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# Supporting Information

# Oxidative Acylation of Sulfoximines with Methylarenes as Acyl Donor **

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**General Information：**

All reactions were carried out in ovendried glassware. All methylarenes and sulfoximines were obtained from commercial sources and used as received. All the reactions were monitored by thin-layer chromatography (TLC); products purification was done using silica gel column chromatography. $^{1}H/^{13}C$ NMR spectra were recorded on Bruker avance 400 MHz and Bruker AMX 400 MHz spectrometer at 400/100 MHz, respectively, in $CDCl_3$ unless otherwise stated, using either TMS or the undeuterated solvent residual signal as the reference. Chemical shifts are given in ppm and are measured relative to $CDCl_3$ as an internal standard. The IR spectra (neat) were recorded with a Nicolet 6700 spectrometer. Mass spectra were obtained by the electrospray ionization time-of-flight (ESI-TOF) mass spectrometry. Flash column chromatography purification of compounds was carried out by gradient elution using ethyl acetate (EA) in light petroleum ether (PE).

**General experimental procedure for N-aroylated sulfoximines:**

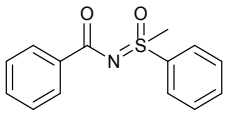
To a mixture of iodine (12.7 mg, 0.05 mmol, 20 mol %) and $FeCl_3 \cdot 6H_2O$ (10.27 mg, 0.038 mmol, 15 mol %) were added methylarenes **1** (5.0 mmol, 20 equiv.), NH-sulfoximine (0.25 mmol), and TBHP (70 wt % in water, 0.27 mL, 2.0 mmol, 8 equiv.). The reaction mixture was stirred at 80 ℃ inside a sealed tube for 24~60 h. After the reaction over (TLC), the contents were cooled to room temperature and then diluted with ethyl acetate (2 mL). The mixture was dried over anhydrous $Na_2SO_4$, filtered and evaporated under reduced pressure to afford the crude product which was further purified by silica gel column chromatography with petroleum ether/ethyl acetate as eluent.

**General experimental procedure for control experiments:**

To a mixture of iodine (12.7 mg, 0.05 mmol, 20 mol %) and $FeCl_3 \cdot 6H_2O$ (10.27 mg, 0.038 mmol, 15 mol %) were added acyl donor (5.0 mmol, 20 equiv. of toluene, benzyl alcohol or benzaldehyde, respectively), NH-sulfoximine (0.25 mmol), TBHP (70 wt % in water, 0.27 mL, 2.0 mmol, 8 equiv.) and radical trapping reagent (0.5 mmol, 2 equiv. of TEMPO or BHT, respectively). The reaction mixture was stirred at 80 ℃ inside a sealed tube and monitored with TLC. After 24 h, the contents were cooled to room temperature and then diluted with ethyl acetate (2 mL). The mixture was dried over anhydrous $Na_2SO_4$, filtered, concentrated and further purified by silica gel column chromatography with petroleum ether/ethyl acetate as eluent.

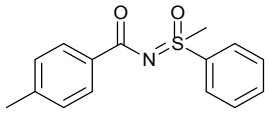
**Characterization of products:**

**N-Benzoyl-S-methyl-S-phenylsulfoximine (3aa)[1]**



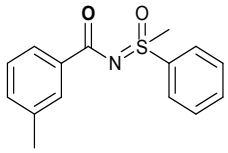
White solid; yield: 93%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.18-8.16 (m, 2H), 8.06-8.04 (m, 2H), 7.70-7.59 (m, 3H), 7.53-7.39 (m, 3H), 3.46 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 174.4, 139.1, 135.6, 133.9, 132.3, 129.8, 129.5, 128.1, 127.3, 44.4.

**N-(4-Methylbenzoyl)-S-methyl-S-phenylsulfoximine (3ab)[1a, 2]**



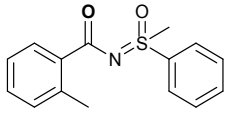
White solid; yield: 95%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.06-8.05 (m, 4H), 7.69-7.66 (m, 1H), 7.62-7.59 (m, 2H), 7.21 (d, $J$ = 7.6 Hz, 2H), 3.45 (s, 3H), 2.40 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 174.4, 142.8, 139.3, 133.9, 133.1, 129.8, 129.6, 128.9, 127.3, 44.5, 21.7.

**N-(3-Methylbenzoyl)-S-methyl-S-phenylsulfoximine (3ac)[1a, 2]**



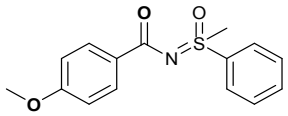
White solid; yield: 94%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.07-8.05 (m, 2H), 7.98-7.96 (m, 2H), 7.70-7.66 (m, 1H), 7.63-7.59 (m, 2H), 7.32-7.28 (m, 2H), 3.46 (s, 3H), 2.40 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 174.6, 139.2, 137.9, 135.7, 133.9, 133.1, 130.1, 129.8, 128.1, 127.3, 126.8, 44.5, 21.5.

**N-(2-Methylbenzoyl)-S-methyl-S-phenylsulfoximine (3ad)[2]**



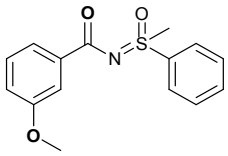
White solid; yield: 60%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.06-8.05 (m, 2H), 7.68-7.60 (m, 3H), 7.34-7.19 (m, 4H), 3.43 (s, 3H), 2.60 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 176.6, 139.4, 139.1, 135.4, 133.9, 131.6, 131.0, 130.7, 129.8, 127.2, 125.5, 44.6, 21.9.

**N-(4-Methoxybenzoyl)-S-methyl-S-phenylsulfoximine (3ae)[1b, 2a]**



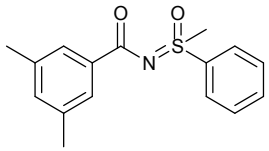
White solid; yield: 96%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.13 (d, *J* = 8.7 Hz, 2H), 8.06-8.04 (m, 2H), 7.70-7.66 (m, 1H), 7.63-7.59 (m, 2H), 6.90 (d, *J* = 8.7 Hz, 2H), 3.85 (s, 3H), 3.46 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 173.8, 162.9, 139.2, 133.7, 131.4, 129.7, 128.3, 127.2, 113.2, 55.4, 44.4.

**N-(3-Methoxybenzoyl)-S-methyl-S-phenylsulfoximine (3af)[2a]**



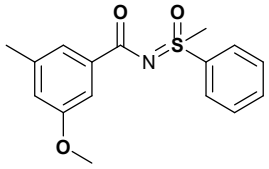
White solid; yield: 84%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.05-8.03 (m, 2H), 7.79-7.77 (m, 1H), 7.68-7.66 (m, 2H), 7.63-7.59 (m, 2H), 7.34-7.30 (m, 1H), 7.07-7.05 (m, 1H), 3.83 (s, 3H), 3.45 (s, 3H).**$^{13}$C NMR (101 MHz, $CDCl_3$):** δ 174.2, 159.5, 139.1, 137.1, 133.9, 129.8, 129.1, 127.3, 122.1, 118.9, 113.9, 55.5, 44.6.

**N-(3,5-dimethylbenzoyl)-S-methyl-S-phenylsulfoximine (3ag)[1a]**



White solid; yield: 92%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.06-8.04 (m, 2H), 7.78 (s, 2H), 7.69-7.58 (m, 3H), 7.15 (s, 1H), 3.45 (s, 3H), 2.35 (s, 6H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 174.7, 139.1, 137.7, 135.5, 133.9, 133.8, 129.7, 127.21, 127.19, 44.4, 21.3.

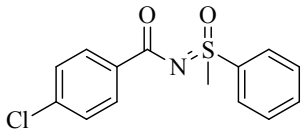
**N-(3-methyl-5-Methoxybenzoyl)-S-methyl-S-phenylsulfoximine (3ah)**



White solid; yield: 92%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.05-8.03 (m, 2H), 7.69-7.60 (m, 4H), 7.49 (s, 1H), 6.88 (s, 1H), 3.81 (s, 3H), 3.44 (s, 3H), 2.36 (s, 3H).; **$^{13}$C NMR (101 MHz, $CDCl_3$ ):** δ 174.4, 159.5, 139.2, 139.1, 136.9, 133.9, 129.8, 127.2, 122.9, 119.6, 111.0, 55.5, 44.4, 21.5; IR (neat, $cm^{-1}$): 1622, 1601, 1589, 1464, 1445, 1333, 1304, 1242, 1206, 1066, 983, 772, 686: HRMS (m/z) [$C_{16}H_{17}NO_3S$ +

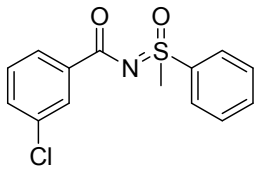
Na]$^+$ Calcd. 326.0827, Found 326.0816.

**N-(4-Chlorobenzoyl)-S-methyl-S-phenylsulfoximine (3ai)[1]**



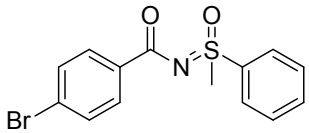
White solid; yield: 84%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.08 (d, *J* = 8.4 Hz, 2H), 8.03-8.01 (m, 2H), 7.69-7.66 (m, 1H), 7.62-7.58 (m, 2H), 7.36 (d, *J* = 8.4 Hz, 2H), 3.45 (s, 3H); **$^{13}$C NMR (101 MHz, $CDCl_3$ ):** δ 173.2, 138.8, 138.5, 134.2, 134.0, 130.9, 129.8, 128.4, 127.2, 44.4.

**N-(3-Chlorobenzoyl)-S-methyl-S-phenylsulfoximine (3ag)[1a]**



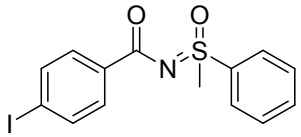
White solid; yield: 84%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.17-8.09 (m, 1H), 8.04-8.02 (m, 3H), 7.70-7.67 (m, 1H), 7.63-7.59 (m, 2H), 7.47-7.46 (m, 1H), 7.35-7.32 (m, 1H), 3.45 (s, 3H).; **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 172.9, 138.7, 137.5, 134.2, 134.1, 132.2, 129.8, 129.6, 129.5, 127.6, 127.2, 44.5.

**N-(4-Bromobenzoyl)-S-methyl-S-phenylsulfoximine (3ak)[1a]**



White solid; yield: 94%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.04-8.01 (m, 4H), 7.71-7.67 (m, 1H), 7.63 – 7.60 (m, 2H), 7.53 (d, *J* = 8.5 Hz, 2H), 3.46 (s, 3H).; **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 173.4, 138.9, 134.7, 134.0, 131.4, 131.2, 129.9, 127.2, 127.1, 44.5.

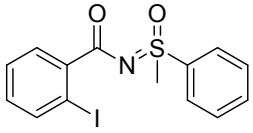
**N-(4-Iodobenzoyl)-S-methyl-S-phenylsulfoximine (3al)[1a]**



White solid; yield: 70%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.04-8.02 (m, 2H), 7.87 (d, *J* = 7.0 Hz, 2H),

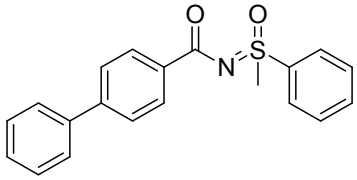
7.76 (d, *J* = 8.2 Hz, 2H), 7.70-7.68 (m, 1H), 7.64-7.60 (m, 2H), 3.46 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 173.6, 138.9, 137.5, 135.3, 134.1, 131.2, 129.9, 127.3, 100.0, 44.5.

**N-(2-Iodobenzoyl)-S-methyl-S-phenylsulfoximine (3am)**



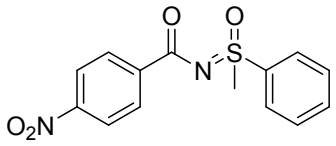
White solid; yield: 43%; **$^{1}$H NMR (400 MHz, $CDCl_3$ ):** δ 8.13-8.08 (m, 2H), 7.93-7.92 (m, 1H), 7.83-7.82 (m, 1H), 7.69-7.63 (m, 3H), 7.38-7.37 (m, 1H), 7.09-7.07 (m, 1H), 3.50 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 175.8, 141.5, 140.7, 138.5, 134.2, 131.5, 130.3, 129.8, 128.0, 127.5, 93.1, 44.3; FT-IR (neat, $cm^{-1}$) 1633, 1460, 1445, 1320, 1263, 1219, 980, 836, 750, 698; HRMS (m/z) $[C_{14}H_{12}NO_2SI + Na]^+$ Calcd. 407.9531, Found 407.9532.

**N-(4-Phenylbenzoyl)-S-methyl-S-phenylsulfoximine (3an)[1b]**



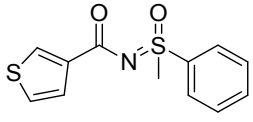
White solid; yield: 75%; **$^{1}$H NMR (400 MHz, $CDCl_3$ ):** δ 8.25 (d, *J* = 8.3 Hz, 2H), 8.09-8.07 (m, 2H), 7.71-7.60 (m, 7H), 7.48-7.44 (m, 2H), 7.40-7.36 (m, 1H), 3.48 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 174.2, 145.0, 140.5, 139.2, 134.6, 134.0, 130.1, 129.8, 129.0, 128.0, 127.4, 127.3, 126.9, 44.5.

**N-(4-Nitrobenzoyl)-S-methyl-S-phenylsulfoximine (3ao)[1]**



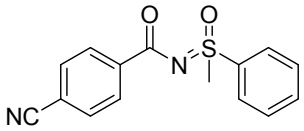
White solid; yield: 64%; **$^{1}$H NMR (400 MHz, $CDCl_3$ ):** δ 8.31 (d, *J* = 8.8 Hz, 2H), 8.25-8.24 (m, 2H), 8.06-8.04 (m, 2H), 7.75-7.71 (m, 1H), 7.67-7.63 (m, 2H), 3.50 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 172.2, 150.2, 141.2, 138.5, 134.3, 130.5, 130.0, 127.2, 123.4, 44.5.

**N-(3-Thiophene)-S-methyl-S-phenylsulfoximine (3ap)**



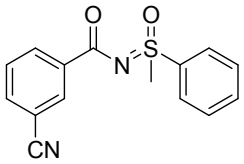
White solid; yield: 30%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.15-7.98 (m, 3H), 7.63-7.49 (m, 4H), 7.20-7.18 (m, 1H), 3.39 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 169.2, 139.3, 138.2, 133.0, 131.1, 128.8, 127.4, 126.3, 124.5, 43.6; IR (neat, $cm^{-1}$): 1712, 1621, 1518, 1447, 1409, 1277, 1222, 1121, 987, 801, 752; HRMS (m/z) $[C_{12}H_{11}N_1O_2S + Na]^+$ Calcd. 288.0129, Found 288.0131.

**N-(4-Cyanobenzoyl)-S-methyl-S-phenylsulfoximine (3aq)**



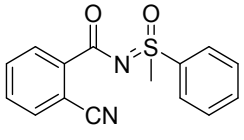
White solid; yield: 67%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.02 (d, *J* = 6.2 Hz, 2H), 7.78-7.77 (m, 1H), 7.62-7.61 (m, 1H), 7.57-7.55 (m, 2H), 7.34-7.32 (m, 1H), 7.27-7.19 (m, 2H), 3.41 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 172.4, 139.6, 138.5, 134.2, 132.0, 130.0, 129.9, 127.2, 118.6, 115.4, 44.4; IR (neat, $cm^{-1}$): 2232, 1632, 1581, 1561, 1325, 1297, 1286, 1132, 1088, 991, 766, 690; HRMS (m/z) $[C_{15}H_{12}N_2O_2S + Na]^+$ Calcd. 307.0517, Found 307.0520.

**N-(3-Cyanobenzoyl)-S-methyl-S-phenylsulfoximine (3ar)**



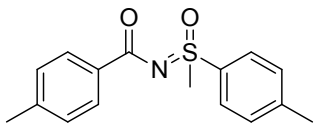
White solid; yield: 75%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.45-8.42 (m, 1H), 8.35 (d, *J* = 7.9 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 2H), 7.77-7.75 (m, 1H), 7.71-7.69 (m, 1H), 7.65-7.62 (m, 2H), 7.54-7.51 (m, 1H), 3.48 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 171.9, 138.4, 136.9, 135.2, 134.3, 133.5, 133.3, 129.9, 129.1, 127.0, 118.5, 112.4, 44.5; IR (neat, $cm^{-1}$): 2231, 1633, 1579, 1447, 1302, 1224, 1119, 986, 857, 755, 684; HRMS (m/z) $[C_{15}H_{12}N_2O_2S + Na]^+$ Calcd. 307.0517, Found 307.0511.

**N-(2-Cyanobenzoyl)-S-methyl-S-phenylsulfoximine (3as)**



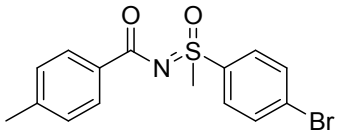
White solid; yield: 59%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.18-8.13 (m, 2H), 7.77-7.75 (m, 1H), 7.70-7.68 (m, 1H), 7.65-7.57 (m, 5H), 3.51 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 171.4, 138.7, 138.2, 134.5, 134.3, 132.4, 131.6, 131.0, 129.9, 127.5, 118.9, 112.4, 44.3; IR (neat, $cm^{-1}$): 2224, 1635, 1591, 1447, 1285, 1223, 1154, 1098, 981, 839, 760, 686; HRMS (m/z) $[C_{15}H_{12}N_2O_2S + Na]^+$ Calcd. 307.0517, Found 307.0520.

**N-(4-Methylbenzoyl)-S-methyl-S-(4-methylphenyl)sulfoximine (3bb)**



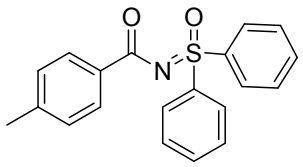
White solid; yield: 87%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.07-8.05 (m, 2H), 7.93-7.91 (m, 2H), 7.39 (d, *J* = 8.2 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 3.44 (s, 3H), 2.45 (s, 3H), 2.39 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 174.4, 144.9, 142.7, 136.1, 133.1, 130.4, 129.6, 128.8, 127.3, 44.6, 21.7 (2 C); IR (neat, $cm^{-1}$): 1705, 1627, 1450, 1406, 1313, 1283, 1222, 1174, 1137. 1097, 1020, 981, 841, 757; HRMS (m/z) $[C_{16}H_{17}NO_2S + Na]^+$ Calcd. 310.0878, Found 310.0885.

**N-(4-Methylbenzoyl)-S-methyl-S-(4-bromophenyl)sulfoximine (3cb)**



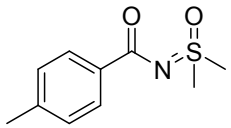
White solid; yield: 95%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.04-7.99 (m, 2H), 7.89-7.88 (m, 2H), 7.72-7.64 (m, 2H), 7.26-7.21 (m, 2H), 3.43 (s, 3H), 2.39 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 174.3, 143.0, 138.4, 135.2, 133.1, 132.8, 129.7, 128.93, 128.89, 44.5, 21.7; IR (neat, $cm^{-1}$): 1623, 1572, 1388, 1323, 1291, 1214, 1145, 1065, 987, 854, 753, 689; HRMS (m/z) $[C_{15}H_{14}NO_2SBr + Na]^+$ Calcd. 373.9826, Found 373.9829.

**N-(4-Methylbenzoyl)-S, S-diphenylsulfoximine (3db)**



White solid; yield: 80%; **$^1$H NMR (400 MHz, $CDCl_3$ ):** δ 8.15-8.13 (m, 2H), 8.07-8.05 (m, 4H), 7.57-7.51 (m, 6H), 7.26-7.23 (m, 2H), 2.41 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$ ):** δ 174.0, 142.9, 140.2, 133.3, 129.7, 129.6, 128.9, 127.8 (2 C), 21.8; IR (neat, $cm^{-1}$): 1635, 1608, 1452, 1377, 1278, 1228, 1140, 1020, 936, 832, 755, 720, 689; HRMS (m/z) $[C_{20}H_{17}N_1O_2S + Na]^+$ Calcd. 358.0878, Found 358.0870.

**N-(4-Methylbenzoyl)-S, S-dimethylsulfoximine (3eb)[3]**

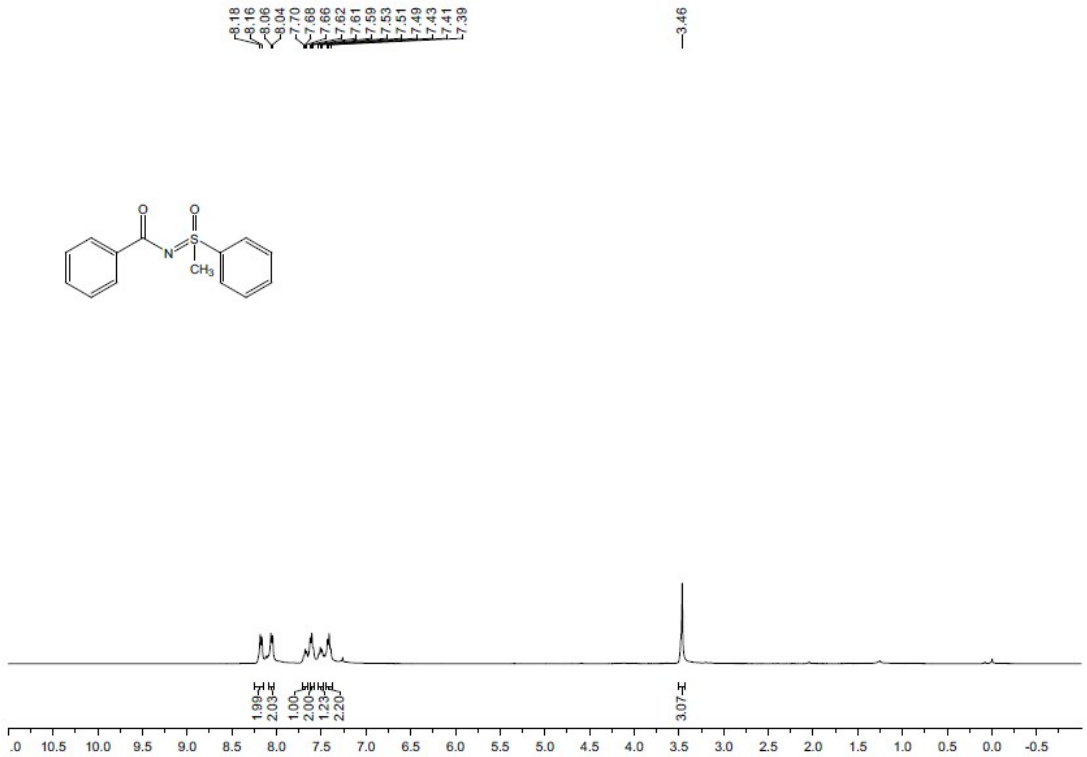


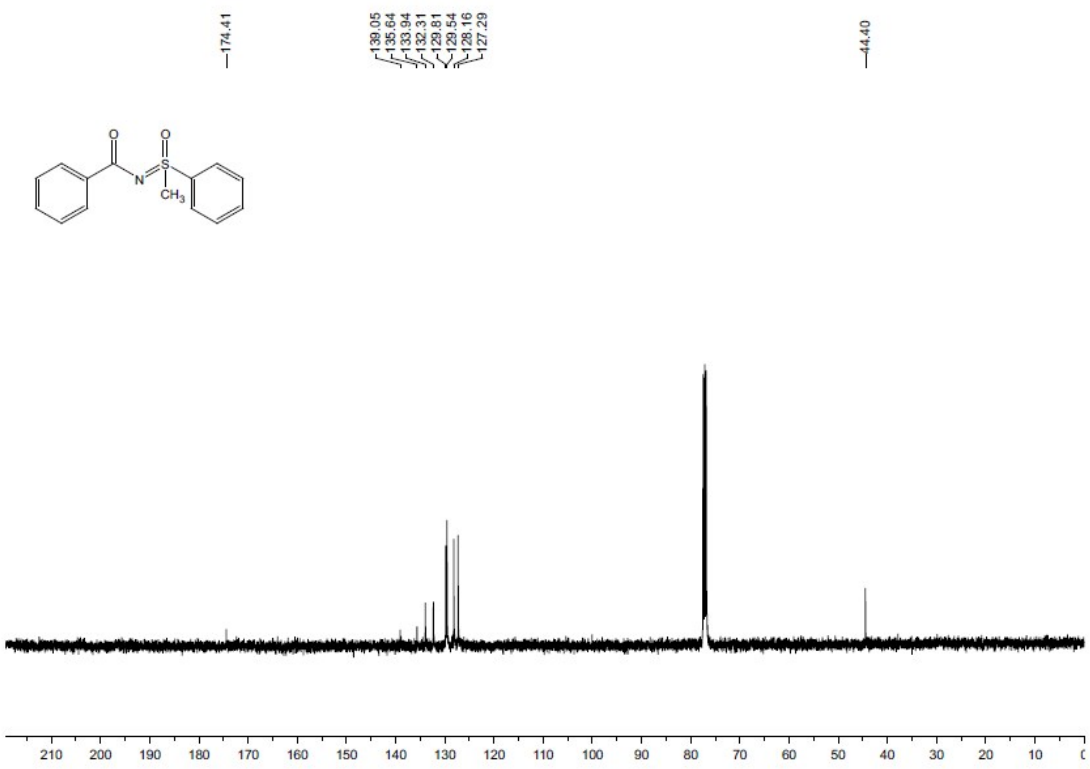
White solid; yield: 28%; **$^{1}$H NMR (400 MHz, $CDCl_3$):** δ 8.02-8.00 (m, 2H), 7.21-7.19 (m, 2H), 3.38 (s, 6H), 2.39 (s, 3H); **$^{13}$C NMR (100 MHz, $CDCl_3$):** δ 174.2, 142.7, 132.8, 129.3, 128.8, 41.8, 21.6.

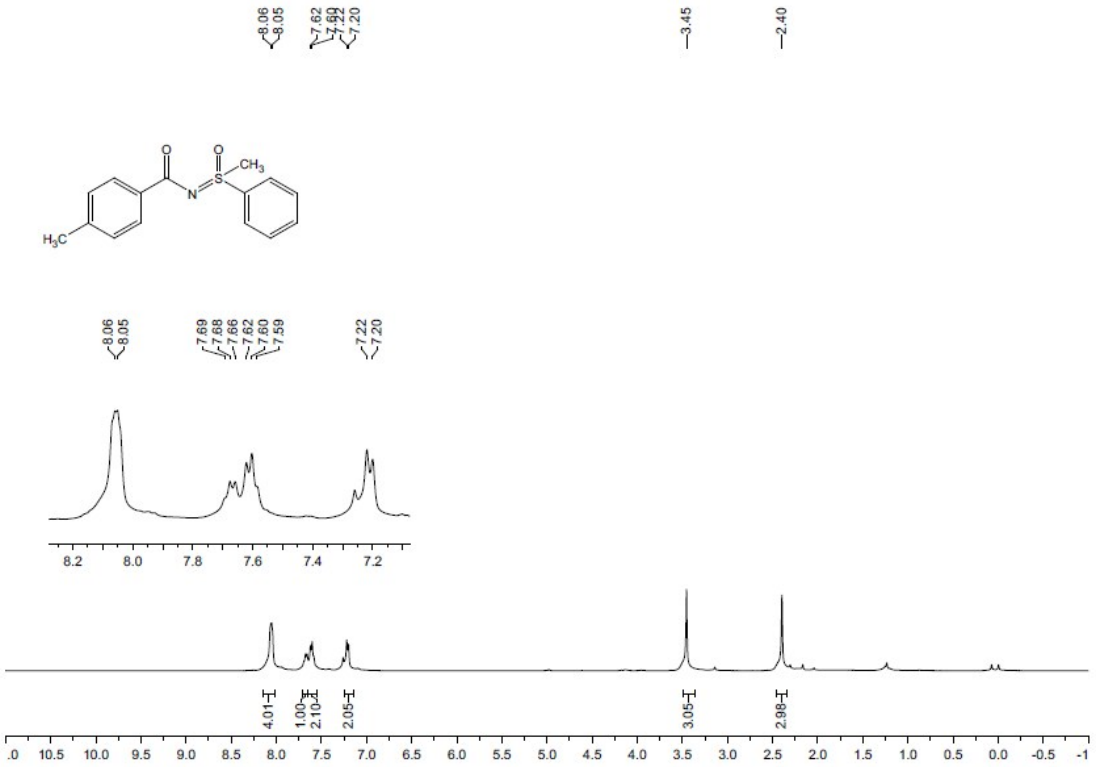
**References:**


1. (a) Priebbenow, D. L.; Bolm, C. *Org.Lett.* **2014,** *16*, 1650-2. (b) Wang, L.; Priebbenow, D. L.; Zou, L.-H.; Bolm, C. *Adv. Synth. Catal.* **2013,** *355*, 1490-1494.
2. (a) Yadav, M. R.; Rit, R. K.; Sahoo, A. K. *Chem. Eur. J.* **2012,** *18*, 5541-5545. (b) Yadav, M. R.; Rit, R. K.; Sahoo, A. K. *Org. Lett.* **2013,** *15*, 1638-1641.
3. Parthasarathy, K.; Bolm, C. *Chem. Eur. J.* **2014,** *20*, 4896-4900.

**Copies of $^{1}$H-NMR & $^{13}$C-NMR spectrum**

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7.2
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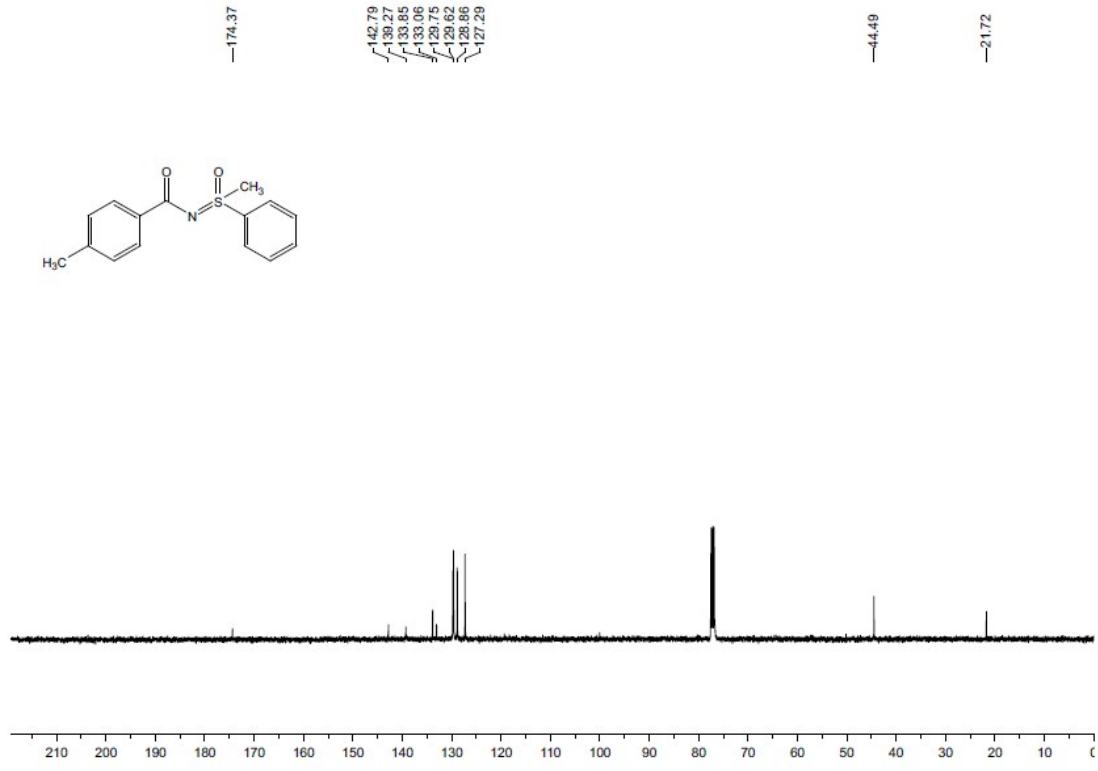
3.05
2.98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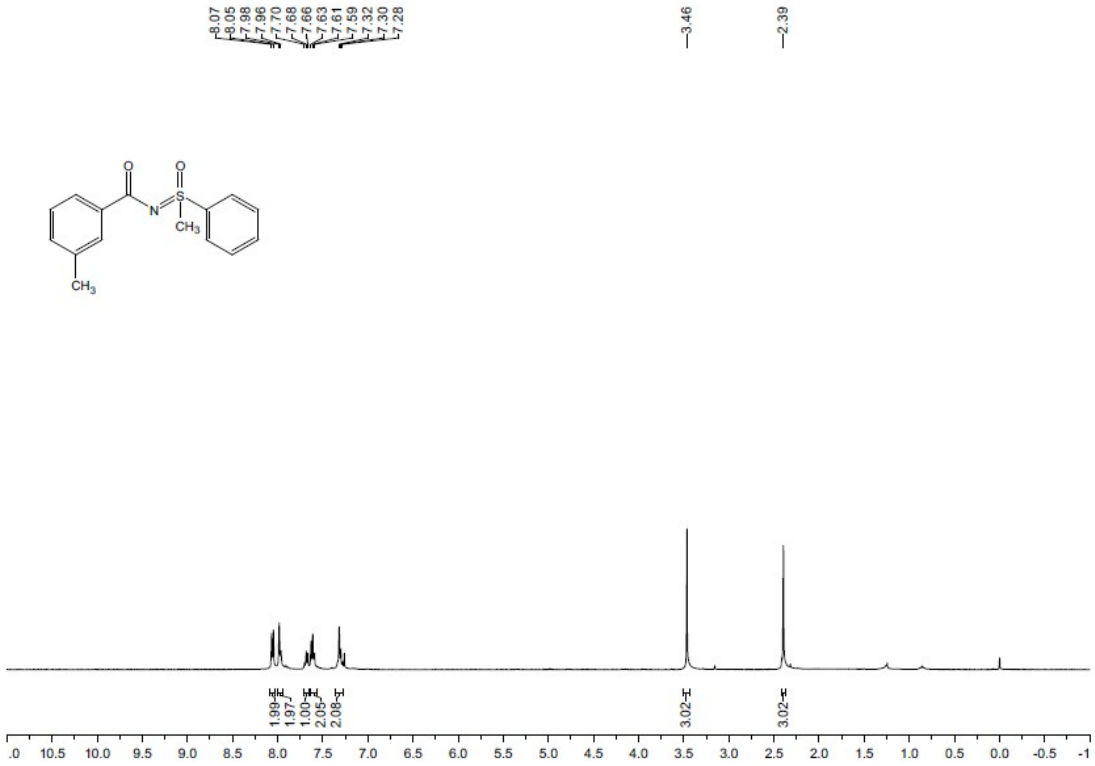
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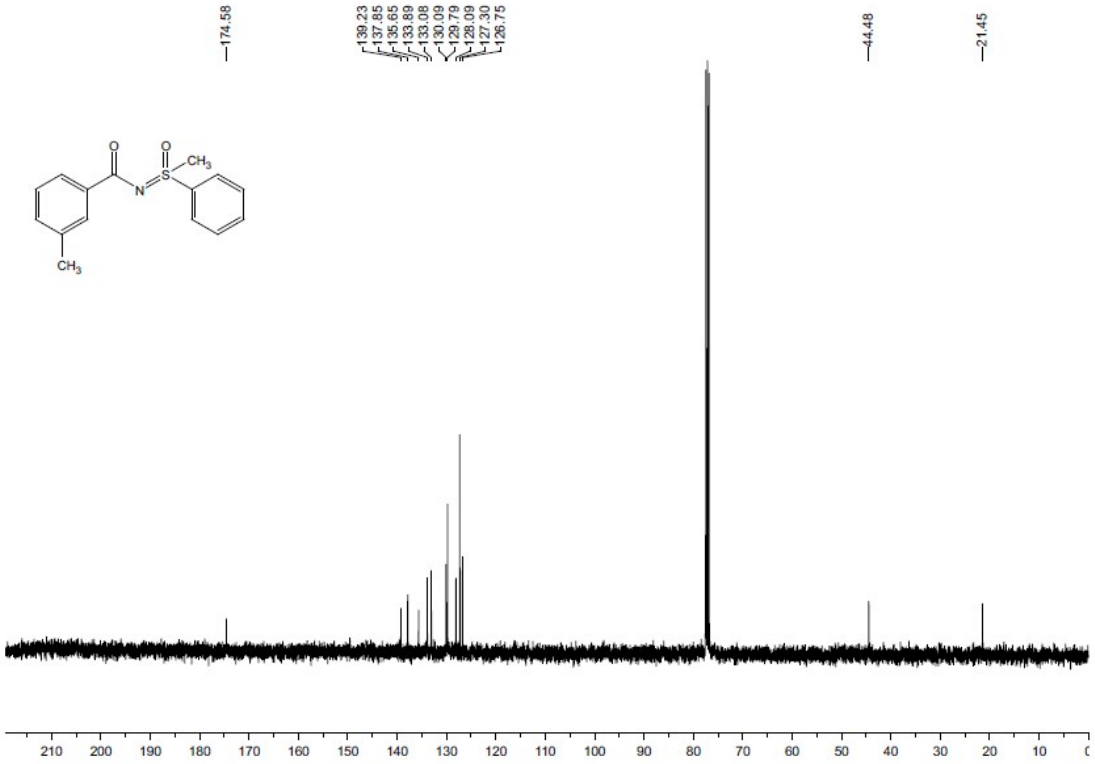
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N
S
CH3
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8.06
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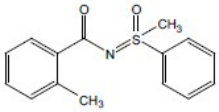
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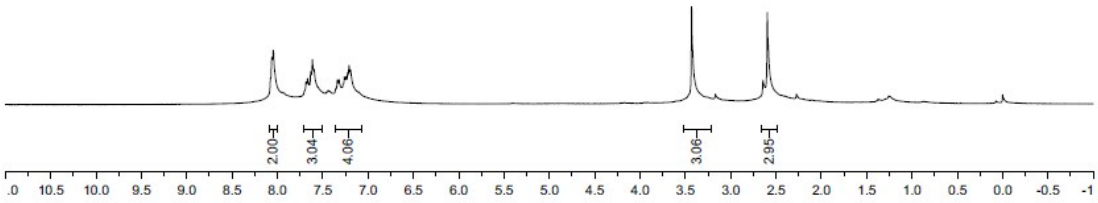
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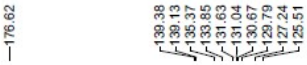
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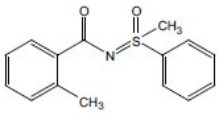
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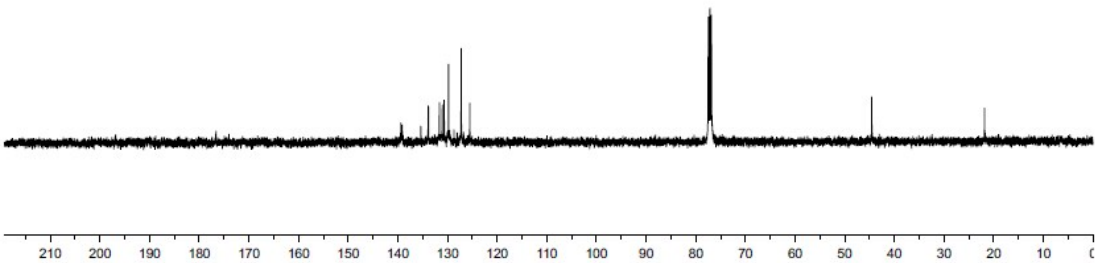
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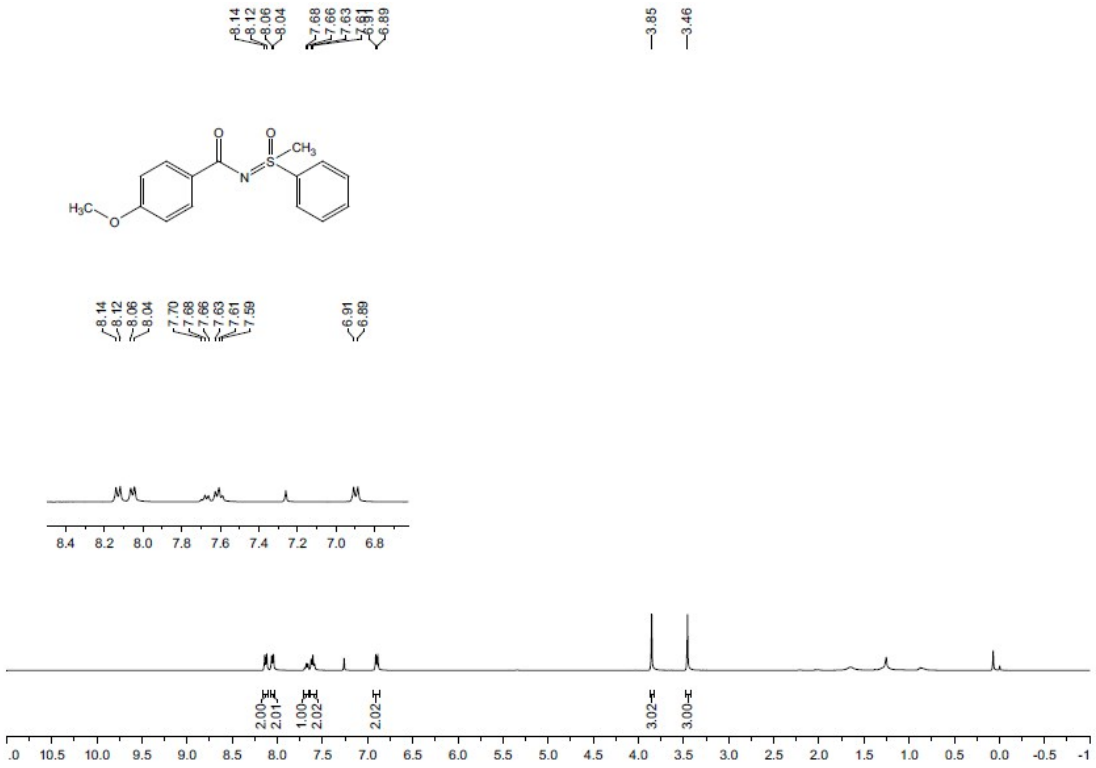
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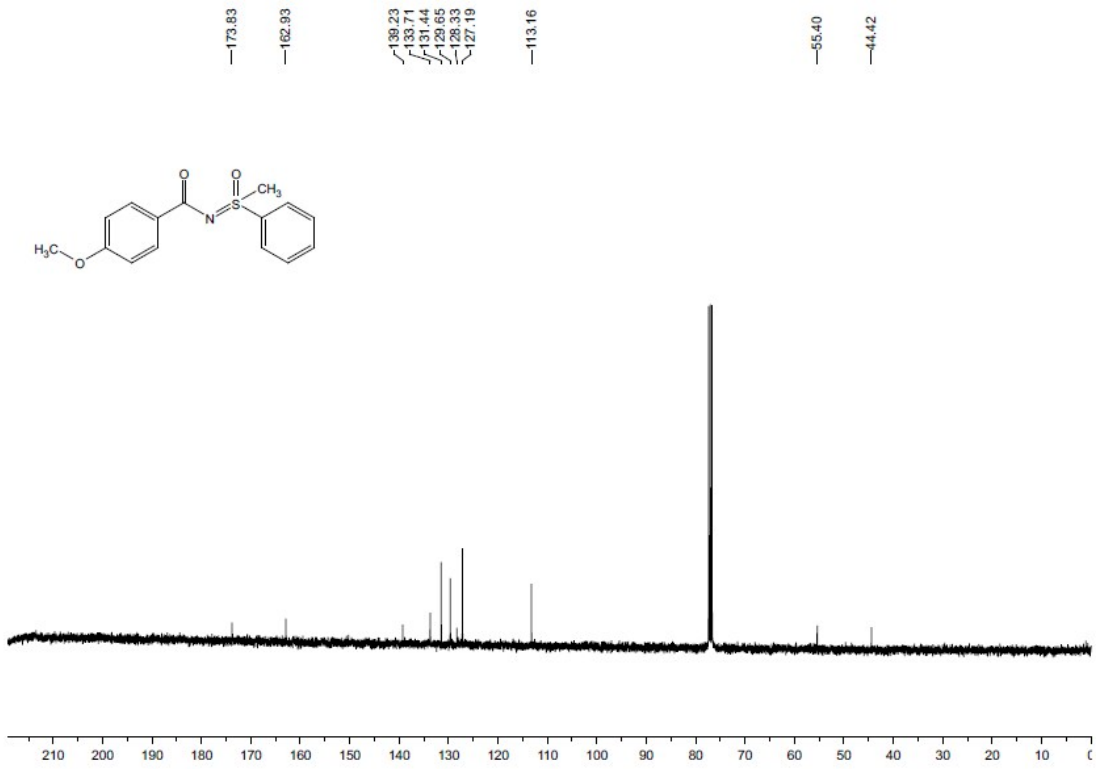
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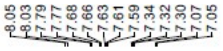
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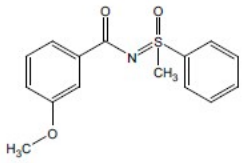
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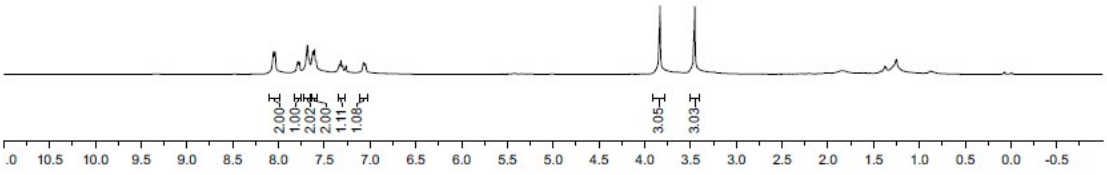
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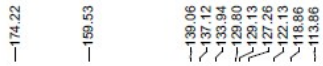
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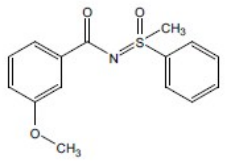
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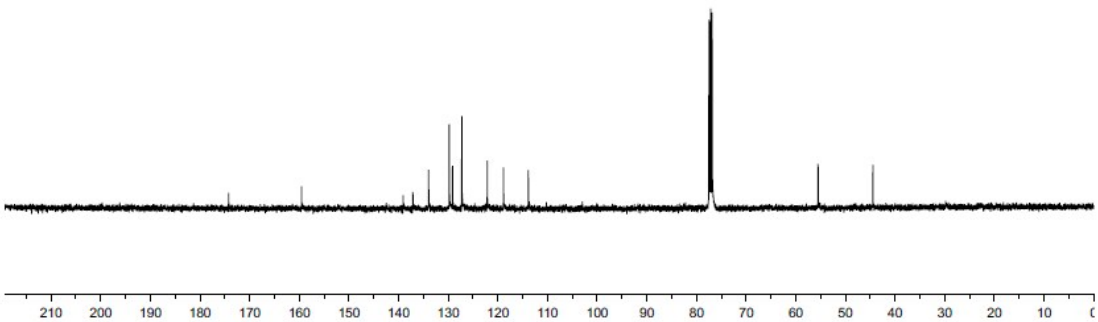
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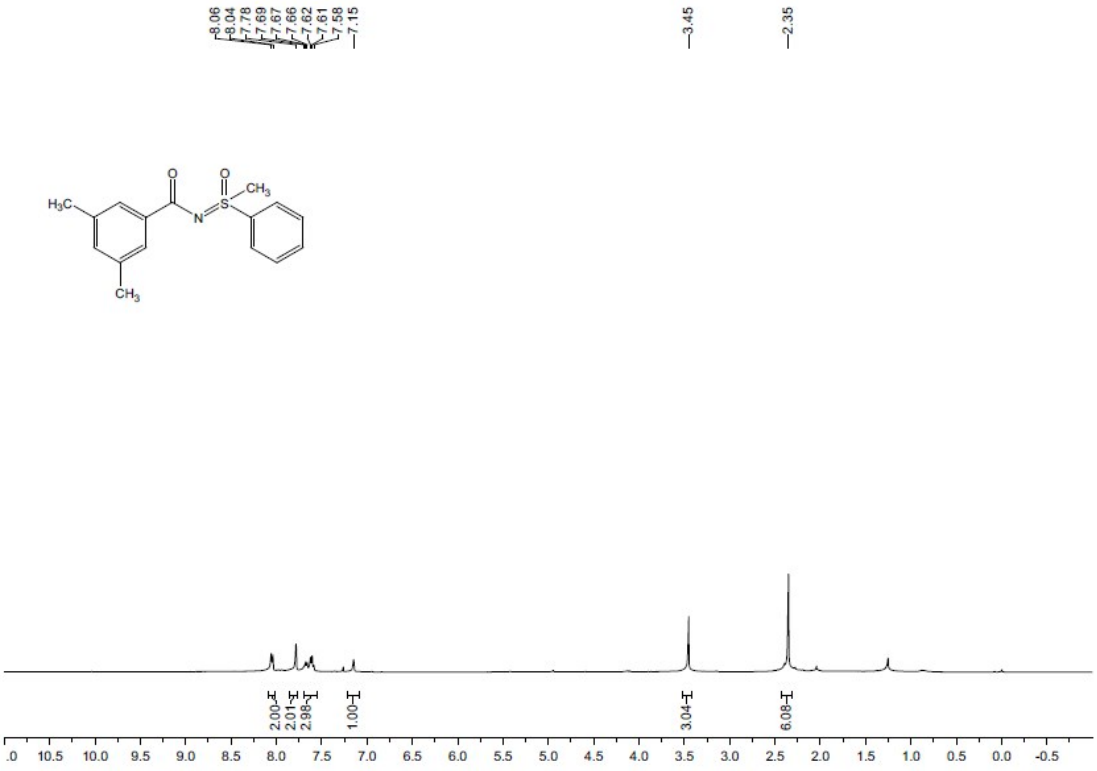
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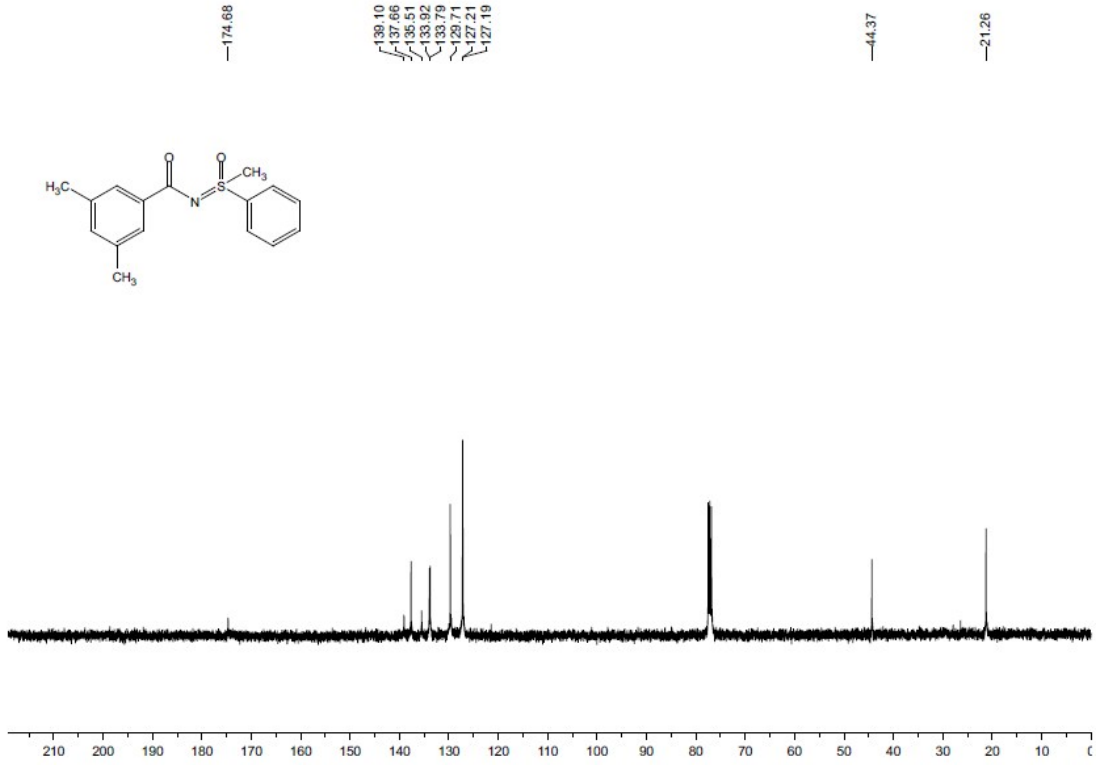
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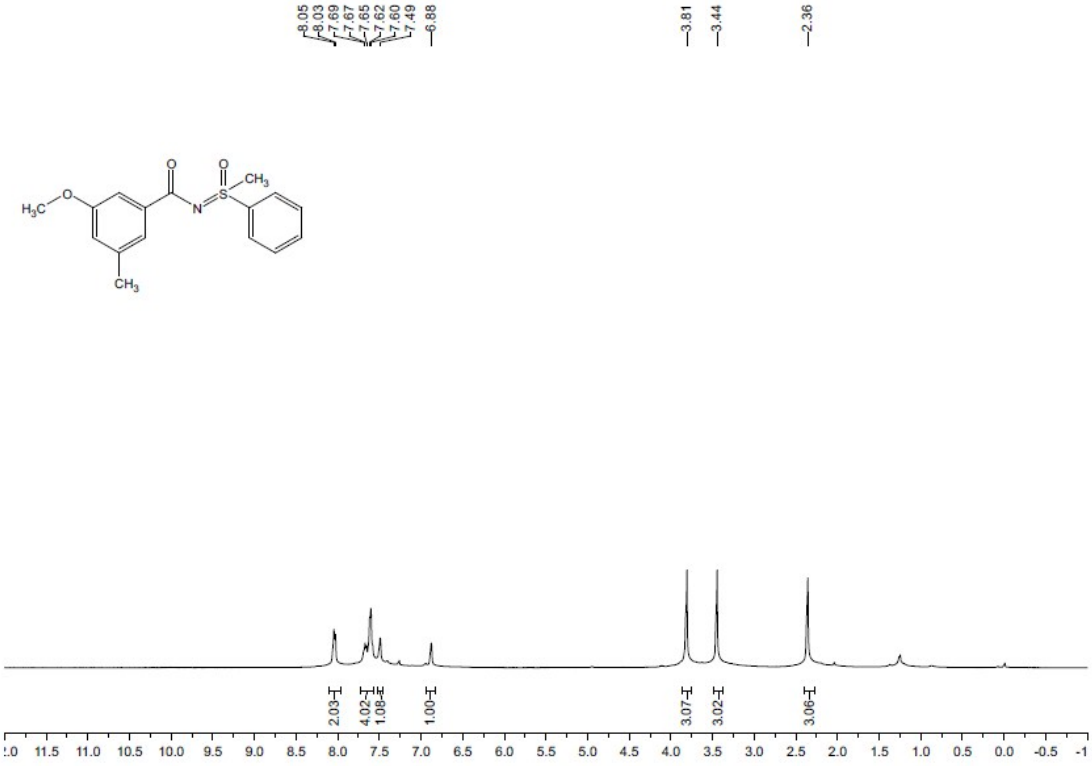
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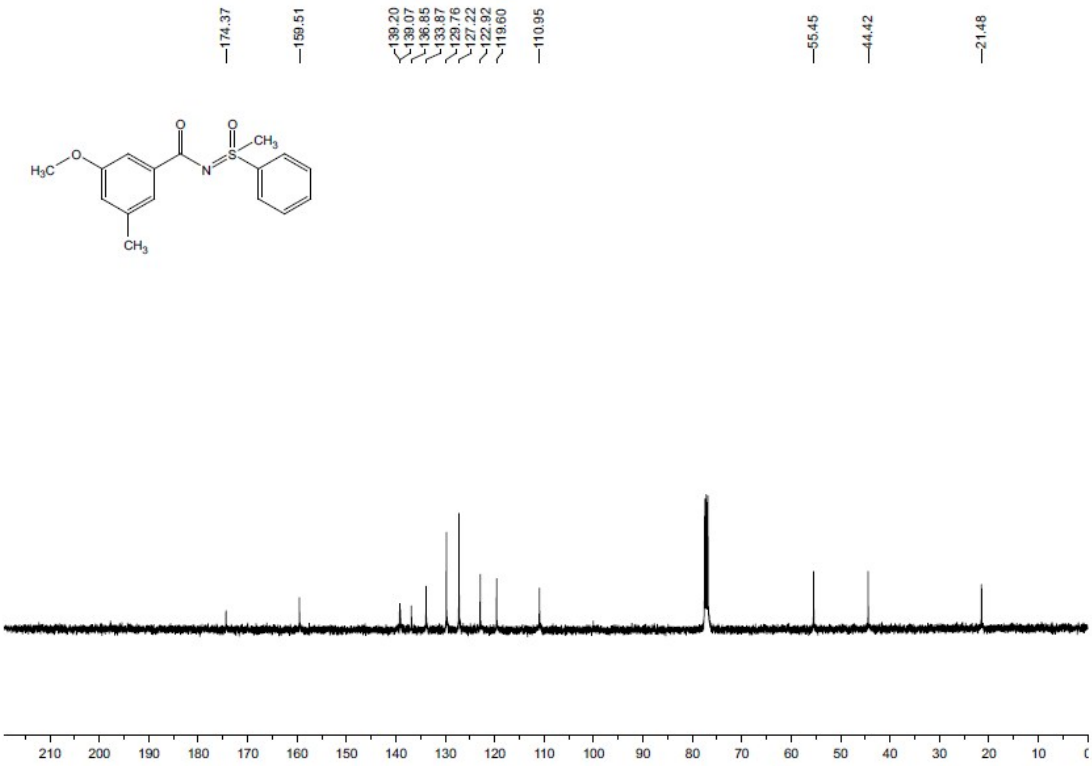
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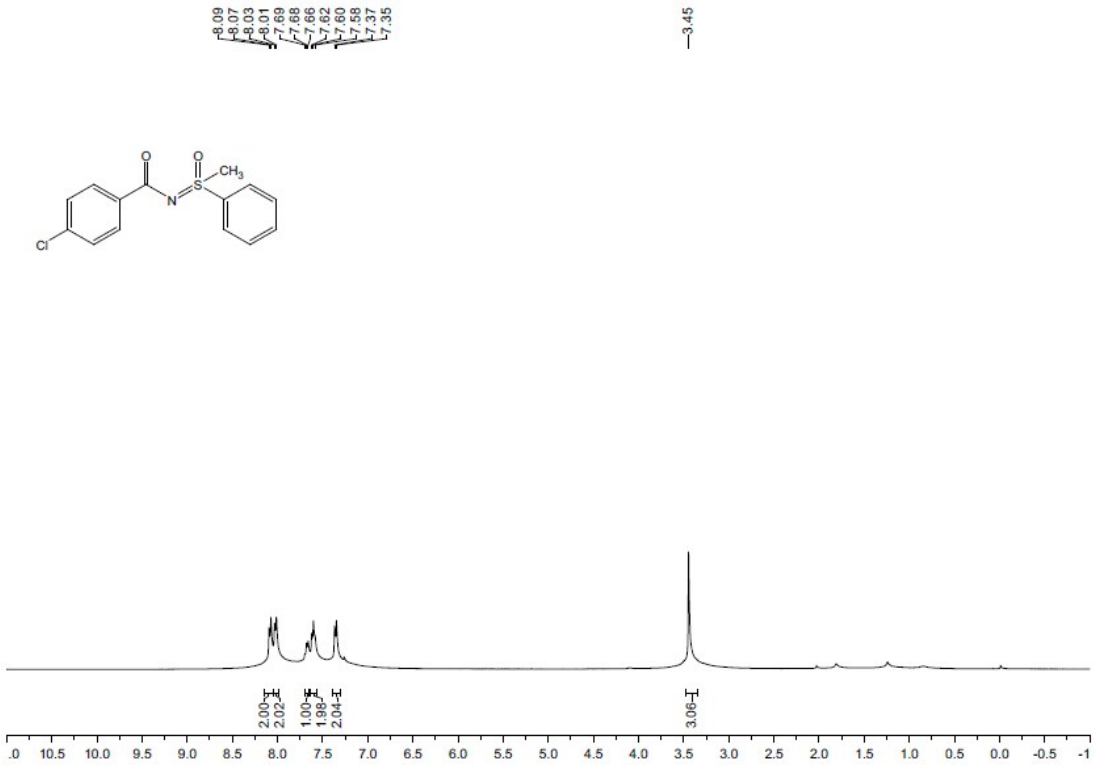
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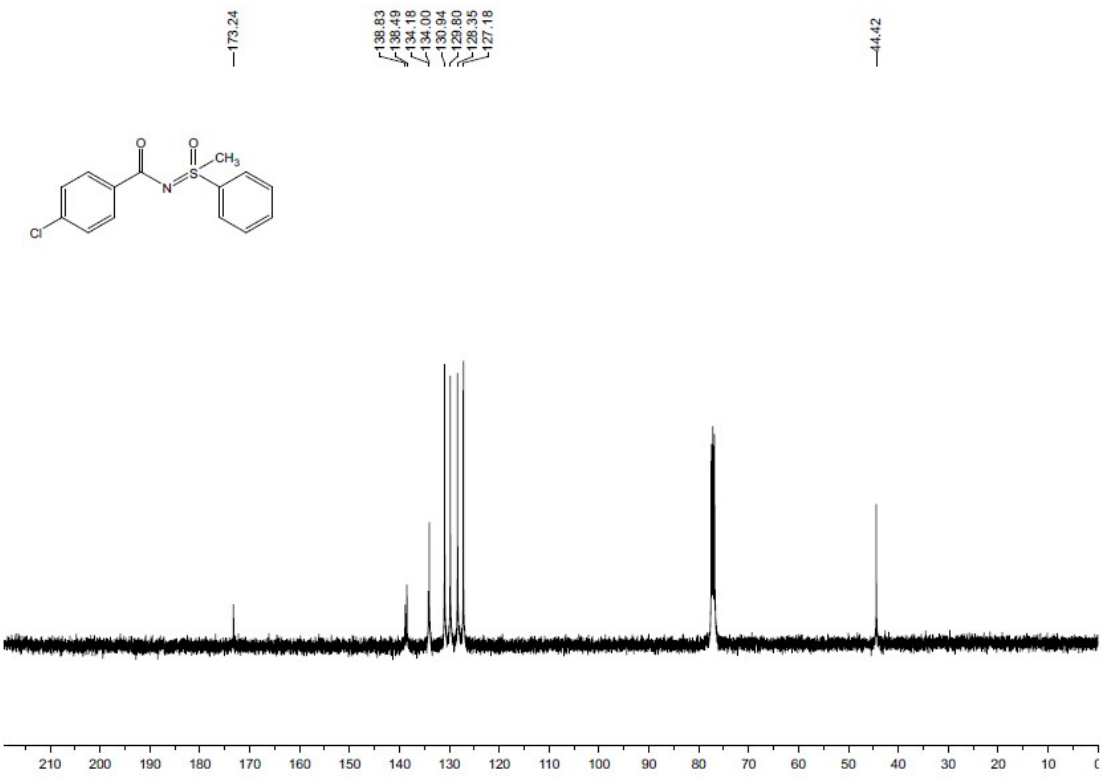
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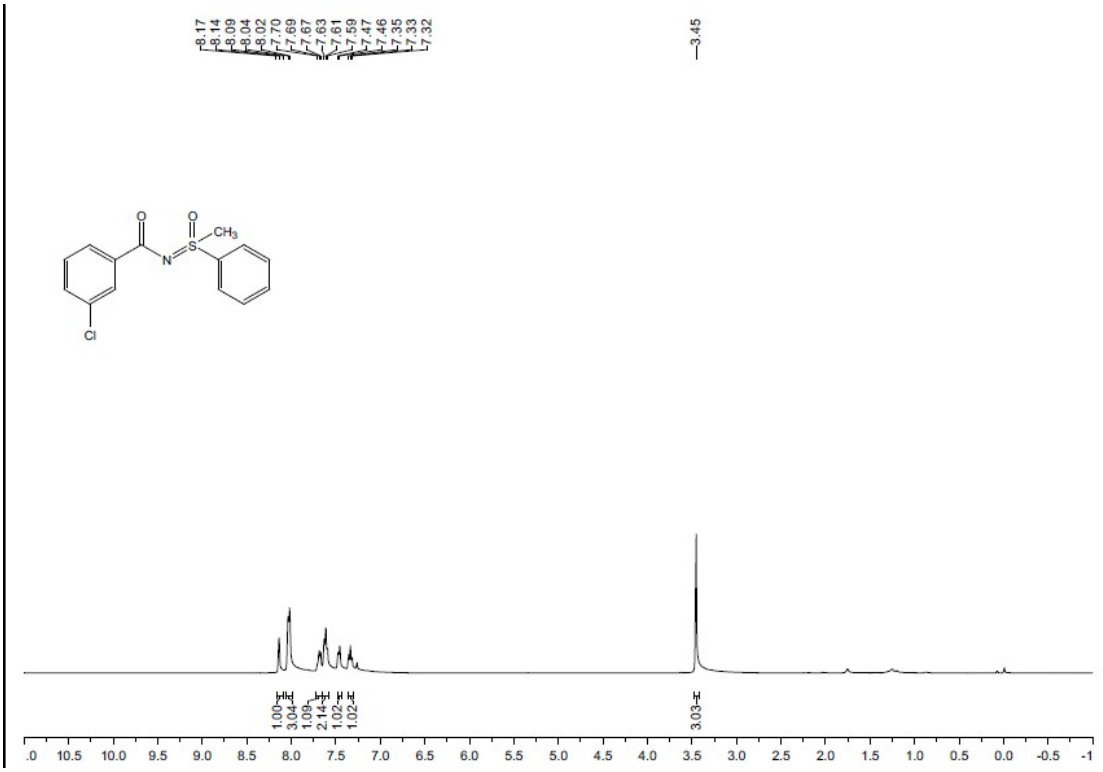
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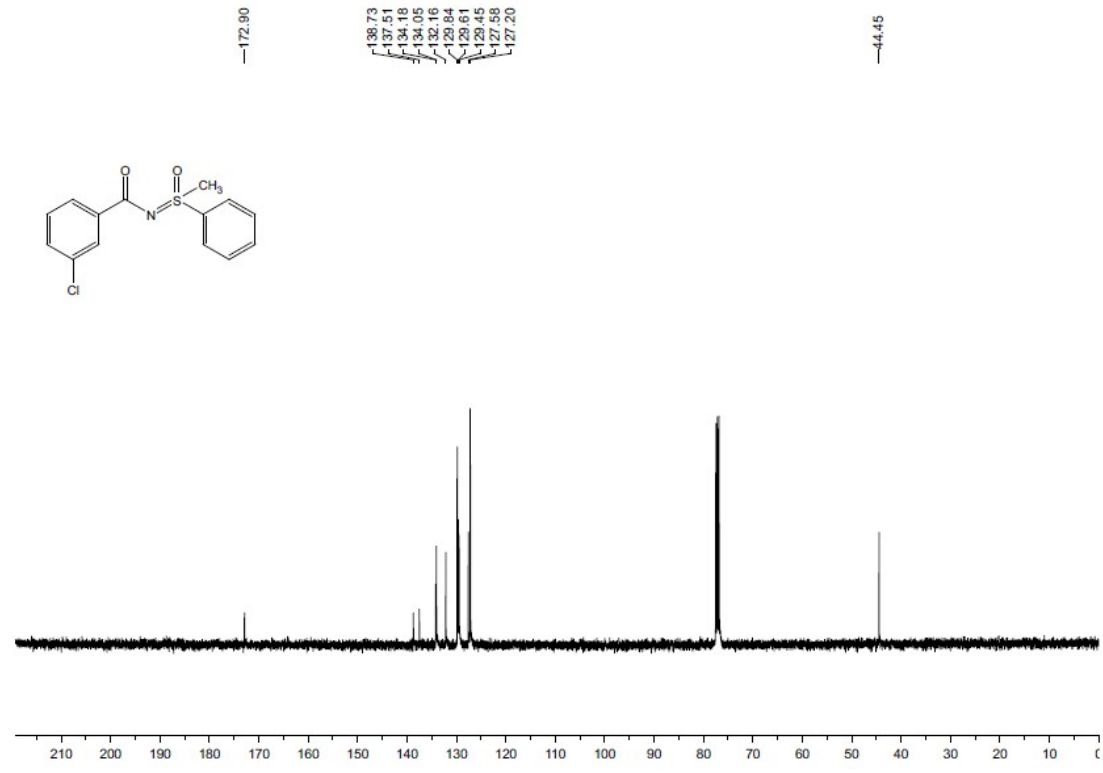
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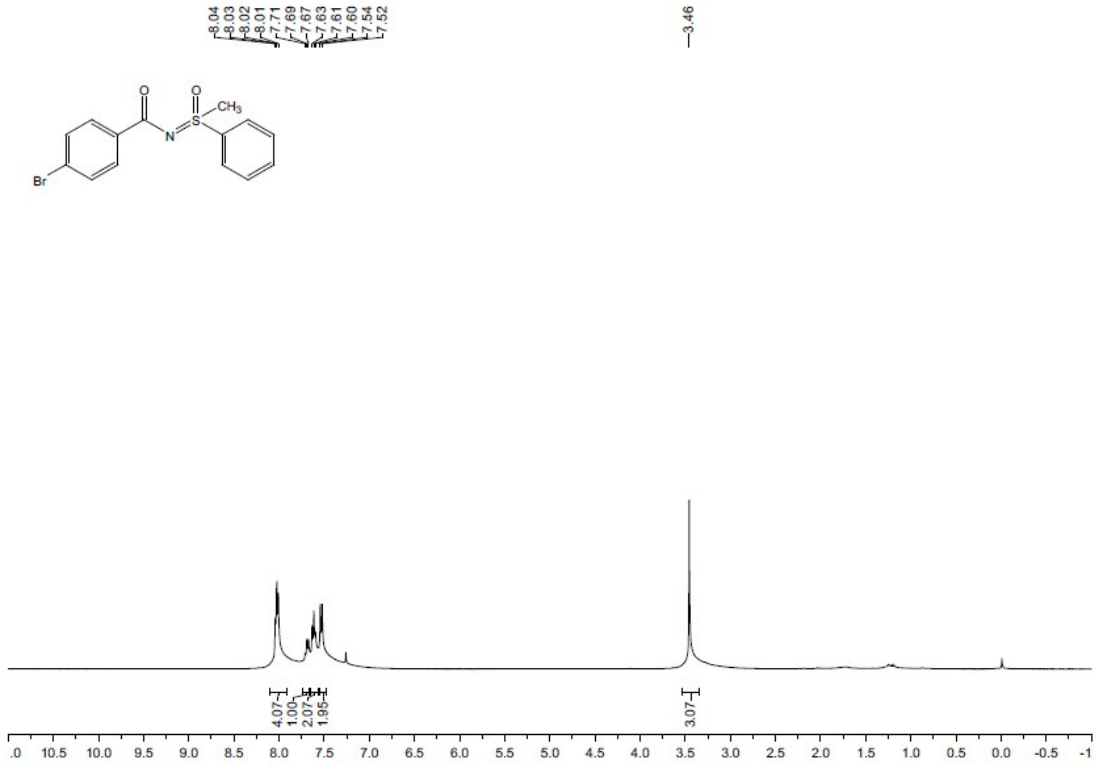
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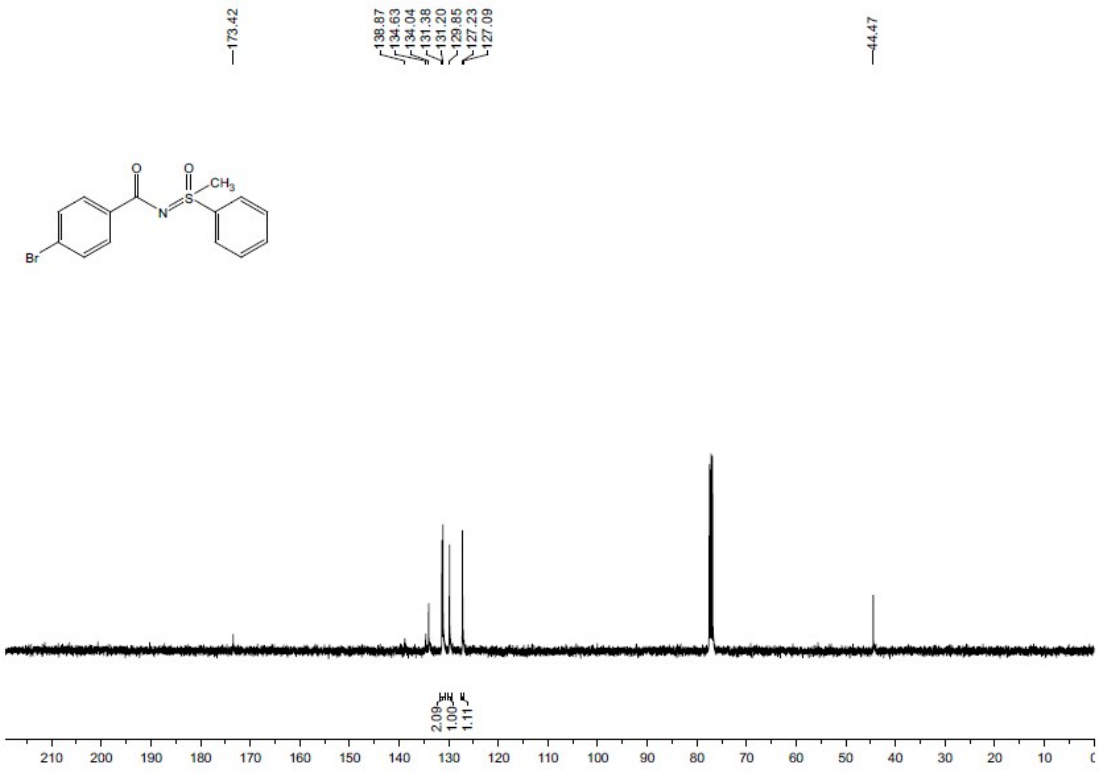
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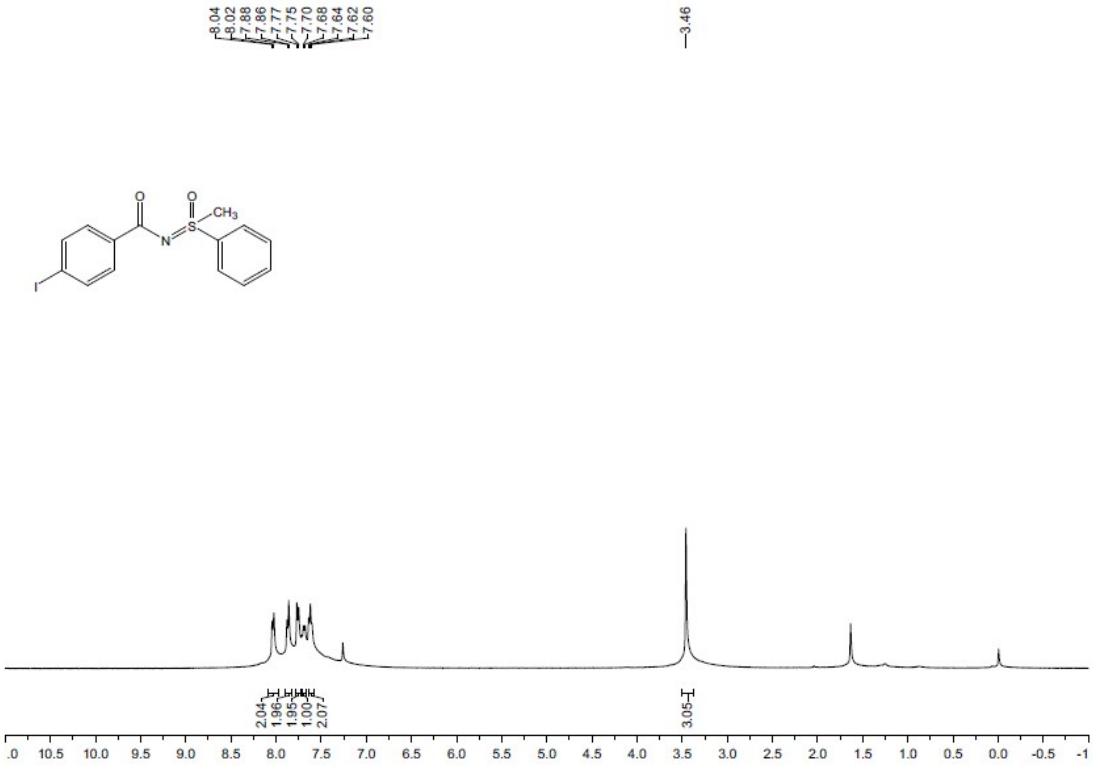
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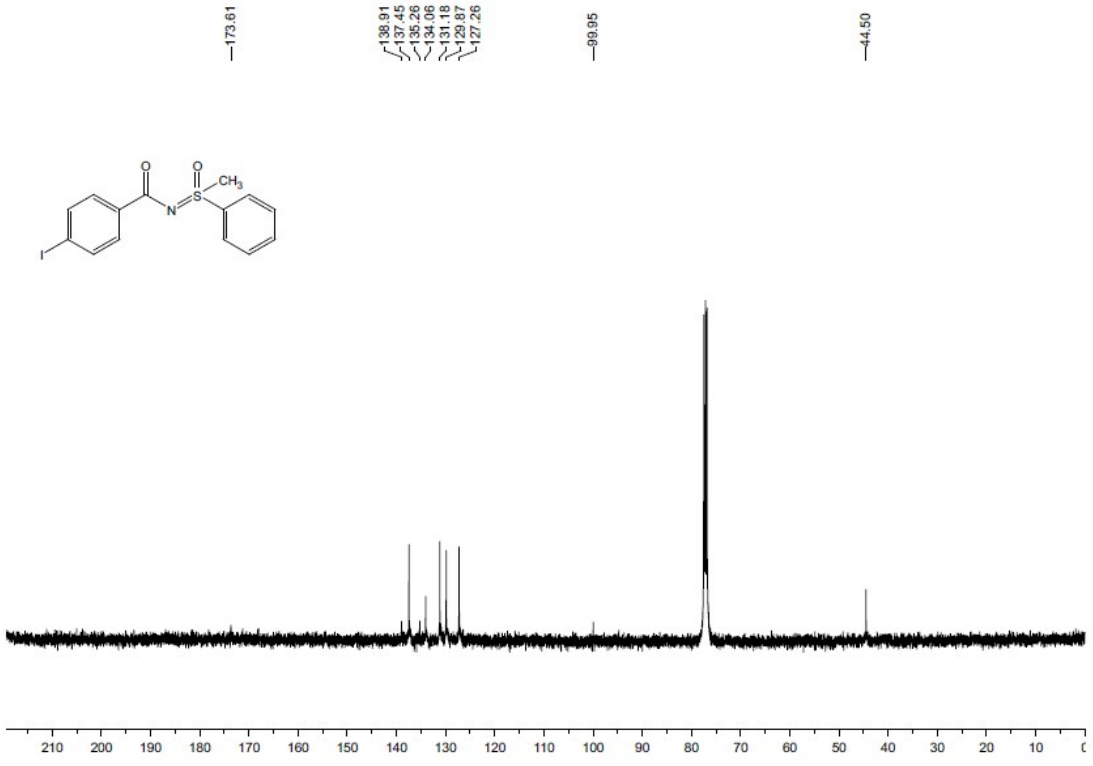
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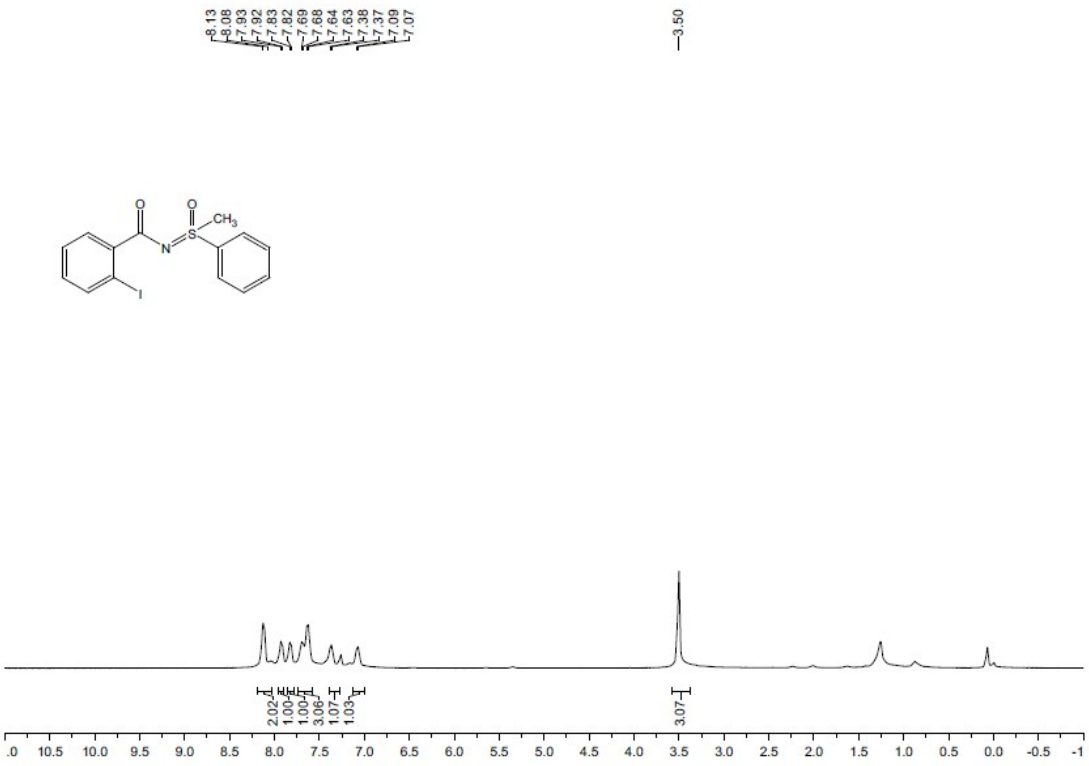
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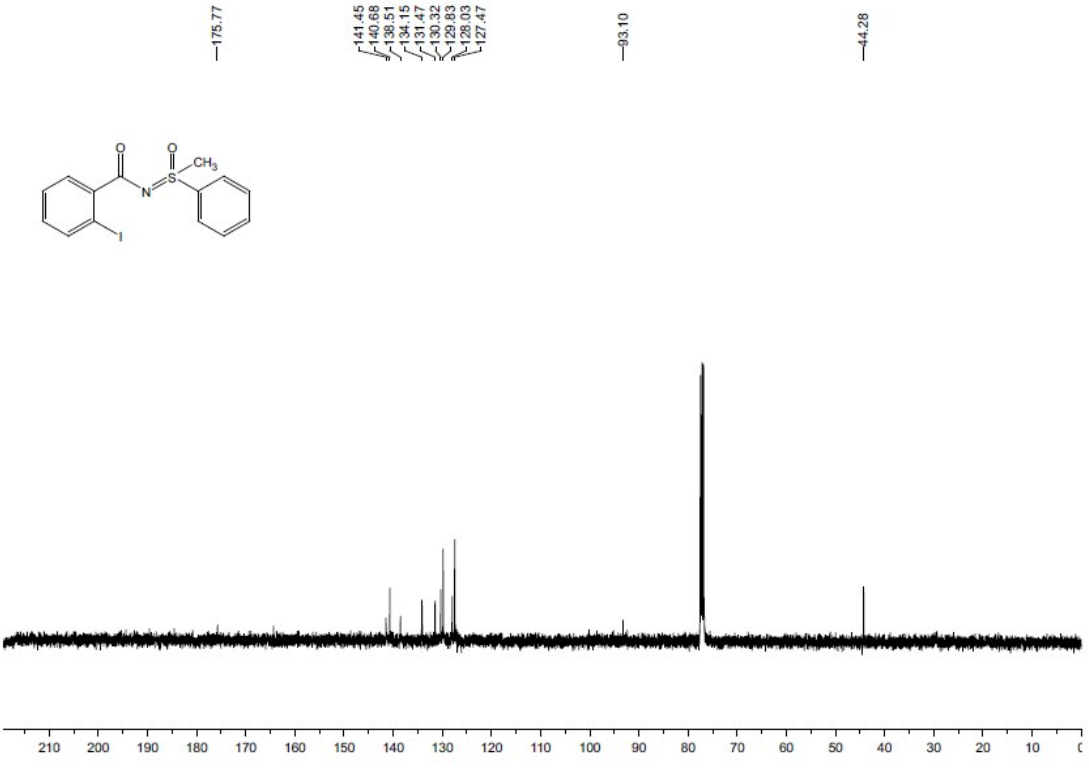
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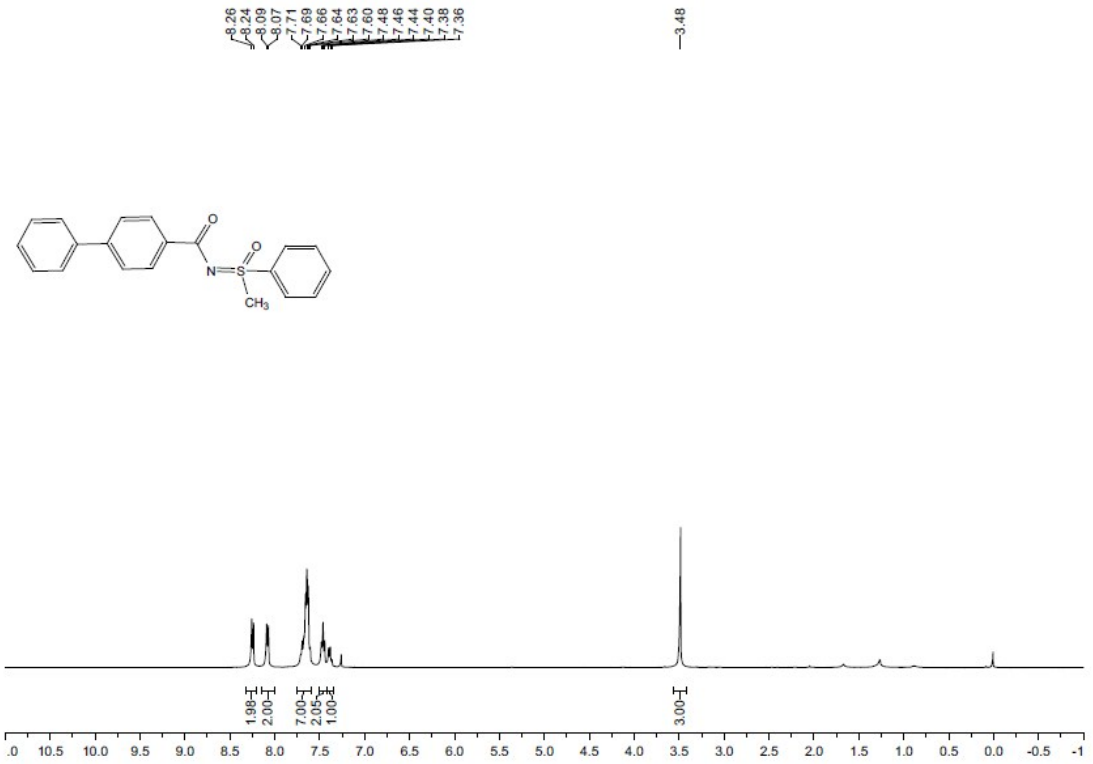
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S
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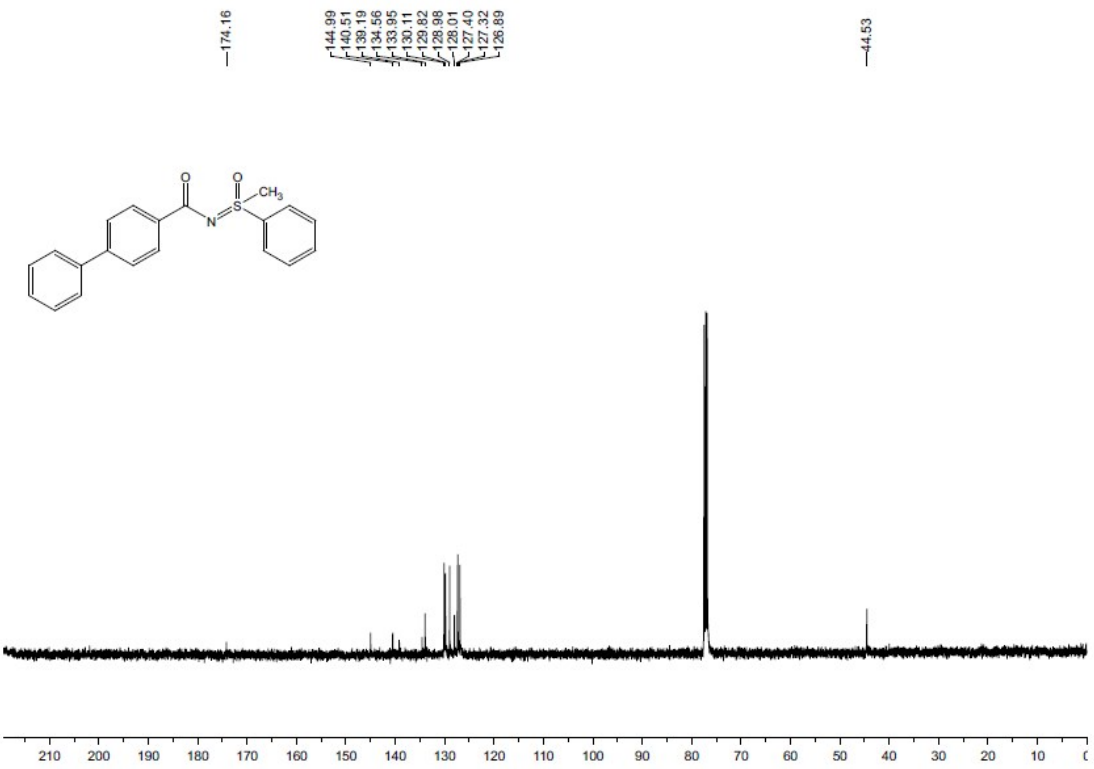
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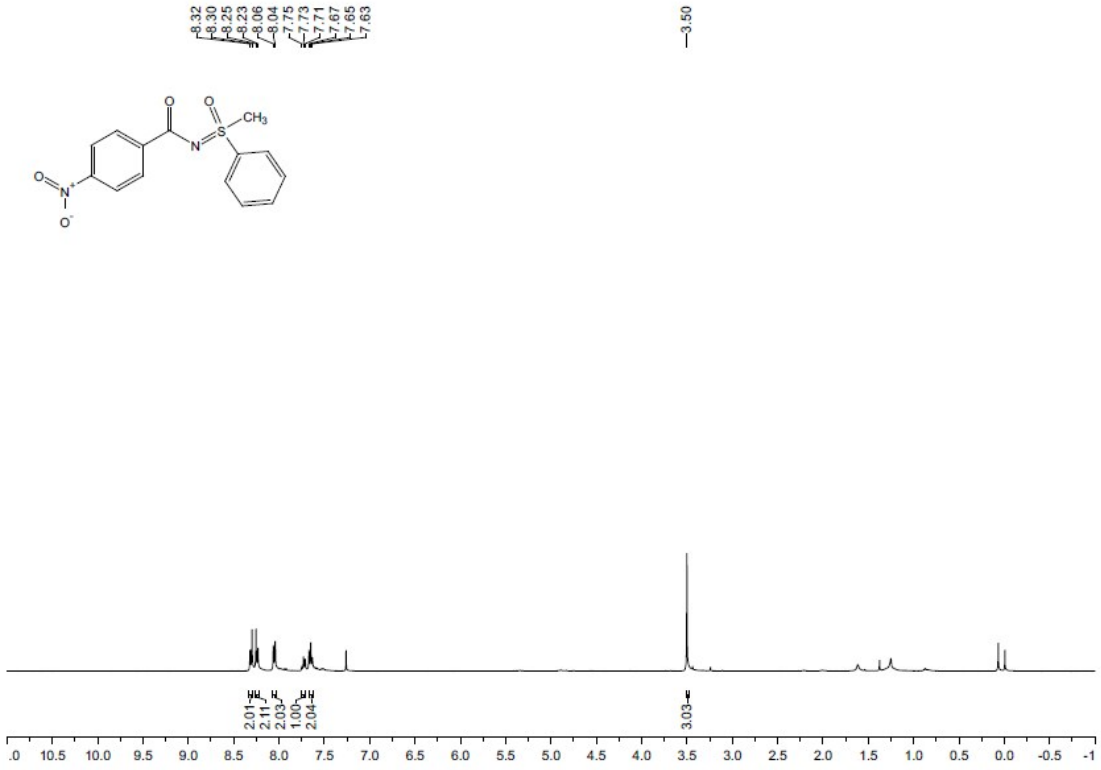
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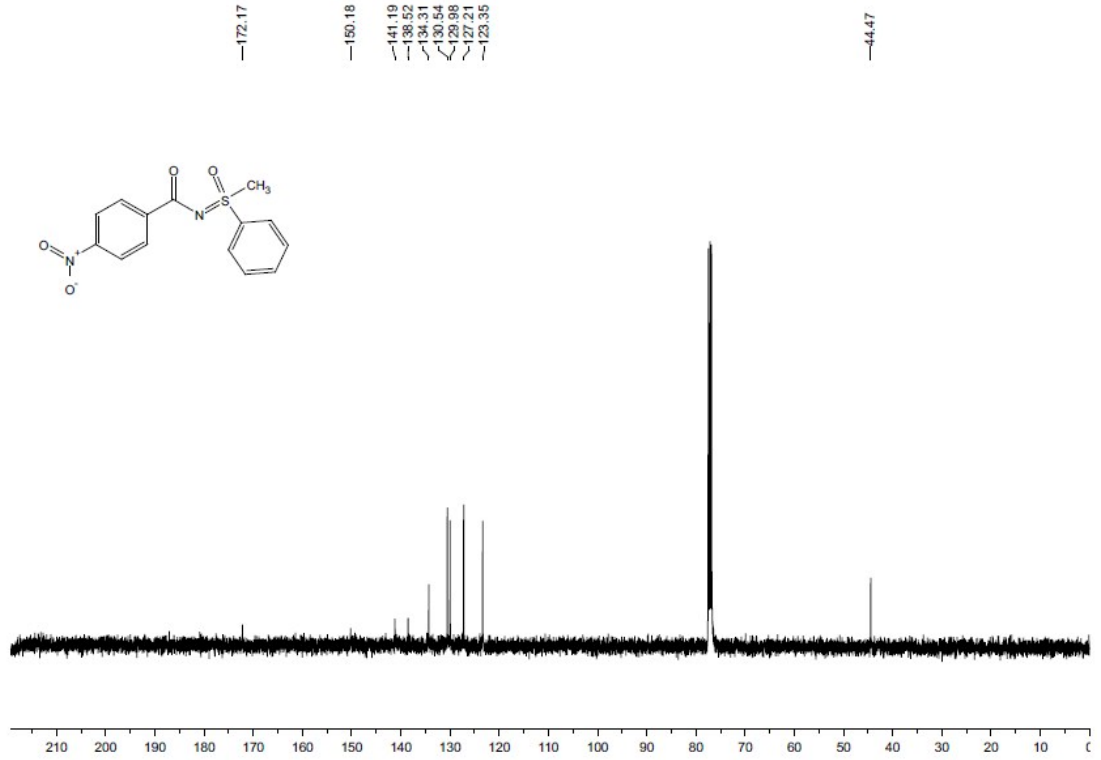
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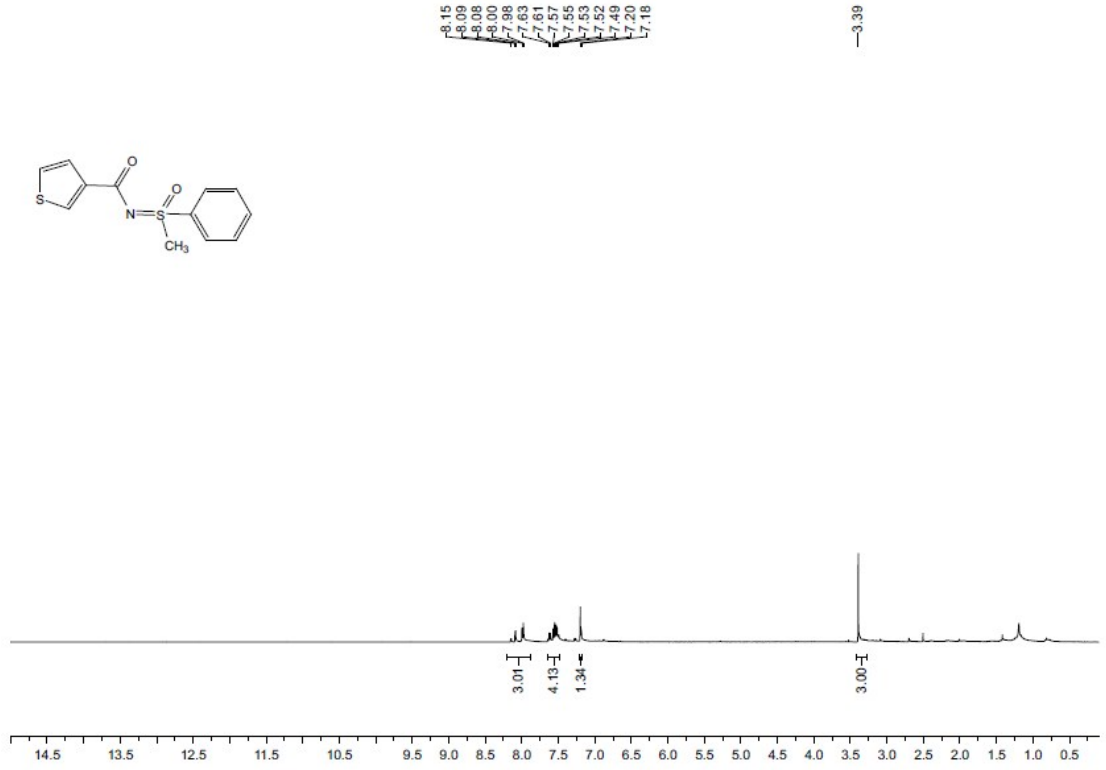
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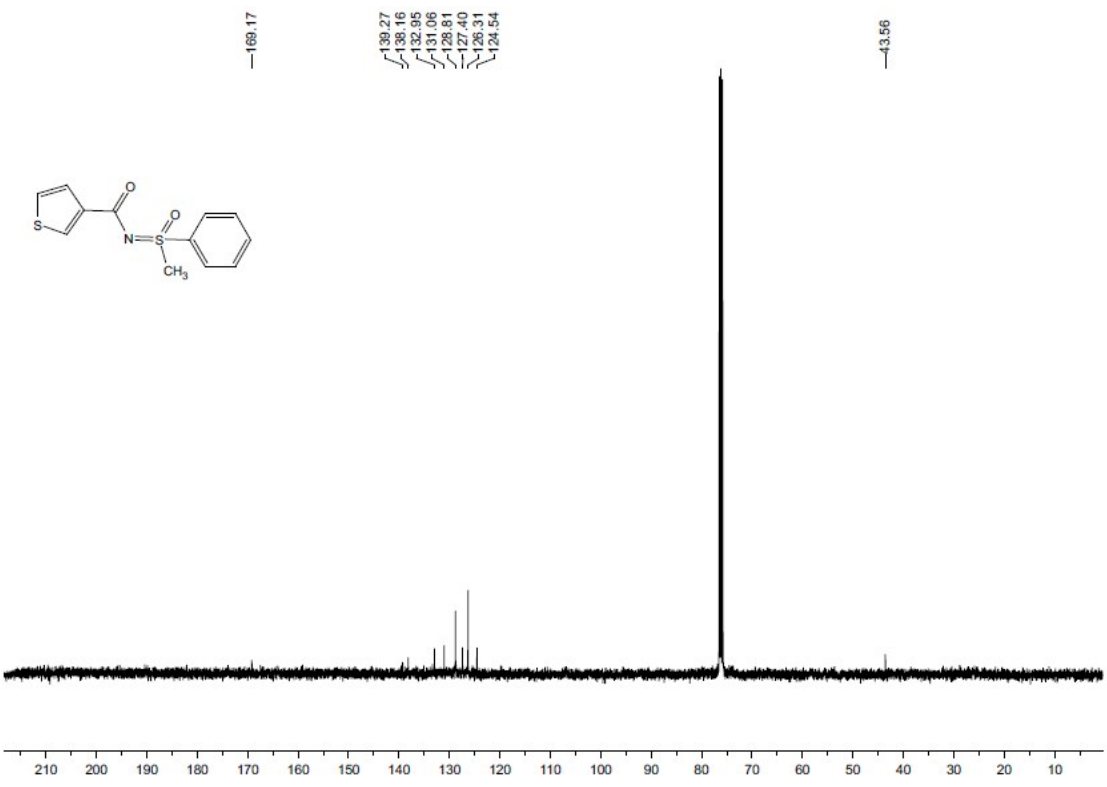
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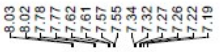
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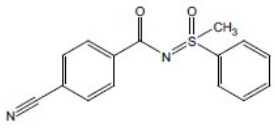
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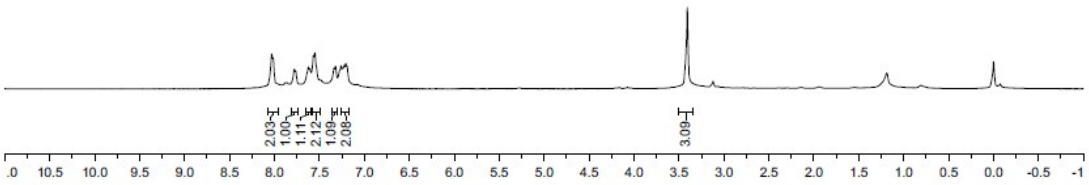
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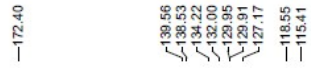
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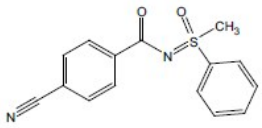
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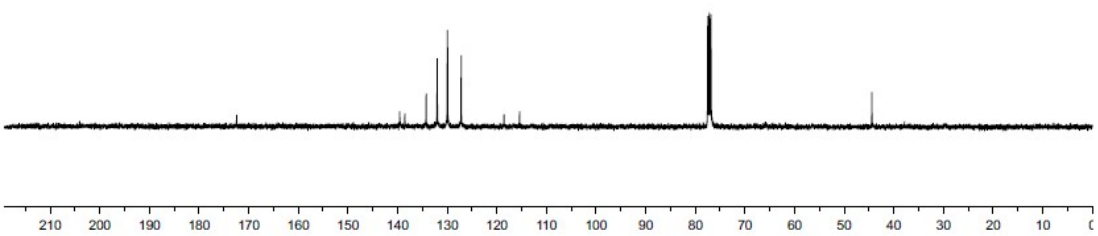
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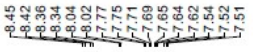
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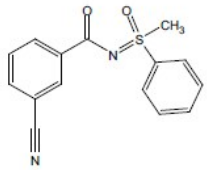
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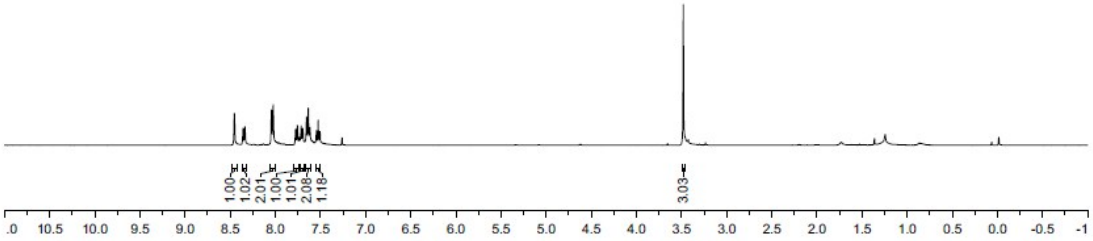
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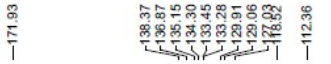
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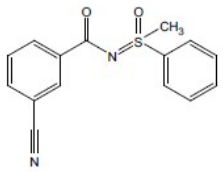
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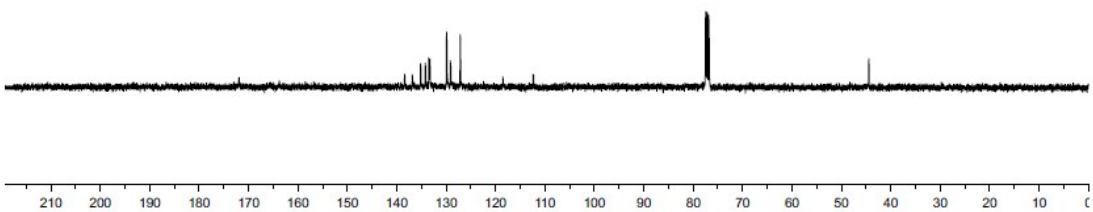
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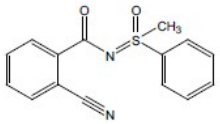
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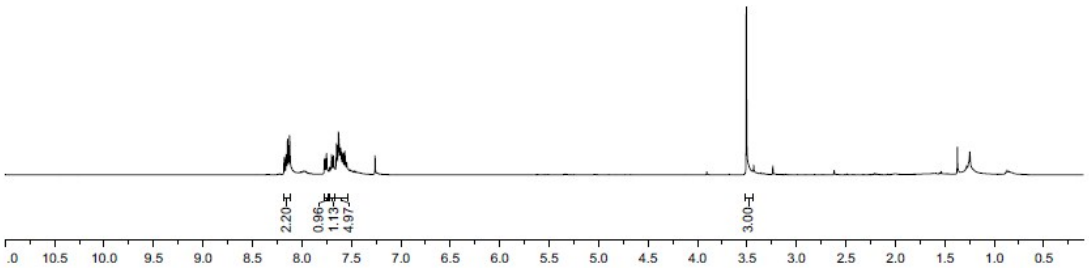
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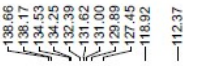
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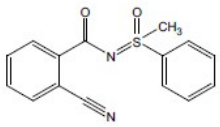
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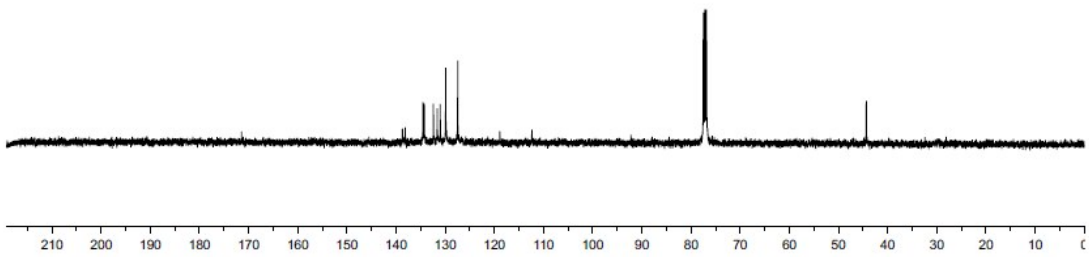
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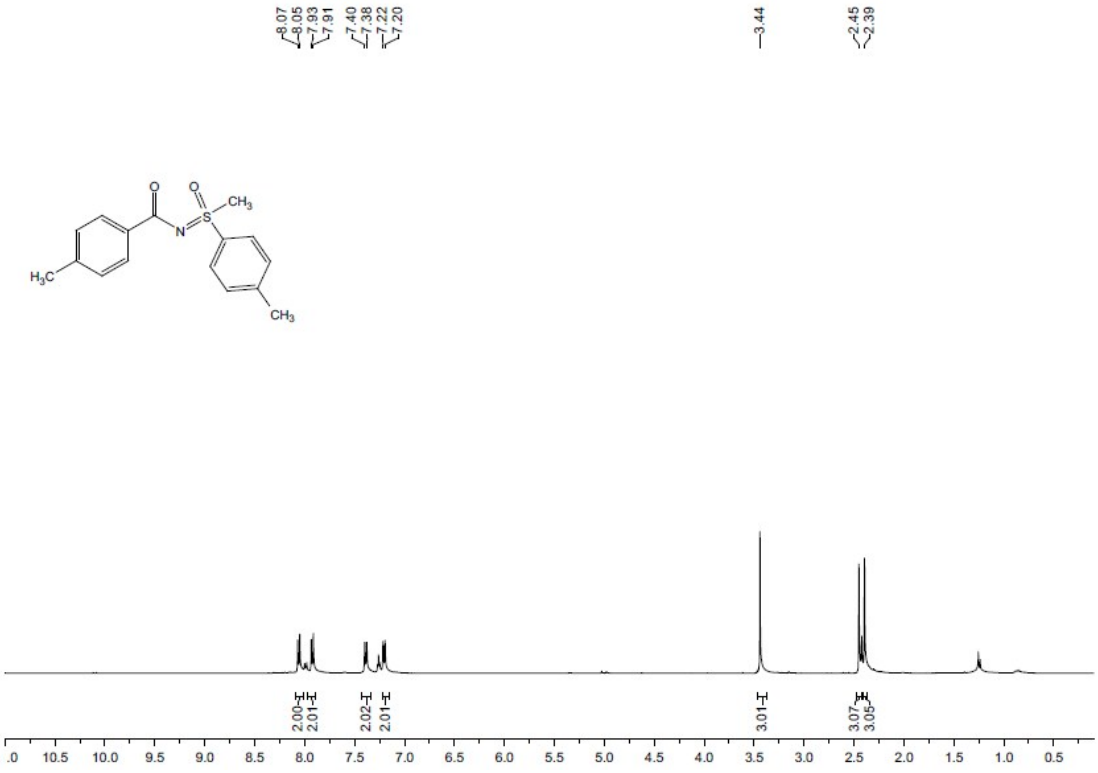
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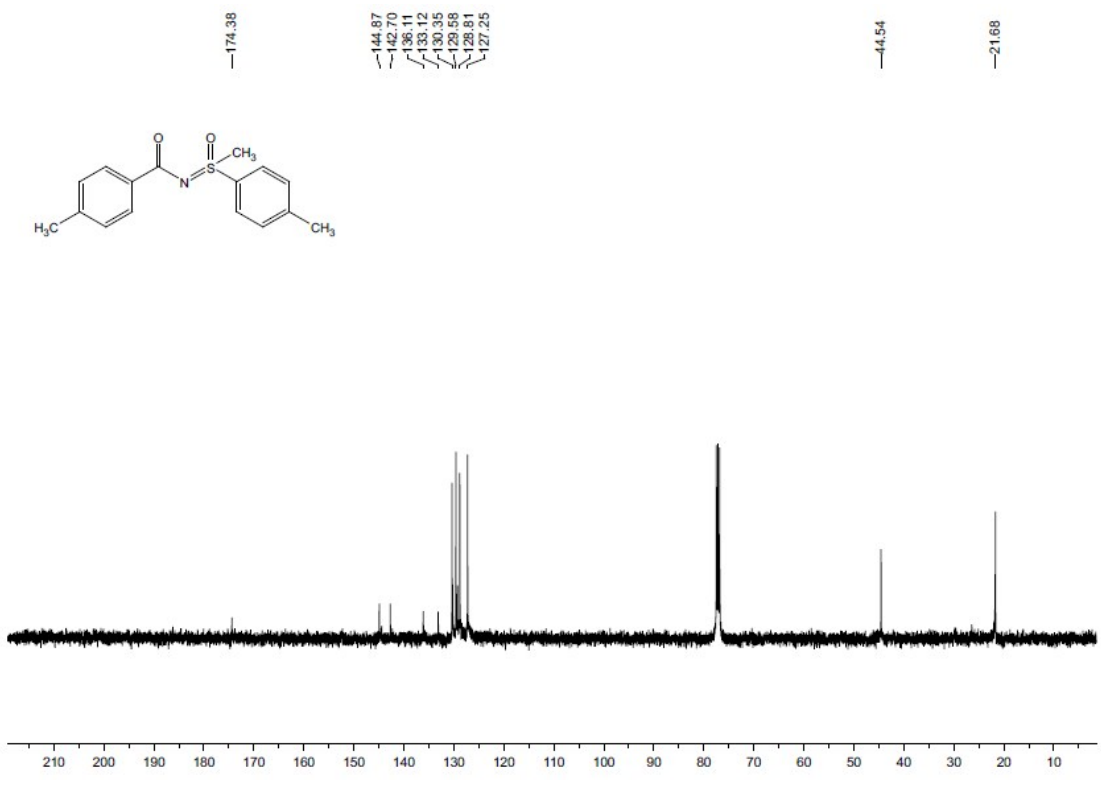
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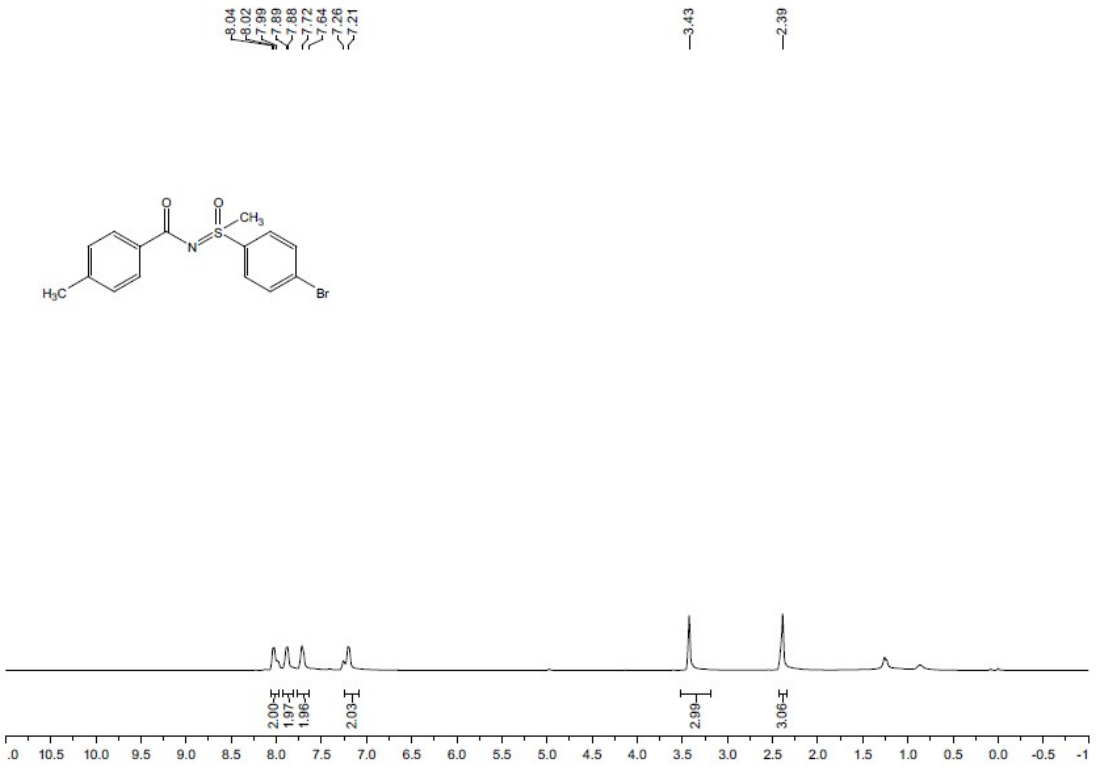
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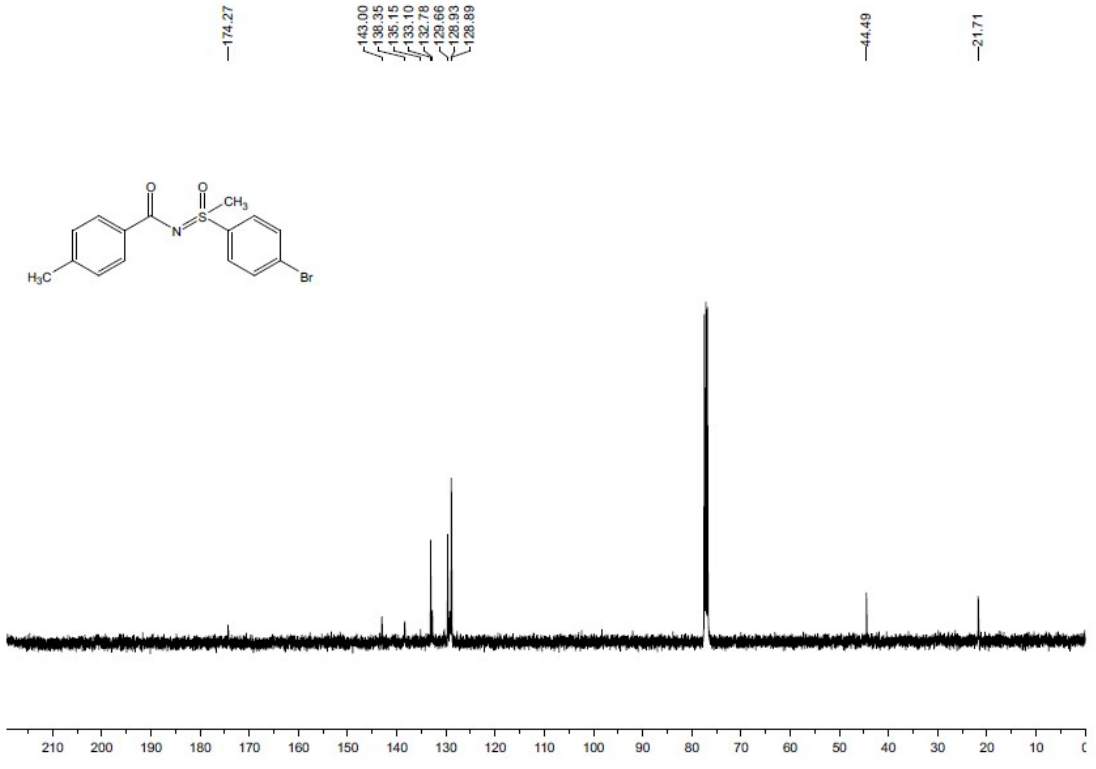
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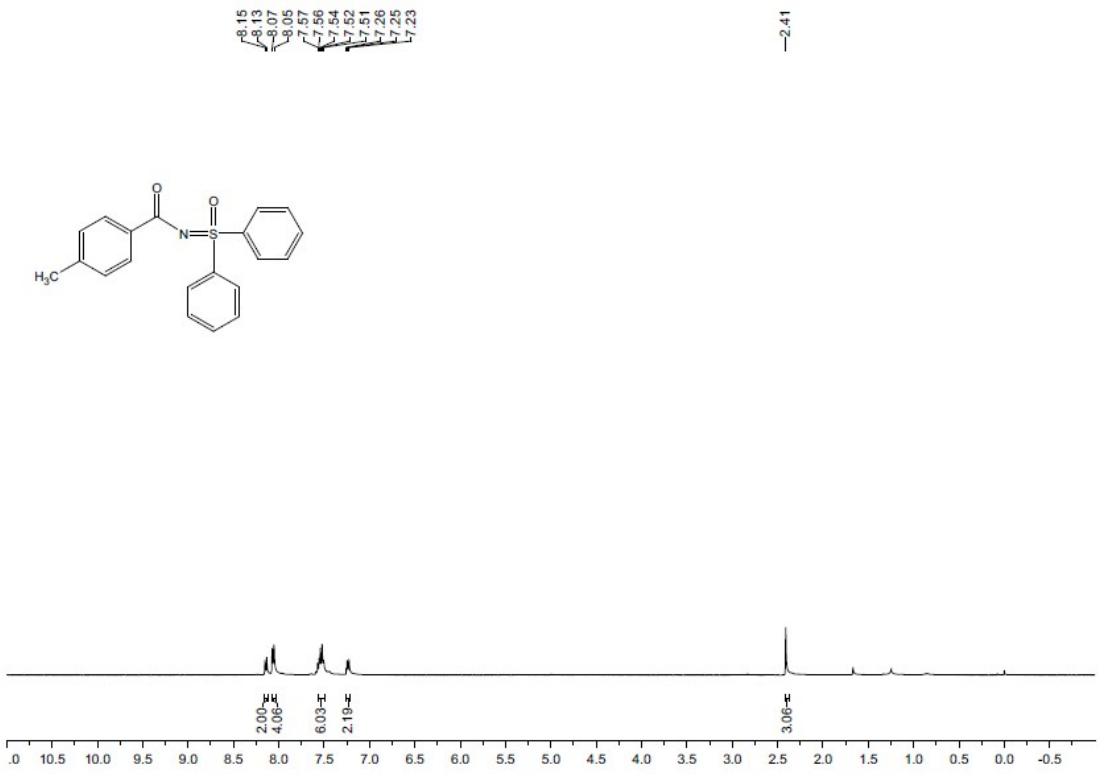
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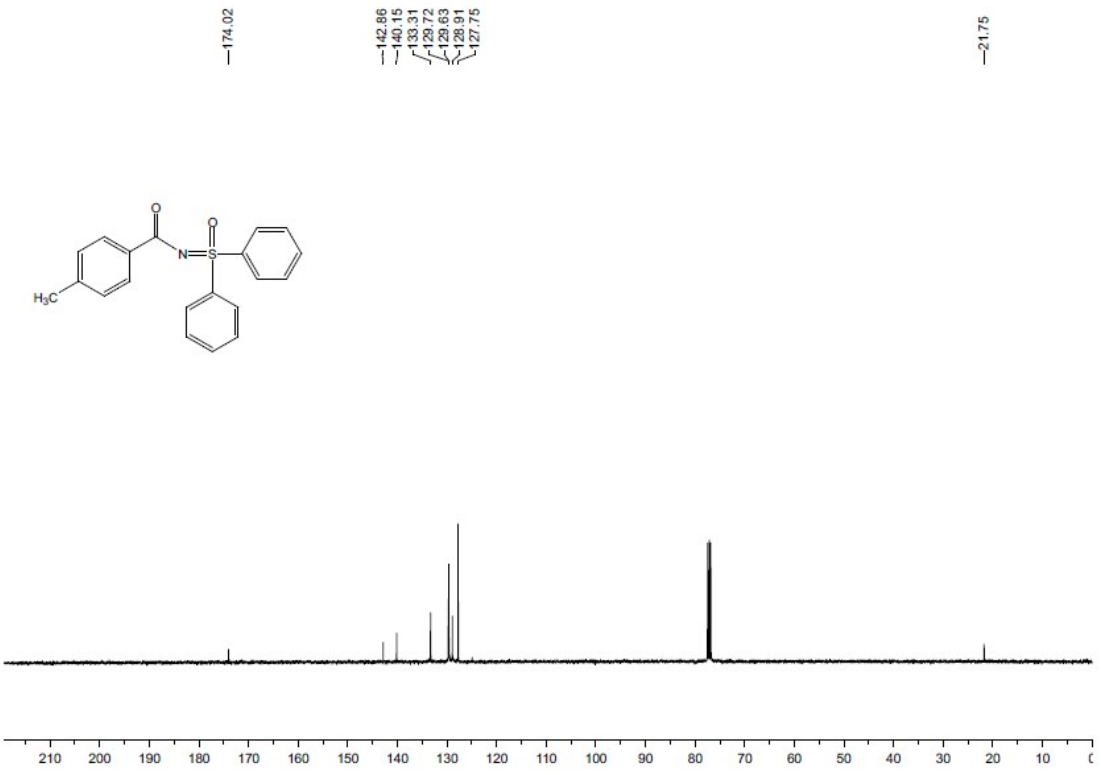
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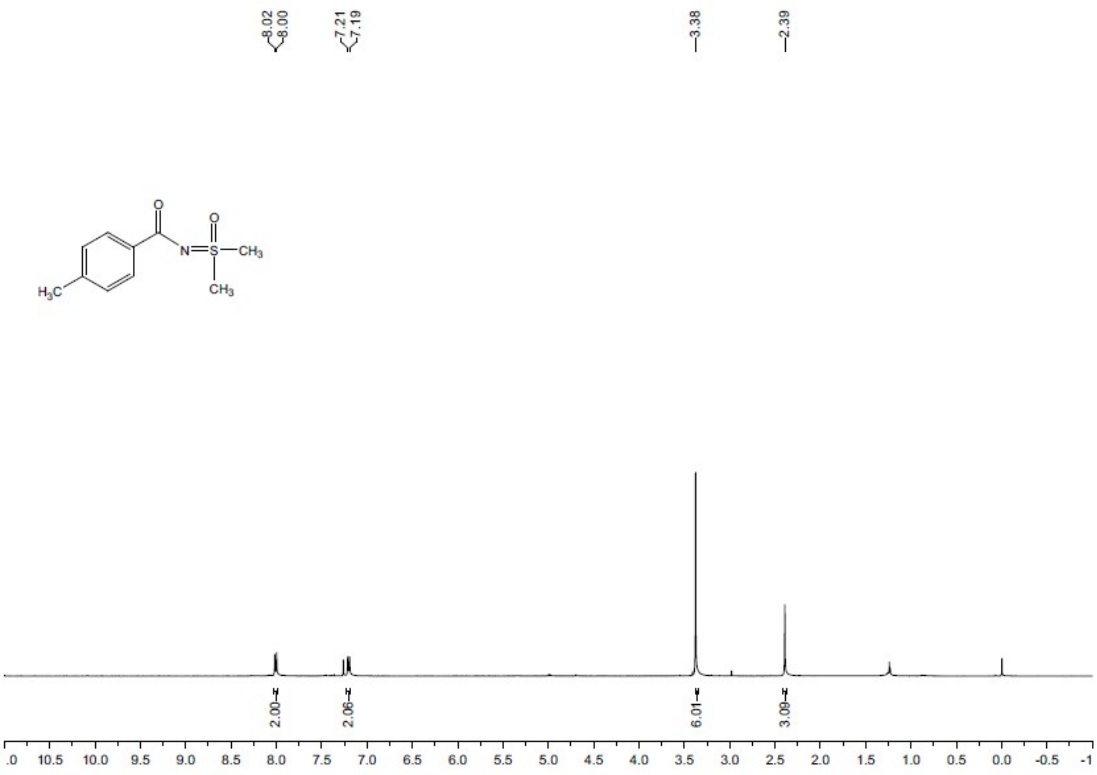
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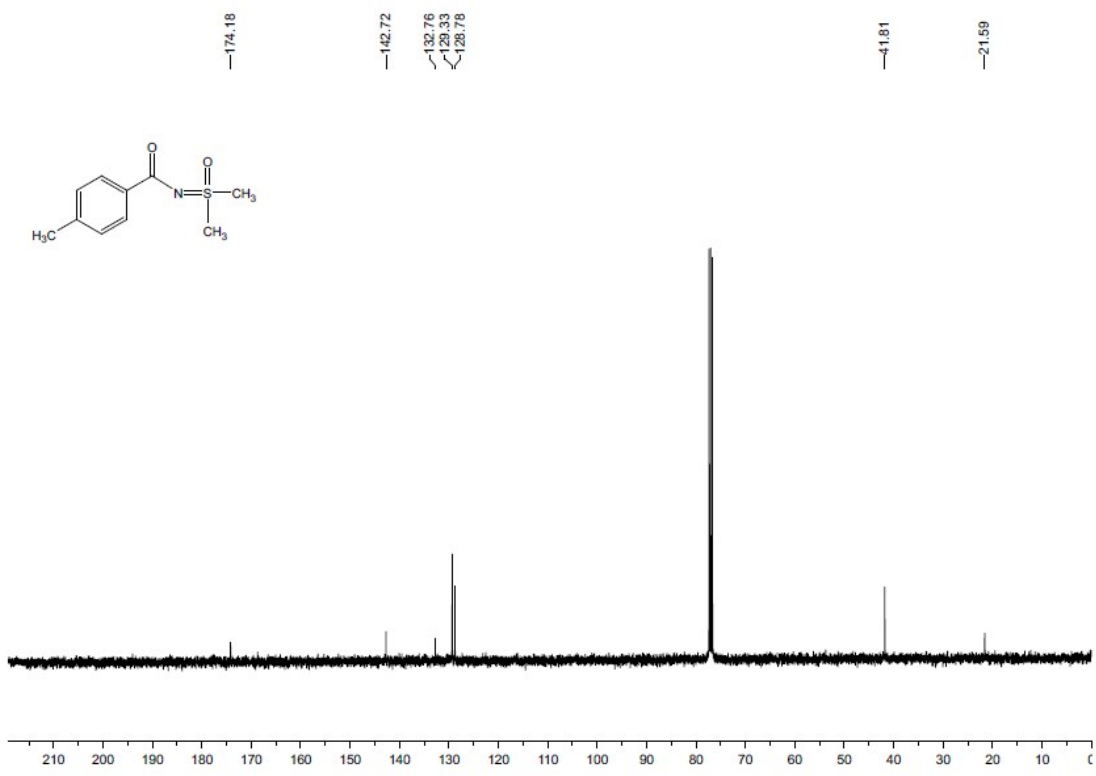
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