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Supporting Information

Copper(II)-Catalyzed Trifluoromethylation of Iodoarenes using Chen Reagent Shiyu Zhao^{a,d}, Yong Guo^{a,d,*}, En-Jian Han^a, Jun Luo^b, Hui-Min Liu^{b,*}, Chao Liu^{a,d}, Weidong Xie^c, Wei Zhang^c, Mengying Wang^c ^aKey Laboratory of Organofluorine Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai 200032, P. R. of China ^bSchool of Perfume and Aroma Technology, Shanghai Institute of Technology, 100 Haiquan Road, Shanghai 201418, P. R. of China ^cSanming Hexafluo Chemicals Co., LTD., Fluorinated New Material Industry Park, Mingxi, Fujian 365200, P. R. of China ^dUniversity of Chinese Academy of Sciences Email addresses: yguo@sioc.ac.cn, szliuhm@sit.edu.cn **Table of Contents** 3. General procedures for trifluoromethylation of iodoarenes.......S3

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2. General information

NMR spectra were obtained on a 400 MHz spectrometer using CDCl₃ as deuterated solvents, with proton, carbon and fluorine resonances at 400 MHz, 100 MHz and 376 MHz, respectively. Chemical shifts were reported in parts per million (ppm) relative to TMS as an internal standard ($\delta_{TMS} = 0$ ppm) for ¹H and ¹³C NMR spectra and CFCl₃ as an external standard (negative for upfield) for ¹⁹F NMR spectra. DMF was distilled from CaH₂. All the other solvents or reagents were used as commercial sources without purification if not noted. All reactions were performed in standard Schlenk tubes and monitored by thin-layer chromatography (TLC), ¹⁹F NMR or GC-MS. Flash column chromatography was carried out using 300-400 mesh silica gel.

3. General procedures for trifluoromethylation of iodoarenes

A Schlenk tube was charged with CuCl₂ (6.7 mg, 0.05 mmol), FSO₂CF₂CO₂Me (240 mg, 1.25 mmol), aryl iodide (0.5 mmol) and DMF (1.5 mL) under nitrogen. The reaction mixture was warmed stepwise to 110°C and then the mixture was stirred at 110 °C for 2 hours. An internal standard (α , α , α -trifluorotoluene or 4-(trifluoromethoxy)benzotrifluoride) was added into the resulting mixture to calculate the ¹⁹F NMR yield. The reaction mixture was added with ethyl acetate (10 mL) or dichloromethane (10 mL) and water (10 mL). After the filterate and washing with water (2 × 10 mL) and brine (2 × 10 mL), the organic phase was dried with anhydrous sodium sulfate. After removal of the solvent under reduced pressure, the crude product was purified by column chromatography on silica gel with an ethyl acetate/petroleum ether mixture as eluent to afford the desired trifluoromethylated product.



1-(trifluoromethyl)naphthalene (3a)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a colorless liquid in 82% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃): δ 8.19 (d, 1H), 8.02 (d, 1H), 8.02–7.82 (q, 2H), 7.69 – 7.55 (m, 2H), 7.54–7.46 (t, 1H). ¹⁹F NMR (376 MHz, CDCl₃) δ -59.7 (s).

4-(trifluoromethyl)-1,1'-biphenyl (3b)²: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a colorless liquid in 85% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 7.70 (s, 4H), 7.61 (d, J = 8.5 Hz, 2H), 7.48 (t, J = 7.9 Hz, 2H), 7.41 (t, J = 7.3 Hz, 1H). ¹⁹F NMR (376 MHz, CDCl₃) δ ppm -62.5 (s).



2-(trifluoromethyl)-1,1'-biphenyl (3c)³: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a colorless liquid in 78% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 7.80 (d, *J* = 8.4 Hz, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 7.53 – 7.46 (m, 1H), 7.44 (m, 3H), 7.41 – 7.37 (m, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -56.8 (s).



1-tert-Butyl-4-(trifluoromethyl)benzene (3d)⁴: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.5 mmol, 3 equiv), and CuCl₂ (0.075 mmol, 0.15 equiv), and the product was obtained as a colorless liquid in 74% yield by silica gel flash column chromatography. ¹H NMR (300 MHz, CDCl₃) δ 7.66 (d, *J* = 8.3 Hz, 2H), 7.60 (d, *J* = 8.3 Hz, 2H), 1.44 (s, 9H). ¹⁹F NMR (376 MHz, CDCl₃) δ -62.7 (s).



1-(4-(trifluoromethyl)phenyl)ethan-1-one (3e)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1equiv), and the product was obtained as a colorless liquid in 90% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 8.04 (d, *J* = 8.2 Hz, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 2.63 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ ppm -62.9 (s).



Methyl 3-(trifluoromethyl)benzoate $(3f)^1$: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a colorless liquid in 86% yield by silica gel flash

column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 8.31 (s, 1H), 8.22 (d, *J* = 7.8 Hz, 1H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.58 (t, *J* = 7.8 Hz, 1H), 3.96 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ ppm -63.0 (s).



Methyl 4-(trifluoromethyl)benzoate (3g)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a colorless liquid in 90% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 8.14 (d, *J* = 8.2 Hz, 2H), 7.69 (d, *J* = 8.2 Hz, 2H), 3.95 (s, 3H).¹⁹ F NMR (376 MHz, CDCl₃) δ -63.4 (s).



Methyl 2-(trifluoromethyl)benzoate (3h)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a colorless liquid in 89% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 7.75 (dq, *J* = 12.7, 3.8 Hz, 2H), 7.59 (d, *J* = 5.5 Hz, 2H), 3.93 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -59.8 (s).



2-(Trifluoromethyl)benzonitrile (3i)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a yellow liquid in 90% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 7.85 (d, *J* = 7.4 Hz, 1H), 7.80 (d, *J* = 7.7 Hz, 1H), 7.77 (d, *J* = 7.4 Hz, 1H), 7.71 (q, *J* = 7.4, 6.5 Hz, 1H). ¹⁹F NMR (376 MHz, CDCl₃) δ -62.1 (s).



4-(Trifluoromethyl)benzonitrile (3j)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the

product was obtained as a colorless liquid in 92% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 7.81 (d, *J* = 8.7 Hz, 2H), 7.76 (d, *J* = 8.6 Hz, 2H). ¹⁹F NMR (376 MHz, CDCl₃) δ -63.6 (s).

1-Nitro-2-(trifluoromethyl)benzene (3k)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a colorless liquid in 82% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 7.92 – 7.86 (m, 1H), 7.84 (dd, J = 5.7, 3.6 Hz, 1H), 7.77 – 7.70 (m, 2H). ¹⁹F NMR (376 MHz, CDCl₃) δ -60.1 (s).



1-Nitro-4-(trifluoromethyl)benzene (3l)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a colorless liquid in 82% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 8.52 (s, 1H), 8.45 (d, *J* = 8.2 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 7.76 (t, *J* = 8.0 Hz, 1H). ¹⁹ F NMR (376 MHz, CDCl₃) δ -63.0 (s).

1-Nitro-4-(trifluoromethyl)benzene (3m)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a white solid in 82% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 8.36 (d, *J* = 8.6 Hz, 2H), 7.84 (d, *J* = 8.7 Hz, 2H). ¹⁹ F NMR(376 MHz, CDCl₃) δ -63.1 (s).



(4-(Trifluoromethyl)phenyl)methanol (3n)⁵: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a colorless liquid in 87% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 7.60 (d, *J* = 8.1 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 2H), 4.73 (s, 2H), 2.47 (s, 1H). ¹⁹F NMR (376 MHz, CDCl₃) δ -62.5 (s).



1-Chloro-4-(trifluoromethyl)benzene (30)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.5mmol, 3 equiv), and CuCl₂ (0.75 mmol, 0.15 equiv). 80% yield was determined by ¹⁹F NMR. Crude ¹⁹F NMR (unlocked): δ –62.2 (s).



4-(trifluoromethyl)benzaldehyde (3p)⁶: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a colorless liquid in 87% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 10.09 (s, 1H), 8.00 (d, *J* = 8.0 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 2H). ¹⁹F NMR (376 MHz, CDCl₃) δ -63.3 (s).



2-(Trifluoromethyl)acetophenone (3q)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.25 mmol, 2.5 equiv), and CuCl₂ (0.05 mmol, 0.1 equiv), and the product was obtained as a colorless liquid in 87% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 7.68 (d, *J* = 8.9 Hz, 1H), 7.63 – 7.50 (m, 2H), 7.45 (d, *J* = 8.2 Hz, 1H), 2.56 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -58.1 (s).



1-Methoxy-4-(trifluoromethyl)benzene (3r)⁷: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.5 mmol, 3 equiv), and CuCl₂ (0.75 mmol, 0.15 equiv),

and the product was obtained as a colorless liquid in 69% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 7.55 (d, *J* = 8.8 Hz, 2H), 6.97 (d, *J* = 8.8 Hz, 2H), 3.85 (s, 3H). ¹⁹F NMR (376 MHz, CDCl₃) δ -61.5 (s).

1-Methoxy-2-(trifluoromethyl)benzene (3s)⁷: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.5 mmol, 3 equiv), and CuCl₂ (0.075 mmol, 0.15 equiv), and the product was obtained as a colorless liquid in 84% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 7.57 (d, *J* = 7.9 Hz, 1H), 7.50 (t, *J* = 7.9 Hz, 1H), 7.01 (dt, *J* = 7.4, 3.0 Hz, 2H), 3.91 (s, 3H).¹⁹F NMR (376 MHz, CDCl₃) δ -62.5 (s).



1-Methyl-4-(trifluoromethyl)benzene (3t)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.5 mmol, 3 equiv), and CuCl₂ (0.075 mmol, 0.15 equiv). 60% yield was determined by ¹⁹F NMR. Crude ¹⁹F NMR (unlocked): δ –61.8 (s).



1-Methyl-2-(trifluoromethyl)benzene (3u)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.5 mmol, 3 equiv), and CuCl₂ (0.075 mmol, 0.1equiv). 51% yield was determined by ¹⁹F NMR. Crude ¹⁹F NMR (unlocked): δ –61.2 (s).



1-Methyl-3-(trifluoromethyl)benzene (3v)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.5mmol, 3 equiv), and CuCl₂ (0.075 mmol, 0.1 equiv). 66% yield was determined by ¹⁹F NMR. Crude ¹⁹F NMR (unlocked): δ –61.8 (s).

5-Chloro-2-(trifluoromethyl)pyrimidine (3w)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.5mmol, 3 equiv), and CuCl₂ (0.075 mmol, 0.1 equiv). 83% yield was determined by ¹⁹F NMR. Crude ¹⁹F NMR (unlocked): δ –69.8 (s).

2-Methoxy-3-(trifluoromethyl)pyridine (3x)¹: The reaction was run on substrate(0.5 mmol), FSO₂CF₂CO₂Me (1. 5mmol, 3 equiv), and CuCl₂ (0.05 mmol, 0.1equiv). and the product was obtained as a colorless liquid in 70% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, Chloroform-d) δ 8.31 (d, J = 4.5 Hz, 1H), 7.84 (d, J = 7.4 Hz, 1H), 7.00 – 6.89 (m, 1H), 4.03 (s, 3H). ¹⁹F NMR (376MHz, CDCl₃) δ - 64.04 (s, 3F).



4-methoxy-2-(trifluoromethyl)pyrimidine (3y)¹: The reaction was run on substrate (0.5 mmol), FSO₂CF₂CO₂Me (1.5 mmol, 3 equiv), and CuCl₂ (0.075 mmol, 0.15 equiv). and the product was obtained as a colorless liquid in 62% yield by silica gel flash column chromatography. ¹H NMR (400 MHz, CDCl₃) δ 8.53 (d, *J* = 5.8 Hz, 1H), 6.87 (d, *J* = 5.8 Hz, 1H).¹⁹F NMR (376 MHz, CDCl₃) δ -71.1 (s).



3-(Trifluoromethyl)thiophene (3z)¹: The reaction was run on substrate (0.5 mmol), $FSO_2CF_2CO_2Me$ (1.5mmol, 3 equiv), and $CuCl_2$ (0.075 mmol, 0.1 equiv). 55% yield was determined by ¹⁹F NMR. Crude ¹⁹F NMR (unlocked): δ –58.6 (s).



2-(trifluoromethyl)pyridine (3aa)¹: The reaction was run on substrate (0.5 mmol), $FSO_2CF_2CO_2Me$ (1.5mmol, 3 equiv), and $CuCl_2$ (0.075 mmol, 0.15 equiv). 75% yield was determined by ¹⁹F NMR. Crude ¹⁹F NMR (unlocked): δ –67.8 (s, 3F).

4. Application of the reaction

Synthesis of 3e on gram scale

An oven-dried two-neck flask was charged with CuCl₂ (134 mg, 1 mmol), FSO₂CF₂CO₂Me (5.76 g, 30 mmol), 4-iodoacetophenone (2.46 g, 10 mmol) and DMF (30 mL) under nitrogen atmosphere. The reaction mixture was warmed stepwise to 110 °C and then the mixture was stirred at 110 °C for 2 hours. Then the reaction mixture was added ethyl acetate (50 mL). After the filtration and washing with water (2 × 50 mL) and brine (2 × 50 mL), the organic phase was dried with anhydrous sodium sulfate. After removal of the solvent under reduced pressure, the crude product was purified by column chromatography on silica gel with an ethyl acetate/petroleum ether mixture as eluent to afford the desired trifluoromethylated product **3e** (1.60 g, 83%).

Synthesis of Prozac⁸



An oven-dried two-neck flask was charged with **4** (1.65g, 10mmol), NEt₃ (1.01g, 10 mmol) and THF (10 mL). The Boc₂O (2.26 g, 12 mmol) was added dropwise via syringe. Then the mixture was stirred at room temperature for 2 h. After removal of the solvent under reduced pressure, the colorless liquid was dried in *vacuo* to afford the *tert*-butyl (3-hydroxy-3-phenylpropyl)(methyl)carbamate **5** (2.62 g, 99% yield).

¹H NMR (400 MHz, CDCl₃) δ 7.38 – 7.21 (m, 5H), 4.60 (dd, *J* = 10.4, 3.4 Hz, 1H), 3.79 (s, 1H), 3.05 (d, *J* = 22.7 Hz, 1H), 2.86 (d, *J* = 2.0 Hz, 3H), 1.93 (dddd, *J* = 11.5, 9.9, 6.3, 4.1 Hz, 2H), 1.46 (d, *J* = 1.5 Hz, 9H).



An oven-dried two-neck flask was charged with **5** (265 mg, 1 mmol), 4iodophenol (330 mg, 1.5 mmol), PPh₃ (394 mg,1.5 mmol) and THF (2 mL). The diisopropylazodicarboxylate (303 mg, 1.5 mmol) was added dropwise via syringe while keeping inner temperature between 0 °C – 5 °C. Then the mixture was allowed to warm to room temperate and stirred at room temperature for overnight. After completion of the reaction as indicated the TLC (the next day), the solvent was removed in *vacuo*. The crude product was purified by silica gel column chromatography to afford the *tert*-butyl (3-(4-iodophenoxy)-3phenylpropyl)(methyl)carbamate **6** (257 mg, 55% yield) as colorless oil.



This substrates was prepared according to the procedure described for 3e. An oven-dried two-neck flask was charged with CuCl₂ (40.2 mg, 0.3 mmol), FSO₂CF₂CO₂Me 6 mmol), *tert*-butyl (3-(4-iodophenoxy)-3-(1.15)g, phenylpropyl)(methyl)carbamate 6 (0.93 g, 2 mmol) and DMF (6 mL) under nitrogen atmosphere. The reaction mixture was warmed stepwise to 110 °C and then the mixture was stirred at 110 °C for 2 hours. Then the reaction mixture was added ethyl acetate (30 mL). After the filtration and washing with water (2×30 mL) and brine (2 \times 10 mL), the organic phase was dried with anhydrous sodium sulfate. After removal of the solvent under reduced pressure, the crude product was purified by column chromatography on silica gel with an ethyl acetate/petroleum ether mixture as eluent to afford the desired trifluoromethylated product tert-butyl methyl(3-phenyl-3-(4-(trifluoromethyl)phenoxy)propyl)carbamate 7 (0.41 g, 50%) and the starting material (0.32 g) was recovered. ¹H NMR (400 MHz, CDCl₃) δ 7.42 (d, J = 8.5 Hz, 2H), 7.38 – 7.21 (m, 5H), 6.88 (d, J = 8.5 Hz, 2H), 5.16 (dd, J = 8.9, 4.1 Hz, 1H), 3.41 (d, J = 47.2 Hz, 2H), 2.85 (s, 3H), 2.25 – 2.02 (m, 2H), 1.38 (d, J = 14.0 Hz, 9H). ¹⁹F NMR (376 MHz, CDCl₃) δ -61.6 (s, 3F).



An oven-dried two-neck flask was charged with 7 (220 mg, 0.54 mmol), TFA (616 mg, 5.4 mmol), CH₂Cl₂ (2 mL). Then the mixture was stirred at room temperature for 2 hours. The excess TFA was evaporated and the residue was dried in *vacuo* to give title compound (160 mg, 96%) as a yellow oil. ¹H NMR (400 MHz, CDCl₃) δ 9.26 (s, 2H), 7.41 (d, *J* = 8.6 Hz, 2H), 7.35 – 7.23 (m, 5H), 6.85 (d, *J* = 8.4 Hz, 2H), 3.13 (s, 2H), 2.61 (s, 3H), 2.45 – 2.19 (m, 2H). ¹⁹F NMR (376 MHz, CDCl₃) δ -61.7 (s, 3F), -75.8 (s, 3F).

5. Mechanistic Studies

Figure S1. CuCF₃ and $[Cu(CF_3)_4]^-$ species region of the ¹⁹F NMR spectrum of the reaction mixture of CuCl₂ with FSO₂CF₂CO₂Me in DMF under nitrogen at 110 °C



-20 -21 -22 -23 -24 -25 -26 -27 -28 -29 -30 -31 -32 -33 -34 -35 -36 -37 -38 -39 -40 -41 -42 -43 -44 -45 -46 -47 -48 -49 -50 -51 -52 -53 -54 -55 -56 -57 -58 -59 -60 f1 (ppm)

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7. NMR data



¹⁹F NMR spectrum of 1-(trifluoromethyl)naphthalene (3a)



¹H NMR spectrum of 4-(trifluoromethyl)-1,1'-biphenyl (3b)



¹H NMR spectrum of 2-(trifluoromethyl)-1,1'-biphenyl (3c)



¹⁹F NMR spectrum of 2-(trifluoromethyl)-1,1'-biphenyl (3c)



30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -20(f1 (ppm)

¹H NMR spectrum of 1-tert-Butyl-4-(trifluoromethyl)benzene (3d)



30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 f1 (ppm)

¹H NMR spectrum of 1-(4-(trifluoromethyl)phenyl)ethan-1-one (3e)





¹H NMR spectrum of methyl 3-(trifluoromethyl)benzoate (3f)



¹H NMR spectrum of methyl 4-(trifluoromethyl)benzoate (3g)



¹H NMR spectrum of methyl 2-(trifluoromethyl)benzoate (3h)



¹H NMR spectrum of 2-(Trifluoromethyl)benzonitrile (3i)



¹H NMR spectrum of 4-(Trifluoromethyl)benzonitrile (3j)



¹H NMR spectrum of 1-nitro-2-(trifluoromethyl)benzene (3k)



¹⁹F NMR spectrum of 1-nitro-2-(trifluoromethyl)benzene (3k)



¹H NMR spectrum of 1-nitro-4-(trifluoromethyl)benzene (3l)



¹H NMR spectrum of 1-Nitro-4-(trifluoromethyl)benzene (3m)



¹H NMR spectrum of (4-(trifluoromethyl)phenyl)methanol (3n)



¹⁹F NMR spectrum of (4-(trifluoromethyl)phenyl)methanol (3n)



30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 fl (ppm)

Crude ¹⁹F NMR spectrum of 1-chloro-4-(trifluoromethyl)benzene (30)



¹⁹F NMR spectrum of 4-(trifluoromethyl)benzaldehyde (3p)



¹⁹F NMR spectrum of 2-(Trifluoromethyl)acetophenone (3q)



¹⁹F NMR spectrum of 1-Methoxy-4-(trifluoromethyl)benzene (3r)



¹⁹F NMR spectrum of 1-methoxy-2-(trifluoromethyl)benzene (3s)



30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200

Crude ¹⁹F NMR spectrum of 1-methyl-4-(trifluoromethyl)benzene (3t)



Crude ¹⁹F NMR spectrum of 1-methyl-2-(trifluoromethyl)benzene (3u)



Crude ¹⁹F NMR spectrum of 1-methyl-3-(trifluoromethyl)benzene (3v)



Crude ¹⁹F NMR spectrum of 5-chloro-2-(trifluoromethyl)pyrimidine (3w)



¹H NMR spectrum of 2-methoxy-3-(trifluoromethyl)pyridine (3x)



¹⁹F NMR spectrum of 2-methoxy-3-(trifluoromethyl)pyridine (3x)



¹H NMR spectrum of 4-methoxy-2-(trifluoromethyl)pyrimidine (3y)



¹⁹F NMR spectrum of 4-methoxy-2-(trifluoromethyl)pyrimidine (3y)



Crude ¹⁹F NMR spectrum of 3-(trifluoromethyl)thiophene (3z)



Crude ¹⁹F NMR spectrum of 2-(trifluoromethyl)pyridine (3aa)



¹H NMR spectrum of tert-butyl (3-hydroxy-3-phenylpropyl)(methyl)carbamate (5)



phenylpropyl)(methyl)carbamate (6)



(trifluoromethyl)phenoxy)propyl)carbamate (7)



(trifluoromethyl)phenoxy)propyl)carbamate (7)



¹H NMR spectrum of N-methyl-3-phenyl-3-(4-(trifluoromethyl)phenoxy)propan-

1-amine trifluoroacetate (8)



¹⁹F NMR spectrum of N-methyl-3-phenyl-3-(4-(trifluoromethyl)phenoxy)propan-

1-amine trifluoroacetate (8)

