Electronic Supplementary Information

Ag-Cu Copromoted Direct C2–H Bond Thiolation of Azoles with Bunte Salts as Sulfur Sources

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General procedure for synthesis of Bunte salts

1. General procedure for synthesis of alkyl Bunte salts: According to the reported literatures,[1] a flask was filled with alkyl halide (10 mmol), sodium thiosulfate (12 mmol, 1.2 equiv.), water (5 mL), and MeOH (15 mL). The mixture was stirred and heated to 65 °C for 1 hour, cooled to room temperature, and then concentrated on the rotary evaporator to remove MeOH and water. The resulting solid was dissolved in MeOH at 50 °C and then filtered to get solids. The solids were washed with n-hexane, filtered, and dried under vacuum.

2. General procedure for synthesis of aryl Bunte salts: According to the reported literatures,[1] a flask was filled with aryl halide (10 mol), anhydrous sodium thiosulfate (15 mmol, 1.5 equiv.) and CuI (1 mmol, 10 mol%) under nitrogen. DMSO (10 mL) was added via syringe, and then adding DMEDA (2 mmol, 20 mol%). The mixture was heated at 80 °C for 10 h. Then the mixture was cooled to room temperature, and saturated aqueous NaCl (10 mL) was added. The mixture was stirred at room temperature for 10 min. Saturated NaCl (9 mL) and n-hexane (10 mL) were added to the mixture. The mixture was filtered and the obtained solids were dried under vacuum.

Experimental procedures of the scale-up reaction.

In a glove box, a 50 mL Schlenk tube equipped with a stir bar was charged with sodium *S*-benzyl thiosulfate **2a** (3 mmol, 1.5 equiv.), $Cu(OAc)_2$ (4 mmol, 2.0 equiv.), $AgNO_3$ (0.4 mmol, 20 mol %). The tube was fitted with a rubber septum, and removed out from the glove box. Then azole (2 mmol) was added through the rubber septum using syringe under the atmosphere of N_2. DMF (20 mL) was added to the Schlenk tube through the rubber septum using a syringe. The septum was replaced by a Teflon screwcap under N_2 flow. The mixture was stirred at 120 ^oC (preheated to 120 ^oC) for 22 h. After cooling, the mixture was diluted with ethyl acetate (20 mL), filtered through a pad of silica gel, followed by washing the pad of the silica gel with the ethyl acetate (30 mL). The organic phase was concentrated under reduced pressure. The residue was then purified by chromatography on silica gel to provide the corresponding product **3a** (64%).

Experimental procedures of mechanistic studies

1. Thiolation of benzothiazole with 3,5-dimethyl-benzenethiol

In a glove box, a 25 mL Schlenk tube equipped with a stir bar was charged with $Cu(OAc)_2$ (0.4 mmol, 2.0 equiv.), $AgNO_3$ (0.04 mmol, 20 mol %). The tube was fitted with a rubber septum, and removed out from the glove box. Then benzothiazole **1a** (0.2 mmol) and 3,5-dimethyl-benzenethiol **2m'** (0.3 mmol, 1.5 equiv.) were added through the rubber septum using syringe under the atmosphere of N_2. DMF (2 mL) was added to the Schlenk tube through the rubber septum using a syringe. The septum was replaced by a Teflon screwcap under N_2 flow. The mixture was stirred at 120 ^oC (preheated to 120 ^oC) for 22 h. After cooling, the mixture was diluted with ethyl acetate (10 mL), filtered through a pad of silica gel, followed by washing the pad of the silica gel with the ethyl acetate (20 mL). The organic phase was concentrated under reduced pressure. The residue was then purified by chromatography on silica gel to provide the corresponding product **3m** (49%).

2. Thiolation of benzothiazole with Cu thiolate

Procedure for synthesis of Cu thiolate: According to the reported literatures,[2] a 25 mL Schlenk tube was charged with 3,5-dimethyl-benzenethiol (20 mmol) and ethanol (10 mL), and then then aqueous copper nitrate (5 mL, 1.0 mol/L) was slowly dropped to the mixture to give a yellow-green suspension. After vigorous stirring for 30 min, filter to get precipitate, and wash the solid with distilled water and ethanol. And then dried in an evacuated vacuum. Finally, the yellow-green powdery precursor was obtained.

(1). In a glove box, a 25 mL Schlenk tube equipped with a stir bar was charged with $Cu(OAc)_2$ (1.0 equiv.), $(3,5\text{-}2MePhS)_2Cu$ (0.3 mmol, 1.5 equiv.), $AgNO_3$ (0.04 mmol, 20 mol %). The tube was fitted with a rubber septum, and removed out from the glove box. Then benzothiazole **1a** (0.2 mmol) and were added through the rubber septum using syringe under the atmosphere of N_2. DMF (2 mL) was added to the Schlenk tube through the rubber septum using a syringe. The septum was replaced by a Teflon screwcap under N_2 flow. The mixture was stirred at 120 ^oC (preheated to 120 ^oC) for 22 h. After cooling, the mixture was diluted with ethyl acetate (10 mL), filtered through a pad of silica gel, followed by washing the pad of the silica gel with the ethyl acetate (20 mL). The organic phase was concentrated under reduced pressure. The residue was then purified by chromatography on silica gel to provide the corresponding product (41%).

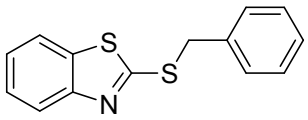
(2). In a glove box, a 25 mL Schlenk tube equipped with a stir bar was charged with $(3,5\text{-}2MePhS)_2Cu$ (0.3 mmol, 1.5 equiv.), $AgNO_3$ (0.04 mmol, 20 mol %). The tube was fitted with a rubber septum, and removed out from the glove box. Then benzothiazole **1a** (0.2 mmol) and were added through the rubber septum using syringe under the atmosphere of N_2. DMF (2 mL) was added to the Schlenk tube through the rubber septum using a syringe. The septum was replaced by a teflon screwcap under N_2 flow. The mixture was stirred at 120 ^oC (preheated to 120 ^oC) for 22 h. After cooling, the mixture was diluted with ethyl acetate (10 mL), filtered through a pad of silica gel, followed by washing the pad of the silica gel with the ethyl acetate (20 mL). Through TLC and GC-MS analysis, only trace amount of corresponding product was observed.

3.The control experiment between benzyl Bunte salt and tolyl Bunte salt.

In a glove box, a 25 mL Schlenk tube equipped with a stir bar was charged with $Cu(OAc)_2$ (0.4 mmol, 2.0 equiv.), $AgNO_3$ (0.04 mmol, 20 mol %). The tube was fitted with a rubber septum, and removed out from the glove box. Then benzothiazole **1a** (0.2 mmol) and benzyl Bunte salt **2b** (0.15 mmol)and tolyl Bunte salt **2k** (0.15 mmol) were added through the rubber septum using syringe under the atmosphere of N_2. DMF (2 mL) was added to the Schlenk tube through the rubber septum using a syringe. The septum was replaced by a Teflon screwcap under N_2 flow. The mixture was stirred at 120 ^oC (preheated to 120 ^oC) for 22 h. After cooling, the mixture was diluted with ethyl acetate (10 mL), filtered through a pad of silica gel, followed by washing the pad of the silica gel with the ethyl acetate (20 mL). The organic phase was concentrated under reduced pressure. The residue was then purified by chromatography on silica gel to provide the corresponding product **3b** (34%) and **3k** (17%).

Characterization of products

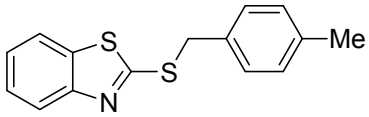
2-(benzylthio)benzo[*d*]thiazole (3a).[3]



3a

39.2 mg (77%), colorless oil (R_f = 0.4, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.1 Hz, 1H), 7.76 (d, *J* = 8.0 Hz, 1H), 7.47 – 7.41 (m, 3H), 7.36 – 7.29 (m, 4H), 4.61 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.4, 153.2, 136.2, 135.3, 129.2, 128.7, 127.8, 126.1, 124.3, 121.6, 121.0, 37.7.

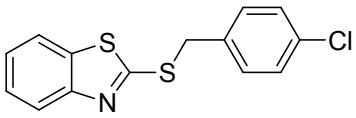
2-((4-methylbenzyl)thio)benzo[*d*]thiazole (3b).[4]



3b

22.1 mg (41%), white solid (R_f = 0.5, V_{Et2O}/V_{PE} = 2:98). m.p. 49 – 51 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 7.9 Hz, 1H), 7.45 – 7.41 (m, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.32 – 7.28 (m, 1H), 7.14 (d, *J* = 7.8 Hz, 2H), 4.58 (s, 2H), 2.34 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 153.2, 137.6, 135.3, 133.0, 129.4, 129.1 126.1, 124.3, 121.6, 121.0, 37.6, 21.2.

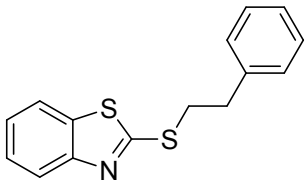
2-((4-chlorobenzyl)thio)benzo[*d*]thiazole (3c).[5]



3c

34.9 mg (60%), white solid (R_f = 0.5, V_{Et2O}/V_{PE} = 2:98). m.p. 80 – 82 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 8.0 Hz, 1H), 7.45 – 7.38 (m, 3H), 7.32 – 7.25 (m, 3H), 4.56 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8, 153.1, 135.4, 135.0, 133.6, 130.5, 128.9, 126.1, 124.4, 121.6, 121.1, 36.9.

2-(phenethylthio)benzo[*d*]thiazole (3d).[6]

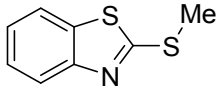


3d

42.5 mg (78%), colorless oil (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.1 Hz, 1H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.34 – 7.22 (m, 6H), 3.6 – 3.56 (m,

2H), 3.15 – 3.11 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.7, 153.3, 139.7, 135.2, 128.7, 128.6, 126.7, 126.0, 124.2, 121.5, 121.0, 35.6, 34.8.

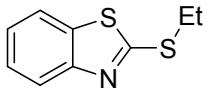
2-(methylthio)benzo[*d*]thiazole (3e).[1]



3e

10.9 mg (30%), yellow oil (R_f = 0.4, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.2 Hz, 1H), 7.76 (d, *J* = 7.9 Hz, 1H), 7.44 – 7.39 (m, 1H), 7.31 – 7.27 (m, 1H), 2.80 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.1, 153.4, 135.2, 126.1, 124.1, 121.4, 121.0, 16.0.

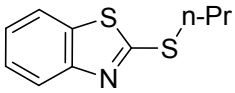
2-(ethylthio)benzo[*d*]thiazole (3f).[7]



3f

21.9 mg (56%), colorless oil (R_f = 0.4, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.1 Hz, 1H), 7.76 (d, *J* = 7.9 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.31 – 7.27(m, 1H), 3.36 (q, *J* = 7.4 Hz, 2H), 1.49 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.1, 153.4, 135.2, 126.0, 124.1, 121.5, 120.9, 28.0, 14.6.

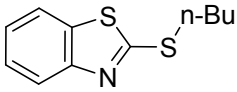
2-(propylthio)benzo[*d*]thiazole (3g).[6]



3g

25.1 mg (60%), colorless oil (R_f = 0.4, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 7.9 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.31 – 7.27 (m, 1H), 3.33 (t, *J* = 7.2 Hz, 2H), 1.91 – 1.82 (m, 2H), 1.09 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.4, 153.4, 135.2, 126.0, 124.1, 121.5, 120.9, 35.6, 22.7, 13.4.

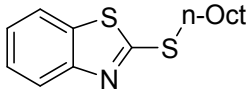
2-(butylthio)benzo[*d*]thiazole (3h).[3]



3h

33.4 mg (75%), yellow oil (R_f = 0.5, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 7.9 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.30 – 7.26 (m, 1H), 3.35 (t, *J* = 7.3 Hz, 2H), 1.85 – 1.75 (m, 2H), 1.56 – 1.46 (m, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.4, 153.4, 135.2, 126.0, 124.1, 121.5, 120.9, 33.3, 31.3, 21.9, 13.6.

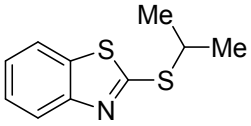
2-(octylthio)benzo[*d*]thiazole (3i).[6]



3i

40.1 mg (72%), colorless oil (R_f = 0.5, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.1 Hz, 1H), 7.75 (d, *J* = 7.5 Hz, 1H), 7.43 – 7.38 (m, 1H), 7.30 – 7.26 (m, 1H), 3.34 (t, *J* = 7.4 Hz, 2H), 1.86 – 1.78 (m, 2H), 1.51 – 1.44 (m, 2H), 1.36 – 1.28 (m, 8H), 0.90 – 0.87 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 167.4, 153.4, 135.2, 126.0, 124.1, 121.5, 120.9, 33.6, 31.8, 29.2, 29.1, 29.1, 28.8, 22.7, 14.1.

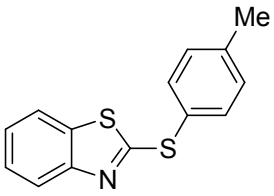
2-(isopropylthio)benzo[*d*]thiazole (3j).[8]



3j

21.3 mg (51%), colorless oil (R_f = 0.4, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.1 Hz, 1H), 7.76 (d, *J* = 7.9 Hz, 1H), 7.43 – 7.40 (m, 1H), 7.31 – 7.28 (m, 1H), 4.14 – 4.03 (m, 1H), 1.51 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.5, 153.5, 135.3, 126.0, 124.2, 121.6, 120.9, 39.5, 23.3.

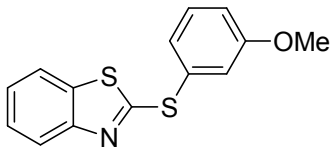
2-(p-tolylthio)benzo[*d*]thiazole (3k).[8]



3k

20.8 mg (41%), colorless oil (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.2 Hz, 1H), 7.64 – 7.62 (m, 3H), 7.42 – 7.38 (m, 1H), 7.30 (d, *J* = 7.9 Hz, 2H), 7.27 – 7.23 (m, 1H), 2.44 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.40, 153.99, 139.73, 135.56, 132.91, 132.26, 129.24, 126.09, 124.20, 121.89, 120.76, 21.19. ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 154.1, 141.2, 135.6, 135.5, 130.8, 126.3, 126.1, 124.2, 121.9, 120.8, 21.5.

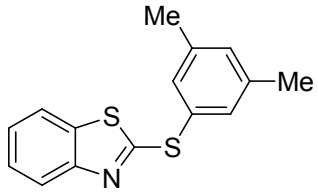
2-((3-methoxyphenyl)thio)benzo[*d*]thiazole (3l).[9]



3l

40.1 mg (73%), colorless oil (R_f = 0.3, V_{Et2O}/V_{PE} = 4:96). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.2 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.43 – 7.37 (m, 2H), 7.33 – 7.25 (m, 3H), 7.06 – 7.03 (m, 1H), 3.83 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.5, 160.4, 153.9, 135.6, 130.8, 130.7, 127.3, 126.2, 124.4, 122.0, 120.8, 120.0, 116.6, 55.5.

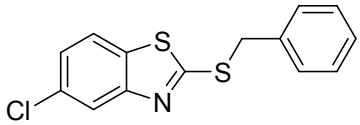
2-((3,5-dimethylphenyl)thio)benzo[*d*]thiazole (3m).[6]



3m

33.6 mg (62%), colorless oil (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.1 Hz, 1H), 7.64 (d, *J* = 7.7 Hz, 1H), 7.41 – 7.37 (m, 1H), 7.35 (s, 2H), 7.27 – 7.23 (m, 1H), 7.13 (s, 1H), 2.36 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.4, 154.0, 139.7, 135.6, 132.9, 132.3, 129.2, 126.1, 124.2, 121.9, 120.8, 21.2.

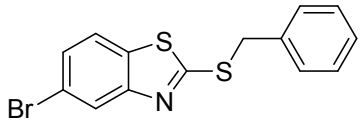
2-(benzylthio)-5-chlorobenzo[*d*]thiazole (4a).[10]



4a

46.3 mg (80%), white solid (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98). m.p. 72 – 73 °C.^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.62 (d, *J* = 8.5 Hz, 1H), 7.45 – 7.43 (m, 2H), 7.35 – 7.24 (m, 4H), 4.58 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.6, 154.0, 136.1, 133.6, 132.1, 129.2, 128.8, 127.9, 124.6, 121.6, 121.4, 37.7.

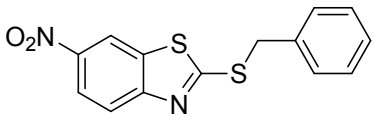
2-(benzylthio)-5-bromobenzo[*d*]thiazole (4b).



4b

41.7 mg (62%), white solid (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98), m.p. 73 – 74 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 1.7 Hz, 1H), 7.59 (d, *J* = 8.5 Hz, 1H), 7.46 – 7.44 (m, 2H), 7.41 – 7.39 (m, 1H)), 7.36 – 7.29 (m, 3H), 4.60 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.5, 154.3, 136.0, 134.2, 129.2, 128.8, 127.9, 127.3, 124.5, 122.0, 119.7, 37.7. $[M + H]^+$ calculated for $C_{14}H_{10}BrNS_2$: 335.9511, found: 335.9506.

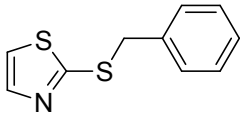
2-(benzylthio)-6-nitrobenzo[*d*]thiazole (4c).[11]



4c

32.3 mg (53%), poor yellow solid (R_f = 0.3, V_{EA}/V_{PE} = 4:96). m.p. 113 – 115 °C.^{1}H NMR (400 MHz, $CDCl_3$) δ .65 (d, J = 2.2 Hz, 1H), 8.30 (dd, J = 9.0, 2.3 Hz, 1H), 7.93 (d, J = 9.0 Hz, 1H), 7.48 – 7.46 (m, 2H), 7.38 – 7.29 (m, 3H), 4.65 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.6, 156.8, 144.1, 135.7, 135.4, 129.2, 128.8, 128.1, 121.9, 121.3, 117.4, 37.8.

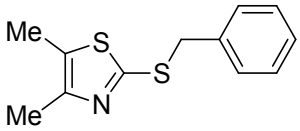
2-(benzylthio)thiazole (4d).[12]



4d

25.3 mg (61%), yellow oil (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 3.3 Hz, 1H), 7.38 – 7.36 (m, 2H), 7.33 – 7.24 (m, 3H)), 7.20 (d, *J* = 3.3 Hz, 1H), 4.43 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.1, 142.8, 136.4, 129.0, 128.6, 127.6, 119.3, 38.9.

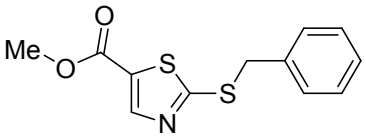
2-(benzylthio)-4,5-dimethylthiazole (4e).[13]



4e

30.1 mg (64%), colorless oil (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ7.36 – 7.34 (m, 2H), 7.32 – 7.23 (m, 3H), 4.32 (s, 2H), 2.29 (s, 3H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.1, 148.6, 136.7, 129.0, 128.6, 127.5, 127.2, 39.3, 14.7, 11.3.

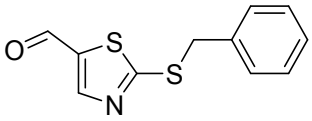
methyl 2-(benzylthio)thiazole-5-carboxylate (4f).



4f

33.2 mg (63%), colorless oil (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98), m.p. 64 – 65 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (s, 1H), 7.41 – 7.39 (m, 2H), 7.35 – 7.28 (m, 3H), 4.48 (s, 2H), 3.87 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 161.3, 148.3, 135.6, 129.0, 128.8, 128.1, 127.9, 52.4, 38.2. [M + H]$^+$ calculated for $C_{12}H_{11}NO_2S_2$: 266.0304, found: 266.0300.

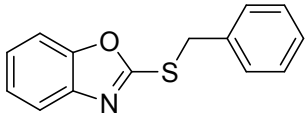
2-(benzylthio)thiazole-5-carbaldehyde (4g).



4g

23.4 mg (50%), yellow oil (R_f = 0.3, V_{EA}/V_{PE} = 10:90). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.89 (s, 1H), 8.21 (s, 1H), 7.43 – 7.42 (m, 2H), 7.38 – 7.27 (m, 3H), 4.52 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 181.0, 175.7, 151.4, 138.7, 135.2, 129.1, 128.8, 128.1, 38.2. $[M + H]^+$ calculated for $C_{11}H_9NOS_2$: 236.0198, found: 236.0195.

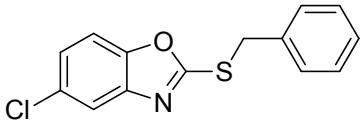
2-(benzylthio)benzo[*d*]oxazole (4h).[5]



4h

27.4 mg (57%), colorless oil (R_f = 0.4, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (dd, J = 7.7, 0.7 Hz, 1H), 7.47 – 7.43(m, 3H), 7.36 – 7.22 (m, 5H), 4.57 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.6, 151.9, 141.9, 135.9, 129.1, 128.8, 127.9, 124.3, 124.0, 118.5, 109.9, 36.6.

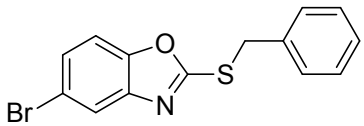
2-(benzylthio)-5-chlorobenzo[*d*]oxazole (4i).[14]



4i

45.6 mg (84%), white solid (R_f = 0.3, V_{Et2O}/V_{PE} = 1:99). m.p. 68 – 70 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 1.9 Hz, 1H), 7.64 (d, *J* = 8.5 Hz, 1H), 7.46 – 7.45 (m, 2H), 7.36 – 7.26 (m, 5H), 4.60 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.6, 154.0, 136.0, 133.6, 132.1, 129.2, 128.8, 127.9, 124.6, 121.6, 121.5, 37.7.

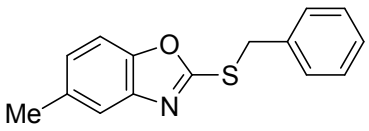
2-(benzylthio)-5-chlorobenzo[*d*]oxazole (4j).



4j

37.1 mg (58%), white solid (R_f = 0.3, V_{Et2O}/V_{PE} = 1:99), m.p. 76 – 77 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 1.8 Hz, 1H), 7.47 – 7.45 (m, 2H), 7.37 – 7.26 (m, 5H), 4.55 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.16, 150.91, 143.50, 135.65, 129.11, 128.82, 128.04, 126.84, 121.53, 117.15, 111.04, 36.63. $[M + H]^+$ calculated for $C_{14}H_{10}BrNOS$: 319.9739, found: 319.9736.

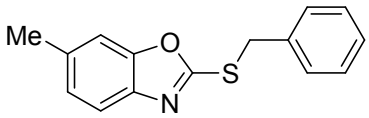
2-(benzylthio)-5-methylbenzo[*d*]oxazole (4k).



4k

22.2 mg (44%), white solid (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98), m.p. 58 – 59 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 – 7.45 (m, 2H), 7.42 (s, 1H), 7.36 – 7.26 (m, 4H), 7.07 – 7.05 (m, 1H), 4.56 (s, 2H), 2.45 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.4, 150.1, 142.1, 136.0, 134.1, 129.1, 128.8, 127.9, 124.9, 118.6, 109.3, 36.6, 21.5. [M + H]$^+$ calculated for $C_{15}H_{13}NOS$: 256.0791, found: 256.0799.

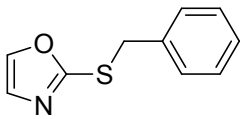
2-(benzylthio)-6-methylbenzo[*d*]oxazole (4l).



4l

28.2 mg (56%), white solid (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98), m.p. 62 – 63 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, *J* = 8.1 Hz, 1H), 7.47 – 7.45 (m, 2H), 7.36 – 7.25 (m, 4H), 7.11 (d, *J* = 8.1 Hz, 1H), 4.56 (s, 2H), 2.46 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 163.6, 152.2, 139.7, 135.9, 134.3, 129.1, 128.8, 127.9, 125.4, 117.3, 110.2, 36.6, 21.7. [M + H]$^+$ calculated for $C_{15}H_{13}NOS$: 256.0791, found: 256.0798.

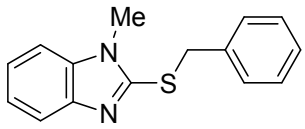
2-(benzylthio)oxazole (4m).



4m

16.7 mg (44%), colorless oil (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (s, 1H), 7.39 – 7.38 (m, 2H), 7.34 – 7.25 (m, 3H), 7.11 (s, 1H), 4.40 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 140.2, 136.3, 128.9, 128.7, 128.4, 127.8, 36.9. [M + H]$^+$ calculated for $C_{10}H_9NOS$: 192.0478, found: 192.0474.

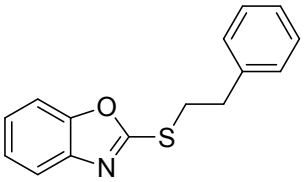
2-(benzylthio)-1-methyl-1H-benzo[*d*]imidazole (4n).[15]



4n

15.2 mg (30%), colorless oil (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98). m.p. 70 – 71 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.72 (m, 1H), 7.41 – 7.36 (m, 2H), 7.31 – 7.23 (m, 6H), 4.62 (s, 2H), 3.58 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.6, 143.0, 136.7, 136.5, 129.1, 128.7, 127.7, 122.1, 122.0, 118.3, 108.6, 37.3, 30.00.

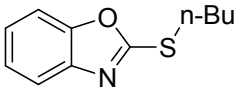
2-(phenethylthio)benzo[*d*]oxazole (4o).



4o

23.1 mg (46%), colorless oil (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.61 (m, 1H), 7.45 – 7.43 (m, 1H), 7.35 – 7.22 (m, 7H), 3.57 – 3.53 (m, 2H), 3.17 – 3.13 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8, 151.9, 142.0, 139.4, 128.7, 128.6, 126.8, 124.3, 123.9, 118.5, 109.9, 35.6, 33.5. $[M + H]^+$ calculated for $C_{15}H_{13}NOS$: 256.0791, found: 256.0795.

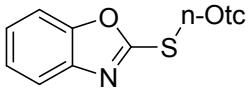
2-(butylthio)benzo[*d*]oxazole (4p).[5]



4p

21.1 mg (51%), colorless oil (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.59 (m, 1H), 7.44 – 7.42 (m, 1H), 7.29 – 7.21 (m, 2H), 3.32 (t, *J* = 7.3 Hz, 2H), 1.81 (dt, *J* = 15.0, 7.5 Hz, 2H), 1.51 (dq, *J* = 14.7, 7.4 Hz, 2H), 0.97 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 151.8, 142.0, 124.2, 123.7, 118.3, 109.8, 32.0, 31.3, 21.8, 13.6.

2-(octylthio)benzo[*d*]oxazole (4q).[16]



4q

23.1 mg (44%), colorless oil (R_f = 0.3, V_{Et2O}/V_{PE} = 2:98). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 – 7.59 (m, 1H), 7.44 – 7.42 (m, 1H), 7.30 – 7.21 (m, 2H), 3.31 (t, *J* = 7.3 Hz, 2H), 1.86 – 1.79 (m, 2H), 1.51 – 1.44 (m, 2H), 1.36 – 1.27 (m, 8H), 0.96 – 0.86 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.3, 151.8, 1421, 124.2, 123.7, 118.4, 109.8, 32.3, 31.8, 29.3, 29.1, 29.1, 28.7, 22.7, 14.1.

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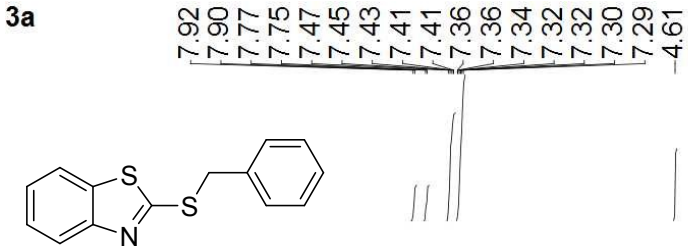
^{1}H and ^{13}C NMR Spectra of compounds

3a



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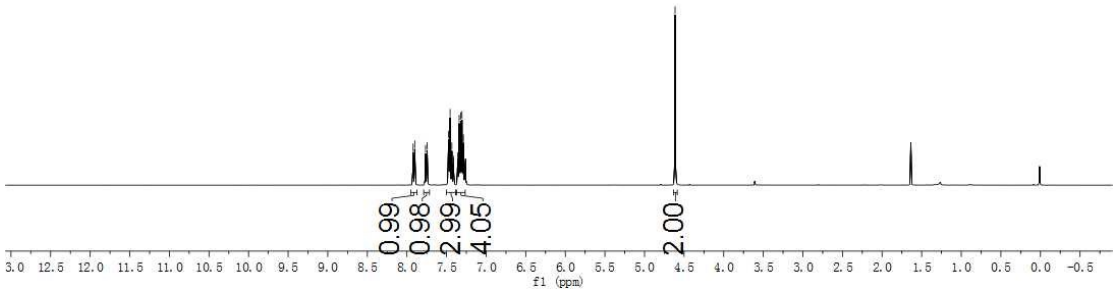

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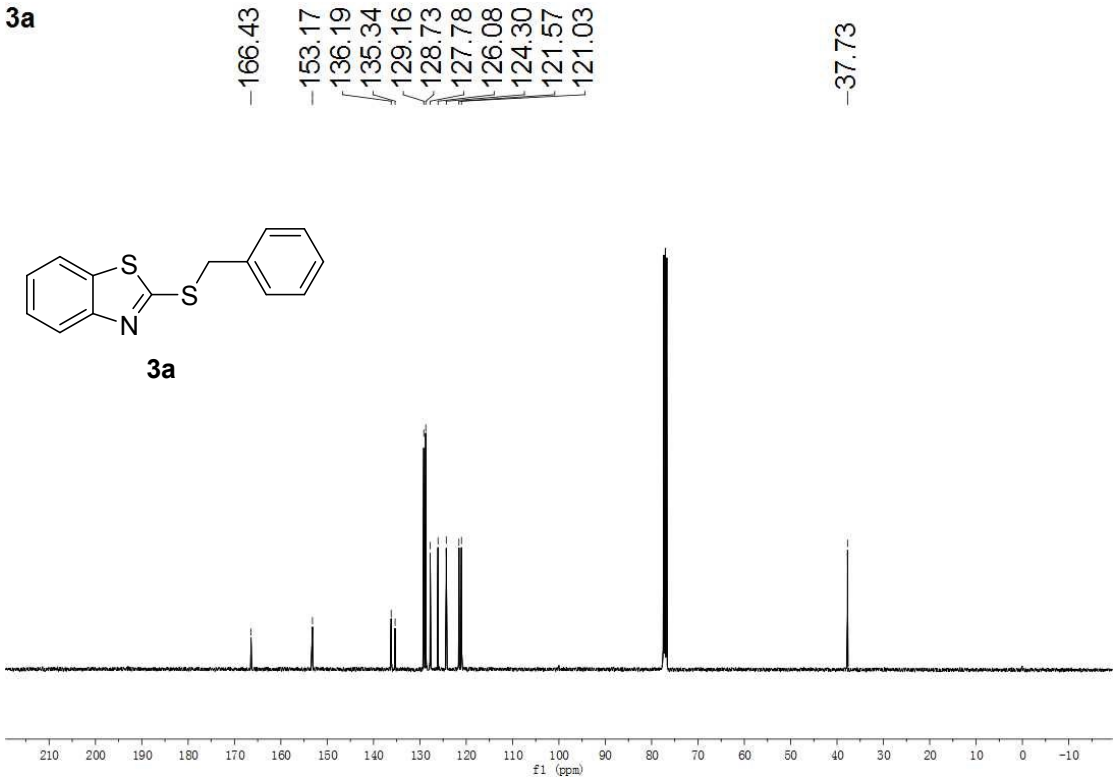
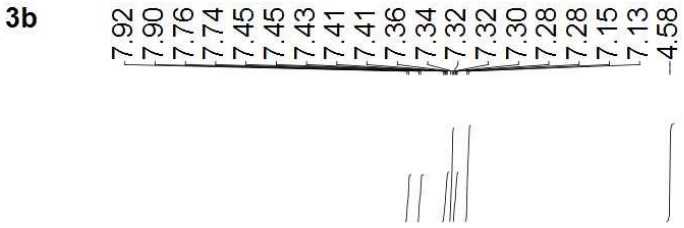


3a

3b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7.45
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7.41
7.41
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7.32
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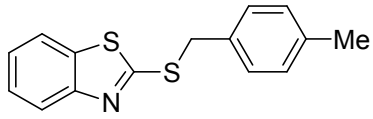
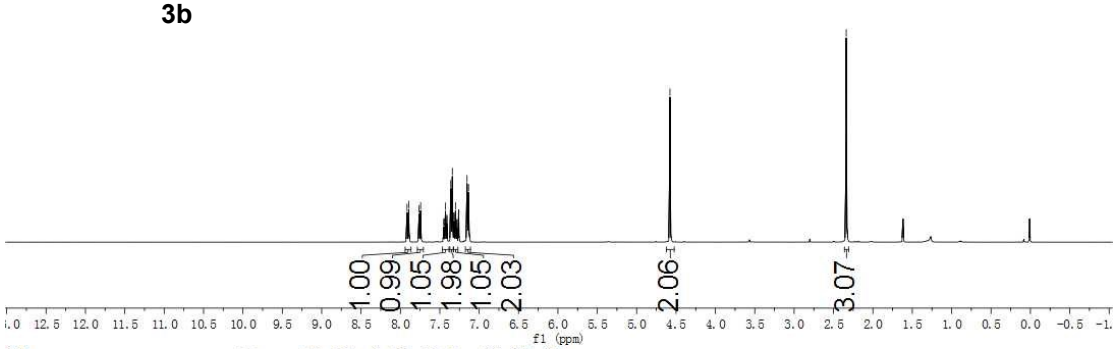
7.28
7.28
7.15
7.13
4.58
2.34


S
S
N
Me

3b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0.99
1.05
1.98
1.05
2.03
2.06
3.07
f1 (ppm)

3b


166.62
153.22
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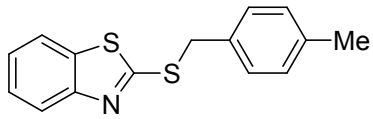
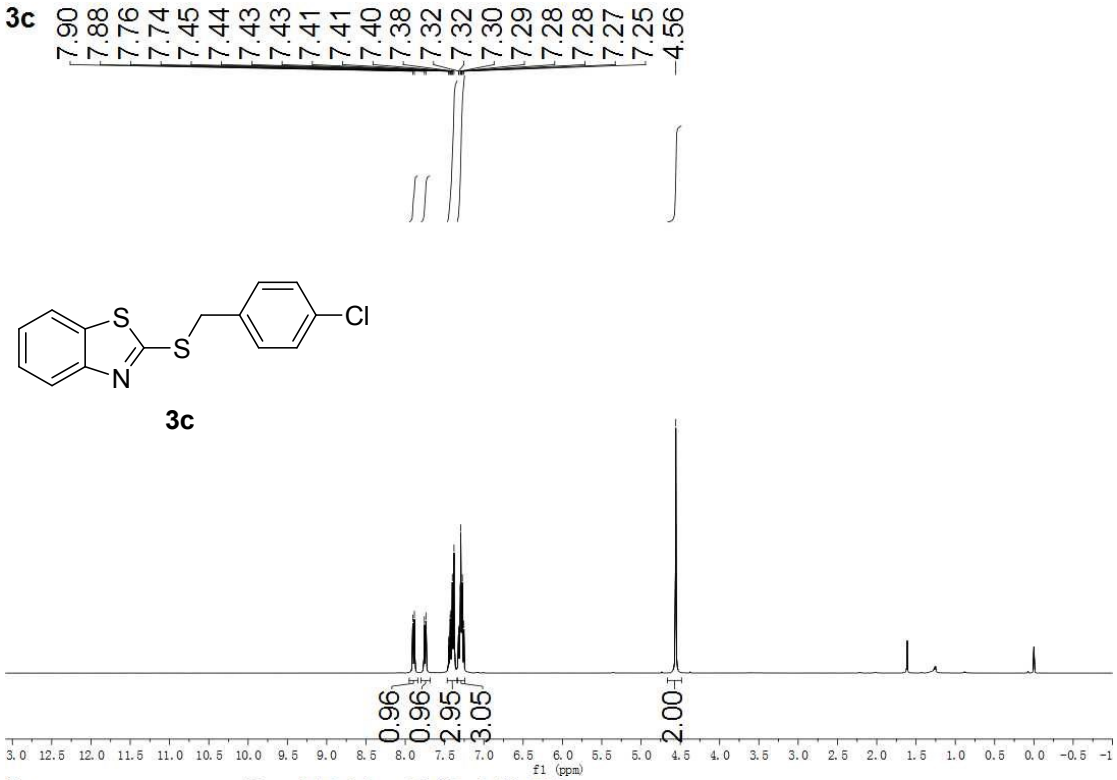
135.34
133.03
129.43
129.07
126.06
124.26
121.56
121.01
37.57
21.18


S
S
N
Me

3b

f1 (ppm)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7.41
7.41
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7.32
7.32
7.30
7.29
7.28
7.28
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7.25
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S
S
N
Cl
3c
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0.96
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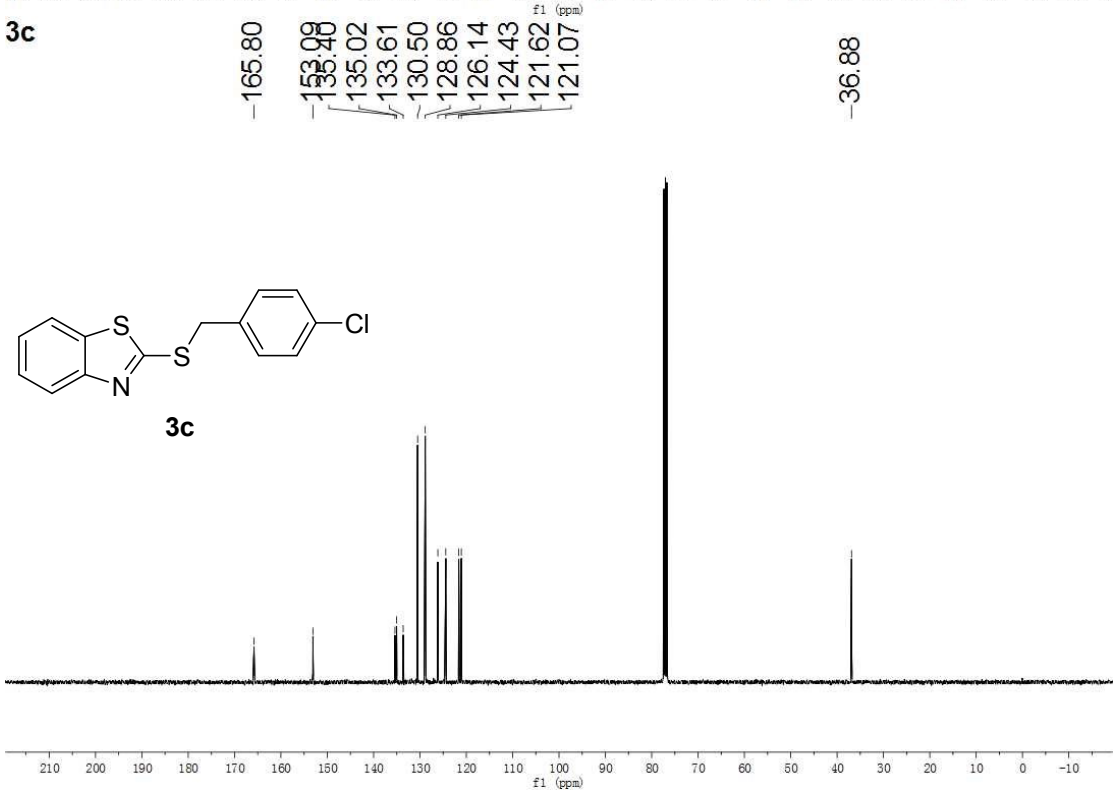
2.00
f1 (ppm)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135.40
135.02
133.61
130.50
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124.43
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121.07
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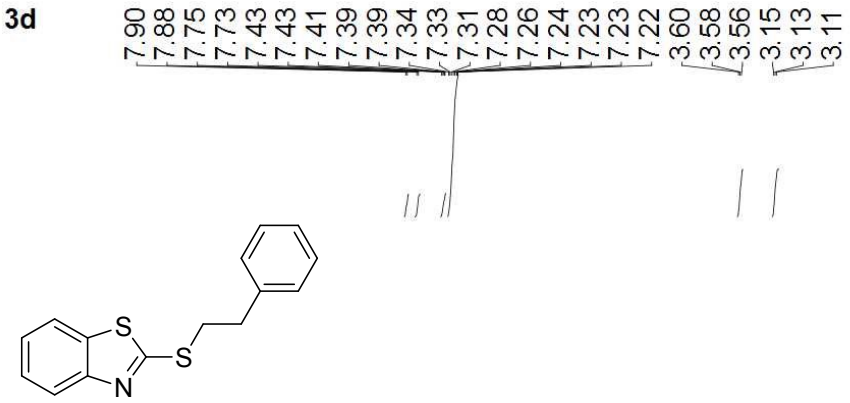
S
S
N
Cl
3c
f1 (ppm)

3d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7.39
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7.34
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7.26
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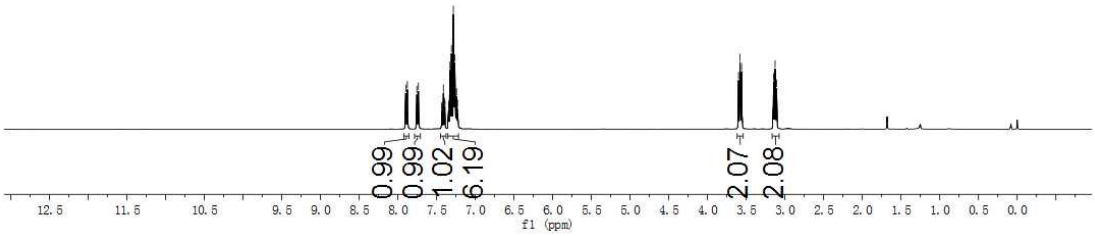
3.13
3.11
S
S
N

3d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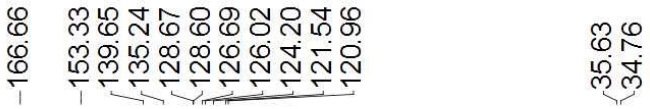
2.07
2.08
f1 (ppm)

3d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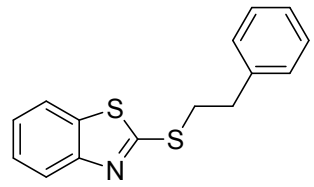
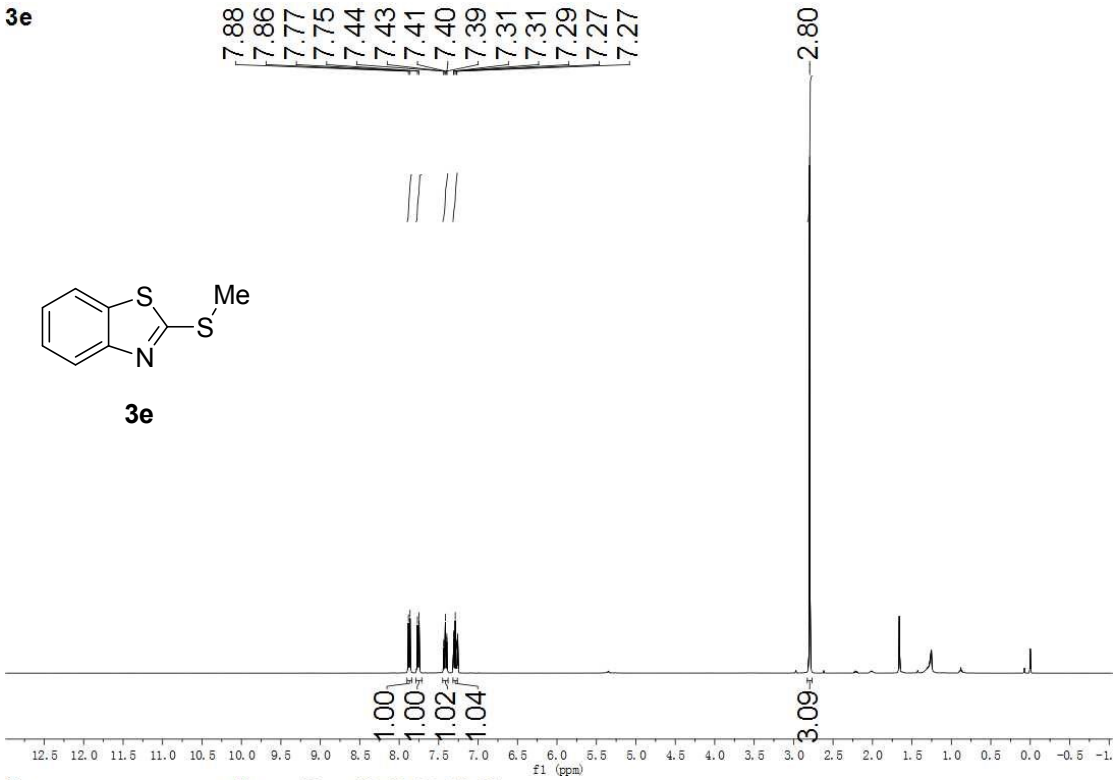
126.69
126.02
124.20
121.54
120.96
35.63
34.76


S
S
N

3d

f1 (ppm)

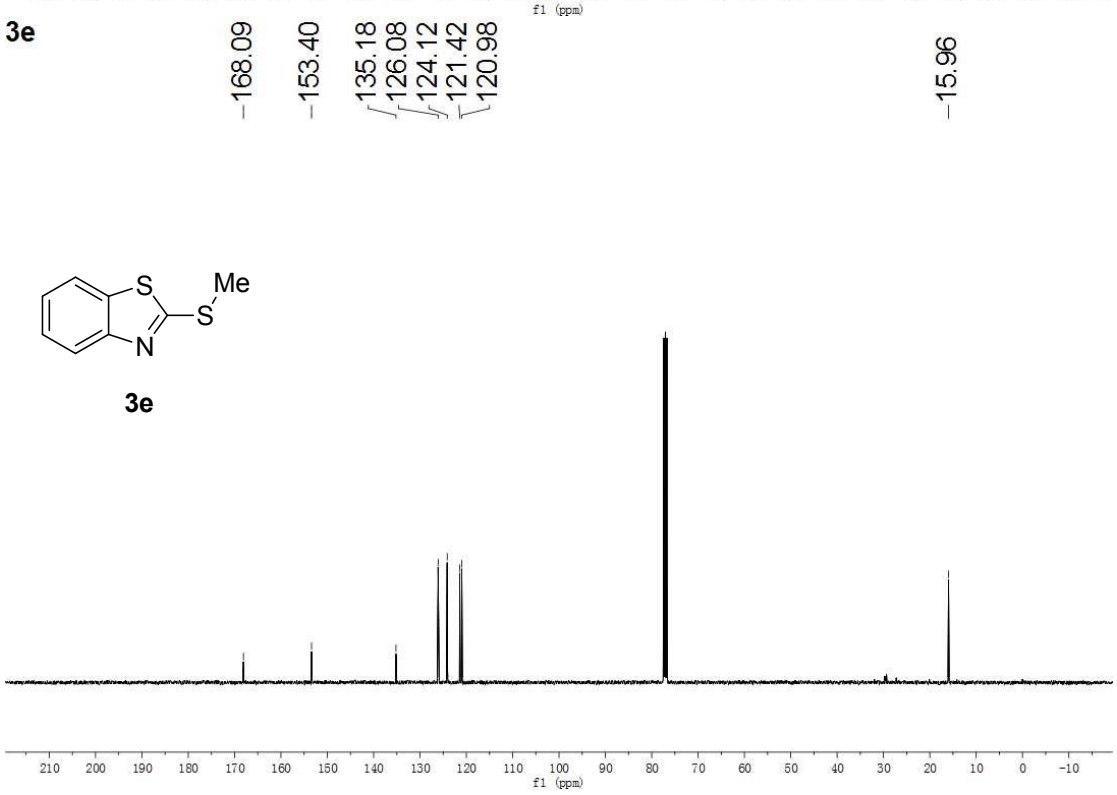
3e


7.88
7.86
7.77
7.75
7.44
7.43
7.41
7.40
7.39
7.31
7.31
7.29
7.27
7.27
2.80
1.00
1.00
1.02
1.04
3.09
f1 (ppm)

S
Me
S
N

3e

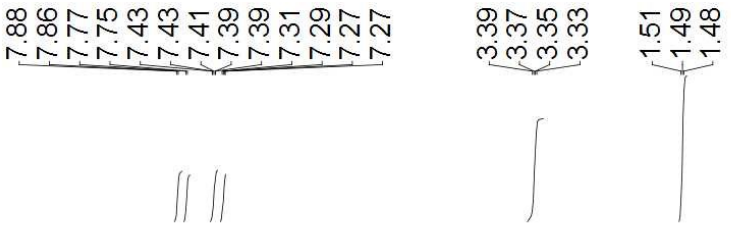
3e

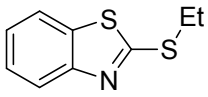

168.09
153.40
135.18
126.08
124.12
121.42
120.98
15.96
f1 (ppm)

S
Me
S
N

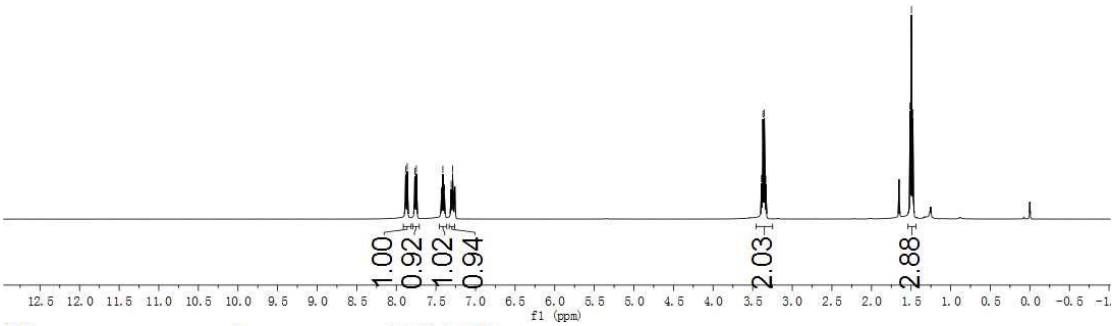
3e

3f

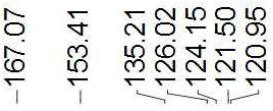

7.88
7.86
7.77
7.75
7.43
7.43
7.41
7.39
7.39
7.31
7.29
7.27
7.27
3.39
3.37
3.35
3.33
1.51
1.49
1.48

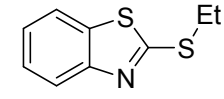

S
Et
S
N

3f


1.00
0.92
1.02
0.94
2.03
2.88
f1 (ppm)

3f

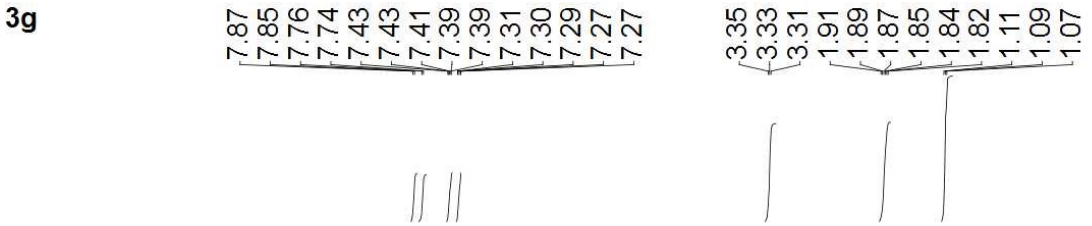

167.07
153.41
135.21
126.02
124.15
121.50
120.95
27.97
14.61

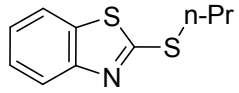

S
Et
S
N

3f

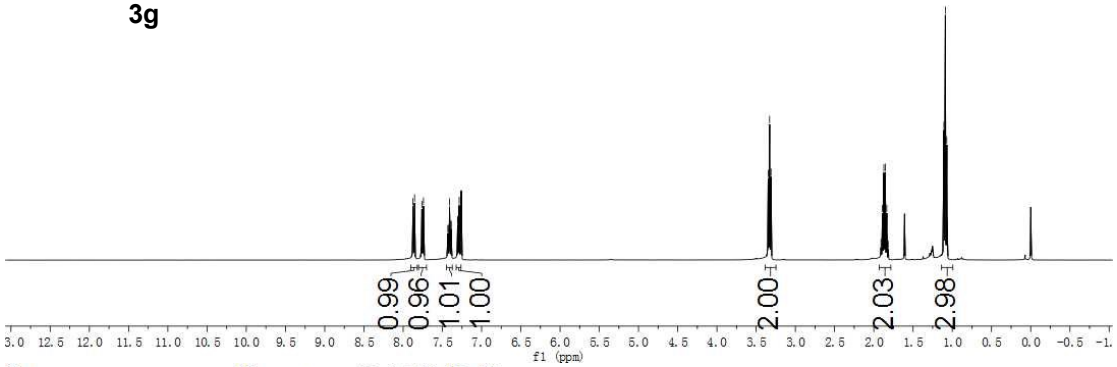
f1 (ppm)

3g

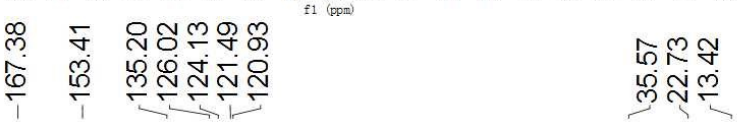

7.87
7.85
7.76
7.74
7.43
7.43
7.41
7.39
7.39
7.31
7.30
7.29
7.27
7.27
3.35
3.33
3.31
1.91
1.89
1.87
1.85
1.84
1.82
1.11
1.09
1.07

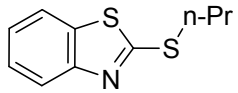

S
n-Pr
S
N

3g


0.99
0.96
1.01
1.00
2.00
2.03
2.98
f1 (ppm)

3g

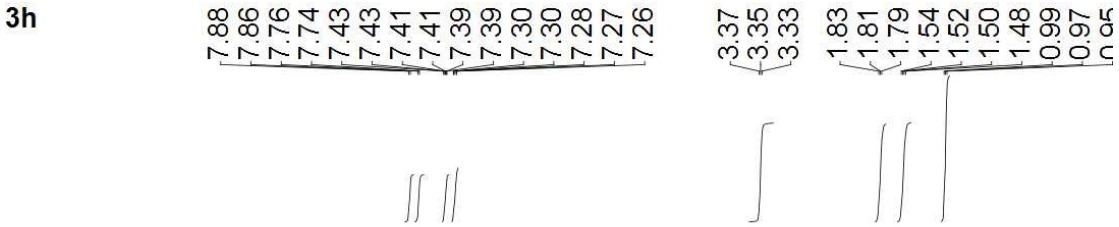

167.38
153.41
135.20
126.02
124.13
121.49
120.93
35.57
22.73
13.42

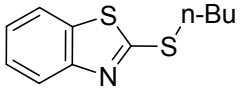

S
n-Pr
S
N

3g

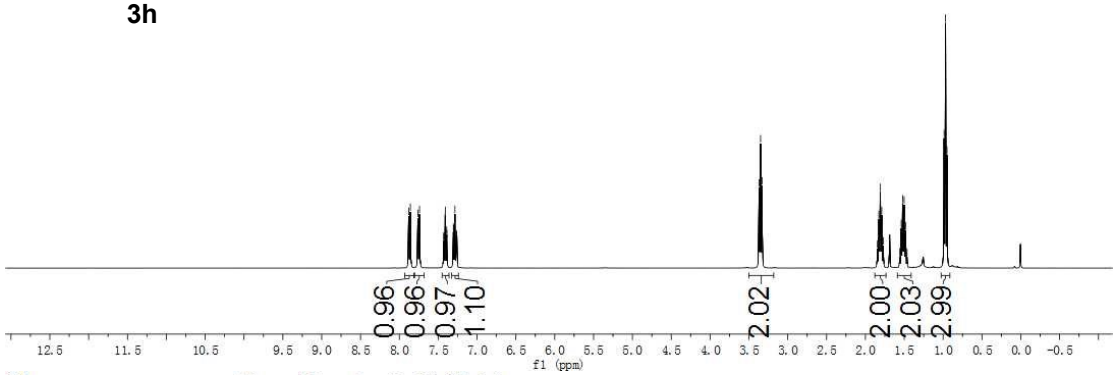
f1 (ppm)

3h


7.88
7.86
7.76
7.74
7.43
7.43
7.41
7.41
7.39
7.39
7.30
7.30
7.28
7.27
7.26
3.37
3.35
3.33
1.83
1.81
1.79
1.54
1.52
1.50
1.48
0.99
0.97

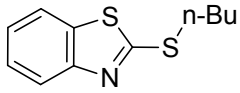

S
n-Bu
S
N

3h

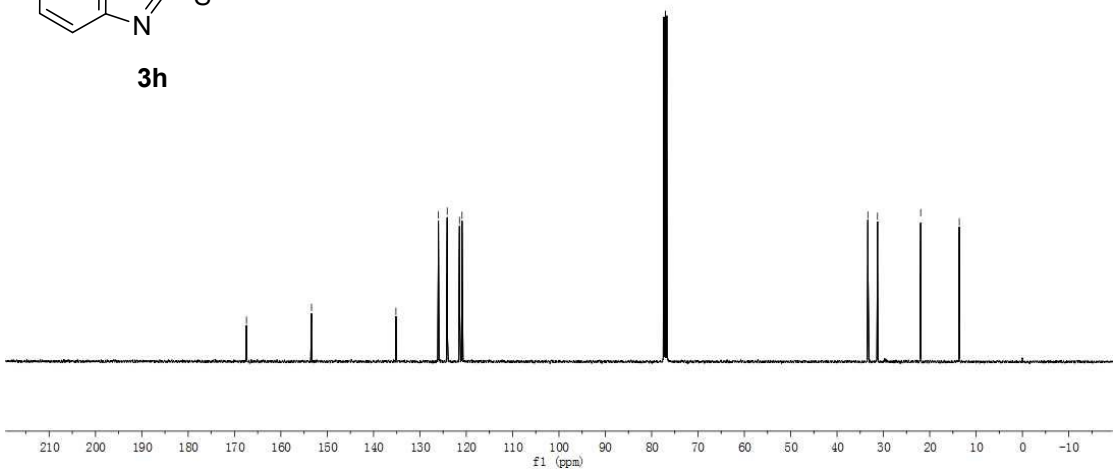

0.96
0.96
0.97
1.10
2.02
2.00
2.03
2.99
f1 (ppm)

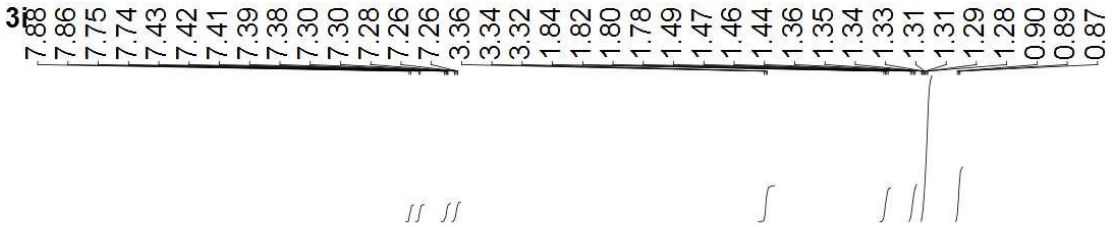
3h

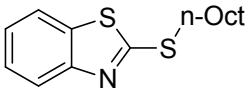

167.42
153.39
135.17
126.00
124.10
121.46
120.92
33.35
31.27
21.95
13.62


S
n-Bu
S
N

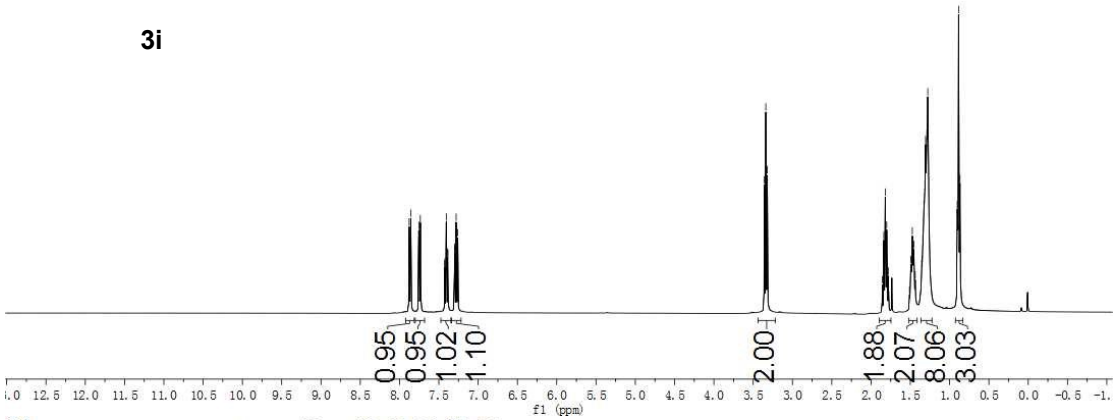
3h


f1 (ppm)


3i
7.88
7.86
7.75
7.74
7.43
7.42
7.41
7.39
7.38
7.30
7.30
7.28
7.26
7.26
3.36
3.34
3.32
1.84
1.82
1.80
1.78
1.49
1.47
1.46
1.44
1.36
1.35
1.34
1.33
1.31
1.31
1.29
1.28
0.90
0.89
0.87

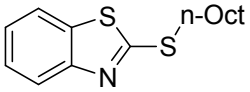

S
n-Oct
S
N

3i

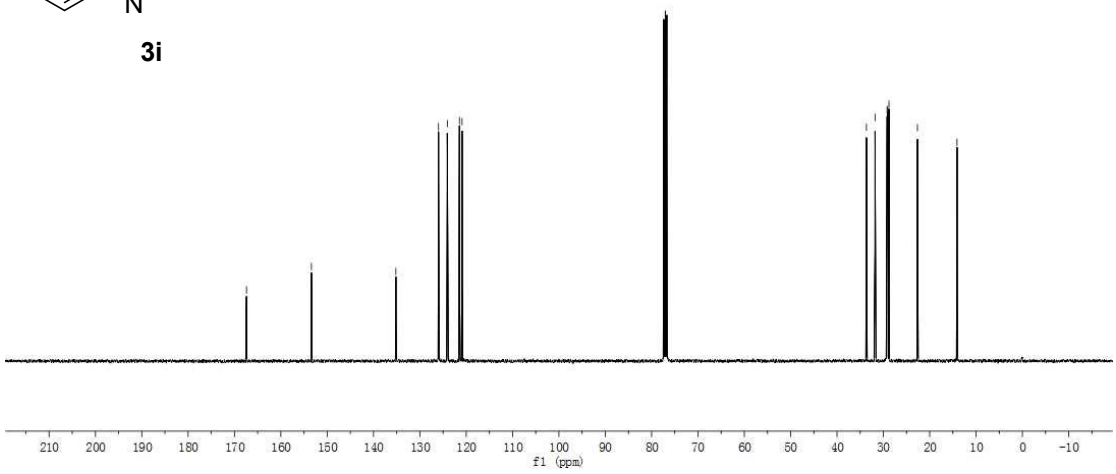

0.95
0.95
1.02
1.10
2.00
1.88
2.07
8.06
3.03
f1 (ppm)

3i

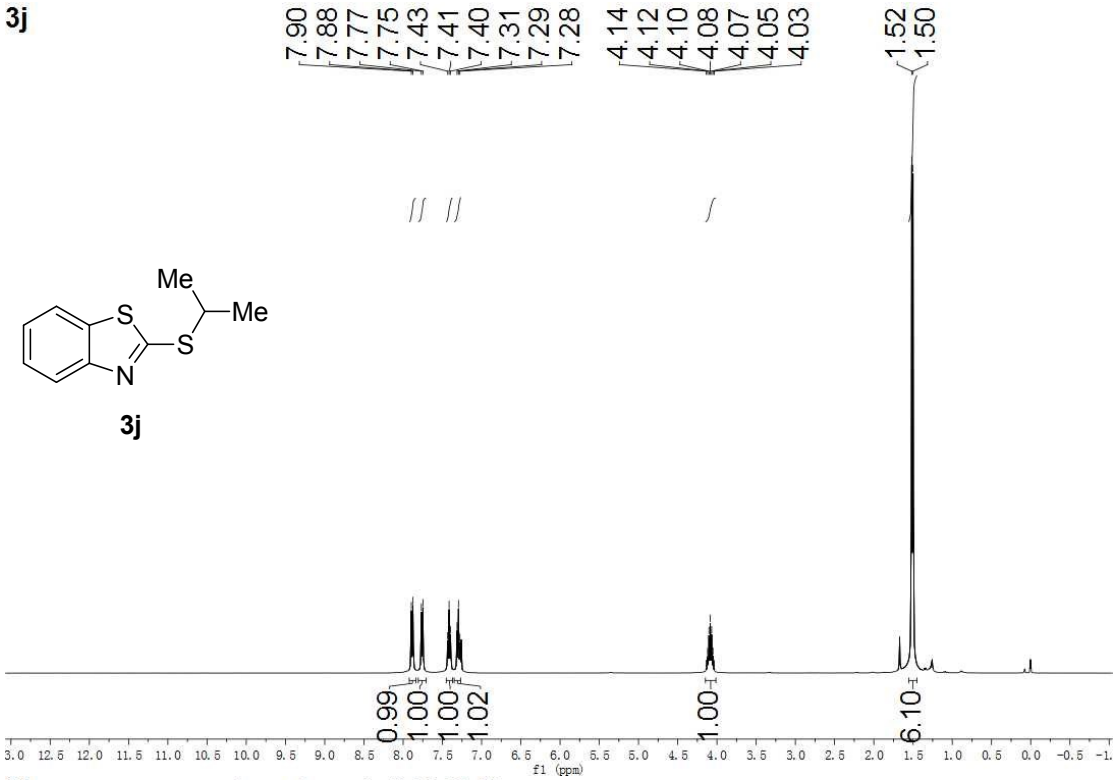

167.41
153.40
135.18
125.98
124.08
121.46
120.90
33.65
31.79
29.21
29.14
29.06
28.79
22.65
14.10


S
n-Oct
S
N

3i


f1 (ppm)

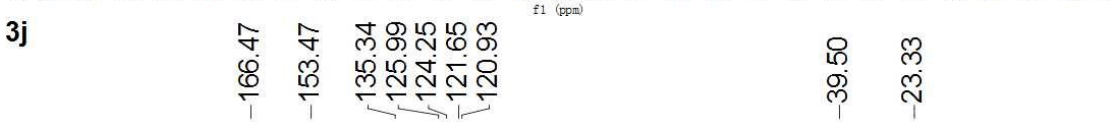
3j

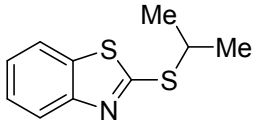

7.90
7.88
7.77
7.75
7.43
7.41
7.40
7.31
7.29
7.28
4.14
4.12
4.10
4.08
4.07
4.05
4.03
1.52
1.50
0.99
1.00
1.00
1.02
1.00
6.10
f1 (ppm)

Me
S
Me
S
N

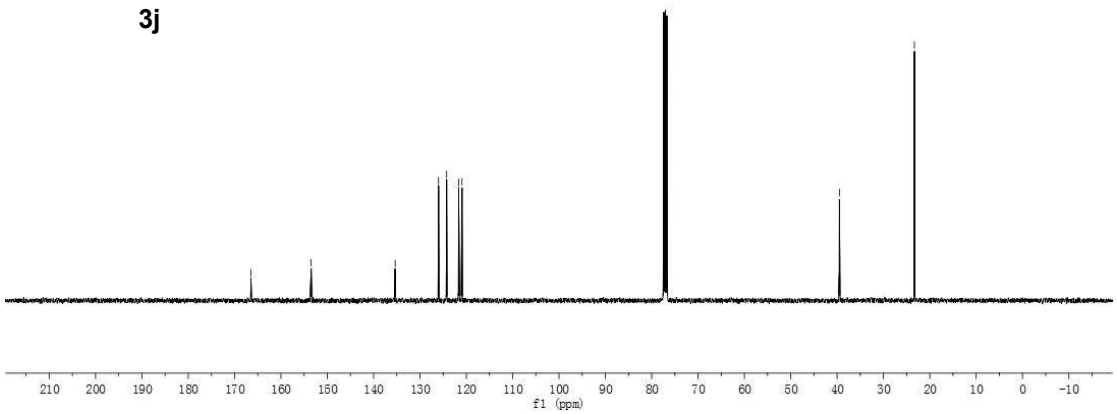
3j

3j

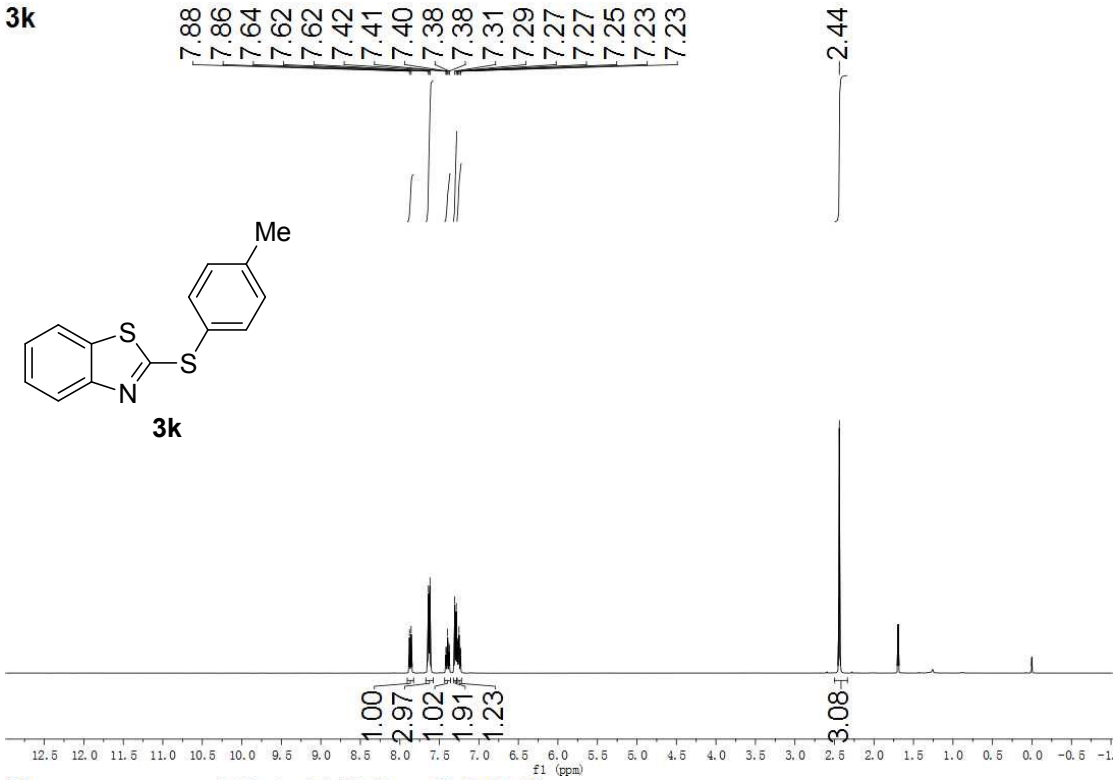

166.47
153.47
135.34
125.99
124.25
121.65
120.93
39.50
23.33


Me
S
Me
S
N

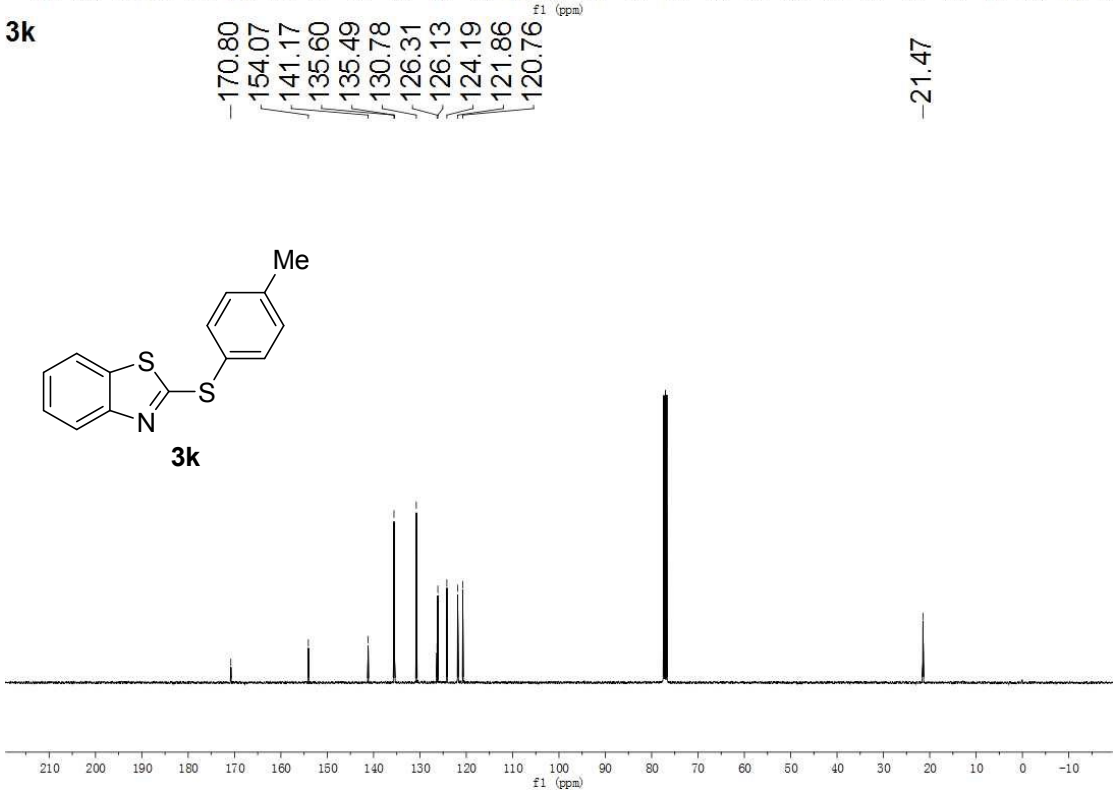
3j

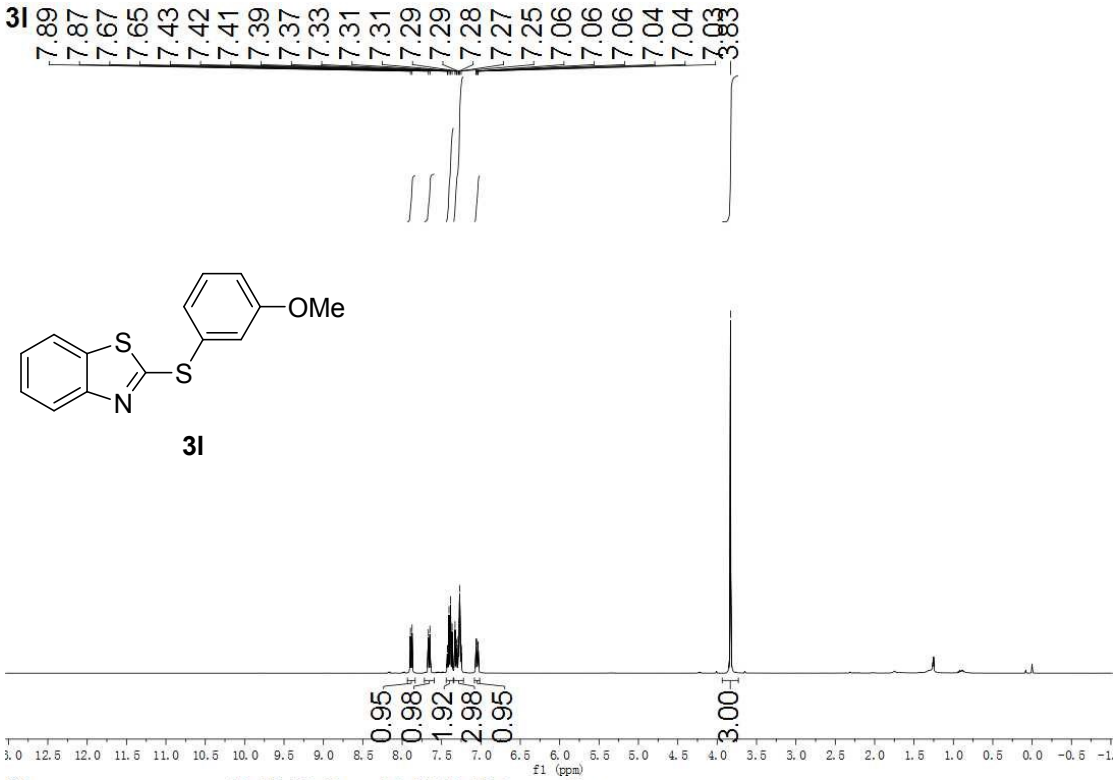

f1 (ppm)

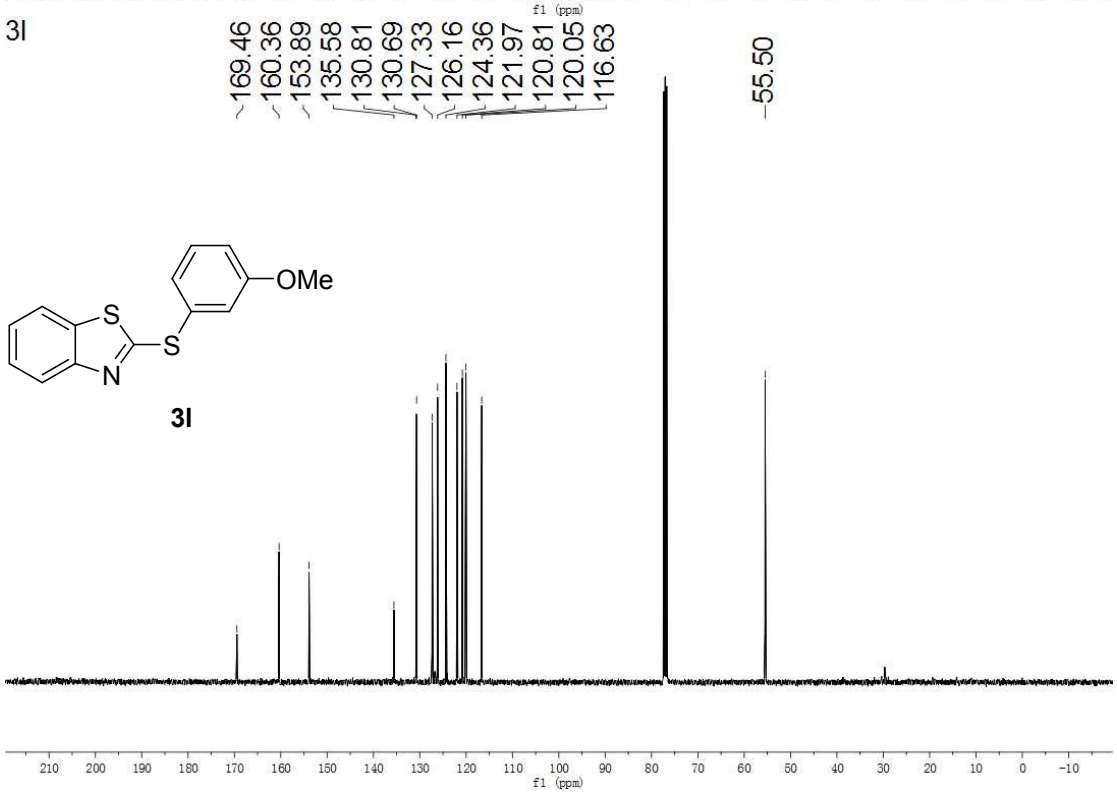
3k


7.88
7.86
7.64
7.62
7.62
7.42
7.41
7.40
7.38
7.38
7.31
7.29
7.27
7.27
7.25
7.23
7.23
2.44
Me
S
S
N
1.00
2.97
1.02
1.91
1.23
3.08
f1 (ppm)

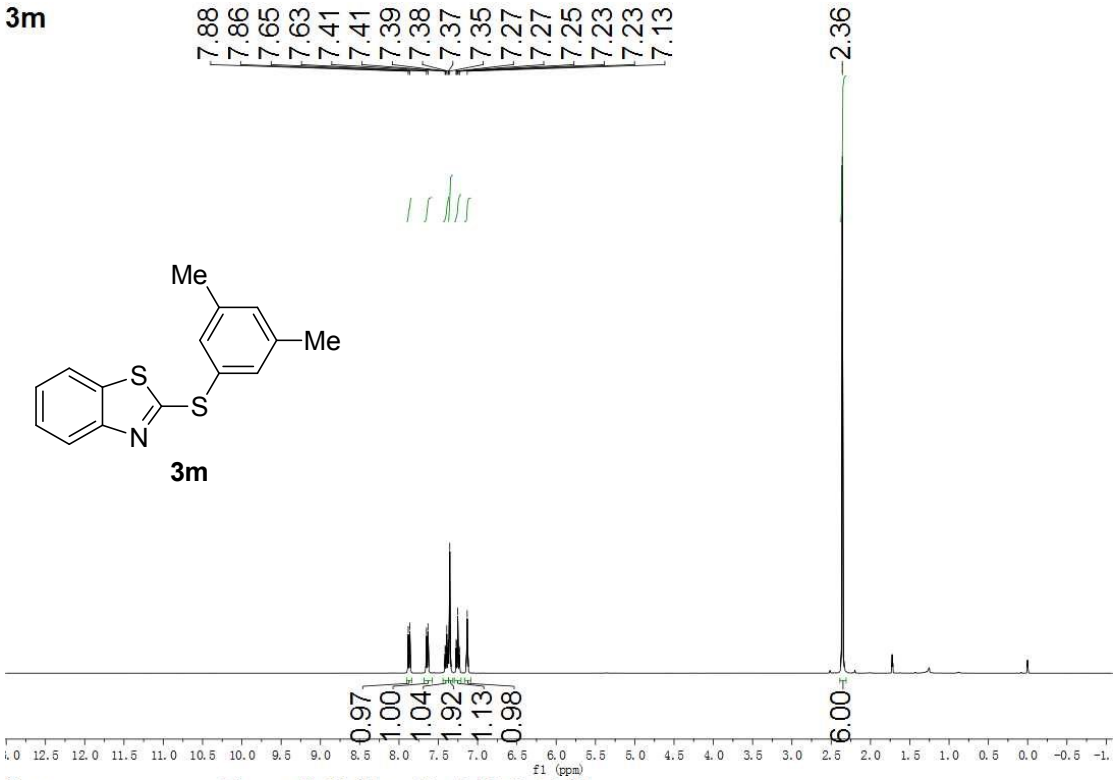
3k


170.80
154.07
141.17
135.60
135.49
130.78
126.31
126.13
124.19
121.86
120.76
21.47
Me
S
S
N
f1 (ppm)


3l
7.89
7.87
7.67
7.65
7.43
7.42
7.41
7.39
7.37
7.33
7.31
7.31
7.29
7.29
7.28
7.27
7.25
7.06
7.06
7.06
7.04
7.04
7.03
3.83
OMe
S
S
N
3l
0.95
0.98
1.92
2.98
0.95
3.00
f1 (ppm)


3l
169.46
160.36
153.89
135.58
130.81
130.69
127.33
126.16
124.36
121.97
120.81
120.05
116.63
55.50
OMe
S
S
N
3l
f1 (ppm)

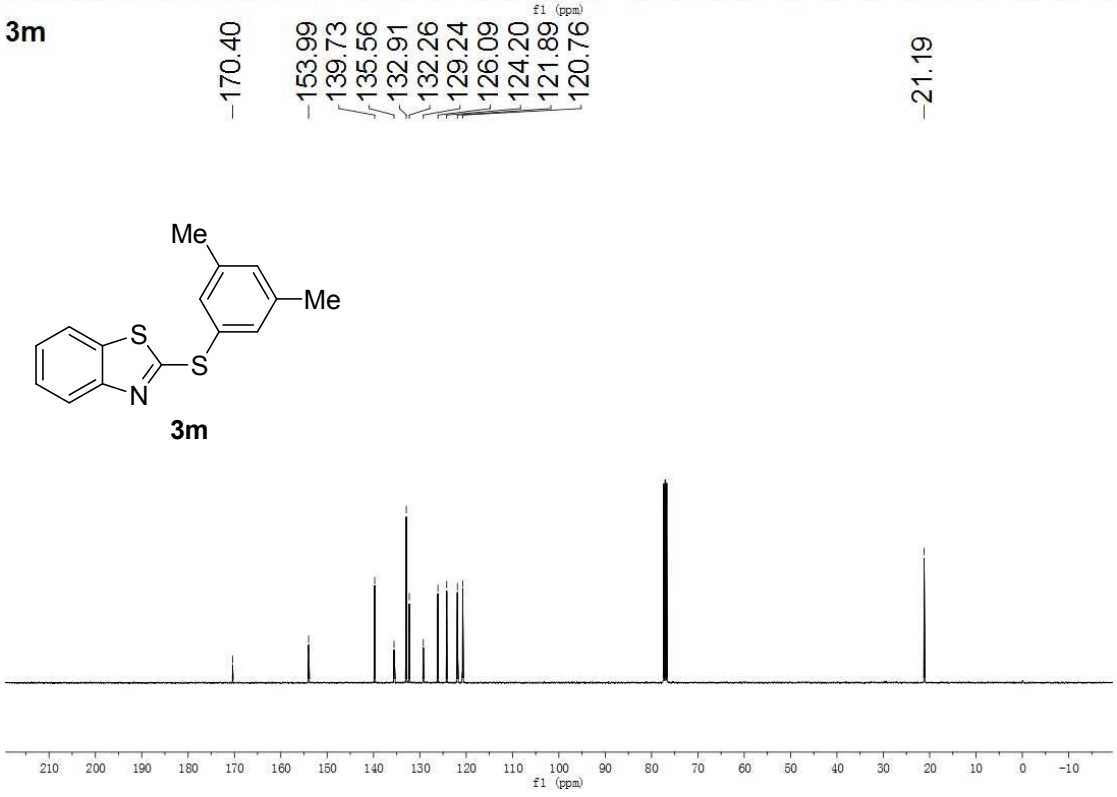
3m


7.88
7.86
7.65
7.63
7.41
7.41
7.39
7.38
7.37
7.35
7.27
7.27
7.25
7.23
7.23
7.13
2.36
0.97
1.00
1.04
1.92
1.13
0.98
6.00
f1 (ppm)

Me
Me
S
S
N

3m

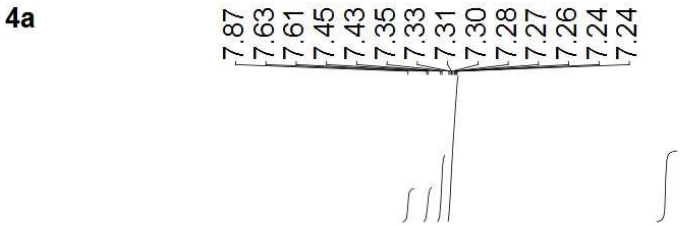
3m

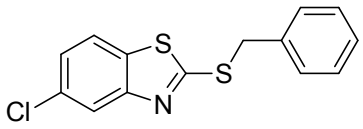

170.40
153.99
139.73
135.56
132.91
132.26
129.24
126.09
124.20
121.89
120.76
21.19
f1 (ppm)

Me
Me
S
S
N

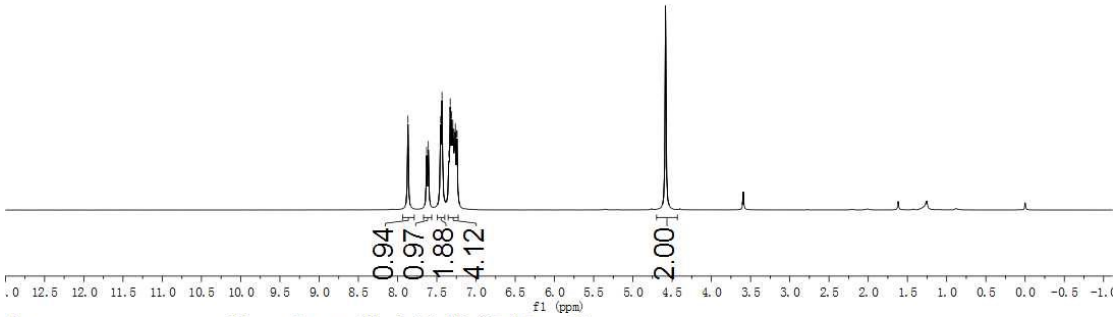
3m

4a

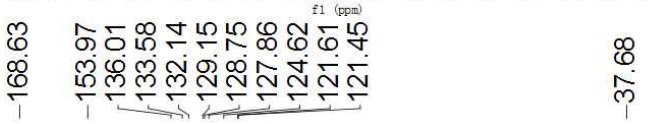

7.87
7.63
7.61
7.45
7.43
7.35
7.33
7.31
7.30
7.28
7.27
7.26
7.24
7.24

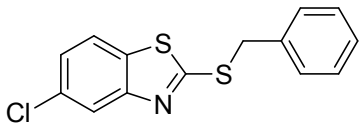

S
S
N
Cl

4a

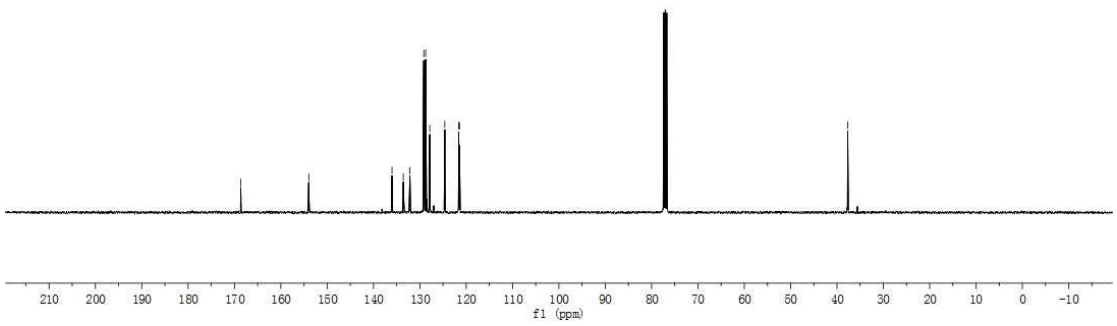

0.94
0.97
1.88
4.12
2.00
f1 (ppm)

4a

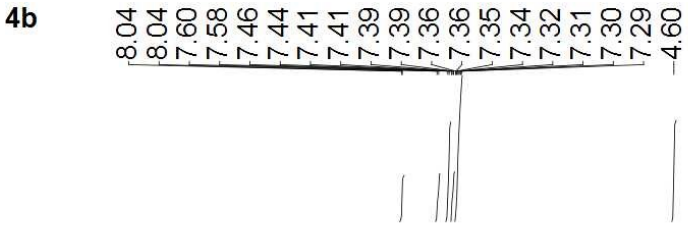

168.63
153.97
136.01
133.58
132.14
129.15
128.75
127.86
124.62
121.61
121.45
37.68

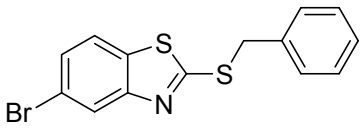

S
S
N
Cl

4a

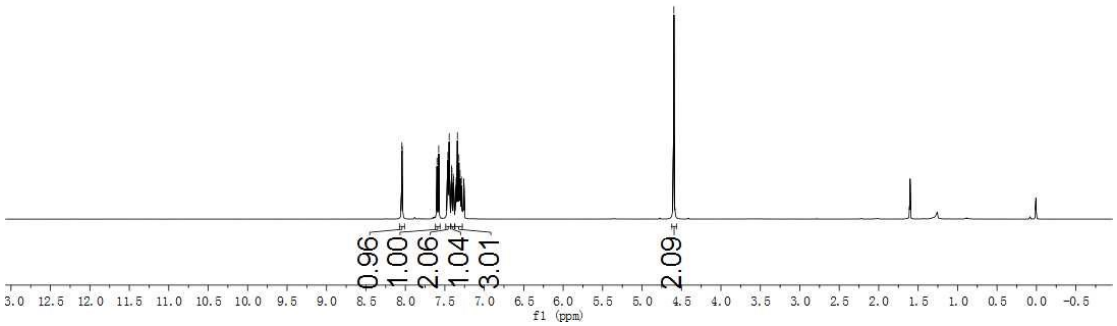

f1 (ppm)

4b

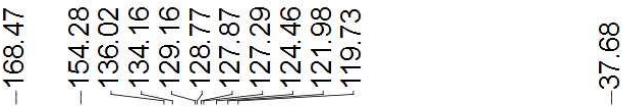

8.04
8.04
7.60
7.58
7.46
7.44
7.41
7.41
7.39
7.39
7.36
7.36
7.35
7.34
7.32
7.31
7.30
7.29
4.60

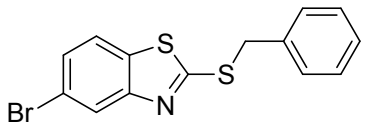

S
S
N
Br

4b


0.96
1.00
2.06
1.04
3.01
2.09
f1 (ppm)

4b

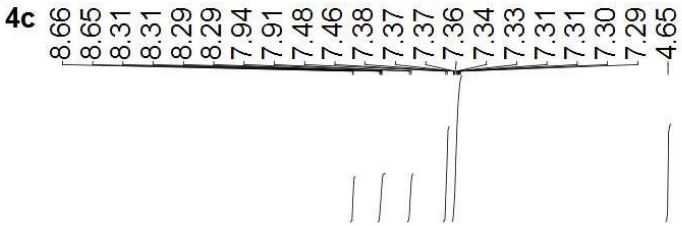

168.47
154.28
136.02
134.16
129.16
128.77
127.87
127.29
124.46
121.98
119.73
37.68

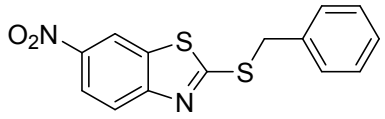

S
S
N
Br

4b

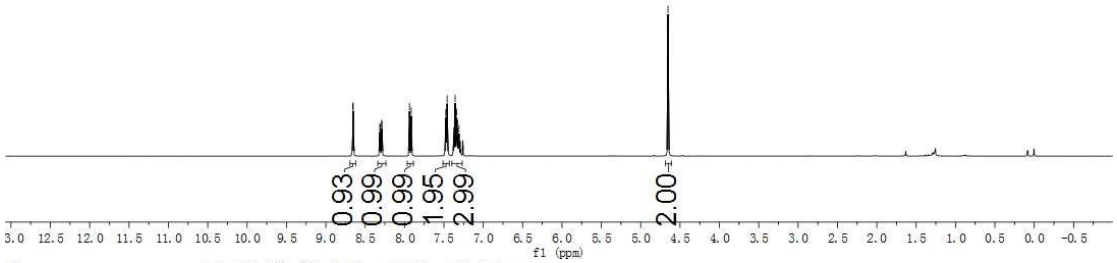
f1 (ppm)

4c


8.66
8.65
8.31
8.31
8.29
8.29
7.94
7.91
7.48
7.46
7.38
7.37
7.37
7.36
7.34
7.33
7.31
7.31
7.30
7.29
4.65

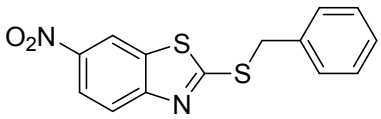

O2N
S
S
N

4c

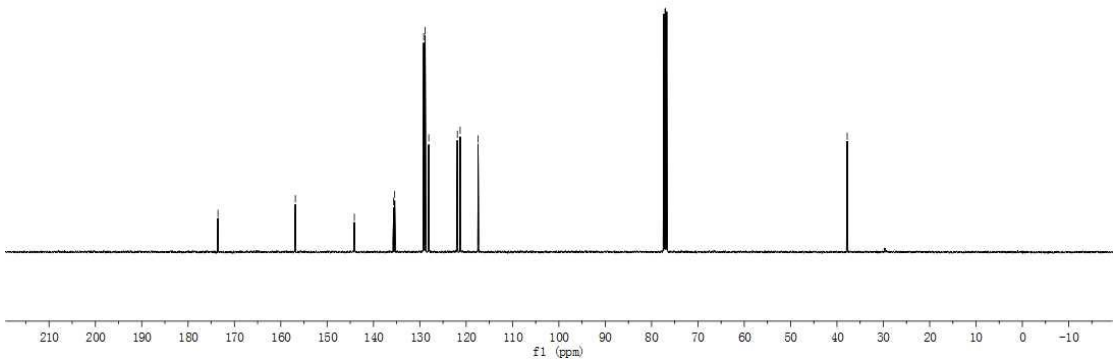

0.93
0.99
0.99
1.95
2.99
2.00
f1 (ppm)

4c

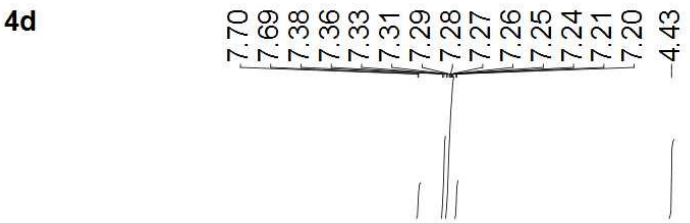

173.55
156.85
144.13
135.66
135.42
129.17
128.85
128.07
121.90
121.29
117.42
37.80

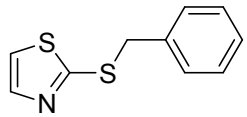

O2N
S
S
N

4c

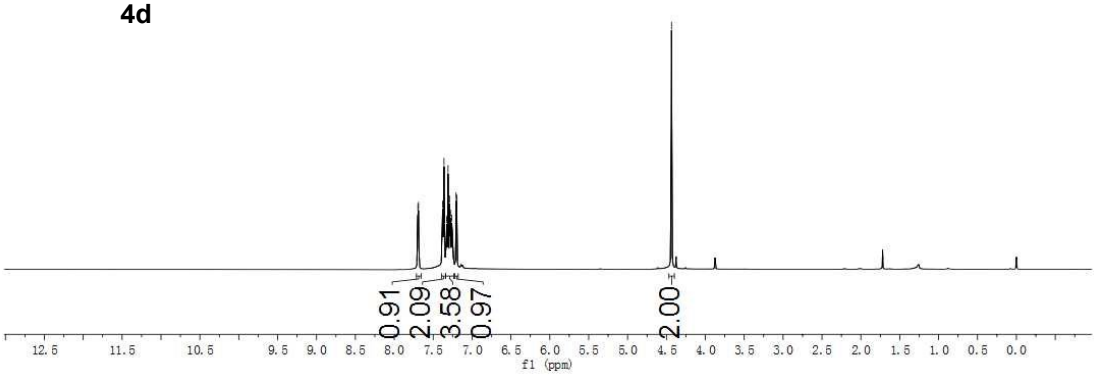

f1 (ppm)

4d


7.70
7.69
7.38
7.36
7.33
7.31
7.29
7.28
7.27
7.26
7.25
7.24
7.21
7.20
4.43

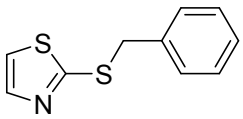


4d

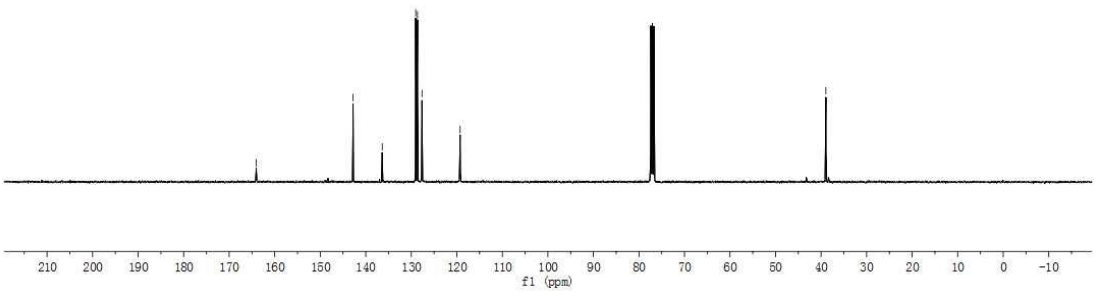

0.91
2.09
3.58
0.97
2.00
12.5
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

4d

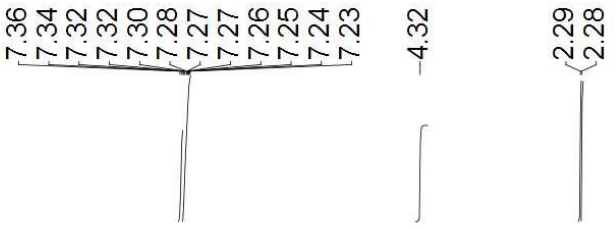

164.06
142.79
136.38
129.03
128.64
127.65
119.28
38.95

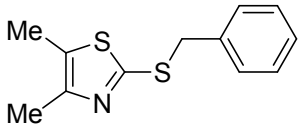


4d

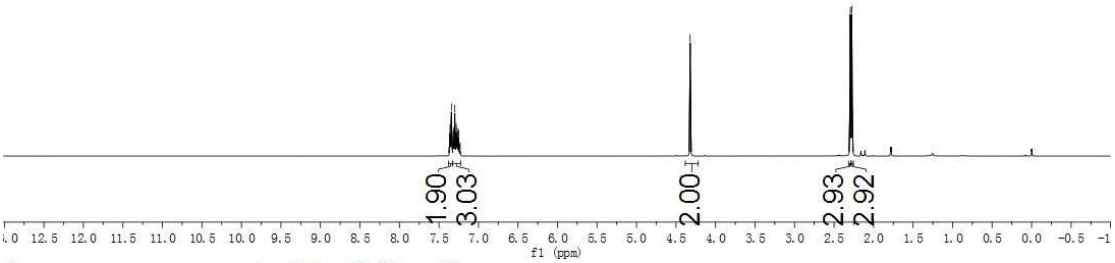

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

4e

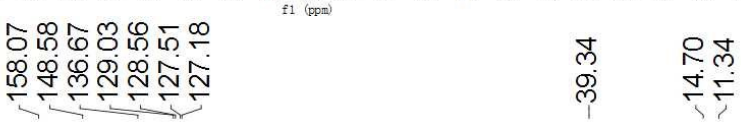

7.36
7.34
7.32
7.32
7.30
7.28
7.27
7.27
7.26
7.25
7.24
7.23
4.32
2.29
2.28

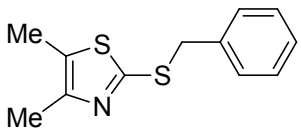

Me
S
S
N
Me

4e

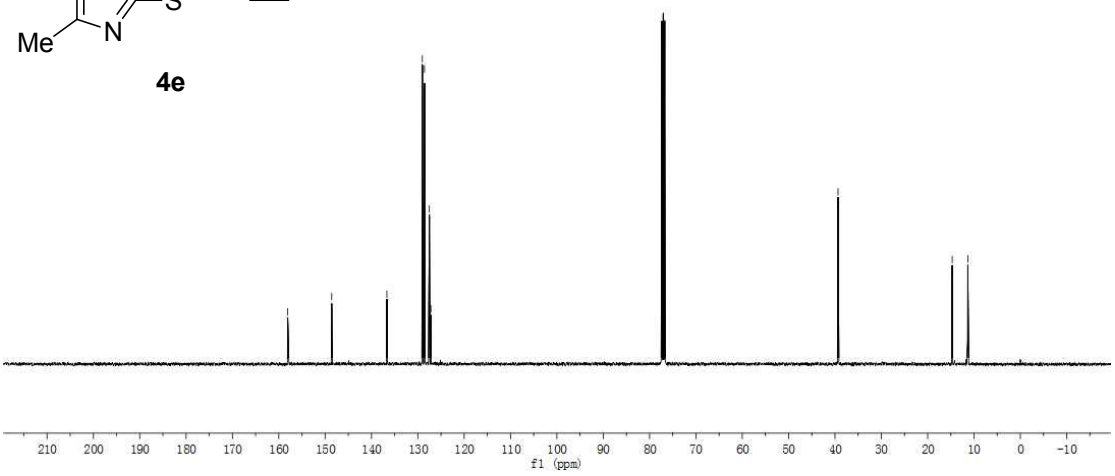

1.90
3.03
2.00
2.93
2.92
f1 (ppm)

4e

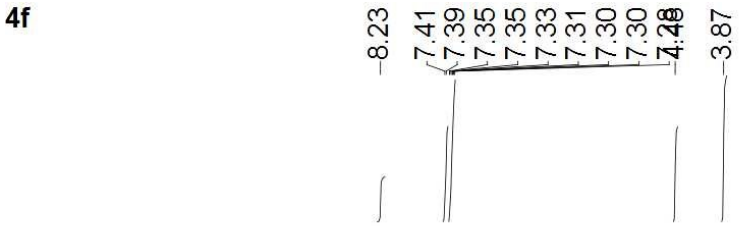

158.07
148.58
136.67
129.03
128.56
127.51
127.18
39.34
14.70
11.34

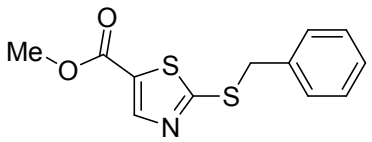

Me
S
S
N
Me

4e

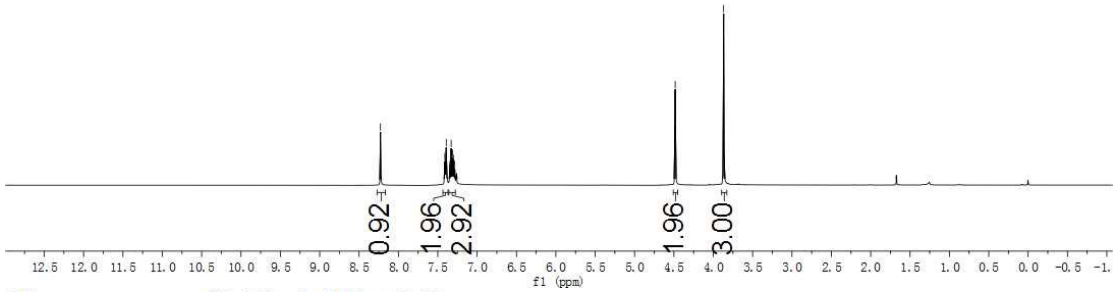

f1 (ppm)

4f

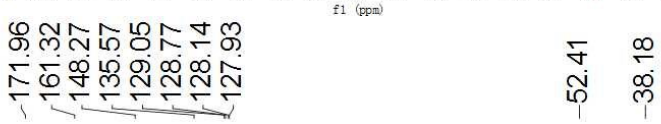

8.23
7.41
7.39
7.35
7.35
7.33
7.31
7.30
7.30
3.87

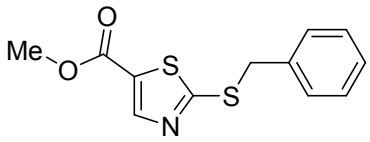

Me
O
O
S
S
N

4f

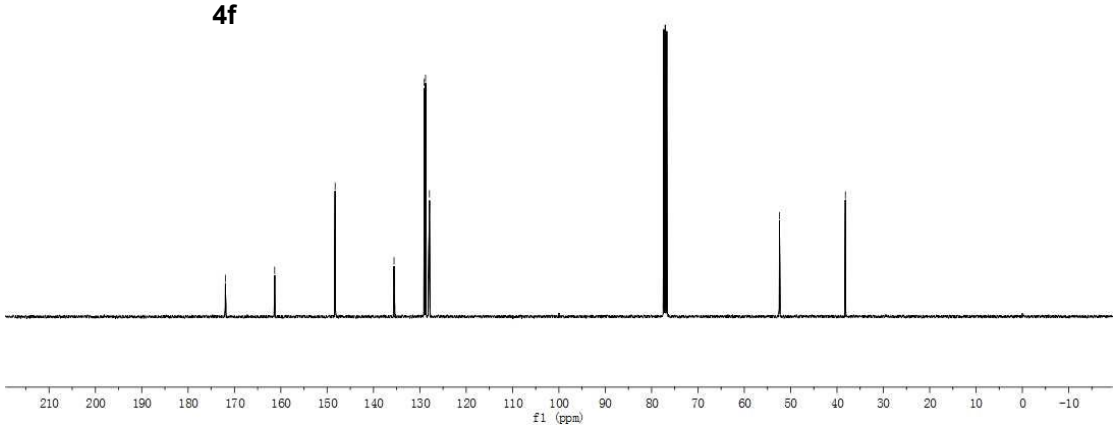

0.92
1.96
2.92
1.96
3.00
f1 (ppm)

4f

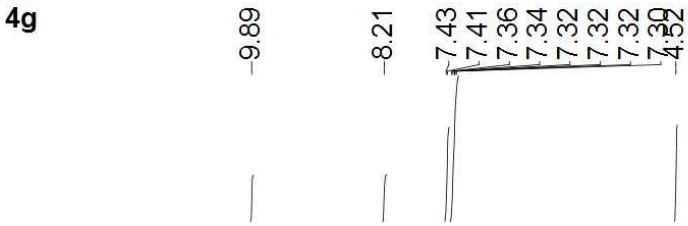

171.96
161.32
148.27
135.57
129.05
128.77
128.14
127.93
52.41
38.18

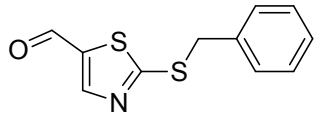

Me
O
O
S
S
N

4f

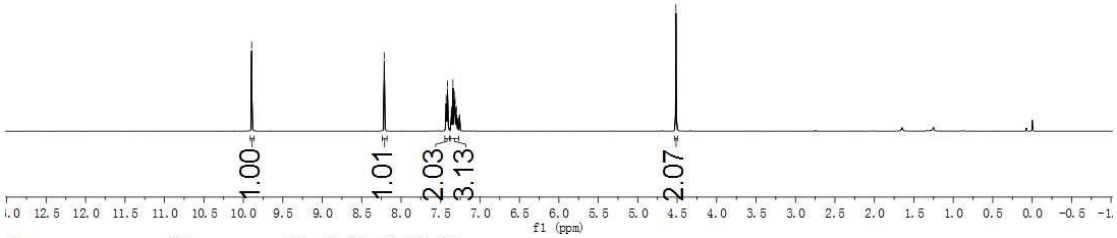

f1 (ppm)

4g


9.89
8.21
7.43
7.41
7.36
7.34
7.32
7.32
7.32
7.30
4.52

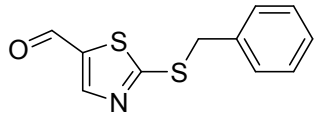

O
S
S
N

4g


1.00
1.01
2.03
3.13
2.07
f1 (ppm)

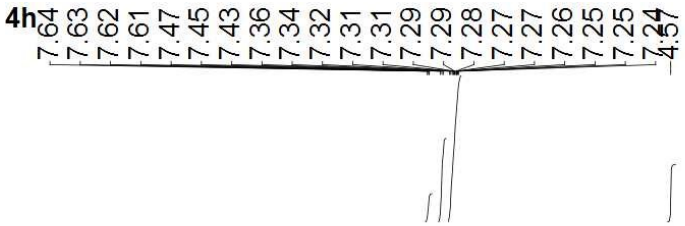
4g


180.96
175.71
151.39
138.74
135.16
129.08
128.85
128.09
38.22


O
S
S
N

4g

f1 (ppm)


4h
7.64
7.63
7.62
7.61
7.47
7.45
7.43
7.36
7.34
7.32
7.31
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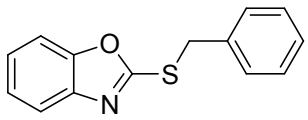
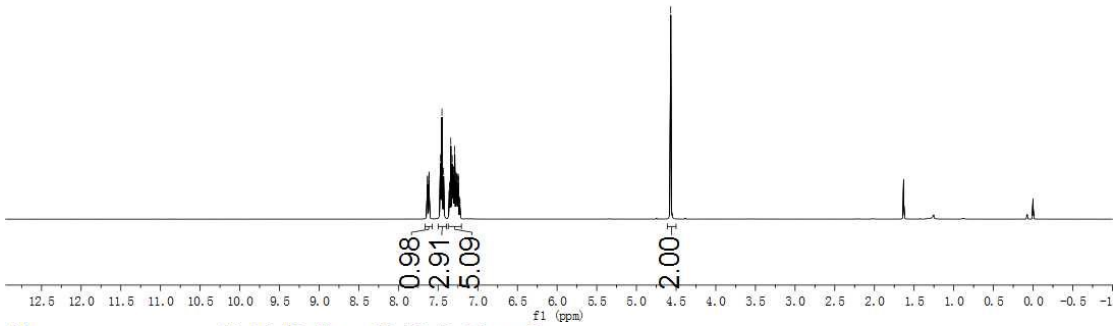
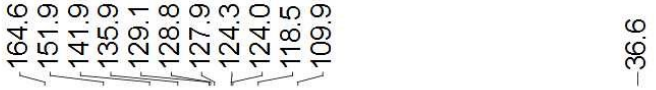
7.27
7.26
7.25
7.25
7.24
4.57

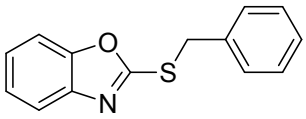

O
S
N

4h


0.98
2.91
5.09
2.00
f1 (ppm)

4h

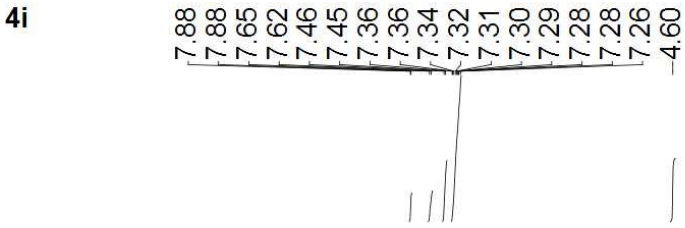

164.6
151.9
141.9
135.9
129.1
128.8
127.9
124.3
124.0
118.5
109.9
36.6

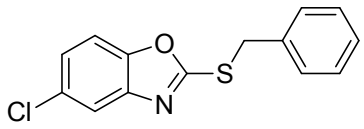

O
S
N

4h

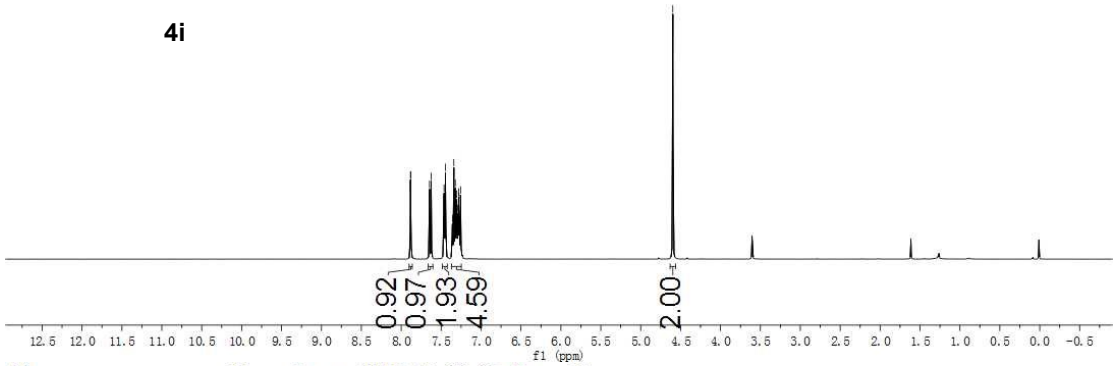
f1 (ppm)

4i

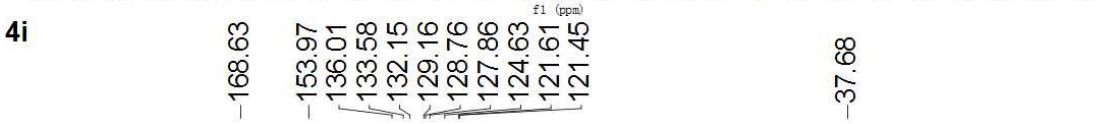

7.88
7.88
7.65
7.62
7.46
7.45
7.36
7.36
7.34
7.32
7.31
7.30
7.29
7.28
7.28
7.26
4.60

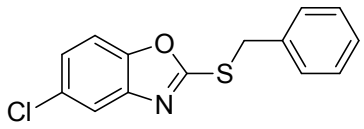

O
S
N
Cl

4i

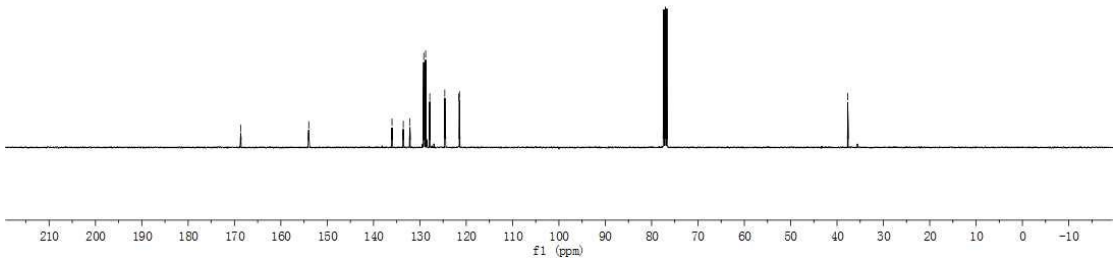

0.92
0.97
1.93
4.59
2.00
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

4i

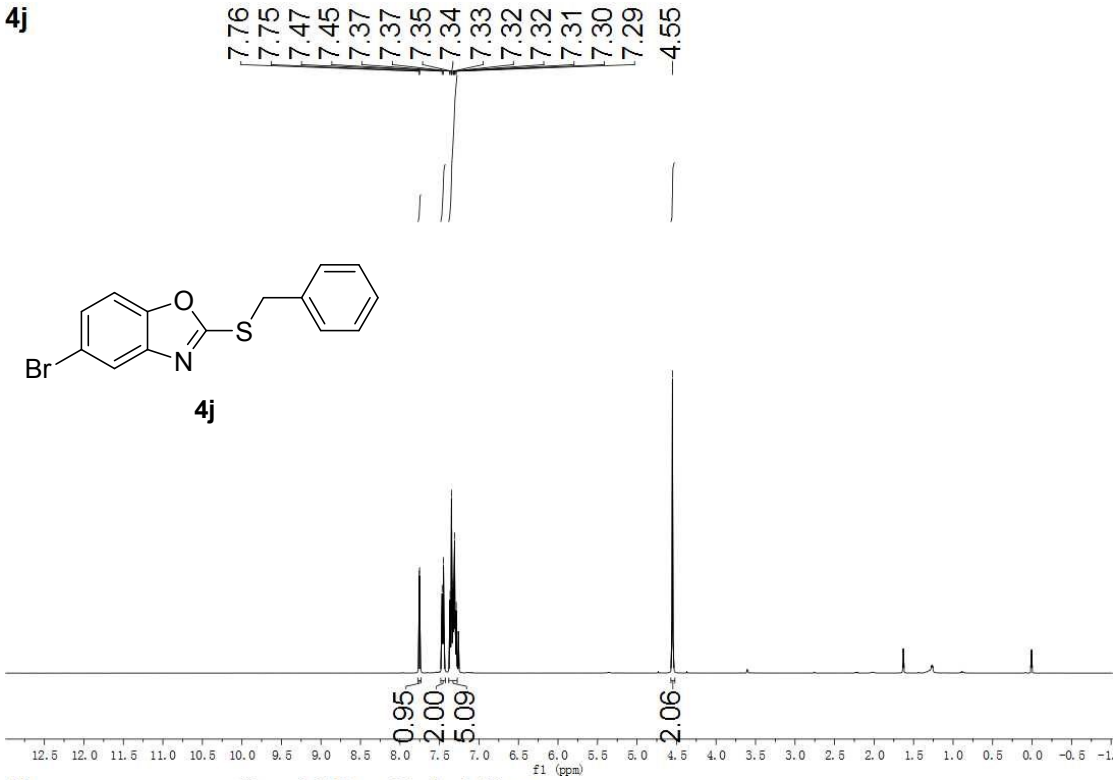

168.63
153.97
136.01
133.58
132.15
129.16
128.76
127.86
124.63
121.61
121.45
37.68


O
S
N
Cl

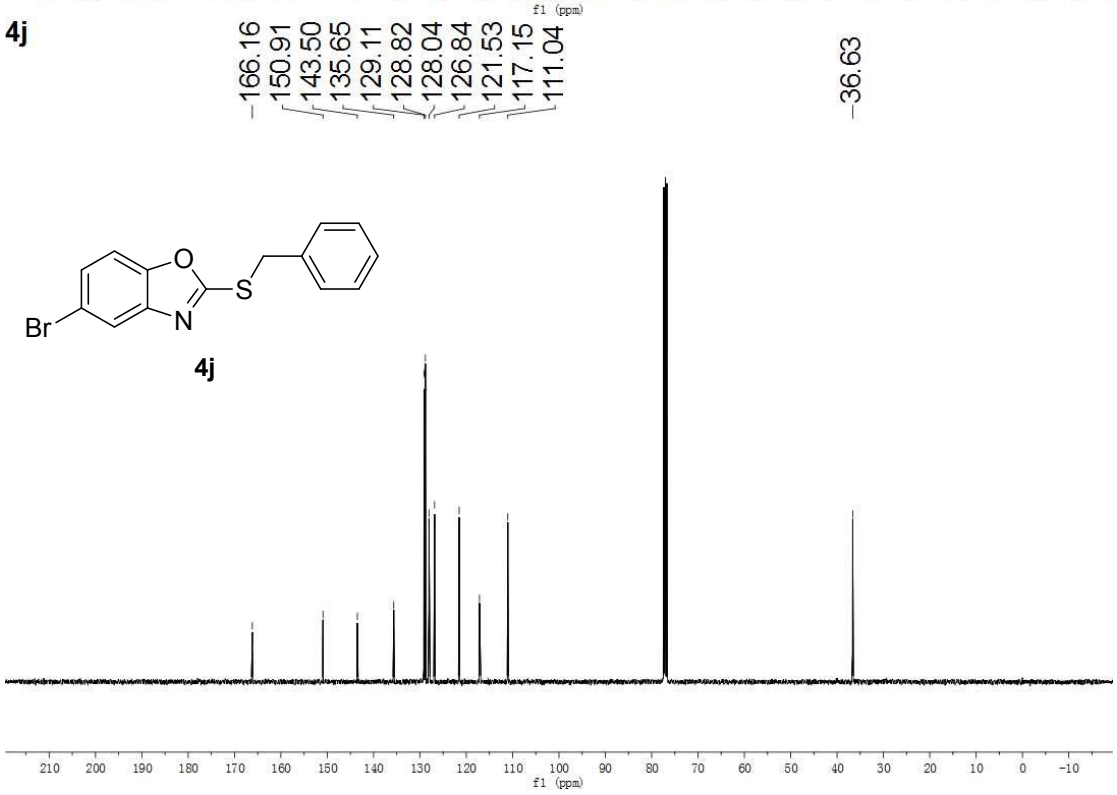
4i


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

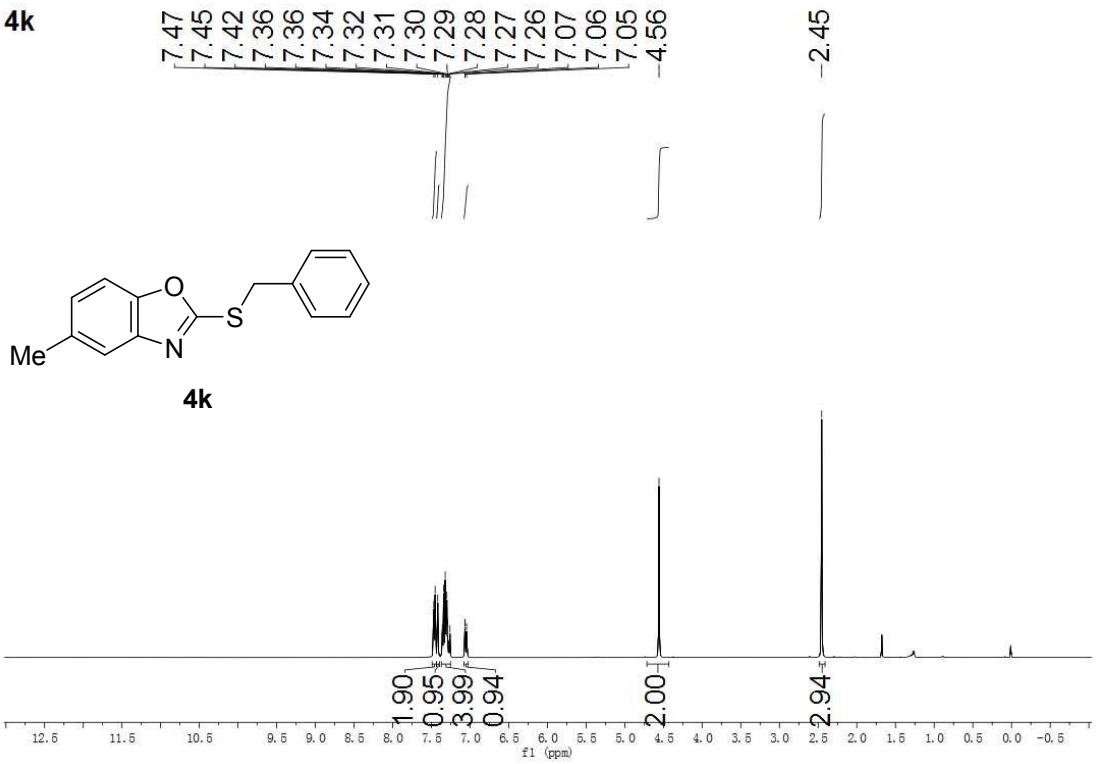
4j


7.76
7.75
7.47
7.45
7.37
7.37
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.29
4.55
O
S
N
Br
0.95
2.00
5.09
2.06
f1 (ppm)

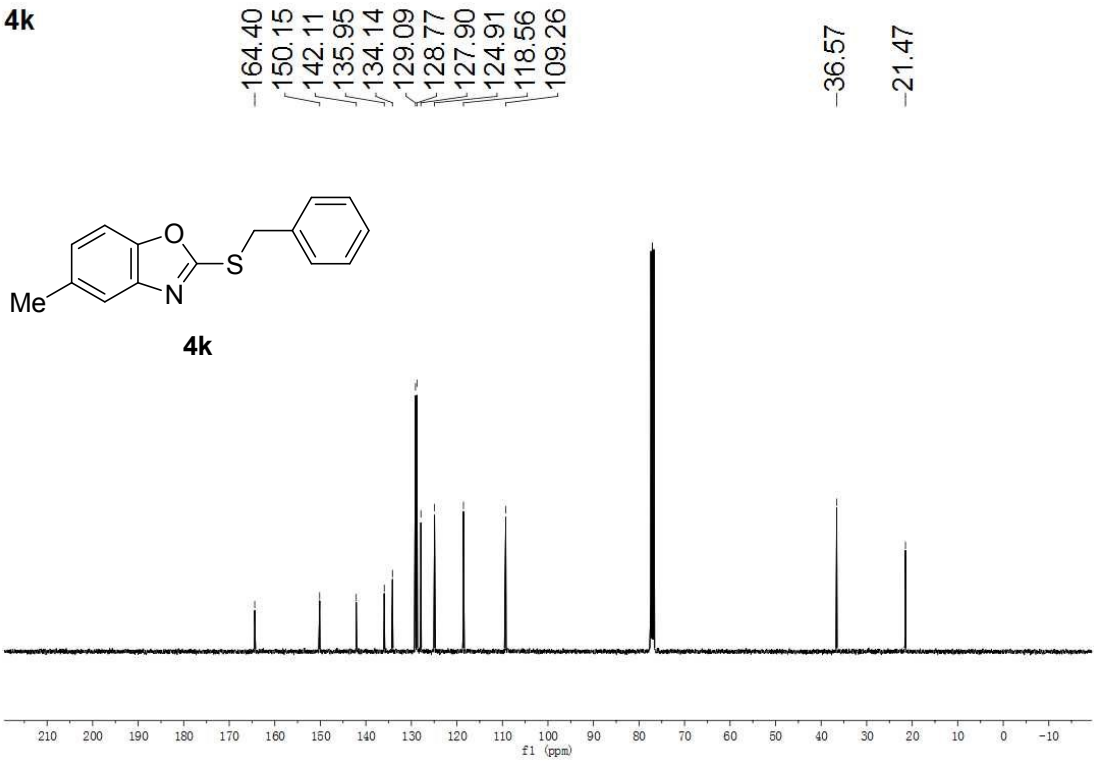
4j


166.16
150.91
143.50
135.65
129.11
128.82
128.04
126.84
121.53
117.15
111.04
36.63
O
S
N
Br
f1 (ppm)

4k

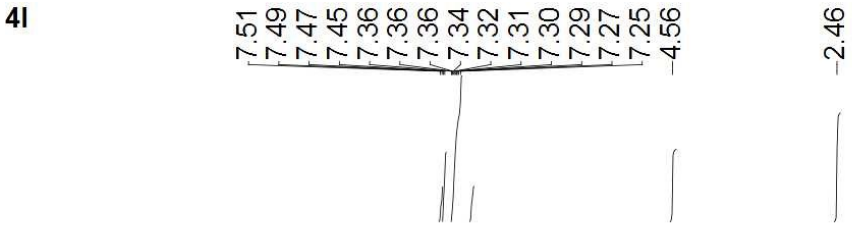

7.47
7.45
7.42
7.36
7.36
7.34
7.32
7.31
7.30
7.29
7.28
7.27
7.26
7.07
7.06
7.05
4.56
2.45
O
S
N
Me
1.90
0.95
3.99
0.94
2.00
2.94
f1 (ppm)

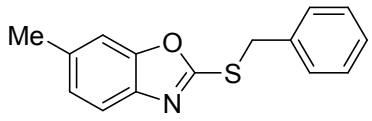
4k


164.40
150.15
142.11
135.95
134.14
129.09
128.77
127.90
124.91
118.56
109.26
36.57
21.47
O
S
N
Me
f1 (ppm)

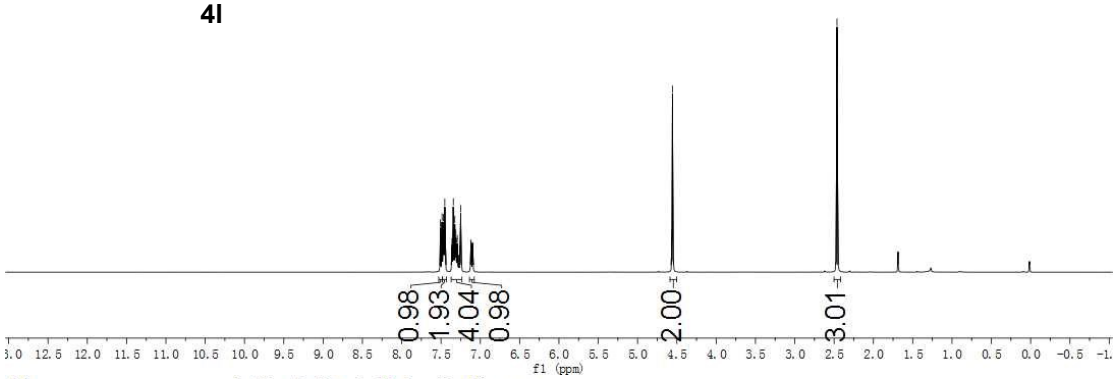
4k

4l

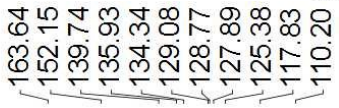

7.51
7.49
7.47
7.45
7.36
7.36
7.36
7.34
7.32
7.31
7.30
7.29
7.27
7.25
4.56
2.46

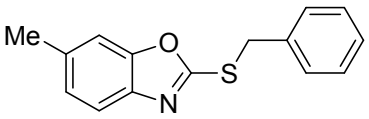

Me
O
S
N

4l

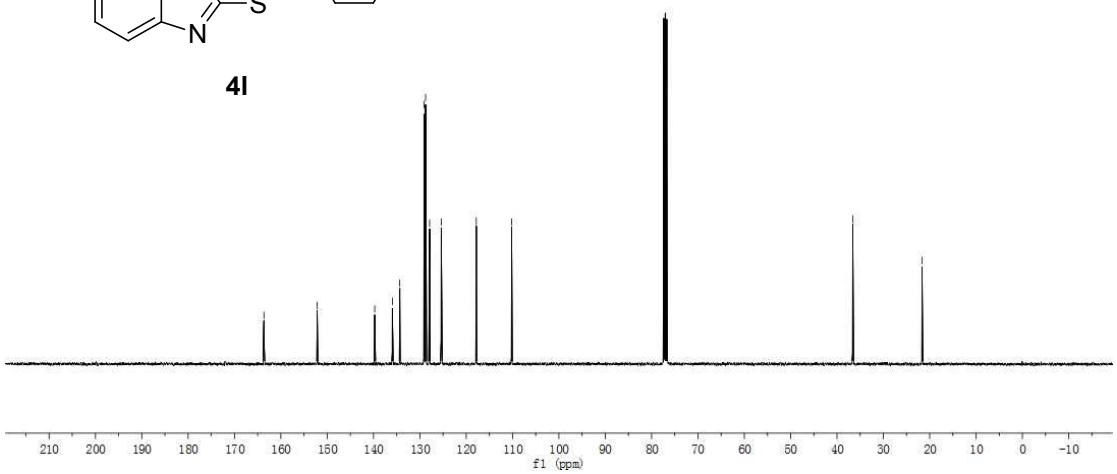

0.98
1.93
4.04
0.98
2.00
3.01
f1 (ppm)

4l

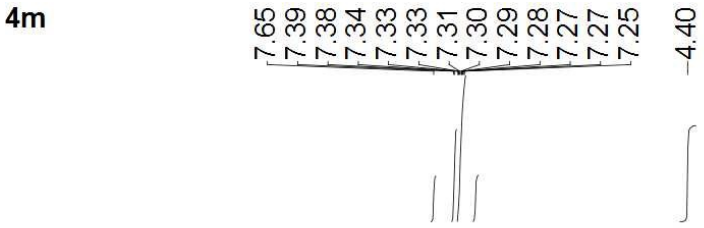

163.64
152.15
139.74
135.93
134.34
129.08
128.77
127.89
125.38
117.83
110.20
36.61
21.65

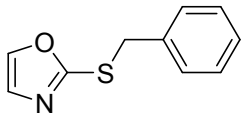

Me
O
S
N

4l

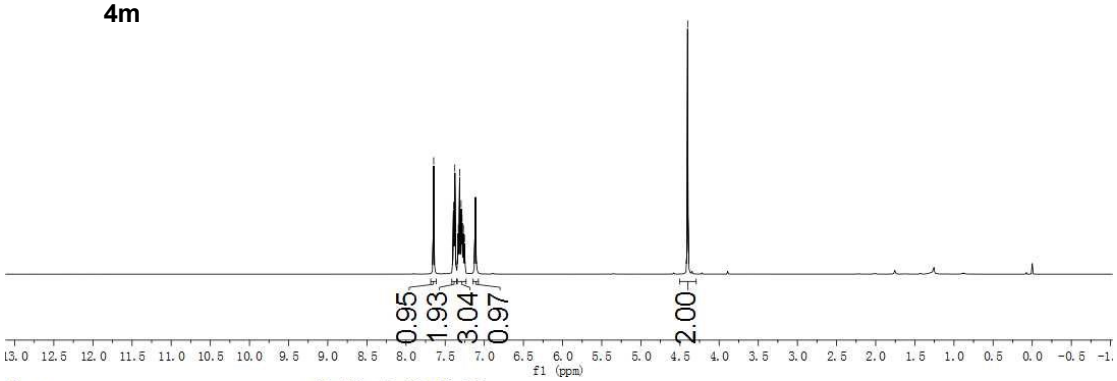

f1 (ppm)

4m

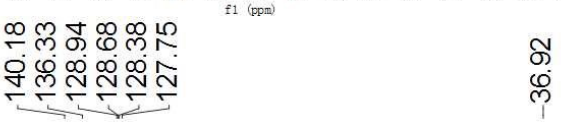

7.65
7.39
7.38
7.34
7.33
7.33
7.31
7.30
7.29
7.28
7.27
7.27
7.25
4.40

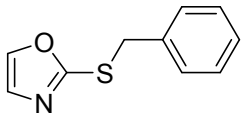

O
S
N

4m

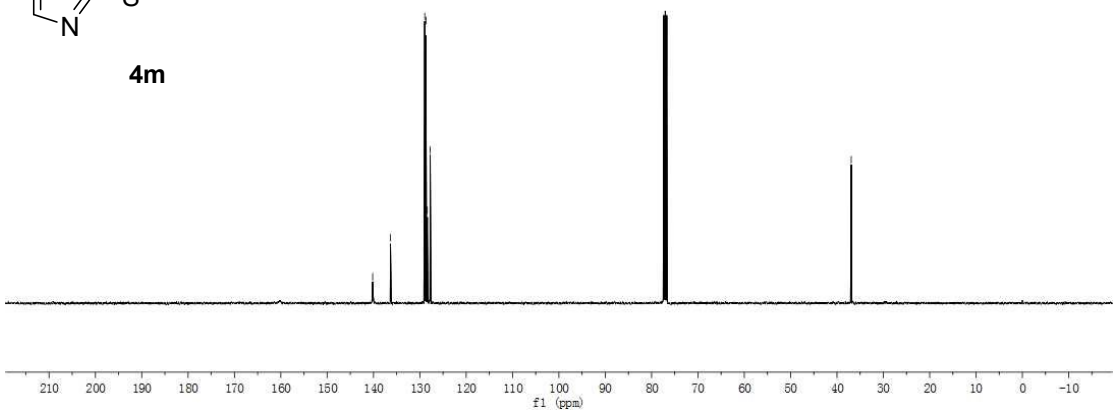

0.95
1.93
3.04
0.97
2.00
f1 (ppm)

4m

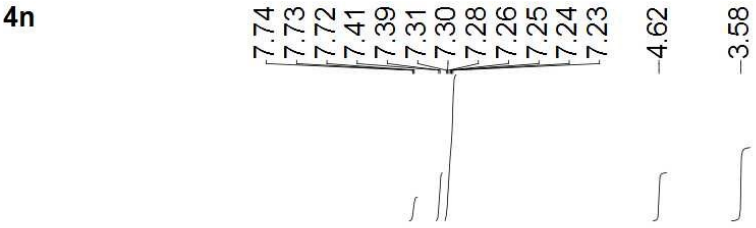

140.18
136.33
128.94
128.68
128.38
127.75
36.92

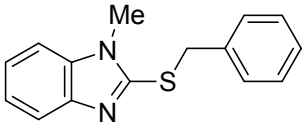

O
S
N

4m

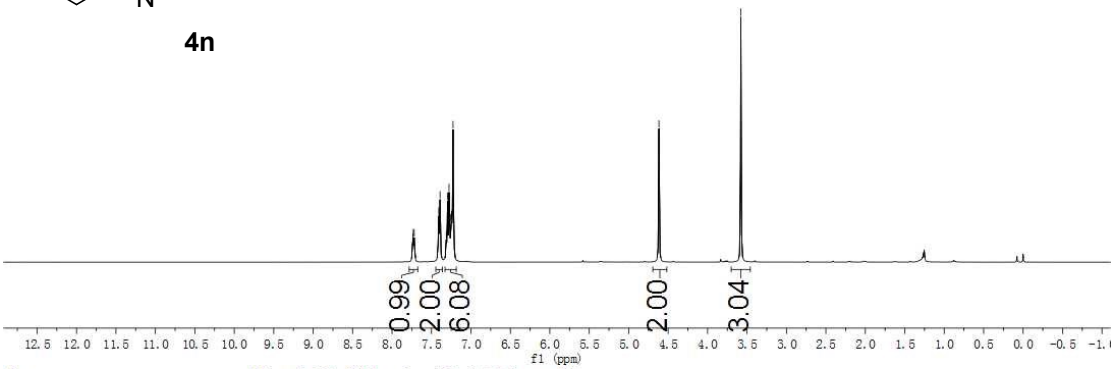

f1 (ppm)

4n

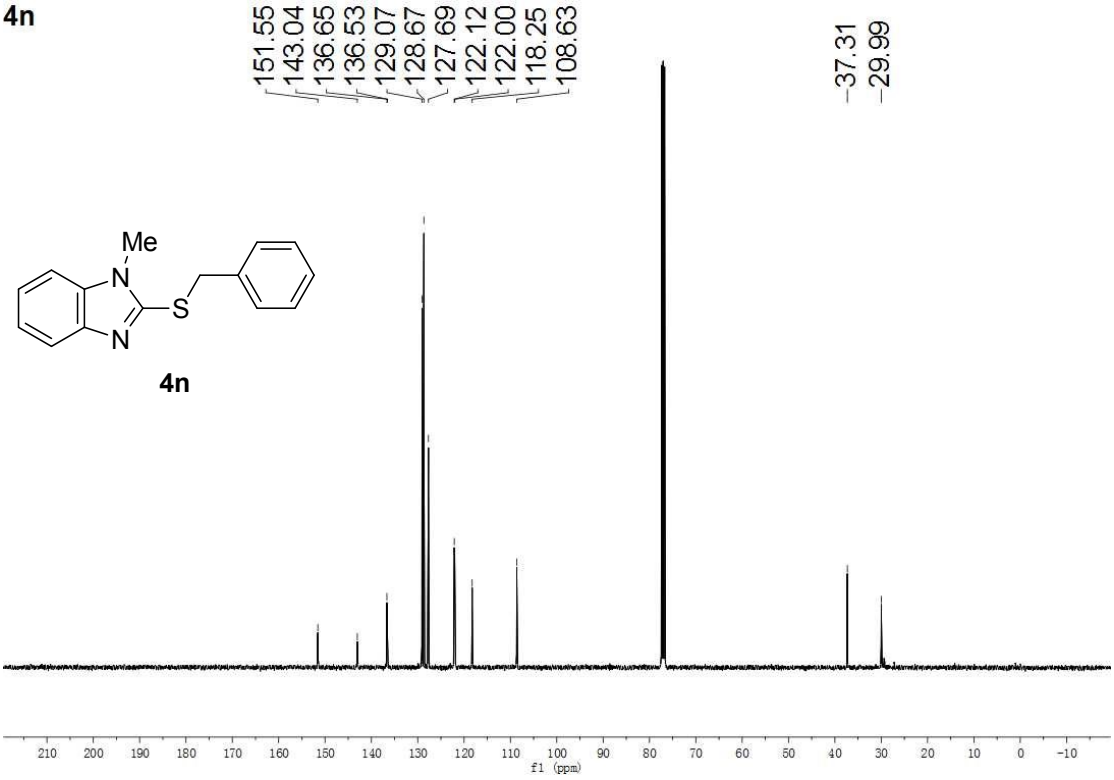

7.74
7.73
7.72
7.41
7.39
7.31
7.30
7.28
7.26
7.25
7.24
7.23
4.62
3.58


Me
N
S
N

4n

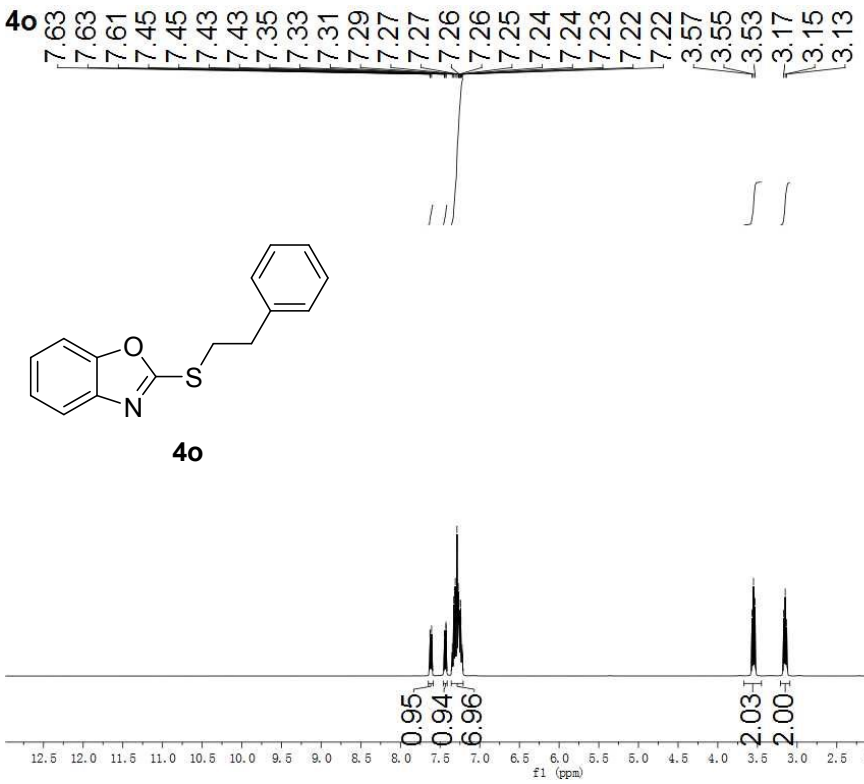

0.99
2.00
6.08
2.00
3.04
f1 (ppm)

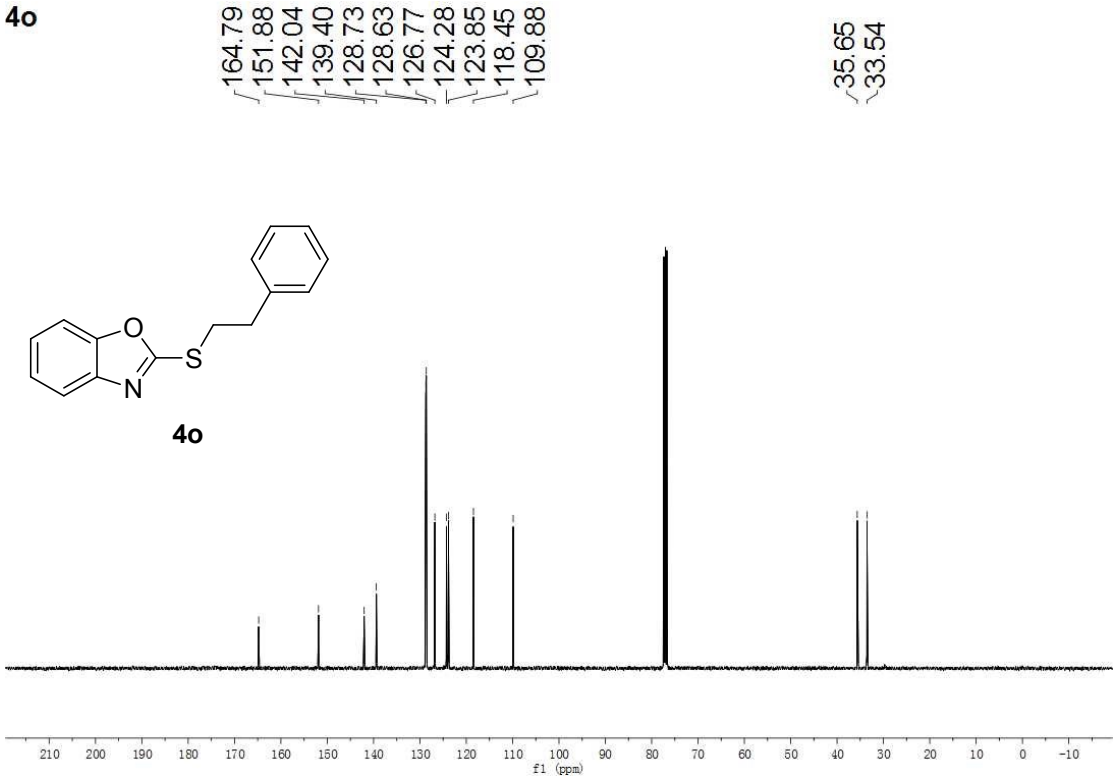
4n

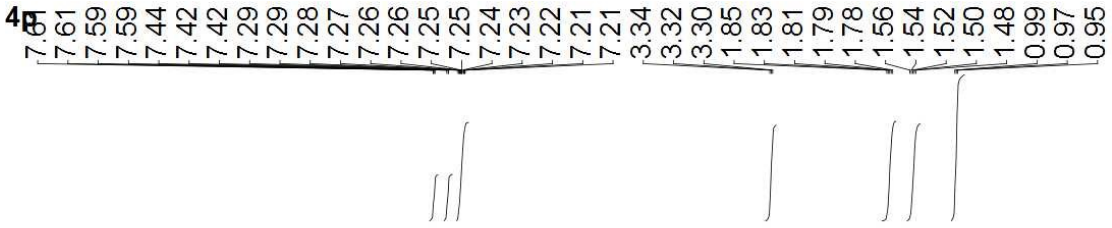

151.55
143.04
136.65
136.53
129.07
128.67
127.69
122.12
122.00
118.25
108.63
37.31
29.99
f1 (ppm)

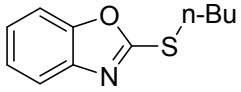
Me
N
S
N

4n

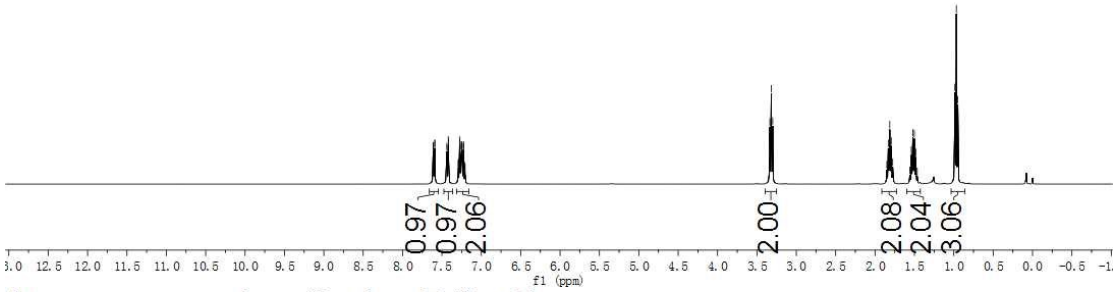

4o
7.63
7.63
7.61
7.45
7.45
7.43
7.43
7.35
7.33
7.31
7.29
7.27
7.27
7.26
7.26
7.25
7.24
7.24
7.23
7.22
7.22
3.57
3.55
3.53
3.17
3.15
3.13
O
S
N
4o
0.95
0.94
6.96
2.03
2.00
f1 (ppm)


4o
164.79
151.88
142.04
139.40
128.73
128.63
126.77
124.28
123.85
118.45
109.88
35.65
33.54
O
S
N
4o
f1 (ppm)


7.61
7.59
7.59
7.44
7.42
7.42
7.29
7.29
7.28
7.27
7.26
7.26
7.25
7.25
7.24
7.23
7.22
7.21
7.21
3.34
3.32
3.30
1.85
1.83
1.81
1.79
1.78
1.56
1.54
1.52
1.50
1.48
0.99
0.97
0.95

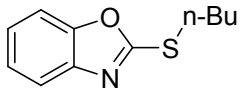

O
S
n-Bu
N

4p

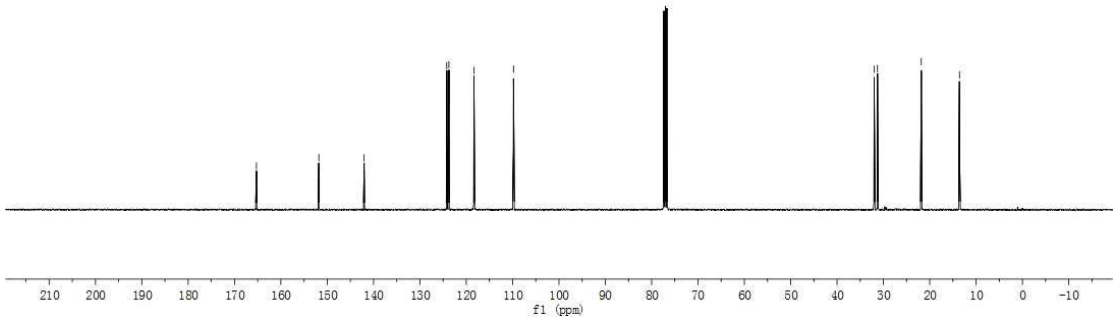

0.97
0.97
2.06
2.00
2.08
2.04
3.06
f1 (ppm)

4p

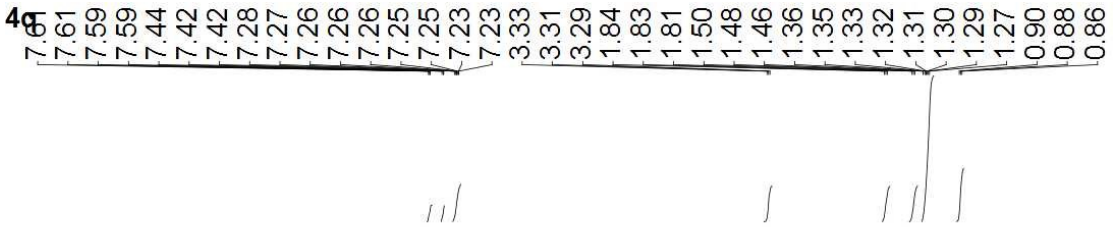

165.27
151.80
142.04
124.20
123.73
118.34
109.80
32.00
31.28
21.83
13.58

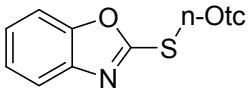

O
S
n-Bu
N

4p

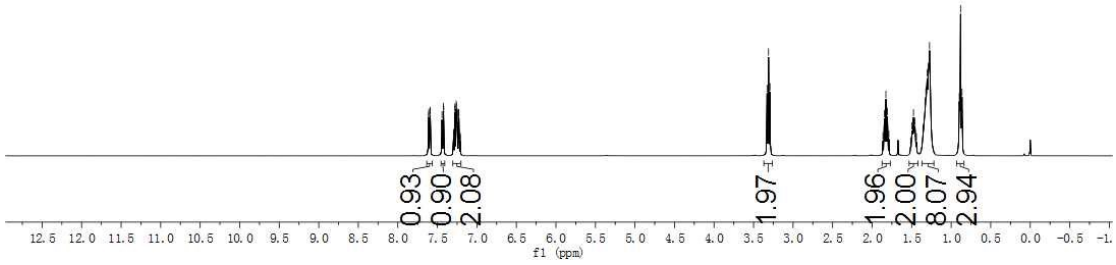

f1 (ppm)

4q


7.61
7.61
7.59
7.59
7.44
7.42
7.42
7.28
7.27
7.26
7.26
7.26
7.25
7.25
7.23
7.23
3.33
3.31
3.29
1.84
1.83
1.81
1.50
1.48
1.46
1.36
1.35
1.33
1.32
1.31
1.30
1.29
1.27
0.90
0.88
0.86

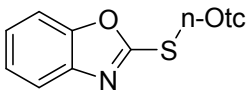

O
S
n-Otc
N

4q


0.93
0.90
2.08
1.97
1.96
2.00
8.07
2.94
f1 (ppm)

4q


165.30
151.82
142.06
124.22
123.75
118.36
109.82
32.32
31.80
29.25
29.14
29.06
28.69
22.66
14.11


O
S
n-Otc
N

4q

f1 (ppm)