Supporting Information

Copper-Mediated Trifluoromethylation Using Phenyl Trifluoromethyl Sulfoxide

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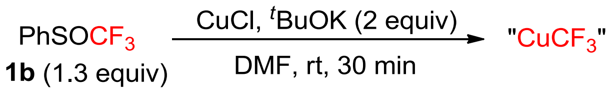
1. General Information

Commercial reagents were used without further purification. All solvents were dried from CaH_2 and purified by distillation before being used. CuCl and CuI were purified according to reported procedures. Phenyl trifluoromethyl sulfone (**1a**) or sulfoxide (**1b**) was obtained by distillation. ^{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 $PhOCF_3$ at δ –57.8 or $PhCF_3$ 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). Mass spectra were obtained on a Finnigan GC-MS 4021 instrument. All reactions were monitored by TLC, ^{19}F NMR spectroscopy, or GC-MS.

2. Preparation of “$CuCF_3$” Generated from $PhSOCF_3$



$$\underset{\textbf{1b}\ (1.3\ \text{equiv})}{PhSOCF_3} \xrightarrow[\text{DMF, rt, 30 min}]{\text{CuCl, }{}^t\text{BuOK (2 equiv)}} \text{"}CuCF_3\text{"}$$

In a glovebox, CuCl (29.7 mg, 0.3 mmol) and ^{t}BuOK (67.2 mg, 0.6 mmol) were added to an oven-dried 10mL Schlenk tube equipped with a stir bar. Then the Schlenk tube was sealed with a septum and brought to the bench. DMF (1 mL) was added and stirred at room temperature for 30 min, then phenyl trifluoromethyl sulfoxide **1b** (75.7 mg, 0.39 mmol) was added at the same temperature for 30 min under argon atmosphere. The reaction was monitored by ^{19}F NMR spectroscopy using $PhOCF_3$ as an internal standard.

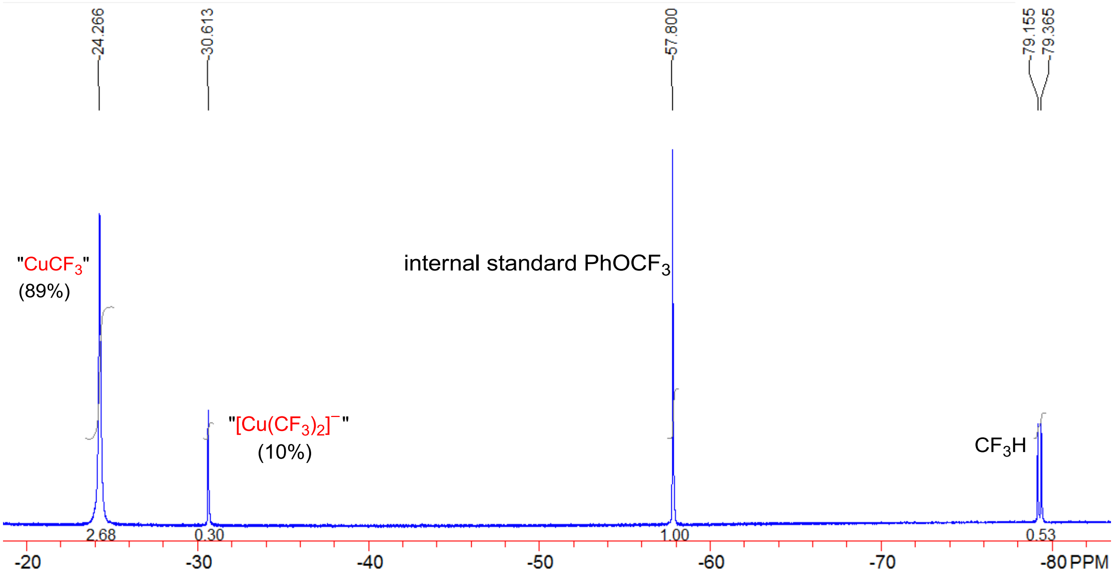


Figure S1. Preparation of “$CuCF_3$” generated from $PhSOCF_3$

3. The Comparison of $PhSO_2CF_3$ and $PhSOCF_3$ in the Generation of “$CuCF_3$”

Experiment Procedures for **A**, **B1** and **B2**:

In a glovebox, CuCl (29.7 mg, 0.3 mmol) and ^{t}BuOK (**A**, **B1**: 67.2 mg, 0.6 mmol; **B2**: 100.8 mg, 0.9 mmol) were added to an oven-dried 10mL Schlenk tube equipped with a stir bar. Then the Schlenk tube was sealed with a septum and brought to the bench. DMF (1 mL) was added and stirred at room temperature for 30 min, and then **1b** (58.2 mg, 0.3 mmol) or **1a** (63mg, 0.3 mmol) was added at the same temperature for 30 min under argon atmosphere. The reaction was monitored by ^{19}F NMR spectroscopy using $PhOCF_3$ as an internal standard.

Experiment Procedure for **C**:

In a glovebox, CuCl (29.7 mg, 0.3 mmol) and ^{t}BuOK (67.2 mg, 0.6 mmol) were added to an oven-dried 10mL Schlenk tube equipped with a stir bar. Then the Schlenk tube was sealed with a septum and brought to the bench. DMF (1 mL) was added and stirred at room temperature for 30 min, then **1b** (58.2 mg, 0.3 mmol) and **1a** (63mg, 0.3 mmol) were added at the same temperature for 30 min under argon atmosphere. The reaction was monitored by ^{19}F NMR spectroscopy using $PhCF_3$ as an internal standard.

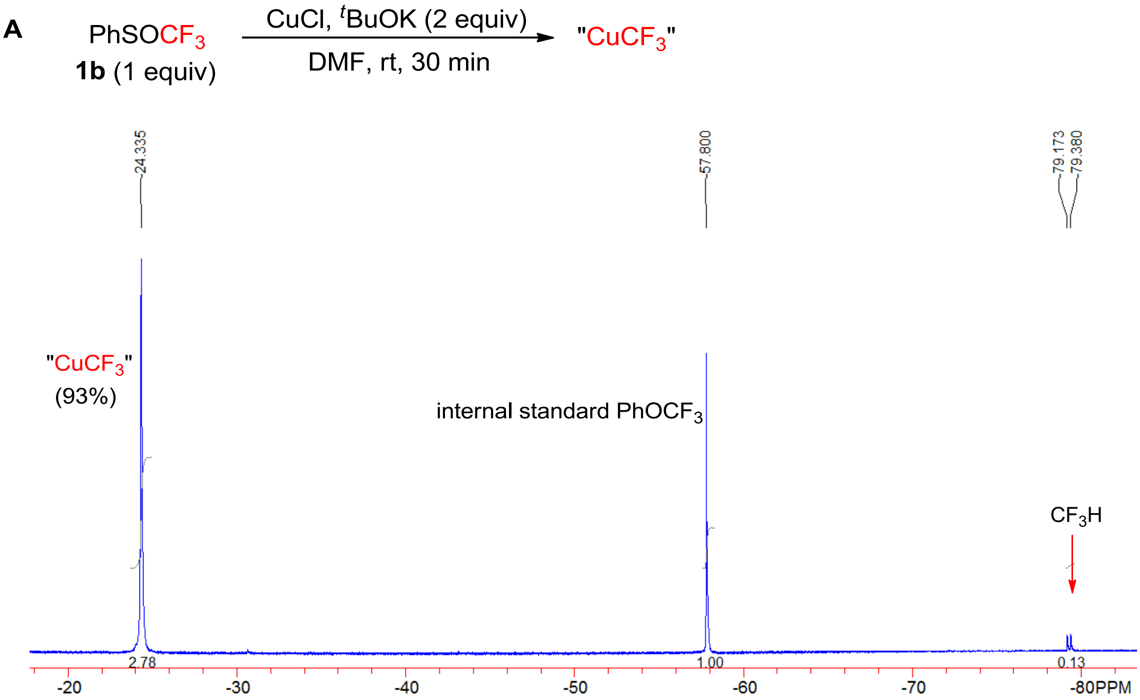


Figure S2. Preparation of “CuCF$_3$” generated from PhSOCF$_3$

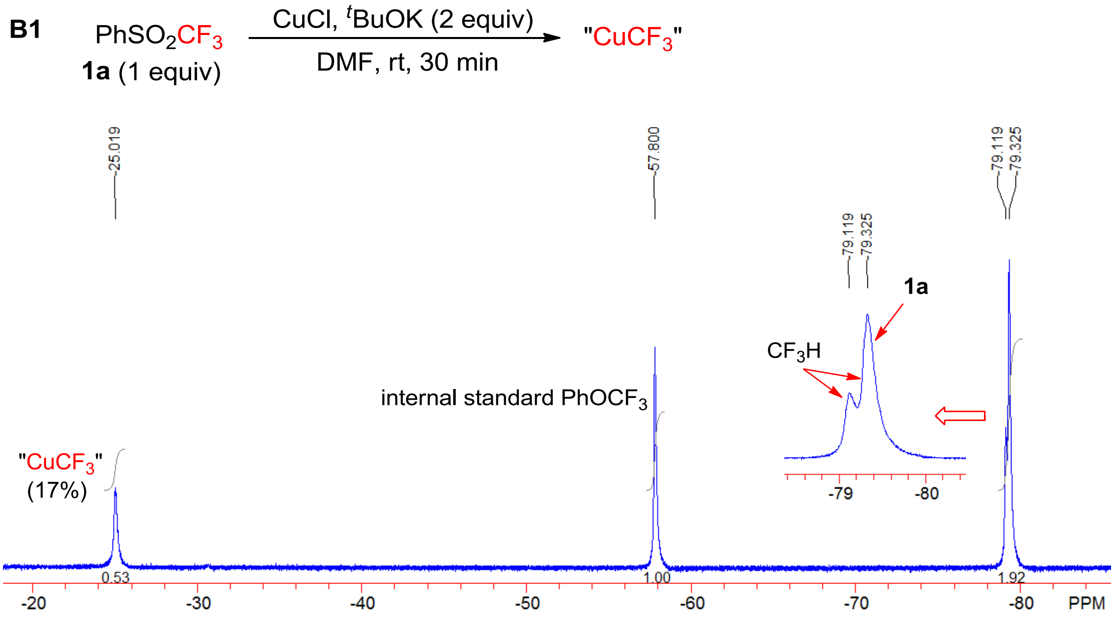


Figure S3. Preparation of “CuCF$_3$” generated from PhSO$_2$CF$_3$

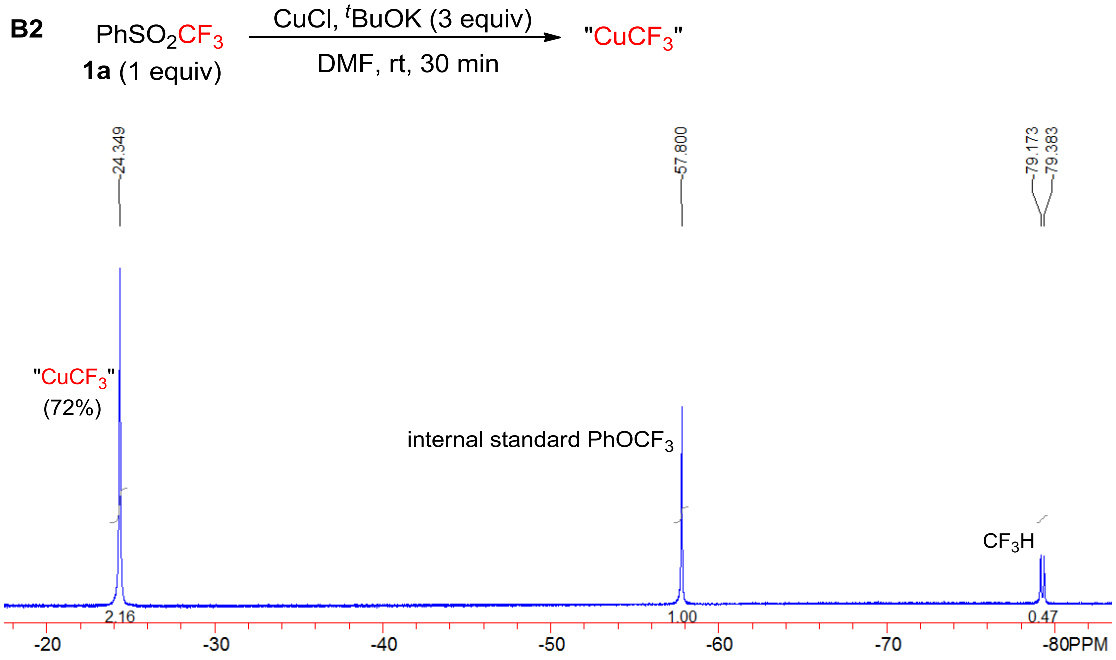


Figure S4. Preparation of "$CuCF_3$" generated from $PhSO_2CF_3$

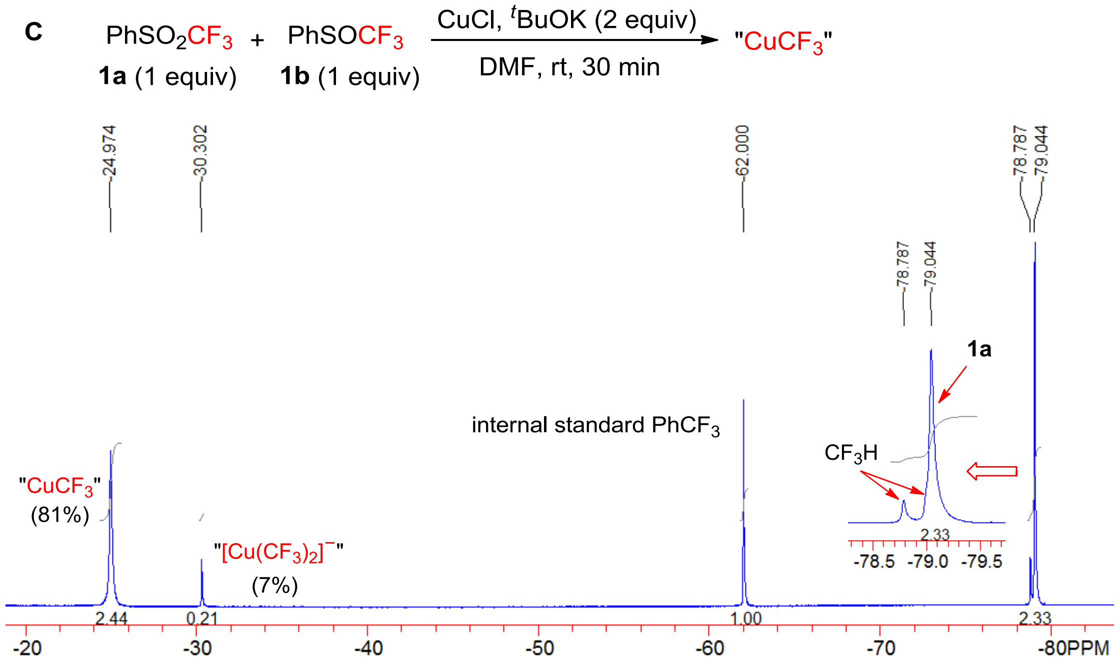


Figure S5. The Comparison of $PhSO_2CF_3$ and $PhSOCF_3$ in the Generation of "$CuCF_3$"

Summary of Results:

(1) $PhSOCF_3$ is more reactive than $PhSO_2CF_3$ to generate "$CuCF_3$" under the standard conditions.

(2) The formation of "$CuCF_3$" generated from $PhSOCF_3$ is fast, less than 30 min.

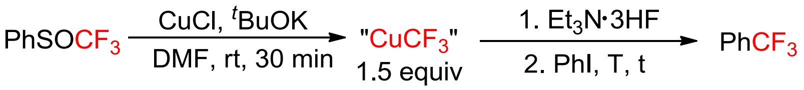
(3) A relatively greater excess of ${}^tBuOK$ (compared to sulfoxide) could promote $PhSO_2CF_3$ to generate "$CuCF_3$".

4. Trifluoromethylation of Aryl Halides with “$CuCF_3$” Generated from $PhSOCF_3$

4.1 Screening Reaction Conditions

In a glovebox, CuCl (29.7 mg, 0.3 mmol) and ^{t}BuOK (67.2 mg, 0.6 mmol) were added to an oven-dried 10mL Schlenk tube equipped with a stir bar. Then the Schlenk tube was sealed with a septum and brought to the bench. DMF (1 mL) was added and stirred at room temperature for 30 min, and then **1b** (75.7 mg, 0.39 mmol) was added at the same temperature for 30 min under argon atmosphere. After the pregenerated “$CuCF_3$” species was stabilized by $Et_3N\cdot 3HF$ (25μL, 0.1 mmol), iodobenzene (40.8 mg, 0.2 mmol) was added. The reaction was monitored by ^{19}F NMR spectroscopy using $PhOCF_3$ as an internal standard.

Table S1. Screening of Reaction Conditions



entry	$Et_3N\cdot 3HF$ (equiv)	T (°C)	t (h)	conversion (%) ("$CuCF_3$")	yield (%) (^{19}F NMR)
1	0.5	20	24	< 2	< 1
2	0.5	50	28	49	50
3	0.42	75	28	77	80
4	0.5	75	22	84	88
5	**0.5**	**80**	**24**	**> 98**	**92**
6	0.6	80	20	> 99	85

4.2 Trifluoromethylation of Aryl Halides with “$CuCF_3$” Generated from $PhSOCF_3$

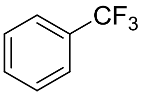
Typical Experiment Procedure on 0.1-mmol Scale (2a, 2d, 2e, 2i, 2k, 2m, 2o-2q):

In a glovebox, CuCl (19.8 mg, 0.2 mmol) and ^{t}BuOK (44.8 mg, 0.4 mmol) were added to an oven-dried 10mL Schlenk tube equipped with a stir bar. Then the Schlenk tube was sealed with a septum and brought to the bench. DMF (1 mL) was added and stirred at room temperature for 30 min, and then **1b** (50.4 mg, 0.26 mmol) was added at the same temperature for 30 min under argon atmosphere. After the pregenerated "$CuCF_3$" species was stabilized by $Et_3N·3HF$ (17μL, 0.067 mmol), iodobenzene (22.4 mg, 0.1 mmol) was added. After stirring at 80℃ for 20 h, **2a** was produced in 86% yield monitored by ^{19}F NMR spectroscopy using $PhOCF_3$ as an internal standard. The reaction mixture was also characterized by GC－MS.

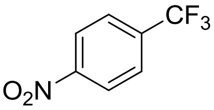
*(Note: for **2a, 2d, 2e, 2i, 2k, 2m**, the substrates were ArI; for **2o-2q**, the substrates were ABr.)*

Typical Experiment Procedure on 0.5-mmol Scale (isolated products: 2b, 2c, 2f-2h, 2j, 2l, 2n):

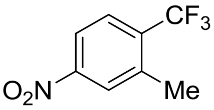
In a glovebox, CuCl (74.3 mg, 0.75 mmol) and ^{t}BuOK (168 mg, 1.5 mmol) were added to an oven-dried 10mL Schlenk tube equipped with a stir bar. Then the Schlenk tube was sealed with a septum and brought to the bench. DMF (2 mL) was added and stirred at room temperature for 30 min, and then **1b** (189 mg, 0.975 mmol) was added at the same temperature for 30 min under argon atmosphere. After the pregenerated "$CuCF_3$" species was stabilized by $Et_3N·3HF$ (63μL, 0.25 mmol), 1-iodo-4-nitrobenzene (125 mg, 0.5 mmol) in 0.5 mL DMF was added, and the mixture was stirred at 80℃ for 20 h. After addition of $NH_3·H_2O$ (33%, 0.5~1 mL), H_2O (10 mL) and Et_2O (5 mL), the organic layer was separated and the aqueous layer was extracted with Et_2O (3×5 mL). The combined organic layer was washed with brine (2×5 mL), dried over $MgSO_4$, filtered and concentrated in vacuo. The residue was purified by chromatography on silica gel (pentane/dichloromethane, 5:1, v/v) to obtain a white solid **2b** (85 mg) in an isolated yield of 89%.



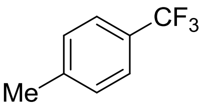
(Trifluoromethyl)benzene (2a)[1] The yield (86%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard. Characterization of **2a** in reaction solution: ^{19}F NMR (unlocked): δ -62.3 (s, 3F). GC—MS (EI): *m/z* = 146.1.



1-Nitro-4-(trifluoromethyl)benzene (2b)[1] White solid; isolated yield: 89% (85 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (d, *J* = 8.0 Hz, 2H), 8.36 (d, *J* = 8.0 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 123.0 (q, $^1J_{C\text{-}F}$ = 271.5 Hz), 124.1, 126.8 (q, $^3J_{C\text{-}F}$ = 3.6 Hz), 136.1 (q, $^2J_{C\text{-}F}$ = 33.0 Hz), 150.1. ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.2 (s, 3F). GC—MS (EI): *m/z* = 191.0.

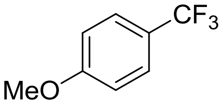


2-Methyl-4-nitro-1-(trifluoromethyl)benzene (2c)[2] Light yellow oil; isolated yield: 85% (88 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.60 (s, 3H), 7.79 (d, *J* = 8.8 Hz, 1H), 8.11 (d, *J* = 8.8 Hz, 1H), 8.14 (s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.4, 120.9, 123.4 (q, $^1J_{C\text{-}F}$ = 272.7 Hz), 126.5, 127.2 (q, $^3J_{C\text{-}F}$ = 5.6 Hz), 134.4 (q, $^2J_{C\text{-}F}$ = 30.6 Hz), 139.3, 149.7. ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.5 (s, 3F). GC—MS (EI): *m/z* = 205.0.

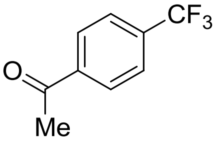


1-Methoxyl-4-(trifluoromethyl)benzene (2d)[1] The yield (89%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard. Characterization of **2d** in reaction solution: ^{19}F NMR (unlocked): δ -61.9 (s, 3F). GC—

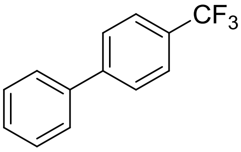
MS (EI): *m/z* = 160.1.



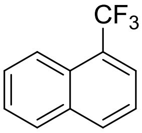
1-Methyl-4-(trifluoromethyl)benzene (2e)[1] The yield (87%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard. Characterization of **2e** in reaction solution: ^{19}F NMR (unlocked): δ -60.9 (s, 3F). GC—MS (EI): *m/z* = 176.0.



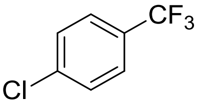
1-(4-(Trifluoromethyl)phenyl)ethanone (2f)[3] Yellowish oil; isolated yield: 75% (70 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.65 (s, 3H), 7.73 (d, *J* = 8.4 Hz, 2H), 8.06 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.7, 123.6 (q, $^{1}J_{C\text{-}F}$ = 271.0 Hz), 125.7 (q, $^{3}J_{C\text{-}F}$ = 3.6 Hz), 128.6, 134.4 (q, $^{2}J_{C\text{-}F}$ = 32.6 Hz), 139.7, 197.0. ^{19}F NMR (376 MHz, $CDCl_3$): δ -63.2 (s, 3F).



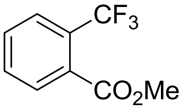
4-(Trifluoromethyl)biphenyl (2g)[3] White solid; isolated yield: 89% (99 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.40-7.44 (m, 1H), 7.47-7.51 (m, 2H), 7.60-7.62 (m, 2H), 7.71 (s, 4H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 124.4 (q, $^{1}J_{C\text{-}F}$ = 270.3 Hz), 125.8 (q, $^{3}J_{C\text{-}F}$ = 3.6 Hz), 127.3, 127.5, 128.5, 129.0, 129.4 (q, $^{2}J_{C\text{-}F}$ = 32.3 Hz), 139.8, 144.8. ^{19}F NMR (376 MHz, $CDCl_3$): δ -62.4 (s, 3F). GC—MS (EI): *m/z* = 222.1.



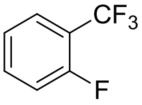
1-(Trifluoromethyl)naphthalene (2h)[1] Colorless oil; isolated yield: 78% (76 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51 (t, *J* = 8.0 Hz, 1H), 7.57-7.66 (m, 2H), 7.88 (d, *J* = 7.2 Hz, 1H), 7.93 (d, *J* = 8.0 Hz, 1H), 8.02 (d, *J* = 8.4 Hz, 1H), 8.22 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 124.2, 124.3, 124.7 (q, $^3J_{C\text{-}F}$ = 5.8 Hz), 124.8 (q, $^1J_{C\text{-}F}$ = 272.0 Hz), 126.1 (q, $^2J_{C\text{-}F}$ = 29.9 Hz), 126.6, 127.7, 128.8, 129.0, 132.8, 133.9. ^{19}F NMR (376 MHz, $CDCl_3$): δ -59.7 (s, 3F). GC—MS (EI): *m/z* = 196.1.



1-Chloro-4-(trifluoromethyl)benzene (2i)[4] The yield (92%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard. Characterization of **2i** in reaction solution: ^{19}F NMR (unlocked): δ -62.2 (s, 3F). GC—MS (EI): *m/z* = 180.0.

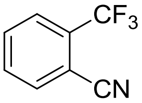


Methyl 2-(Trifluoromethyl)benzoate (2j)[1] Colorless oil; isolated yield: 76% (78 mg). ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.92 (s, 3H), 757-7.95 (m, 2H), 7.72-7.74 (m, 1H), 7.76-7.78 (m, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 52.7, 123.4 (q, $^1J_{C\text{-}F}$ = 271.8 Hz), 126.7 (q, $^3J_{C\text{-}F}$ = 5.1 Hz), 128.8 (q, $^2J_{C\text{-}F}$ = 32.3 Hz), 130.1, 131.1, 131.2 (2C), 167.3. ^{19}F NMR (376 MHz, $CDCl_3$): δ -59.8 (s, 3F). GC—MS (EI): *m/z* = 204.1.

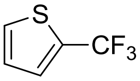


2-Fluoro-2-(trifluoromethyl)benzene (2k)[4] The yield (90%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard.

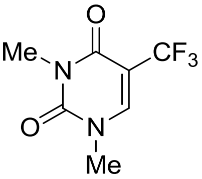
Characterization of **2k** in reaction solution: ^{19}F NMR (unlocked): δ -61.0 (d, *J* =12.0 Hz 3F), -116.5 (m, 1F). GC—MS (EI): *m/z* = 164.0.



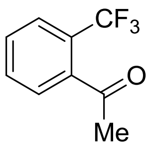
2-(Trifluoromethyl)benzonitrile (2l)[1] Pale yellow liquid; isolated yield: 73% (63 mg). ^{1}H NMR (400 MHz, CDCl$_3$): δ 7.68-7.72 (m, 1H), 7.75 (t, *J* = 7.2 Hz, 1H), 7.81 (d, *J* = 7.6 Hz, 1H), 7.85 (d, *J* = 7.6 Hz, 1H). ^{13}C NMR (100 MHz, CDCl$_3$): δ 110.2, 115.5, 122.4 (q, $^1J_{C\text{-}F}$ = 272.0 Hz), 126.7 (q, $^3J_{C\text{-}F}$ = 4.6 Hz), 132.3, 132.6, 133.0, 134.7. ^{19}F NMR (376 MHz, CDCl$_3$): δ -62.0 (s, 3F). GC—MS (EI): *m/z* = 171.0.



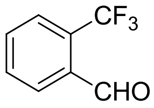
2-(Trifluoromethyl)thiophene (2m)[1] The yield (89%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard. Characterization of **2m** in reaction solution: ^{19}F NMR (unlocked): δ -54.6 (s, 3F). GC—MS (EI): *m/z* = 152.0.



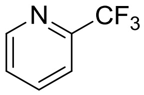
1,3-Dimethyl-5-(trifluoromethyl)pyrimidine-2,4(1H,3H)-dione (2n)[5] White solid; isolated yield: 78% (81 mg). ^{1}H NMR (400 MHz, CDCl$_3$): δ 3.37 (s, 3H), 3.49 (s, 3H), 7.66 (s, 1H). ^{13}C NMR (100 MHz, CDCl$_3$): δ 27.9, 37.7, 104.2 (q, $^2J_{C\text{-}F}$ = 33.1 Hz), 122.6 (q, $^1J_{C\text{-}F}$ = 268.1 Hz), 143.4 (q, $^3J_{C\text{-}F}$ = 5.8 Hz), 150.9, 158.7. ^{19}F NMR (376 MHz, CDCl$_3$): δ -63.8 (s, 3F). GC—MS (EI): *m/z* = 208.1.



1-(2-(Trifluoromethyl)phenyl)ethanone (2o)[1] The yield (88%) was determined by ^{19}F NMR spectroscopy using (trifluoromethyl)benzene as an internal standard. Characterization of **2o** in reaction solution: ^{19}F NMR (unlocked): δ -57.7 (s, 3F). GC—MS (EI): *m/z* = 188.0.

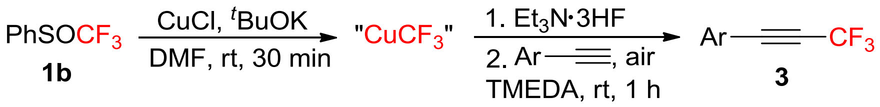


2-(Trifluoromethyl)benzaldehyde (2p)[1] The yield (78%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard. Characterization of **2p** in reaction solution: ^{19}F NMR (unlocked): δ -56.2 (s, 3F). GC—MS (EI): *m/z* = 174.0.



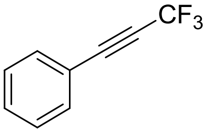
2-(Trifluoromethyl)pyridine (2q)[1] The yield (57%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard. Characterization of **2q** in reaction solution: ^{19}F NMR (unlocked): δ -67.7 (s, 3F). GC—MS (EI): *m/z* = 147.1.

5. Trifluoromethylation of Terminal Alkynes with "$CuCF_3$" Generated from $PhSOCF_3$

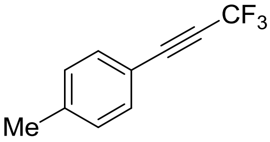


Typical Experiment Procedure (3a-3c):

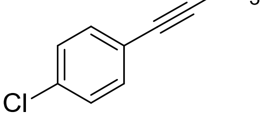
In a glovebox, CuCl (19.8 mg, 0.2 mmol) and ^{t}BuOK (44.8 mg, 0.4 mmol) were added to an oven-dried 10mL Schlenk tube equipped with a stir bar. Then the Schlenk tube was sealed with a septum and brought to the bench. DMF (0.5 mL) was added and stirred at room temperature for 30 min, and then **1b** (50.4 mg, 0.26 mmol) was added at the same temperature for 30 min under argon atmosphere. After the pregenerated "$CuCF_3$" species was stabilized by Et_3N 3HF (17µL, 0.067 mmol), TMEDA (23 mg, 0.2 mmol) was added. 1-chloro-4-ethynylbenzene (13.7 mg, 0.1 mmol) in 0.5 mL DMF was added via syringe under air atmosphere for 1~1.5 h. After stirring at room temperature for 15 min, **3c** was produced in 67% yield monitored by ^{19}F NMR spectroscopy using $PhCF_3$ as an internal standard.



(3,3,3-Trifluoroprop-1-yn-1-yl)benzene (3a)[6] The yield (65%) was determined by ^{19}F NMR spectroscopy using (trifluoromethyl)benzene as an internal standard. Characterization of **3a** in reaction solution: ^{19}F NMR (unlocked): δ -49.2 (s, 3F).

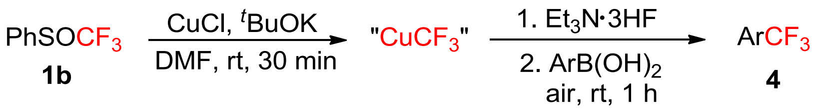


1-Methyl-4-(3,3,3-trifluoroprop-1-yn-1-yl)benzene (3b)[6] The yield (66%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard. Characterization of **3b** in reaction solution: ^{19}F NMR (unlocked): δ -49.2 (s, 3F). GC－MS (EI): *m/z* = 184.1.



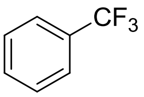
1-Chloro-4-(3,3,3-trifluoroprop-1-yn-1-yl)benzene (3c)[6] The yield (67%) was determined by ^{19}F NMR spectroscopy using (trifluoromethyl)benzene as an internal standard. Characterization of **3c** in reaction solution: ^{19}F NMR (unlocked): δ -49.4 (s, 3F).

6. Trifluoromethylation of Arylboronic Acids with “CuCF$_3$” Generated from PhSOCF$_3$

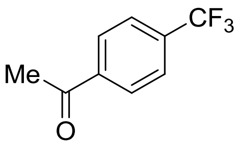


Typical Experiment Procedure (4a-4c):

In a glovebox, CuCl (19.8 mg, 0.2 mmol) and ^{t}BuOK (44.8 mg, 0.4 mmol) were added to an oven-dried 10mL Schlenk tube equipped with a stir bar. Then the Schlenk tube was sealed with a septum and brought to the bench. DMF (0.5 mL) was added and stirred at room temperature for 30 min, and then **1b** (50.4 mg, 0.26 mmol) was added at the same temperature for 30 min under argon atmosphere. After the pregenerated “CuCF$_3$” species was stabilized by Et$_3$N·3HF (17μL, 0.067 mmol), phenylboronic acid (12.2 mg, 0.1 mmol) in 0.5 mL DMF was added under air atmosphere. After stirring at room temperature for 1 h, **4a** was produced in 81% yield monitored by ^{19}F NMR spectroscopy using PhOCF$_3$ as an internal standard.

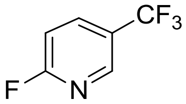


(Trifluoromethyl)benzene (4a)[1] The yield (81%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard. Characterization of **4a** in reaction solution: ^{19}F NMR (unlocked): δ -62.3 (s, 3F).



1-(4-(Trifluoromethyl)phenyl)ethanone (4b)[1] The yield (72%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard.

Characterization of **4b** in reaction solution: ^{19}F NMR (unlocked): δ -62.7 (s, 3F). GC－MS (EI): *m/z* = 188.0.



2-Fluoro-5-(trifluoromethyl)pyridine (4c)[7] The yield (95%) was determined by ^{19}F NMR spectroscopy using (trifluoromethoxyl)benzene as an internal standard. Characterization of **4c** in reaction solution: ^{19}F NMR (unlocked): δ -61.6 (s, 3F), -63.2 (s, 1F). GC－MS (EI): *m/z* = 165.0.

7. References

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3. Chu, L.; Qing, F.-L. *Org. Lett.* **2010**, *12*, 5060.
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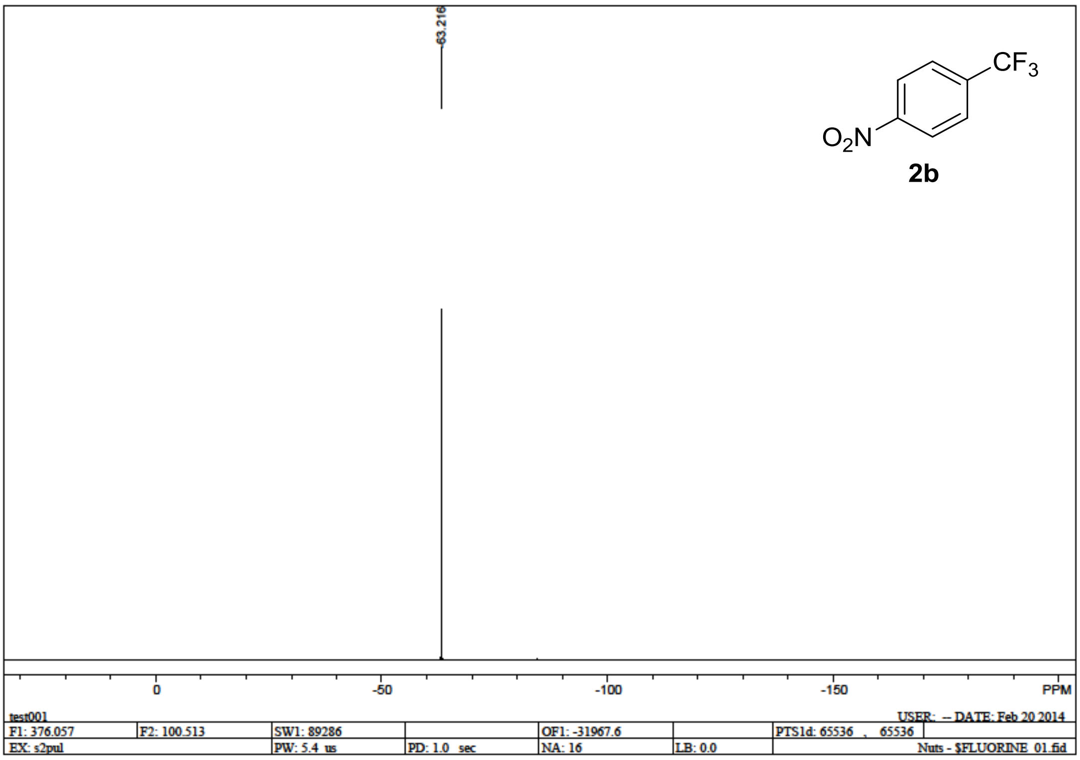
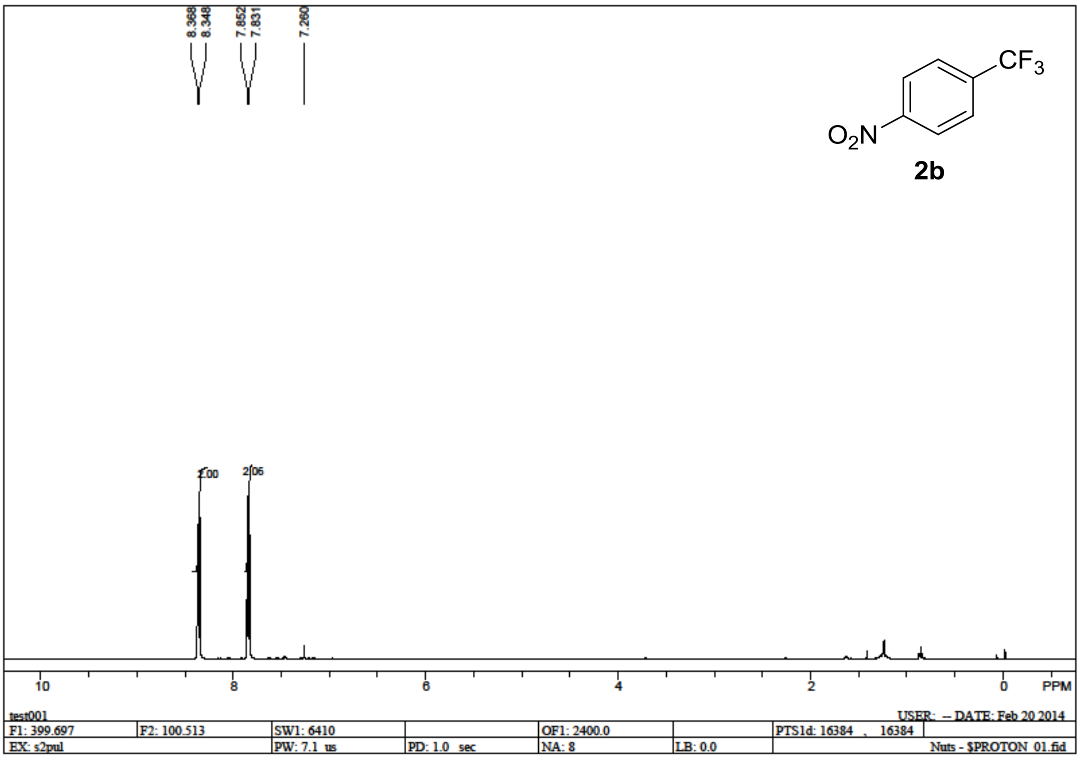
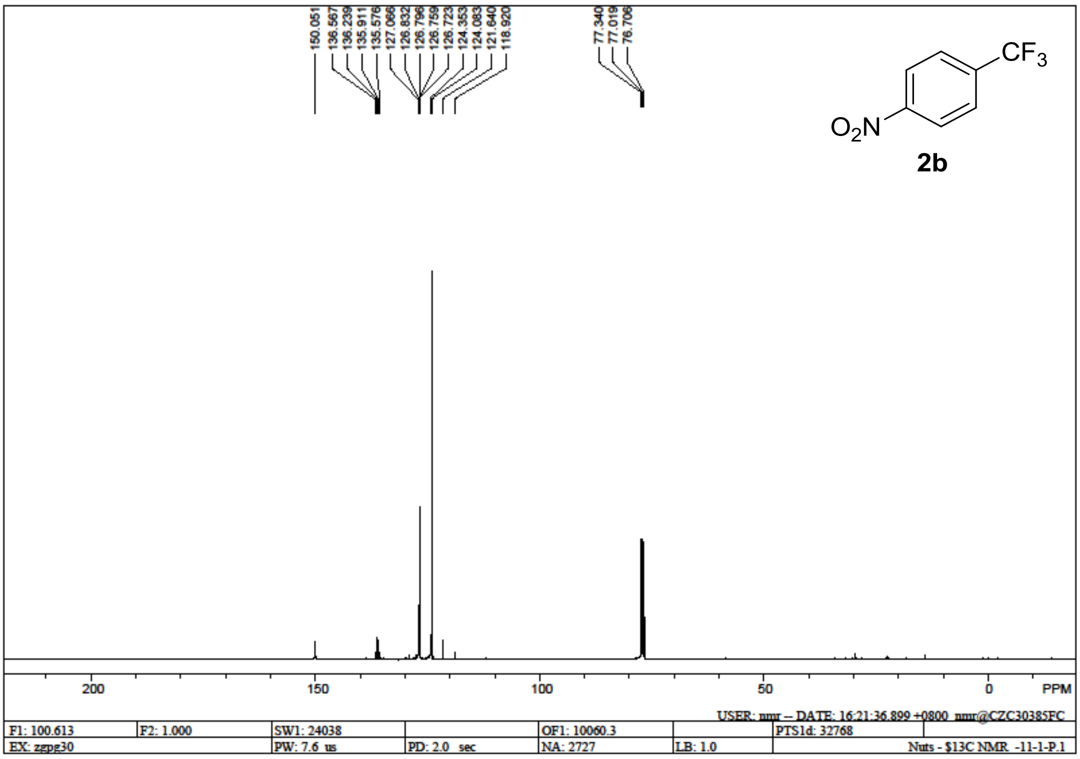
7. Sun, H.; DiMagno, S. G. *Angew. Chem., Int. Ed.* **2006**, *45*, 2720.

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



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121.640
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77.340
77.019
76.706
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2b
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150
100
50
0
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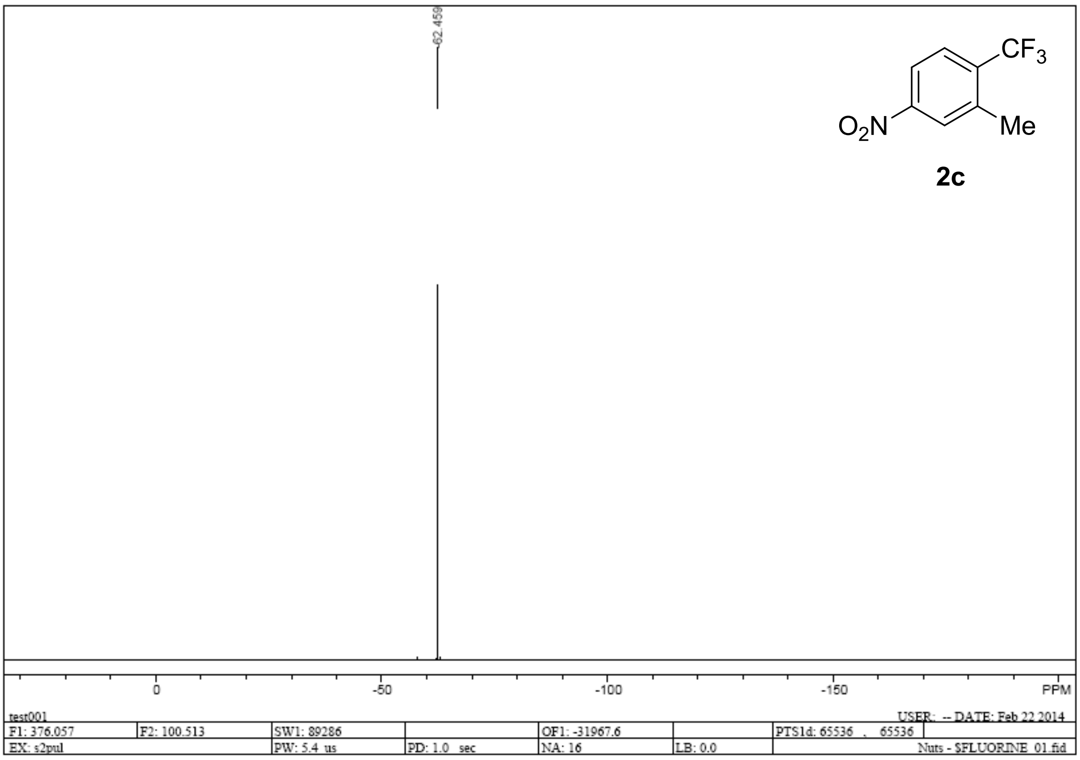
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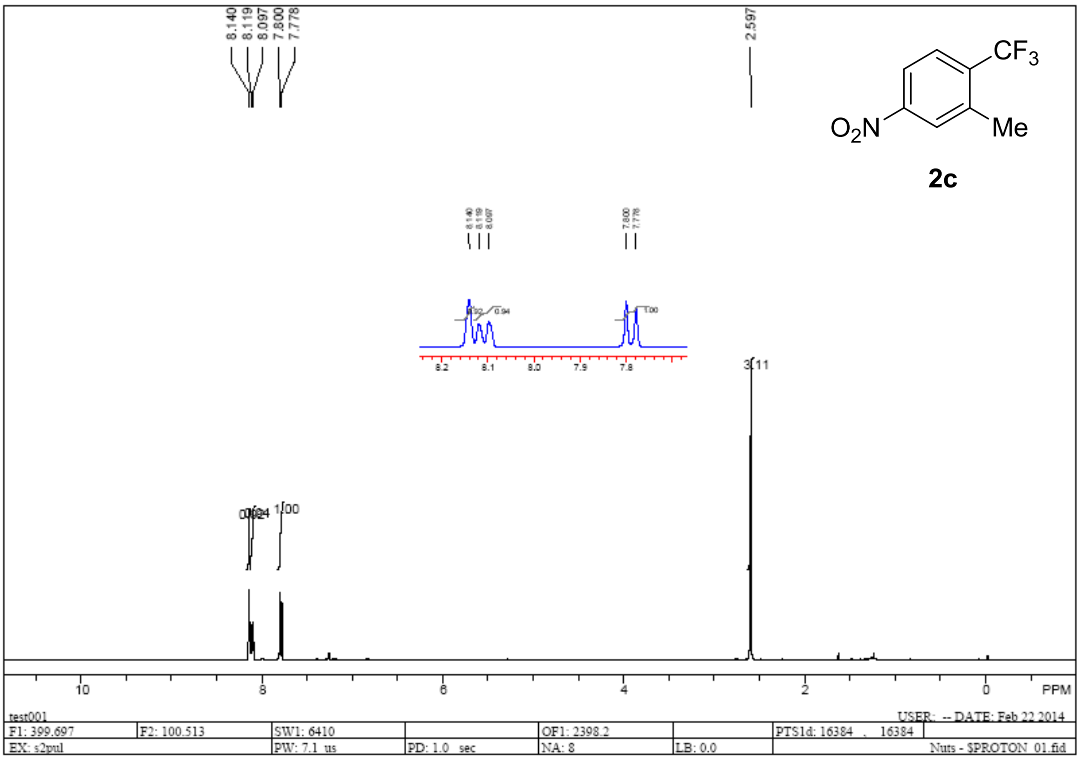
Nuts - $FLUORINE_01.fid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8.2
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8
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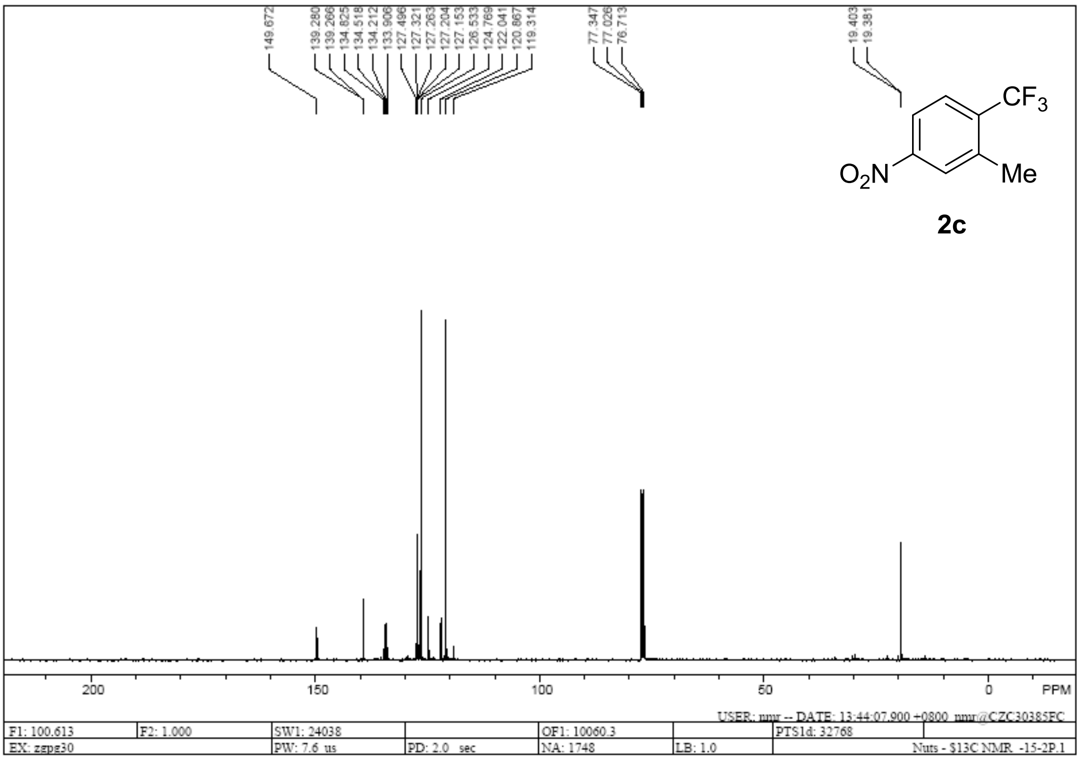
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120.867
119.314
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19.403
19.381
CF3
O2N
Me
2c
200
150
100
50
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PPM
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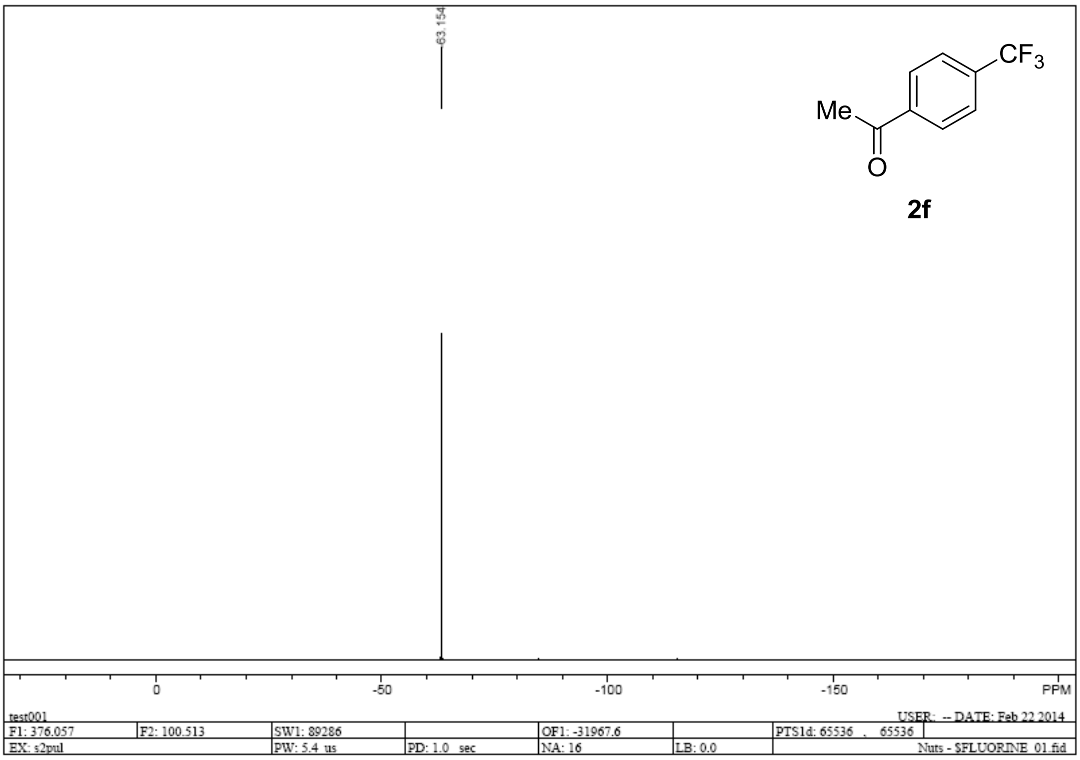
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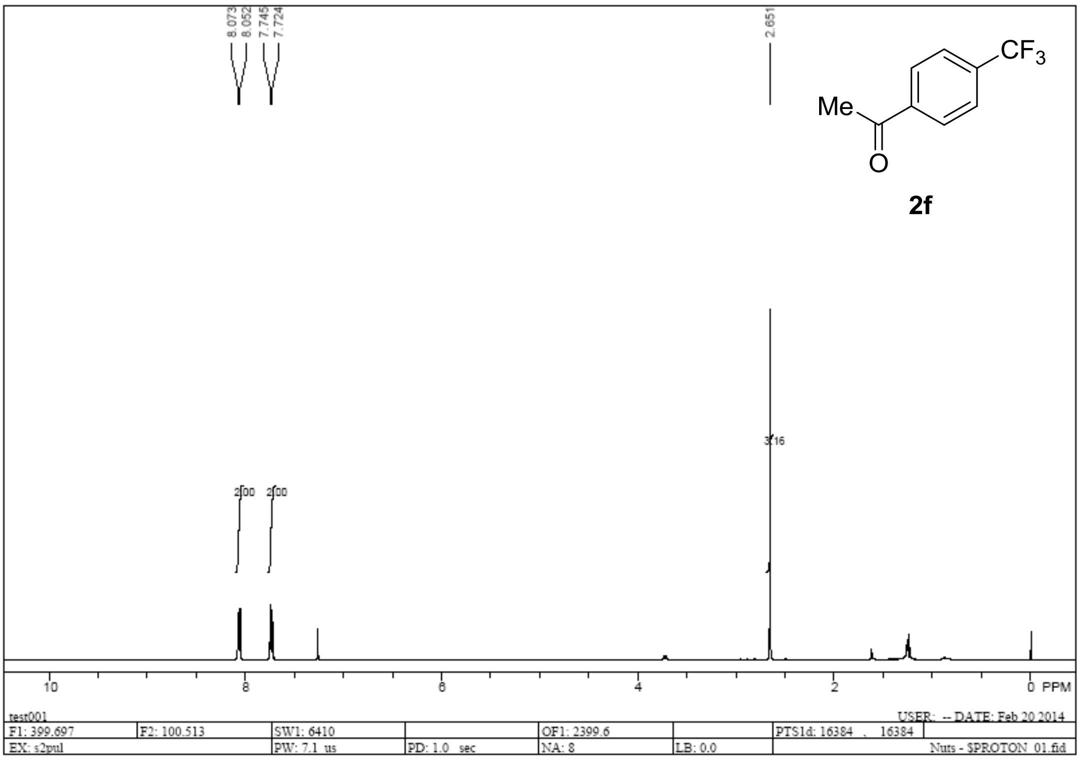
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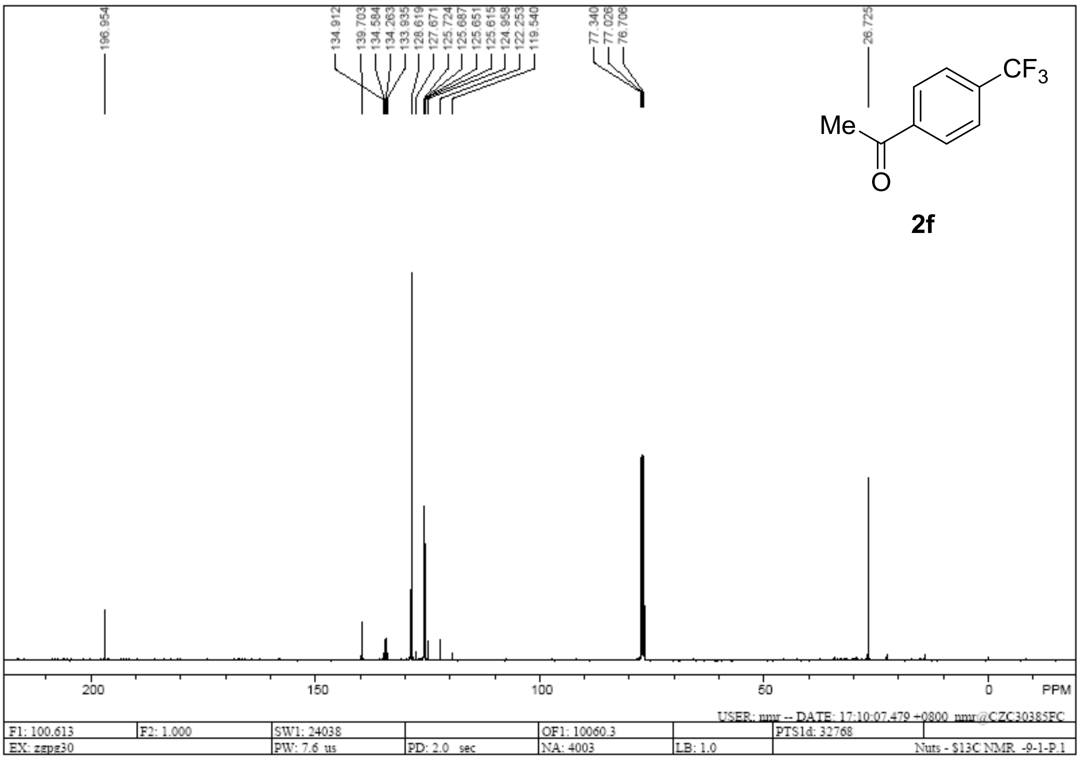
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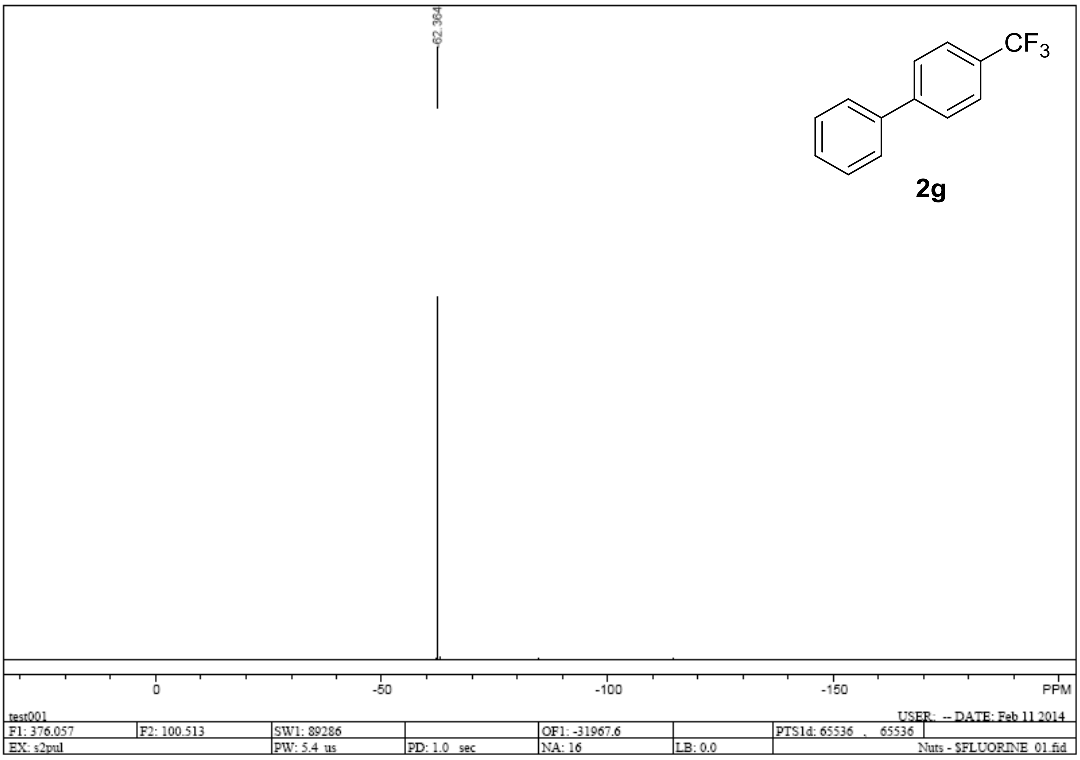
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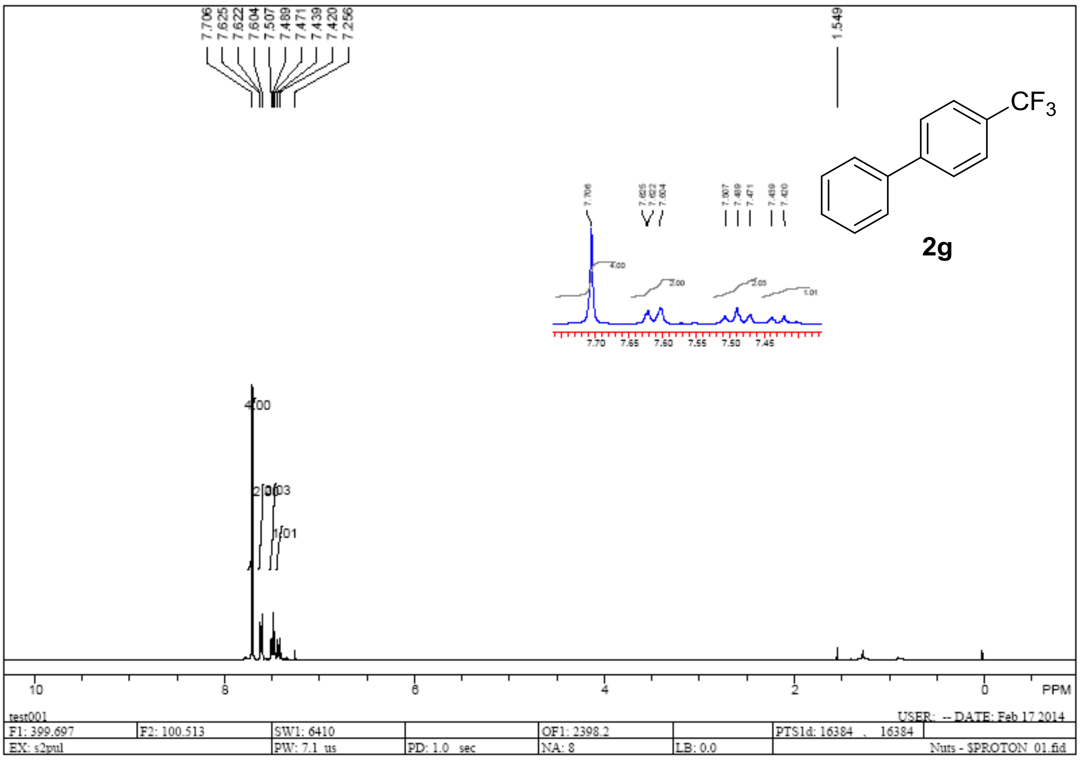
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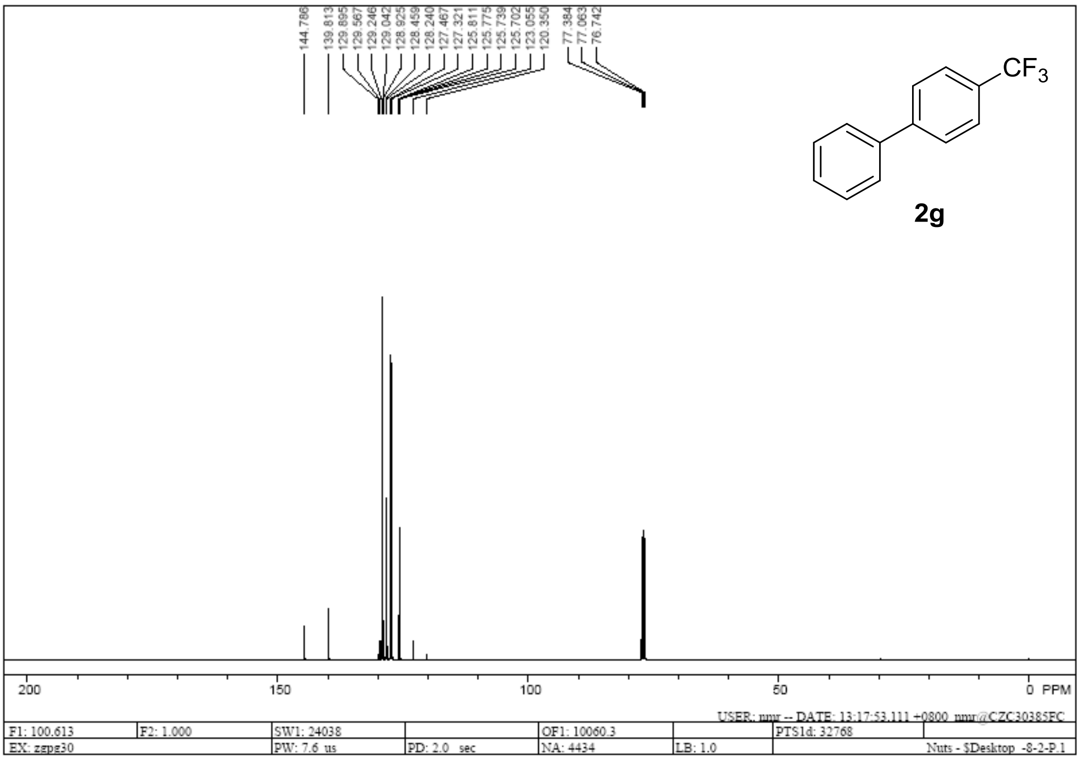
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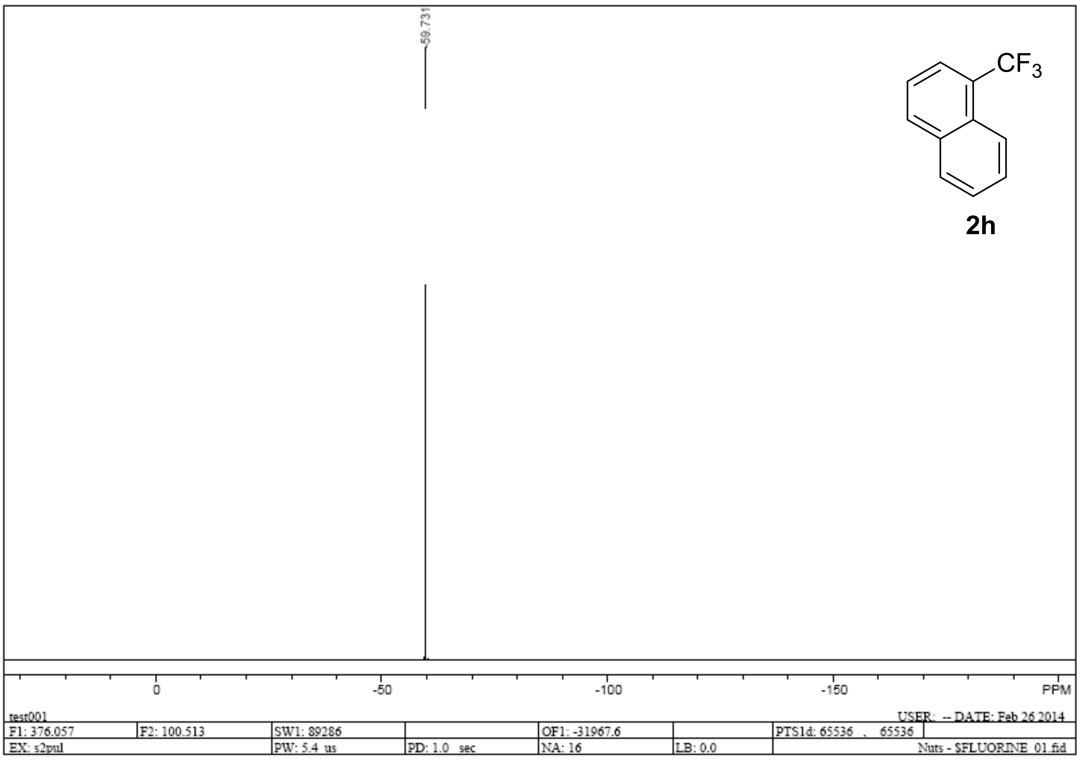
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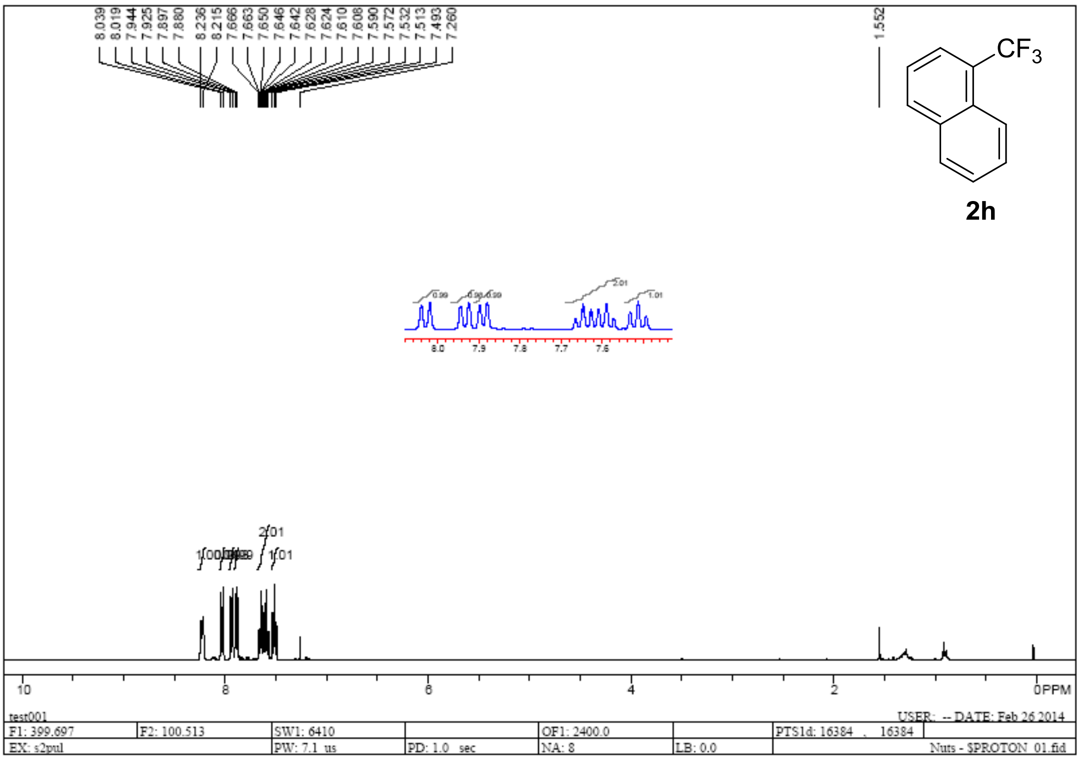
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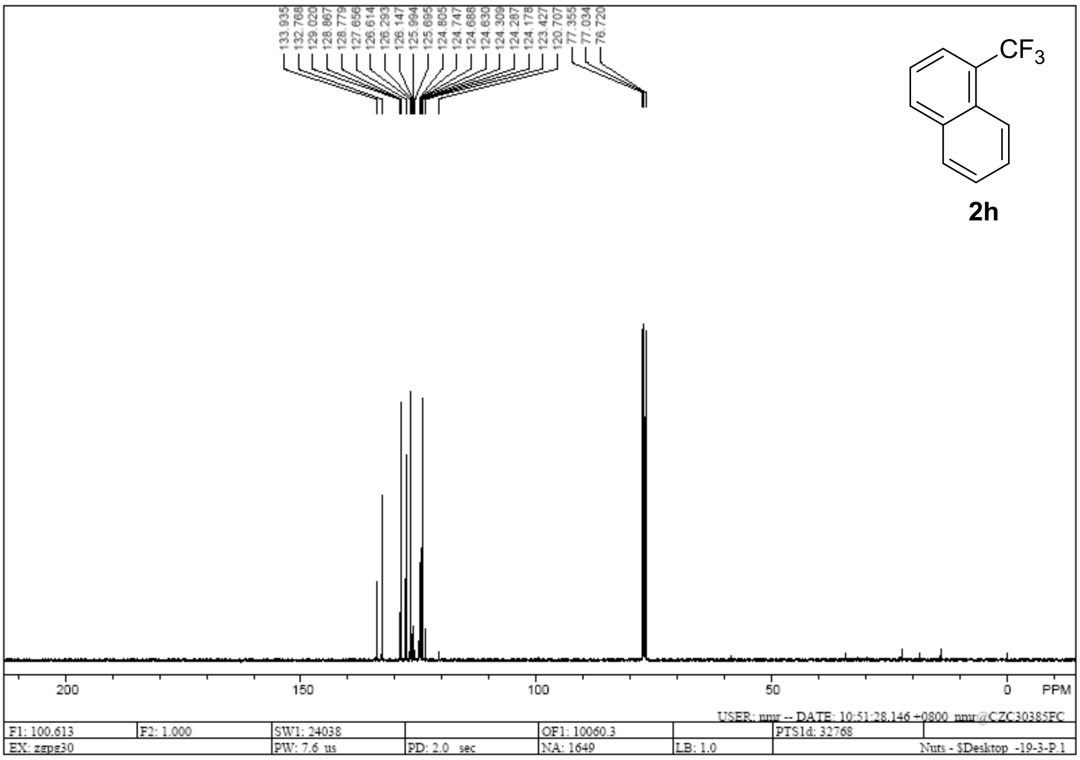
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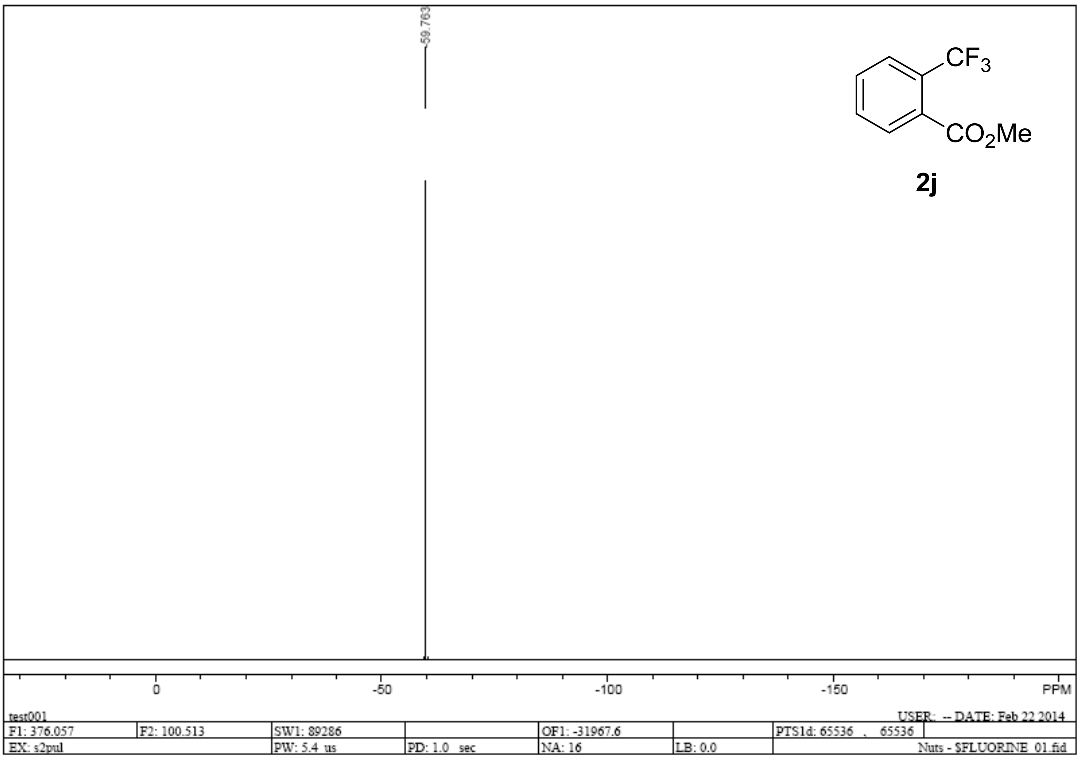
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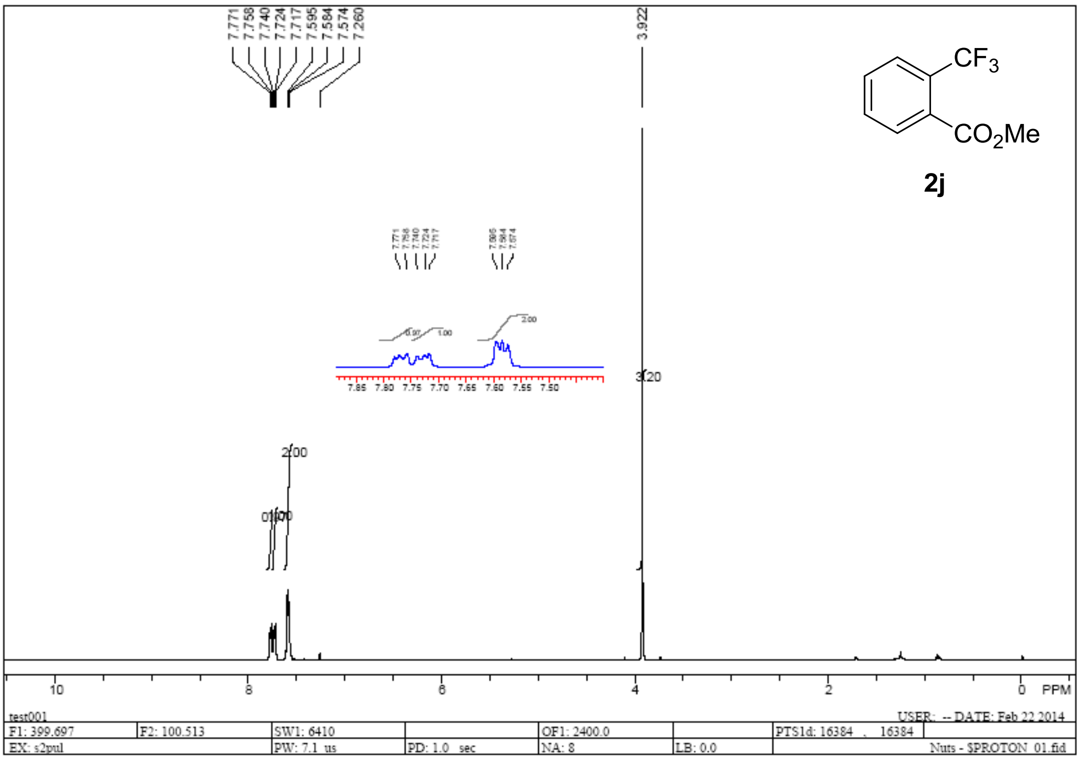
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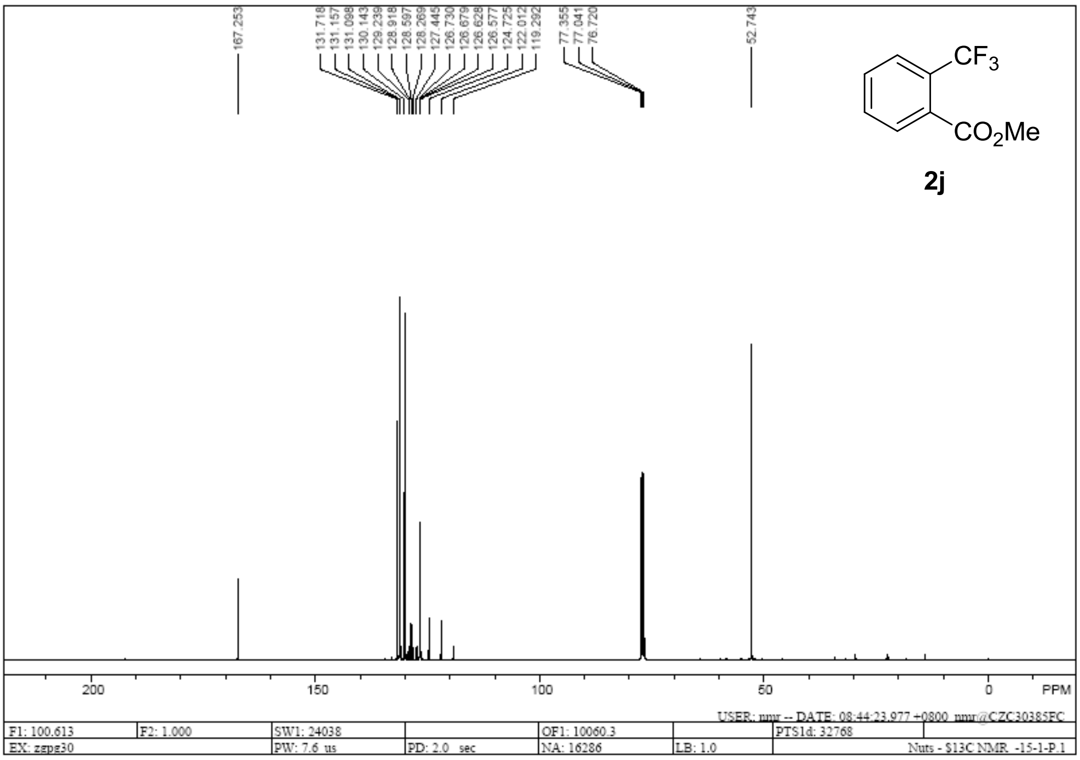
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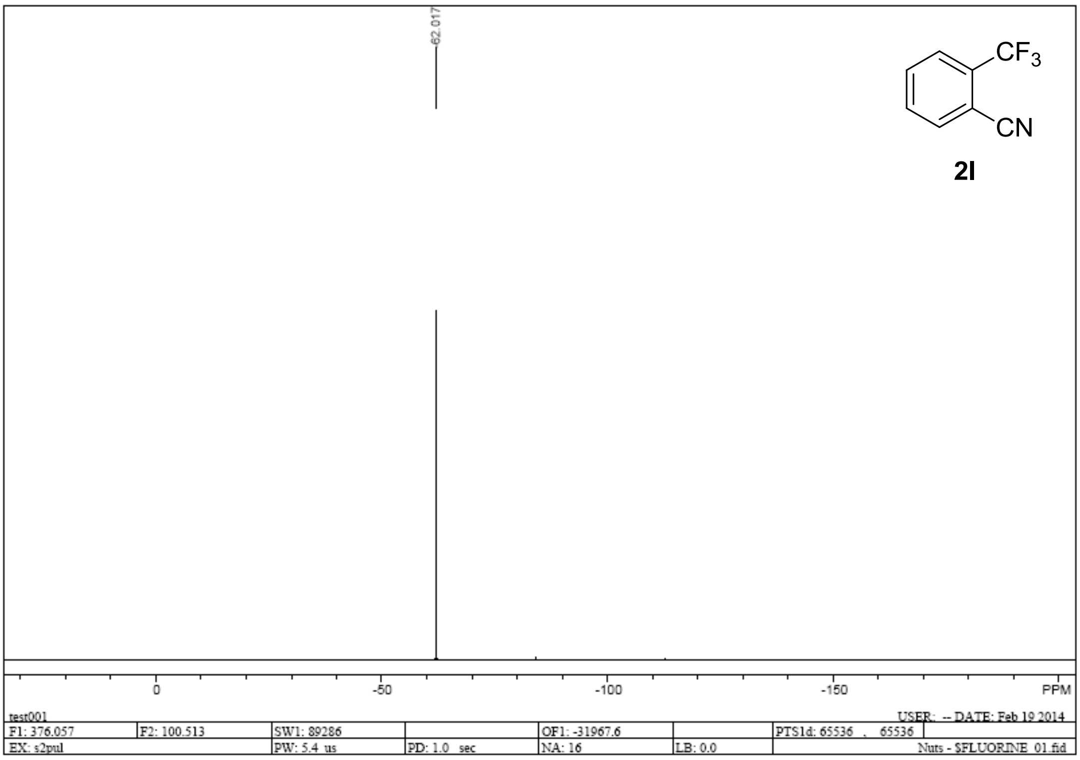
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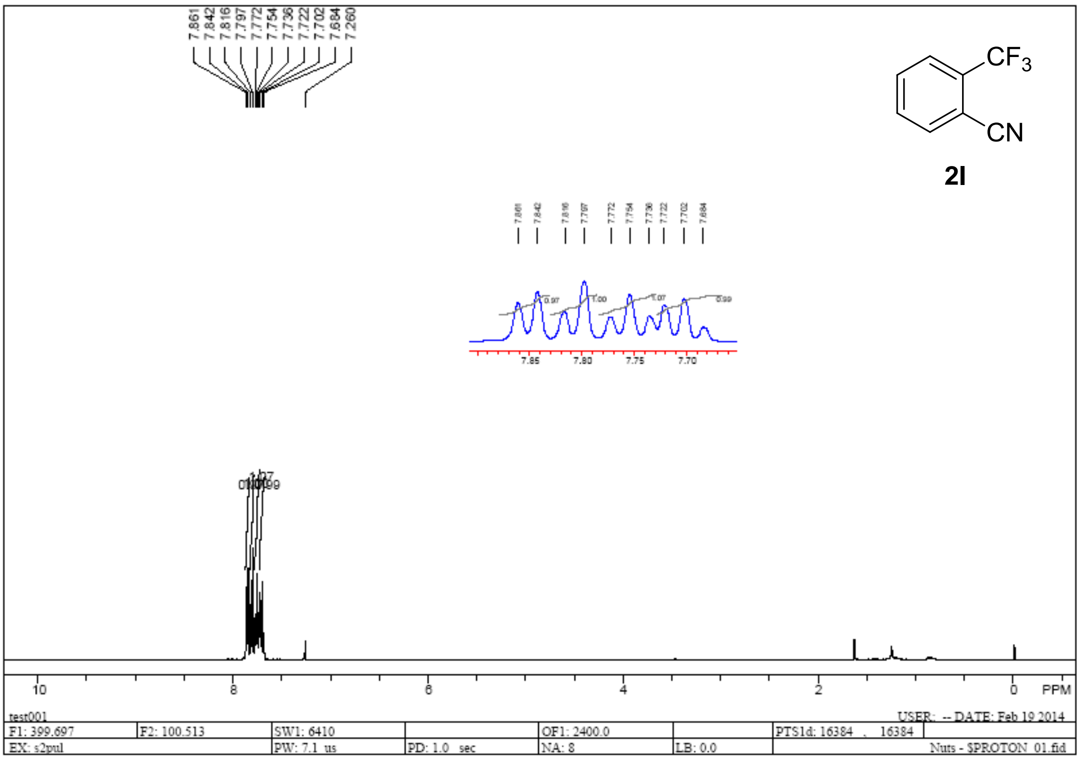
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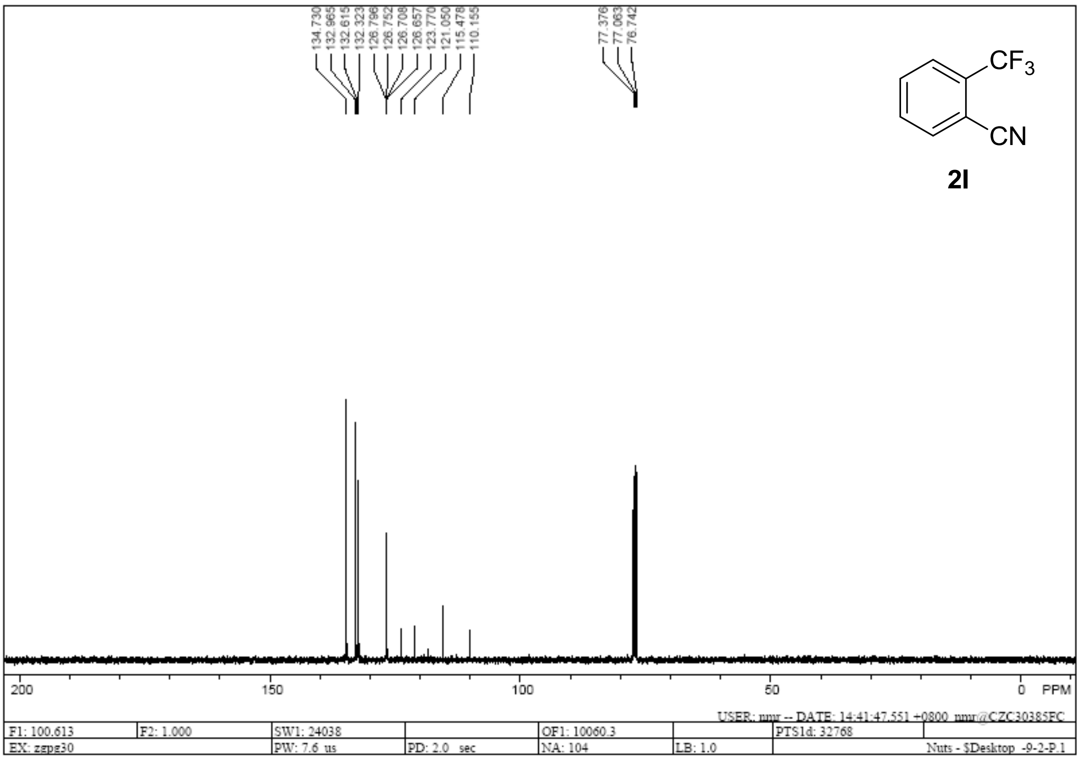
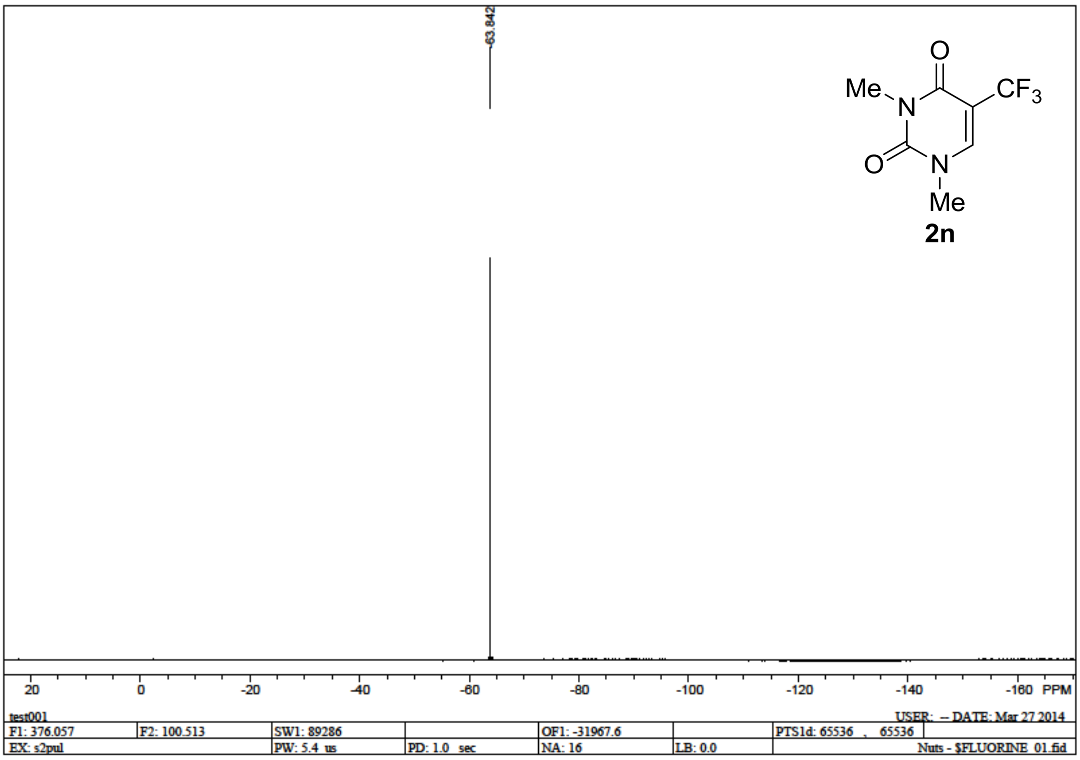
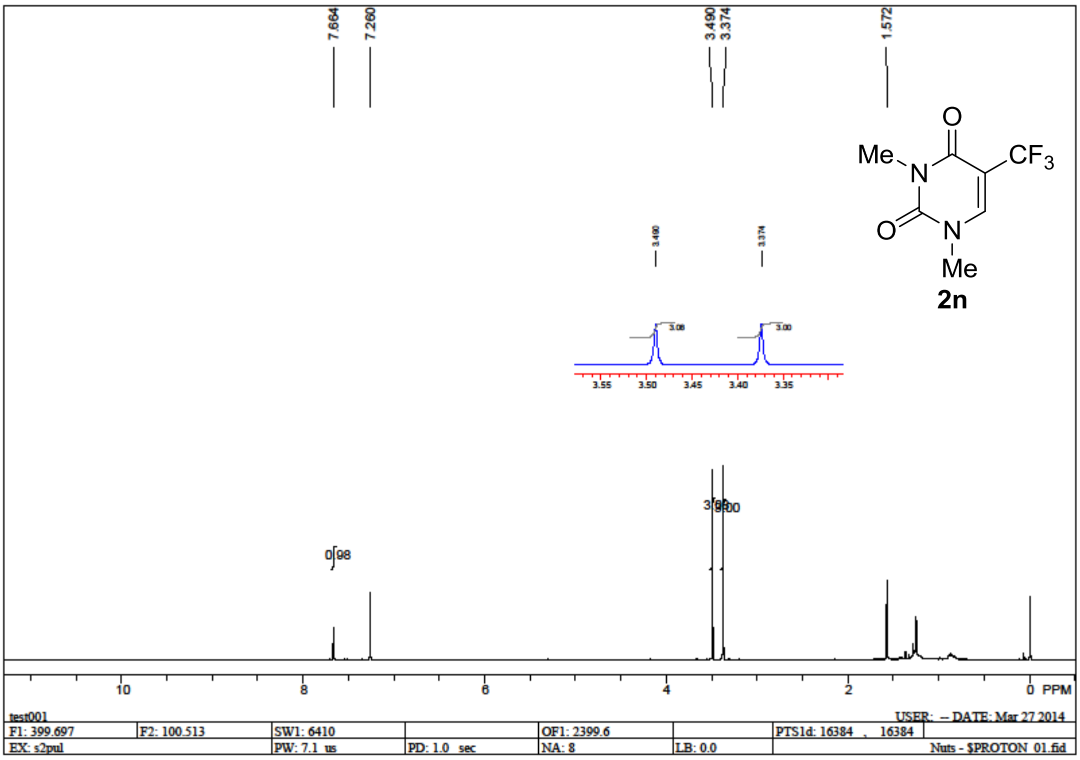
0.99
7.85
7.80
7.75
7.70
10
8
6
4
2
0
PPM
test001
USER: -- DATE: Feb 19 2014
F1: 399.697
F2: 100.513
SW1: 6410
OF1: 2400.0
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON_01.fid

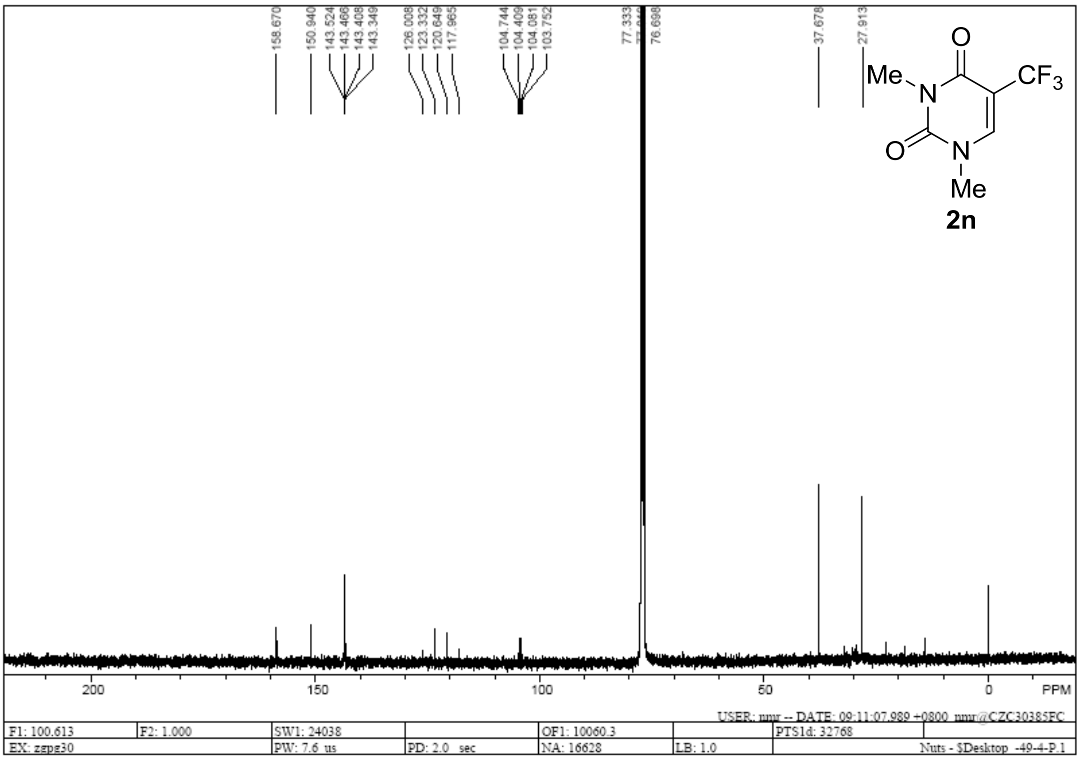

134.730
132.965
132.615
132.323
126.796
126.752
126.708
126.657
123.770
121.050
115.478
110.155
77.376
77.063
76.742
CF3
CN
200
150
100
50
0 PPM
USER: nmr -- DATE: 14:41:47.551 +0800 nmr@CZC30385FC
F1: 100.613
F2: 1.000
SW1: 24038
OF1: 10060.3
PTS1d: 32768
EX: zgpg30
PW: 7.6 us
PD: 2.0 sec
NA: 104
LB: 1.0
Nuts - $Desktop -9-2-P.1

2l


-63.842
O
Me
N
CF3
O
N
Me
20
0
-20
-40
-60
-80
-100
-120
-140
-160 PPM
test001
USER: -- DATE: Mar 27 2014
F1: 376.057
F2: 100.513
SW1: 89286
OF1: -31967.6
PTS1d: 65536 , 65536
EX: s2pul
PW: 5.4 us
PD: 1.0 sec
NA: 16
LB: 0.0
Nuts - $FLUORINE 01.fid

2n


7.664
7.260
3.490
3.374
1.572
0.98
3.08
3.00
3.55
3.50
3.45
3.40
3.35
10
8
6
4
2
0 PPM
Me
N
O
CF3
2n
test001
USER: -- DATE: Mar 27 2014
F1: 399.697
F2: 100.513
SW1: 6410
OF1: 2399.6
PTS1d: 16384 , 16384
EX: s2pul
PW: 7.1 us
PD: 1.0 sec
NA: 8
LB: 0.0
Nuts - $PROTON 01.fid


158.670
150.940
143.524
143.466
143.408
143.349
126.008
123.332
120.649
117.965
104.744
104.409
104.081
103.752
77.333
76.698
37.678
27.913
Me
N
O
CF3
2n
200
150
100
50
0
PPM
USER: nmr -- DATE: 09:11:07.989 +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: 16628
LB: 1.0
Nuts - $Desktop -49-4-P.1