Supporting Information

Copper-Mediated Aerobic (Phenylsulfonyl)difluoromethylation of Arylboronic Acids with Difluoromethy Phenyl Sulfone

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Table of Contents

1. General Information 3

2. Preparation of "$PhSO_2CF_2Cu$" Generated from $PhSO_2CF_2H$ 3

3. Transformation of "$[(PhSO_2CF_2)_2Cu]^-$" into "$PhSO_2CF_2Cu$" 4

4. The Stability of "$PhSO_2CF_2Cu$" under Different Conditions 5

5.(Phenylsulfonyl)difluoromethylation of Arylboronic Acids with "$PhSO_2CF_2Cu$" Generated from $PhSO_2CF_2H$ 6

6. Synthesis of Difluoromethylated Aromatics by Reductive Desulfonylation 21

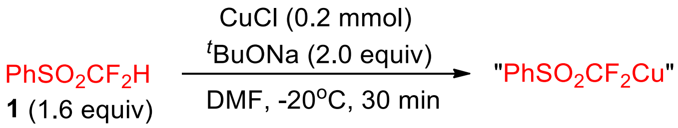
7. References 22

8. ^{19}F, ^{1}H and ^{13}C NMR Spectra of isolated Products 24

1. General Information

Commercial reagents were used without further purification. DMF and NMP were distilled over CaH_2, and stored over activated molecular sieve. CuCl and CuI were purified according to reported procedures.[1] Difluoromethyl phenyl sulfone (**1**) was prepared using known procedure.[2] ^{1}H, ^{13}C and ^{19}F NMR spectra were recorded on a 400 MHz NMR spectrometer. ^{1}H NMR spectroscopy chemical shifts were determined relative to internal Me_4Si (TMS) at δ 0.0 or to the signal of the residual protonated solvent $CDCl_3$ δ 7.26. ^{13}C NMR spectroscopy chemical shifts were determined relative to internal TMS at δ 0.0. For the isolated compounds, ^{19}F NMR spectroscopy chemical shifts were determined relative to $CFCl_3$ at δ 0.0; for the reaction mixtures, ^{19}F NMR spectroscopy chemical shifts were determined relative to $PhCF_3$ at δ –62.0. Data for ^{1}H, ^{13}C and ^{19}F NMR spectra are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet, br = broad). FT-IR spectra were obtained with a Nicolet 380 spectrophotometer. Mass spectra were obtained on an Agilent LC-MS 1100 instrument. High resolution mass data were recorded on a Thermo Fisher Scientific LTQ FT Ultra instrument. GC–MS data were recorded on a Finnigan 4021 instrument. Elemental analysis was performed with Elementer Vario EL III instrument. Melting points were recorded on a SGW X-4 melting point apparatus and are uncorrected. All reactions were monitored by TLC or ^{19}F NMR spectroscopy.

2. Preparation of “$PhSO_2CF_2Cu$” Generated from $PhSO_2CF_2H$



In a glovebox, CuCl (20 mg, 0.2 mmol) and ^{t}BuONa (38.5 mg, 0.4 mmol) were added to an oven-dried 10-mL Schlenk tube equipped with a stirring bar. The Schlenk tube was sealed with a septum and brought to the bench. DMF (1 mL) was added and stirred vigorously at room temperature for 10 min, and then difluoromethyl phenyl sulfone (**1**) (45 μL, 0.32 mmol) was added at −20℃ for 30 min under an argon atmosphere. The reaction was monitored by ^{19}F NMR spectroscopy using $PhCF_3$ (25 μL) as an internal standard (Figure S1).

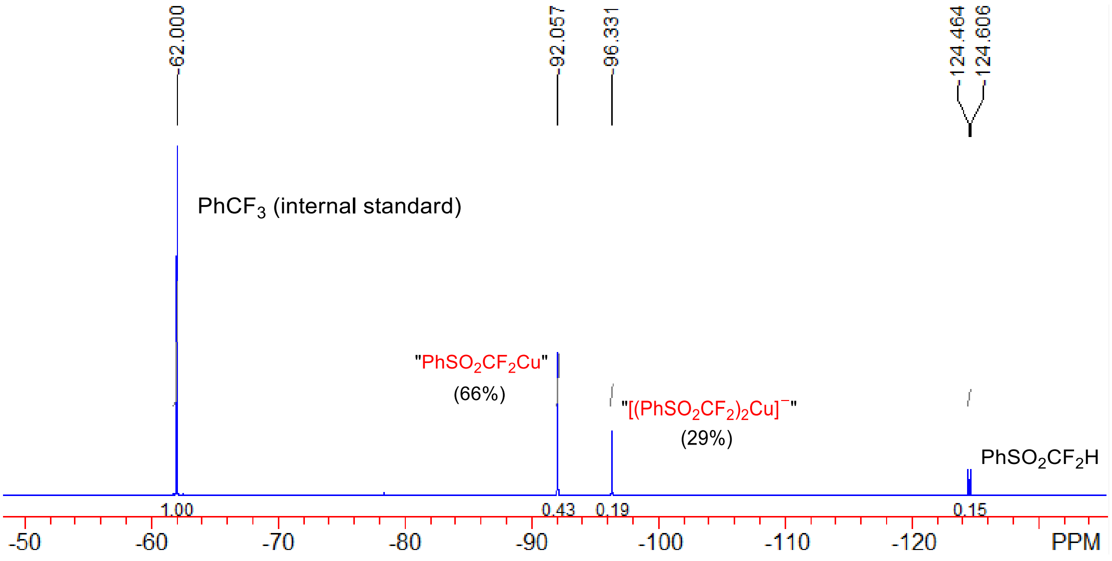
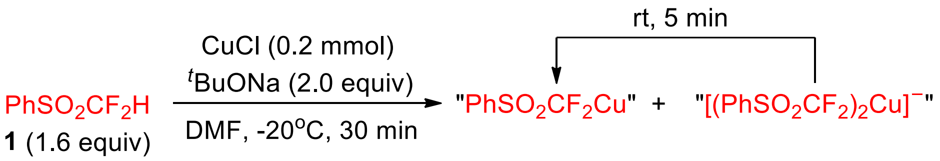


Figure S1. Preparation of "$PhSO_2CF_2Cu$" generated from $PhSO_2CF_2H$

3. Transformation of "$[(PhSO_2CF_2)_2Cu]^-$" into $[PhSO_2CF_2Cu]$



In a glovebox, CuCl (20 mg, 0.2 mmol) and ^{t}BuONa (38.5 mg, 0.4 mmol) were added to an oven-dried 10-mL Schlenk tube equipped with a stirring bar. The Schlenk tube was sealed with a septum and brought to the bench. DMF (1 mL) was added and stirred vigorously at rt for 10 min, and then difluoromethyl phenyl sulfone (**1**) (45 μL, 0.32 mmol) was added at −20℃ for 30 min under an argon atmosphere. The reaction was monitored by ^{19}F NMR spectroscopy using $PhCF_3$ (25 μL,) as an internal standard (Figure S2, **a**). The same sample was monitored again by ^{19}F NMR spectroscopy at rt after 5 min (Figure S2, **b**).

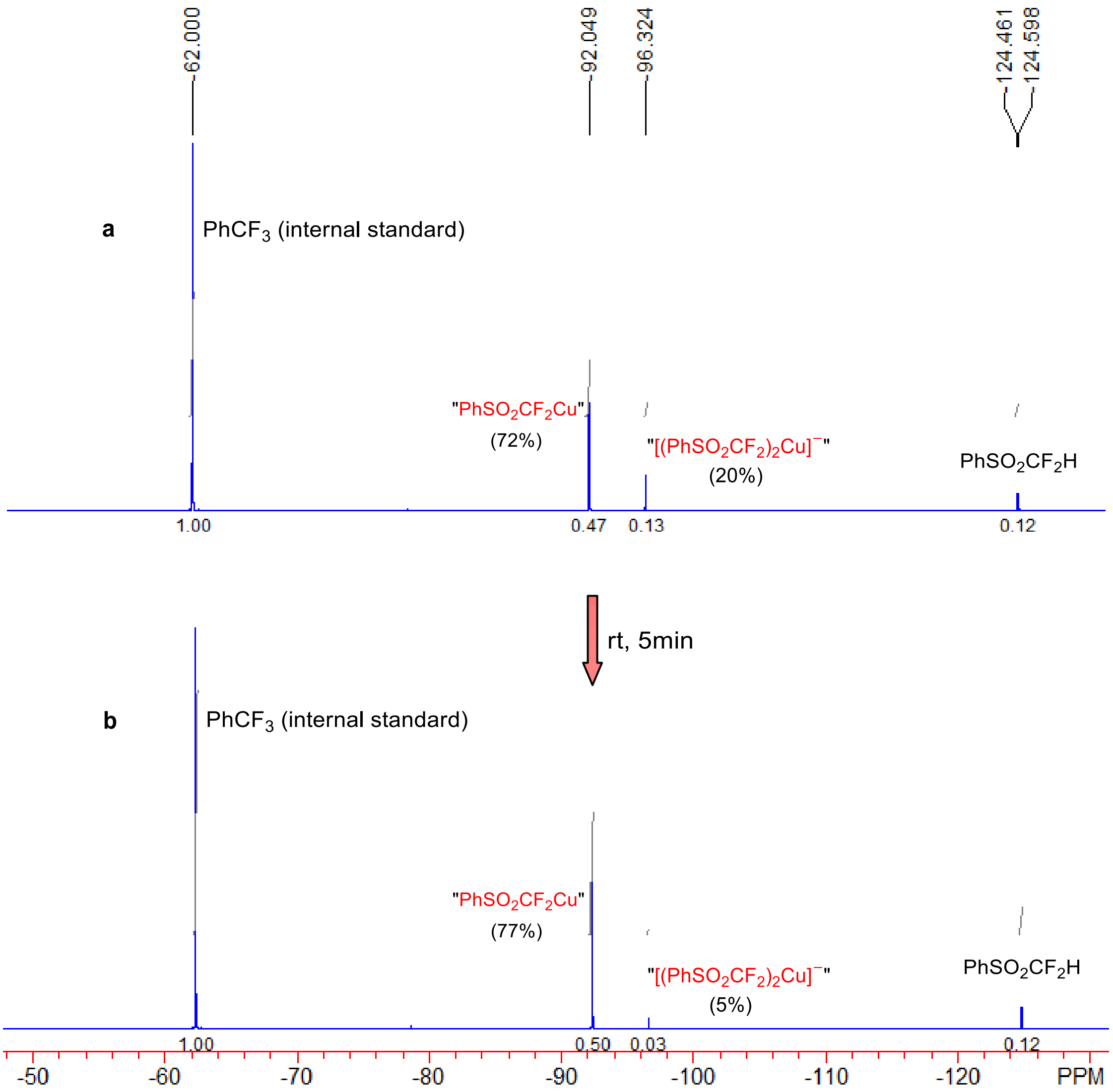
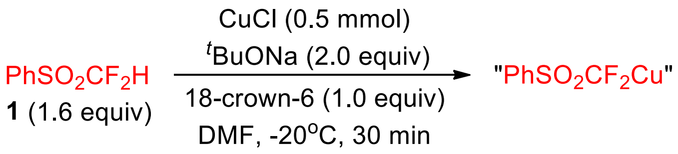


Figure S2. Transformation of "[$(PhSO_2CF_2)_2Cu]^-$" into "$PhSO_2CF_2Cu$"

4. The Stability of "$PhSO_2CF_2Cu$" under Different Conditions



In a glovebox, CuCl (50 mg, 0.5 mmol, 1.0 equiv) and ^{t}BuONa (96 mg, 1.0 mmol) were added to an oven-dried 10-mL Schlenk tube equipped with a stirring bar. The Schlenk tube was sealed with a septum and brought to the bench. DMF (2 mL) was added and stirred vigorously at rt for 20 min, and then difluoromethyl phenyl sulfone (**1**) (113 μL, 0.8 mmol) and 18-crowm-6 (132 mg, 0.5 mmol) was added at -20℃ for 30 min under an argon atmosphere. The reaction was monitored at rt after 5 min by ^{19}F NMR spectroscopy using $PhCF_3$ (25.5 μL) as an internal standard (81% yield for "$PhSO_2CF_2Cu$"). The same sample was stored in refrigerator (about -12℃) and was monitored again by ^{19}F NMR spectroscopy after 5 h, 13 h, 24 h, 37 h, 61 h, 109 h (Figure S3).

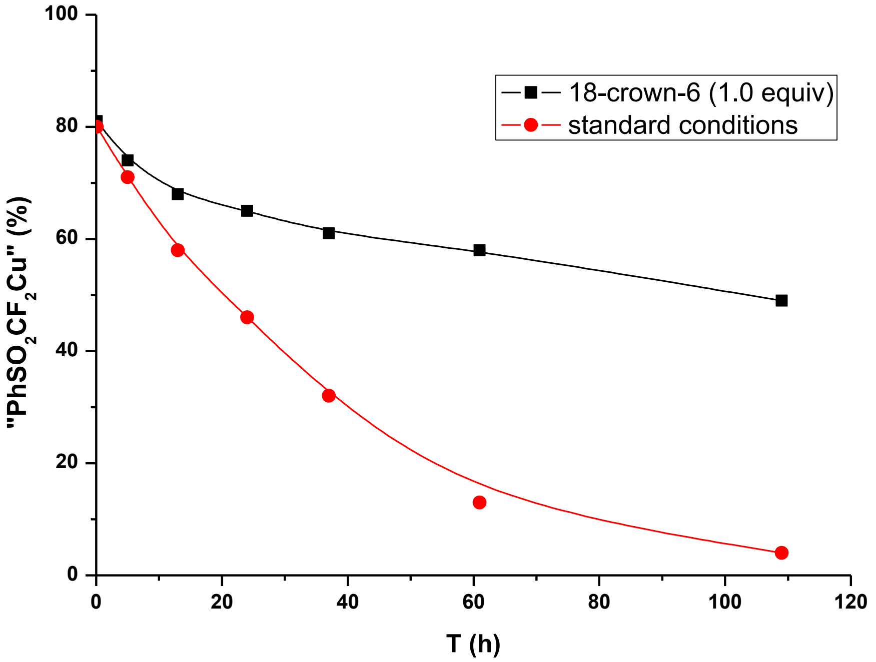


Figure S3. The stability of "$PhSO_2CF_2Cu$" under different conditions

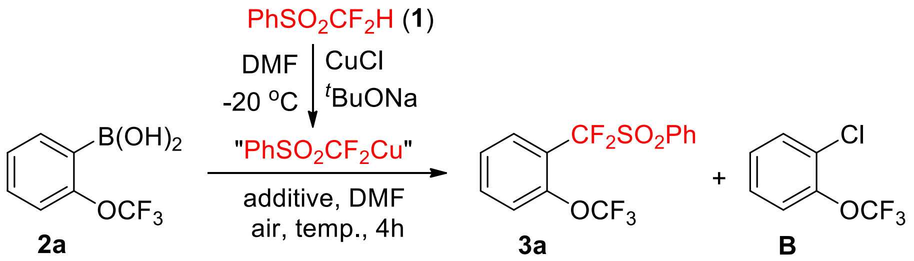
5. (Phenylsulfonyl)difluoromethylation of Arylboronic Acids with "$PhSO_2CF_2Cu$" Generated from $PhSO_2CF_2H$

5.1 Screening of Reaction Conditions

In a glovebox, CuCl (50 mg, 0.5 mmol) and *t*BuONa (96 mg, 1.0 mmol) were added to an oven-dried 10-mL Schlenk tube equipped with a stirring bar. The Schlenk tube was sealed with a septum and brought to the bench. DMF (2 mL) was added and stirred vigorously at rt for 20 min, and then difluoromethyl phenyl sulfone (**1**) (113 μL, 0.8 mmol) was added at -20℃ for 45 min under an argon atmosphere. The pregenerated "$PhSO_2CF_2Cu$" and additive were added respectively into

(2-(trifluoromethoxy)phenyl)boronic acid (**2a**) (purity 98%, 42 mg, 0.2 mmol, 1.0 equiv) in DMF (2 mL) for 4 h under an air atmosphere. The reaction mixture was monitored by ^{19}F NMR spectroscopy using $PhCF_3$ as an internal standard.

Table S1. Screening of Reaction Conditions



entry	additive (equiv)	temp.	yield[a] of **3a** (**B**) (%)
1	–	0 °C	16 (28)
2	–	rt	67 (18)
3	$Et_3N\cdot 3HF$ (0.8)	rt	0 (0)
4	H_2O (0.5)	rt	68 (19)
5	H_2O (1.0)	rt	60 (21)
6	1,10-phen (1.0)	rt	0 (0)
7[b]	18-crowm-6 (2.5)	rt	68 (11)
8	K_3PO_4 (1.0)	rt	68 (18)
9	KOAc (1.0)	rt	60 (27)
10[c]	$Cu(OAc)_2$ (5 mol %)	rt	69 (19)
11	$AgNO_3$ (0.5)	rt	72 (15)
12	$AgNO_3$ (1.0)	rt	73 (10)
13	$AgNO_3$ (0.5) + $Cu(OAc)_2\cdot H_2O$ (0.2)	rt	75 (7)
14[d]	$AgNO_3$ (0.5) + $Cu(OAc)_2\cdot H_2O$ (0.2)	rt	77 (9)
15[d]	$AgNO_3$ (0.6) + $Cu(OAc)_2\cdot H_2O$ (0.3)	rt	80 (7)
16[e]	$AgNO_3$ (0.6) + $Cu(OAc)_2\cdot H_2O$ (0.3)	rt	0 (–)

[a] Yields were determined by ^{19}F NMR spectroscopy.

[b] 18-crowm-6 was added after the addition of **1** in the generation of “$PhSO_2CF_2Cu$”.

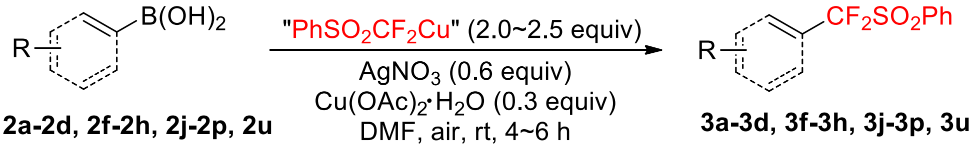
[c] The reaction was conducted for 3 h and **1** (3.2 equiv) was used.

[d] The reaction was conducted with 0.4 mmol of **2a** for 6 h.

[e] The reaction was conducted under argon atmosphere.

5.2 (Phenylsulfonyl)difluoromethylation of Arylboronic Acids with “$PhSO_2CF_2Cu$” Generated from $PhSO_2CF_2H$

Method A



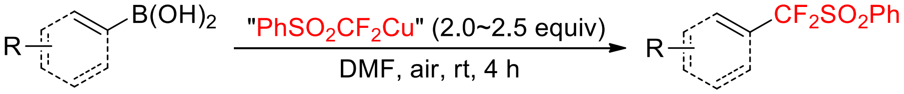
Standard procedure for 0.2 mmol scale:

In a glovebox, CuCl (50 mg, 0.5 mmol) and ^{t}BuONa (96 mg, 1.0 mmol) were added to an oven-dried 10-mL Schlenk tube equipped with a stirring bar. The Schlenk tube was sealed with a septum and brought to the bench. DMF (2 mL) was added and stirred vigorously at rt for 20 min, and then difluoromethyl phenyl sulfone (**1**) (113 μL, 0.8 mmol) was added at –20℃ for 45 min under an argon atmosphere. The pregenerated “$PhSO_2CF_2Cu$”, $AgNO_3$ (20.5 mg, 0.12 mmol), and $Cu(OAc)_2 \cdot H_2O$ (12 mg, 0.06 mmol) were added respectively into a solution of arylboronic acid (0.2 mmol, 1.0 equiv) in DMF (2 mL) at rt for 4 h under an air atmosphere. After addition of dichloromethane (5 mL), 1N HCl solution (1 mL), and H_2O (10 mL), the organic layer was separated and the aqueous layer was extracted with dichloromethane (3×5 mL). The combined organic layer was washed with brine (2×10 mL), dried over $MgSO_4$, filtered and concentrated in vacuo. The residue was purified by column chromatography on silica gel.

Standard procedure for 0.4 mmol scale:

In a glovebox, CuCl (100 mg, 1.0 mmol) and ^{t}BuONa (192 mg, 2.0 mmol) were added to an oven-dried 10-mL Schlenk tube equipped with a stirring bar. The Schlenk tube was sealed with a septum and brought to the bench. DMF (4 mL) was added and stirred vigorously at rt for 20 min, and then difluoromethyl phenyl sulfone (**1**) (113 μL, 1.6 mmol) was added at -20℃ for 45 min under an argon atmosphere. The pregenerated “$PhSO_2CF_2Cu$”, $AgNO_3$ (41 mg, 0.24 mmol), and $Cu(OAc)_2 \cdot H_2O$ (24 mg, 0.12 mmol) were added respectively into a solution of arylboronic acid (0.4 mmol, 1.0 equiv) in DMF (4 mL) at rt for 6 h under an air atmosphere. After addition of dichloromethane (10 mL), 1N HCl solution (1.5 mL), and H_2O (10 mL), the organic layer was separated and the aqueous layer was extracted with dichloromethane (3 × 10 mL). The combined organic layer was washed with brine (2 × 20 mL), dried over $MgSO_4$, filtered and concentrated in vacuo. The residue was purified by column chromatography on silica gel.

Method B

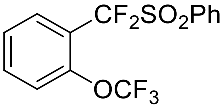


2e, 2i, 2q-2t **3e, 3i, 3q-3t**

Standard procedure:

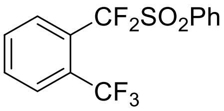
In a glovebox, CuCl (50 mg, 0.5 mmol) and ^{t}BuONa (96 mg, 1.0 mmol) were added to an oven-dried 10-mL Schlenk tube equipped with a stirring bar. The Schlenk tube was sealed with a septum and brought to the bench. DMF (2 mL) was added and stirred vigorously at rt for 20 min, and then difluoromethyl phenyl sulfone (**1**) (113 μL, 0.8 mmol) was added at -20℃ for 45 min under an argon atmosphere. The pregenerated “$PhSO_2CF_2Cu$” was added into a solution of arylboronic acid (0.2 mmol, 1.0 equiv) in DMF (2 mL) at rt for 4 h under an air atmosphere. After addition of dichloromethane (5 mL), 1N HCl solution (1 mL), H_2O (10 mL) and the organic layer was separated and the aqueous layer was extracted with dichloromethane (3 × 5 mL). The combined organic layer was washed with brine (2 × 10 mL), dried over $MgSO_4$, filtered and concentrated in vacuo. The residue was purified by column chromatography on silica gel.

(**Note**: The generation of “$PhSO_2CF_2Cu$” is crucial for obtaining all products in good yields.)



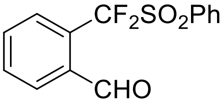
1-(Difluoro(phenylsulfonyl)methyl)-2-(trifluoromethoxy)benzene (3a)

For 0.4 mmol scale, the standard procedure of method A was followed to provide **3a** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (105 mg, 75%). M.p.: 93-95 °C. IR (KBr): 3092, 1609, 1493, 1449, 1341, 1251, 1172, 1061, 945, 773, 763, 598 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38-7.44 (m, 2H, ArH), 7.60-7.64 (m, 3H, ArH), 7.70 (d, *J* = 7.6 Hz, 1H, ArH), 7.78 (t, *J* = 7.4 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.2 (t, *J* = 21.5 Hz), 120.2 (q, *J* = 257.9 Hz), 120.9 (q, *J* = 1.5 Hz), 121.2 (t, *J* = 287.7 Hz), 126.4, 129.3, 130.8 (t, *J* = 6.9 Hz), 131.0, 132.7, 134.1, 135.5, 147.8 (q, *J* = 1.4 Hz). ^{19}F NMR (376 MHz, $CDCl_3$): δ –56.6 (s, 3F), –98.4 (s, 2F). MS (ESI, m/z): 369.9 $(M+NH_4)^+$, 374.8 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{14}H_{13}O_3NF_5S$ $(M+NH_4)^+$: 370.0527, found: 370.0531.



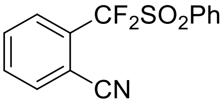
1-(Difluoro(phenylsulfonyl)methyl)-2-(trifluoromethyl)benzene (3b)

For 0.2 mmol scale, the standard procedure of method A was followed to provide **3b** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (44 mg, 65%). M.p.: 117-118 °C. IR (KBr): 3067, 1584, 1448, 1351, 1304, 1284, 1172, 1037, 933, 772, 720, 685, 589, 544 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (t, *J* = 7.6 Hz, 2H, ArH), 7.72-7.74 (m, 2H, ArH), 7.78 (t, *J* = 7.6 Hz, 1H, ArH), 7.90-7.98 (m, 2H, ArH), 8.03 (d, *J* = 7.8 Hz, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 121.5 (t, *J* = 288.0 Hz), 122.7 (q, *J* = 272.2 Hz), 125.1 (t, *J* = 22.6 Hz), 127.9 (q, *J* = 6.6 Hz), 129.4, 129.5 (q, *J* = 32.8 Hz), 131.0, 131.7 (t, *J* = 7.7 Hz), 131.8, 132.5, 132.7, 135.5. ^{19}F NMR (376 MHz, $CDCl_3$): δ –58.0 (t, *J* = 18.8 Hz, 3F), –94.4 (q, *J* = 19.1 Hz, 2F). MS (ESI, m/z): 353.9 $(M+NH_4)^+$, 358.8 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{14}H_{10}O_2F_5S$ $(M+H)^+$: 337.0311, found: 337.0316.



2-(Difluoro(phenylsulfonyl)methyl)benzaldehyde (3c)

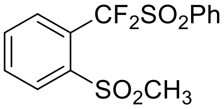
For 0.2 mmol scale, the standard procedure of method A was followed to provide **3c** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (39 mg, 66%). M.p.: 102-103 °C. IR (KBr): 3080, 2929, 1696, 1596, 1457, 1340, 1249, 1170, 1064, 939, 823, 761, 687, 595 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 7.66 (t, J = 7.8 Hz, 2H, ArH), 7.72-7.74 (m, 3H, ArH), 7.81 (t, J = 7.6 Hz, 1H, ArH), 8.03 (d, J = 7.8 Hz, 2H, ArH), 8.18 (d, J = 6.0 Hz, 1H, ArH), 10.50 (s, 1H, CHO). ^{13}C NMR (100 MHz, $CDCl_3$): δ 122.6 (t, J = 286.6 Hz), 127.1 (t, J = 21.5 Hz), 129.0, 129.5 (t, J = 8.8 Hz), 129.6, 131.0, 132.0, 132.8, 133.1, 135.9, 136.3, 190.4 (t, J = 5.8 Hz). ^{19}F NMR (376 MHz, $CDCl_3$): δ –92.8 (s, 2F). MS (ESI, m/z): 296.8 $(M+H)^+$, 313.9 $(M+NH_4)^+$, 318.9 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{14}H_{11}O_3F_2S$ $(M+H)^+$: 297.0390, found: 297.0391.



2-(Difluoro(phenylsulfonyl)methyl)benzonitrile (3d)

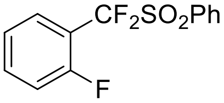
For 0.2 mmol scale, the standard procedure of method A was followed to provide **3d** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (41 mg, 70%). M.p.: 149-150 °C. IR (KBr): 3075, 2237, 1579, 1446, 1340, 1287, 1170, 1060, 939, 770, 711, 597, 543 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 7.67 (t, J = 8.0 Hz, 2H, ArH), 7.71-7.84 (m, 5H, ArH), 8.07 (d, J = 8.0 Hz, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 112.3 (t, J = 3.6 Hz), 116.1, 120.8 (t, J = 287.7 Hz), 128.9 (t, J = 21.8 Hz), 129.6, 130.1 (t, J = 6.5 Hz), 131.2, 131.8, 132.6, 132.7, 135.1, 136.0. ^{19}F

NMR (376 MHz, $CDCl_3$): δ –99.6 (s, 2F). MS (ESI, m/z): 293.9 $(M+H)^+$, 310.9 $(M+NH_4)^+$, 315.8 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{14}H_{13}O_2N_2F_2S$ $(M+NH_4)^+$: 311.0656, found: 311.0660.



1-(Difluoro(phenylsulfonyl)methyl)-2-(methylsulfonyl)benzene (3e)

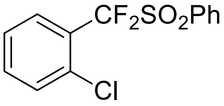
For 0.2 mmol scale, the standard procedure of method B was followed to provide **3e** by column chromatography on silica gel (petroleum ether/EtOAc, 10:1 to 5:1, v/v) as a white solid (44 mg, 64%). M.p.: 164-165 °C. IR (KBr): 3118, 2937, 1583, 1454, 1353, 1319, 1249, 1169, 1143, 1047, 949, 775, 732, 686, 597 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 3.29 (s, 3H, CH_3), 7.65 (t, J = 7.6 Hz, 2H, ArH), 7.80-7.83 (m, 3H, ArH), 8.01-8.06 (m, 3H, ArH), 8.42-8.46 (m, 1H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 45.0 (t, J = 4.3 Hz), 121.6 (t, J = 288.6 Hz), 125.3 (t, J = 22.6 Hz), 129.5, 131.1, 131.91 (t, J = 7.6 Hz), 131.92, 132.3, 133.1, 133.3, 135.8, 141.2. ^{19}F NMR (376 MHz, $CDCl_3$): δ –90.9 (s, 2F). MS (ESI, m/z): 346.9 $(M+H)^+$, 363.9 $(M+NH_4)^+$, 368.8 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{14}H_{13}O_4F_2S_2$ $(M+H)^+$: 347.0215, found: 347.0218.



1-(Difluoro(phenylsulfonyl)methyl)-2-fluorobenzene (3f)

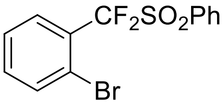
For 0.2 mmol scale, the standard procedure of method A was followed to provide **3f** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (43 mg, 75%). M.p.: 105-106 °C. IR (KBr): 3079, 1614, 1493, 1449, 1340, 1261, 1171, 1106, 1062, 939, 764, 687, 597, 545 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 7.16-7.20 (m, 1H, ArH), 7.26-7.30 (m, 1H, ArH), 7.55-7.64 (m, 4H, ArH), 7.77 (t, J = 7.6 Hz, 1H, ArH), 8.01 (d, J = 7.6 Hz, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 114.5 (td, $^2J_{F\text{-}C}$ = 22.2 Hz, $^2J_{F\text{-}C}$ = 10.9 Hz), 117.2 (d, $^2J_{F\text{-}C}$ = 21.2 Hz), 121.2 (td, $^1J_{F\text{-}C}$ = 286.6

Hz, ${}^3J_{F\text{-}C}$ = 3.7 Hz), 124.2 (d, ${}^3J_{F\text{-}C}$ = 3.6 Hz), 129.3, 130.2 (t, ${}^3J_{F\text{-}C}$ = 6.6 Hz), 131.0, 132.6, 134.7 (d, ${}^3J_{F\text{-}C}$ = 8.7 Hz), 135.5, 160.7 (dt, ${}^1J_{F\text{-}C}$ = 257.4 Hz, ${}^3J_{F\text{-}C}$ = 2.9 Hz,). ^{19}F NMR (376 MHz, $CDCl_3$): δ –99.7 (d, *J* = 22.9 Hz 2F), –110.8 (m, 1F). MS (ESI, m/z): 303.9 $(M+NH_4)^+$, 308.8 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{13}H_{13}O_2NF_3S$ $(M+NH_4)^+$: 304.0610, found: 304.0614.



1-Chloro-2-(difluoro(phenylsulfonyl)methyl)benzene (3g)

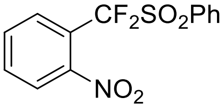
For 0.2 mmol scale, the standard procedure of method A was followed to provide **3g** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (42 mg, 70%). M.p.: 101-102 °C. IR (KBr): 3084, 1592, 1473, 1453, 1341, 1245, 1166, 1107, 1042, 938, 759, 728, 687, 596, 541 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.38-7.41 (m, 1H, ArH), 7.48-7.49 (m, 2H, ArH), 7.62 (t, *J* = 7.8 Hz, 2H, ArH), 7.67 (d, *J* = 8.0 Hz, 1H, ArH), 7.77 (t, *J* = 7.2 Hz, 1H, ArH), 8.00 (d, *J* = 8.0 Hz, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 121.6 (t, *J* = 288.0 Hz), 124.7 (t, *J* = 20.7 Hz), 126.7, 129.4, 131.0, 131.2 (t, *J* = 7.6 Hz), 132.2, 132.8, 133.4, 134.1 (t, *J* = 2.5 Hz), 135.5. ^{19}F NMR (376 MHz, $CDCl_3$): δ –97.2 (s, 2F). MS (ESI, m/z): 319.8 $(M+NH_4)^+$, 324.7 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{13}H_{13}O_2NClF_2S$ $(M+NH_4)^+$: 320.0315, found: 320.0318.



1-Bromo-2-(difluoro(phenylsulfonyl)methyl)benzene (3h)

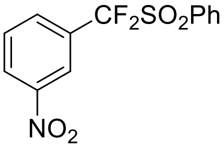
For 0.2 mmol scale, the standard procedure of method A was followed to provide **3h** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (49 mg, 71%). M.p.: 119-121 °C. IR (KBr): 3067, 1590, 1450, 1340, 1245, 1164, 1108, 1029, 933, 755, 723, 686, 592 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ

7.37-7.45 (m, 2H, ArH), 7.61 (t, *J* = 7.6 Hz, 2H, ArH), 7.66-7.72 (m, 2H, ArH), 7.77 (t, *J* = 7.4 Hz, 1H, ArH), 8.00 (d, *J* = 8.0 Hz, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 121.4 (t, *J* = 288.4 Hz), 121.6 (t, *J* = 2.5 Hz), 126.4 (t, *J* = 20.8 Hz), 127.3, 129.4, 131.0, 131.5 (t, *J* = 7.6 Hz), 132.8, 133.4, 135.5, 135.8. ^{19}F NMR (376 MHz, $CDCl_3$): δ –96.7 (s, 2F). MS (ESI, m/z): 363.7 $(M+NH_4)^+$, 368.8 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{13}H_{13}O_2NBrF_2S$ $(M+NH_4)^+$: 363.9809, found: 363.9813.



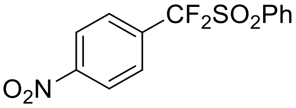
1-(Difluoro(phenylsulfonyl)methyl)-2-nitrobenzene (3i)

For 0.2 mmol scale, the standard procedure of method B was followed to provide **3i** by column chromatography on silica gel (petroleum ether/EtOAc, 15:1 to 10:1, v/v) as a white solid (44 mg, 70%). M.p.: 128-129 °C. IR (KBr): 3101, 1543, 1452, 1368, 1253, 1175, 1108, 1058, 939, 853, 765, 686, 599, 540 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61-7.65 (m, 3H, ArH), 7.70-7.75 (m, 2H, ArH), 7.79 (t, *J* = 7.6 Hz, 1H, ArH), 7.91 (d, *J* = 7.2 Hz, 1H, ArH), 8.00 (d, *J* = 8.0 Hz, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.4 (t, *J* = 22.9 Hz), 120.4 (t, *J* = 288.0 Hz), 124.3, 129.5, 130.8 (t, *J* = 6.5 Hz), 131.1, 131.4, 132.2, 133.8, 135.9, 149.7. ^{19}F NMR (376 MHz, $CDCl_3$): δ –96.0 (s, 2F). MS (ESI, m/z): 335.8 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{13}H_{10}O_4NF_2S$ $(M+H)^+$: 314.0290, found: 314.0293.



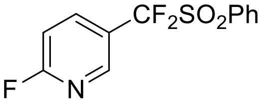
1-(Difluoro(phenylsulfonyl)methyl)-3-nitrobenzene (3j)

For 0.2 mmol scale, the standard procedure of method A was followed to provide **3j** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (43 mg, 69%). M.p.: 138-140 °C. IR (KBr): 3101, 1628, 1541, 1448, 1358, 1267, 1167, 1066, 978, 712, 595, 544 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (t, *J* = 7.8 Hz, 2H, ArH), 7.74 (t, *J* = 8.0 Hz, 1H, ArH), 7.81 (t, *J* = 7.6 Hz, 1H, ArH), 8.02-8.04 (m, 3H, ArH), 8.46 (d, *J* = 8.4 Hz, 1H, ArH), 8.52 (s, 1H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 120.6 (t, *J* = 285.8 Hz), 123.2 (t, *J* = 6.6 Hz), 127.2, 128.8 (t, *J* = 23.0 Hz), 129.6, 130.1, 131.0, 131.9, 133.7 (t, *J* = 5.4 Hz), 135.9, 148.2. ^{19}F NMR (376 MHz, $CDCl_3$): δ −102.4 (s, 2F). MS (ESI, m/z): 335.9 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{13}H_{13}O_4N_2F_2S$ $(M+NH_4)^+$: 331.0555, found: 331.0559.



1-(Difluoro(phenylsulfonyl)methyl)-4-nitrobenzene (3k)

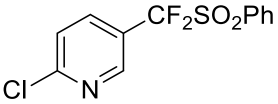
For 0.2 mmol scale, the standard procedure of method A was followed to provide **3k** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (38 mg, 61%). M.p.: 153-155 °C. IR (KBr): 3122, 1613, 1537, 1448, 1344, 1272, 1166, 1094, 1065, 858, 731, 685, 594 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 (t, *J* = 7.6 Hz, 2H, ArH), 7.83 (t, *J* = 7.4 Hz, 1H, ArH), 7.90 (d, *J* = 8.8 Hz, 2H, ArH), 8.03 (d, *J* = 8.0 Hz, 2H, ArH), 8.37 (d, *J* = 8.8 Hz, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 120.8 (t, *J* = 285.9 Hz), 123.7, 129.4 (t, *J* = 5.8 Hz), 129.6, 131.0, 132.0, 132.8 (t, *J* = 22.3 Hz), 135.9, 150.4. ^{19}F NMR (376 MHz, $CDCl_3$): δ −102.7 (s, 2F). MS (ESI, m/z): 335.8 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{13}H_{13}O_4N_2F_2S$ $(M+NH_4)^+$: 331.0554, found: 331.0559.



5-(Difluoro(phenylsulfonyl)methyl)-2-fluoropyridine (3l)

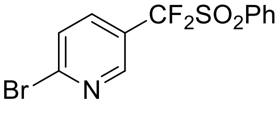
For 0.4 mmol scale, the standard procedure of method A was followed to provide **3l** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (82 mg, 71%). M.p.: 133-134 °C. IR (KBr): 3062, 1601, 1487, 1447, 1397, 1338, 1264, 1169, 1071, 952, 846, 753, 716, 685, 606 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ

7.11 (dd, J = 8.6 Hz, J = 2.6 Hz, 1H, ArH), 7.67 (t, J = 8.0 Hz, 2H, ArH), 7.82 (t, J = 7.6 Hz, 1H, ArH), 8.03 (d, J = 8.0 Hz, 2H, ArH), 8.11-8.15 (m, 1H, ArH), 8.53 (s, 1H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 110.0 (d, $^2J_{F\text{-}C}$ = 37.2 Hz), 120.7 (t, $^1J_{F\text{-}C}$ = 285.1 Hz), 121.2 (td, $^2J_{F\text{-}C}$ = 23.3 Hz, $^4J_{F\text{-}C}$ = 4.4 Hz), 129.6, 131.0, 131.8, 135.9, 141.1 (dt, $^3J_{F\text{-}C}$ = 9.5 Hz, $^3J_{F\text{-}C}$ = 4.7 Hz,), 148.1 (dt, $^3J_{F\text{-}C}$ = 16.8 Hz, $^3J_{F\text{-}C}$ = 6.6 Hz,), 165.8 (d, $^1J_{F\text{-}C}$ = 244.3 Hz). ^{19}F NMR (376 MHz, $CDCl_3$): δ –61.5 (d, J = 4.1 Hz, 1F), –102.5 (s, 2F). MS (ESI, m/z): 287.8 $(M+H)^+$. HRMS (ESI): calcd. For $C_{12}H_9O_2NF_3S$ $(M+H)^+$: 288.0296, found: 288.0301.



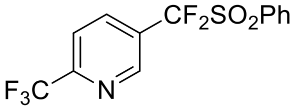
2-Chloro-5-(difluoro(phenylsulfonyl)methyl)pyridine (3m)

For 0.2 mmol scale, the standard procedure of method A was followed to provide **3m** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (49 mg, 81%). M.p.: 137-139 ^{o}C. IR (KBr): 3049, 1589, 1461, 1339, 1277, 1168, 1116, 1070, 842, 741, 685, 598 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.48 (d, J = 8.4 Hz, 1H, ArH), 7.64 (t, J = 7.8 Hz, 2H, ArH), 7.79 (t, J = 7.4 Hz, 1H, ArH), 7.94 (dd, J = 8.4 Hz, J = 2.0 Hz, 1H, ArH), 8.00 (d, J = 8.0 Hz, 2H, ArH), 8.63 (s, 1H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 120.7 (t, J = 285.2 Hz), 122.2 (t, J = 23.0 Hz), 124.4, 129.6, 131.0, 131.7, 135.9, 138.1 (t, J = 5.1 Hz), 148.9 (t, J = 6.5 Hz), 155.8. ^{19}F NMR (376 MHz, $CDCl_3$): δ –103.1 (s, 2F). MS (ESI, m/z): 303.8 $(M+H)^+$. HRMS (ESI): calcd. For $C_{12}H_9O_2NClF_2S$ $(M+H)^+$: 304.0002, found: 304.0005.



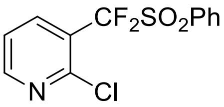
2-Bromo-5-(difluoro(phenylsulfonyl)methyl)pyridine (3n)

For 0.2 mmol scale, the standard procedure of method A was followed to provide **3n** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (54 mg, 78%). M.p.: 138-139 °C. IR (KBr): 3045, 1582, 1456, 1339, 1276, 1169, 1097, 1068, 954, 844, 736, 685, 601, 541 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63-7.67 (m, 3H, ArH), 7.79-7.85 (m, 2H, ArH), 8.01 (d, *J* = 8.0 Hz, 2H, ArH), 8.61 (s, 1H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 120.7 (t, *J* = 285.8 Hz), 122.6 (t, *J* = 22.9 Hz), 128.2, 129.6, 131.0, 131.8, 135.9, 137.6 (t, *J* = 5.1 Hz), 146.8 (t, *J* = 1.8 Hz), 149.1 (t, *J* = 6.2 Hz). ^{19}F NMR (376 MHz, $CDCl_3$): δ –103.2 (s, 2F). MS (ESI, m/z): 347.7 $(M+H)^+$. HRMS (ESI): calcd. For $C_{12}H_9O_2NBrF_2S$ $(M+H)^+$: 347.9495, found: 347.9500.



5-(Difluoro(phenylsulfonyl)methyl)-2-(trifluoromethyl)pyridine (3o)

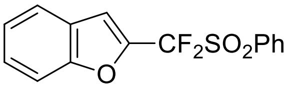
For 0.2 mmol scale, the standard procedure of method A was followed to provide **3o** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (55 mg, 82%). M.p.: 112-113 °C. IR (KBr): 3058, 1582, 1448, 1340, 1280, 1171, 1101, 1024, 956, 861, 723, 686, 609, 583, 539 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 (t, *J* = 7.8 Hz, 2H, ArH), 7.81-7.87 (m, 2H, ArH), 8.04 (d, *J* = 8.0 Hz, 2H, ArH), 8.23 (d, *J* = 8.4 Hz, 1H, ArH), 8.99 (s, 1H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 121.0 (q, *J* = 273.2 Hz), 120.2 (q, *J* = 2.1 Hz), 120.3 (t, *J* = 285.8 Hz), 126.2 (t, *J* = 23.2 Hz), 129.6, 131.1, 131.6, 136.0, 137.5 (t, *J* = 5.5 Hz), 148.9 (t, *J* = 6.2 Hz), 151.5 (q, *J* = 35.2). ^{19}F NMR (376 MHz, $CDCl_3$): δ −68.3 (s, 3F), −103.4 (s, 2F). MS (ESI, m/z): 337.8 $(M+H)^+$. HRMS (ESI): calcd. For $C_{13}H_9O_2NF_5S$ $(M+H)^+$: 338.0264, found: 338.0269.



2-Chloro-3-(difluoro(phenylsulfonyl)methyl)pyridine (3p)

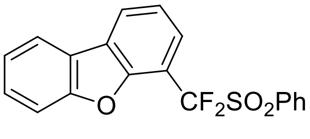
For 0.2 mmol scale, the standard procedure of method A was followed to provide

3p by column chromatography on silica gel (petroleum ether/EtOAc, 20:1 to 10:1, v/v) as a white solid (44 mg, 73%). M.p.: 142-143 °C. IR (KBr): 3080, 1582, 1449, 1410, 1341, 1284, 1176, 1116, 1046, 937, 808, 743, 687, 597, 547 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 7.40 (dd, *J* = 8.0 Hz, *J* = 4.8 Hz, 1H, ArH), 7.63 (t, *J* = 7.8 Hz, 2H, ArH), 7.78 (t, *J* = 7.4 Hz, 1H, ArH), 7.99 (d, *J* = 7.6 Hz, 2H, ArH), 8.02 (dd, *J* = 7.6 Hz, *J* = 2.0 Hz, 1H, ArH), 8.57 (d, *J* = 4.8 Hz, 1H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 120.5 (t, *J* = 287.6 Hz), 122.0, 122.4 (t, *J* = 22.2 Hz), 129.6, 131.0, 132.2, 135.9, 140.3 (t, *J* = 7.0 Hz), 150.1, 152.7. ^{19}F NMR (376 MHz, $CDCl_3$): δ –98.9 (s, 2F). MS (ESI, m/z): 303.8 $(M+H)^+$. HRMS (ESI): calcd. For $C_{12}H_9O_2NClF_2S$ $(M+H)^+$: 304.0002, found: 304.0005.



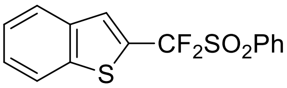
2-(Difluoro(phenylsulfonyl)methyl)benzofuran (3q)

For 0.2 mmol scale, the standard procedure of method B was followed to provide **3q** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (39 mg, 63%). M.p.: 106-108 °C. IR (KBr): 3075, 1582, 1449, 1351, 1298, 1166, 1064, 979, 881, 753, 682, 626, 575 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 7.30-7.34 (m, 2H, ArH), 7.43 (t, *J* = 7.8 Hz, 1H, ArH), 7.56 (d, *J* = 8.0 Hz, 1H, ArH), 7.61 (t, *J* = 7.8 Hz, 2H, ArH), 7.67 (d, *J* = 8.0 Hz, 1H, ArH), 7.77 (t, *J* = 7.4 Hz, 1H, ArH), 8.02 (d, *J* = 7.2 Hz, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 112.2, 112.5 (t, *J* = 3.3 Hz), 117.4 (t, *J* = 283.3 Hz), 122.5, 124.1, 126.5, 127.2, 129.5, 131.0, 132.6, 135.7, 141.6 (t, *J* = 30.3 Hz), 156.1. ^{19}F NMR (376 MHz, $CDCl_3$): δ –102.9 (s, 2F). MS (ESI, m/z): 325.9 $(M+NH_4)^+$. HRMS (ESI): calcd. For $C_{15}H_{14}O_3NF_2S$ $(M+NH_4)^+$: 326.0655, found: 326.0657.



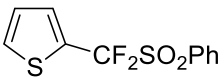
4-(Difluoro(phenylsulfonyl)methyl)dibenzo[*b,d*]furan (3r)

For 0.2 mmol scale, the standard procedure of method B was followed to provide **3r** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (43 mg, 60%). M.p.: 186-188 ^{o}C. IR (KBr): 3071, 1581, 1478, 1423, 1338, 1282, 1193, 1169, 1045, 966, 848, 758, 684, 599, 538 cm^{-1}. ^{1}H NMR (400 MHz, CDCl$_3$): δ 7.37 (t, *J* = 7.4 Hz, 1H, ArH), 7.44-7.57 (m, 5H, ArH), 7.69 (t, *J* = 7.8 Hz, 2H, ArH), 7.95 (d, *J* = 7.6 Hz, 1H, ArH), 8.00 (d, *J* = 8.0 Hz, 2H, ArH), 8.15 (d, *J* = 7.6 Hz, 1H, ArH). ^{13}C NMR (100 MHz, CDCl$_3$): δ 111.6 (t, *J* = 23.4 Hz), 112.1, 120.7, 121.7 (t, *J* = 286.5 Hz), 122.6, 122.7, 123.3, 125.0, 126.0, 127.0 (t, *J* = 7.4 Hz), 128.1, 129.1, 131.1, 132.9, 135.3, 153.5 (t, *J* = 2.2 Hz), 156.4. ^{19}F NMR (376 MHz, CDCl$_3$): δ −100.0 (s, 2F). MS (ESI, m/z): 375.9 (M+NH$_4$)$^+$, 380.9 (M+Na)$^+$. HRMS (ESI): calcd. For $C_{19}H_{16}O_3NF_2S$ (M+NH$_4$)$^+$: 376.0808, found: 376.0813.



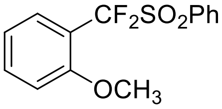
2-(Difluoro(phenylsulfonyl)methyl)benzo[*b*]thiophene (3s)

For 0.2 mmol scale, the standard procedure of method B was followed to provide **3s** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a pink solid (49 mg, 76%). M.p.: 141-143 ^{o}C. IR (KBr): 3066, 1581, 1523, 1448, 1346, 1238, 1167, 1036, 830, 751, 682, 600, 531 cm^{-1}. ^{1}H NMR (400 MHz, CDCl$_3$): δ 7.40-7.47 (m, 2H, ArH), 7.61 (t, *J* = 7.8 Hz, 2H, ArH), 7.76 (t, *J* = 7.6 Hz, 1H, ArH), 7.80 (s, 1H, ArH), 7.87 (d, *J* = 9.2 Hz, 2H, ArH), 8.03 (d, *J* = 8.0 Hz, 2H, ArH). ^{13}C NMR (100 MHz, CDCl$_3$): δ 120.7 (t, *J* = 284.0 Hz), 122.5, 125.2, 125.3, 126.7, 127.4 (t, *J* = 26.2 Hz), 129.3 (t, *J* = 5.8 Hz), 129.4, 131.0, 132.5, 135.5, 138.3, 141.6. ^{19}F NMR (376 MHz, CDCl$_3$): δ −93.6 (s, 2F). MS (ESI, m/z): 346.7 (M+Na)$^+$. HRMS (ESI): calcd. For $C_{15}H_{14}O_2NF_2S_2$ (M+NH$_4$)$^+$: 342.0425, found: 342.0429.



2-(Difluoro(phenylsulfonyl)methyl)thiophene (3t)

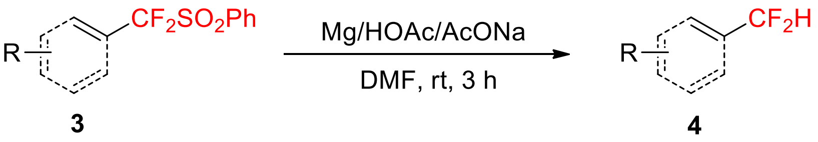
For 0.2 mmol scale, the standard procedure of method B was followed to provide **3t** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (30 mg, 55%). M.p.: 99-100 °C. IR (KBr): 3131, 1525, 1424, 1339, 1259, 1171, 1093, 1033, 863, 719, 686, 602, 539 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.15-7.17 (m, 1H, ArH), 7.54-7.55 (m, 1H, ArH), 7.60-7.64 (m, 3H, ArH), 7.77 (t, *J* = 7.4 Hz, 1H, ArH), 8.01 (d, *J* = 7.6 Hz, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 120.8 (t, *J* = 283.6 Hz), 127.3 (t, *J* = 27.0 Hz), 127.7, 129.3, 130.9, 131.5, 132.0 (t, *J* = 5.5 Hz), 132.6, 135.4. ^{19}F NMR (376 MHz, $CDCl_3$): δ –92.8 (s, 2F). MS (ESI, m/z): 291.8 $(M+NH_4)^+$, 296.7 $(M+Na)^+$. HRMS (ESI): calcd. For $C_{11}H_{12}O_2NF_2S_2$ $(M+NH_4)^+$: 292.0269, found: 292.0272.



1-(Difluoro(phenylsulfonyl)methyl)-2-methoxybenzene (3u)

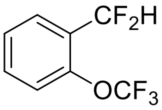
For 0.2 mmol scale, the standard procedure of method A was followed to provide **3u** by column chromatography on silica gel (petroleum ether/EtOAc, 20:1, v/v) as a white solid (27 mg, 45%). M.p.: 83-84 °C. IR (KBr): 3045, 2847, 1604, 1585, 1495, 1450, 1333, 1300, 1247, 1162, 1045, 924, 753, 688, 596, 530 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.69 (s, 3H, OCH_3), 6.94 (d, *J* = 8.4 Hz, 1H, ArH), 7.02 (t, *J* = 7.4 Hz, 1H, ArH), 7.50 (t, *J* = 8.2 Hz, 2H, ArH), 7.56 (t, *J* = 7.4 Hz, 2H, ArH), 7.71 (t, *J* = 7.6 Hz, 1H, ArH), 7.93 (d, *J* = 7.6 Hz, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.9, 112.4, 115.1(t, *J* = 20.8 Hz), 120.3, 122.5 (t, *J* = 287.3 Hz), 129.0, 130.2 (t, *J* = 7.6 Hz), 130.8, 133.8, 134.1, 135.0, 158.8 (t, *J* = 2.1 Hz). ^{19}F NMR (376 MHz, $CDCl_3$): δ –97.5 (s, 2F). MS (ESI, m/z): 316.0 $(M+NH_4)^+$. Anal. calcd. For $C_{14}H_{12}F_2O_3S$ (%): C, 56.37; H, 4.05. Found: C, 56.39; H, 3.95.

6. Synthesis of Difluoromethylated Aromatics by Reductive Desulfonylation



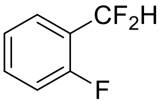
Standard procedure:

The reductive desulfonylation procedure was according to our previous report.[3] HOAc/NaOAc (1:1) solution (1.5 mL) was added into a suspension of **3** (0.2 mmol, 1.0 equiv), Magnesium turning (72 mg, 3.0 mmol) in DMF (2 mL) at rt under an argon atmosphere. The reaction was monitored by TLC until the starting material **3** was consumed completely.



1-(Difluoromethyl)-2-(trifluoromethoxy)benzene (4a)

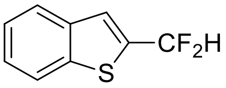
According to standard procedure, after stirring at rt for 3 h, $PhCF_3$ (26.5 μL,) as an internal standard was added into the reaction mixture, and monitored by ^{19}F NMR spectroscopy in 76% yield. Characterization of **4a**: ^{19}F NMR (376 MHz, unlocked): δ −56.9 (s, 3F), −113.2 (d, J = 54.5 Hz, 2F). GC—MS (EI): m/z = 212.2.



1-(Difluoromethyl)-2-fluorobenzene (4b) [4]

According to standard procedure, after stirring at rt for 3 h, $PhCF_3$ (26 μL) as an internal standard was added into the reaction mixture, and monitored by ^{19}F NMR spectroscopy in 86% yield. Characterization of **4b**: ^{19}F NMR (376 MHz, unlocked): δ −113.1 (dd, $^{2}J_{H\text{-}F}$ = 54.3 Hz, $^{4}J_{H\text{-}F}$ = 3.9 Hz, 2F), −119.4 (m, 1F). GC—MS (EI): m/z =

146.1.



2-(Difluoromethyl)benzo[*b*]thiophene (4c)

HOAc/NaOAc (1:1) solution (1.5 mL) was added into a suspension of **3s** (0.2 mmol, 1.0 equiv), Magnesium turning (72 mg, 3.0 mmol) in DMF (2 mL) at rt under an argon atmosphere. After stirring at rt for 3 h, dichloromethane (5 mL), and H_2O (10 mL) was added, and then the organic layer was separated and the aqueous layer was extracted with dichloromethane (3×5 mL). The combined organic layer was washed with brine (2×10 mL), dried over $MgSO_4$, filtered and concentrated in vacuo to obtain the crude product. The crude product was purified by a flash cloum chromatography on silica gel using pentane as eluent to afford **4c** as light yellow oil (25 mg, 68%). IR (KBr): 2924, 2852, 1461, 1369, 1260, 1150, 1061, 1036, 801, 745, 689 cm^{-1}. ^1H NMR (400 MHz, $CDCl_3$): δ 6.93 (t, J = 55.8 Hz, 1H, CF_2H), 7.41-7.43 (m, 2H, ArH), 7.53 (s, 1H, ArH), 7.82-7.89 (m, 2H, ArH). ^{13}C NMR (100 MHz, $CDCl_3$): δ 111.9 (t, J = 236.2 Hz), 122.7, 124.5 (t, J = 7.3 Hz), 124.7, 124.9, 125.9, 136.4 (t, J = 25.5 Hz), 138.3, 140.2. ^{19}F NMR (376 MHz, $CDCl_3$): δ –104.0 (dd, $^2J_{H\text{-}F}$ = 52.3 Hz, $^4J_{H\text{-}F}$ = 2.6 Hz, 2F). MS (EI, m/z): 184 (M^+, 100). HRMS (EI): calcd. For $C_9H_6F_2S$ (M^+): 184.0158, found: 184.0156.

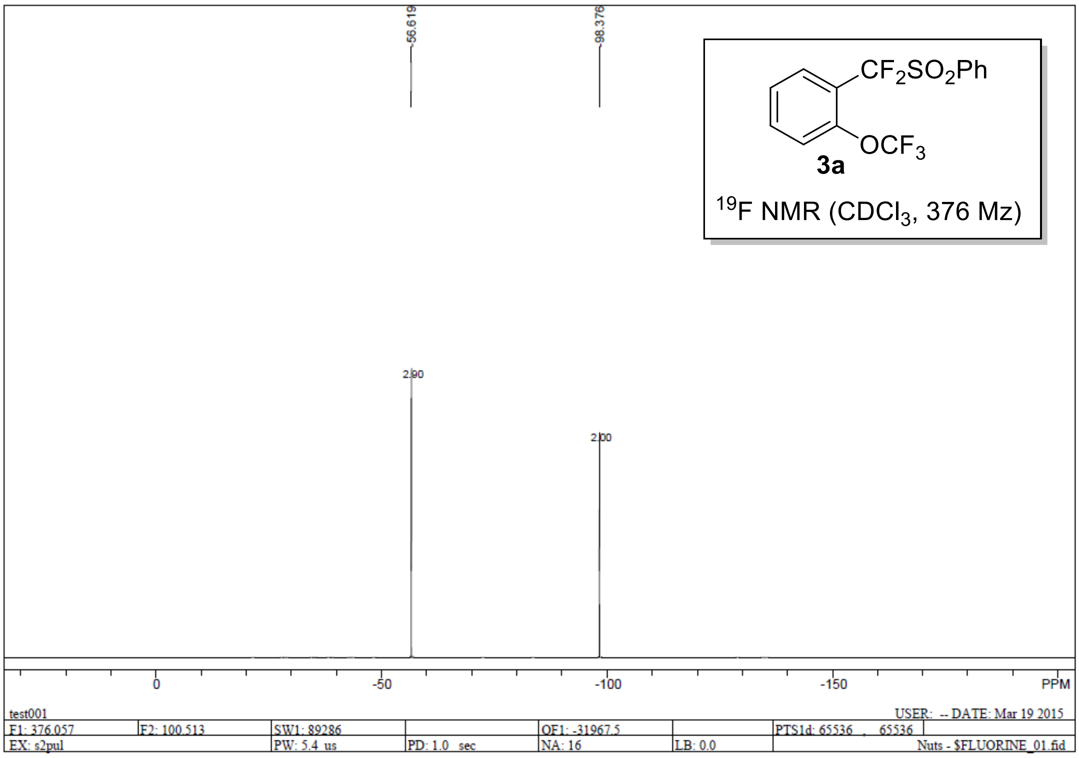
(**Not**e: The product **4c** was isolated in a moderate yield because of its volatility.)

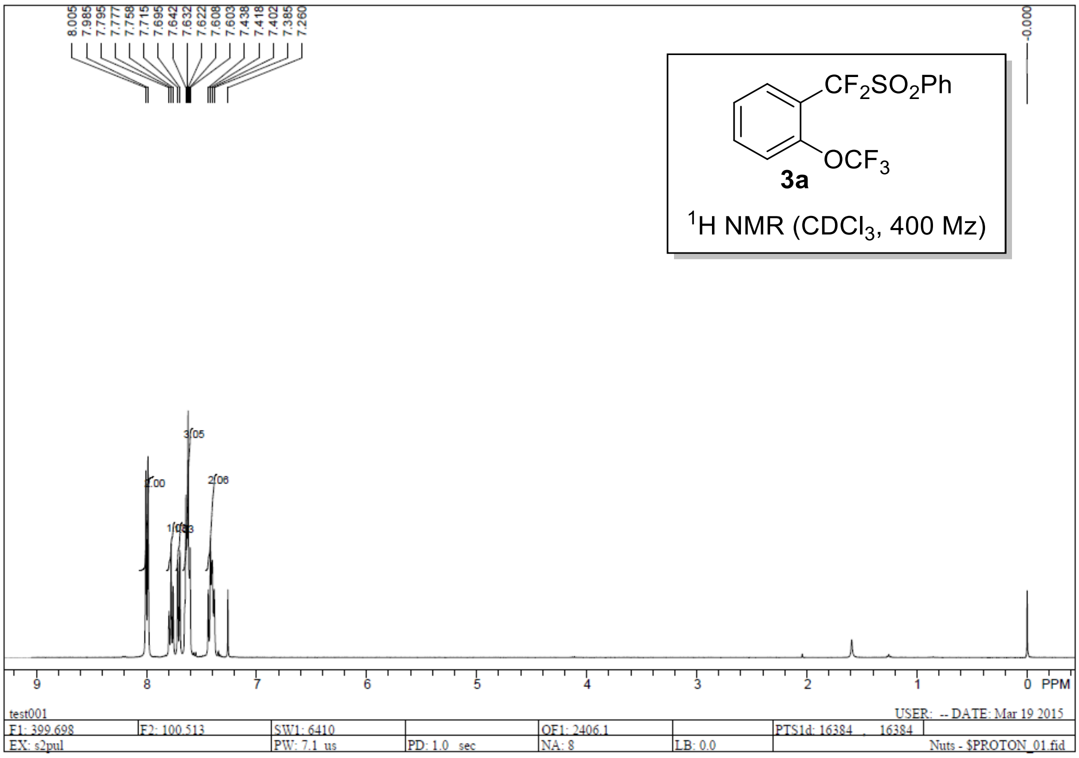
7. References

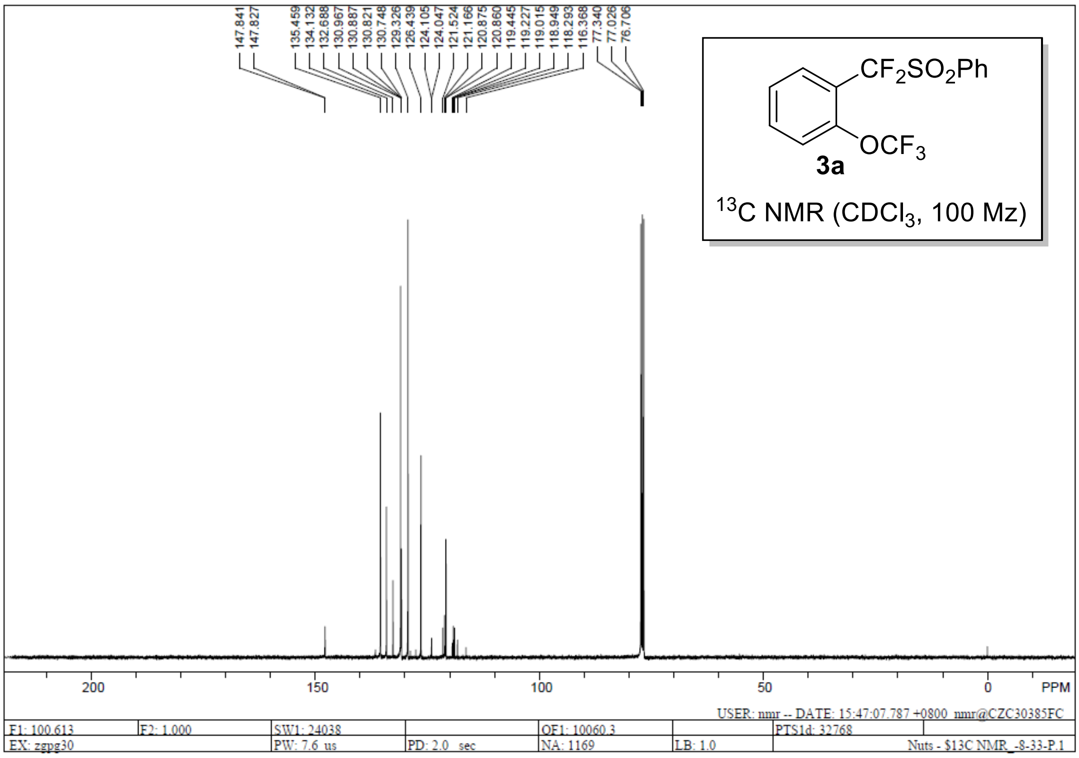
1. W. L. F. Armarego and C. L. L. Chai, *Purification of laboratory chemicals (fifth edition)*; Elsevier Science: USA, 2003.
2. (a) J. Hine and J. J. Porter, *J. Am. Chem. Soc.*, 1960, **82**, 6178; (b) G. K. S. Prakash, J. Hu, and G. A. Olah, *J. Org. Chem.*, 2003, **68**, 4457.
3. C. Ni and J. Hu, *Tetrahedron Lett.*, 2005, **46**, 8273.

4. D. A. Burgess and I. D. Rae, *Aust. J. Chem.*, 1977, **30**, 1611.

8. ^{19}F, ^{1}H and ^{13}C NMR Spectra of isolated Products



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124.105
124.047
121.524
121.166
120.875
120.860
119.445
119.227
119.015
118.949
118.293
116.368
77.340
77.026
76.706
CF2SO2Ph
OCF3
3a
13C NMR (CDCl3, 100 Mz)
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150
100
50
0
PPM
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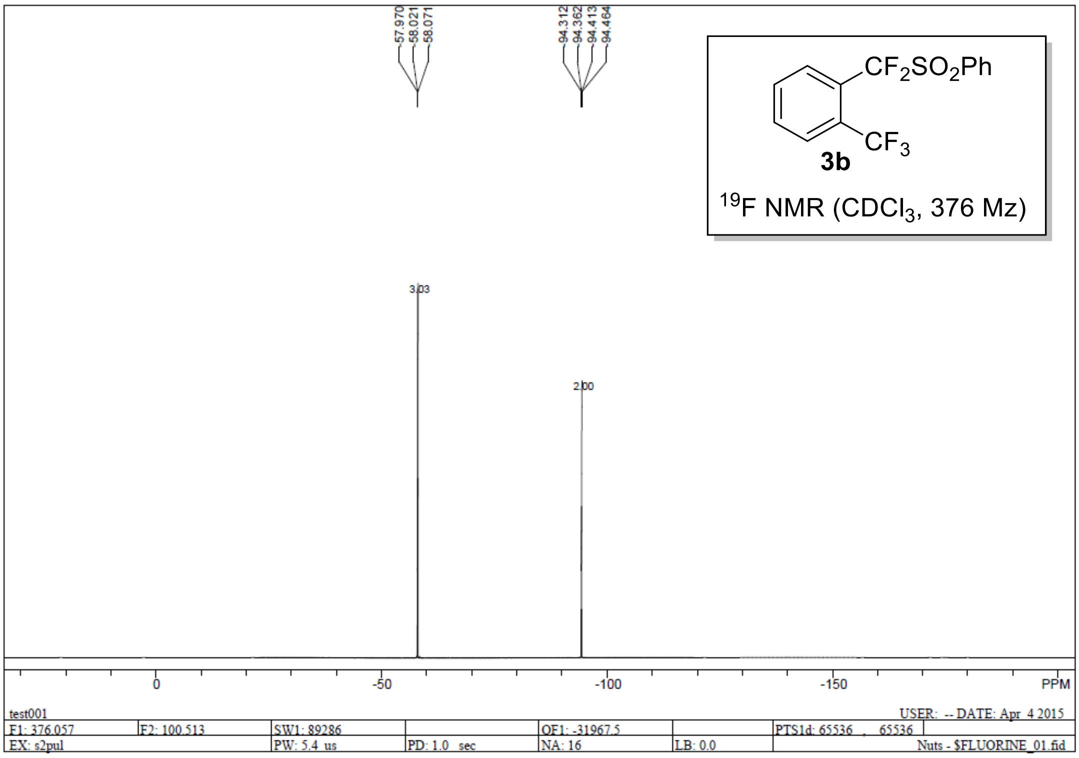
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-94.464
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3b
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2.00
0
-50
-100
-150
PPM
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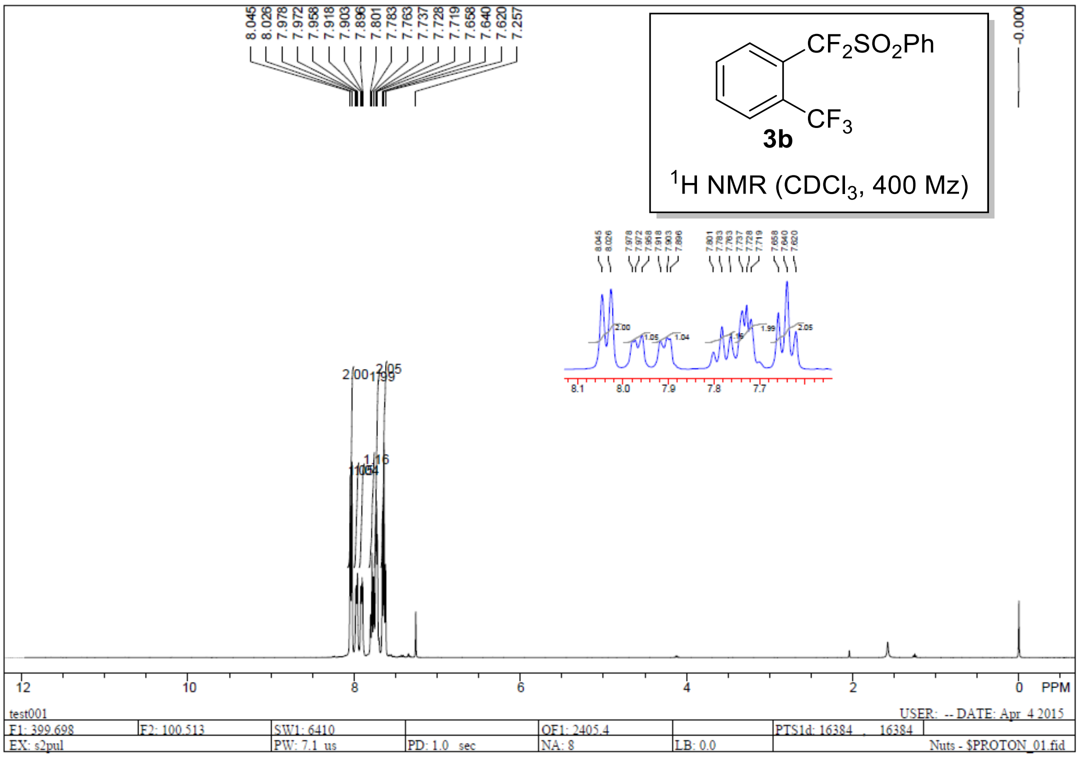
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7.958
7.918
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7.896
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7.728
7.719
7.658
7.640
7.620
7.257
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CF2SO2Ph
CF3
3b
1H NMR (CDCl3, 400 Mz)
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1.05
1.04
1.16
1.99
2.05
8.1
8.0
7.9
7.8
7.7
12
10
8
6
4
2
0
PPM
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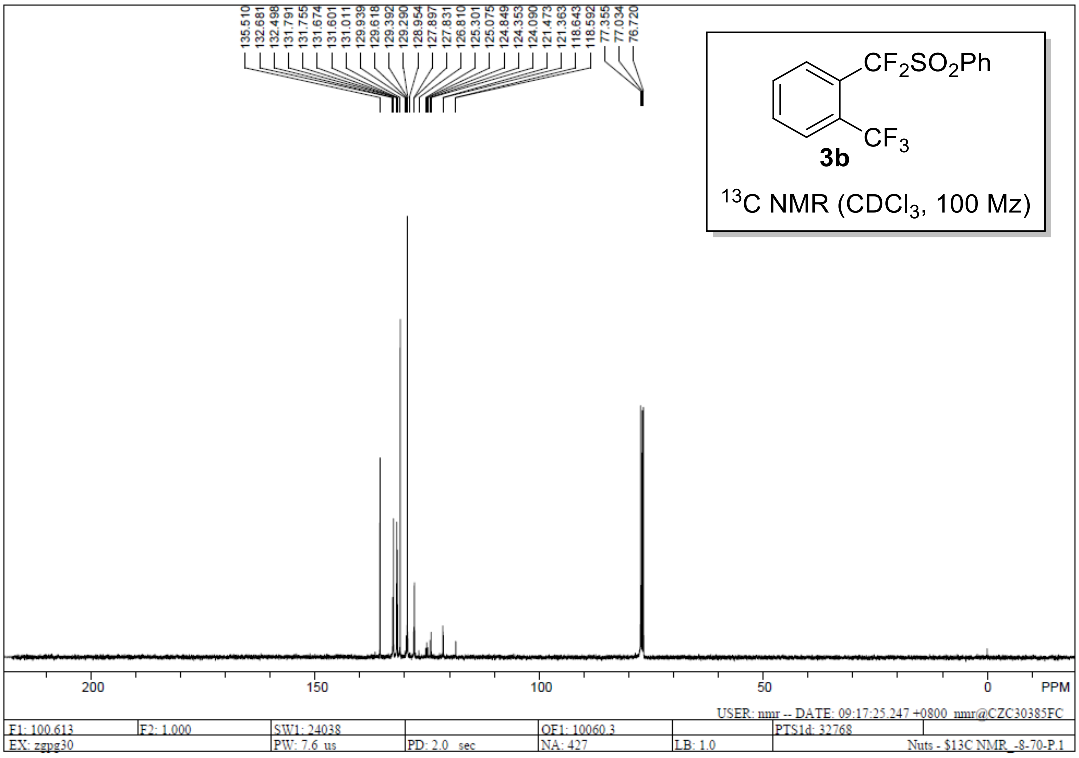
Nuts - $PROTON_01.fid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128.954
127.897
127.831
126.810
125.301
125.075
124.849
124.353
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121.473
121.363
118.643
118.592
77.355
77.034
76.720
CF2SO2Ph
CF3
3b
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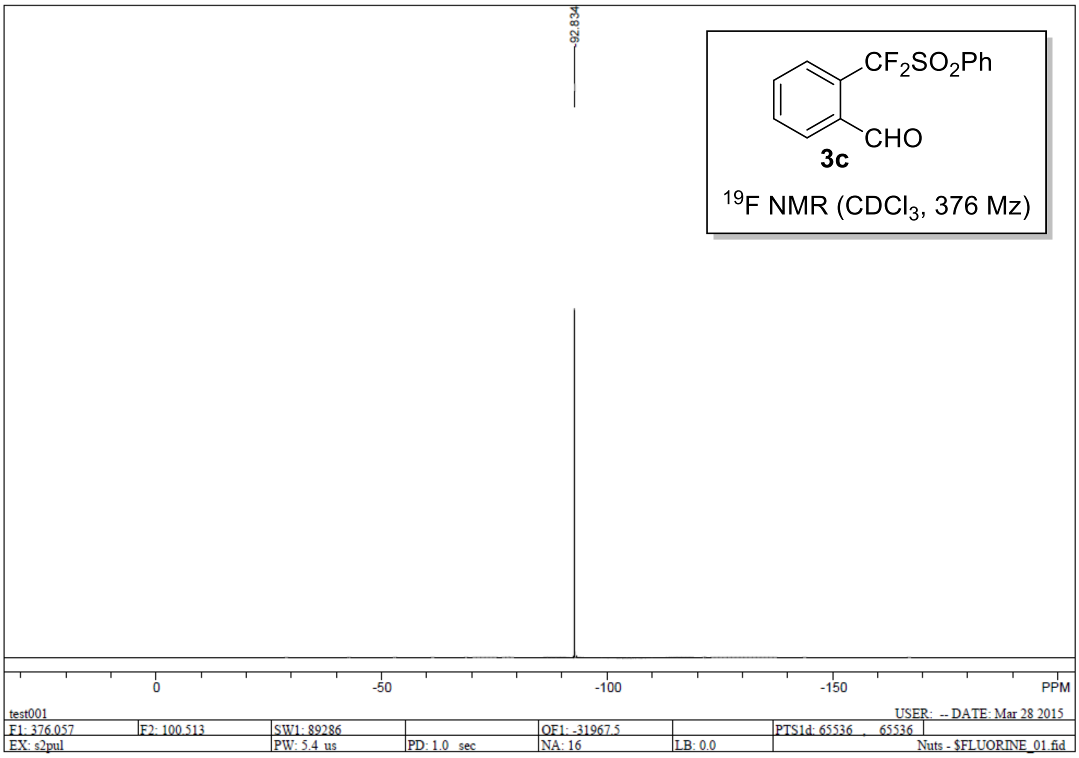

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PPM
test001
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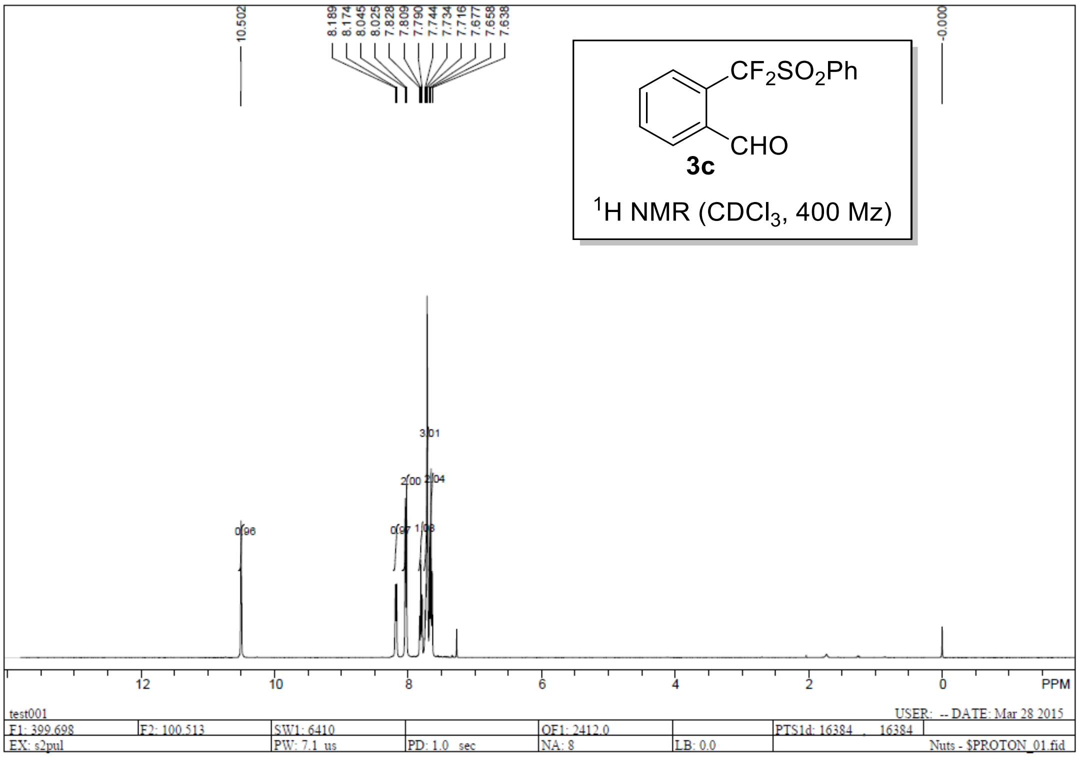
LB: 0.0
Nuts - $FLUORINE_01.fid



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7.658
7.638
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CHO
3c
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1.08
3.01
2.04
12
10
8
6
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2
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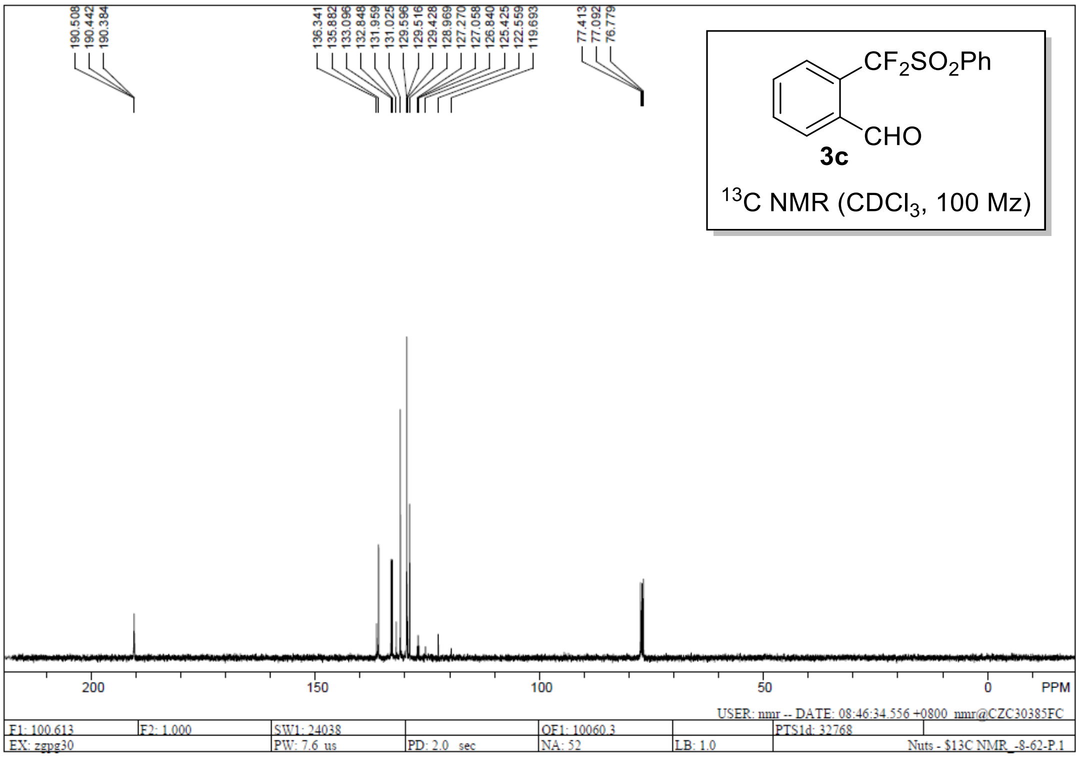
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119.693
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77.092
76.779
CF2SO2Ph
CHO
3c
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50
0
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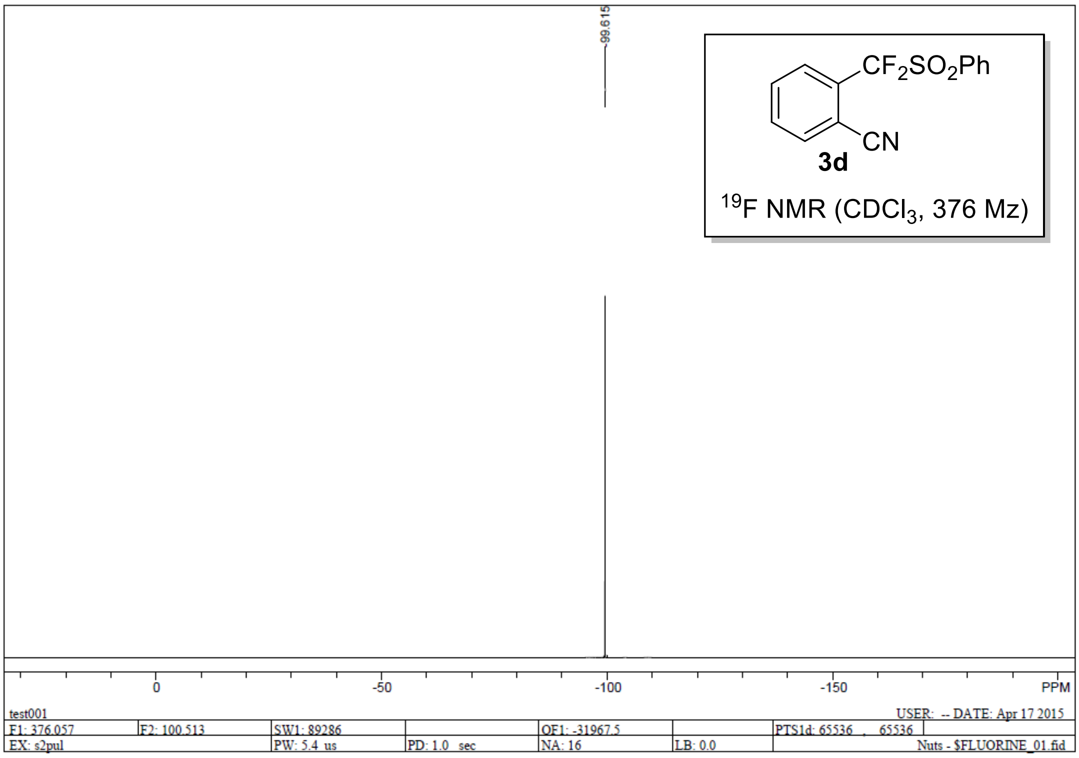
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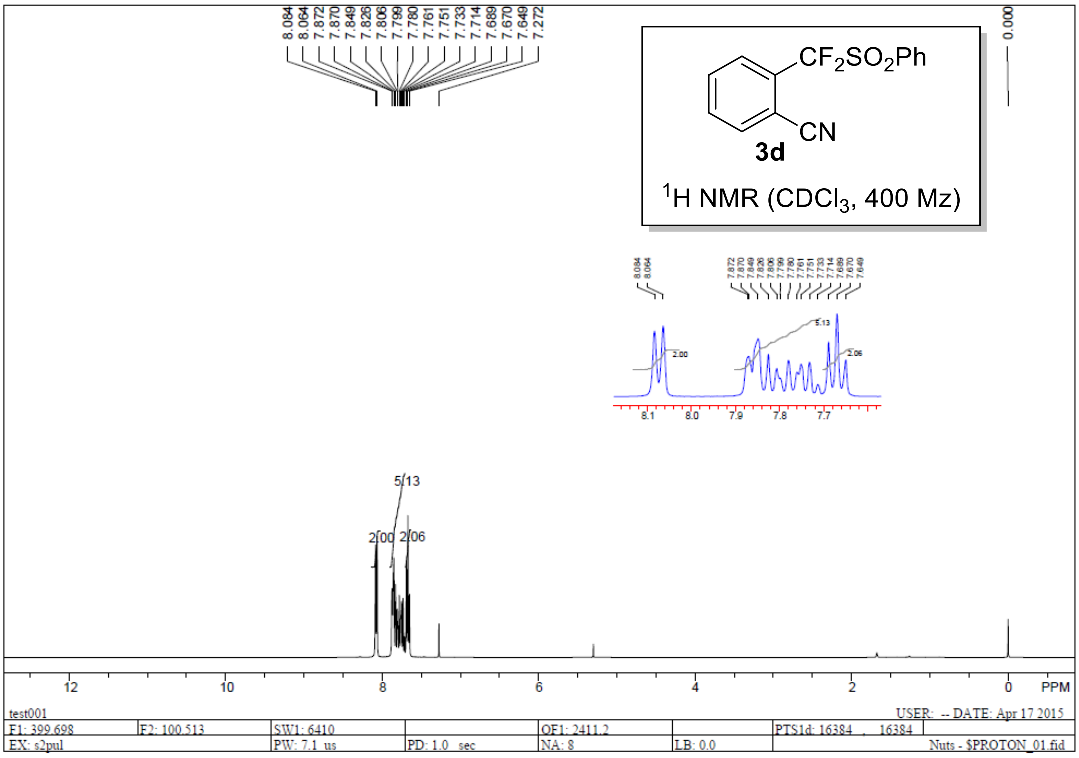
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7.272
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CF2SO2Ph
CN
3d
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7.9
7.8
7.7
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10
8
6
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2
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PPM
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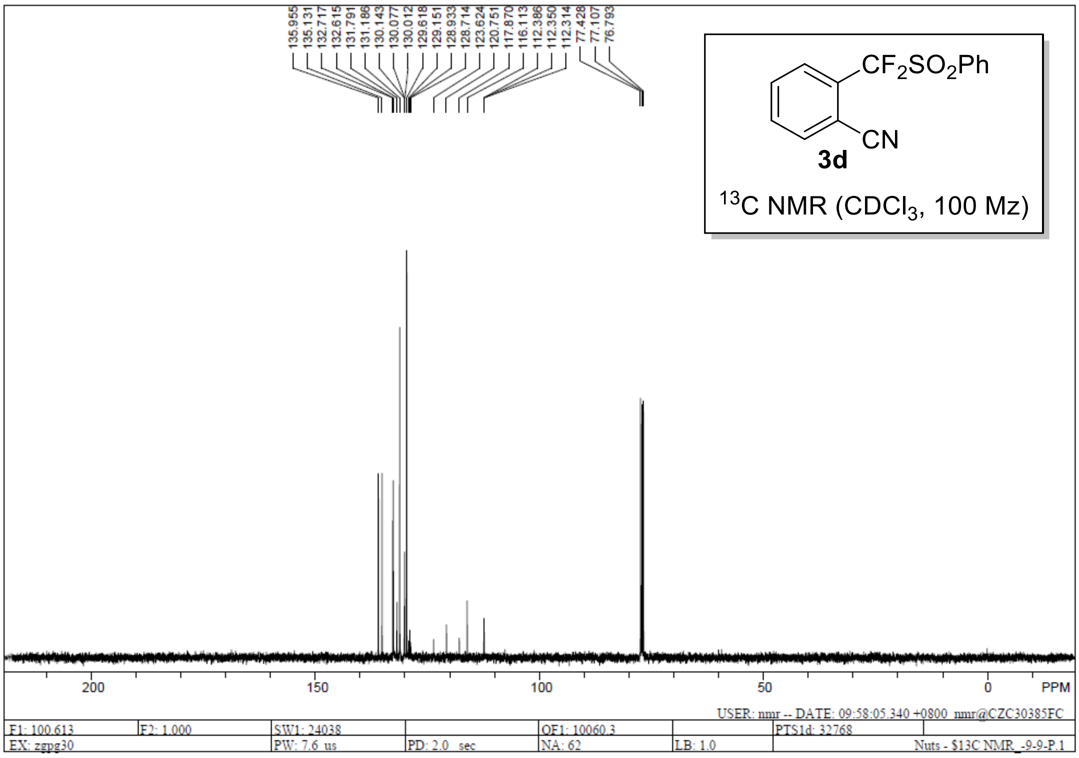
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112.314
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CF2SO2Ph
CN
3d
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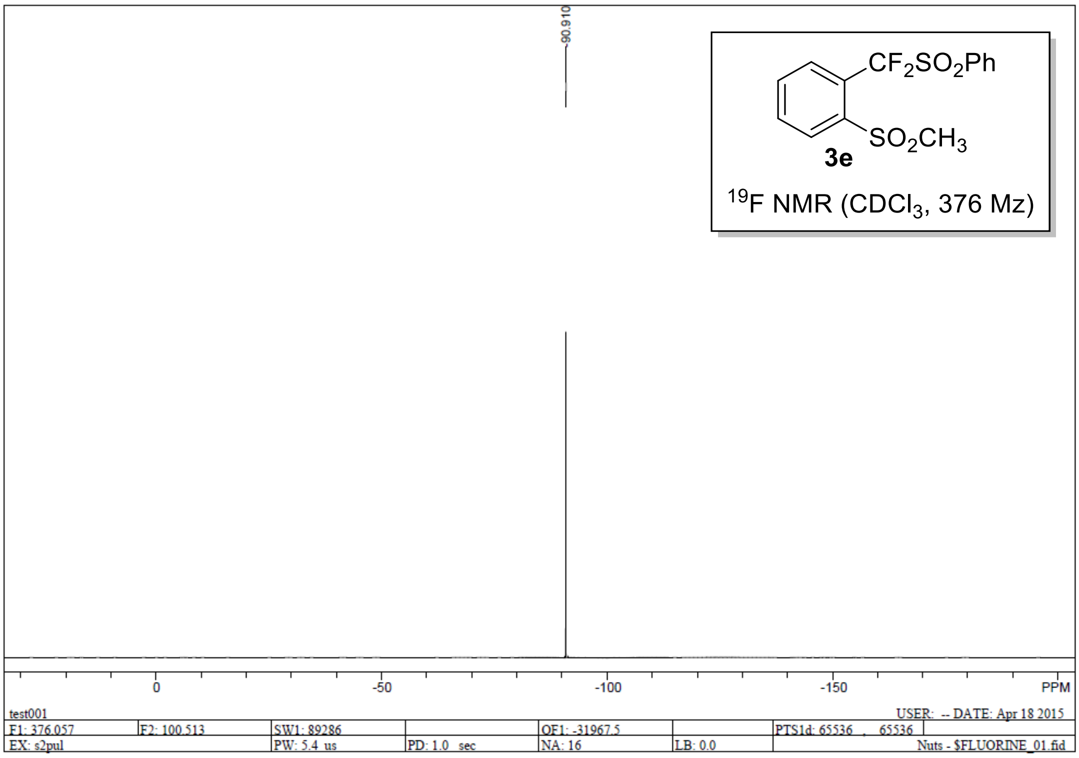
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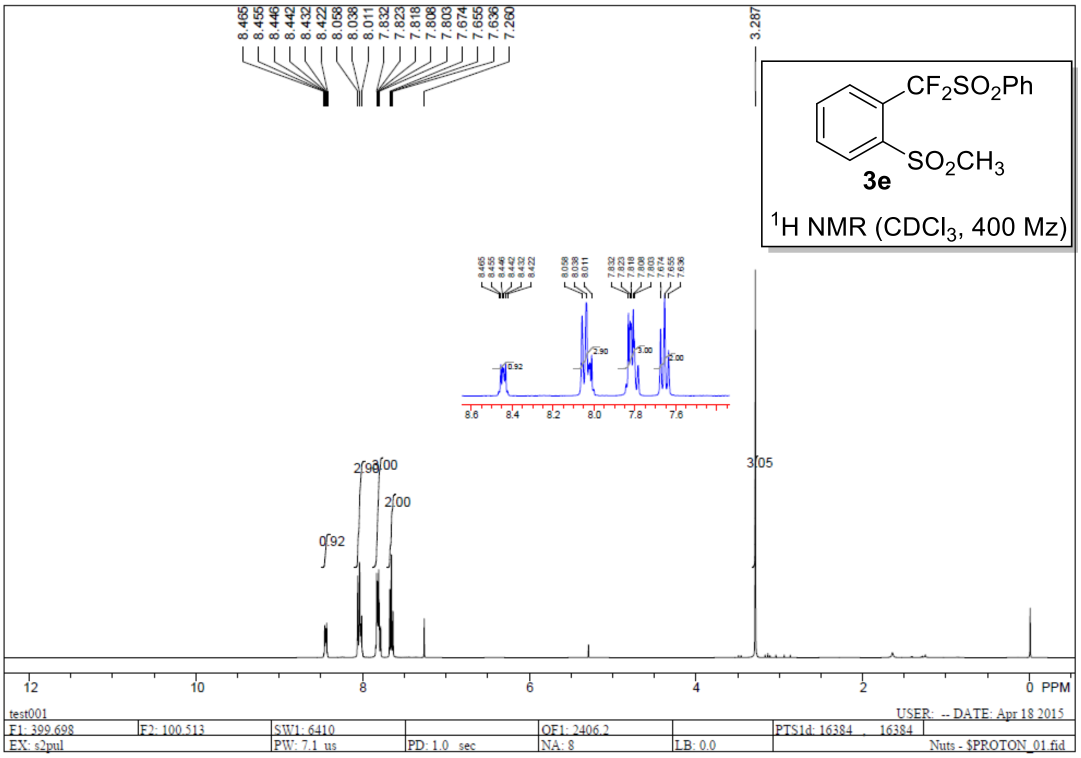
LB: 0.0
Nuts - $FLUORINE_01.fid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7.808
7.803
7.674
7.655
7.636
7.260
3.287
CF2SO2Ph
SO2CH3
3e
1H NMR (CDCl3, 400 Mz)
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8.4
8.2
8.0
7.8
7.6
12
10
8
6
4
2
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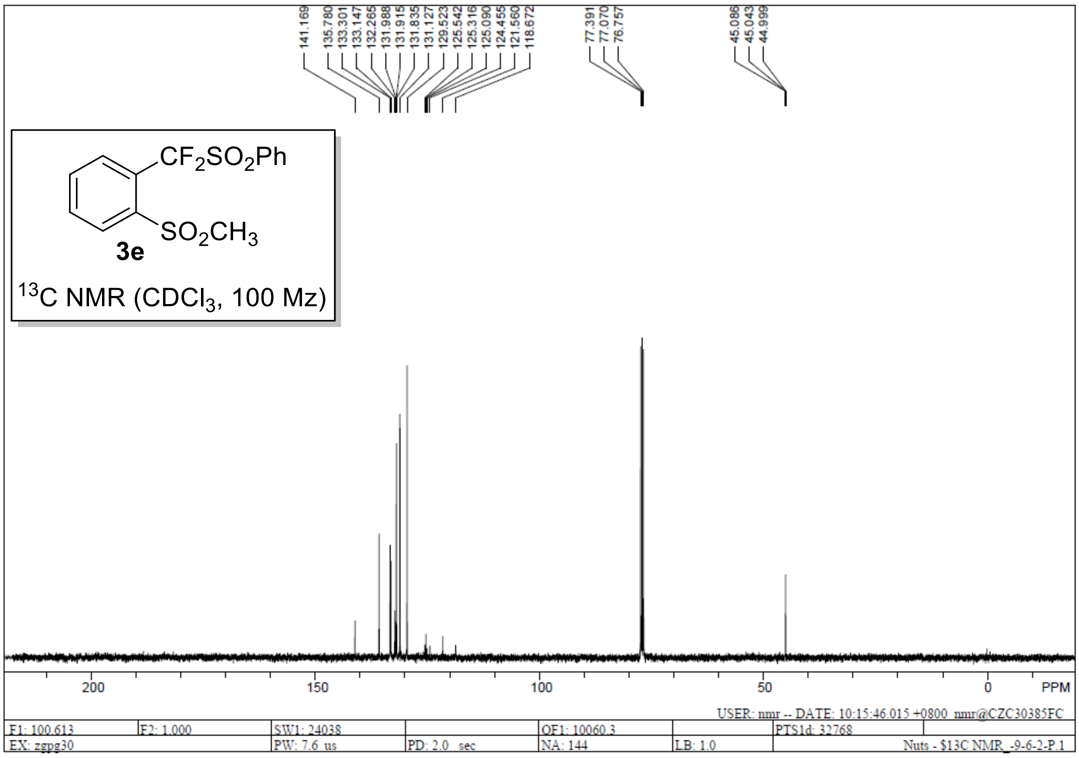
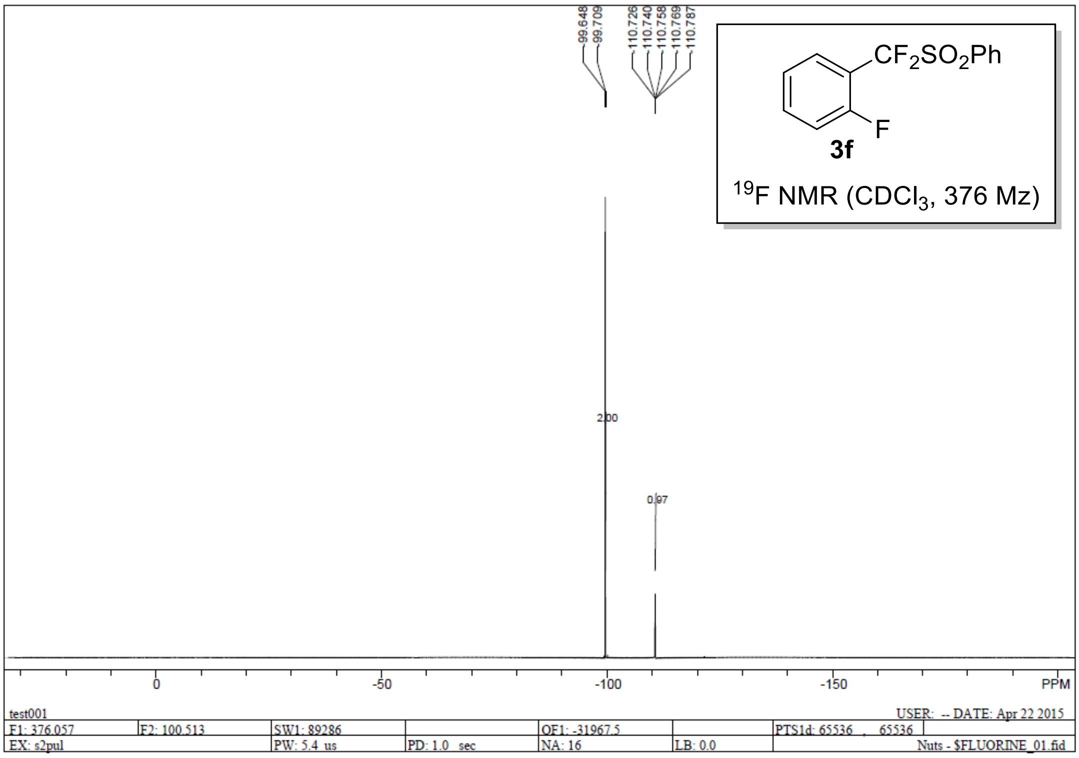


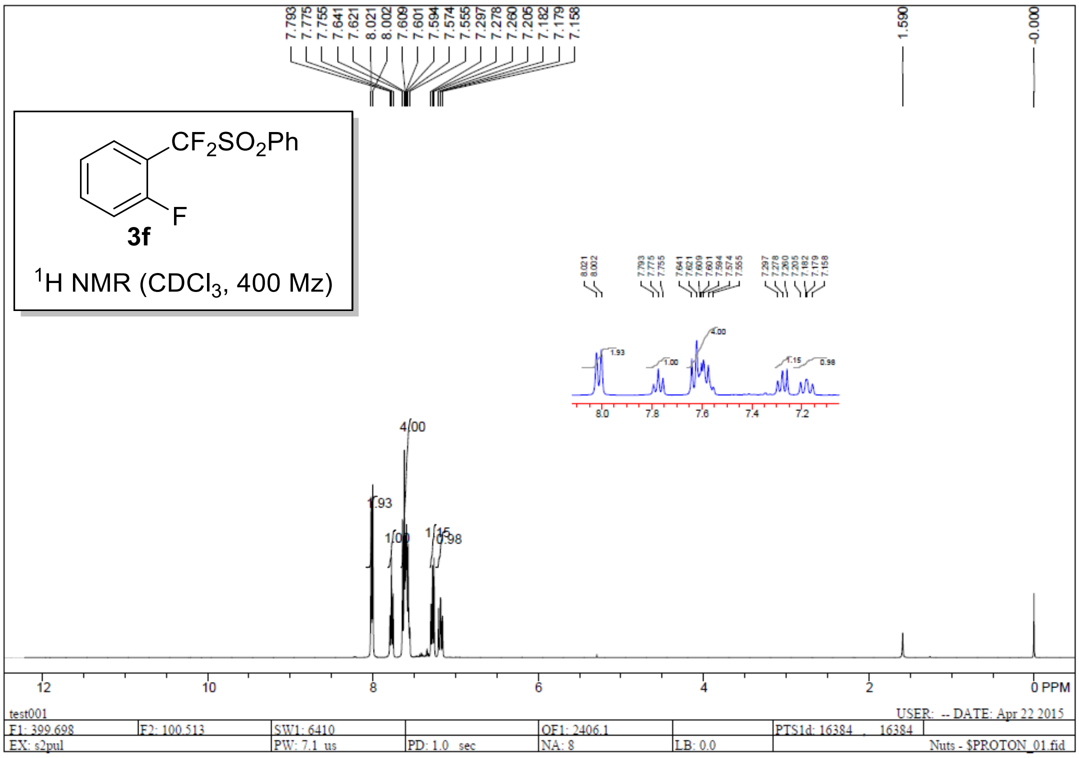
3e

^{13}C NMR (CDCl$_3$, 100 Mz)



3f

^{19}F NMR (CDCl$_3$, 376 Mz)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7.609
7.601
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7.297
7.278
7.260
7.205
7.182
7.179
7.158
1.590
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F
3f
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4.00
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7.8
7.6
7.4
7.2
12
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8
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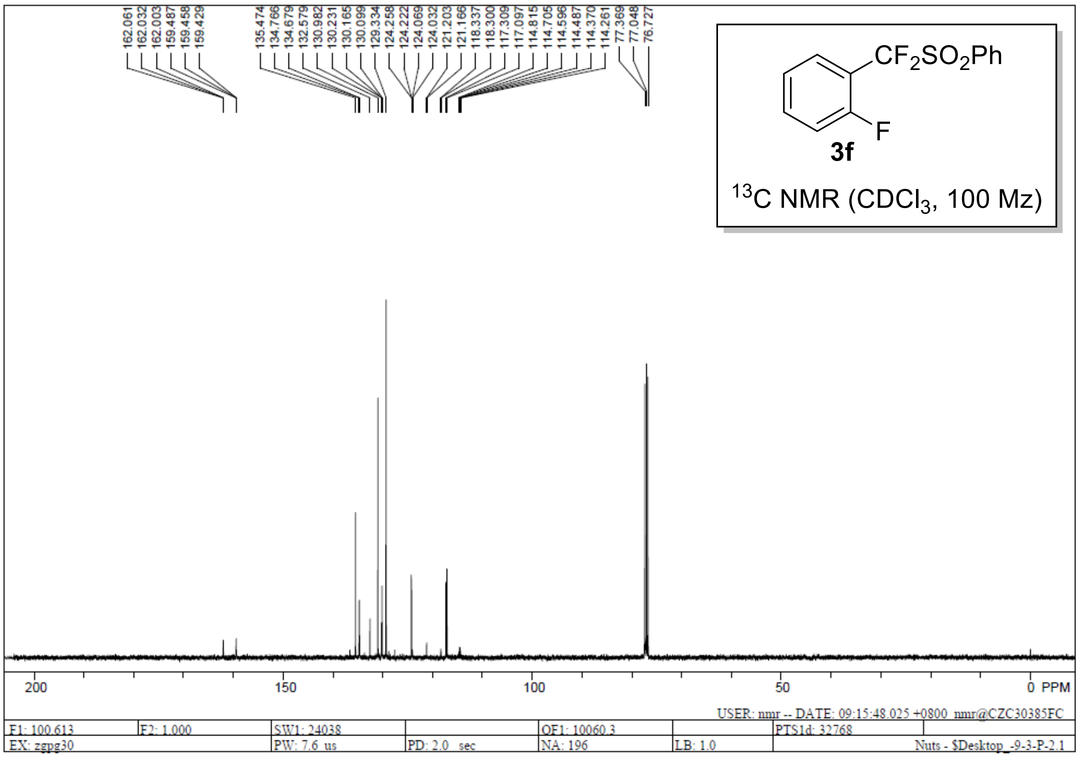
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124.222
124.069
124.032
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121.166
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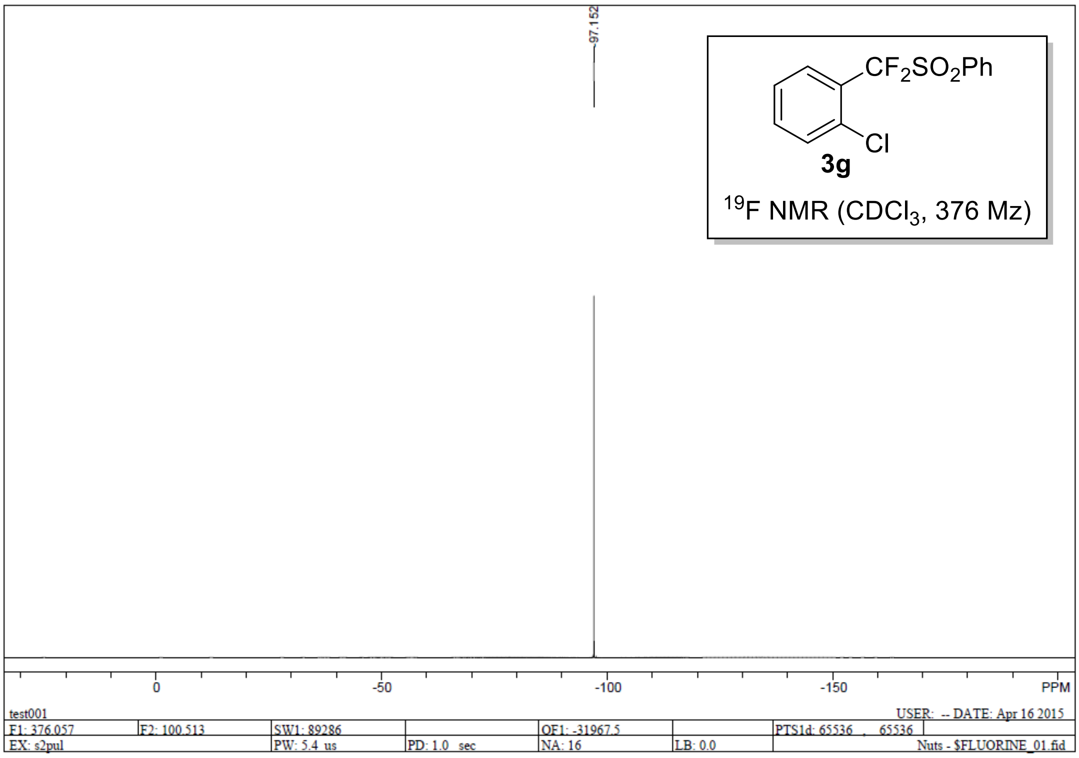
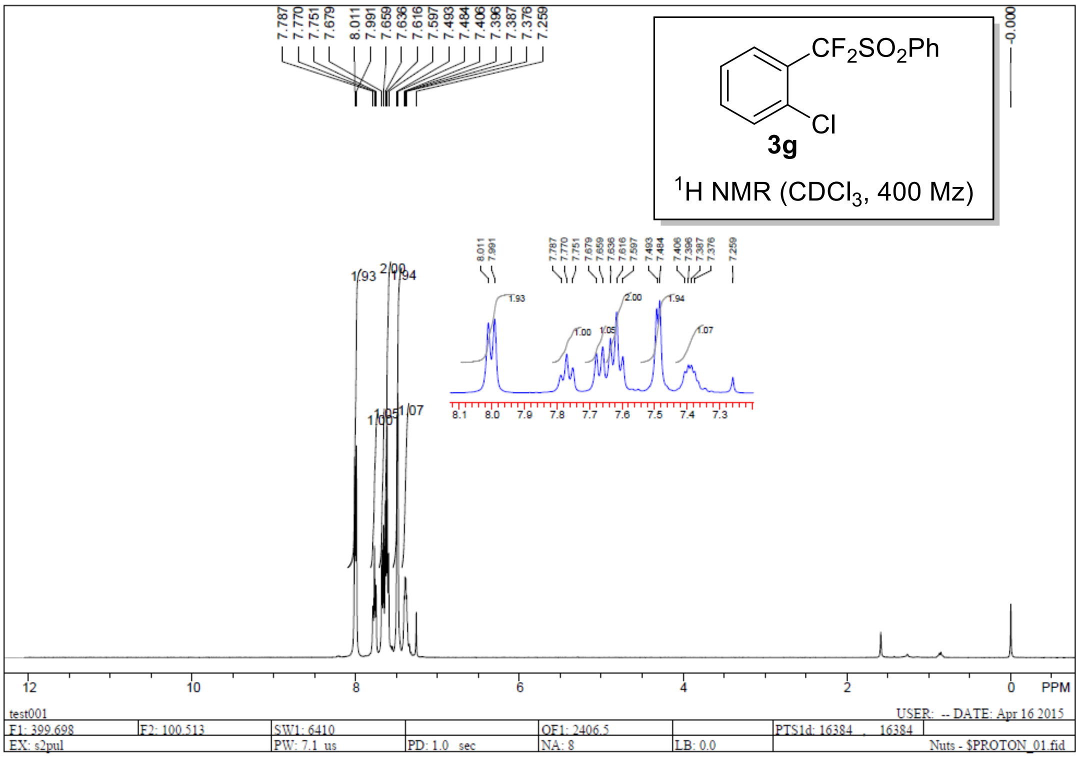
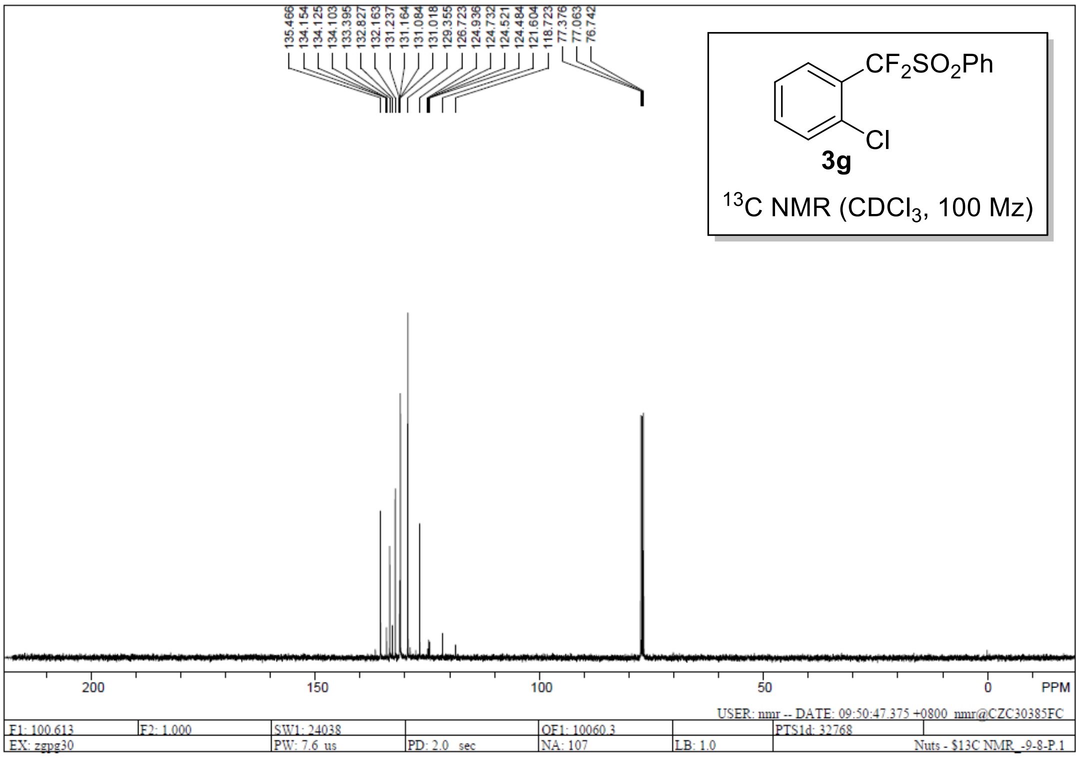
114.596
114.487
114.370
114.261
77.369
77.048
76.727
CF$_2$SO$_2$Ph
F
3f
^{13}C NMR (CDCl$_3$, 100 Mz)
200
150
100
50
0 PPM
USER: nmr -- DATE: 09:15:48.025 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 196
LB: 1.0
Nuts - $Desktop_-9-3-P-2.1

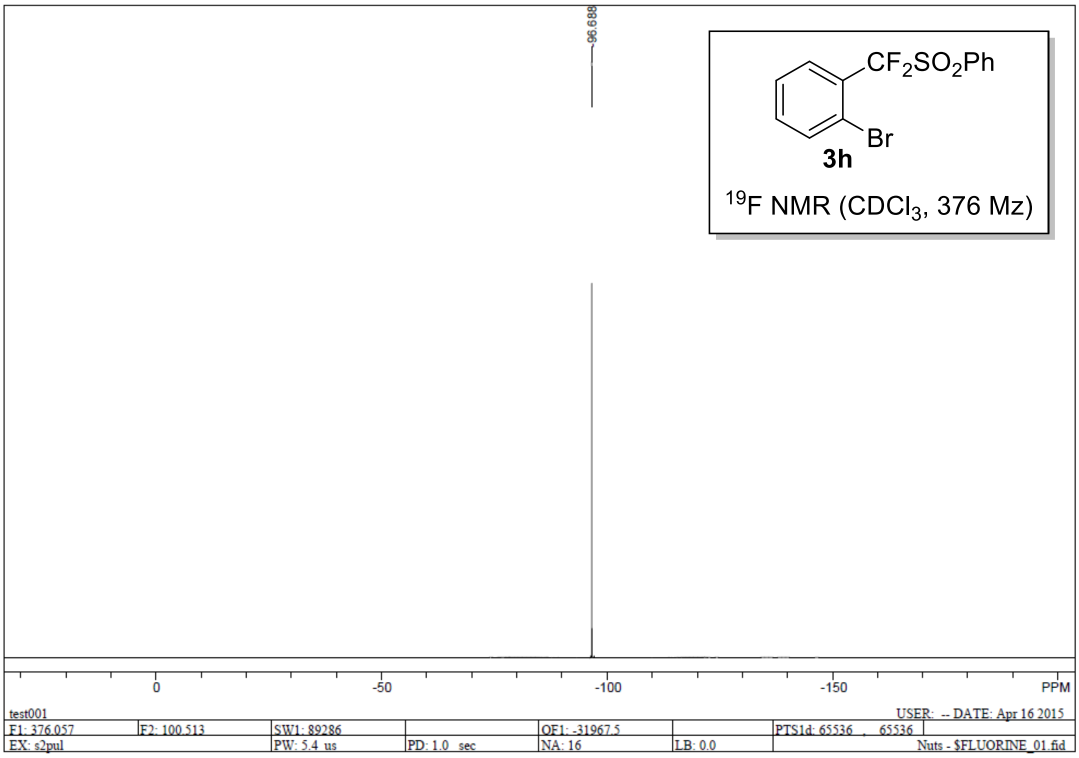

-97.152
CF2SO2Ph
Cl
3g
19F NMR (CDCl3, 376 Mz)
0
-50
-100
-150
PPM
test001
USER: -- DATE: Apr 16 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid


7.787
7.770
7.751
7.679
8.011
7.991
7.659
7.636
7.616
7.597
7.493
7.484
7.406
7.396
7.387
7.376
7.259
-0.000
CF2SO2Ph
Cl
3g
1H NMR (CDCl3, 400 Mz)
1.93
2.00
1.94
1.00
1.05
1.07
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
12
10
8
6
4
2
0
PPM
test001
USER: -- DATE: Apr 16 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2406.5
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid



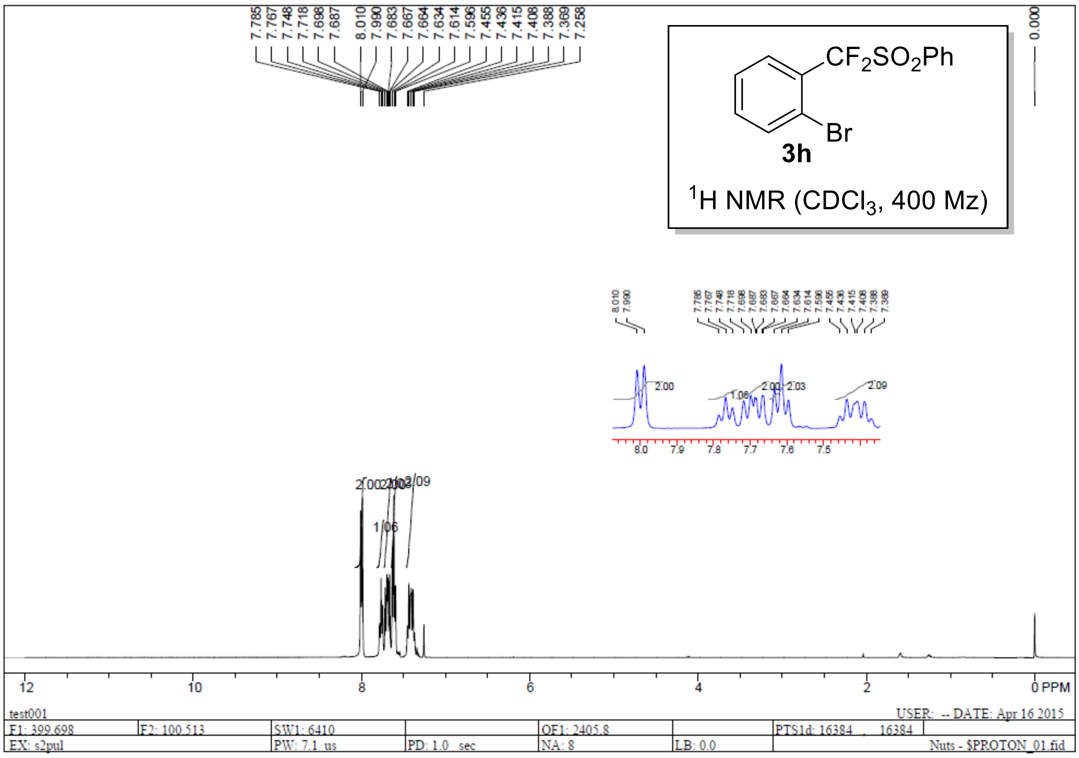
3g

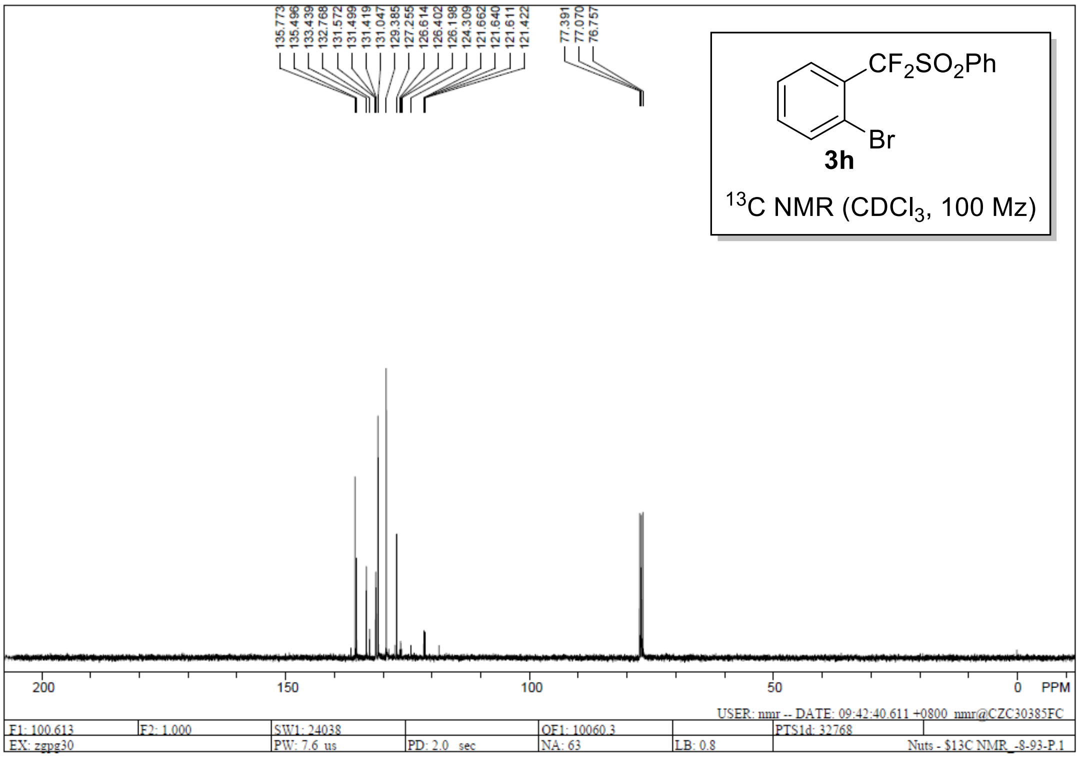
^{13}C NMR ($CDCl_3$, 100 Mz)

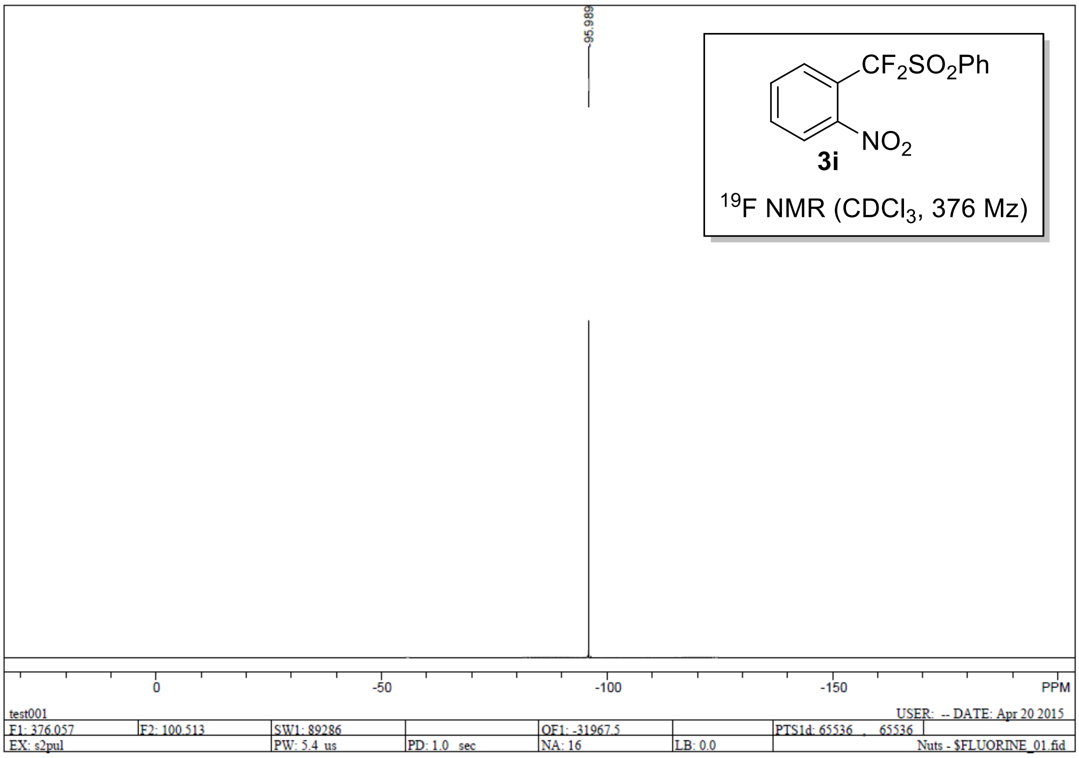


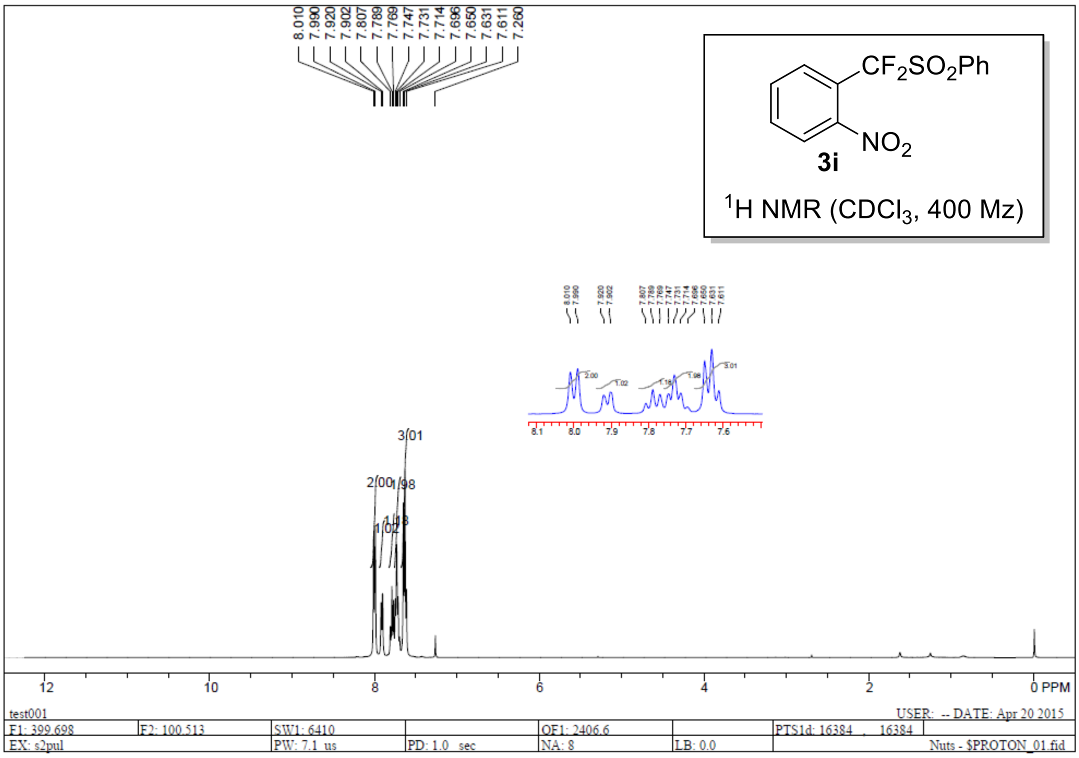
3h

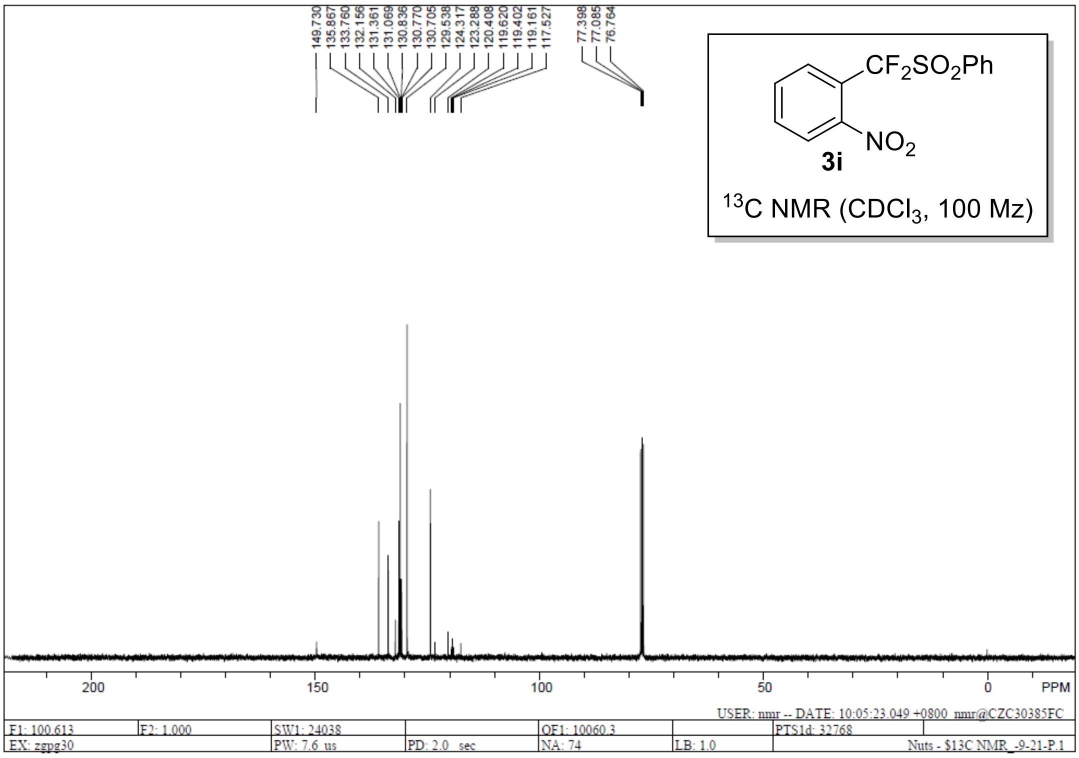
^{19}F NMR ($CDCl_3$, 376 Mz)

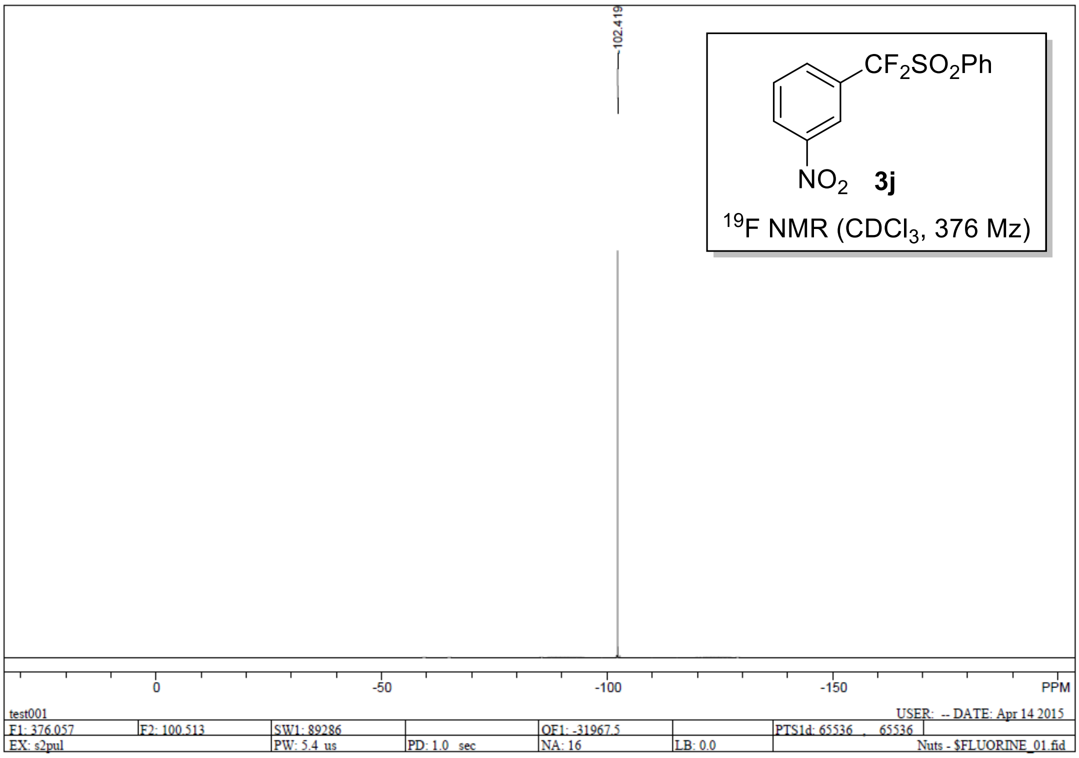

7.785
7.767
7.748
7.718
7.698
7.687
8.010
7.990
7.683
7.667
7.664
7.634
7.614
7.596
7.455
7.436
7.415
7.408
7.388
7.369
7.258
0.000
CF2SO2Ph
Br
3h
1H NMR (CDCl3, 400 Mz)
2.00
1.06
2.00
2.03
2.09
8.0
7.9
7.8
7.7
7.6
7.5
12
10
8
6
4
2
0 PPM
test001
USER: -- DATE: Apr 16 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2405.8
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

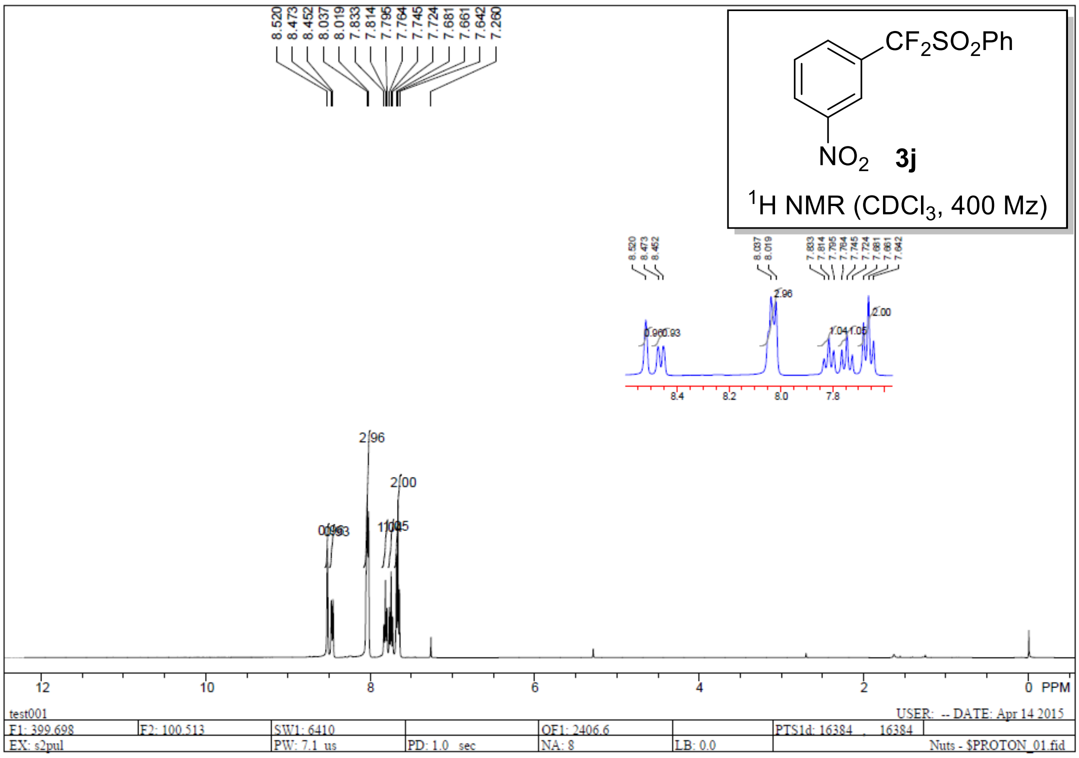

135.773
135.496
133.439
132.768
131.572
131.499
131.419
131.047
129.385
127.255
126.614
126.402
126.198
124.309
121.662
121.640
121.611
121.422
77.391
77.070
76.757
CF2SO2Ph
Br
3h
13C NMR (CDCl3, 100 Mz)
200
150
100
50
0
PPM
USER: nmr -- DATE: 09:42:40.611 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 63
LB: 0.8
Nuts - $13C NMR_-8-93-P.1

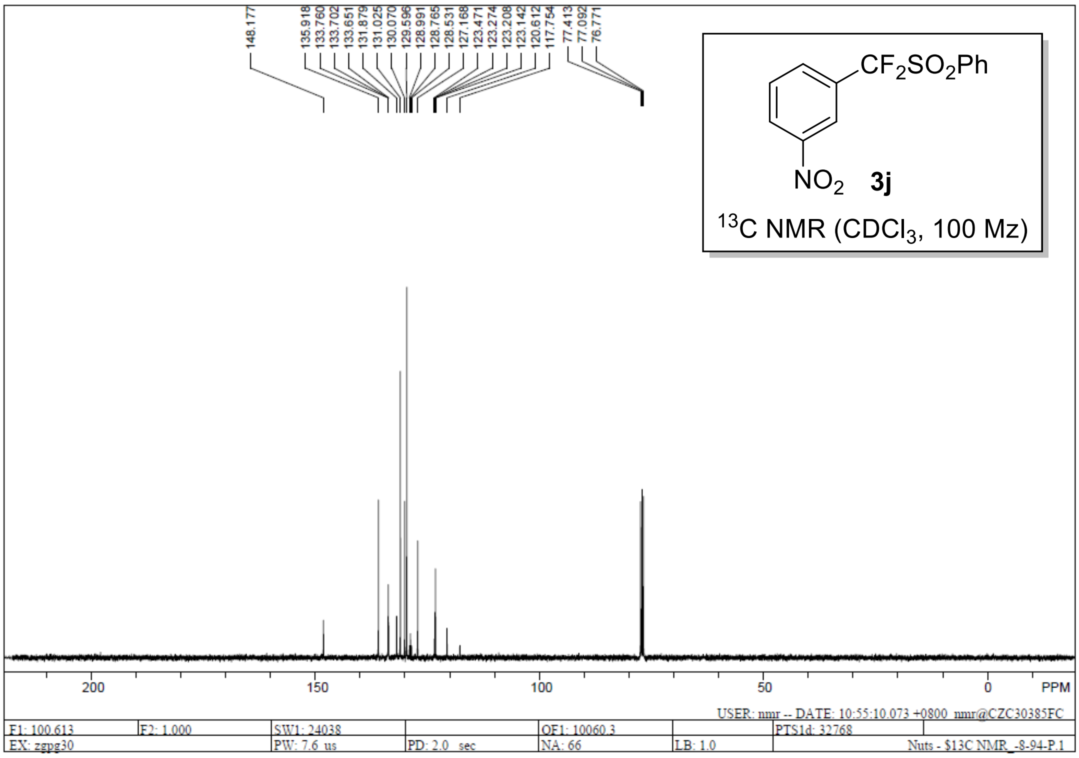

-95.989
CF2SO2Ph
NO2
3i
19F NMR (CDCl3, 376 Mz)
0
-50
-100
-150
PPM
test001
USER: -- DATE: Apr 20 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid

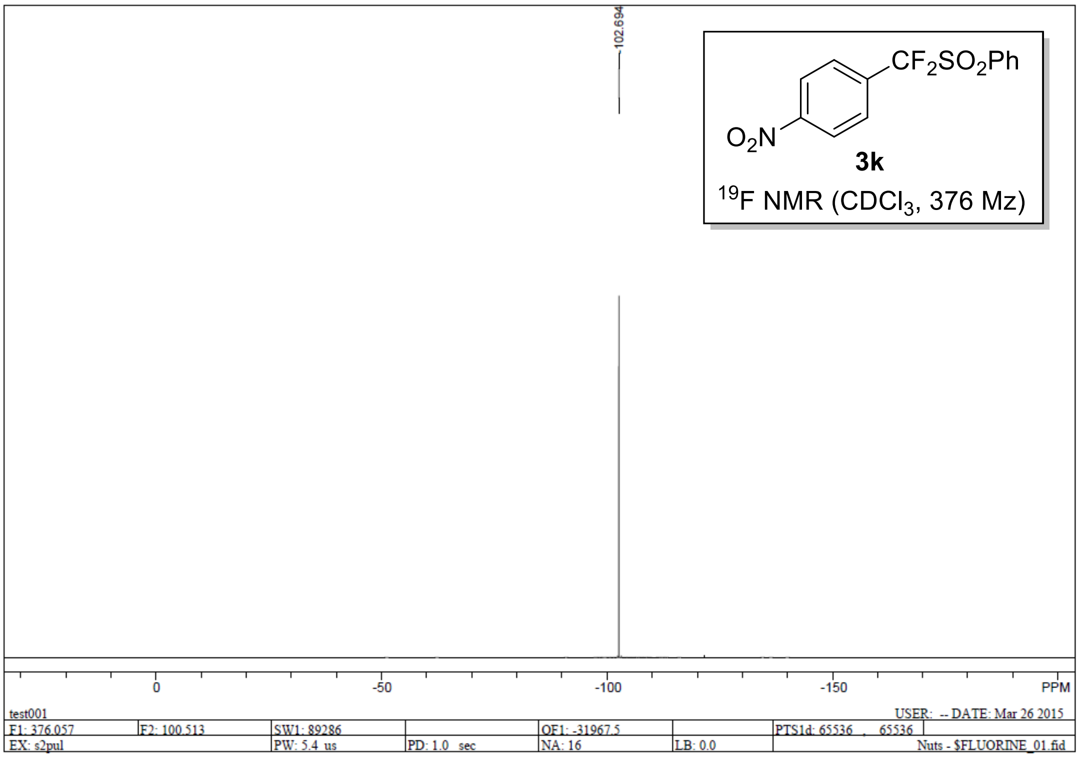

8.010
7.990
7.920
7.902
7.807
7.789
7.769
7.747
7.731
7.714
7.696
7.650
7.631
7.611
7.260
CF2SO2Ph
NO2
3i
1H NMR (CDCl3, 400 Mz)
2.00
1.02
1.18
1.98
3.01
8.1
8.0
7.9
7.8
7.7
7.6
12
10
8
6
4
2
0 PPM
test001
USER: -- DATE: Apr 20 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2406.6
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

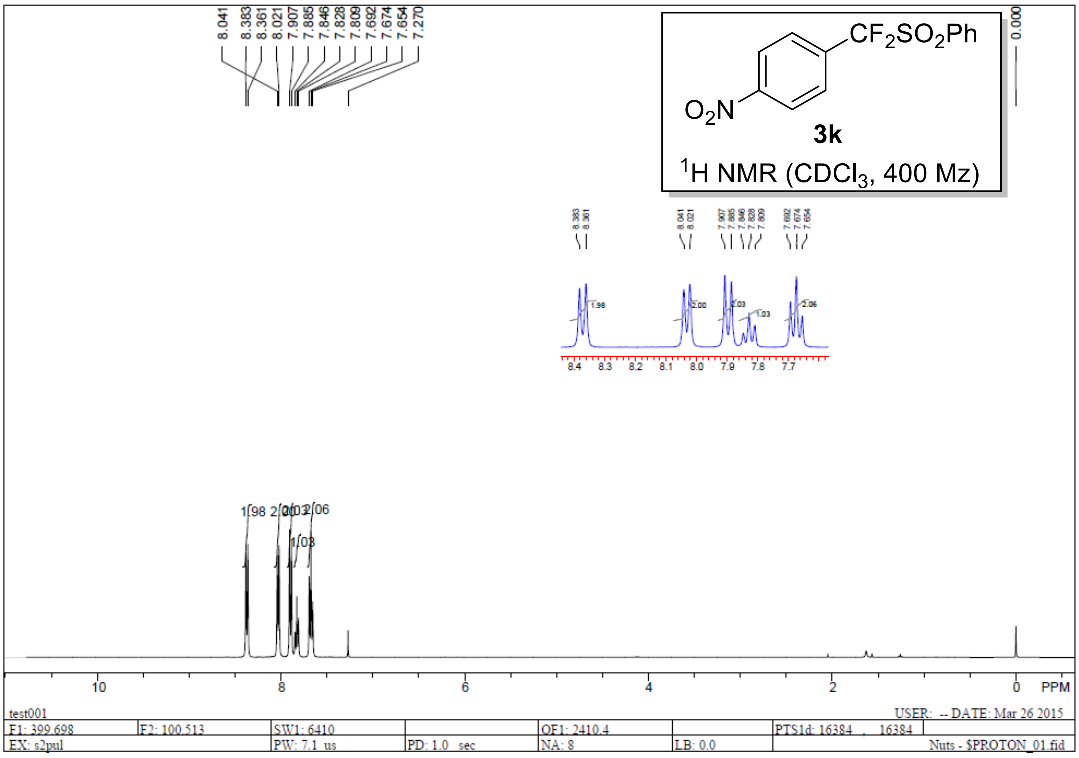

149.730
135.867
133.760
132.156
131.361
131.069
130.836
130.770
130.705
129.538
124.317
123.288
120.408
119.620
119.402
119.161
117.527
77.398
77.085
76.764
CF2SO2Ph
NO2
3i
13C NMR (CDCl3, 100 Mz)
200
150
100
50
0
PPM
USER: nmr -- DATE: 10:05:23.049 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 74
LB: 1.0
Nuts - $13C NMR_-9-21-P.1

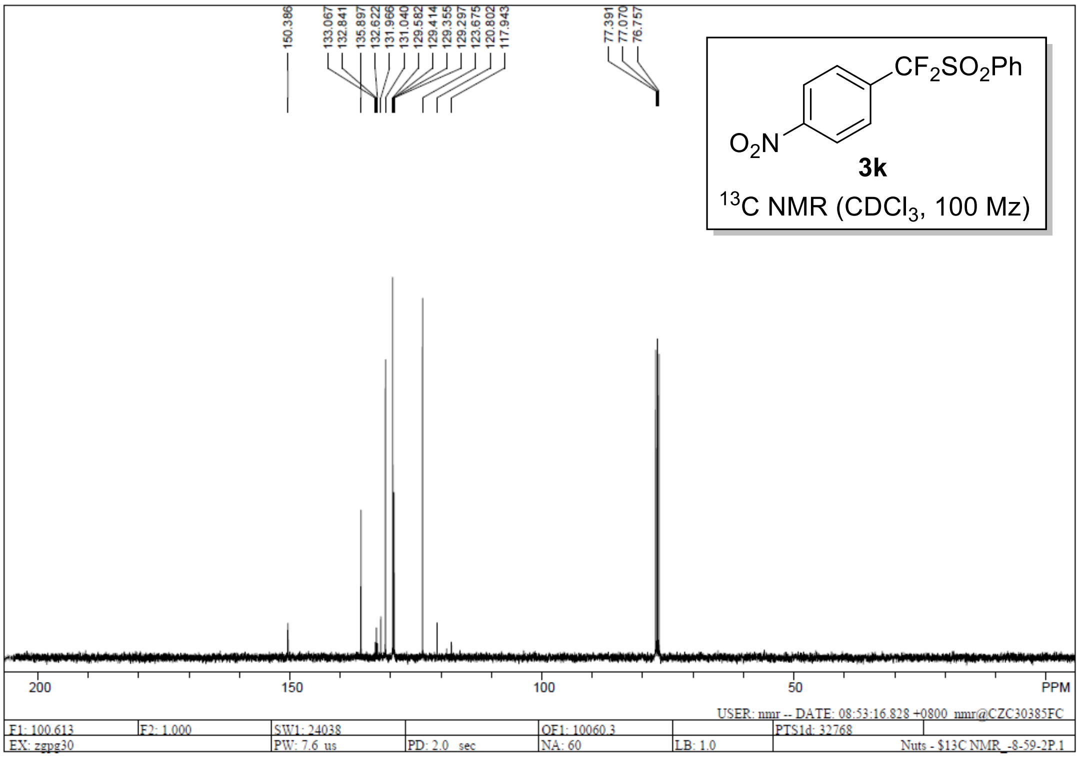

-102.419
CF2SO2Ph
NO2
3j
19F NMR (CDCl3, 376 Mz)
0
-50
-100
-150
PPM
test001
USER: -- DATE: Apr 14 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid

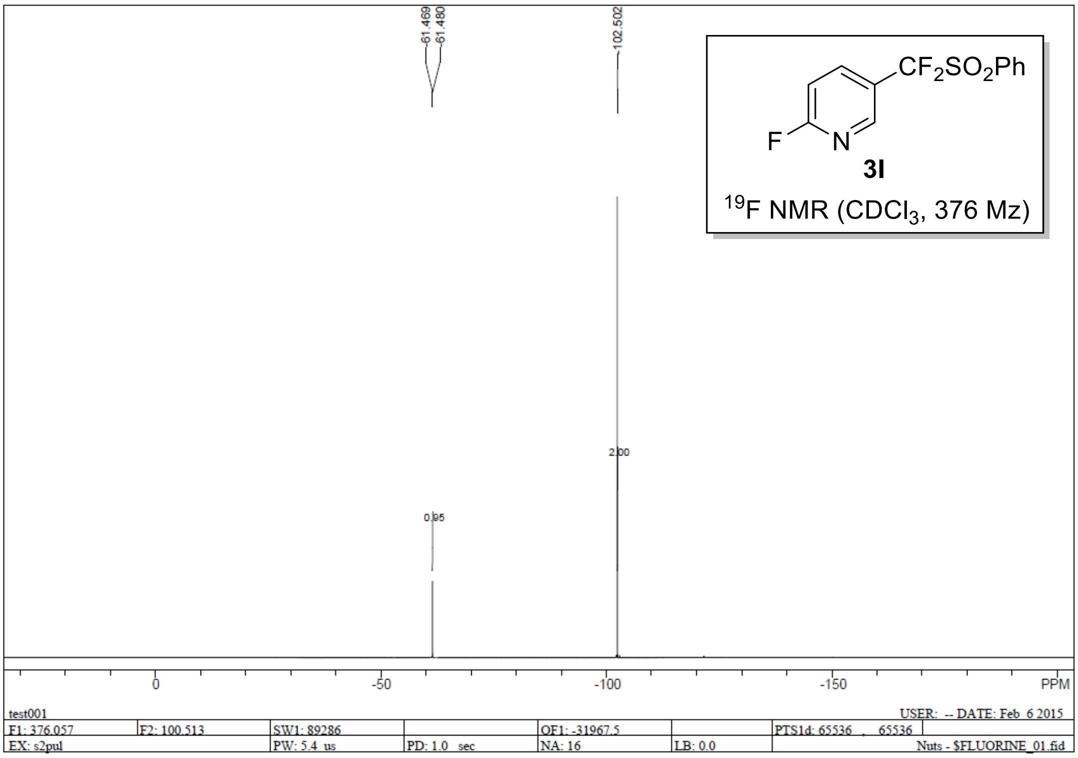

8.520
8.473
8.452
8.037
8.019
7.833
7.814
7.795
7.764
7.745
7.724
7.681
7.661
7.642
7.260
CF2SO2Ph
NO2
3j
1H NMR (CDCl3, 400 Mz)
2.96
2.00
0.96
0.93
1.04
1.05
8.4
8.2
8.0
7.8
12
10
8
6
4
2
0
PPM
test001
USER: -- DATE: Apr 14 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2406.6
PTS1d: 16384 . 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

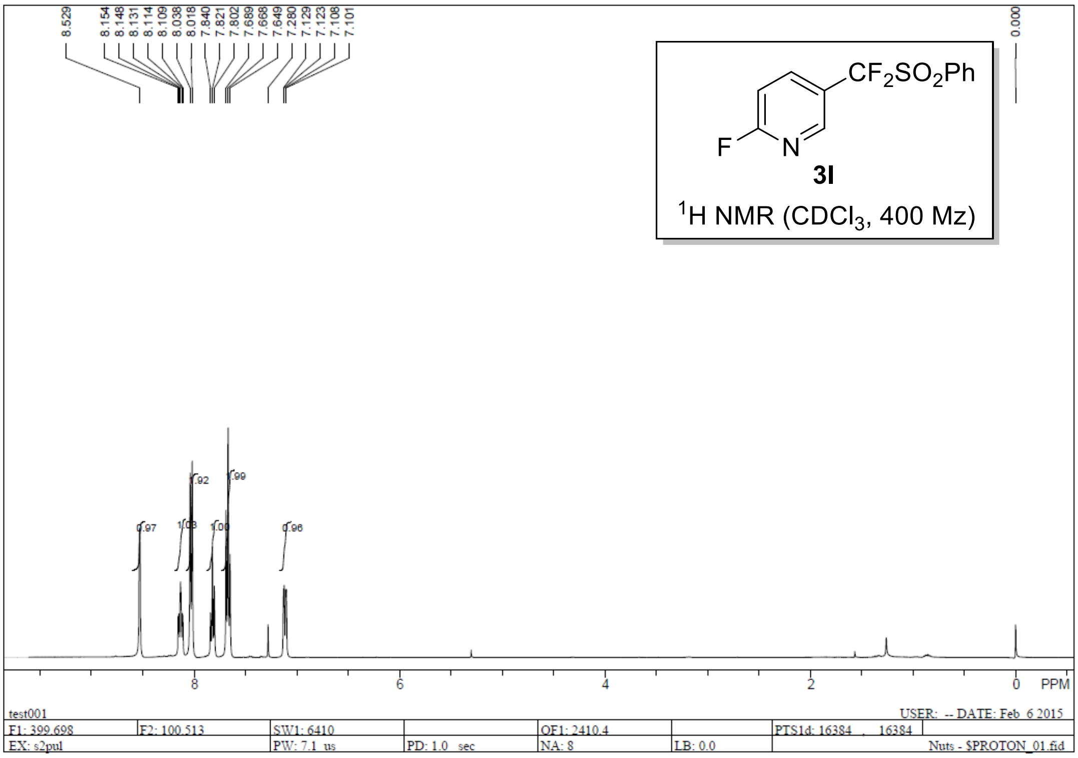

148.177
135.918
133.760
133.702
133.651
131.879
131.025
130.070
129.596
128.991
128.765
128.531
127.168
123.471
123.274
123.208
123.142
120.612
117.754
77.413
77.092
76.771
CF2SO2Ph
NO2
3j
13C NMR (CDCl3, 100 Mz)
200
150
100
50
0
PPM
USER: nmr -- DATE: 10:55:10.073 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 66
LB: 1.0
Nuts - $13C NMR_-8-94-P.1

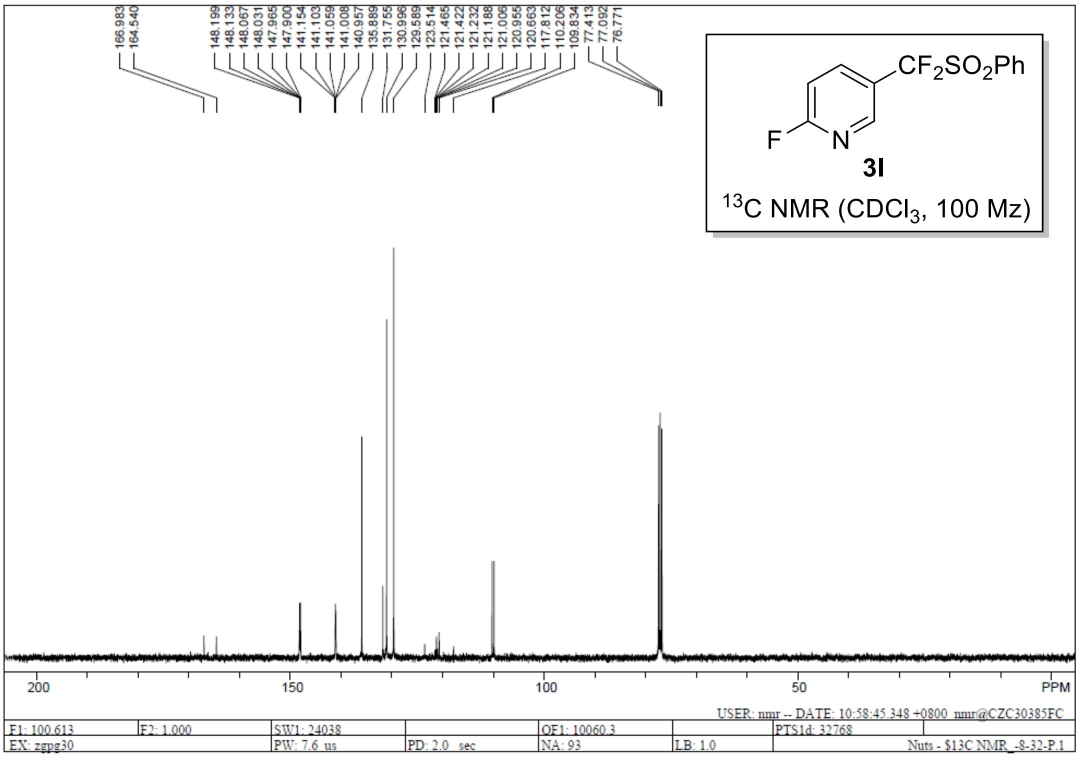

-102.694
CF_2SO_2Ph
O_2N
3k
^{19}F NMR ($CDCl_3$, 376 Mz)
0
-50
-100
-150
PPM
test001
USER: -- DATE: Mar 26 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid

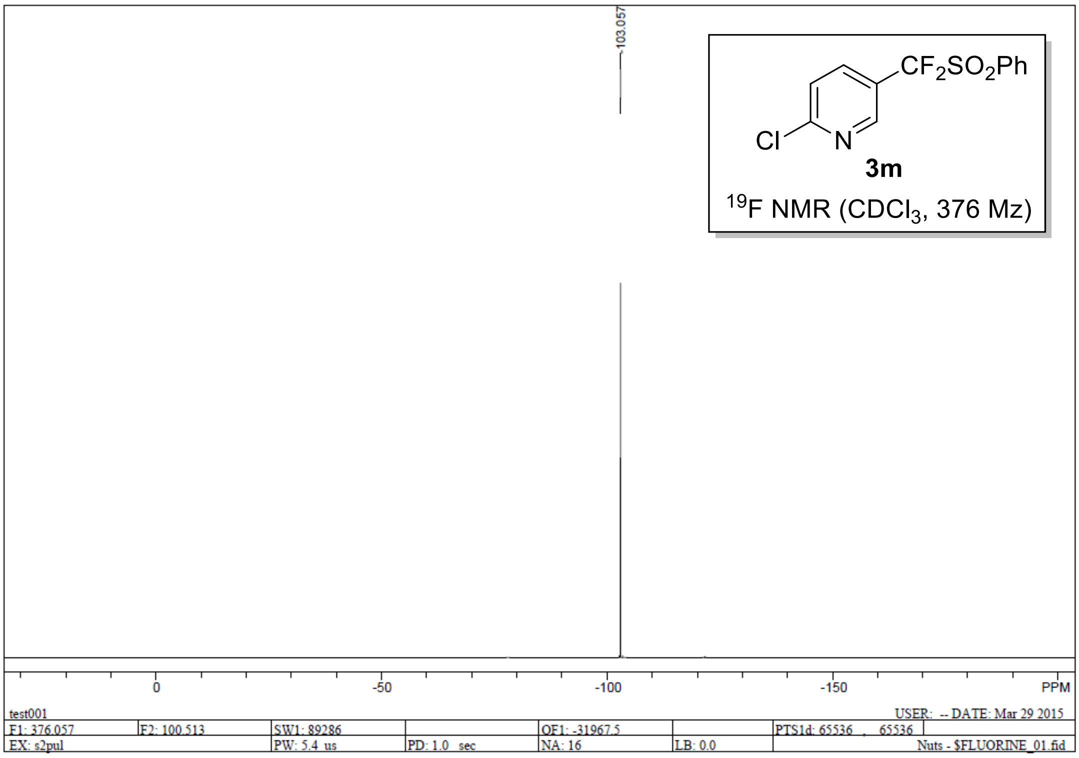

8.041
8.383
8.361
8.021
7.907
7.885
7.846
7.828
7.809
7.692
7.674
7.654
7.270
0.000
CF_2SO_2Ph
O_2N
3k
^{1}H NMR ($CDCl_3$, 400 Mz)
1.98
2.00
2.03
1.03
2.06
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
10
8
6
4
2
0
PPM
test001
USER: -- DATE: Mar 26 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2410.4
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid


150.386
133.067
132.841
135.897
132.622
131.966
131.040
129.582
129.414
129.355
129.297
123.675
120.802
117.943
77.391
77.070
76.757
CF2SO2Ph
O2N
3k
13C NMR (CDCl3, 100 Mz)
200
150
100
50
PPM
USER: nmr -- DATE: 08:53:16.828 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 60
LB: 1.0
Nuts - $13C NMR_-8-59-2P.1

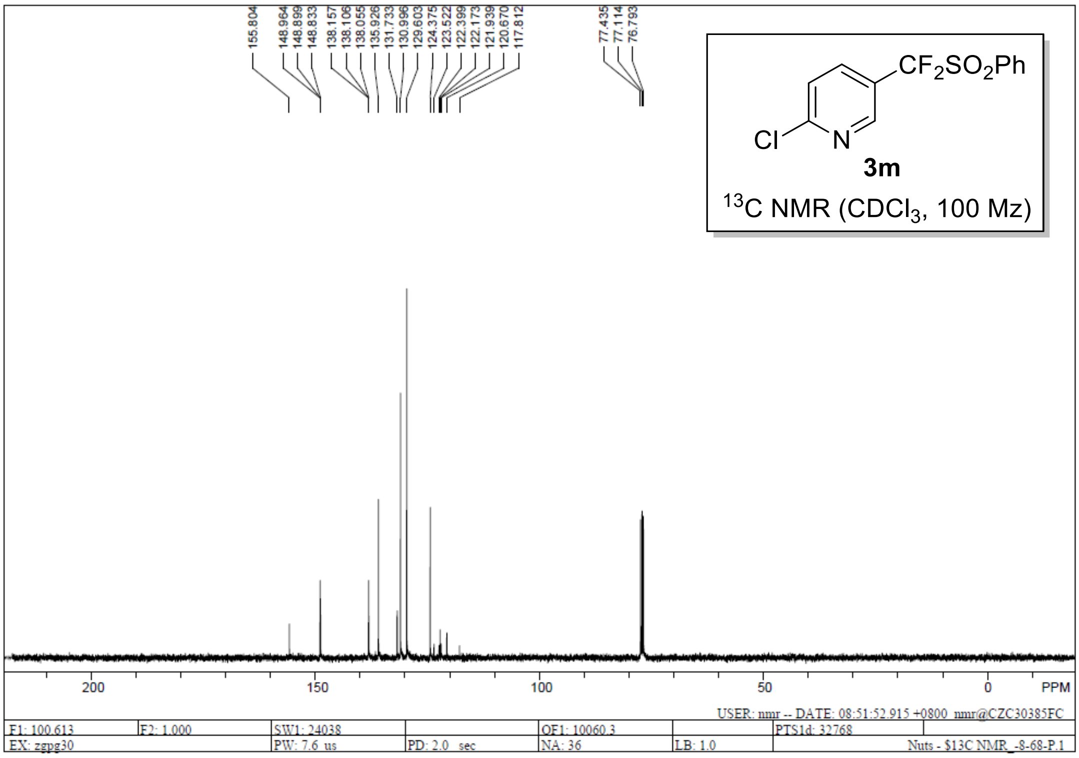

-61.469
-61.480
-102.502
CF2SO2Ph
F
N
3l
19F NMR (CDCl3, 376 Mz)
2.00
0.95
0
-50
-100
-150
PPM
test001
USER: -- DATE: Feb 6 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid


8.529
8.154
8.148
8.131
8.114
8.109
8.038
8.018
7.840
7.821
7.802
7.689
7.668
7.649
7.280
7.129
7.123
7.108
7.101
0.000
CF$_2$SO$_2$Ph
F
N
3l
^{1}H NMR (CDCl$_3$, 400 Mz)
0.97
1.03
1.92
1.00
1.99
0.96
8
6
4
2
0
PPM
test001
USER: -- DATE: Feb 6 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2410.4
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid


166.983
164.540
148.199
148.133
148.067
148.031
147.965
147.900
141.154
141.103
141.059
141.008
140.957
135.889
131.755
130.996
129.589
123.514
121.465
121.422
121.232
121.188
121.006
120.955
120.663
117.812
110.206
109.834
77.413
77.092
76.771
CF$_2$SO$_2$Ph
F
N
3l
^{13}C NMR (CDCl$_3$, 100 Mz)
200
150
100
50
PPM
USER: nmr -- DATE: 10:58:45.348 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 93
LB: 1.0
Nuts - $13C NMR_-8-32-P.1

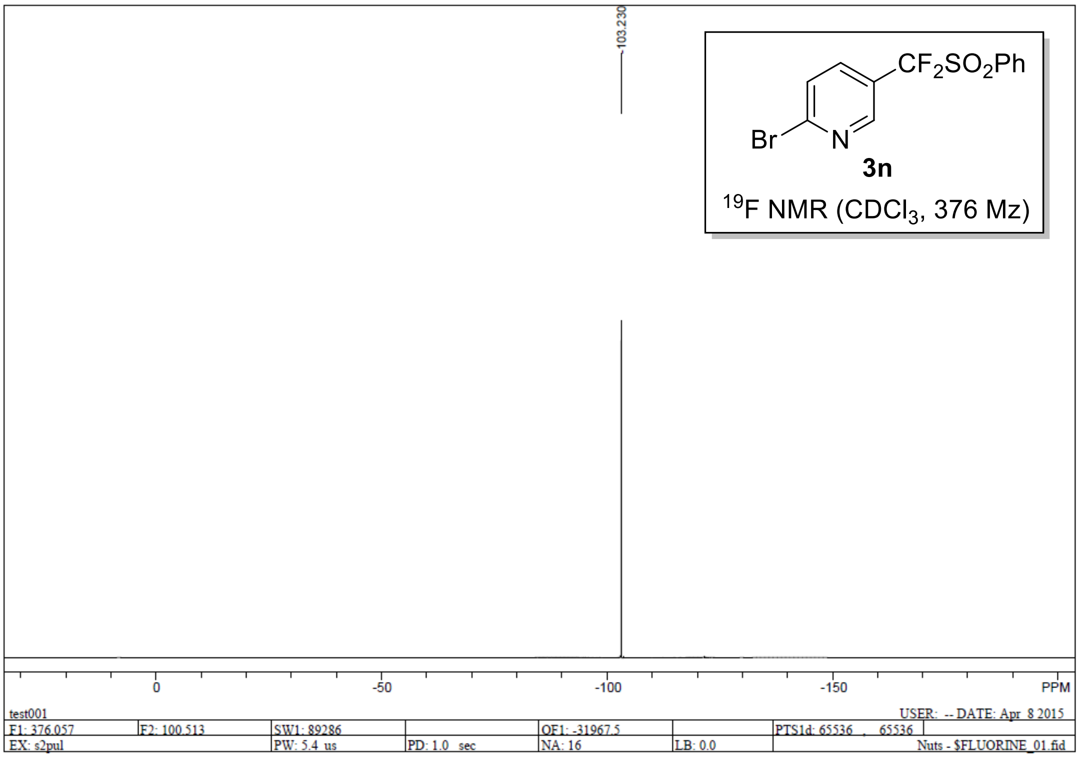

-103.057
CF2SO2Ph
Cl
N
3m
19F NMR (CDCl3, 376 Mz)
0
-50
-100
-150
PPM
test001
USER: -- DATE: Mar 29 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid


8.631
8.007
7.987
7.958
7.952
7.936
7.932
7.807
7.789
7.770
7.656
7.637
7.617
7.490
7.469
7.260
CF2SO2Ph
Cl
N
3m
1H NMR (CDCl3, 400 Mz)
1.99
1.01
1.00
2.01
0.99
8.0
7.9
7.8
7.7
7.6
7.5
0.97
1.99
2.01
1.01
1.00
0.99
12
10
8
6
4
2
0
PPM
test001
USER: -- DATE: Mar 29 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2406.6
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid



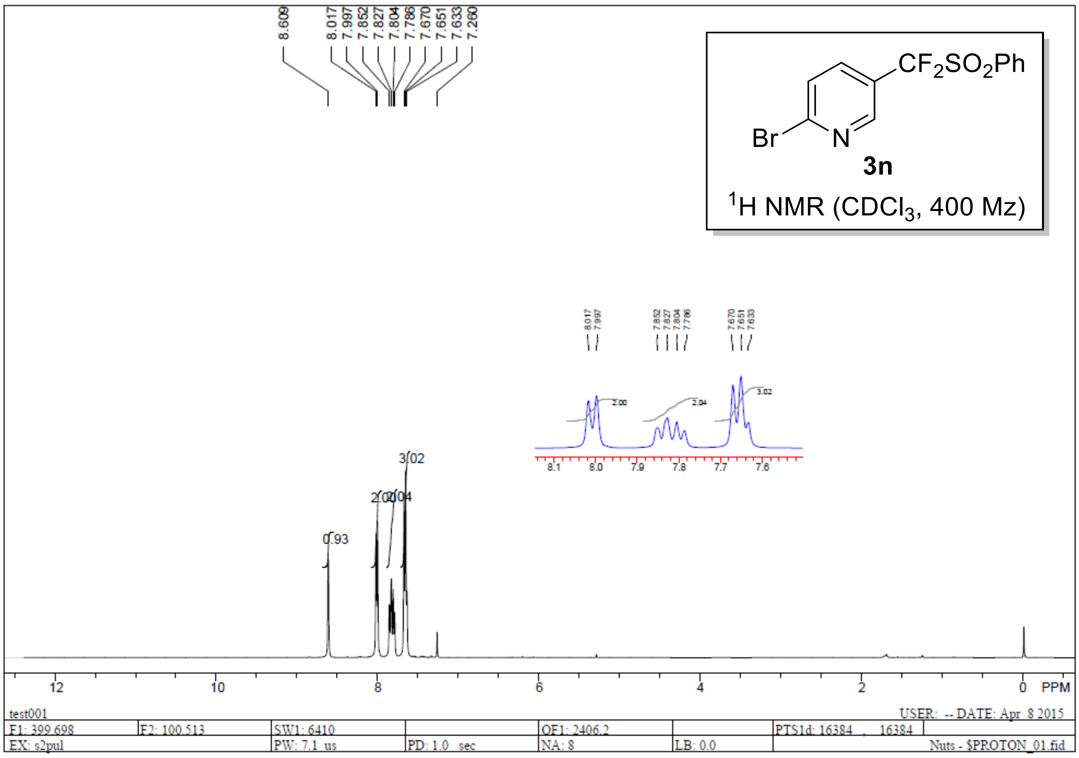
3m

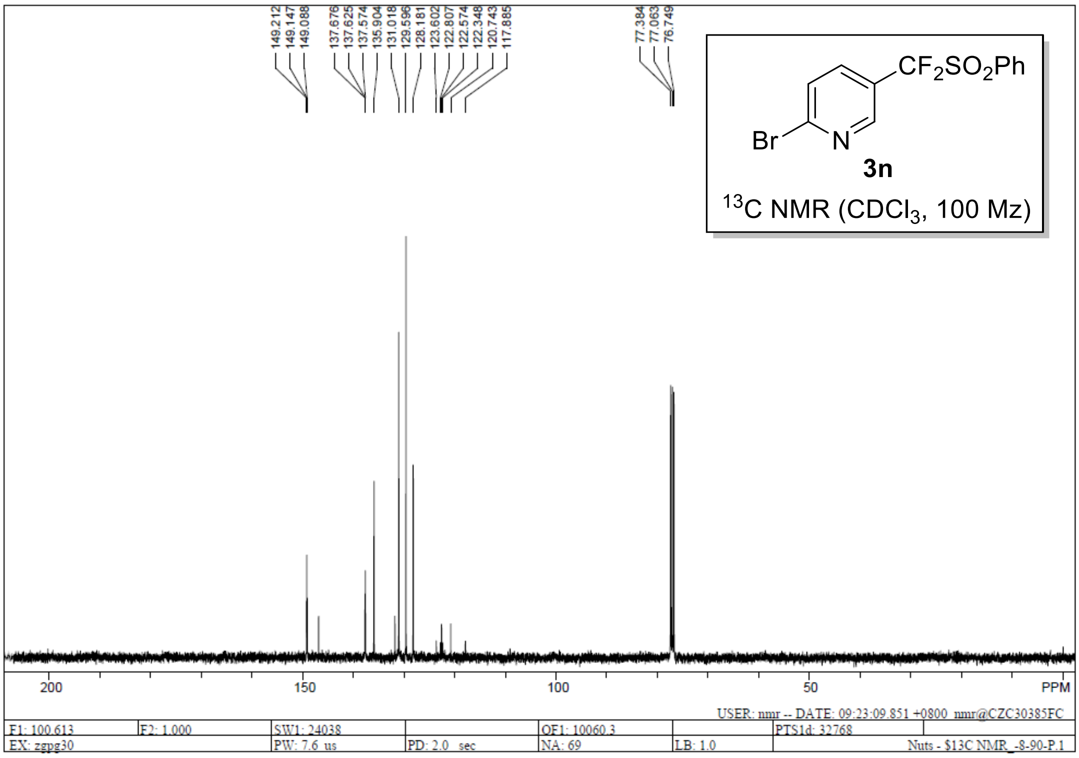
^{13}C NMR (CDCl$_3$, 100 Mz)

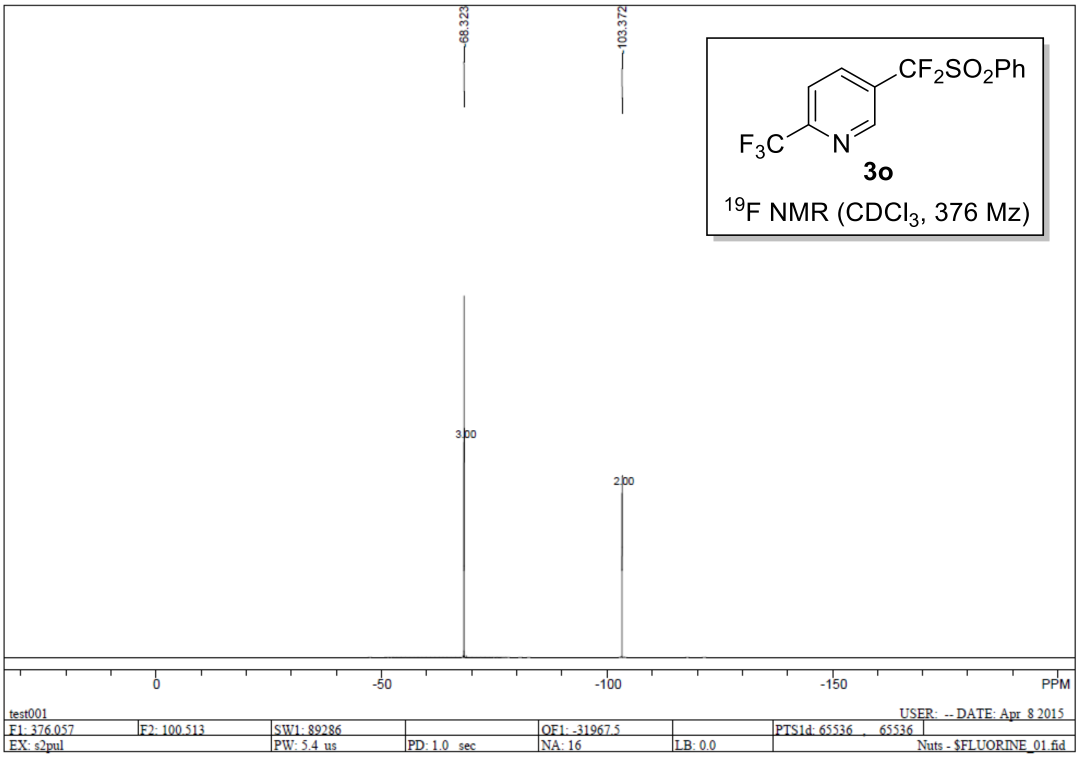


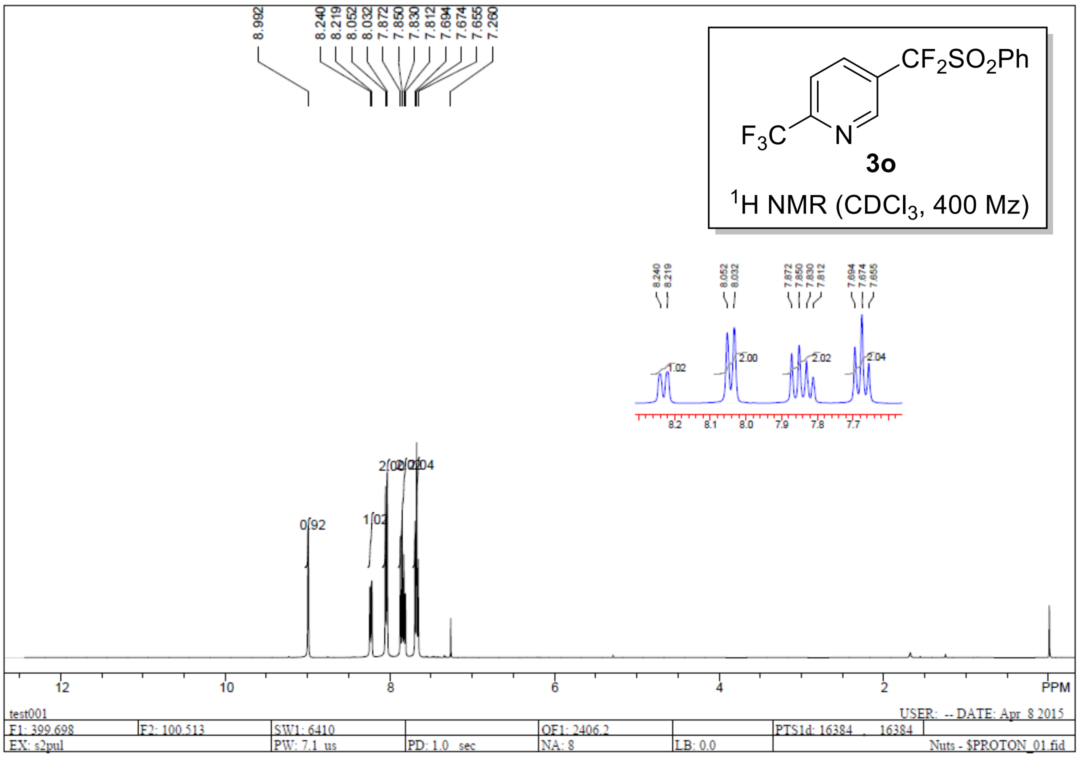
3n

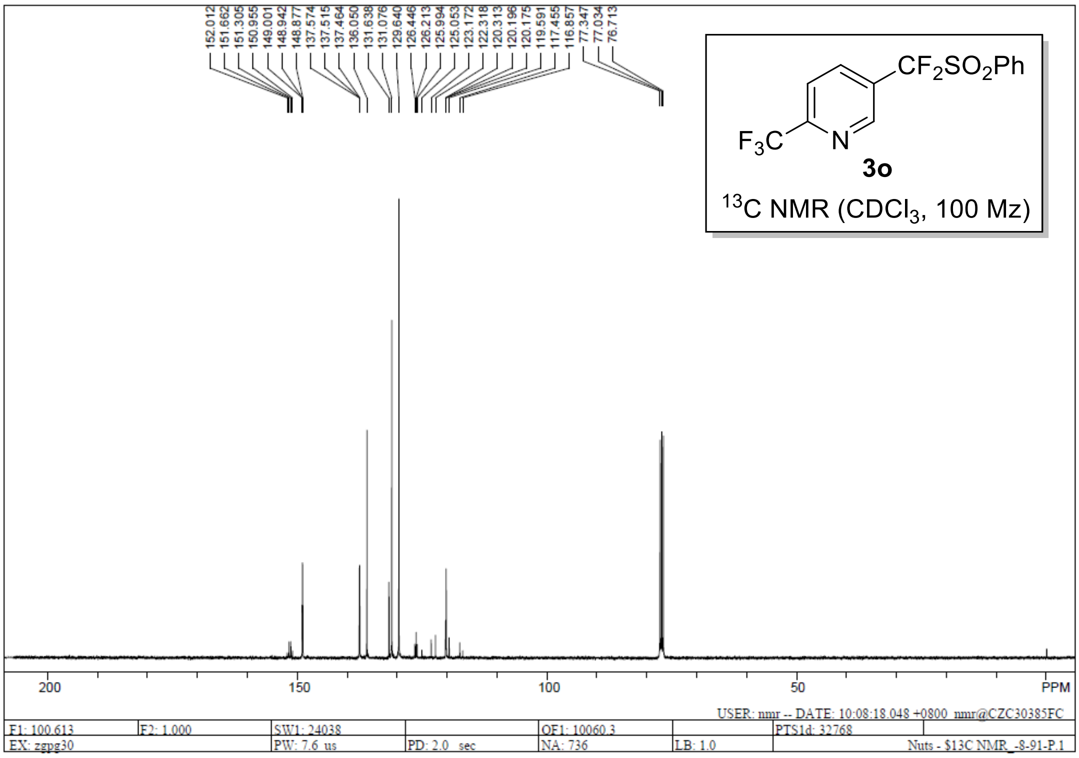
^{19}F NMR (CDCl$_3$, 376 Mz)


8.609
8.017
7.997
7.852
7.827
7.804
7.786
7.670
7.651
7.633
7.260
CF2SO2Ph
Br
N
3n
1H NMR (CDCl3, 400 Mz)
2.00
2.04
3.02
8.1
8.0
7.9
7.8
7.7
7.6
0.93
12
10
8
6
4
2
0
PPM
test001
USER: -- DATE: Apr 8 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2406.2
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid


149.212
149.147
149.088
137.676
137.625
137.574
135.904
131.018
129.596
128.181
123.602
122.807
122.574
122.348
120.743
117.885
77.384
77.063
76.749
CF2SO2Ph
Br
N
3n
13C NMR (CDCl3, 100 Mz)
200
150
100
50
PPM
USER: nmr -- DATE: 09:23:09.851 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 69
LB: 1.0
Nuts - $13C NMR_-8-90-P.1

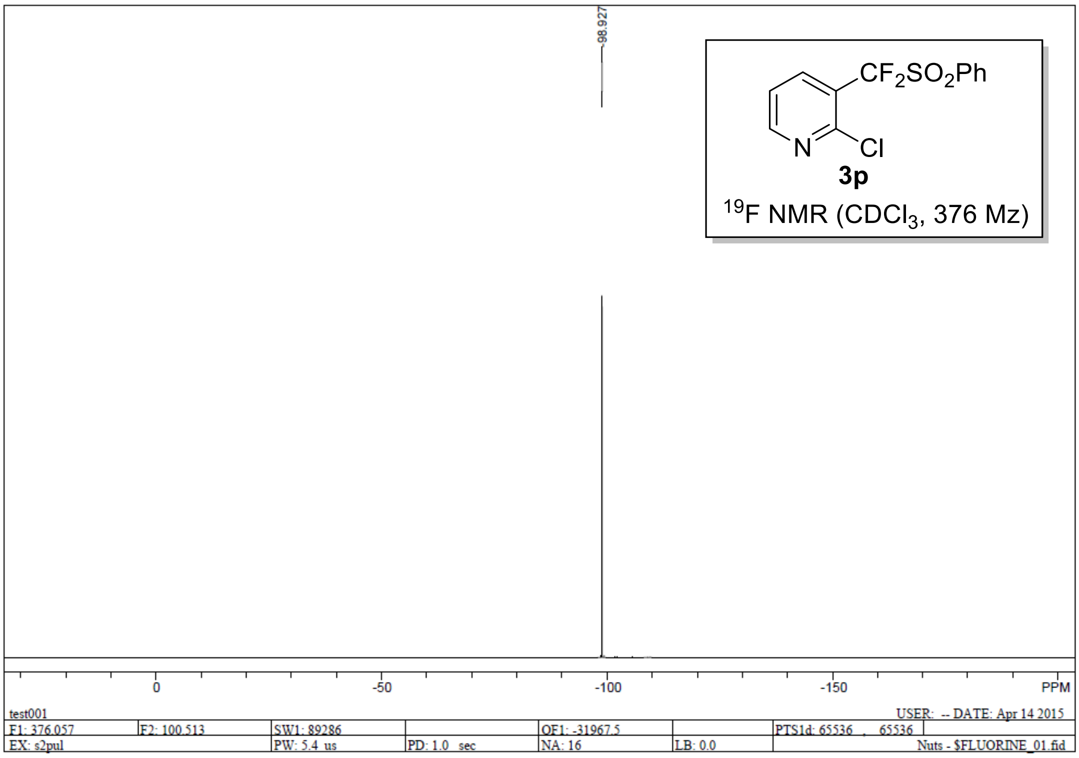

-68.323
-103.372
CF2SO2Ph
F3C
N
3o
19F NMR (CDCl3, 376 Mz)
3.00
2.00
0
-50
-100
-150
PPM
test001
USER: -- DATE: Apr 8 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid


8.992
8.240
8.219
8.052
8.032
7.872
7.850
7.830
7.812
7.694
7.674
7.655
7.260
CF2SO2Ph
F3C
N
3o
1H NMR (CDCl3, 400 Mz)
1.02
2.00
2.02
2.04
8.2
8.1
8.0
7.9
7.8
7.7
0.92
1.02
2.00
2.02
2.04
12
10
8
6
4
2
PPM
test001
USER: -- DATE: Apr 8 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2406.2
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid



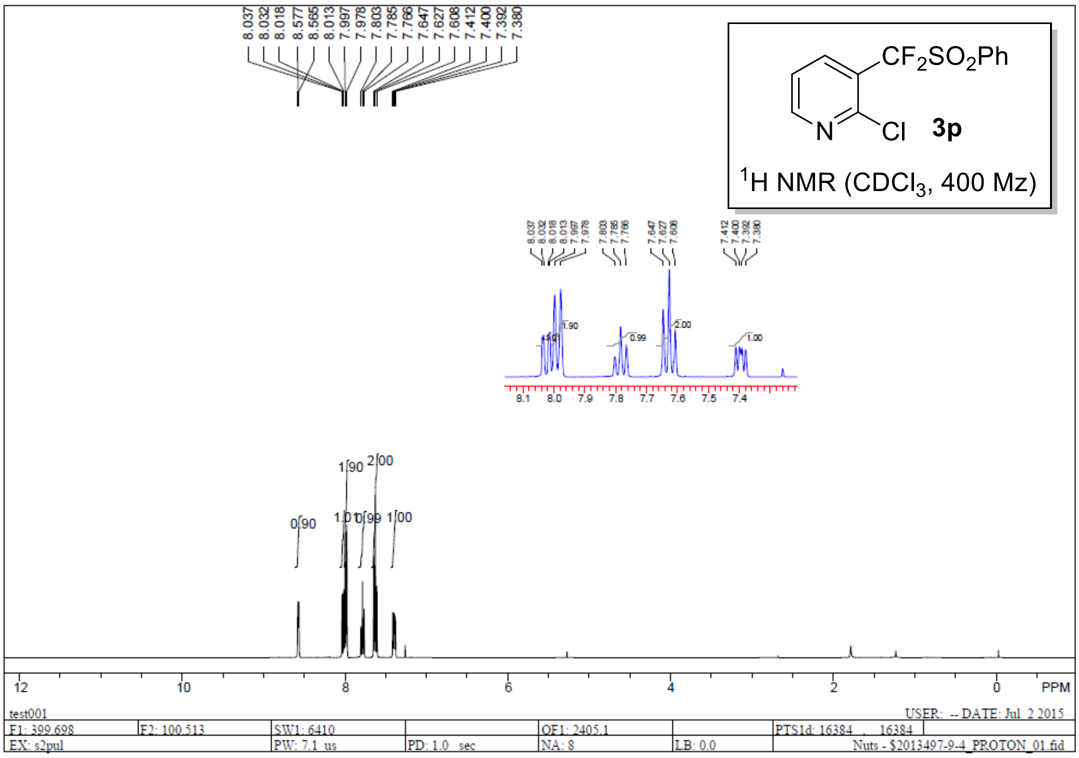
3o

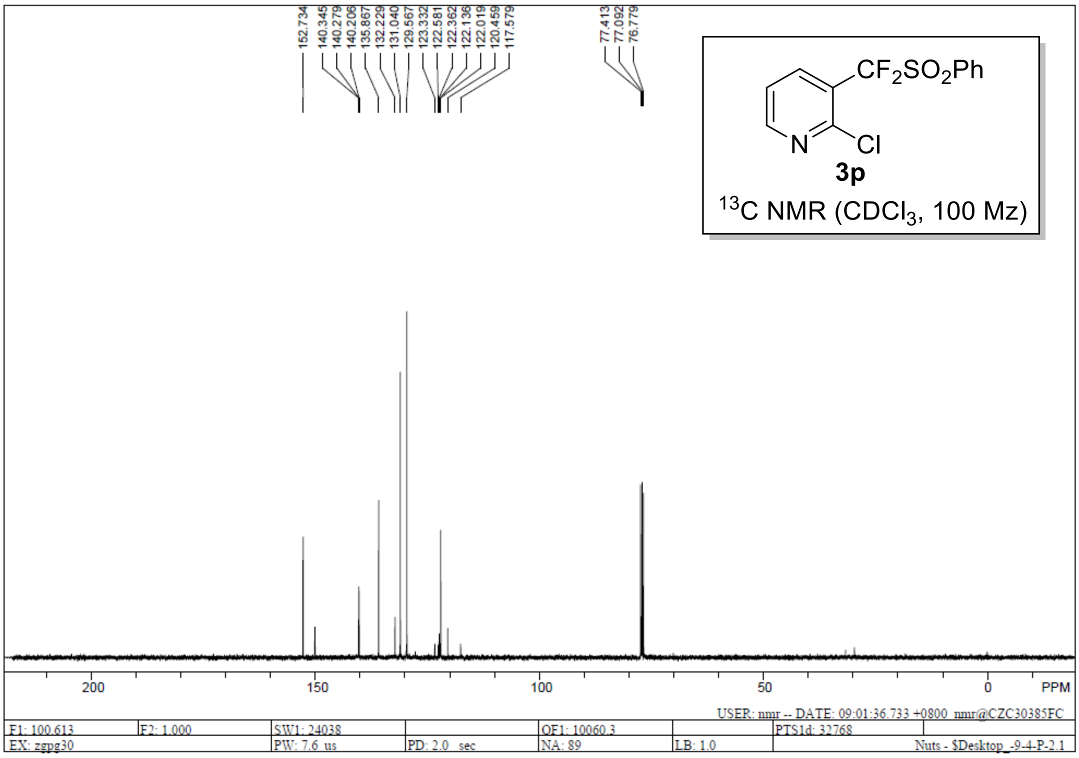
^{13}C NMR ($CDCl_3$, 100 Mz)

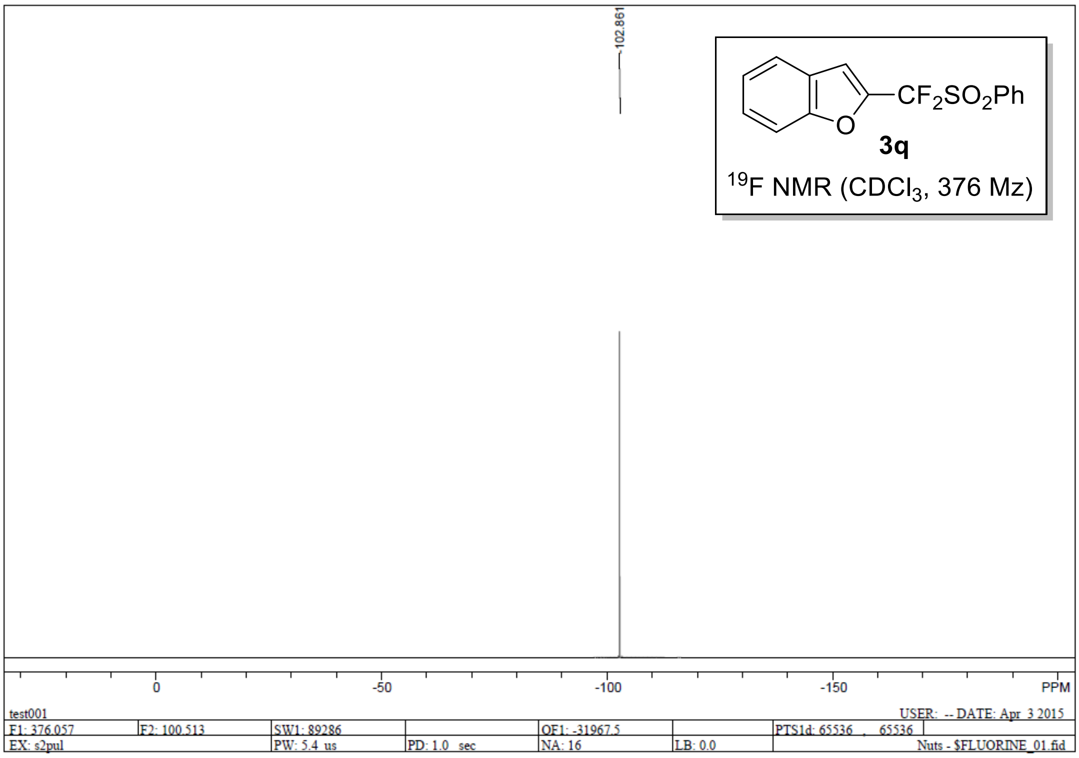


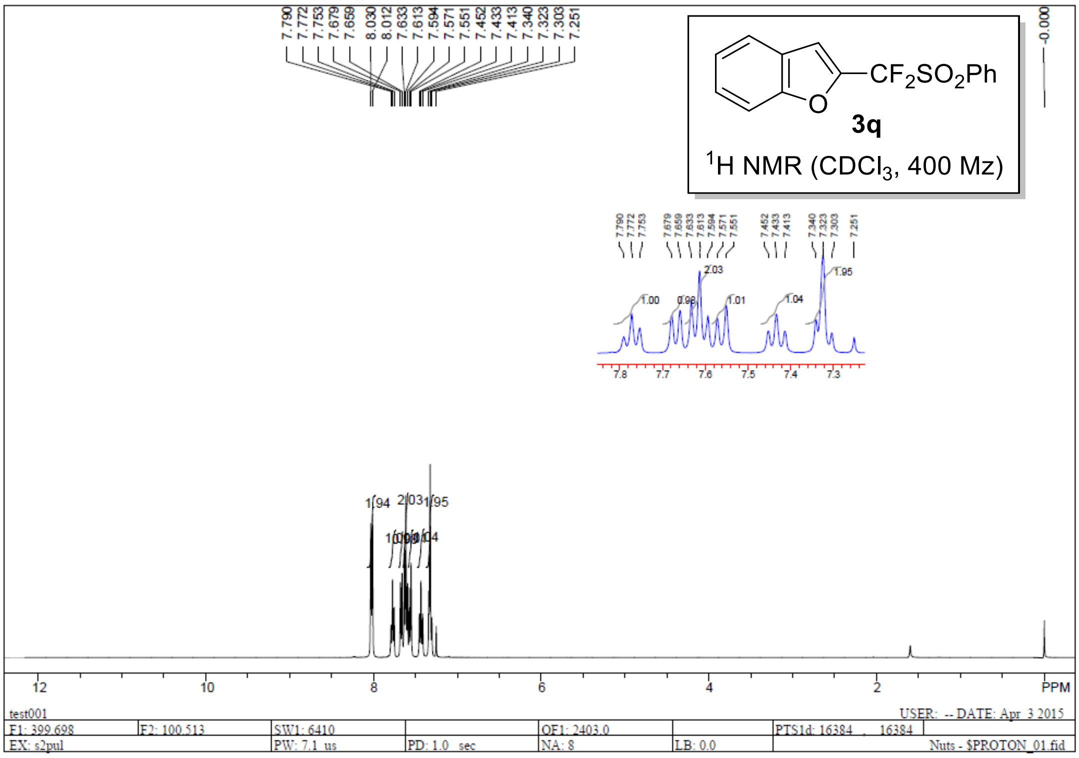
3p

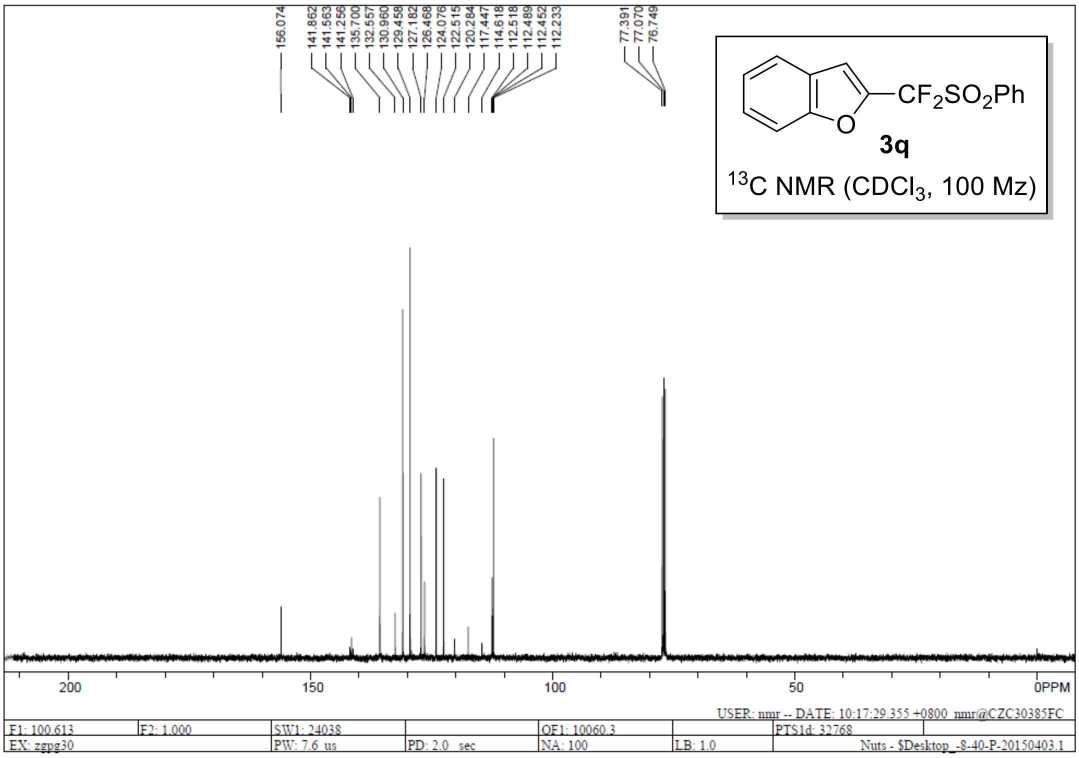
^{19}F NMR ($CDCl_3$, 376 Mz)

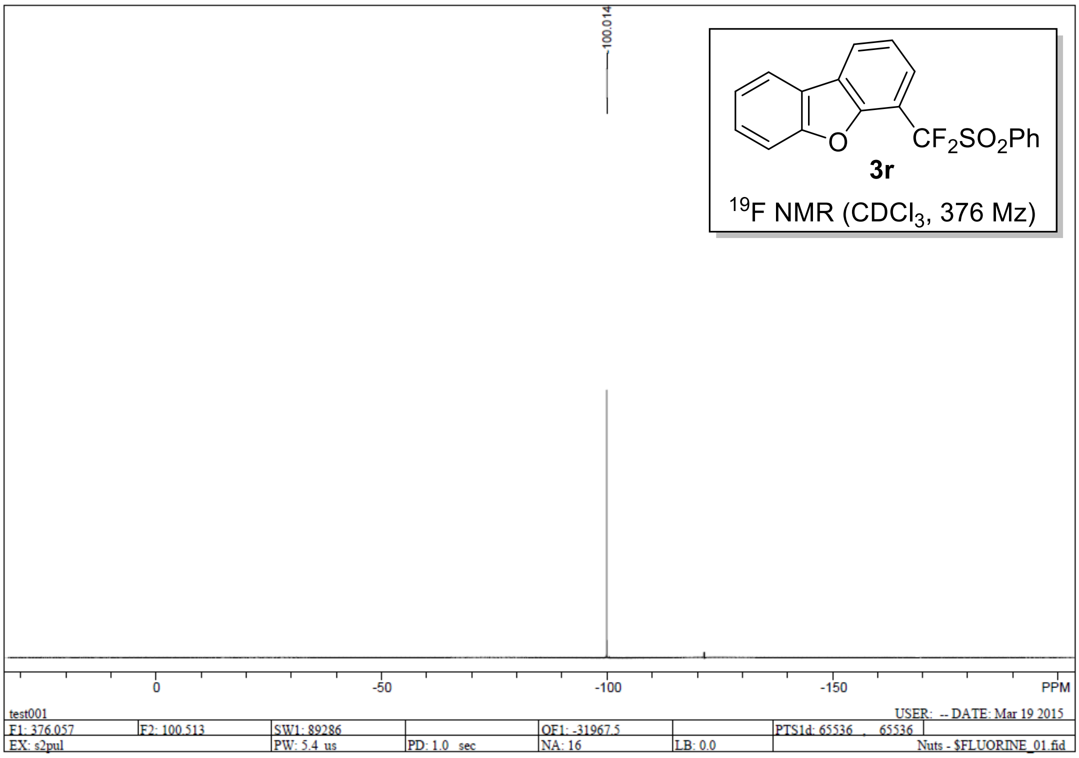

8.037
8.032
8.018
8.577
8.565
8.013
7.997
7.978
7.803
7.785
7.766
7.647
7.627
7.608
7.412
7.400
7.392
7.380
CF2SO2Ph
N
Cl
3p
1H NMR (CDCl3, 400 Mz)
1.01
1.90
0.99
2.00
1.00
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
0.90
1.90
2.00
1.01
0.99
1.00
12
10
8
6
4
2
0
PPM
test001
USER: -- DATE: Jul 2 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2405.1
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $2013497-9-4_PROTON_01.fid

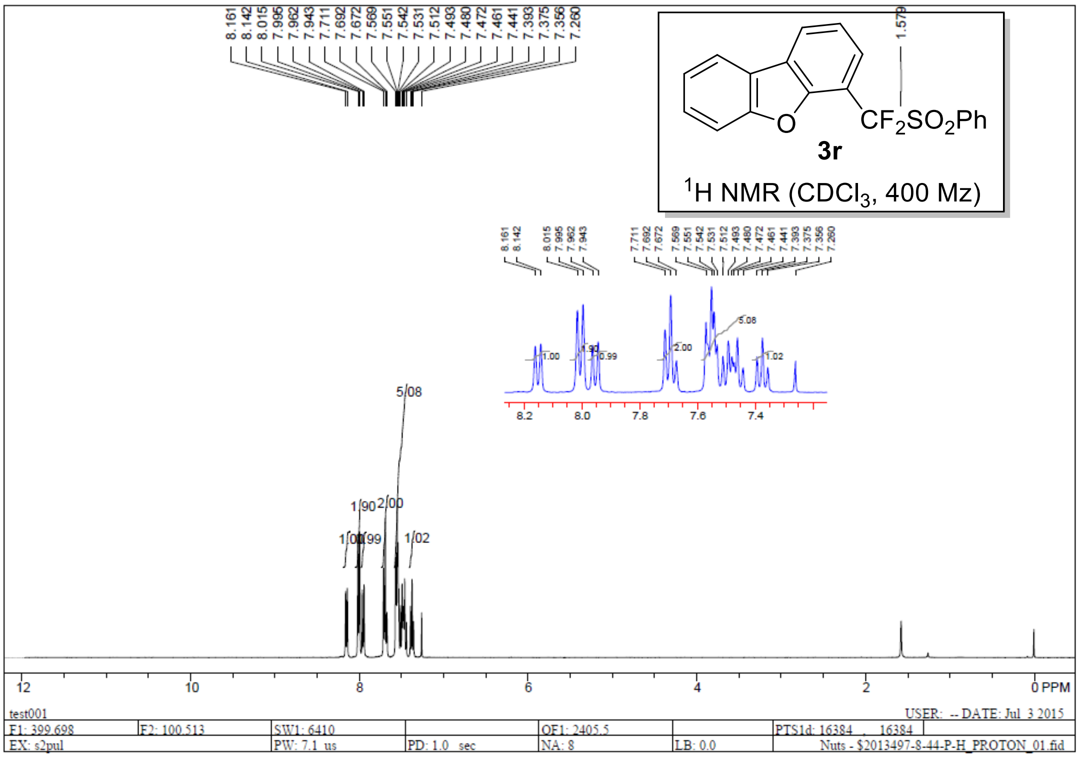

152.734
140.345
140.279
140.206
135.867
132.229
131.040
129.567
123.332
122.581
122.362
122.136
122.019
120.459
117.579
77.413
77.092
76.779
CF2SO2Ph
N
Cl
3p
13C NMR (CDCl3, 100 Mz)
200
150
100
50
0
PPM
USER: nmr -- DATE: 09:01:36.733 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 89
LB: 1.0
Nuts - $Desktop_-9-4-P-2.1

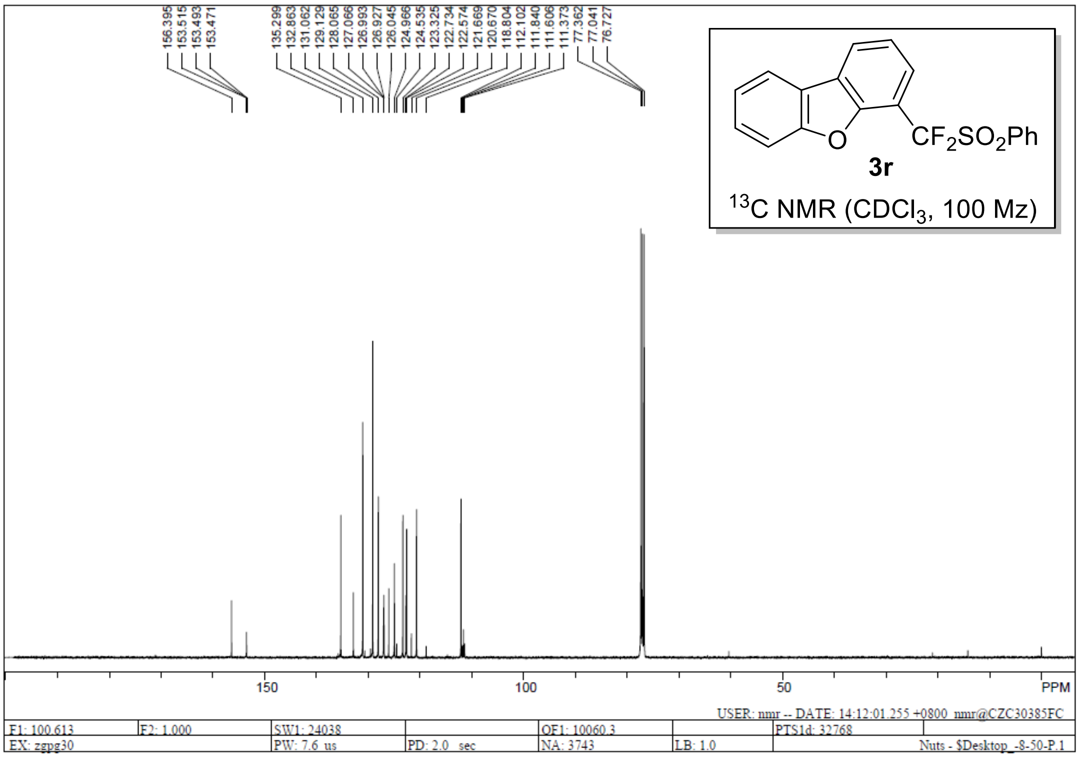

-102.861
CF2SO2Ph
O
3q
19F NMR (CDCl3, 376 Mz)
0
-50
-100
-150
PPM
test001
USER: -- DATE: Apr 3 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid

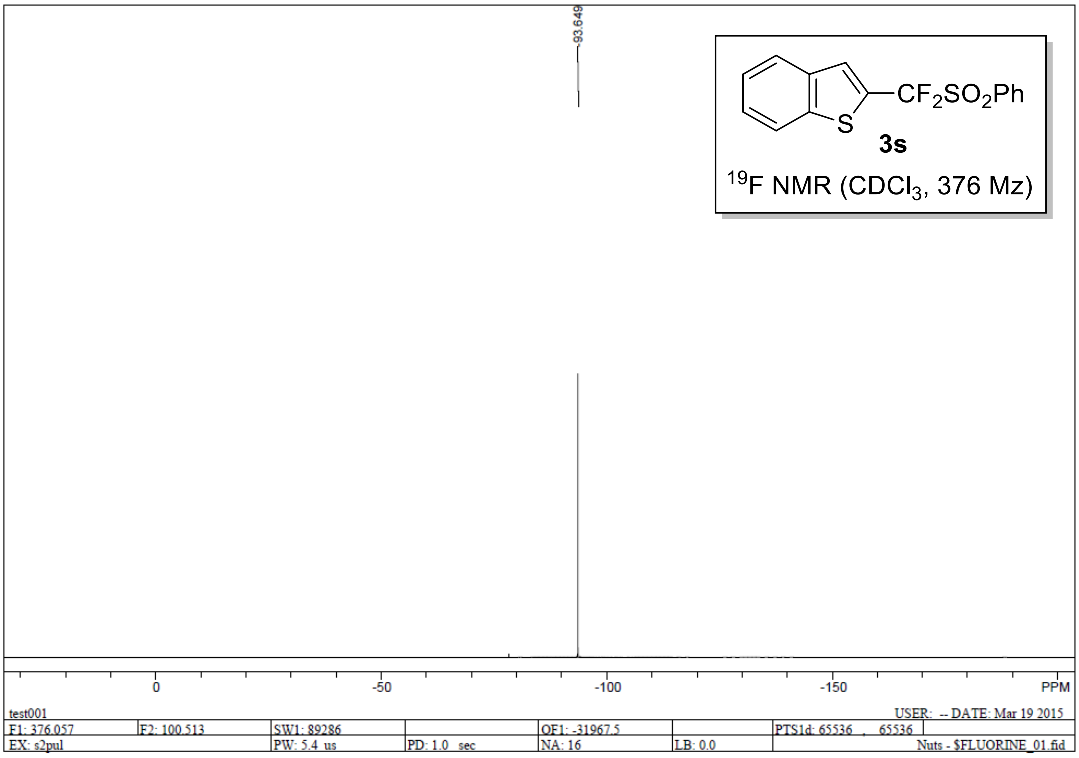

7.790
7.772
7.753
7.679
7.659
8.030
8.012
7.633
7.613
7.594
7.571
7.551
7.452
7.433
7.413
7.340
7.323
7.303
7.251
-0.000
CF2SO2Ph
O
3q
1H NMR (CDCl3, 400 Mz)
1.00
0.98
2.03
1.01
1.04
1.95
7.8
7.7
7.6
7.5
7.4
7.3
1.94
12
10
8
6
4
2
PPM
test001
USER: -- DATE: Apr 3 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2403.0
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

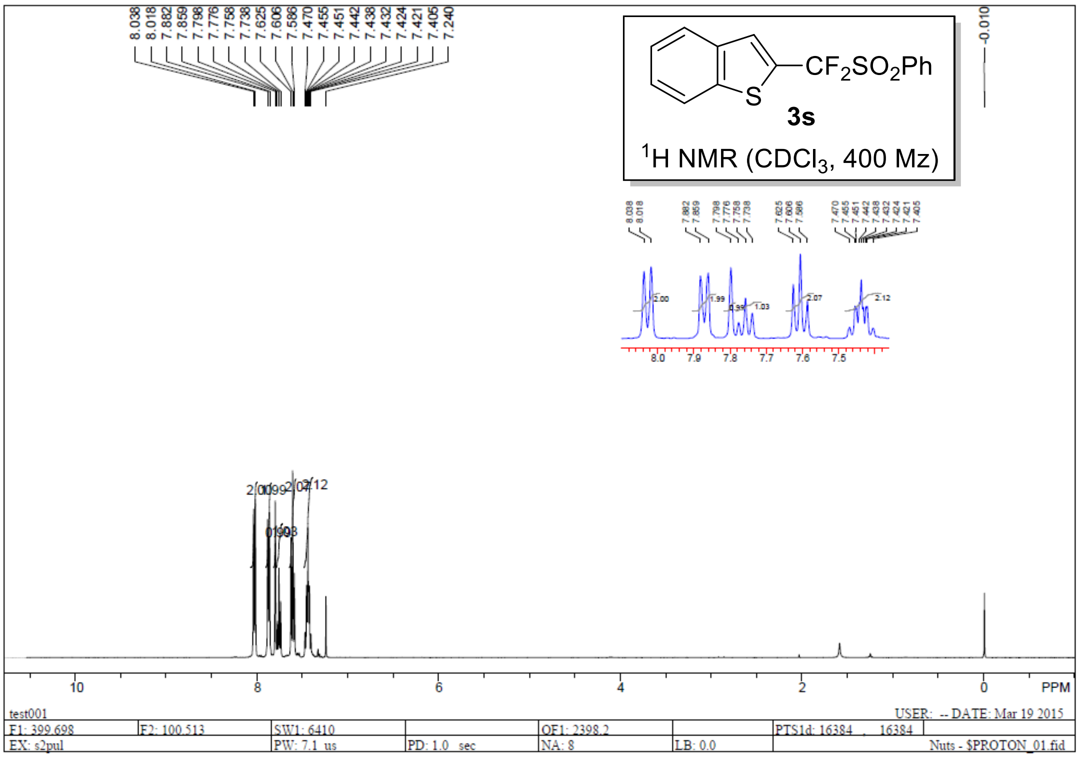

156.074
141.862
141.563
141.256
135.700
132.557
130.960
129.458
127.182
126.468
124.076
122.515
120.284
117.447
114.618
112.518
112.489
112.452
112.233
77.391
77.070
76.749
CF2SO2Ph
O
3q
13C NMR (CDCl3, 100 Mz)
200
150
100
50
0PPM
USER: nmr -- DATE: 10:17:29.355 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 100
LB: 1.0
Nuts - $Desktop_-8-40-P-20150403.1

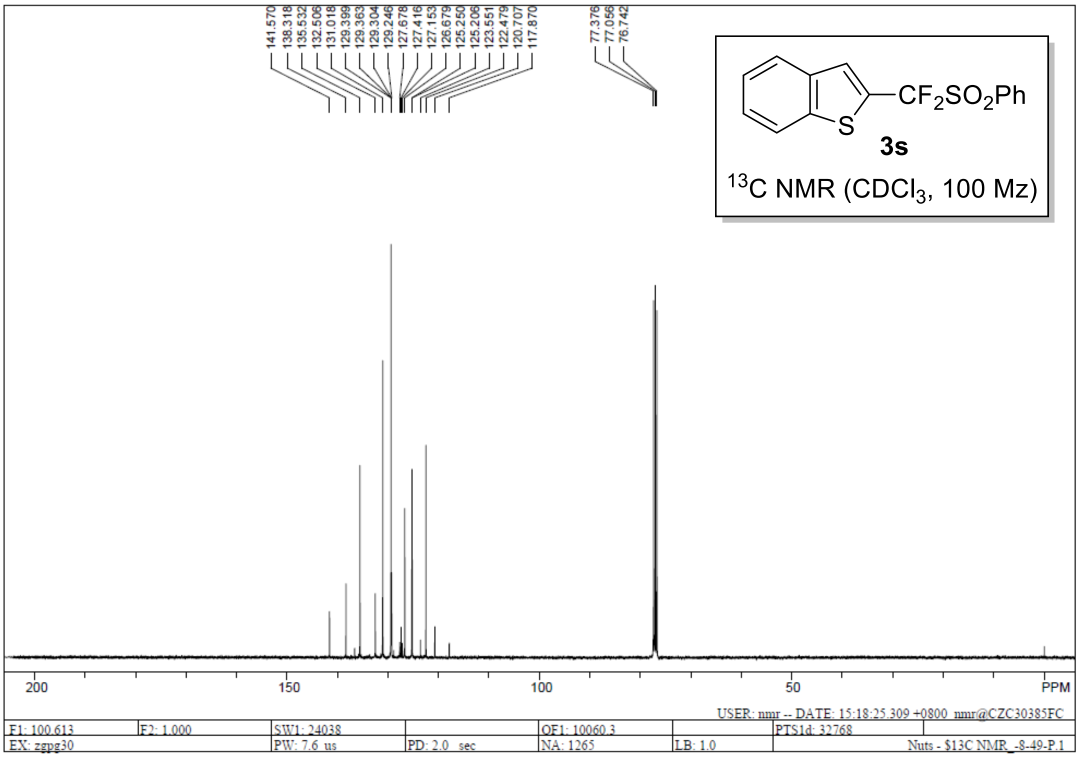

100.014
O
CF2SO2Ph
3r
19F NMR (CDCl3, 376 Mz)
0
-50
-100
-150
PPM
test001
USER: -- DATE: Mar 19 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid

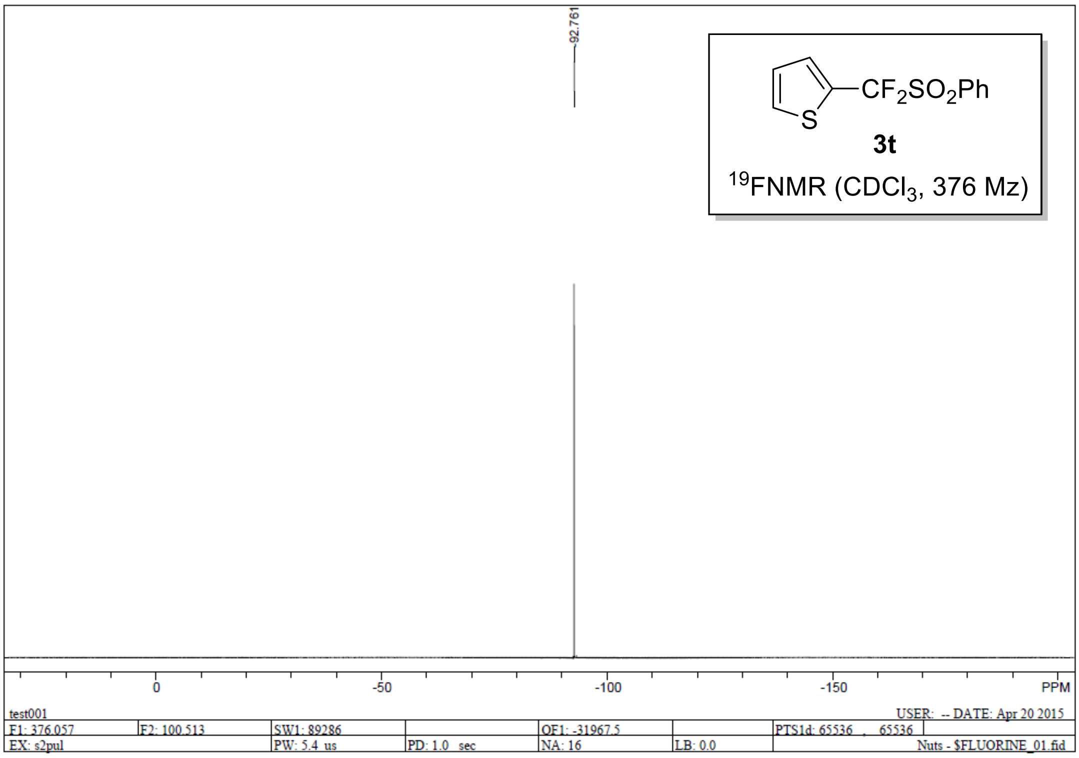

8.161 8.142 8.015 7.995 7.962 7.943 7.711 7.692 7.672 7.569 7.551 7.542 7.531 7.512 7.493 7.480 7.472 7.461 7.441 7.393 7.375 7.356 7.260
1.579
CF2SO2Ph
O
3r
1H NMR (CDCl3, 400 Mz)
1.00 1.90 0.99 2.00 5.08 1.02
8.2 8.0 7.8 7.6 7.4
12 10 8 6 4 2 0 PPM
test001
USER: -- DATE: Jul 3 2015
F1: 399.698 F2: 100.513 SW1: 6410 OF1: 2405.5 PTS1d: 16384 16384
EX: s2pul PW: 7.1 us PD: 1.0 sec NA: 8 LB: 0.0 Nuts - $2013497-8-44-P-H_PROTON_01.fid

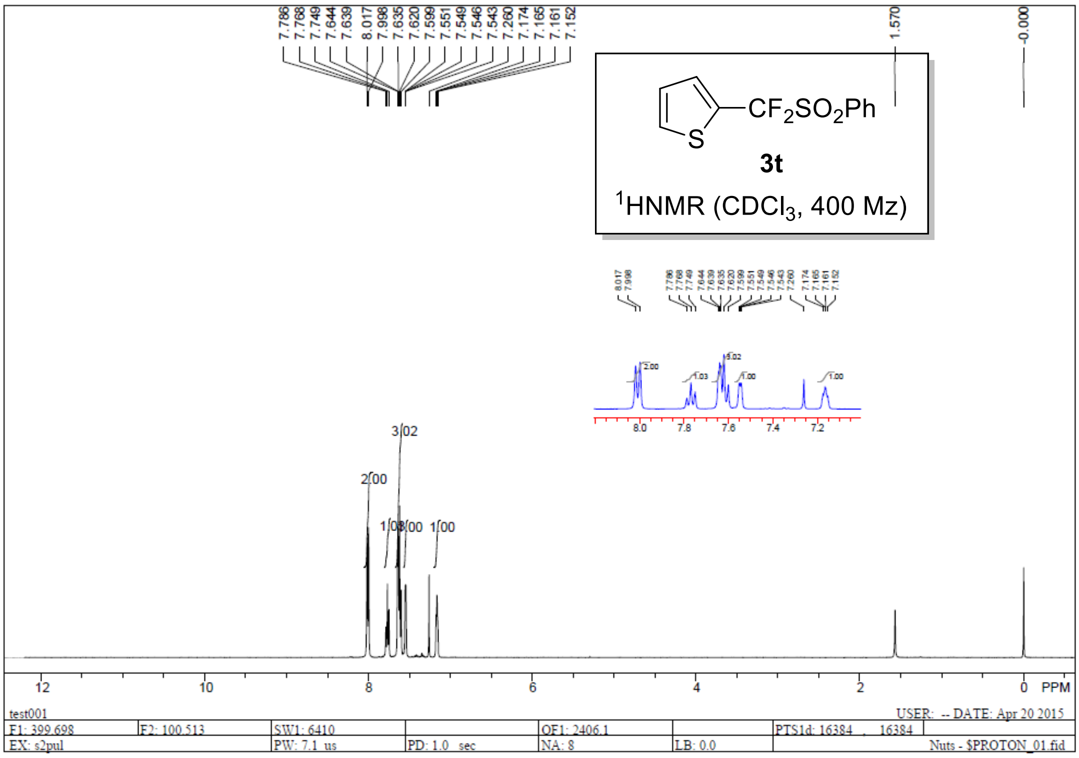

156.395 153.515 153.493 153.471 135.299 132.863 131.062 129.129 128.065 127.066 126.993 126.927 126.045 124.966 124.535 123.325 122.734 122.574 121.669 120.670 118.804 112.102 111.840 111.606 111.373 77.362 77.041 76.727
CF2SO2Ph
O
3r
13C NMR (CDCl3, 100 Mz)
150 100 50 PPM
USER: nmr -- DATE: 14:12:01.255 +0800 nmr@CZC30385FC
F1: 100.613 F2: 1.000 SW1: 24038 OF1: 10060.3 PTS1d: 32768
EX: zgpg30 PW: 7.6 us PD: 2.0 sec NA: 3743 LB: 1.0 Nuts - $Desktop_-8-50-P.1

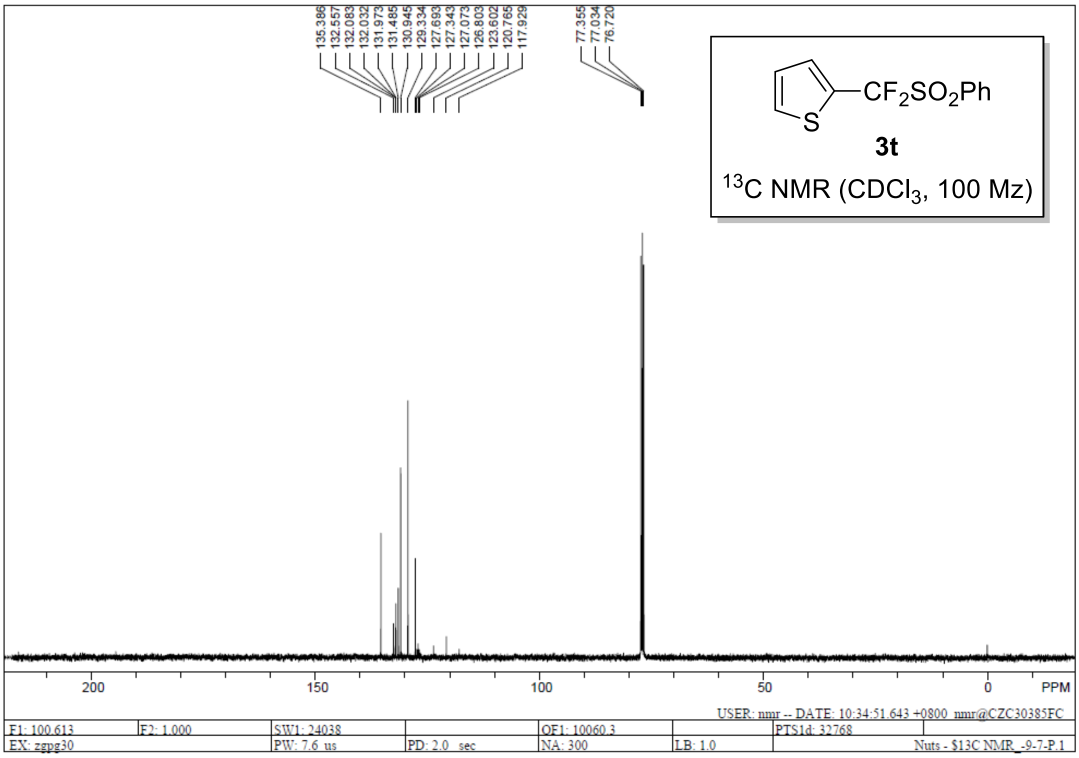

-93.649
CF$_2$SO$_2$Ph
S
3s
^{19}F NMR (CDCl$_3$, 376 Mz)
0
-50
-100
-150
PPM
test001
USER: -- DATE: Mar 19 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid

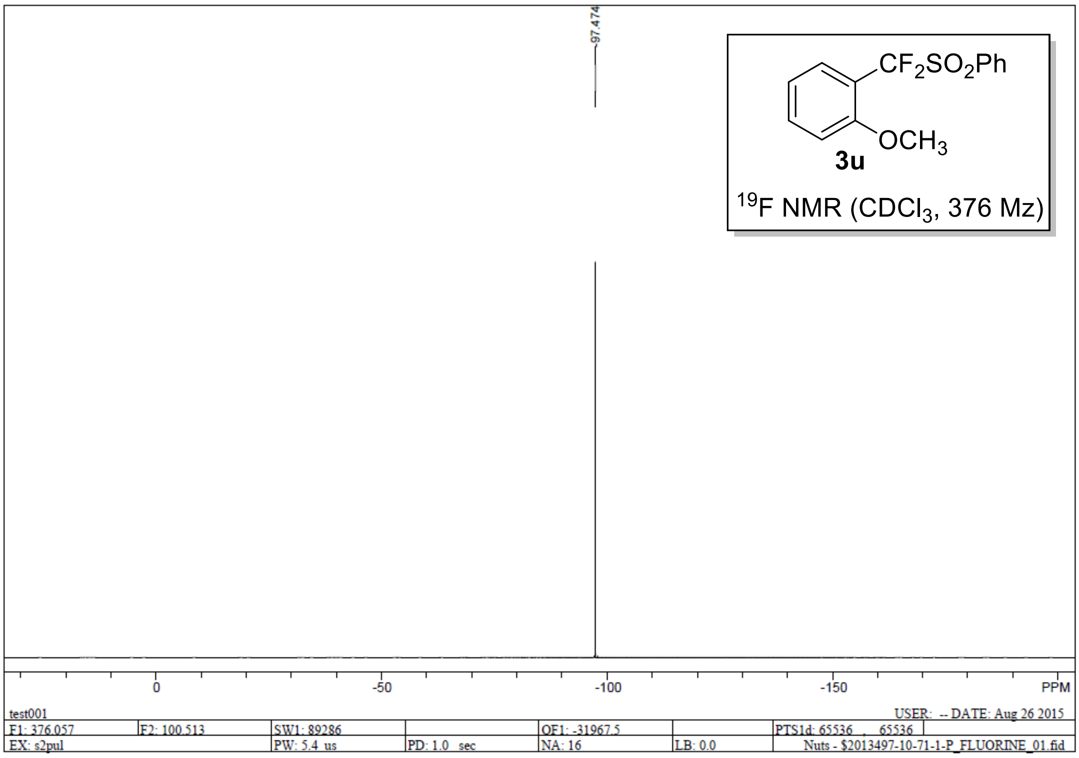

8.038
8.018
7.882
7.859
7.798
7.776
7.758
7.738
7.625
7.606
7.586
7.470
7.455
7.451
7.442
7.438
7.432
7.424
7.421
7.405
7.240
-0.010
CF$_2$SO$_2$Ph
S
3s
^{1}H NMR (CDCl$_3$, 400 Mz)
2.00
1.99
0.99
1.03
2.07
2.12
8.0
7.9
7.8
7.7
7.6
7.5
10
8
6
4
2
0
PPM
test001
USER: -- DATE: Mar 19 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2398.2
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

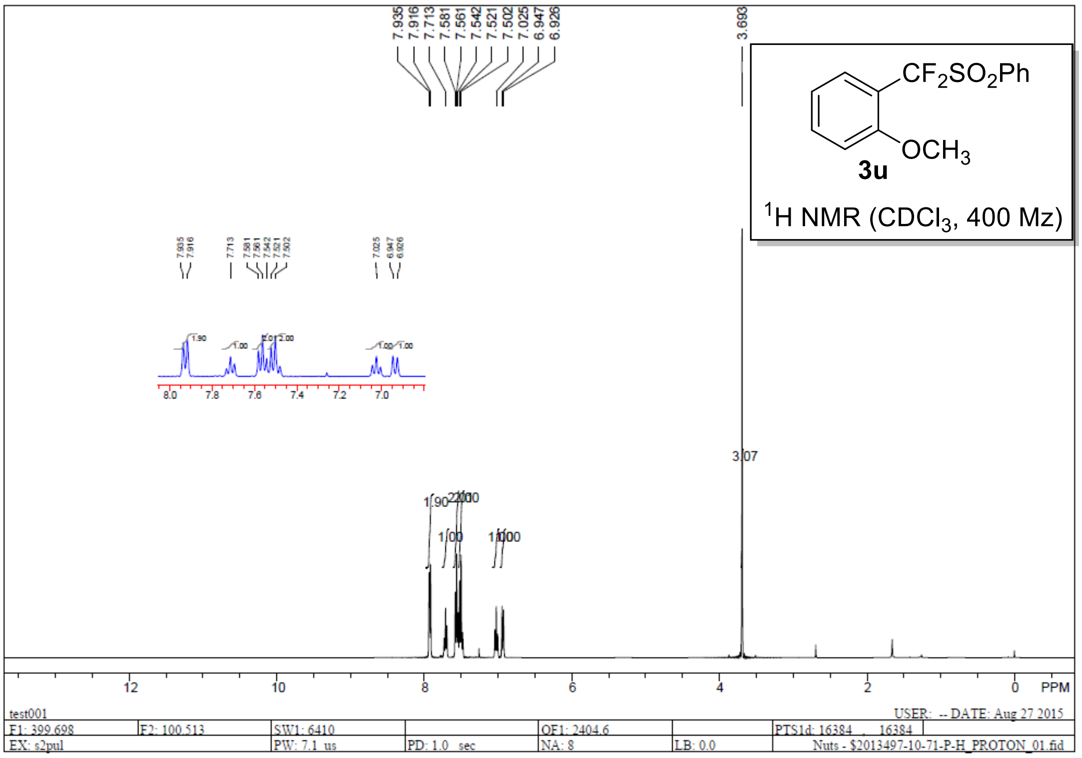

141.570
138.318
135.532
132.506
131.018
129.399
129.363
129.304
129.246
127.678
127.416
127.153
126.679
125.250
125.206
123.551
122.479
120.707
117.870
77.376
77.056
76.742
CF2SO2Ph
S
3s
13C NMR (CDCl3, 100 Mz)
200
150
100
50
PPM
USER: nmr -- DATE: 15:18:25.309 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 1265
LB: 1.0
Nuts - $13C NMR_-8-49-P.1

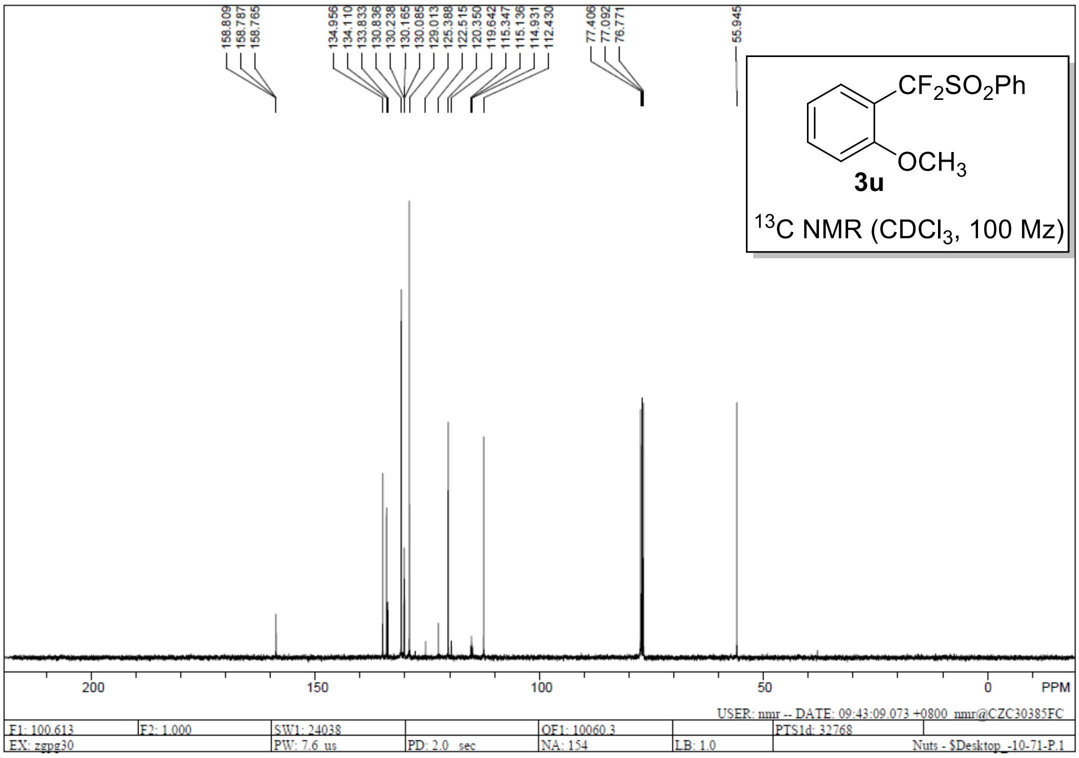

-92.761
CF2SO2Ph
S
3t
19FNMR (CDCl3, 376 Mz)
0
-50
-100
-150
PPM
test001
USER: -- DATE: Apr 20 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE_01.fid

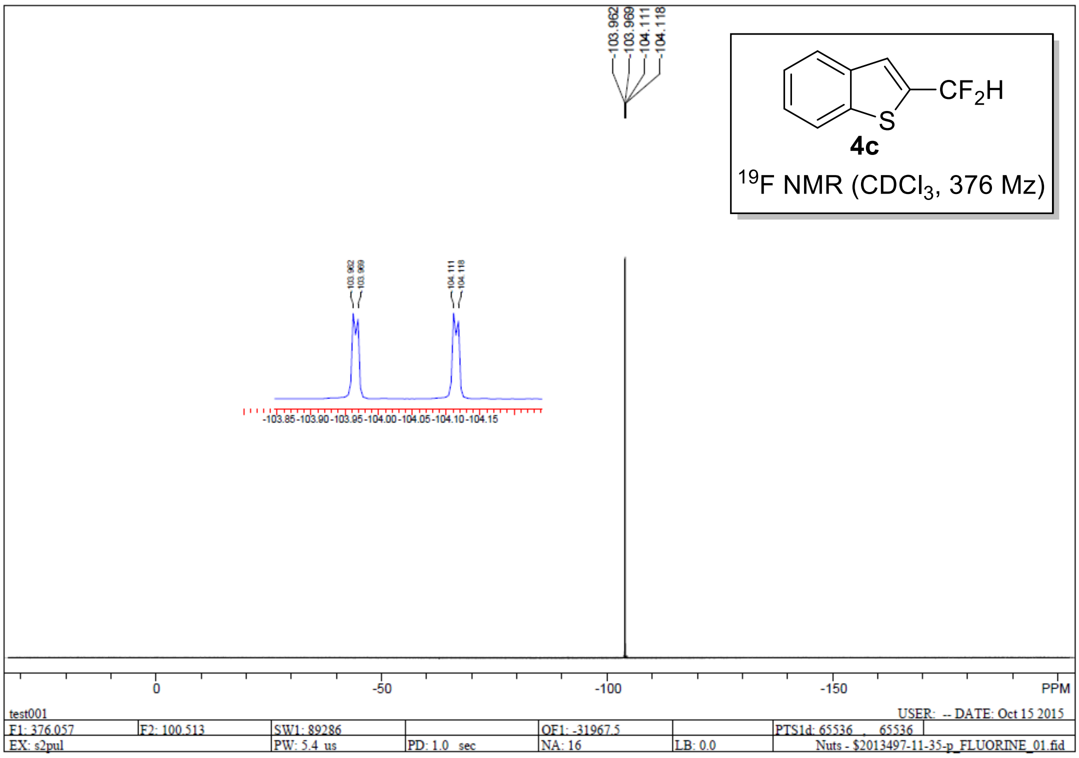

7.786
7.768
7.749
7.644
7.639
8.017
7.998
7.635
7.620
7.599
7.551
7.549
7.546
7.543
7.260
7.174
7.165
7.161
7.152
1.570
-0.000
CF2SO2Ph
S
3t
1HNMR (CDCl3, 400 Mz)
2.00
1.03
3.02
1.00
1.00
8.0
7.8
7.6
7.4
7.2
12
10
8
6
4
2
0
PPM
test001
USER: -- DATE: Apr 20 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2406.1
PTS1d: 16384 . 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

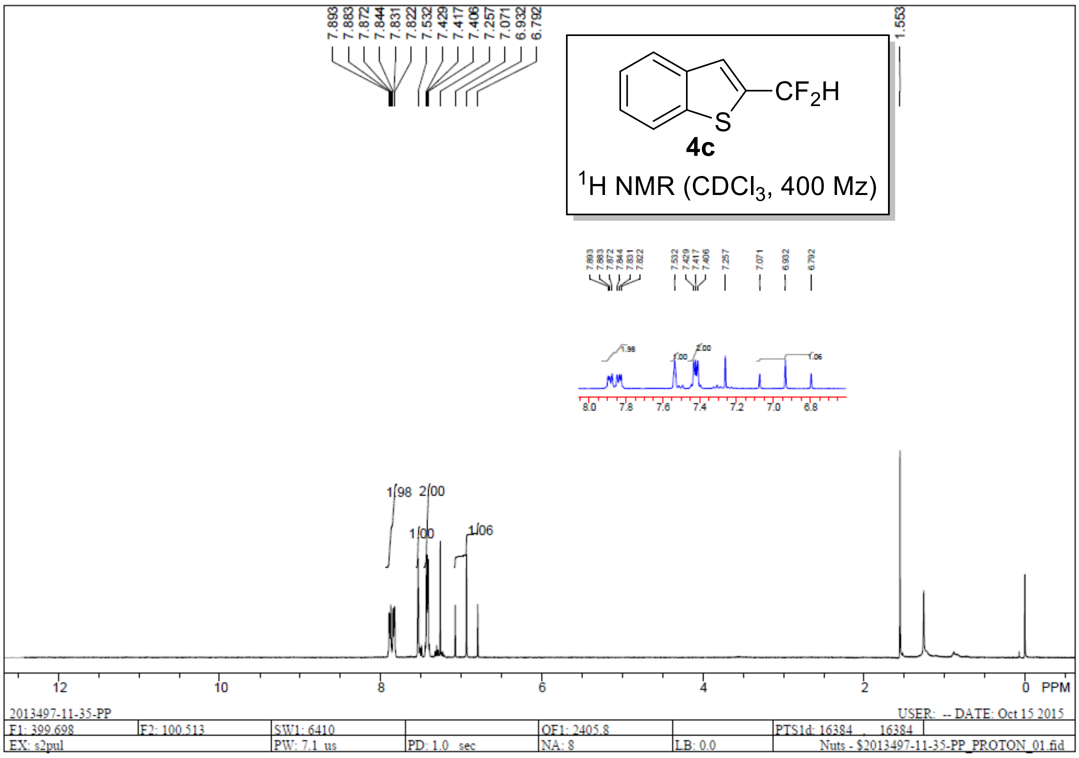

135.386
132.557
132.083
132.032
131.973
131.485
130.945
129.334
127.693
127.343
127.073
126.803
123.602
120.765
117.929
77.355
77.034
76.720
CF2SO2Ph
S
3t
13C NMR (CDCl3, 100 Mz)
200
150
100
50
0
PPM
USER: nmr -- DATE: 10:34:51.643 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 300
LB: 1.0
Nuts - $13C NMR_-9-7-P.1

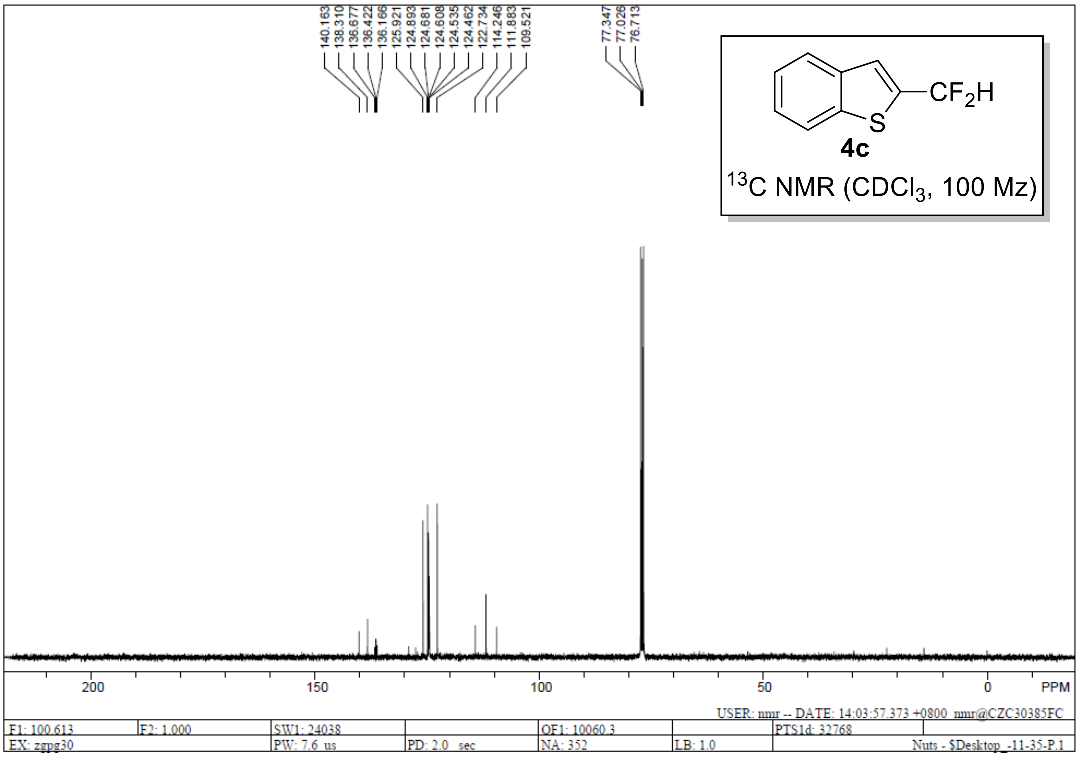

-97.474
CF2SO2Ph
OCH3
3u
19F NMR (CDCl3, 376 Mz)
0
-50
-100
-150
PPM
test001
USER: -- DATE: Aug 26 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $2013497-10-71-1-P_FLUORINE_01.fid


7.935
7.916
7.713
7.581
7.561
7.542
7.521
7.502
7.025
6.947
6.926
3.693
CF2SO2Ph
OCH3
3u
1H NMR (CDCl3, 400 Mz)
1.90
1.00
2.01
2.00
1.00
1.00
8.0
7.8
7.6
7.4
7.2
7.0
3.07
12
10
8
6
4
2
0
PPM
test001
USER: -- DATE: Aug 27 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2404.6
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $2013497-10-71-P-H_PROTON_01.fid


158.809
158.787
158.765
134.956
134.110
133.833
130.836
130.238
130.165
130.085
129.013
125.388
122.515
120.350
119.642
115.347
115.136
114.931
112.430
77.406
77.092
76.771
55.945
CF2SO2Ph
OCH3
3u
13C NMR (CDCl3, 100 Mz)
200
150
100
50
0
PPM
USER: nmr -- DATE: 09:43:09.073 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 154
LB: 1.0
Nuts - $Desktop_-10-71-P.1


-103.962
-103.969
-104.111
-104.118
CF2H
S
4c
19F NMR (CDCl3, 376 Mz)
103.962
103.969
104.111
104.118
-103.85
-103.90
-103.95
-104.00
-104.05
-104.10
-104.15
0
-50
-100
-150
PPM
test001
USER: -- DATE: Oct 15 2015
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.5
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $2013497-11-35-p_FLUORINE_01.fid


7.893
7.883
7.872
7.844
7.831
7.822
7.532
7.429
7.417
7.406
7.257
7.071
6.932
6.792
1.553
CF$_2$H
S
4c
^{1}H NMR (CDCl$_3$, 400 Mz)
1.98
1.00
2.00
1.06
8.0
7.8
7.6
7.4
7.2
7.0
6.8
12
10
8
6
4
2
0
PPM
2013497-11-35-PP
USER: -- DATE: Oct 15 2015
F1: 399.698
F2: 100.513
SW1: 6410
OF1: 2405.8
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $2013497-11-35-PP_PROTON_01.fid


140.163
138.310
136.677
136.422
136.166
125.921
124.893
124.681
124.608
124.535
124.462
122.734
114.246
111.883
109.521
77.347
77.026
76.713
CF$_2$H
S
4c
^{13}C NMR (CDCl$_3$, 100 Mz)
200
150
100
50
0
PPM
USER: nmr -- DATE: 14:03:57.373 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 352
LB: 1.0
Nuts - $Desktop_-11-35-P.1