Supporting Information
for

Photocatalytic Difunctionalisations of Alkenes with *N*–SCN Sulfoximines

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1. General information

Unless otherwise noted, the reagents were purchased from commercial suppliers and used without purification. Reactions were tracked by thin layer chromatography (TLC) using TLC plates from Merck. Column chromatography was performed using silica gel 60 (63 - 200 μm) from Merck. ^{1}H NMR spectra were recorded on an Agilent 400 or 600 MHz spectrometer in deuterated chloroform. The chemical shifts were given in ppm relative to the residual peak of the non-deuterated solvent was used as internal standard ($CDCl_3$ 7.26 ppm). ^{1}H NMR data are reported as follows: chemical shift, multiplicity (s = singlet, d =doublet, t = triplet, q = quartet, hept = heptet, m = multiplet, br = broad), coupling constants (in Hz), integration. ^{13}C {^{1}H} NMR data were collected at 100 or 150 MHz with complete proton decoupling ($CDCl_3$ δ 77.16 ppm). IR spectra were recorded on a Perkin Elmer 100 FT/IR spectrometer, and the wave numbers of the absorption peaks are given in cm^{-1}. Mass (MS) were acquired on a Finnigan SSQ 7000 spectrometer [electron ionization (EI), 70 eV. High resolution mass spectra (HRMS) analyses were recorded on a Thermo Scientific LTQ Orbitrap XL with positive ion mode. Visible light was provided by irradiation with blue-LEDs (5 W, 455 nm). The microwave reactor (CEM Discover) was purchased from CEM Company. The respective temperature (90 °C) was measured externally. N–Bromo sulfoximines **1** were prepared according to literature procedures.[1]

2. Synthesis of *N*–SCN sulfoximines

2.1. Using *N*–Br sulfoximines 1 as starting materials

1 **2**

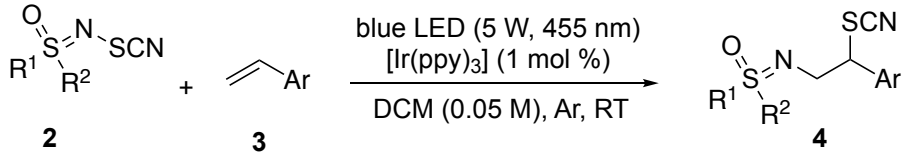
The *N*–bromo sulfoximine **1** (0.2 mmol) and NH_4SCN (22.8 mg, 0.3 mmol, 1.5 equiv) was added to a 5.0 mL sealable reaction tube. Then, DCM (1.0 mL) was added and the reaction was stirred for 16 h at 25 ºC in the air atmosphere. The product was purified by flash column chromatography (ethyl acetate/ *n*-pentane = 1/4 to 1/1) to give the corresponding *N*–SCN sulfoximine **2**.

Note: The *N*–SCN sulfoximines were transferred to the small glass bottle. Then, they were kept under vacuum until them were used in the next step.

2.2. Using *N*–H sulfoximines as starting materials

The *N*–H sulfoximine (0.2 mmol), NH_4SCN (22.8 mg, 0.3 mmol, 1.5 equiv) and NBS (0.24 mmol, 42.7 mg) were added to a 5.0 mL sealable reaction tube. Then, DCM (1.0 mL) was added and the reaction was stirred for 16 h at 25 °C in the air atmosphere. The isolation of **2** was performed as described under 2.1.

3. General method for the synthesis of 4 (as illustrated for 4aa)

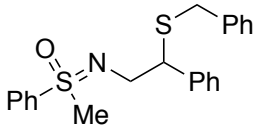


Under argon, freshly prepared *N*–SCN sulfoximine **2a** (31.8 mg, 0.15 mmol, 1.0 equiv), styrene **3a** (78.2 mg, 0.75 mmol, 5.0 equiv) and *fac*-[Ir(ppy)$_3$] (1.0 mg, 1.0 mol%, 0.01 equiv) were added into a 5.0 mL sealable reaction tube. Then, DCM (3 mL, 0.05 mL·mmol^{-1} of *N*–SCN sulfoximine) was added, and the mixture was stirred under argon with blue-LED irradiation (5 W) at room temperature for 40 h. Subsequently, the product was purified by flash column chromatography (ethyl acetate/ *n*-pentane = 1/2) to give **4aa** in 72% yield. The diastereomeric ratio of **4** was determined by ^{1}H NMR of the crude product mixture.

Note: In all reactions freshly prepared N–SCN sulfoximines were used.

4. Conversions of 4aa into thioether 5 and disulfide 6

[(2-(Benzylthio)-2-phenylethyl)imino](methyl)(phenyl)- λ^6-sulfanone (5)

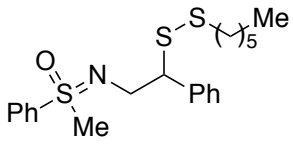


A mixture of **4aa** (15.6 mg, 0.05 mmol), lithium aluminum hydride (5.4 mg, 0.14 mmol), benzylbromide (15.0 uL, 0.125 mmol) in THF (0.6 mL) was stirred in air at room temperature for 48 h. Purification by column chromatography (*n*-pentane: ethyl acetate = 2:1) gave 14.8 mg (78%) of product **5** as a light yellow oil.

Note: The protocol followed a literature procedure applied for converting related compounds.[2] Accordingly, we expected to isolate the corresponding dimerized disulfide. That product, however, remained undetected.

^{1}H NMR (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.80 (d, *J* = 7.7 Hz, 1H), 7.56 (dd, *J* = 16.5, 7.5 Hz, 2H), 7.50 (t, *J* = 7.7 Hz, 1H), 7.42 (t, *J* = 7.7 Hz, 1H), 7.33 – 7.18 (m, 10H), 3.98 – 3.86 (m, 1H), 3.60 – 3.48 (m, 2H), 3.44 – 3.38 (m, 1H), 3.22 – 3.07 (m, 1H), 2.97 (s, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 141.2, 141.0, 139.3, 139.0, 138.3, 132.9, 132.7, 129.4, 129.3, 129.0, 129.0, 128.7, 128.6, 128.5, 128.4, 128.3, 128.3, 127.2, 127.1, 126.8, 126.8, 52.0, 51.6, 49.5, 49.5, 45.0, 44.8, 35.7, 35.7. **MS** (EI, 70 eV): *m/z* (%) = 168.0 (78), 141.0 (53), 125.0 (16), 124.0 (12), 121.0 (14), 104.1 (12), 91.1 (100). **MS** (ESI) $[M+Na]^+$: 404.11 (ESI) (*m/z*) $[C_{22}H_{23}NOS_2Na]^+$: Calcd. 404.1119. found, 404.1096. **IR** (ATR): *ν* = 3570, 3027, 2917, 2845, 2667, 2330, 2108, 1900, 1815, 1726, 1595, 1489, 1447, 1239, 1136, 1082, 974, 737, 696.

[(2-(Hexylthio)-2-phenylethyl)imino](methyl)(phenyl)- λ⁶-sulfanone (6)



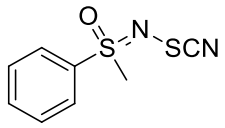
A mixture of **4aa** (15.6 mg, 0.05 mmol), 1-bromohexane (12.4 mg, 0.075 mmol), thiourea (4.6 mg, 0.06 mmol), K_3PO_4 (12.7 mg, 0.06 mmol), KI (12.4 mg, 0.075 mmol) and TBAH (49.0 mg, 0.075 mmol, 40% in water) in water (1.0 mL) was put into the cavity of the microwave reactor (with a power of 50 W at 90 °C for 10 min). Then, the reaction mixture was extracted by DCM (3 x 2.0 mL). The combined organic extract was concentrated, and the product was purified by column chromatography (*n*-pentane : ethyl acetate = 2:1) to give 6.5 mg (32%) of **6** as a light yellow oil.

Note: The protocol followed a procedure reported in the literature.[3]

^{1}H NMR (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.89 – 7.86 (m, 1H), 7.72 – 7.69 (m, 1H), 7.62 – 7.47 (m, 4H), 7.31 – 7.26 (m, 4H), 4.11 – 4.03 (m, 1H), 3.63 (dd, *J* = 12.7, 5.9 Hz, 0.5H), 3.51 (dd, *J* = 12.8, 6.8 Hz, 0.5H), 3.39 (dd, *J* = 12.8, 7.5 Hz, 0.5H), 3.27 (dd, *J* = 12.6, 8.7 Hz, 0.5H), 3.03 (d, *J* = 4.4 Hz, 3H), 2.35 – 2.29 (m, 1H), 2.19 – 2.15 (m, 1H), 1.51 – 1.42 (m, 2H), 1.28 – 1.23 (m, 4H), 1.20 – 1.17 (m, 2H), 0.87 – 0.85 (m, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 140.2, 132.9, 132.8, 129.4, 129.3, 128.7, 128.6, 128.6, 128.5, 128.3, 128.2, 127.4, 57.9, 57.6, 48.2, 47.5, 45.0, 45.0, 38.9, 38.7, 31.3, 28.9, 28.9, 28.1, 22.5, 14.0. **MS** (EI, 70 eV): *m/z* (%) =258.0 (52), 168.0 (80), 141.0 (100), 125.0 (16), 124.0 (13), 91.1 (33). **MS** (ESI) $[M+H]^+$: 408.15 (ESI) (*m/z*) $[C_{21}H_{30}NOS_3]^+$: Calcd. 408.1490. found, 408.1484. **IR** (ATR): *v* =3879, 3364, 3185, 2925, 2857, 2672, 2330, 2101, 1992, 1910, 1732, 1675, 1595, 1451, 1243, 1138, 1081,975, 741, 694.

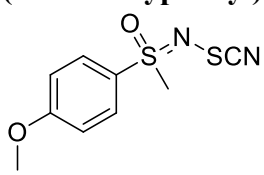
5. Characterisation Data

Methyl(phenyl)(thiocyanatoimino)-λ⁶-sulfanone (2a)



Colorless oil, 38.2 mg, 90% yield, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.94 – 7.89 (m, 2H), 7.75 (t, *J* = 7.5 Hz, 1H), 7.66 (t, *J* = 7.9 Hz, 2H), 3.31 (s, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$) δ 135.8, 134.8, 130.0, 128.6, 115.3, 43.8, 43.8. **MS** (EI, 70 eV): *m/z* (%) = 212.0 (100, M^+), 186.0 (14), 156.0 (15), 140.1 (90), 125.0 (76), 97.1 (22), 77.2 (25). **IR** (ATR): *v* = 3524, 3008, 2918, 2326, 2193, 2132, 2053, 1925, 1740, 1571, 1448, 1321, 1217, 1091, 973, 744, 678. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_8H_8N_2OS_2Na]^+$: 234.9976, found, 234.9977.

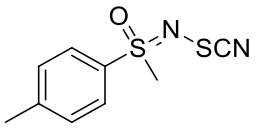
(4-Methoxyphenyl)(methyl)(thiocyanatoimino)-λ⁶-sulfanone (2b)



Colorless oil, 25.1 mg, 52% yield, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 8.8, 1.5 Hz, 2H), 7.10 (dd, *J* = 8.8, 1.5 Hz, 2H), 3.91 (d, *J* = 1.5 Hz, 3H), 3.28 (d, *J* = 1.5 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 164.6, 130.9, 126.4, 115.5, 115.2, 55.9, 44.2. **MS** (EI, 70 eV): *m/z* (%) = 242.0 (9, M^+), 155.1 (100),

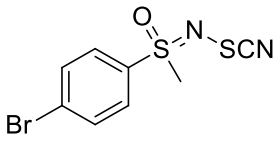
76.3 (3). **IR** (ATR): *v* = 3492, 3002, 2914, 2666, 2299, 2054, 1910, 1638, 1546, 1447, 1400, 1322, 1219, 1101, 1007, 843,743, 681. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_9H_{10}N_2O_2S_2Na]^+$: 265.0081, found, 265.0077.

Methyl(thiocyanatoimino)(*p*-tolyl)-λ^6-sulfanone (**2c**)



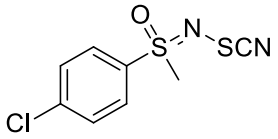
Colorless oil, 26.2 mg, 58% yield, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.2 Hz, 2H), 3.29 (s, 3H), 2.48 (s, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$) δ 146.1, 132.6, 130.6, 128.6, 115.4, 44.0, 21.8. **MS** (EI, 70 eV): *m/z* (%) = 226.0 (18, M^+),194.1 (18), 139.0 (64), 91.2 (29), 77.2 (23), 65.3 (57), 63.2 (41), 58.2 (13), 46.2 (100). **IR** (ATR): *v* = 3893, 3745, 2922, 2344, 2095, 1746, 1597, 1397, 1215, 1091, 969, 795, 692. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_9H_{10}N_2OS_2Na]^+$: 249.0232, found, 249.0127.

(4-Bromophenyl)(methyl)(thiocyanatoimino)-λ^6-sulfanone (**2d**)



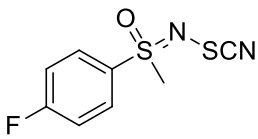
Colorless oil, 44.1 mg, 76% yield, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.82 – 7.73 (m, 4H), 3.29 (s, 3H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$) δ 134.8, 133.3, 130.4, 130.1, 115.0, 43.9. **MS** (EI, 70 eV): *m/z* (%) = 289.9 (72, M^+), 219.9 (100), 218.0 (97), 204.9 (80), 202.9 (78), 156.9 (16), 155.0 (16), 75.2 (28), 50.2 (40). **IR** (ATR): *v* = 3876, 2913, 2337, 2101, 1740, 1528, 1349, 1221, 1094, 975, 854, 728. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_8H_7N_2OS_2BrNa]^+$: 312.9081, found, 312.9076

(4-Chlorophenyl)(methyl)(thiocyanatoimino)-λ^6-sulfanone (**2e**)



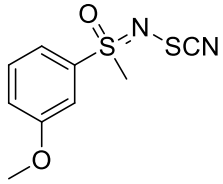
Colorless oil, 31.9 mg, 65% yield, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88 – 7.80 (m, 2H), 7.66 – 7.56 (m, 2H), 3.30 (s, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 141.8, 134.2, 130.3, 130.0, 115.0, 43.9. **MS** (EI, 70 eV): *m/z* (%) = 245.9 (85, M^+), 176.0 (41), 174.0 (85), 160.9 (52), 158.9 (100), 130.9 (19), 128.0 (20), 126.0 (12), 111.0 (19). **IR** (ATR): *v* = 3542, 3299, 3078, 3016, 2923, 2661, 2310, 2134, 2055, 1915, 1573, 1472, 1395, 1318, 1218, 1085, 975, 829, 773, 685. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_8H_7N_2OS_2FNa]^+$: 268.9586, found 268.9581.

(4-Fluorophenyl)(methyl)(thiocyanatoimino)-λ^6-sulfanone (**2f**)



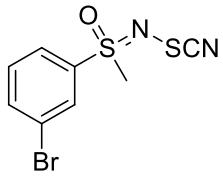
Colorless oil, 31.1 mg, 68% yield, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.97 – 7.92 (m, 2H), 7.34 (t, *J* = 8.5 Hz, 2H), 3.32 (s, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$) δ 166.4 (*J* = 258 Hz), 131.6 (*J* = 10.5 Hz), 131.5 (*J* = 3 Hz), 117.5 (*J* = 22.5 Hz), 115.1, 44.0. **MS** (EI, 70 eV): *m/z* (%) = 230.0 (6, M^+), 158.0 (34), 143.0 (58), 110.1 (97), 95.2 (68), 83.1 (48), 75.2 (55), 63.2 (23), 59.2 (33), 50.2 (46), 46.2 (100). **IR** (ATR): *v* = 3859, 3742, 3525, 3307, 3071, 3015, 2922, 2668, 2325, 2125, 1995, 1898, 1743, 1634, 1567, 1458, 1404, 1313, 1219, 1096, 974, 780, 680. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_8H_7N_2OS_2ClNa]^+$: 252.9882, found 252.9878

(3-Methoxyphenyl)(methyl)(thiocyanatoimino)-λ⁶-sulfanone (2g)



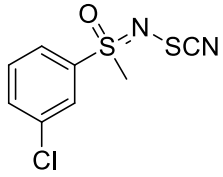
Colorless oil, 24.7 mg, 51% yield, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.55 (td, *J* = 8.1, 1.9 Hz, 1H), 7.47 (d, *J* = 7.7 Hz, 1H), 7.39 (d, *J* = 1.4 Hz, 1H), 7.25 (d, *J* = 8.3 Hz, 1H), 3.90 (d, *J* = 2.0 Hz, 3H), 3.30 (d, *J* = 1.9 Hz, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$) δ 160.5, 136.9, 131.0, 121.4, 120.6, 115.3, 112.9, 55.9, 55.9, 43.9, 43.9. **MS** (EI, 70 eV): *m/z* (%) = 242.2 (7, M^+), 155.0 (19), 124.1 (11), 95.1 (13), 92.1 (40), 78.2 (13), 77.1 (50), 64.2 (58), 63.2 (81), 46.1 (100). **IR** (ATR): *v* = 3743, 3625, 3303, 3073, 3015, 2924, 2666, 2320, 2134, 1993, 1904, 1741, 1570, 1461, 1405, 1318, 1220, 1097, 977, 778, 680. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_9H_{10}N_2O_2S_2Na]^+$ 265.0081, found 265.0079.

(3-Bromophenyl)(methyl)(thiocyanatoimino)-λ⁶-sulfanone (2h)



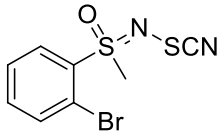
Colorless oil, 40.1 mg, 69% yield, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.07 (t, *J* = 1.7 Hz, 1H), 7.90 – 7.81 (m, 2H), 7.54 (t, *J* = 8.0 Hz, 1H), 3.33 (s, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 137.9, 137.7, 131.5, 131.4, 127.1, 124.0, 114.9, 43.8, 43.8. **MS** (EI, 70 eV): *m/z* (%) = 289.9 (56, M^+), 219.9 (100), 218.0 (90), 204.9 (74), 202.9 (72), 156.9 (15), 155.0 (15), 75.2 (30), 50.2 (36). CHN-elemental analysis: Calcd. for $C_8H_7N_2OS_2Br$, C = 33.00, H = 2.42, N = 9.62, found C = 32.75, H = 2.55, N = 9.48. **IR** (ATR): *v* = 3616, 3021, 2924, 2341, 2116, 1743, 1570, 1406, 1217, 1095, 968, 776, 689. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_8H_7N_2OS_2BrNa]^+$ 312.9081, found 312.9075

(3-Chlorophenyl)(methyl)(thiocyanatoimino)-λ⁶-sulfanone (2i)



Colorless oil, 32.4 mg, 66% yield, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.92 (t, *J* = 1.9 Hz, 1H), 7.82 – 7.79 (m, 1H), 7.72 – 7.70(m, 1H), 7.61 (t, *J* = 7.9 Hz, 1H), 3.33 (s, 3H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$) δ 137.6, 136.3, 134.9, 131.2, 128.6, 126.6, 114.9, 43.8. **MS** (EI, 70 eV): *m/z* (%) =176.1 (18), 174.1 (54), 161.1 (14), 159.1 (36), 131.1 (22), 128.2 (28), 126.1 (36), 113.1 (21), 111.1 (67), 99.2 (21), 45.3 (100). **IR** (ATR): *v* = 3867, 3532, 3298, 3073, 3013, 2921, 2657, 2319, 2127, 2063, 1898, 1636, 1574, 1460, 1408, 1318, 1220, 1115, 976, 788, 678. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_8H_7N_2OS_2ClNa]^+$ 268.9586, found 268.9581

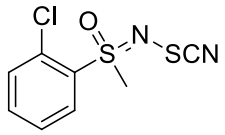
(2-Bromophenyl)(methyl)(thiocyanatoimino)-λ⁶-sulfanone (2j)



Colorless oil, 46.4 mg, 80% yield, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 8.27 (dd, *J* = 7.9, 1.3 Hz, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.70 – 7.48 (m, 2H), 3.54 (s, 3H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$) δ 136.1, 135.8, 134.8, 133.4, 128.6, 120.7, 114.1, 41.9. **MS** (EI, 70 eV): *m/z* (%) = 289.9 (99, M^+), 220.0 (100), 218.0 (100), 204.9 (86), 202.9 (86), 139.1 (61), 75.2 (26). CHN-elemental analysis: Calcd. for $C_8H_7N_2OS_2Br$, C = 33.00, H = 2.42, N = 9.62, found C = 32.78, H = 2.54, N = 9.44. **IR** (ATR): *v* = 3624, 3305, 3083, 3010, 2925, 2329, 2136, 2055, 1917, 1738, 1632, 1568, 1434, 1315, 1217, 1097, 1029,

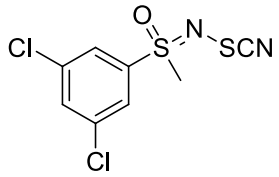
975, 758, 681. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_8H_7N_2OS_2BrNa]^+$ 312.9081, found 312.9075

(2-Chlorophenyl)(methyl)(thiocyanatoimino)-λ^6-sulfanone (**2k**)



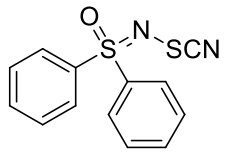
Colorless oil, 30.1 mg, 61% yield, ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.24 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.69 (td, *J* = 7.8, 1.5 Hz, 1H), 7.65 – 7.57 (m, 2H), 3.53 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 136.0, 133.1, 133.0, 132.5, 132.4, 128.0, 114.2, 42.2, 42.2. **MS** (EI, 70 eV): *m/z* (%) = 245.9 (8, M^+), 176.0 (6), 174.0 (18), 161.0 (10), 159.0 (27), 133.0 (6.2), 131.0 (18), 76.2 (12), 75.1 (64), 741.1 (19), 63.1 (34), 50.2 (68), 46.1 (100). **MS** (EI, 70 eV): *m/z* (%) = 246.2 (2, M^+), 176.1 (18), 174.1 (74), 159.1 (41), 131.1 (27), 128.2 (38), 126.1 (36), 113.1 (21), 111.1 (100). CHN-elemental analysis: Calcd. for $C_8H_7N_2OS_2Cl$, C = 38.94, H = 2.86, N = 11.35, found C = 38.73, H = 3.02, N = 11.38. **IR** (ATR): *v* = 3899, 3743, 3621, 3525, 3013, 2929, 2677, 2316, 2114, 1999, 1901, 1741, 1589, 1540, 1368, 1218, 1094, 975, 808, 763, 692. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_8H_7N_2OS_2ClNa]^+$ 268.9586, found 268.9583.

(3,5-Dichlorophenyl)(methyl)(thiocyanatoimino)-λ^6-sulfanone (**2l**)



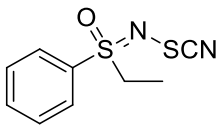
Colorless oil, 47.0 mg, 84% yield, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.79 (d, *J* = 1.8 Hz, 2H), 7.71 (t, *J* = 1.6 Hz, 1H), 3.35 (s, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$) δ 138.9, 137.1, 134.8, 126.9, 114.6, 43.8, 43.8. **MS** (EI, 70 eV): *m/z* (%) = 279.9 (18, M^+), 209.9 (25), 207.9 (37), 194.9 (30), 192.9 (44), 163.9 (17), 161.9 (28), 147.1 (12), 145.0 (23), 111.0 (16), 109.0 (38), 75.1 (68), 46.2 (100). CHN-elemental analysis: Calcd. for $C_8H_6N_2OS_2Cl_2$, C = 34.17, H = 2.15, N = 9.96, found C = 34.50, H = 2.25, N = 9.74. **IR** (ATR): *v* = 3893, 3742, 3614, 2961, 2334, 2098, 1897, 1722, 1532, 1360, 1247, 1118, 1001, 864, 764. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_8H_6N_2OS_2Cl_2Na]^+$ 302.9196, found 302.9193.

Diphenyl(thiocyanatoimino)-λ^6-sulfanone (**2m**)



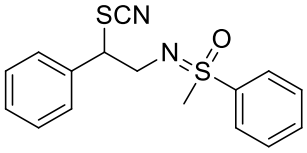
Colorless oil, 42.2 mg, 77% yield, **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.00 – 7.95 (m, 4H), 7.65 (t, *J* = 7.5 Hz, 2H), 7.58 (t, *J* = 7.8 Hz, 4H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$) δ 137.6, 134.2, 129.7, 128.5, 115.2. **MS** (EI, 70 eV): *m/z* (%) = 274.0 (100, M^+), 202.0 (93), 186.1 (15), 174.0 (34), 154.1 (74), 109.1 (38), 77.2 (23). CHN-elemental analysis: Calcd. for $C_{13}H_{10}N_2OS_2$, C = 56.91, H = 3.67, N = 10.21, found C = 56.76, H = 3.52, N = 9.96. **IR** (ATR): *v* = 3751, 3457, 3079, 3015, 3933, 2651, 2450, 2281, 2138, 2090, 2037, 1990, 1941, 1739, 1623, 1577, 1445, 1367, 1220, 1085, 948, 727, 684. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_{13}H_{10}N_2OS_2Na]^+$ 297.0132, found 297.0128.

Ethyl(phenyl)(thiocyanatoimino)-λ^6-sulfanone (2n)



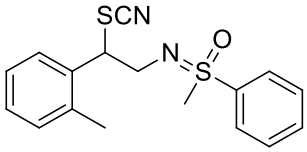
Colorless oil, 35.3 mg, 78% yield, **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.88 – 7.83 (m, 2H), 7.76 – 7.69 (m, 1H), 7.67 – 7.61 (m, 2H), 3.51 – 3.28 (m, 2H), 1.28 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (101 MHz, $CDCl_3$) δ 134.7, 133.8, 129.9, 129.3, 115.4, 50.5, 7.1. **MS** (EI, 70 eV): *m/z* (%) = 226.0 (73, M^+), 154.0 (37),126.0 (100), 125.0 (38), 78.2 (37), 77.2 (26). **IR** (ATR): *v* = 3854, 3745, 3462, 2930, 2314, 2061, 1901, 1741, 1547, 1450, 1365, 1218, 1099, 960, 734, 677. **HRMS** (ESI) (*m/z*) $[M+Na]^+$: Calcd. $[C_9H_{10}N_2OS_2Na]^+$ 249.0132, found 249.0126.

Methyl(phenyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4aa)



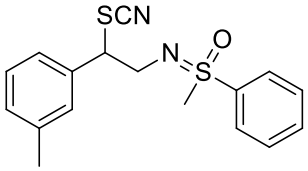
Light yellow oil, 34.2 mg, 72% yield. *dr* = 1:1. **^{1}H NMR** (400 MHz, $CDCl_3$, mixture of diastereomers) δ 7.89 – 7.78 (m, 2H), 7.66 – 7.49 (m, 3H), 7.39 – 7.26 (m, 5H), 4.81 – 4.54 (m, 1H), 3.59 – 3.50 (m, 1H), 3.41 – 3.30 (m, 1H), 3.09 (d, *J* = 8.9 Hz, 3H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$, mixture of diastereomers) δ 138.9, 138.6, 137.4, 137.3, 133.3, 133.3, 129.6, 129.6, 128.9, 128.8, 128.5, 128.4, 128.0, 127.8, 112.3, 112.3, 56.9, 55.9, 48.5, 48.4, 45.1, 44.8. **MS** (EI, 70 eV): *m/z* (%) = 287.0 (20), 168.0 (100), 141.0 (61), 132.0 (19), 125.0 (19), 77.1 (19). **MS** (ESI) $[M+H]^+$: 317.08. **HRMS** (ESI) (*m/z*) $[C_{16}H_{17}N_2OS_2]^+$: Calcd. 317.0782, found, 317.0761. **IR** (ATR): *v* =3522, 3011, 2926, 2838, 2607, 2337, 2143, 2092, 1907, 1785, 1607, 1510, 1448, 1238, 1139, 1029, 973, 892, 833, 743.

Methyl(phenyl)((2-thiocyanato-2-(*o*-tolyl)ethyl)imino)-λ^6-sulfanone (4ab)



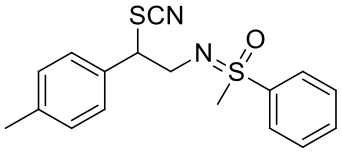
Light yellow oil, 18.8 mg, 38% yield, *dr* = 1:1. **^{1}H NMR** (400 MHz, $CDCl_3$, mixture of diastereomers) δ 7.95 – 7.81 (m, 2H), 7.68 – 7.49 (m, 3H), 7.35 – 7.22 (m, 1H), 7.21 – 7.12 (m, 3H), 4.87 – 4.71 (m, 1H), 3.62 – 3.52 (m, 1H), 3.48 – 3.35 (m, 1H), 3.10 (d, *J* = 12.5 Hz, 3H), 2.36 (d, *J* = 2.9 Hz, 3H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$, mixture of diastereomers) δ 139.2, 138.6, 136.5, 136.3, 135.1, 133.3, 133.2, 130.8, 130.8, 129.7, 129.6, 128.6, 128.4, 126.7, 126.7, 126.6, 126.5, 112.1, 52.8, 51.5, 48.3, 48.2, 45.1, 44.8. **MS** (EI, 70 eV): *m/z* (%) = 168.0 (100), 141.1 (63), 77.1 (18). **MS** (ESI) $[M+H]^+$: 331.09 (ESI) (*m/z*) $[C_{17}H_{19}N_2OS_2]^+$: Calcd. 331.0939. found, 331.0936. **IR** (ATR): *v* = 3533, 3019, 2924, 2849, 2334, 2147, 1997, 1911, 1736, 1591, 1450, 1235, 1140, 1087, 973, 887, 742, 688.

Methyl(phenyl)((2-thiocyanato-2-(*m*-tolyl)ethyl)imino)-λ^6-sulfanone (4ac)



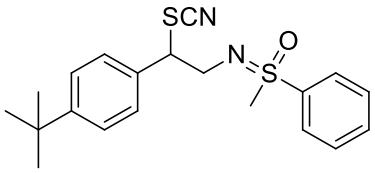
Light yellow oil, 25.3 mg, 51% yield, *dr* = 1:1. **^{1}H NMR** (400 MHz, $CDCl_3$, mixture of diastereomers) δ 7.92 – 7.75 (m, 2H), 7.66 – 7.45 (m, 3H), 7.24 – 7.19 (m, 1H), 7.15 – 7.09 (m, 3H), 4.58 – 4.50 (m, 1H), 3.58 – 3.51 (m, 1H), 3.40 – 3.29 (m, 1H), 3.09 (d, *J* = 9.0 Hz, 3H), 2.31 (d, *J* = 5.2 Hz, 3H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$, mixture of diastereomers) δ 139.0, 138.7, 138.6, 137.2, 133.3, 133.2, 129.7, 129.6, 129.6, 128.7, 128.6, 128.5, 128.5, 128.4, 125.1, 124.8, 112.4, 57.0, 56.0, 48.6, 48.4, 45.1, 44.8, 21.4. **MS** (EI, 70 eV): *m/z* (%) = 168.0 (100), 141.1 (63), 125.0 (20), 77.1 (15). **MS** (ESI) $[M+H]^+$: 331.09 (ESI) (*m/z*) $[C_{17}H_{19}N_2OS_2]^+$: Calcd. 331.0939. found, 331.0915. **IR** (ATR): *v* = 3526, 3019, 2921, 2847, 2671, 2330, 2142, 1999, 1895, 1602, 1446, 1237, 1140, 1085, 974, 881, 785, 742, 696.

Methyl(phenyl)((2-thiocyanato-2-(*p*-tolyl)ethyl)imino)-λ^6-sulfanone (4ad)



Light yellow oil, 25.7 mg, 52% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.89 (d, *J* = 7.8 Hz, 1H), 7.84 (d, *J* = 7.8 Hz, 1H), 7.63 (q, *J* = 7.4 Hz, 1H), 7.56 (dt, *J* = 15.2, 7.7 Hz, 2H), 7.27 – 7.23 (m, 1H), 7.21 (d, *J* = 8.1 Hz, 1H), 7.17 – 7.12 (m, 2H), 4.57 (ddd, *J* = 24.9, 8.6, 5.7 Hz, 1H), 3.60 – 3.50 (m, 1H), 3.40 – 3.31 (m, 1H), 3.11 (d, *J* = 12.9 Hz, 3H), 2.33 (d, *J* = 9.6 Hz, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 139.0, 138.8, 138.6, 134.3, 134.2, 133.3, 133.3, 129.7, 129.6, 129.6, 129.5, 128.6, 128.4, 127.9, 127.7, 112.5, 112.5, 56.9 55.9, 48.6, 48.4, 45.1, 44.8, 21.2, 21.2. **MS** (EI, 70 eV): *m/z* (%) = 168.0 (100), 141.0 (46), 125.0 (11). **MS** (ESI) $[M+H]^+$: 331.09 (ESI) (*m/z*) $[C_{17}H_{19}N_2OS_2]^+$: Calcd. 331.0939. found, 331.0934. **IR** (ATR): *v* =3611, 3019, 2923, 2847, 2341, 2149, 2001, 1910, 1737, 1612, 1513, 1446, 1234, 1139, 1086, 892, 818, 740.

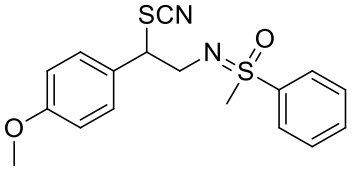
({2-[4-(*tert*-butyl)phenyl]-2-thiocyanatoethyl}imino)(methyl)(phenyl)-λ^6-sulfanone (4ae)



Light yellow oil, 33.5 mg, 60% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.90 – 7.86 (m, 1H), 7.86 – 7.83 (m, 1H), 7.66 – 7.60 (m, 1H), 7.58 – 7.54 (m, 2H), 7.38 – 7.32 (m, 2H), 7.29 (d, *J* = 8.4 Hz, 1H), 7.26 – 7.23 (m, 1H), 4.61 – 4.54 (m, 1H), 3.58 – 3.52 (m, 1H), 3.41 – 3.32 (m, 1H), 3.12 (d, *J* = 11.9 Hz, 3H), 1.29 (d, *J* = 9.5 Hz, 9H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 151.89, 138.94, 138.61, 134.23, 134.22, 133.31, 133.27, 129.64, 129.60, 128.61, 128.42, 127.62, 127.46, 125.81, 125.77, 112.56, 112.55, 56.78, 55.78, 48.68, 48.43, 45.08, 44.83, 34.64, 34.62, 31.24, 31.22. **MS** (EI, 70 eV): *m/z* (%) = 168.0 (100), 141.1 (65), 125.0 (19), 117.0 (16), 91.1 (12), 77.1 (12). **MS** (ESI) $[M+Na]^+$: 395.12 (ESI) (*m/z*) $[C_{20}H_{24}N_2OS_2Na]^+$: Calcd. 395.1227. found, 395.1216. **IR** (ATR): *v* =

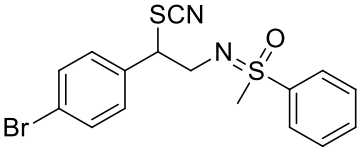
3746, 3612, 2957, 2331, 2149, 1913, 1738, 1609, 1510, 1453, 1408, 1366, 1235, 1139, 973, 896, 836, 742, 687.

{[2-(4-Methoxyphenyl)-2-thiocyanatoethyl]imino}(methyl)(phenyl)-λ^6-sulfanone (4af)



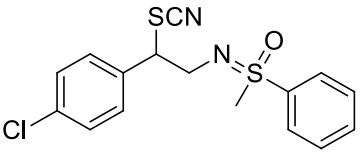
Light yellow oil, 25.0 mg, 50% yield, *dr* = 1:1. **^{1}H NMR** (400 MHz, $CDCl_3$, mixture of diastereomers) δ 7.91 – 7.83 (m, 2H), 7.65 – 7.53 (m, 3H), 7.27 (dd, *J* = 17.6, 8.2 Hz, 2H), 6.86 (dd, *J* = 8.5, 6.4 Hz, 2H), 4.63 – 4.54 (m, 1H), 3.79 (d, *J* = 6.0 Hz, 3H), 3.58 – 3.50 (m, 1H), 3.42 – 3.31 (m, 1H), 3.11 (d, *J* = 8.1 Hz, 3H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$, mixture of diastereomers) δ 159.9, 133.3, 133.2, 129.6, 129.6, 129.3, 129.1, 128.6, 128.4, 114.2, 112.5, 56.8, 55.8, 55.3, 48.6, 48.4, 45.1, 44.8. **MS** (EI, 70 eV): *m/z* (%) = 287.0 (20), 168.0 (100), 141.0 (61), 132.0 (19), 125.0 (19), 91.1 (12), 77.1 (18). **MS** (ESI) $[M+H]^+$: 347.09 (ESI) (*m/z*) $[C_{17}H_{19}N_2O_2S_2]^+$: Calcd. 347.0888. found, 347.0882. **IR** (ATR): *v* = 3522, 3011, 2926, 2838, 2670, 2337, 2143, 2092, 1907, 1758, 1607, 1510, 1448, 1238, 1139, 1029, 973, 892, 833, 743, 687.

{[2-(4-Bromophenyl)-2-thiocyanatoethyl]imino}(methyl)(phenyl)-λ^6-sulfanone (4ag)



Light yellow oil, 39.0 mg, 66% yield, *dr* = 1:1. **^{1}H NMR** (400 MHz, $CDCl_3$, mixture of diastereomers) δ 7.87 – 7.78 (m, 2H), 7.67 – 7.60 (m, 1H), 7.59 – 7.52 (m, 2H), 7.49 – 7.45 (m, 2H), 7.27 – 7.18 (m, 2H), 4.59 – 4.46 (m, 1H), 3.55 – 3.48 (m, 1H), 3.38 – 3.25 (m, 1H), 3.08 (d, *J* = 10.1 Hz, 3H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$, mixture of diastereomers) δ 138.8, 138.6, 136.5, 133.4, 133.3, 132.0, 129.7, 129.6, 129.5, 128.5, 128.3, 122.9, 56.0, 55.0, 48.1, 45.1, 44.9. **MS** (EI, 70 eV): *m/z* (%) = 169.0 (19), 168.0 (100), 141.0 (77), 124.9 (28), 124.0 (11), 97.0 (11). **MS** (ESI) $[M+Na]^+$: 416.97 (ESI) (*m/z*) $[C_{16}H_{15}N_2OS_2BrNa]^+$: Calcd. 416.9707. found, 416.9718. **IR** (ATR): *v* = 3786, 3458, 3060, 3019, 2924, 2848, 2663, 2501, 2327, 2144, 2083, 1994, 1957, 1739, 1586, 1485, 1445, 1405, 1368, 1228, 1140, 1075, 1008, 978, 889, 826, 783, 742, 688.

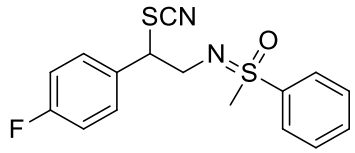
{[2-(4-Chlorophenyl)-2-thiocyanatoethyl]imino}(methyl)(phenyl)-λ^6-sulfanone (4ah)



Light yellow oil, 27.8 mg, 53% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.85 (dd, *J* = 17.6, 7.5 Hz, 2H), 7.67 – 7.61 (m, 1H), 7.57 (q, *J* = 7.6 Hz, 2H), 7.33 – 7.25 (m, 4H), 4.60 – 4.52 (m, 1H), 3.56 – 3.49 (m, 1H), 3.39 – 3.28 (m, 1H), 3.10 (d, *J* = 15.0 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 138.8, 138.6, 136.0, 135.9, 134.8, 133.4, 133.4, 129.7, 129.7, 129.4, 129.3, 129.1, 129.1, 128.5, 128.4, 112.0, 112.0, 56.0, 55.0, 48.3, 48.2, 45.1, 44.9. **MS** (EI, 70 eV): *m/z* (%) = 168.0 (100), 141.1 (45), 125.0 (25). **MS** (ESI) $[M+Na]^+$: 373.02 (ESI) (*m/z*) $[C_{16}H_{15}N_2OS_2ClNa]^+$:

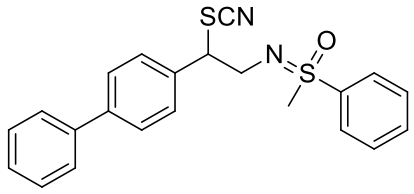
Calcd. 373.0212. found, 373.0201. **IR** (ATR): *v* = 3461, 3021, 2923, 2319, 2147, 2057, 1907, 1737, 1590, 1485, 1235, 1135, 1088, 974, 740, 831, 740, 685.

{[2-(4-Fluorophenyl)-2-thiocyanatoethyl]imino}(methyl)(phenyl)-λ^6-sulfanone (4ai)



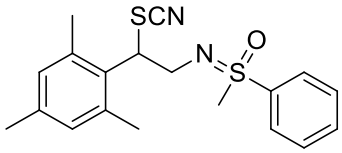
Light yellow oil, 25.0 mg, 50% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.89 – 7.81 (m, 2H), 7.68 – 7.61 (m, 1H), 7.57 (q, *J* = 7.6 Hz, 2H), 7.40 – 7.34 (m, 1H), 7.32 (dd, *J* = 8.6, 5.2 Hz, 1H), 7.03 (q, *J* = 8.5 Hz, 2H), 4.64 – 4.53 (m, 1H), 3.58 – 3.51 (m, 1H), 3.40 – 3.29 (m 1H), 3.11 (d, *J* = 12.9 Hz, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 163.6, 163.6, 161.9, 161.9, 138.8, 138.6, 133.4, 133.4, 129.9, 129.9, 129.8, 129.7, 129.7, 128.5, 128.4, 115.9, 115.8, 112.2, 112.1, 56.1, 55.1, 48.5, 48.3, 45.1, 45.0. **MS** (EI, 70 eV): *m/z* (%) = 168.0 (100), 141.1 (54), 125.0 (17). **MS** (ESI) $[M+Na]^+$: 357.05 (ESI) (*m/z*) $[C_{16}H_{15}N_2OS_2FNa]^+$: Calcd. 357.0508. found, 357.0492. **IR** (ATR): *v* = 2918, 2336, 2122, 1898, 1740, 1604, 1501, 1225, 976, 741.

({2[(1,1'-Biphenyl)-4-yl]-2-thiocyanatoethyl}imino)(methyl)(phenyl)-λ^6-sulfanone (4aj)



Light yellow oil, 24.1 mg, 41% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.93 – 7.79 (m, 2H), 7.64 (dd, *J* = 14.4, 7.2 Hz, 1H), 7.60 – 7.52 (m, 6H), 7.47 – 7.39 (m, 4H), 7.35 (dd, *J* = 13.3, 7.1 Hz, 1H), 4.71 – 4.57 (m, 1H), 3.63 – 3.59 (m, 1H), 3.47 – 3.37 (m, 1H), 3.13 (d, *J* = 15.1 Hz, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 141.8, 140.3, 140.3, 138.9, 138.6, 136.3, 136.3, 133.4, 133.3, 129.7, 129.6, 128.8, 128.8, 128.6, 128.5, 128.4, 128.3, 127.6, 127.6, 127.5, 127.1, 112.4, 112.3, 56.7, 55.6, 48.5, 48.4, 45.1, 44.9. **MS** (EI, 70 eV): *m/z* (%) = 168.0 (100), 141.1 (47), 125.0 (15), 77.1 (17), 58.1 (25). **MS** (ESI) $[M+Na]^+$: 415.09 (ESI) (*m/z*) $[C_{22}H_{20}N_2OS_2Na]^+$: Calcd. 415.09147. found, 415.08948. **IR** (ATR): *v* =3534, 3029, 2922, 2853, 2148, 1724, 1599, 1483, 1447, 1407, 1236, 1138, 1083, 974, 839, 738, 691.

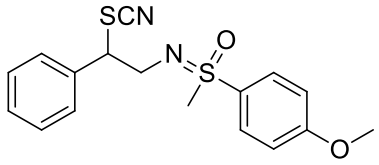
[(2-Mesityl-2-thiocyanatoethyl)imino](methyl)(phenyl)-λ^6-sulfanone (4ak)



Light yellow oil, 16.5 mg, 33% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.94 (d, *J* = 7.5 Hz, 1H), 7.86 (d, *J* = 7.5 Hz, 1H), 7.67 – 7.51 (m, 3H), 6.80 (dd, *J* = 27.3, 5.3 Hz, 2H), 5.33 – 5.14 (m, 1H), 3.71 – 3.55 (m, 1H), 3.44 – 3.37 (m, 1H), 3.18 – 3.17 (m, 3H), 2.44 – 2.26 (m, 6H), 2.22 – 2.21 (m, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 138.3, 137.4, 137.4, 137.1, 137.0, 133.5, 133.4, 131.4, 131.3, 129.8, 129.7, 129.6, 129.5, 129.5, 128.6, 128.4, 113.1, 113.0, 53.8, 52.4, 47.0, 46.2, 44.9, 44.7, 21.3, 21.3, 21.1, 20.9. **MS** (EI, 70 eV): *m/z* (%) = 190.1 (10), 168.0 (79), 145.1 (16), 141.0 (100), 133.1 (26), 125.0 (67), 117.1(32), 115.1 (33), 91.1 (47), 77.2 (67), 51.2 (54). **MS** (ESI)

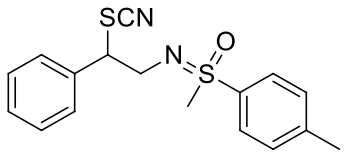
$[M+Na]^+$: 359.12 (ESI) (*m/z*) $[C_{19}H_{23}N_2OS_2]^+$: Calcd. 359.1252. found, 359.1238. **IR** (ATR): *v* = 3523, 2926, 2336, 2144, 1912, 1727, 1606, 1452, 1229, 1137, 971, 858, 743, 678.

(4-Methoxyphenyl)(methyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4ba)



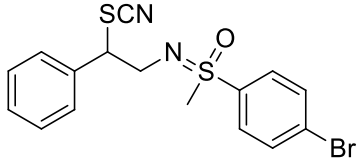
Light yellow oil, 42.0 mg, 81% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.77 (dd, *J* = 21.5, 8.8 Hz, 2H), 7.39 – 7.29 (m, 5H), 7.01 (dd, *J* = 11.0, 8.8 Hz, 2H), 4.62 – 4.56 (m, 1H), 3.87 (s, 3H), 3.56 – 3.52 (m, 1H), 3.42 – 3.31 (m, 1H), 3.08 (d, *J* = 15.7 Hz, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 163.5, 163.5, 137.5, 137.4, 130.7, 130.6, 130.0, 129.6, 128.9, 128.8, 128.0, 127.9, 114.9, 114.8, 112.4, 112.4, 57.0, 56.0, 55.8, 48.6, 48.4, 45.5, 45.2. **MS** (EI, 70 eV): *m/z* (%) = 198.0 (90), 171.0 (96), 154.9 (100), 139.0 (13), 91.1 (41), 77.1 (18), 63.1 (11). **MS** (ESI) $[M+H]^+$: 347.09 (ESI) (*m/z*) $[C_{17}H_{19}N_2O_2S_2]^+$: Calcd. 347.0888. found, 347.0873. **IR** (ATR): *v* = 3556, 3018, 2923, 2845, 2570, 2325, 2147, 1901, 1722, 1588, 1492, 1454, 1410, 1306, 1245, 1135, 1091, 1021, 973, 891, 834, 766, 699.

Methyl[(2-phenyl-2-thiocyanatoethyl)imino](*p*-tolyl)-λ^6-sulfanone (4ca)



Light yellow oil, 35.1 mg, 71% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.73 (dd, *J* = 20.3, 8.2 Hz, 2H), 7.42 – 7.28 (m, 7H), 4.62 – 4.58 (m, 1H), 3.59 – 3.49 (m, 1H), 3.41 – 3.31 (m, 1H), 3.09 (d, *J* = 14.5 Hz, 3H), 2.45 (d, *J* = 1.9 Hz, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 144.3, 144.2, 137.4, 137.4, 135.8, 135.4, 130.3, 130.3, 128.9, 128.8, 128.6, 128.5, 128.0, 127.9, 112.4, 112.4, 57.0, 56.0, 48.6, 48.4, 45.2, 45.0, 21.6. **MS** (EI, 70 eV): *m/z* (%) = 182.0 (100), 155.0 (48), 139.0 (18), 91.1 (17). **MS** (ESI) $[M+H]^+$: 331.09 (ESI) (*m/z*) $[C_{17}H_{19}N_2OS_2]^+$: Calcd. 331.0939. found, 331.0924. **IR** (ATR): *v* = 3542, 3059, 3029, 2923, 2841, 2660, 2324, 2211, 2178, 2146, 2084, 1992, 1940, 1808, 1725, 1595, 1538, 1492, 1451, 1404, 1323, 1139, 1086, 1032, 979, 887, 816, 762, 699.

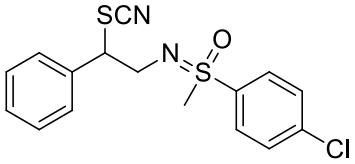
(4-Bromophenyl)(methyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4da)



Light yellow oil, 39.1 mg, 66% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.74 – 7.65 (m, 4H), 7.38 – 7.31 (m, 5H), 4.62 – 4.53 (m, 1H), 3.59 – 3.54 (m, 1H), 3.40 – 3.30 (m, 1H), 3.10 (d, *J* = 16.4 Hz, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 138.1, 137.8, 137.2, 137.1, 133.0, 132.9, 130.2, 130.0, 129.0, 128.9, 128.9, 128.7, 128.6, 128.0, 127.8, 112.2, 112.2, 56.7, 55.7, 48.5, 48.4, 45.1, 44.9. **MS** (EI, 70 eV): *m/z* (%) = 247.9 (100), 245.9 (98), 221.0 (60), 219.0 (59), 204.9 (27), 202.9 (26), 118.1 (26), 91.1 (43). **MS** (ESI) $[M+Na]^+$: 416.97 (ESI) (*m/z*)

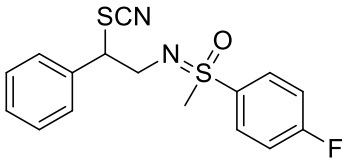
$[C_{16}H_{15}N_2OS_2BrNa]^+$: Calcd. 416.9707. found, 416.9715. **IR** (ATR): *v* = 3528, 3029, 2920, 2846, 2149, 1921, 1730, 1570, 1464, 1386, 1239, 1140, 1070, 972, 823, 765.

(4-Chlorophenyl)(methyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4ea)



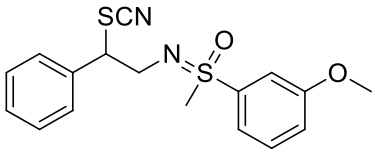
Light yellow oil, 32.3 mg, 62% yield, *dr* = 1:1. **^{1}H NMR** (400 MHz, $CDCl_3$, mixture of diastereomers) δ 7.81 – 7.71 (m, 2H), 7.55 – 7.47 (m, 2H), 7.37 – 7.29 (m, 5H), 4.60 – 4.51 (m, 1H), 3.60 – 3.52 (m, 1H), 3.40 – 3.28 (m, 1H), 3.08 (d, *J* = 10.2 Hz, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 140.8, 140.0, 137.5, 137.2, 137.2, 130.1, 130.0, 129.9, 129.0, 128.9, 128.9, 128.0, 127.8, 112.2, 112.2, 56.68, 56.67, 55.7, 48.5, 48.4, 45.1, 44.9. **MS** (EI, 70 eV): *m/z* (%) = 203.9 (36), 201.9 (100), 176.9 (22), 174.9 (60), 159.9 (12), 158.9 (25), 118.0 (17), 91.1 (26). **MS** (ESI) $[M+Na]^+$: 373.02 (ESI) (*m/z*) $[C_{16}H_{15}N_2OS_2ClNa]^+$: Calcd. 373.0212. found, 373.0200. **IR** (ATR): *v* = 3543, 3067, 3027, 2923, 2844, 2563, 2324, 2149, 2055, 1925, 1811, 1728, 1576, 1466, 1393, 1238, 1141, 1082, 975, 889, 829, 769, 699.

(4-Fluorophenyl)(methyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4fa)



Light yellow oil, 27.6 mg, 55% yield, *dr* = 1:1. **^{1}H NMR** (400 MHz, $CDCl_3$, mixture of diastereomers) δ 7.91 – 7.75 (m, 2H), 7.37 – 7.29 (m, 4H), 7.25 – 7.18 (m, 2H), 4.60 – 4.53 (m, 1H), 3.60 – 3.51 (m, 1H), 3.41 – 3.29 (m, 1H), 3.08 (d, *J* = 10.4 Hz, 3H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$, mixture of diastereomers) δ 166.8, 164.3, 137.2, 137.2, 134.9, 134.6, 131.4, 131.3, 131.2, 131.1, 128.9, 128.9, 128.9, 128.0, 127.8, 117.0, 117.0, 116.8, 116.7, 112.2, 112.1, 56.7, 55.7, 48.5, 48.4, 45.3, 45.0. **MS** (EI, 70 eV): *m/z* (%) = 185.9 (100), 158.9 (47), 142.9 (15). **MS** (ESI) $[M+H]^+$: 335.07, (ESI) (*m/z*) $[C_{16}H_{16}N_2OS_2F]^+$: Calcd. 335.0688. found, 335.0674. **IR** (ATR): *v* = 3066, 3030, 2924, 2848, 2207, 2150, 2052, 1986, 1909, 1739, 1588, 1490, 1453, 1404, 1367, 1229, 1138, 1085, 981, 838, 765, 699.

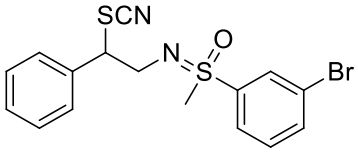
(3-Methoxyphenyl)(methyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4ga)



Light yellow oil, 20.8 mg, 40% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.50 – 7.42 (m, 2H), 7.41 – 7.30 (m, 6H), 7.16 – 7.13 (m, 1H), 4.63 – 4.56 (m, 1H), 3.86 (d, *J* = 4.6 Hz, 3H), 3.60 – 3.53 (m, 1H), 3.44 – 3.34 (m, 1H), 3.11 (d, *J* = 13.3 Hz, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 160.4, 160.4, 140.2, 139.9, 137.4, 137.3, 130.7, 130.6, 128.9, 128.9, 128.0, 127.9, 120.5, 120.3, 119.8, 119.6, 113.0, 112.3, 56.9, 55.9, 55.7, 48.6, 48.4, 45.1, 44.8. **MS** (EI, 70 eV): *m/z* (%) = 198.0 (100), 171.0 (96), 155.0 (63), 148.0 (18), 121.0 (29), 108.0 (29), 91.1 (82), 77.1 (58). **MS** (ESI) $[M+H]^+$: 347.09 (ESI) (*m/z*) $[C_{17}H_{19}N_2O_2S_2]^+$: Calcd. 347.0888. found,

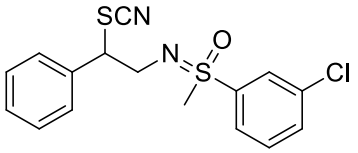
347.0877. **IR** (ATR): *v* = 3589, 3018, 2925, 2846, 2331, 2147, 1892, 1772, 1593, 1470, 1239, 1138, 1084, 1034, 972, 864, 767, 692.

(3-Bromophenyl)(methyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4ha)



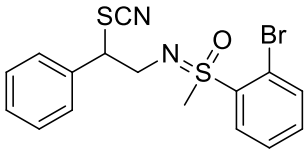
Light yellow oil, 26.0 mg, 44% yield, *dr* = 1:1. **^{1}H NMR** (400 MHz, $CDCl_3$, mixture of diastereomers) δ 7.98 (dt, *J* = 16.7, 1.8 Hz, 1H), 7.80 – 7.70 (m, 2H), 7.41 (q, *J* = 8.0 Hz, 1H), 7.35 – 7.30 (m, 5H), 4.59 – 4.53 (m, 1H), 3.61 – 3.52 (m, 1H), 3.41 – 3.30 (m, 1H), 3.09 (d, *J* = 11.2 Hz, 3H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$, mixture of diastereomers) δ 141.2, 141.0, 137.1, 136.4, 136.3, 131.6, 131.3, 131.1, 131.1, 129.0, 128.9, 128.9, 128.0, 127.8, 127.0, 126.9, 123.7, 123.6, 112.1, 112.1, 56.6, 55.6, 48.5, 48.3, 45.1, 44.9. **MS** (EI, 70 eV): *m/z* (%) = 247.9 (100), 245.9 (99), 220.9 (40), 218.9 (41), 204.9 (10), 202.8 (9), 91.1 (13). **MS** (ESI) $[M+Na]^+$: 416.97 (ESI) (*m/z*) $[C_{16}H_{15}N_2OS_2BrNa]^+$: Calcd. 416.9707. found, 416.9718. **IR** (ATR): *v* = 3063, 3027, 2925, 2845, 2328, 2149, 1889, 1737, 1568, 1493, 1454, 1404, 1366, 1235, 1140, 1098, 979, 889, 834, 774, 732, 699, 678.

(3-Chlorophenyl)(methyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4ia)



Light yellow oil, 22.6 mg, 43% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.84 (dt, *J* = 28.8, 1.6 Hz, 1H), 7.72 (dd, *J* = 27.1, 7.8 Hz, 1H), 7.62 – 7.56 (m, 1H), 7.53 – 7.48 (m, 1H), 7.37 – 7.32 (m, 5H), 4.61 – 4.56 (m, 1H), 3.61 – 3.53 (m, 1H), 3.42 – 3.33 (m, 1H), 3.11 (d, *J* = 17.2 Hz, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 141.1, 140.7, 137.1, 135.9, 135.9, 133.5, 133.5, 130.9, 130.9, 129.00, 128.9, 128.9, 128.7, 128.5, 128.0, 127.8, 126.7, 126.5, 112.2, 112.1, 56.6, 55.6, 48.5, 48.3, 45.1, 44.9. **MS** (EI, 70 eV): *m/z* (%) = 222.2 (42), 204.0 (53), 202.0 (100), 177.0 (22), 175.0 (58), 159.0 (16), 118.1 (49), 104.1 (10), 91.1 (30). **MS** (ESI) $[M+Na]^+$: 373.02 (ESI) (*m/z*) $[C_{16}H_{15}N_2OS_2ClNa]^+$: Calcd. 373.0212. found, 373.0197. **IR** (ATR): *v* =3525, 3065, 3028, 2923, 2849, 2688, 2339, 2149, 2061, 1887, 1731, 1577, 1454, 1408, 1241, 1139, 1077, 975, 891, 840, 758, 696.

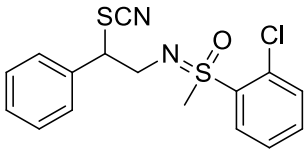
(2-Bromophenyl)(methyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4ja)



Light yellow oil, 22.5 mg, 38% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 8.21 – 8.17 (m, 1H), 7.81 – 7.73 (m, 1H), 7.56 – 7.50 (m, 1H), 7.48 – 7.42 (m, 1H), 7.38 – 7.30 (m, 5H), 4.62 – 4.57 (m, 1H), 3.53 – 3.44 (m, 1H), 3.36 – 3.28 (m, 4H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 137.7, 137.7, 137.2, 137.2, 135.8, 135.7, 134.4, 133.3, 133.2, 128.9, 128.9, 128.9, 128.5, 128.4, 128.0, 127.9, 120.7, 120.7, 112.3, 112.3, 56.5, 55.7, 48.6, 48.5, 42.7, 42.6. **MS** (EI, 70 eV): *m/z* (%) = 393.9 (2, M^+), 247.9 (100), 245.9 (96), 220.9 (59), 218.9 (60), 204.9 (15), 202.8 (14). **MS** (ESI) $[M+Na]^+$: 416.97 (ESI) (*m/z*) $[C_{16}H_{15}N_2OS_2BrNa]^+$: Calcd. 416.9707. found, 416.9712. **IR** (ATR): *v* = 3533,

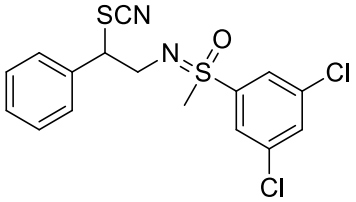
3028, 2923, 2845, 2693, 2326, 2148, 1992, 1940, 1734, 1569, 1492, 1441, 1235, 1141, 1093, 1025, 972, 878, 832, 758, 700.

(2-Chlorophenyl)(methyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4ka)



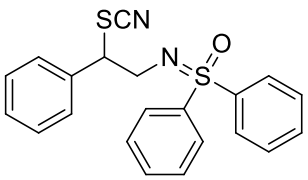
Light yellow oil, 27.3 mg, 52% yield, *dr* = 1:1. **^{1}H NMR** (400 MHz, $CDCl_3$, mixture of diastereomers) δ 8.17 – 8.09 (m, 1H), 7.55 – 7.52 (m, 2H), 7.49 – 7.43 (m, 1H), 7.35 – 7.26 (m, 5H), 4.58 – 4.53 (m, 1H), 3.54 – 3.44 (m, 1H), 3.36 – 3.24 (m, 4H). **^{13}C NMR** (101 MHz, $CDCl_3$, mixture of diastereomers) δ 137.2, 136.1, 134.4, 132.9, 132.9, 132.3, 132.2, 132.1, 128.9, 127.9, 127.9, 127.8, 127.7, 112.2, 56.4, 55.7, 48.6, 48.6, 43.1, 42.3. **MS** (EI, 70 eV): *m/z* (%) = 203.9 (38), 202.0 (100), 176.9 (27), 174.9 (66), 160.0 (10), 158.9 (12), 91.1 (16). **MS** (ESI) $[M+Na]^+$: 373.02 (ESI) (*m/z*) $[C_{16}H_{15}N_2OS_2ClNa]^+$: Calcd. 373.0212. found, 373.0198. **IR** (ATR): *v* = 3836, 3508, 3065, 2922, 2845, 2681, 2328, 2145, 1882, 1739, 1573, 1493, 1445, 1243, 1142, 1029, 969, 761, 700.

(3,5-Dichlorophenyl)(methyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4la)



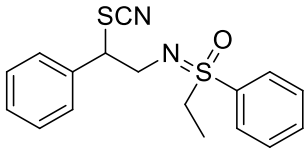
Light yellow oil, 33.6 mg, 58% yield, *dr* = 1:1 **^{1}H NMR** (400 MHz, $CDCl_3$, mixture of diastereomers) δ 7.72 (d, *J* = 1.8 Hz, 1H), 7.66 (d, *J* = 1.8 Hz, 1H), 7.59 – 7.57 (m, 1H), 7.37 – 7.29 (m, 5H), 4.59 – 4.50 (m, 1H), 3.63 – 3.53 (m, 1H), 3.42 – 3.31 (m, 1H), 3.09 (d, *J* = 13.6 Hz, 3H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$, mixture of diastereomers) δ 142.6, 142.3, 136.9, 136.9, 136.6, 136.6, 133.3, 133.3, 129.1, 129.0, 128.9, 127.9, 127.8, 126.9, 126.7, 112.0, 111.9, 56.4, 55.3, 48.5, 48.2, 45.0, 44.9. **MS** (EI, 70 eV): *m/z* (%) = 238.0 (63), 235.9 (100), 211.0 (31), 208.9 (50), 194.9 (9), 192.9 (15), 118.1 (21), 91.1 (31). **MS** (ESI) $[M+H]^+$: 385.00 (ESI) (*m/z*) $[C_{16}H_{15}N_2OS_2Cl_2]^+$: Calcd. 385.0003. found, 384.9990. **IR** (ATR): *v* = 3479, 3057, 2923, 2149, 1743, 1568, 1408, 1241, 1139, 980, 780, 699.

Diphenyl((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (4ma)



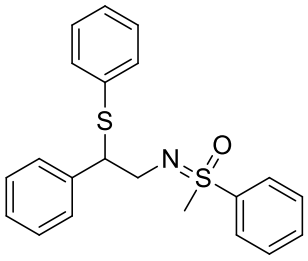
Light yellow oil, 25.6 mg, 46% yield. **^{1}H NMR** (400 MHz, $CDCl_3$) δ7.95 – 7.91 (m, 4H), 7.58 – 7.47 (m, 6H), 7.41 – 7.33 (m, 5H), 4.71 (dd, *J* = 8.2, 5.7 Hz, 1H), 3.67 – 3.58 (m, 2H). **^{13}C {^{1}H} NMR** (101 MHz, $CDCl_3$) δ 140.1, 139.8, 137.6, 132.8, 129.3, 129.3, 128.9, 128.8, 128.5, 128.3, 128.1, 128.0, 112.4, 56.8, 48.2. **MS** (EI, 70 eV): *m/z* (%) = 230.1 (82), 203.1 (62), 186.1 (20), 154.1 (24), 125.0 (29), 121.0 (23), 118.1 (40), 109.0 (55), 104.1 (23), 97.1 (34), 91.1 (100), 89.1 (27), 78.2 (28), 77.2 (94), 65.2 (62). **MS** (ESI) $[M+H]^+$: 379.09 (ESI) (*m/z*) $[C_{21}H_{19}N_2OS_2]^+$: Calcd. 379.0939. found, 379.0920. **IR** (ATR): *v* =3596, 3061, 2920, 2846, 2334, 2149, 2055, 1901, 1739, 1585, 1447, 1365, 1245, 1142, 1083, 996, 896, 835, 728.

Ethyl(phenyl)((2-phenyl-2-thiocyanatoethyl)imino)-λ^6-sulfanone (**4na**)



Light yellow oil, 27.2 mg, 55% yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.80 (dd, *J* = 20.3, 7.8 Hz, 2H), 7.65 – 7.60 (m, 1H), 7.55 (dd, *J* = 16.6, 8.1 Hz, 2H), 7.40 – 7.30 (m, 5H), 4.66 – 4.59 (m, 1H), 3.62 – 3.55 (m, 1H), 3.43 – 3.38 (m, 1H), 3.25 – 3.11 (m, 2H), 1.24 (dt, *J* = 12.5, 7.4 Hz, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 137.5, 137.5, 137.2, 136.9, 133.3, 133.2, 129.6, 129.5, 129.3, 129.1, 128.8, 128.8, 128.1, 127.9, 112.5, 112.5, 57.3, 56.2, 51.1, 50.9, 48.4, 48.2, 7.2, 7.2. **MS** (EI, 70 eV): *m/z* (%) = 183.0 (21), 182.0 (100), 155.0 (61), 125.0 (14), 109.0 (14), 91.0 (12). **MS** (ESI) $[M+Na]^+$: 353.08. (ESI) (*m/z*) $[C_{17}H_{18}N_2OS_2Na]^+$: Calcd. 353.0758. found, 353.0746. **IR** (ATR): *v* = 3905, 2928, 2677, 2336, 2096, 1743, 1448, 1226, 895, 725.

Methyl(phenyl)((2-phenyl-2-(phenylthio)ethyl)imino)-λ^6-sulfanone (**7**)

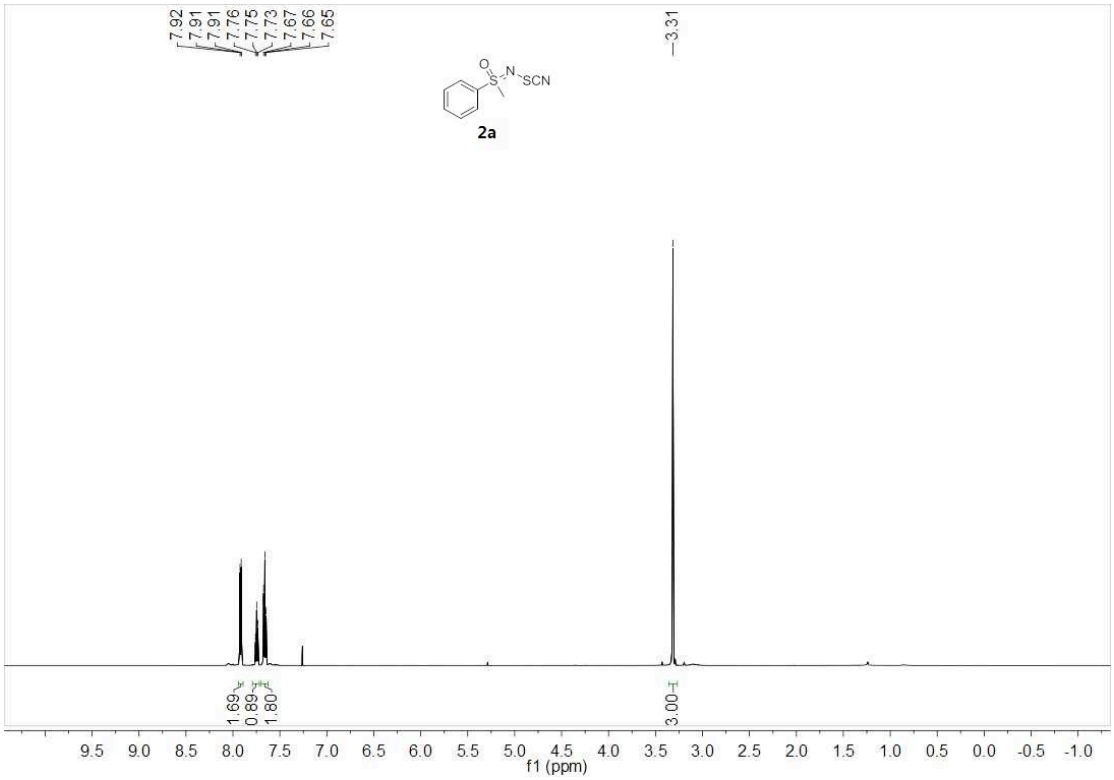


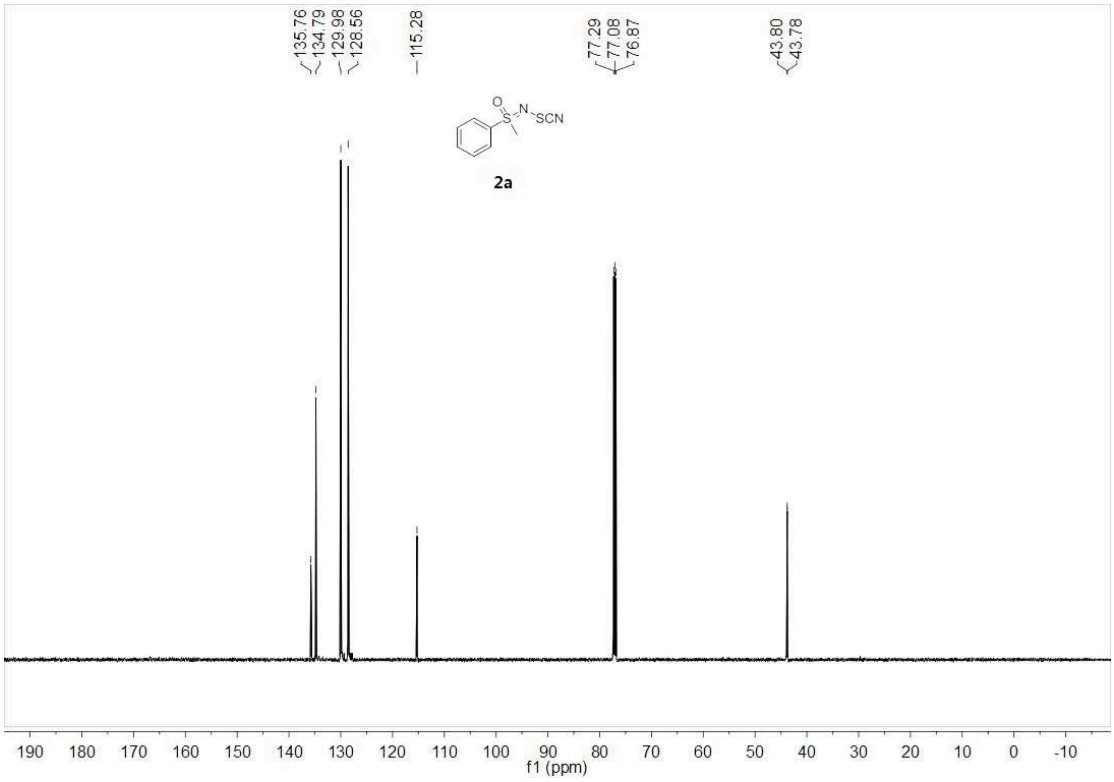
Light yellow oil, 6.6 mg, 12% yield, yield, *dr* = 1:1. **^{1}H NMR** (600 MHz, $CDCl_3$, mixture of diastereomers) δ 7.72 – 7.66 (m, 2H), 7.52 – 7.47 (m, 1H), 7.37 (t, *J* = 7.8 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 2H), 7.22 – 7.16 (m, 7H), 7.12 – 7.07 (m, 1H), 4.29 (dd, *J* = 7.5, 6.5 Hz, 1H), 3.52 (dd, *J* = 13.0, 6.3 Hz, 1H), 3.29 (dd, *J* = 9.4, 3.6 Hz, 1H), 3.11 (s, 3H). **^{13}C {^{1}H} NMR** (151 MHz, $CDCl_3$, mixture of diastereomers) δ 143.5, 139.7, 136.9, 134.8, 132.7, 130.0, 129.0, 128.7, 128.6, 128.6, 128.1, 127.1, 127.1, 125.4, 58.1, 45.0, 43.5. **MS** (EI, 70 eV): *m/z* (%) = 244.1 (100), 141.1 (82), 125.0 (27), 123.1 (27), 91.1 (17), 77.2 (49). **MS** (ESI) $[M+H]^+$: 368.11 (ESI) (*m/z*) $[C_{21}H_{22}NOS_2]^+$: Calcd. 368.1143 found, 368.1127. **IR** (ATR): *v* = 3440, 3061, 2923, 2858, 2662, 2322, 2101, 1995, 1908, 1729, 1581, 1448, 1355, 1313, 1226, 1129, 976, 847, 739, 693.

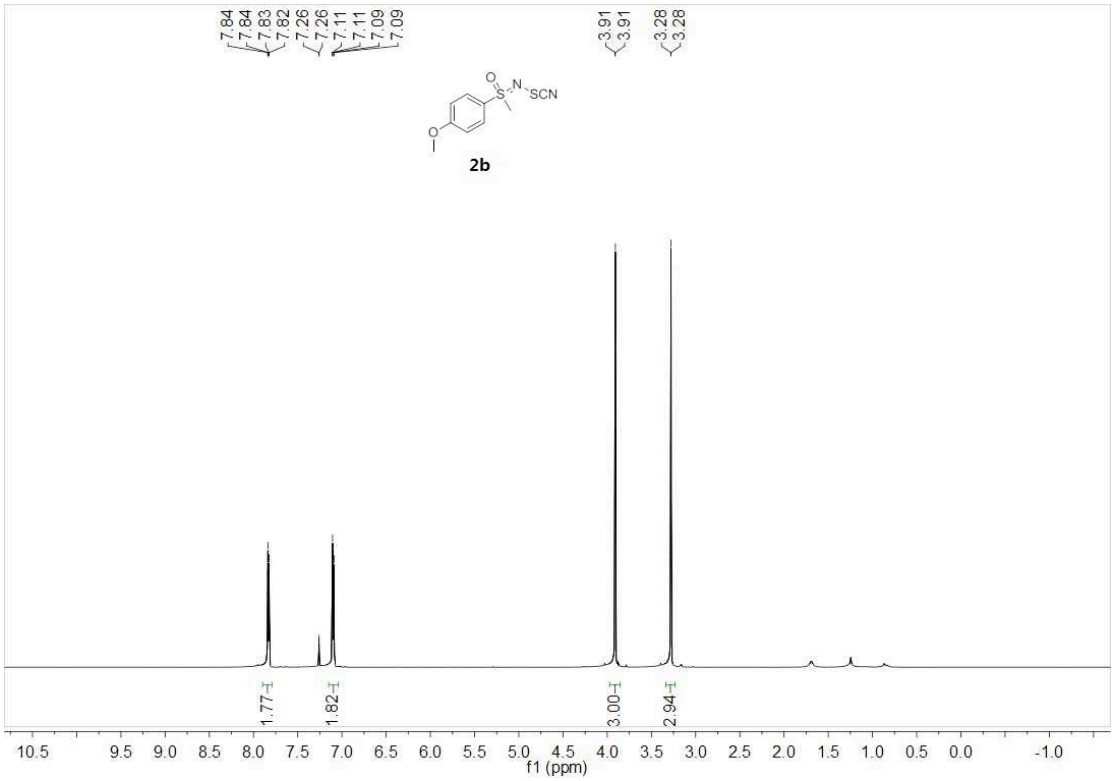
6. References

[1] C. Bohnen and C. Bolm, *Org. Lett.,* 2015, **17**, 3011.
[2] Z. Liang, F. Wang, P. Chen and G. Liu, *Org. Lett*., 2015, **17**, 2438.
[3] X. Lu, H. Wang, R. Gao, D. Sun and X. Bi, *RSC Adv.,* 2014, **4**, 28794.

7. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of compounds 2 and 4-7



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7.84
7.83
7.82
7.26
7.26
7.11
7.09
7.09
3.91
3.91
3.28
3.28
SCN
2b
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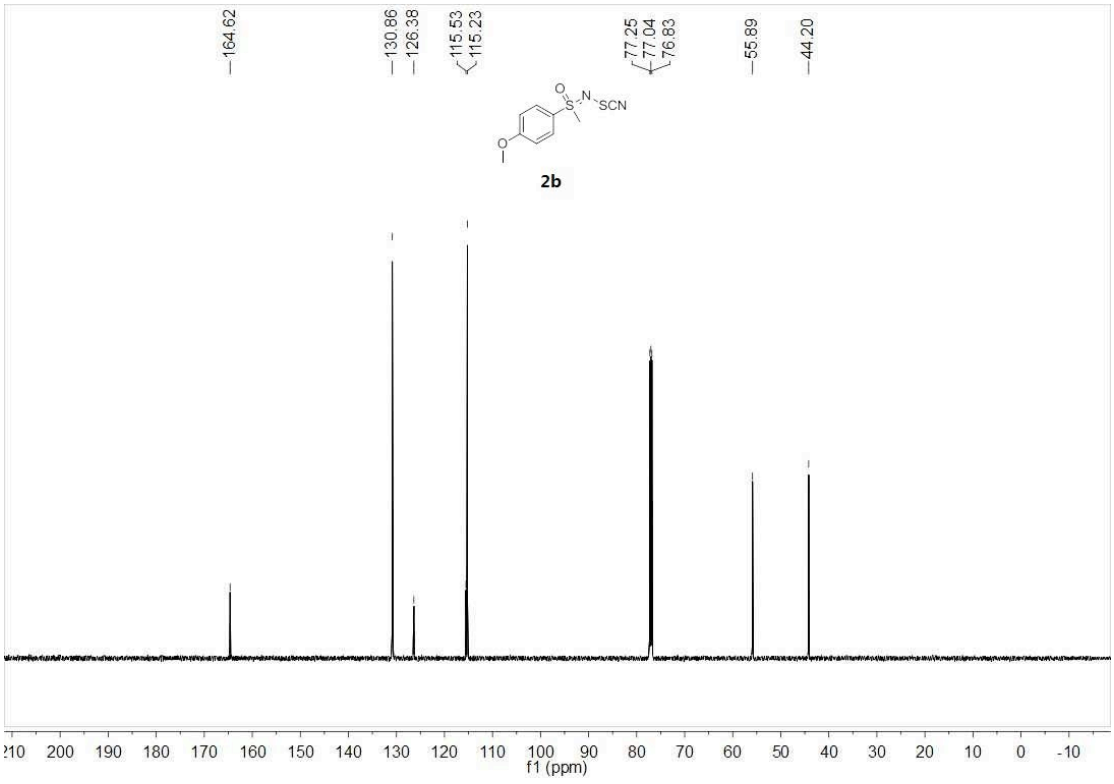
1.82
3.00
2.94
f1 (ppm)


164.62
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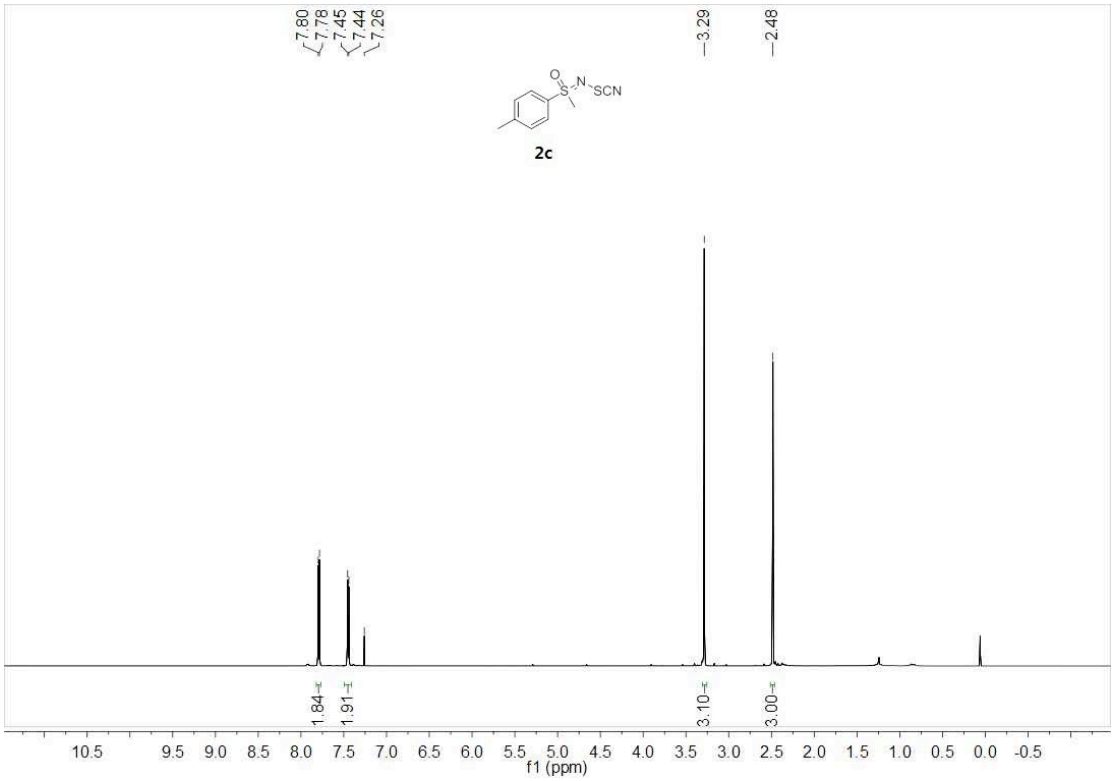
126.38
115.53
115.23
77.25
77.04
76.83
55.89
44.20
SCN
2b
f1 (ppm)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SCN
2c
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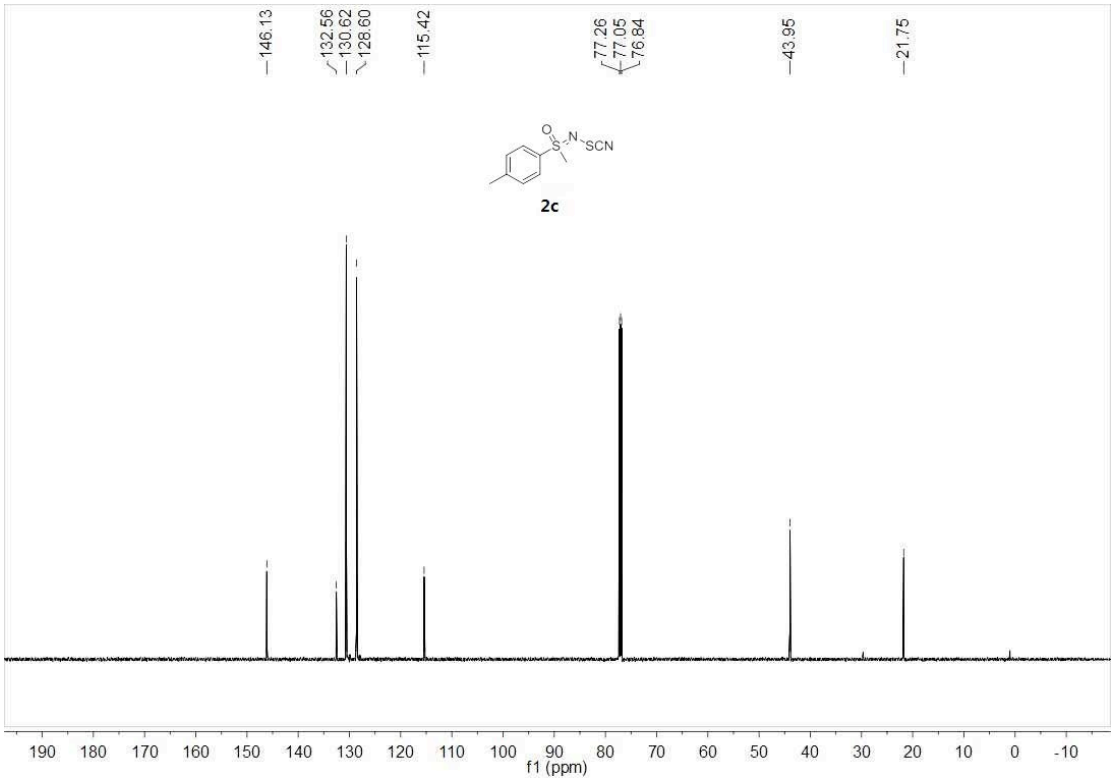
1.91
3.10
3.00
f1 (ppm)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77.26
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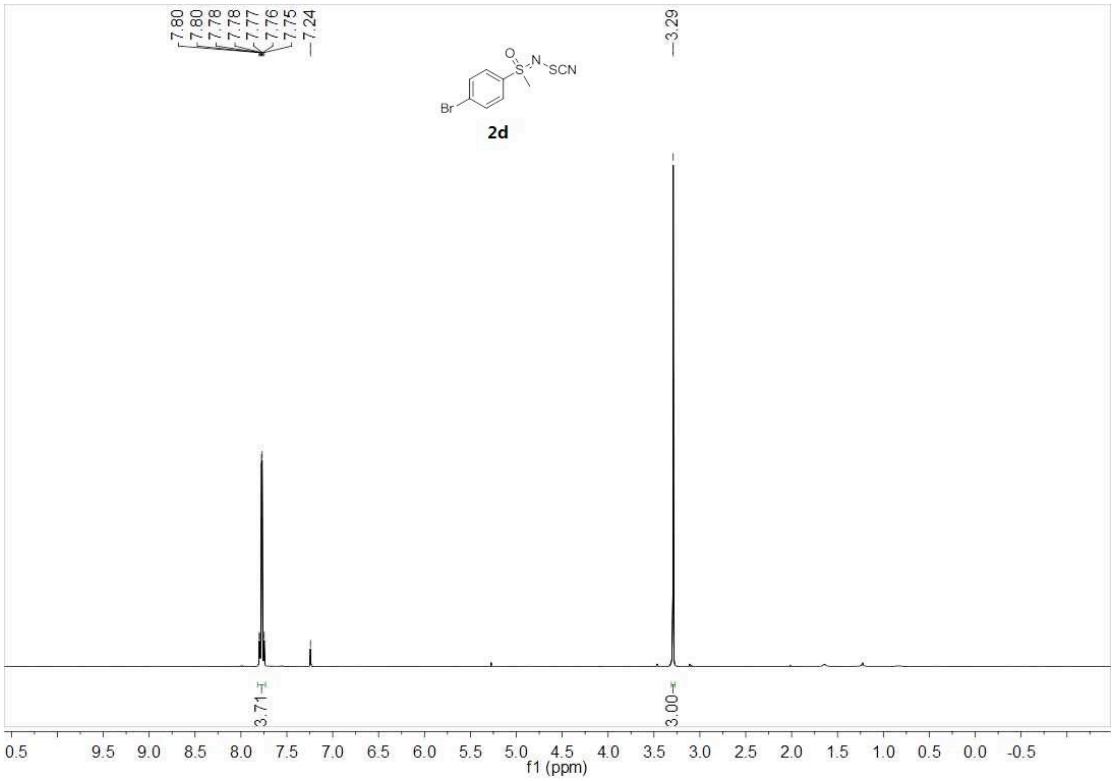
76.84
43.95
21.75
SCN
2c
f1 (ppm)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7.77
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7.24
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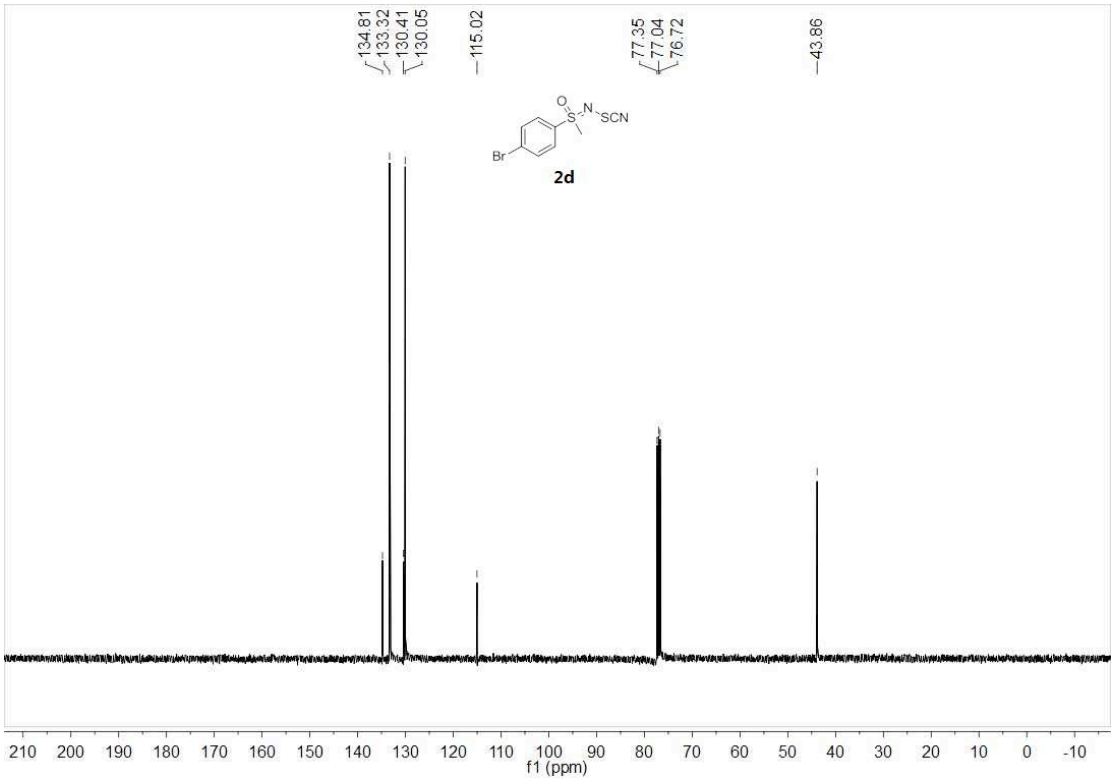
Br
SCN
2d
3.71
3.00
f1 (ppm)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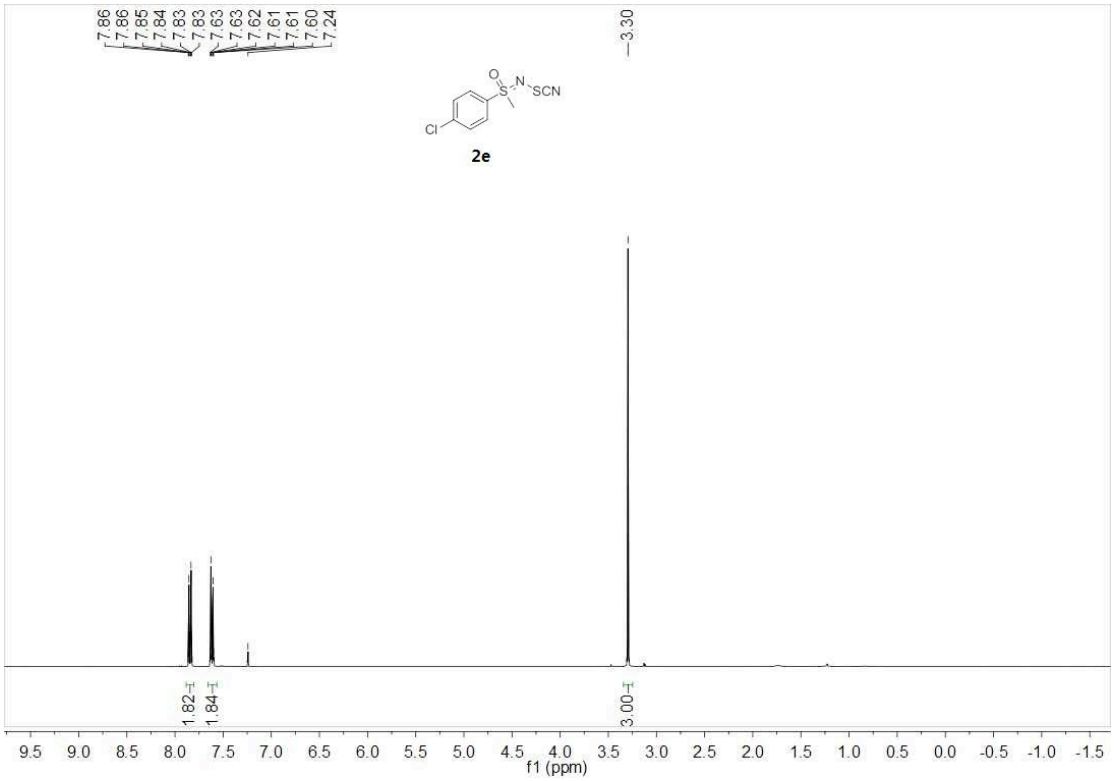
77.35
77.04
76.72
43.86
Br
SCN
2d
f1 (ppm)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7.83
7.83
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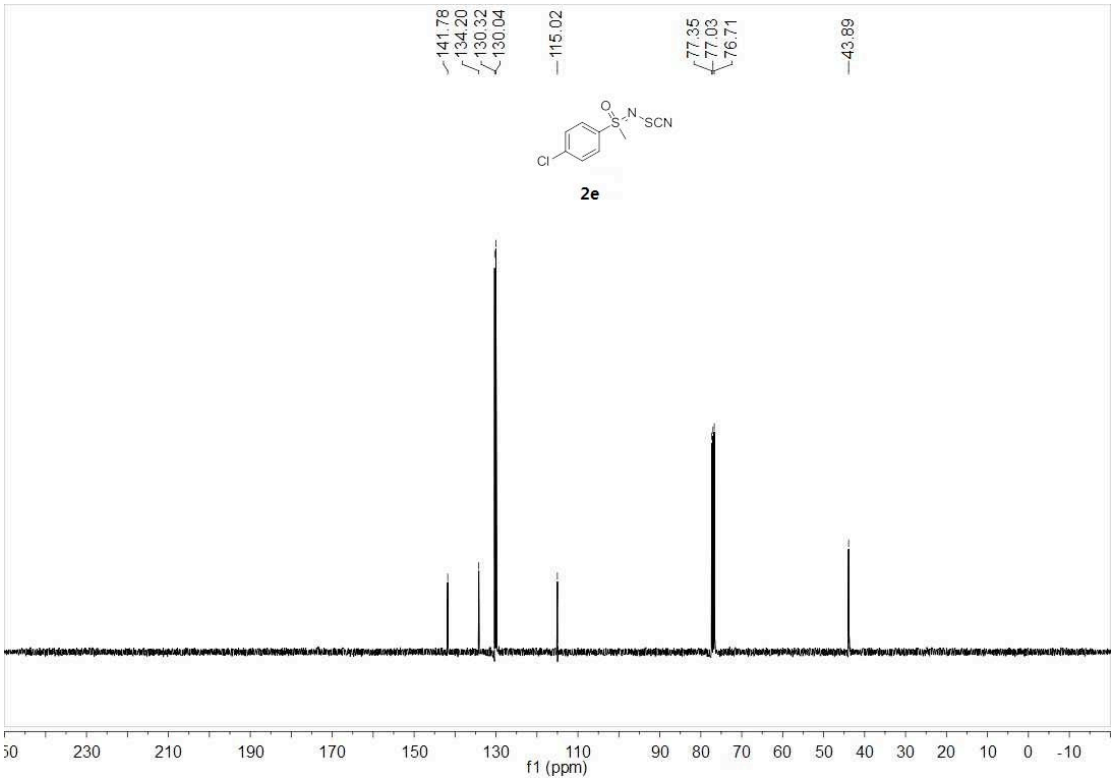
7.63
7.62
7.61
7.61
7.60
7.24
3.30
O
S
N
SCN
Cl
2e
1.82
1.84
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)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S
N
SCN
Cl
2e
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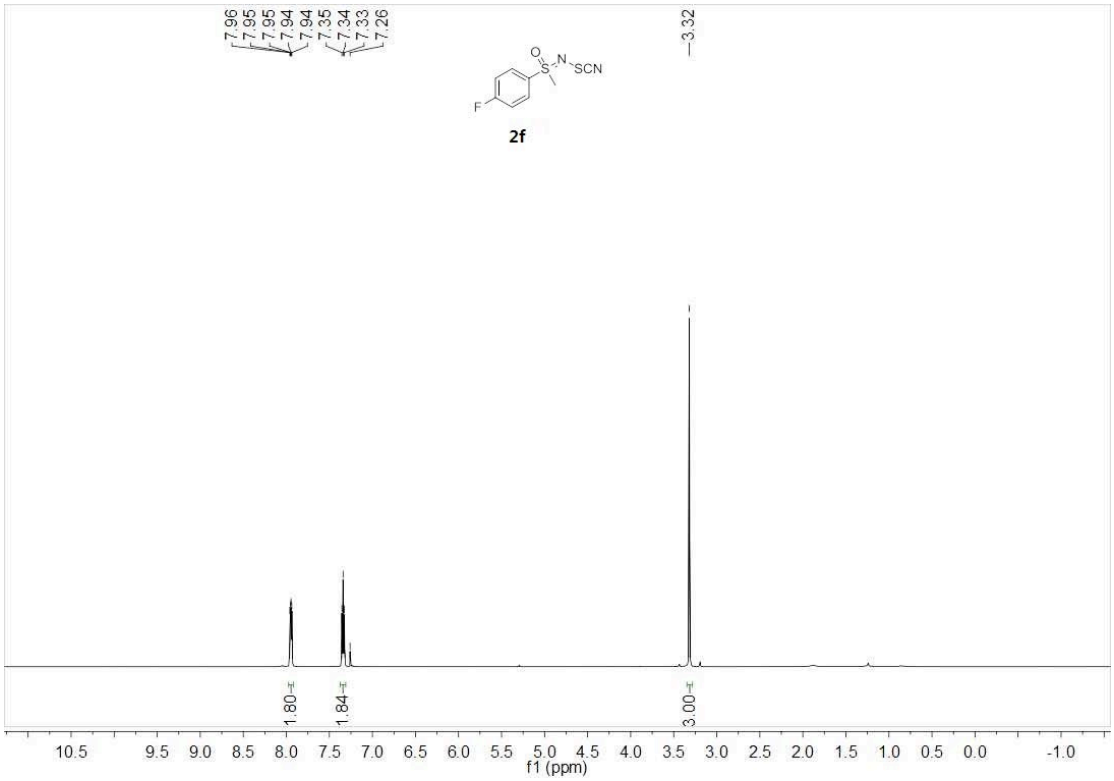
f1 (ppm)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2f
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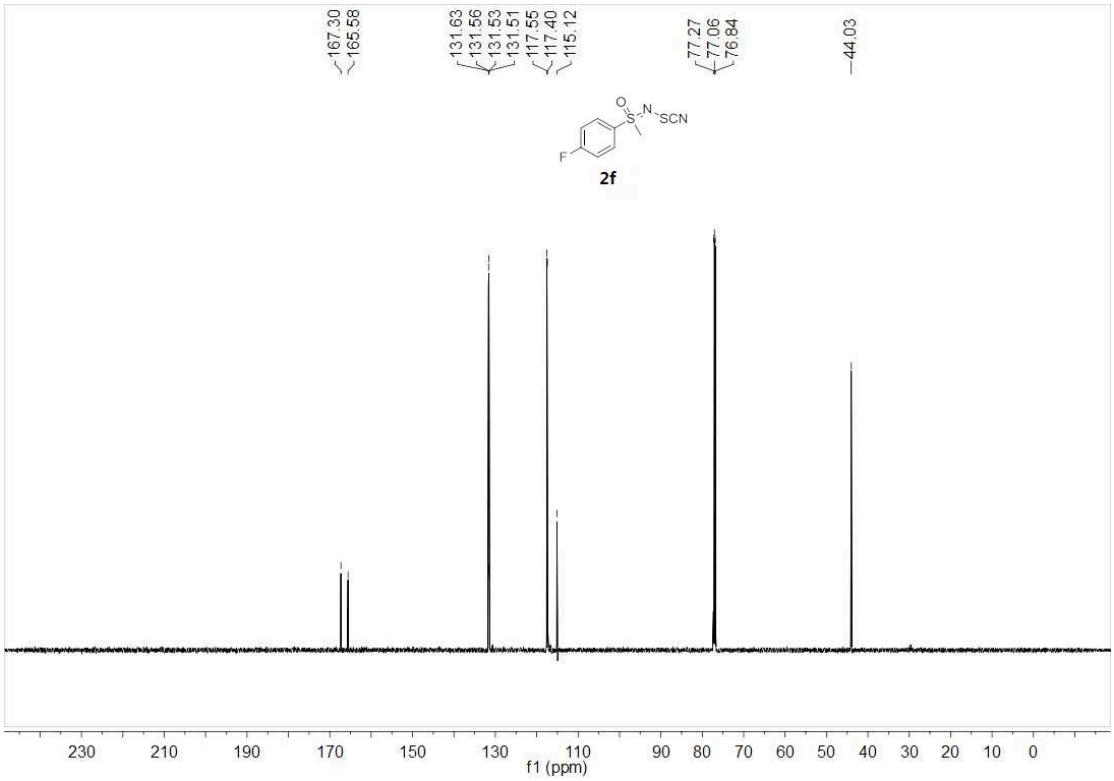
1.84
3.00
f1 (ppm)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165.58
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117.40
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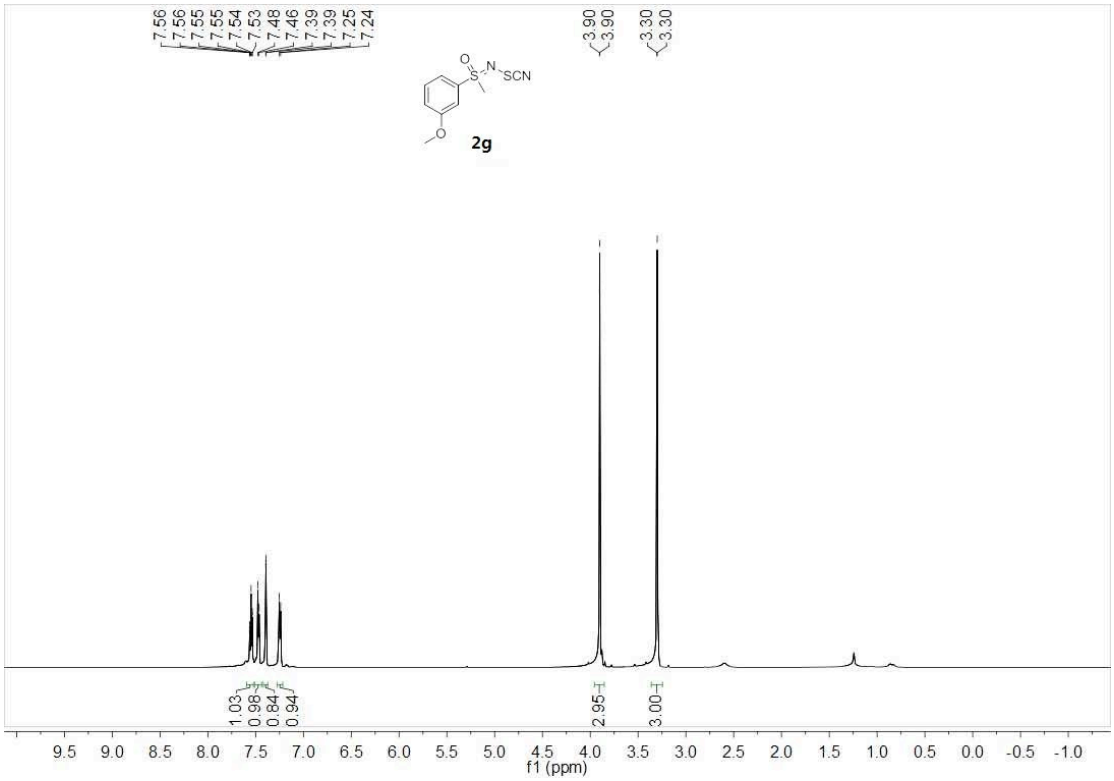
77.27
77.06
76.84
44.03
2f
f1 (ppm)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7.24
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3.90
3.30
3.30
O
S
N
SCN
2g
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0.84
0.94
2.95
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
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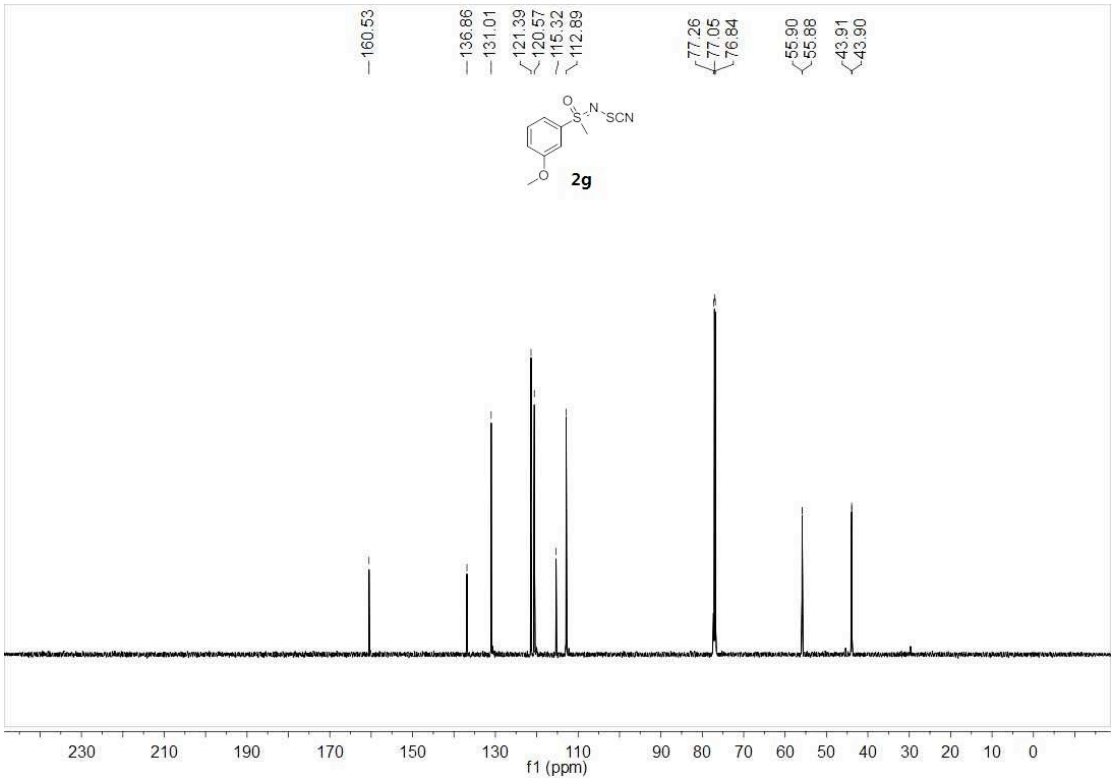
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N
SCN
2g
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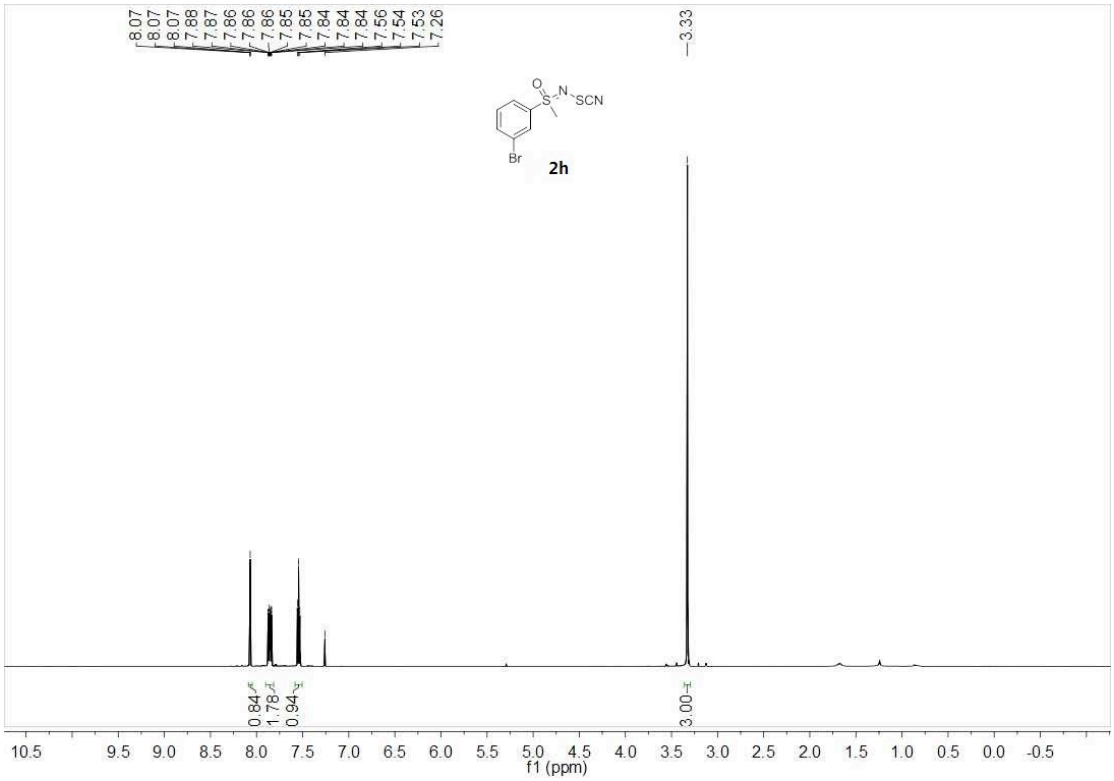
f1 (ppm)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7.26
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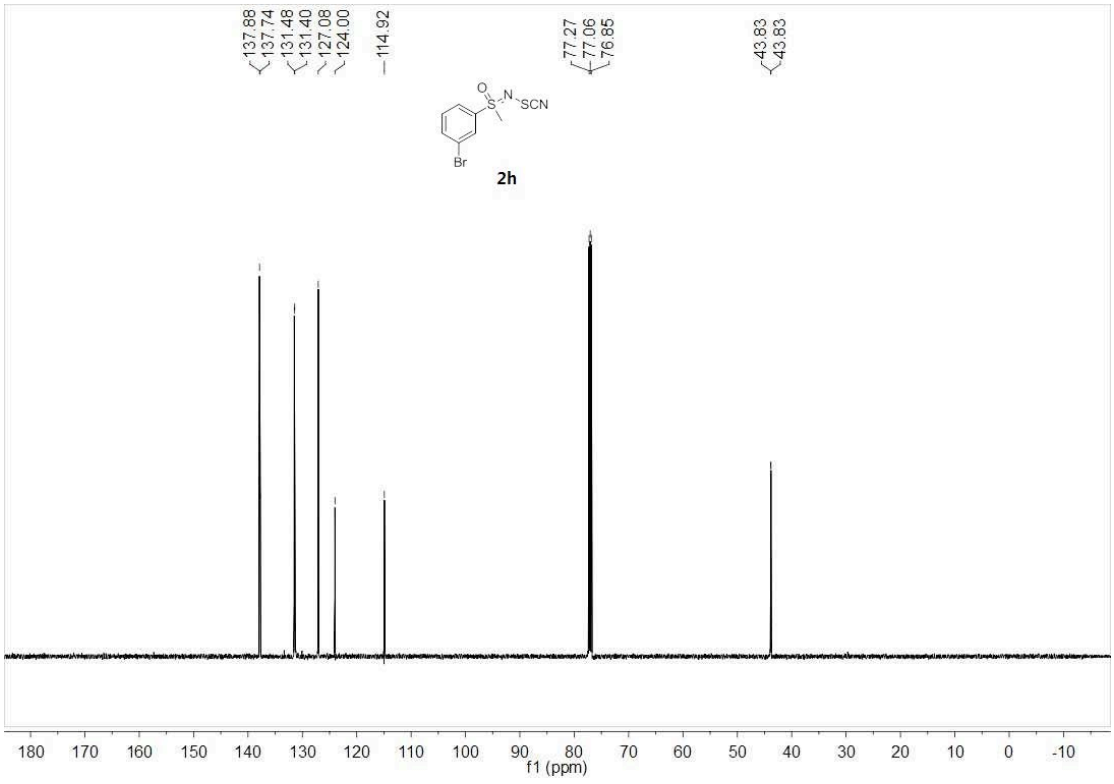
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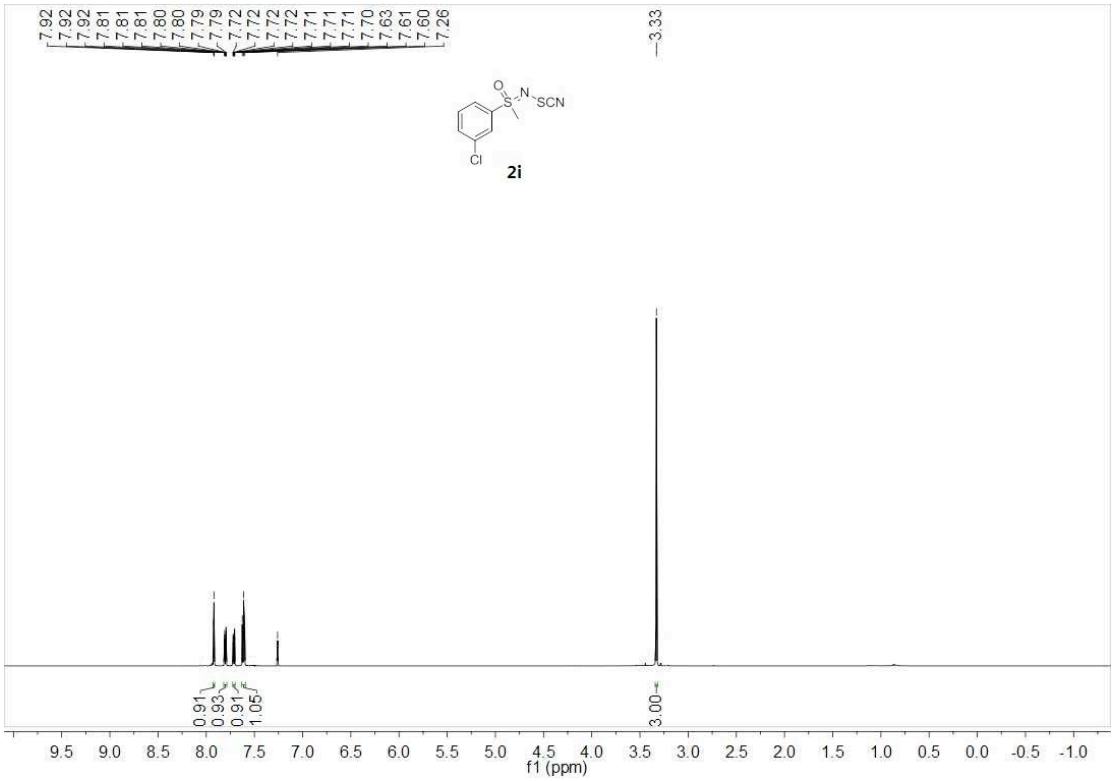
f1 (ppm)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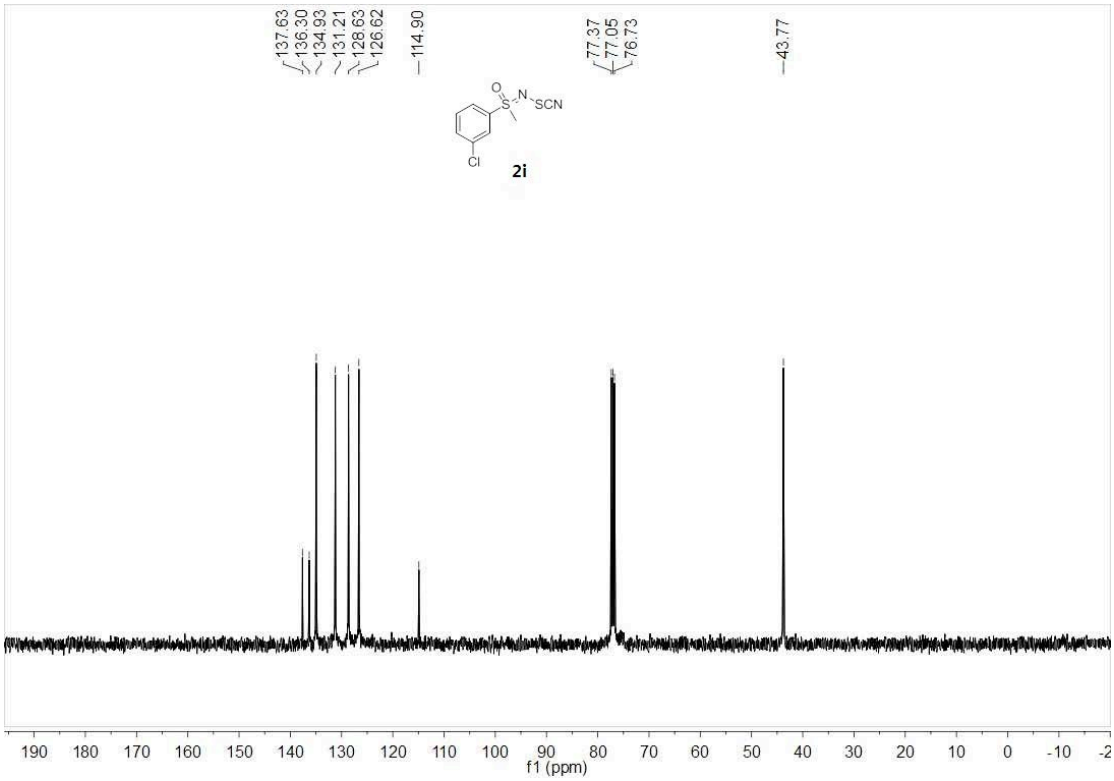
f1 (ppm)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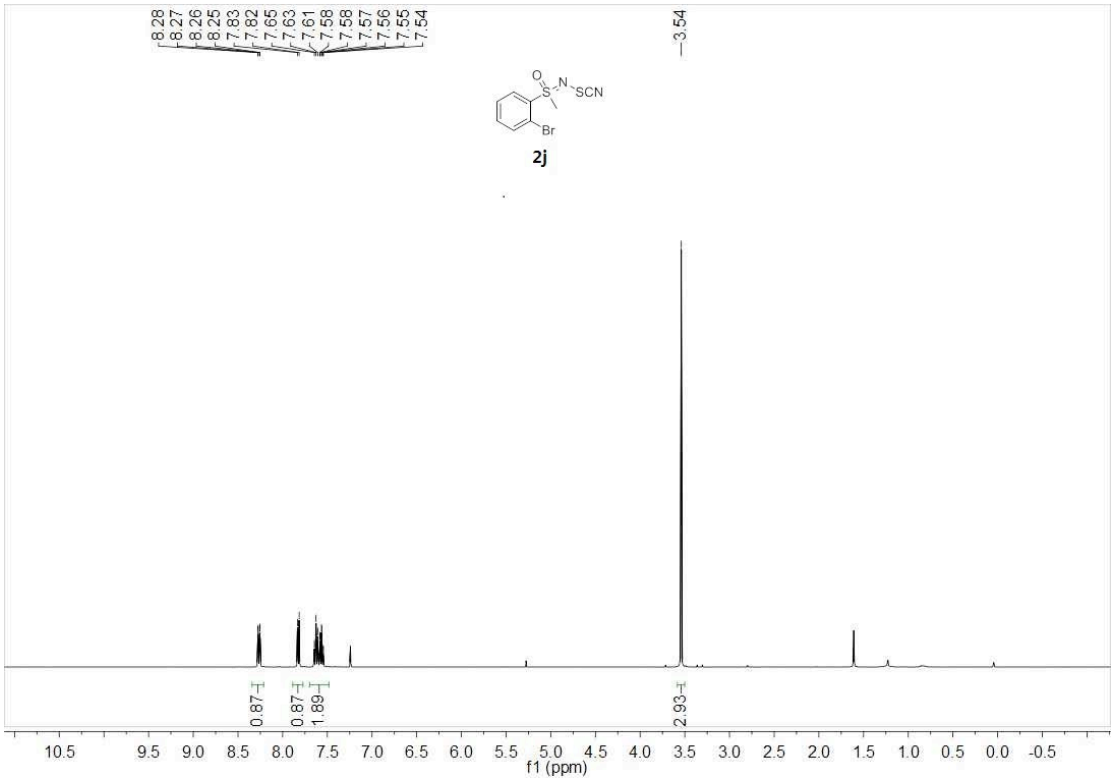
2i
f1 (ppm)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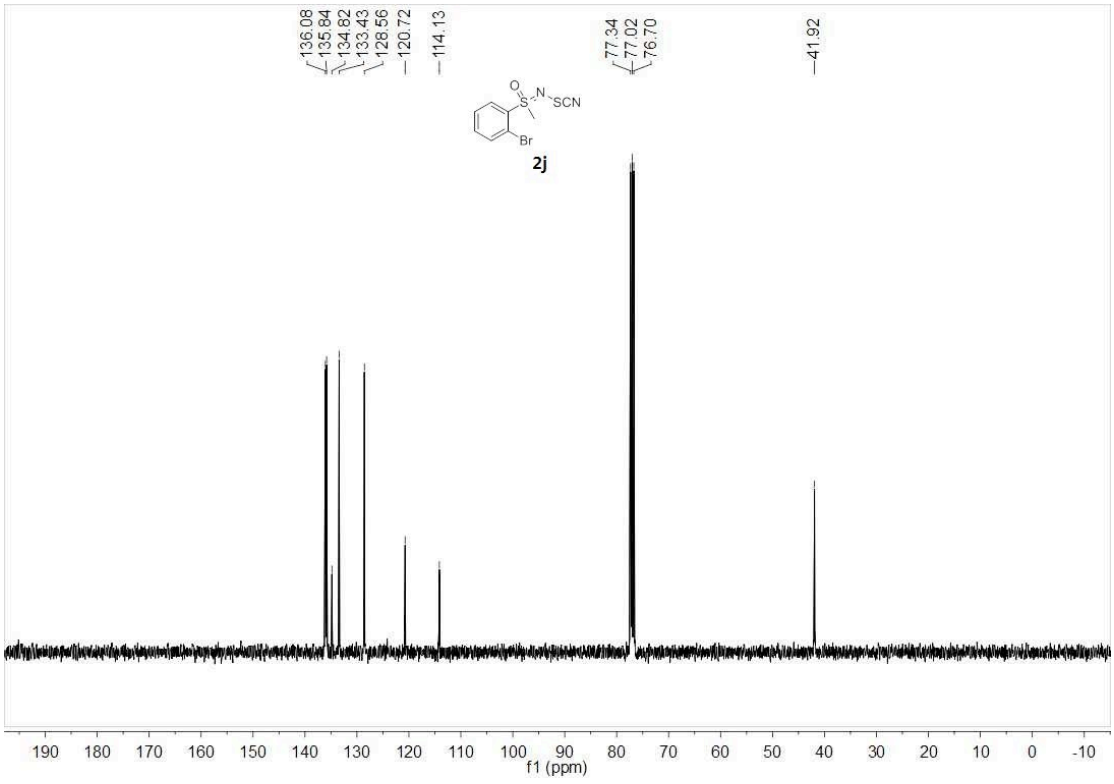
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41.92
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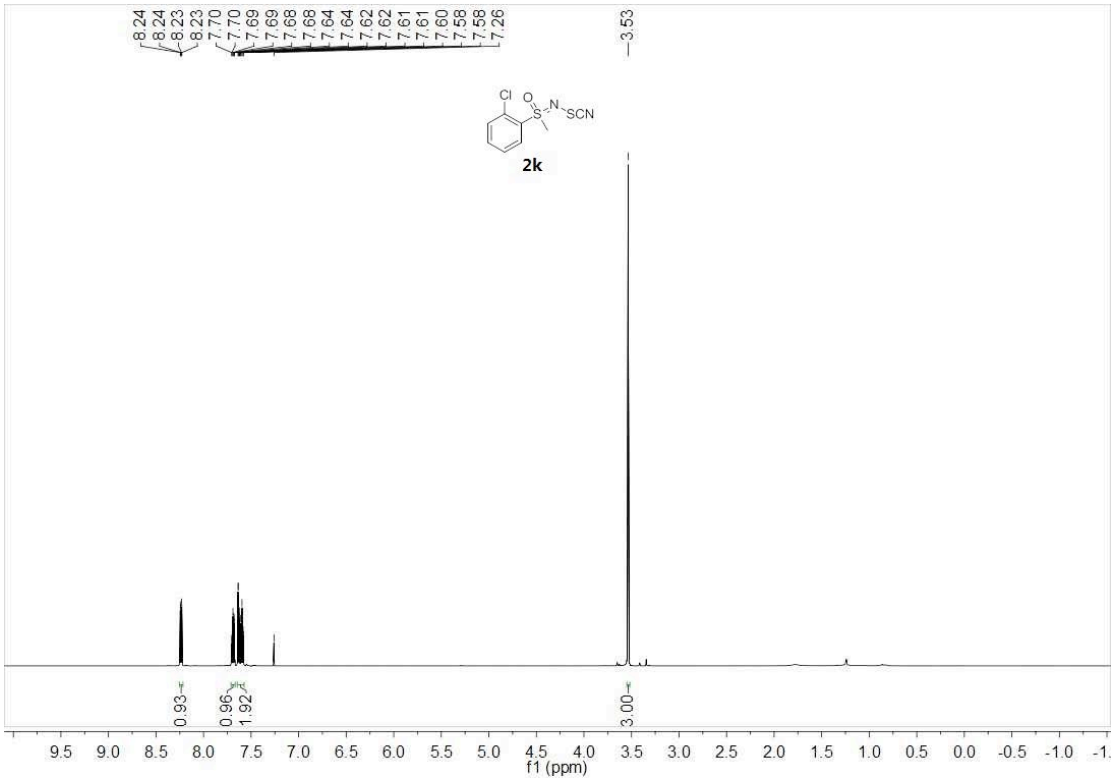
2j
f1 (ppm)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7.58
7.58
7.26
3.53
Cl
O
S
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SCN
2k
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1.92
3.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
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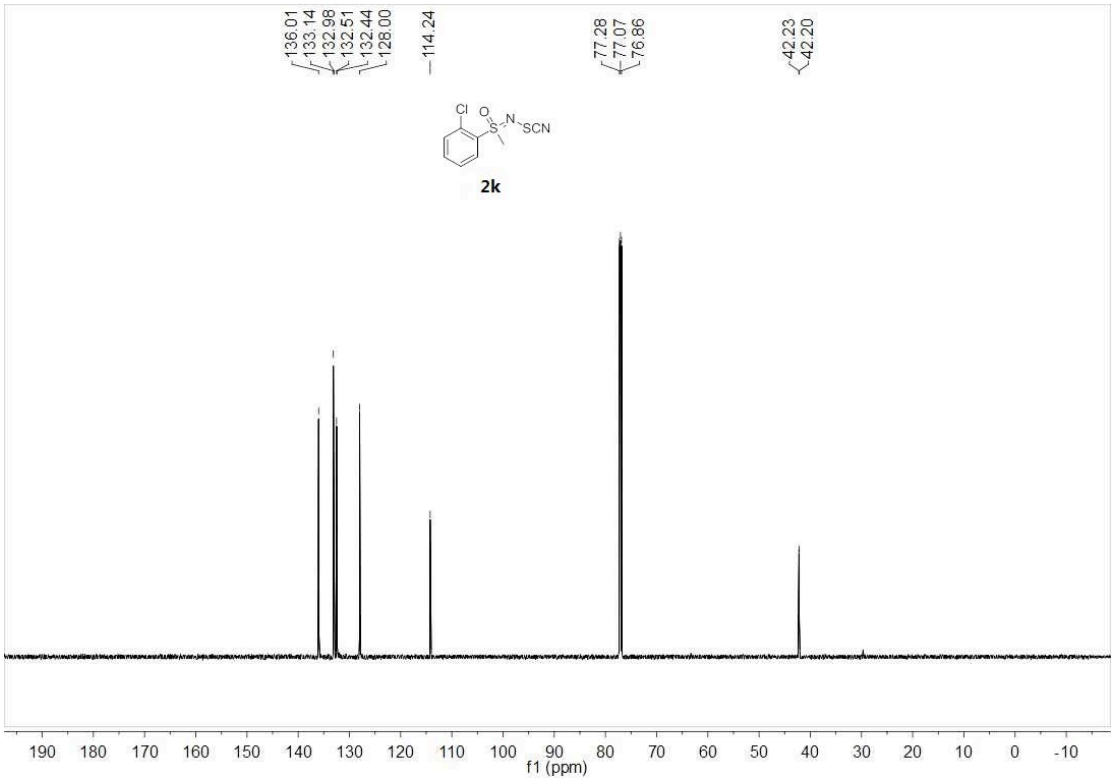
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O
S
N
SCN
2k
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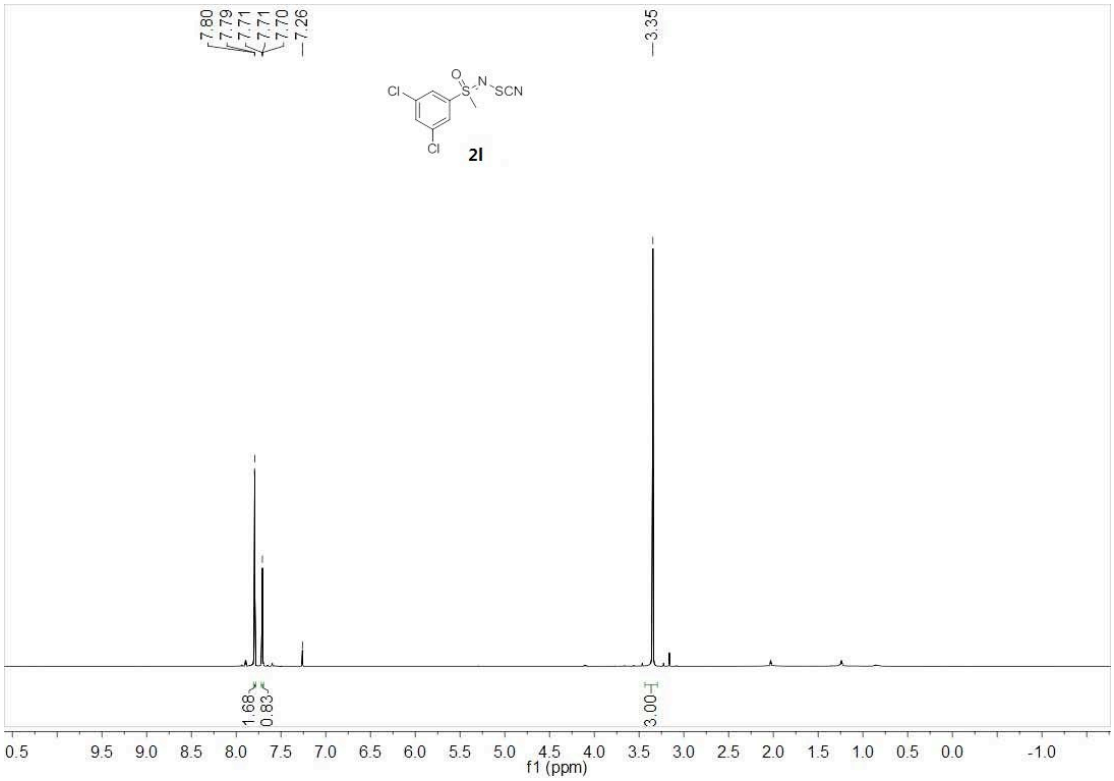
f1 (ppm)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N
SCN
Cl
2l
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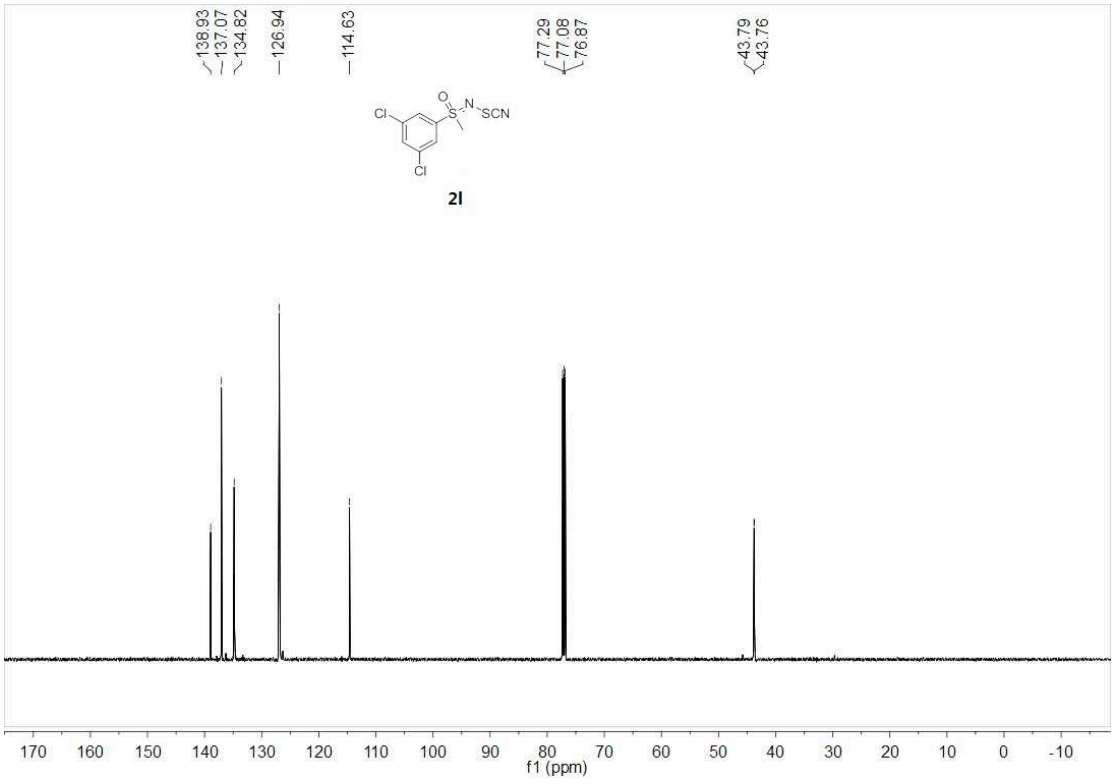
3.00
f1 (ppm)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43.76
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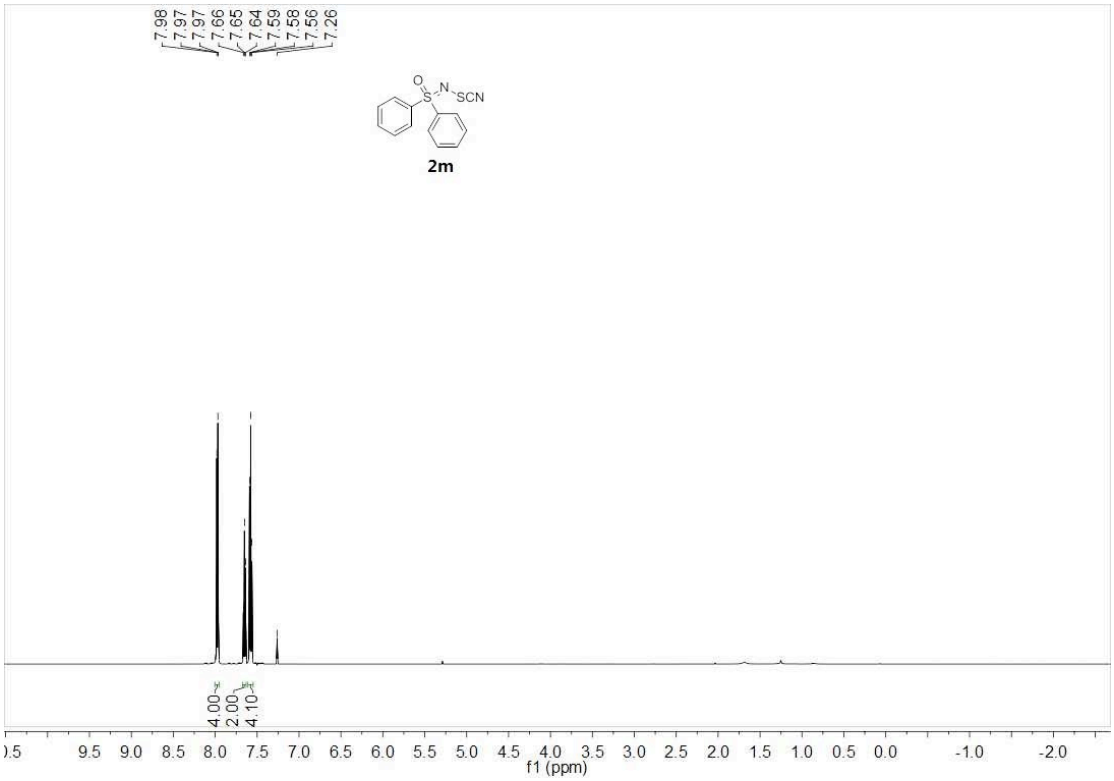
O
N
SCN
Cl
2l
f1 (ppm)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7.97
7.97
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7.26
SCN
2m
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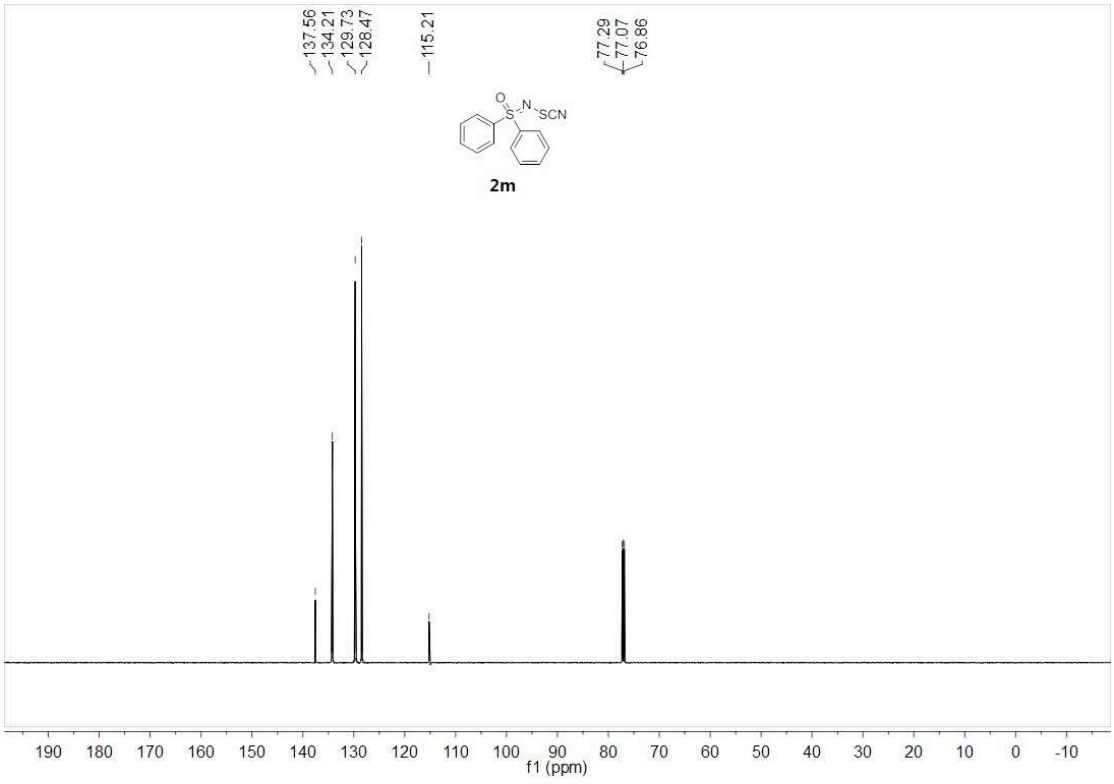
4.10
f1 (ppm)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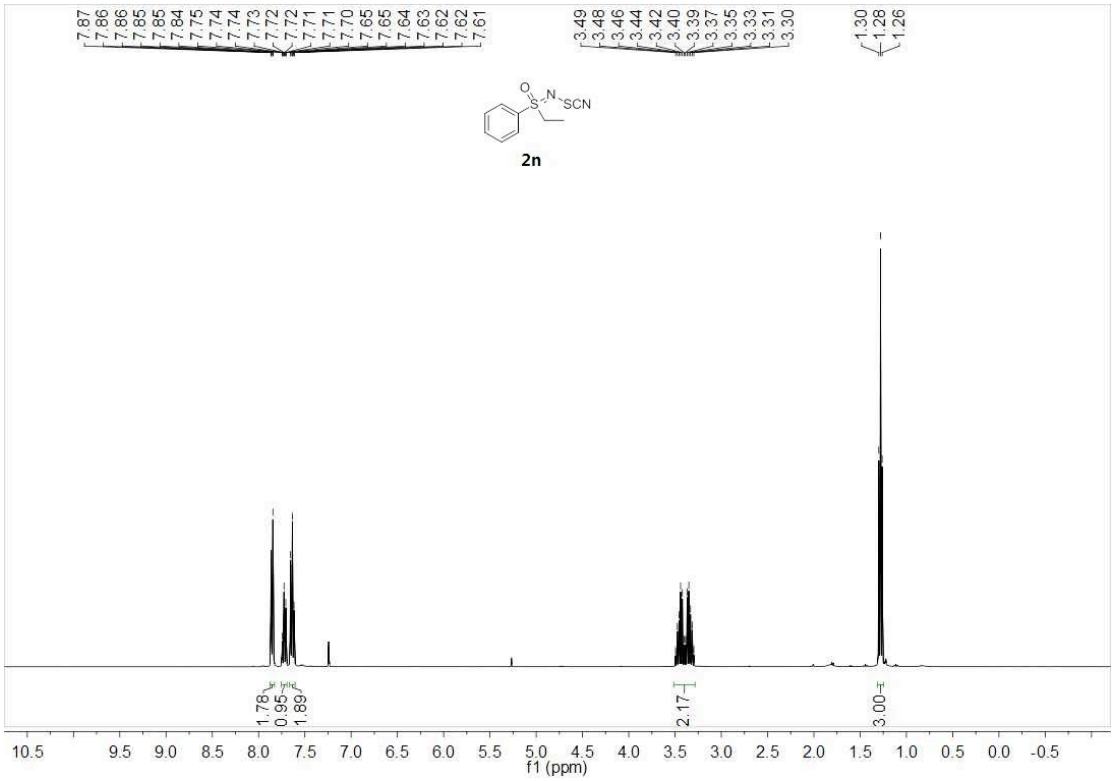
SCN
2m
f1 (ppm)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3.42
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3.37
3.35
3.33
3.31
3.30
1.30
1.28
1.26
SCN
2n
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3.00
10.5
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9.0
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8.0
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7.0
6.5
6.0
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5.0
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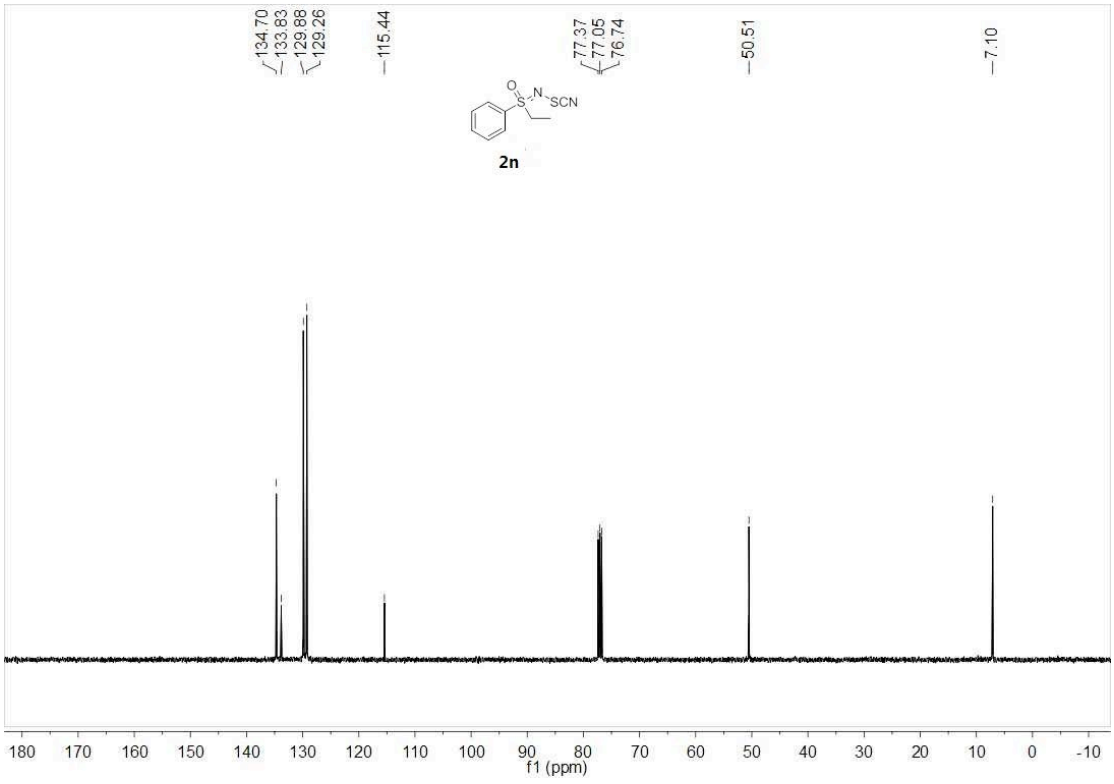
-0.5
f1 (ppm)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SCN
2n
180
170
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100
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40
30
20
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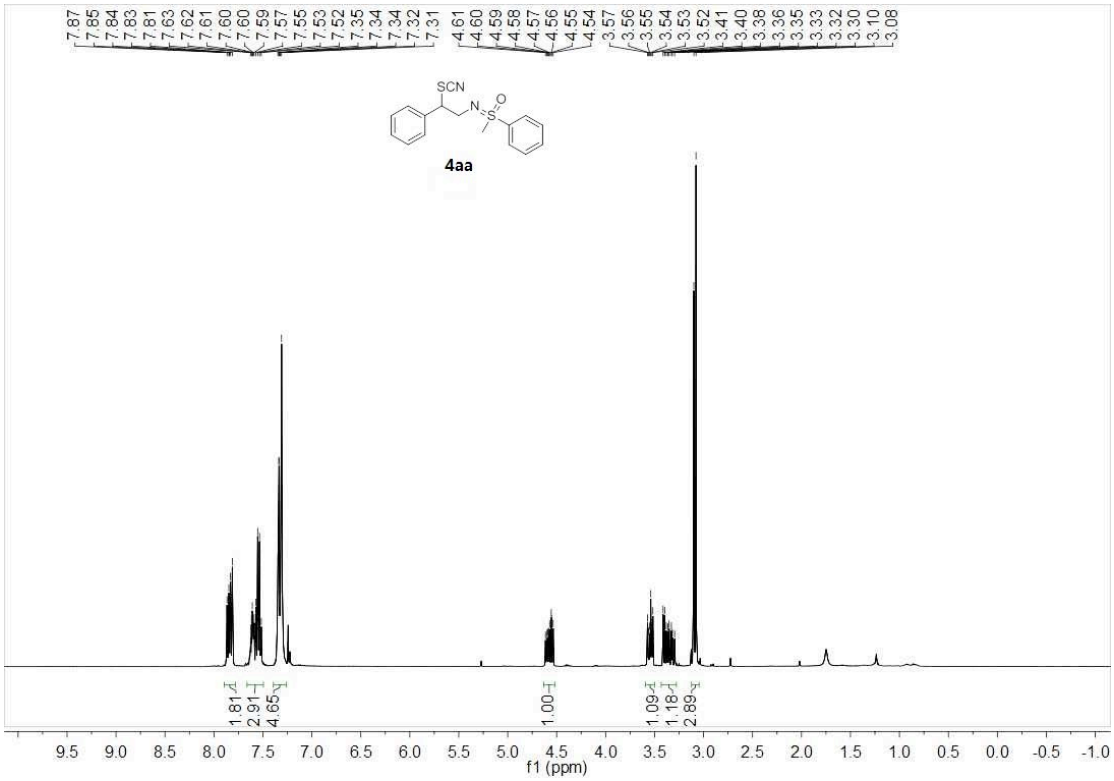
0
-10
f1 (ppm)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7.55
7.53
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7.35
7.34
7.34
7.32
7.31
4.61
4.60
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4.57
4.56
4.55
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3.57
3.56
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3.54
3.53
3.52
3.41
3.40
3.38
3.36
3.35
3.33
3.32
3.30
3.10
3.08
SCN
N
S
O
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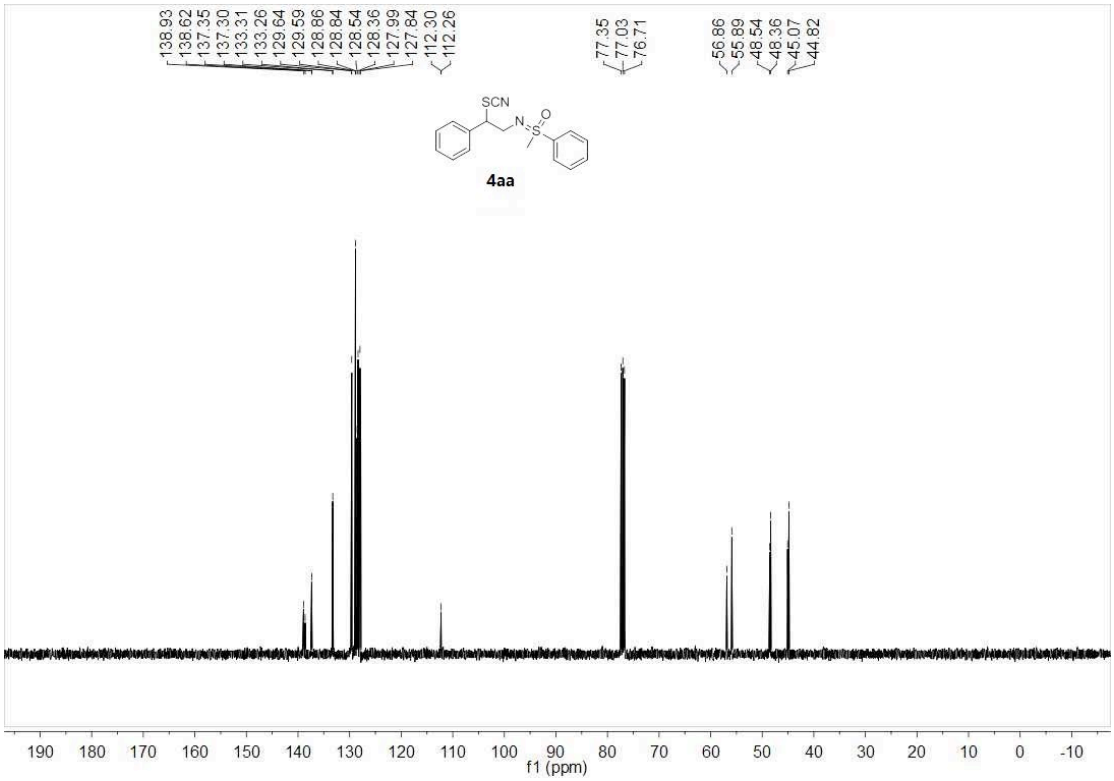
1.81
2.91
4.65
1.00
1.09
1.18
2.89
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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112.30
112.26
77.35
77.03
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56.86
55.89
48.54
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SCN
N
S
O
4aa
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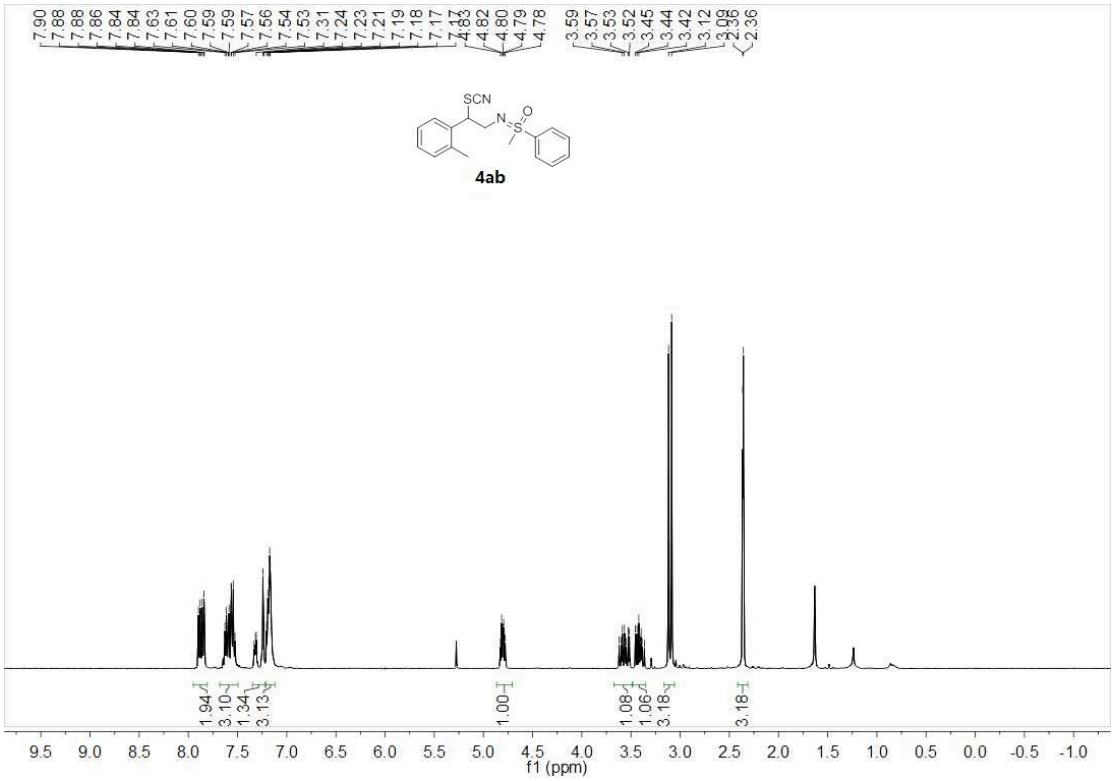
f1 (ppm)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7.31
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7.17
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3.12
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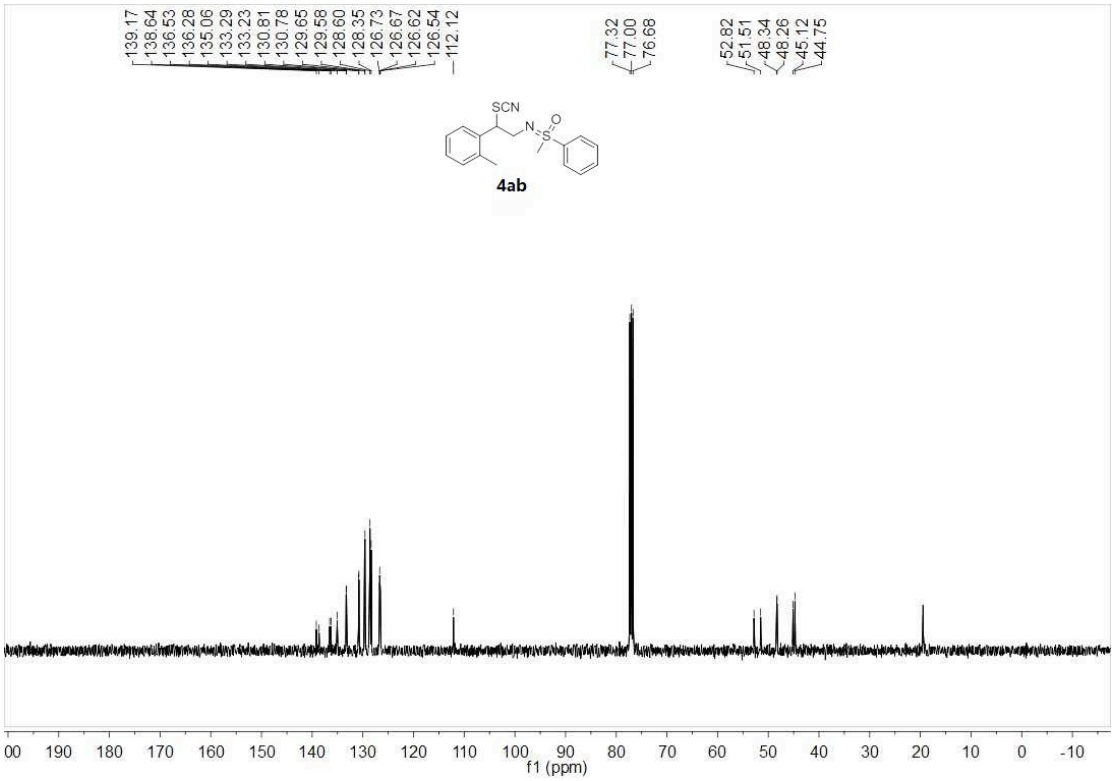
S
O
4ab
1.94
3.10
1.34
3.13
1.00
1.08
1.06
3.18
3.18
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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48.34
48.26
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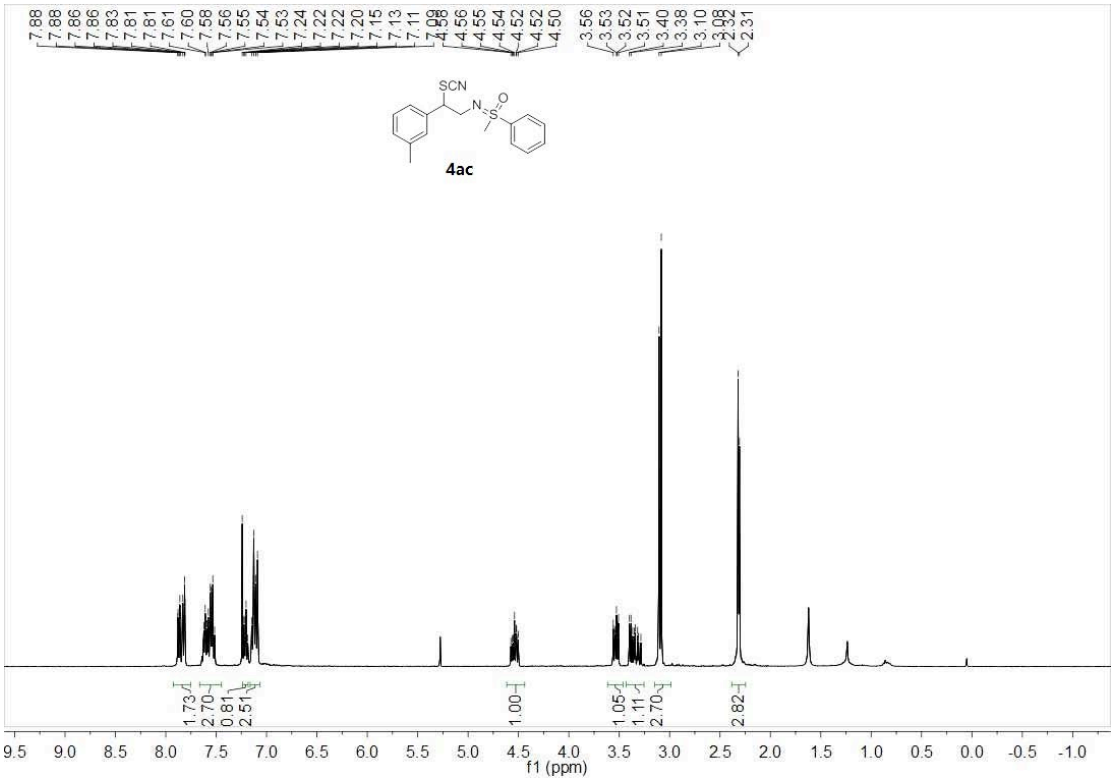
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.86
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4.50
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3.10
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2.31
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N
S
O
4ac
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2.70
0.81
2.51
1.00
1.05
1.11
2.70
2.82
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 -1.0
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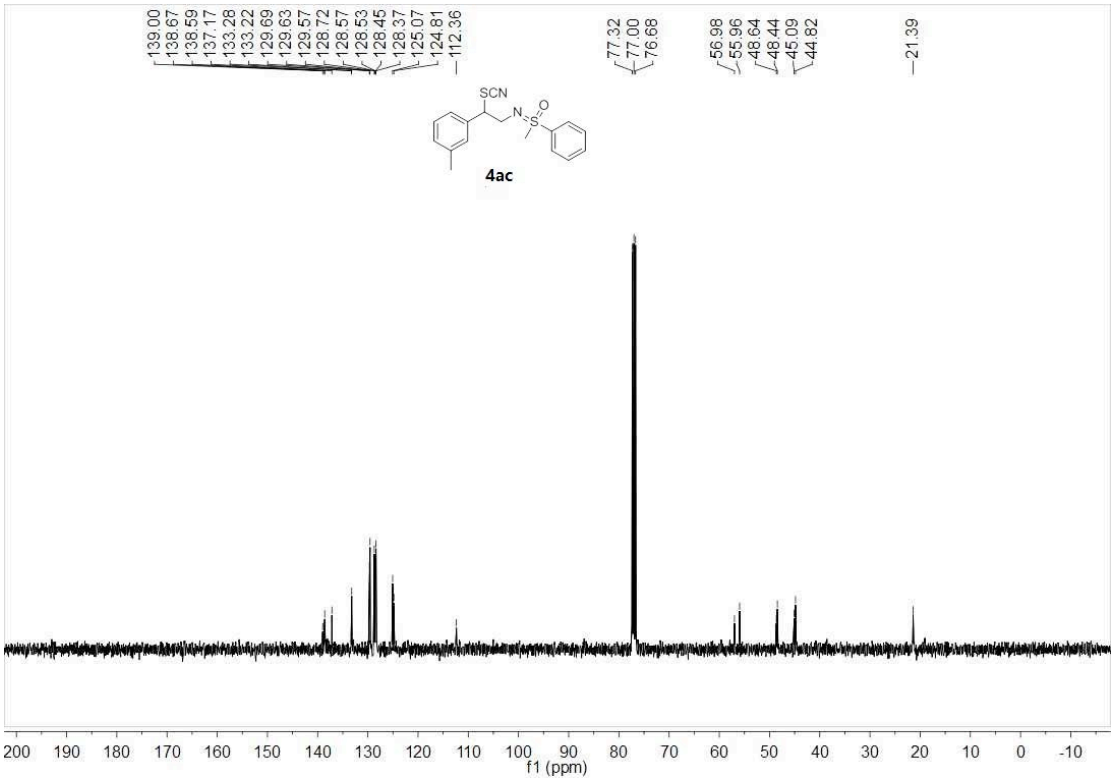
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125.07
124.81
112.36
77.32
77.00
76.68
56.98
55.96
48.64
48.44
45.09
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SCN
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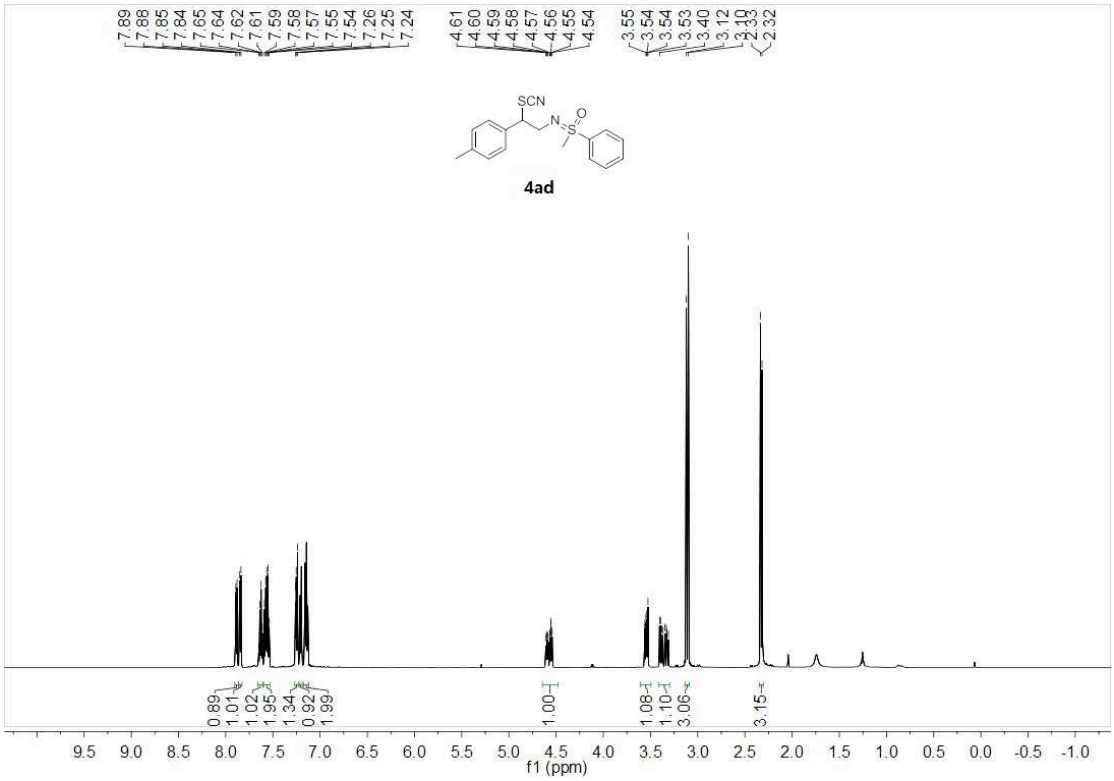
f1 (ppm)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3.55
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3.54
3.53
3.40
3.12
3.10
2.33
2.32
SCN
N
S
O
4ad
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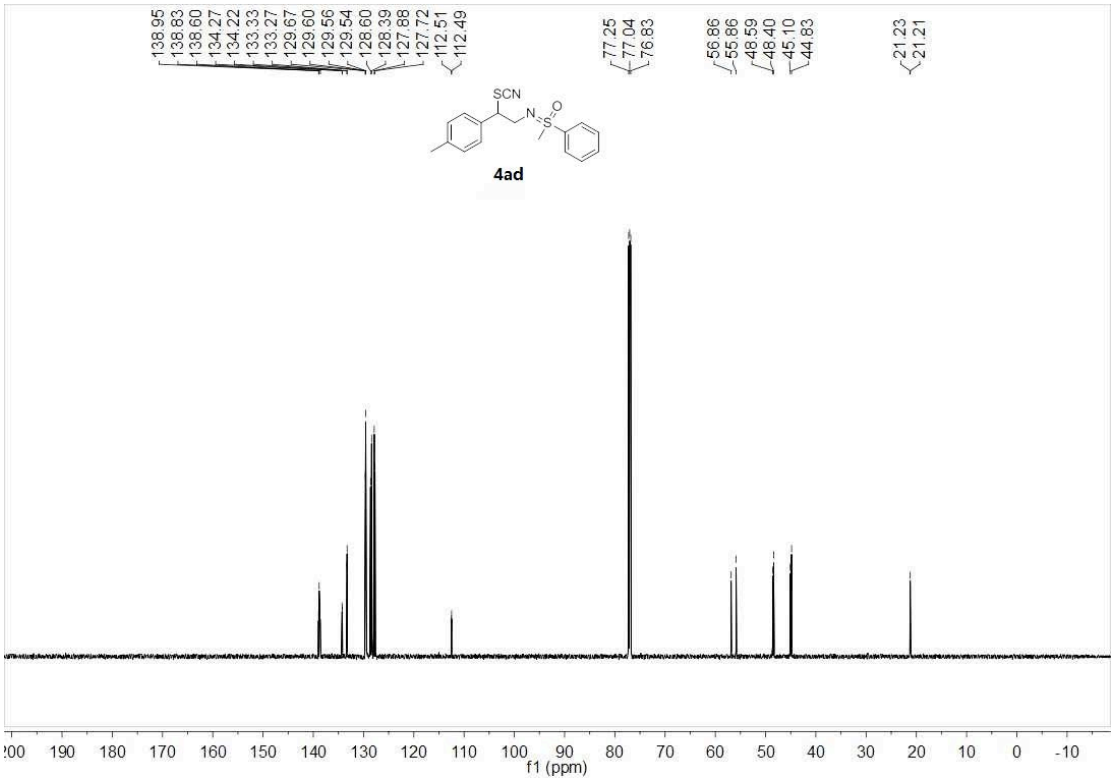
1.01
1.02
1.95
1.34
0.92
1.99
1.00
1.08
1.10
3.06
3.15
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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77.04
76.83
56.86
55.86
48.59
48.40
45.10
44.83
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S
O
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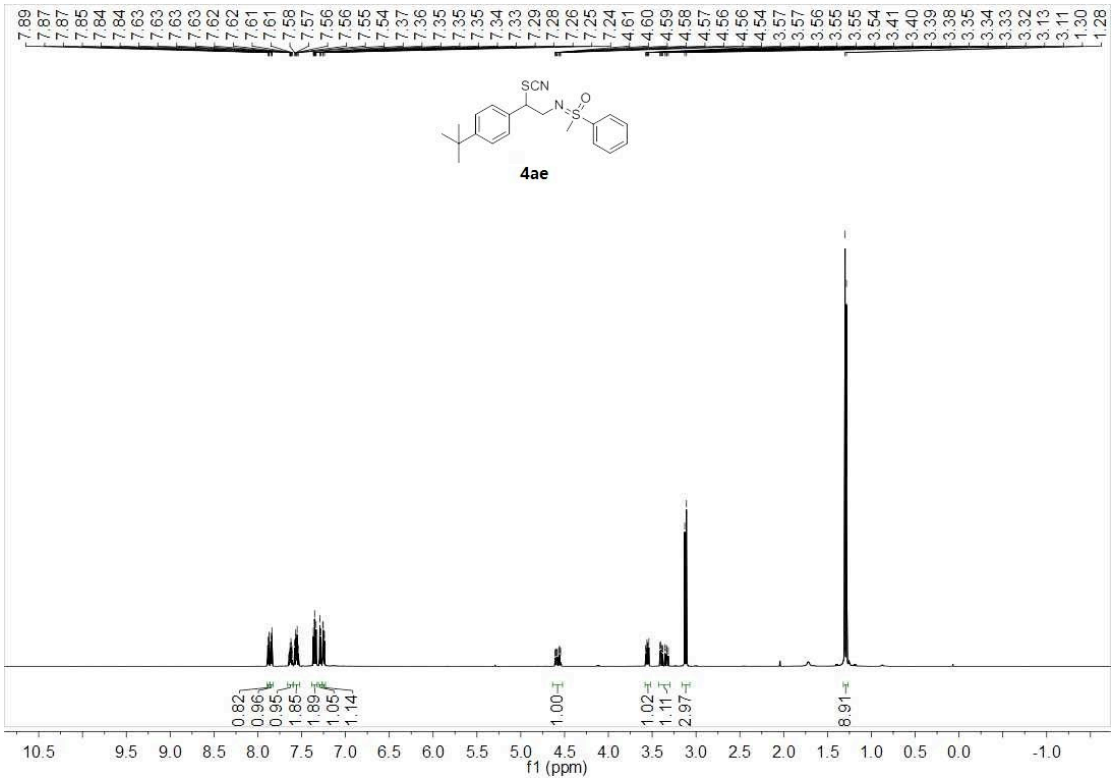
f1 (ppm)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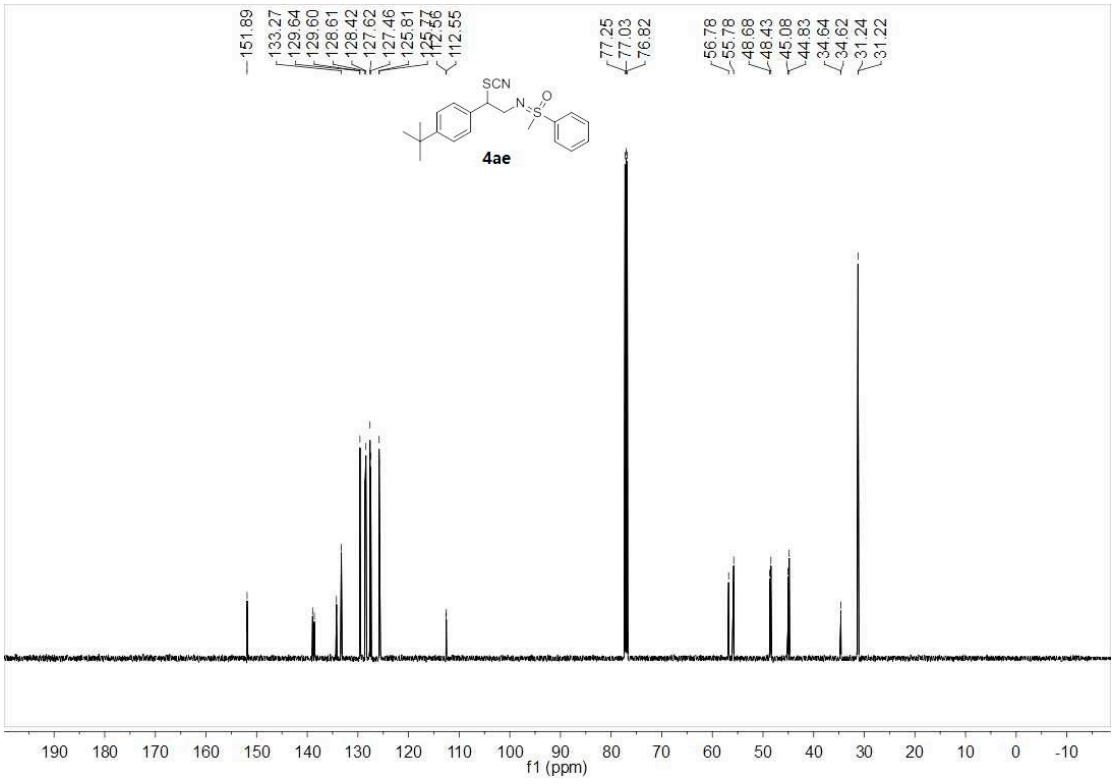
SCN
N
S
O
4ae
0.82 0.96 0.95 1.85 1.89 1.05 1.14 1.00 1.02 1.11 2.97 8.91
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)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77.25 77.03 76.82
56.78 55.78 48.68 48.43 45.08 44.83 34.64 34.62 31.24 31.22
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N
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O
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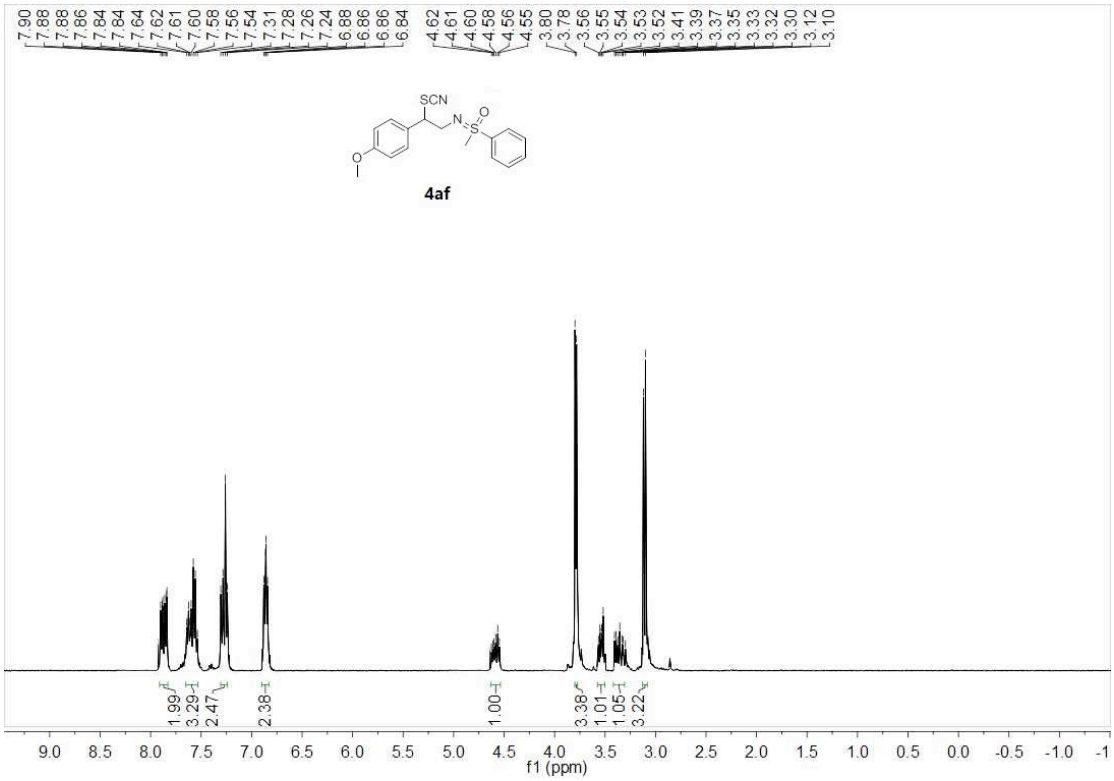
f1 (ppm)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6.86
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4.60
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S
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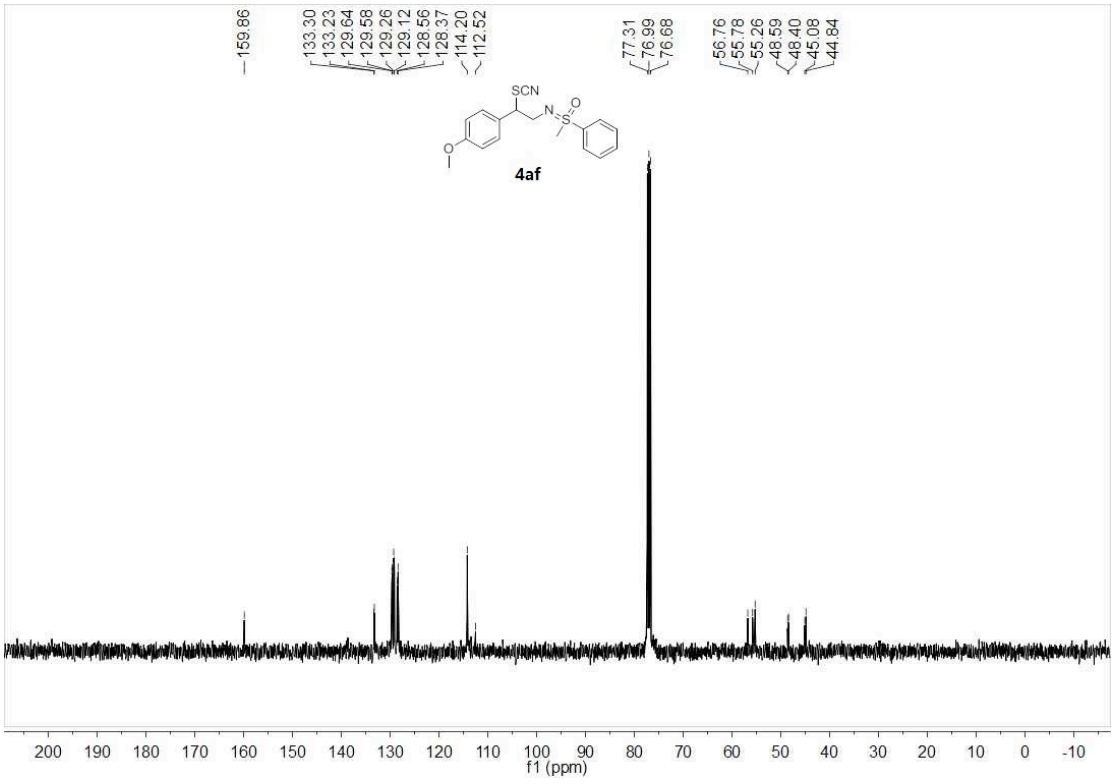
3.22
f1 (ppm)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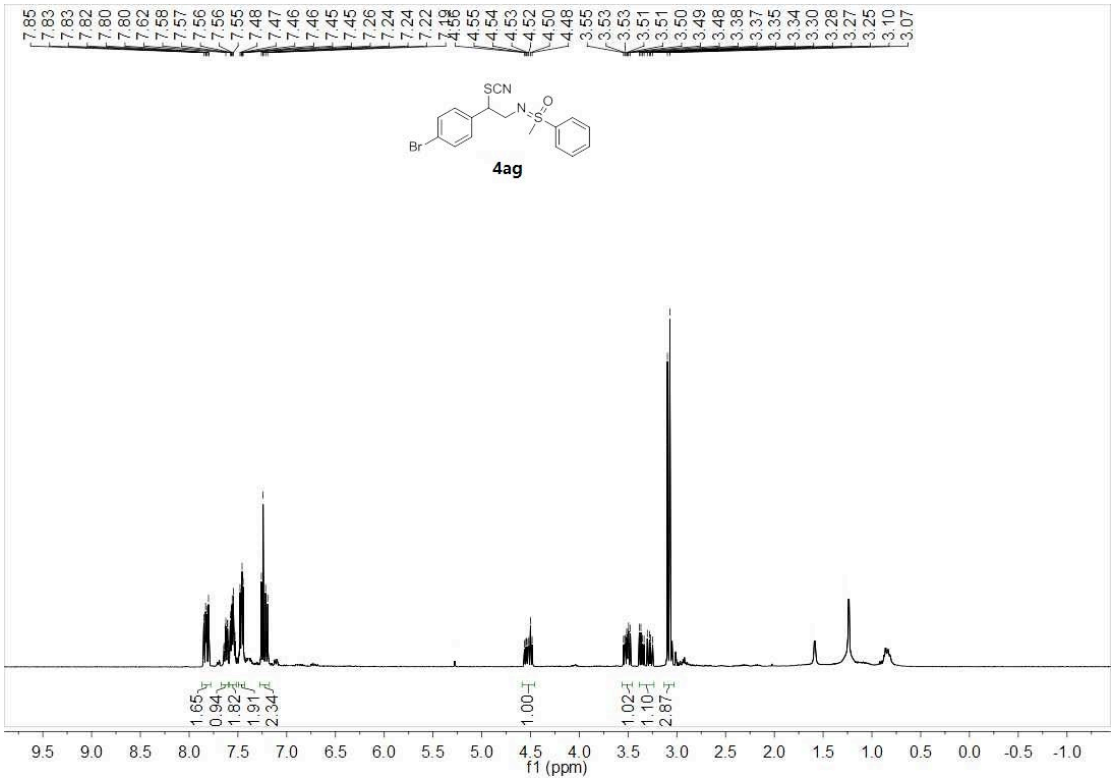
45.08
44.84
SCN
N
S
O
O
4af
f1 (ppm)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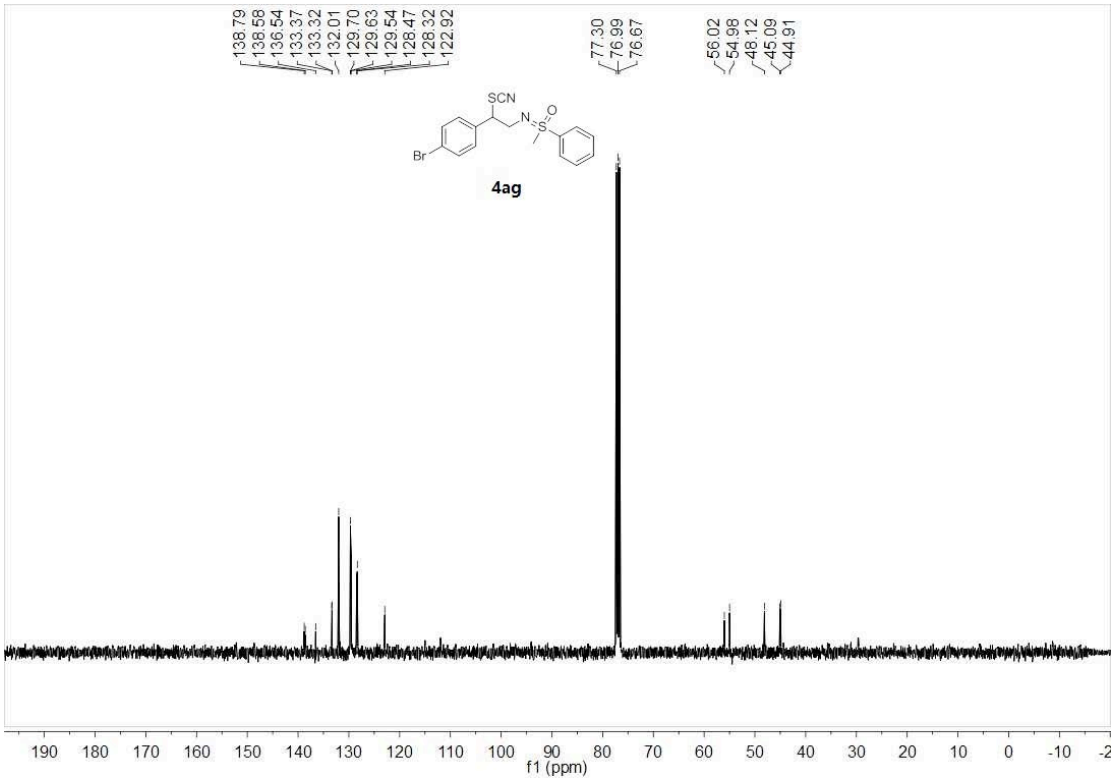
SCN
N
S
O
Br
4ag
1.65 0.94 1.82 1.91 2.34 1.00 1.02 1.10 2.87
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)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77.30 76.99 76.67
56.02 54.98 48.12 45.09 44.91
SCN
N
S
O
Br
4ag
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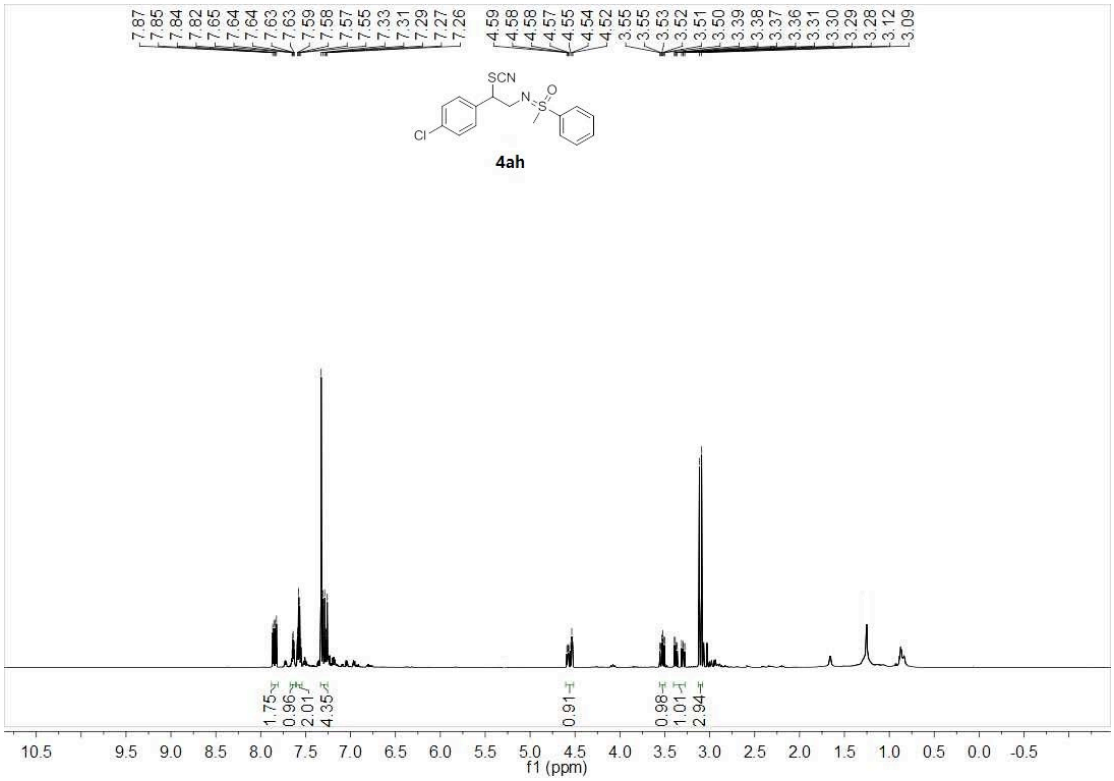
f1 (ppm)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SCN
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S
O
Cl
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0.98
1.01
2.94
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6.5
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5.0
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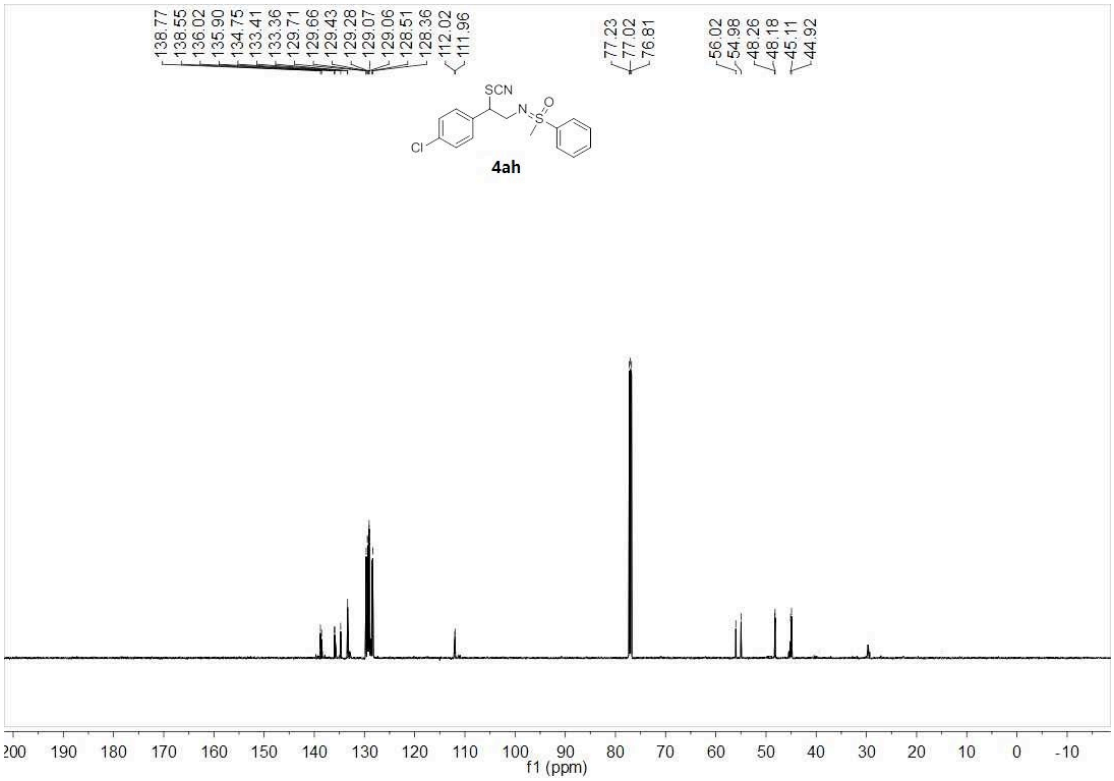
-0.5
f1 (ppm)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128.36
112.02
111.96
77.23
77.02
76.81
56.02
54.98
48.26
48.18
45.11
44.92
SCN
N
S
O
Cl
4ah
200
190
180
170
160
150
140
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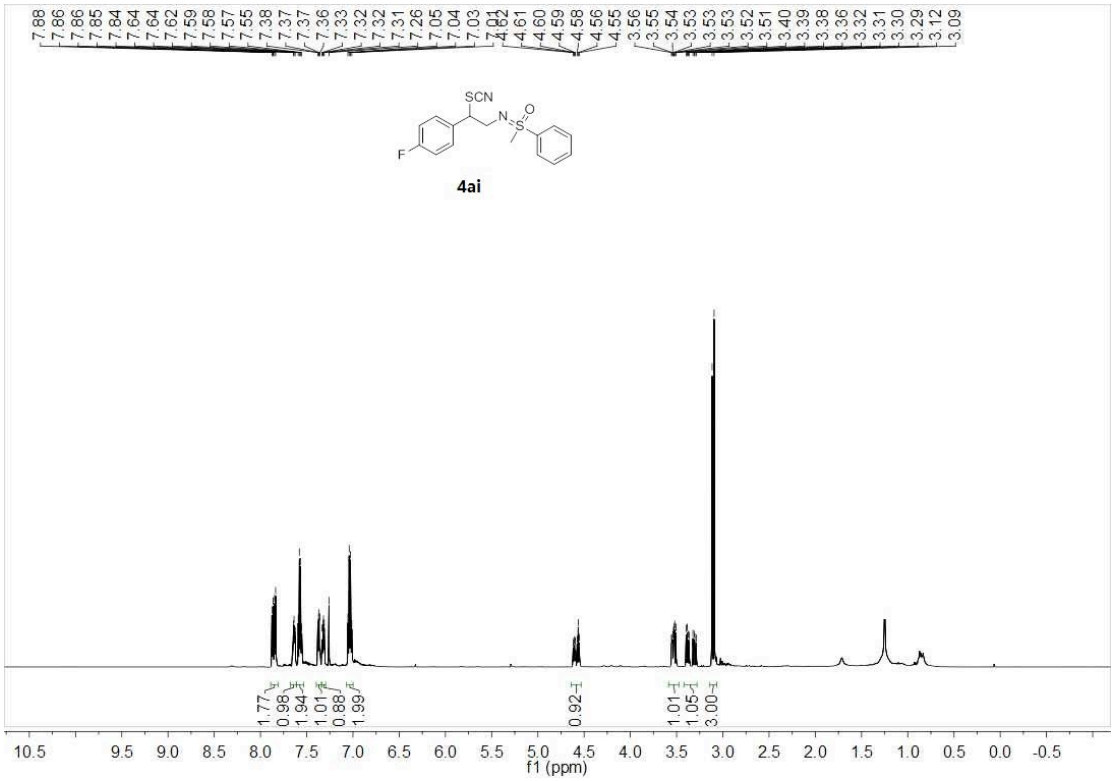
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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3.39
3.38
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3.31
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3.29
3.12
3.09
SCN
N
S
O
F
4ai
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0.88
1.99
0.92
1.01
1.05
3.00
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9.5
9.0
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8.0
7.5
7.0
6.5
6.0
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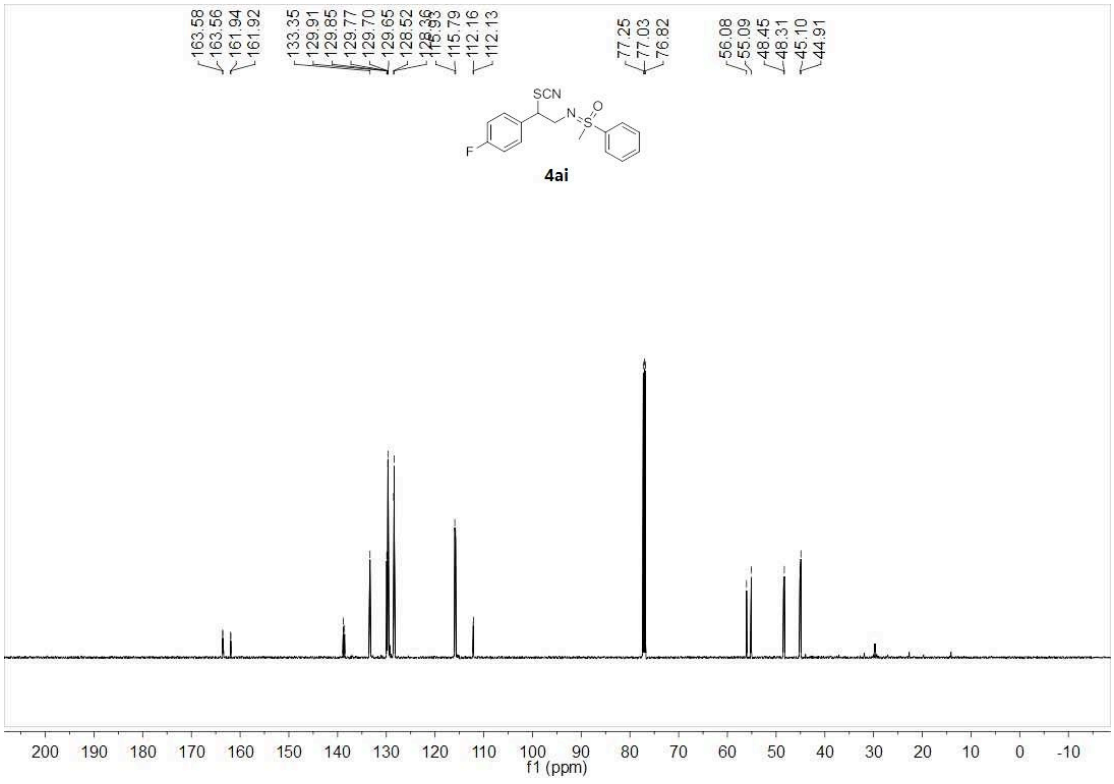
f1 (ppm)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112.16
112.13
77.25
77.03
76.82
56.08
55.09
48.45
48.31
45.10
44.91
SCN
N
S
O
F
4ai
200
190
180
170
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100
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40
30
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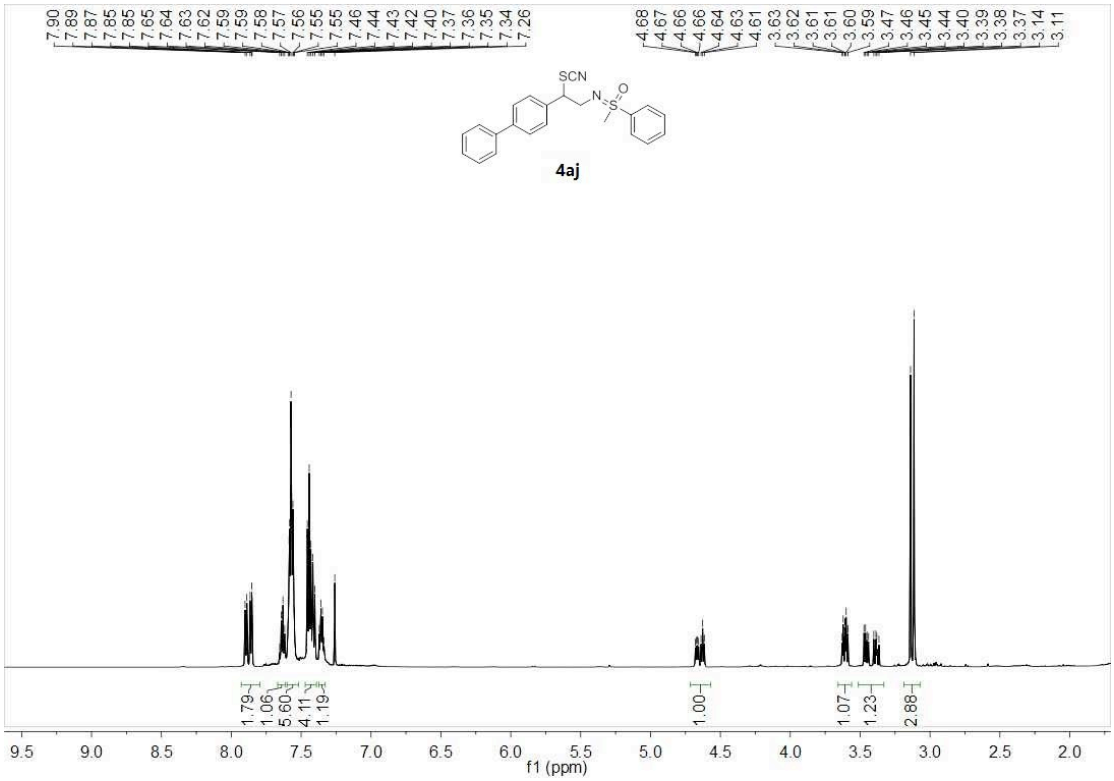
-10
f1 (ppm)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7.56
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7.55
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7.43
7.42
7.40
7.37
7.36
7.35
7.34
7.26
4.68
4.67
4.66
4.66
4.64
4.63
4.61
3.63
3.62
3.61
3.61
3.60
3.59
3.47
3.46
3.45
3.44
3.40
3.39
3.38
3.37
3.14
3.11
SCN
N
S
O
4aj
1.79
1.06
5.60
4.11
1.19
1.00
1.07
1.23
2.88
9.5
9.0
8.5
8.0
7.5
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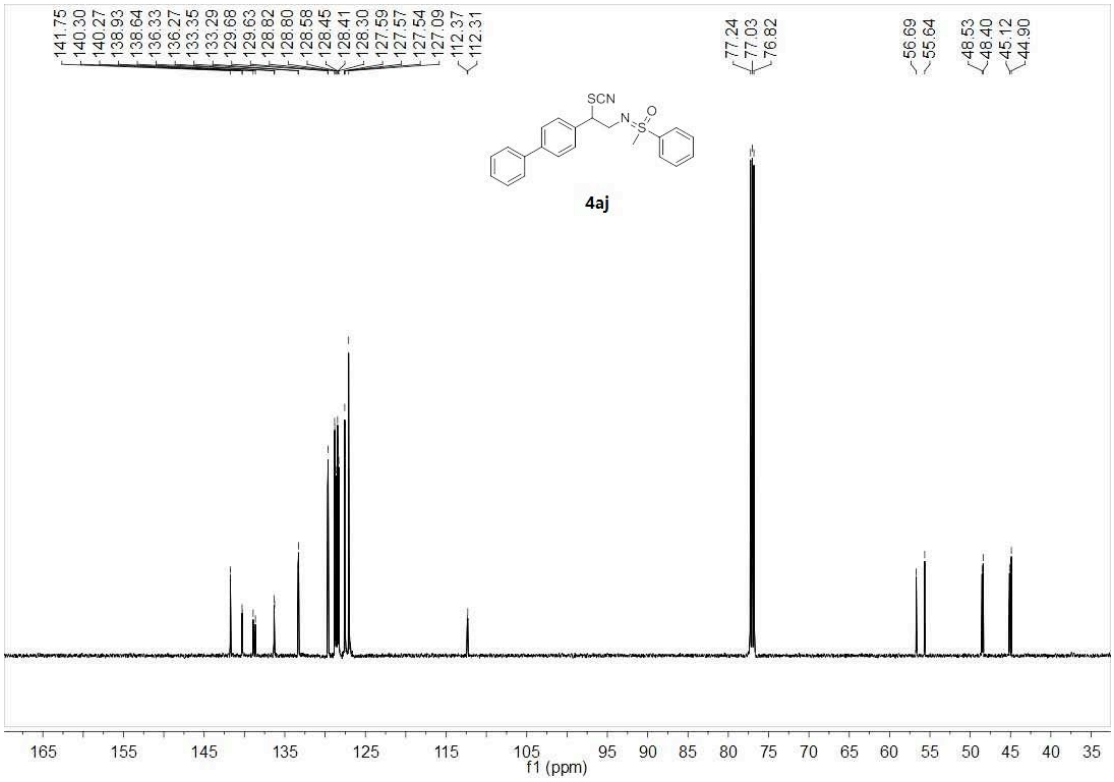
2.5
2.0
f1 (ppm)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127.57
127.54
127.09
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112.31
77.24
77.03
76.82
56.69
55.64
48.53
48.40
45.12
44.90
SCN
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S
O
4aj
165
155
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80
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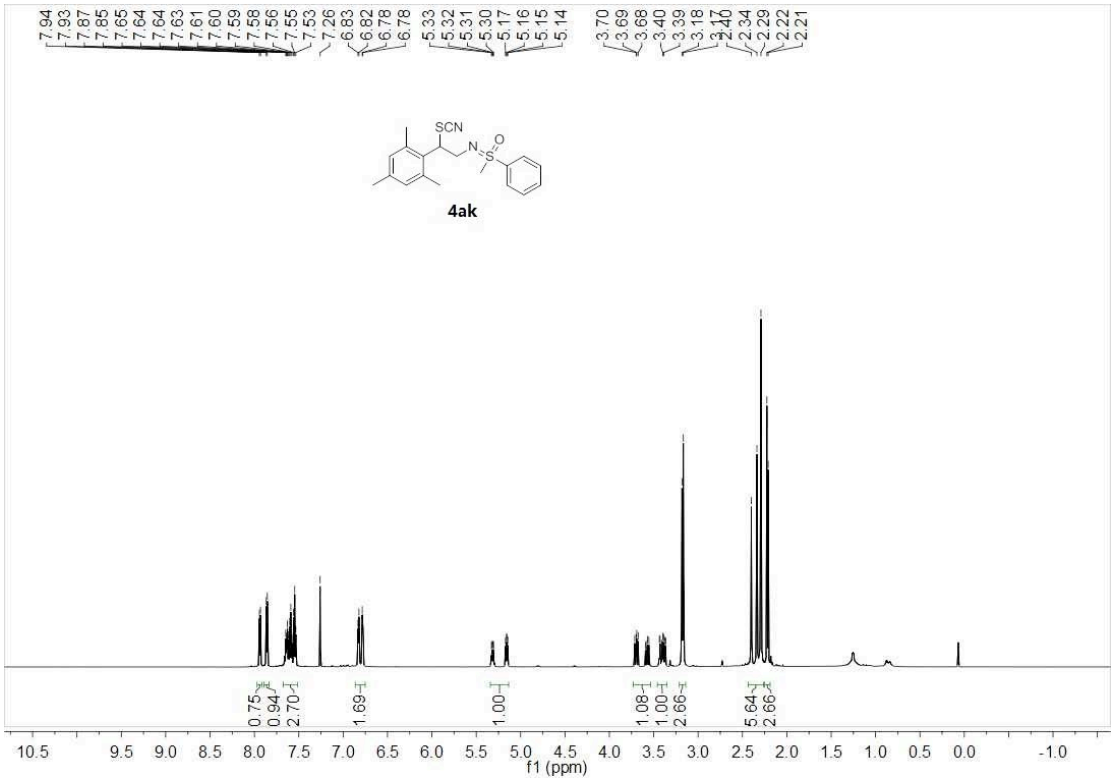
f1 (ppm)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7.56
7.55
7.53
7.26
6.83
6.82
6.78
6.78
5.33
5.32
5.31
5.30
5.17
5.16
5.15
5.14
3.70
3.69
3.68
3.40
3.39
3.18
3.17
2.40
2.34
2.29
2.22
2.21
SCN
N
S
O
4ak
0.75
0.94
2.70
1.69
1.00
1.08
1.00
2.66
5.64
2.66
10.5
9.5
9.0
8.5
8.0
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6.5
6.0
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5.0
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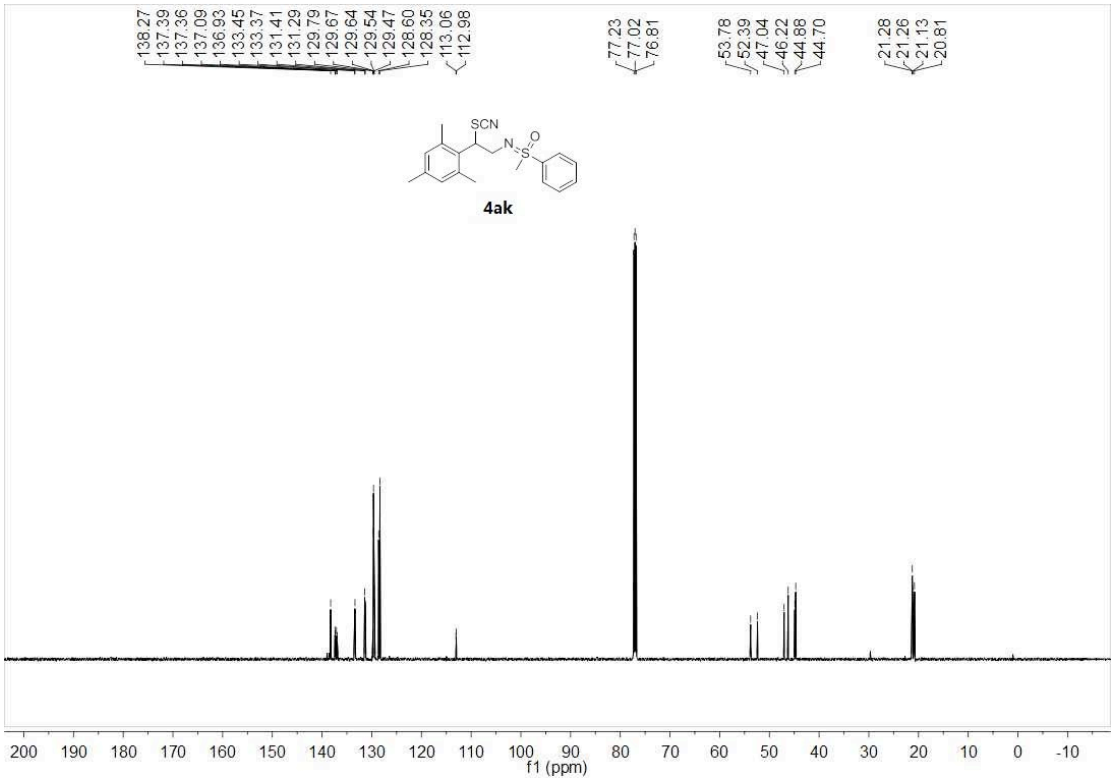
f1 (ppm)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128.60
128.35
113.06
112.98
77.23
77.02
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53.78
52.39
47.04
46.22
44.88
44.70
21.28
21.26
21.13
20.81
SCN
N
S
O
4ak
200
190
180
170
160
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120
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100
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80
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40
30
20
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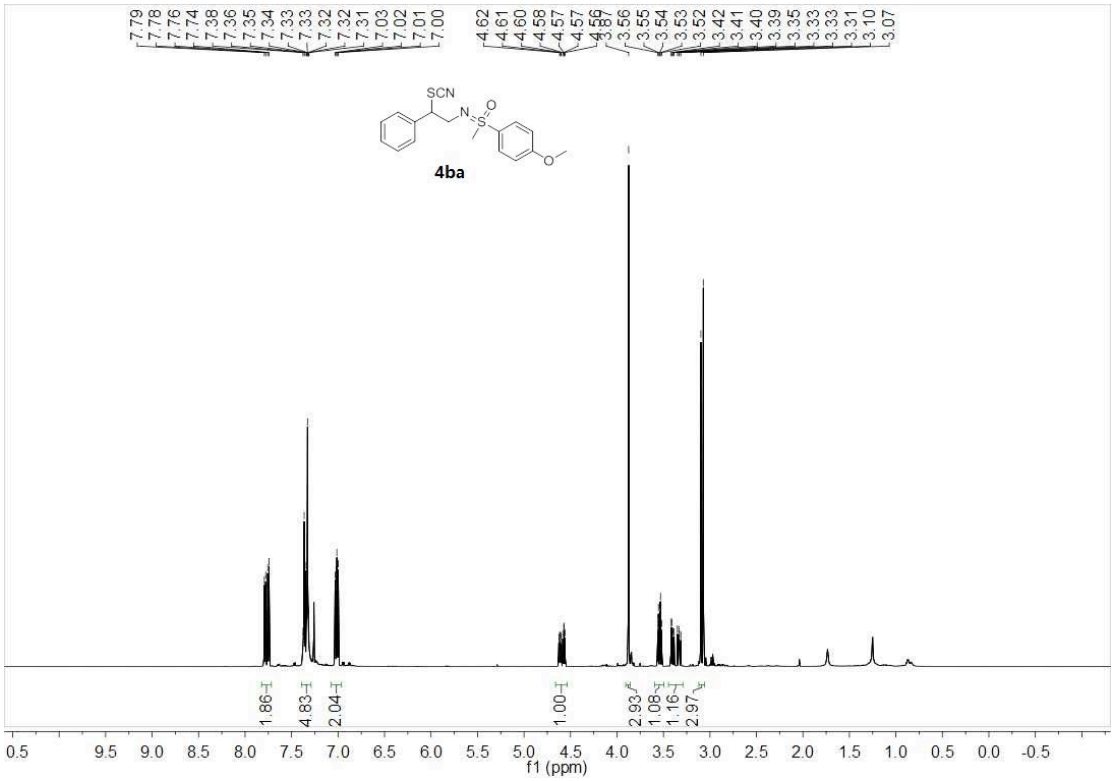
0
-10
f1 (ppm)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7.00
4.62
4.61
4.60
4.58
4.57
4.57
4.56
3.87
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3.55
3.54
3.53
3.52
3.42
3.41
3.40
3.39
3.35
3.33
3.33
3.31
3.10
3.07
SCN
N
S
O
O
4ba
1.86
4.83
2.04
1.00
2.93
1.08
1.16
2.97
0.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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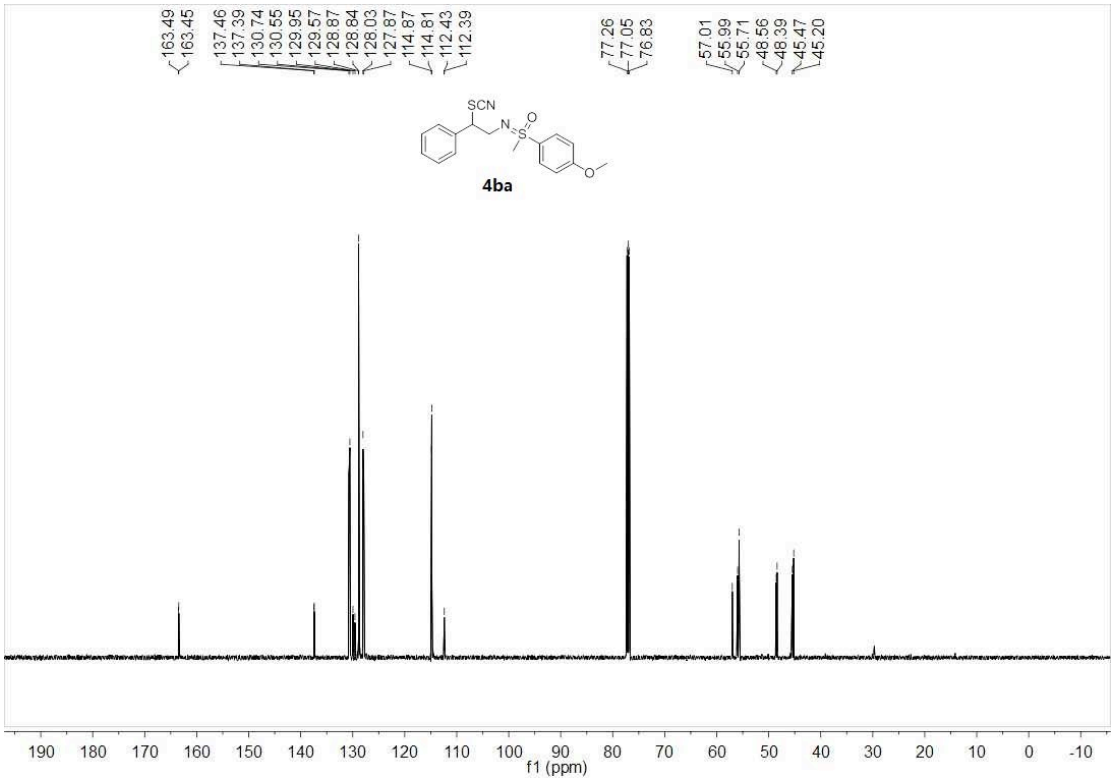
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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127.87
114.87
114.81
112.43
112.39
77.26
77.05
76.83
57.01
55.99
55.71
48.56
48.39
45.47
45.20
SCN
N
S
O
O
4ba
190
180
170
160
150
140
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120
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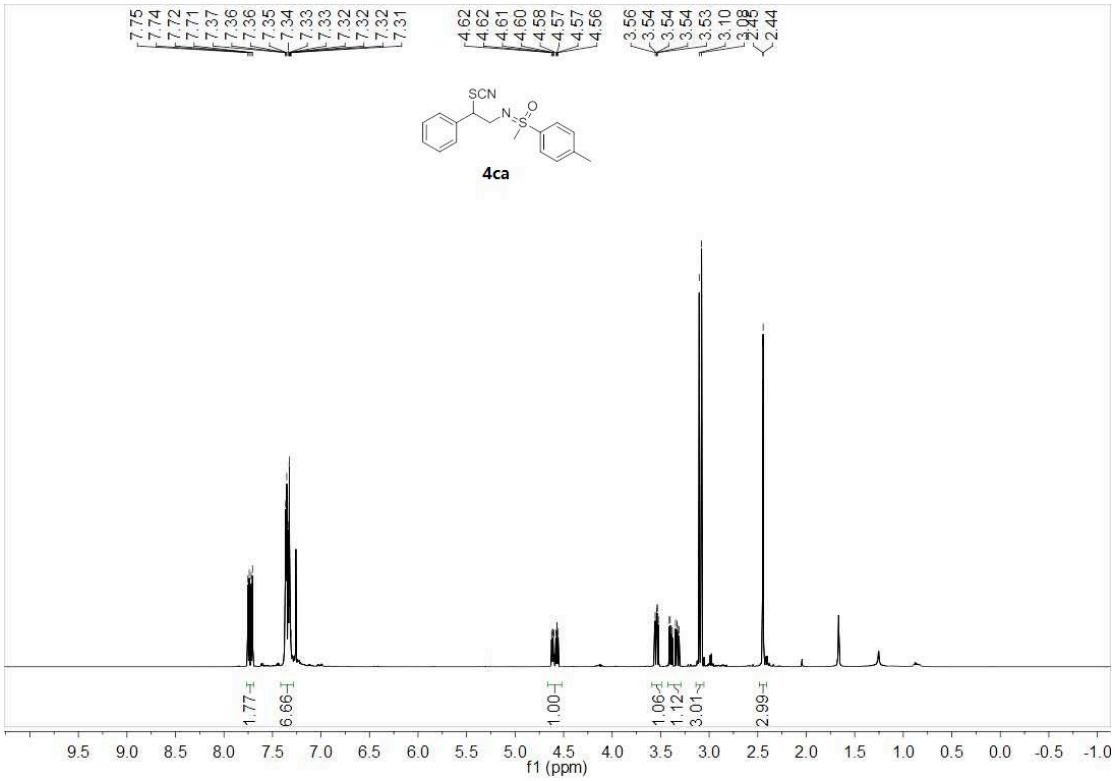
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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4.60
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4.57
4.56
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3.53
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SCN
4ca
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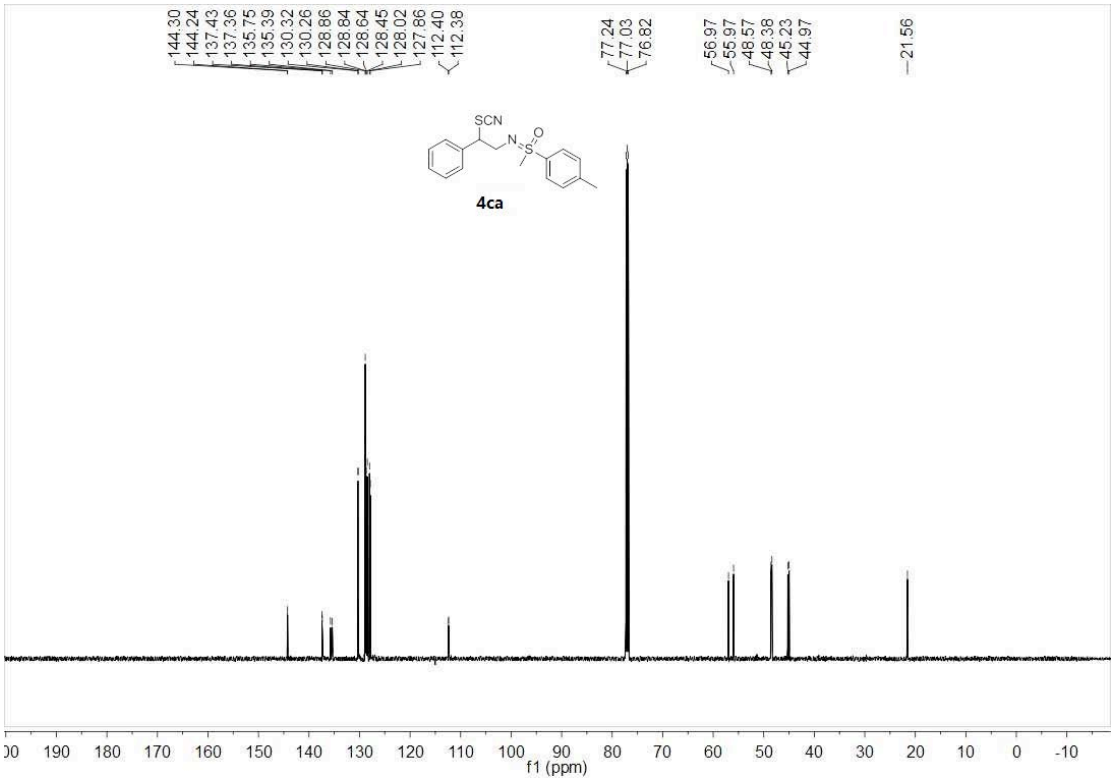
1.12
3.01
2.99
f1 (ppm)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128.84
128.64
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127.86
112.40
112.38
77.24
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55.97
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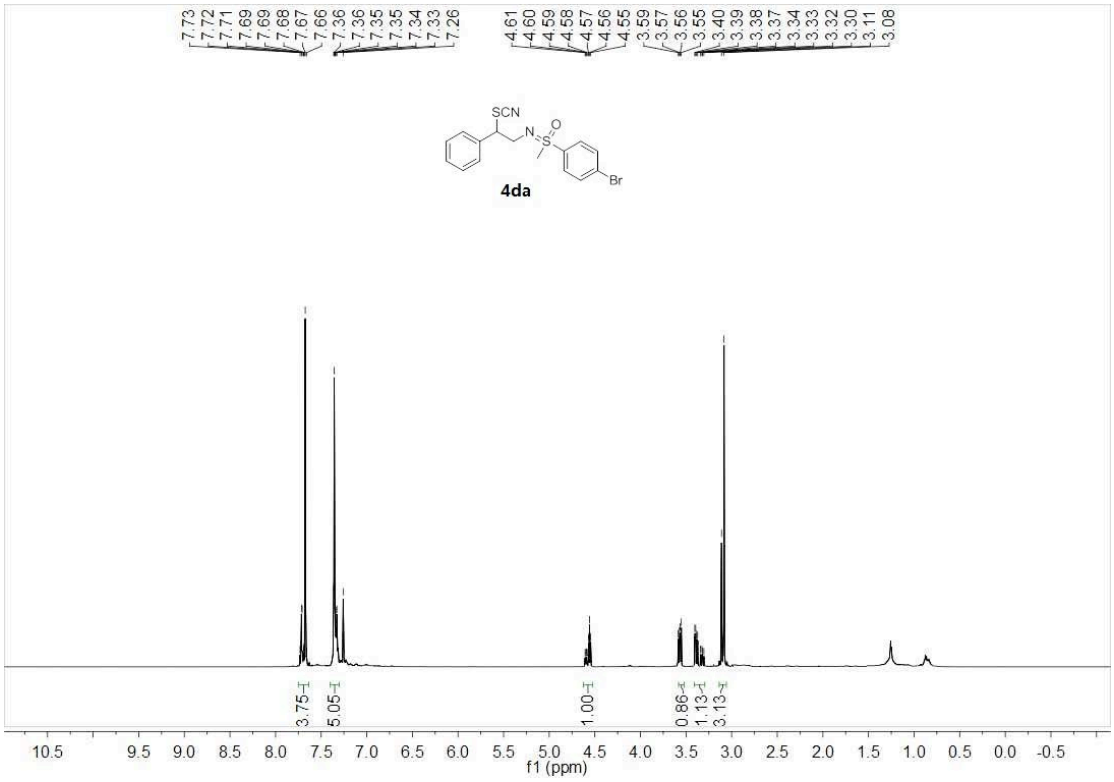
48.38
45.23
44.97
21.56
SCN
4ca
f1 (ppm)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7.34
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4.60
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4.58
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4.56
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3.59
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3.40
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3.38
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3.34
3.33
3.32
3.30
3.11
3.08
SCN
N
S
O
Br
4da
3.75
5.05
1.00
0.86
1.13
3.13
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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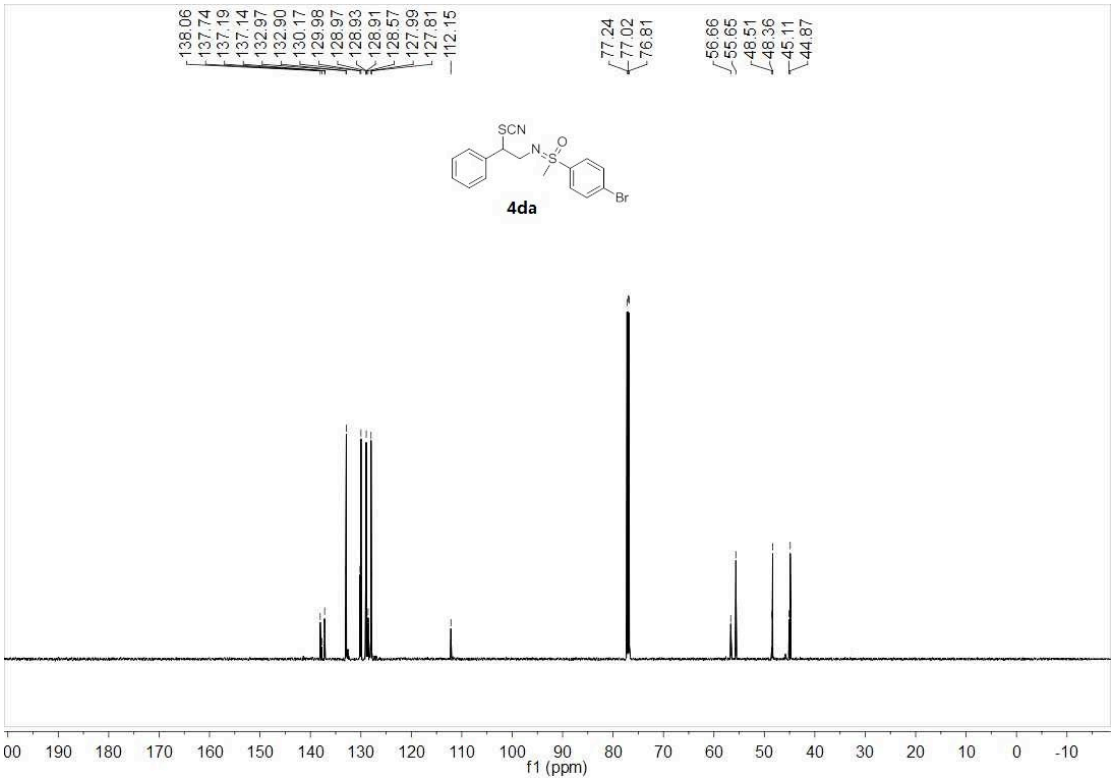
0.5
0.0
-0.5
f1 (ppm)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128.57
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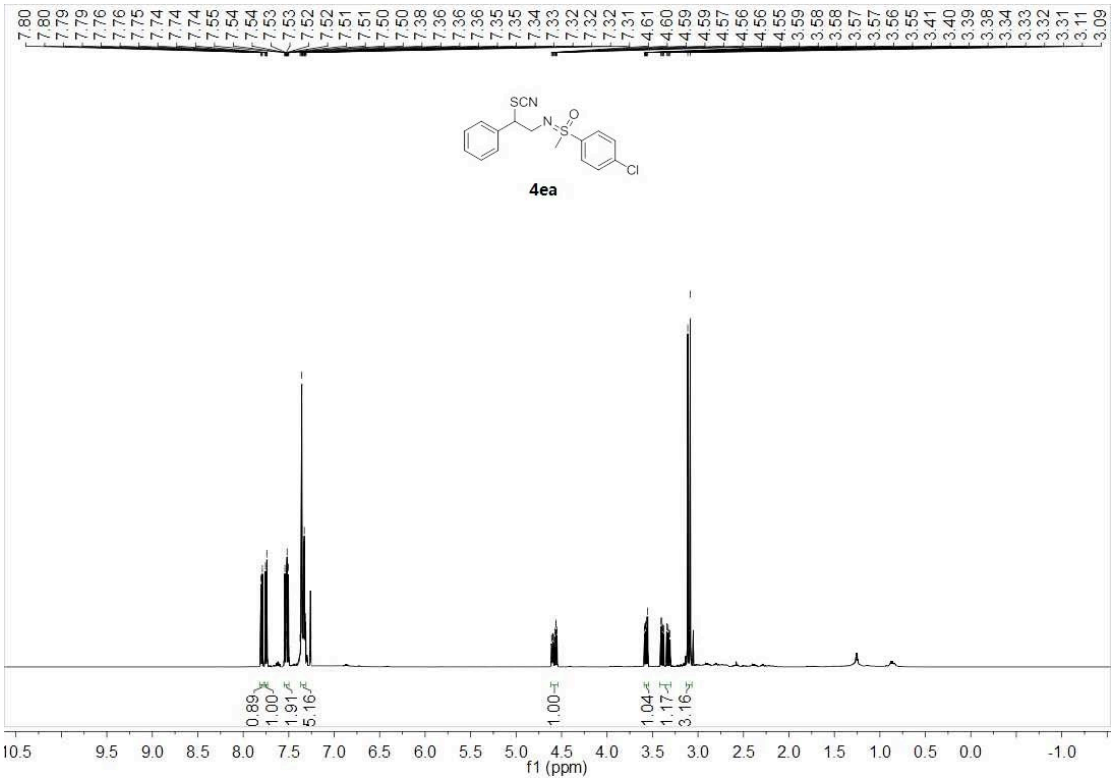
127.81
112.15
77.24
77.02
76.81
56.66
55.65
48.51
48.36
45.11
44.87
SCN
N
S
O
Br
4da
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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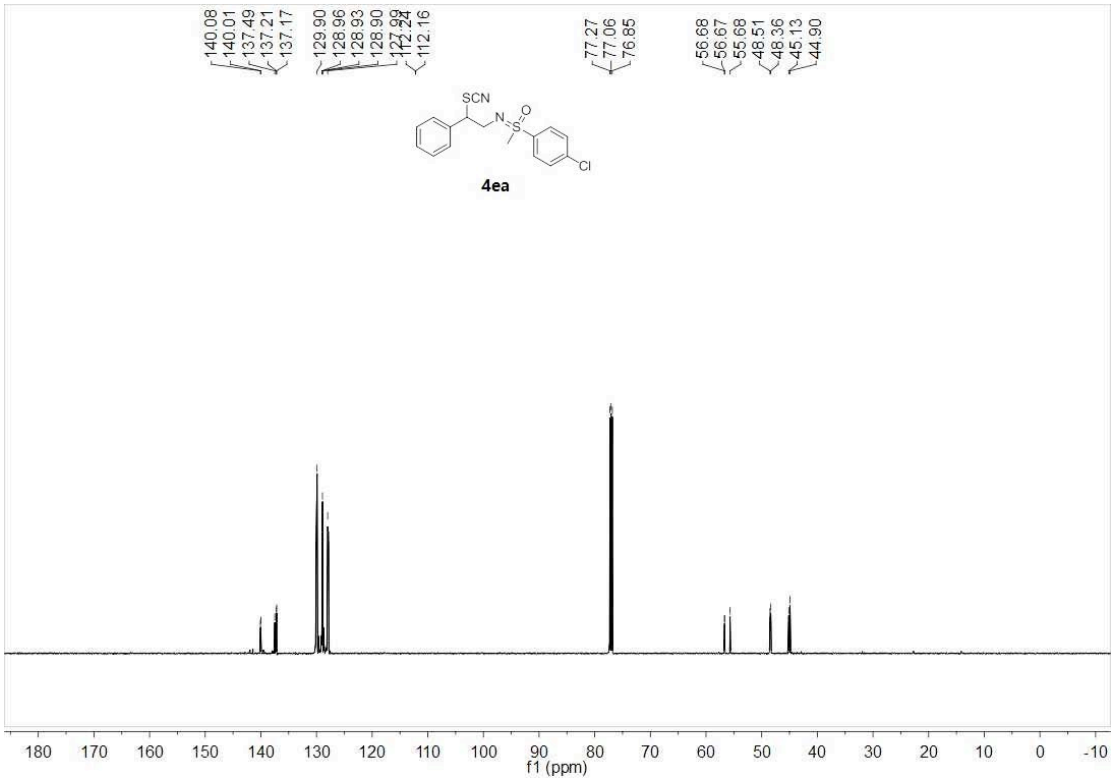
SCN
N
S
O
Cl
4ea
0.89 1.00 1.91 5.16 1.00 1.04 1.17 3.16
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)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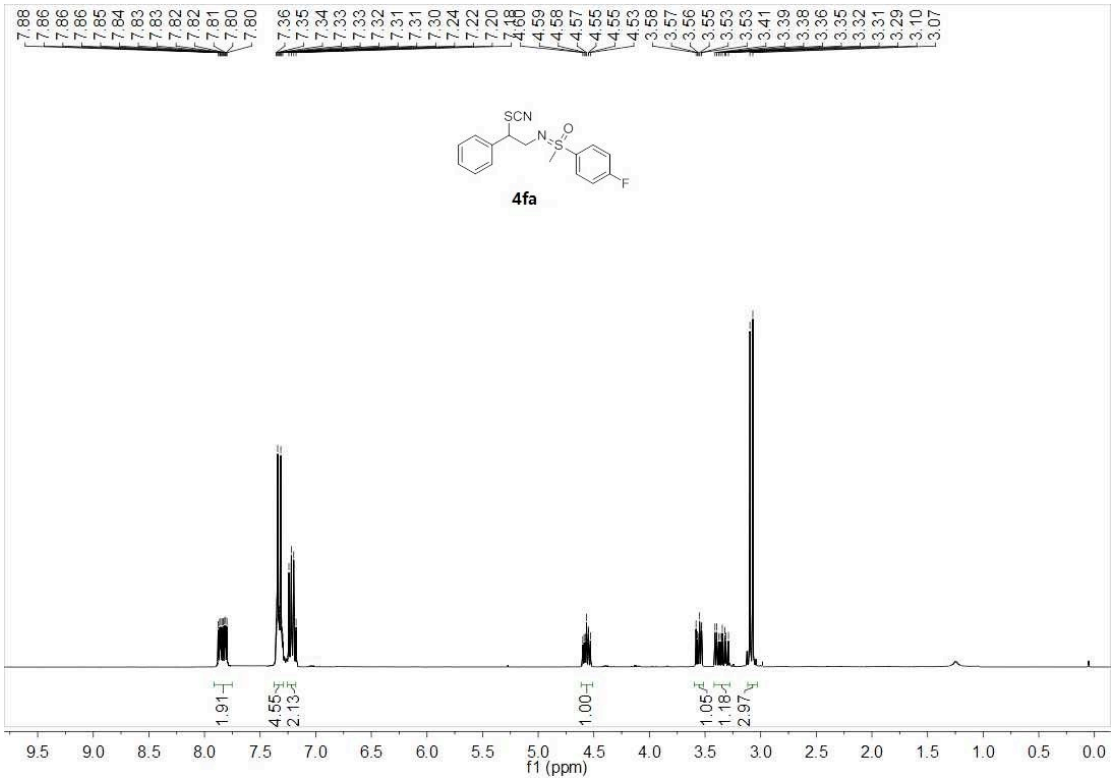
SCN
N
S
O
Cl
4ea
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.80
7.80
7.36
7.35
7.34
7.33
7.33
7.32
7.31
7.31
7.30
7.24
7.22
7.20
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4.58
4.57
4.55
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3.57
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3.55
3.53
3.53
3.41
3.39
3.38
3.36
3.35
3.32
3.31
3.29
3.10
3.07
SCN
N
S
O
F
4fa
1.91
4.55
2.13
1.00
1.05
1.18
2.97
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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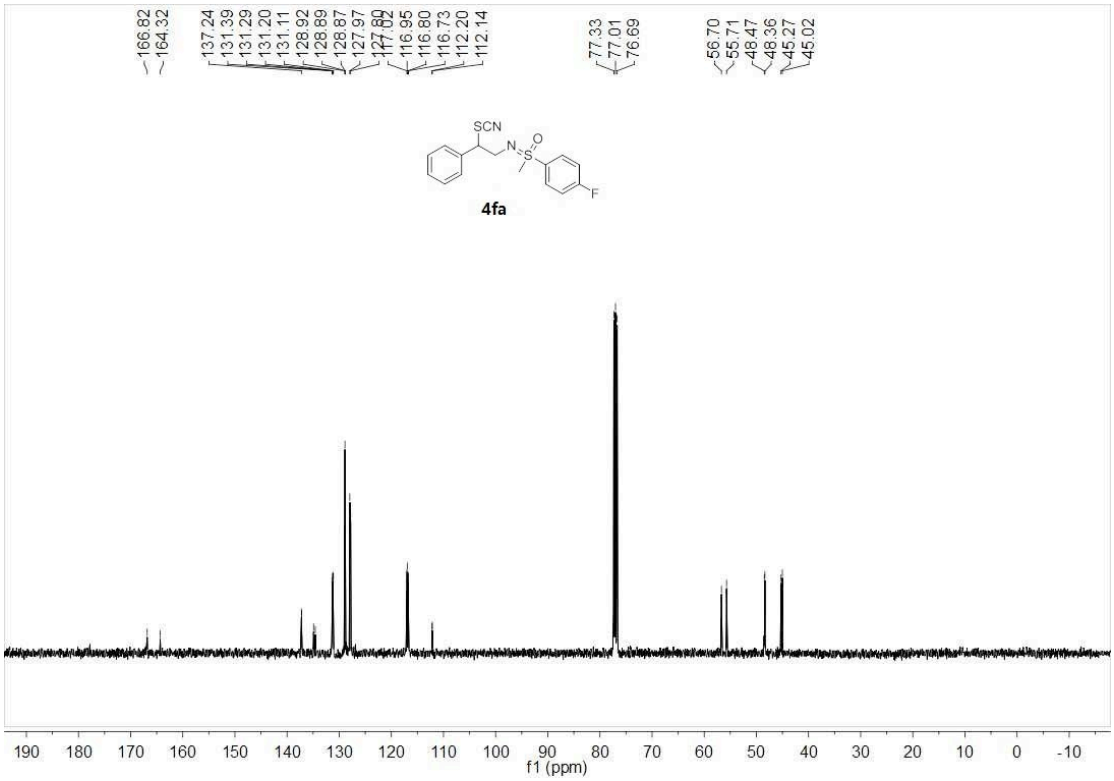
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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128.87
127.97
127.80
127.02
116.95
116.80
116.73
112.20
112.14
77.33
77.01
76.69
56.70
55.71
48.47
48.36
45.27
45.02
SCN
N
S
O
F
4fa
190
180
170
160
150
140
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120
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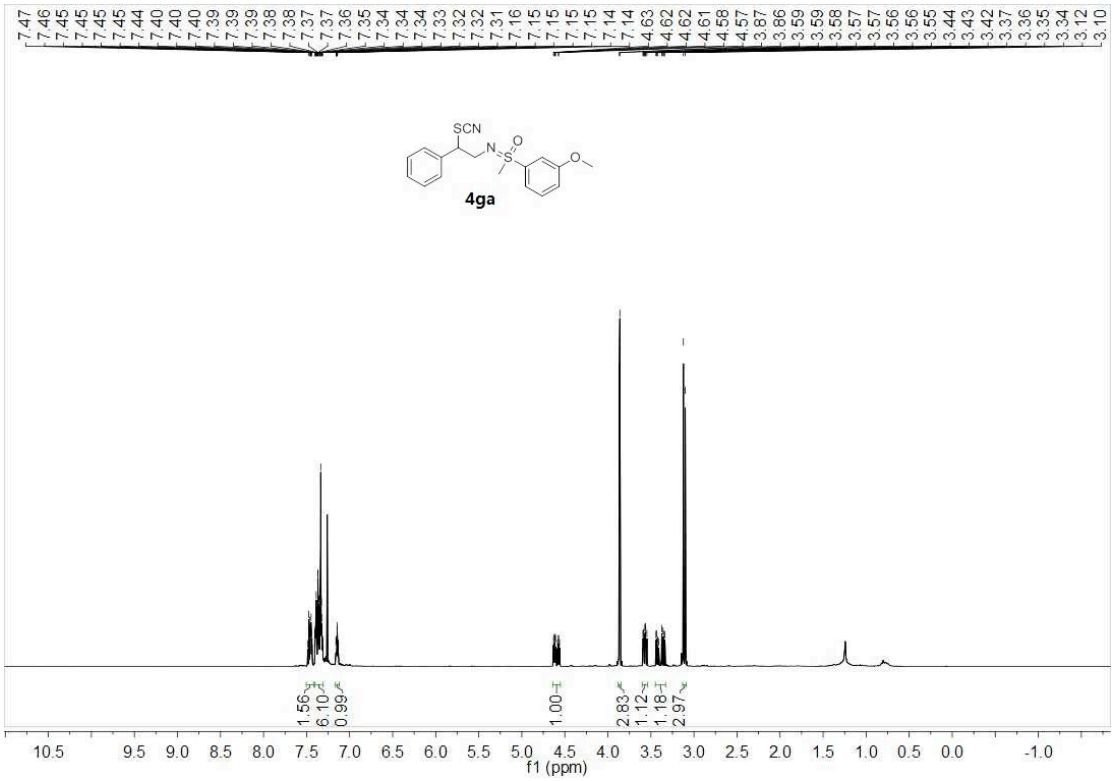
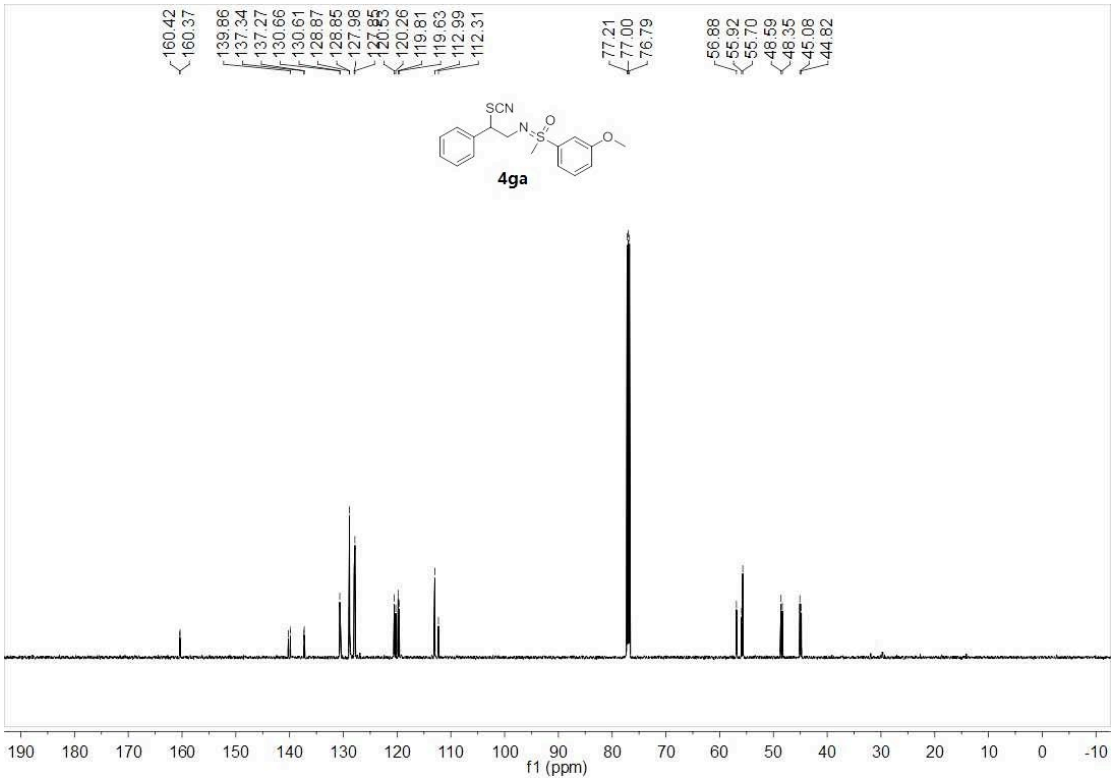
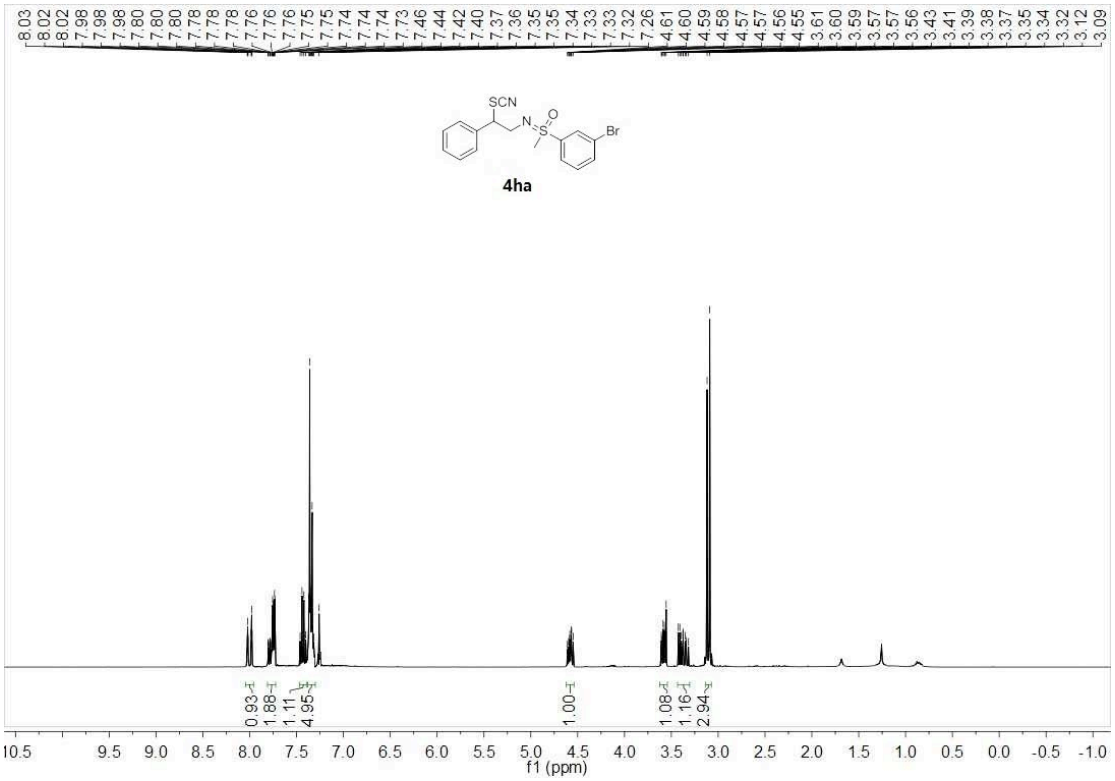
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


4ga
f1 (ppm)


4ga
f1 (ppm)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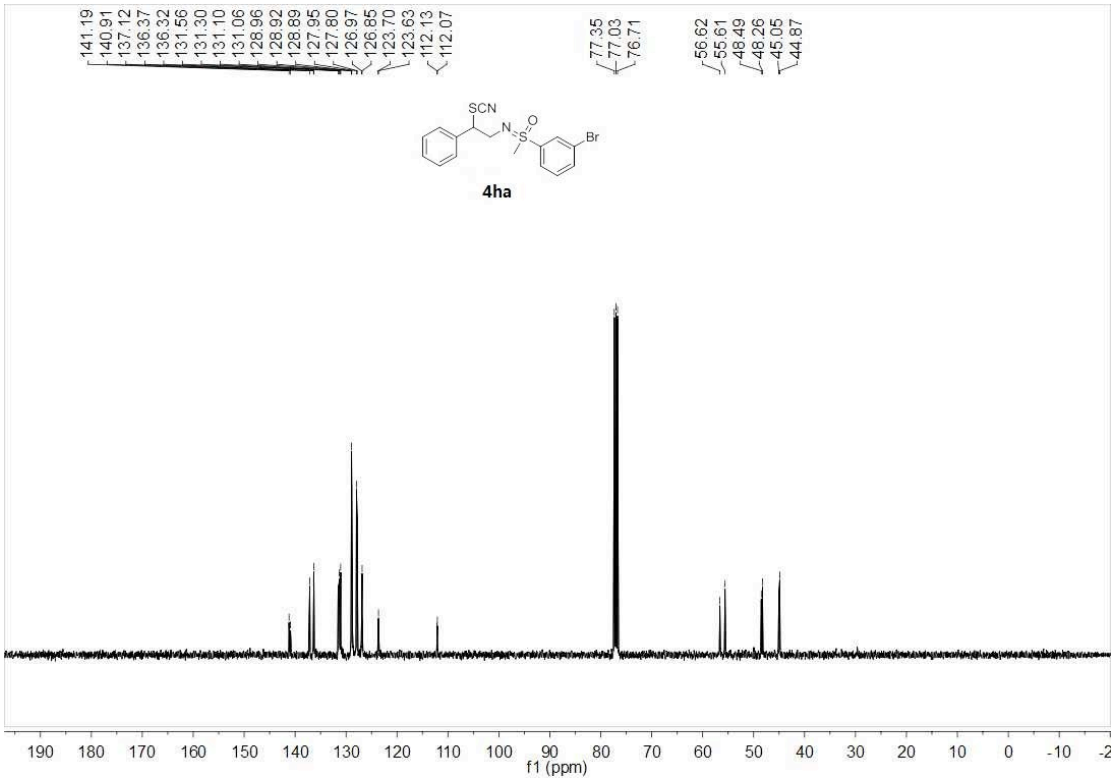
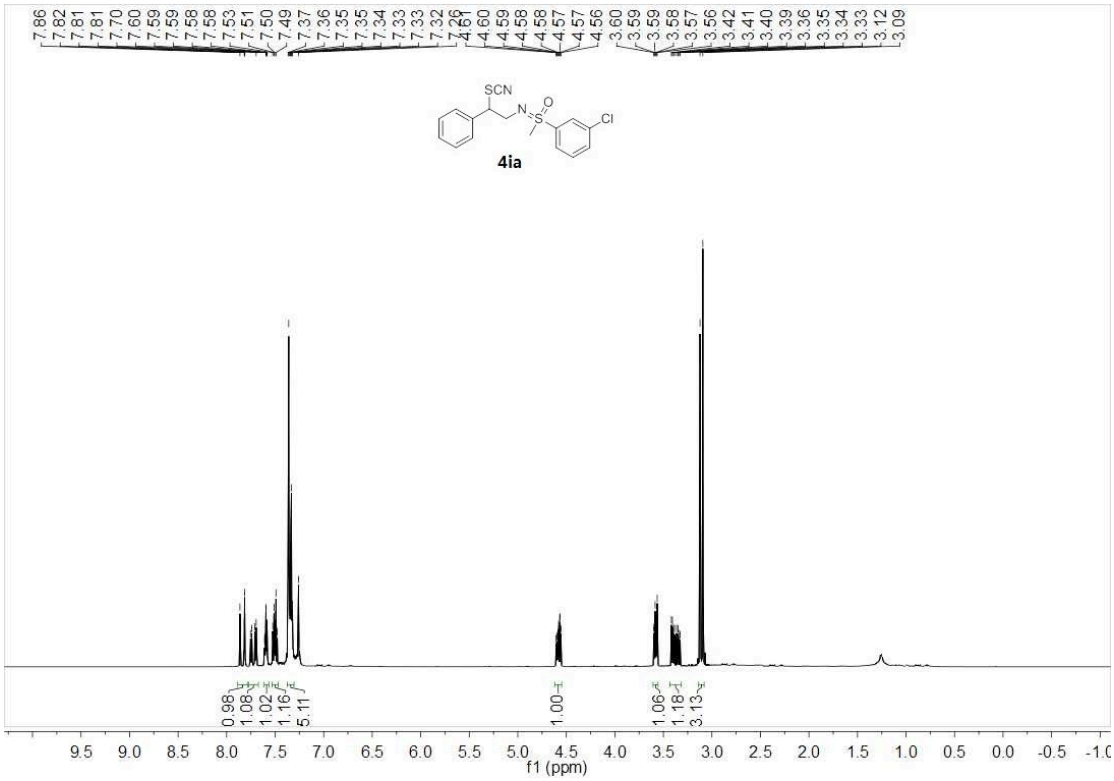
SCN
N
S
O
Br
4ha
0.93
1.88
1.11
4.95
1.00
1.08
1.16
2.94
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


141.19 140.91 137.12 136.37 136.32 131.56 131.30 131.10 131.06 128.96 128.92 128.89 127.95 127.80 126.97 126.85 123.70 123.63 112.13 112.07
77.35 77.03 76.71
56.62 55.61 48.49 48.26 45.05 44.87
SCN
N
S
O
Br
4ha
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -2
f1 (ppm)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3.39
3.36
3.35
3.34
3.33
3.12
3.09
SCN
N
O
S
Cl
4ia
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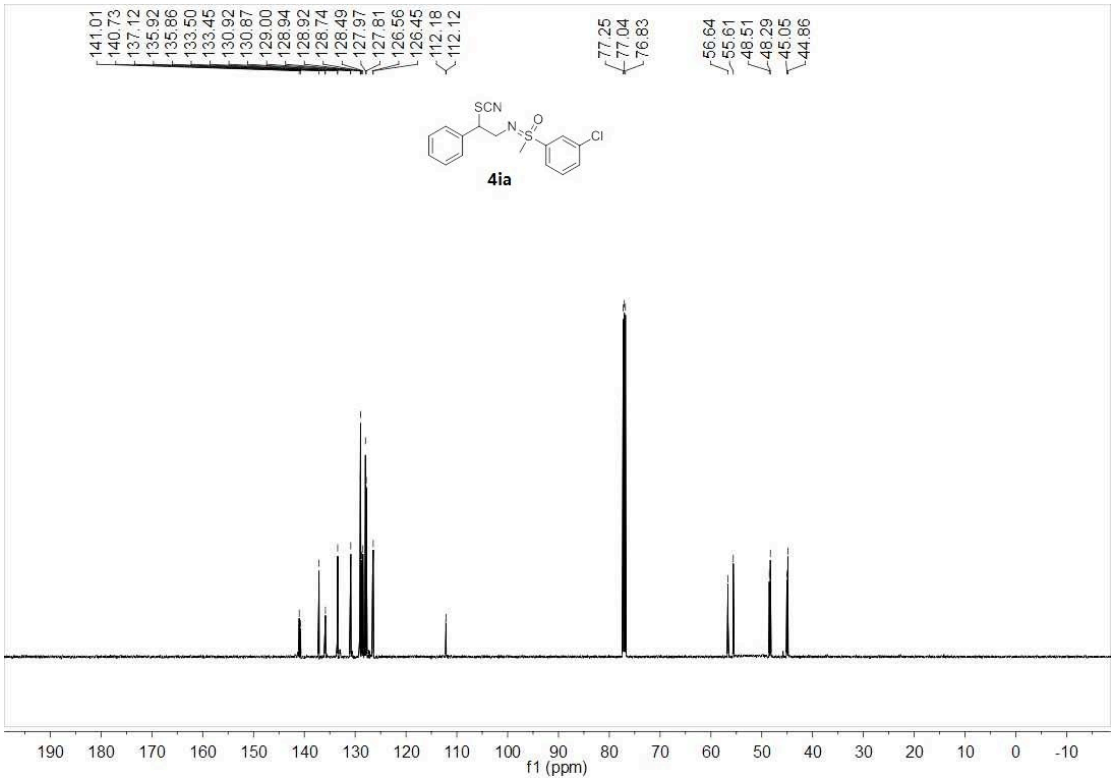
1.08
1.02
1.16
5.11
1.00
1.06
1.18
3.13
f1 (ppm)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135.92
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133.50
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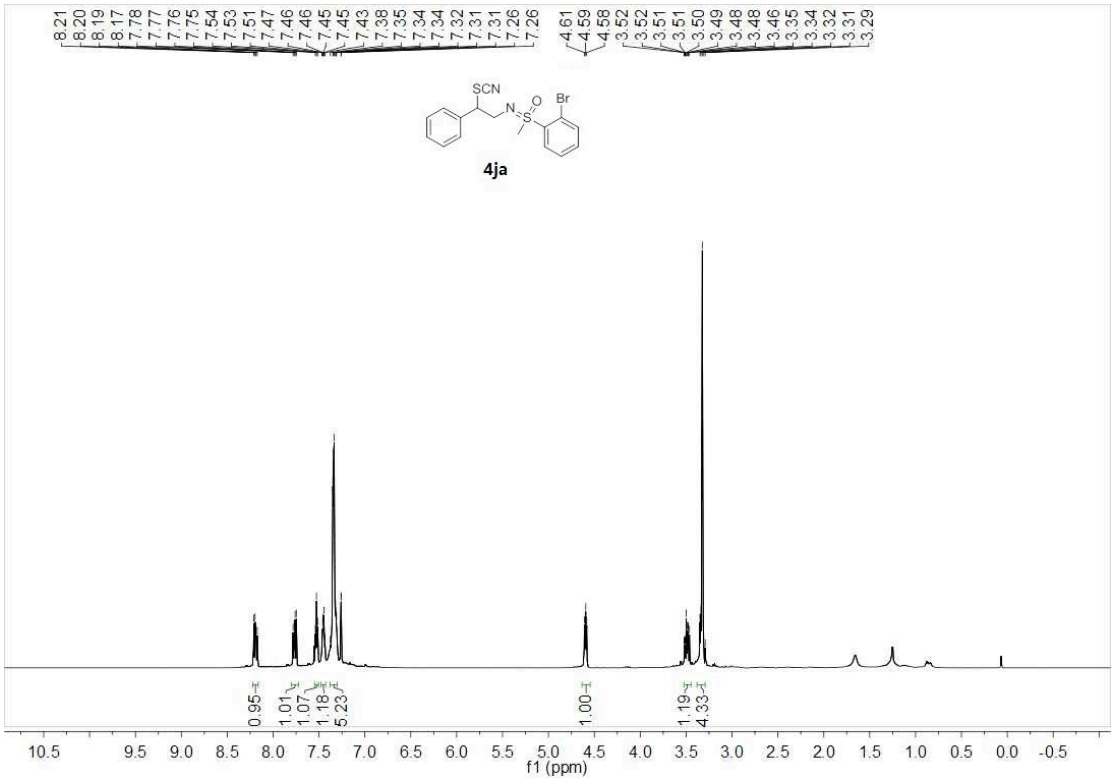
130.92
130.87
129.00
128.94
128.92
128.74
128.49
127.97
127.81
126.56
126.45
112.18
112.12
77.25
77.04
76.83
56.64
55.61
48.51
48.29
45.05
44.86
SCN
N
O
S
Cl
4ia
f1 (ppm)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8.19
8.17
7.78
7.77
7.76
7.75
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7.46
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7.45
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7.31
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3.50
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3.48
3.46
3.35
3.34
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3.31
3.29
SCN
N
S
O
Br
4ja
0.95
1.01
1.07
1.18
5.23
1.00
1.19
4.33
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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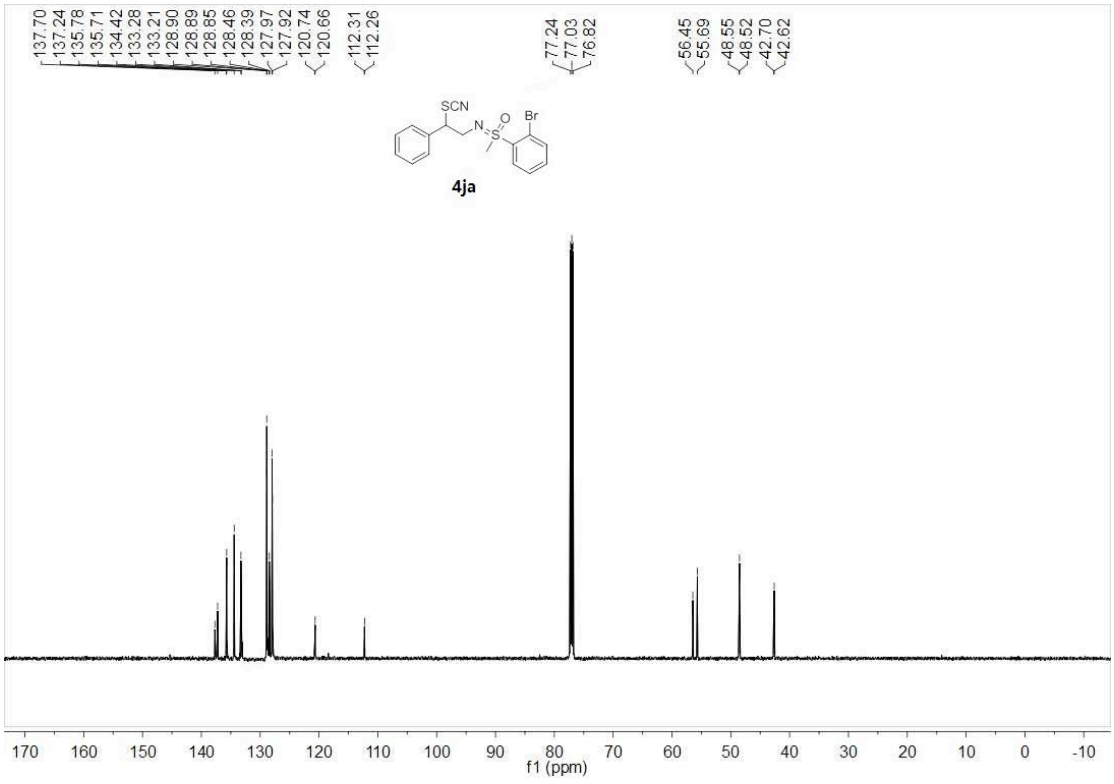
-0.5
f1 (ppm)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128.46
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127.92
120.74
120.66
112.31
112.26
77.24
77.03
76.82
56.45
55.69
48.55
48.52
42.70
42.62
SCN
N
S
O
Br
4ja
170
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120
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100
90
80
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60
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40
30
20
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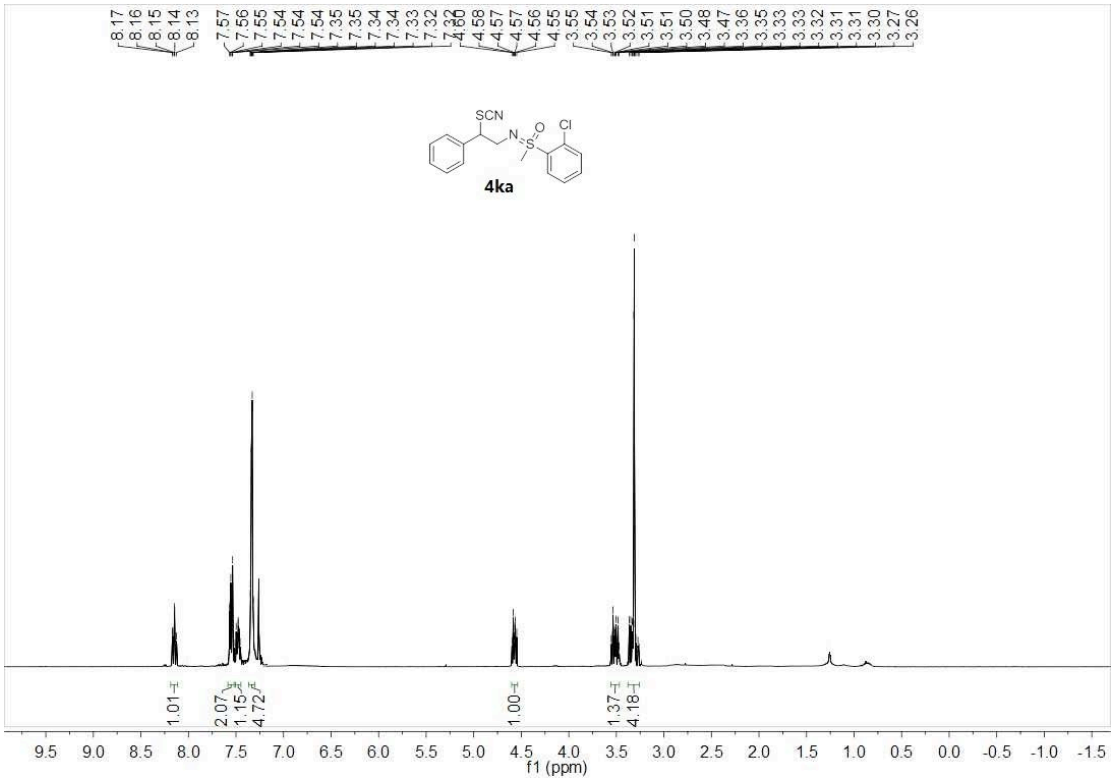
0
-10
f1 (ppm)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7.55
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7.35
7.34
7.34
7.33
7.32
4.60
4.58
4.57
4.57
4.56
4.55
3.55
3.54
3.53
3.52
3.51
3.51
3.50
3.48
3.47
3.36
3.35
3.33
3.33
3.32
3.31
3.31
3.30
3.27
3.26
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S
O
Cl
4ka
1.01
2.07
1.15
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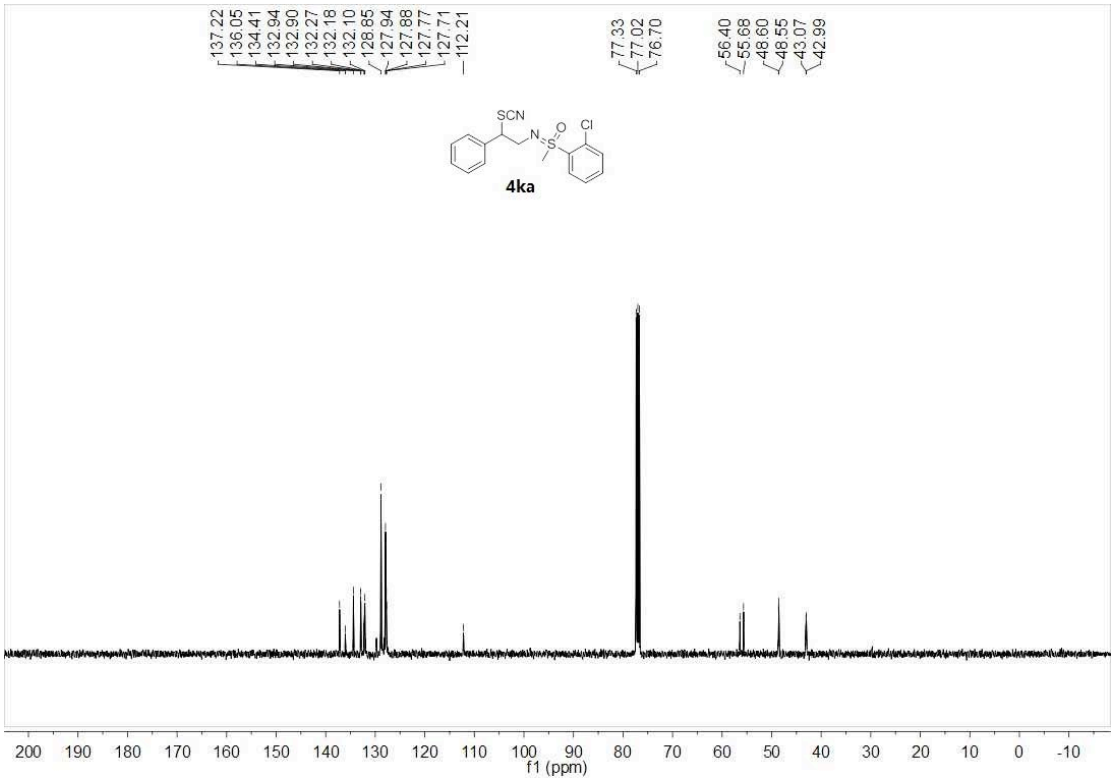
1.00
1.37
4.18
f1 (ppm)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127.94
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127.77
127.71
112.21
77.33
77.02
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43.07
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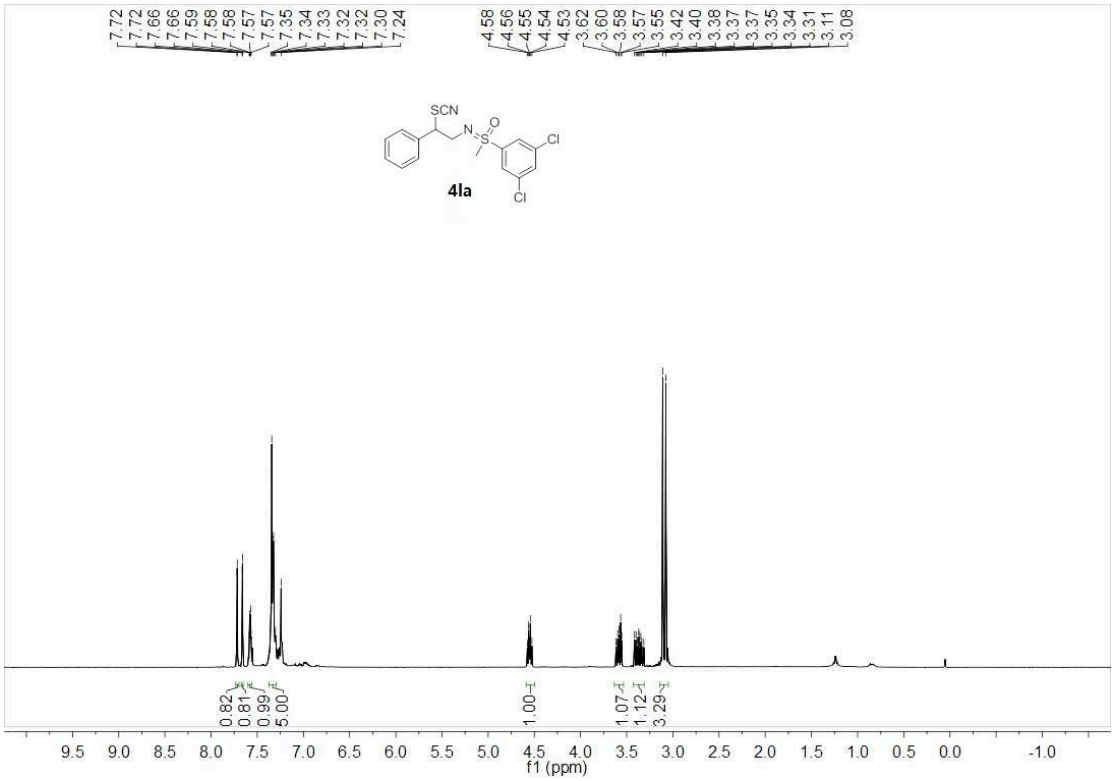
SCN
N
S
O
Cl
4ka
f1 (ppm)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7.57
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7.34
7.33
7.32
7.32
7.30
7.24
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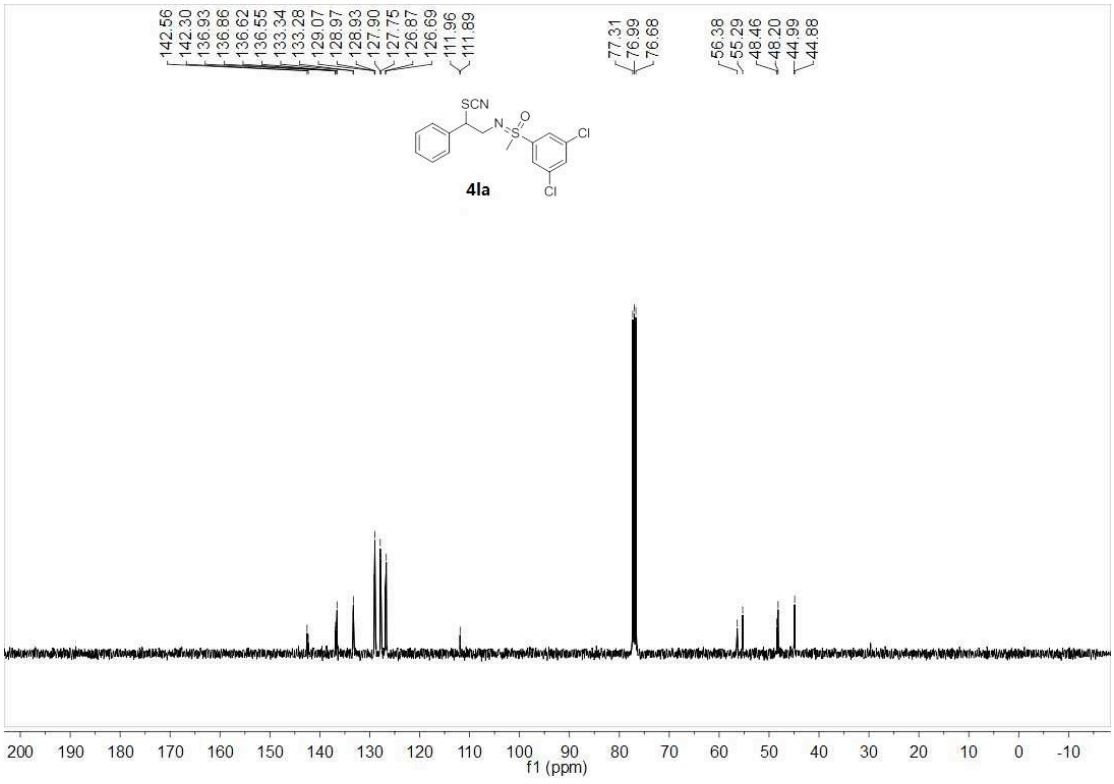
4.56
4.55
4.54
4.53
3.62
3.60
3.58
3.57
3.55
3.42
3.40
3.38
3.37
3.37
3.35
3.34
3.31
3.11
3.08
SCN
N
S
O
Cl
Cl
4la
0.82
0.81
0.99
5.00
1.00
1.07
1.12
3.29
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)


142.56
142.30
136.93
136.86
136.62
136.55
133.34
133.28
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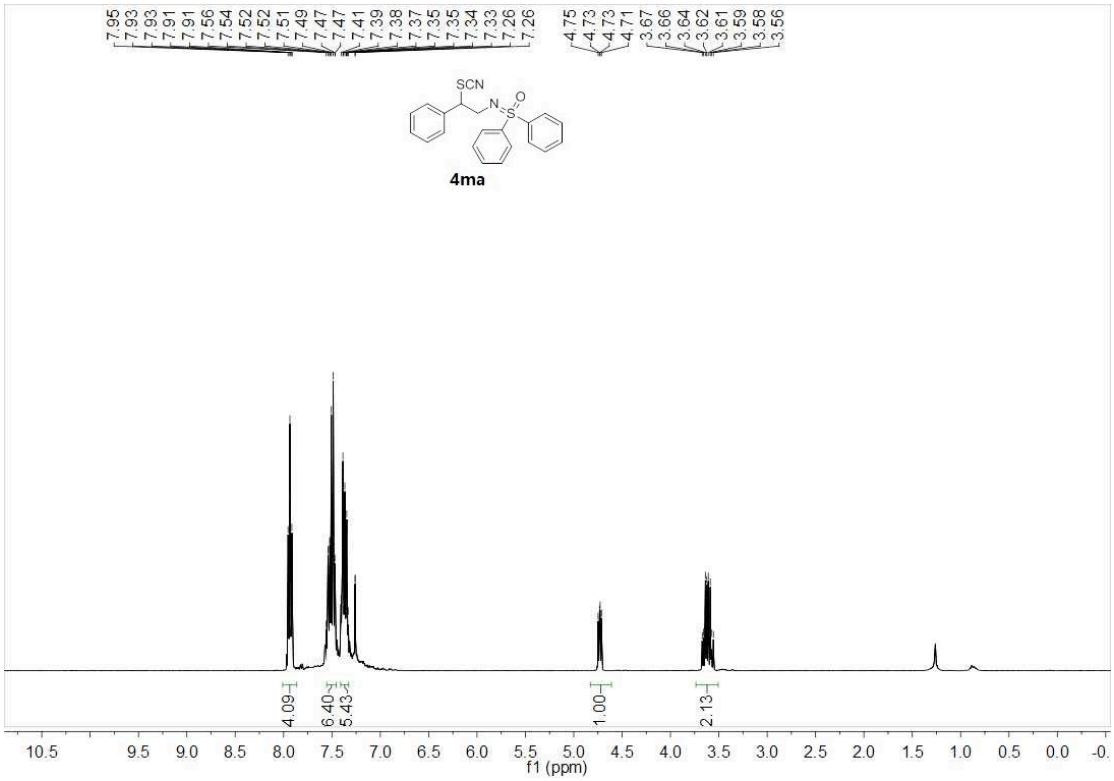
128.97
128.93
127.90
127.75
126.87
126.69
111.96
111.89
77.31
76.99
76.68
56.38
55.29
48.46
48.20
44.99
44.88
SCN
N
S
O
Cl
Cl
4la
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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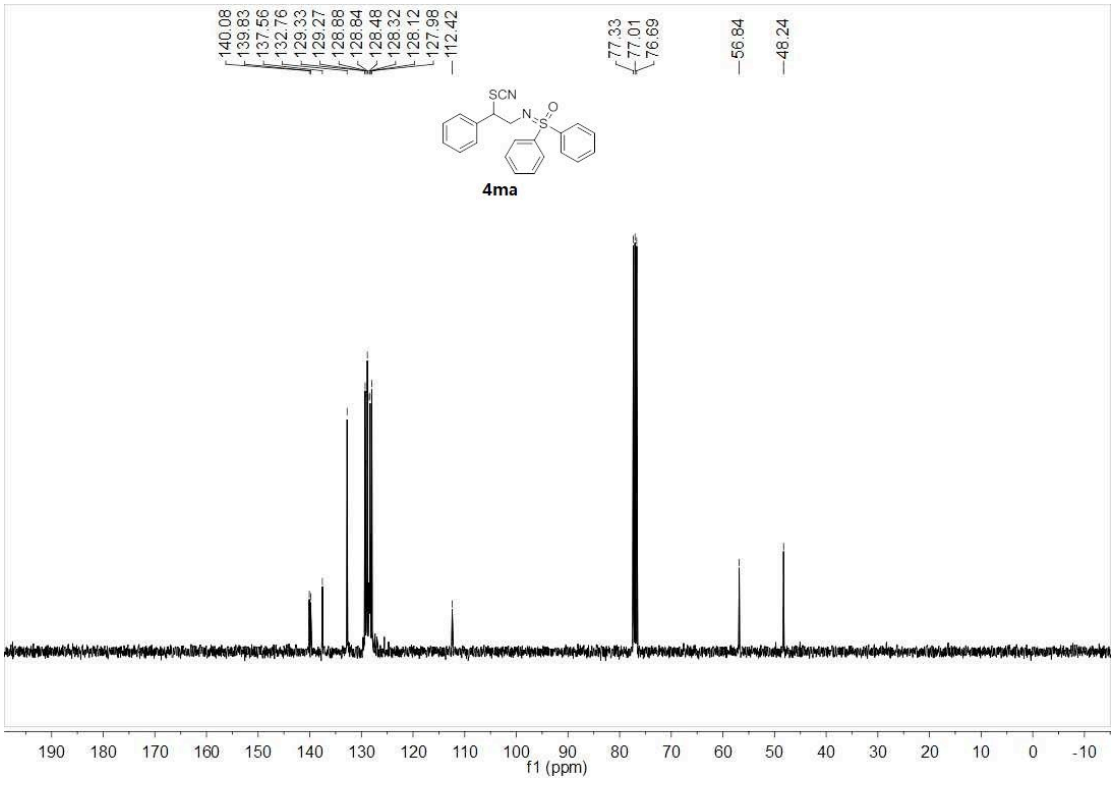
7.49
7.47
7.47
7.41
7.39
7.38
7.37
7.35
7.35
7.34
7.33
7.26
7.26
4.75
4.73
4.73
4.71
3.67
3.66
3.64
3.62
3.61
3.59
3.58
3.56
SCN
N
S
O
4ma
4.09
6.40
5.43
1.00
2.13
f1 (ppm)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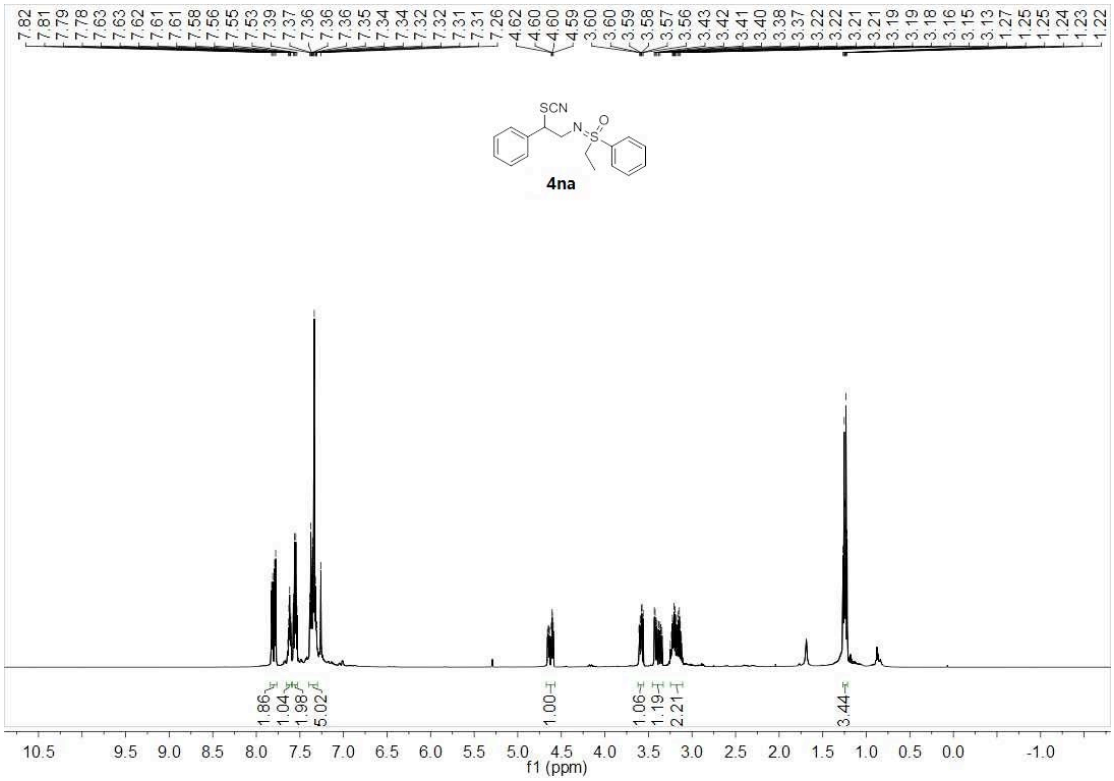
139.83
137.56
132.76
129.33
129.27
128.88
128.84
128.48
128.32
128.12
127.98
112.42
77.33
77.01
76.69
56.84
48.24
SCN
N
S
O
4ma
f1 (ppm)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S
O
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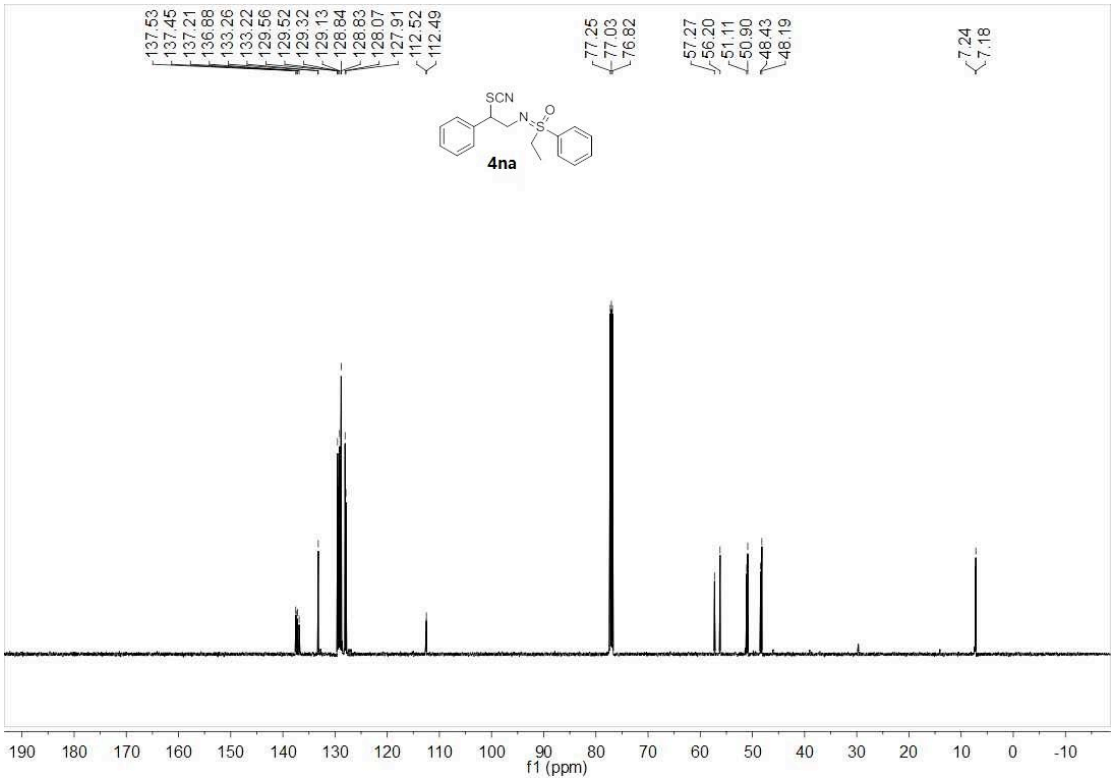
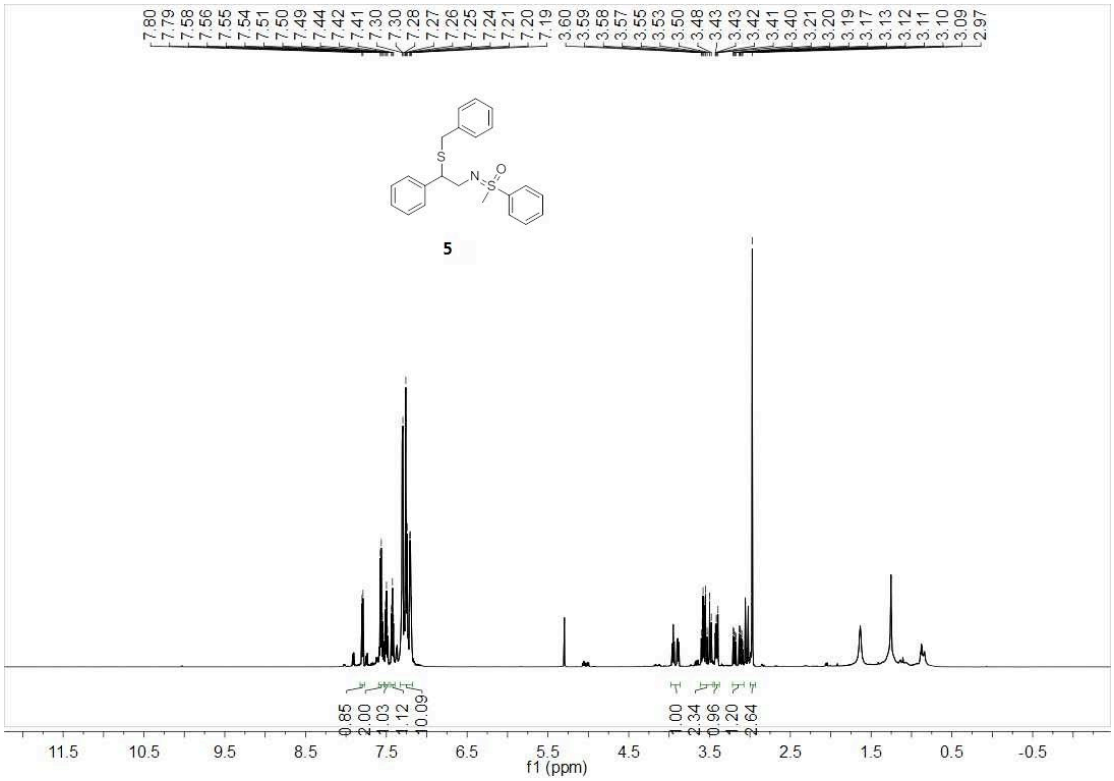
5.02
1.00
1.06
1.19
2.21
3.44
f1 (ppm)


SCN
N
S
O
4na
f1 (ppm)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7.44
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7.41
7.30
7.30
7.28
7.27
7.26
7.25
7.24
7.21
7.20
7.19
3.60
3.59
3.58
3.57
3.55
3.53
3.50
3.48
3.43
3.43
3.42
3.41
3.40
3.21
3.20
3.19
3.17
3.13
3.12
3.11
3.10
3.09
2.97
S
N
O
S
5
0.85
2.00
1.03
1.12
10.09
7.00
2.34
0.96
1.20
2.64
11.5
10.5
9.5
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6.5
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4.5
3.5
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1.5
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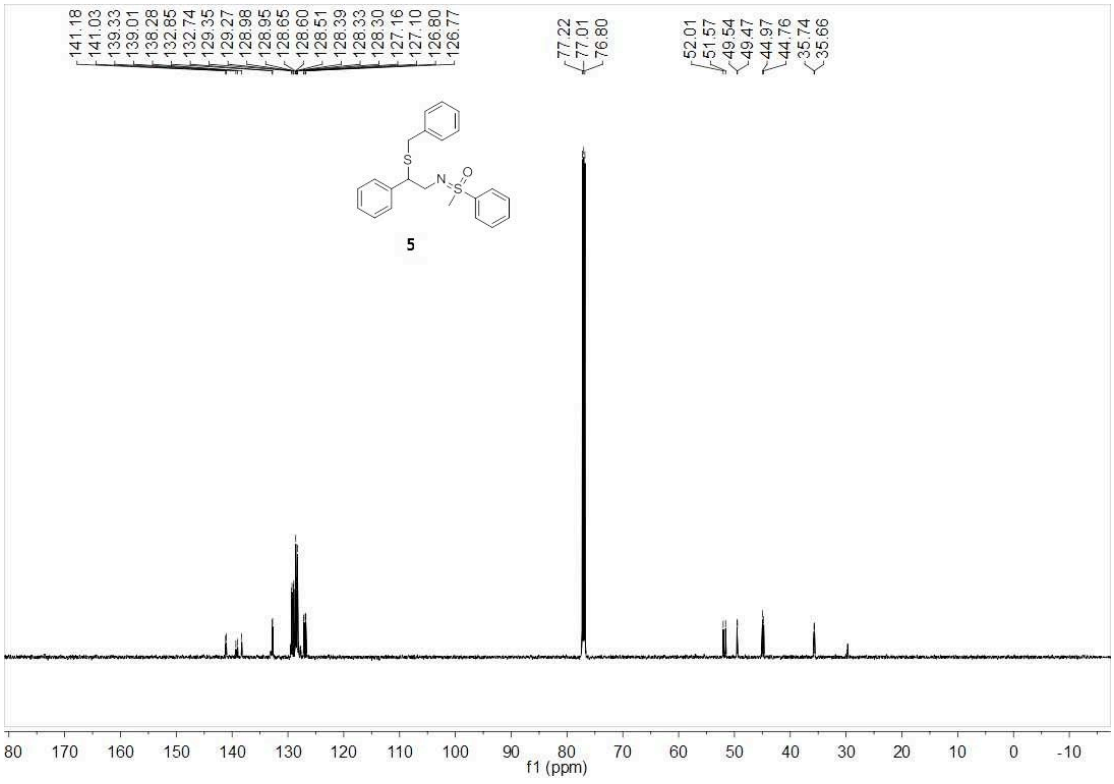
-0.5
f1 (ppm)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129.35
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128.98
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128.60
128.51
128.39
128.33
128.30
127.16
127.10
126.80
126.77
77.22
77.01
76.80
52.01
51.57
49.54
49.47
44.97
44.76
35.74
35.66
S
N
O
S
5
80
170
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120
110
100
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80
70
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40
30
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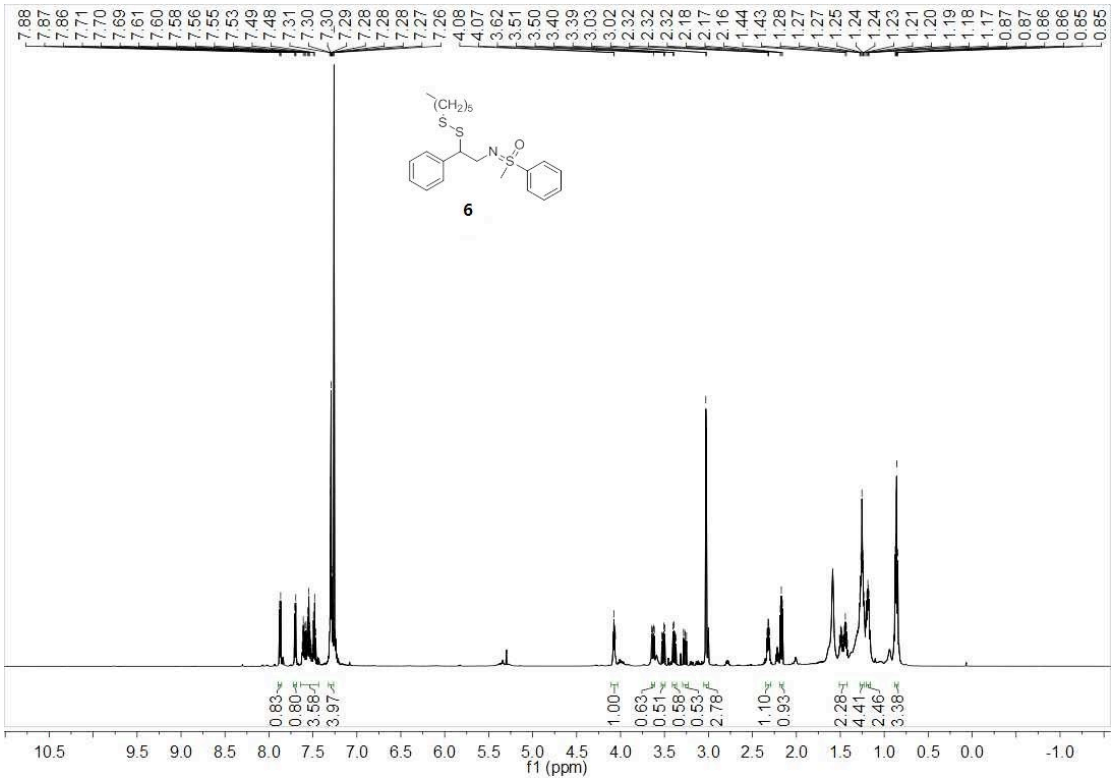
0
-10
f1 (ppm)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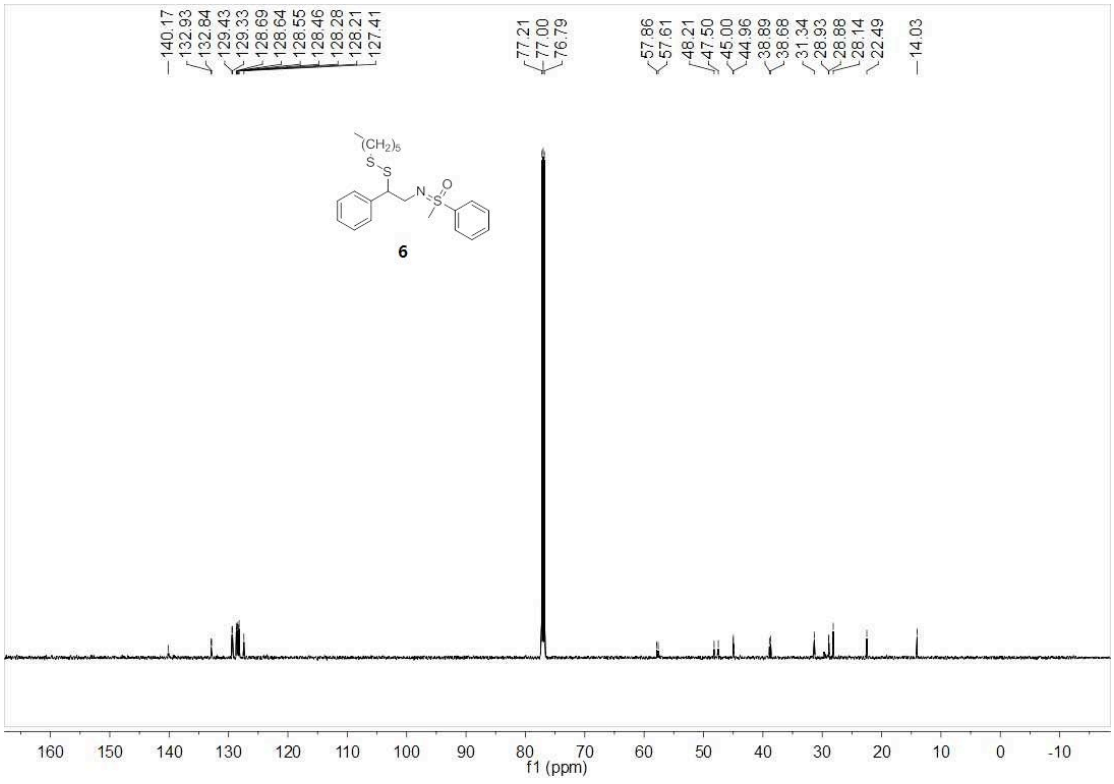
4.08 4.07 3.62 3.51 3.50 3.40 3.39 3.03 3.02 2.32 2.32 2.18 2.17 2.16 1.44 1.43 1.28 1.27 1.27 1.25 1.24 1.24 1.23 1.21 1.20 1.19 1.18 1.17 0.87 0.87 0.86 0.86 0.85 0.85
6
0.83 0.80 3.58 3.97 1.00 0.63 0.51 0.58 0.53 2.78 1.10 0.93 2.28 4.41 2.46 3.38
10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)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77.21 77.00 76.79
57.86 57.61 48.21 47.50 45.00 44.96 38.89 38.68 31.34 28.93 28.88 28.14 22.49 14.03
6
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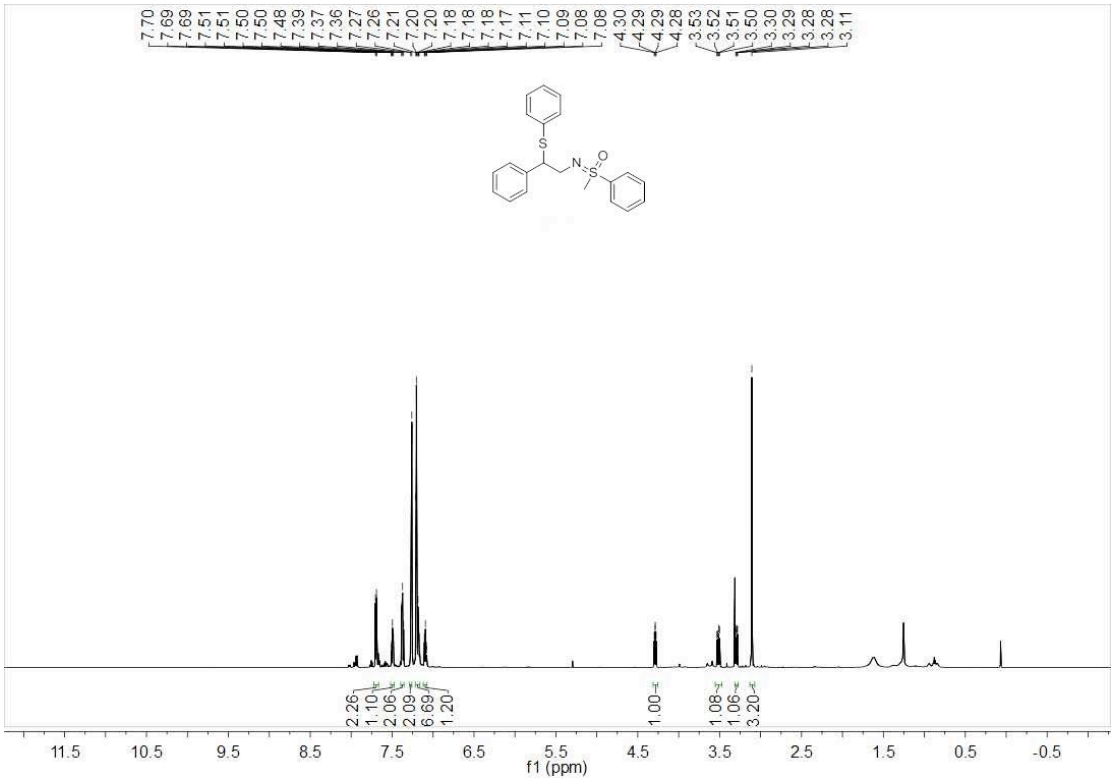
f1 (ppm)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7.21
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7.20
7.18
7.18
7.18
7.17
7.11
7.10
7.09
7.08
7.08
4.30
4.29
4.29
4.28
3.53
3.52
3.51
3.50
3.30
3.29
3.28
3.28
3.11
S
N
O
2.26
1.10
2.06
2.09
6.69
1.20
1.00
1.08
1.06
3.20
11.5
10.5
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6.5
5.5
4.5
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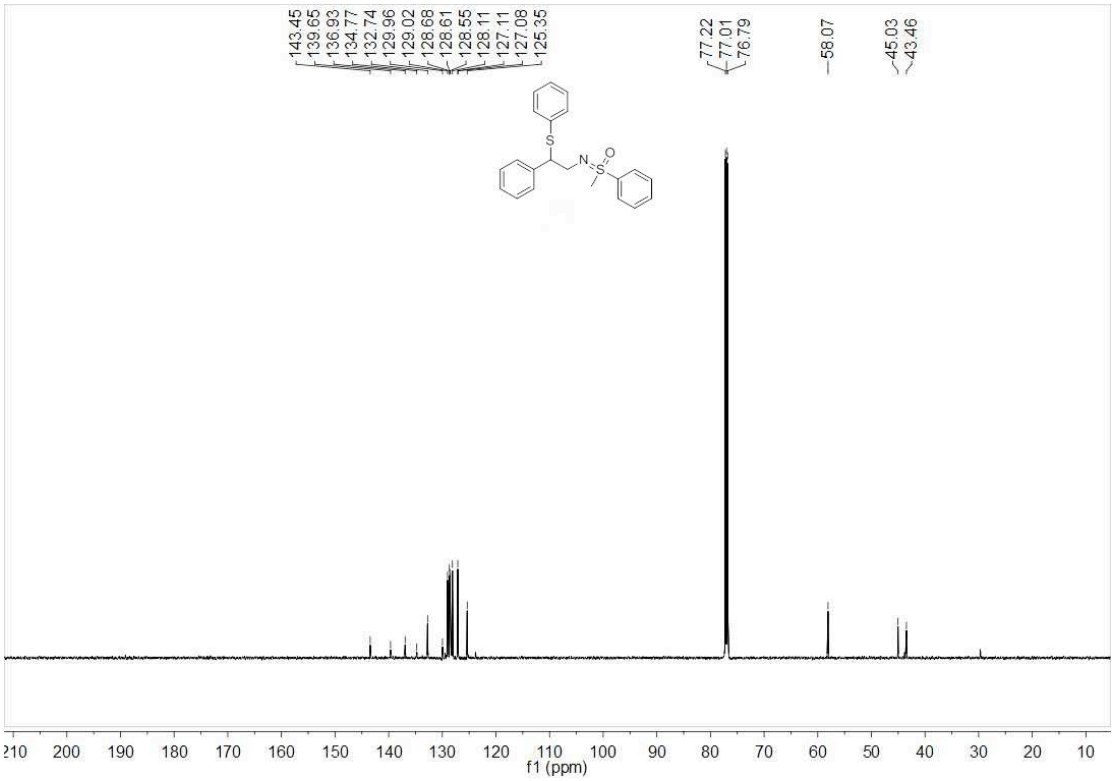
1.5
0.5
-0.5
f1 (ppm)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134.77
132.74
129.96
129.02
128.68
128.61
128.55
128.11
127.11
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77.22
77.01
76.79
58.07
45.03
43.46
S
N
O
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200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)