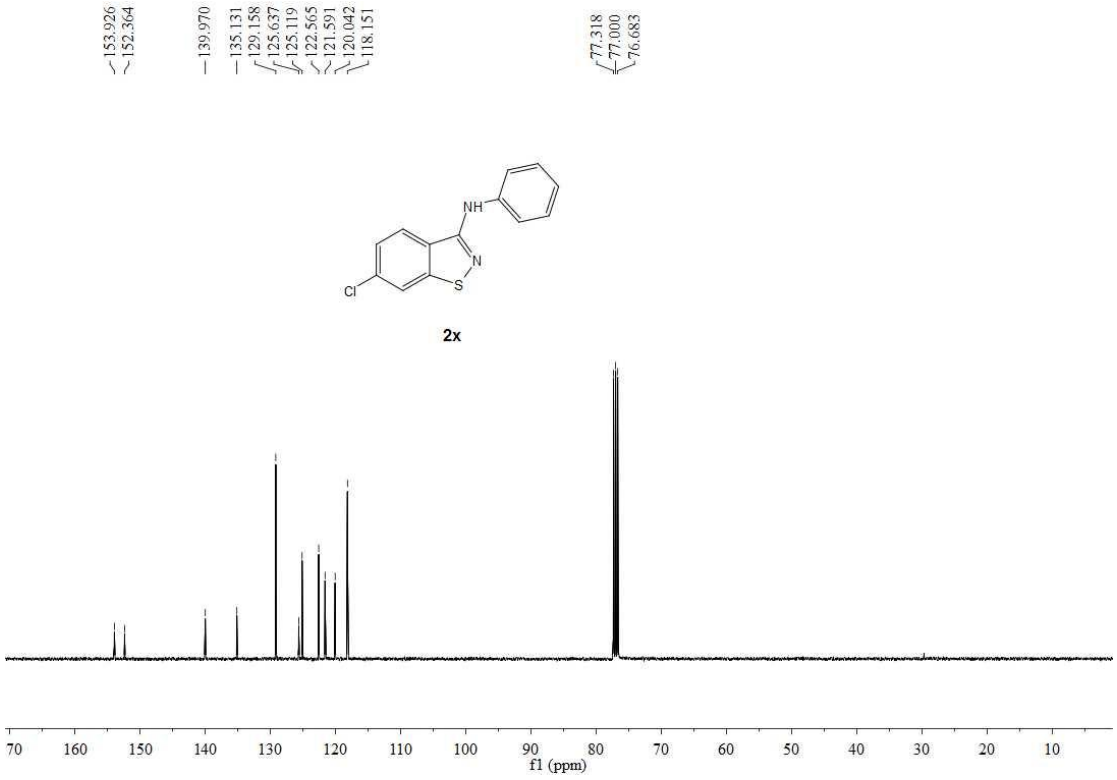

7.759
7.756
7.737
7.620
7.600
7.382
7.377
7.364
7.346
7.342
7.327
7.299
7.281
7.248
7.059
7.040
7.022
7.001
2.529
0.000
NH
N
S
CH3
2v
2.03
1.00
4.10
1.05
0.96
3.05
f1 (ppm)

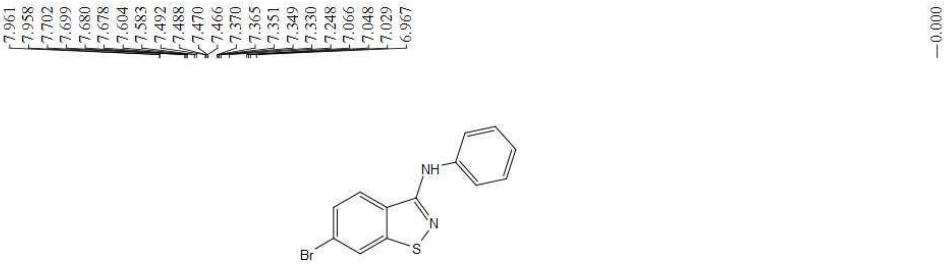

155.049
151.375
140.287
130.677
129.122
128.228
126.916
125.006
122.223
118.207
118.035
77.318
77.000
76.683
19.864
NH
N
S
CH3
2v
f1 (ppm)


7.739
7.727
7.716
7.708
7.689
7.499
7.494
7.478
7.473
7.378
7.360
7.339
7.251
7.168
7.163
7.147
7.142
7.125
7.120
7.071
7.053
7.034
6.964
0.000
NH
N
S
F
2w
3.09
1.00
2.03
1.06
1.09
1.00
f1 (ppm)

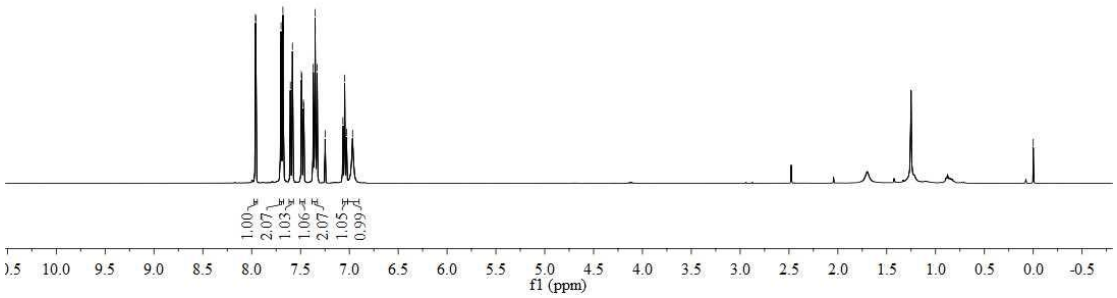

164.076
161.579
153.850
152.867
152.765
140.048
129.149
123.828
122.517
122.280
122.178
118.160
113.685
113.431
106.590
106.338
77.317
77.000
76.682
NH
N
S
F
2w
f1 (ppm)

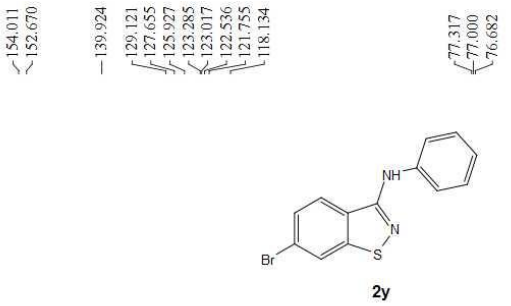

7.817
7.813
7.716
7.714
7.694
7.672
7.387
7.384
7.380
7.368
7.366
7.358
7.351
7.347
7.342
7.255
7.085
7.082
7.080
7.064
7.048
7.045
7.043
7.002
0.000
NH
N
S
Cl
2x
1.00
3.04
3.06
1.05
0.96
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


153.926
152.364
139.970
135.131
129.158
125.637
125.119
122.565
121.591
120.042
118.151
77.318
77.000
76.683
NH
N
S
Cl
2x
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

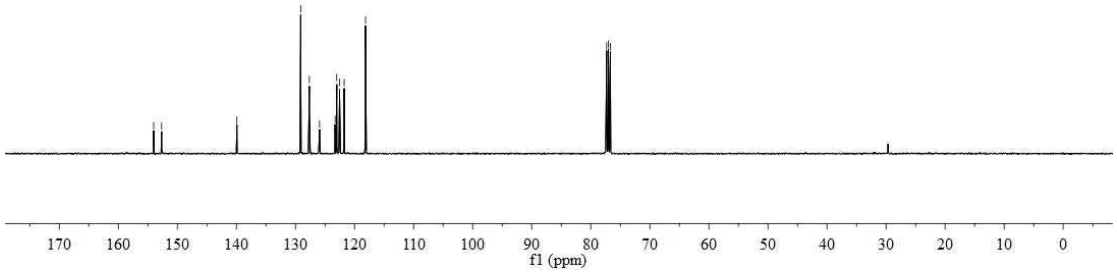

7.961
7.958
7.702
7.699
7.680
7.678
7.604
7.583
7.492
7.488
7.470
7.466
7.370
7.365
7.351
7.349
7.330
7.248
7.066
7.048
7.029
6.967
0.000
NH
N
S
Br

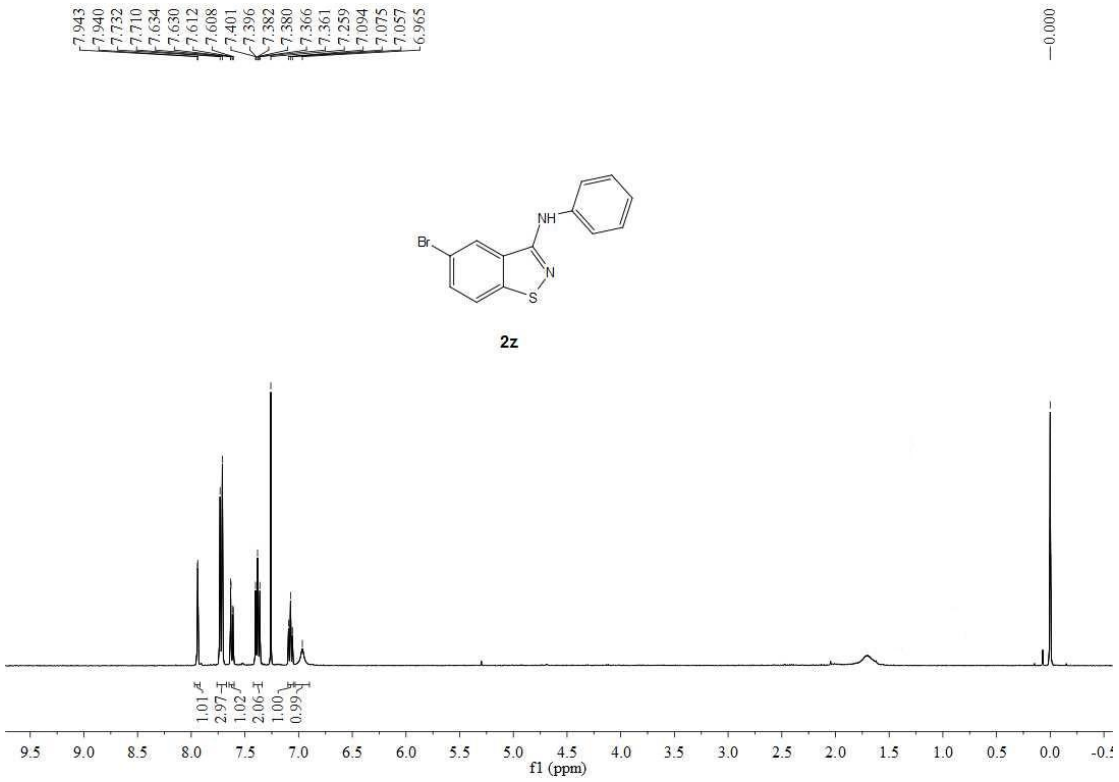
2y

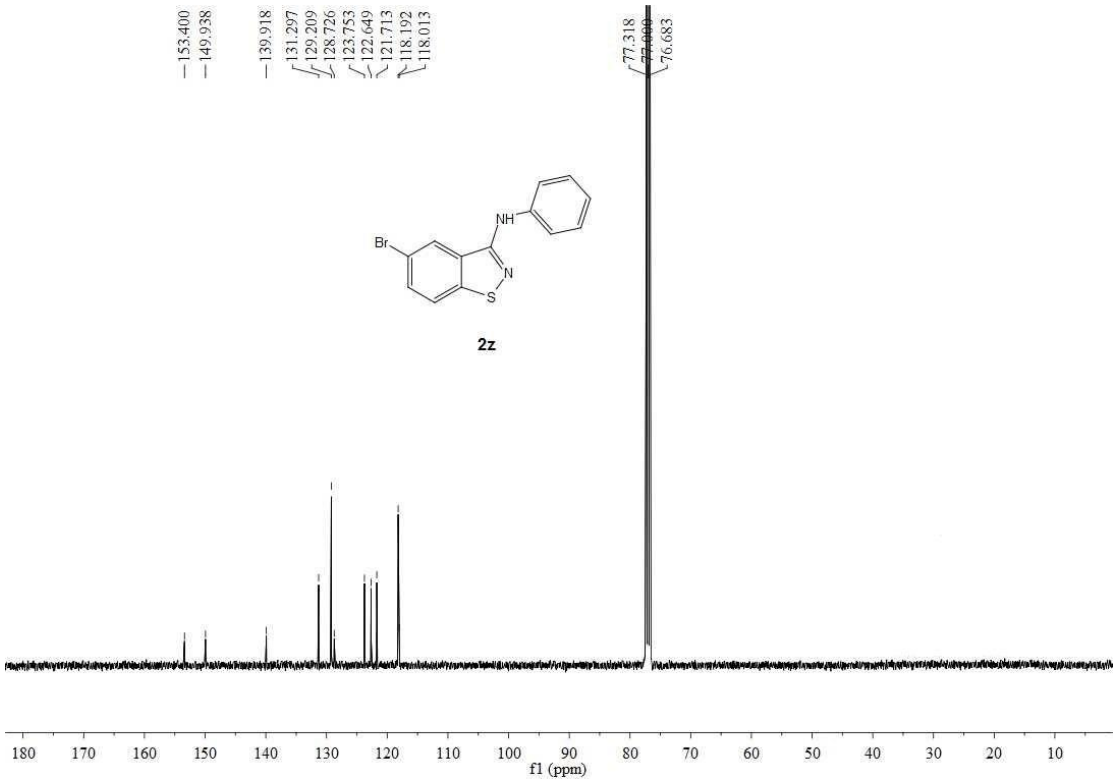

1.00
2.07
1.03
1.06
2.07
1.05
0.99
f1 (ppm)

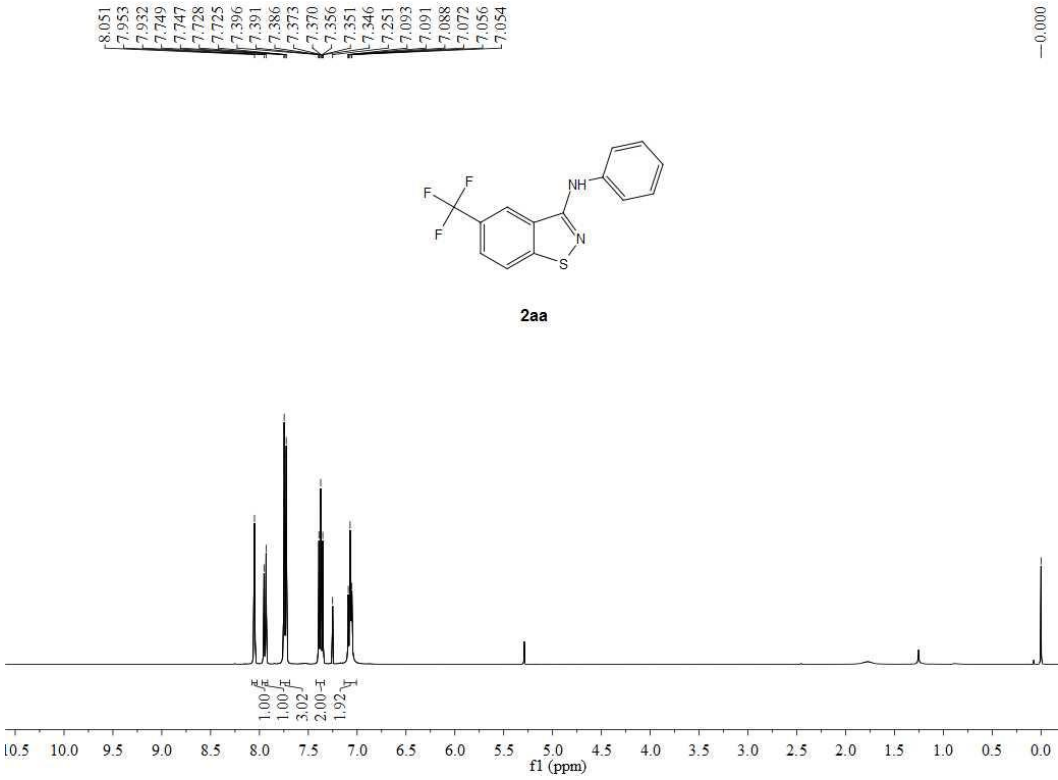

154.011
152.670
139.924
129.121
127.655
125.927
123.285
123.017
122.536
121.755
118.134
77.317
77.000
76.682
NH
N
S
Br

2y

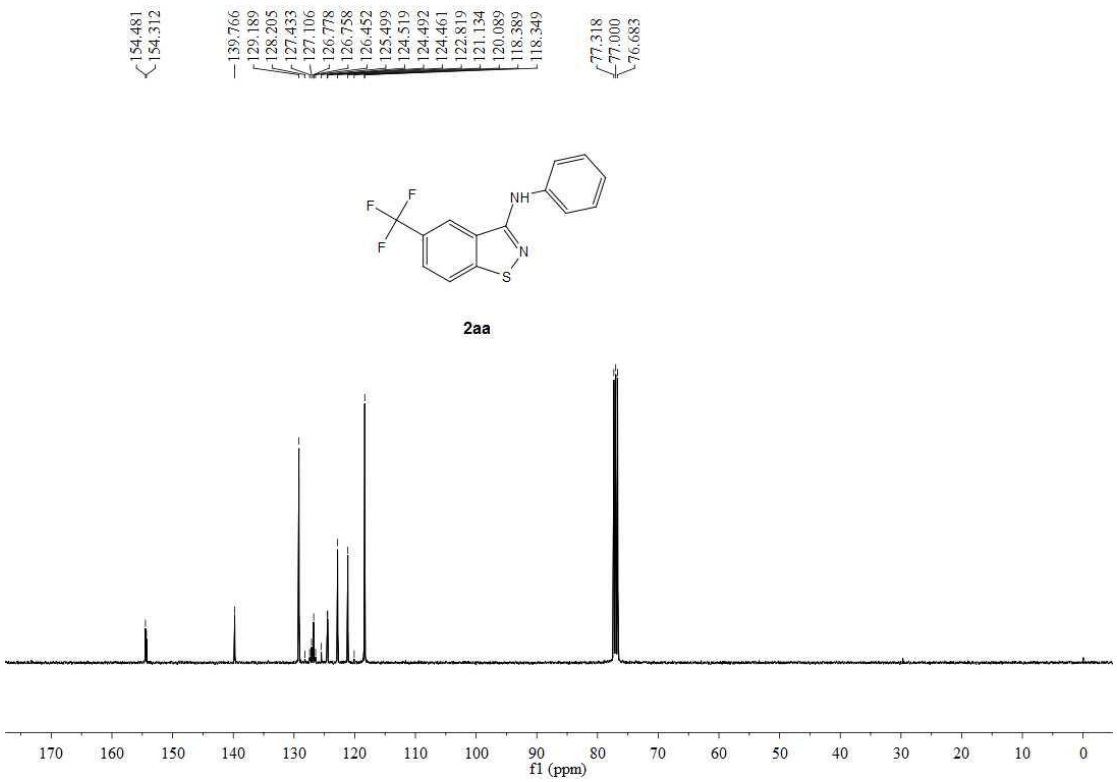

f1 (ppm)


7.943
7.940
7.732
7.710
7.634
7.630
7.612
7.608
7.401
7.396
7.382
7.380
7.366
7.361
7.259
7.094
7.075
7.057
6.965
0.000
NH
Br
N
S
2z
1.01
2.97
1.02
2.06
1.00
0.99
f1 (ppm)

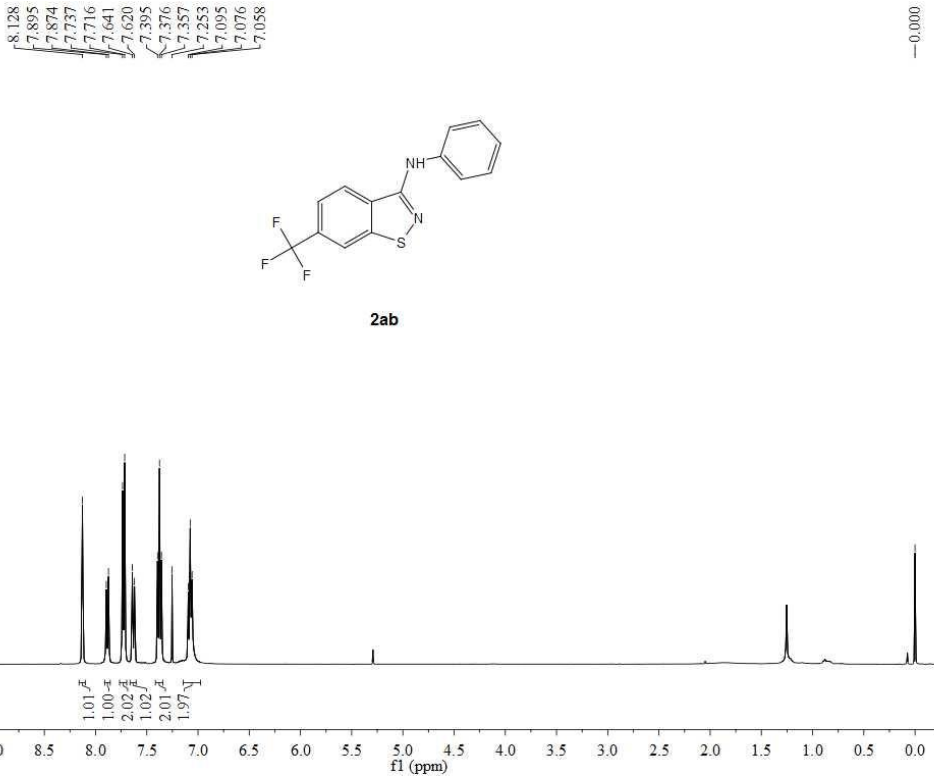

153.400
149.938
139.918
131.297
129.209
128.726
123.753
122.649
121.713
118.192
118.013
77.318
77.000
76.683
NH
Br
N
S
2z
f1 (ppm)

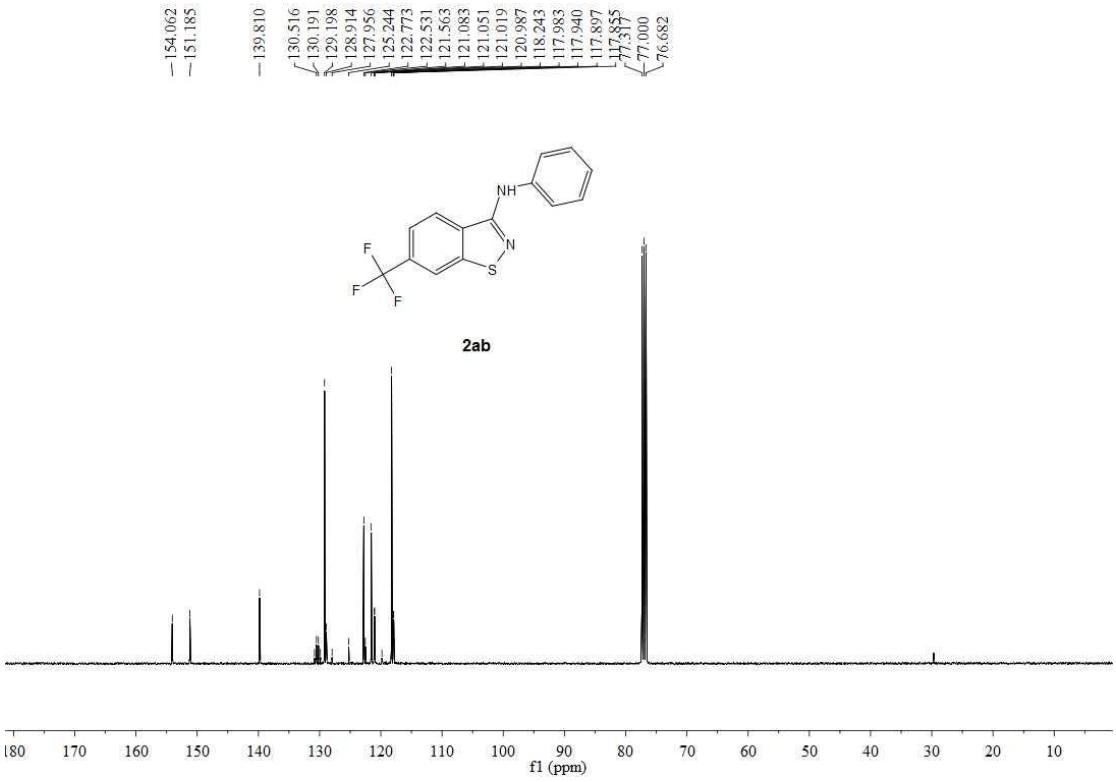

8.051
7.953
7.932
7.749
7.747
7.728
7.725
7.396
7.391
7.386
7.373
7.370
7.356
7.351
7.346
7.251
7.093
7.091
7.088
7.072
7.056
7.054
0.000
F
F
F
NH
N
S
1.00
1.00
3.02
2.00
1.92
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

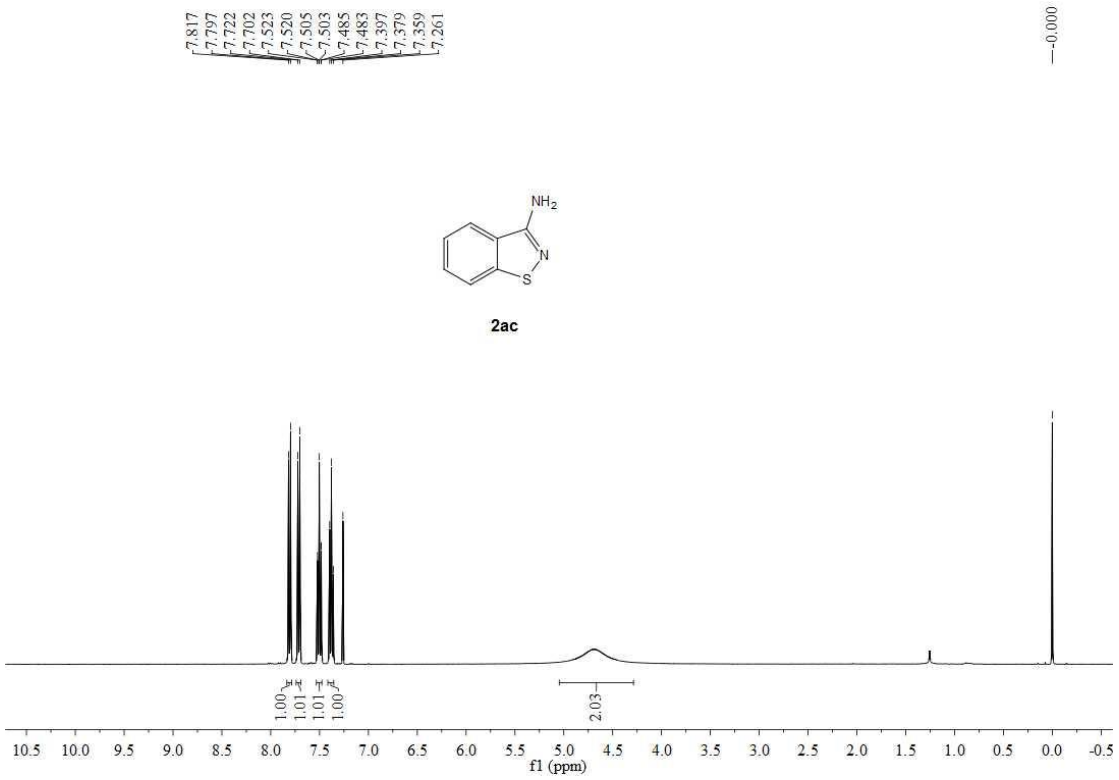
2aa

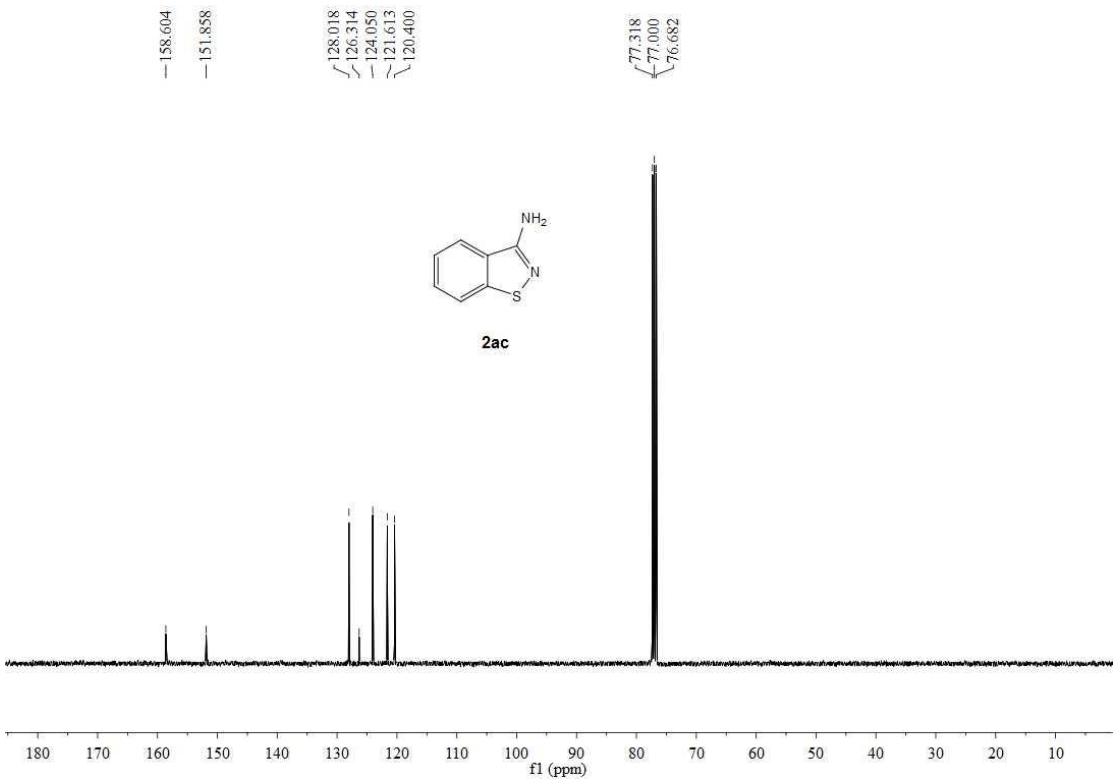

154.481
154.312
139.766
129.189
128.205
127.433
127.106
126.778
126.758
126.452
125.499
124.519
124.492
124.461
122.819
121.134
120.089
118.389
118.349
77.318
77.000
76.683
F
F
F
NH
N
S
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

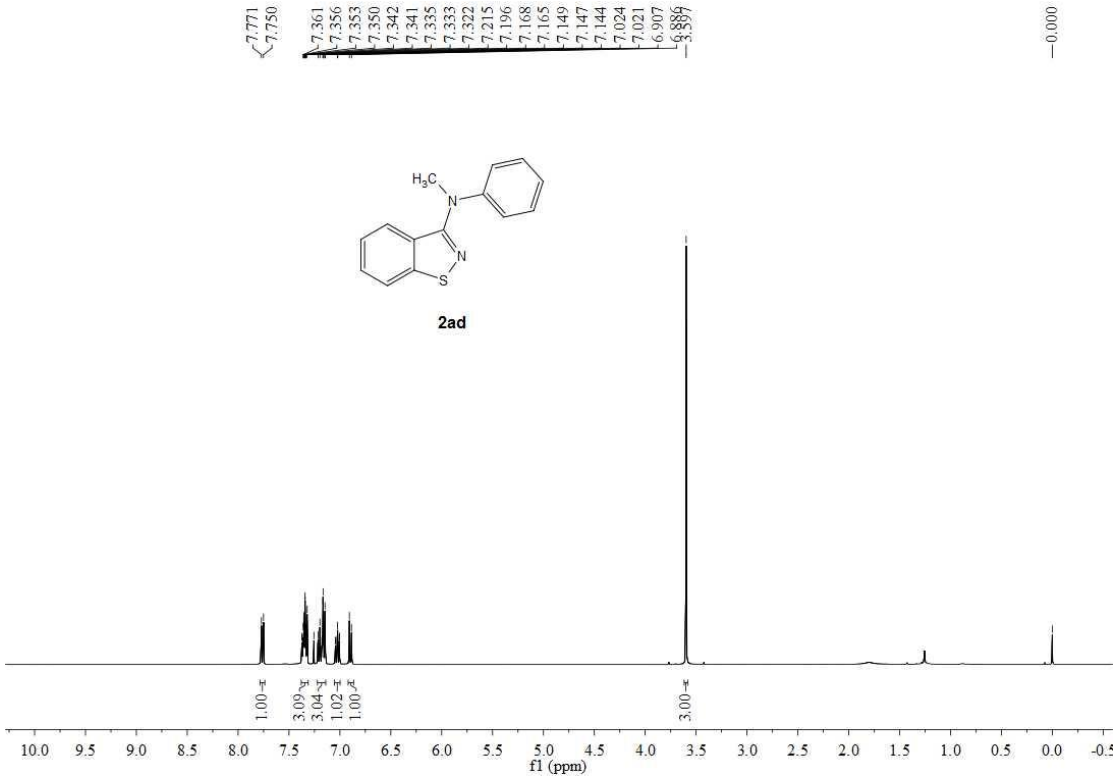
2aa

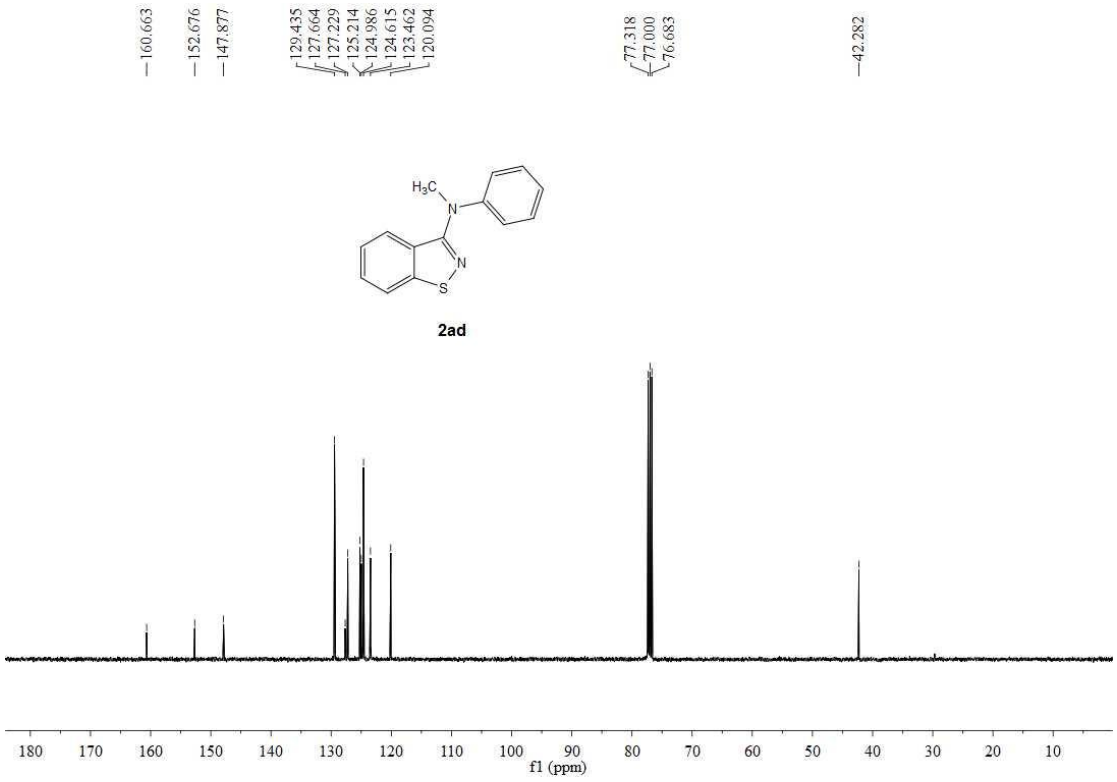

8.128
7.895
7.874
7.737
7.716
7.641
7.620
7.395
7.376
7.357
7.253
7.095
7.076
7.058
0.000
NH
N
S
F
F
F
2ab
1.01
1.00
2.02
1.02
2.01
1.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

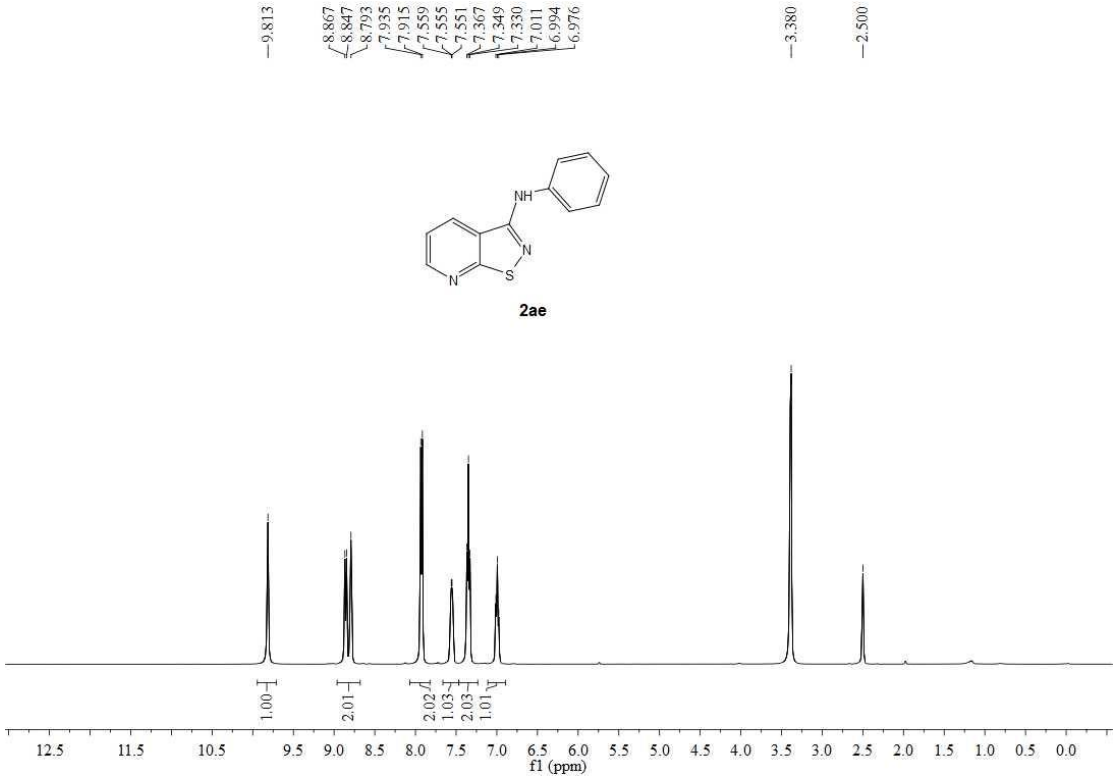

154.062
151.185
139.810
130.516
130.191
129.198
128.914
127.956
125.244
122.773
122.531
121.563
121.083
121.051
121.019
120.987
118.243
117.983
117.940
117.897
117.855
77.317
77.000
76.682
NH
N
S
F
F
F
2ab
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

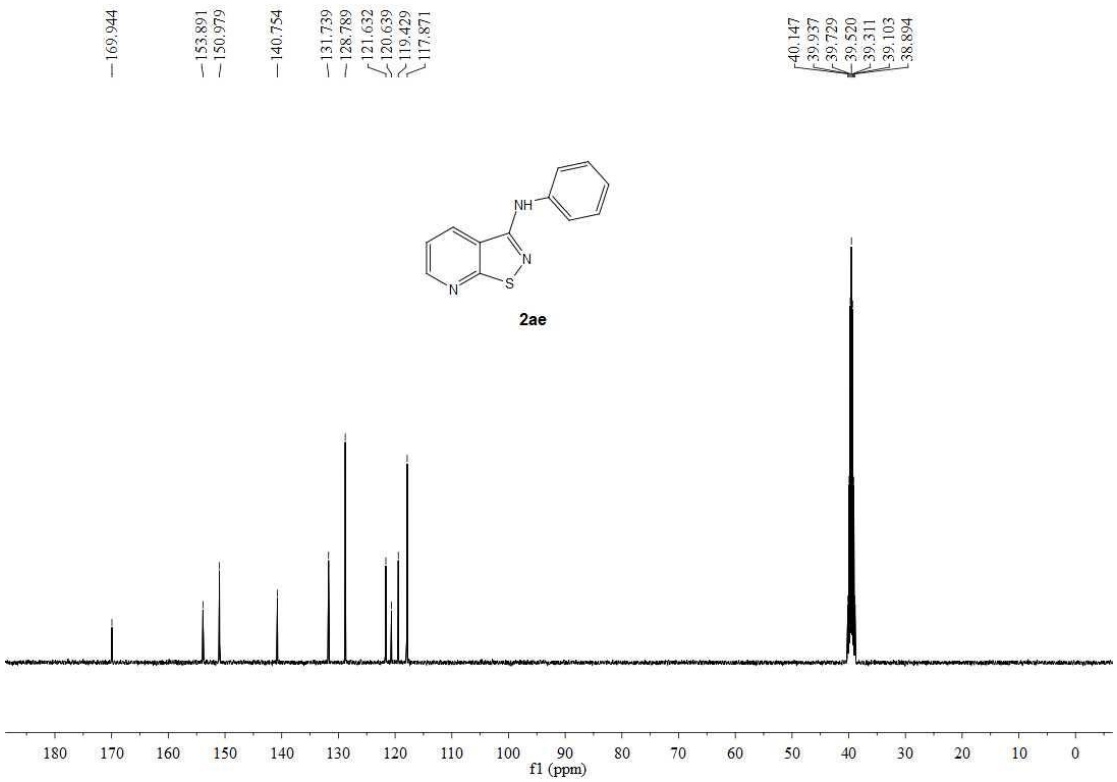

7.817
7.797
7.722
7.702
7.523
7.520
7.505
7.503
7.485
7.483
7.397
7.379
7.359
7.261
0.000
NH2
N
S
2ac
1.00
1.01
1.01
1.00
2.03
f1 (ppm)

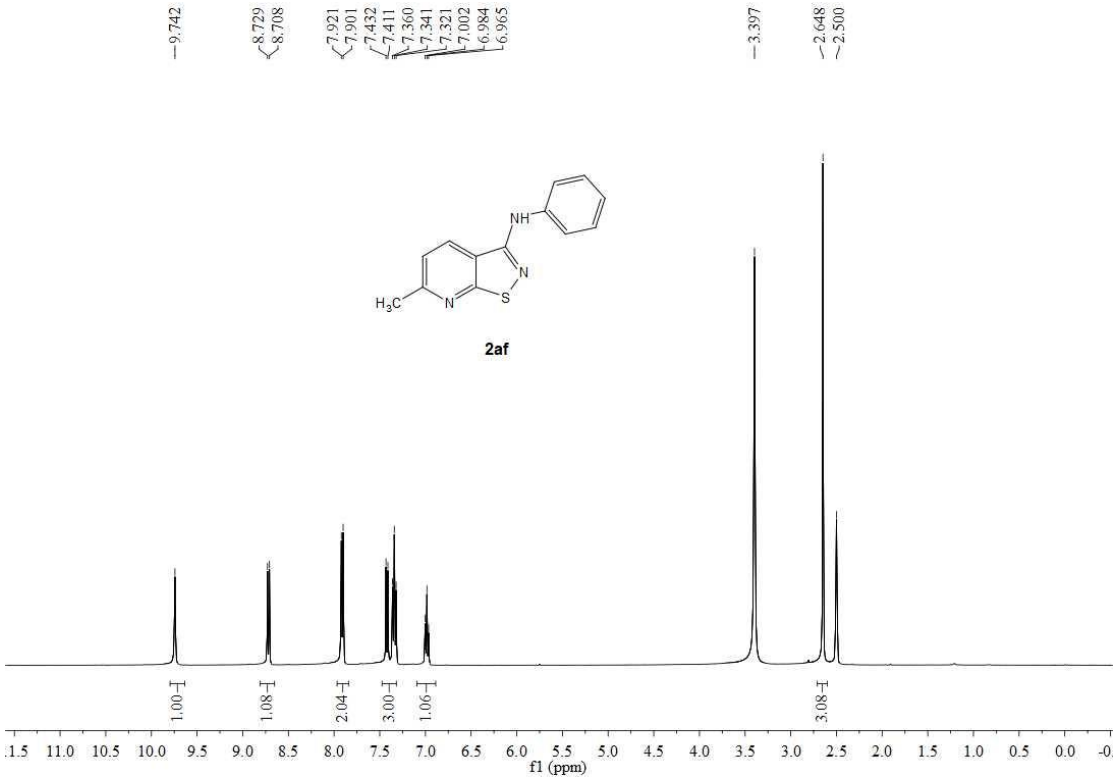

158.604
151.858
128.018
126.314
124.050
121.613
120.400
77.318
77.000
76.682
NH2
N
S
2ac
f1 (ppm)

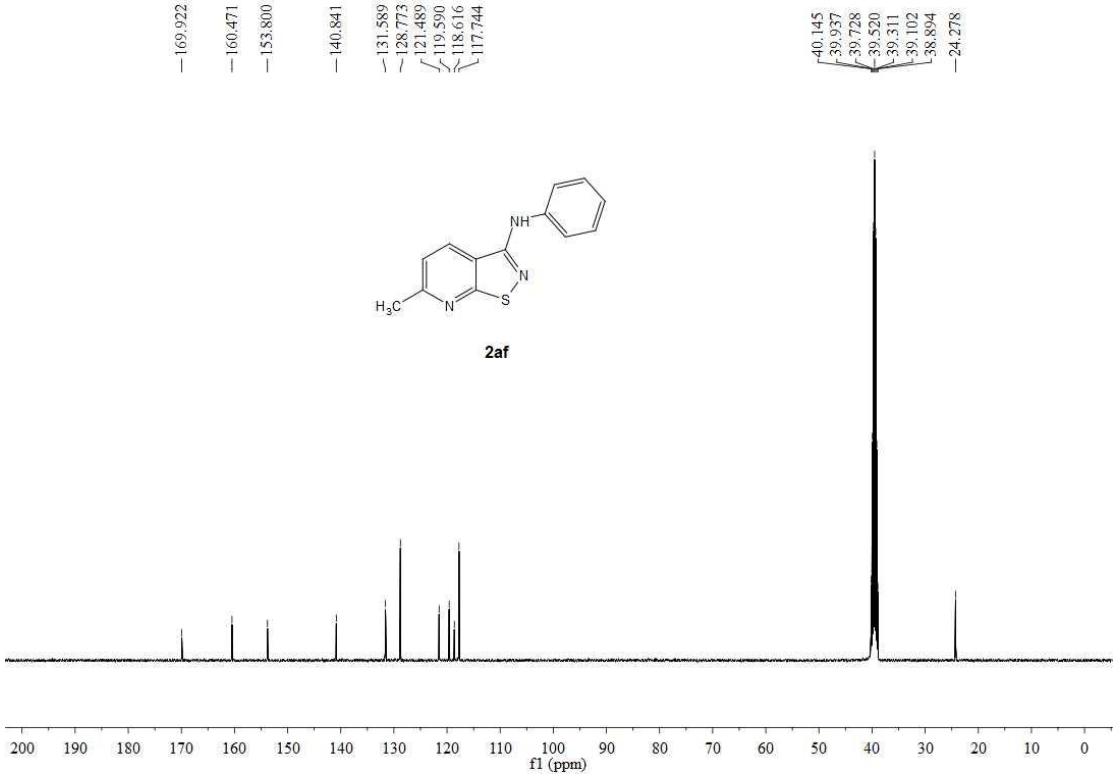

7.771
7.750
7.361
7.356
7.353
7.350
7.342
7.341
7.335
7.333
7.322
7.215
7.196
7.168
7.165
7.149
7.147
7.144
7.024
7.021
6.907
6.886
3.597
0.000
H3C
N
N
S
2ad
1.00
3.09
3.04
1.02
1.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

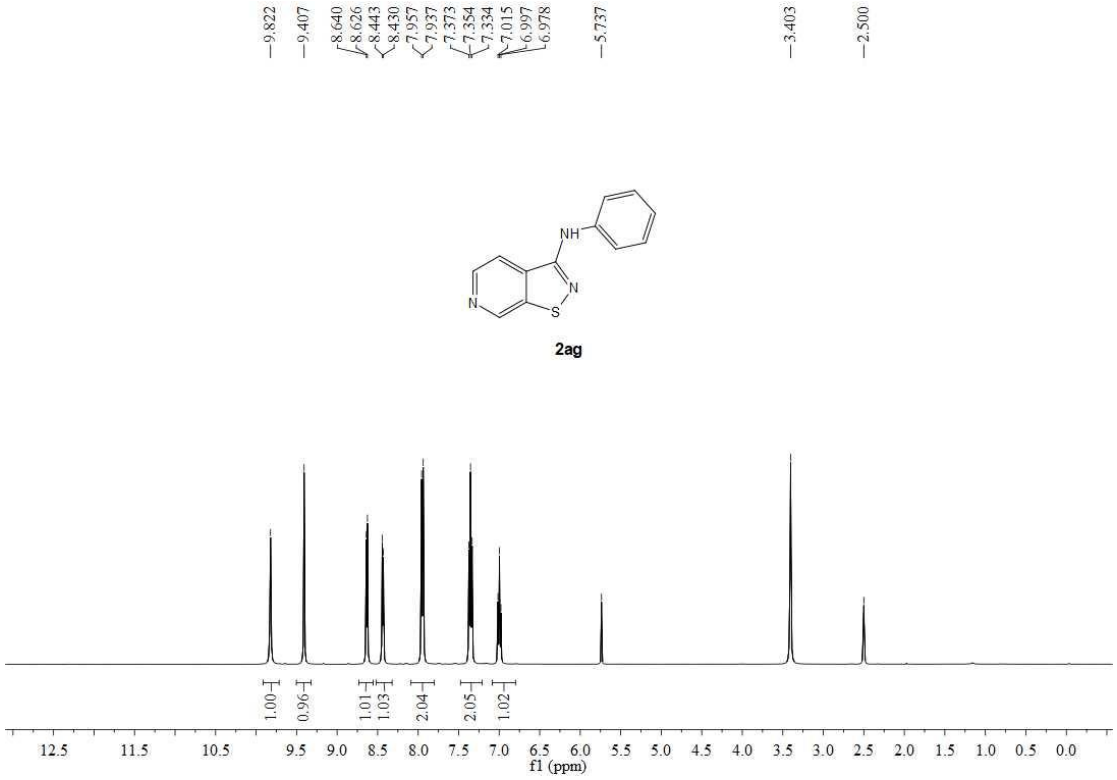

160.663
152.676
147.877
129.435
127.664
127.229
125.214
124.986
124.615
123.462
120.094
77.318
77.000
76.683
42.282
H3C
N
N
S
2ad
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

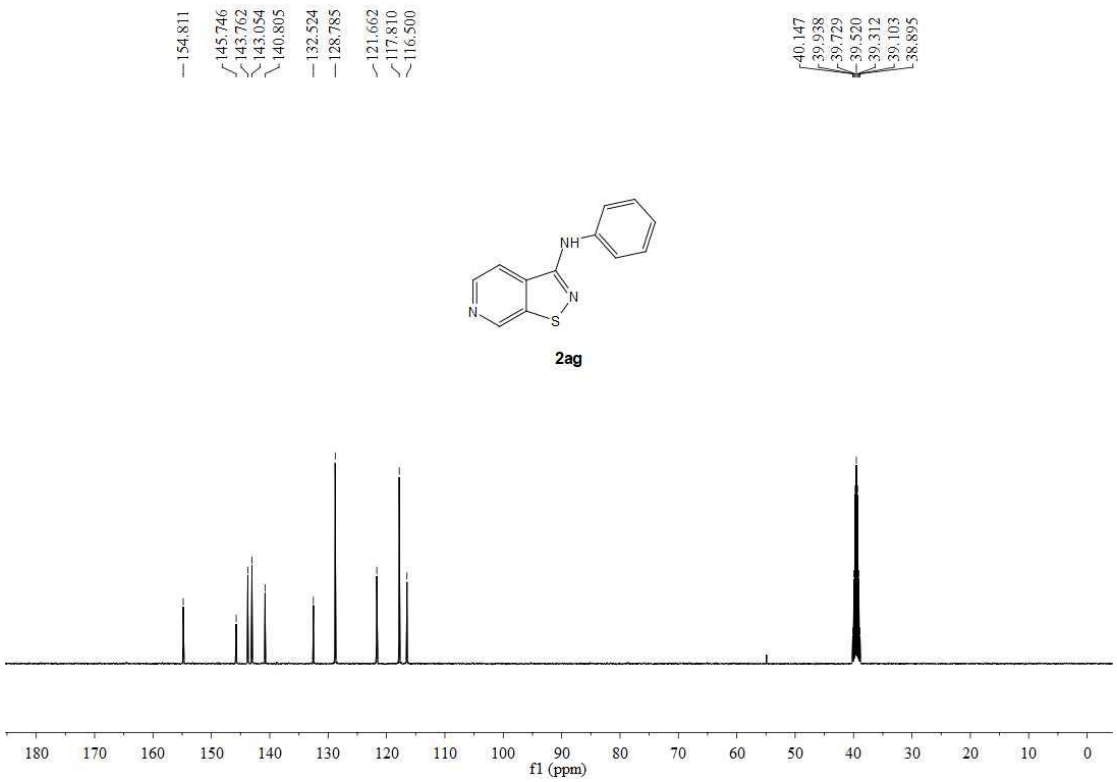

9.813
8.867
8.847
8.793
7.935
7.915
7.559
7.555
7.551
7.367
7.349
7.330
7.011
6.994
6.976
3.380
2.500
NH
N
S
N
2ae
1.00
2.01
2.02
1.03
2.03
1.01
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

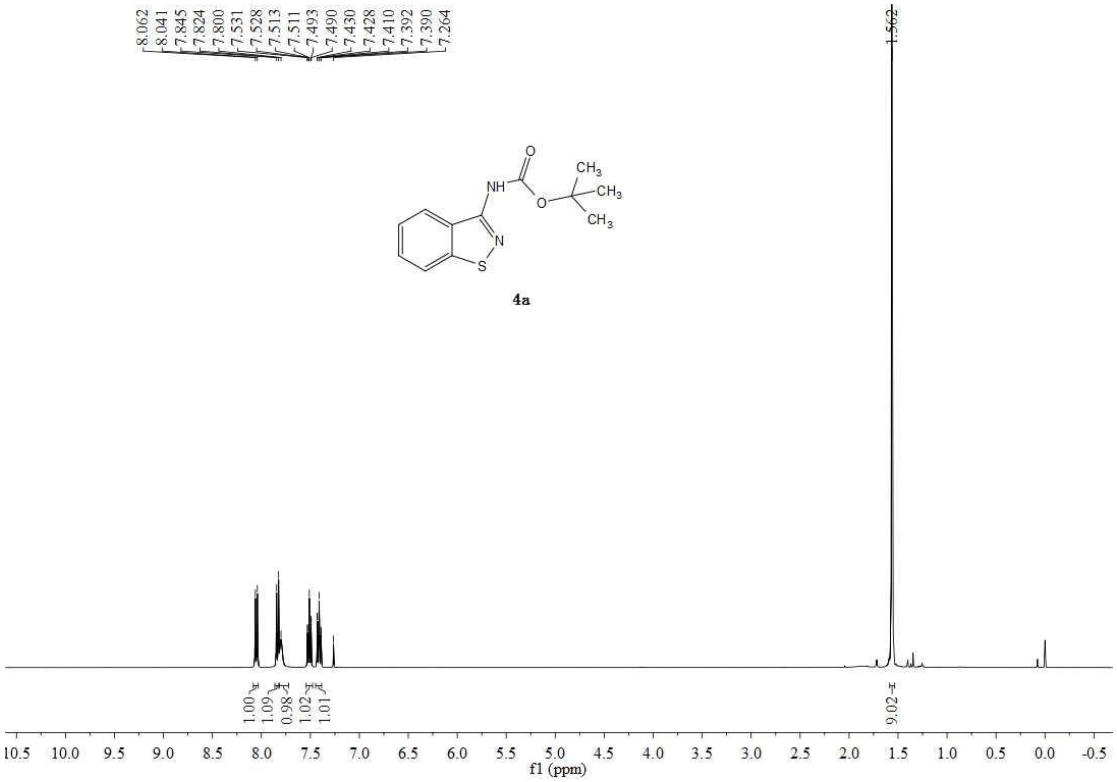

169.944
153.891
150.979
140.754
131.739
128.789
121.632
120.639
119.429
117.871
40.147
39.937
39.729
39.520
39.311
39.103
38.894
NH
N
S
N
2ae
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

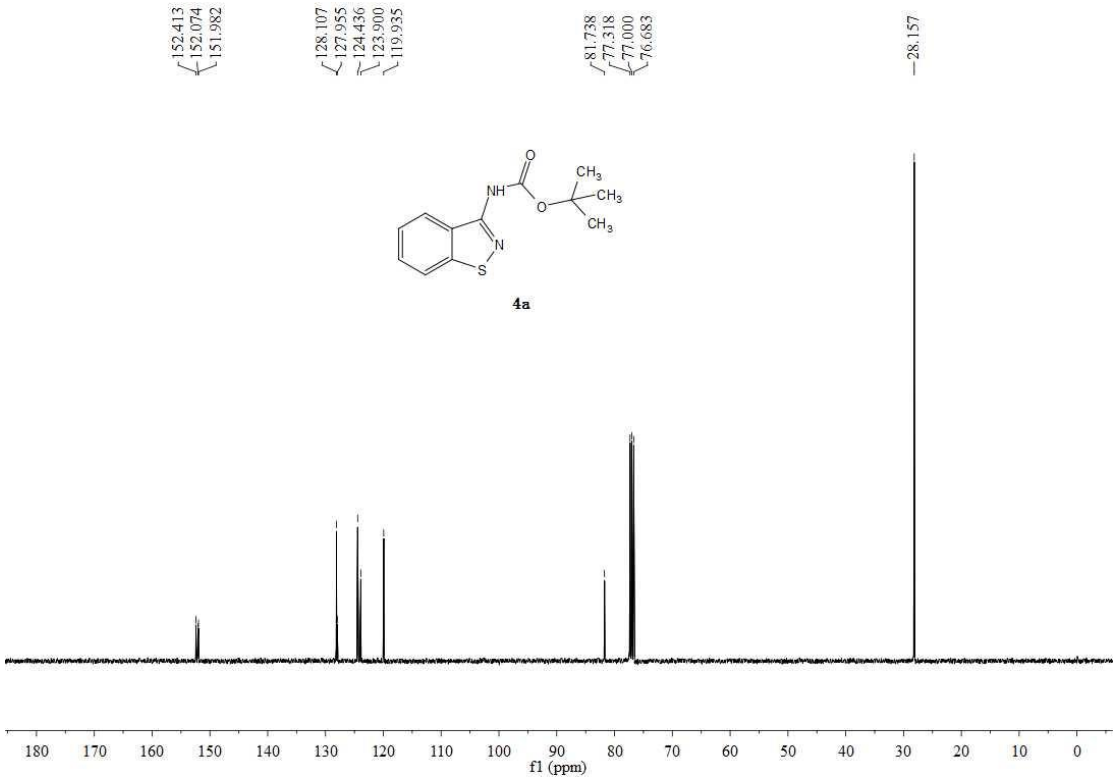

9.742
8.729
8.708
7.921
7.901
7.432
7.411
7.360
7.341
7.321
7.002
6.984
6.965
3.397
2.648
2.500
NH
N
S
N
H3C
2af
1.00
1.08
2.04
3.00
1.06
3.08
f1 (ppm)

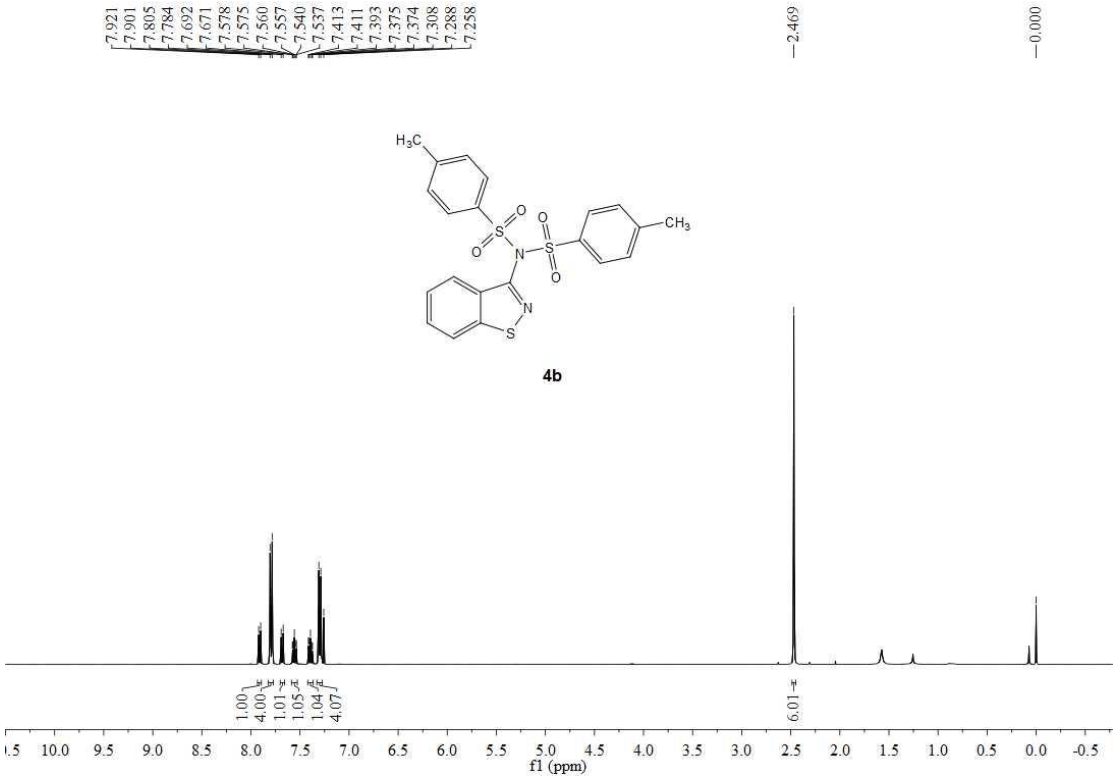

169.922
160.471
153.800
140.841
131.589
128.773
121.489
119.590
118.616
117.744
40.145
39.937
39.728
39.520
39.311
39.102
38.894
24.278
NH
N
S
N
H3C
2af
f1 (ppm)

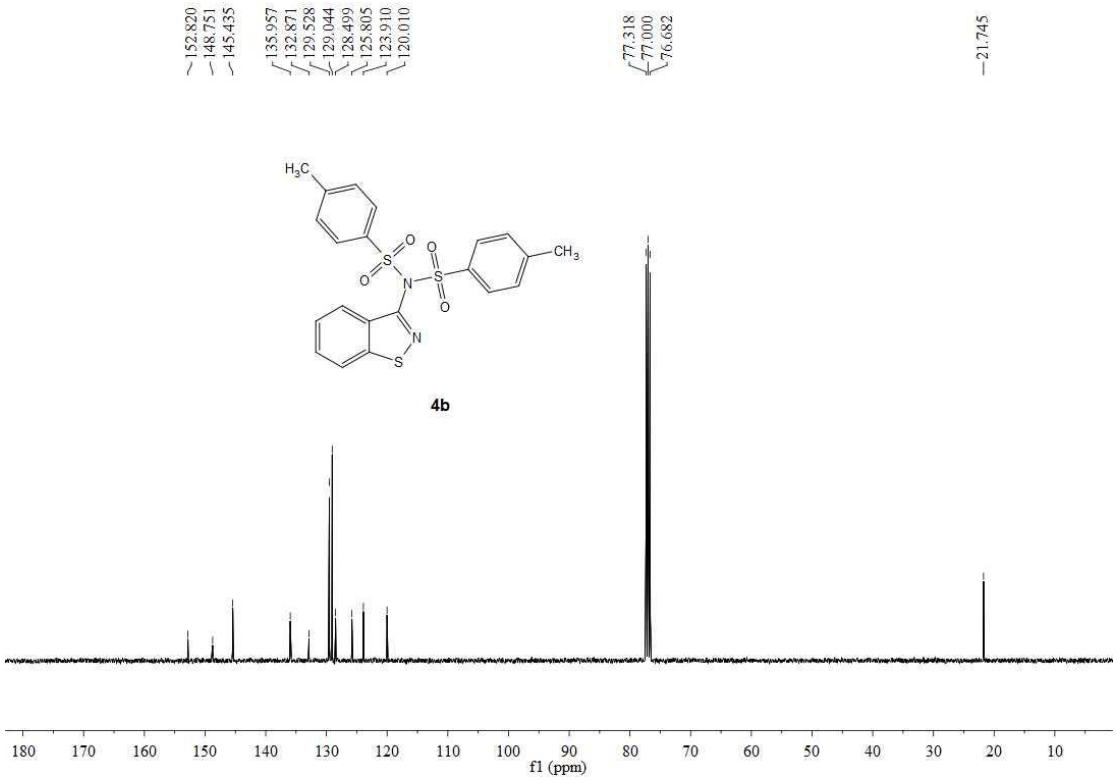

9.822
9.407
8.640
8.626
8.443
8.430
7.957
7.937
7.373
7.354
7.334
7.015
6.997
6.978
5.737
3.403
2.500
NH
N
N
S
2ag
1.00
0.96
1.01
1.03
2.04
2.05
1.02
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

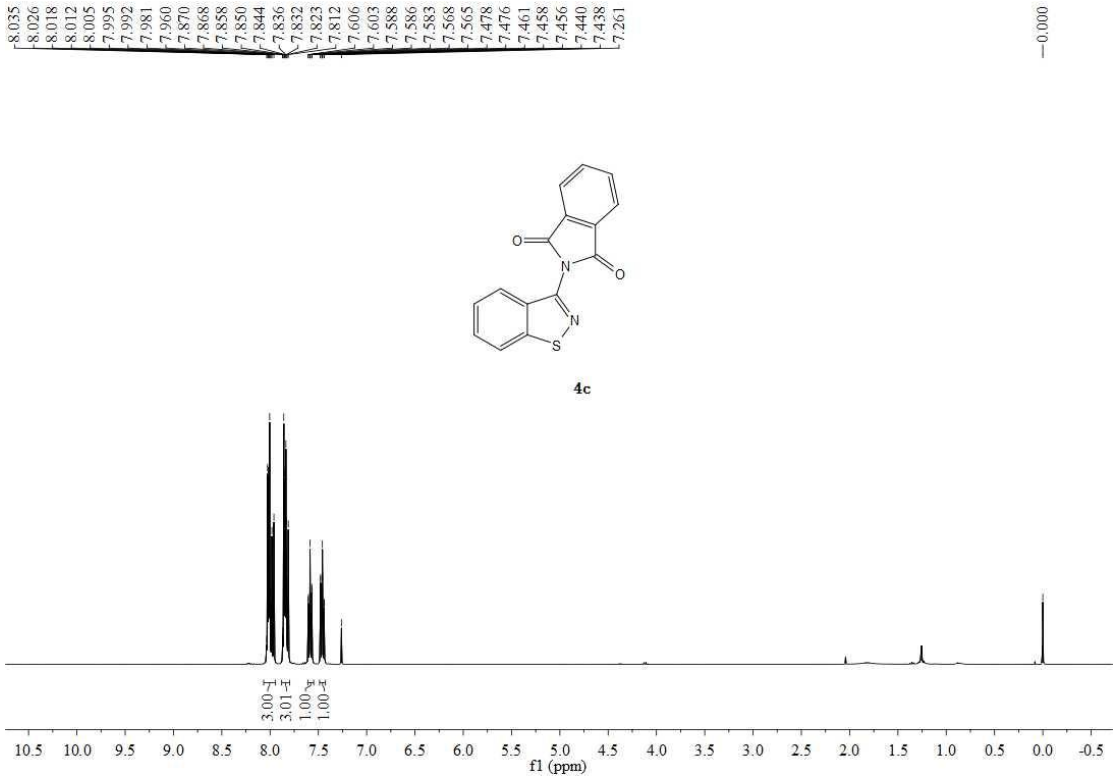

154.811
145.746
143.762
143.054
140.805
132.524
128.785
121.662
117.810
116.500
40.147
39.938
39.729
39.520
39.312
39.103
38.895
NH
N
N
S
2ag
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

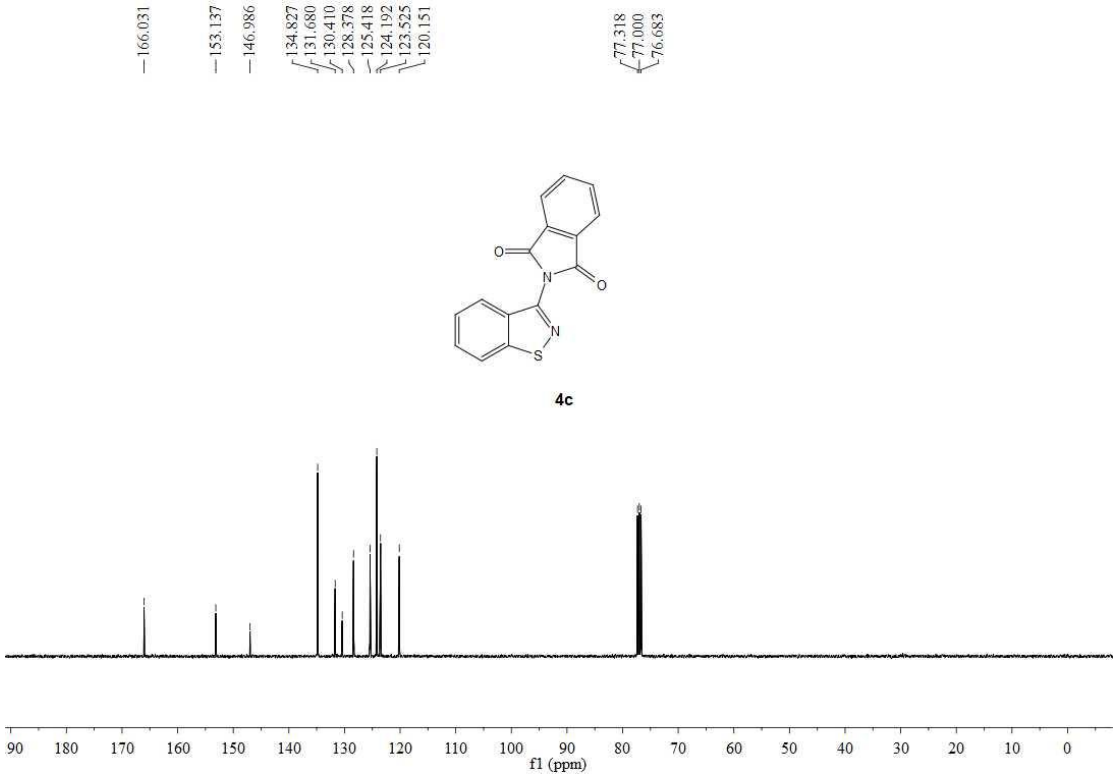

8.062
8.041
7.845
7.824
7.800
7.531
7.528
7.513
7.511
7.493
7.490
7.430
7.428
7.410
7.392
7.390
7.264
1.562
NH
O
O
CH3
CH3
CH3
N
S
4a
1.00
1.09
0.98
1.02
1.01
9.02
f1 (ppm)

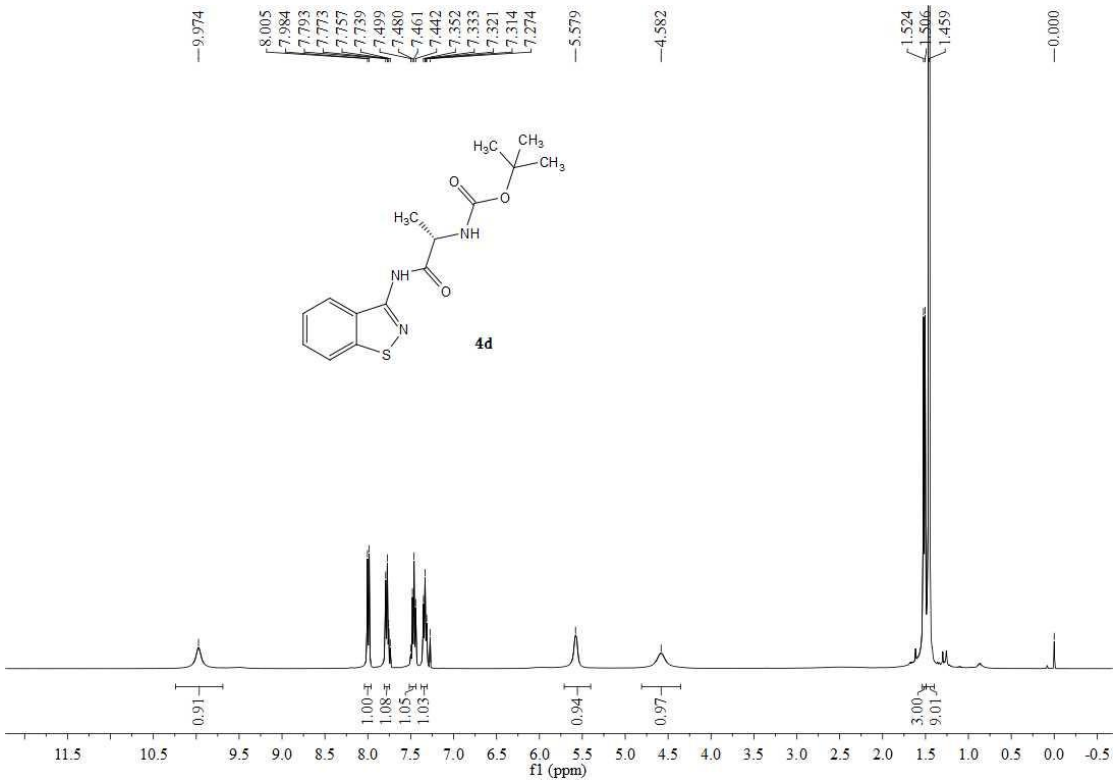

152.413
152.074
151.982
128.107
127.955
124.436
123.900
119.935
81.738
77.318
77.000
76.683
28.157
NH
O
O
CH3
CH3
CH3
N
S
4a
f1 (ppm)

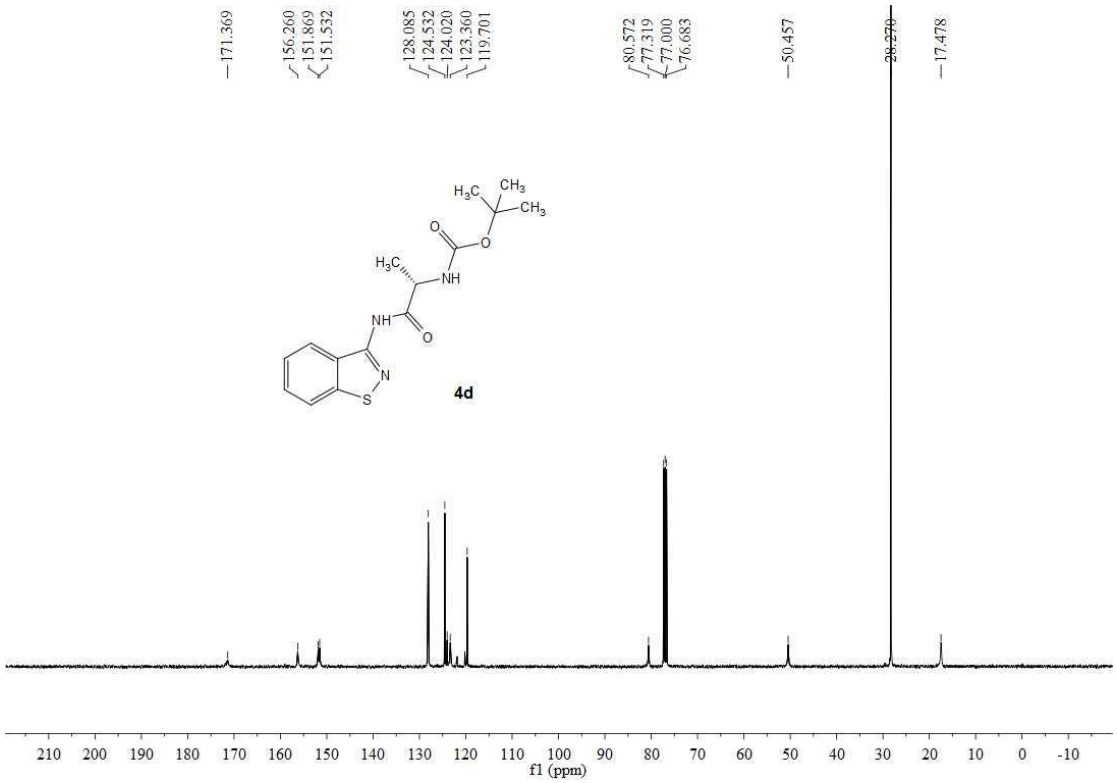

7.921
7.901
7.805
7.784
7.692
7.671
7.578
7.575
7.560
7.557
7.540
7.537
7.413
7.411
7.393
7.375
7.374
7.308
7.288
7.258
2.469
0.000
4b
1.00
4.00
1.01
1.05
1.04
4.07
6.01
f1 (ppm)


152.820
148.751
145.435
135.957
132.871
129.528
129.044
128.499
125.805
123.910
120.010
77.318
77.000
76.682
21.745
4b
f1 (ppm)


8.035
8.026
8.018
8.012
8.005
7.995
7.992
7.981
7.960
7.870
7.868
7.858
7.850
7.844
7.836
7.832
7.823
7.812
7.606
7.603
7.588
7.586
7.583
7.568
7.565
7.478
7.476
7.461
7.458
7.456
7.440
7.438
7.261
0.000
O
N
O
N
S
4c
3.00
3.01
1.00
1.00
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 -0.5
f1 (ppm)


166.031
153.137
146.986
134.827
131.680
130.410
128.378
125.418
124.192
123.525
120.151
77.318
77.000
76.683
O
N
O
N
S
4c
90 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.974
8.005
7.984
7.793
7.773
7.757
7.739
7.499
7.480
7.461
7.442
7.352
7.333
7.321
7.314
7.274
5.579
4.582
1.524
1.506
1.459
0.000
4d
0.91
1.00
1.08
1.05
1.03
0.94
0.97
3.00
9.01
f1 (ppm)


171.369
156.260
151.869
151.532
128.085
124.532
124.020
123.360
119.701
80.572
77.319
77.000
76.683
50.457
28.270
17.478
4d
f1 (ppm)