Supporting Information

Elemental sulfur mediated 2-substituted benzothiazole formation from 2-aminobenzenethiols and arylacetylenes or styrenes under metal-free conditions

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1. General information

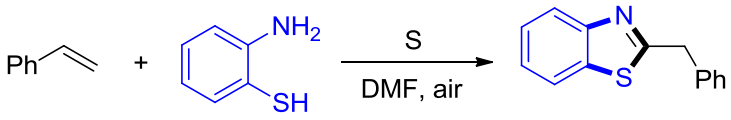
Column chromatography was performed using silica gel 48-75 μm. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker-AV (400 and 100 MHz, respectively) instrument internally referenced to tetramethylsilane (TMS) or chloroform signals. Mass spectra were measured on Agilent 5975 GC-MS instrument (EI). High-resolution mass spectra were recorded at the Institute of Chemistry, Chinese Academy of Sciences. 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. Most reagents were obtained from commercial suppliers and used without further purification.

2. General procedure for benzothiazole synthesis

From arylacetylenes: Ethynylbenzene (**1a**, 23 μL, 0.2 mmol), 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol) , sulfur (12.8 mg, 0.4 mmol), *N*,*N*-dimethylformamide (0.6 mL) were added to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred at 110 ^{o}C for 15 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (5 mL) and washed with saturated sodium chloride solution. The organic layer was separated and the aqueous layer was extracted with ethyl acetate for three times. The combined organic layer was dried over magnesium sulfate and filtered. The volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3aa** as yellow solid (39 mg , 87% yield).

From styrenes: Styrene (**1l**, 24 μL, 0.2 mmol), 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol), sulfur (19.2 mg, 0.6 mmol), $KHCO_3$ (40 mg, 0.4 mmol), *N*,*N*-dimethylformamide (0.6 mL) were added to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred at 110 ^{o}C for 15 h. After cooling to room temperature, the reaction was diluted with ethyl acetate (5 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate for three times. The combined organic layer was dried over magnesium sulfate and filtered. The volatiles were removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3aa** as yellow solid (35 mg , 77% yield).

Table S1 Optimization of the reaction conditions for styrene substrates[a]



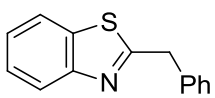
1m **2a** **3ma**

entry	additive	solvent	yield[b] (%)
1	——	DMF	34
2	$KHCO_3$	DMF	56
3	Cs_2CO_3	DMF	25
4	K_2HPO_4	DMF	22
5	C_2H_5ONa	DMF	51
6	$Na_2S_2O_3$	DMF	32
7	$KHCO_3$	NMP	44
8	$KHCO_3$	toluene	8
9	$KHCO_3$	PhCl	11
10	$KHCO_3$	DMSO	trace
11[c]	$KHCO_3$	DMF	66
12[d]	$KHCO_3$	DMF	67
13[e]	$KHCO_3$	DMF	78

[a] Reaction conditions: **1m** (0.2 mmol), **2a** (0.4 mmol), additive (0.2 mmol), solvent (0.6 mL), S (0.4 mmol), 110 °C, under air, 15 h. [b] GC yield. [c] S (0.6 mmol). [d] $KHCO_3$ (0.4 mmol). [e] S (0.6 mmol), $KHCO_3$ (0.4 mmol).

3. Characterization data of products

2-Benzylbenzo[d]thiazole (3aa, CAS: 6265-94-7)[1]



For the ethynylbenzene: The reaction was conducted with ethynylbenzene (**1a**, 23 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product

3aa as yellow solid (39 mg, 87% yield), mp 105-106 ^{o}C.

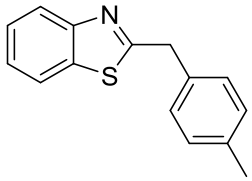
For the styrene: The reaction was conducted with styrene Styrene (**1l**, 24 μL, 0.2 mmol), 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3aa** as yellow solid (35 mg , 77% yield), mp 105-106 ^{o}C.

For the (*E*)-(2-bromovinyl)benzene: The reaction was conducted with (*E*)-(2-bromovinyl)benzene (**1m**, 36.4 μL , 0.2 mmol), 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3aa** as yellow solid (37 mg, 83% yield), mp 105-106 ^{o}C.

For the (*E*)-(2-nitrovinyl)benzene: The reaction was conducted with (*E*)-(2-nitrovinyl)benzene (**1n**, 30 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3aa** as yellow solid (32 mg, 71% yield), mp 105-106 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.2 Hz, 1H), 7.75 (d, J = 8.0 Hz, 1H), 7.45 – 7.39 (m, 1H), 7.37 – 7.31 (m, 4H), 7.31 – 7.23 (m, 2H), 4.41 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.1, 171.1, 153.1, 137.1, 135.5, 129.0, 128.8, 127.2, 125.9, 124.7, 122.6, 121.4, 77.3, 77.0, 76.7, 40.5.

2-(4-Methylbenzyl)benzo[d]thiazole (3ba, CAS: 37859-31-7)[2]

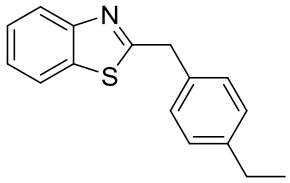


For the 1-ethynyl-4-methylbenzene: The reaction was conducted with 1-ethynyl-4-methylbenzene (**1b**, 24 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3ba** as yellow oil (39 mg, 82% yield).

For the 1-methyl-4-vinylbenzene: The reaction was conducted with 1-methyl-4-vinylbenzene (**1o**, 24 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3ba** as yellow oil (34 mg, 72% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.2 Hz, 1H), 7.81 – 7.75 (m, 1H), 7.47 – 7.42 (m, 1H), 7.36 – 7.30 (m, 1H), 7.28 – 7.21 (m, 1H), 7.17 (d, J = 8.3 Hz, 2H), 7.10 (d, J = 7.4 Hz, 1H), 4.40 (s, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 153.1, 137.0, 135.6, 134.1, 129.5, 129.0, 125.9, 124.8, 122.7, 121.5, 77.3, 77.0, 76.7, 40.2, 21.1.

2-(4-Ethylbenzyl)benzo[d]thiazole (3ca)



The reaction was conducted with 1-ethyl-4-ethynylbenzene (**1c**, 29 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate =40:1) to yield the desired product **3ca** as yellow oil (36 mg, 72% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.2 Hz, 1H), 7.81 – 7.75 (m, 1H), 7.47 – 7.41 (m, 1H), 7.35 – 7.26 (m, 3H), 7.18 (d, J = 8.0 Hz, 2H), 4.40 (s, 2H), 2.68 – 2.60 (m, 2H), 1.23 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 153.2, 143.4, 135.6, 134.3, 129.1, 128.3, 125.9, 124.7, 122.7, 121.5, 77.3, 77.0, 76.7, 40.2, 28.5, 15.5; HRMS (ESI) m/z calcd for $C_{16}H_{16}NS^+$ $(M+H)^+$ 254.09980, found 254.10004.

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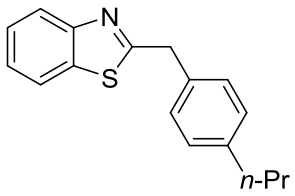
2-(4-Butylbenzyl)benzo[d]thiazole (3da)

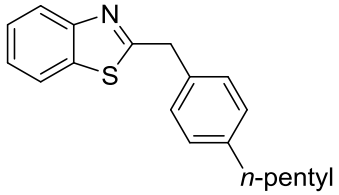


The reaction was conducted with 2-(4-propylbenzyl)benzo[d]thiazole (**1d**, 30 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3da** as yellow oil (38 mg, 67 % yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.2 Hz, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.47 – 7.41 (m, 1H), 7.36 – 7.24 (m, 3H), 7.16 (d, J = 8.0 Hz, 2H), 4.41 (s, 2H), 2.61 – 2.53 (m, 2H), 1.68 – 1.57

(m, 2H), 0.93 (t, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 153.1, 141.8, 135.6, 134.3, 129.0, 128.9, 125.9, 124.8, 122.7, 121.5, 77.3, 77.0, 76.7, 40.2, 37.7, 24.5, 13.8; HRMS (ESI) m/z calcd for $C_{17}H_{18}NS^+$ $(M+H)^+$ 268.11545, found 268.11511.

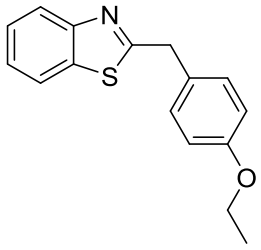
2-(4-Pentylbenzyl)benzo[d]thiazole (3ea)



The reaction was conducted with 1-ethynyl-4-pentylbenzene (**1e**, 35 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3ea** as yellow oil (37 mg, 62% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.1 Hz, 1H), 7.77 (d, J = 8.0 Hz, 1H), 7.48 – 7.41 (m, 1H), 7.36 – 7.23 (m, 3H), 7.16 (d, J = 8.0 Hz, 2H), 4.40 (s, 2H), 2.61 – 2.52 (m, 2H), 1.65 – 1.54 (m, 2H), 1.36 – 1.27 (m, 4H), 0.88 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 153.2, 142.1, 135.6, 134.29, 129.0, 128.9, 125.9, 124.7, 122.7, 121.5, 77.3, 77.0, 76.7, 40.2, 35.5, 31.5, 31.1, 22.5, 14.0; HRMS (ESI) m/z calcd for $C_{19}H_{21}NSNa^+$ $(M+Na)^+$ 318.12869, found 318.12860.

2-(4-Ethoxybenzyl)benzo[d]thiazole (3fa)

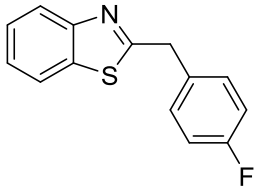


The reaction was conducted with 1-ethoxy-4-ethynylbenzene (**1f**, 30 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 60:1) to yield the desired product **3fa** as yellow oil (38 mg, 70% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.2 Hz, 1H), 7.81 – 7.75 (m, 1H), 7.47 – 7.41 (m, 1H), 7.36

– 7.24 (m, 3H), 6.90 – 6.84 (m, 2H), 4.37 (s, 2H), 4.06 – 3.98 (m, 2H), 1.41 (t, J = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.3, 158.3, 153.2, 135.6, 130.2, 129.1, 125.9, 124.7, 122.7, 121.5, 114.8, 77.3, 77.0, 76.7, 63.4, 39.8, 14.8; HRMS (ESI) m/z calcd for $C_{16}H_{16}NOS^+$ $(M+H)^+$ 270.09471, found 270.09445.

2-(4-Fluorobenzyl)benzo[d]thiazole (3ga, CAS: 37859-33-9)[3]

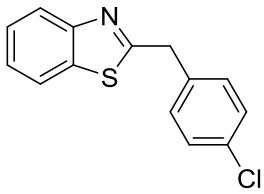


For the 1-ethynyl-4-fluorobenzene: The reaction was conducted with 1-ethynyl-4-fluorobenzene (**1g**, 25 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 70:1) to yield the desired product **3ga** as yellow solid (40 mg, 82 % yield), mp 51-51 ^{o}C.

For the 1-fluoro-4-vinylbenzene: The reaction was conducted with 1-fluoro-4-vinylbenzene (**1p**, 25 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3ga** as yellow solid (24 mg, 50% yield). mp 51-51 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.1 Hz, 1H), 7.81 – 7.76 (m, 1H), 7.49 – 7.42 (m, 1H), 7.37 – 7.29 (m, 3H), 7.07 – 6.99 (m, 2H), 4.40 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 163.3 (d, J = 244.4 Hz), 153.2, 135.5, 132.9 (d, J = 3.3 Hz), 130.7 (d, J = 80.5 Hz), 126.0, 124.9, 122.8, 121.5, 115.8 (d, J = 21.3 Hz), 77.3, 77.0, 76.7, 39.7.

2-(4-Chlorobenzyl)benzo[d]thiazole (3ha, CAS: 17142-76-6)[4]



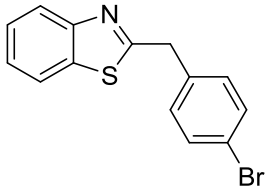
For the 1-chloro-4-ethynylbenzene: The reaction was conducted with 1-chloro-4-ethynylbenzene (**1h**, 28 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired

product **3ha** as yellow oil (39 mg, 76% yield).

For the 1-chloro-4-vinylbenzene: The reaction was conducted with 1-chloro-4-vinylbenzene (**1q**, 28 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3ha** as yellow oil (35 mg, 68% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.1 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.50 – 7.42 (m, 1H), 7.39 – 7.26 (m, 5H), 4.41 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 153.1, 135.6, 135.5, 133.3, 130.5, 129.0, 126.1, 125.0, 122.8, 121.5, 77.3, 77.0, 76.7, 39.8.

2-(4-Bromobenzyl)benzo[d]thiazole (3ia, CAS: 37859-32-8)[5]

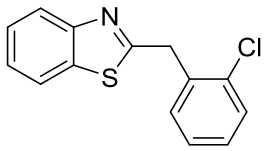


For the 1-bromo-4-ethynylbenzene: The reaction was conducted with 1-bromo-4-ethynylbenzene (**1i**, 36 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3ia** as yellow solid (49 mg, 82% yield), mp 55-56 ^{o}C.

For the 1-bromo-4-vinylbenzene: The reaction was conducted with 1-bromo-4-vinylbenzene (**1r**, 36.4 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3ia** as yellow solid (50 mg, 82% yield), mp 55-56 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.1 Hz, 1H), 7.81 (d, J = 7.9 Hz, 1H), 7.47 (t, J = 6.9 Hz, 3H), 7.36 (t, J = 7.5 Hz, 1H), 7.25 (d, J = 8.6 Hz, 2H), 4.40 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 153.1, 136.1, 135.5, 132.0, 130.8, 126.1, 125.0, 122.8, 121.6, 121.4, 77.3, 77.0, 76.7, 39.9.

2-(2-Chlorobenzyl)benzo[d]thiazole (3ja)[4]



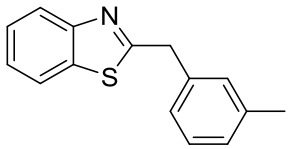
For the 1-chloro-2-ethynylbenzene: The reaction was conducted with 1-chloro-2-ethynylbenzene (**1j**, 28 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3ja** as yellow oil (43 mg, 83% yield).

For the 1-chloro-2-vinylbenzene: The reaction was conducted with 1-chloro-2-vinylbenzene (**1t**, 28 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3ja** as yellow oil (42 mg, 82% yield).

For the (*E*)-1-chloro-2-(2-nitrovinyl)benzene: The reaction was conducted with (*E*)-1-chloro-2-(2-nitrovinyl)benzene (**1u**, 37 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3ja** as yellow oil (34 mg, 65 % yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.49 – 7.42 (m, 1H), 7.39 – 7.30 (m, 2H), 7.28 – 7.22 (m, 3H), 4.40 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 153.1, 139.0, 135.6, 134.6, 130.1, 129.2, 127.5, 127.3, 126.1, 125.0, 122.8, 121.5, 77.3, 77.0, 76.7, 40.0; HRMS (ESI) m/z calcd for $C_{14}H_{11}ClNS^+$ $(M+H)^+$ 260.02952, found 260.02930.

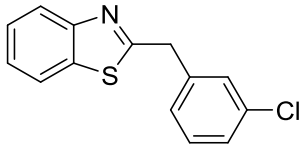
2-(3-Methylbenzyl)benzo[d]thiazole (3ka)



The reaction was conducted with 1-ethynyl-3-methylbenzene (**1k**, 24μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3ka** as yellow oil (37 mg, 77% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.2 Hz, 1H), 7.81 – 7.75 (m, 1H), 7.47 – 7.42 (m, 1H), 7.36 – 7.30 (m, 1H), 7.28 – 7.21 (m, 1H), 7.17 (d, J = 8.3 Hz, 2H), 7.10 (d, J = 7.4 Hz, 1H), 4.40 (s, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 153.2, 138.5, 137.0, 135.6, 129.9, 128.7, 128.1, 126.1, 125.9, 124.8, 122.7, 121.5, 77.3, 77.0, 76.7, 40.5, 21.4; HRMS (ESI) m/z calcd for $C_{15}H_{14}NS^+$ $(M+H)^+$ 240.08415, found 240.08415.

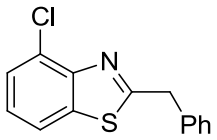
2-(3-Chlorobenzyl)benzo[d]thiazole (3sa)



The reaction was conducted with 1-chloro-3-vinylbenzene (**1s**, 28 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3sa** as yellow oil (44 mg, 85% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.50 – 7.43 (m, 1H), 7.39 – 7.31 (m, 2H), 7.29 – 7.23 (m, 3H), 4.40 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.8, 153.1, 139.0, 135.6, 134.6, 130.1, 129.2, 127.5, 127.3, 126.1, 125.0, 122.8, 121.5, 77.3, 77.0, 76.7, 40.0; HRMS (ESI) m/z calcd for $C_{14}H_{11}ClNS^+$ $(M+H)^+$ 260.02952, found 260.02933.

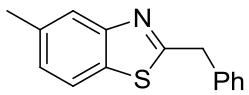
2-Benzyl-4-chlorobenzo[d]thiazole (3ab, CAS: 1239844-05-3)[3]



The reaction was conducted with acetylene (**1a**, 23 μL, 0.2 mmol) and 4-chlorobenzo[d]thiazole (**2b**, 68 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3ab** as yellow oil (37 mg, 72% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.63 (m, 1H), 7.49 – 7.45 (m, 1H), 7.39 – 7.33 (m, 4H), 7.33 – 7.28 (m, 1H), 7.28 – 7.22 (m, 1H), 4.50 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.0, 150.1, 137.1, 136.9, 129.2, 128.9, 127.5, 127.4, 126.2, 125.3, 120.0, 77.3, 77.0, 76.7, 40.7.

2-Benzyl-5-methylbenzo[d]thiazole (3ac)

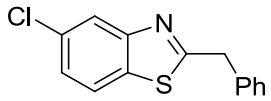


The reaction was conducted with acetylene (**1a**, 23 μL, 0.2 mmol) and 2-amino-4-methylbenzenethiol (**2c**, 56 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product

3ac as yellow oil (35 mg, 73% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 1H), 7.64 (d, J = 8.2 Hz, 1H), 7.38 – 7.31 (m, 4H), 7.30 – 7.25 (m, 1H), 7.17 – 7.13 (m, 1H), 4.42 (s, 2H), 2.48 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.3, 153.5, 137.2, 136.0, 132.5, 129.1, 128.8, 127.2, 126.4, 122.7, 121.0, 77.3, 77.0, 76.7, 40.6, 21.4; HRMS (ESI) m/z calcd for $C_{15}H_{14}NS^+$ $(M+H)^+$ 240.08415, found 240.08420.

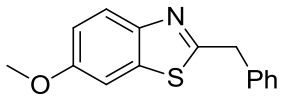
2-Benzyl-5-chlorobenzo[d]thiazole (3ad, CAS: 1857-54-1)[3]



The reaction was conducted with acetylene (**1a**, 23 μL, 0.2 mmol) and 2-amino-4-chlorobenzenethiol (**2d**, 62 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) yield the desired product **3ad** as yellow solid (35 mg, 67% yield), mp 69-70 ^{o}C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.7 Hz, 1H), 7.73 (d, J = 2.0 Hz, 1H), 7.41 – 7.37 (m, 1H), 7.37 – 7.32 (m, 4H), 7.32 – 7.26 (m, 1H), 4.41 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 151.7, 136.8, 130.7, 129.1, 128.9, 127.5, 126.7, 123.5, 121.1, 77.3, 77.0, 76.7, 40.5.

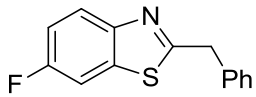
2-Benzyl-6-methoxybenzo[d]thiazole (3ae)



The reaction was conducted with and acetylene (**1a**, 23 μL, 0.2 mmol) and 2-amino-5-methoxybenzenethiol (**2e**, 62 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **3ae** as yellow oil (35 mg, 68% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (d, J = 8.9 Hz, 1H), 7.39 – 7.32 (m, 4H), 7.31 – 7.26 (m, 1H), 7.24 (d, J = 2.5 Hz, 1H), 7.08 – 7.01 (m, 1H), 4.40 (s, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 157.4, 147.5, 137.3, 136.9, 129.1, 128.8, 127.3, 123.1, 115.1, 104.2, 77.3, 77.0, 76.7, 55.8, 40.4; HRMS (ESI) m/z calcd for $C_{15}H_{14}NOS^+$ $(M+H)^+$ 256.07906, found 256.07962.

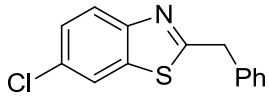
2-Benzyl-6-fluorobenzo[d]thiazole (3af)



The reaction was conducted with and acetylene (**1a**, 23 μL, 0.2 mmol) and 2-amino-5-fluorobenzenethiol (**2f**, 57 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3af** as yellow oil (37 mg, 76% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 – 7.89 (m, 1H), 7.48 – 7.42 (m, 1H), 7.38 – 7.33 (m, 4H), 7.33 – 7.26 (m, 1H), 7.21 – 7.13 (m, 1H), 4.41 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.9, 161.4 (d, J = 243.6 Hz), 149.8, 136.9, 136.6 (d, J = 11.0 Hz), 129.1 (d, J = 22.0 Hz), 127.4, 123.6 (d, J = 9.3 Hz), 114.7 (d, J = 24.5 Hz), 107.8 (d, J = 26.5 Hz), 77.3, 77.0, 76.7, 40.5; HRMS (ESI) m/z calcd for $C_{14}H_{12}FNS^+$ $(M+H)^+$ 245.06690, found 244.05894.

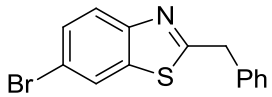
2-Benzyl-6-chlorobenzo[d]thiazole (3ag)



The reaction was conducted with acetylene (**1a**, 23 μL, 0.2 mmol) and 2-amino-5-chlorobenzenethiol (**2g**, 63 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3ag** as yellow oil (44 mg, 85% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.7 Hz, 1H), 7.73 (d, J = 2.0 Hz, 1H), 7.41 – 7.37 (m, 1H), 7.37 – 7.32 (m, 4H), 7.32 – 7.26 (m, 1H), 4.41 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 151.7, 136.8, 130.7, 129.1, 128.9, 127.5, 126.7, 123.5, 121.1, 77.3, 77.0, 76.7, 40.5; HRMS (ESI) m/z calcd for $C_{14}H_{11}ClNS^+$ $(M+H)^+$ 260.02952, found 260.02930.

2-Benzyl-6-bromobenzo[d]thiazole (3ah)

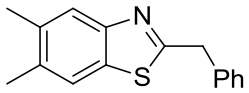


The reaction was conducted with acetylene (**1a**, 23 μL, 0.2 mmol) and 2-amino-5-bromobenzenethiol (**2h**, 82 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product

3ah as yellow liquid (35 mg, 58% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (t, J = 2.2 Hz, 1H), 7.84 (d, J = 8.7 Hz, 1H), 7.57 – 7.52 (m, 1H), 7.36 (d, J = 4.5 Hz, 4H), 7.34 – 7.28 (m, 1H), 4.41 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 152.1, 137.3, 136.8, 129.4, 129.1, 128.9, 127.5, 124.0, 123.9, 118.4, 77.3, 77.0, 76.7, 40.5; HRMS (ESI) m/z calcd for $C_{14}H_{11}BrNS^+$ $(M+H)^+$ 303.97901, found 303.97818.

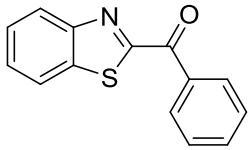
2-(6-Bromoquinolin-2-yl)-6-(*tert*-butyl)benzo[d]thiazole (3ai)



The reaction was conducted with 4-tert-butylaniline acetylene (**1a**, 23 μL, 0.2 mmol) and 2-amino-4,5-dimethylbenzenethiol (**2i**, 61 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **3ai** as yellow oil (45 mg, 90% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (s, 1H), 7.51 (s, 1H), 7.38 – 7.24 (m, 5H), 4.40 (s, 2H), 2.35 (d, J = 13.3 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.9, 151.9, 137.4, 135.1, 134.2, 133.0, 129.1, 128.8, 127.2, 122.9, 121.4, 77.3, 77.0, 76.7, 40.5, 20.1, 20.0; HRMS (ESI) m/z calcd for $C_{16}H_{16}NS^+$ $(M+H)^+$ 254.09980, found 254.09978.

Benzo[d]thiazol-2-yl(phenyl)methanone (4a, CAS: 1629-75-0)[6]

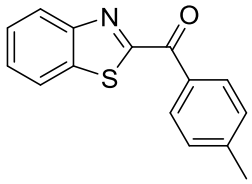


Acetylene (23 μL, 0.2 mmol), 2-aminobenzenethiol (50 μL, 0.4 mmol), sulfur (12.8 mg, 0.4 mmol), *N*,*N*-dimethylformamide (0.5 mL) were added to a 10 mL oven-dried reaction vessel. The sealed reaction vessel was stirred at 110 ^{o}C for 15 h. And then cuprous iodide (3.8 mg, 20 mol%), acetic acid (24 μL, 0.4 mmol), dimethyl sulfoxide (0.5 mL) were added to the reaction vessel. The sealed reaction vessel was stirred at 110 ^{o}C for 24 h under O_2. After cooling to room temperature, the reaction was diluted with ethyl acetate (5 mL) and washed with saturated sodium chloride solution. The organic layer was separated, and the aqueous layer was extracted with ethyl acetate for three times. The combined organic layer was dried over magnesium sulfate , the volatiles were

removed under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **4a** as white solid (40 mg , 83% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 – 8.53 (m, 2H), 8.28 – 8.23 (m, 1H), 8.06 – 8.01 (m, 1H), 7.72 – 7.65 (m, 1H), 7.63 – 7.52 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.3, 167.1, 153.9, 137.0, 134.9, 133.8, 131.2, 128.5, 127.6, 126.9, 125.7, 122.1, 77.3, 77.0, 76.7.

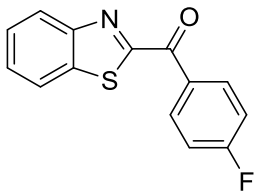
Benzo[d]thiazol-2-yl(*p*-tolyl)methanone (4b, CAS: 33429-09-3)[6]



The reaction was conducted with 1-ethynyl-4-methylbenzene (**1b**, 24 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 40:1) to yield the desired product **4b** as yellow solid (41 mg, 81% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 – 8.45 (m, 2H), 8.26 – 8.21 (m, 1H), 8.01 (d, J = 7.8 Hz, 1H), 7.61 – 7.50 (m, 2H), 7.36 (d, J = 8.1 Hz, 2H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.9, 167.4, 153.9, 145.0, 137.0, 132.4, 131.4, 129.2, 127.5, 126.8, 125.6, 122.1, 77.3, 77.0, 76.7, 21.8.

Benzo[d]thiazol-2-yl(4-fluorophenyl)methanone (4c)[6]

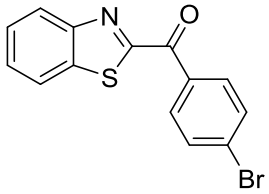


The reaction was conducted with 1-ethynyl-4-fluorobenzene (**1g**, 25 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **4c** as white solid (40 mg, 78 % yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 – 8.61 (m, 2H), 8.28 – 8.18 (m, 1H), 8.05 – 7.96 (m, 1H), 7.63 – 7.50 (m, 2H), 7.29 – 7.19 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 183.5, 167.7 (d, J = 255.2

Hz), 153.8, 137.0, 134.2 (d, *J* = 9.4 Hz), 131.3 (d, *J* = 2.9 Hz), 127.7, 127.0, 125.7, 122.2, 115.8 (d, *J* = 21.7 Hz), 77.3, 77.0, 76.7.

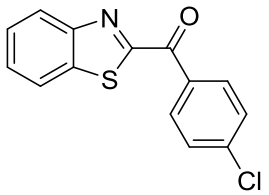
Benzo[d]thiazol-2-yl(4-bromophenyl)methanone (4d, CAS: 140935-32-6)[7]



The reaction was conducted with 1-bromo-4-ethynylbenzene (**1i**, 36 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **4d** as white solid (45 mg, 71% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 – 8.45 (m, 2H), 8.26 – 8.22 (m, 1H), 8.03 (d, *J* = 7.9 Hz, 1H), 7.71 (d, *J* = 8.6 Hz, 2H), 7.64 – 7.53 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.2, 166.8, 153.8, 137.1, 133.7, 132.8, 131.9, 129.5, 127.8, 127.0, 125.8, 122.2, 77.3, 77.0, 76.7.

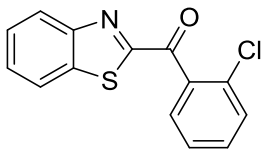
Benzo[d]thiazol-2-yl(4-chlorophenyl)methanone (4e, CAS: 33429-11-7)[6]



The reaction was conducted with 1-chloro-4-ethynylbenzene (**1h**, 28 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **4e** as white solid (40 mg, 74% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 – 8.54 (m, 2H), 8.27 – 8.21 (m, 1H), 8.05 – 8.00 (m, 1H), 7.63 – 7.52 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.0, 166.8, 153.8, 140.6, 137.0, 133.2, 132.7, 128.8, 127.8, 127.0, 125.7, 122.2, 77.3, 77.0, 76.7.

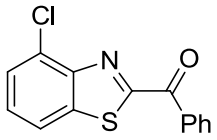
Benzo[d]thiazol-2-yl(2-chlorophenyl)methanone (4f, CAS: 443988-37-1)[6]



The reaction was conducted with 1-chloro-2-ethynylbenzene (**1j**, 28 μL, 0.2 mmol) and 2-aminobenzenethiol (**2a**, 50 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **4f** as white solid (41 mg, 75% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 – 8.13 (m, 1H), 8.06 – 7.98 (m, 1H), 7.79 – 7.73 (m, 1H), 7.60 – 7.49 (m, 4H), 7.46 – 7.40 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.6, 165.9, 153.7, 137.4, 136.0, 132.6, 132.4, 130.8, 130.5, 128.0, 127.1, 126.5, 125.9, 122.3, 77.3, 77.0, 76.7.

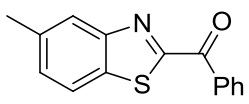
(4-Chlorobenzo[d]thiazol-2-yl)(phenyl)methanone (4g)[3]



The reaction was conducted with acetylene (**1a**, 23 μL , 0.2 mmol) and 4-chlorobenzo[d]thiazole (**2b**, 68 μL, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **4g** as white solid (44 mg, 80% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 – 8.64 (m, 2H), 7.93 – 7.86 (m, 1H), 7.72 – 7.65 (m, 1H), 7.63 – 7.55 (m, 3H), 7.50 – 7.43 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.5, 167.8, 151.0, 138.4, 134.6, 134.2, 131.5, 130.6, 128.6, 128.1, 127.1, 120.7, 77.3, 77.0, 76.7.

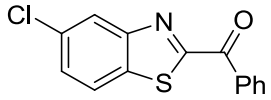
(5-Methylbenzo[d]thiazol-2-yl)(phenyl)methanone (4h)[8]



The reaction was conducted with acetylene (**1a**, 23 μL, 0.2 mmol) and 2-amino-4-methylbenzenethiol (**2c**, 56 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **4h** as yellow liquid (38 mg, 71% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 – 8.52 (m, 2H), 8.05 (s, 1H), 7.90 (d, J = 8.3 Hz, 1H), 7.71 – 7.64 (m, 1H), 7.56 (t, J = 7.6 Hz, 2H), 7.42 – 7.37 (m, 1H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 185.4, 167.1, 154.4, 137.1, 135.1, 134.1, 133.8, 131.3, 129.5, 128.5, 125.4, 121.6, 77.3, 77.0, 76.7, 21.5.

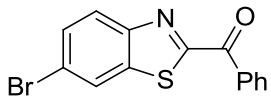
(5-Chlorobenzo[d]thiazol-2-yl)(phenyl)methanone (4i, CAS: 32729-67-2)[7]



The reaction was conducted with acetylene (**1a**, 23 μL, 0.2 mmol) and 2-amino-4-chlorobenzenethiol (**2d**, 62 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **4i** as white solid (38 mg, 71% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 – 8.51 (m, 2H), 8.25 (d, J = 1.8 Hz, 1H), 7.95 (d, J = 8.6 Hz, 1H), 7.72 – 7.65 (m, 1H), 7.61 – 7.50 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.9, 168.9, 154.6, 135.2, 134.6, 134.1, 133.0, 131.3, 128.6, 128.2, 125.2, 122.9, 77.3, 77.0, 76.7.

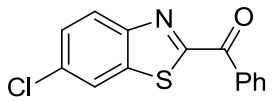
(6-Bromobenzo[d]thiazol-2-yl)(phenyl)methanone (4j)[6]



The reaction was conducted with acetylene (**1a**, 23 μL, 0.2 mmol) and 2-amino-5-bromobenzenethiol (**2h**, 82 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **34j** as white solid (38 mg, 71% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 – 8.52 (m, 2H), 8.18 (d, J = 1.9 Hz, 1H), 8.10 (d, J = 8.8 Hz, 1H), 7.72 – 7.65 (m, 2H), 7.57 (t, J = 7.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.9, 167.6, 152.7, 138.5, 134.7, 134.1, 131.2, 130.7, 128.5, 126.8, 124.7, 121.9, 77.3, 77.0, 76.7.

(6-Chlorobenzo[d]thiazol-2-yl)(phenyl)methanone (4k)[6]



The reaction was conducted with acetylene (**1a**, 23 μL, 0.2 mmol) and 2-amino-5-chlorobenzenethiol (**2g**, 63 mg, 0.4 mmol). The residue was purified by column chromatography on silica gel (petroleum ether/ethyl acetate = 50:1) to yield the desired product **4k** as white solid (43 mg, 78 % yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 – 8.50 (m, 2H), 8.18 – 8.10 (m, 1H), 8.05 – 7.95 (m, 1H), 7.72 – 7.63 (m, 1H), 7.60 – 7.50 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 184.9, 167.7, 152.4, 138.1, 134.7, 134.1, 134.0, 131.2, 128.5, 128.0, 126.5, 121.7, 77.3, 77.0, 76.7.

4. References

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[3] X. S. Fan, Y. He, Y. Y. Wang, Z. K. Xue, X. Y. Zhang, J. J. Wang, *Tetrahedron Lett.* **2011**, *52*, 899.

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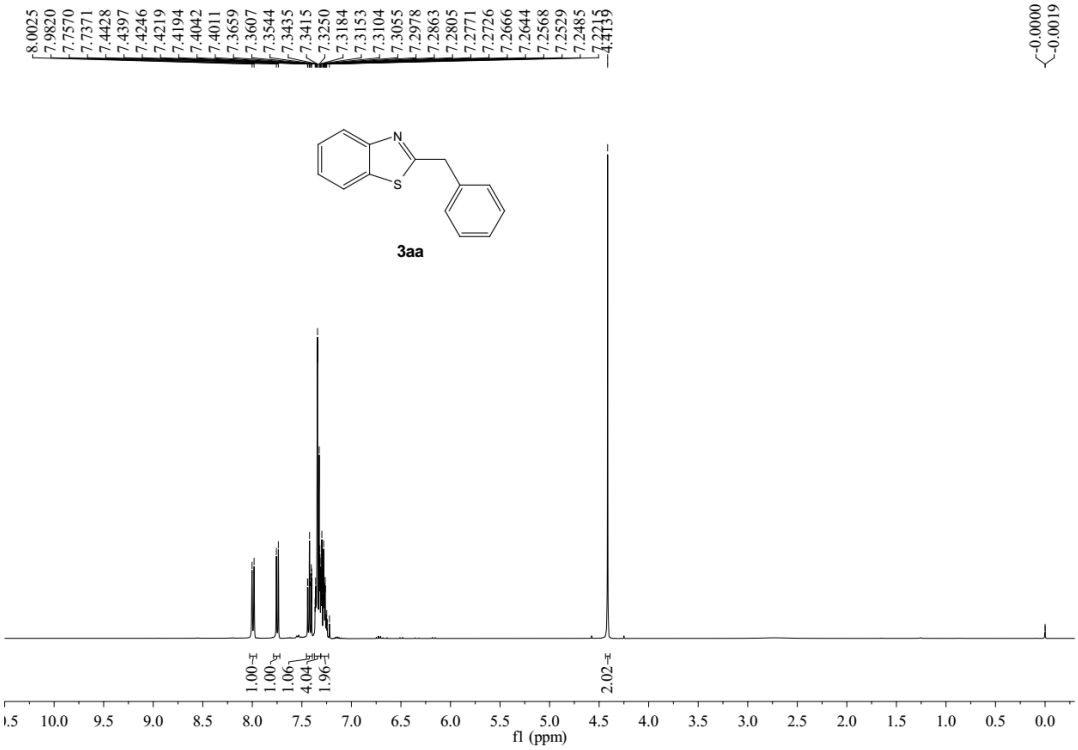
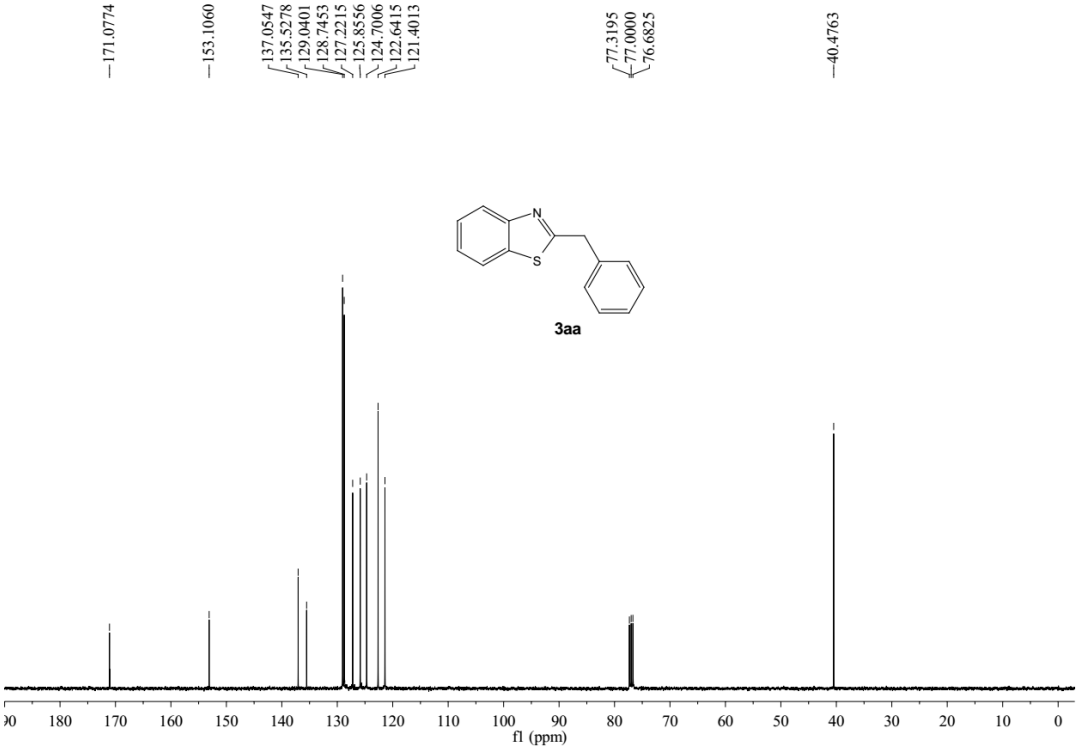
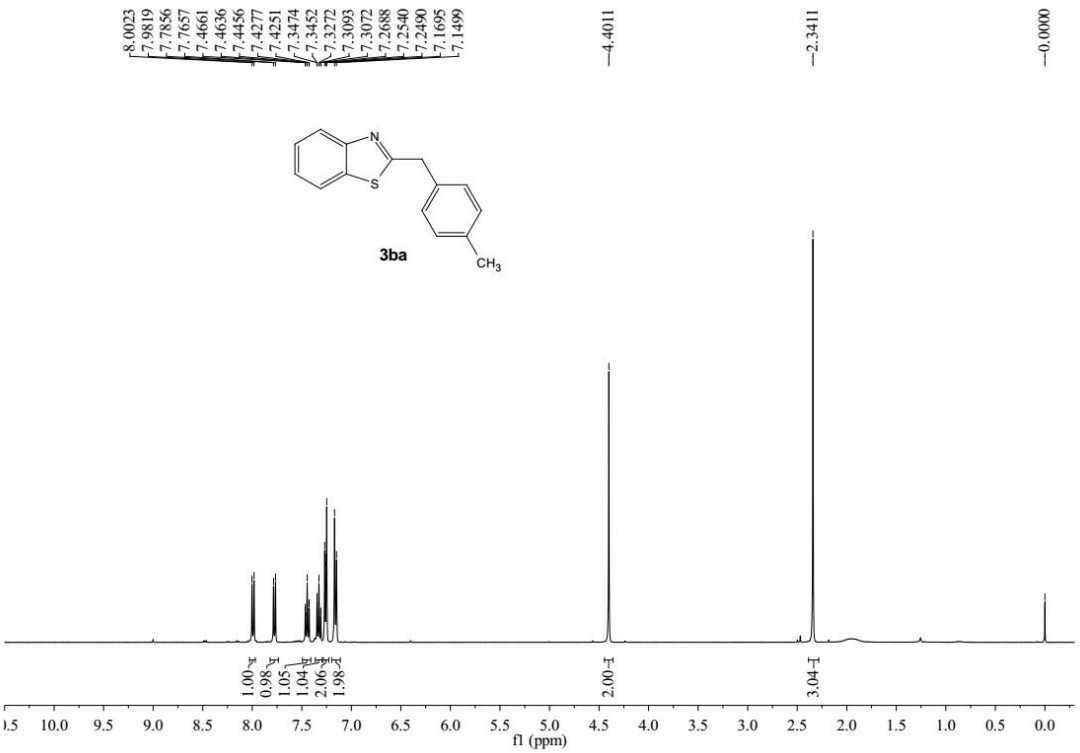
5. ^{1}H and ^{13}C NMR spectra for all products



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7.3452
7.3272
7.3093
7.3072
7.2688
7.2540
7.2490
7.1695
7.1499
4.4011
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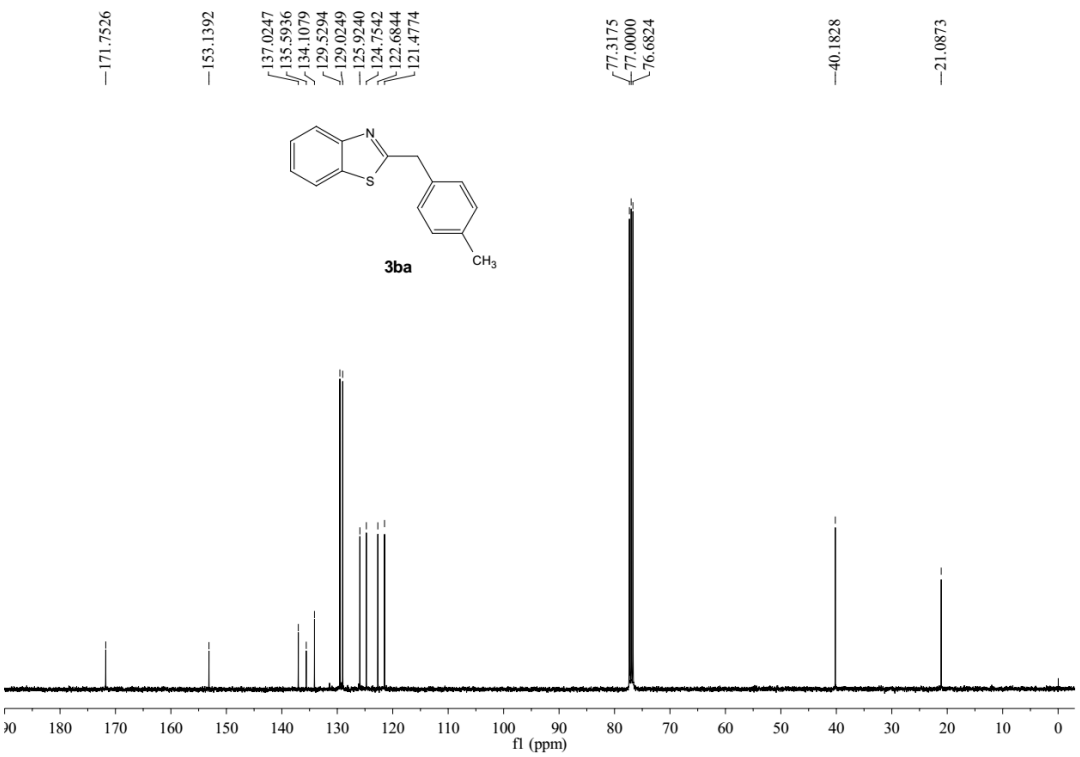
1.00
0.98
1.05
1.04
2.06
1.98
2.00
3.04
f1 (ppm)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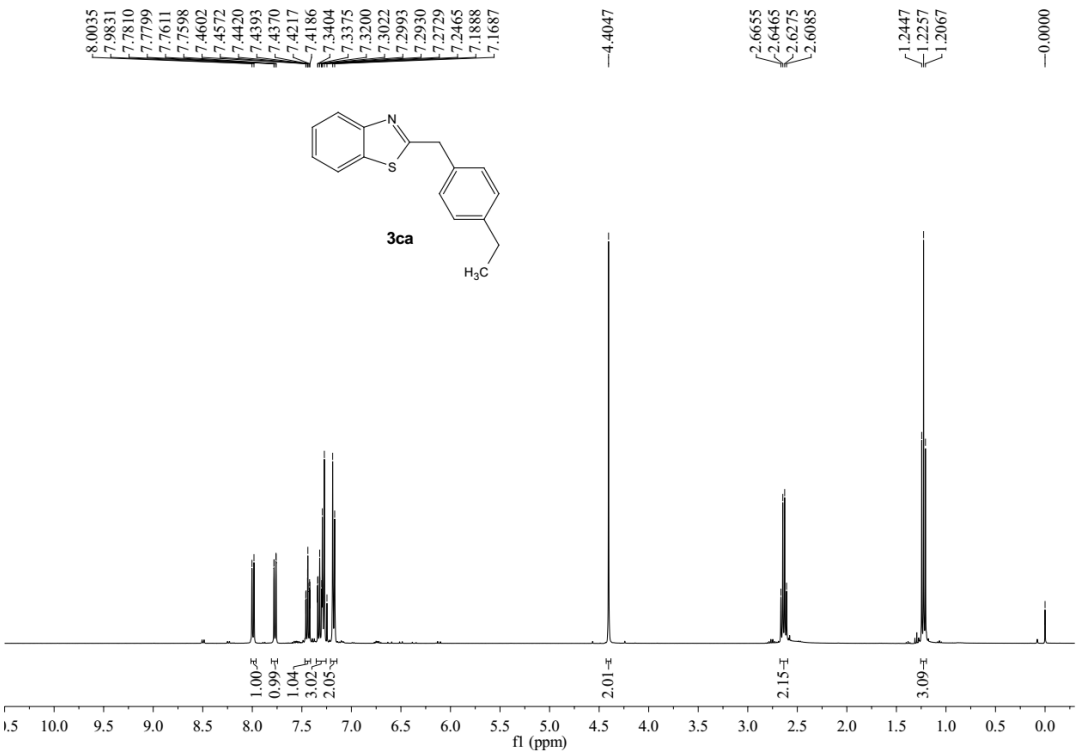
3ba
f1 (ppm)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7.4217
7.4186
7.3404
7.3375
7.3200
7.3022
7.2993
7.2930
7.2729
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7.1888
7.1687
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2.6465
2.6275
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1.2257
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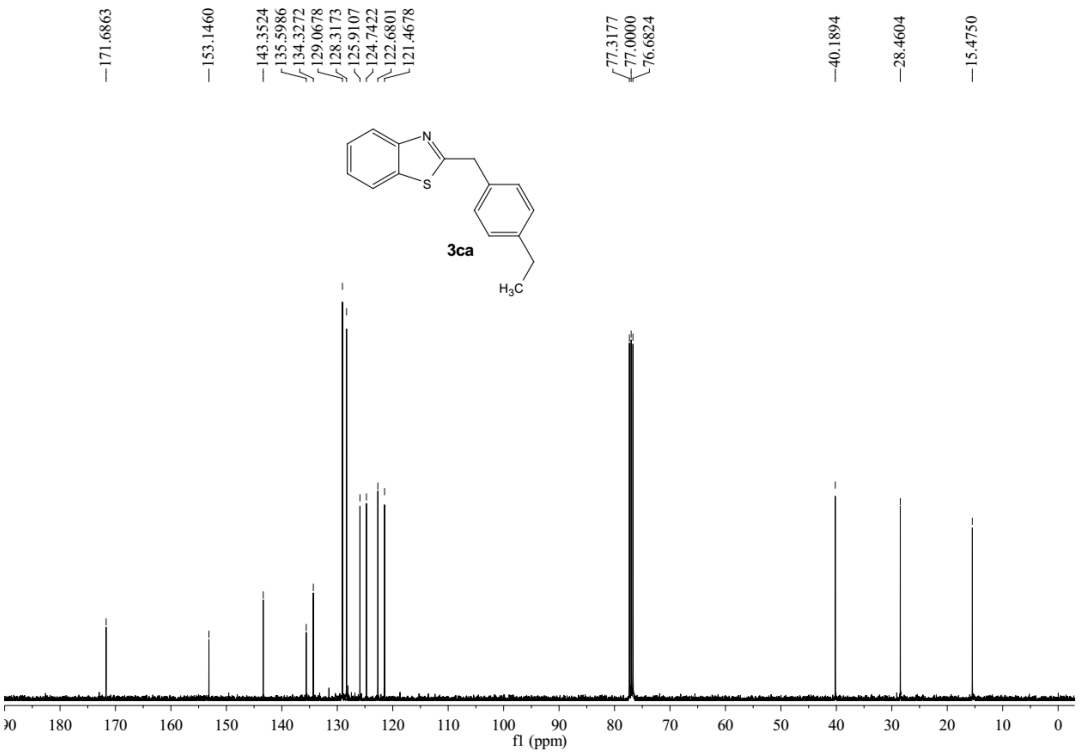
0.99
1.04
3.02
2.05
2.01
2.15
3.09
fl (ppm)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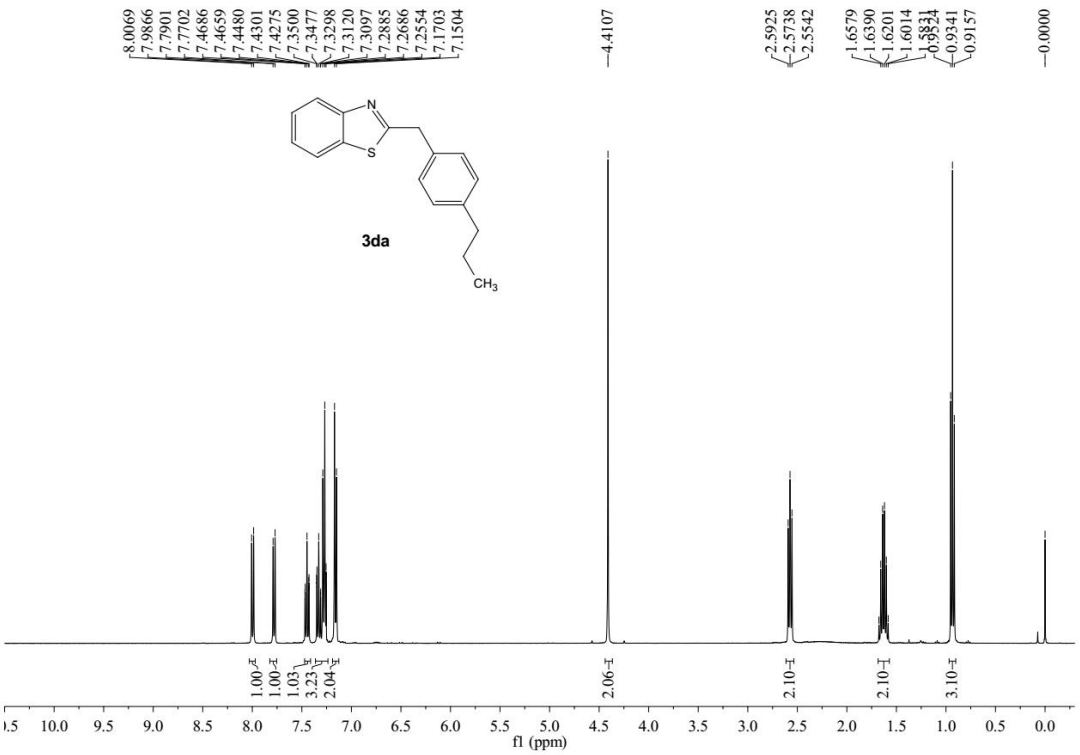
3ca
fl (ppm)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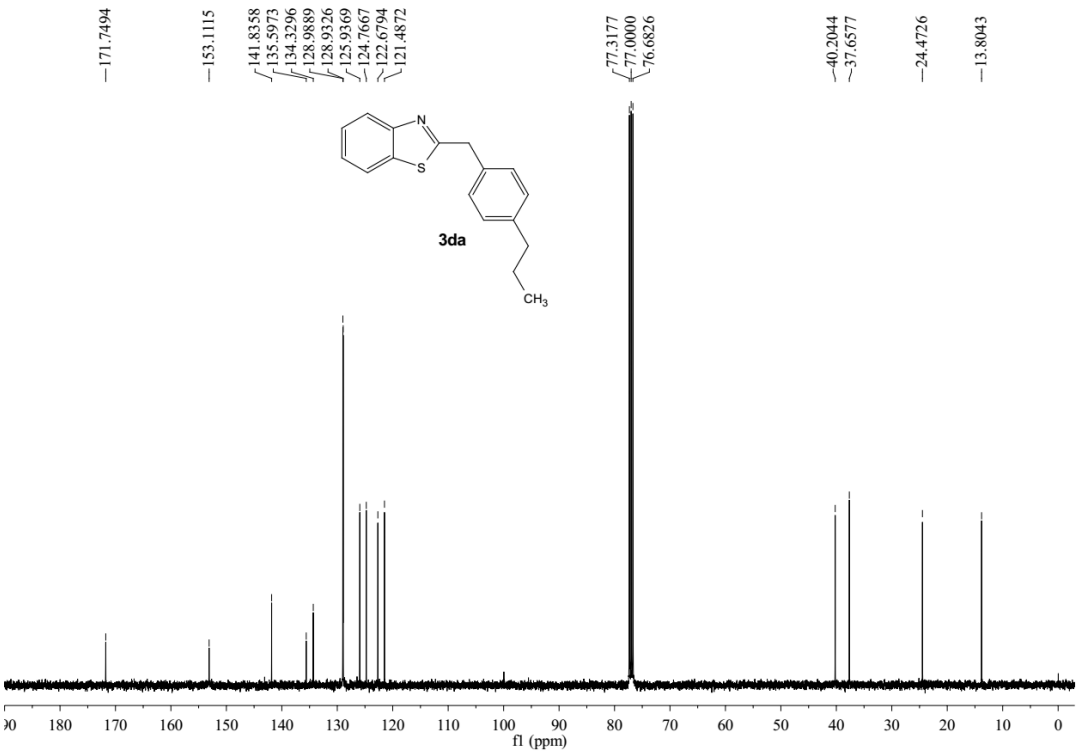
fl (ppm)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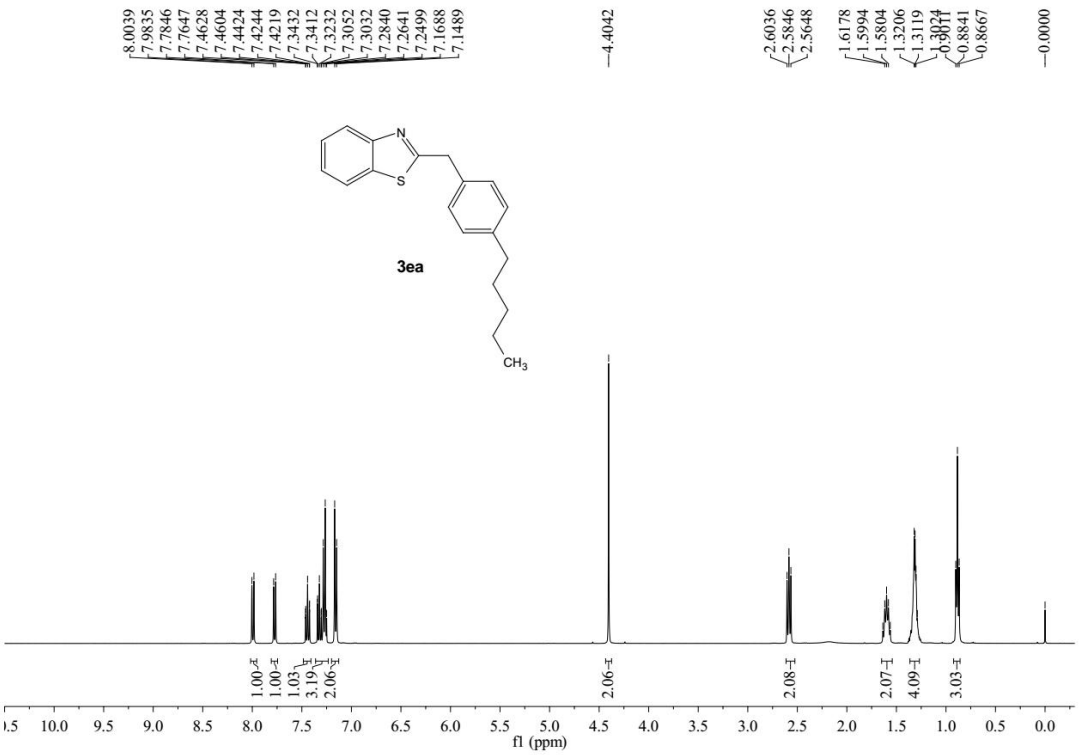
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7.2840
7.2641
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4.4042
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2.5648
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1.5804
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1.3024
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0.8667
0.0000
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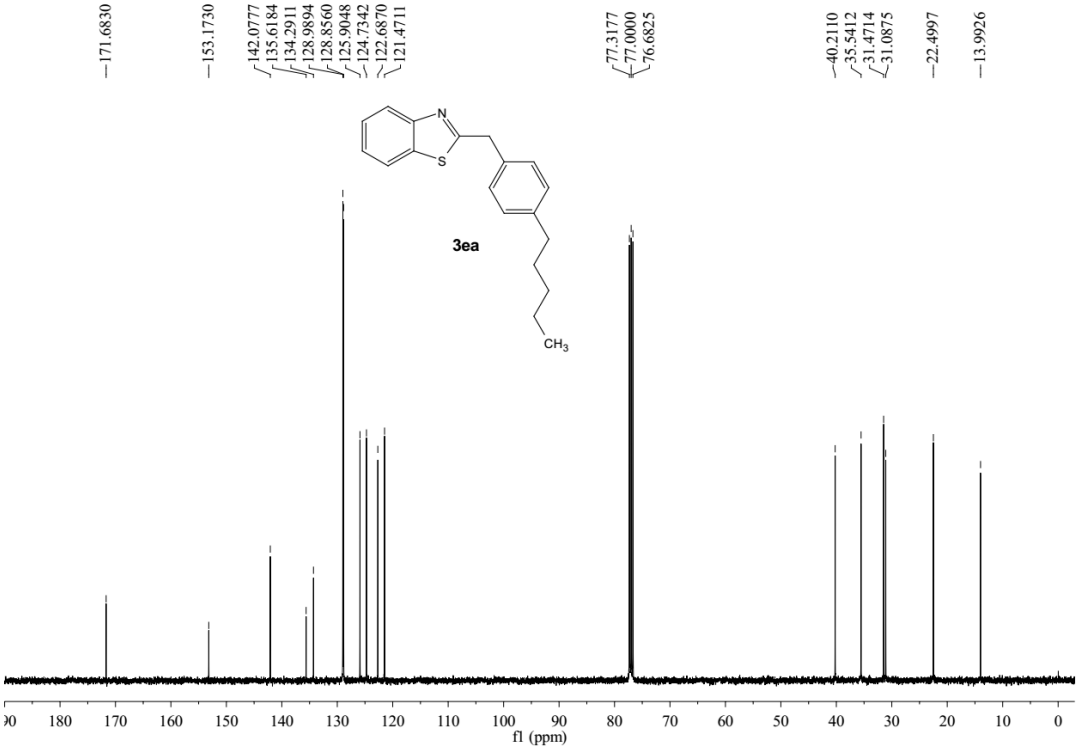
2.06
2.08
2.07
4.09
3.03
fl (ppm)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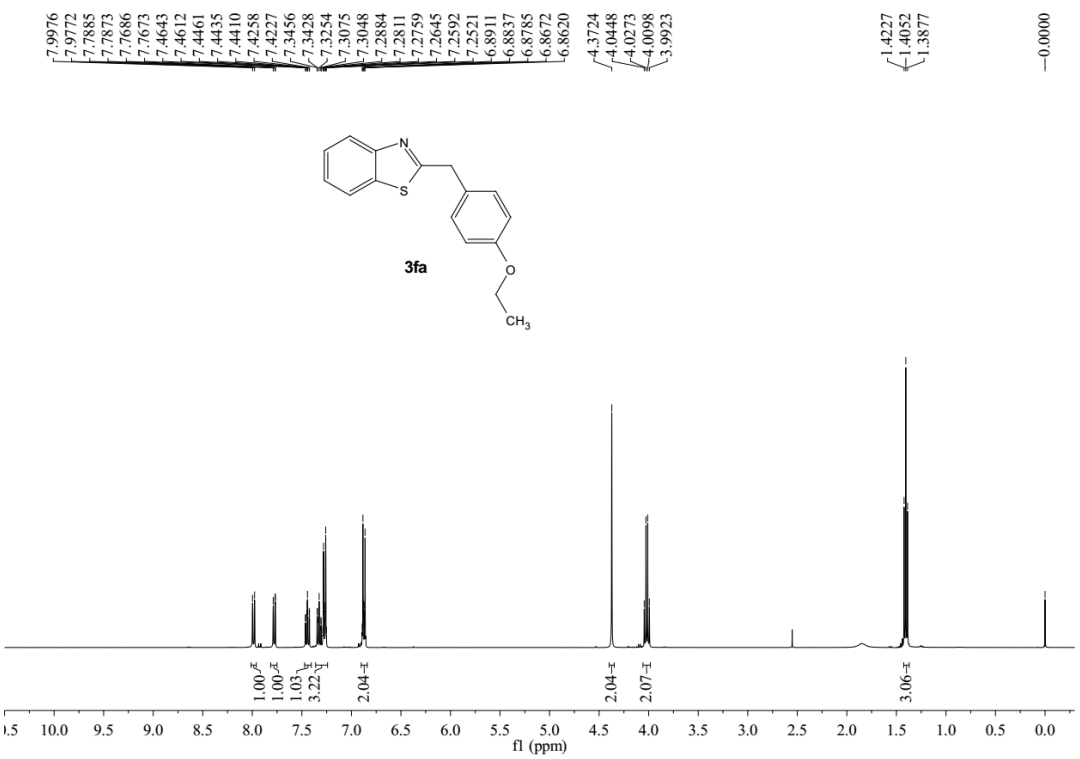
fl (ppm)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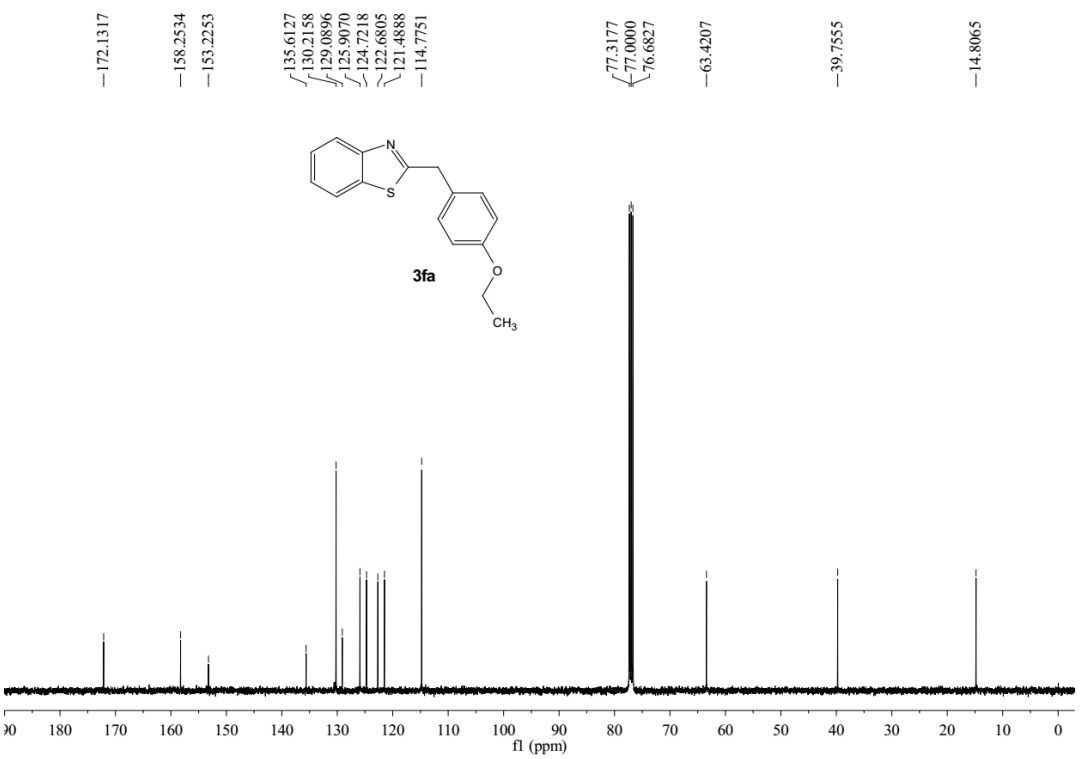
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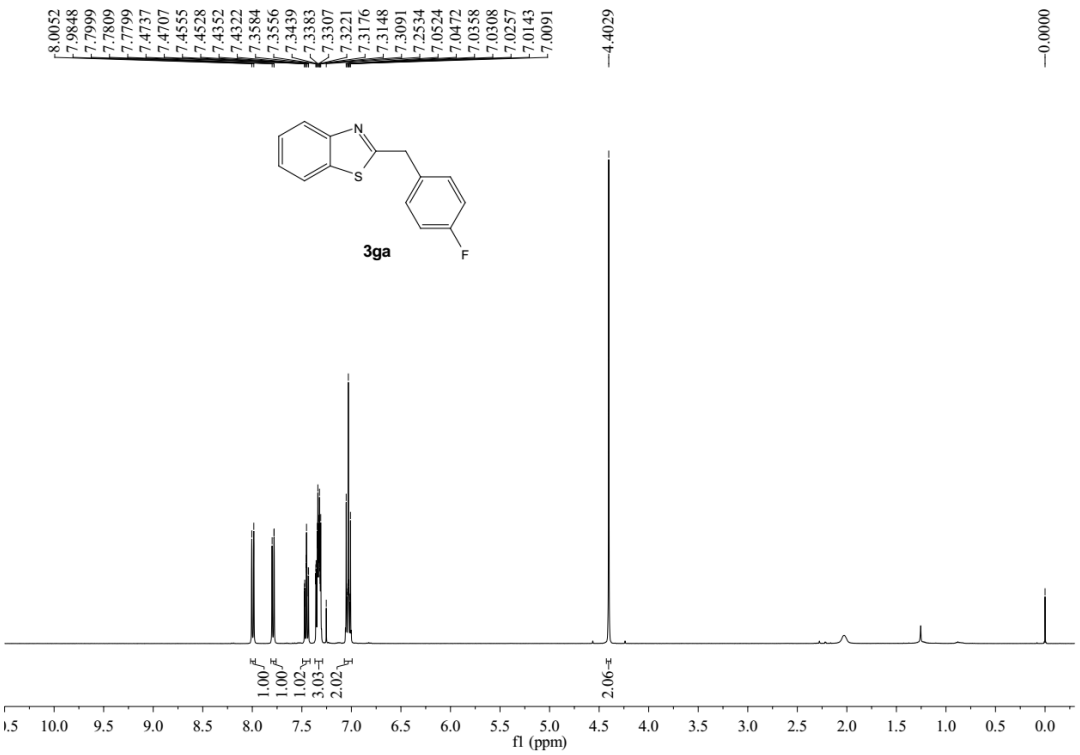
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7.0472
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7.0308
7.0257
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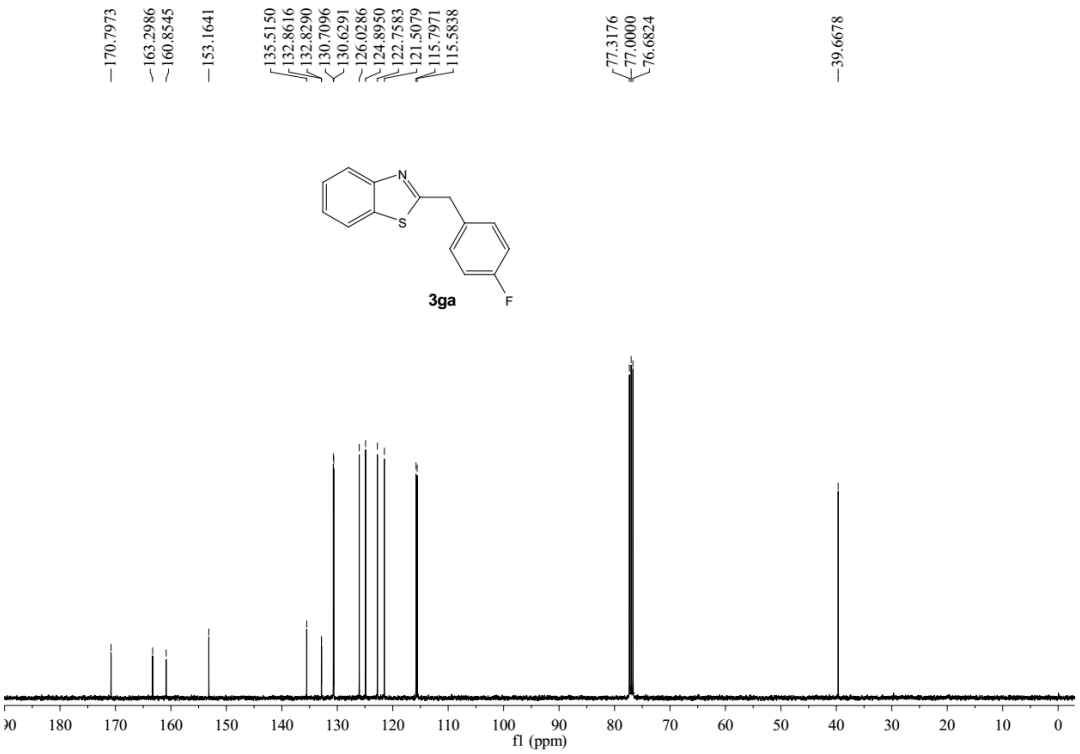
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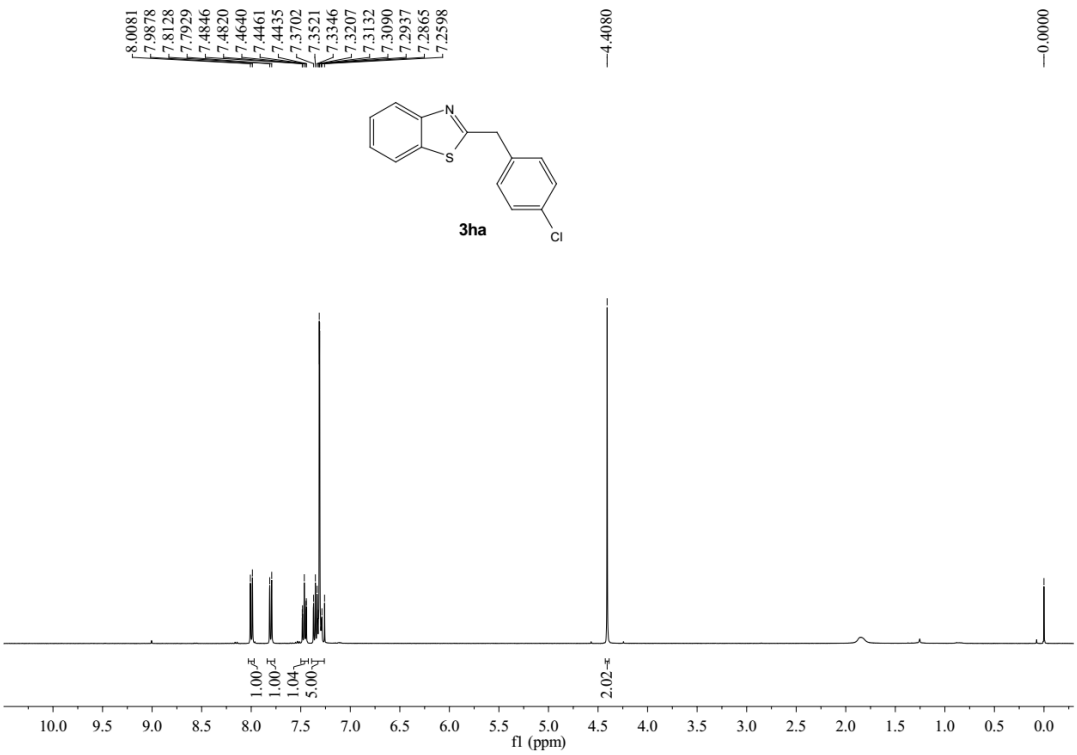
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5.00
2.02
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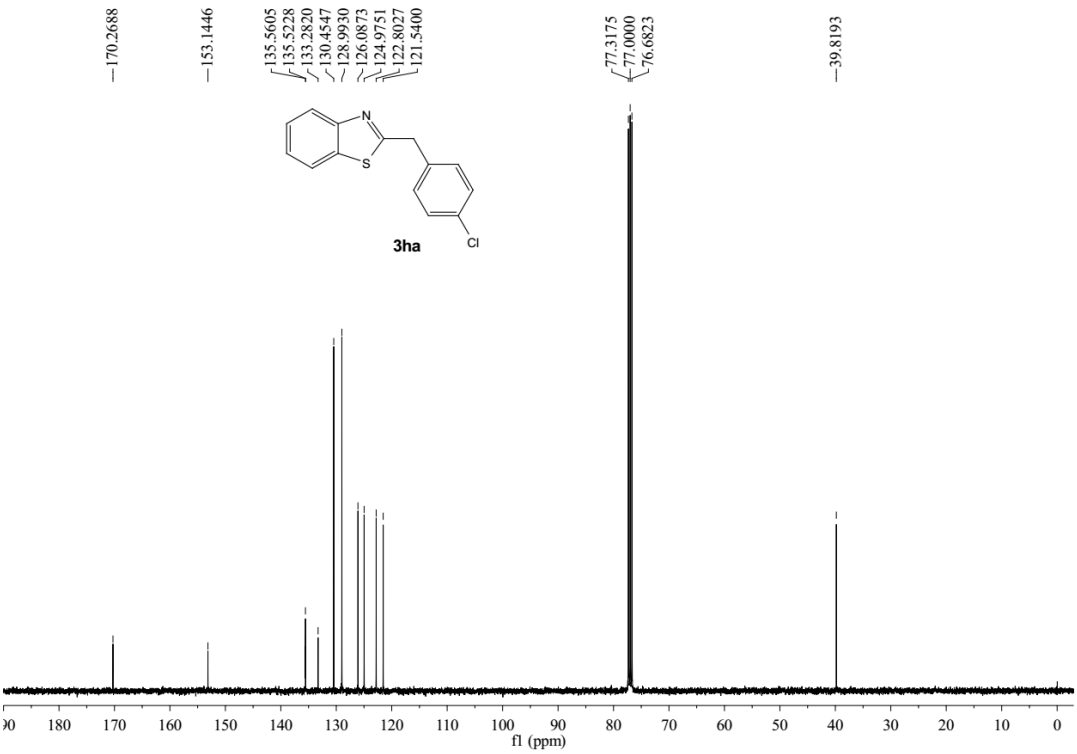
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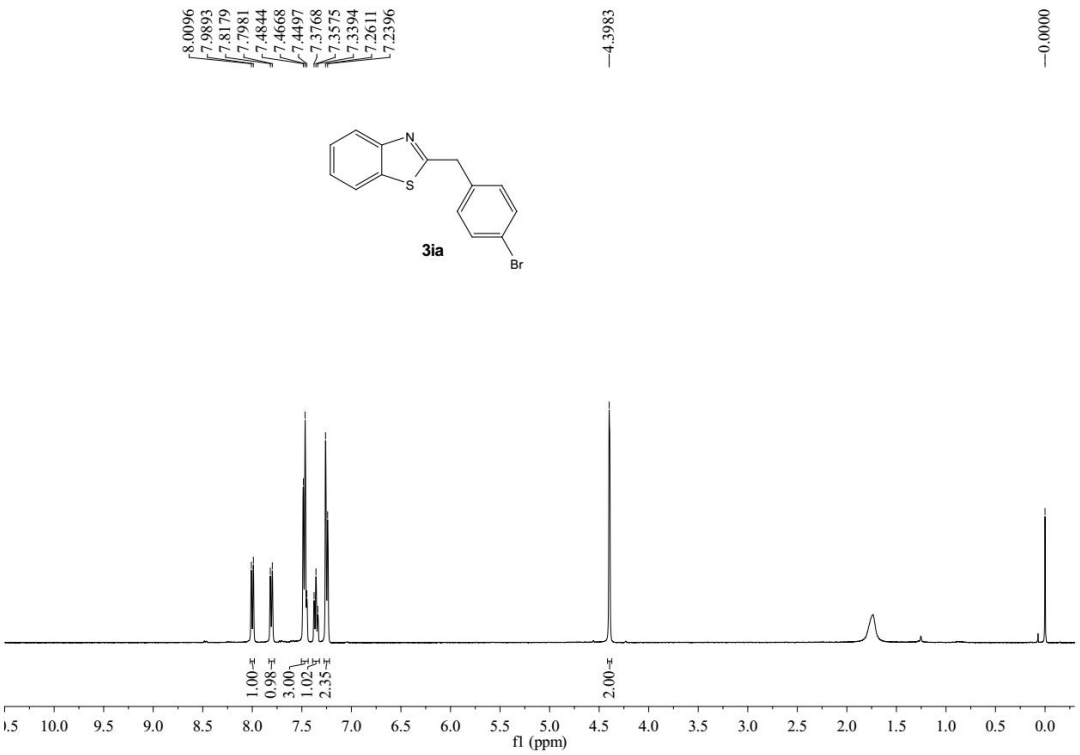
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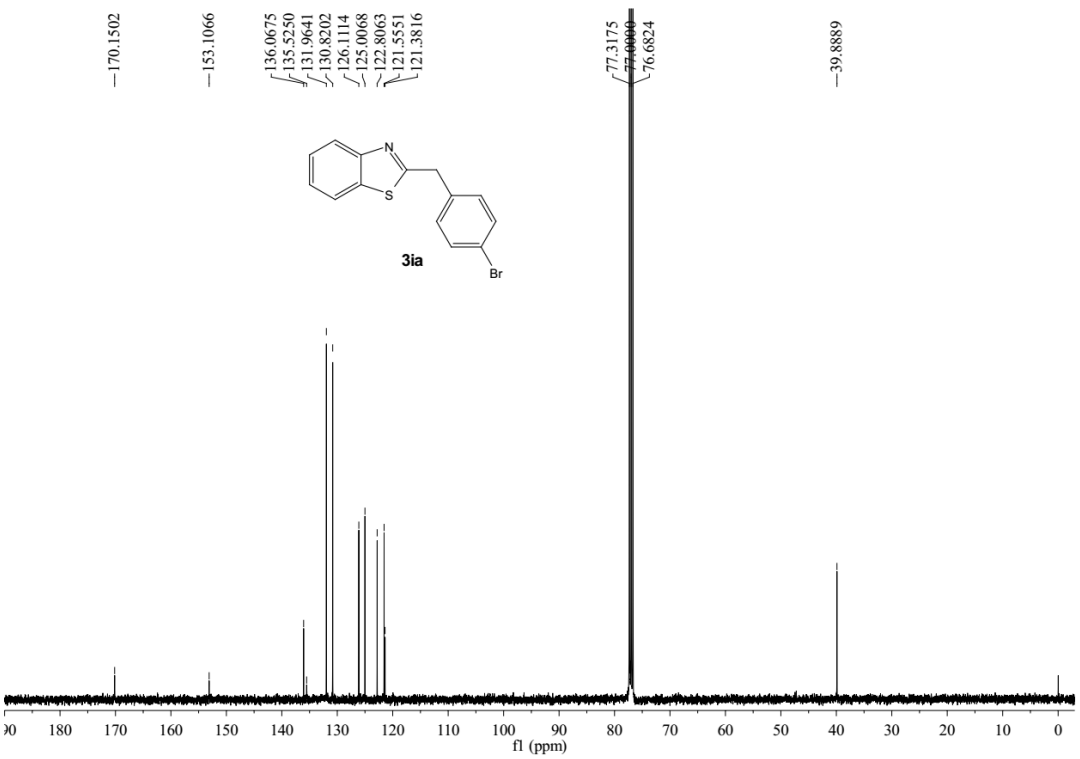
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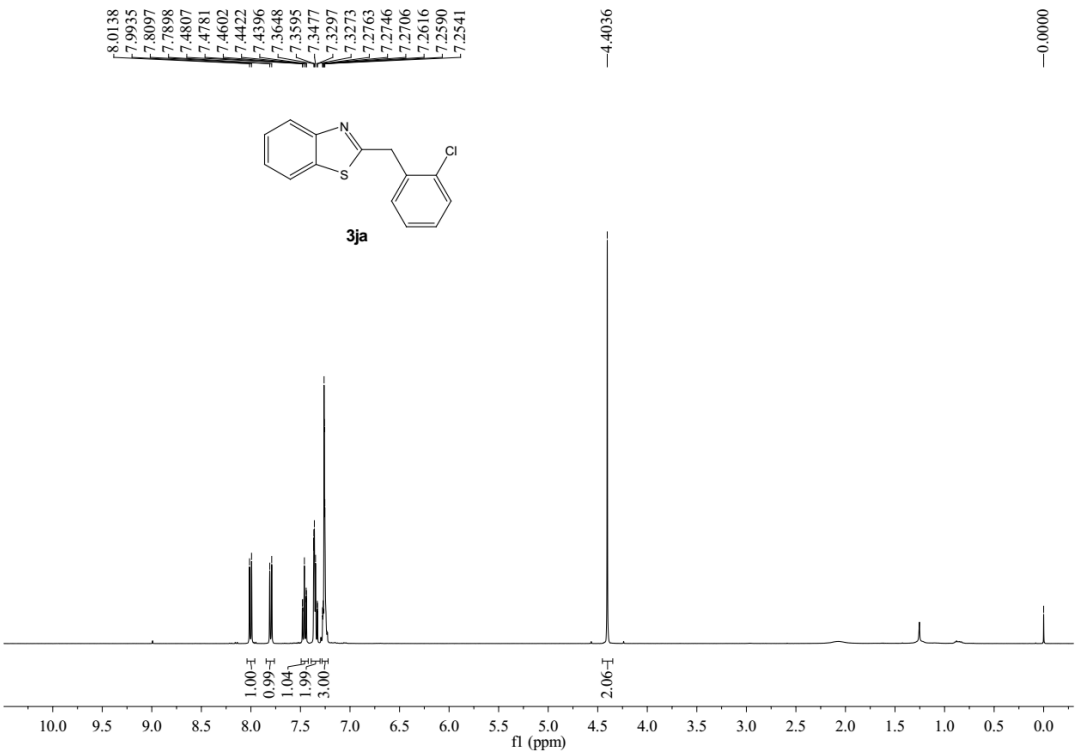
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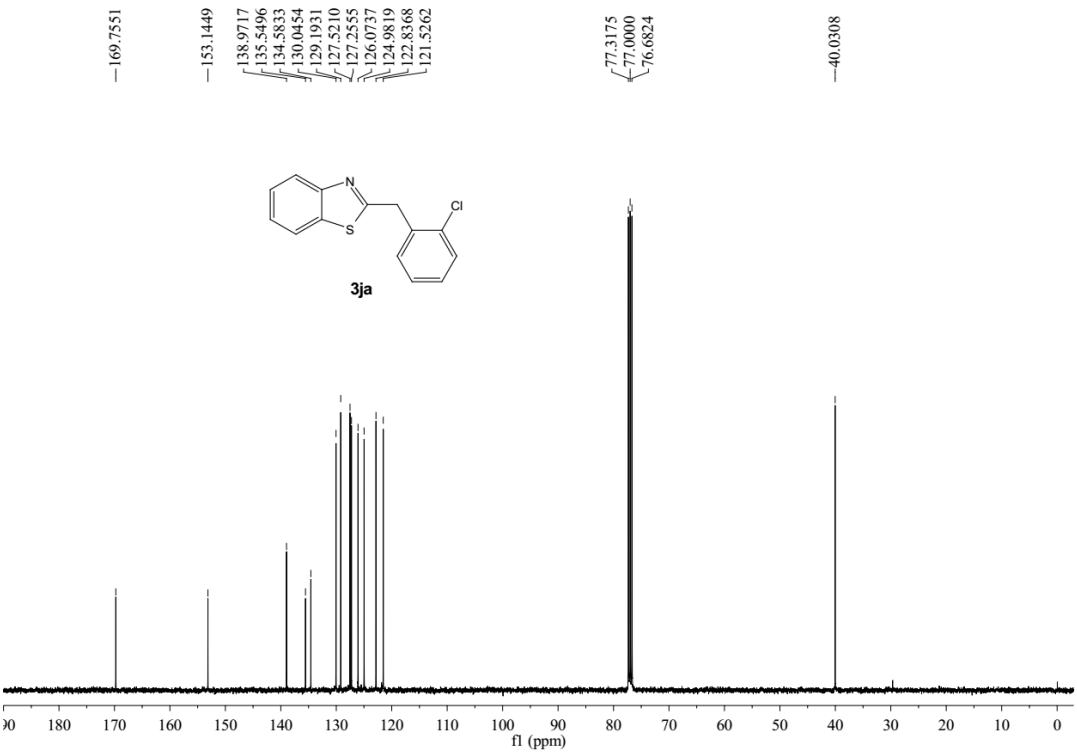
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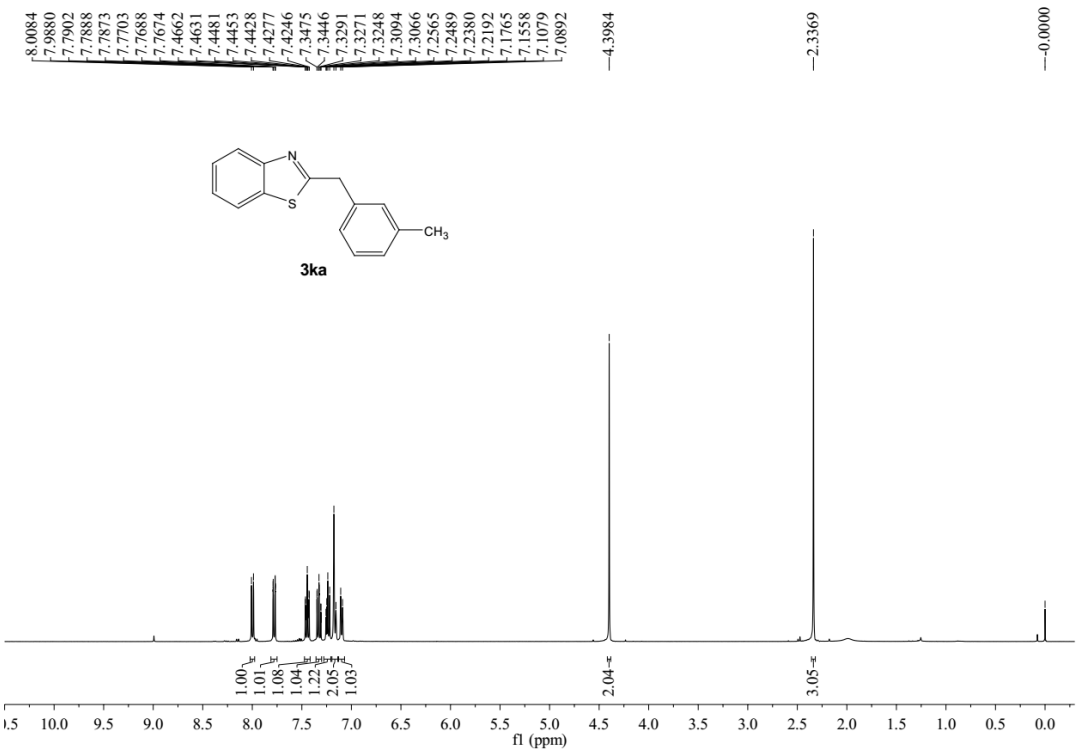
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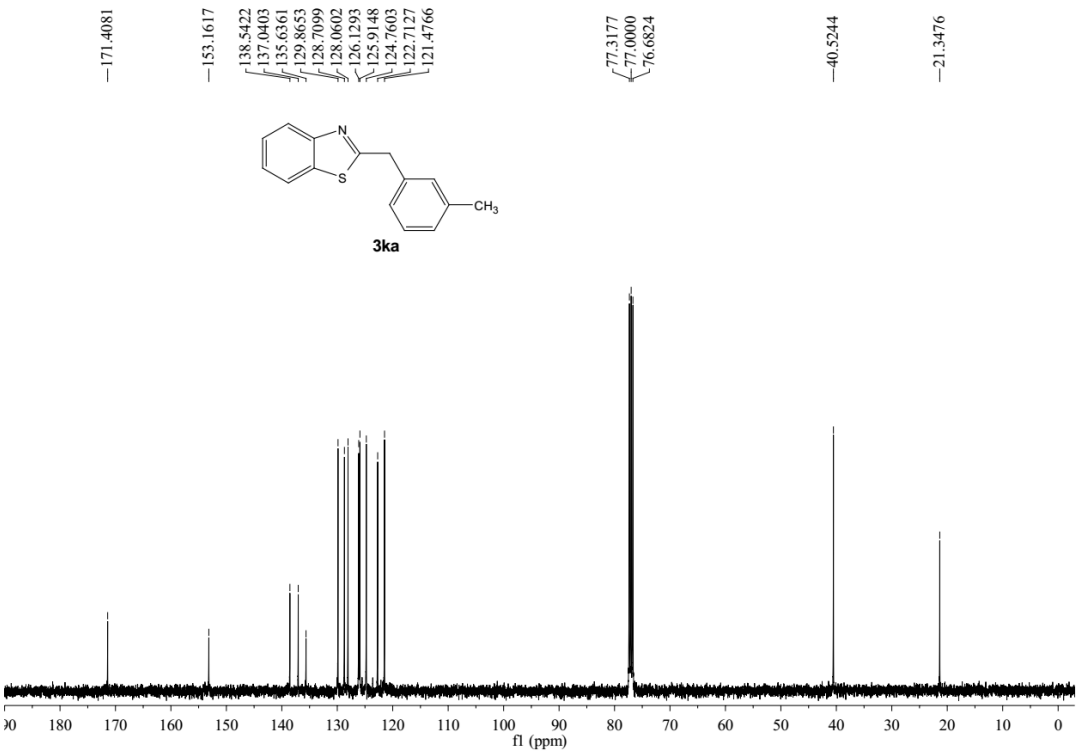
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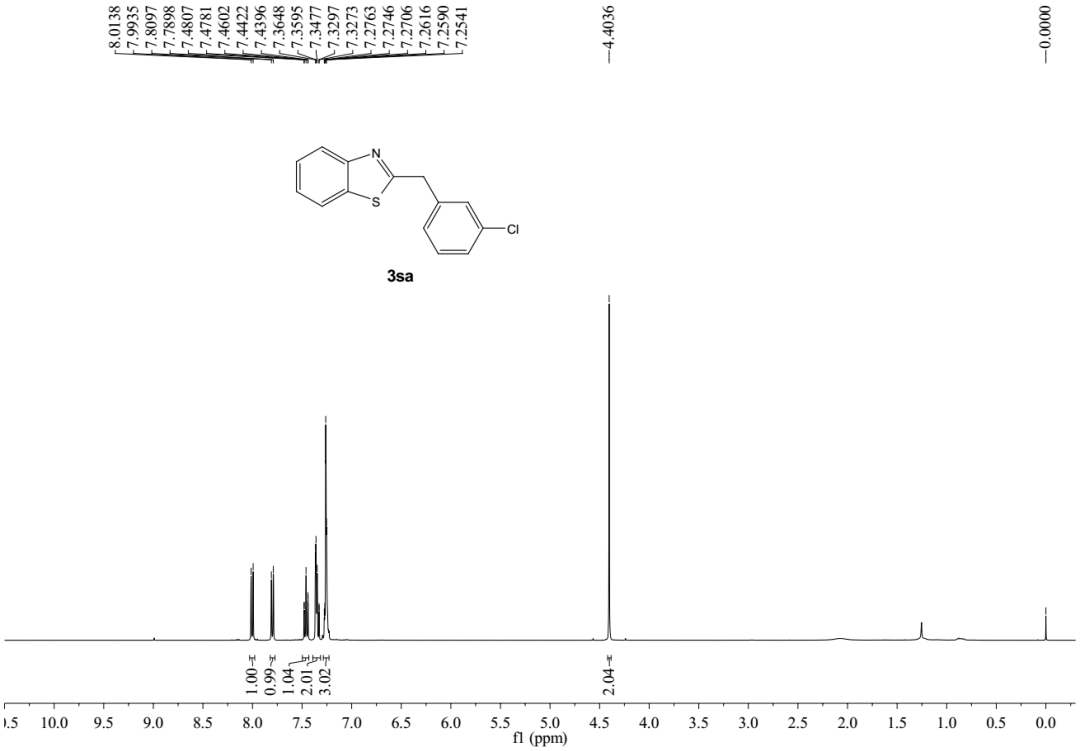
f1 (ppm)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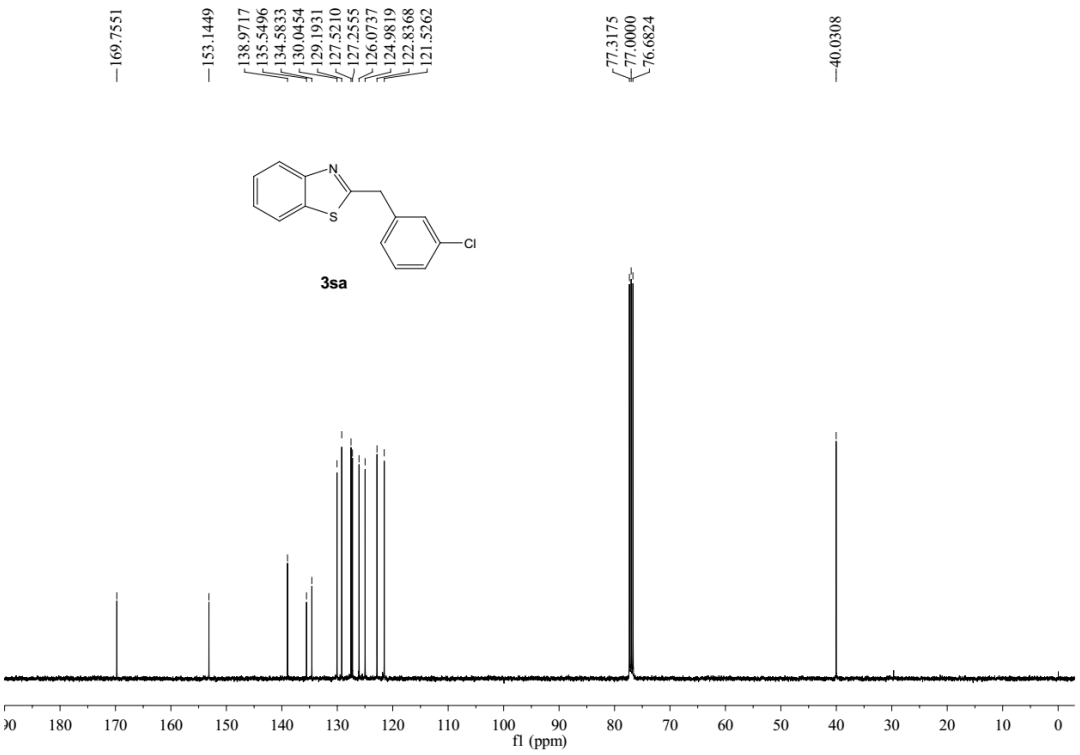
f1 (ppm)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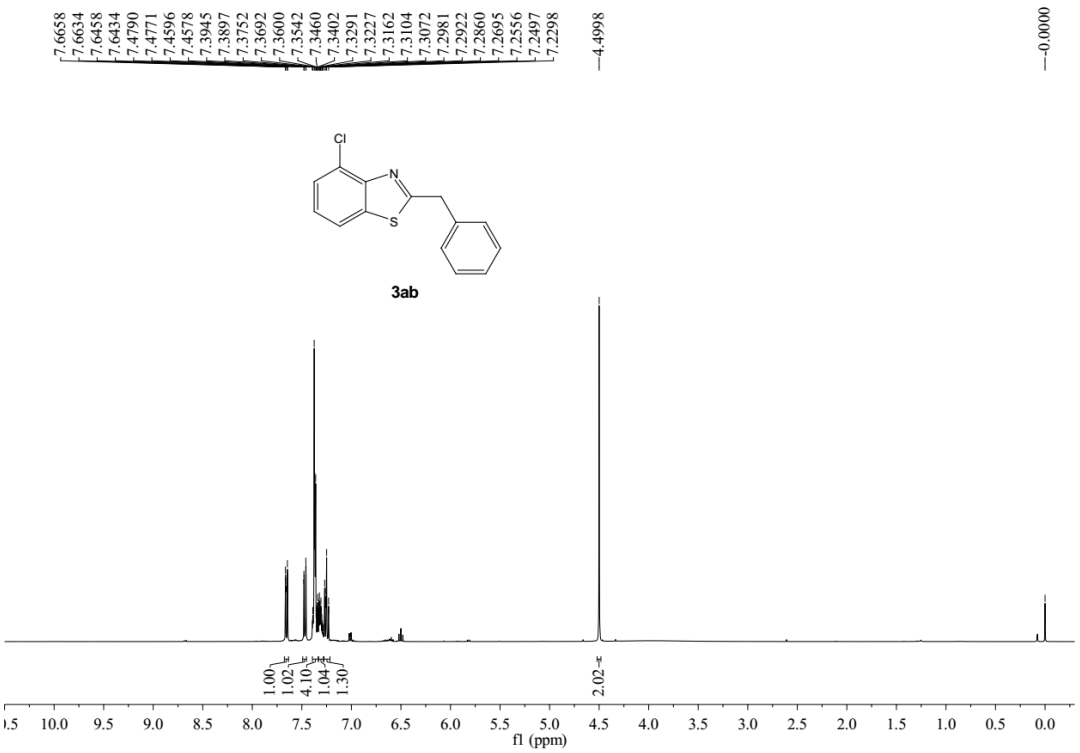
77.0000
76.6824
40.0308
N
S
Cl
3sa
f1 (ppm)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7.4596
7.4578
7.3945
7.3897
7.3752
7.3692
7.3600
7.3542
7.3460
7.3402
7.3291
7.3227
7.3162
7.3104
7.3072
7.2981
7.2922
7.2860
7.2695
7.2556
7.2497
7.2298
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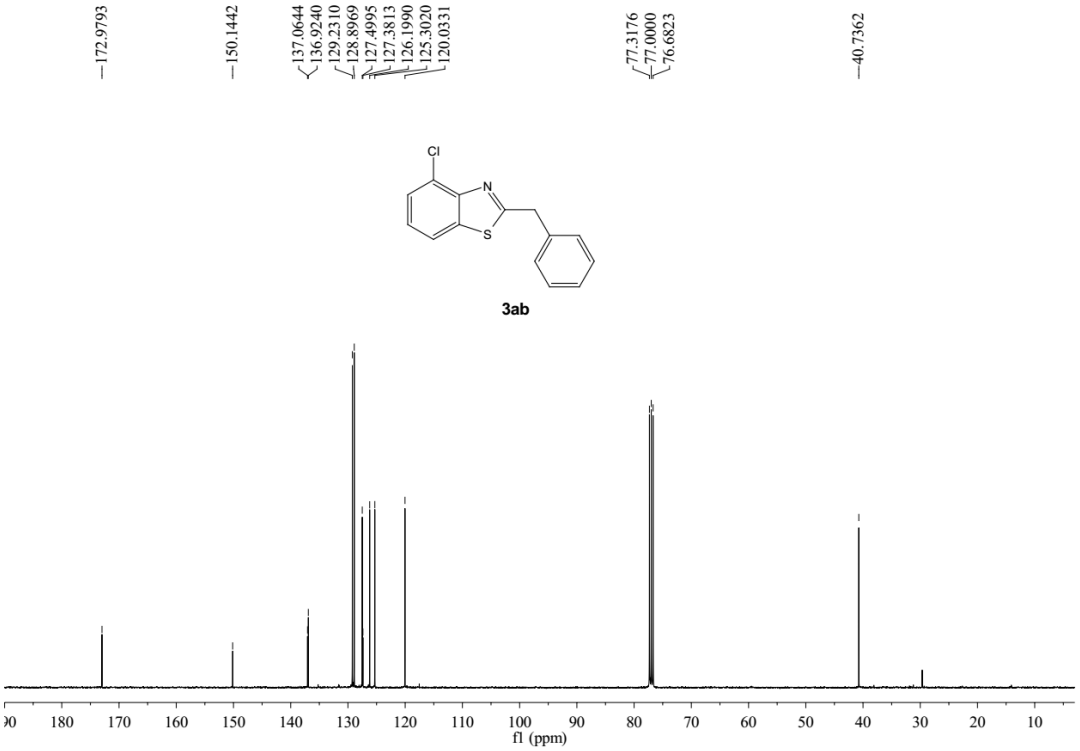
Cl
N
S
3ab
1.00
1.02
4.10
1.04
1.30
2.02
f1 (ppm)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129.2310
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127.4995
127.3813
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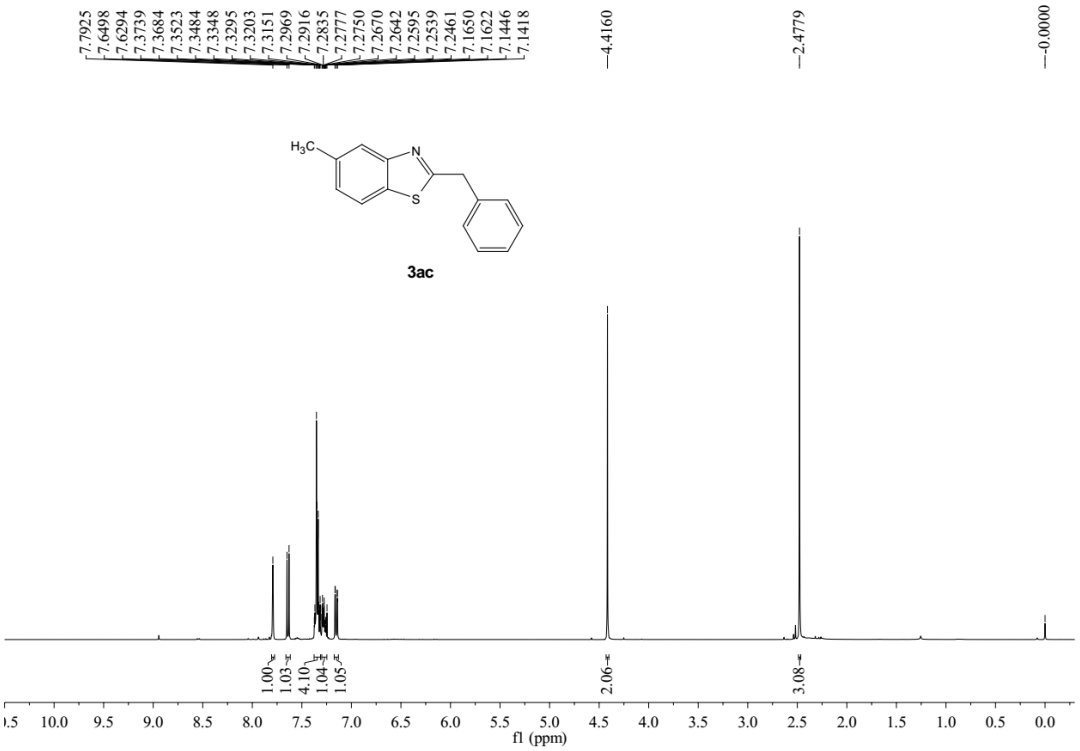
120.0331
77.3176
77.0000
76.6823
40.7362
Cl
N
S
3ab
f1 (ppm)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7.3523
7.3484
7.3348
7.3295
7.3203
7.3151
7.2969
7.2916
7.2835
7.2777
7.2750
7.2670
7.2642
7.2595
7.2539
7.2461
7.1650
7.1622
7.1446
7.1418
4.4160
2.4779
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S
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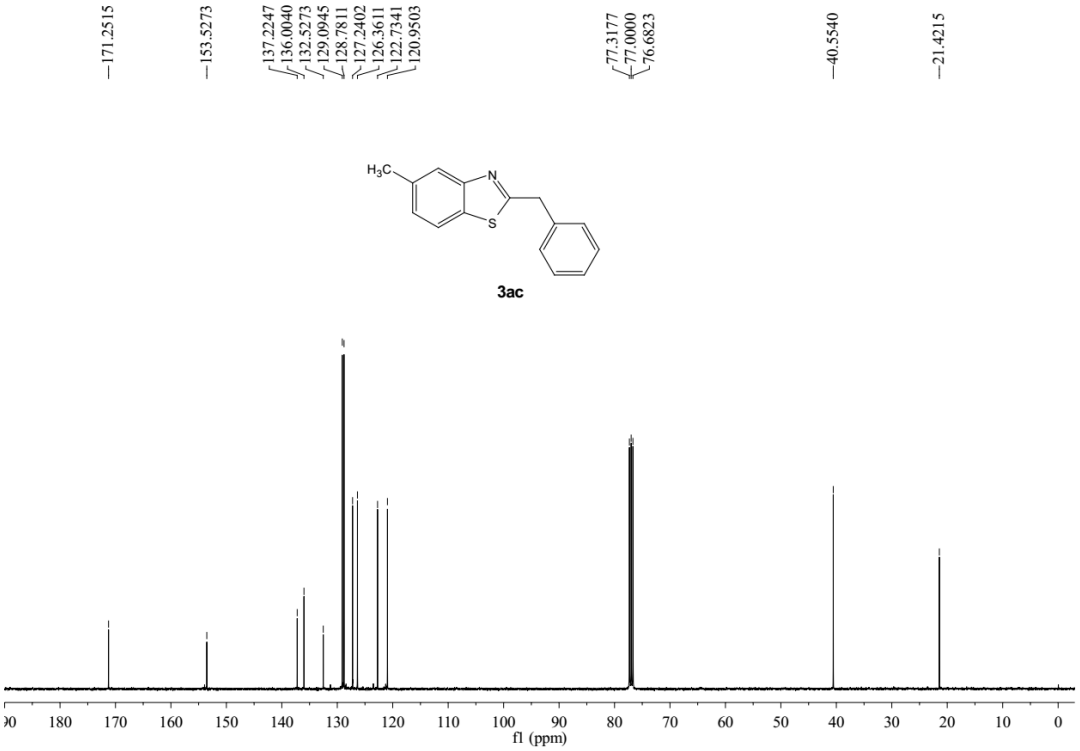
1.03
4.10
1.04
1.05
2.06
3.08
fl (ppm)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126.3611
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77.0000
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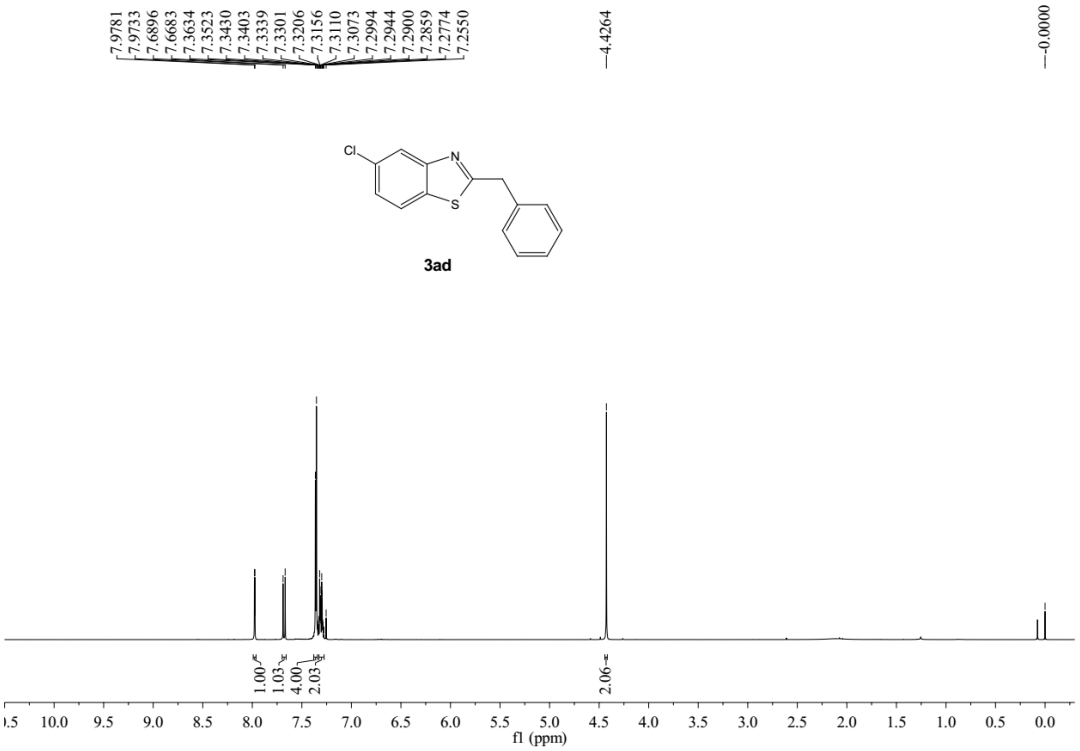
N
S
3ac
fl (ppm)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7.6896
7.6683
7.3634
7.3523
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7.3339
7.3301
7.3206
7.3156
7.3110
7.3073
7.2994
7.2944
7.2900
7.2859
7.2774
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4.4264
0.0000
Cl
N
S
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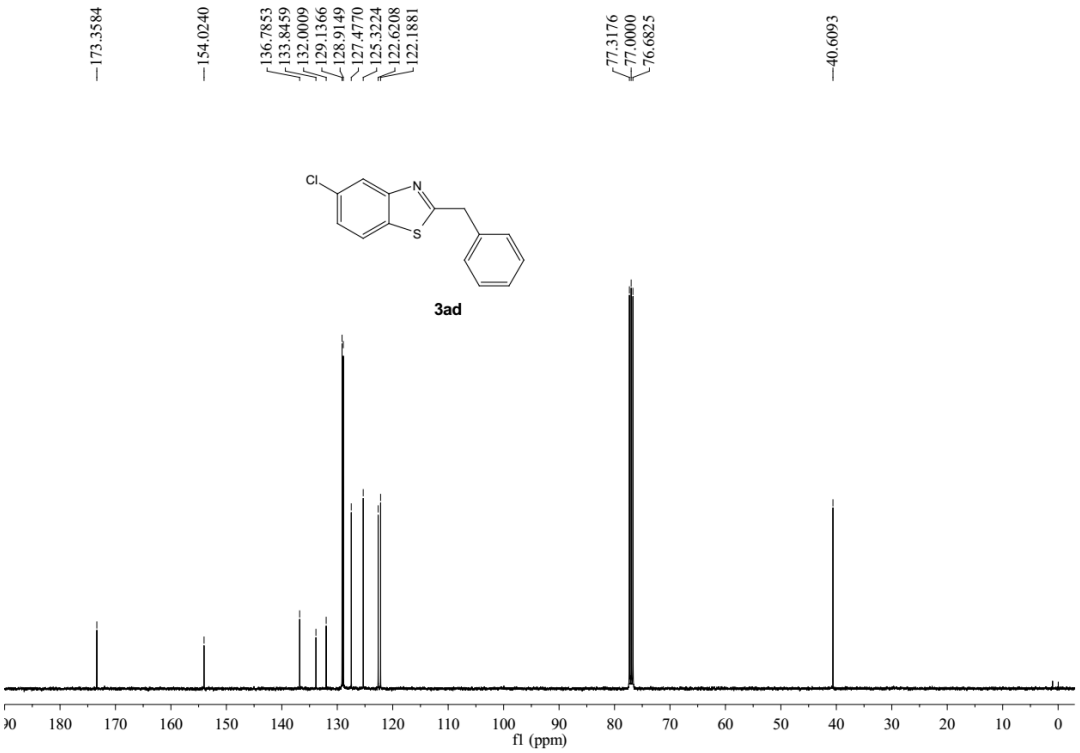
1.00
1.03
4.00
2.03
2.06
f1 (ppm)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128.9149
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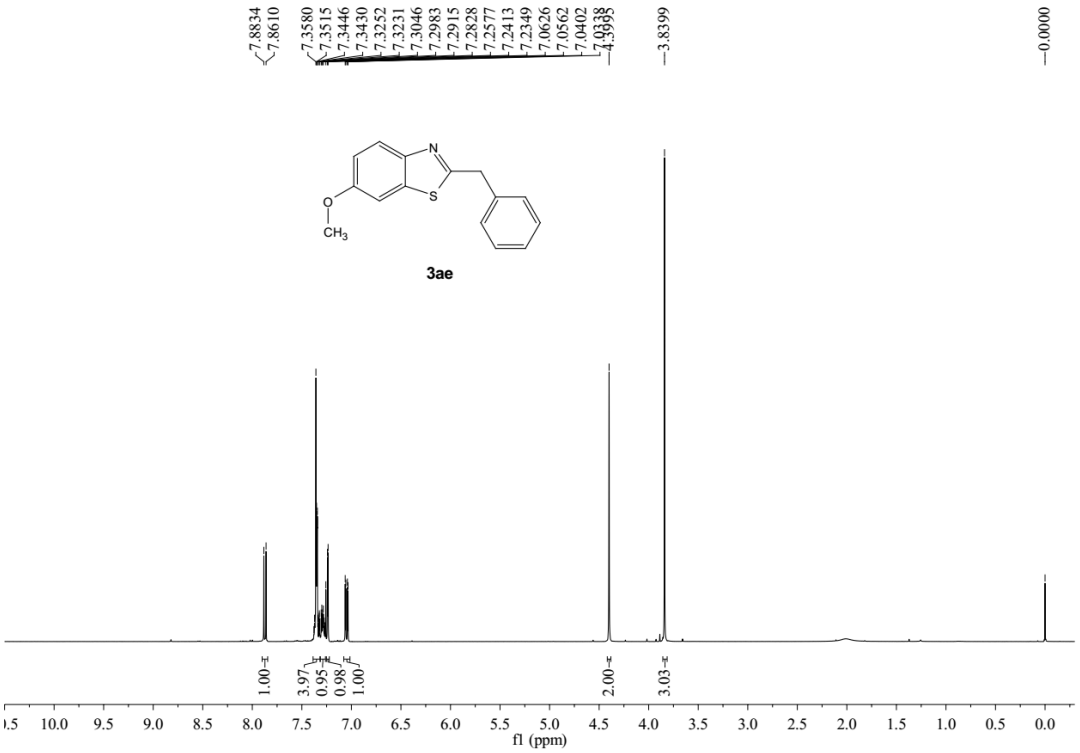
77.0000
76.6825
40.6093
Cl
N
S
3ad
f1 (ppm)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7.3580
7.3515
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7.3252
7.3231
7.3046
7.2983
7.2915
7.2828
7.2577
7.2413
7.2349
7.0626
7.0562
7.0402
7.0338
4.3993
3.8399
0.0000
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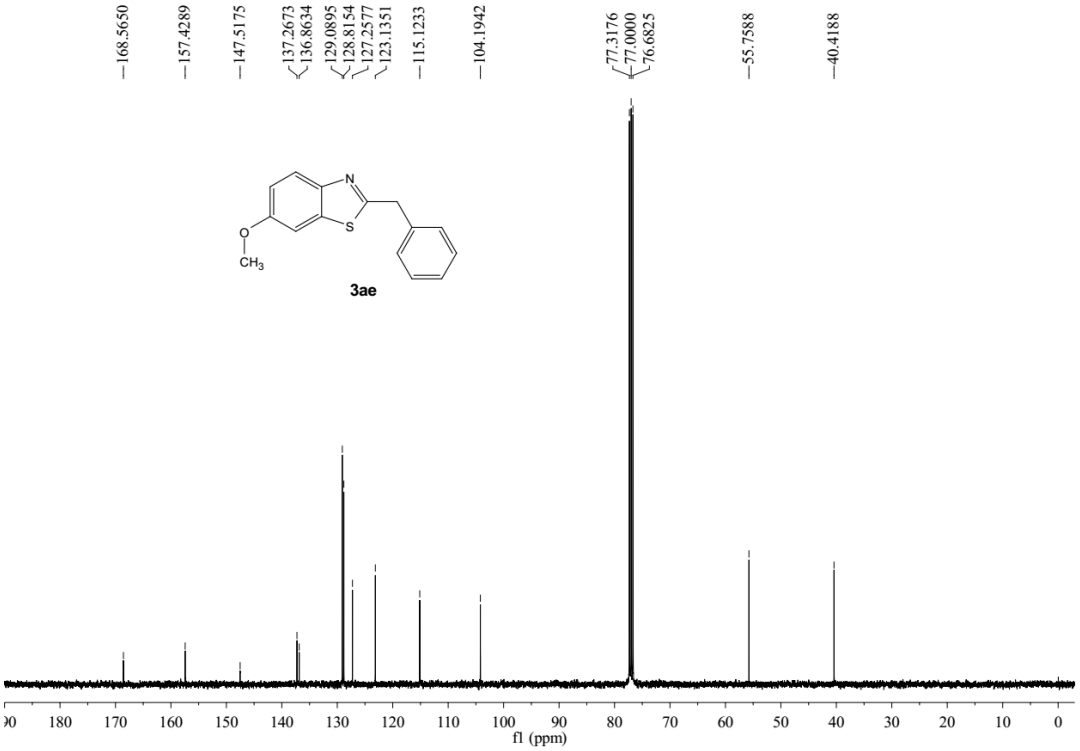
S
O
CH3
3ae
1.00
3.97
0.95
0.98
1.00
2.00
3.03
f1 (ppm)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147.5175
137.2673
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129.0895
128.8154
127.2577
123.1351
115.1233
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77.0000
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55.7588
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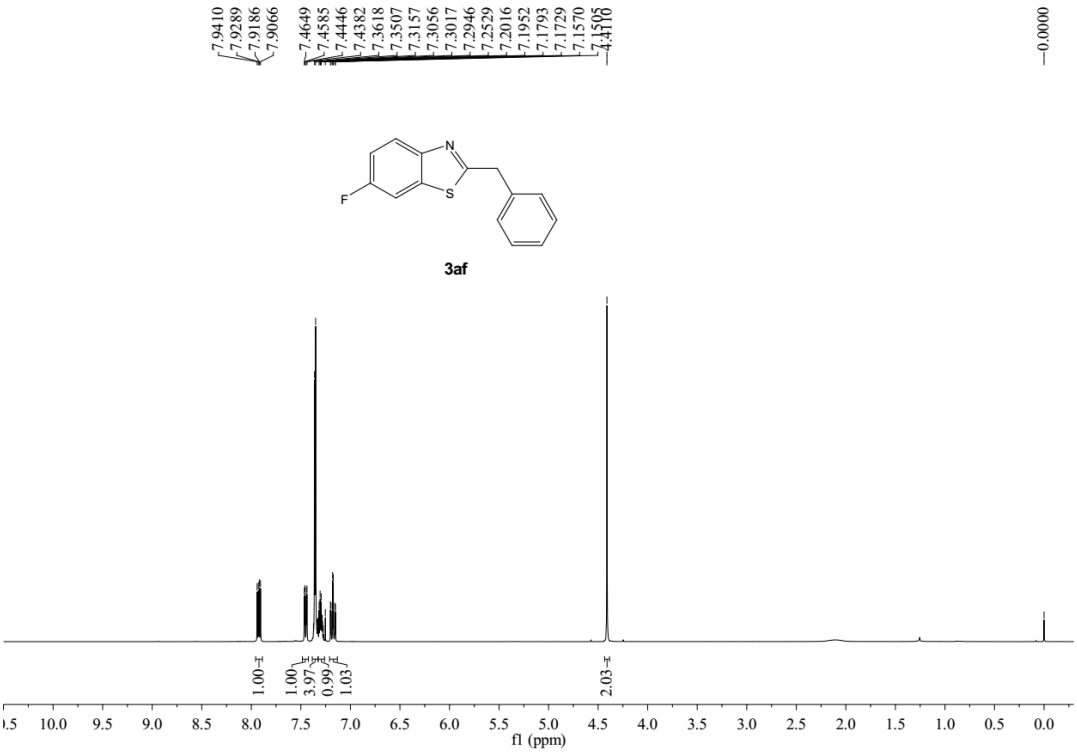
N
S
O
CH3
3ae
f1 (ppm)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7.9186
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7.4649
7.4585
7.4446
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7.3618
7.3507
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7.3056
7.3017
7.2946
7.2529
7.2016
7.1952
7.1793
7.1729
7.1570
7.1505
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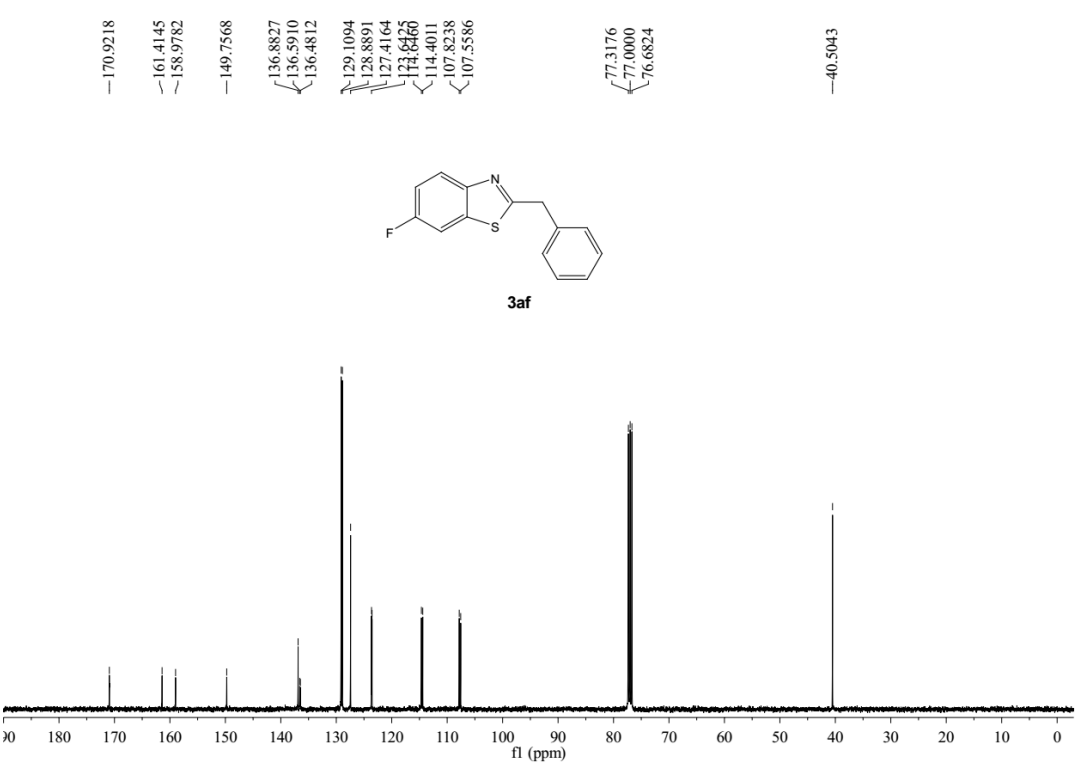
N
S
F
1.00
1.00
3.97
0.99
1.03
2.03
f1 (ppm)

3af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161.4145
158.9782
149.7568
136.8827
136.5910
136.4812
129.1094
128.8891
127.4164
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107.8238
107.5586
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77.0000
76.6824
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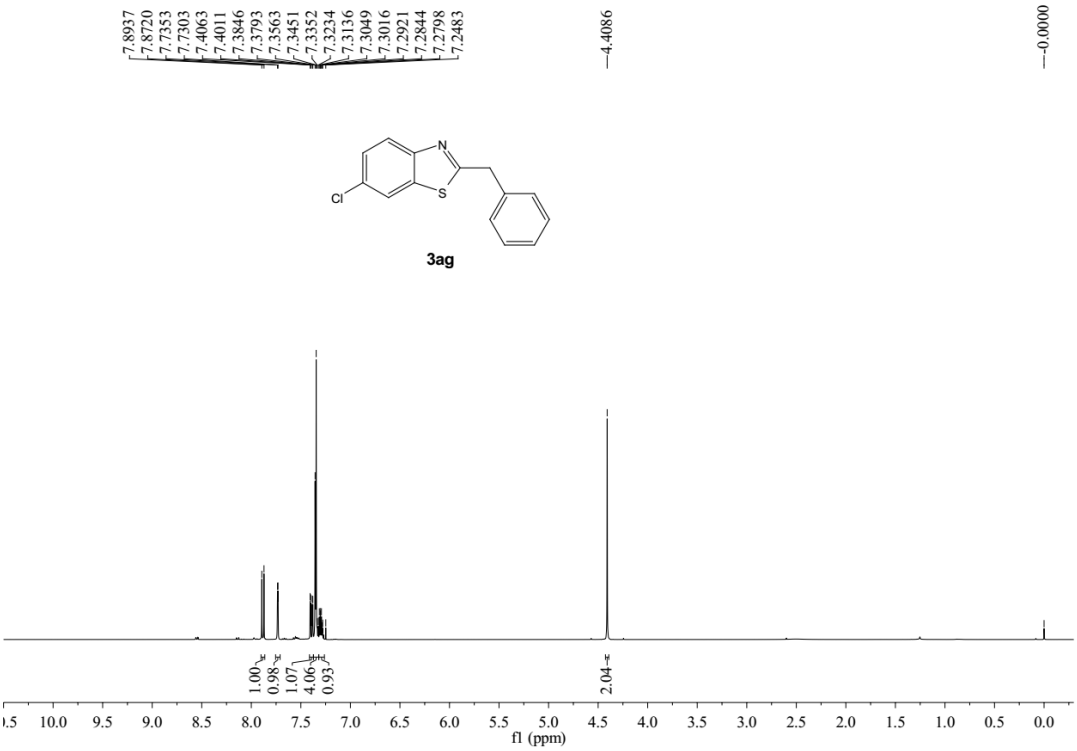
N
S
F
f1 (ppm)

3af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7.7303
7.4063
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7.3846
7.3793
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7.3352
7.3234
7.3136
7.3049
7.3016
7.2921
7.2844
7.2798
7.2483
4.4086
0.0000
N
S
Cl
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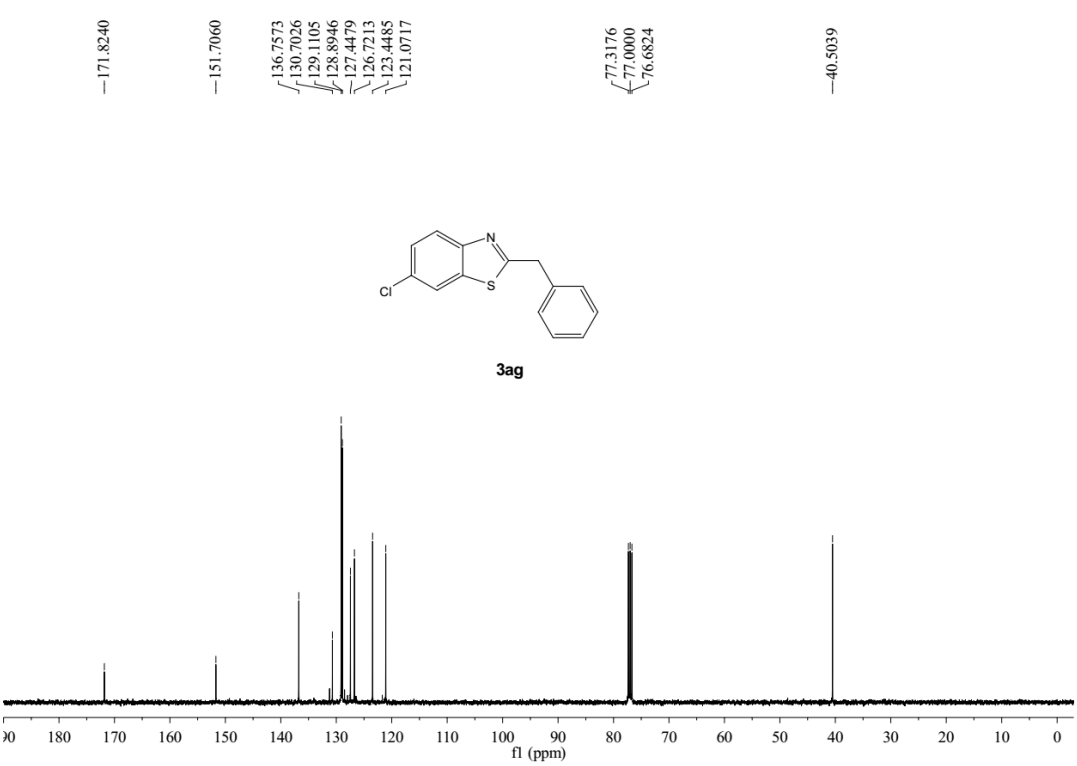
0.98
1.07
4.06
0.93
2.04
f1 (ppm)

3ag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129.1105
128.8946
127.4479
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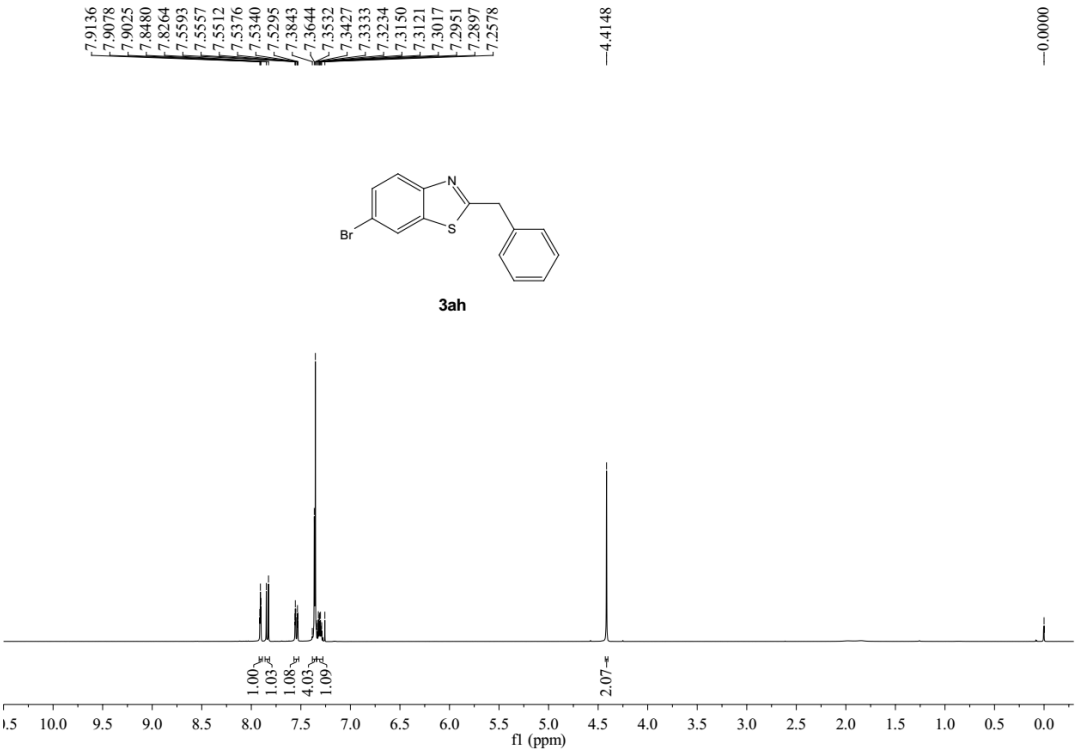
121.0717
77.3176
77.0000
76.6824
40.5039
N
S
Cl
f1 (ppm)

3ag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7.9025
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7.8264
7.5593
7.5557
7.5512
7.5376
7.5340
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7.3843
7.3644
7.3532
7.3427
7.3333
7.3234
7.3150
7.3121
7.3017
7.2951
7.2897
7.2578
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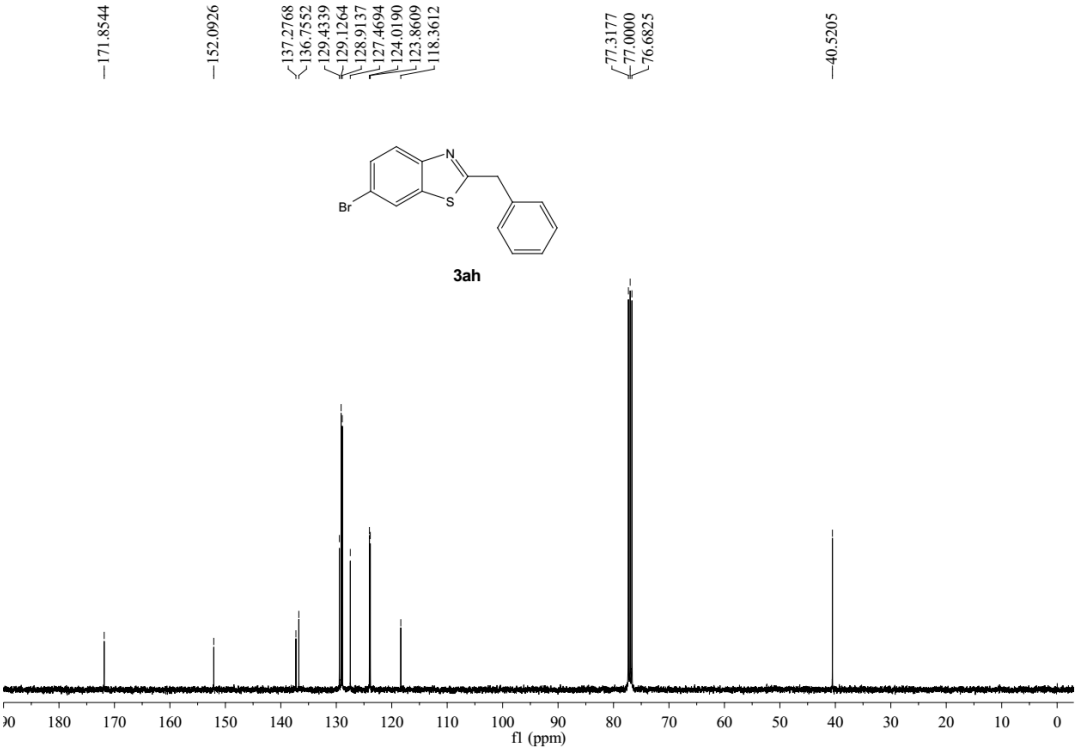
Br
N
S
3ah
1.00
1.03
1.08
4.03
1.09
2.07
f1 (ppm)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77.0000
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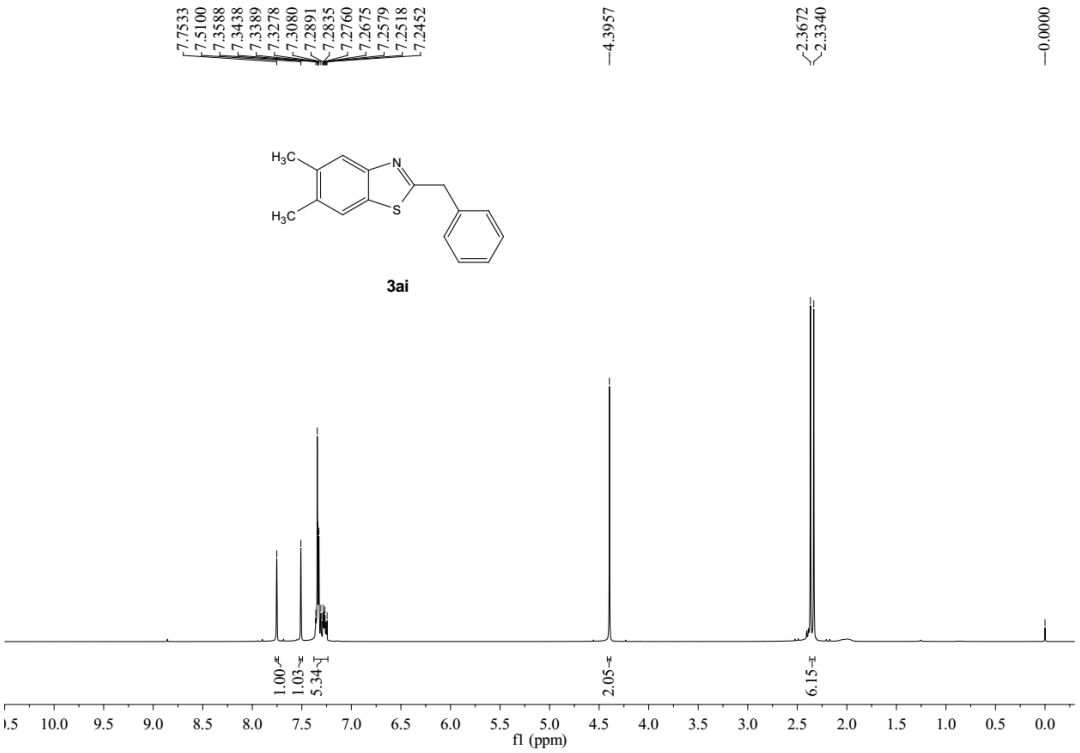
Br
N
S
3ah
f1 (ppm)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7.3588
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7.3389
7.3278
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7.2891
7.2835
7.2760
7.2675
7.2579
7.2518
7.2452
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2.3340
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3ai
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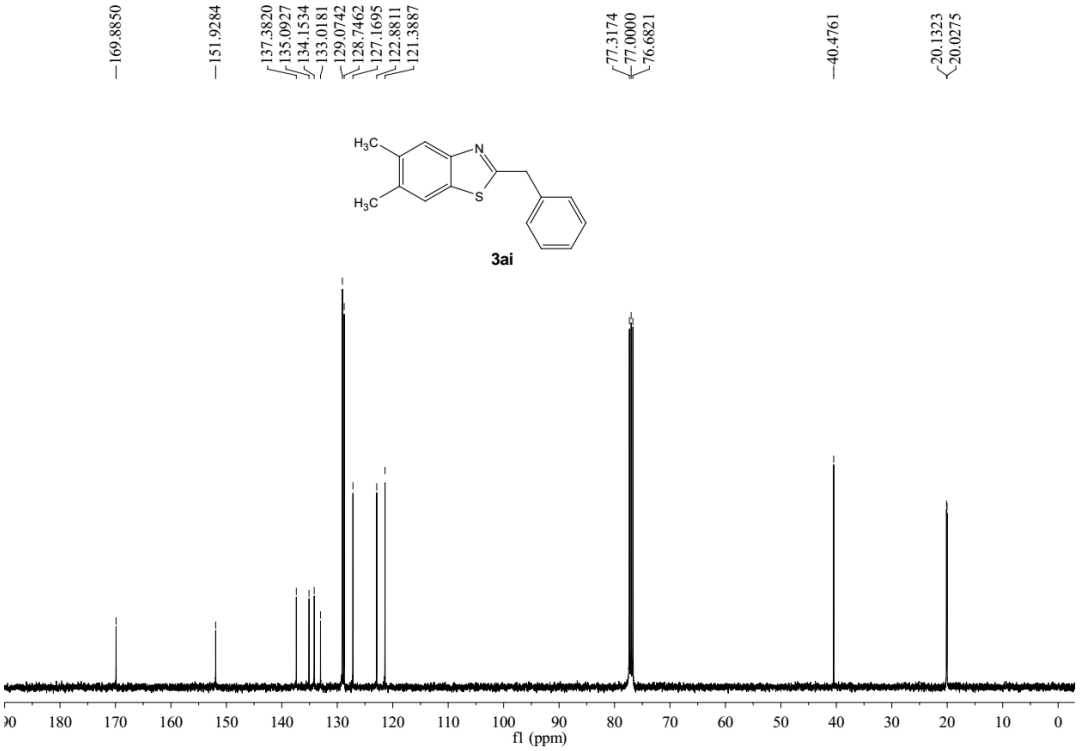
1.03
5.34
2.05
6.15
fl (ppm)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77.0000
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20.1323
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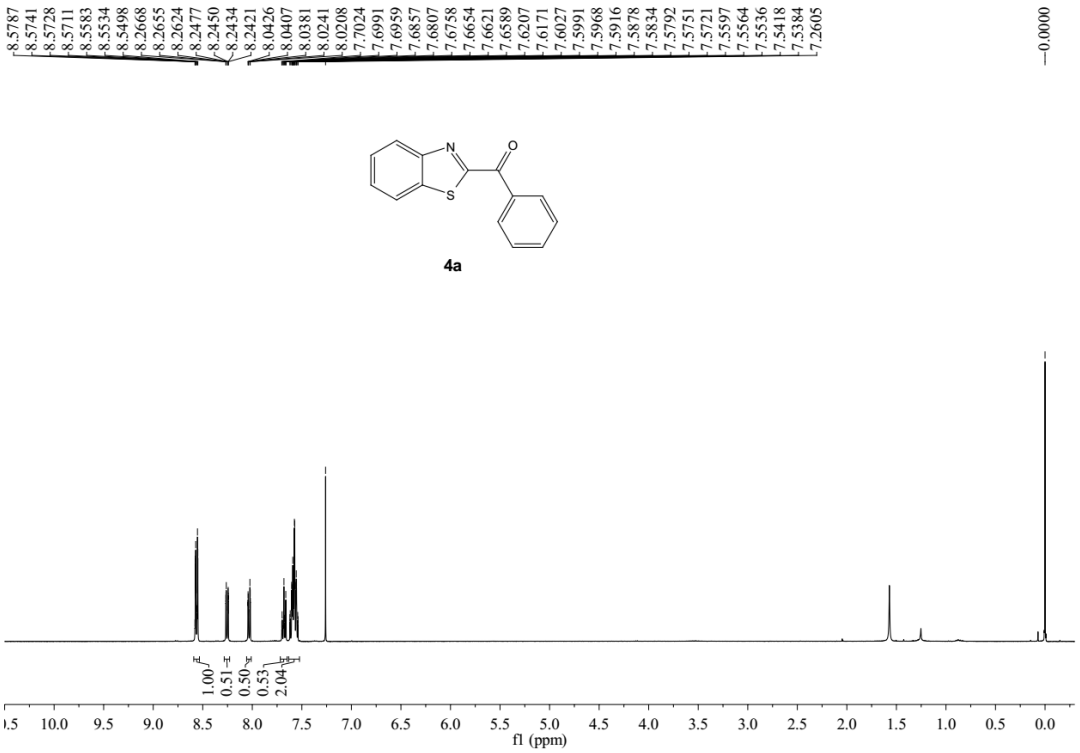
3ai
fl (ppm)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8.5498
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8.2655
8.2624
8.2477
8.2450
8.2434
8.2421
8.0426
8.0407
8.0381
8.0241
8.0208
7.7024
7.6991
7.6959
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7.6807
7.6758
7.6654
7.6621
7.6589
7.6207
7.6171
7.6027
7.5991
7.5968
7.5916
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7.5834
7.5792
7.5751
7.5721
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7.5564
7.5536
7.5418
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O
S
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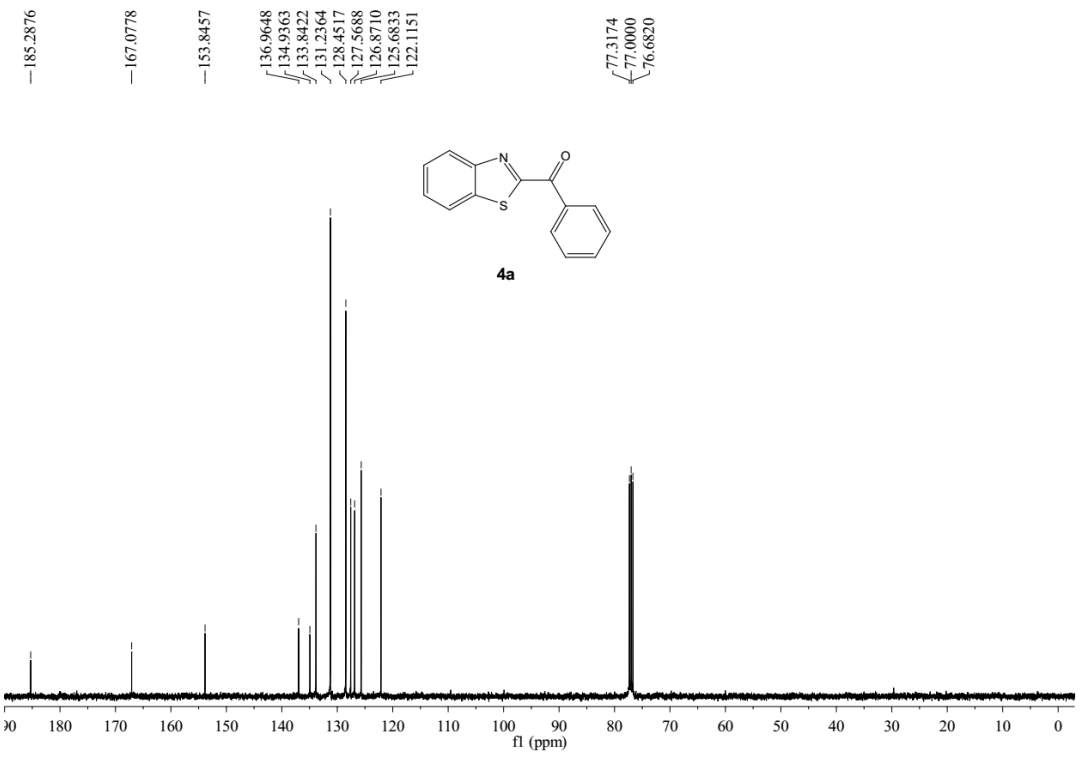
0.50
0.53
2.04
f1 (ppm)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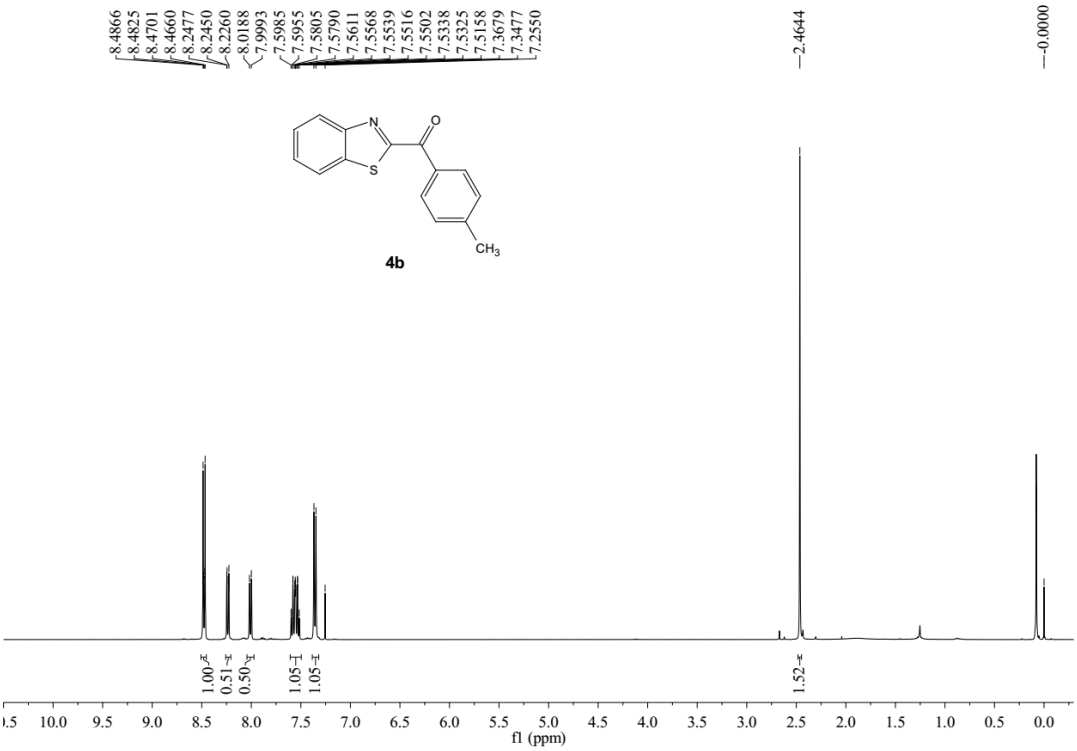
125.6833
122.1151
77.3174
77.0000
76.6820
N
O
S
4a
f1 (ppm)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8.2260
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7.5955
7.5805
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7.5611
7.5568
7.5539
7.5516
7.5502
7.5338
7.5325
7.5158
7.3679
7.3477
7.2550
2.4644
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S
CH3
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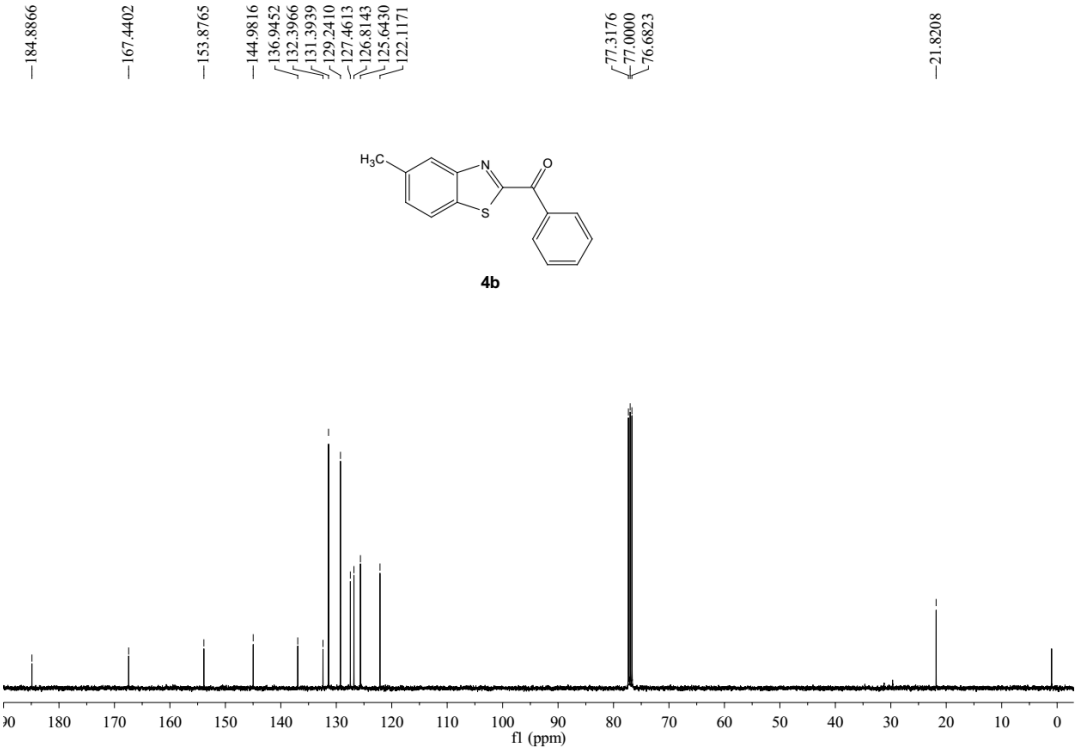
1.05
1.05
1.52
f1 (ppm)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131.3939
129.2410
127.4613
126.8143
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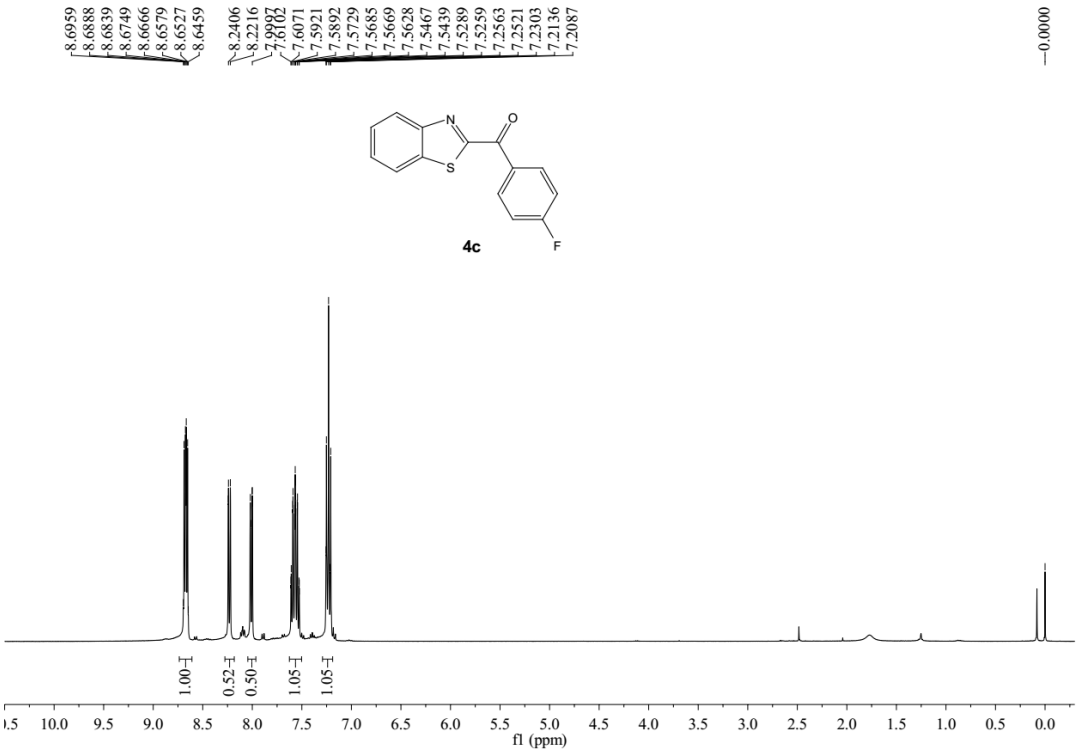
77.3176
77.0000
76.6823
21.8208
H3C
N
O
S
4b
f1 (ppm)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7.5921
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7.5669
7.5628
7.5467
7.5439
7.5289
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7.2563
7.2521
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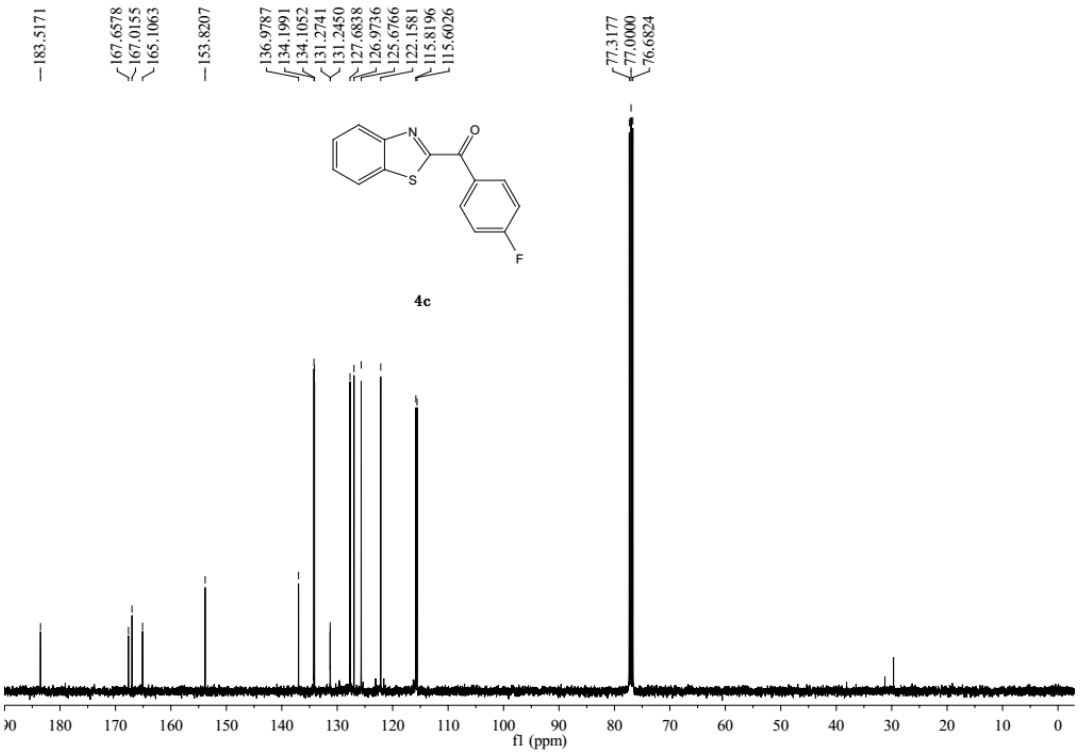
1.05
f1 (ppm)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134.1991
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127.6838
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77.0000
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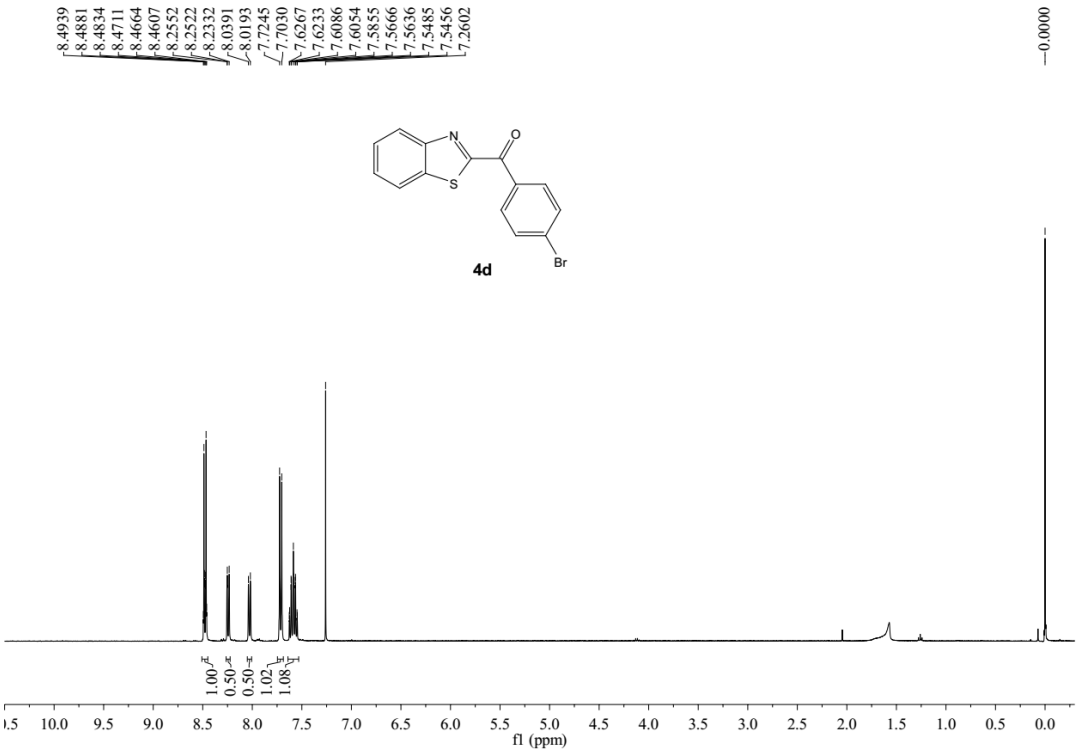
4c
f1 (ppm)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8.0391
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7.7245
7.7030
7.6267
7.6233
7.6086
7.6054
7.5855
7.5666
7.5636
7.5485
7.5456
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O
S
Br
4d
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0.50
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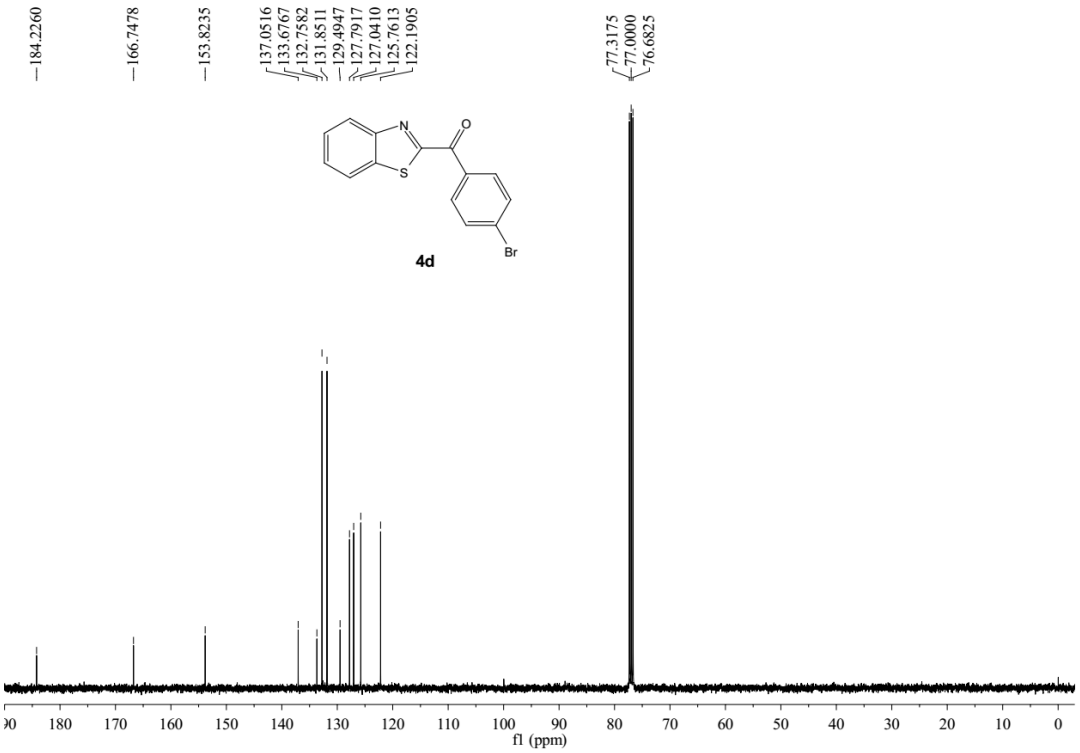
1.08
f1 (ppm)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122.1905
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77.0000
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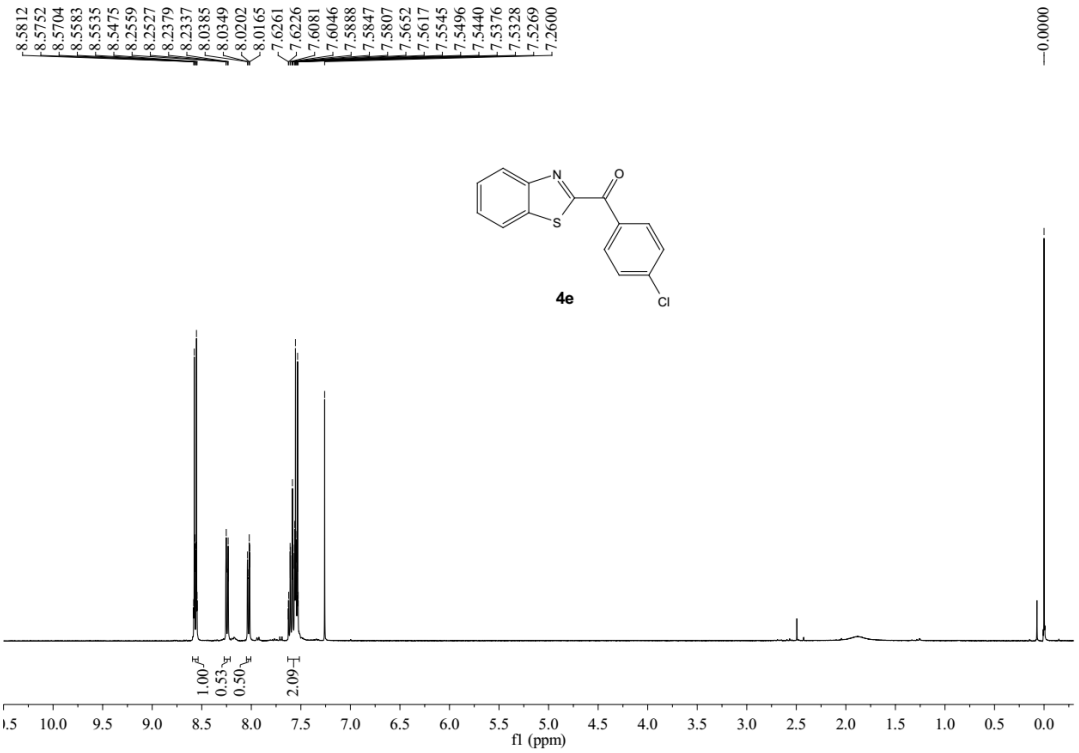
N
O
S
Br
4d
f1 (ppm)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8.0349
8.0202
8.0165
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7.6226
7.6081
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7.5888
7.5847
7.5807
7.5652
7.5617
7.5545
7.5496
7.5440
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7.5269
7.2600
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4e
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0.53
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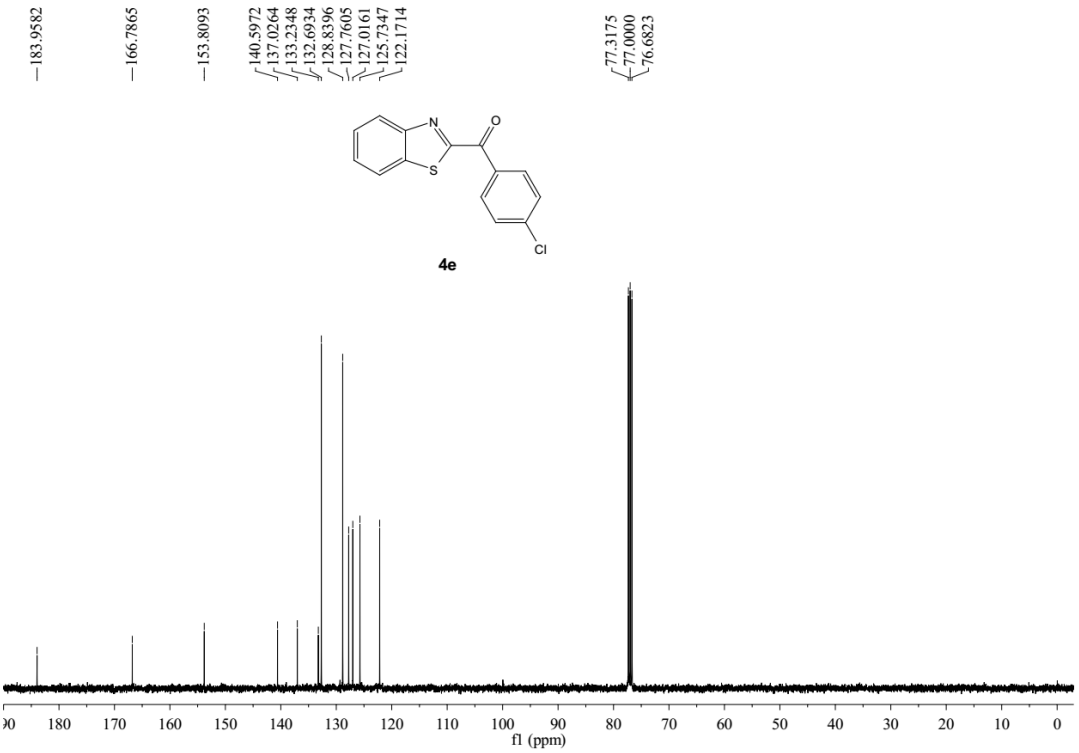
2.09
f1 (ppm)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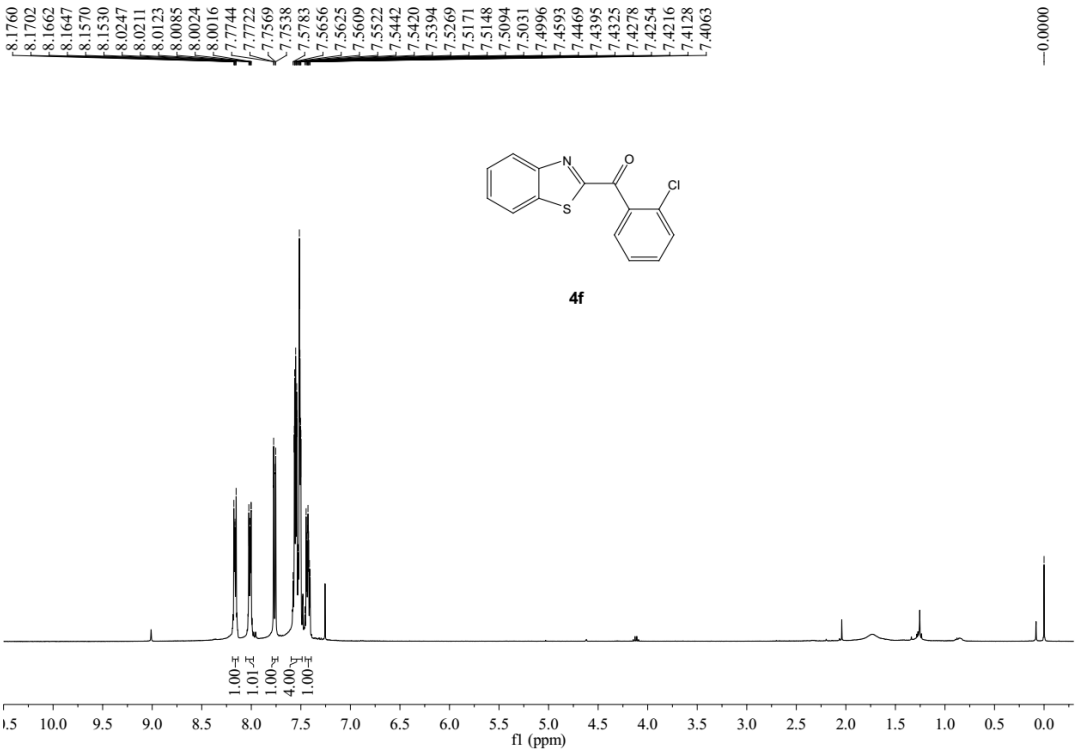
77.0000
76.6823
4e
f1 (ppm)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8.1662
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8.0024
8.0016
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7.7722
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7.7538
7.5783
7.5656
7.5625
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7.5522
7.5442
7.5420
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7.5269
7.5171
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7.5094
7.5031
7.4996
7.4593
7.4469
7.4395
7.4325
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7.4216
7.4128
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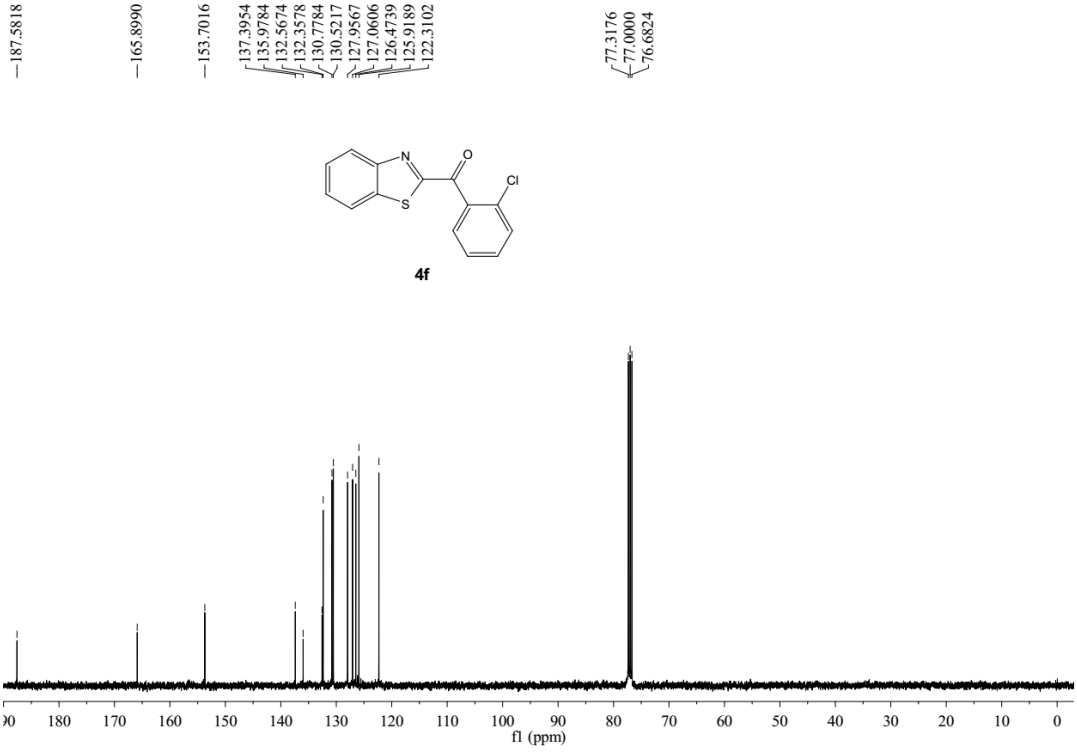
N
O
S
Cl
1.00
1.01
1.00
4.00
1.00
fl (ppm)

4f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122.3102
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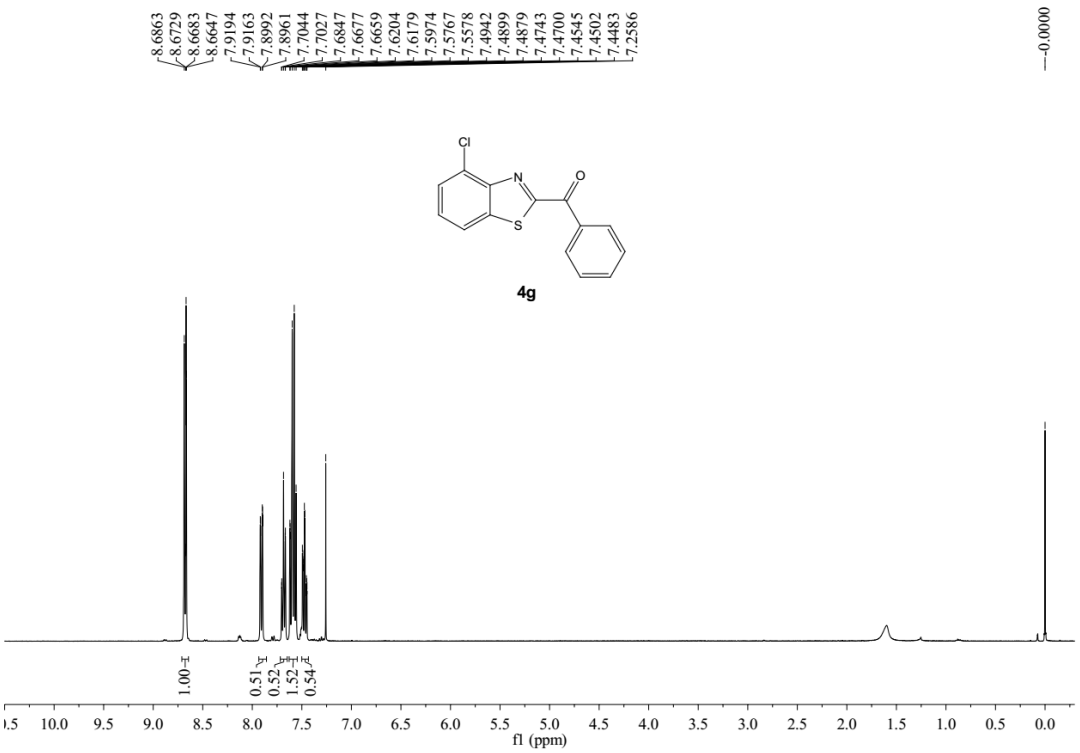
77.0000
76.6824
N
O
S
Cl
fl (ppm)

4f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7.7027
7.6847
7.6677
7.6659
7.6204
7.6179
7.5974
7.5767
7.5578
7.4942
7.4899
7.4879
7.4743
7.4700
7.4545
7.4502
7.4483
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Cl
N
O
S
4g
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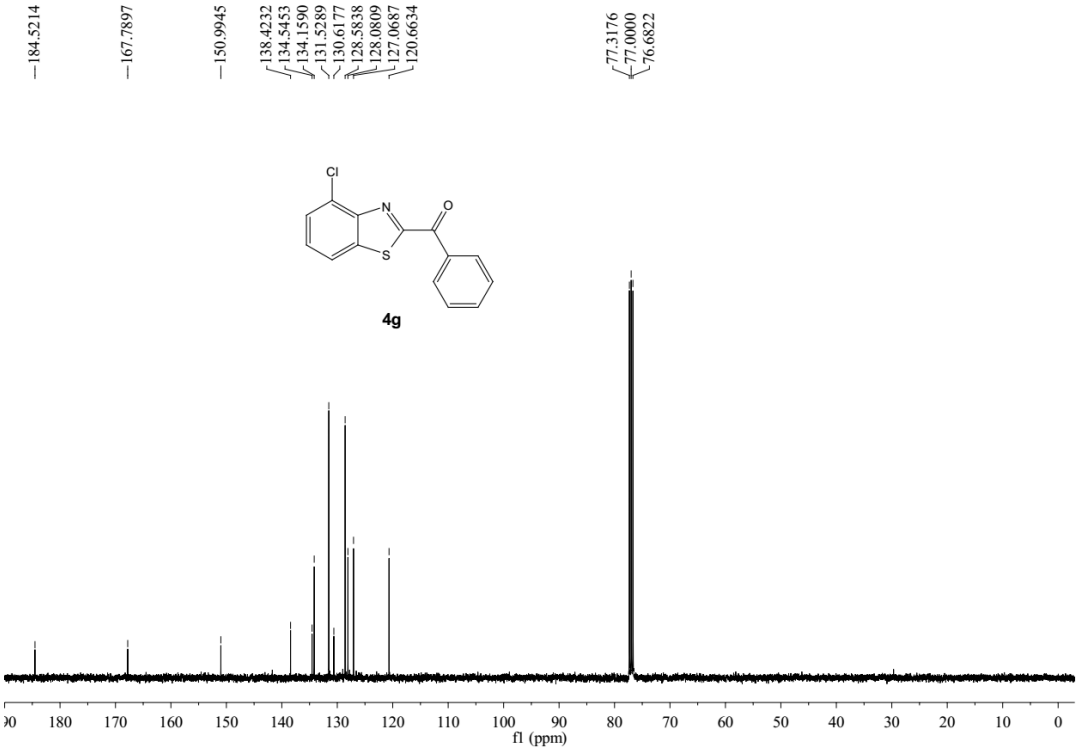
0.52
1.52
0.54
f1 (ppm)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134.5453
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131.5289
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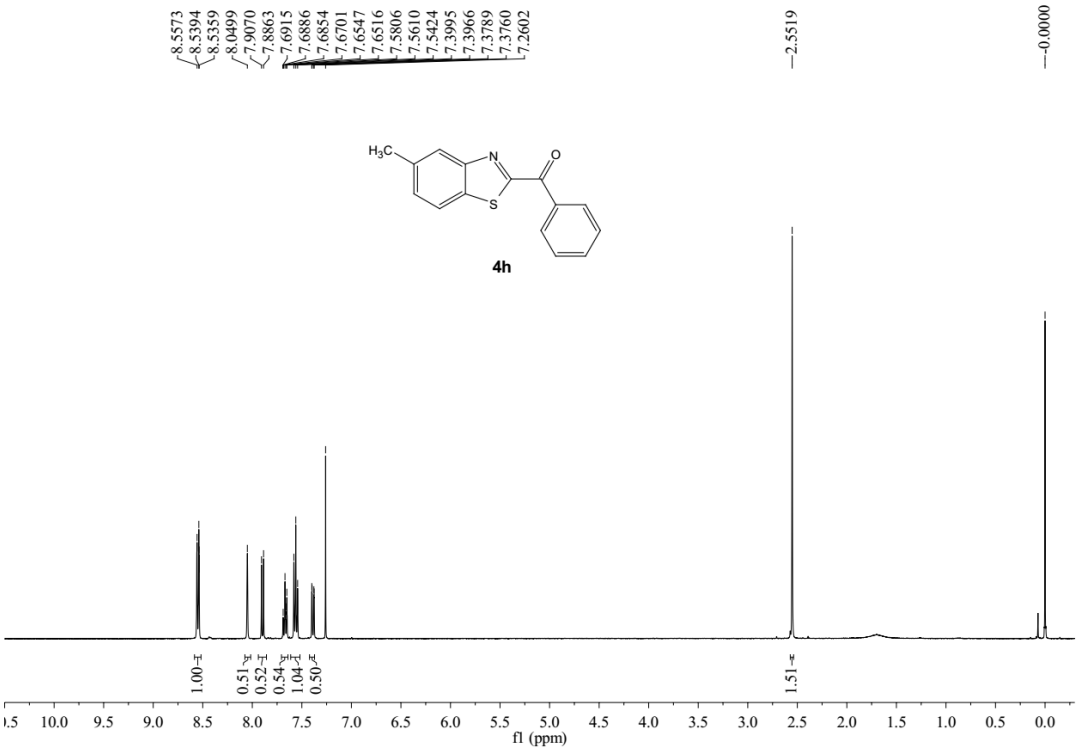
77.0000
76.6822
Cl
N
O
S
4g
f1 (ppm)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7.6915
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7.6854
7.6701
7.6547
7.6516
7.5806
7.5610
7.5424
7.3995
7.3966
7.3789
7.3760
7.2602
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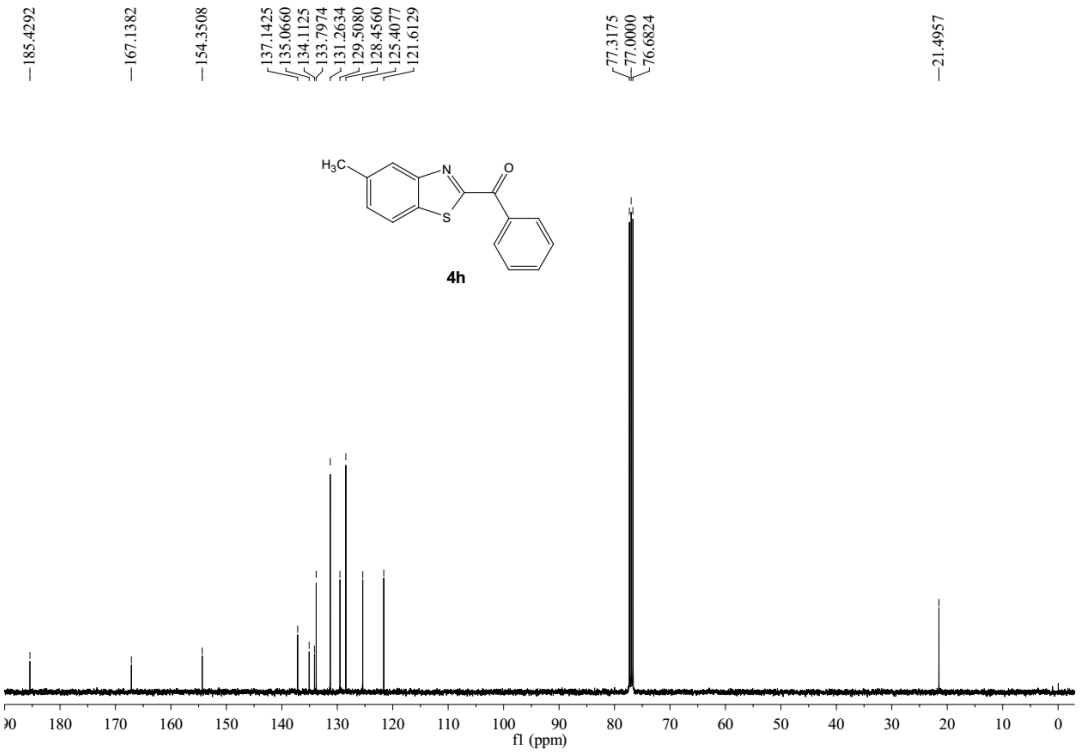
0.0000
4h
1.00
0.51
0.52
0.54
1.04
0.50
1.51
fl (ppm)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167.1382
154.3508
137.1425
135.0660
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133.7974
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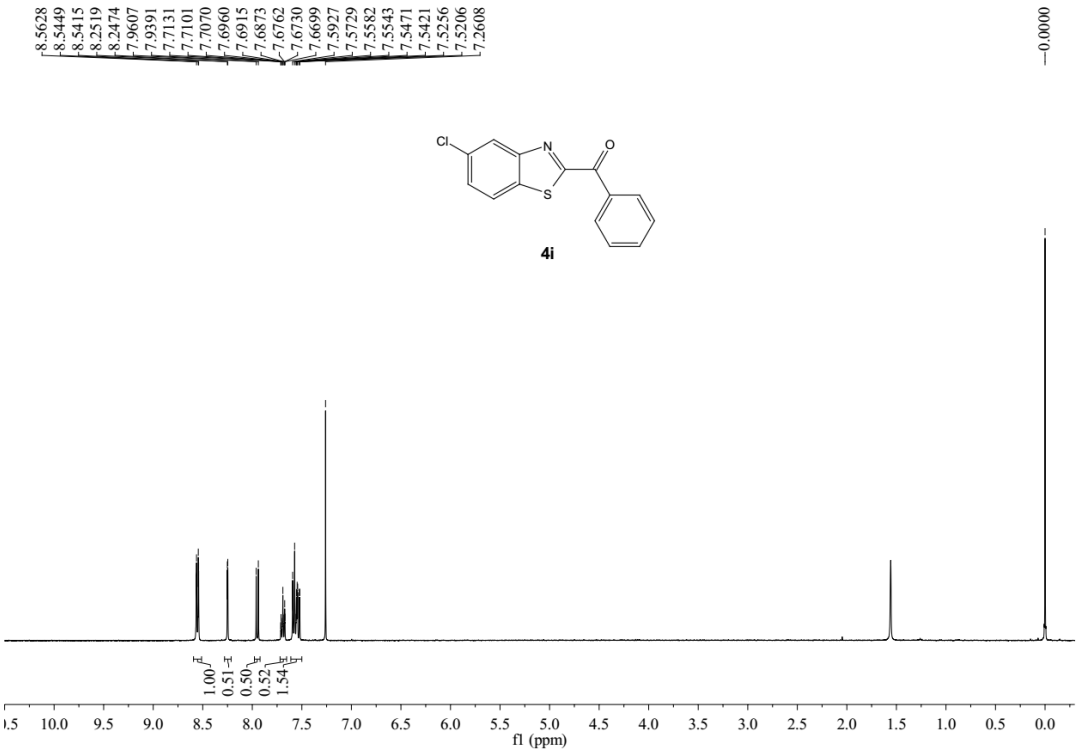
125.4077
121.6129
77.3175
77.0000
76.6824
21.4957
4h
fl (ppm)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8.2474
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7.6960
7.6915
7.6873
7.6762
7.6730
7.6699
7.5927
7.5729
7.5582
7.5543
7.5471
7.5421
7.5256
7.5206
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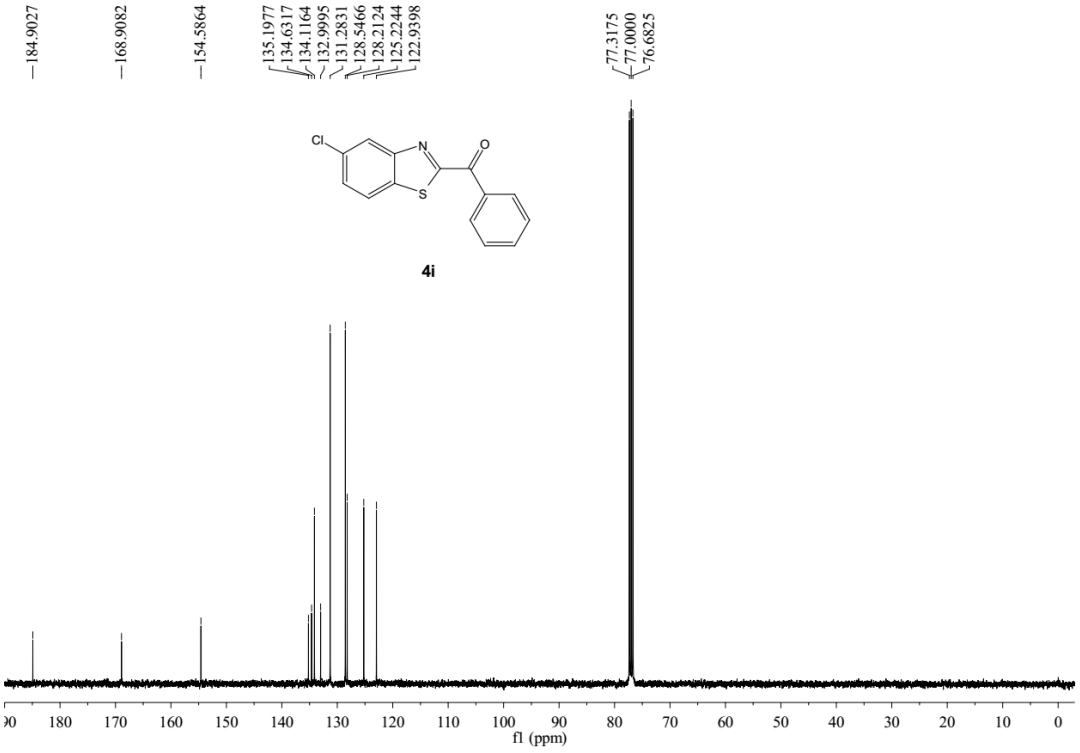
Cl
N
O
S
4i
1.00
0.51
0.50
0.52
1.54
f1 (ppm)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122.9398
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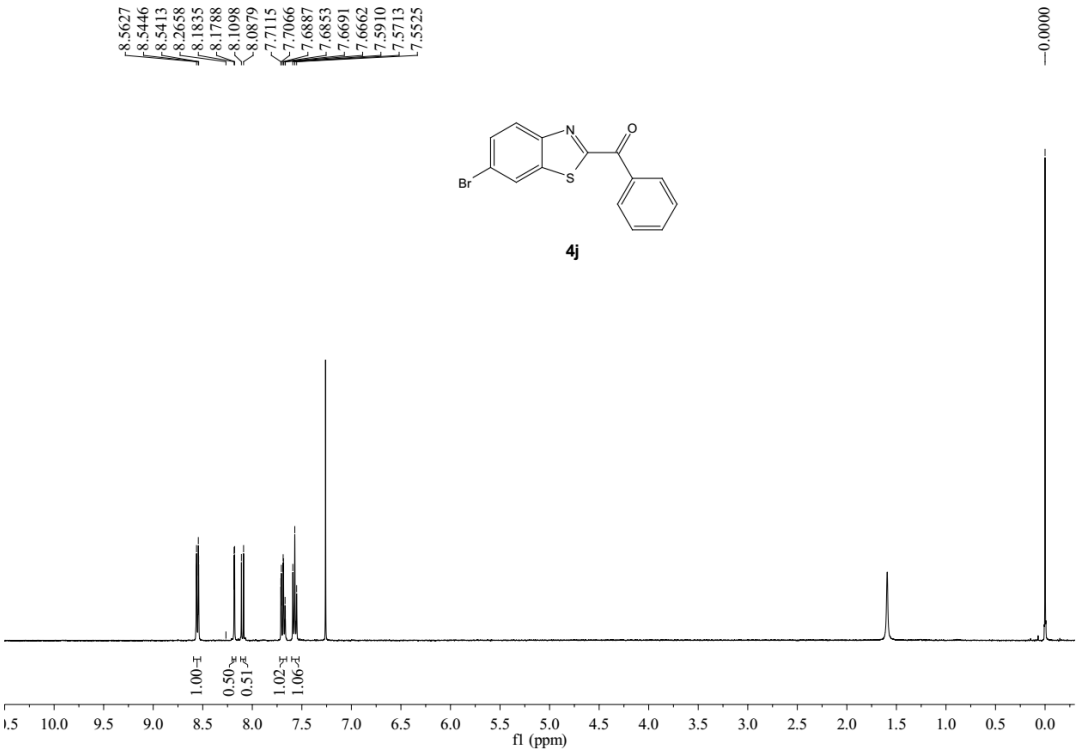
77.0000
76.6825
Cl
N
O
S
4i
f1 (ppm)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7.6887
7.6853
7.6691
7.6662
7.5910
7.5713
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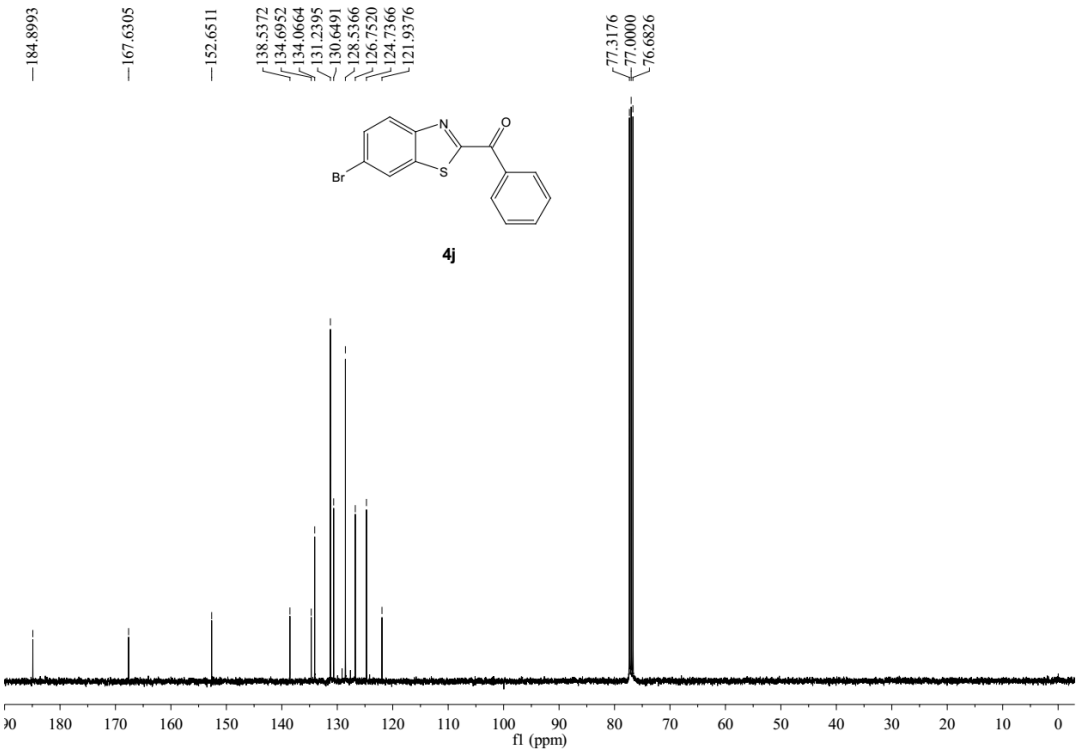
N
O
S
Br
4j
1.00
0.50
0.51
1.02
1.06
f1 (ppm)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131.2395
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128.5366
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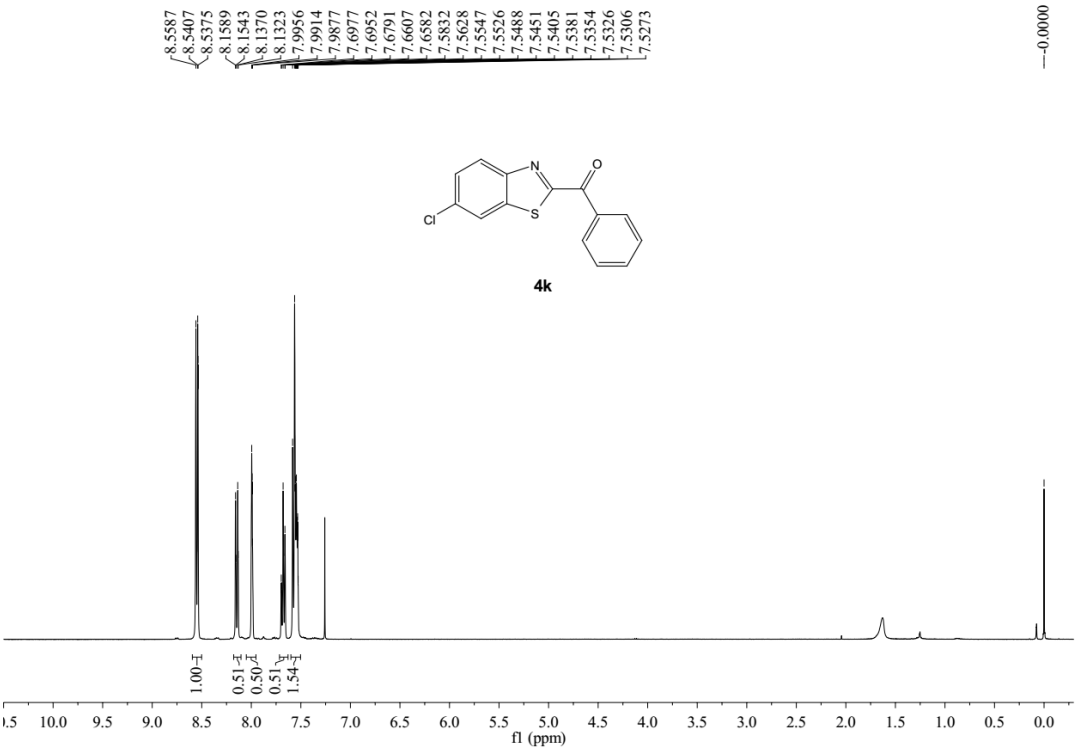
121.9376
77.3176
77.0000
76.6826
N
O
S
Br
4j
f1 (ppm)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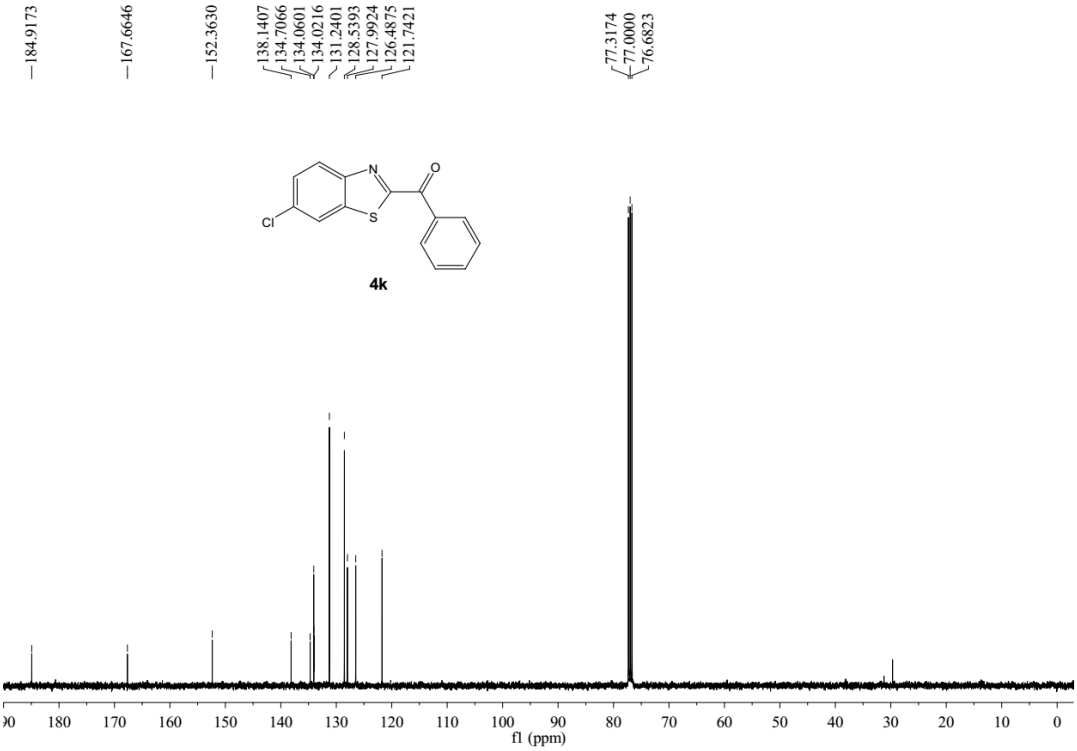
8.5375
8.1589
8.1543
8.1370
8.1323
7.9956
7.9914
7.9877
7.6977
7.6952
7.6791
7.6607
7.6582
7.5832
7.5628
7.5547
7.5526
7.5488
7.5451
7.5405
7.5381
7.5354
7.5326
7.5306
7.5273
0.0000
N
O
Cl
S
4k
1.00
0.51
0.50
0.51
1.54
f1 (ppm)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134.0601
134.0216
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128.5393
127.9924
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121.7421
77.3174
77.0000
76.6823
N
O
Cl
S
4k
f1 (ppm)