Supporting Information

Copper-catalyzed S-methylation of sulfonyl hydrazides with TBHP for the synthesis of methyl sulfones in water

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Contents:

General Remarks

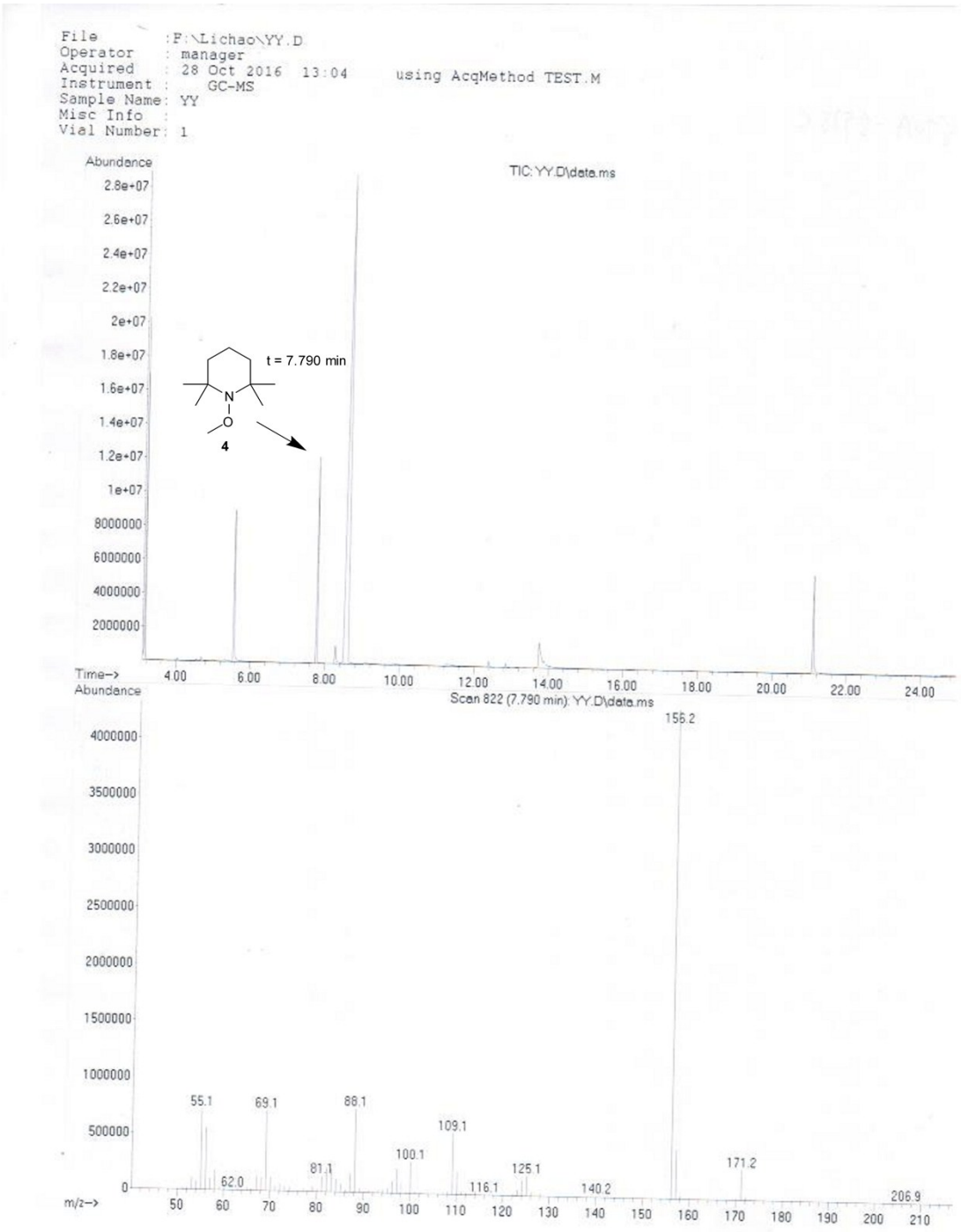
All substrates were purchased commercially without further purification. The yields were determined based on sulfonyl hydrazides.

^{1}H and ^{13}C NMR spectra were recorded on a Bruker AC-300 FT spectrometer at 400 MHz and 100 MHz, respectively, with tetramethylsilane as an internal reference. Chemical shifts (δ) and coupling constants (*J*) were expressed in ppm and Hz, respectively. High resolution mass spectra (HRMS) were recorded on a LC-TOF spectrometer (Micromass). GC-MS samples were recorded on an Agilent Technologies 7890A-5975C GC-MS system.

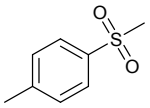
General procedures for the synthesis of Arylsulfonyl Hydrazides

Arylsulfonyl hydrazides **2b**-**2s** were prepared according to the literature procedure.[1] To a solution of an arylsulfonyl chloride (3.0 mmol) in tetrahyrdofuran (15 mL), was added hydrazine monohydrate (375 mg, 7.5 mmol) dropwise under nitrogen at 0 °C. After vigorous stirring for 30 min at 0 °C, the reaction mixture was added ethyl acetate (60 mL), and washed with saturated brine (3 x 10 mL). The organic layer was dried over sodium sulfate, filtered, concentrated and added to hexane (12 mL) over 5 min. The mixture was filtered, and the collected solid was dried in vacuum.

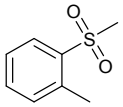
GC-MS analysis for the TEMPO−CH_3 adduct 4



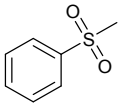
Characterization data of products



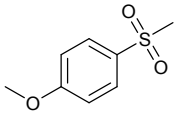
1-methyl-4-(methylsulfonyl)benzene (3aa).[1] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a white solid (88 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 7.84-7.82 (d, 2H, *J* = 8.0 Hz), 7.38-7.36 (d, 2H, *J* = 8.0 Hz), 3.04 (s, 3H), 2.46 (s, 3H); ^{13}C NMR (100 MHz, CDCl3): 144.7, 137.7, 130.0, 127.3, 44.6, 21.6.



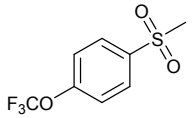
1-methyl-2-(methylsulfonyl)benzene (3ba).[1] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a light yellow oil (83 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 8.04-8.02 (m, 1H), 7.53-7.51 (m, 1H), 7.40-7.28 (m, 2H), 3.08 (s, 3H), 2.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 138.7, 137.5, 133.7, 132.7, 129.2, 126.7, 43.7, 20.3.



methylsulfonylbenzene (3ca). [1] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a light yellow oil (78 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 7.97-7.94 (m, 2H), 7.69-7.65 (m, 1H), 7.60-7.56 (m, 2H), 3.04 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 140.6, 133.7, 129.4, 127.3, 44.5.

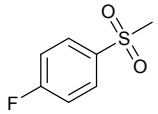


1-methoxy-4-(methylsulfonyl)benzene (3da).[1] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a light yellow solid (81 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 7.89-7.85 (m, 2H), 7.05-7.01 (m, 2H), 3.89 (s, 3H), 3.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 163.7, 132.3, 129.5, 114.5, 55.7, 44.8.

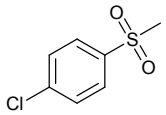


1-(methylsulfonyl)-4-(trifluoromethoxy)benzene (3ea).[2] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a light yellow oil (70% yield). ^{1}H NMR (400 MHz, $CDCl_3$): 3.07 (s, 3H),

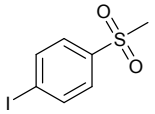
7.41 (d, J = 8.1 Hz, 2H), 8.02 (d, J = 8.7 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 43.5, 120.2, 120.5 (q, J = 258.3 Hz), 128.8, 137.8, 152.0 (q, J = 1.5 Hz).



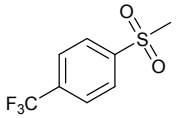
1-fluoro-4-(methylsulfonyl)benzene (3fa).[1] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a light yellow oil (90 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 8.00-7.96 (m, 2H), 7.28-7.24 (m, 2H), 3.07 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 165.8 (d, J = 254 Hz), 136.7 (d, J = 3 Hz), 130.3 (d, J = 10 Hz), 116.7 (d, J = 23 Hz), 44.7.



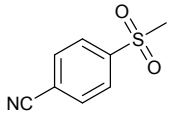
1-chloro-4-(methylsulfonyl)benzene (3ga).[1] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a white solid (84 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 7.91-7.88 (m, 2H), 7.57-7.54 (m, 2H), 3.06 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 140.5, 139.1, 129.7, 128.9, 44.5.



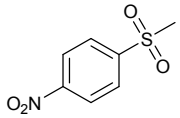
1-iodo-4-(methylsulfonyl)benzene (3ha).[3] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a white solid (58 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 7.96-7.94 (d, 2H, J = 8.0 Hz), 7.67-7.65 (d, 2H, J = 8.0 Hz), 3.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 140.2, 138.7, 128.8, 101.6, 44.5.



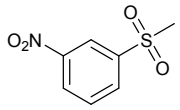
1-(methylsulfonyl)-4-(trifluoromethyl)benzene (3ia).[4] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a white solid (73 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 8.12-8.10 (d, 2H, J = 8.0 Hz), 7.87-7.85 (d, 2H, J = 8 Hz), 3.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 144.0, 135.6 (, J = 33 Hz), 128.1, 126.6 (q, J = 7 Hz), 123.1 (q, J = 272 Hz), 44.3.



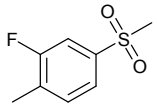
4-(methylsulfonyl)benzonitrile (3ja). [5] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a white solid (56 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 8.03-8.01 (d, 2H, J = 8.0 Hz), 7.84-7.82 (d, 2H, J = 8.0 Hz), 3.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 143.5, 132.2, 127.2, 116.6, 116.0, 43.2.



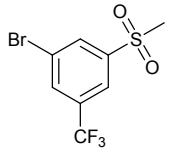
1-(methylsulfonyl)-4-nitrobenzene (3ka).[1] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a white solid (73 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 8.45-8.43 (d, 2H, J = 8.0 Hz), 8.18-8.16 (d, 2H, J = 8.0 Hz), 3.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 150.9, 146.0, 129.0, 124.6, 44.3.



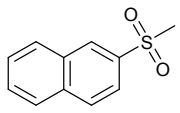
1-(methylsulfonyl)-3-nitrobenzene (3la). [6] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a light yellow solid (65 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 8.81 (s, 1H), 8.55-8.52 (m, 1H), 8.32-8.29 (m, 1H), 7.86-7.82 (m, 1H), 3.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 148.5, 142.6, 133.0, 130.9, 128.3, 122.9, 44.4.



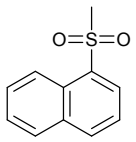
2-fluoro-1-methyl-4-(methylsulfonyl)benzene (3na). The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a colorless oil (77 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 7.65-7.57 (m, 2H), 7.43-7.39 (m, 1H), 3.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 160.9 (d, J = 249 Hz), 139.72, 132.5 (d, J = 6 Hz), 131.9 (d, J = 18 Hz), 122.9 (d, J = 4 Hz), 114.3 (d, J = 26 Hz), 44.5, 14.8 (d, J = 4 Hz). HRMS $[M+H]^+$ calcd. for $C_8H_{10}FO_2S$: 189.0386, found : 189.0388.



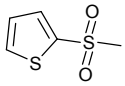
1-bromo-3-(methylsulfonyl)-5-(trifluoromethyl)benzene (3oa). [7] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a white solid (68 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 8.29 (s, 1H), 8.15 (s, 1H), 8.05 (s, 1H), 3.13 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 143.4, 133.8, 133.7 (q, J = 68 Hz), 133.6 (q, J = 3 Hz), 124.1, 123.2 (q, J = 3 Hz), 122.2 (q, J = 271 Hz), 44.4.



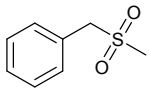
2-(methylsulfonyl)naphthalene (3pa). [8] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a white solid (81 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 8.53 (s, 1H), 8.03-8.00 (m, 2H), 7.95-7.80 (m, 2H), 7.71-7.62 (m, 2H), 3.13 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): 137.5, 135.3, 132.2, 129.7, 129.42, 129.3, 129.1, 128.0, 127.8, 122.1, 44.6.



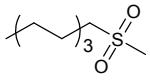
1-(methylsulfonyl)naphthalene (3qa). [5] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a light blue oil (59 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 8.74-8.72 (m, 1H), 8.35-8.33 (m, 1H), 8.14-8.12 (m, 1H), 7.99-7.97 (m, 1H), 7.74-7.70 (m, 1H), 7.65-7.58 (m, 2H), 3.22 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): 135.6, 135.2, 134.2, 129.7, 129.3, 128.8, 128.7, 127.1, 124.5, 123.9, 44.3.



2-(methylsulfonyl)thiophene (3ra).[5] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a light yellow oli (69 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 7.73-7.71 (m, 2H), 7.17-7.15 (m, 1H), 3.19 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 141.8, 133.7, 133.5, 127.9, 46.1.



(methylsulfonylmethyl)benzene (3sa).[9] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a light yellow solid (71 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 7.40 (m, 5H), 4.25 (s, 2H), 2.75 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 130.9, 130.5, 129.2, 129.0, 61.3, 39.0.



1-(methylsulfonyl)octane (3ta). [10] The title compound was prepared according to the general procedure and purified by column chromatography (Petroleum Ether: EtOAc = 3:1) to give a white solid (62 % yield). ^{1}H NMR (400 MHz, $CDCl_3$): 3.02-2.98 (m, 2H), 2.89 (s, 3H), 1.89-1.81 (m, 2H), 1.46-1.41 (m, 2H), 1.32-1.28 (m, 8H), 0.90-0.87 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 54.9, 40.4, 31.7, 29.0, 28.9, 28.4, 22.6, 22.5, 14.1.

Reference

[1] G. Yuan, J. Zheng, X. Gao, X. Li, L. Huang, H. Chen and H. Jiang, *Chem. Commun.*, 2012, **48**, 7513.
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[8] B. Yu, A.-H. Liu, L.-N. He, B. Li, Z.-F. Diao and Y.-N. Li, *Green Chem.*, 2012, **14**, 957.
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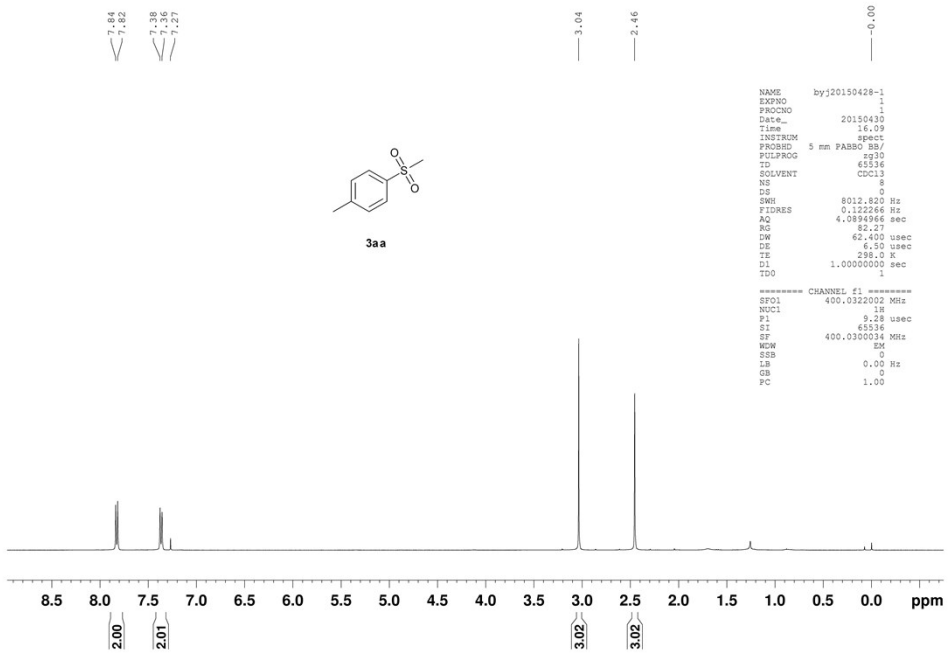
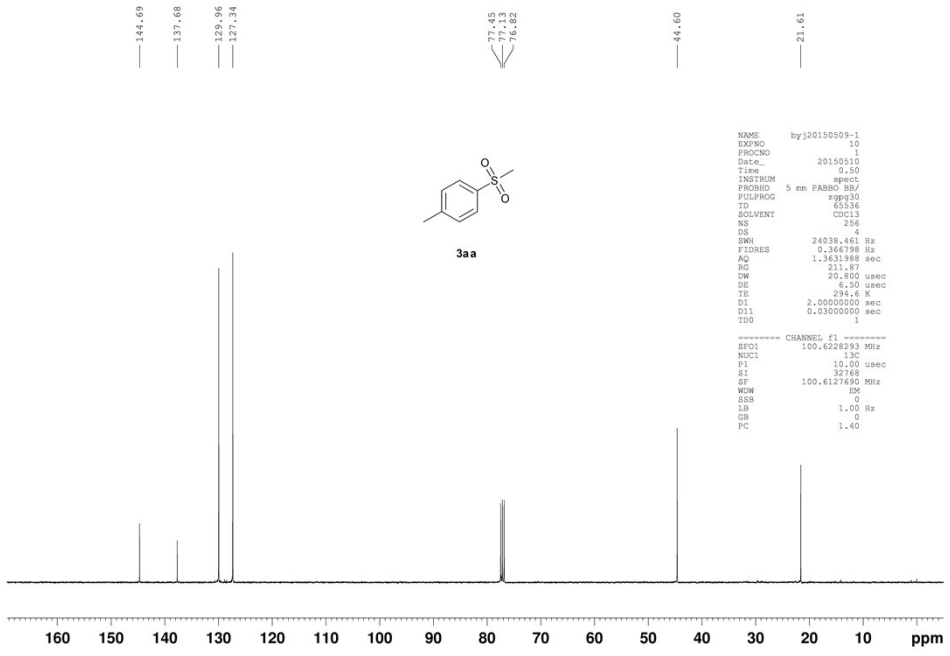
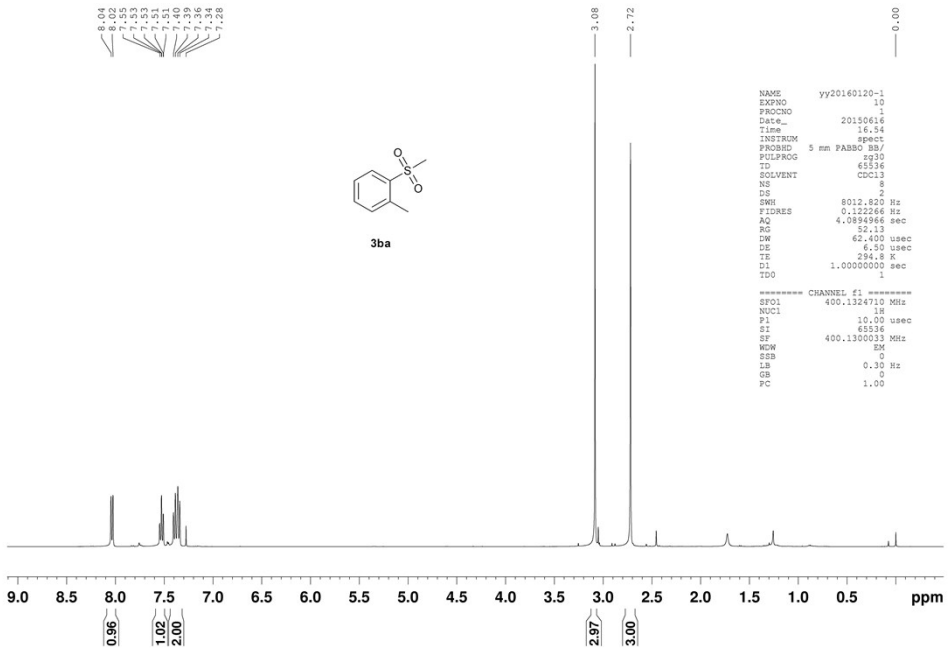
[10] K. Kamata, T. Hirano and N. Mizuno, *Chem. Commun.*, 2009, 3958.

NMR Spectra of products



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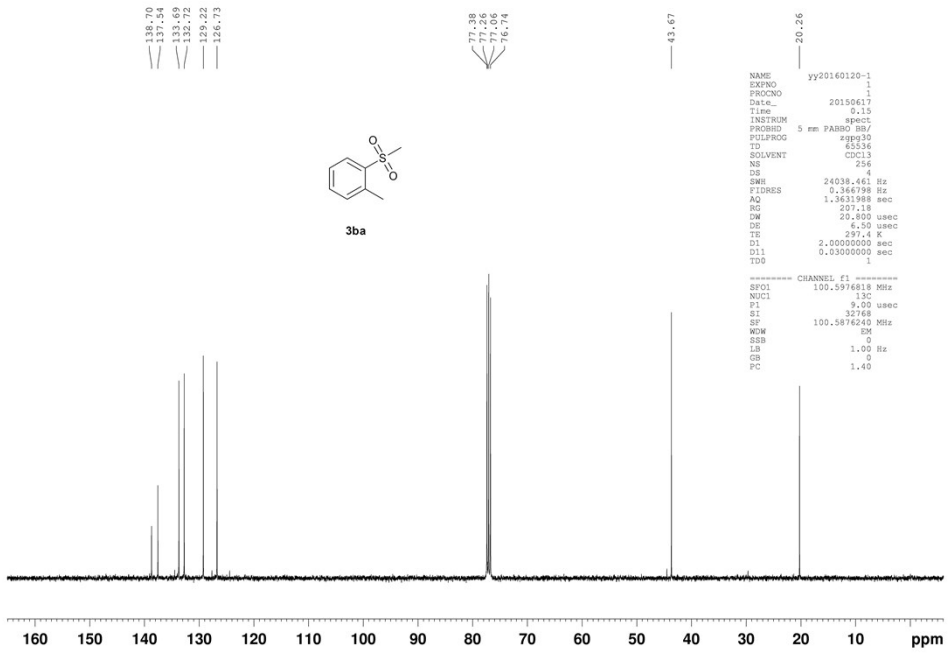
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PC 1.40
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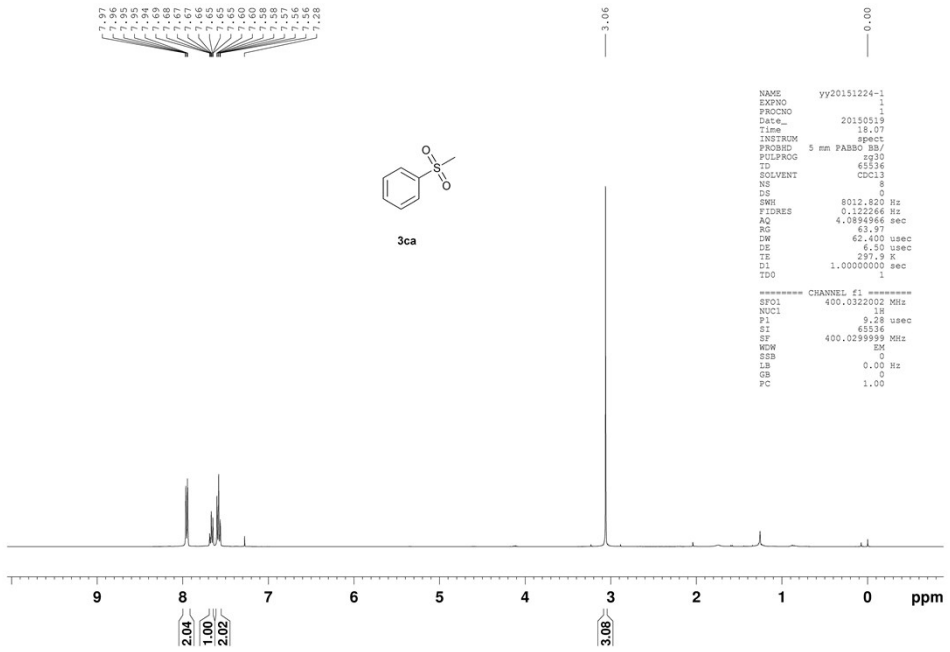
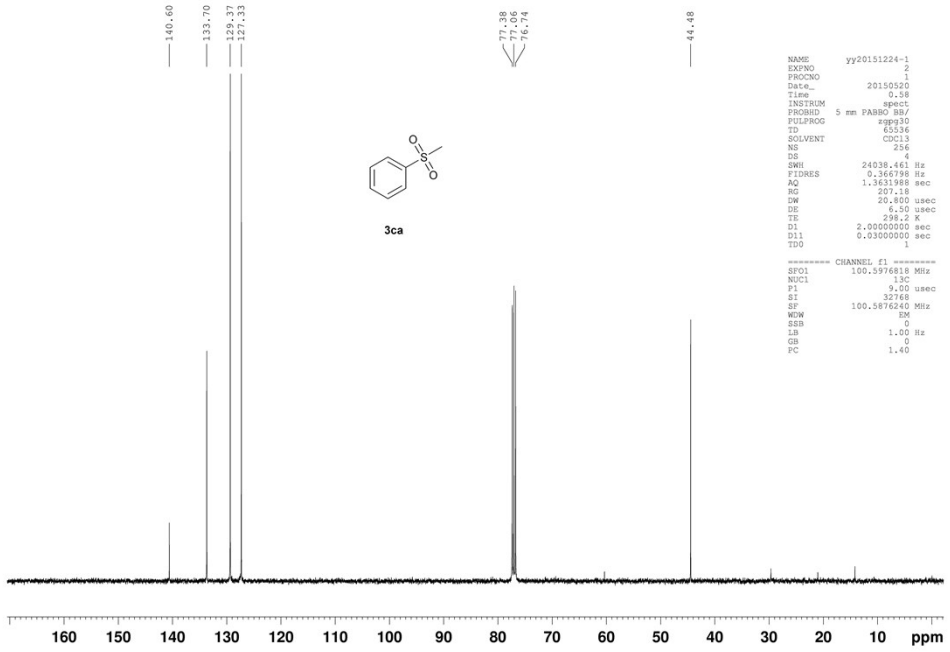
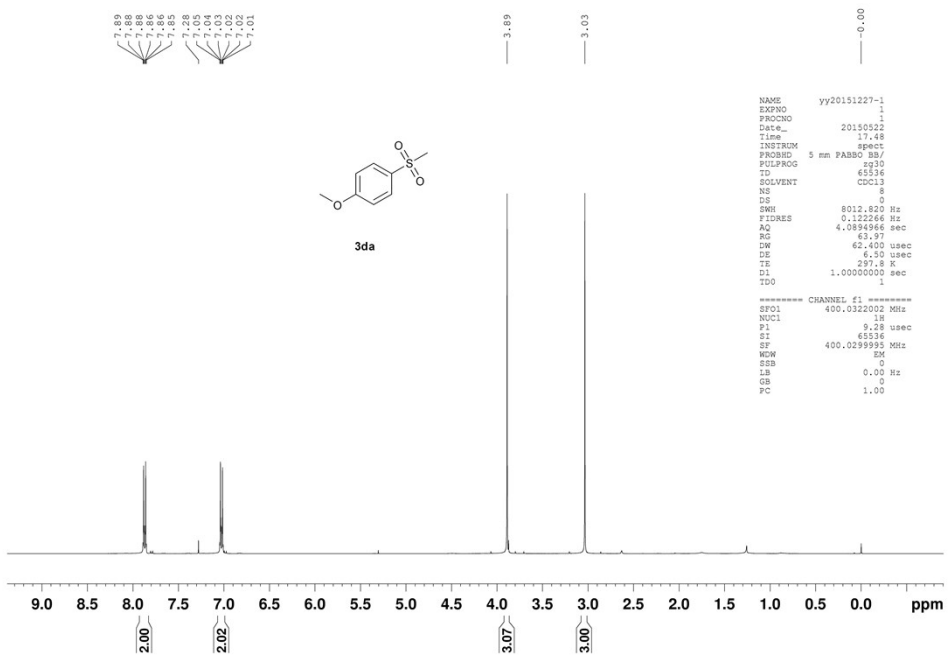
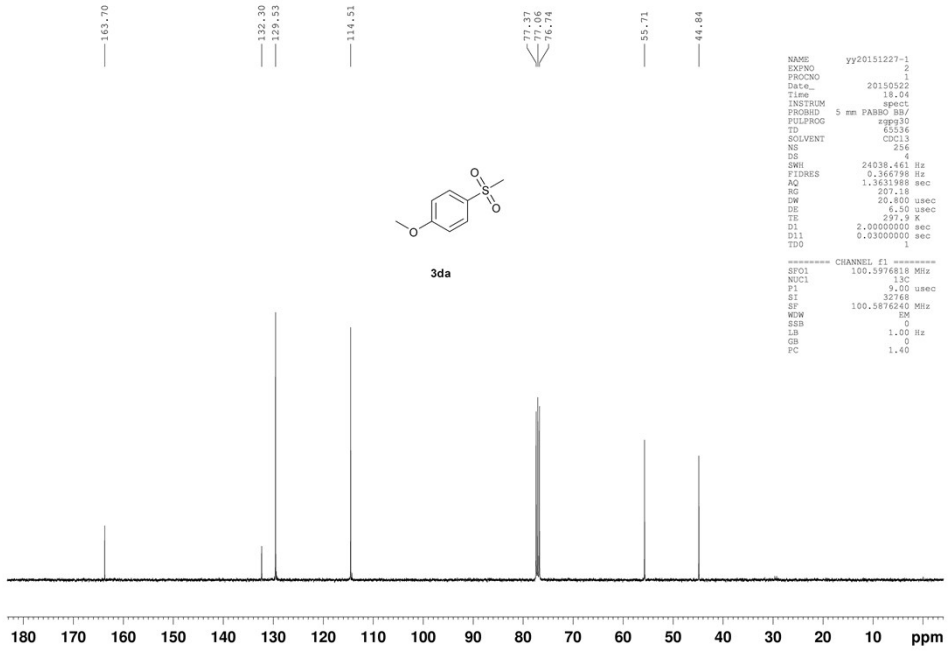
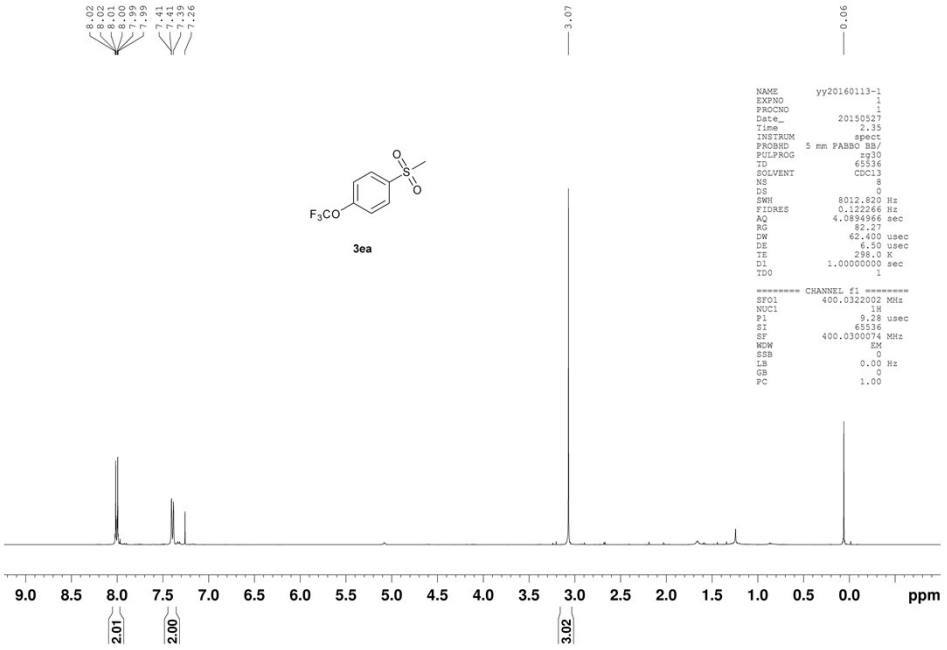
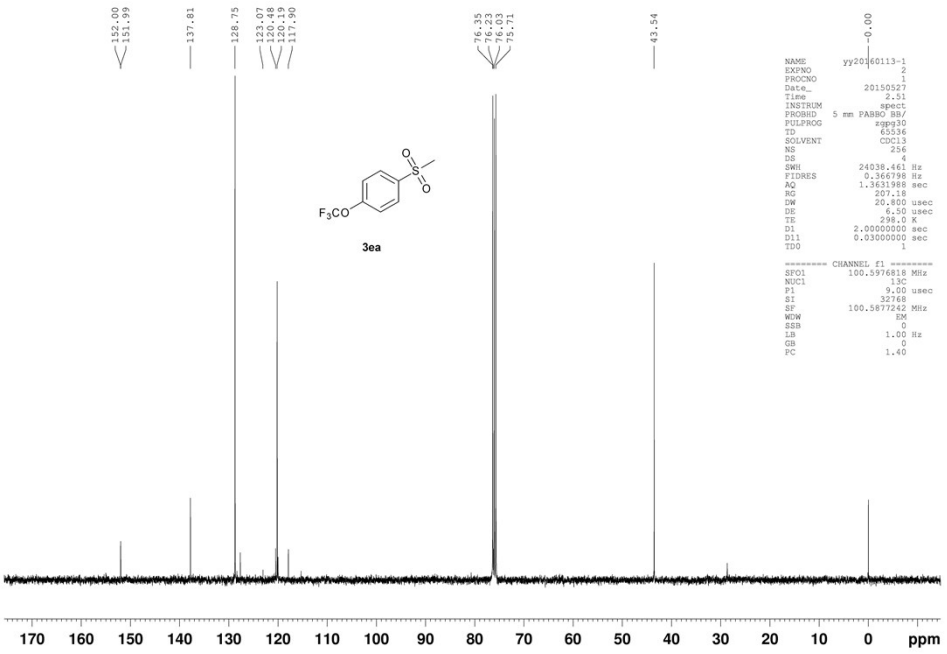

7.97
7.96
7.95
7.95
7.94
7.69
7.68
7.67
7.67
7.66
7.65
7.65
7.65
7.60
7.58
7.57
7.56
7.56
7.28
3.06
0.00
3ca
NAME yy20151224-1
EXPNO 1
PROCNO 1
Date_ 20150519
Time 18.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 63.97
DW 62.400 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TDO 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0299999 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.04
1.00
2.02
3.08

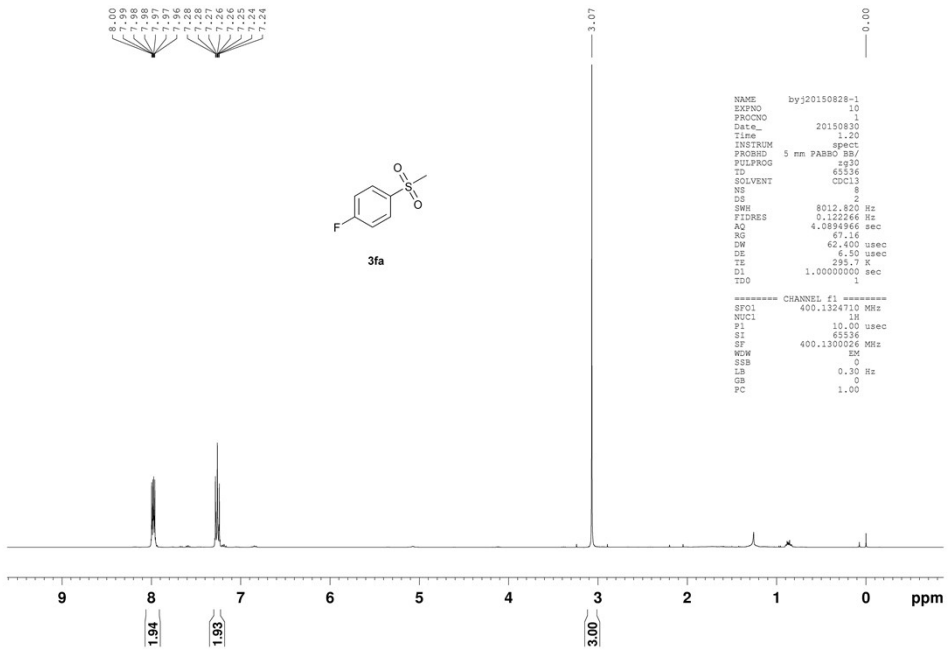

140.60
133.70
129.37
127.33
77.38
77.06
76.74
44.48
3ca
NAME yy20151224-1
EXPNO 2
PROCNO 1
Date_ 20150520
Time 0.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5876240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

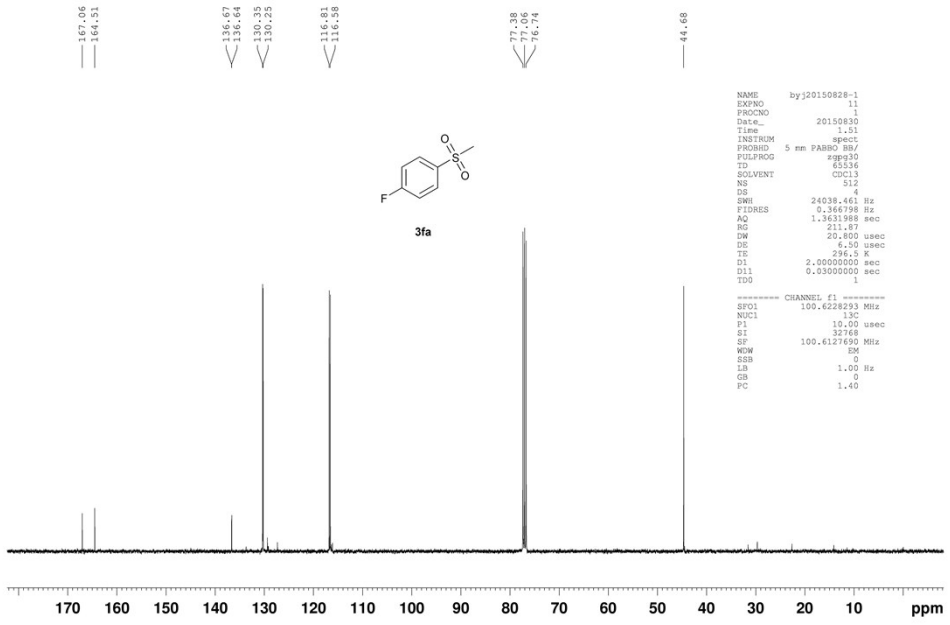

7.89
7.88
7.88
7.86
7.86
7.85
7.28
7.05
7.04
7.03
7.02
7.02
7.01
3.89
3.03
-0.00
3da
NAME yy20151227-1
EXPNO 1
PROCNO 1
Date_ 20150522
Time 17.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 63.97
DW 62.400 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0299995 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
2.02
3.07
3.00

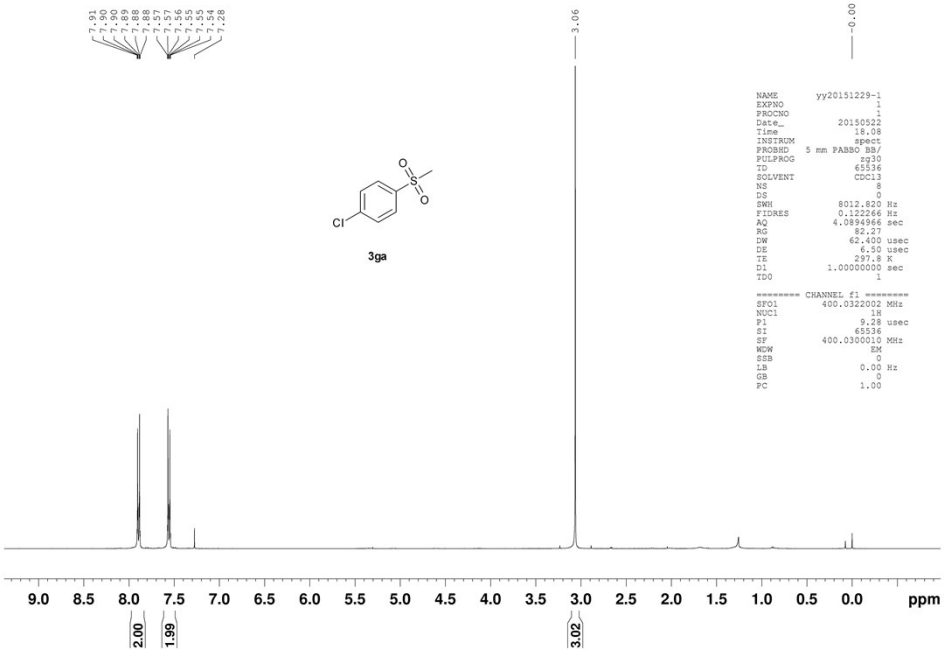

163.70
132.30
129.53
114.51
77.37
77.06
76.74
55.71
44.84
3da
NAME yy20151227-1
EXPNO 2
PROCNO 1
Date_ 20150522
Time 18.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5876240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

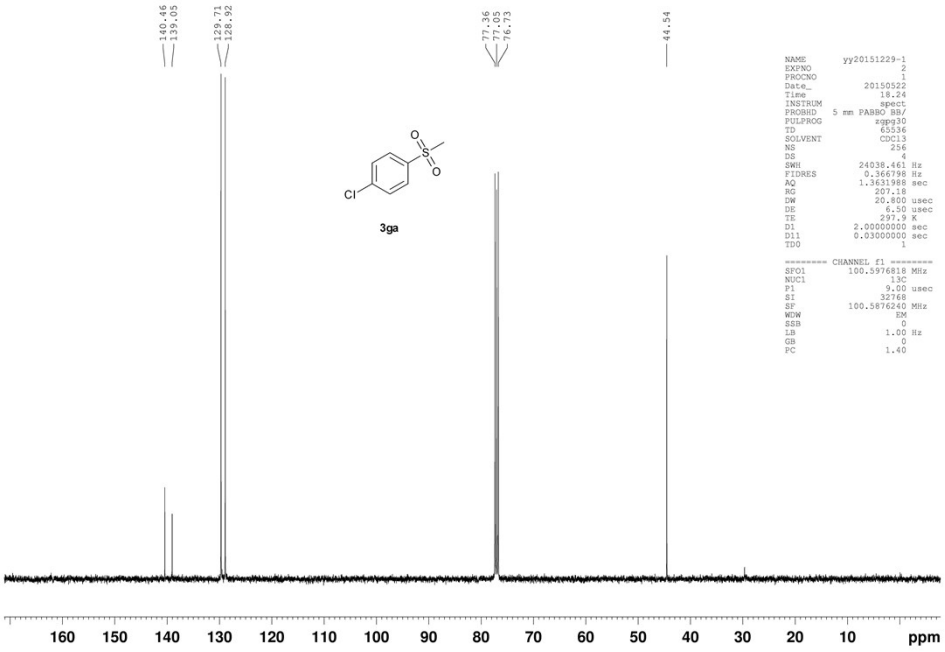

8.02
8.02
8.01
8.00
7.99
7.99
7.41
7.41
7.39
7.26
3.07
0.06
NAME yy20160113-1
EXPNO 1
PROCNO 1
Date_ 20150527
Time 2.35
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 82.27
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0300074 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
F3CO
3ea
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.01
2.00
3.02

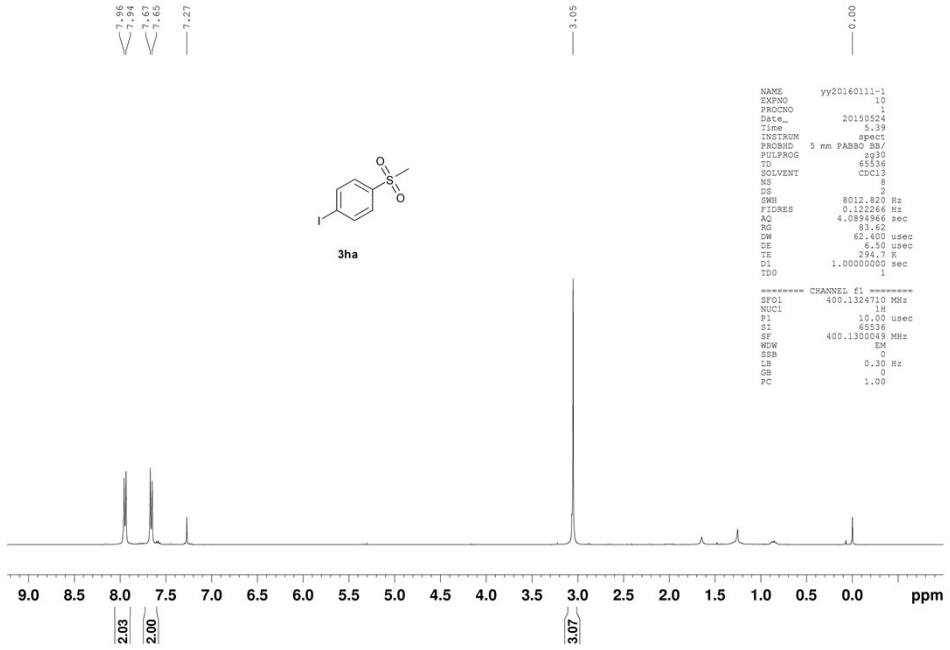

152.00
151.99
137.81
128.75
123.07
120.48
120.19
117.90
76.35
76.23
76.03
75.71
43.54
0.00
NAME yy20160113-1
EXPNO 2
PROCNO 1
Date_ 20150527
Time 2.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5877242 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
F3CO
3ea
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

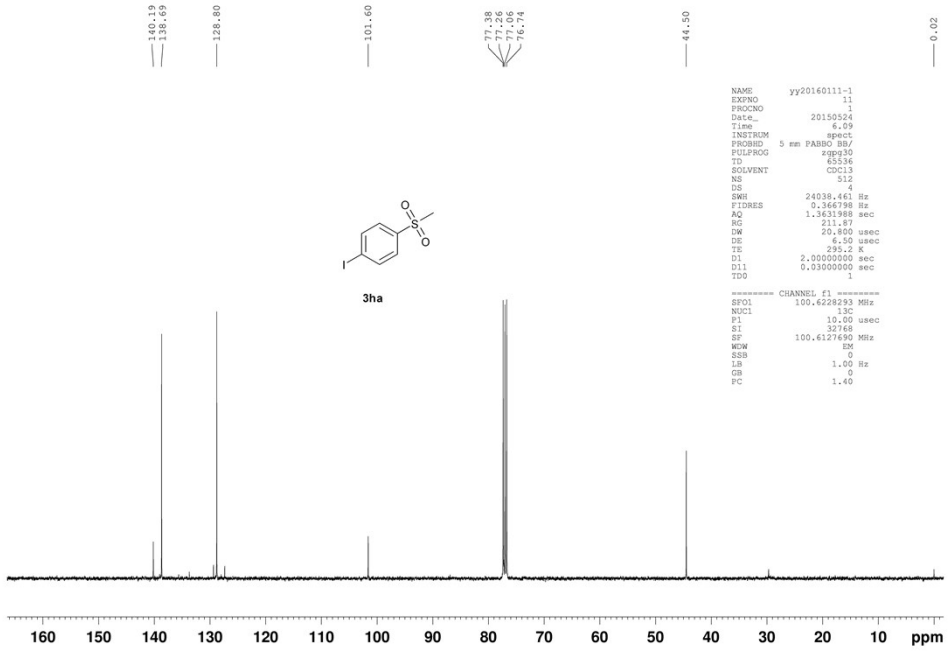

8.00
7.99
7.98
7.98
7.97
7.97
7.96
7.28
7.27
7.26
7.26
7.25
7.24
7.24
3.07
0.00
3fa
NAME byj20150828-1
EXPNO 10
PROCNO 1
Date_ 20150830
Time 1.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 67.16
DW 62.400 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
SI 65536
SF 400.1300026 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
1.94
1.93
3.00

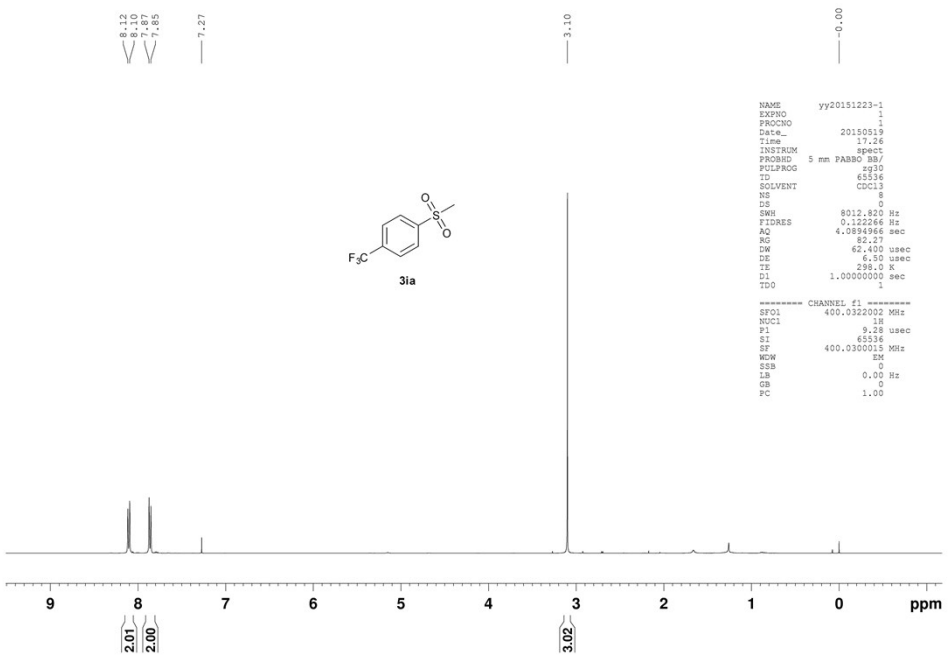

167.06
164.51
136.67
136.64
130.35
130.25
116.81
116.58
77.38
77.06
76.74
44.68
3fa
NAME byj20150828-1
EXPNO 11
PROCNO 1
Date_ 20150830
Time 1.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 211.87
DW 20.800 usec
DE 6.50 usec
TE 296.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

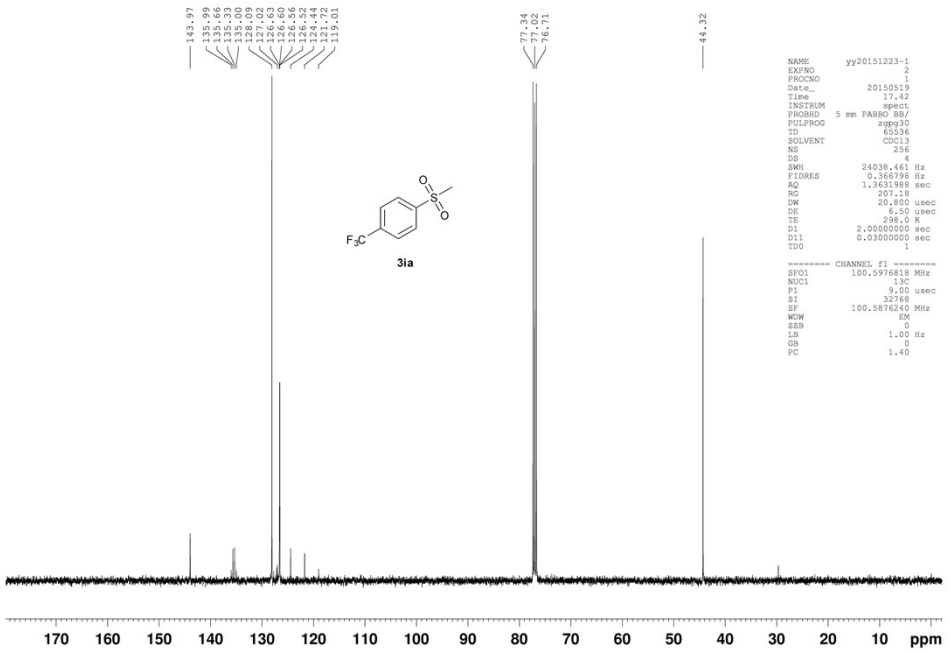

7.91
7.90
7.90
7.89
7.88
7.88
7.57
7.56
7.55
7.55
7.54
7.28
3.06
-0.00
NAME yy20151229-1
EXPNO 1
PROCNO 1
Date_ 20150522
Time 18.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 82.27
DW 62.400 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0300010 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Cl
O
S
O
3ga
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
1.99
3.02

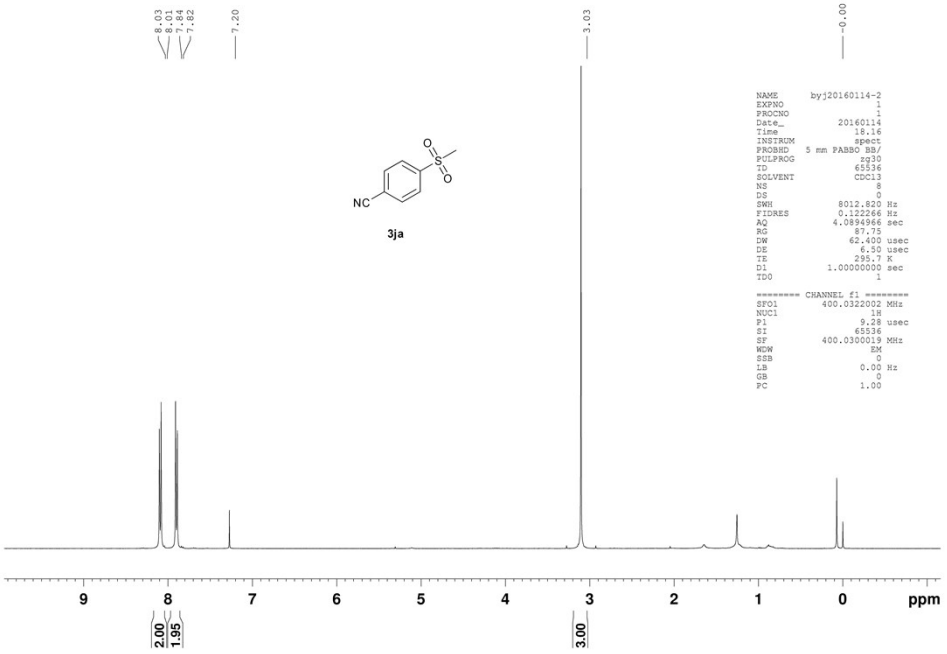

140.46
139.05
129.71
128.92
77.36
77.05
76.73
44.54
NAME yy20151229-1
EXPNO 2
PROCNO 1
Date_ 20150522
Time 18.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5876240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Cl
O
S
O
3ga
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

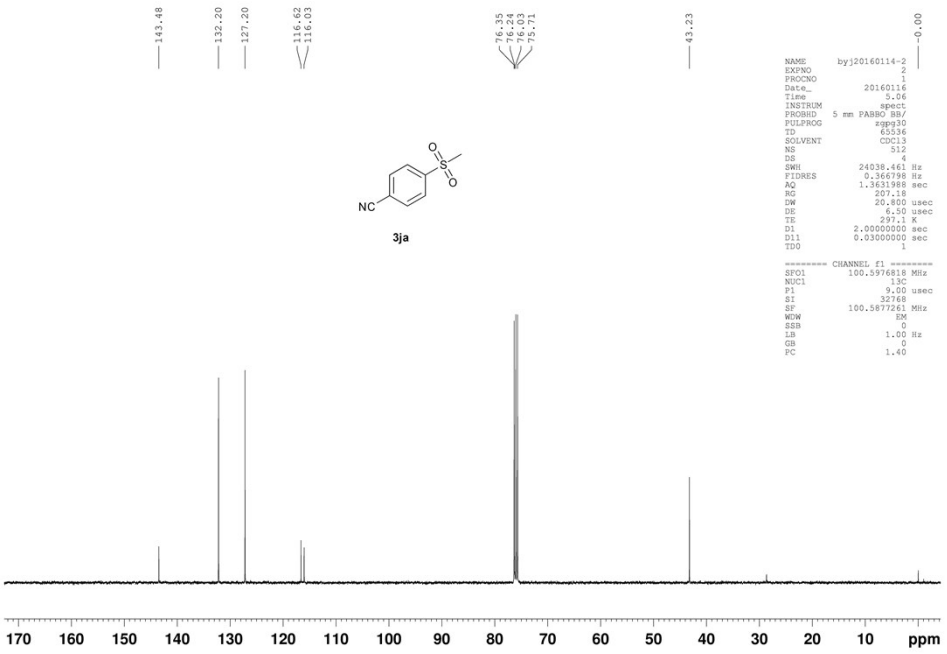

7.96
7.94
7.67
7.65
7.27
3.05
0.00
NAME yy20160111-1
EXPNO 10
PROCNO 1
Date_ 20150524
Time 5.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 83.62
DW 62.400 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
SI 65536
SF 400.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
3ha
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.03
2.00
3.07

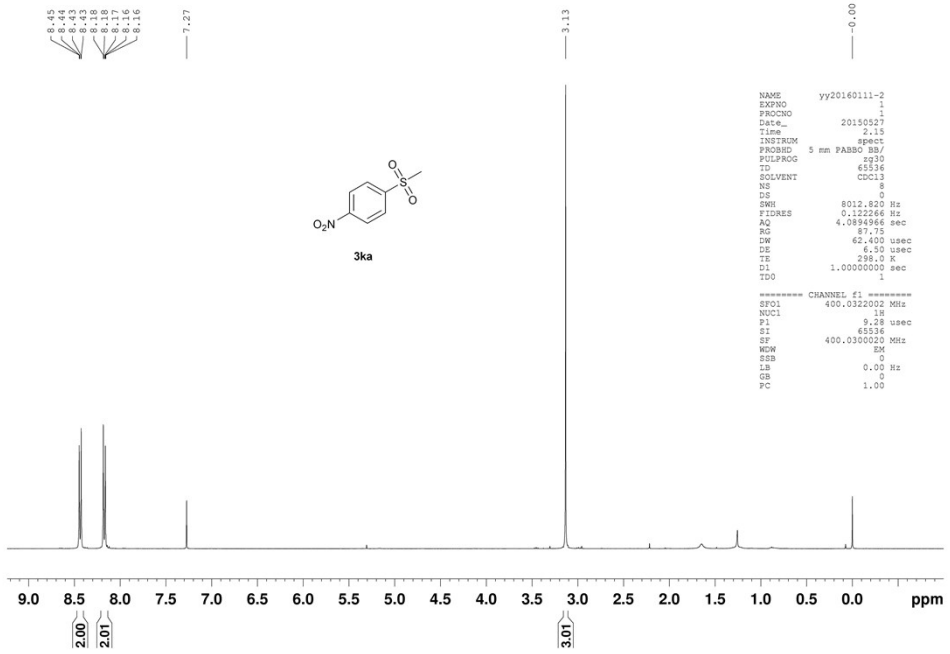

140.19
138.69
128.80
101.60
77.38
77.26
77.06
76.74
44.50
0.02
NAME yy20160111-1
EXPNO 11
PROCNO 1
Date_ 20150524
Time 6.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 211.87
DW 20.800 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
3ha
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

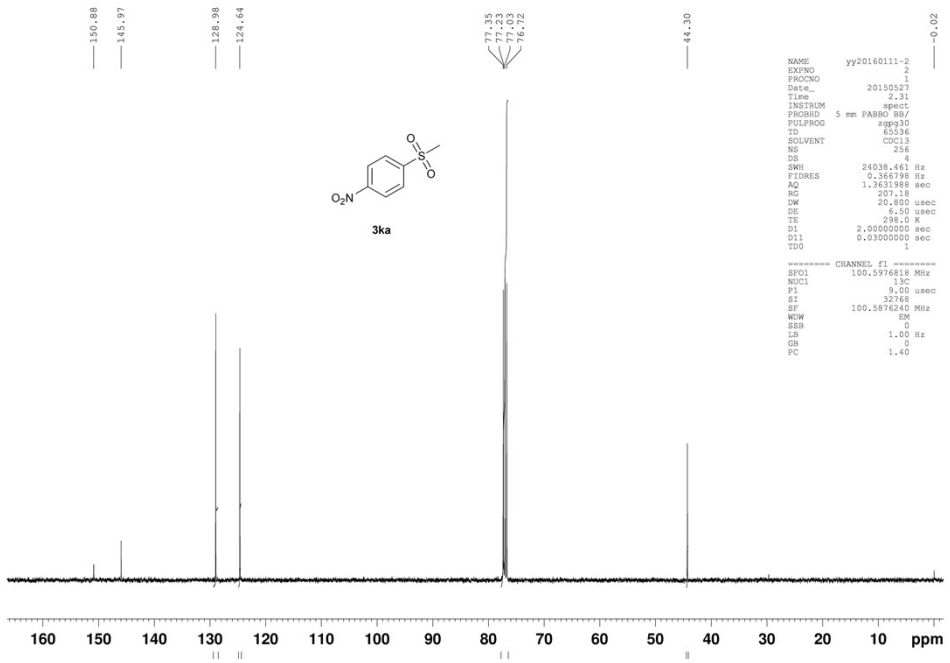

8.12
8.10
7.87
7.85
7.27
3.10
0.00
3ia
NAME yy20151223-1
EXPNO 1
PROCNO 1
Date_ 20150519
Time 17.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 82.27
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0300015 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.01
2.00
3.02

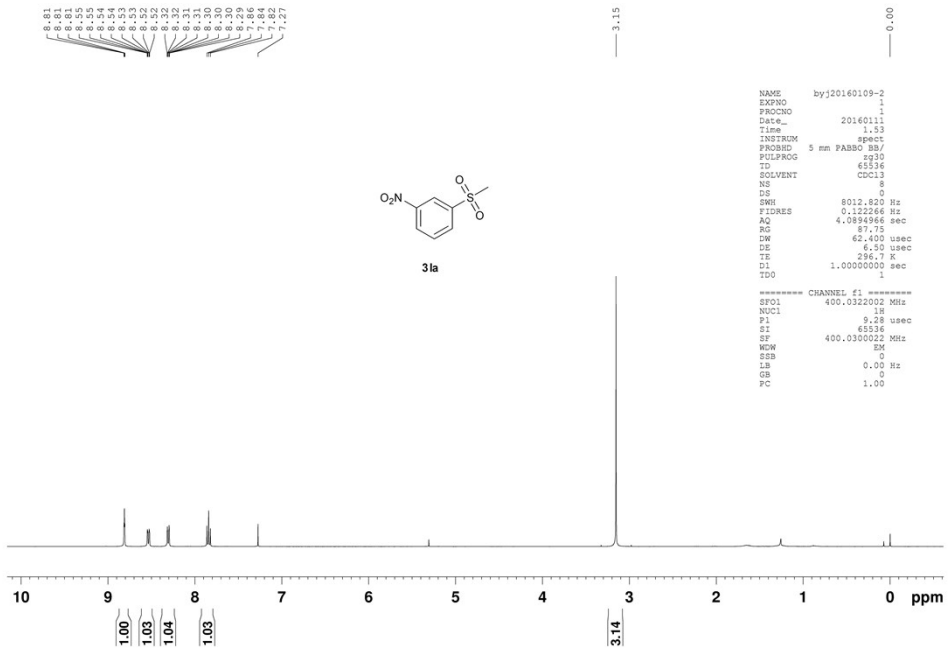

143.97
135.99
135.66
135.33
135.00
128.09
127.72
126.63
126.60
126.56
126.53
124.44
121.72
119.01
77.34
77.02
76.71
44.32
3ia
NAME yy20151223-1
EXPNO 2
PROCNO 1
Date_ 20150519
Time 17.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5876240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

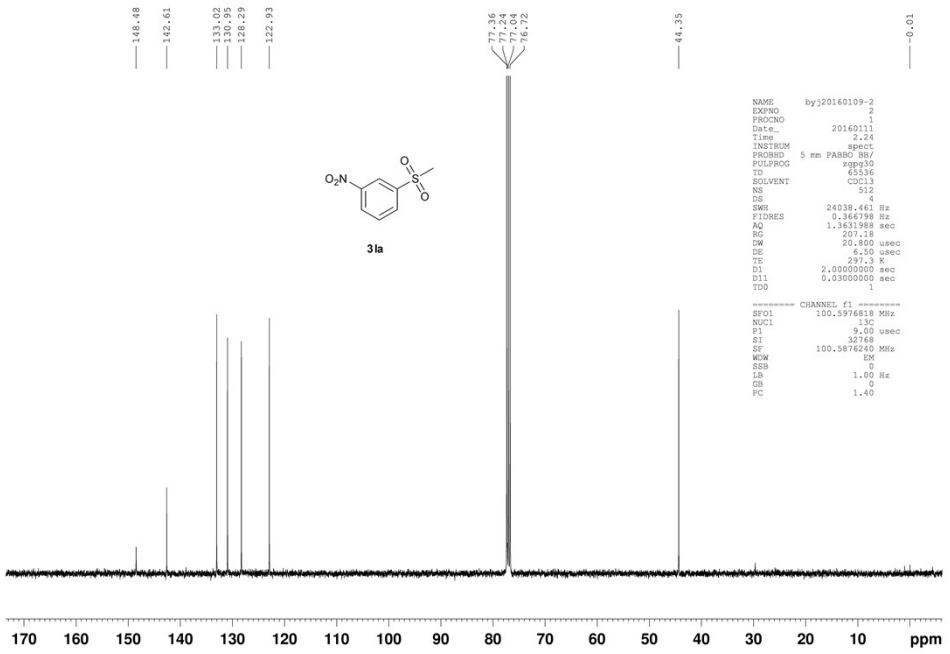

8.03
8.01
7.84
7.82
7.20
3.03
-0.00
NC
3ja
NAME byj20160114-2
EXPNO 1
PROCNO 1
Date_ 20160114
Time 18.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 87.75
DW 62.400 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0300019 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.00
1.95
3.00

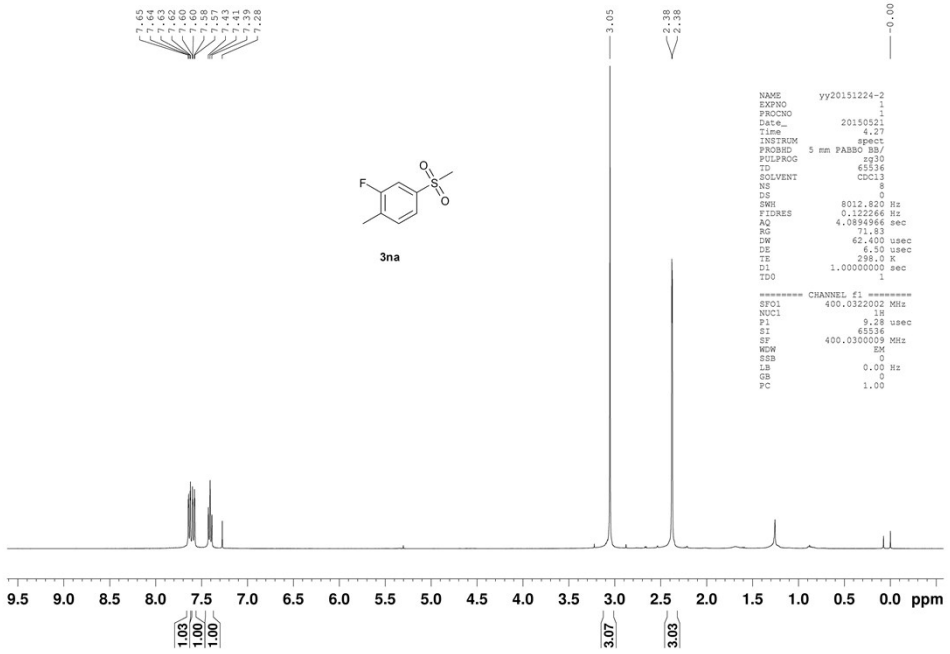

143.48
132.20
127.20
116.62
116.03
76.35
76.24
76.03
75.71
43.23
-0.00
NC
3ja
NAME byj20160114-2
EXPNO 2
PROCNO 1
Date_ 20160116
Time 5.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5877261 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

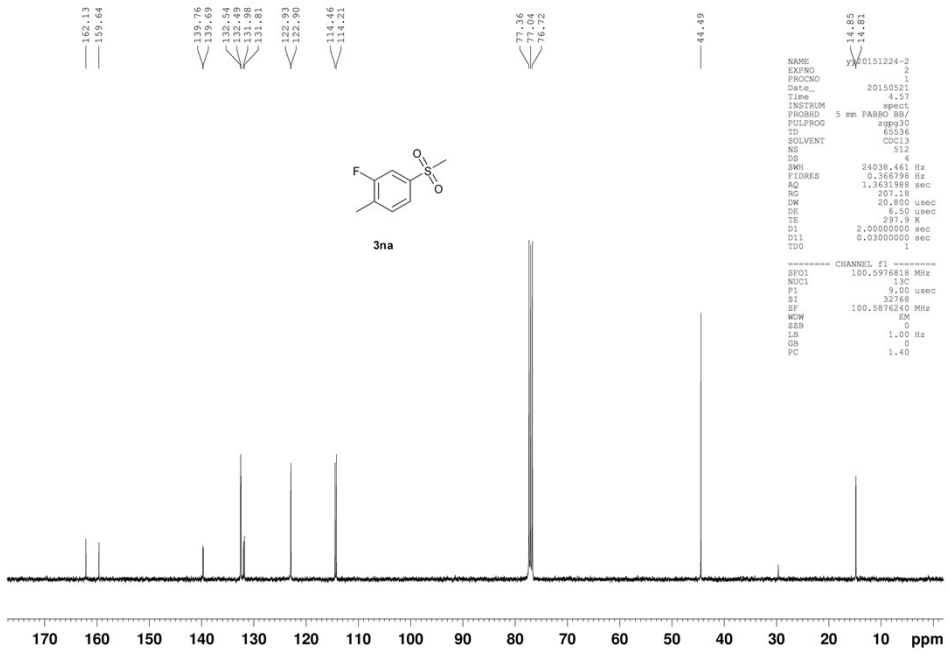

8.45
8.44
8.43
8.18
8.18
8.17
8.16
8.16
7.27
3.13
0.00
NAME yy20160111-2
EXPNO 1
PROCNO 1
Date_ 20150527
Time 2.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 87.75
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0300020 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
3ka
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
2.01
3.01

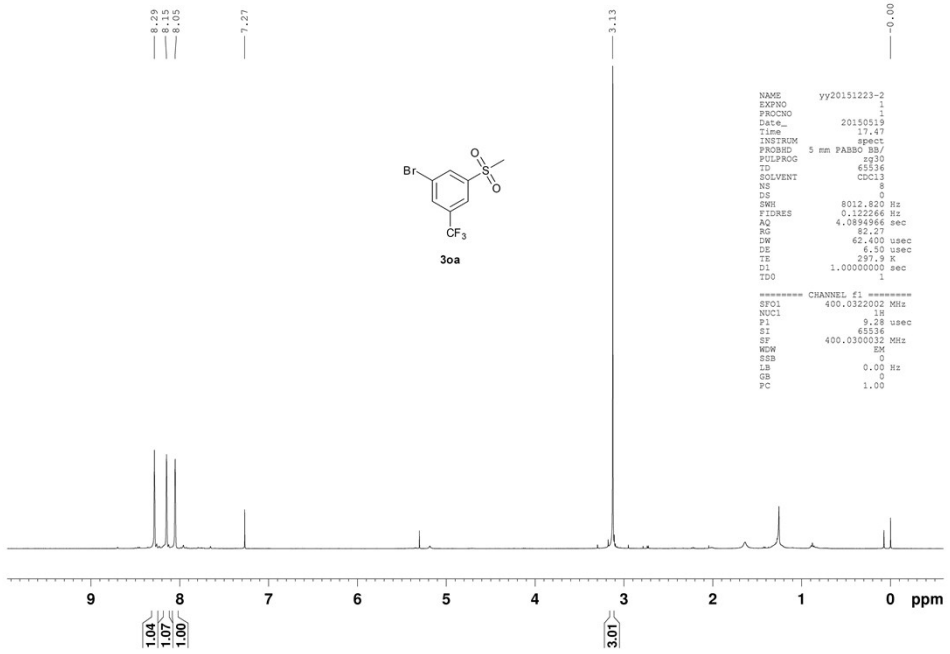

150.88
145.97
128.98
124.64
77.35
77.23
77.03
76.72
44.30
0.02
NAME yy20160111-2
EXPNO 2
PROCNO 1
Date_ 20150527
Time 2.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5876240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
3ka
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

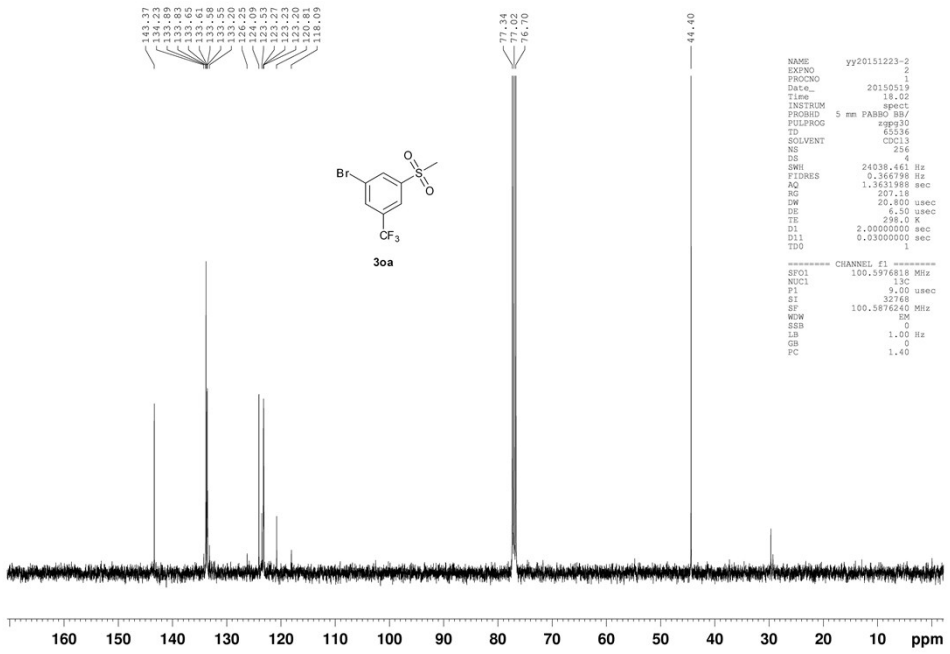

8.81
8.81
8.81
8.55
8.55
8.54
8.54
8.53
8.53
8.52
8.52
8.32
8.32
8.31
8.31
8.30
8.30
8.30
8.29
7.86
7.84
7.82
7.27
3.15
0.00
NAME byj20160109-2
EXPNO 1
PROCNO 1
Date_ 20160111
Time 1.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 87.75
DW 62.400 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0300022 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
O2N
3 la
10 9 8 7 6 5 4 3 2 1 0 ppm
1.00
1.03
1.04
1.03
3.14

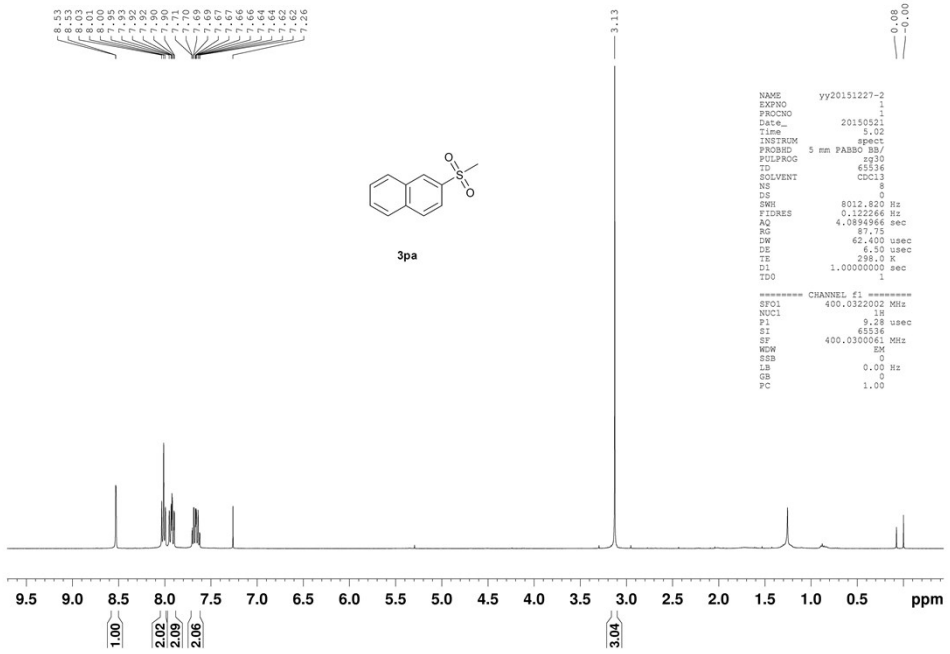

148.48
142.61
133.02
130.95
128.29
122.93
77.36
77.24
77.04
76.72
44.35
-0.01
NAME byj20160109-2
EXPNO 2
PROCNO 1
Date_ 20160111
Time 2.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5876240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
O2N
3 la
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

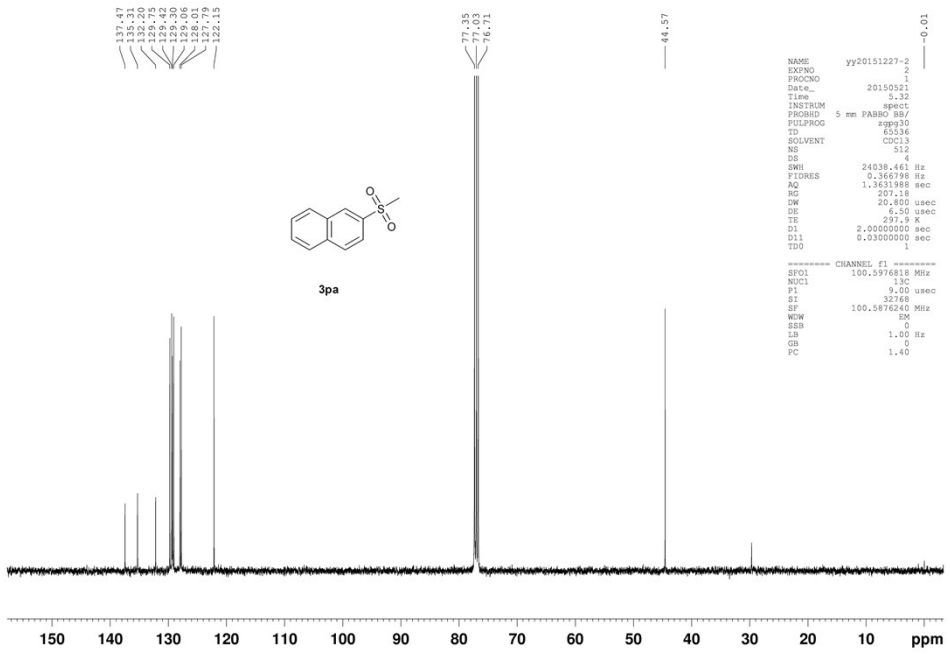

7.65
7.64
7.63
7.62
7.60
7.60
7.59
7.57
7.43
7.41
7.29
7.28
3.05
2.38
2.38
-0.00
F
O
S
O
3na
NAME yy20151224-2
EXPNO 1
PROCNO 1
Date_ 20150521
Time 4.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 71.83
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0300009 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.03
1.00
1.00
3.07
3.03

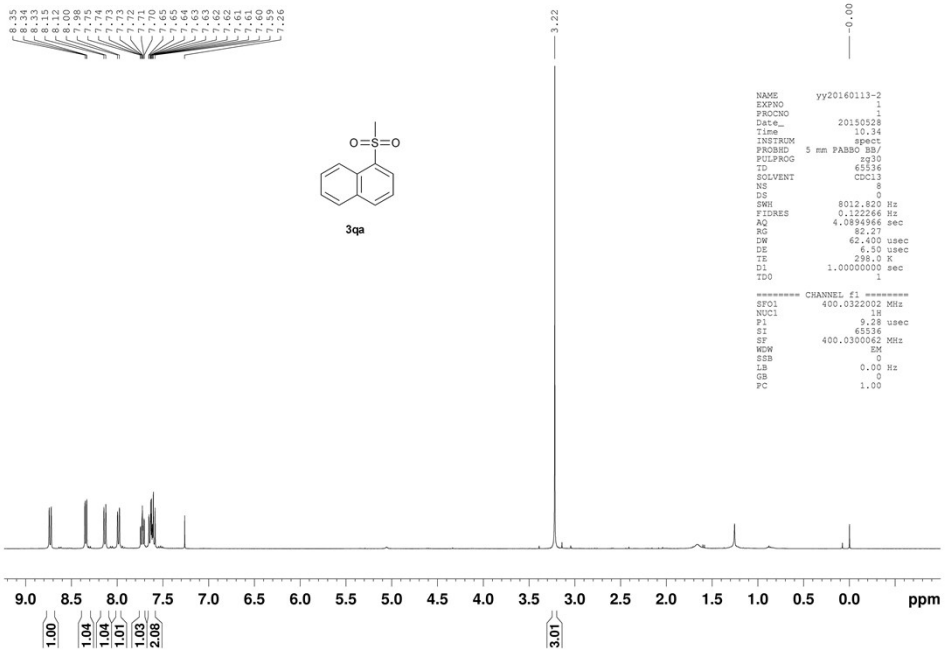

162.13
159.64
139.76
139.69
132.54
132.49
131.98
131.81
122.93
122.90
114.46
114.21
77.36
77.04
76.72
44.49
14.85
14.81
F
O
S
O
3na
NAME yy20151224-2
EXPNO 2
PROCNO 1
Date_ 20150521
Time 4.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5876240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

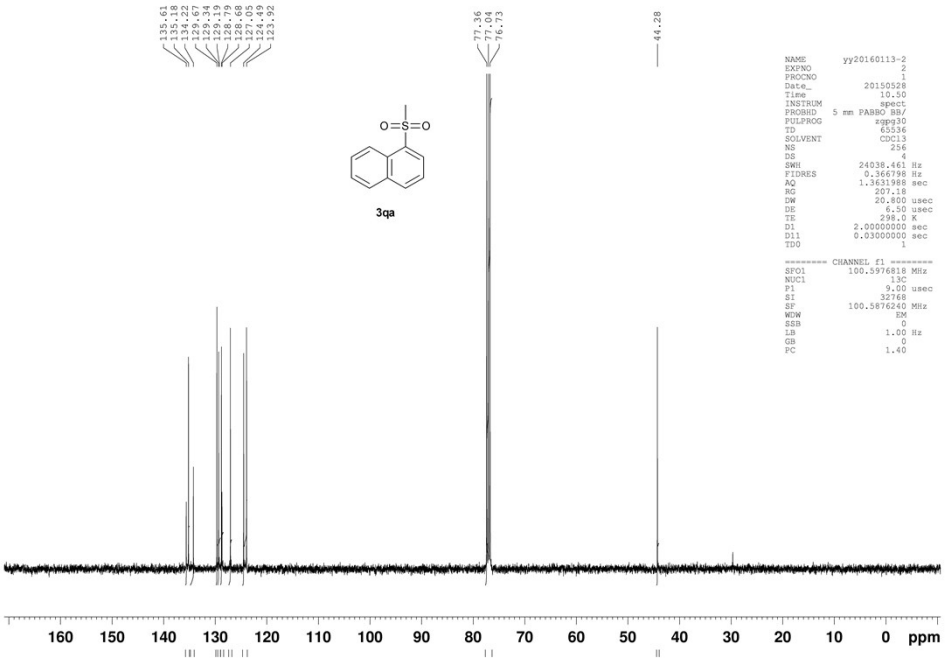

8.29
8.15
8.05
7.27
3.13
0.00
Br
O
S
O
CF3
3oa
NAME yy20151223-2
EXPNO 1
PROCNO 1
Date_ 20150519
Time 17.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 82.27
DW 62.400 usec
DE 6.50 usec
TE 297.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0300032 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
1.04
1.07
1.00
3.01

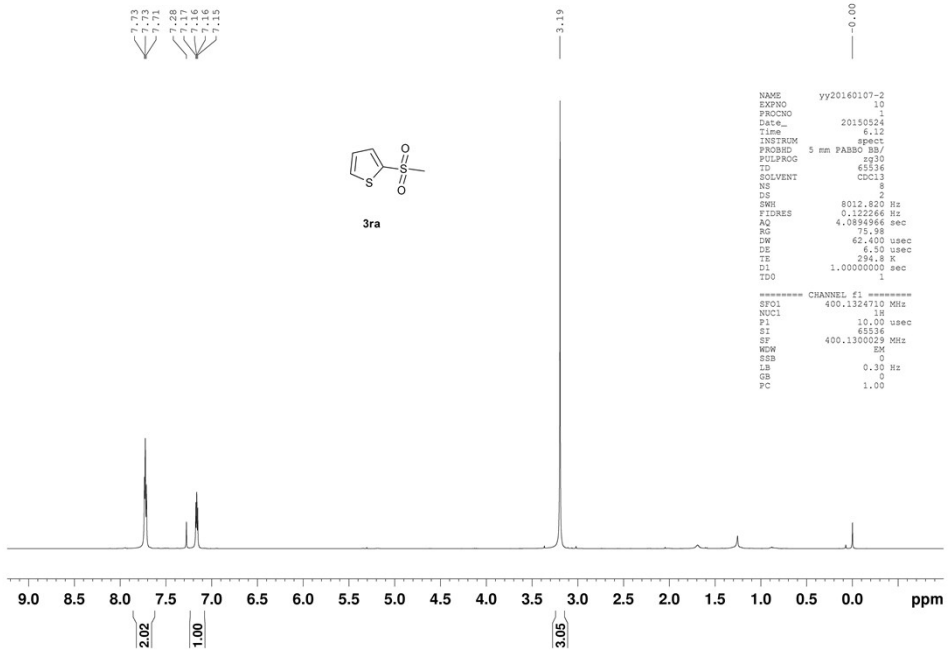

143.37
134.23
133.89
133.83
133.65
133.61
133.58
133.55
133.50
126.25
124.09
123.53
123.27
123.23
123.20
120.81
118.09
77.34
77.02
76.70
44.40
Br
O
S
O
CF3
3oa
NAME yy20151223-2
EXPNO 2
PROCNO 1
Date_ 20150519
Time 18.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5876240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

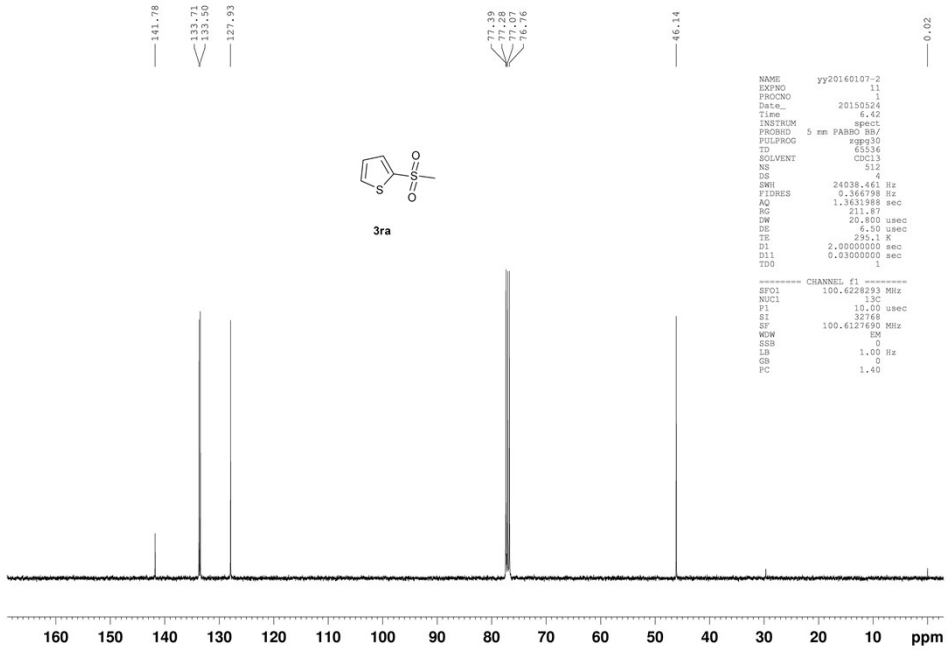

8.53
8.53
8.03
8.01
8.00
7.95
7.93
7.92
7.90
7.90
7.71
7.70
7.69
7.69
7.67
7.66
7.66
7.64
7.64
7.62
7.62
7.26
3.13
0.08
-0.00
3pa
NAME yy20151227-2
EXPNO 1
PROCNO 1
Date_ 20150521
Time 5.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 87.75
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0300061 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
2.02
2.09
2.06
3.04

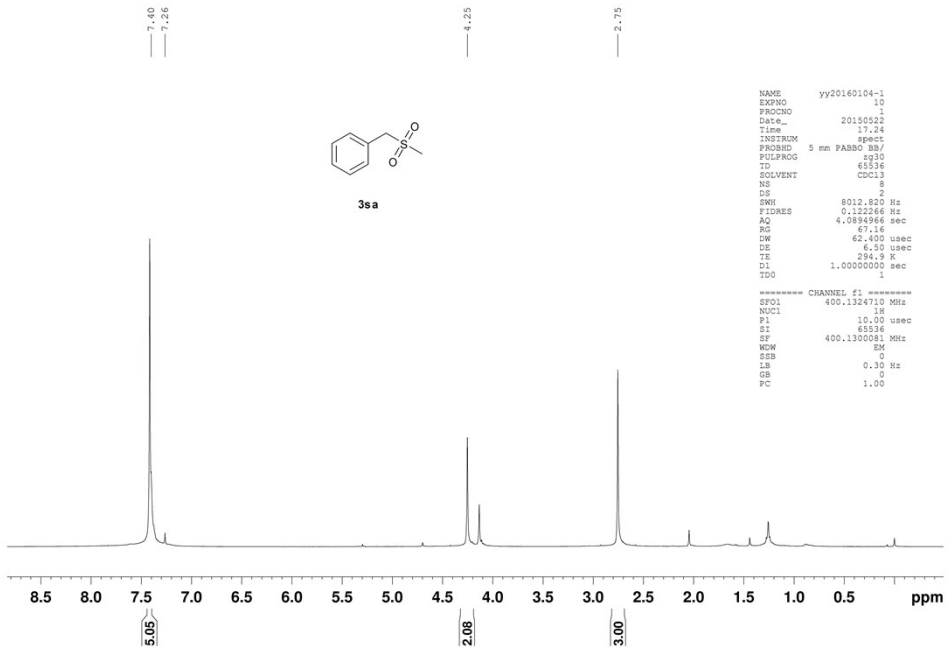

137.47
135.31
132.20
129.75
129.32
129.30
129.06
128.01
127.79
122.15
77.35
77.03
76.71
44.57
-0.01
3pa
NAME yy20151227-2
EXPNO 2
PROCNO 1
Date_ 20150521
Time 5.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5876240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

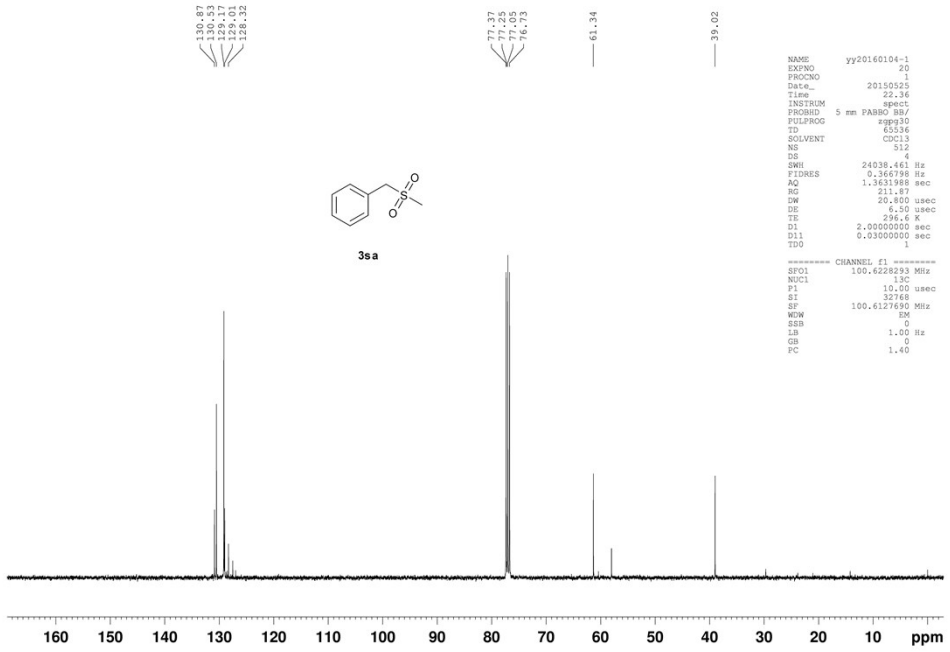

8.35
8.34
8.33
8.15
8.12
8.00
7.98
7.75
7.74
7.73
7.73
7.72
7.71
7.70
7.65
7.65
7.64
7.63
7.62
7.62
7.61
7.61
7.60
7.59
7.26
3.22
-0.00
O=S=O
3qa
NAME yy20160113-2
EXPNO 1
PROCNO 1
Date_ 20150528
Time 10.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 82.27
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.0322002 MHz
NUC1 1H
P1 9.28 usec
SI 65536
SF 400.0300062 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.04
1.04
1.01
1.03
2.08
3.01

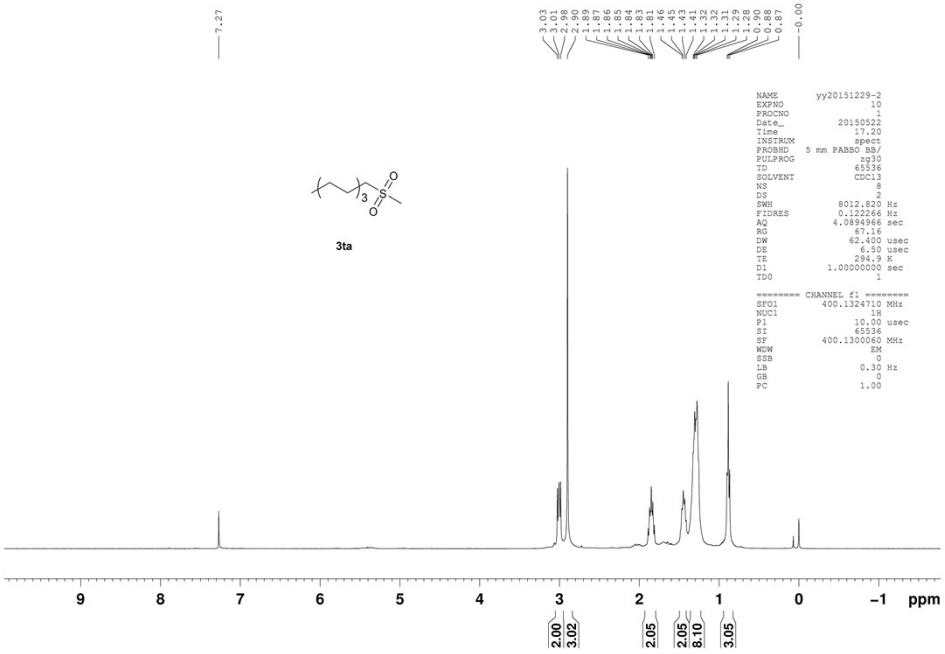

135.61
135.18
133.22
129.67
129.34
129.19
128.79
128.68
127.05
124.49
123.92
77.36
77.04
76.73
44.28
O=S=O
3qa
NAME yy20160113-2
EXPNO 2
PROCNO 1
Date_ 20150528
Time 10.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 207.18
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.5976818 MHz
NUC1 13C
P1 9.00 usec
SI 32768
SF 100.5876240 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

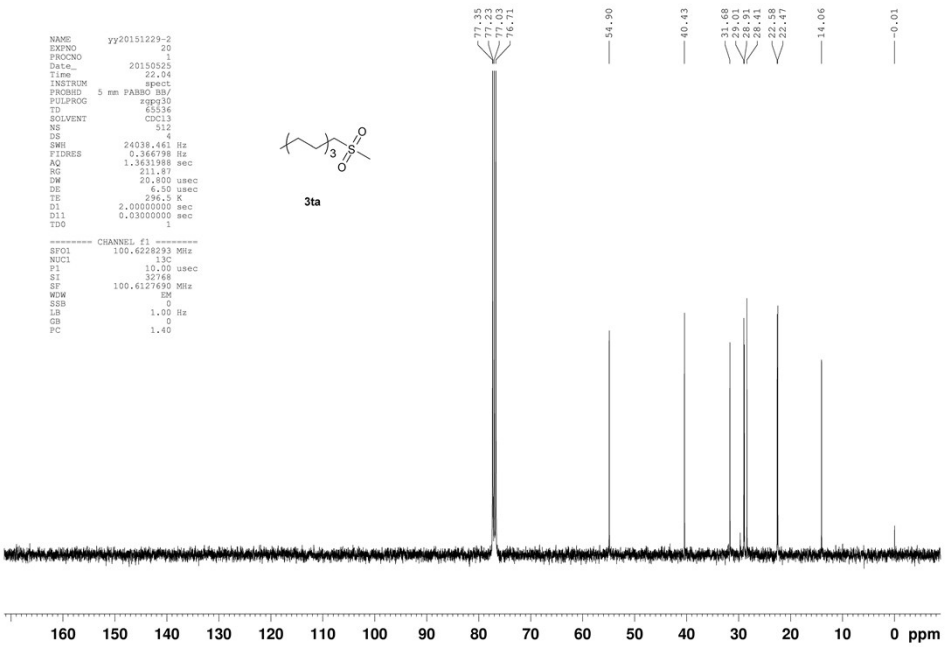

7.73
7.73
7.71
7.28
7.17
7.16
7.16
7.15
3.19
-0.00
3ra
NAME yy20160107-2
EXPNO 10
PROCNO 1
Date_ 20150524
Time 6.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 75.98
DW 62.400 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
SI 65536
SF 400.1300029 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.02
1.00
3.05


141.78
133.71
133.50
127.93
77.39
77.28
77.07
76.76
46.14
0.02
3ra
NAME yy20160107-2
EXPNO 11
PROCNO 1
Date_ 20150524
Time 6.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 211.87
DW 20.800 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.40
7.26
4.25
2.75
3sa
NAME yy20160104-1
EXPNO 10
PROCNO 1
Date_ 20150522
Time 17.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 67.16
DW 62.400 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
SI 65536
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
5.05
2.08
3.00


130.87
130.53
129.17
129.01
128.32
77.37
77.25
77.05
76.73
61.34
39.02
3sa
NAME yy20160104-1
EXPNO 20
PROCNO 1
Date_ 20150525
Time 22.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 211.87
DW 20.800 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


7.27
3.03
3.01
2.98
2.90
1.89
1.87
1.86
1.85
1.84
1.83
1.61
1.46
1.45
1.43
1.41
1.32
1.31
1.29
1.28
0.90
0.88
0.87
-0.00
3ta
NAME yy20151229-2
EXPNO 10
PROCNO 1
Date_ 20150522
Time 17.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 67.16
DW 62.400 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 10.00 usec
SI 65536
SF 400.1300060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
-1
ppm
2.00
3.02
2.05
2.05
8.10
3.05


77.35
77.23
77.03
76.71
54.90
40.43
31.68
29.01
28.91
28.41
22.58
22.47
14.06
-0.01
3ta
NAME yy20151229-2
EXPNO 20
PROCNO 1
Date_ 20150525
Time 22.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 211.87
DW 20.800 usec
DE 6.50 usec
TE 296.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm