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Supporting Information

Ligand Free Iron-Catalyzed C (sp^3)-H Amination of Methylarenes with N-Fluorobenzenesulfonimide

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General information

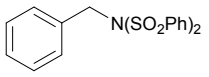
All chemicals were commercial available and used without purification. All reactions were carried out in air and monitored by thin layer chromatography (TLC). ^{1}H and ^{13}C NMR were measured on a Bruker AVANCE III 400 using tetramethylsilane as an internal standard. In the NMR data, chemical shift (δ, ppm) and integration are recorded. The abbreviations are as follows: s = singlet, d = doublet, t = triplet, m = multiplet. Hertz (Hz) is used for coupling constant (J). HRMS were measured on Agilent 1290-6540 Ultra High Performance Liquid Chromatography-Q-Time of Flight/ High Resolution Mass Spectrometer.

General procedure for the amination reactions of methylarenes

1, 2-Dichlorobenzene (20 mL) was added to a mixture of iron (III) oxalate hexahydrate (0.05 mmol, 10 mol%), methylarenes (0.5 mmol), N-fluorobenzenesulfonimide (NFSI, 0.75 mmol, 1.5 eq). The mixture was stirred and heated in electric heating sleeve at reflux. After the complete consumption of NFSI, the mixture was concentrated in vacuo, and the crude product was purified by a silica gel column chromatography.

Characterization data of compounds 3

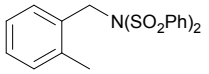
N-benzyl-N-(phenylsulfonyl)benzenesulfonamide (3a)



3a

3a was obtained according to the general procedure using toluene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 6). Yield: 113.4 mg (59%); white solid. $^{1}HNMR$ (400 MHz, CDCl3): δ7.77-7.79 (m, 4H), 7.55-7.59 (m, 2H), 7.36-7.44 (m, 6H), 7.21-7.25 (m, 3H), 4.94 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.0, 134.5, 133.6, 129.2, 128.8, 128.4, 128.1, 52.5. MS m/z: 410.2 ($[M+Na]^+$).

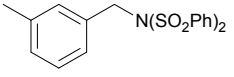
N-(2-methylbenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3b)



3b

3b was obtained according to the general procedure using o-xylene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 6). Yield: 97.8 mg (49%); white solid. $^{1}HNMR$ (400 MHz, CDCl3): δ7.79-7.81 (m, 4H), 7.56-7.60 (m, 2H), 7.41-7.45 (m, 4H), 7.21 (d, J = 7.76 Hz, 1H), 7.11 (t, J = 7.36 Hz, 1H), 7.04 (d, J = 7.36 Hz, 1H), 6.95 (t, J = 7.36 Hz, 1H), 5.02 (s, 2H), 2.30 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.1, 136.4, 133.6, 132.1, 130.3, 129.3, 128.8, 128.1, 127.8, 126.0, 50.1, 19.2. MS m/z: 424.2 ($[M+Na]^+$).

N-(3-methylbenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3c)

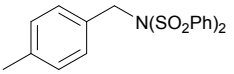


3c

3c was obtained according to the general procedure using m-xylene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 6). Yield: 78.1 mg (39%); white solid. $^{1}HNMR$ (400 MHz, CDCl3): δ 7.78-7.81 (m, 4H), 7.55-7.59 (m, 2H), 7.41-7.46 (m, 4H), 7.04-7.16 (m,

4H), 4.91 (s, 2H), 2.21 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.1, 138.1, 134.2, 133.6, 129.6, 128.8, 128.3, 128.1, 126.2, 52.6, 21.2. MS m/z: 424.2 ($[M+Na]^+$).

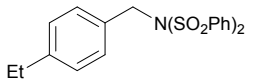
N-(4-methylbenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3d)



3d

3d was obtained according to the general procedure using p-xylene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 6). Yield: 104.1 mg (52%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ7.77-7.80 (m, 4H), 7.57 (t, J = 7.48 Hz, 2H), 7.42 (t, J = 7.88Hz, 4H), 7.25 (d, J = 7.88 Hz, 2H), 7.03 (d, J = 7.88 Hz, 2H), 4.90 (s, 2H), 2.33 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 140.1, 137.9, 133.5, 131.5, 129.2, 129.0, 128.8, 128.1, 52.3, 21.1. MS m/z: 424.2 ($[M+Na]^+$).

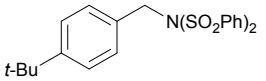
N-(4-ethylbenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3e)



3e

3e was obtained according to the general procedure using 1-ethyl-4-methylbenzene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 8). Yield: 24.5 mg (12%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.76-7.78 (m, 4H), 7.56 (t, J = 7.48 Hz, 2H), 7.41 (t, J = 8.00 Hz, 4H), 7.28 (d, J = 8.00 Hz, 2H), 7.05 (d, J = 8.00 Hz, 2H), 4.91 (s, 2H), 2.62 (q, J = 7.60 Hz, 2H), 1.23 (t, J = 7.60 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 144.4, 140.2, 133.5, 131.6, 129.4, 128.8, 128.1, 127.9, 52.4, 28.6, 15.9. MS m/z: 438.2 ($[M+Na]^+$).

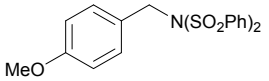
N-(4-(tert-butyl)benzyl)-N-(phenylsulfonyl)benzenesulfonamide (3f)



3f

3f was obtained according to the general procedure using 1-(tert-butyl)-4-methylbenzene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 8). Yield: 178.2 mg (80%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.75-7.77 (m, 4H), 7.52-7.57 (m, 2H), 7.38-7.72 (m, 4H), 7.29 (d, J = 8.40 Hz, 2H), 7.24 (d, J = 8.40 Hz, 2H), 4.93 (s, 2H), 1.31 (s, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.2, 140.2, 133.5, 131.3, 129.1, 128.7, 128.1, 125.3, 52.4, 34.6, 31.4. HRMS: calculated for $C_{23}H_{25}NO_4S_2$ ($[M+Na]^+$), 466.1123, found, 466.1118.

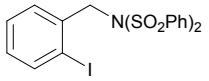
N-(4-methoxylbenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3g)



3g

3g was obtained according to the general procedure using 1-methoxy-4-methylbenzene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 3.5). Yield: 66.6 mg (32%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.80-7.82 (m, 4H), 7.57-7.62 (m, 2H), 7.44-7.48 (m, 4H), 7.34 (d, J = 8.76 Hz, 2H), 6.79 (d, J = 8.76 Hz, 2H), 4.90 (s, 2H), 3.83 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.5, 140.1, 133.6, 130.8, 128.8, 128.1, 126.6, 113.8, 55.4, 52.1. MS m/z: 440.1 ($[M+Na]^+$).

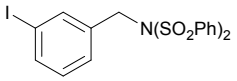
N-(2-iodobenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3h)



3h

3h was obtained according to the general procedure using 1-iodo-2-methylbenzene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 6.5). Yield: 109.2 mg (43%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.89-7.92 (m, 4H), 7.77-7.79 (m, 1H), 7.60-7.64 (m, 2H), 7.46-7.50 (m, 4H), 7.11-7.13 (m, 1H), 7.00-7.04 (m, 1H), 6.85-6.90 (m, 1H), 5.04 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.6, 139.3, 136.6, 133.9, 129.2, 129.0, 128.8, 128.4, 128.1, 97.4, 57.4. MS m/z: 536.1 ($[M+Na]^+$).

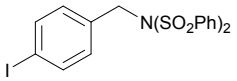
N-(3-iodobenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3i)



3i

3i was obtained according to the general procedure using 1-iodo-3-methylbenzene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 6). Yield: 104.2 mg (41%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.81-7.83 (m, 4H), 7.56-7.62 (m, 4H), 7.44-7.48 (m, 4H), 7.30 (d, J = 7.76 Hz, 1H), 6.95 (t, J = 7.76Hz, 1H), 4.87 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.8, 137.7, 137.2, 136.8, 133.9, 130.1, 129.0, 128.2, 128.1, 94.2, 51.6. HRMS: calculated for $C_{19}H_{16}INO_4S_2$ ($[M+H]^+$), 513.9643, found, 513.9639.

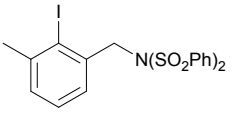
N-(4-iodobenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3j)



3j

3j was obtained according to the general procedure using 1-iodo-4-methylbenzene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 6.5). Yield: 108.7 mg (42%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.78-7.81 (m, 4H), 7.60 (t, J = 7.56 Hz, 2H), 7.54 (d, J = 8.32 Hz, 2H), 7.45 (t, J = 7.56 Hz, 4H), 7.09 (d, J = 8.32 Hz, 2H), 4.86 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.8, 137.5, 134.3, 133.8, 131.1, 128.9, 128.1, 93.9, 51.9. MS m/z: 536.0 ($[M+Na]^+$).

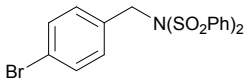
N-(2-iodo-3-methylbenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3k)



3k

3k was obtained according to the general procedure using 2-iodo-1, 3-dimethylbenzene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 4.5). Yield: 108.3 mg (41%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.91-7.93 (m, 4H), 7.61-7.65 (m, 2H), 7.47-7.51 (m, 4H), 7.08 (dd, J = 7.48, 1.40 Hz, 1H), 6.91 (t, J = 7.48 Hz, 1H), 6.88 (dd, J = 7.72, 1.48 Hz, 1H), 5.07 (s, 2H), 2.46 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 142.1, 139.5, 137.1, 134.0, 128.9, 128.9, 128.5, 127.6, 125.8, 104.4, 58.6, 29.4. HRMS: calculated for $C_{20}H_{18}INO_4S_2$ ($[M+H]^+$), 527.9800, found, 527.9792.

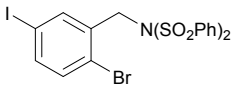
N-(4-bromobenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3l)



3l

3l was obtained according to the general procedure using 1-bromo-4-methylbenzene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 6.5). Yield: 176.1 mg (76%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.79-7.81 (m, 4H), 7.60 (t, J = 7.44 Hz, 2H), 7.45 (t, J = 8.00 Hz, 4H), 7.35 (d, J = 8.00 Hz, 2H), 7.23 (d, J = 8.00 Hz, 2H), 4.87 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.9, 133.8, 133.6, 131.5, 130.9, 128.9, 128.1, 122.3, 51.8. MS m/z: 488.1 ($[M+Na]^+$).

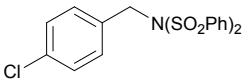
N-(2-bromo-5-iodobenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3m)



3m

3m was obtained according to the general procedure using 1-bromo-4-iodo-2-methylbenzene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 5). Yield: 85.2 mg (29%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.94-7.96 (m, 4H), 7.65-7.69 (m, 2H), 7.52-7.56 (m, 4H), 7.36 (dd, J = 8.32, 2.08 Hz, 1H), 7.29 (d, J = 2.08 Hz, 1H), 7.20 (d, J = 8.32 Hz, 1H), 5.03 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.3, 138.1, 137.8, 136.0, 134.3, 134.1, 129.2, 128.3, 122.2, 92.5, 51.7. HRMS: calculated for $C_{19}H_{15}BrINO_4S_2$ ($[M+Na]^+$), 613.8569, found, 613.8565.

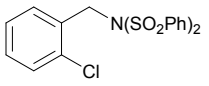
N-(4-chlorobenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3n)



3n

3n was obtained according to the general procedure using 1-chloro-4-methylbenzene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 6.5). Yield: 120.5 mg (57%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.79-7.81 (m, 4H), 7.58-7.62 (m, 2H), 7.44-7.48 (m, 4H), 7.30 (d, J = 8.48 Hz, 2H), 7.19-7.21 (m, 2H), 4.89 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.9, 134.1, 133.8, 133.1, 130.6, 128.9, 128.5, 128.1, 51.7. MS m/z: 444.1 ($[M+Na]^+$).

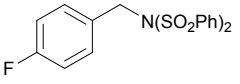
N-(2-chlorobenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3o)



3o

3o was obtained according to the general procedure using 1-chloro-2-methylbenzene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 6). Yield: 113.3 mg (54%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.89-7.91 (m, 4H), 7.58-7.63 (m, 2H), 7.45-7.49 (m, 4H), 7.28-7.30 (m, 1H), 7.18 (d, J = 7.76 Hz, 1H), 7.11-7.15 (m, 1H), 6.95-6.99 (m, 1H), 5.15 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.7, 133.9, 132.8, 132.3, 129.4, 129.4, 128.9, 128.8, 128.3, 126.6, 49.8. MS m/z: 444.1 ($[M+Na]^+$).

N-(4-fluorobenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3p)

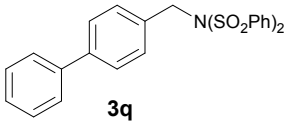


3p

3p was obtained according to the general procedure using 1-fluoro-4-methylbenene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 5). Yield: 116.6 mg (58%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.78-7.81 (m, 4H), 7.57-7.61 (m, 2H), 7.43-7.47 (m, 4H), 7.34-7.38 (m, 2H), 6.90-6.95 (m, 2H), 4.90 (s, 2H). ^{13}C NMR (100

MHz, $CDCl_3$): δ 163.8, 161.4, 139.9, 133.7, 131.2, 131.1, 130.4, 130.4, 128.9, 128.1, 115.4, 115.2, 51.7. HRMS: calculated for $C_{19}H_{16}FNO_4S_2$ ([M+Na]$^+$), 428.0403, found, 428.0398.

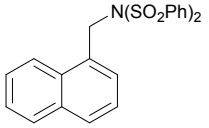
N-([1, 1'-biphenyl]-4-ylmethyl)-N-(phenylsulfonyl)benzenesulfonamide (3q)



3q

3q was obtained according to the general procedure using 4-methyl-1, 1'-biphenyl and purified by column chromatography (ethyl acetate: petroleum ether = 1: 4.5). Yield: 151.7 mg (66%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.81-7.83 (m, 4H), 7.55-7.59 (m, 4H), 7.38-7.48 (m, 11H), 4.99 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.0, 140.6, 140.1, 133.6, 133.5, 129.7, 128.9, 128.8, 128.1, 127.5, 127.1, 127.1, 52.3. MS m/z: 486.2 ([M+Na] $^+$).

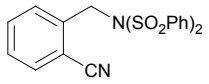
N-(naphthalen-1-ylmethyl)-N-(phenylsulfonyl)benzenesulfonamide (3r)



3r

3r was obtained according to the general procedure using 1-methylnaphthalene and purified by column chromatography (ethyl acetate: petroleum ether = 1: 4.5). Yield: 95.0 mg (43%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 8.10 (d, J = 8.0 Hz, 1H), 7.75-7.81 (m, 5H), 7.68 (d, J = 8.0 Hz, 1H), 7.42-7.53 (m, 4H), 7.34-7.38 (m, 5H), 7.22 (t, J = 8.0 Hz, 1H), 5.53 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.8, 133.5, 133.4, 131.1, 129.2, 128.7, 128.7, 128.6, 128.0, 127.9, 126.5, 125.7, 124.9, 122.7, 50.7. MS m/z: 460.2 ([M+Na] $^+$).

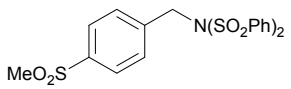
N-(2-cyanobenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3s)



3s

3s was obtained according to the general procedure using 2-methylbenzonitrile and purified by column chromatography (ethyl acetate: petroleum ether = 1: 4). Yield: 73.7 mg (35%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.85-7.87 (m, 4H), 7.61-7.65 (m, 3H), 7.46-7.50 (m, 4H), 7.41-7.44 (m, 1H), 7.31-7.38 (m, 2H), 5.18 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 139.3, 138.7, 134.1, 132.8, 132.7, 129.1, 128.9, 128.3, 128.2, 116.9, 111.7, 50.0. HRMS: calculated for $C_{20}H_{16}N_2O_4S_2$ ([M+H]$^+$), 413.0629, found, 413.0623.

N-(4-(methylsulfonyl)benzyl)-N-(phenylsulfonyl)benzenesulfonamide (3t)

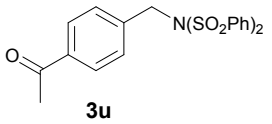


3t

3t was obtained according to the general procedure using 1-methyl-4-(methylsulfonyl)benzene and purified by column chromatography (ethyl acetate: petroleum ether = 2: 1.5). Yield: 107.4 mg (46%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.82-7.84 (m, 4H), 7.79 (d, J = 8.36 Hz, 2H), 7.62 (t, J = 7.48 Hz, 2H), 7.51 (d, J = 8.36 Hz, 2H), 7.45-7.49 (m, 4H), 5.01 (s, 2H), 3.04 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 141.0, 140.3, 139.5, 134.1, 129.6, 129.1, 128.1, 127.5, 51.6, 44.4. HRMS: calculated for

$C_{20}H_{19}NO_6S_3$ ([M+H]$^+$), 466.0452, found, 466.0446.

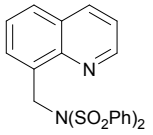
N-(4-acetylbenzyl)-N-(phenylsulfonyl)benzenesulfonamide (3u)



3u

3u was obtained according to the general procedure using 1-(p-tolyl)ethan-1-one and purified by column chromatography (ethyl acetate: petroleum ether = 1: 3.5). Yield: 69.7 mg (32%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 7.80-7.83 (m, 6H), 7.59 (t, J = 7.48 Hz, 2H), 7.44 (t, J = 8.00 Hz, 6H), 4.97 (s, 2H), 2.59 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.6, 139.9, 139.7, 136.7, 133.9, 129.0, 128.9, 128.4, 128.1, 51.9, 26.7. MS m/z: 430.2 ([M+H] $^+$).

N-(phenylsulfonyl)-N-(quinolin-8-ylmethyl)benzenesulfonamide (5a)

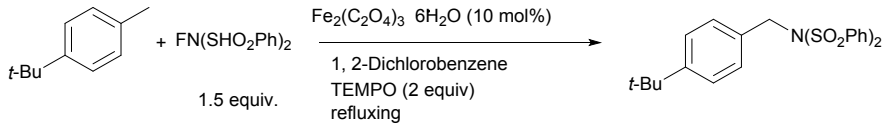


5a

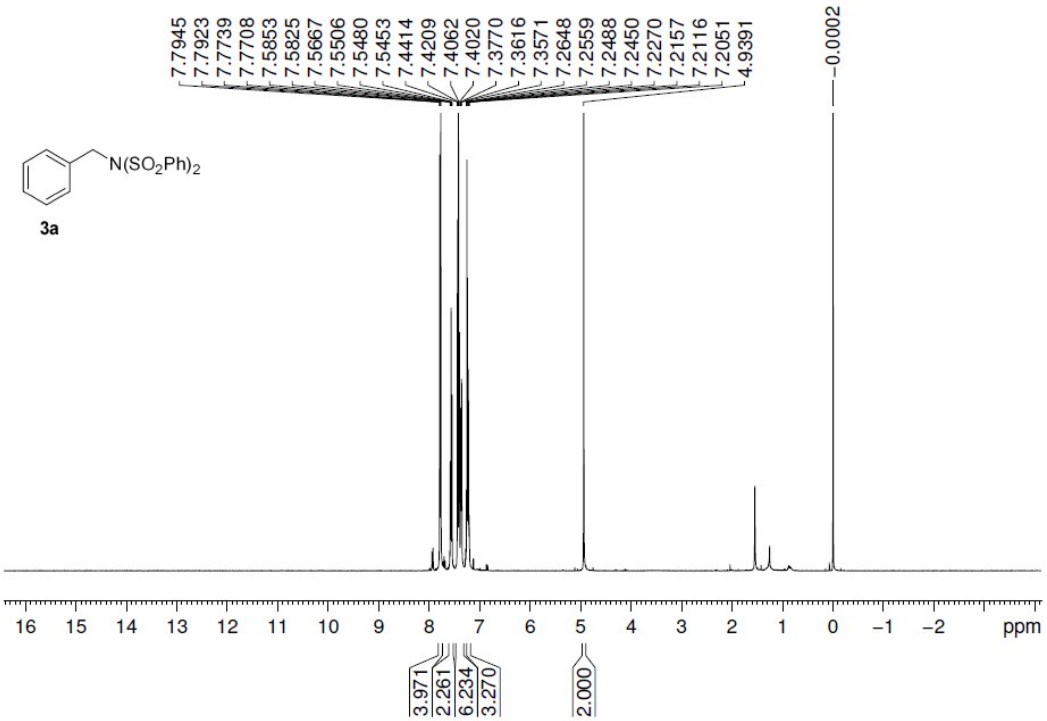
5a was obtained according to the general procedure using 8-methylquinoline and purified by column chromatography (ethyl acetate: petroleum ether = 1: 2). Yield: 103.4 mg (47%); white solid. ^{1}HNMR (400 MHz, CDCl3): δ 8.91 (dd, J = 4.16, 1.68 Hz, 1H), 8.15 (dd, J = 8.32, 1.68 Hz, 1H), 7.89-7.92 (m, 4H), 7.68 (d, J = 8.32 Hz, 1H), 7.58-7.63 (m, 2H), 7.50-7.53 (m, 1H), 7.42-7.47 (m, 5H),7.29 (t, J = 7.72 Hz, 1H), 5.82 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.5, 145.6, 139.7, 136.3, 133.8, 133.0, 128.9, 128.4, 128.1, 128.0, 127.3, 126.0, 121.2, 49.1. HRMS: calculated for $C_{22}H_{18}N_2O_4S_2$ ([M+H]$^+$), 439.0786, found, 439.0784.

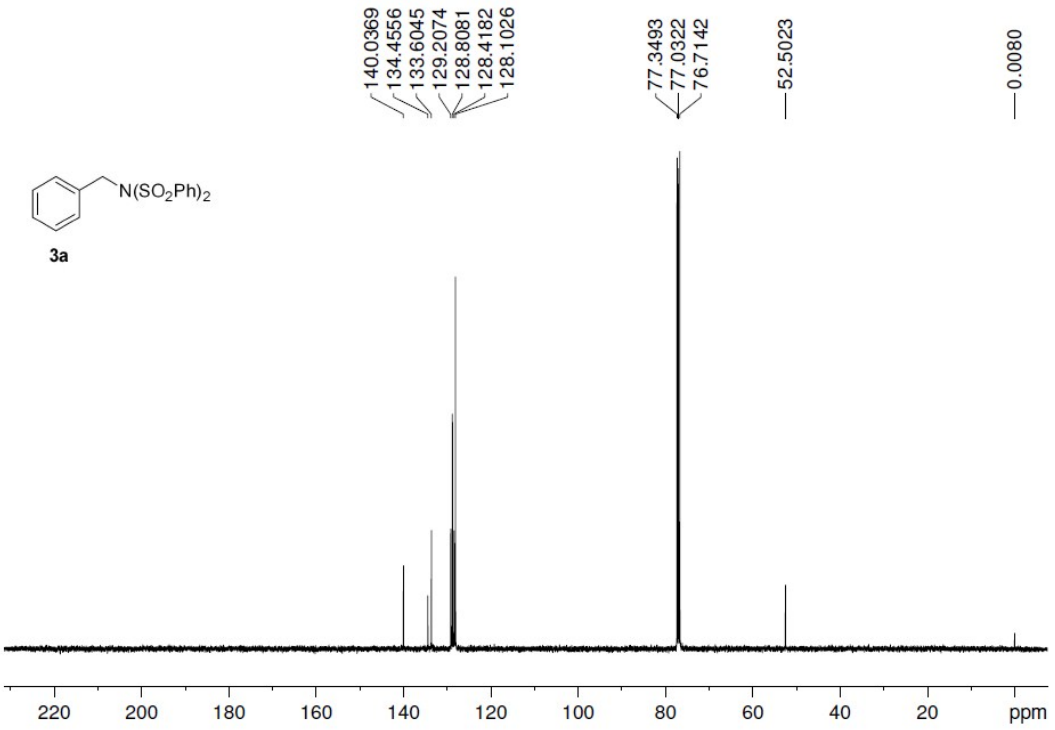
The radical-trapping experiment

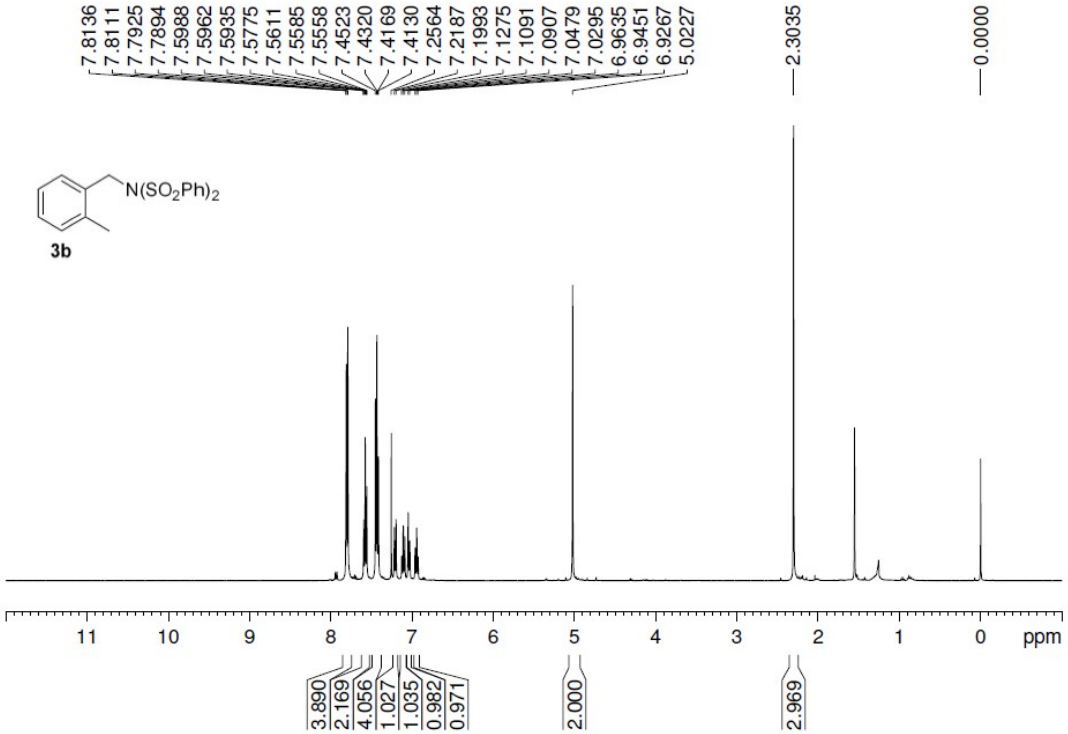
2 equiv of 2, 2, 6, 6-tetramethylpiperidyl-1-oxyl (TEMPO) was added in the amination reaction under the standard reaction conditions. No product could be detected by thin layer chromatography.

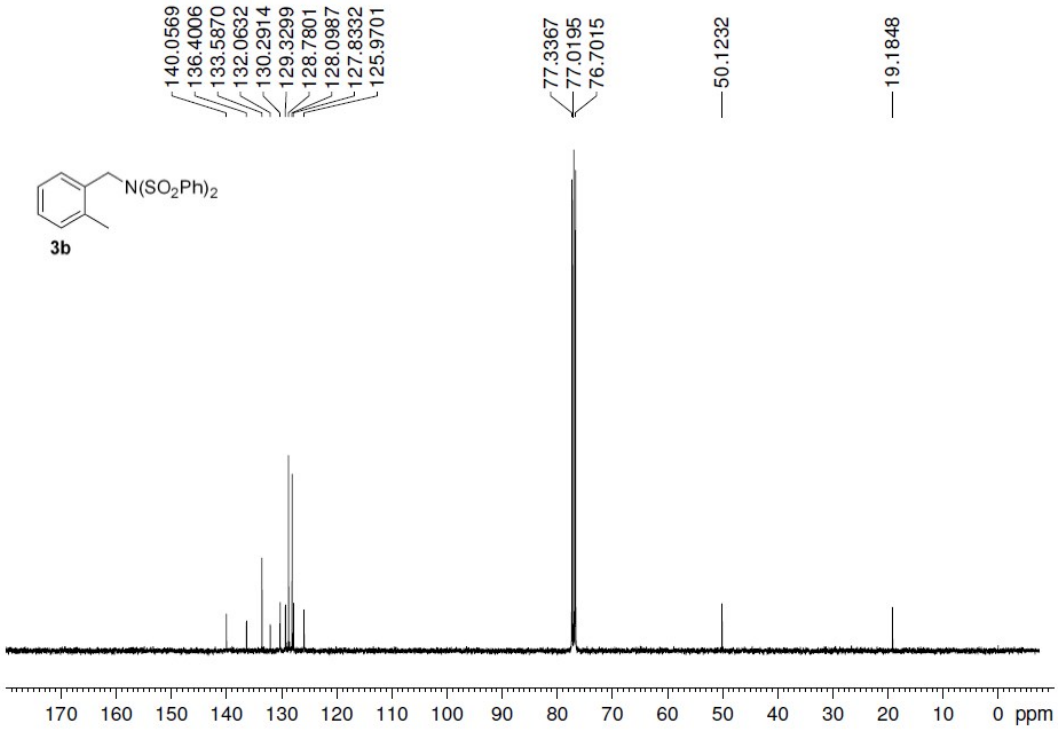


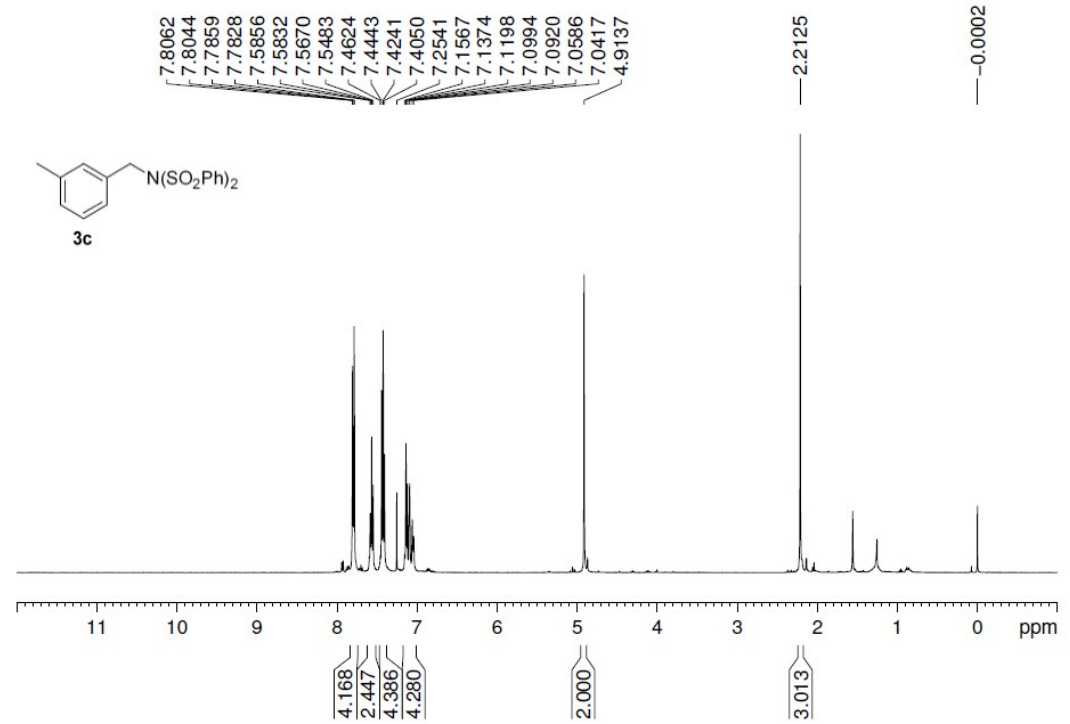
1f, 0.5 mmol **2**, 0.75 mmol **3f**, 0%

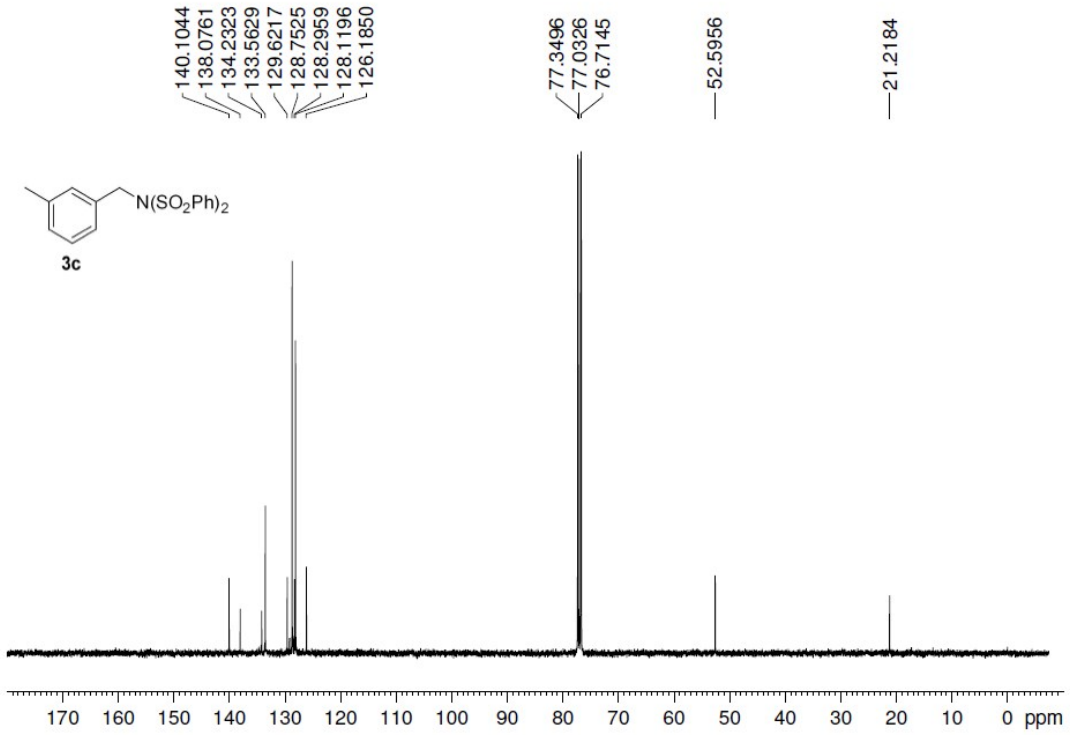

7.7945
7.7923
7.7739
7.7708
7.5853
7.5825
7.5667
7.5506
7.5480
7.5453
7.4414
7.4209
7.4062
7.4020
7.3770
7.3616
7.3571
7.2648
7.2559
7.2488
7.2450
7.2270
7.2157
7.2116
7.2051
4.9391
0.0002
N(SO2Ph)2
3a
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
3.971
2.261
6.234
3.270
2.000

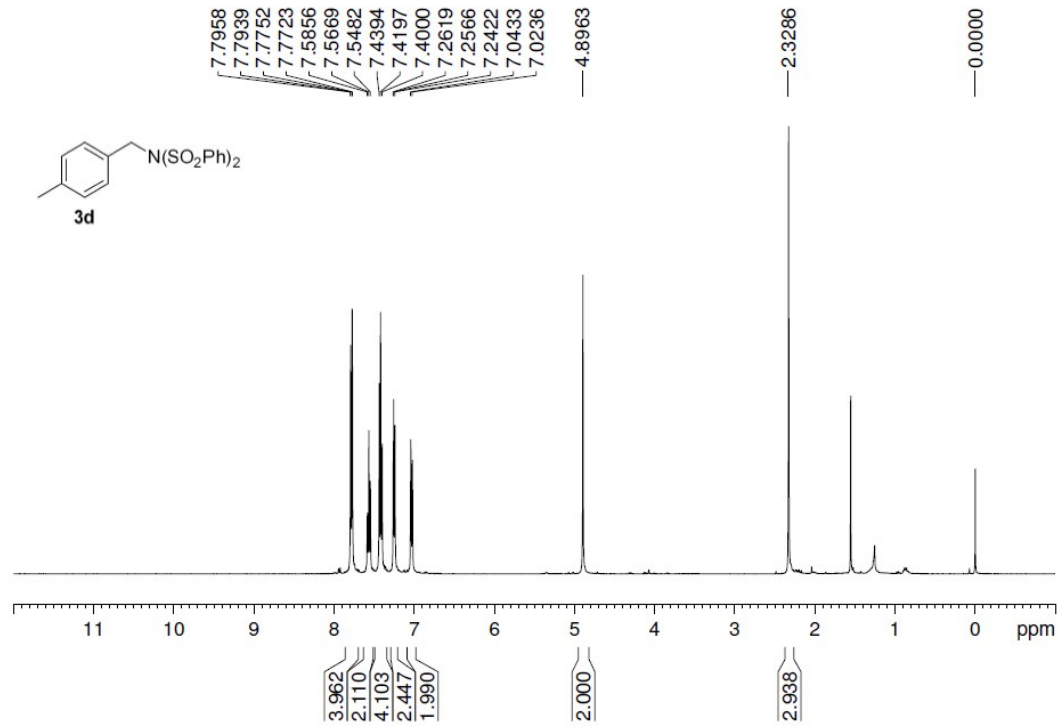

140.0369
134.4556
133.6045
129.2074
128.8081
128.4182
128.1026
77.3493
77.0322
76.7142
52.5023
0.0080
N(SO2Ph)2
3a
220 200 180 160 140 120 100 80 60 40 20 ppm


7.8136
7.8111
7.7925
7.7894
7.5988
7.5962
7.5935
7.5775
7.5611
7.5585
7.5558
7.4523
7.4320
7.4169
7.4130
7.2564
7.2187
7.1993
7.1275
7.1091
7.0907
7.0479
7.0295
6.9635
6.9451
6.9267
5.0227
2.3035
0.0000
N(SO2Ph)2
3b
11 10 9 8 7 6 5 4 3 2 1 0 ppm
3.890
2.169
4.056
1.027
1.035
0.982
0.971
2.000
2.969


140.0569
136.4006
133.5870
132.0632
130.2914
129.3299
128.7801
128.0987
127.8332
125.9701
77.3367
77.0195
76.7015
50.1232
19.1848
N(SO2Ph)2
3b
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


7.8062
7.8044
7.7859
7.7828
7.5856
7.5832
7.5670
7.5483
7.4624
7.4443
7.4241
7.4050
7.2541
7.1567
7.1374
7.1198
7.0994
7.0920
7.0586
7.0417
4.9137
2.2125
0.0002
N(SO2Ph)2
3c
11
10
9
8
7
6
5
4
3
2
1
0
ppm
4.168
2.447
4.386
4.280
2.000
3.013


140.1044
138.0761
134.2323
133.5629
129.6217
128.7525
128.2959
128.1196
126.1850
77.3496
77.0326
76.7145
52.5956
21.2184
N(SO2Ph)2
3c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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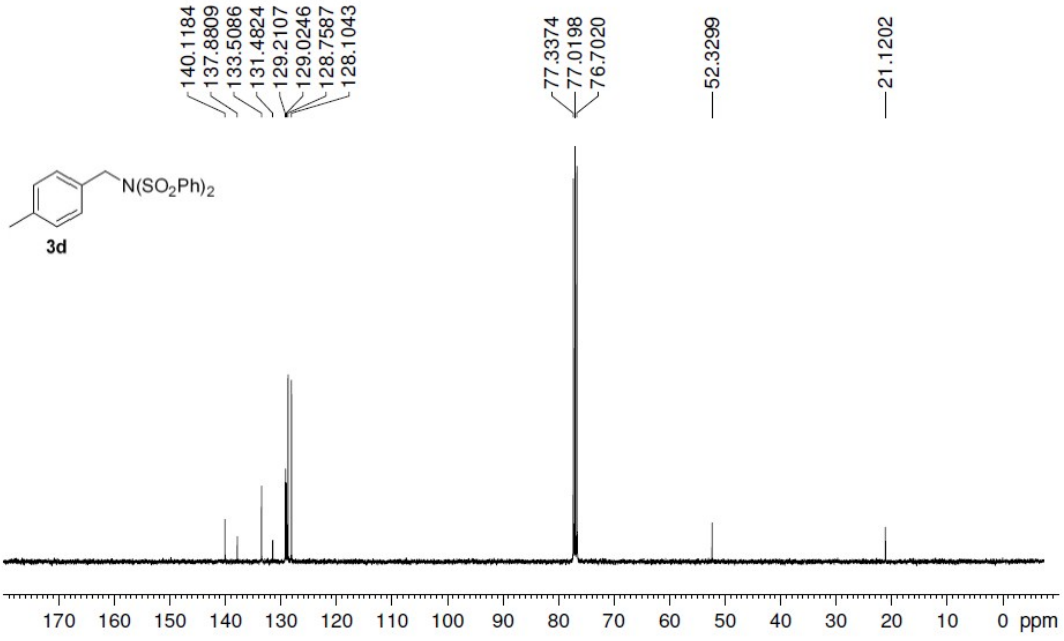
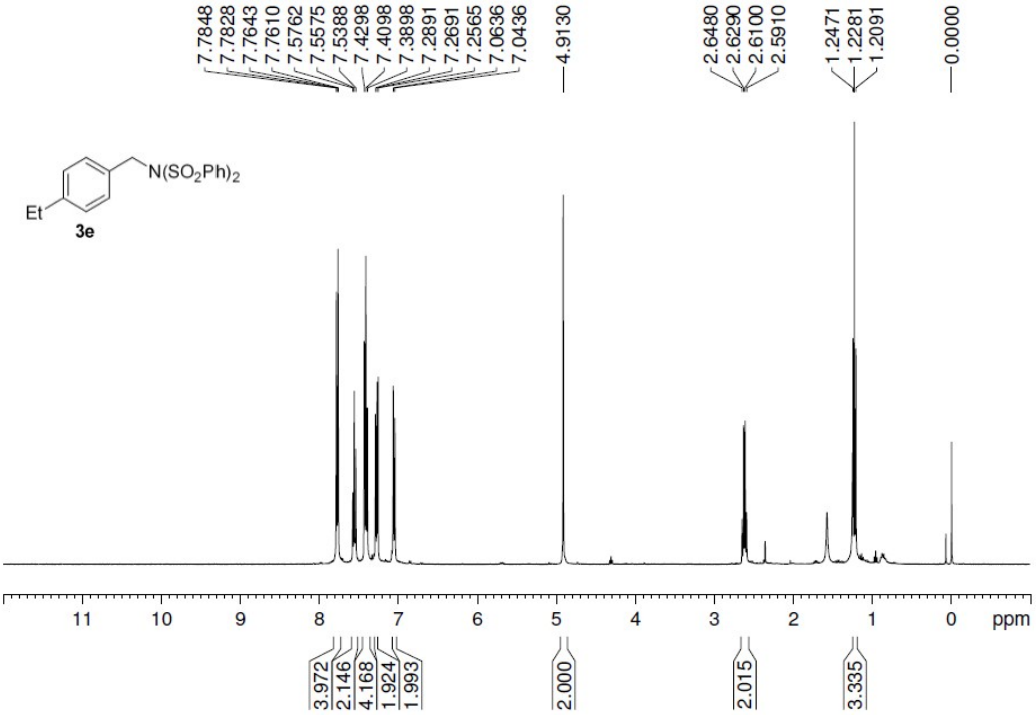
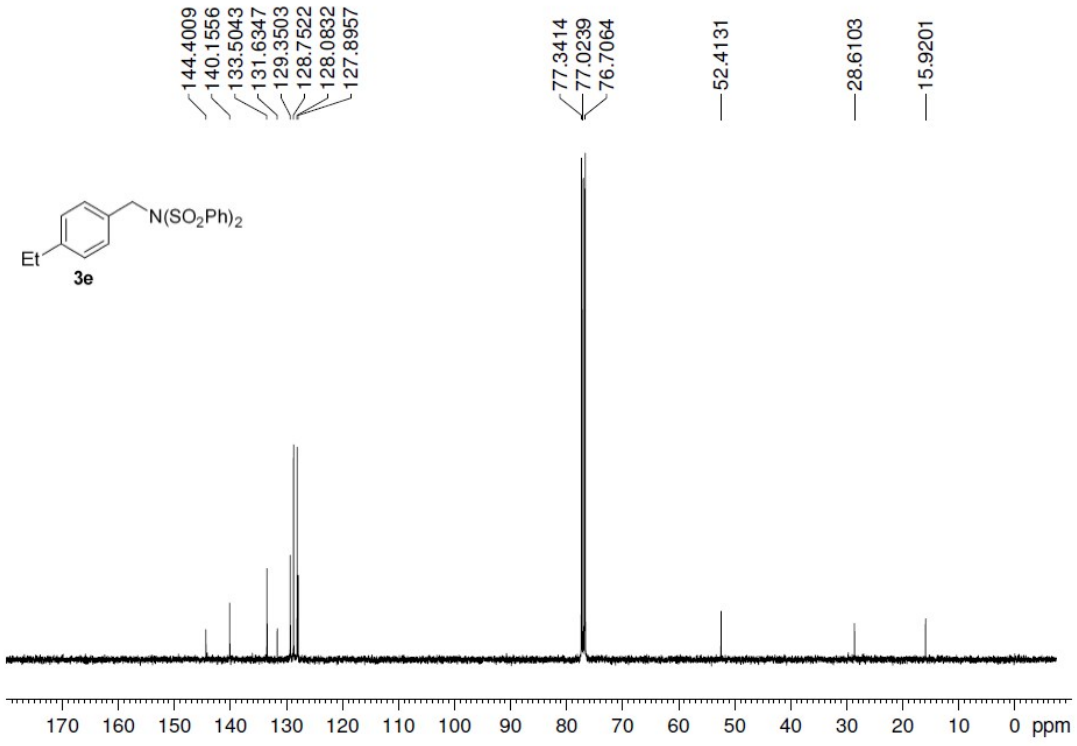
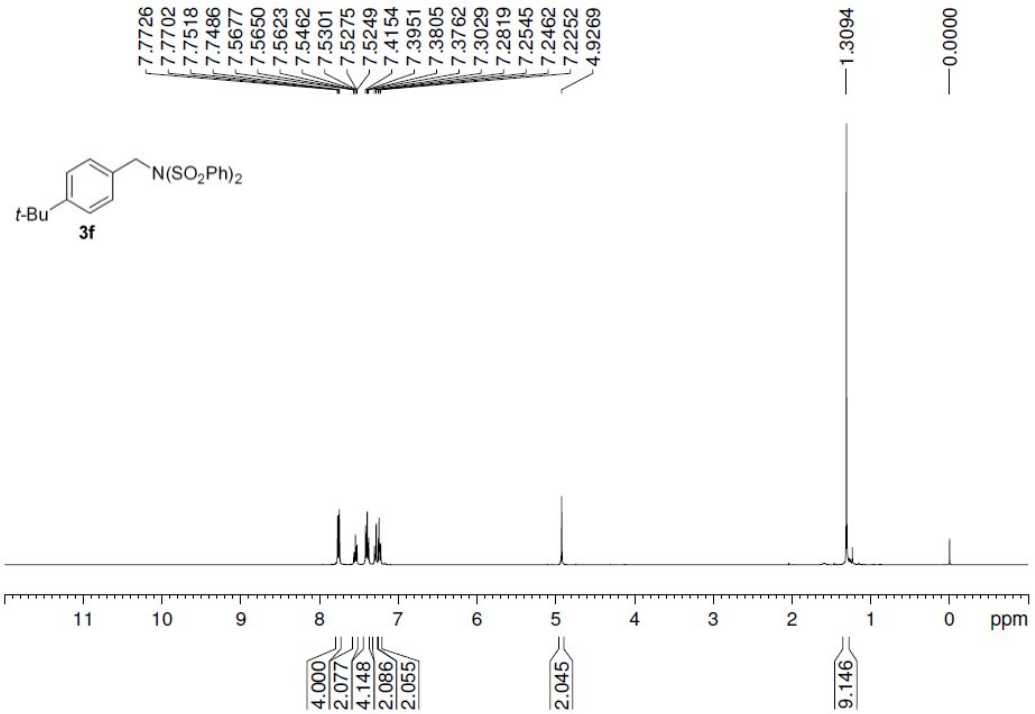
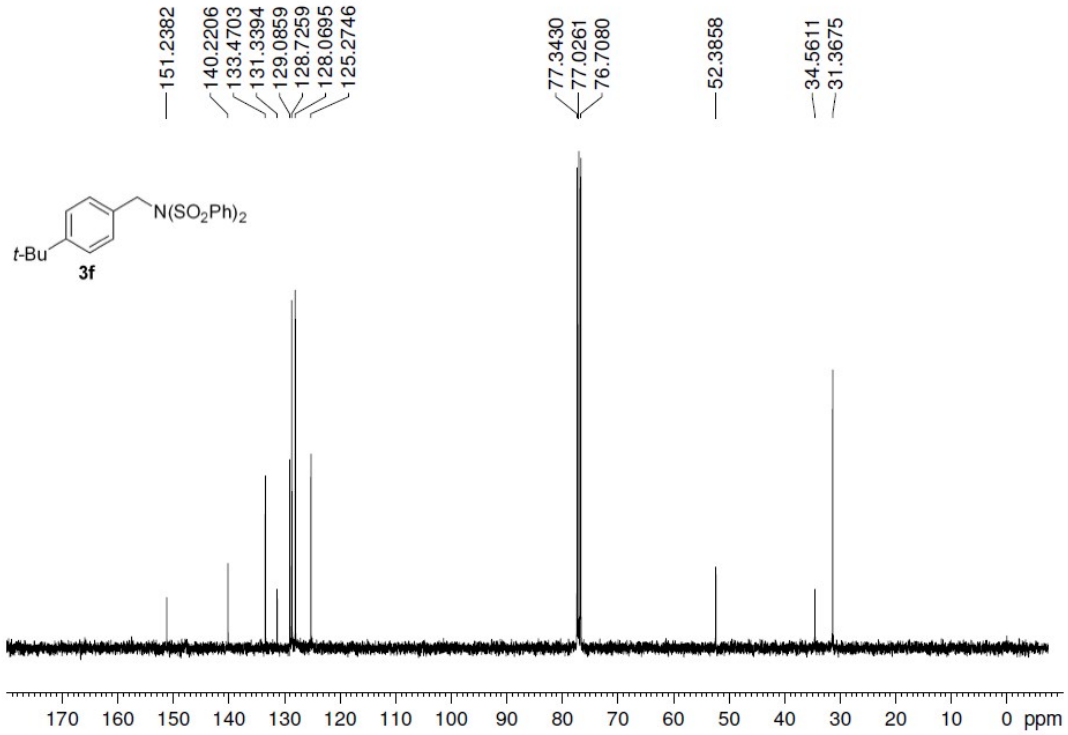
7.7939
7.7752
7.7723
7.5856
7.5669
7.5482
7.4394
7.4197
7.4000
7.2619
7.2566
7.2422
7.0433
7.0236
4.8963
2.3286
0.0000
N(SO2Ph)2
3d
11 10 9 8 7 6 5 4 3 2 1 0 ppm
3.962
2.110
4.103
2.447
1.990
2.000
2.938

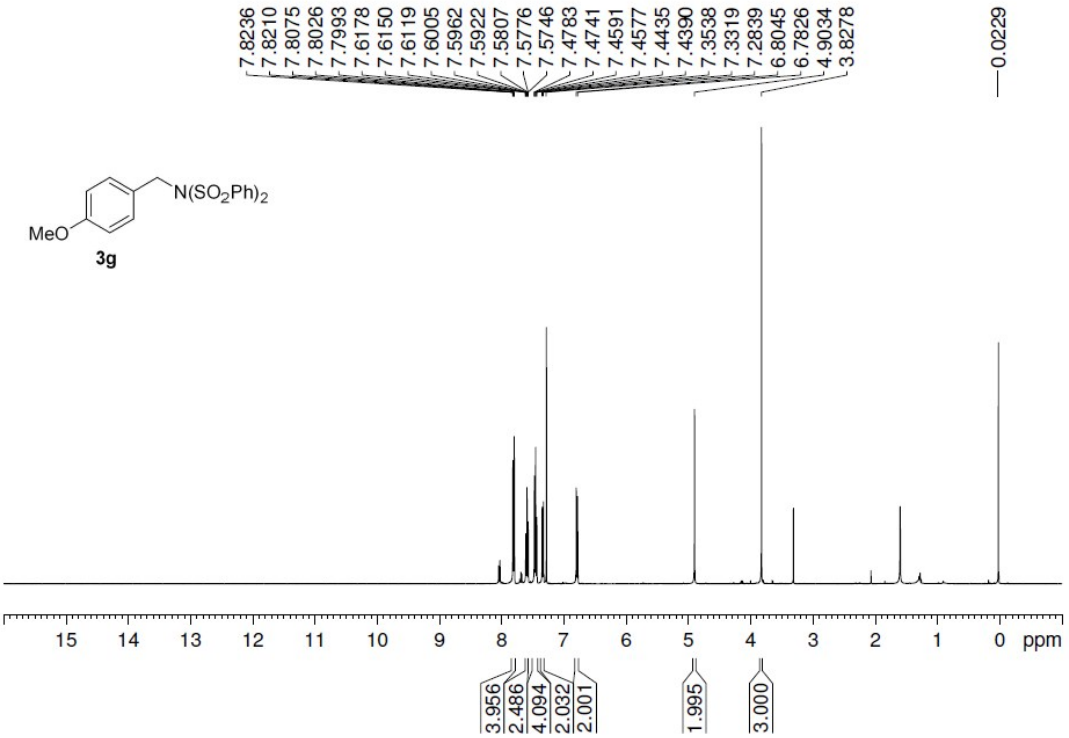

140.1184
137.8809
133.5086
131.4824
129.2107
129.0246
128.7587
128.1043
77.3374
77.0198
76.7020
52.3299
21.1202
N(SO2Ph)2
3d
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

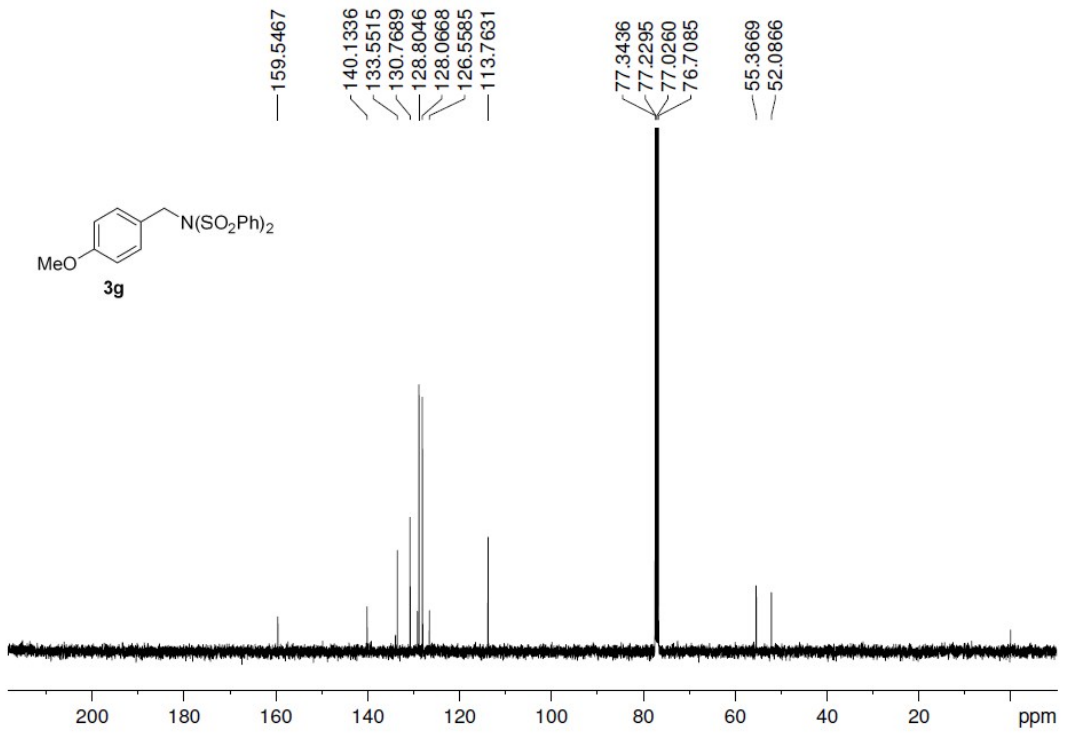

7.7848
7.7828
7.7643
7.7610
7.5762
7.5575
7.5388
7.4298
7.4098
7.3898
7.2891
7.2691
7.2565
7.0636
7.0436
4.9130
2.6480
2.6290
2.6100
2.5910
1.2471
1.2281
1.2091
0.0000
N(SO2Ph)2
Et
3e
11 10 9 8 7 6 5 4 3 2 1 0 ppm
3.972
2.146
4.168
1.924
1.993
2.000
2.015
3.335

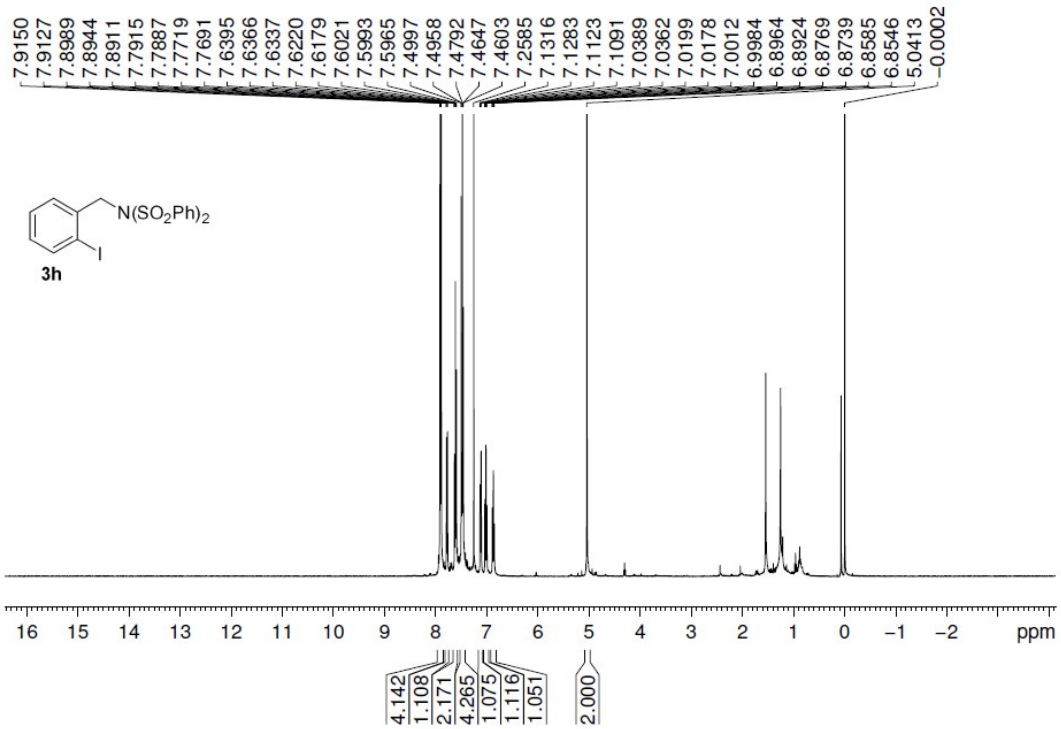

144.4009
140.1556
133.5043
131.6347
129.3503
128.7522
128.0832
127.8957
77.3414
77.0239
76.7064
52.4131
28.6103
15.9201
N(SO2Ph)2
Et
3e
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

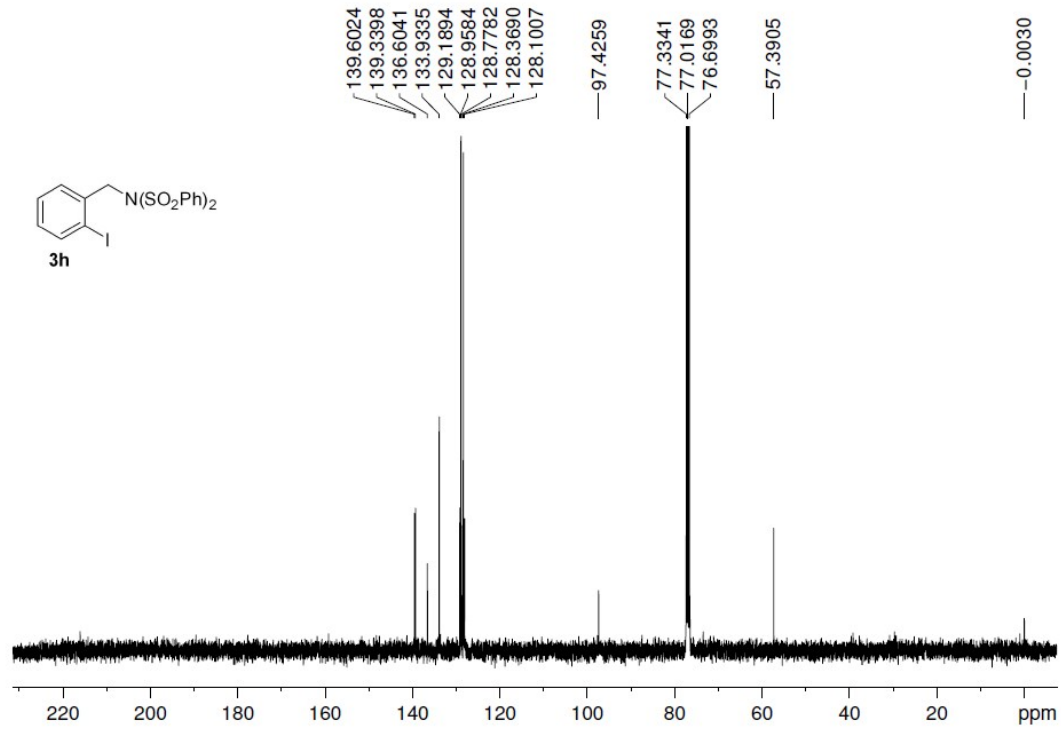

7.7726
7.7702
7.7518
7.7486
7.5677
7.5650
7.5623
7.5462
7.5301
7.5275
7.5249
7.4154
7.3951
7.3805
7.3762
7.3029
7.2819
7.2545
7.2462
7.2252
4.9269
1.3094
0.0000
N(SO2Ph)2
t-Bu
3f
11 10 9 8 7 6 5 4 3 2 1 0 ppm
4.000
2.077
4.148
2.086
2.055
2.045
9.146

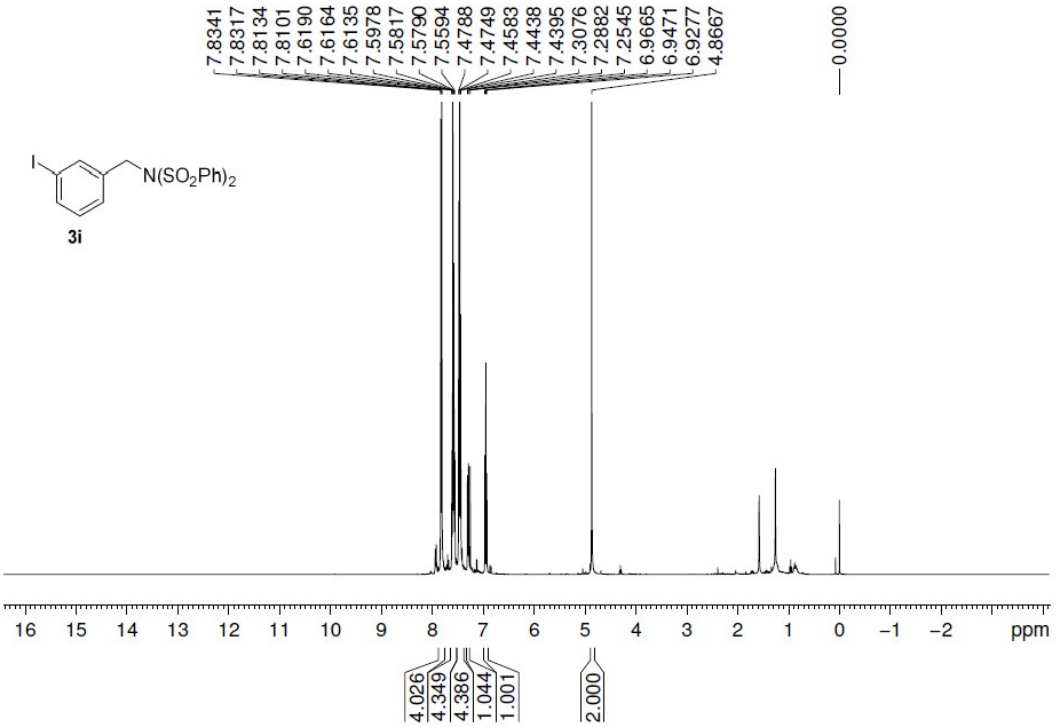

151.2382
140.2206
133.4703
131.3394
129.0859
128.7259
128.0695
125.2746
77.3430
77.0261
76.7080
52.3858
34.5611
31.3675
N(SO2Ph)2
t-Bu
3f
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

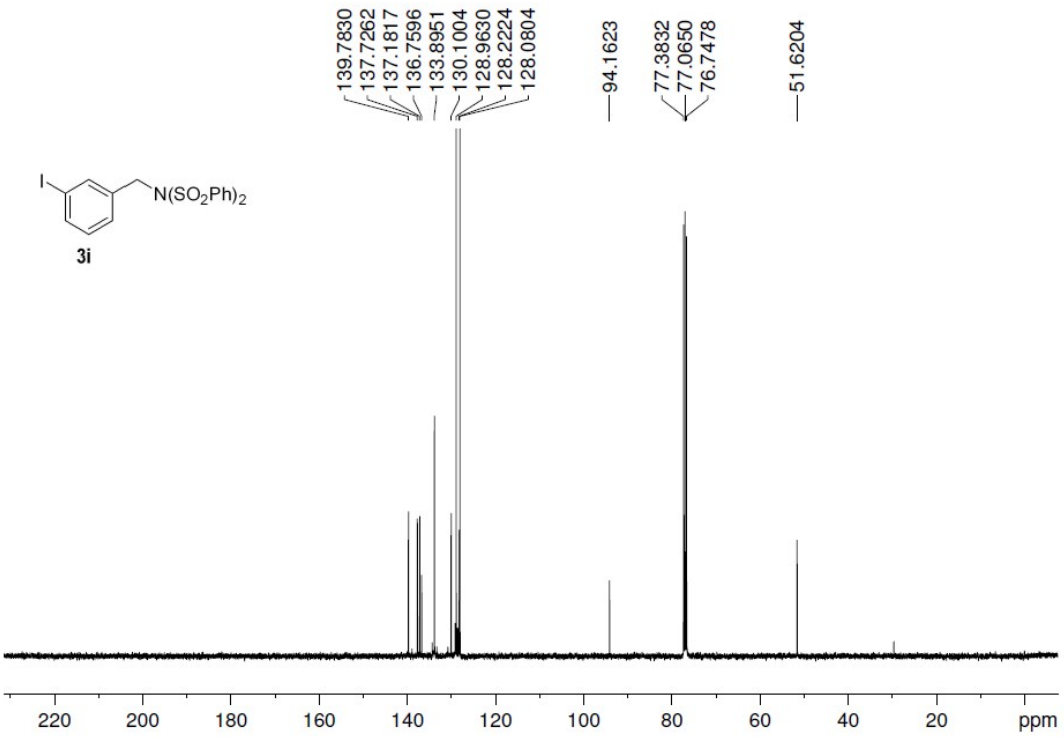

7.8236
7.8210
7.8075
7.8026
7.7993
7.6178
7.6150
7.6119
7.6005
7.5962
7.5922
7.5807
7.5776
7.5746
7.4783
7.4741
7.4591
7.4577
7.4435
7.4390
7.3538
7.3319
7.2839
6.8045
6.7826
4.9034
3.8278
0.0229
N(SO2Ph)2
MeO
3g
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
3.956
2.486
4.094
2.032
2.001
1.995
3.000

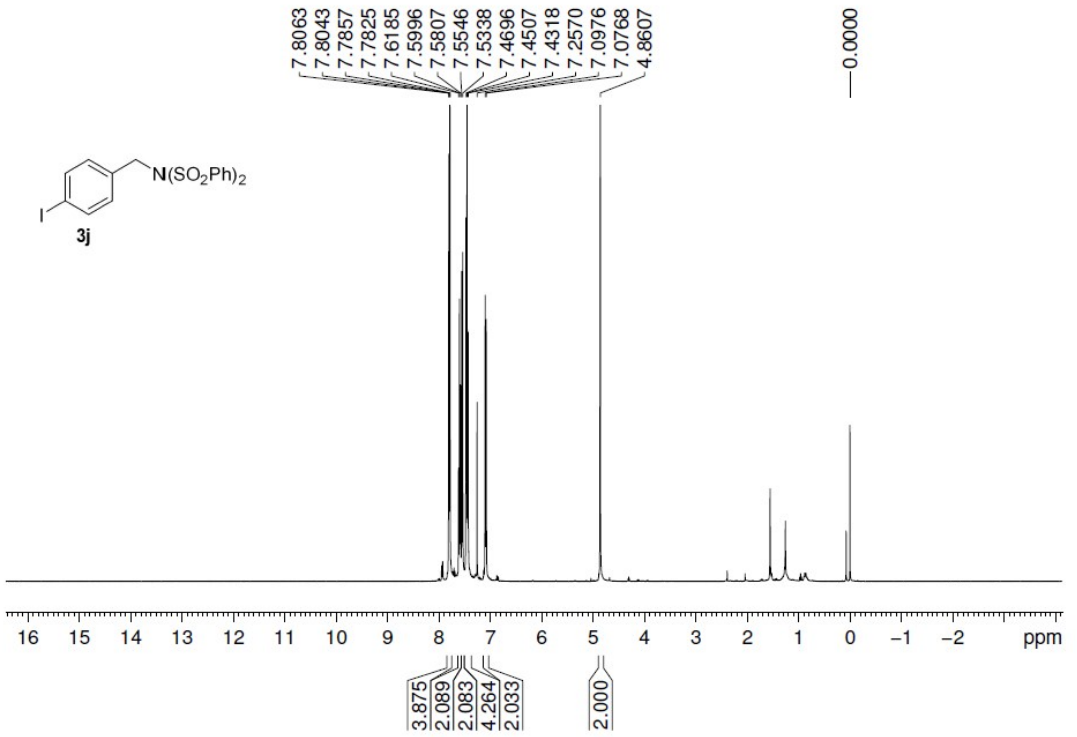

159.5467
140.1336
133.5515
130.7689
128.8046
128.0668
126.5585
113.7631
77.3436
77.2295
77.0260
76.7085
55.3669
52.0866
N(SO2Ph)2
MeO
3g
200 180 160 140 120 100 80 60 40 20 ppm

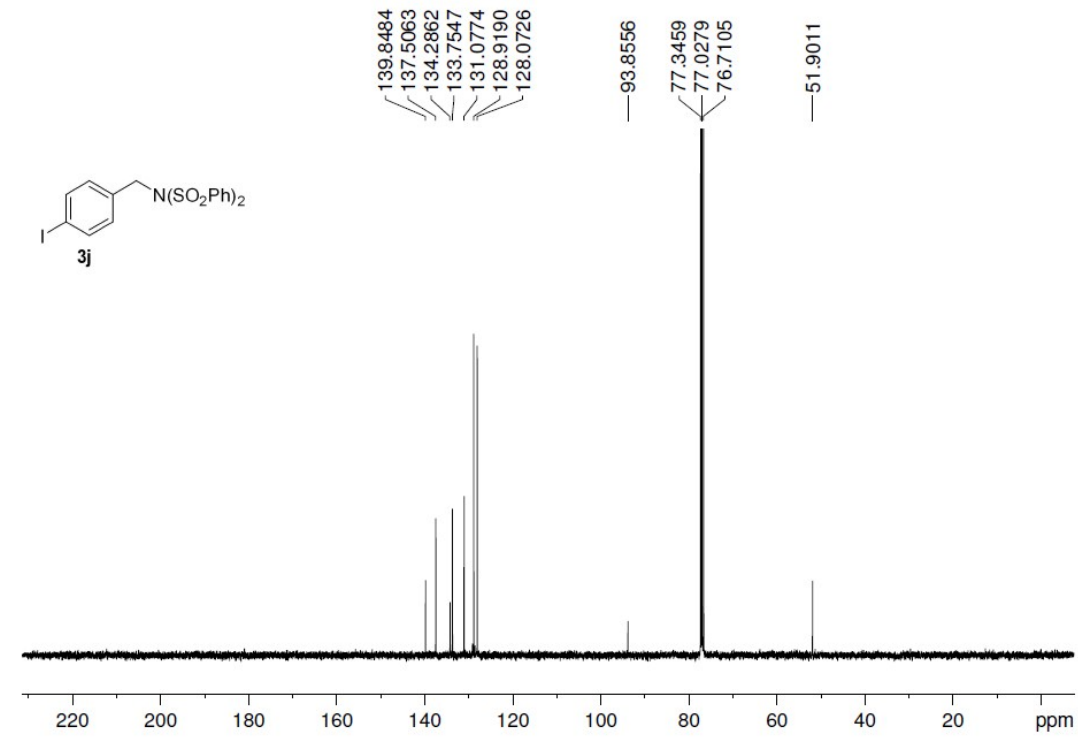

7.9150
7.9127
7.8989
7.8944
7.8911
7.7915
7.7887
7.7719
7.7691
7.6395
7.6366
7.6337
7.6220
7.6179
7.6021
7.5993
7.5965
7.4997
7.4958
7.4792
7.4647
7.4603
7.2585
7.1316
7.1283
7.1123
7.1091
7.0389
7.0362
7.0199
7.0178
7.0012
6.9984
6.8964
6.8924
6.8769
6.8739
6.8585
6.8546
5.0413
−0.0002
N(SO2Ph)2
I
3h
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
4.142
1.108
2.171
4.265
1.075
1.116
1.051
2.000

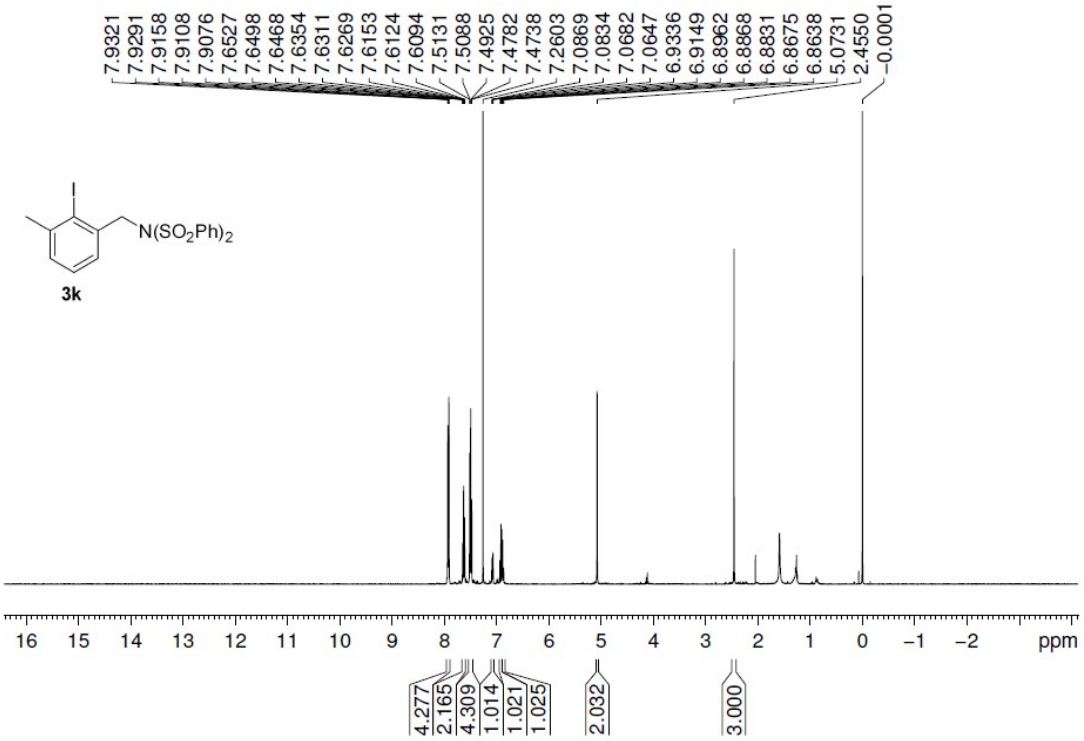

139.6024
139.3398
136.6041
133.9335
129.1894
128.9584
128.7782
128.3690
128.1007
97.4259
77.3341
77.0169
76.6993
57.3905
−0.0030
N(SO2Ph)2
I
3h
220 200 180 160 140 120 100 80 60 40 20 ppm

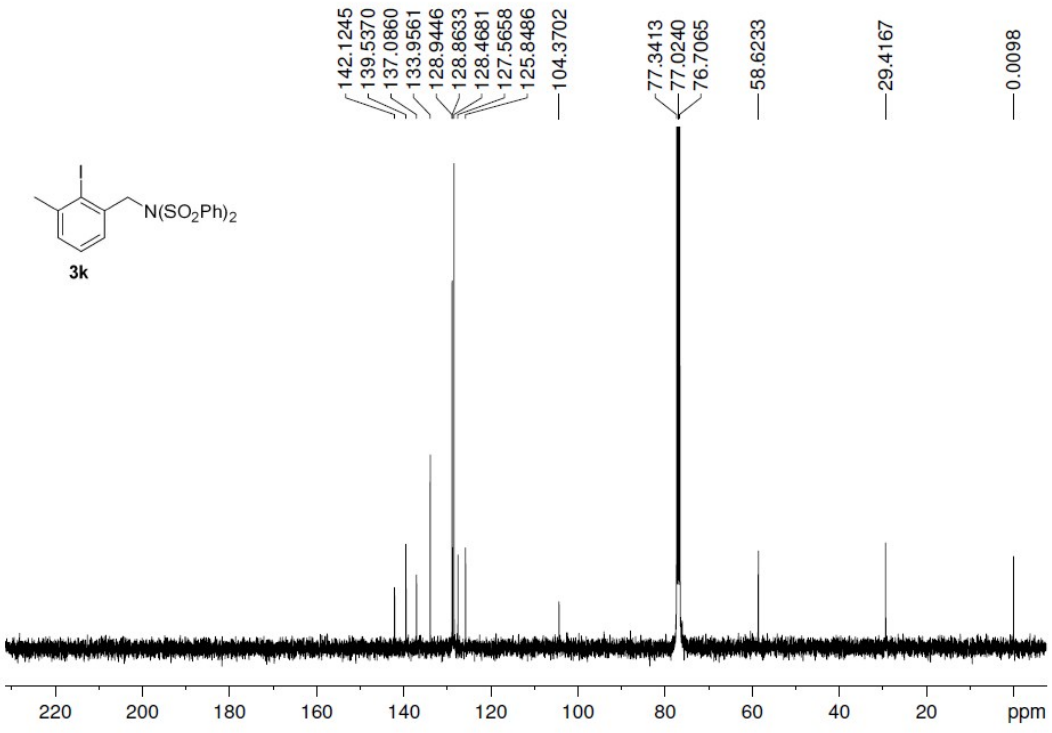

7.8341
7.8317
7.8134
7.8101
7.6190
7.6164
7.6135
7.5978
7.5817
7.5790
7.5594
7.4788
7.4749
7.4583
7.4438
7.4395
7.3076
7.2882
7.2545
6.9665
6.9471
6.9277
4.8667
0.0000
I
N(SO2Ph)2
3i
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
4.026
4.349
4.386
1.044
1.001
2.000

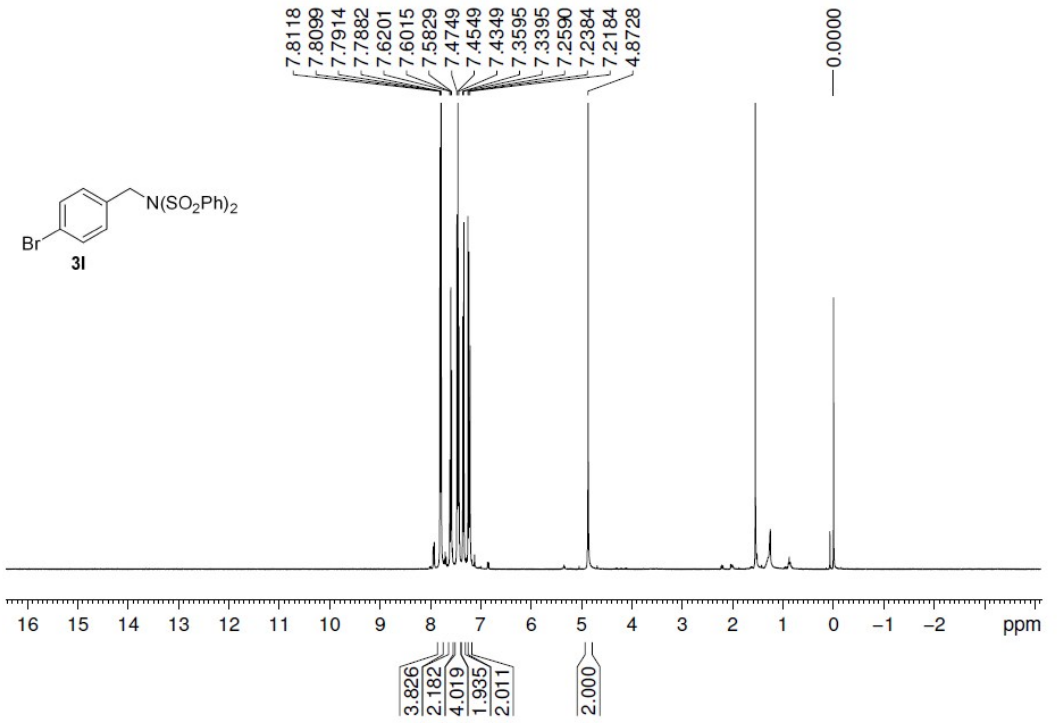

139.7830
137.7262
137.1817
136.7596
133.8951
130.1004
128.9630
128.2224
128.0804
94.1623
77.3832
77.0650
76.7478
51.6204
I
N(SO2Ph)2
3i
220 200 180 160 140 120 100 80 60 40 20 ppm

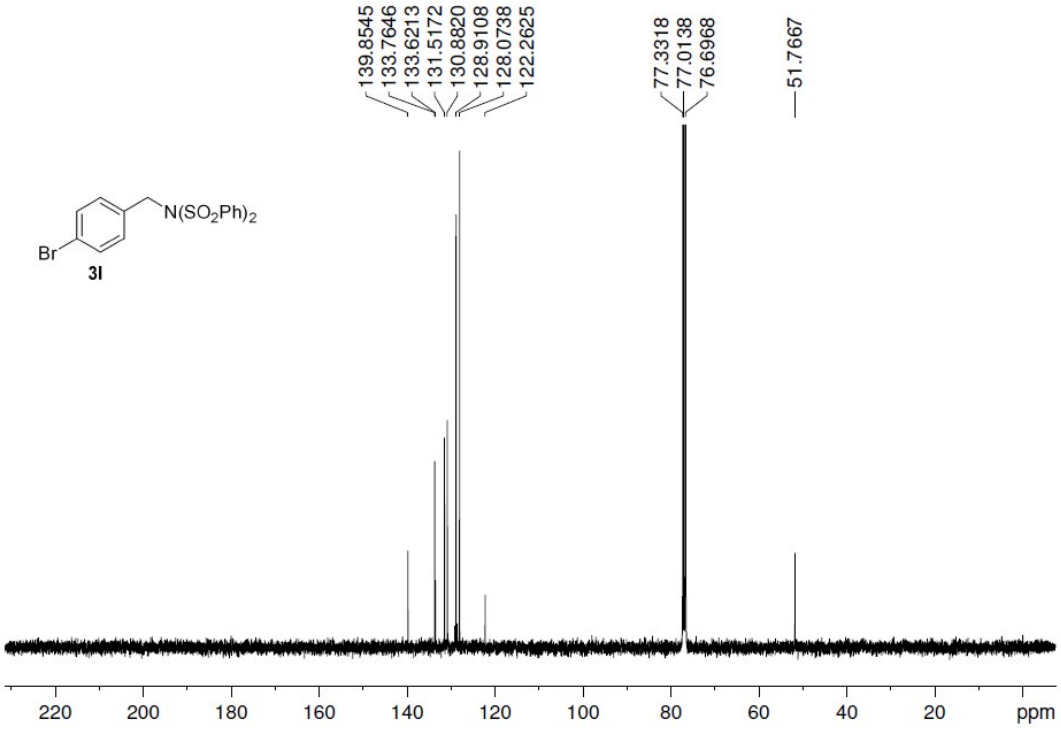

7.8063
7.8043
7.7857
7.7825
7.6185
7.5996
7.5807
7.5546
7.5338
7.4696
7.4507
7.4318
7.2570
7.0976
7.0768
4.8607
0.0000
N(SO2Ph)2
I
3j
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
3.875
2.089
2.083
4.264
2.033
2.000

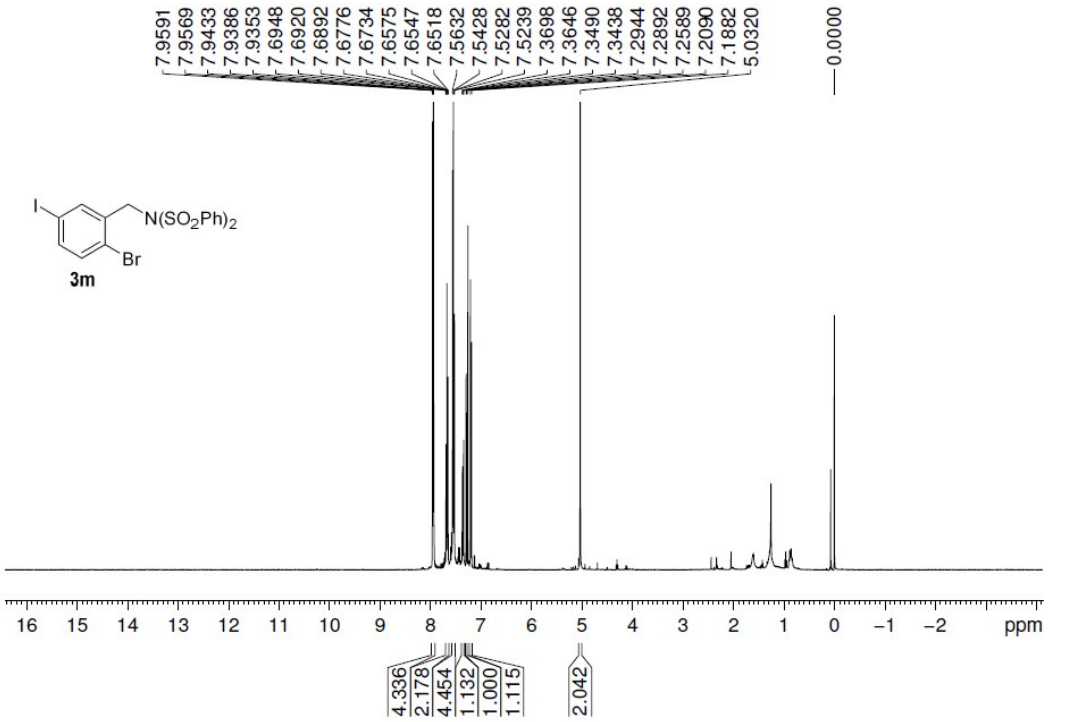

139.8484
137.5063
134.2862
133.7547
131.0774
128.9190
128.0726
93.8556
77.3459
77.0279
76.7105
51.9011
N(SO2Ph)2
I
3j
220 200 180 160 140 120 100 80 60 40 20 ppm

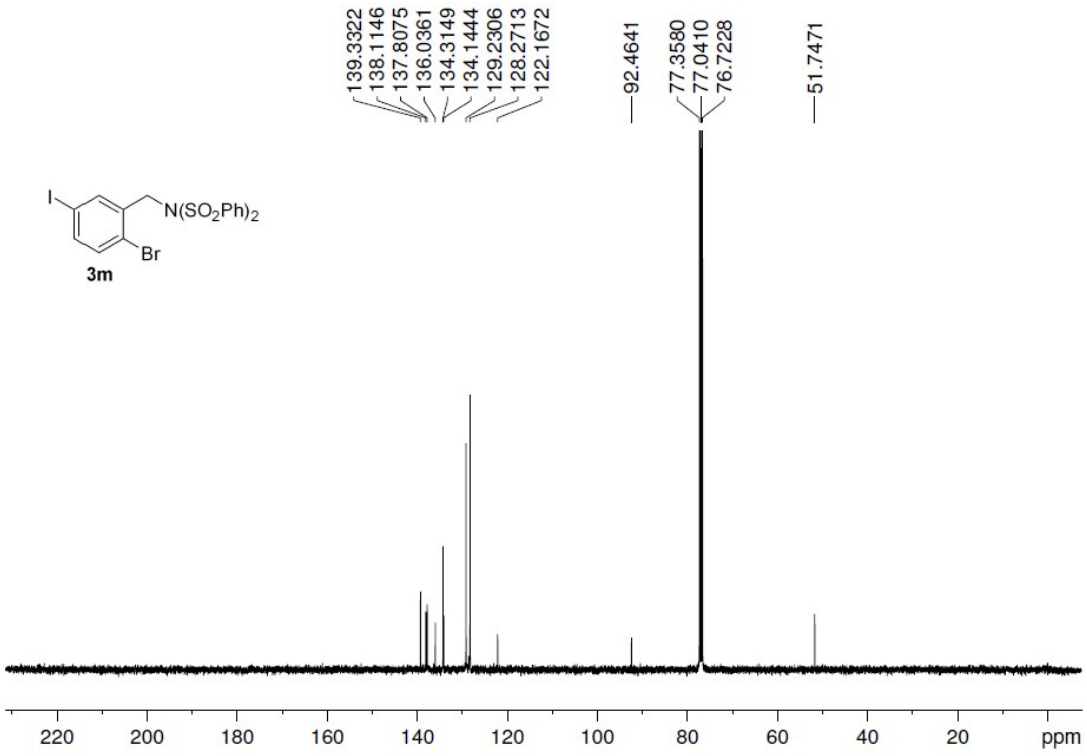

7.9321
7.9291
7.9158
7.9108
7.9076
7.6527
7.6498
7.6468
7.6354
7.6311
7.6269
7.6153
7.6124
7.6094
7.5131
7.5088
7.4925
7.4782
7.4738
7.2603
7.0869
7.0834
7.0682
7.0647
6.9336
6.9149
6.8962
6.8868
6.8831
6.8675
6.8638
5.0731
2.4550
0.0001
N(SO2Ph)2
3k
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
4.277
2.165
4.309
1.014
1.021
1.025
2.032
3.000

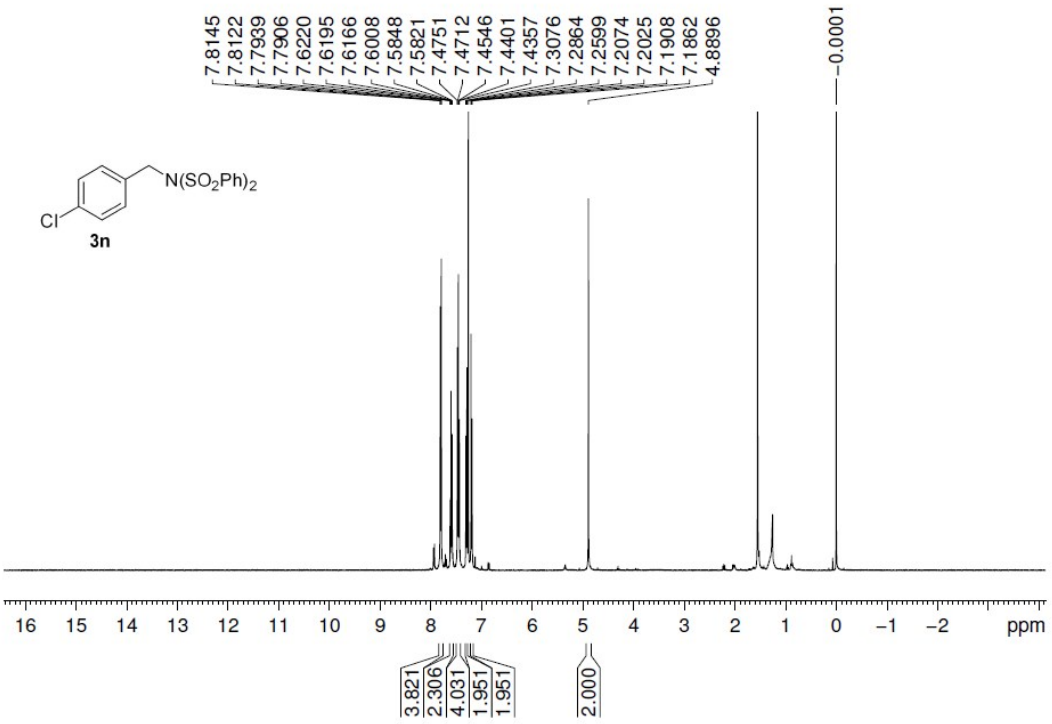

142.1245
139.5370
137.0860
133.9561
128.9446
128.8633
128.4681
127.5658
125.8486
104.3702
77.3413
77.0240
76.7065
58.6233
29.4167
0.0098
N(SO2Ph)2
3k
220 200 180 160 140 120 100 80 60 40 20 ppm

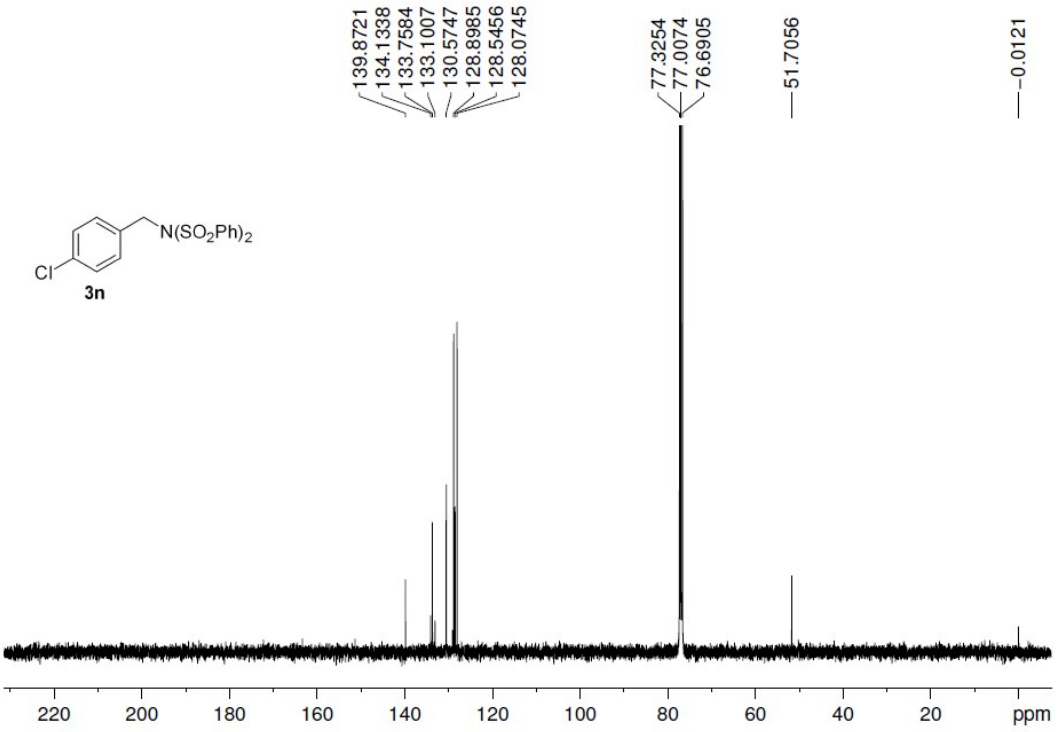

7.8118
7.8099
7.7914
7.7882
7.6201
7.6015
7.5829
7.4749
7.4549
7.4349
7.3595
7.3395
7.2590
7.2384
7.2184
4.8728
0.0000
N(SO2Ph)2
Br
3l
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
3.826
2.182
4.019
1.935
2.011
2.000

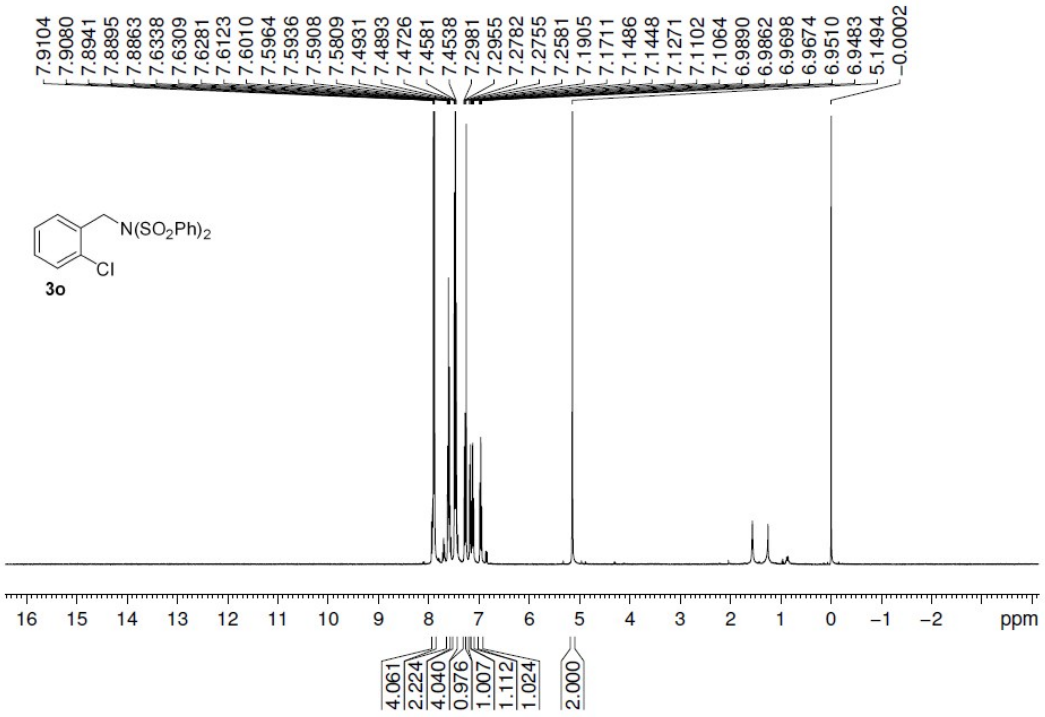

139.8545
133.7646
133.6213
131.5172
130.8820
128.9108
128.0738
122.2625
77.3318
77.0138
76.6968
51.7667
N(SO2Ph)2
Br
3l
220 200 180 160 140 120 100 80 60 40 20 ppm

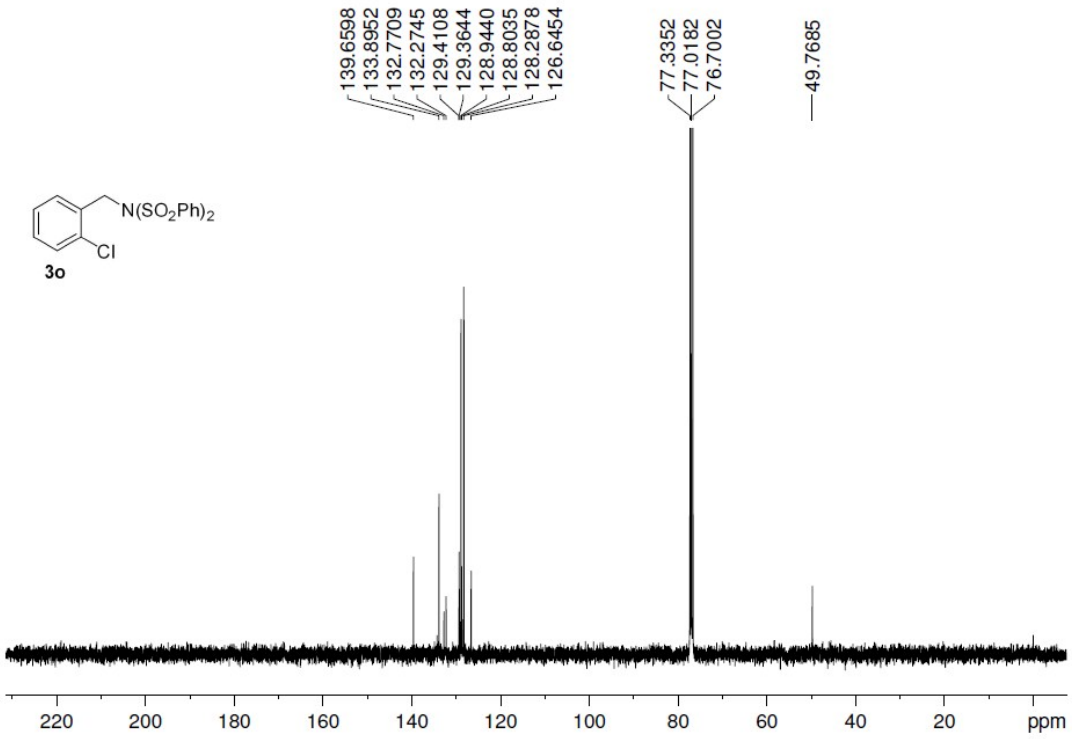

7.9591
7.9569
7.9433
7.9386
7.9353
7.6948
7.6920
7.6892
7.6776
7.6734
7.6575
7.6547
7.6518
7.5632
7.5428
7.5282
7.5239
7.3698
7.3646
7.3490
7.3438
7.2944
7.2892
7.2589
7.2090
7.1882
5.0320
0.0000
I
N(SO2Ph)2
Br
3m
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
4.336
2.178
4.454
1.132
1.000
1.115
2.042

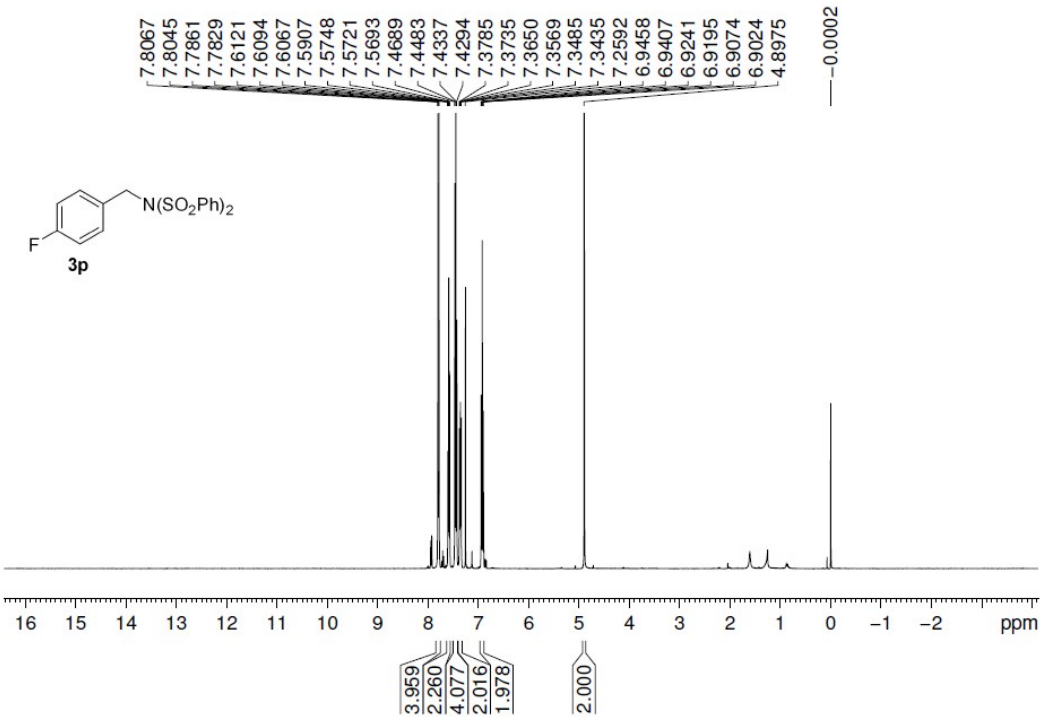

139.3322
138.1146
137.8075
136.0361
134.3149
134.1444
129.2306
128.2713
122.1672
92.4641
77.3580
77.0410
76.7228
51.7471
I
N(SO2Ph)2
Br
3m
220 200 180 160 140 120 100 80 60 40 20 ppm

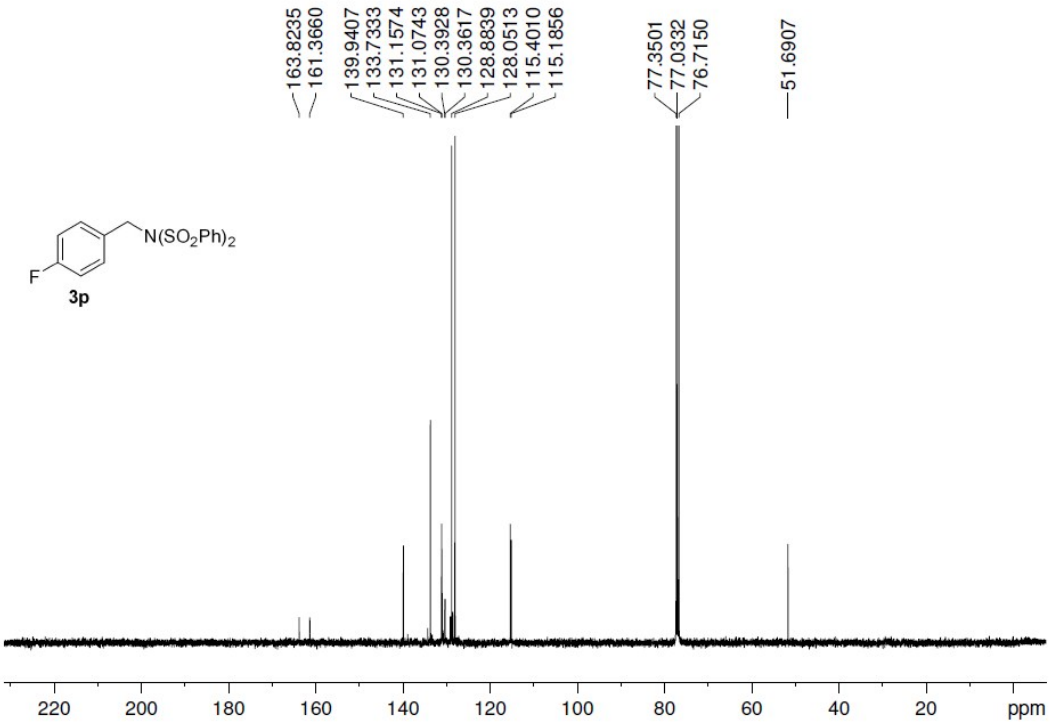

7.8145
7.8122
7.7939
7.7906
7.6220
7.6195
7.6166
7.6008
7.5848
7.5821
7.4751
7.4712
7.4546
7.4401
7.4357
7.3076
7.2864
7.2599
7.2074
7.2025
7.1908
7.1862
4.8896
0.0001
N(SO2Ph)2
Cl
3n
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
3.821
2.306
4.031
1.951
1.951
2.000

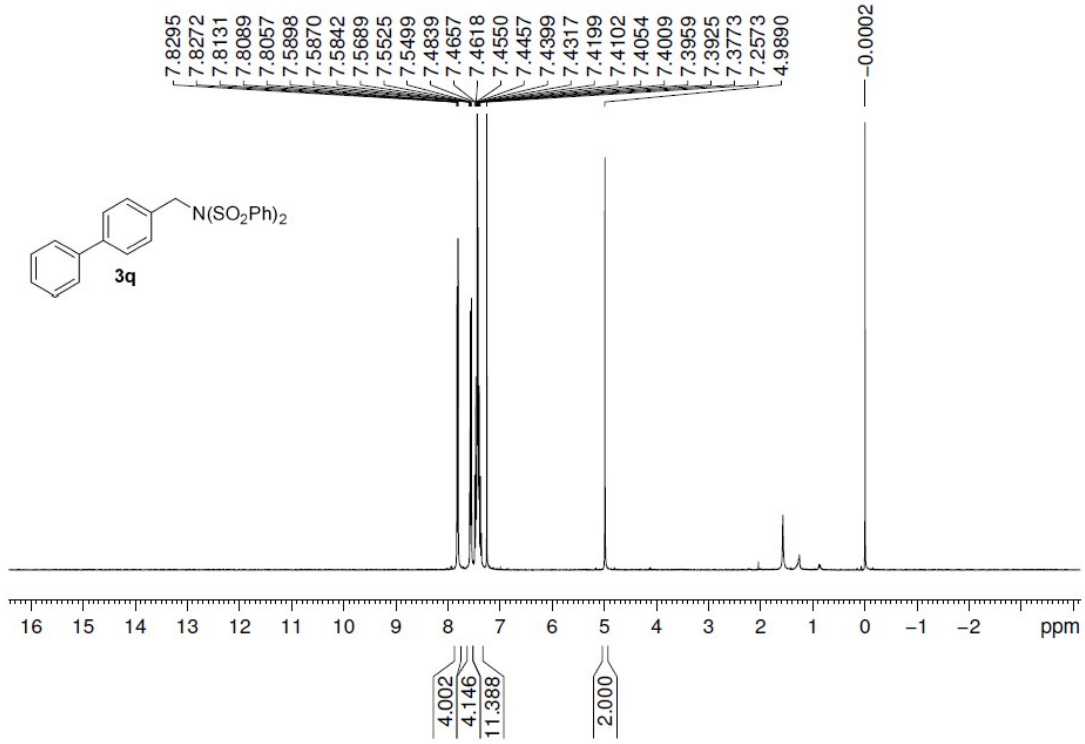

139.8721
134.1338
133.7584
133.1007
130.5747
128.8985
128.5456
128.0745
77.3254
77.0074
76.6905
51.7056
0.0121
N(SO2Ph)2
Cl
3n
220 200 180 160 140 120 100 80 60 40 20 ppm

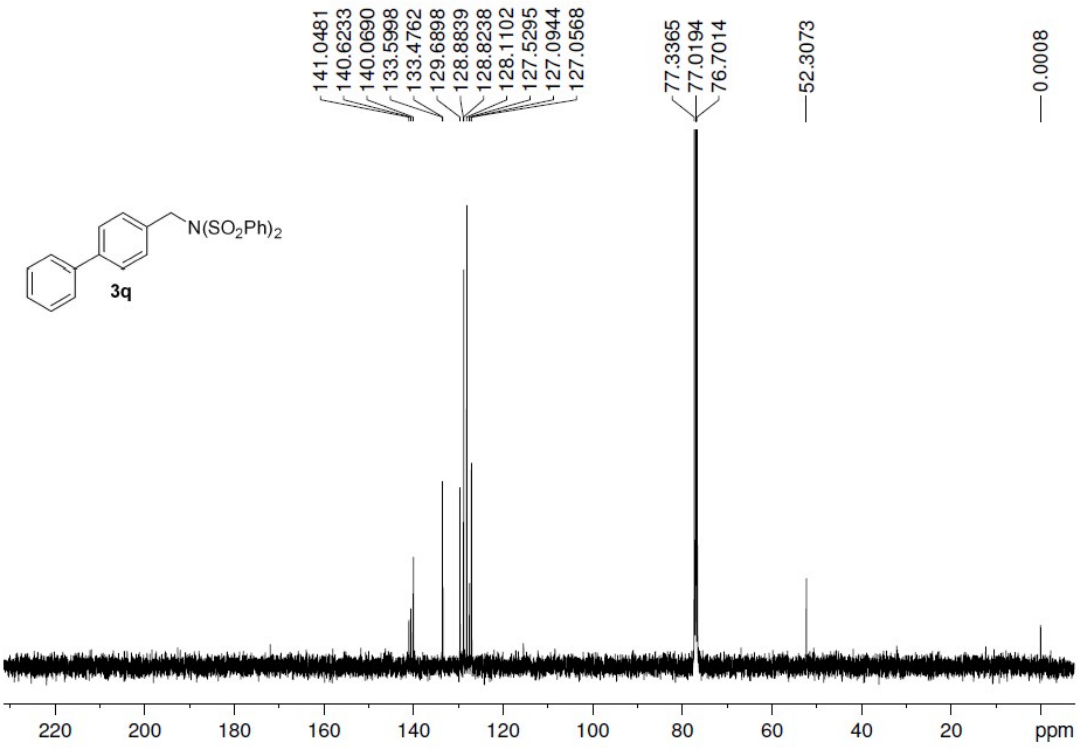

7.9104
7.9080
7.8941
7.8895
7.8863
7.6338
7.6309
7.6281
7.6123
7.6010
7.5964
7.5936
7.5908
7.5809
7.4931
7.4893
7.4726
7.4581
7.4538
7.2981
7.2955
7.2782
7.2755
7.2581
7.1905
7.1711
7.1486
7.1448
7.1271
7.1102
7.1064
6.9890
6.9862
6.9698
6.9674
6.9510
6.9483
5.1494
0.0002
N(SO2Ph)2
Cl
3o
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
4.061
2.224
4.040
0.976
1.007
1.112
1.024
2.000

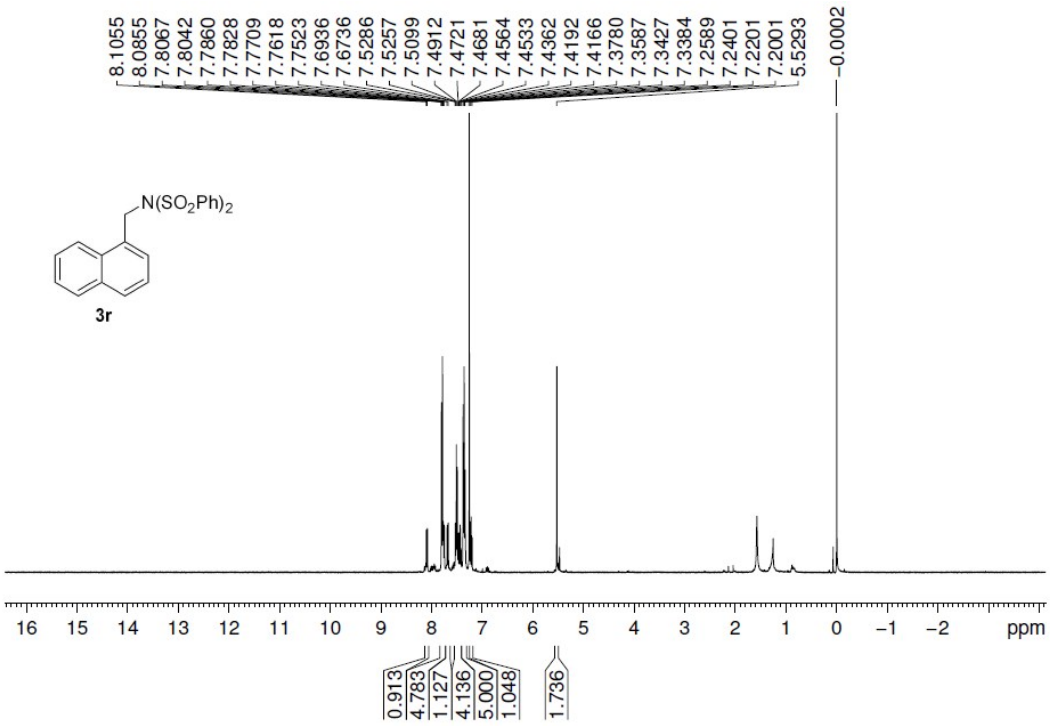

139.6598
133.8952
132.7709
132.2745
129.4108
129.3644
128.9440
128.8035
128.2878
126.6454
77.3352
77.0182
76.7002
49.7685
N(SO2Ph)2
Cl
3o
220 200 180 160 140 120 100 80 60 40 20 ppm

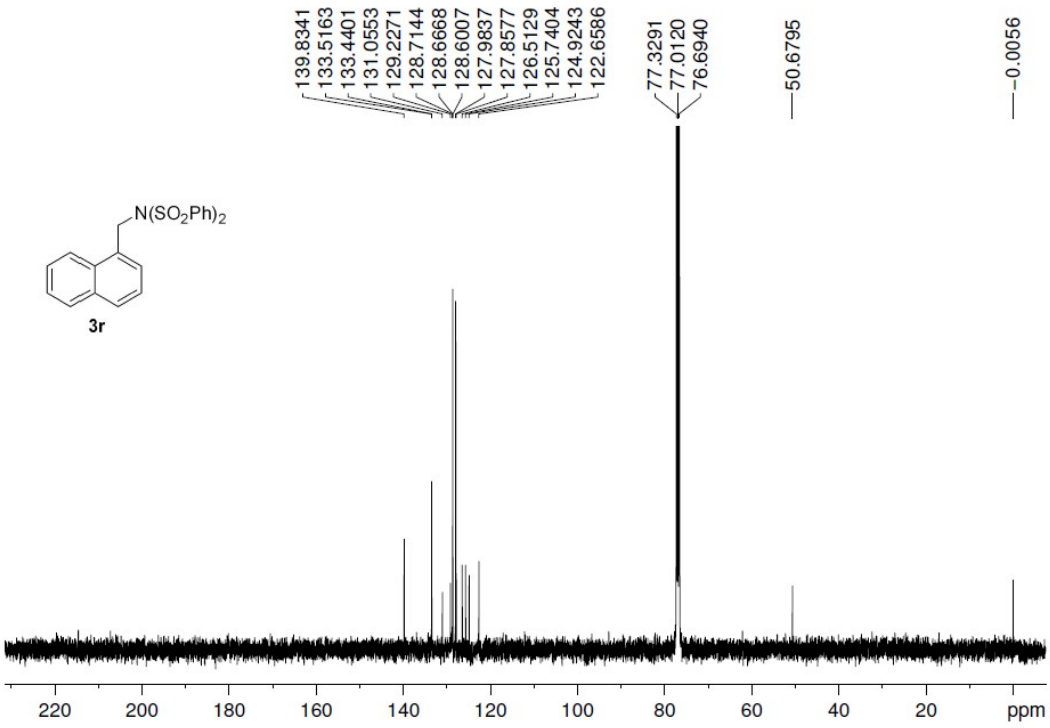

7.8067
7.8045
7.7861
7.7829
7.6121
7.6094
7.6067
7.5907
7.5748
7.5721
7.5693
7.4689
7.4483
7.4337
7.4294
7.3785
7.3735
7.3650
7.3569
7.3485
7.3435
7.2592
6.9458
6.9407
6.9241
6.9195
6.9074
6.9024
4.8975
0.0002
N(SO2Ph)2
F
3p
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
3.959
2.260
4.077
2.016
1.978
2.000

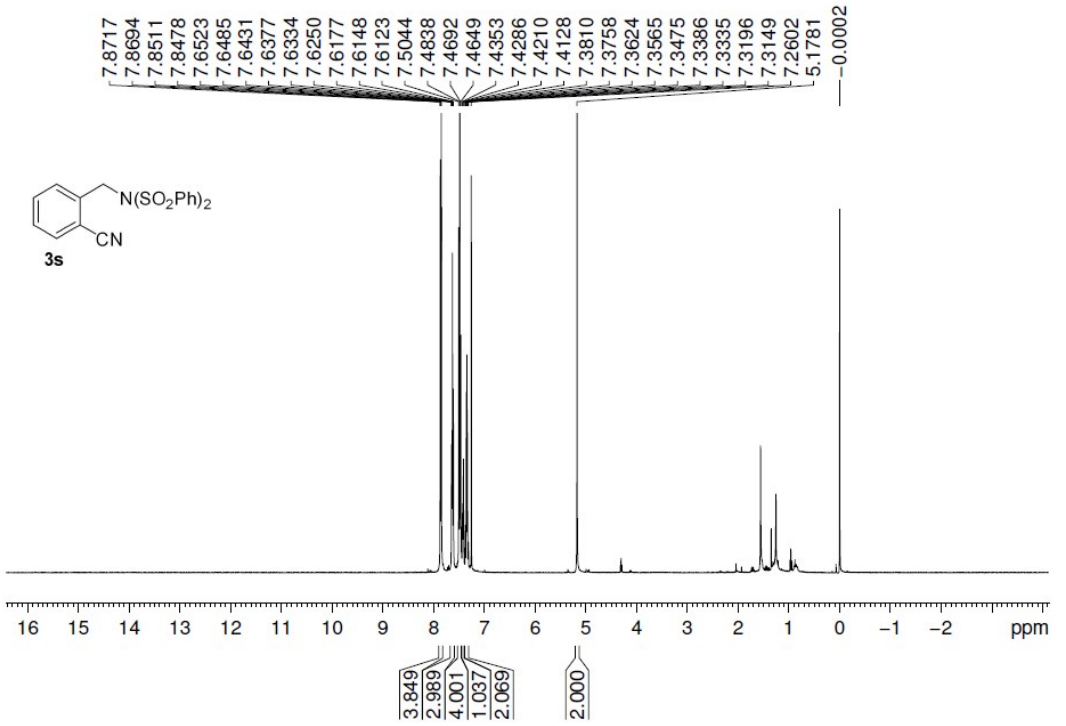

163.8235
161.3660
139.9407
133.7333
131.1574
131.0743
130.3928
130.3617
128.8839
128.0513
115.4010
115.1856
77.3501
77.0332
76.7150
51.6907
N(SO2Ph)2
F
3p
220 200 180 160 140 120 100 80 60 40 20 ppm

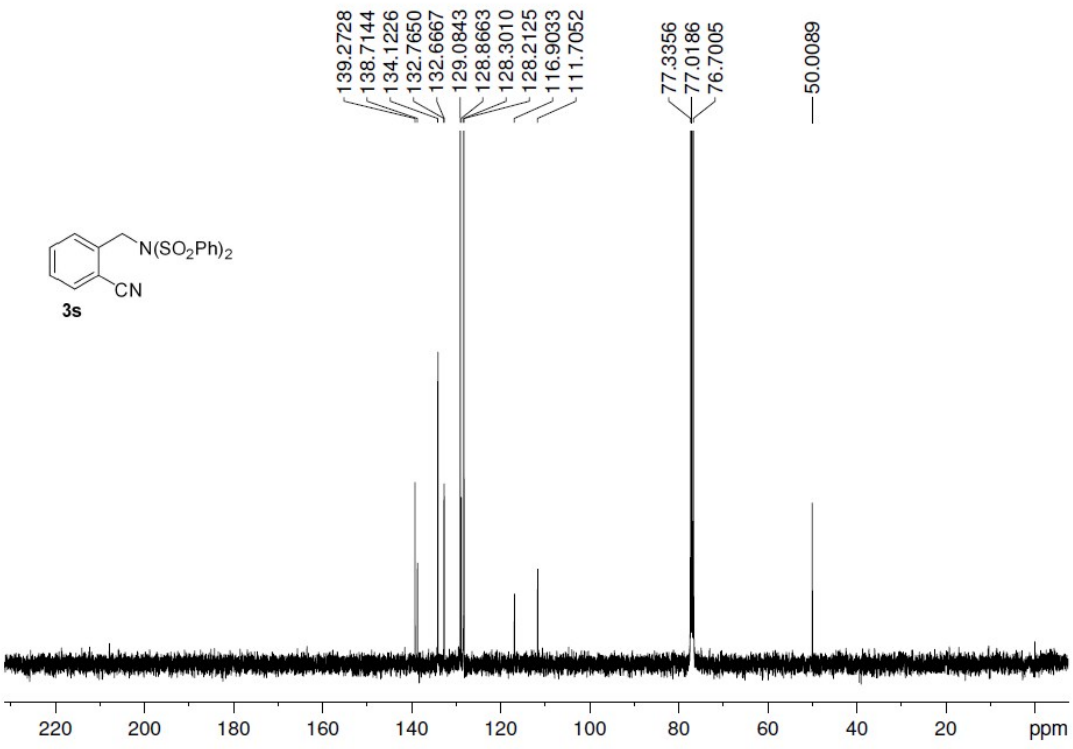

7.8295
7.8272
7.8131
7.8089
7.8057
7.5898
7.5870
7.5842
7.5689
7.5525
7.5499
7.4839
7.4657
7.4618
7.4550
7.4457
7.4399
7.4317
7.4199
7.4102
7.4054
7.4009
7.3959
7.3925
7.3773
7.2573
4.9890
0.0002
N(SO2Ph)2
3q
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
4.002
4.146
11.388
2.000

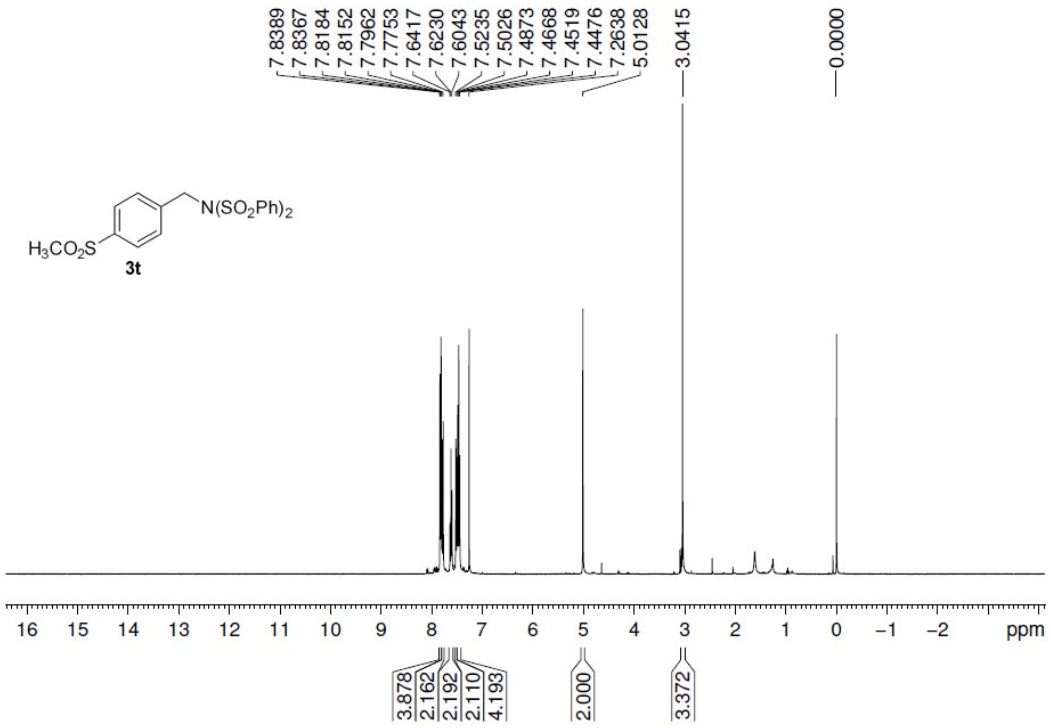

141.0481
140.6233
140.0690
133.5998
133.4762
129.6898
128.8839
128.8238
128.1102
127.5295
127.0944
127.0568
77.3365
77.0194
76.7014
52.3073
0.0008
N(SO2Ph)2
3q
220 200 180 160 140 120 100 80 60 40 20 ppm

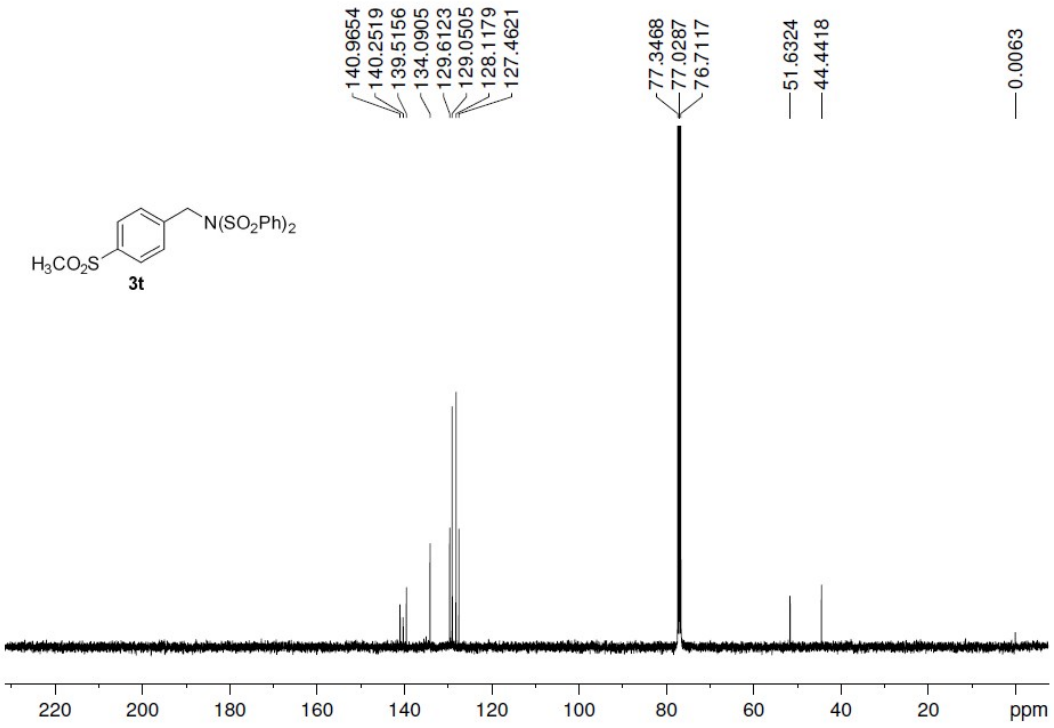

8.1055
8.0855
7.8067
7.8042
7.7860
7.7828
7.7709
7.7618
7.7523
7.6936
7.6736
7.5286
7.5257
7.5099
7.4912
7.4721
7.4681
7.4564
7.4533
7.4362
7.4192
7.4166
7.3780
7.3587
7.3427
7.3384
7.2589
7.2401
7.2201
7.2001
5.5293
0.0002
N(SO2Ph)2
3r
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
0.913
4.783
1.127
4.136
5.000
1.048
1.736

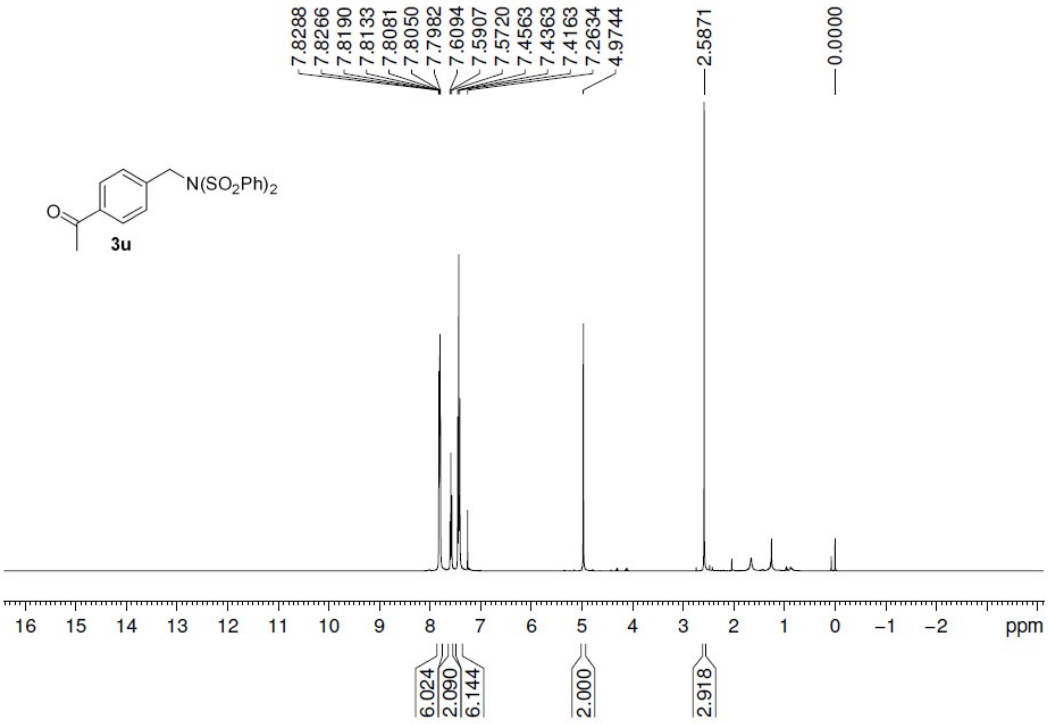

139.8341
133.5163
133.4401
131.0553
129.2271
128.7144
128.6668
128.6007
127.9837
127.8577
126.5129
125.7404
124.9243
122.6586
77.3291
77.0120
76.6940
50.6795
0.0056
N(SO2Ph)2
3r
220 200 180 160 140 120 100 80 60 40 20 ppm

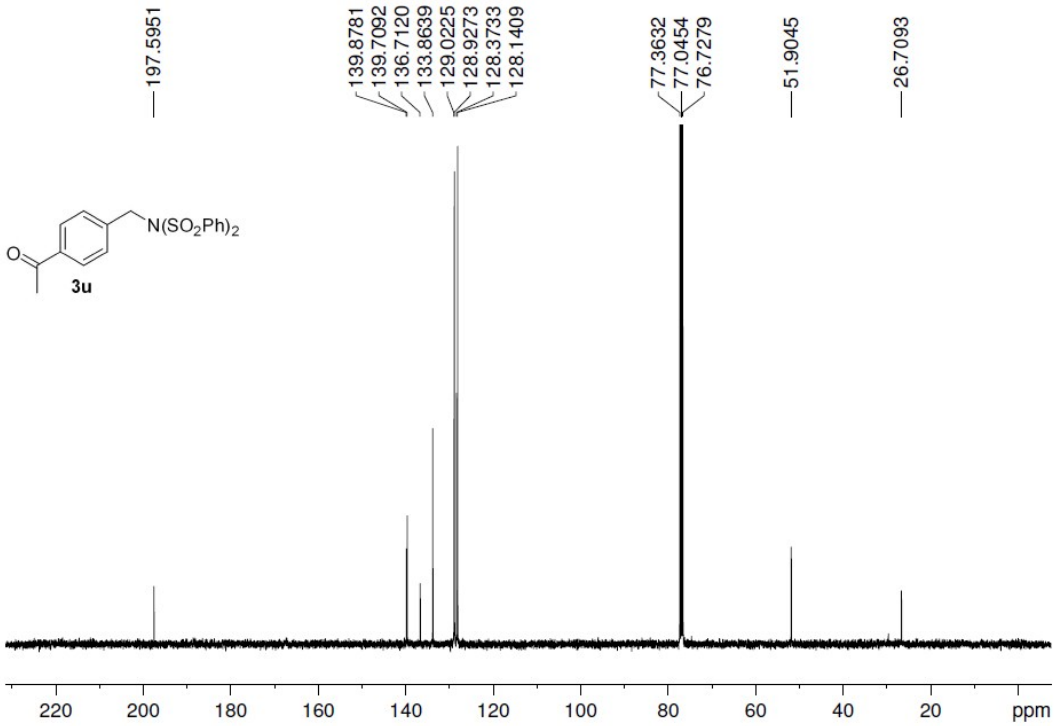

7.8717
7.8694
7.8511
7.8478
7.6523
7.6485
7.6431
7.6377
7.6334
7.6250
7.6177
7.6148
7.6123
7.5044
7.4838
7.4692
7.4649
7.4353
7.4286
7.4210
7.4128
7.3810
7.3758
7.3624
7.3565
7.3475
7.3386
7.3335
7.3196
7.3149
7.2602
5.1781
0.0002
N(SO2Ph)2
CN
3s
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
3.849
2.989
4.001
1.037
2.069
2.000

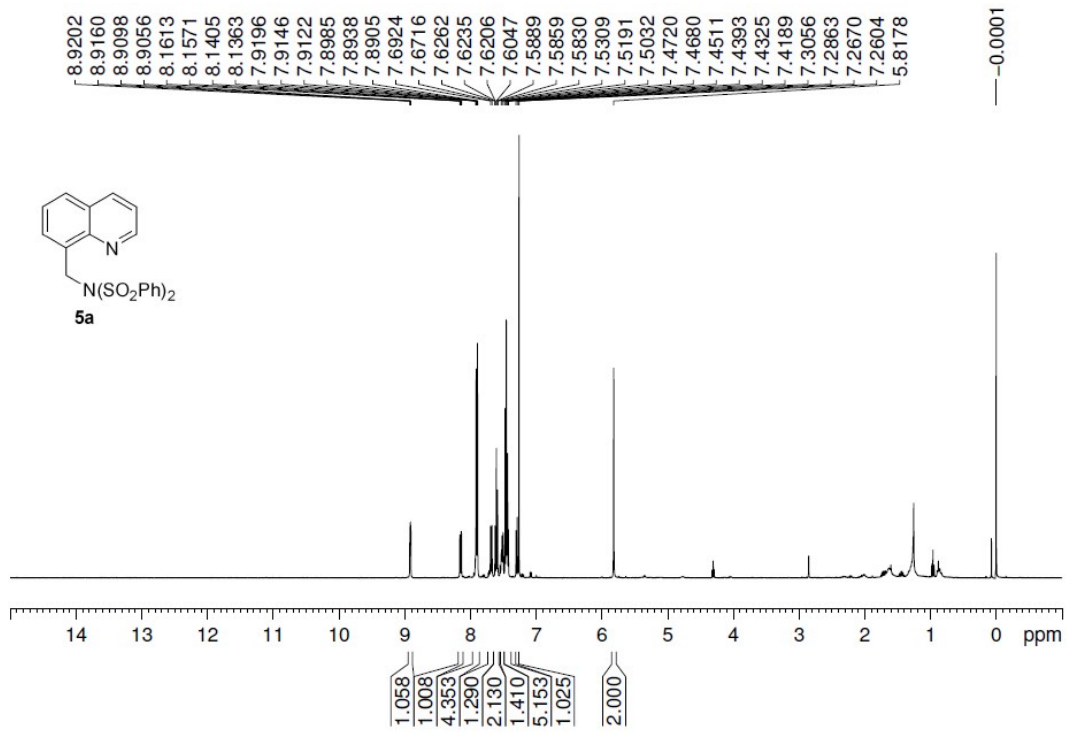

139.2728
138.7144
134.1226
132.7650
132.6667
129.0843
128.8663
128.3010
128.2125
116.9033
111.7052
77.3356
77.0186
76.7005
50.0089
N(SO2Ph)2
CN
3s
220 200 180 160 140 120 100 80 60 40 20 ppm

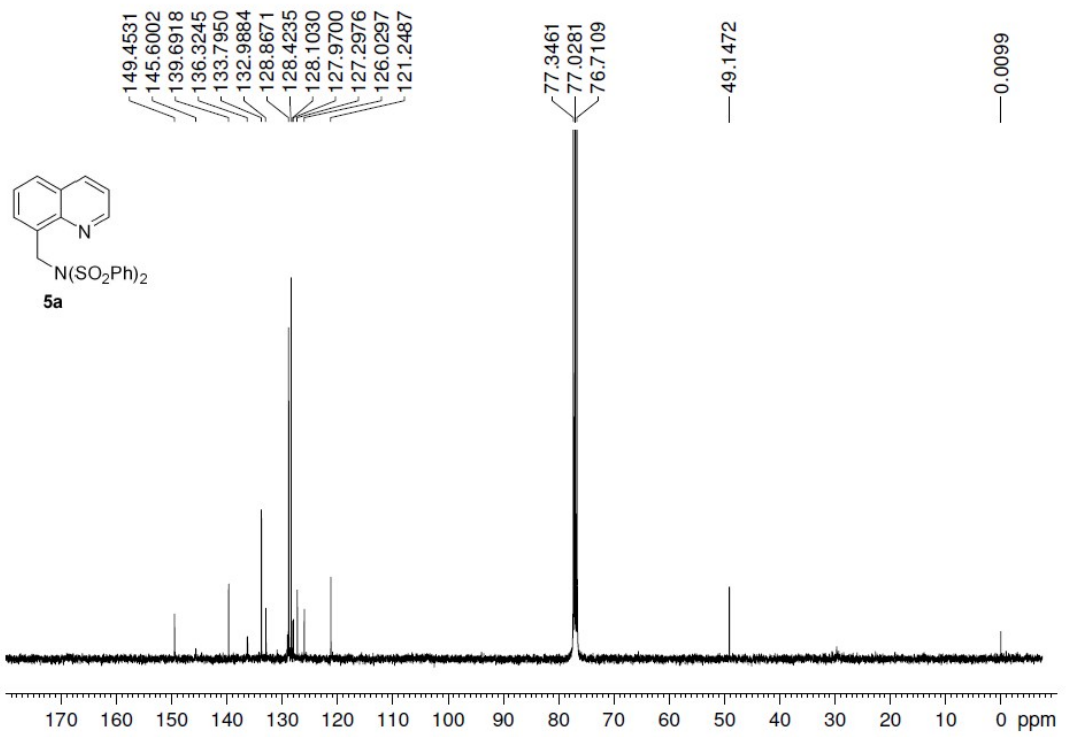

7.8389
7.8367
7.8184
7.8152
7.7962
7.7753
7.6417
7.6230
7.6043
7.5235
7.5026
7.4873
7.4668
7.4519
7.4476
7.2638
5.0128
3.0415
0.0000
N(SO2Ph)2
H3CO2S
3t
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
3.878
2.162
2.192
2.110
4.193
2.000
3.372


140.9654
140.2519
139.5156
134.0905
129.6123
129.0505
128.1179
127.4621
77.3468
77.0287
76.7117
51.6324
44.4418
0.0063
N(SO2Ph)2
H3CO2S
3t
220 200 180 160 140 120 100 80 60 40 20 ppm


7.8288
7.8266
7.8190
7.8133
7.8081
7.8050
7.7982
7.6094
7.5907
7.5720
7.4563
7.4363
7.4163
7.2634
4.9744
2.5871
0.0000
N(SO2Ph)2
O
3u
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 −1 −2 ppm
6.024
2.090
6.144
2.000
2.918


197.5951
139.8781
139.7092
136.7120
133.8639
129.0225
128.9273
128.3733
128.1409
77.3632
77.0454
76.7279
51.9045
26.7093
N(SO2Ph)2
O
3u
220 200 180 160 140 120 100 80 60 40 20 ppm


8.9202
8.9160
8.9098
8.9056
8.1613
8.1571
8.1405
8.1363
7.9196
7.9146
7.9122
7.8985
7.8938
7.8905
7.6924
7.6716
7.6262
7.6235
7.6206
7.6047
7.5889
7.5859
7.5830
7.5309
7.5191
7.5032
7.4720
7.4680
7.4511
7.4393
7.4325
7.4189
7.3056
7.2863
7.2670
7.2604
5.8178
0.0001
N
N(SO2Ph)2
5a
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
1.058
1.008
4.353
1.290
2.130
1.410
5.153
1.025
2.000


149.4531
145.6002
139.6918
136.3245
133.7950
132.9884
128.8671
128.4235
128.1030
127.9700
127.2976
126.0297
121.2487
77.3461
77.0281
76.7109
49.1472
0.0099
N
N(SO2Ph)2
5a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm