Supporting Information
for

N-Arylations of Sulfoximines with 2-Arylpyridines by Copper-Mediated Dual N-H/C-H Activation

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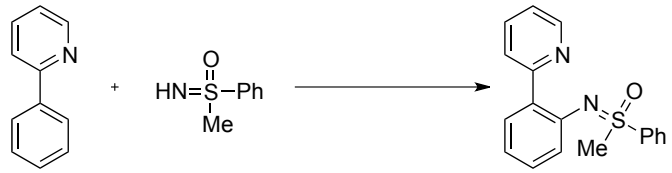
General information

All reagents were purchased from Sigma-Aldrich, Acros or Alfa Aesar and were used without further purification. The substituted 2-phenylpyridines were prepared by following the literature procedure for the Suzuki coupling of the corresponding aryl boronic acid with 2-bromopyridine.[S1] Sulfoximines were prepared according to literature procedures by treating sulfoxides with sodium azide and concentrated sulfuric acid.[S2]

All product mixtures were analyzed by thin layer chromatography using aluminum foil backed silica TLC plates with a fluorescent indicator from Merck. UV-active compounds were detected with a UV lamp (λ = 254 nm). For flash column chromatography, silica gel was used as the stationary phase. ^{1}H and ^{13}C NMR spectra were recorded either on a Varian V-NMRS 600, Varian V-NMRS 400 in deuterated chloroform at 25 °C. Chemical shifts (d) are reported in ppm, and spin-spin coupling constants (*J*) are given in Hz, while multiplicities are abbreviated by br s (broad singlet), s (singlet), d (doublet), t (triplet), q (quartet) and m (multiplet). High resolution mass spectra (HRMS) were recorded on a Thermo Scientific LTQ Orbitrap XL spectrometer [electrospray ionisation (ESI) in positive ion mode]. Analytical high-performance liquid chromatography (HPLC) measurements for the determination of enantiomers were performed with an Agilent 1100-series system and a chiral stationary phase (Chiralcel AD-H: 250 mm × 4.6 mm) from Chiral Technologies Inc. Melting points (M.P.) were determined in open-end capillary tubes on a Büchi B-540 melting point apparatus.

Specific Experimental:

Table S1. Reaction condition screening for oxidative coupling between 2-phenylpyridine and sulfoximine

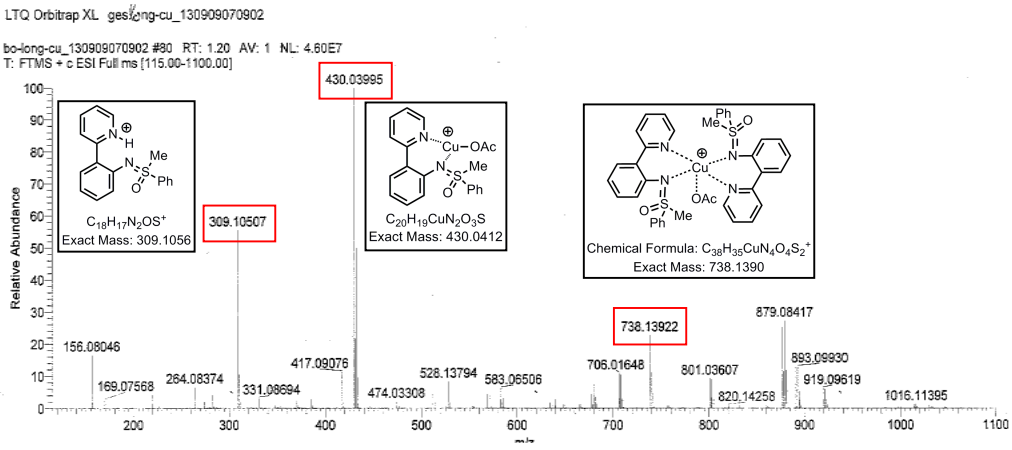


4a **5a** **6a**

Entry[a]	Metal (Equiv)	Oxidant	Solvent	Temp. (°C)	Additive (Equiv)	Yield (%)
1	$Cu(OAc)_2•H_2O$ (1.0)	air	CH_3CN	130	-	26
2	$CuBr_2$ (1.0)	air	CH_3CN	130	-	-
3	$CuCl_2$ (1.0)	air	CH_3CN	130	-	trace
4	$Pd(OAc)_2$ (0.10)	air	CH_3CN	130	-	-
5	$Pd(OAc)_2$ (0.10)	$K_2S_2O_8$	DCE	130	-	-
6	CuBr (0.10)	*t*-BuO-O*t*-Bu	PhMe	120	-	-
7	CuBr (0.10)	*t*-BuO-O*t*-Bu	neat	130	-	-
8	$Cu(OAc)_2•H_2O$ (1.0)	air	DMF	130	-	trace
9	$Cu(OAc)_2•H_2O$ (1.0)	air	DMSO	130	-	trace
10	$Cu(OAc)_2•H_2O$ (1.0)	air	1,4-dioxane	130	-	trace
11	$Cu(OAc)_2•H_2O$ (1.0)	air	PhMe	130	-	trace
12	$Cu(OAc)_2•H_2O$ (1.0)	air	xylene	145	-	trace
13	$Cu(OAc)_2•H_2O$ (1.0)	air	anisole	160	-	trace
14	$Cu(OAc)_2•H_2O$ (1.0)	O_2	CH_3CN	130	-	38
15	$Cu(OAc)_2•H_2O$ (1.0)	O_2	CH_3CH_2CN	150	-	55
16	$Cu(OAc)_2•H_2O$ (1.0)	O_2	CH_3CH_2CN	150	pyridine (1.0)	-
17	**$Cu(OAc)_2•H_2O$ (1.0)**	**O_2**	**CH_3CH_2CN**	**150**	**AcOH (0.5)**	**80**
18	**$Cu(OAc)_2•H_2O$ (1.0)**	**O_2**	**CH_3CH_2CN**	**150**	**2-nitrobenzoic acid (0.5)**	**74**
19	$Cu(OAc)_2•H_2O$ (0.20)	O_2	CH_3CH_2CN	150	AcOH (0.5)	22

a Reactions were performed on a 0.5 mmol scale.

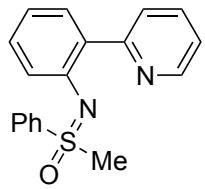
MS analysis of the reaction mixture prior to work-up:



General Procedure A: To a 20 mL sealable reaction tube with a magnetic stirring bar was added $Cu(OAc)_2 \bullet H_2O$ (100 mg, 0.50 mmol) and the reaction tube was back filled with molecular oxygen. To this reaction vessel was then added a solution containing the substituted 2-aryl pyridine (0.50 mmol), the sulfoximine (1.0 mmol), glacial acetic acid (15 mg, 0.25 mmol) and propanenitrile (1 mL). The tube was sealed and heated to 150 ^oC for 24 h. After this time, the reaction mixture was cooled to room temperature and diluted with CH_2Cl_2 (15 mL) The organic phase was washed with Na_2S (10 mL, saturated aqueous solution) and separated. The aqueous phase was then extracted with additional CH_2Cl_2 (2 x 15 mL). The combined organic phases were filtered over a short pad of celite, and the solvent then concentrated under vacuum. Purification by silica gel column chromatography afforded the arylated sulfoximine **6**.

General Procedure B: As General Procedure A, but with the use of 2-nitrobenzoic acid (42 mg, 0.25 mmol) instead of glacial acetic acid.

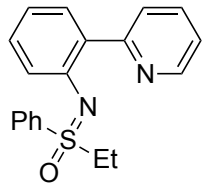
***N*-(2-Pyridinylphenyl)-*S*-methyl-*S*-phenylsulfoximine (6a)**



General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 123 mg (80%), colorless viscous oil. ^1H NMR (600 MHz, $CDCl_3$) δ = 8.72 (s, 1H), 8.00 (d, *J* = 7.2 Hz, 1H), 7.78 – 7.70(m, 3H), 7.61 (d, *J* = 7.2 Hz, 1H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.25 – 7.11 (m, 3H), 7.03 (t, *J* = 7.2 Hz, 1H), 3.07 (s, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$) δ = 158.6, 149.1, 142.3, 139.4, 135.1, 133.1, 130.7, 129.3, 129.1, 128.4, 125.5, 123.3, 122.4, 121.3, 45.0 ppm; ESI-HRMS (*m/z*) $[C_{18}H_{16}N_2OS + H]^+$ Calcd. 309.1056, Found 309.1064.

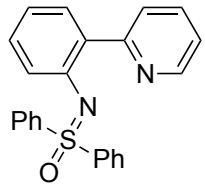
Following General Procedure A with enantiopure (*S*)-**5a** afforded optically active **6a**, $\{[\alpha]_D^{20} = -149.4$ (sample of 10.0 mg in 2 mL $CHCl_3)\}$ in a comparable yield to that reported for the reaction of racemic **5a**. HPLC: t_r = 12.6 min (minor), t_r = 14.9 min (major); Chiralcel AD-H, 0.8 mL/min, *n*-heptane/isopropanol = 85/15, λ = 254 nm, 20 °C; e.r. = >99.5:0.5

***N*-(2-Pyridinylphenyl)-*S*-ethyl-*S*-phenylsulfoximine (6b)**



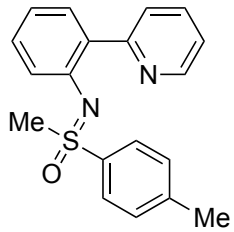
General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 116 mg (72%), colorless viscous oil. ^1H NMR (400 MHz, $CDCl_3$) δ = 8.73 (d, *J* = 4.4 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.76 – 7.70 (m, 3H), 7.60 (dd, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 7.53 (tt, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 2H), 7.25 – 7.20 (m, 1H), 7.15 (dd, *J* = 8.0 Hz, *J* = 1.2 Hz, 1H), 7.08 (td, *J* = 7.8 Hz, *J* = 1.2 Hz, 1H), 6.99 (td, *J* = 7.8 Hz, *J* = 1.2 Hz, 1H), 3.20 (q, *J* = 7.2 Hz, 2H), 1.12 (t, *J* = 7.2 Hz, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.6, 149.1, 142.5, 137.1, 134.9, 134.7, 133.1, 130.6, 129.3, 129.2, 129.1, 125.7, 122.8, 122.0, 121.2, 51.8, 7.8 ppm; ESI-HRMS (*m/z*) $[C_{19}H_{18}N_2OS + H]^+$ Calcd. 323.1213, Found 323.1223.

_N_-(2-Pyridinylphenyl)-_S,S_-diphenylsulfoximine (6c)



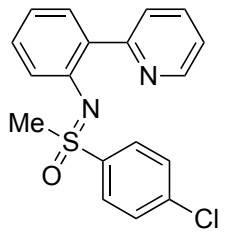
General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 127 mg (69%), white solid, m.p. 120 – 121 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.82 – 8.78 (m, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.87 – 7.82 (m, 4H), 7.78 (td, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 7.58 (dd, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 7.43 (tt, *J* = 7.6 Hz, *J* = 1.6 Hz, 2H), 7.38 – 7.32 (m, 4H), 7.31 – 7.27 (m, 1H), 7.23 (dd, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H), 7.08 (td, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 6.99 (td, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.9, 149.2, 142.1, 140.8, 135.2, 135.1, 132.5, 130.5, 129.1, 128.5, 125.9, 123.2, 122.2, 121.4 ppm; ESI-HRMS (*m/z*) $[C_{23}H_{18}N_2OS + H]^+$ Calcd. 371.1213, Found 371.1222.

_N_-(2-Pyridinylphenyl)-_S_-methyl-_S_-(4-methylphenyl)sulfoximine (6d)



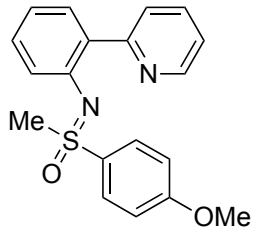
General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 124 mg (77%), colorless viscous oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.73 – 8.70 (m, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.72 (td, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 7.65 – 7.58 (m, 3H), 7.25 – 7.15 (m, 4H), 7.13 (td, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 7.02 (td, *J* = 7.6 Hz, *J* = 1.2 Hz, 1H), 3.05 (s, 3H), 2.37 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.6, 149.1, 144.0, 142.5, 136.3, 135.0, 134.9, 130.6, 129.9, 129.1, 128.4, 125.6, 123.3, 122.3, 121.3, 45.2, 21.5 ppm; ESI-HRMS (*m/z*) $[C_{19}H_{18}N_2OS + H]^+$ Calcd. 323.1213, Found 323.1222.

_N_-(2-Pyridinylphenyl)-_S_-methyl-_S_-(4-chlorophenyl)sulfoximine (6e)



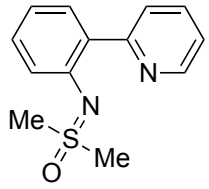
General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 140 mg (82%), pale yellow viscous oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.73 – 8.70 (m, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.73 (td, *J* = 7.8 Hz, *J* = 1.8 Hz, 1H), 7.68 (d, *J* = 9.0 Hz, 2H), 7.58 (dd, *J* = 7.8 Hz, *J* = 1.8 Hz, 1H), 7.39 (d, *J* = 9.0 Hz, 2H), 7.26 – 7.22 (m, 1H), 7.20 – 7.13 (m, 2H), 7.05 (td, *J* = 7.8 Hz, *J* = 1.8 Hz, 1H), 3.08 (s, 3H) ppm; ^{13}C NMR (150MHz, $CDCl_3$) δ = 158.6, 149.1, 141.9, 139.9, 137.9, 135.2, 135.1, 130.7, 129.9, 129.6, 129.2, 125.4, 123.3, 122.7, 121.4, 45.1 ppm; ESI-HRMS (*m/z*) $[C_{18}H_{15}N_2ClOS + H]^+$ Calcd. 343.0666, Found 343.0678.

_N_-(2-Pyridinylphenyl)-_S_-methyl-_S_-(4-methoxyphenyl)sulfoximine (6f)



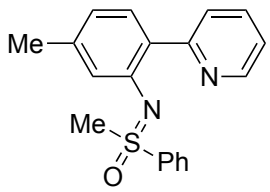
General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 103 mg (61%), pale yellow viscous oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.73 (d, *J* = 4.0 Hz, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.73 (td, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 7.68 (d, *J* = 8.8 Hz, 2H), 7.61 (dd, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 7.25 – 7.11(m,3H), 7.03 (td, *J* = 7.6 Hz, *J* = 1.6 Hz, 1H), 7.68 (d, *J* = 8.8 Hz, 2H), 3.82 (s, 3H), 3.06 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ = 163.3, 158.6, 149.1, 142.6, 135.1, 134.9, 130.6, 130.5, 129.1, 125.5, 123.3, 122.3, 121.3, 114.5, 55.6, 45.4 ppm; ESI-HRMS (*m/z*) $[C_{19}H_{18}N_2O_2S + H]^+$ Calcd. 339.1162, Found 339.1169.

***N*-(2-Pyridinylphenyl)-*S*,*S*-dimethylsulfoximine (6g)**



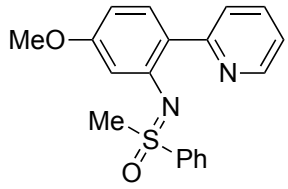
General procedure B was followed using ethyl acetate/pentane (1:1) as eluent; yield: 68 mg (55%), colorless viscous oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.64 (d, *J* = 4.0 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.70 – 7.60 (m, 2H), 7.32 – 7.25 (m, 2H), 7.21 – 7.10 (m, 2H), 2.96 (s, 6H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.4, 149.0, 142.2, 135.4, 135.2, 130.8, 129.3, 125.1, 124.3, 123.1, 121.3, 41.8 ppm; ESI-HRMS (*m/z*) $[C_{13}H_{14}N_2OS + H]^+$ Calcd. 247.0900, Found 247.0905.

***N*-(2-Pyridinyl-5-methylphenyl)-*S*-methyl-*S*-phenylsulfoximine (6h)**



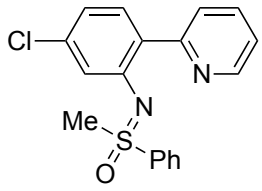
General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 119 mg (74%), colorless viscous oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.71 (s, 1H), 7.99 (d, *J* = 7.2 Hz, 1H), 7.79 – 7.68 (m, 3H), 7.56 – 7.49 (m, 2H), 7.43 (t, *J* = 7.2 Hz, 2H), 7.25 – 7.19 (m, 1H), 7.04 (s, 1H), 6.86 (d, *J* = 7.6 Hz, 2H), 3.07 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ = 158.6, 149.0, 142.0, 139.5, 139.2, 135.1, 133.1, 132.2, 130.5, 129.2, 128.3, 125.5, 124.1, 123.5, 121.1, 44.8, 21.2 ppm; ESI-HRMS (*m/z*) $[C_{19}H_{18}N_2OS + H]^+$ Calcd. 323.1213, Found 323.1226.

***N*-(2-Pyridinyl-5-methoxyphenyl)-*S*-methyl-*S*-phenylsulfoximine (6i)**



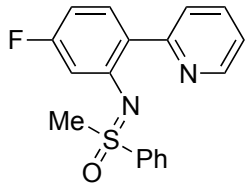
General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 108 mg (64%), pale yellow viscous oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.69 (d, *J* = 4.0 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.79 – 7.75 (m, 2H), 7.70 (td, *J* = 8.0 Hz, *J* = 1.6 Hz, 1H), 7.59 (d, *J* = 8.0 Hz, 1H), 7.57 – 7.50 (m, 1H), 7.44 (t, *J* = 8.0 Hz, 2H), 7.21 – 7.16 (m, 1H), 6.77 (d, *J* = 2.4 Hz, 1H), 6.61 (dd, *J* = 8.0 Hz, *J* = 2.4 Hz, 1H), 3.72 (s, 3H), 3.09 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ = 160.1, 158.2, 149.0, 143.4, 139.3, 135.0, 133.1, 131.6, 129.3, 128.3, 127.9, 125.3, 120.8, 108.6, 108.5, 55.2, 45.0 ppm; ESI-HRMS (*m/z*) $[C_{19}H_{18}N_2O_2S + H]^+$ Calcd. 339.1162, Found 339.1169.

***N*-(2-Pyridinyl-5-chlorophenyl)-*S*-methyl-*S*-phenylsulfoximine (6j)**



General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 139 mg (81%), pale yellow viscous oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.72 (s, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 7.78 – 7.71 (m, 3H), 7.59 – 7.53 (m, 2H), 7.46 (t, *J* = 7.8 Hz, 2H), 7.26 – 7.13 (m, 1H), 7.20 (d, *J* = 1.2 Hz, 1H), 7.00 (dd, *J* = 7.8 Hz, *J* = 1.2 Hz, 1H), 3.11 (s, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$) δ = 157.5, 149.2, 143.6, 138.9, 135.3, 134.4, 133.4, 133.3, 131.6, 129.5, 128.3, 125.4, 122.8, 122.4, 121.6, 45.3 ppm; ESI-HRMS (*m/z*) $[C_{18}H_{15}ClN_2OS + H]^+$ Calcd. 343.0666, Found 343.0677.

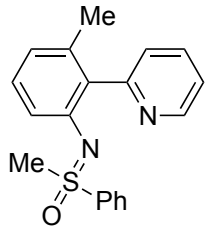
***N*-(2-Pyridinyl-5-fluorophenyl)-*S*-methyl-*S*-phenylsulfoximine (6k)**



General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 138 mg (85%), pale yellow viscous oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.71 (d, *J* = 4.0 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 7.79 – 7.70 (m, 3H), 7.62 – 7.53 (m, 2H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.26 – 7.20 (m, 1H), 6.91 (dd, *J* = 10.8 Hz, *J* = 2.4 Hz, 1H), 6.71 (td, *J* = 8.4 Hz, *J* = 2.4 Hz, 1H), 3.11 (s, 3H) ppm; ^{13}C NMR (100 MHz, $CDCl_3$) δ = 164.1, 161.6, 157.7, 149.1, 144.0,

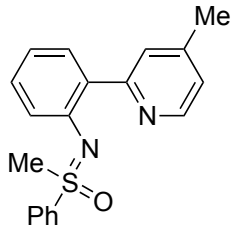
143.9, 138.9, 135.2, 133.4, 131.9, 131.8, 131.1, 131.0, 129.4, 128.3, 125.4, 121.3, 109.8, 109.6, 109.3, 109.0, 45.4 ppm; ESI-HRMS (*m/z*) $[C_{18}H_{15}FN_2OS + H]^+$ Calcd. 327.0962, Found 327.0972.

_N_-(2-Pyridinyl-3-methylphenyl)-_S_-methyl-_S_-phenylsulfoximine (6l)



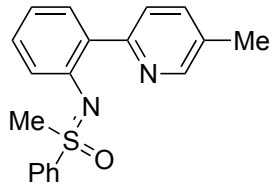
General procedure B was followed using ethyl acetate/pentane (1:1) as eluent; yield: 92 mg (57%), colorless viscous oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.79 (d, *J* = 4.2 Hz, 1H), 7.87 (t, *J* = 7.2 Hz, 1H), 7.67 (d, *J* = 7.2 Hz, 2H), 7.54 (t, *J* = 7.2 Hz, 1H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 2H), 7.36 (t, *J* = 5.4 Hz, 1H), 7.12 – 7.06 (m, 2H), 6.90 (d, *J* = 7.2 Hz, 1H), 3.01 (s, 3H), 2.09 (s, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$) δ = 159.0, 148.1, 143.0, 139.6, 137.1, 133.0, 129.2, 128.9, 128.4, 126.3, 124.1, 121.6, 120.4, 44.1, 20.2 ppm; ESI-HRMS (*m/z*) $[C_{19}H_{18}N_2OS + H]^+$ Calcd. 323.1213, Found 323.1226.

_N_-[2-(4-Methylpyridinyl)phenyl]-_S_-methyl-_S_-phenylsulfoximine (6m)



General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 116 mg (72%), colorless viscous oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.59 (d, *J* = 4.8 Hz, 1H), 7.83 – 7.79 (m, 3H), 7.60 – 7.53 (m, 2H), 7.45 (t, *J* = 7.8 Hz, 2H), 7.22 (d, *J* = 7.8 Hz, 1H), 7.16 (td, *J* = 7.8 Hz, *J* = 1.8 Hz, 1H), 7.09 (d, *J* = 4.8 Hz, 1H), 7.04 (t, *J* = 7.8 Hz, 1H), 3.07 (s, 3H), 2.43 (s, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$) δ = 158.3, 148.7, 146.2, 142.2, 139.5, 135.1, 133.1, 130.7, 129.3, 129.1, 128.4, 126.4, 123.4, 122.5, 122.4, 44.6, 21.2; ESI-HRMS (*m/z*) $[C_{19}H_{18}N_2OS + H]^+$ Calcd. 323.1213, Found 323.1225.

_N_-[2-(5-Methylpyridinyl)phenyl]-_S_-methyl-_S_-phenylsulfoximine (6n)



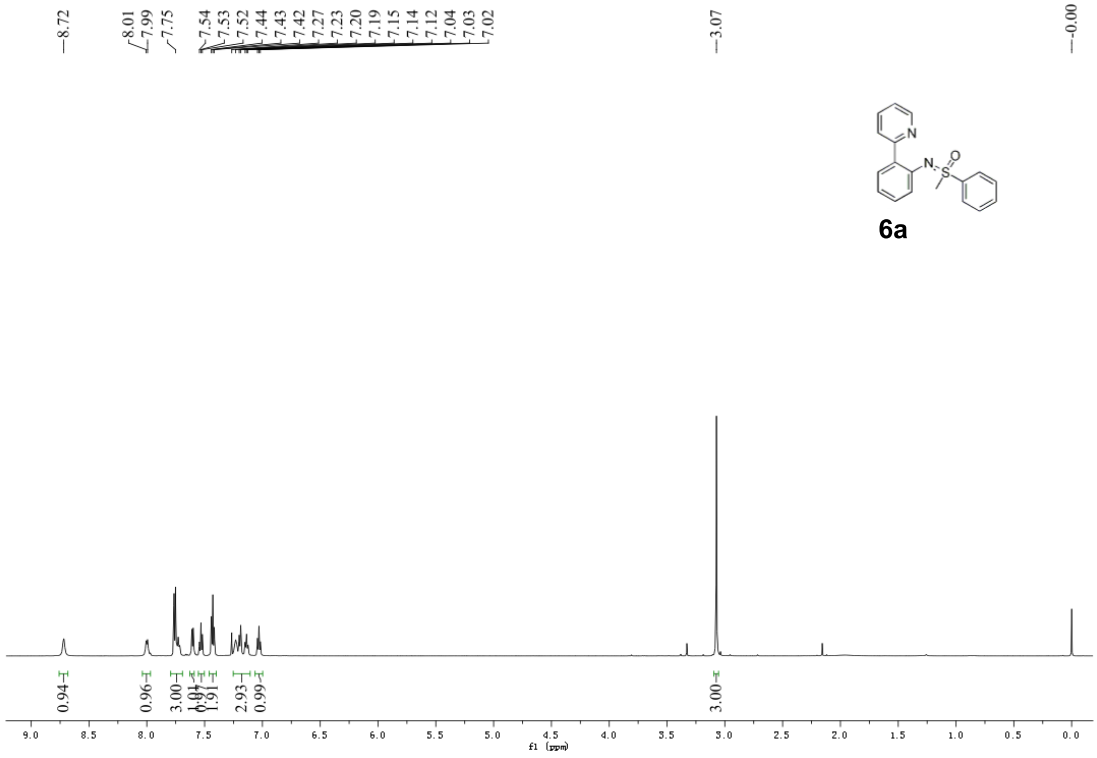
General procedure A was followed using ethyl acetate/pentane (1:1) as eluent; yield: 121 mg (75%), colorless viscous oil. ^{1}H NMR (600 MHz, $CDCl_3$) δ = 8.56 (s, 1H), 7.91 (d, *J* = 7.8 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 2H), 7.60 – 7.52 (m, 3H), 7.44 (t, *J* = 7.8 Hz, 2H), 7.17 (dd, *J* = 7.8 Hz, *J* = 1.2 Hz, 1H), 7.12 (td, *J* = 7.8 Hz, *J* = 1.8 Hz, 1H), 7.02 (td, *J* = 7.8 Hz, *J* = 1.2 Hz, 1H), 3.09 (s, 3H), 2.41(s, 3H) ppm; ^{13}C NMR (150 MHz, $CDCl_3$) δ = 155.6, 149.3, 142.3, 139.4, 135.9, 133.1, 130.7, 130.6, 129.3, 129.0, 128.4, 124.9, 123.2, 122.4, 45.1, 18.3 ppm; ESI-HRMS (*m/z*) $[C_{19}H_{18}N_2OS + H]^+$ Calcd. 323.1213, Found 323.1222.

References:

[S1] Littke, A. F.; Dai, C.; Fu, G. C. *J. Am. Chem. Soc.* **2000**, *122*, 4020.

[S2] Eis, K.; Prien, O.; Luecking, U.; Guenther, J.; Zopf, D.; Brohm, D.; Vöhringer, V.; Woltering, E.; Beck, H.; Lobell, M.; Li, V. M.-J.; Greschat, S. *WO 2008/141843 A1* (Bayer Schering Pharma AG).

NMR Spectra: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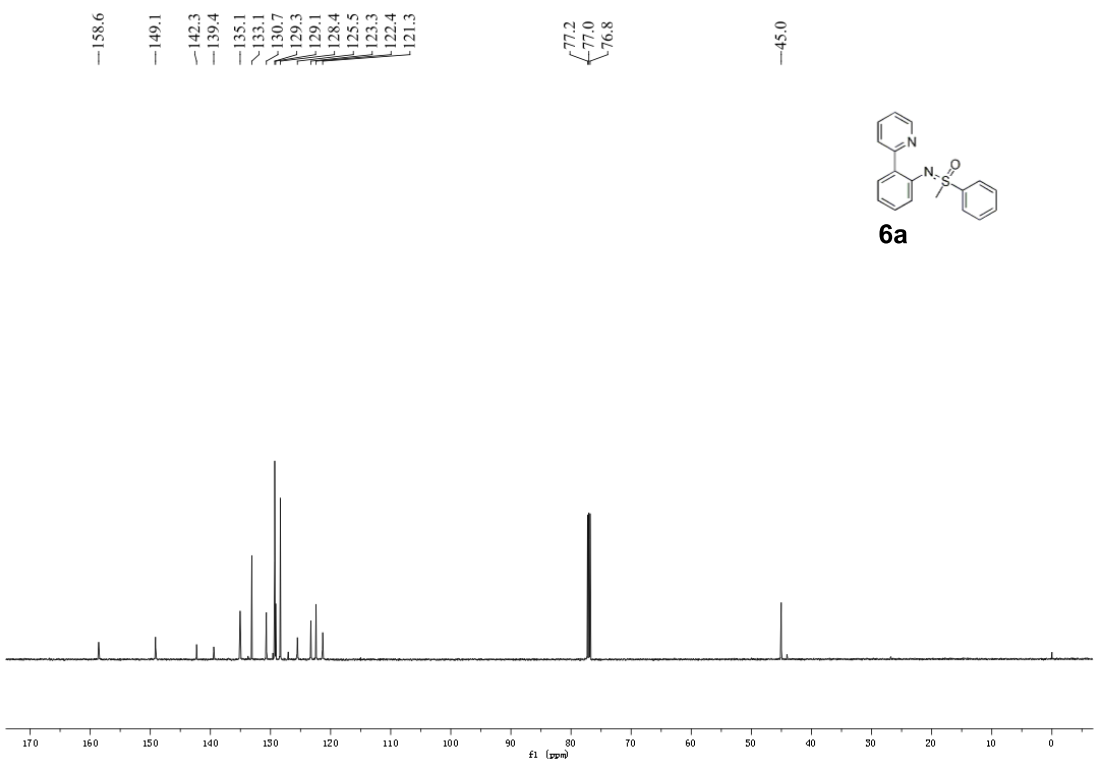
7.99
7.75
7.54
7.53
7.52
7.44
7.43
7.42
7.27
7.23
7.20
7.19
7.15
7.14
7.12
7.04
7.03
7.02
3.07
0.00
6a
0.94
0.96
3.00
1.91
2.93
0.99
3.00
f1 (ppm)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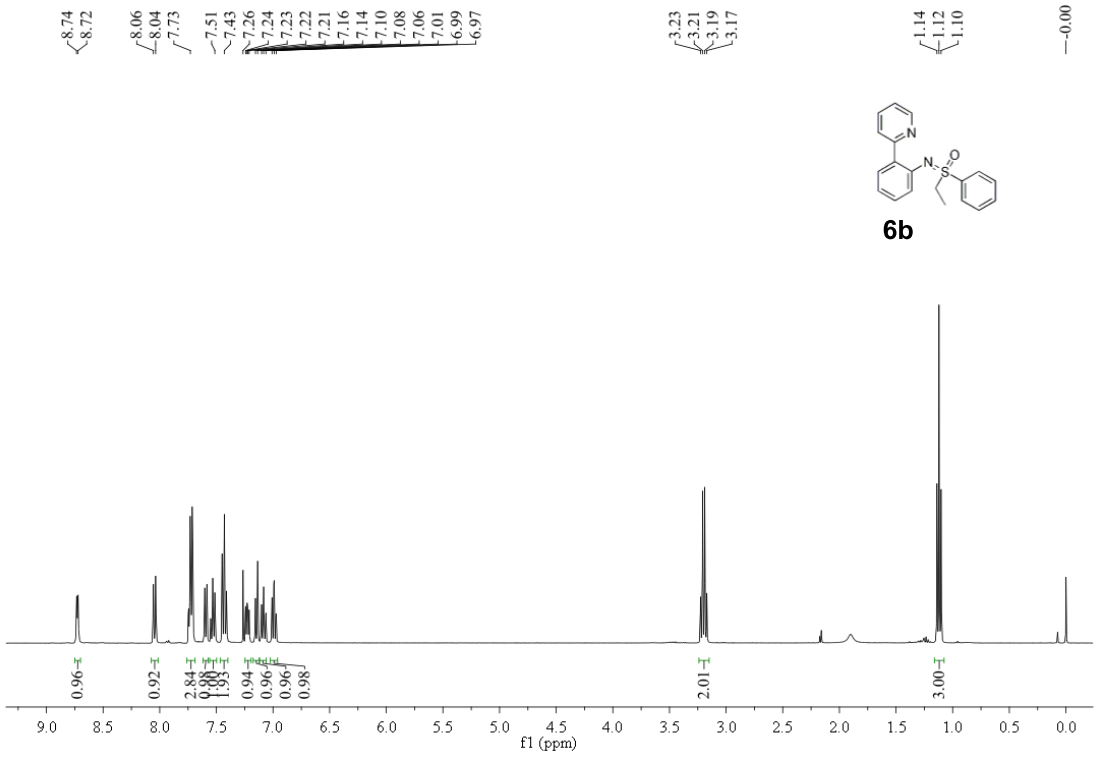
142.3
139.4
135.1
133.1
130.7
129.3
129.1
128.4
125.5
123.3
122.4
121.3
77.2
77.0
76.8
45.0
6a
f1 (ppm)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7.23
7.22
7.21
7.16
7.14
7.10
7.08
7.06
7.01
6.99
6.97
3.23
3.21
3.19
3.17
1.14
1.12
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0.96
0.98
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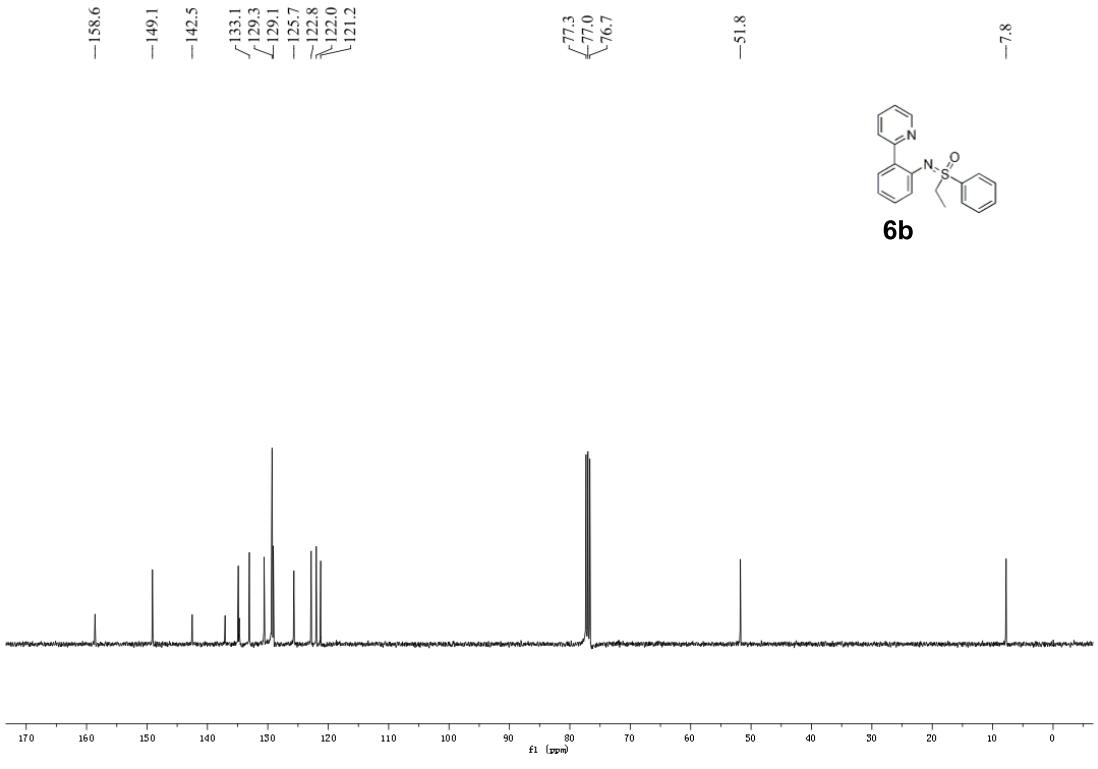
3.00
f1 (ppm)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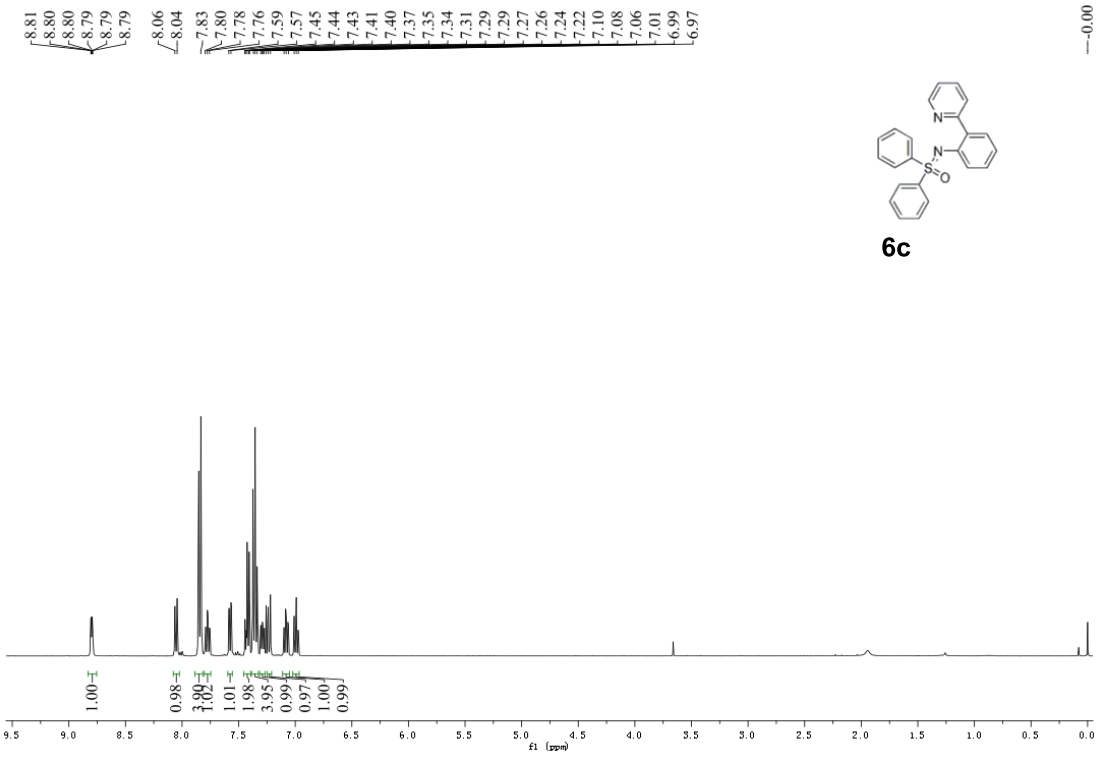
142.5
133.1
129.3
129.1
125.7
122.8
122.0
121.2
77.3
77.0
76.7
51.8
7.8
6b
f1 (ppm)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7.76
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7.45
7.44
7.43
7.41
7.40
7.37
7.35
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7.29
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7.27
7.26
7.24
7.22
7.10
7.08
7.06
7.01
6.99
6.97
0.00
6c
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0.98
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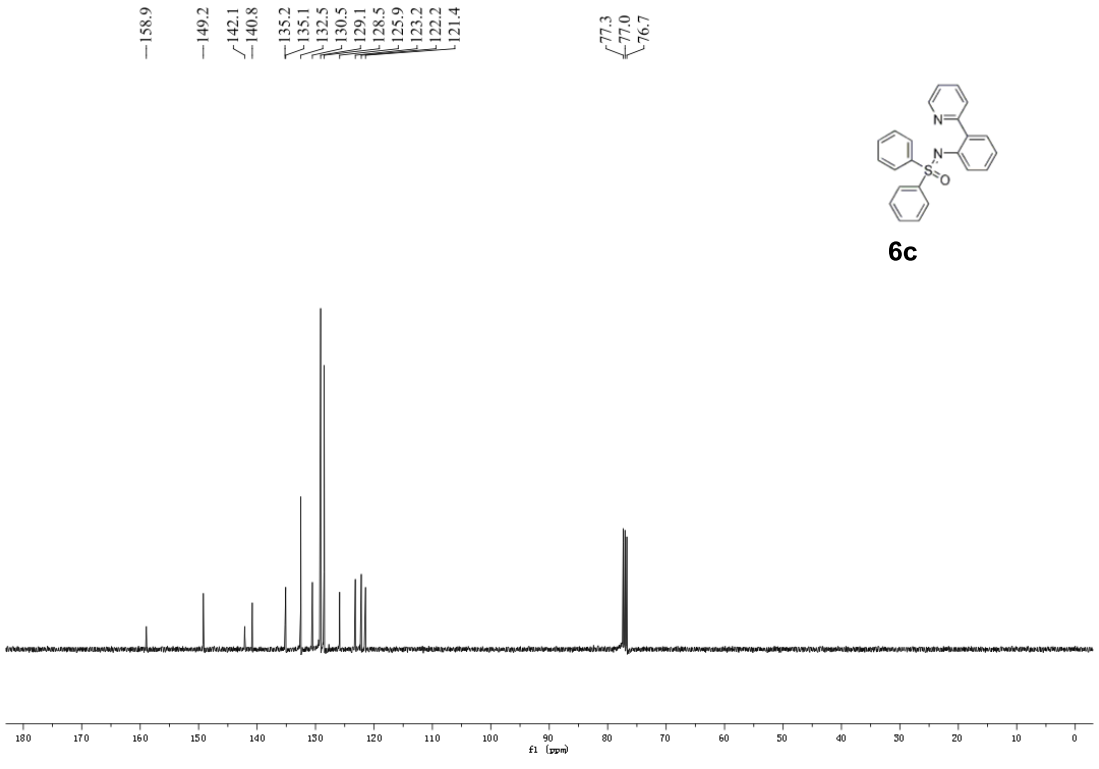
3.02
1.01
1.98
3.95
0.99
0.97
1.00
0.99
f1 (ppm)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132.5
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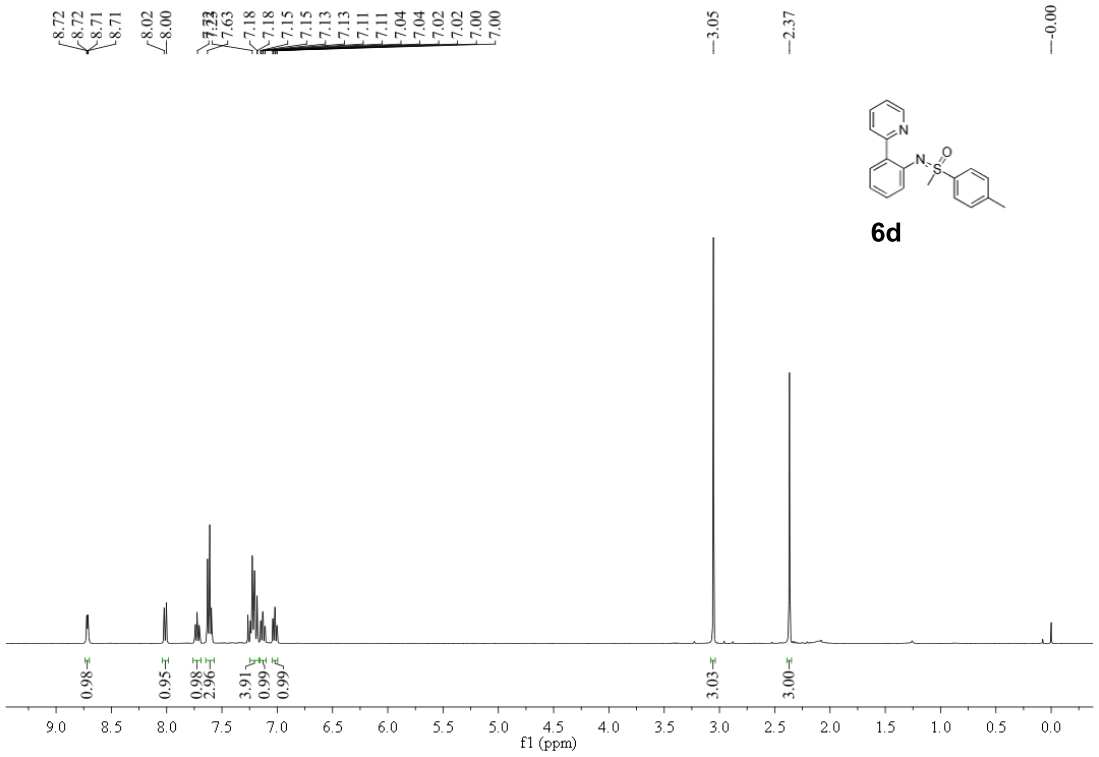
129.1
128.5
125.9
123.2
122.2
121.4
77.3
77.0
76.7
6c
f1 (ppm)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7.13
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7.04
7.04
7.02
7.02
7.00
7.00
3.05
2.37
0.00
6d
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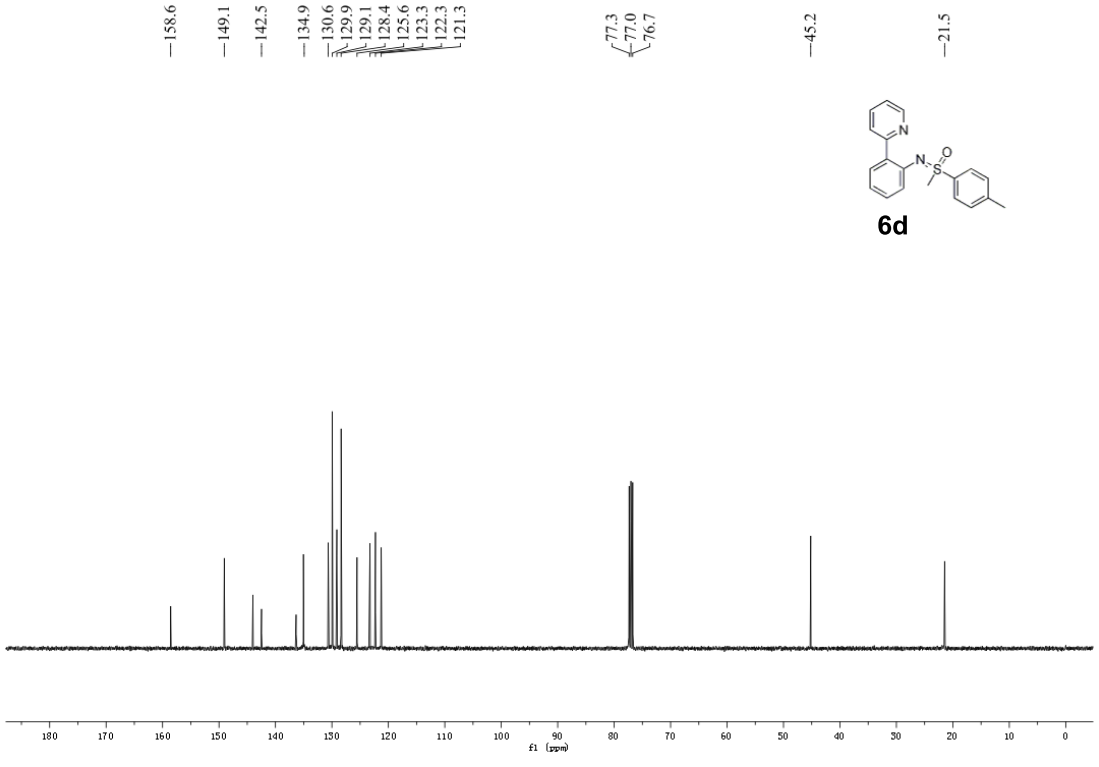
0.98
2.96
3.91
0.99
0.99
3.03
3.00
f1 (ppm)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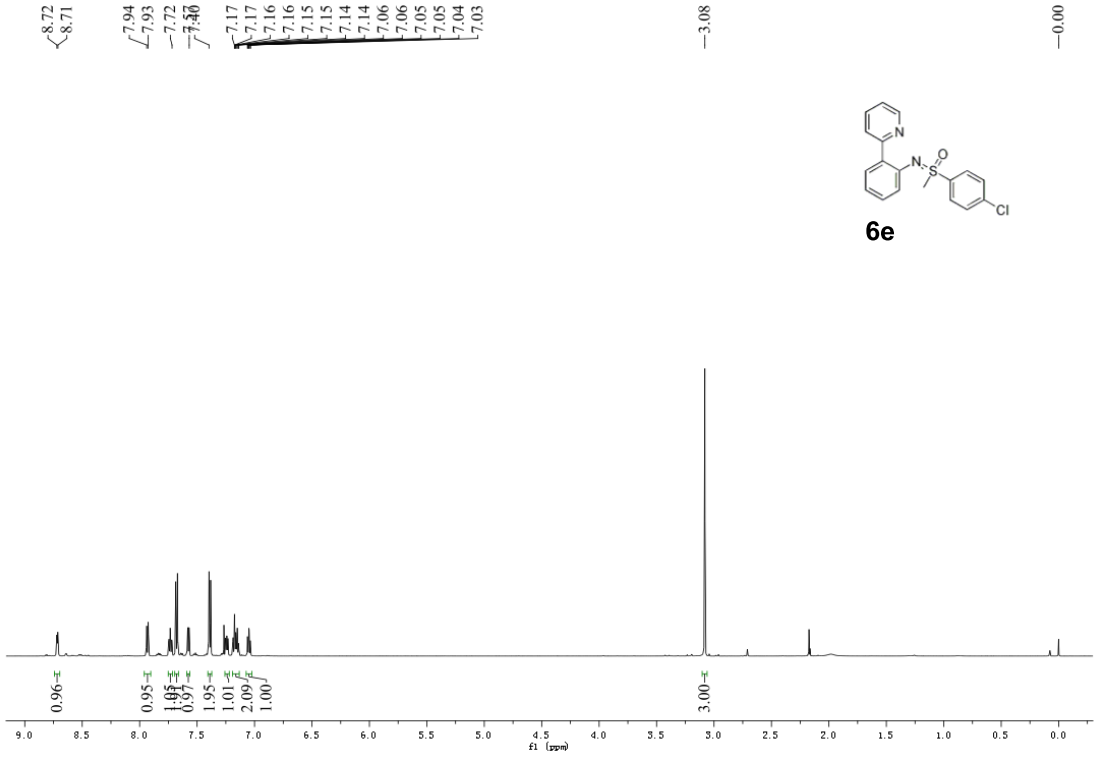
129.9
129.1
128.4
125.6
123.3
122.3
121.3
77.3
77.0
76.7
45.2
21.5
6d
f1 (ppm)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7.15
7.14
7.14
7.06
7.05
7.05
7.04
7.03
3.08
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1.95
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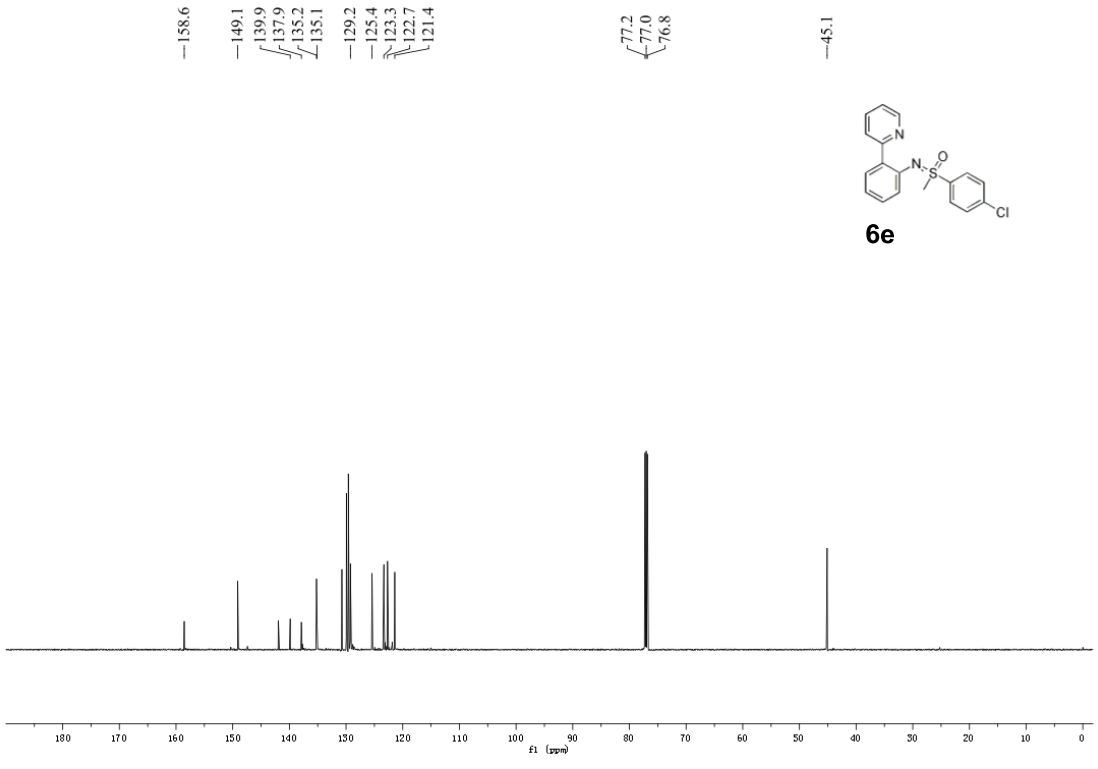
f1 (ppm)

6e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139.9
137.9
135.2
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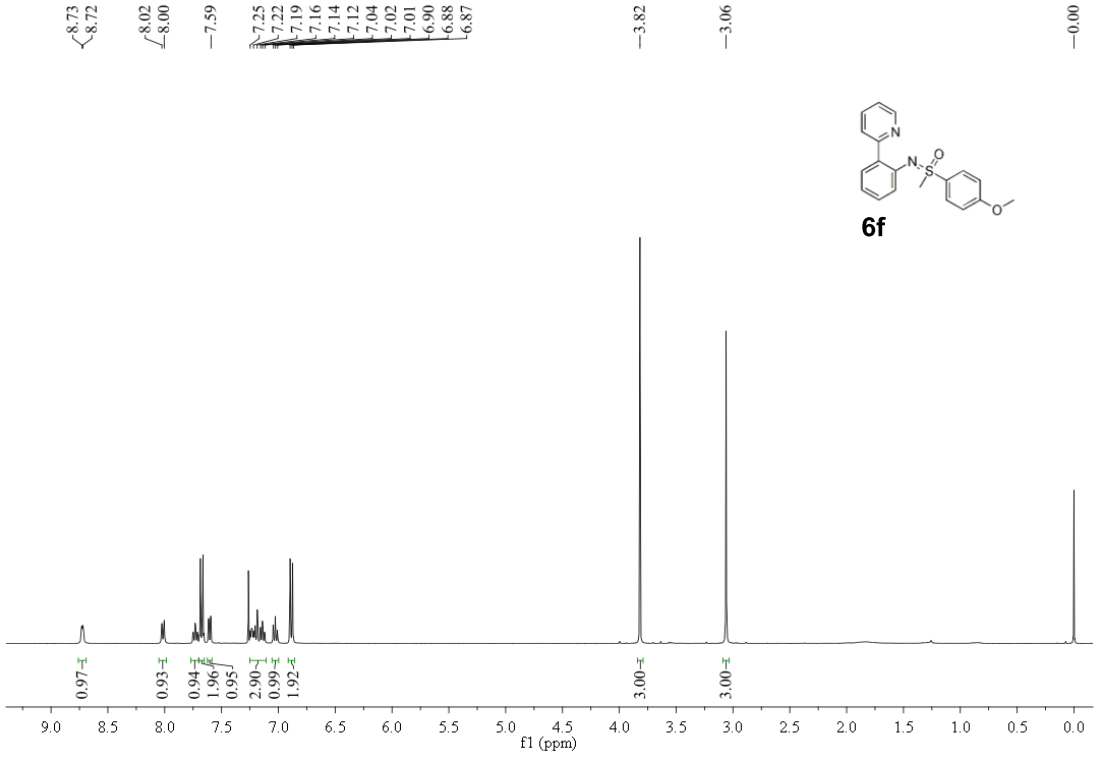
129.2
125.4
123.3
122.7
121.4
77.2
77.0
76.8
45.1
f1 (ppm)

6e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7.02
7.01
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6.88
6.87
3.82
3.06
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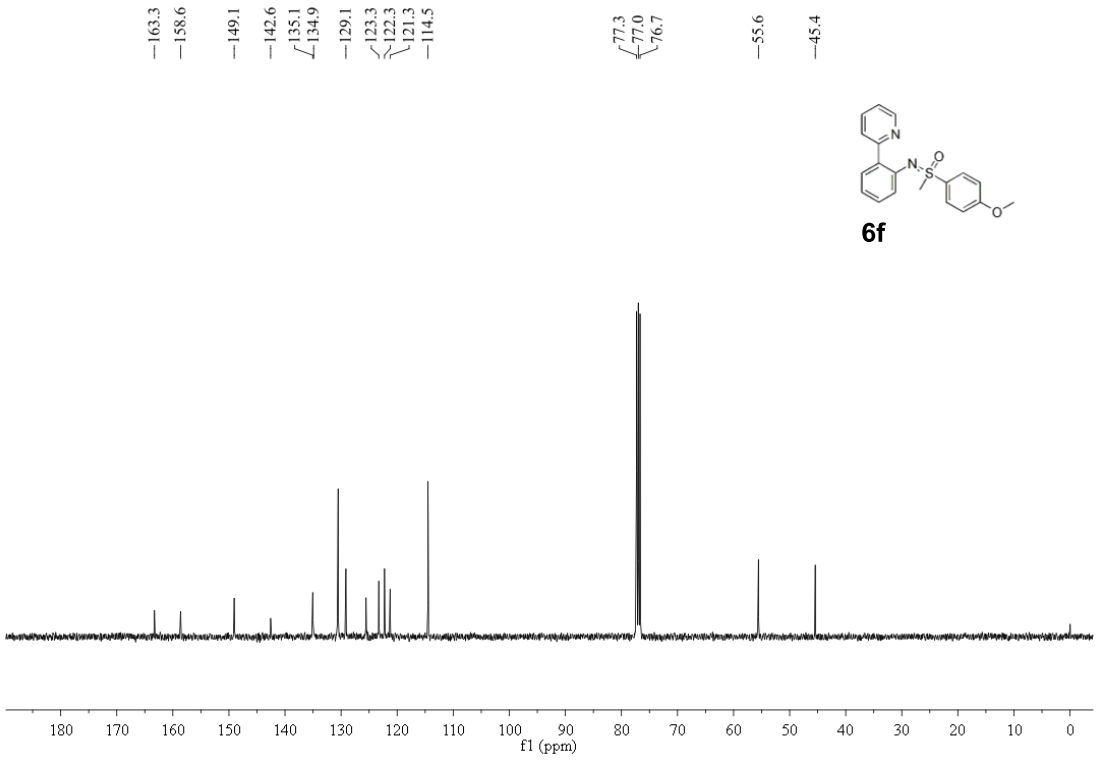
f1 (ppm)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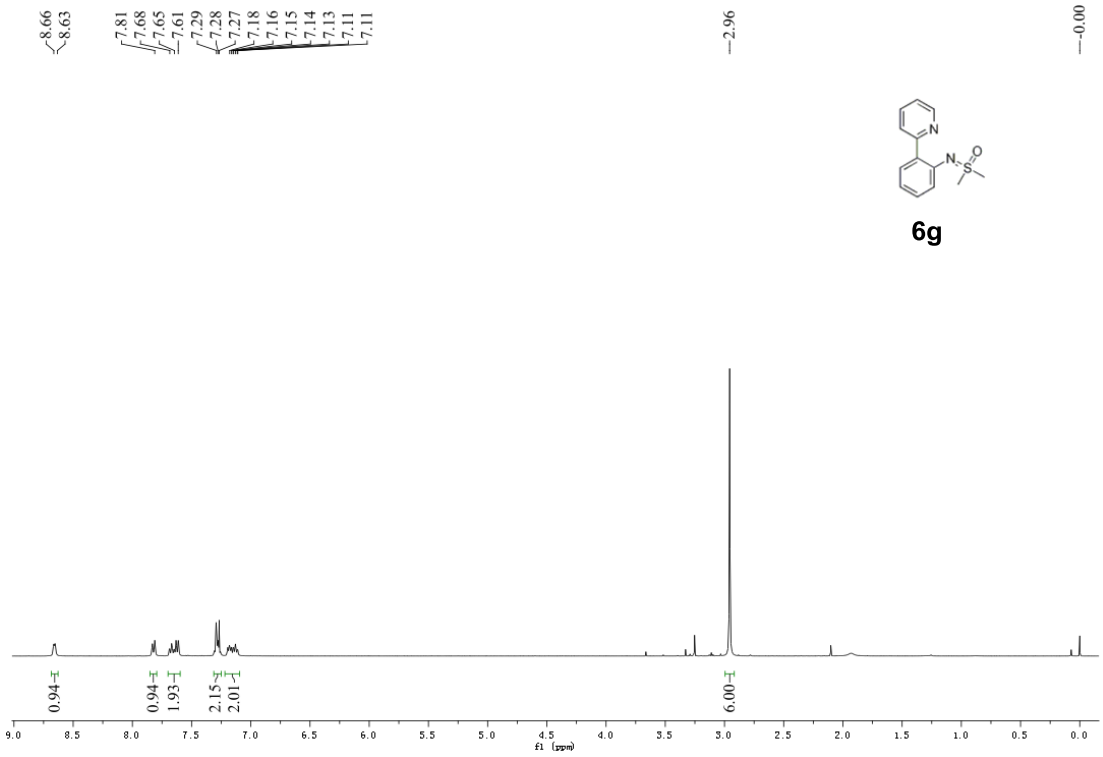
76.7
55.6
45.4
6f
f1 (ppm)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7.13
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7.11
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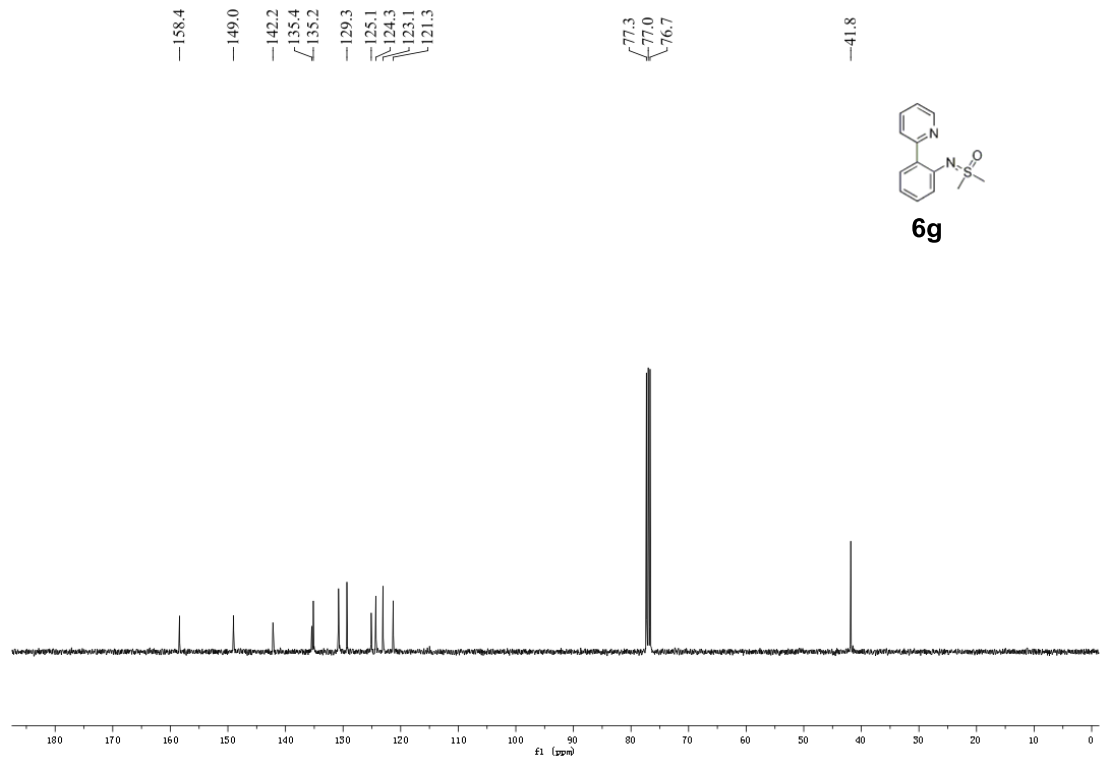
0.94
1.93
2.15
2.01
6.00
f1 (ppm)

6g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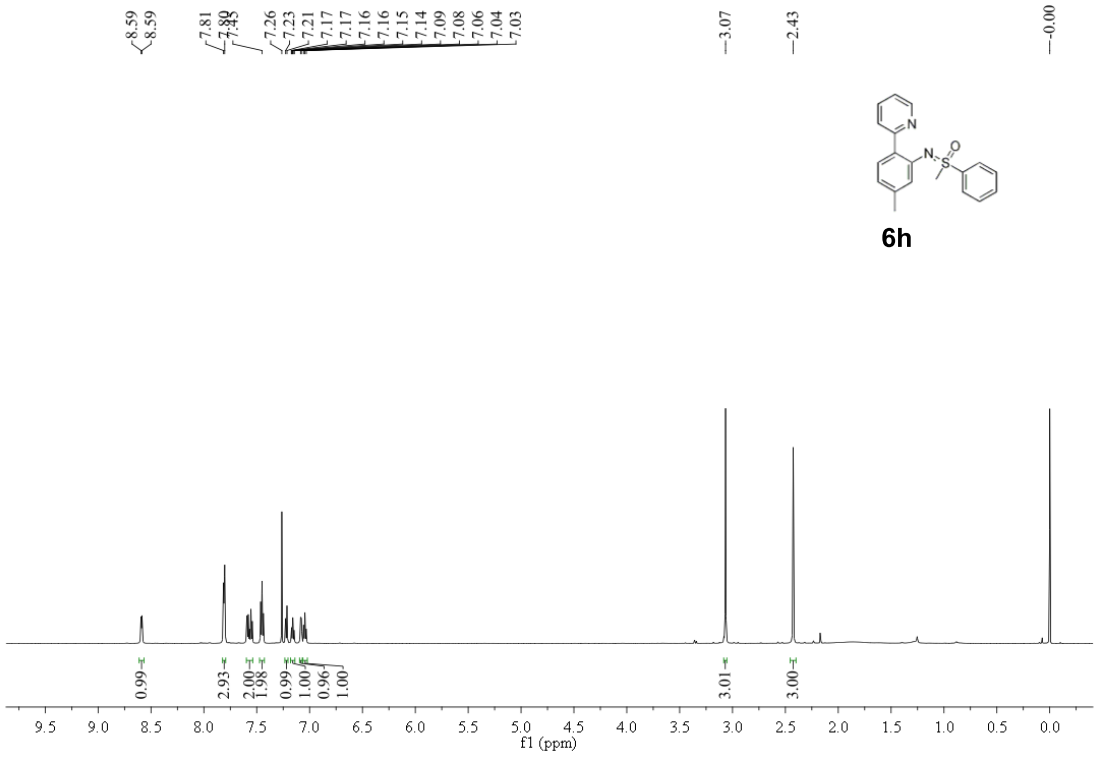
77.0
76.7
41.8
f1 (ppm)

6g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7.14
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7.08
7.06
7.04
7.03
3.07
2.43
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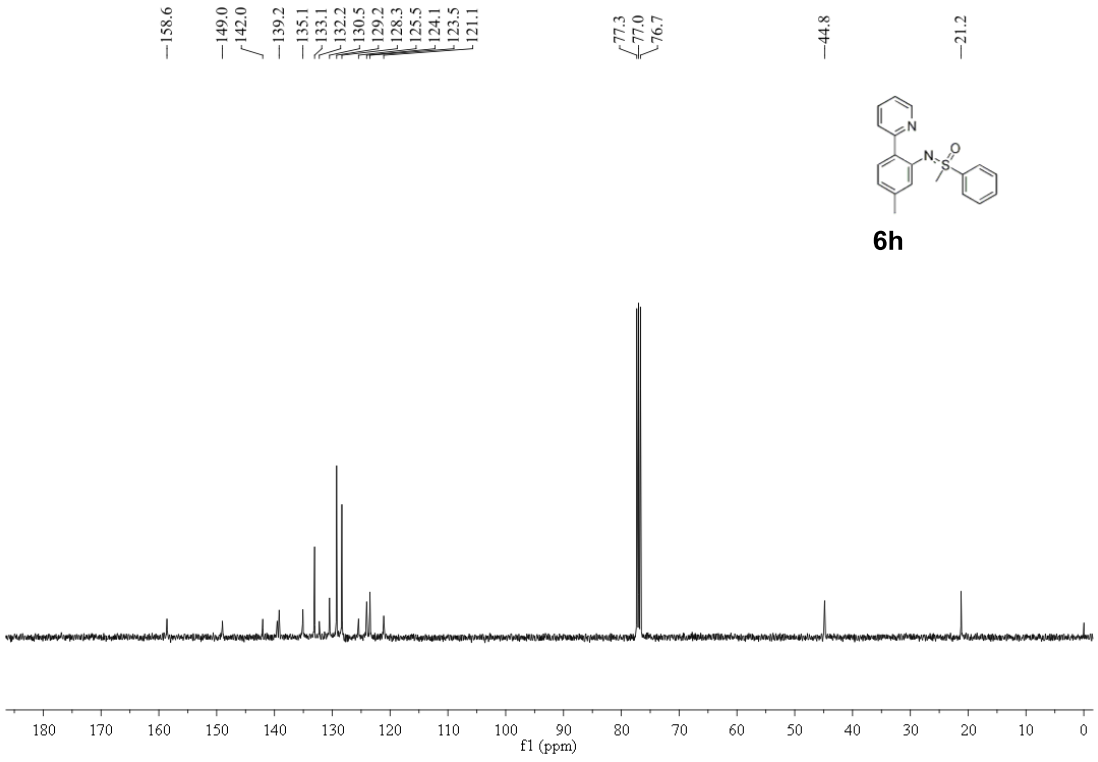
3.00
f1 (ppm)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132.2
130.5
129.2
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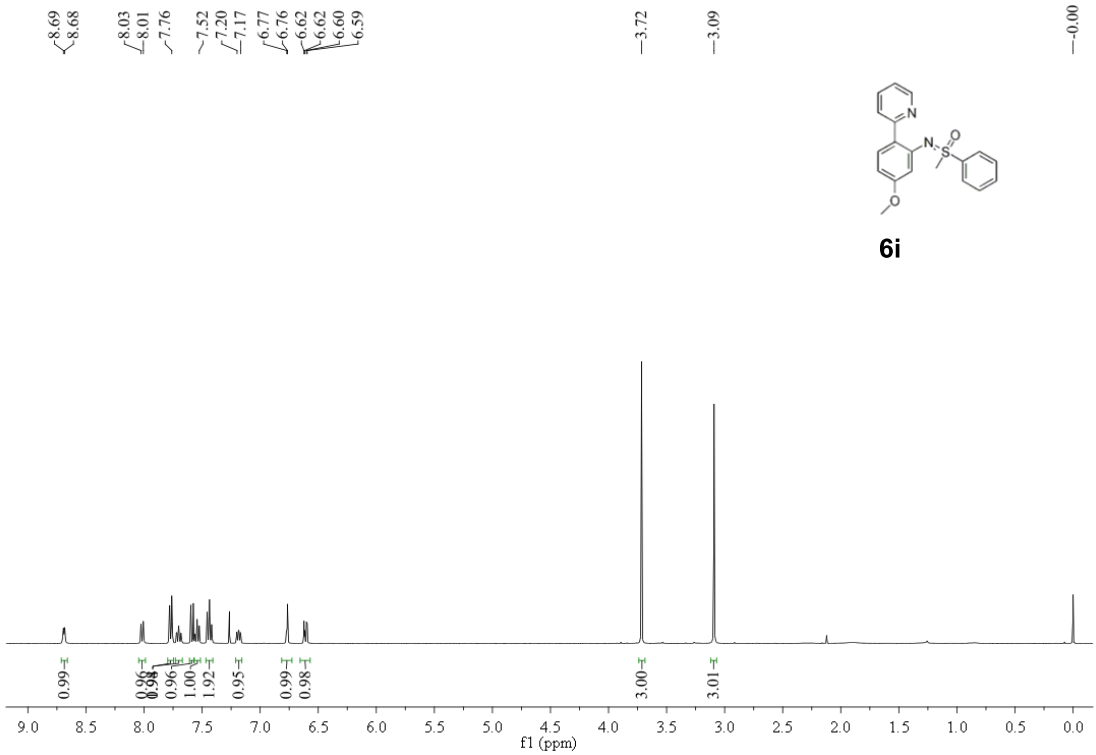
124.1
123.5
121.1
77.3
77.0
76.7
44.8
21.2
6h
f1 (ppm)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3.09
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1.00
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3.00
3.01
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8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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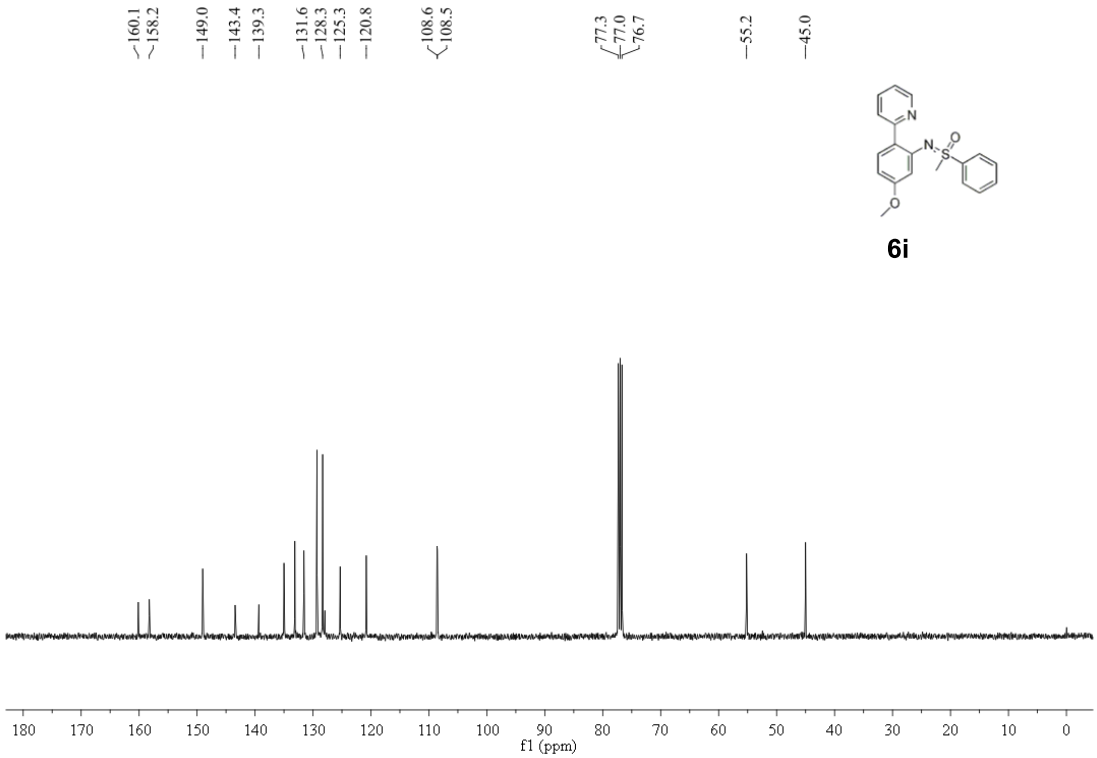
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

6i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77.0
76.7
55.2
45.0
180
170
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140
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120
110
100
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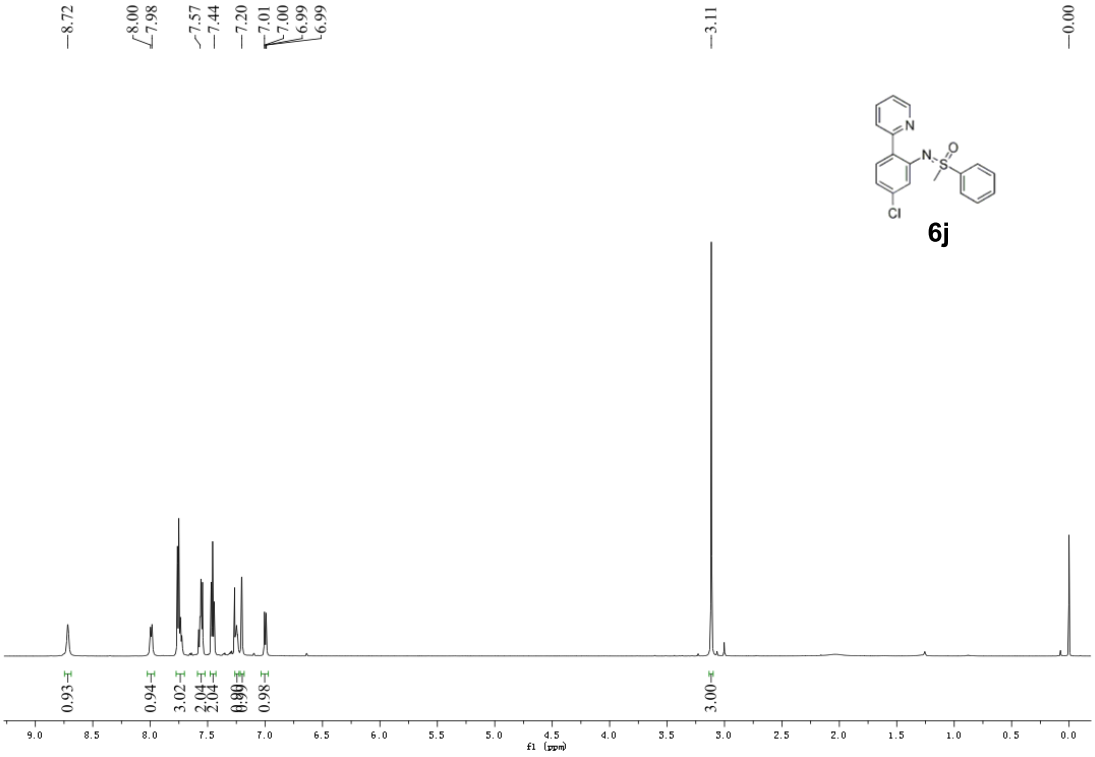
80
70
60
50
40
30
20
10
0
f1 (ppm)

6i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0.94
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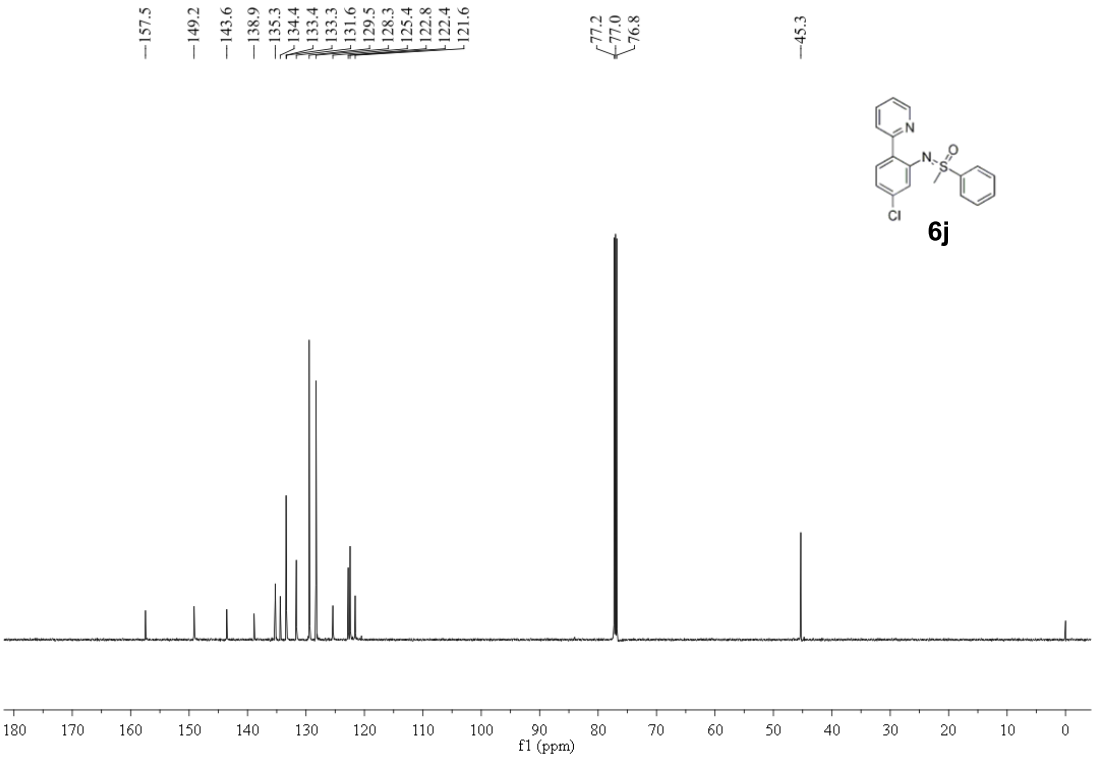
0.98
3.00
f1 (ppm)

6j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122.8
122.4
121.6
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76.8
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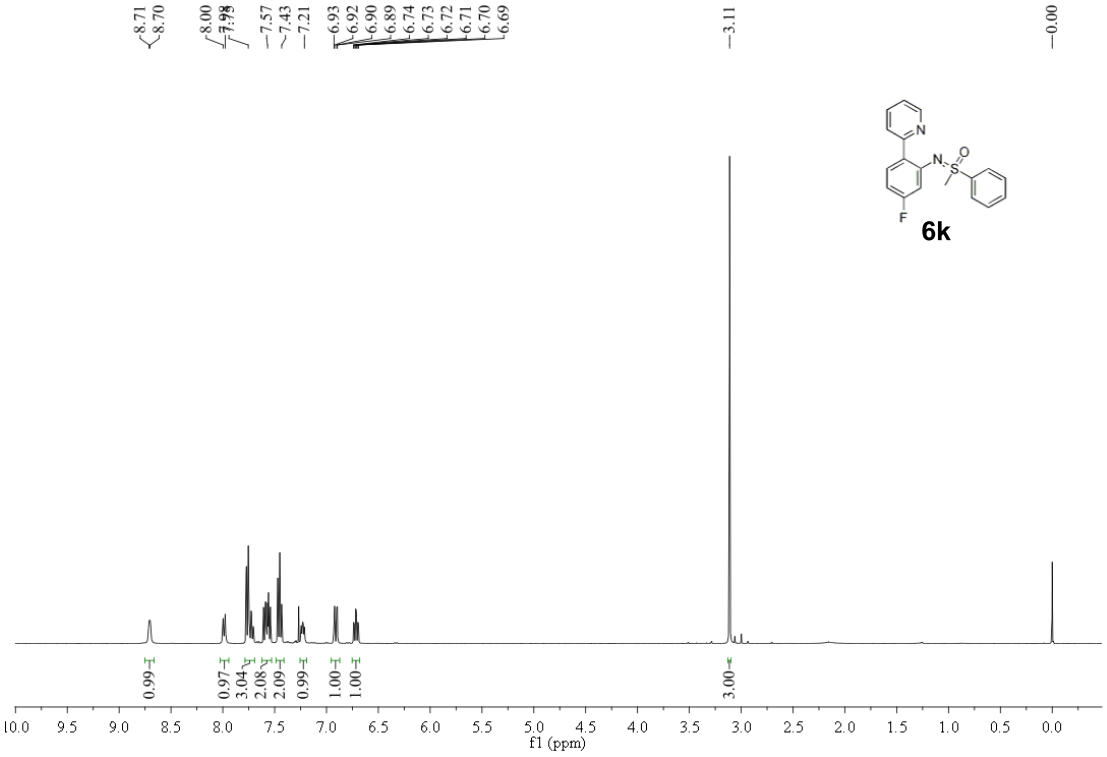
f1 (ppm)

6j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3.11
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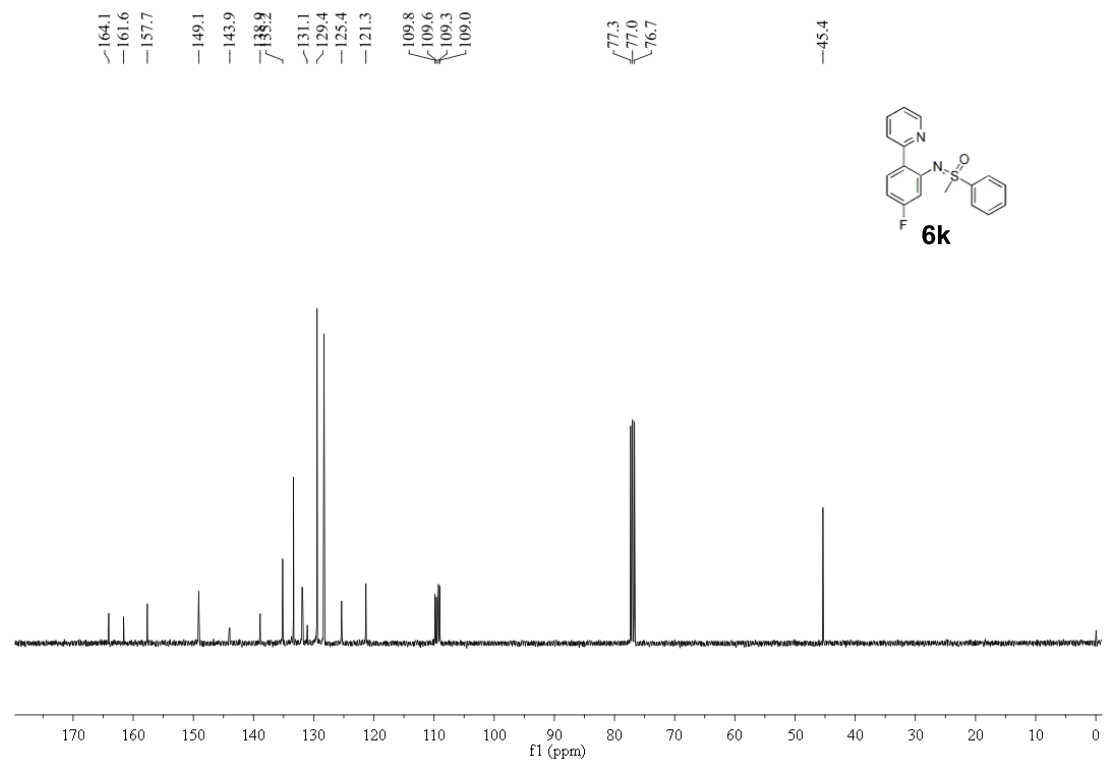
1.00
3.00
f1 (ppm)
6k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109.3
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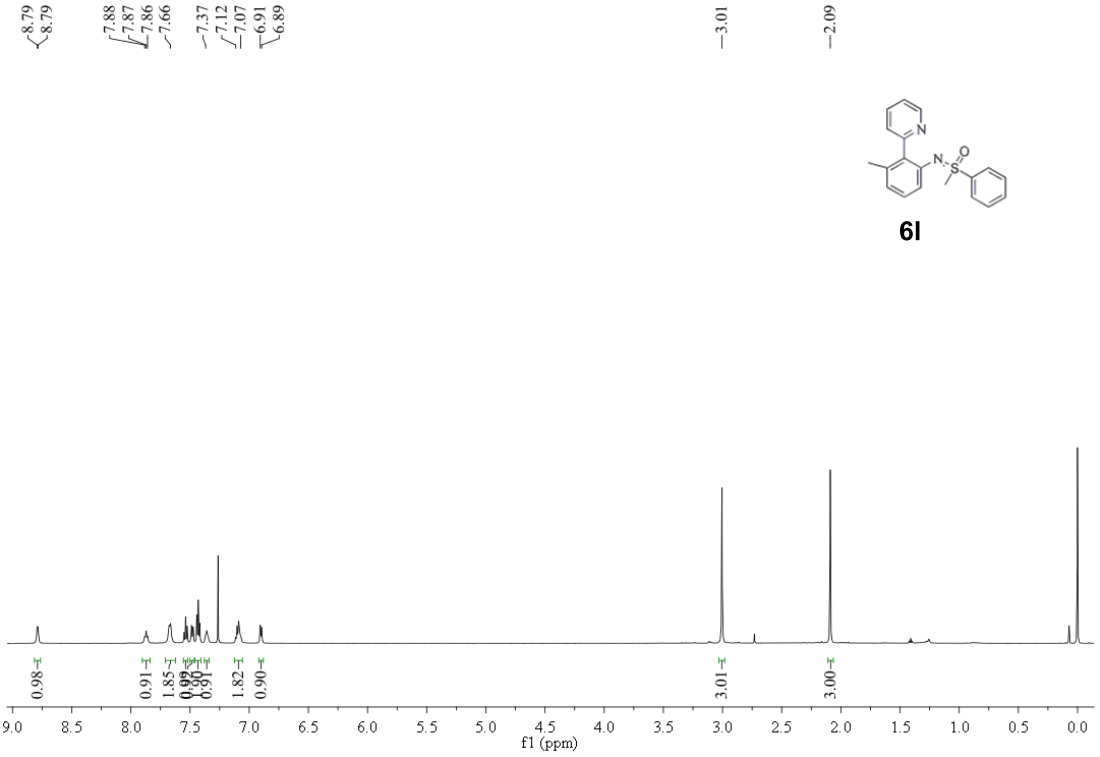
77.0
76.7
45.4
f1 (ppm)
6k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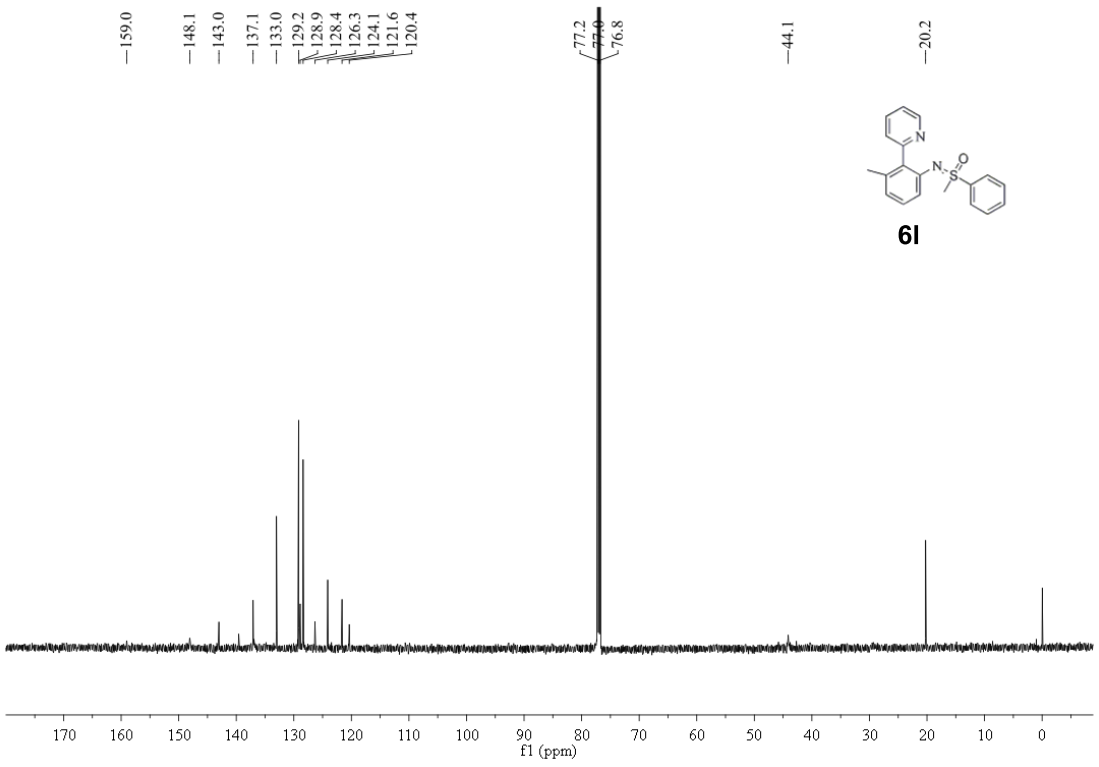
3.00
f1 (ppm)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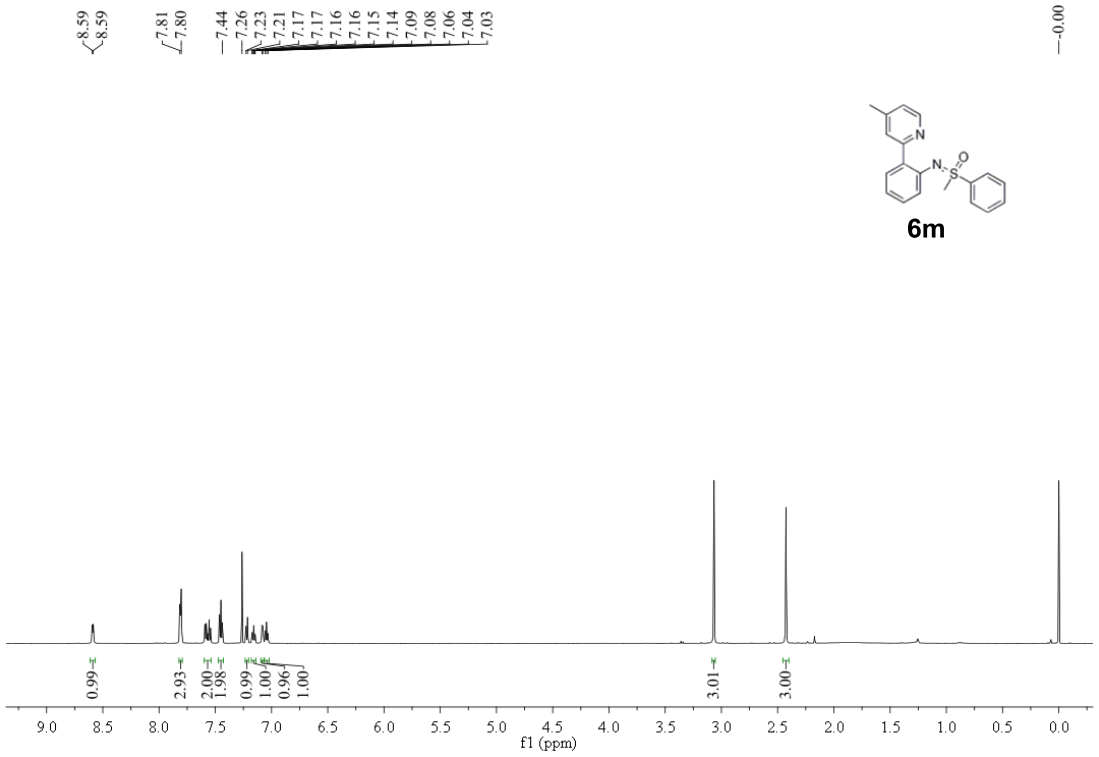
77.0
76.8
44.1
20.2
6l
f1 (ppm)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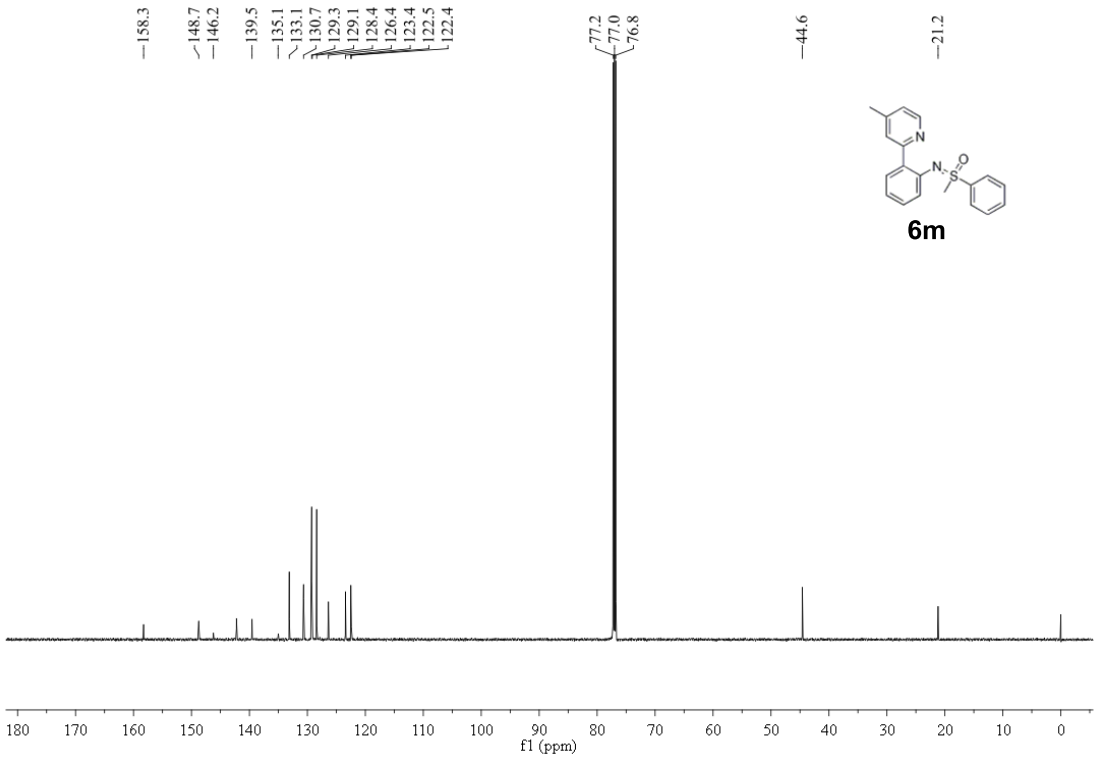
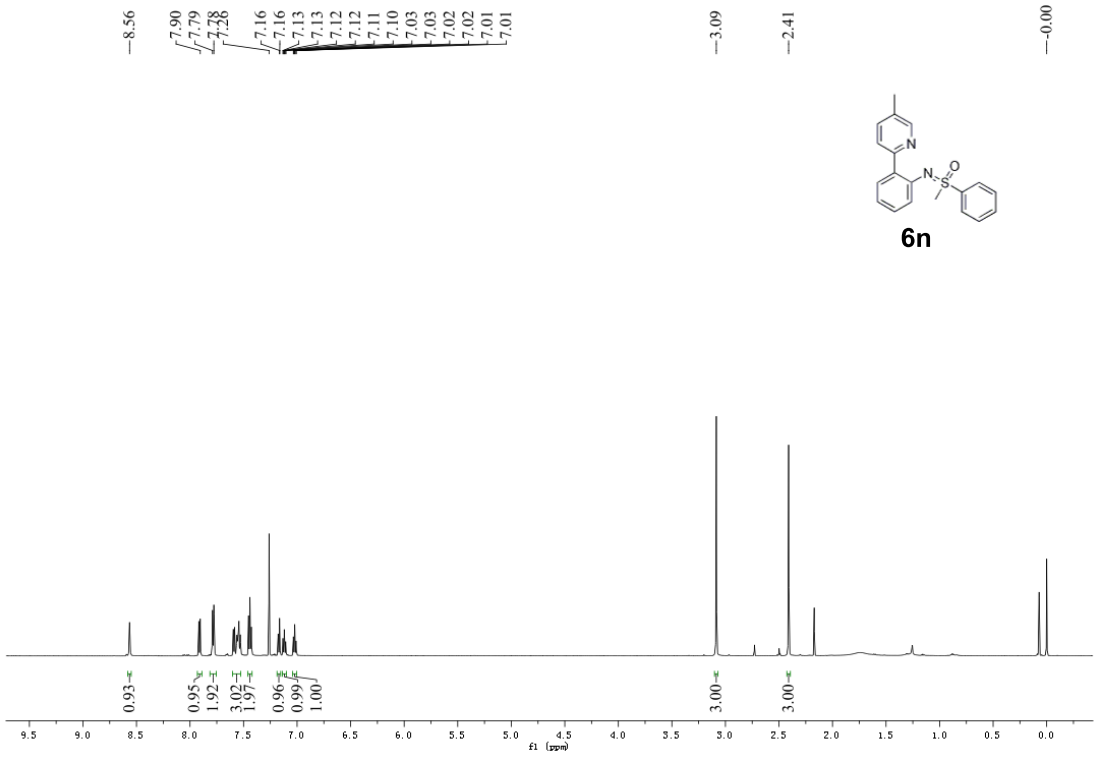
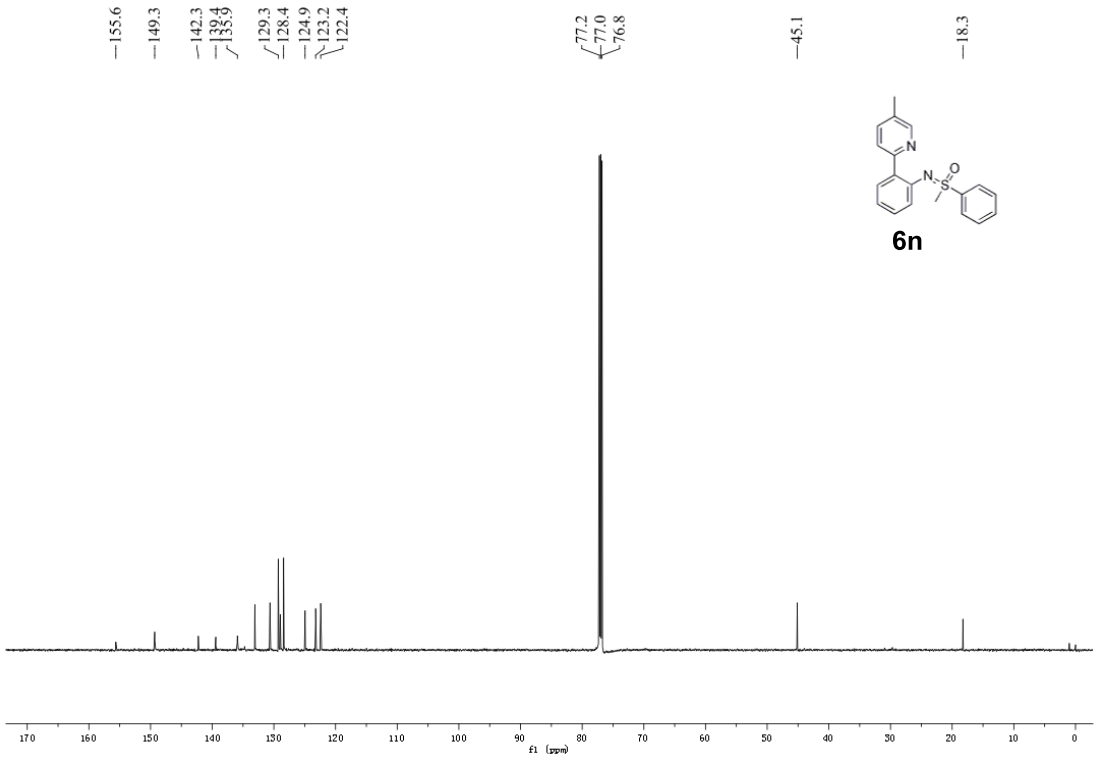
7.81
7.80
7.44
7.26
7.23
7.21
7.17
7.17
7.16
7.16
7.15
7.14
7.09
7.08
7.06
7.04
7.03
0.00
6m
0.99
2.93
2.00
1.98
0.99
1.00
0.96
1.00
3.01
3.00
f1 (ppm)


158.3
148.7
146.2
139.5
135.1
133.1
130.7
129.3
129.1
128.4
126.4
123.4
122.5
122.4
77.2
77.0
76.8
44.6
21.2
6m
f1 (ppm)


8.56
7.90
7.79
7.78
7.26
7.16
7.16
7.13
7.13
7.12
7.12
7.11
7.10
7.03
7.03
7.02
7.02
7.01
7.01
3.09
2.41
0.00
6n
0.93
0.95
1.92
3.02
1.97
0.96
0.99
1.00
3.00
3.00
f1 (ppm)


155.6
149.3
142.3
139.4
135.9
129.3
128.4
124.9
123.2
122.4
77.2
77.0
76.8
45.1
18.3
6n
f1 (ppm)