

Supporting information

**Copper-Mediated Trifluoromethylation of ArylBoronic Acids by
Trifluoromethyl Sulfonium Salts**

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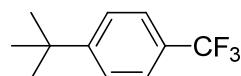
Experimental Details

1. General

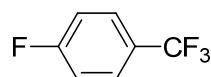
Unless otherwise stated, NMR spectra were recorded in CDCl_3 at 300 MHz (^1H NMR) and 282 MHz (^{19}F NMR). All chemical shifts are reported in ppm relative to TMS or CFCl_3 (positive for downfield shifts) as external standards. DMF ($\geq 99.5\%$) and Cu ($\geq 99.0\%$) were used without purification. *S*-(Trifluoromethyl)diphenylsulfonium triflate $[\text{Ph}_2\text{SCF}_3]^+[\text{OTf}]^-$ was synthesized according to the literature procedure.¹ Other reagents were purchased from commercial sources.

2. General Procedure for the Trifluoromethylation of Aryl- and Alkenylboronic Acids (**1a-q**).

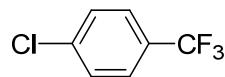
In a 5 mL sealed tube, biphen-4-ylboronic acid (39.9 mg, 0.201 mmol) and $[\text{Ph}_2\text{SCF}_3]^+[\text{OTf}]^-$ (162 mg, 0.4 mmol) were dissolved in DMF (3 mL). Copper powder (26.3 mg, 0.4 mmol) and NaHCO_3 (17.1 mg, 0.2 mmol) were added. The reaction mixture was then stirred at 50 °C for 11 h. After dilution with diethyl ether (30 mL), the reaction mixture was washed with water (3×20 mL), dried over anhydrous sodium sulfate and evaporated under reduced pressure. The crude product was purified by column chromatography (eluent: pentane), providing 4-(trifluoromethyl)biphenyl **2c**^{2a} (22.6 mg, 0.102 mmol, 51% yield) as a white solid. ^1H NMR (300 MHz, CD_3COCD_3): δ 7.90 (d, $J = 8.3$ Hz, 2H), 7.81 (d, $J = 8.3$ Hz, 2H), 7.74 (dm, $J = 7.6$ Hz, 2H), 7.52 (t, $J = 7.6$ Hz, 2H), 7.44 (t, $J = 7.4$ Hz, 1H). ^{19}F NMR (282 MHz, CD_3COCD_3): -63.3 (s, 3F).



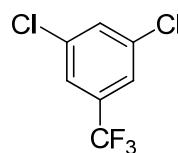
1-*tert*-Butyl-4-trifluoromethylbenzene (**2b**)^{2b}: Colorless oil. ^1H NMR (300MHz, CDCl_3): δ 7.55 (d, $J = 8.3$ Hz, 2H), 7.49 (d, $J = 8.3$ Hz, 2H), 1.34 (s, 9H). ^{19}F NMR (282MHz, CDCl_3): δ -62.0 (s, 3F).



1-Fluoro-4-(trifluoromethyl)benzene (**2d**)^{2c}: ^{19}F NMR (282MHz, CDCl_3): -60.7 (s, 3F). GC-MS (m/z): 164.0 (t = 2.542 min).



1-Chloro-4-(trifluoromethyl)benzene (**2e**)^{2d}: Yellow oil. H NMR (300MHz, CDCl_3): δ 7.48 (d, $J = 8.8$ Hz, 2H), 7.41 (d, $J = 8.8$ Hz, 2H). ^{19}F NMR (282MHz, CDCl_3): δ -61.4 (s, 3F).

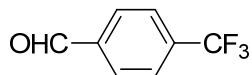


1,3-Dichloro-5-(trifluoromethyl)benzene (**2f**)^{2e}: Colorless oil. H NMR (300MHz, CDCl_3): δ

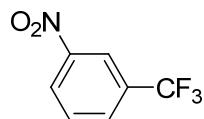
7.55 (s, 1H), 7.52 (s, 2H). ^{19}F NMR (282MHz, CDCl_3): -62.7 (s, 3F).



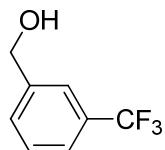
4-(Trifluoromethyl)benzonitrile (**2g**)^{2d}: White solid. ^1H NMR (300MHz, CDCl_3): δ 7.75 (d, J = 8.5 Hz, 2H), 7.70 (d, J = 8.5 Hz, 2H). ^{19}F NMR (282MHz, CDCl_3): δ -63.9 (s, 3F).



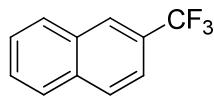
4-(Trifluoromethyl)benzaldehyde (**2h**)^{2f}: Colorless oil. ^1H NMR (300MHz, CDCl_3): δ 10.09 (s, 1H), 8.00 (d, J = 7.9 Hz, 2H), 7.80 (d, J = 7.9 Hz, 2H). ^{19}F NMR (282MHz, CDCl_3): δ -62.7 (s, 3F).



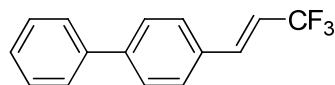
1-Nitro-3-(trifluoromethyl)benzene (**2i**)^{2b}: Yellow oil. ^1H NMR (300MHz, CDCl_3): δ 8.53 (s, 1H), 8.45 (d, J = 8.3 Hz, 1H), 7.99 (d, J = 7.9 Hz), 7.75 (t, J = 8.1Hz, 1H). ^{19}F NMR (282MHz, CDCl_3): δ -62.6 (s, 3F).



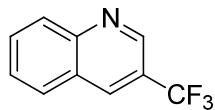
(3-(Trifluoromethyl)phenyl)methanol (**2j**)^{2g}: Yellow oil. ^1H NMR (300MHz, CDCl_3): δ 7.64 (s, 1H), 7.56-7.54 (m, 2H), 7.47 (t, J = 7.4Hz, 1H), 4.76 (d, J = 5.4Hz, 2H), 1.91 (t, J = 5.4Hz, 1H). ^{19}F NMR (282MHz, CDCl_3): δ -62.4 (s, 3F).



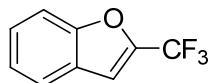
2-(Trifluoromethyl)naphthalene (**2k**)^{2b}: White solid. ^1H NMR (300MHz, CDCl_3): δ 8.16 (s, 1H), 7.97-7.90 (m, 3H), 7.66-7.57 (m, 3H). ^{19}F NMR (282MHz, CDCl_3): δ -62.6 (s, 3F).



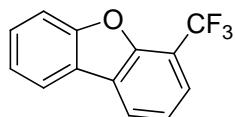
4-(3,3,3-Trifluoroprop-1-enyl)biphenyl (**2l**)^{2h,2j}: White solid. ^1H NMR (300MHz, CDCl_3): δ 7.55 (m, 4H), 7.46 (d, J = 8.5Hz, 2H), 7.38 (tm, J = 7.7Hz, 2H), 7.31 (m, 1H), 7.12 (dq, J = 16.2Hz, J = 1.8Hz, 1H), 6.17 (dq, J = 16.1Hz, J = 6.5Hz, 1H). ^{19}F NMR (282MHz, CDCl_3): δ -63.6 (d, J = 6.5Hz, 3F).



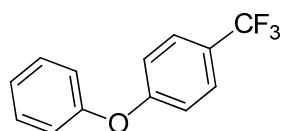
3-(Trifluoromethyl)quinoline (**2m**)²ⁱ: White solid. ¹H NMR (300MHz, CDCl₃): δ 9.11 (d, *J* = 1.5 Hz, 1H), 8.46 (s, 1H), 8.20 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 8.1 Hz, 1H), 7.87 (tm, *J* = 7.2Hz, 1H), 7.68 (t, *J* = 7.2Hz, 1H). ¹⁹F NMR (282MHz, CDCl₃): δ -61.4 (s, 3F).



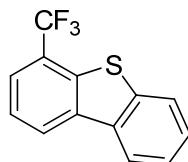
2-(Trifluoromethyl)benzofuran (**2n**)^{2b}: Colorless oil. ¹H NMR (300MHz, CDCl₃): δ 7.68 (d, *J* = 7.9Hz, 1H), 7.58 (dm, *J* = 8.3Hz, 1H), 7.45 (tm, *J* = 7.7Hz, 1H), 7.34 (tm, *J* = 7.2Hz, 1H), 7.18 (m, 1H). ¹⁹F NMR (282MHz, CDCl₃): δ -65.2 (s, 3F).



4-(Trifluoromethyl)dibenzofuran (**2o**)^{2j}: White solid. ¹H NMR (300MHz, CDCl₃): δ 8.13 (d, *J* = 7.7 Hz, 1H), 7.98 (d, *J* = 7.5 Hz, 1H), 7.70 (d, *J* = 7.7 Hz, 1H), 7.67 (d, *J* = 8.5 Hz, 1H), 7.53 (t, *J* = 7.8 Hz, 1H), 7.45-7.38 (m, 2H). ¹⁹F NMR (282MHz, CDCl₃): δ -60.8 (s, 3F).



1-Phenoxy-4-(trifluoromethyl)benzene (**2p**)^{2k}: White solid. ¹H NMR (300MHz, CDCl₃): δ 7.53 (d, *J* = 8.7 Hz, 2H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.15-7.05 (m, 5H). ¹⁹F NMR (282MHz, CDCl₃): δ -61.6 (s, 3F).



4-(Trifluoromethyl)dibenzothiophene (**2q**): White solid. ¹H NMR (300MHz, CDCl₃): δ 8.21 (d, *J* = 7.9Hz, 1H), 8.08 (m, 1H), 7.78 (m, 1H), 7.67 (d, *J* = 7.7Hz, 1H), 7.42(m, 3H). ¹⁹F NMR (282MHz, CDCl₃): δ -62.7 (s, 3F). ¹³C NMR (100MHz, CDCl₃): δ 139.5 (q, *J* = 1.5Hz), 137.4, 136.4, 134.3, 127.6, 125.2 (q, *J* = 33Hz), 124.8, 124.7, 124.3 (q, *J* = 5.2 Hz), 124.3, 124.2 (q, *J* = 273Hz), 122.6, 121.7. EI (m/z, %): 253 (14.7), 252 (100), 251 (14.0), 233 (12.1), 202 (9.4), 184 (52.2), 139 (18.1), 126 (10.0). IR (KBr): 1455, 1445, 1403, 1335, 1302, 1254, 1200, 1174, 1133, 1108, 1074, 1030, 799, 748 cm⁻¹. HRMS for C₁₃H₇F₃S: 252.0221; Found: 252.0223.

References

- (1) (a) E. Magnier, J. C. Blazejewski, M. Tordeux and C. Wakselman, *Angew. Chem. Int. Ed.* 2006, **45**, 1279; (b) Y. Mace, B. Raymondeau, C. Pradet, J. -C. Blazejewski and E. Magnier, *Eur. J. Org. Chem.* 2009, 1390; (c) C. -P. Zhang, H. -P. Cao, Z. -L. Wang, C. -T. Zhang, Q. -Y. Chen and J. -C. Xiao, *Synlett.* 2010, **7**, 1089; (d) C. -P. Zhang, Z. -L. Wang, Q. -Y. Chen, C. -T. Zhang, Y. -C. Gu and J. -C. Xiao, *Angew. Chem. Int. Ed.* 2011, **50**, 1896.
- (2) (a) S. Gao, Z. Zheng, L. Jian and R. Cao, *Chem. Commun.* 2010, **46**, 7584; (b) L. Chu and F. -L. Qing, *Org. Lett.* 2010, **12**, 5060; (c) D. Naumann and J. Kischkowitz, *J. Fluorine Chem.* 1990, **47**, 283; (d) M. Oishi, H. Kondo and H. Amii, *Chem. Commun.* 2009, 1909; (e) J. M. Paratian, E. Labbe, S. Sibille and J. Perichon, *J. Organomet. Chem.* 1995, **489**, 137; (f) P. V. Ramachandran and A. Chatterjee, *Org. Lett.* 2008, **10**, 1195; (g) K. Miyamoto, N. Tada and M. Ochiai, *J. Am. Chem. Soc.* 2007, **129**, 2772; (h) S. Furuta and T. Hiyama, *Synlett* 1996, 1199; (i) J. M. Paratian, S. Sibille and J. Perichon, *J. Chem. Soc. Chem. Commun.* 1992, 53; (j) J. Xu, D. -F. Luo, B. Xiao, Z. -J. Liu, T. -J. Gong, Y. Fu and L. Liu, *Chem. Commun.* 2011, 4300; (k) T. D. Senecal, A. T. Parsons and S. L. Buchwald, *J. Org. Chem.* 2011, **76**, 1174.

¹⁹F NMR and MS Analysis of Reaction Mixtures

The NMR experiments listed in Table 1 were run directly without any further purification of the reaction mixtures. All the experiments were done in the reaction solvents, using [OTf]⁻ (from [Ph₂SCF₃]⁺[OTf]⁻) as the internal standard.

Table 1, entry 1 (¹⁹F NMR in DMF)

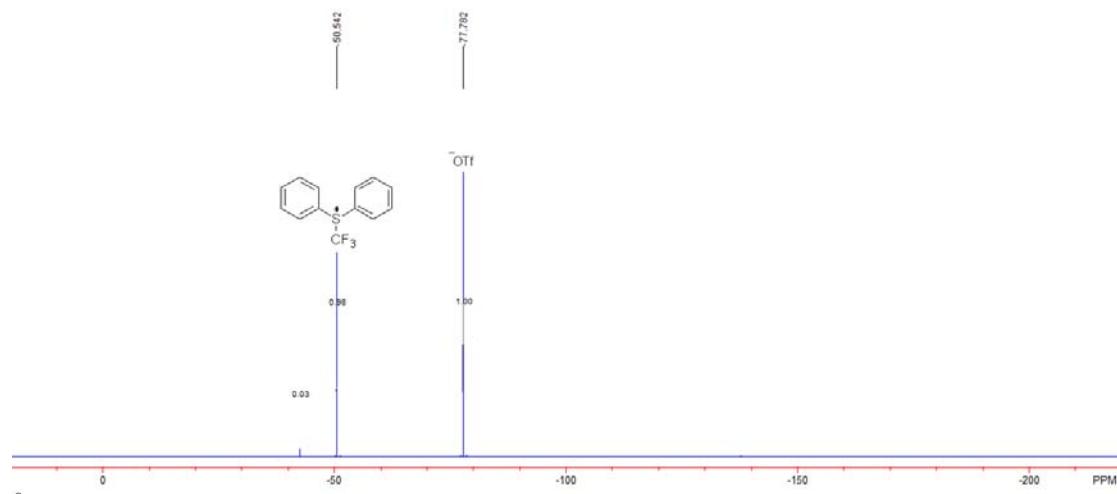


Table 1, entry 2 (¹⁹F NMR in DMF)

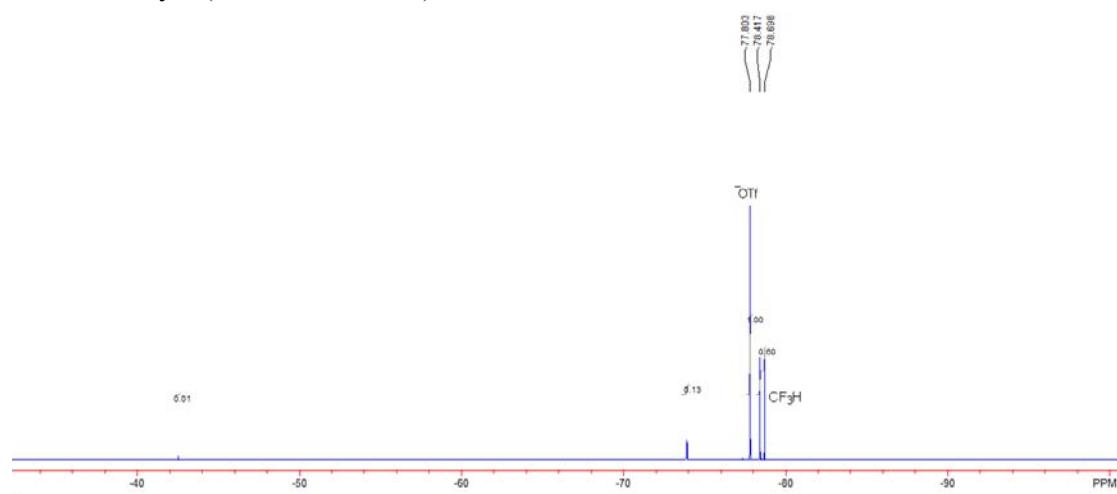


Table 1, entry 3 (¹⁹F NMR in DMF)

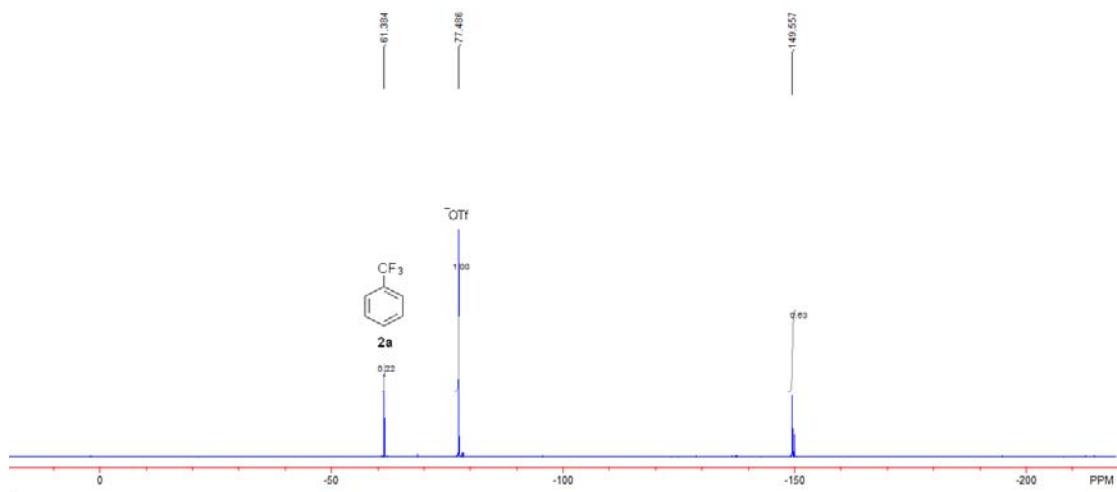


Table 1, entry 4 (^{19}F NMR in DMF)

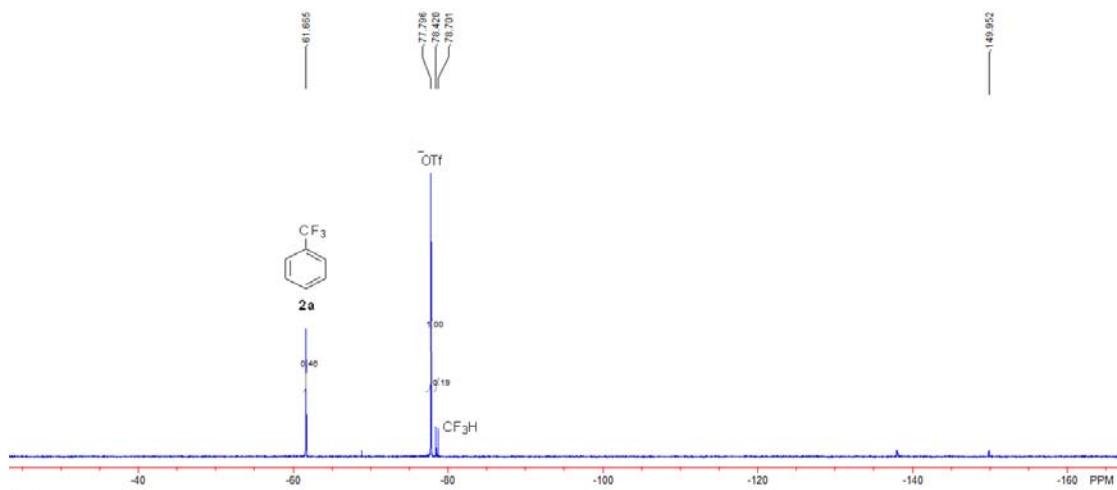


Table 1, entry 5 (^{19}F NMR in DMF)

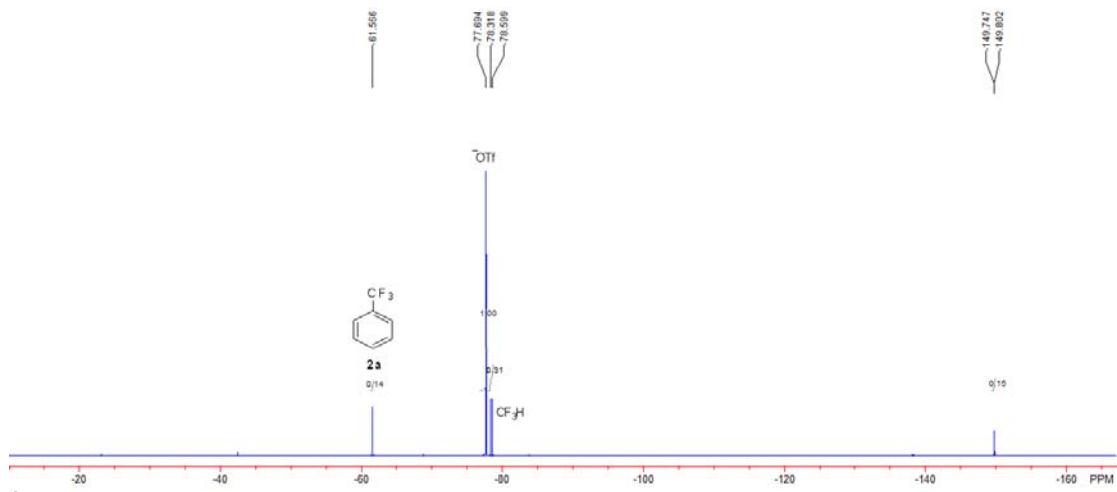


Table 1, entry 6 (^{19}F NMR in DMF)

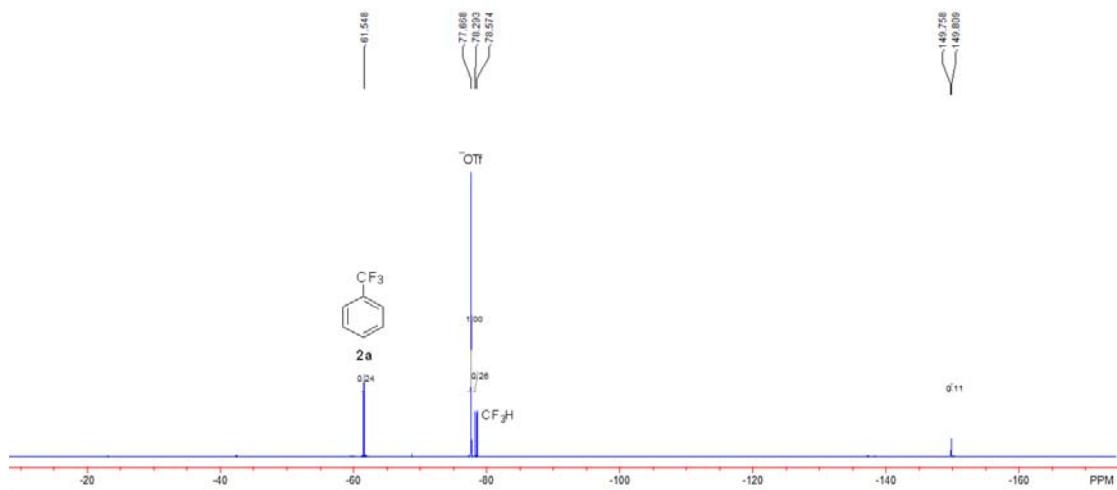


Table 1, entry 7 (^{19}F NMR in DMF)

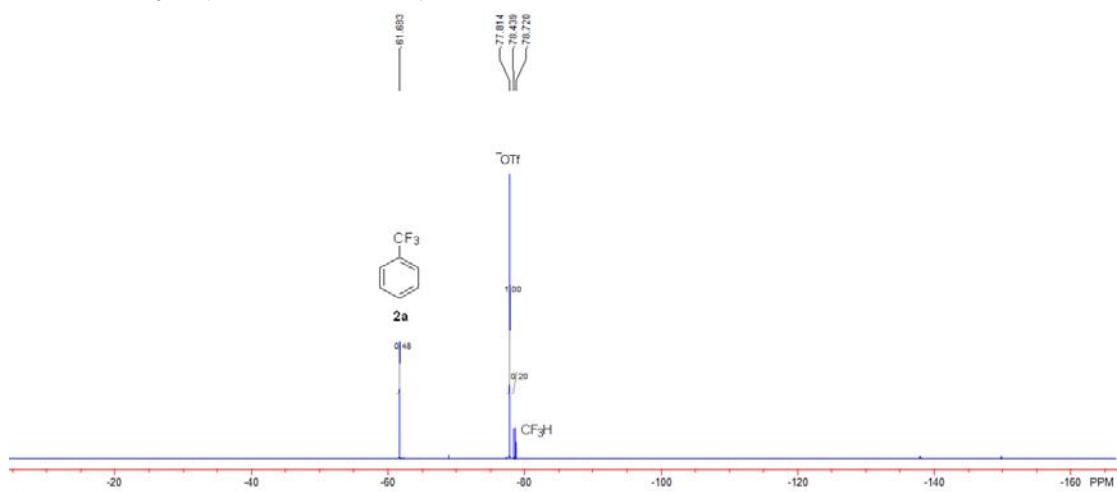


Table 1, entry 8 (^{19}F NMR in DMF)

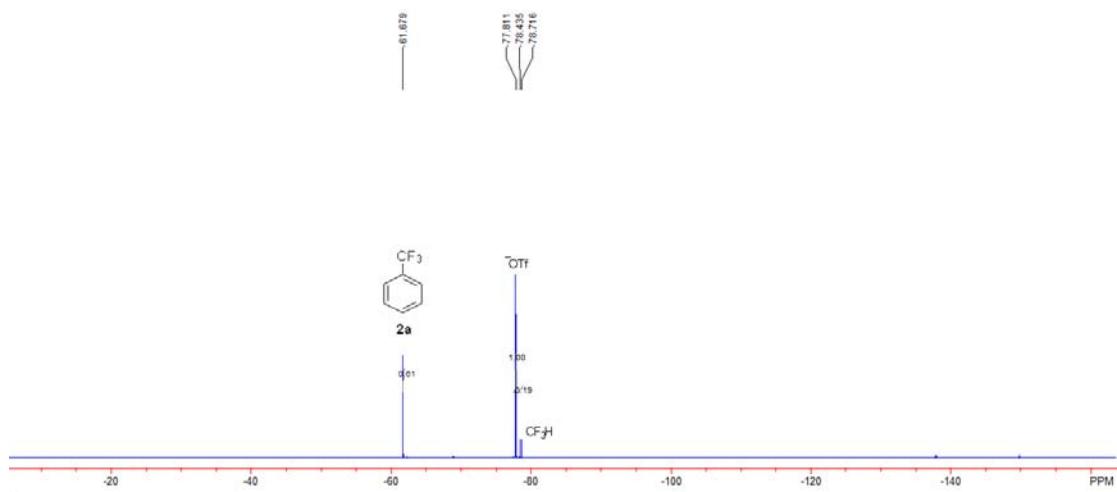


Table 1, entry 9 (^{19}F NMR in DMF)

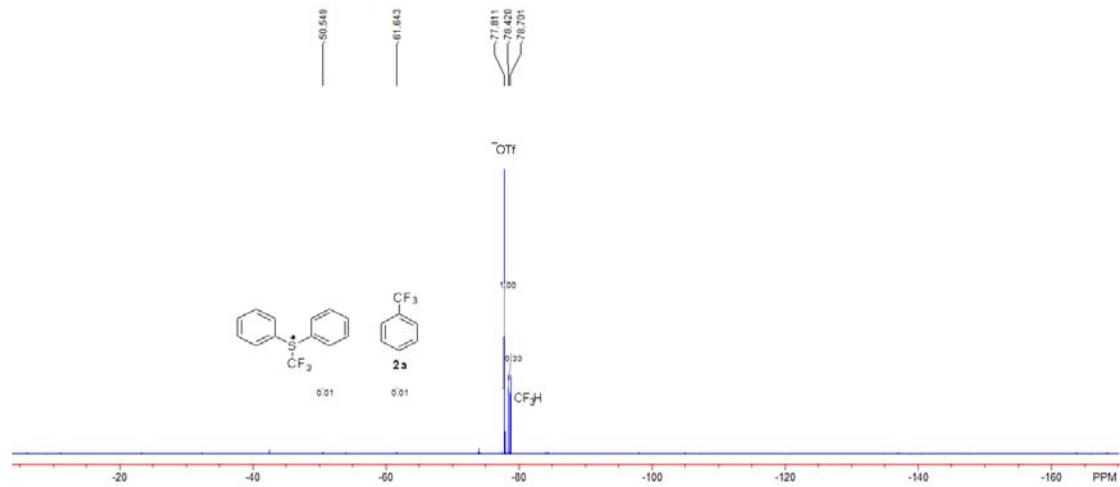


Table 1, entry 10 (¹⁹F NMR in CH₃CN)

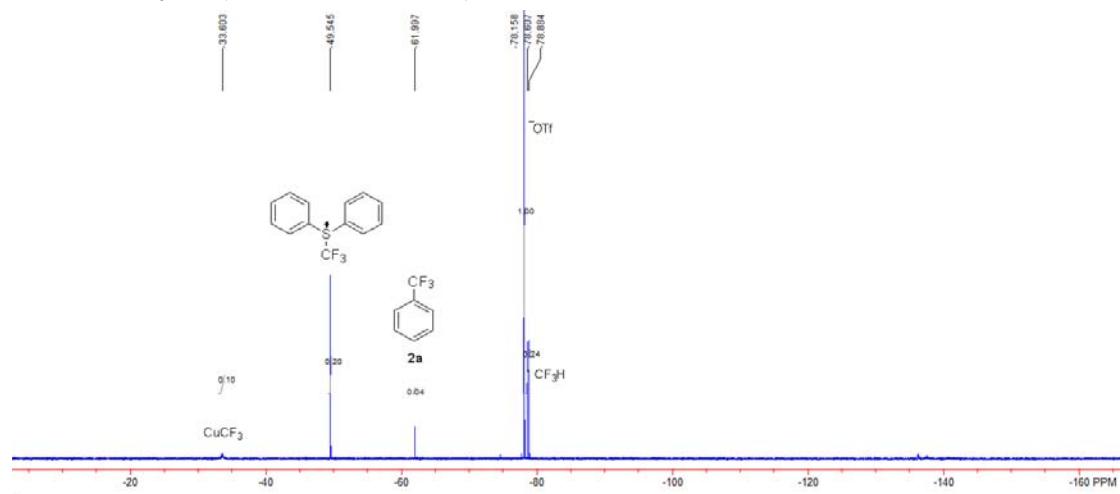


Table 1, entry 11 (¹⁹F NMR in DCM)

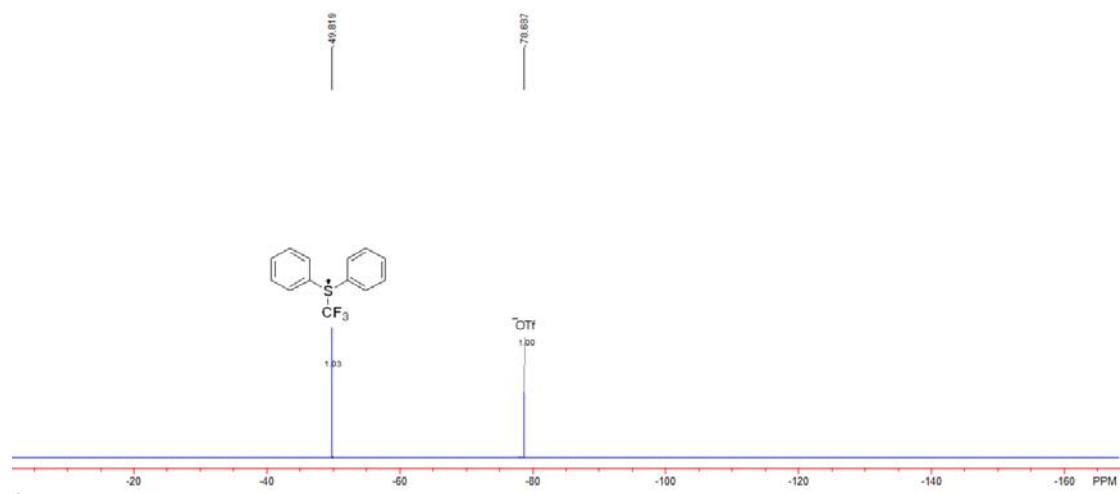


Table 1, entry 12 (¹⁹F NMR in DMSO)

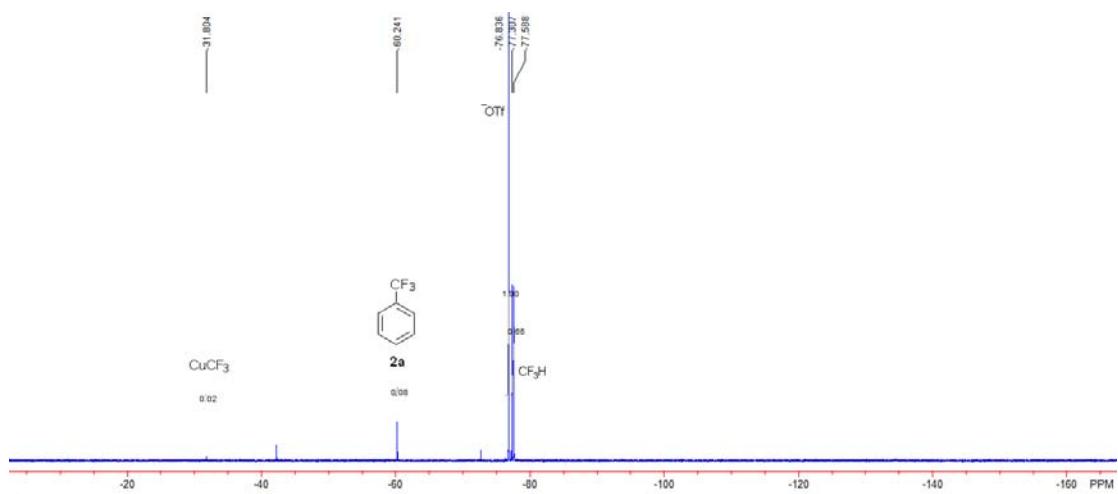


Table 1, entry 13 (¹⁹F NMR in THF)

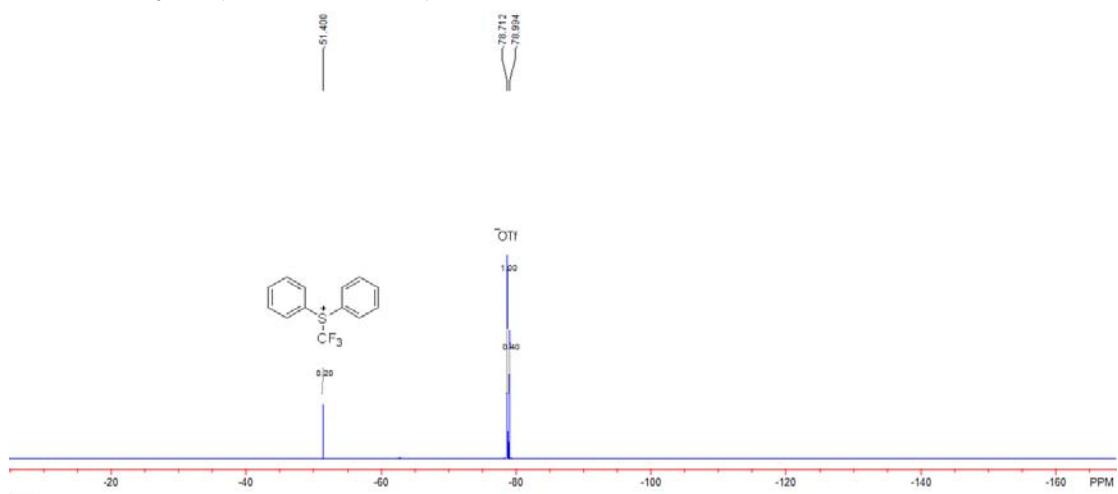


Table 1, entry 14 (¹⁹F NMR in DMF)

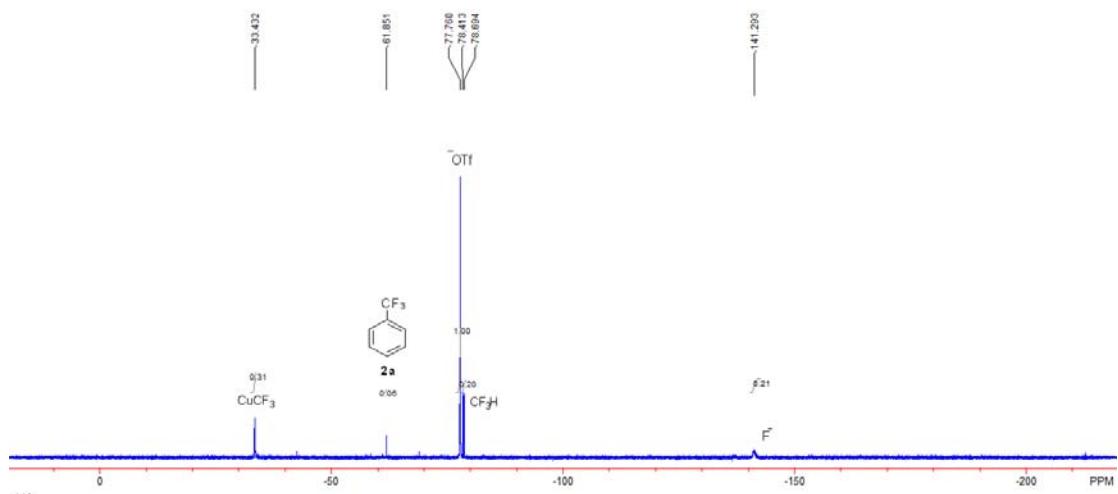


Table 1, entry 15 (¹⁹F NMR in DMF)

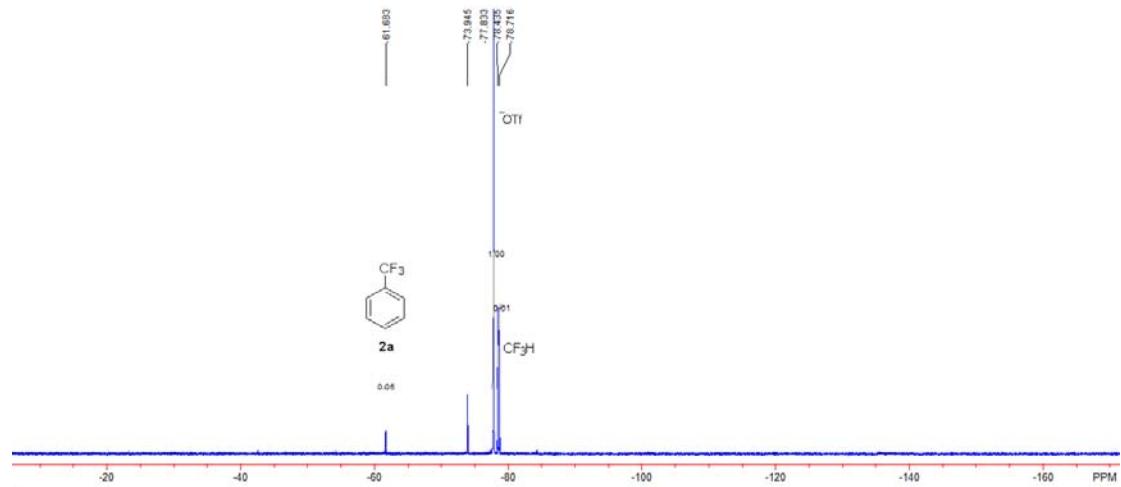


Table 1, entry 16 (^{19}F NMR in DMF)

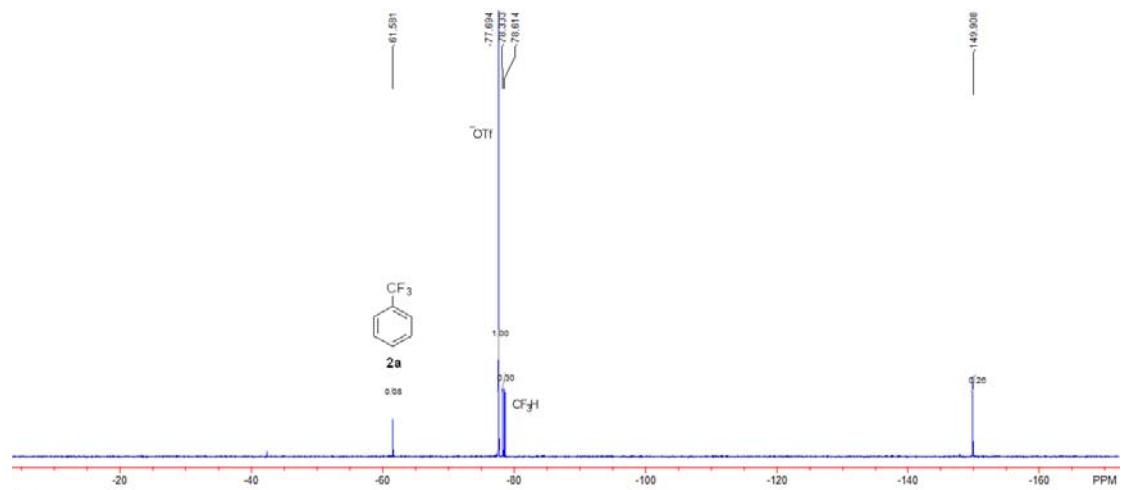


Table 1, entry 17 (^{19}F NMR in DMF)

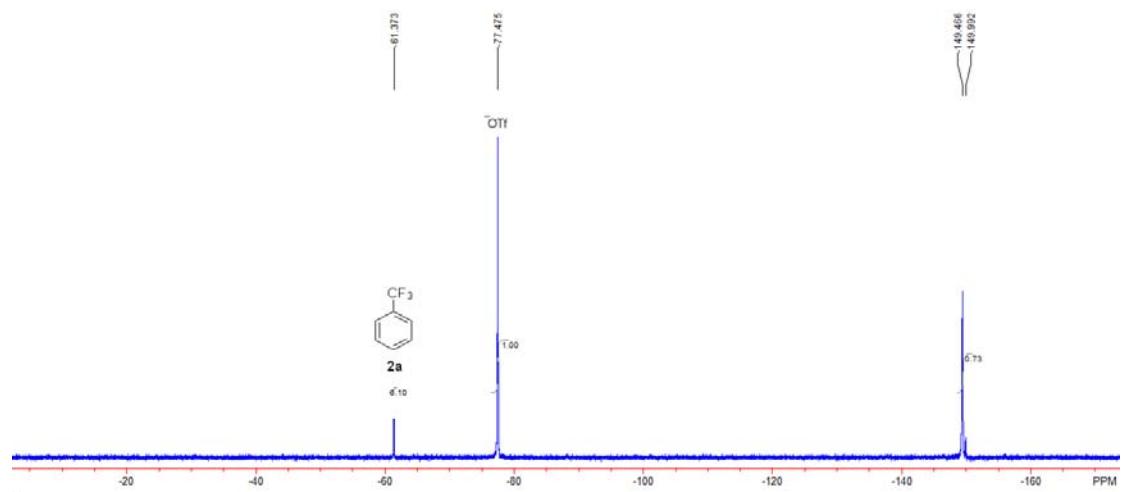


Table 1, entry 18 (^{19}F NMR in DMF)

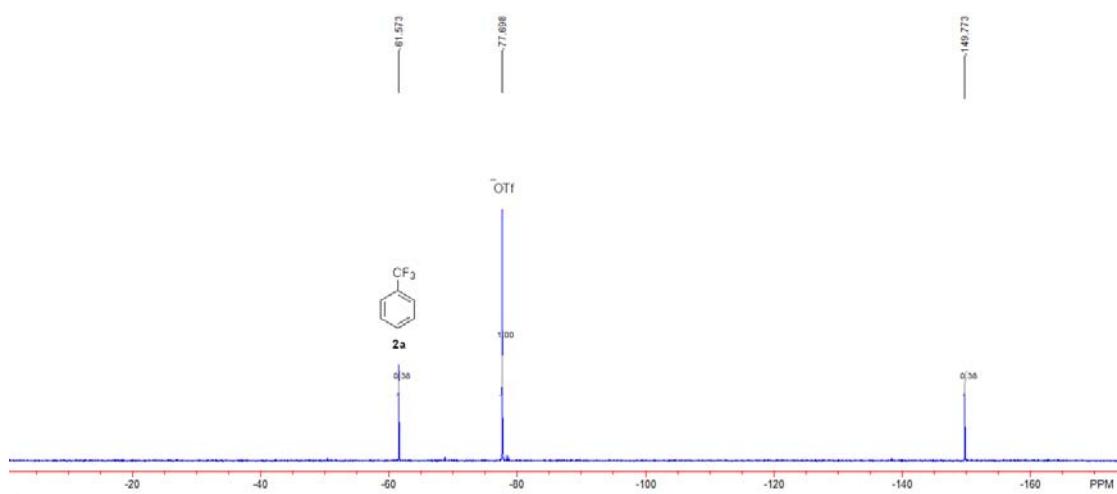


Table 1, entry 19 (¹⁹F NMR in DMF)

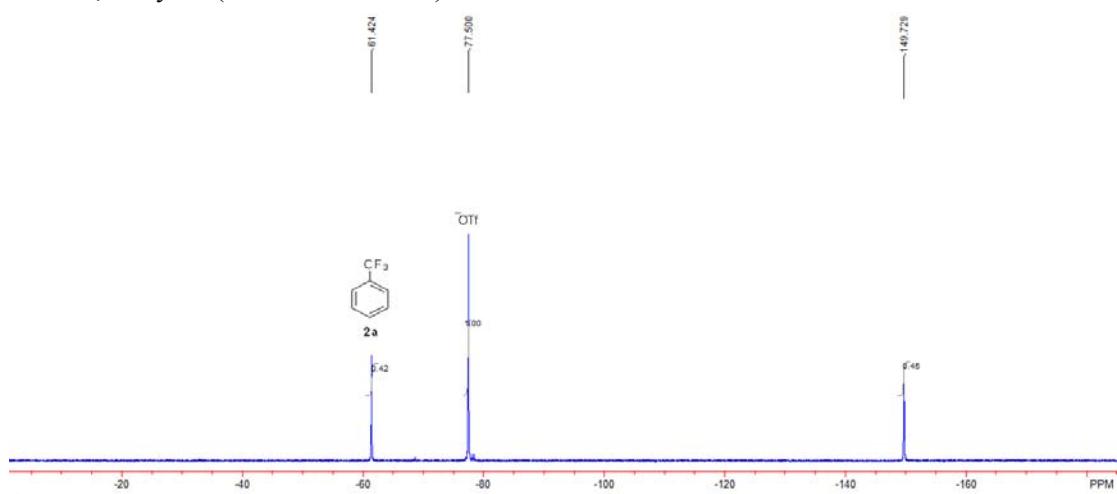
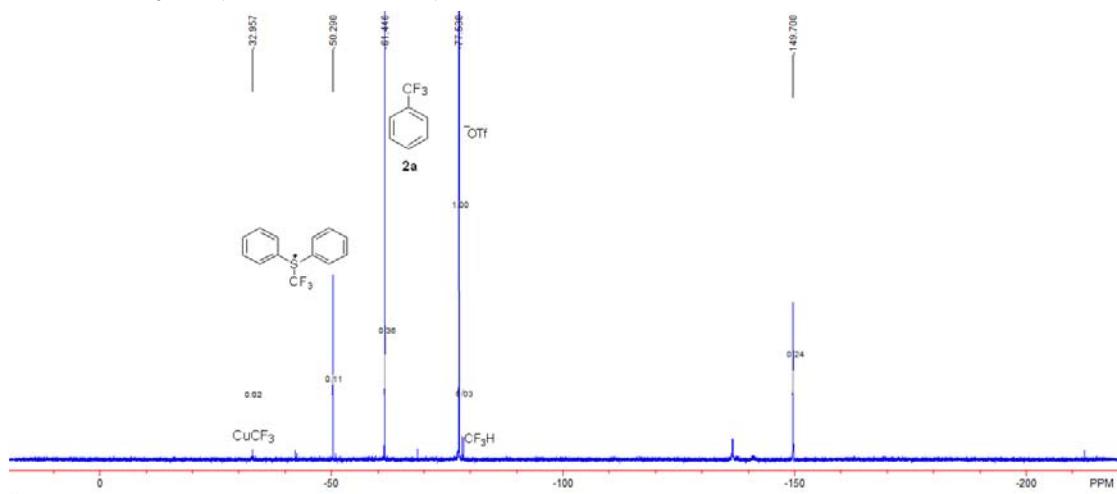


Table 1, entry 20 (¹⁹F NMR in DMF)



MS analysis of the reaction mixture (Table 1, entry 20)

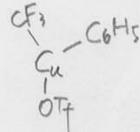
MSD1 SPC, scan=38, time=0.636 of 2010753-1.D
数据文件: : D:\DATA\2010753-1.D
样品名称 :

操作者 :
仪器 : 仪器 1 位置 : 样品瓶 21
进样日期 : 2011-4-18 10:41:45 进样次数 : 1
进样量 : 3.0 μ l
采集方法 : D:\METHOD\STANDBY.M
最后修改 : 2011-4-18 10:40:46
分析方法 : D:\METHOD\STANDBY.M
最后修改 : 2011-3-24 9:35:16

ES-API, Pos, Scan

ES-API, Pos, Scan, Frag : 70

| m/z | 丰度 | m/z | 丰度 | m/z | 丰度 |
|--------|-----------------------|--------|---------------------------------------|--------|------|
| 44.20 | 0.2 | 188.00 | 0.1 | 291.90 | 0.1 |
| 46.10 | 2.0 | 189.10 | 0.1 | 296.90 | 0.1 |
| 47.00 | 0.1 | 194.90 | 1.2 | 297.80 | 0.1 |
| 58.10 | 1.2 | 195.70 | 0.1 | 298.80 | 0.1 |
| 59.00 | 0.1 | 196.80 | 0.2 | 301.00 | 0.5 |
| 62.90 | 0.1 | 199.80 | 0.1 | 302.10 | 0.1 |
| 65.00 | 0.3 | 200.10 | 0.1 | 303.00 | 0.2 |
| 73.10 | 18.6 | 201.90 | 0.1 | 304.00 | 0.1 |
| 74.10 | 1.4 | 209.00 | 15.8 | 305.90 | 0.3 |
| 75.00 | 0.1 | 210.00 | Cu ₂ CF ₃ 1.0 | 307.90 | 0.2 |
| 80.10 | 0.2 | 211.00 | C ₆ H ₅ 7.3 | 309.90 | 0.1 |
| 90.10 | 0.1 | 212.00 | 0.5 | 317.00 | 0.1 |
| 96.10 | 100.0 | 212.90 | 0.1 | 322.00 | 0.3 |
| 97.10 | 3.7 | 214.30 | 0.1 | 322.80 | 0.1 |
| 98.20 | 0.2 | 215.20 | 0.1 | 323.80 | 0.1 |
| 100.40 | 0.1 | 216.10 | 0.1 | 324.70 | 0.1 |
| 100.90 | 0.2 | 216.80 | 0.1 | 325.10 | 0.1 |
| 119.10 | 0.1 | 217.30 | 0.1 | 326.90 | 0.3 |
| 121.60 | 0.2 | 218.00 | 0.2 | 328.10 | 0.1 |
| 122.10 | 0.1 | 220.30 | 0.1 | 329.00 | 0.1 |
| 131.90 | CuCF ₃ 2.3 | 224.00 | 0.1 | 331.00 | 1.4 |
| 134.00 | 1.1 | 225.00 | 0.1 | 331.90 | 0.4 |
| 134.90 | 0.1 | 226.10 | 0.1 | 333.00 | 0.1 |
| 136.00 | 0.1 | 228.00 | 5.5 | 337.90 | 0.1 |
| 137.10 | 0.1 | 229.00 | 0.4 | 340.60 | 0.1 |
| 138.20 | 0.1 | 230.00 | 2.2 | 341.10 | 0.1 |
| 138.70 | 0.1 | 231.00 | 0.2 | 342.80 | 0.1 |
| 139.40 | 0.1 | 232.10 | 0.1 | 345.10 | 0.1 |
| 141.10 | 7.2 | 252.80 | 0.1 | 350.10 | 0.1 |
| 142.00 | 3.4 | 255.00 | ④ 94.0 | 351.90 | 0.1 |
| 145.00 | 1.7 | 256.00 | Ph ₂ SCF ₃ 13.6 | 357.90 | 11.9 |
| 145.80 | 0.1 | 257.00 | 5.4 | 358.90 | 1.4 |
| 146.90 | 0.8 | 258.00 | 0.7 | 359.90 | 6.4 |
| 148.10 | 0.1 | 259.20 | 0.1 | 361.00 | 0.7 |
| 149.10 | 0.1 | 262.10 | 0.1 | 362.00 | 0.4 |
| 149.80 | 0.1 | 263.00 | 2.3 | 363.00 | 0.4 |
| 153.30 | 0.1 | 264.10 | 0.6 | 364.20 | 0.1 |
| 164.00 | 4.4 | 264.90 | 0.2 | 366.10 | 0.1 |
| 164.90 | 0.3 | 265.20 | 0.2 | 366.90 | 0.2 |
| 165.90 | 1.9 | 265.90 | 0.1 | 368.90 | 0.1 |
| 166.80 | 0.1 | 267.90 | 0.8 | 370.20 | 0.1 |
| 169.10 | 2.3 | 269.00 | 4.4 | 388.80 | 0.2 |
| 170.10 | 0.1 | 270.00 | 0.8 | 390.00 | 0.1 |
| 177.00 | 6.6 | 271.00 | 0.3 | 390.90 | 0.1 |
| 177.90 | 0.6 | 283.10 | 3.6 | 391.80 | 0.1 |
| 179.00 | 2.9 | 284.00 | 0.7 | 393.00 | 0.1 |
| 180.00 | 0.3 | 284.90 | 0.4 | 400.00 | 0.3 |
| 180.90 | 0.4 | 286.10 | 0.0 | 401.80 | 0.2 |
| 183.00 | 0.2 | 287.00 | 0.2 | 420.80 | 0.1 |
| 186.00 | 3.1 | 289.90 | 0.1 | 423.00 | 0.1 |
| 187.10 | 0.5 | 290.60 | 0.1 | 426.20 | 0.1 |



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MSD1 SPC, scan=35, time=0.619 of 2010753-1-N.D
数据文件: : D:\DATA\2010753-1-N.D
样品名称 :

=====

操作者 : 仪器 1 位置 : 样品瓶 21
进样日期 : 2011-4-18 15:36:55 进样次数 : 1
进样量 : 5.0 μ l

采集方法 : D:\METHOD\STANDBY.M
最后修改 : 2011-4-18 15:36:03
(调用后修改)

分析方法 : D:\METHOD\STANDBY.M
最后修改 : 2011-3-24 9:35:16

ES- API, Neg. Scan

| m/z | 丰度 | m/z | 丰度 | m/z | 丰度 |
|--------|-----------------------------------|--------|-----|--------|-----|
| 79.90 | 0.6 | 492.80 | 1.8 | 912.80 | 0.2 |
| 87.00 | 0.2 | 493.60 | 0.2 | 914.30 | 0.2 |
| 98.20 | 0.3 | 494.90 | 0.2 | 914.70 | 0.2 |
| 99.10 | 1.1 | 509.80 | 5.9 | 916.40 | 0.2 |
| 111.00 | 0.2 | 510.60 | 0.4 | | |
| 149.00 | 100.0 | 511.80 | 3.3 | | |
| 150.00 | OTf | 512.60 | 0.2 | | |
| 151.00 | 5.3 | 513.70 | 0.6 | | |
| 200.80 | Cu(CF ₃) ₂ | 523.70 | 0.2 | | |
| 202.80 | 0.4 | 534.80 | 0.3 | | |
| 249.80 | 0.5 | 539.70 | 0.2 | | |
| 251.80 | 0.5 | 551.80 | 1.1 | | |
| 263.80 | 0.2 | 553.60 | 0.9 | | |
| 269.90 | 1.6 | 582.10 | 0.2 | | |
| 271.00 | 0.8 | 593.80 | 0.2 | | |
| 271.80 | 0.4 | 595.80 | 0.1 | | |
| 280.90 | 0.5 | 610.80 | 0.2 | | |
| 281.80 | Cu(CF ₃) ₂ | 612.60 | 0.3 | | |
| 282.90 | 0.4 | 622.70 | 0.2 | | |
| 320.90 | 11.4 | 624.60 | 0.2 | | |
| 321.90 | 0.4 | 636.50 | 0.2 | | |
| 322.80 | 1.3 | 664.80 | 0.6 | | |
| 338.90 | 28.8 | 665.60 | 0.2 | | |
| 339.80 | 1.2 | 666.70 | 0.2 | | |
| 340.90 | 13.9 | 681.70 | 2.4 | | |
| 341.80 | 0.7 | 682.70 | 0.4 | | |
| 343.90 | 14.9 | 683.80 | 1.1 | | |
| 344.80 | 1.1 | 684.50 | 0.2 | | |
| 346.00 | 1.6 | 685.80 | 0.2 | | |
| 349.90 | 0.3 | 723.70 | 0.5 | | |
| 360.80 | 1.3 | 725.70 | 0.3 | | |
| 362.90 | 0.9 | 740.60 | 0.7 | | |
| 379.80 | 4.6 | 742.60 | 0.5 | | |
| 380.80 | 0.2 | 744.50 | 0.2 | | |
| 381.80 | 3.1 | 752.80 | 0.3 | | |
| 383.90 | 0.2 | 754.70 | 0.4 | | |
| 391.70 | 0.3 | 756.40 | 0.1 | | |
| 393.80 | 0.2 | 765.60 | 0.1 | | |
| 414.80 | 0.2 | 782.40 | 0.1 | | |
| 418.80 | 0.8 | 836.50 | 0.2 | | |
| 420.80 | 0.2 | 837.00 | 0.2 | | |
| 421.60 | 0.2 | 853.70 | 0.5 | | |
| 422.70 | 0.2 | 855.60 | 0.4 | | |
| 441.70 | 0.1 | 857.60 | 0.2 | | |
| 442.80 | 0.3 | 870.20 | 0.3 | | |
| 443.10 | 0.3 | 870.60 | 0.4 | | |
| 470.70 | 0.5 | 872.60 | 0.4 | | |
| 471.90 | 1.5 | 874.40 | 0.2 | | |
| 472.80 | 0.4 | 874.70 | 0.2 | | |
| 473.20 | 0.3 | 895.60 | 0.3 | | |
| 473.90 | 0.8 | 897.50 | 0.2 | | |

ESI

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Copies of NMR Spectra for 2b-q

