

**VO<sup>2+</sup>@SiO<sub>2</sub>@Fe<sub>3</sub>O<sub>4</sub> Core/Shell-mediated C-H aerobic and oxidant induced  
oxidation of alkylbenzenes (including toluene derivatives) at room temperature  
in water**

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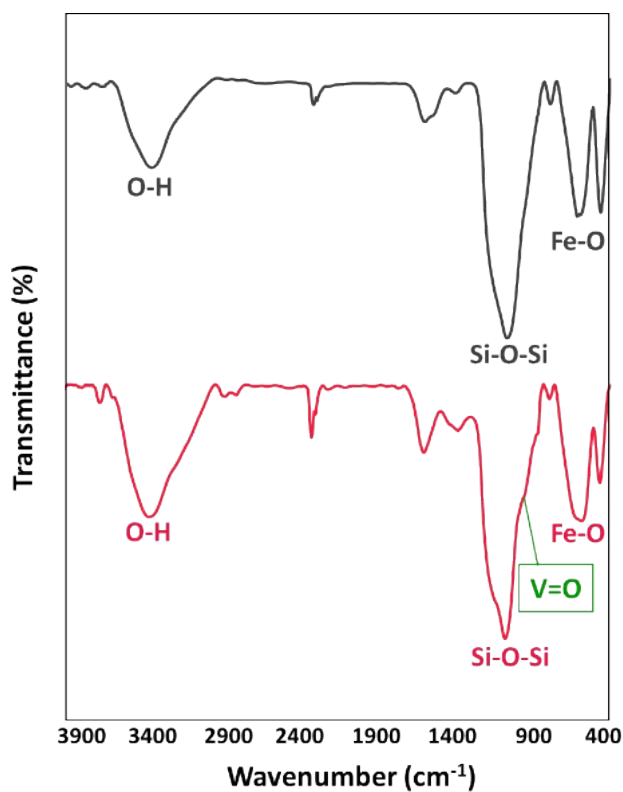


Figure S1. FTIR spectra of A) SiO<sub>2</sub>@Fe<sub>3</sub>O<sub>4</sub> and B) VO<sup>2+</sup>@SiO<sub>2</sub>@Fe<sub>3</sub>O<sub>4</sub>.

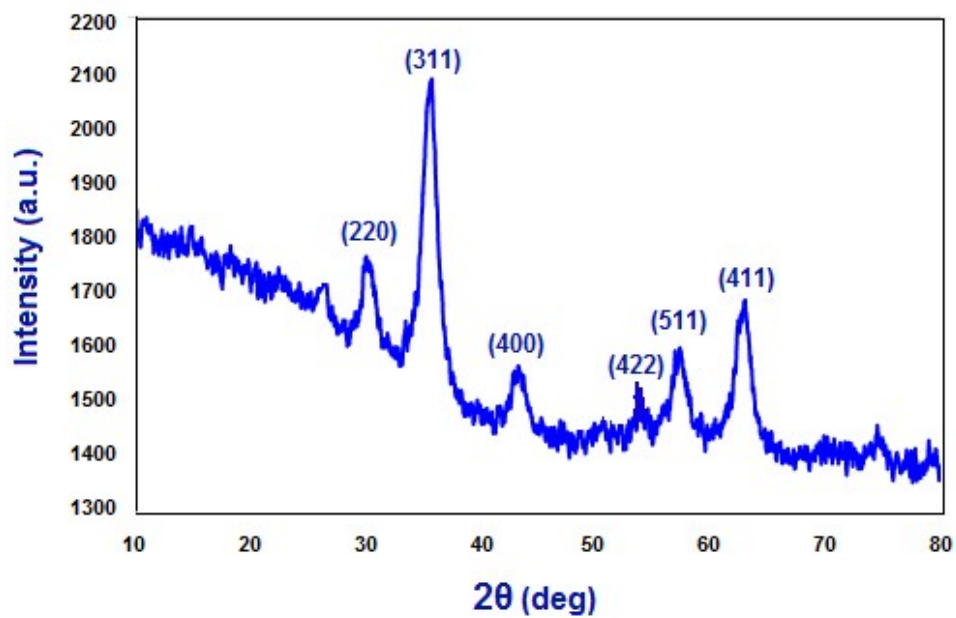
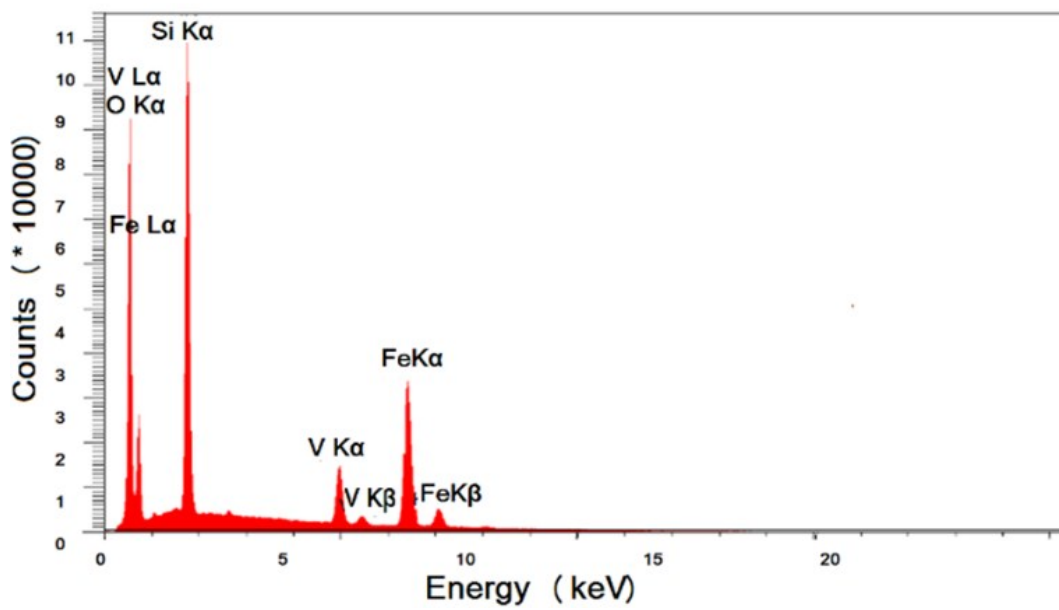
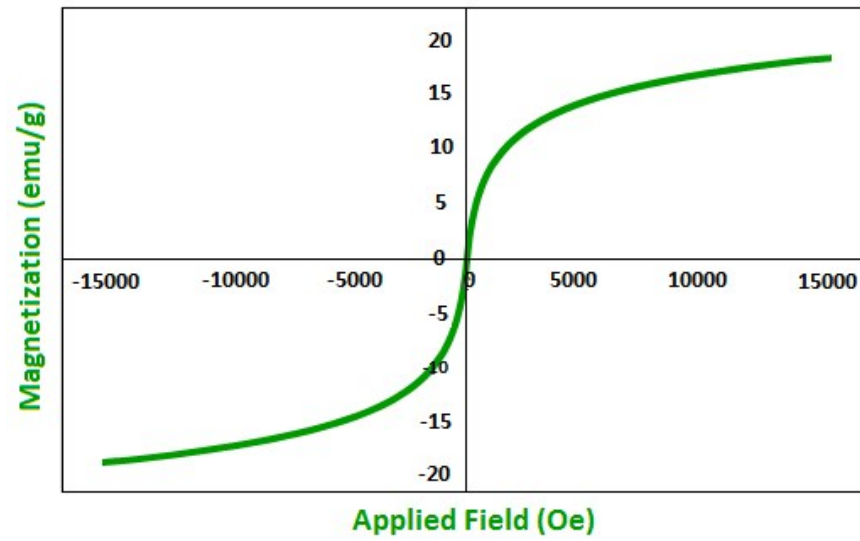


Figure S2. XRD pattern of  $\text{VO}^{2+}@SiO_2@Fe_3O_4$ .



**Figure S3.** Energy-dispersive X-ray spectroscopy of  $\text{VO}^{2+}@SiO_2@Fe_3O_4$ .

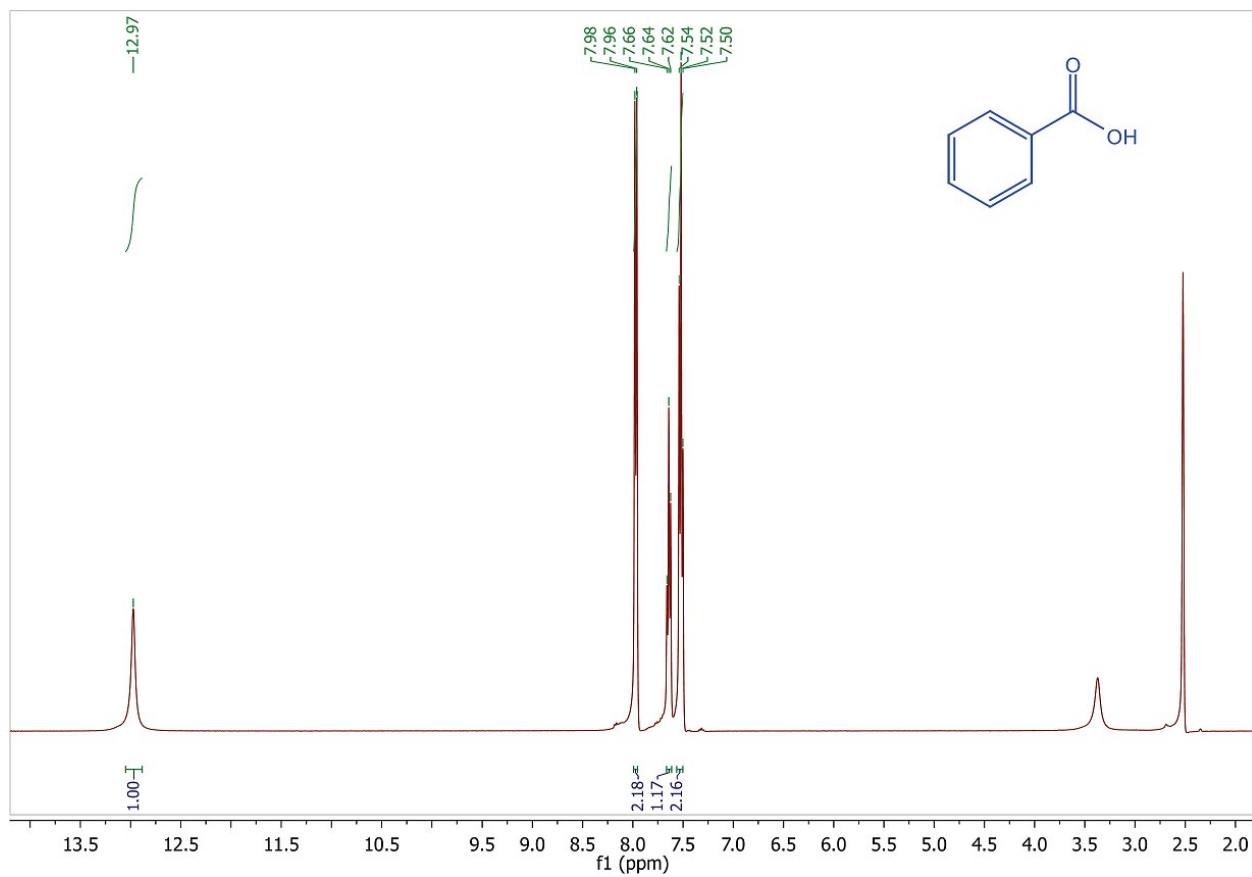


**Figure 5.** Magnetization curve of  $\text{VO}^{2+}@SiO_2@Fe_3O_4$ .

## <sup>1</sup>H NMR spectra for all synthesized compounds

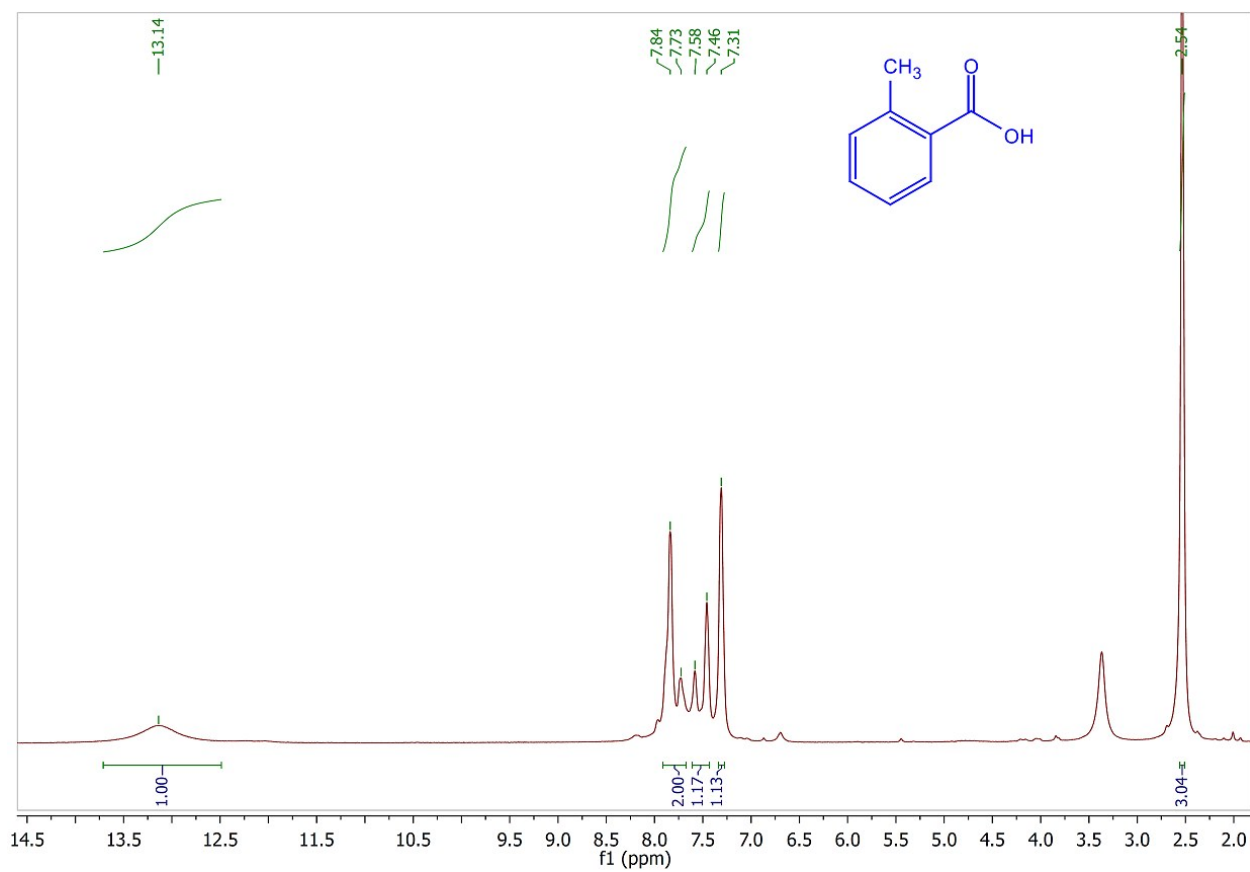
### 1. Benzoic acid

<sup>1</sup>H NMR (400 MHz, *d*<sub>6</sub>-DMSO): δ (ppm) = 12.97 (s, 1H), 7.97 (d, *J* = 8 Hz, 2H), 7.64 (t, *J* = 8 Hz, 1H), 7.52 (t, *J* = 8 Hz, 2H).



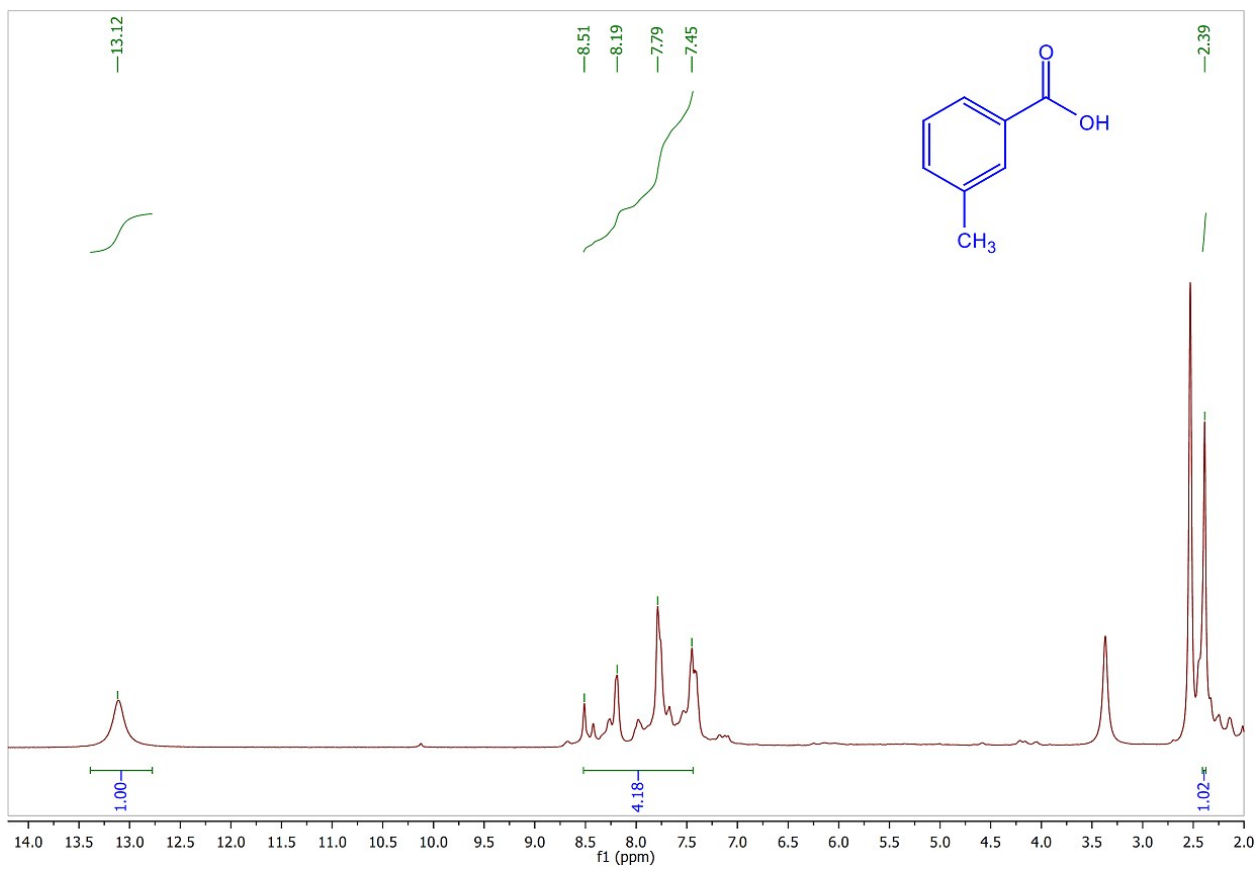
## 2. 2-Methylbenzoic acid

$^1\text{H NMR}$  (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 13.14 (s, 1H), 7.84-7.31 (m, 4H), 2.54 (s, 1H).



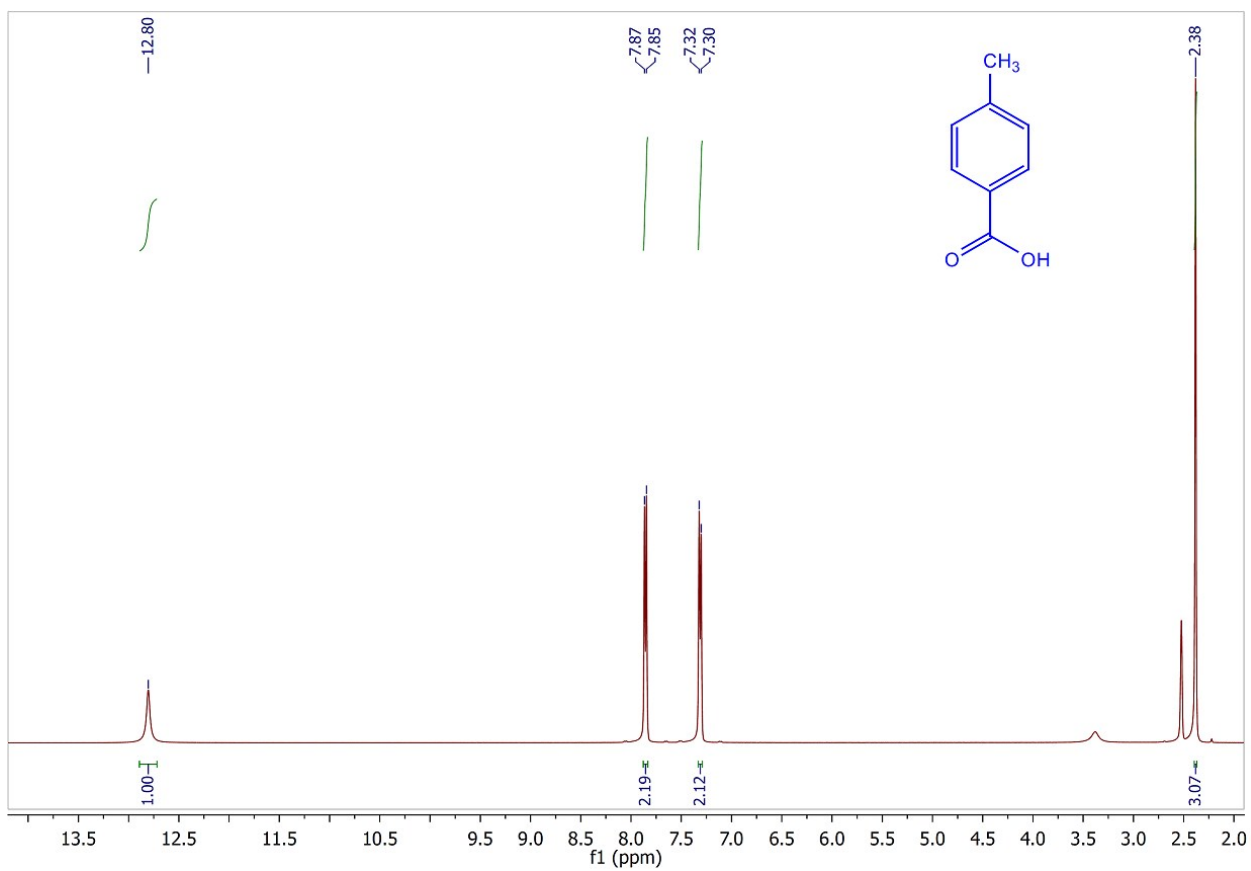
### 3. 3-Methylbenzoic acid

$^1\text{H}$  NMR (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 13.12 (s, 1H), 8.51- 7.45 (m, 4H), 2.39 (s, 3H).



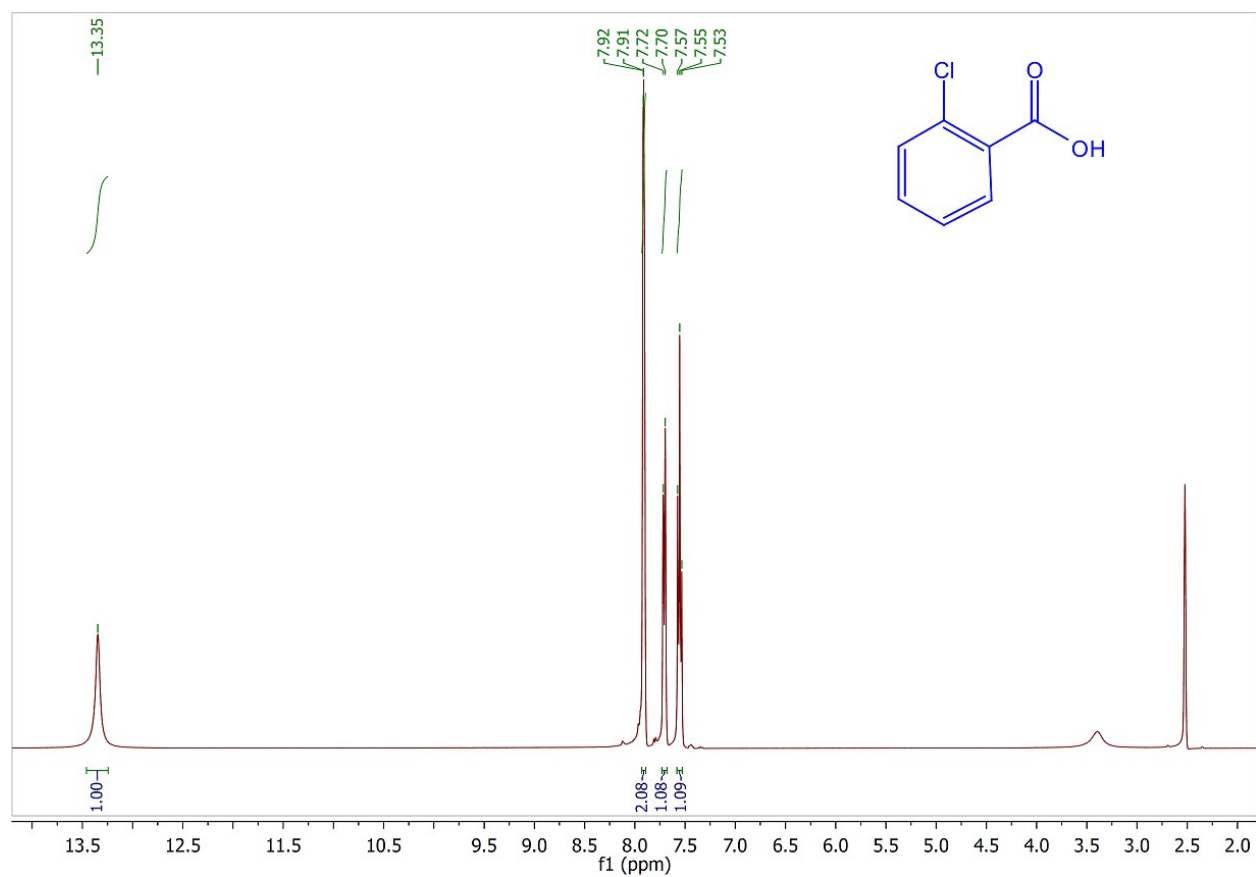
#### 4. 4-Methylbenzoic acid

$^1\text{H}$  NMR (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 12.80 (s, 1H), 7.86 (d,  $J$  = 8 Hz, 2H), 7.31 (d,  $J$  = 8 Hz, 2H), 2.38 (s, 3H).



## 5. 2-Chlorobenzoic acid

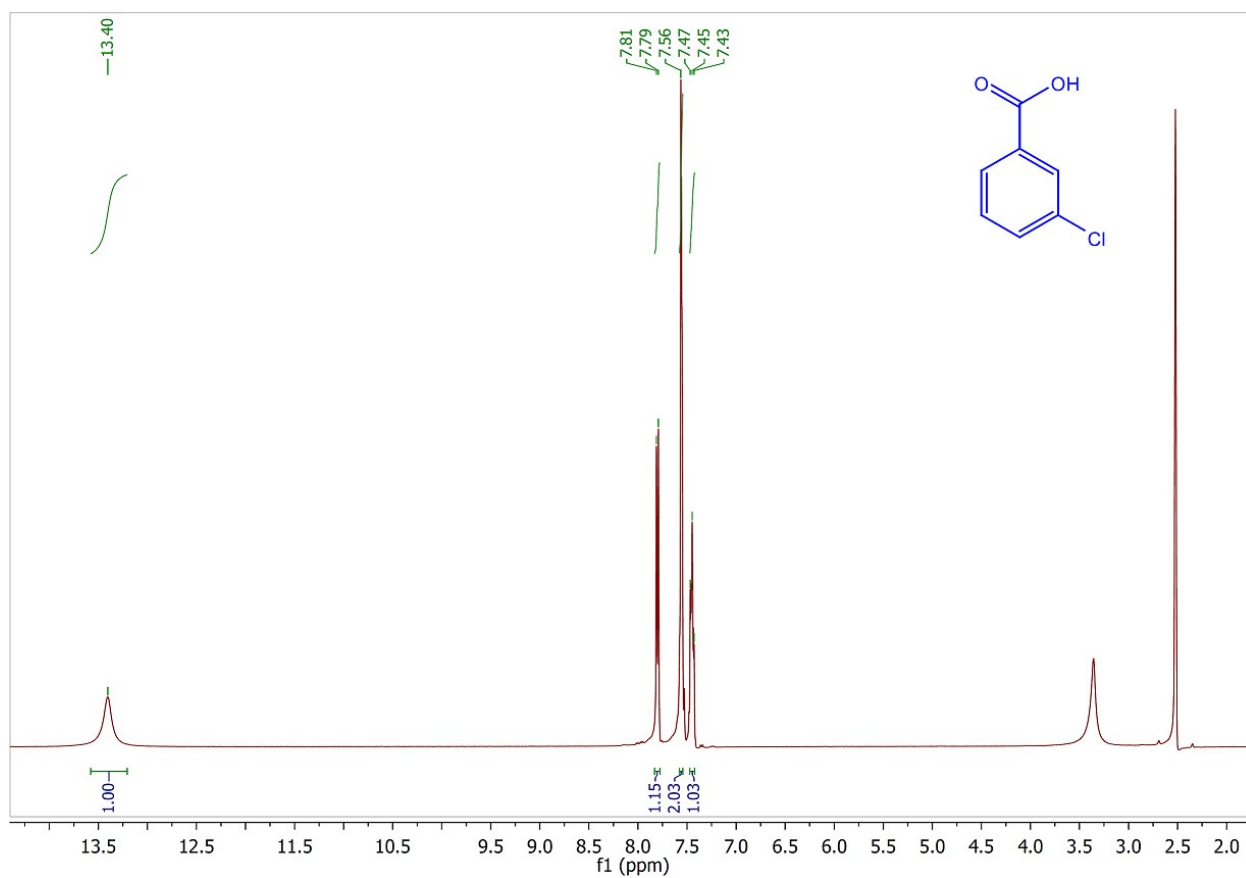
$^1\text{H}$  NMR (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 13.35 (s, 1H), 7.91-7.92 (m, 2H), 7.71 (d,  $J$ = 8 Hz, 1H), 7.55 (t,  $J$ = 8 Hz, 1H).





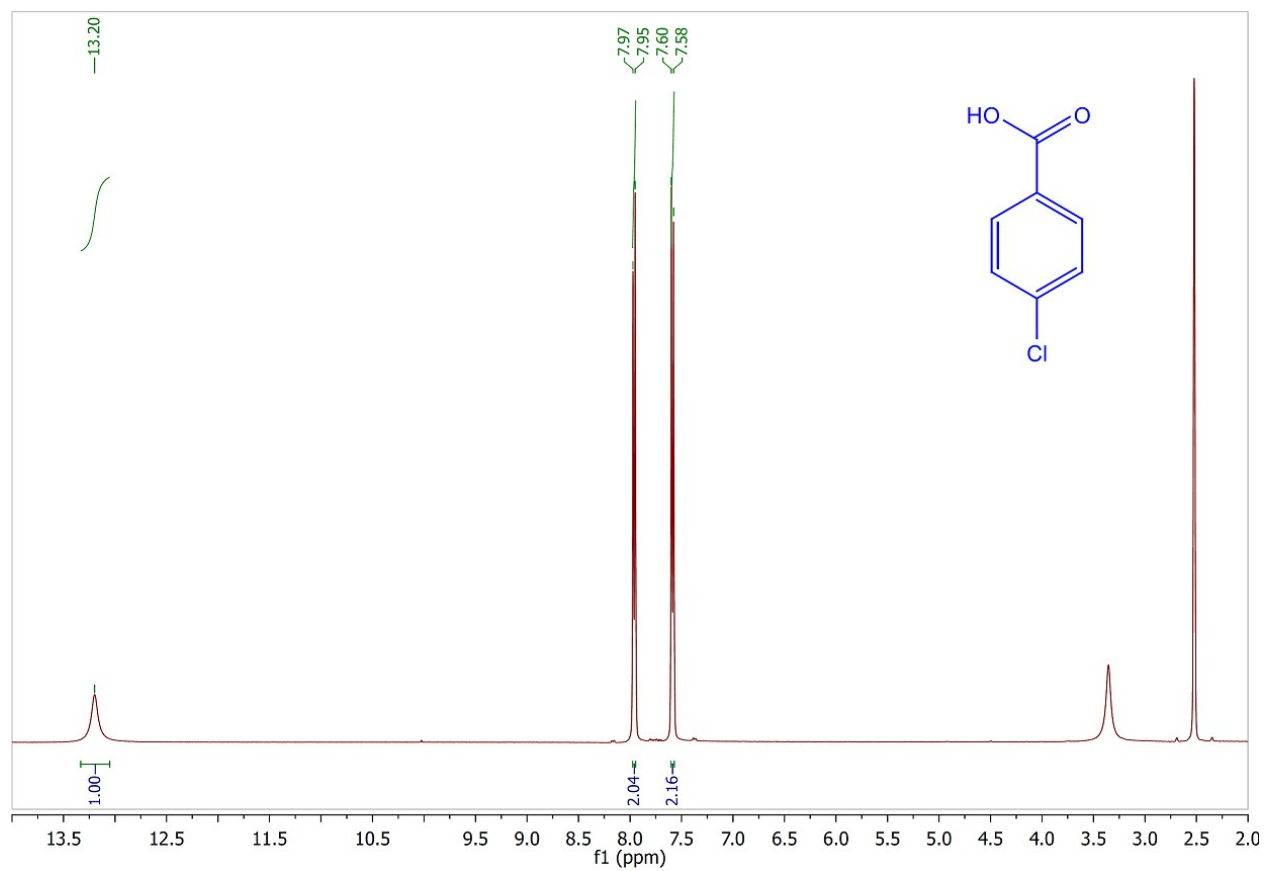
## 6. 3-Chlorobenzoic acid

$^1\text{H}$  NMR (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 13.40 (s, 1H), 7.80 (d,  $J$ = 8 Hz, 1H), 7.56 (s, 2H), 7.45 (t,  $J$ = 8 Hz, 1H).



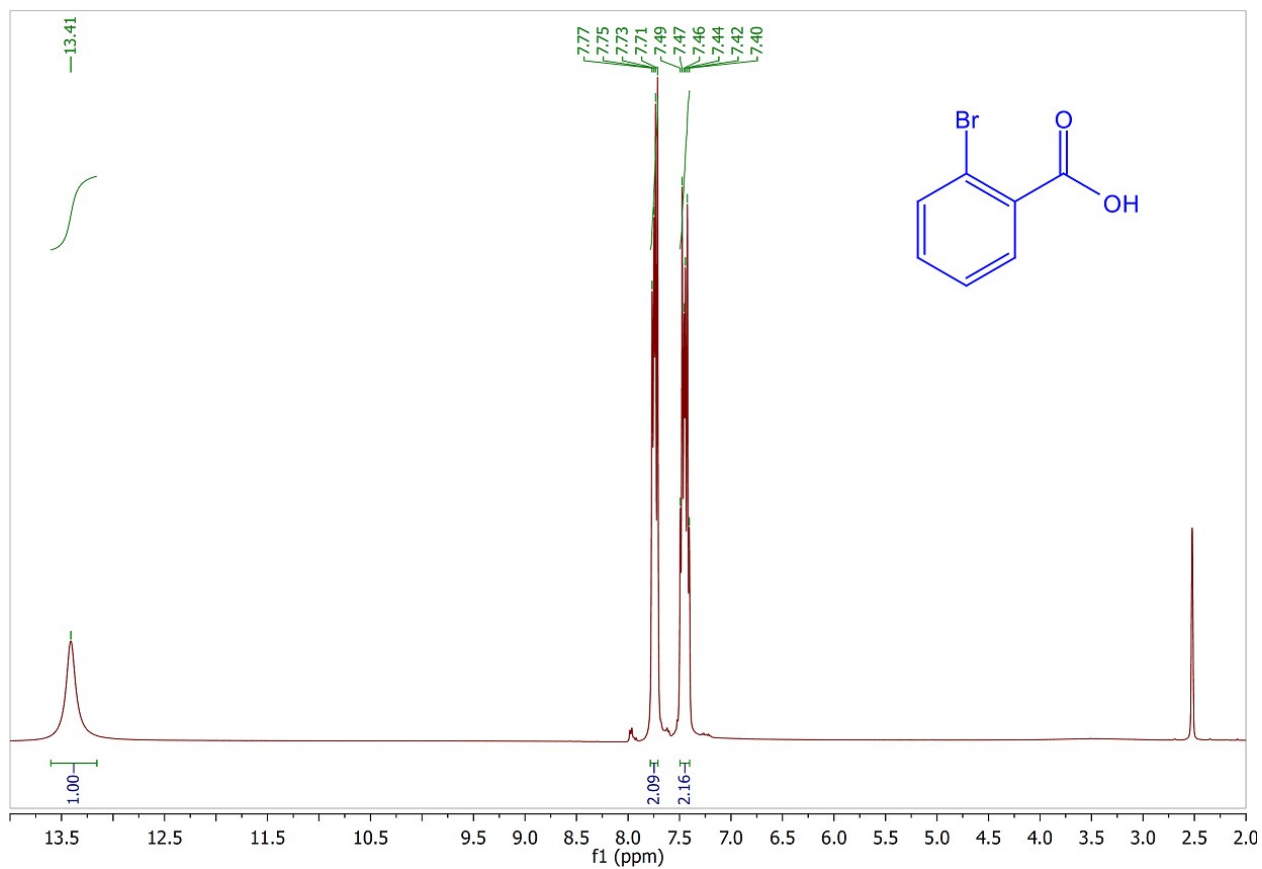
## 7. 4-Chlorobenzoic acid

$^1\text{H}$  NMR (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 13.20 (s, 1H), 7.96 (d,  $J$  = 8 Hz, 2H), 7.59 (d,  $J$  = 8 Hz, 2H).



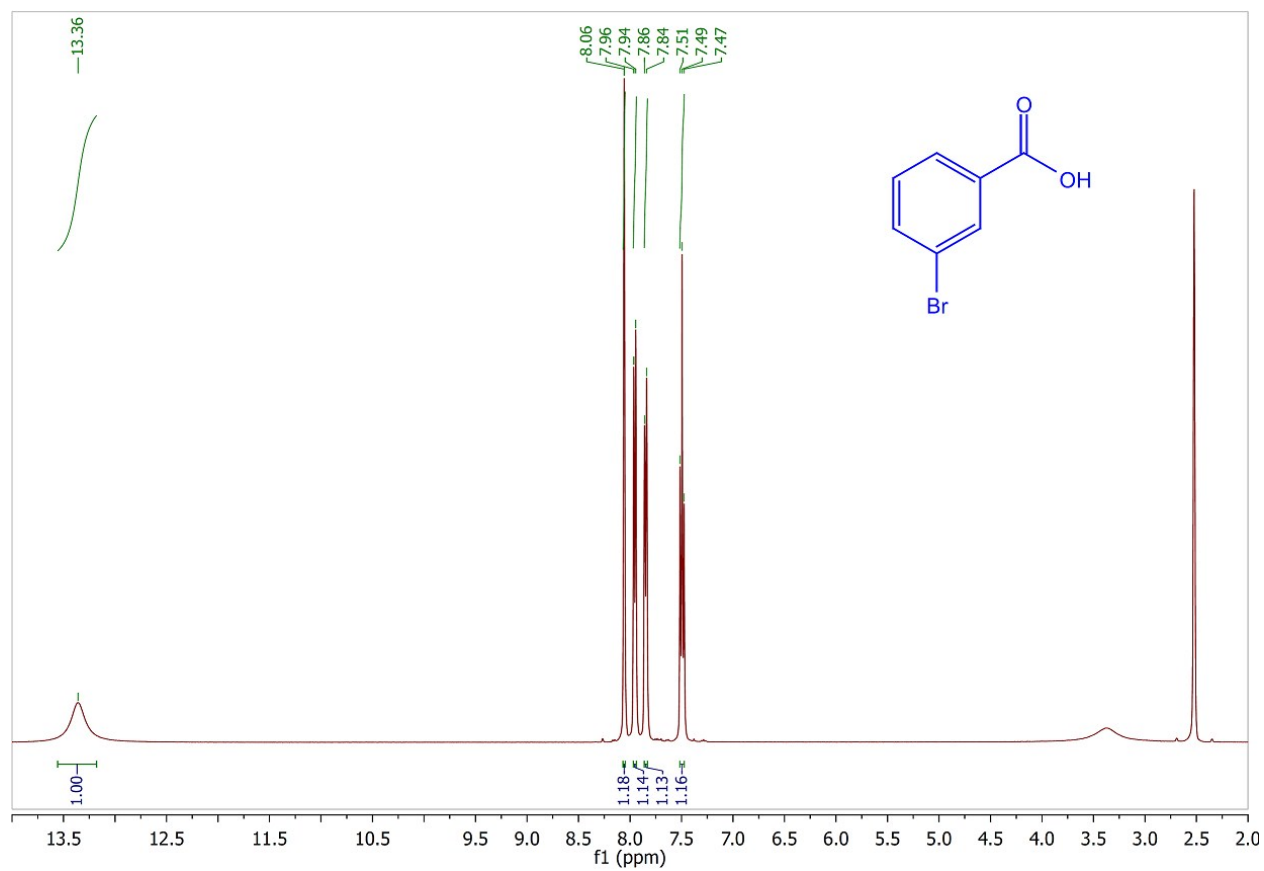
## 8. 2-Bromobenzoic acid

$^1\text{H}$  NMR (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 13.41 (s, 1H), 7.77- 7.71 (m, 2H), 7.49- 7.40 (m, 2H).



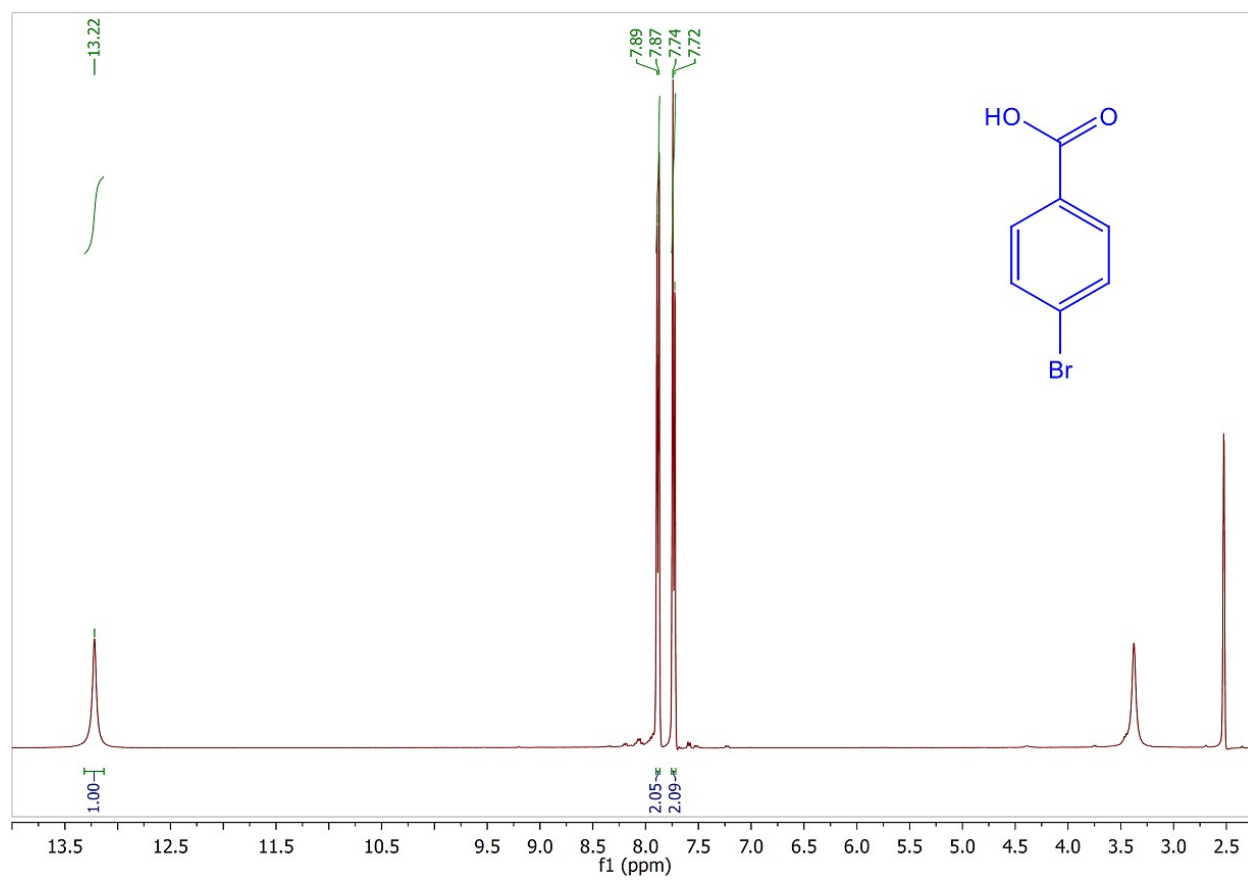
## 9. 3-Bromobenzoic acid

$^1\text{H}$  NMR (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 13.36 (s, 1H), 8.06 (s, 1H), 7.95 (d,  $J=8$  Hz, 1H), 7.85 (d,  $J=8$  Hz, 1H), 7.49 (t,  $J=8$  Hz, 1H).



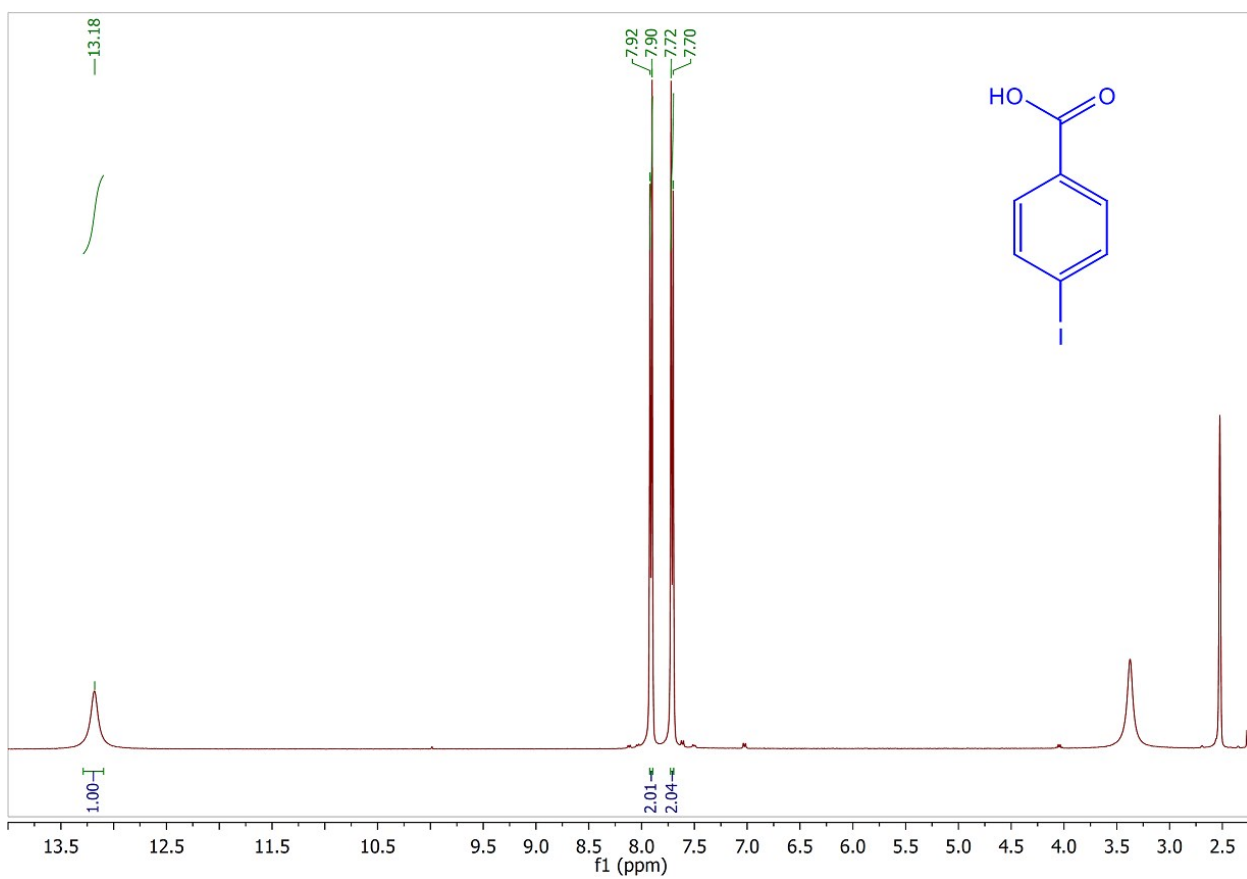
## 10. 4-Bromobenzoic acid

$^1\text{H}$  NMR (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 13.22 (s, 1H), 7.88 (d,  $J=8$  Hz, 2H), 7.73 (d,  $J=8$  Hz, 2H).



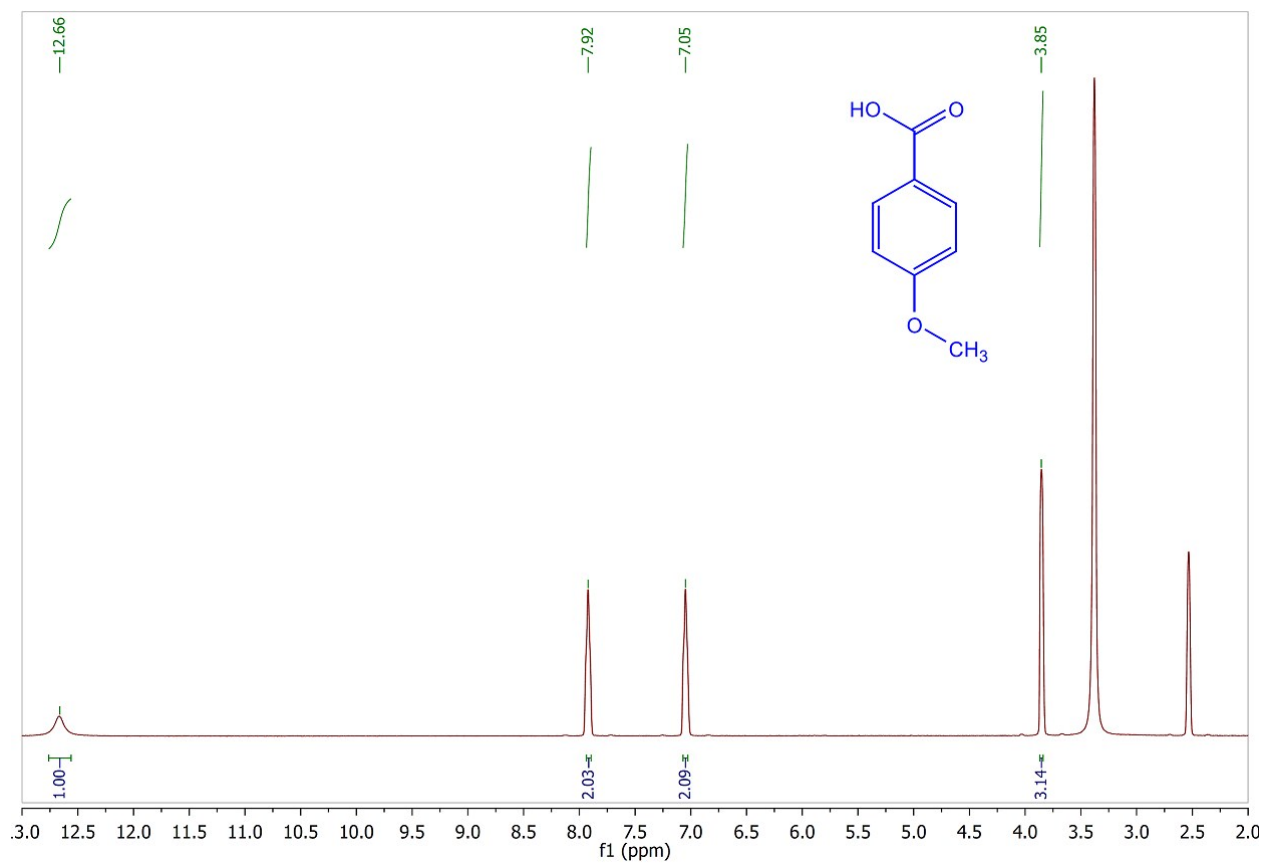
## 11. 4-Iodobenzoic acid

$^1\text{H}$  NMR (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 13.18 (s, 1H), 7.91 (d,  $J$  = 8 Hz, 2H), 7.71 (d,  $J$  = 8 Hz, 2H).



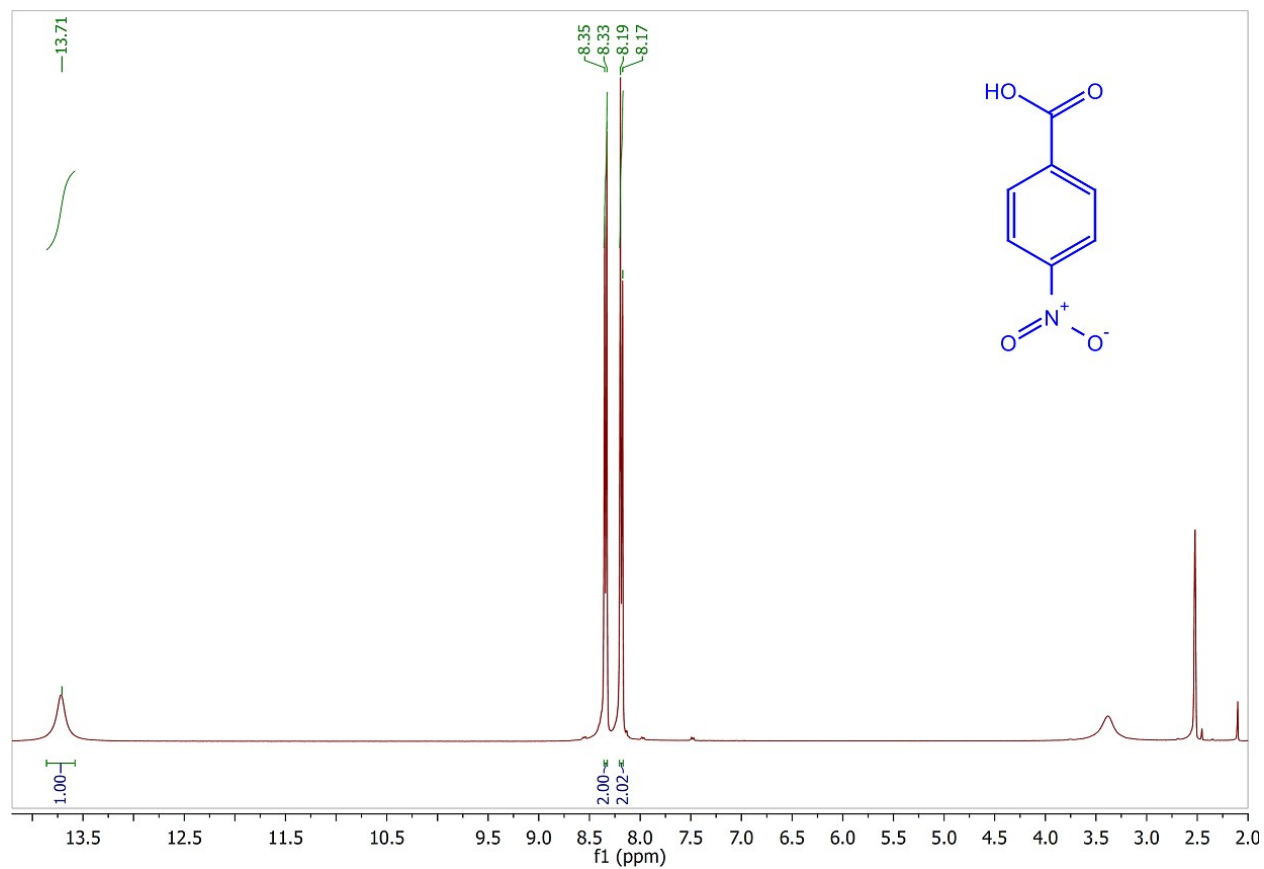
## 12. 4-Methoxybenzoic acid

$^1\text{H NMR}$  (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 12.66 (s, 1H), 7.92 (s, 2H), 7.05 (s, 2H), 3.85 (s, 3H).



### 13. 4-Nitrobenzoic acid

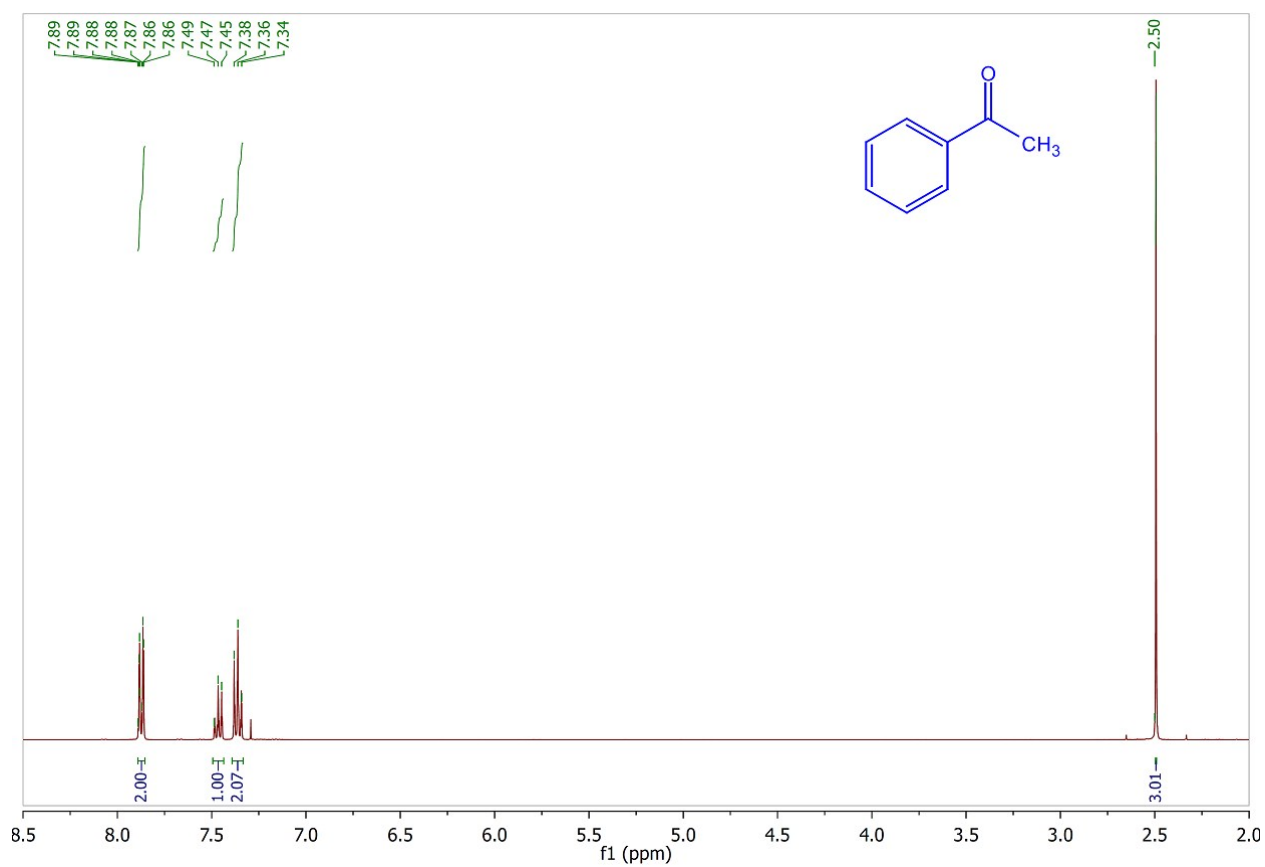
$^1\text{H}$  NMR (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 13.71 (s, 1H), 8.34 (d,  $J$  = 8 Hz, 2H), 8.18 (d,  $J$  = 8 Hz, 2H).





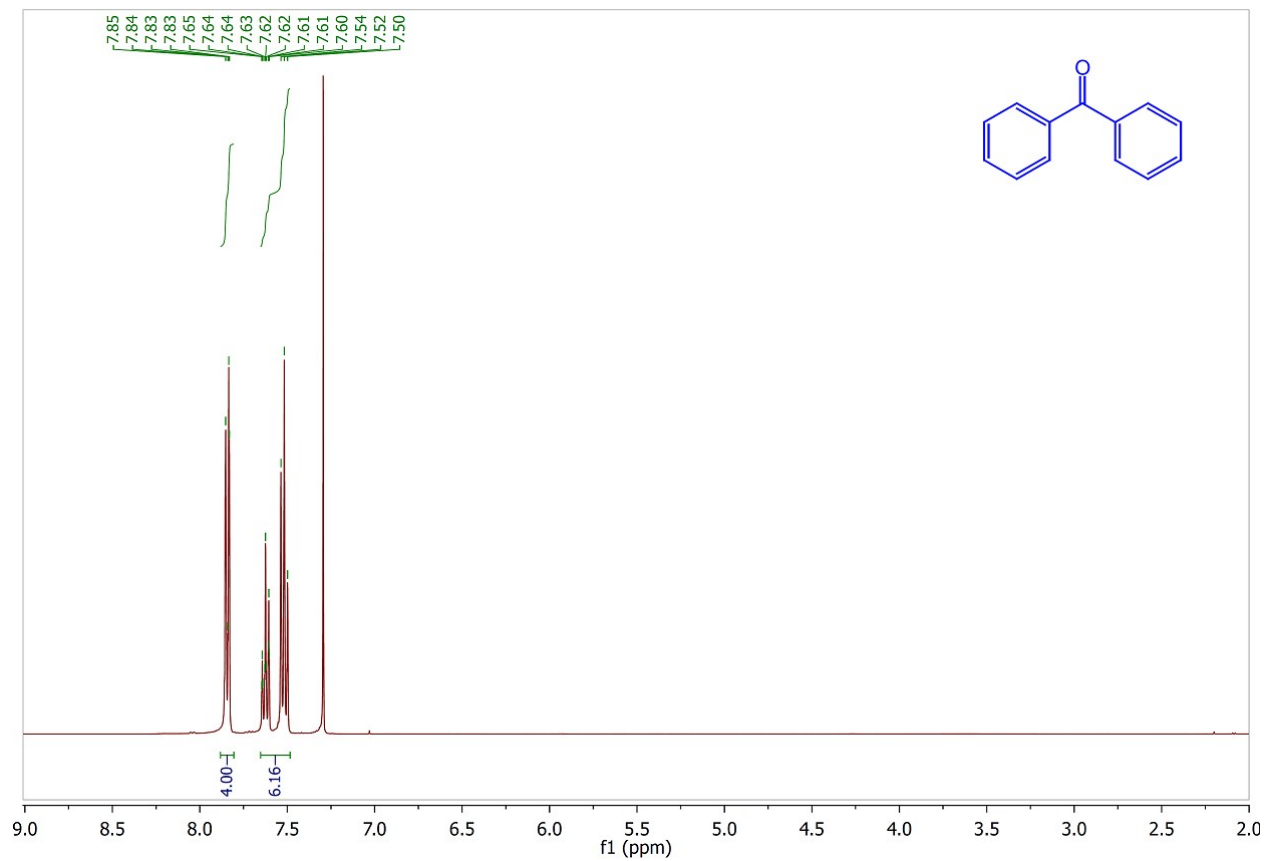
## 14. Acetophenone

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) = 7.89-7.86 (m, 2H), 7.47 (t,  $J=8$  Hz, 1H), 7.36 (t,  $J=8$  Hz, 2H), 2.50 (s, 3H).



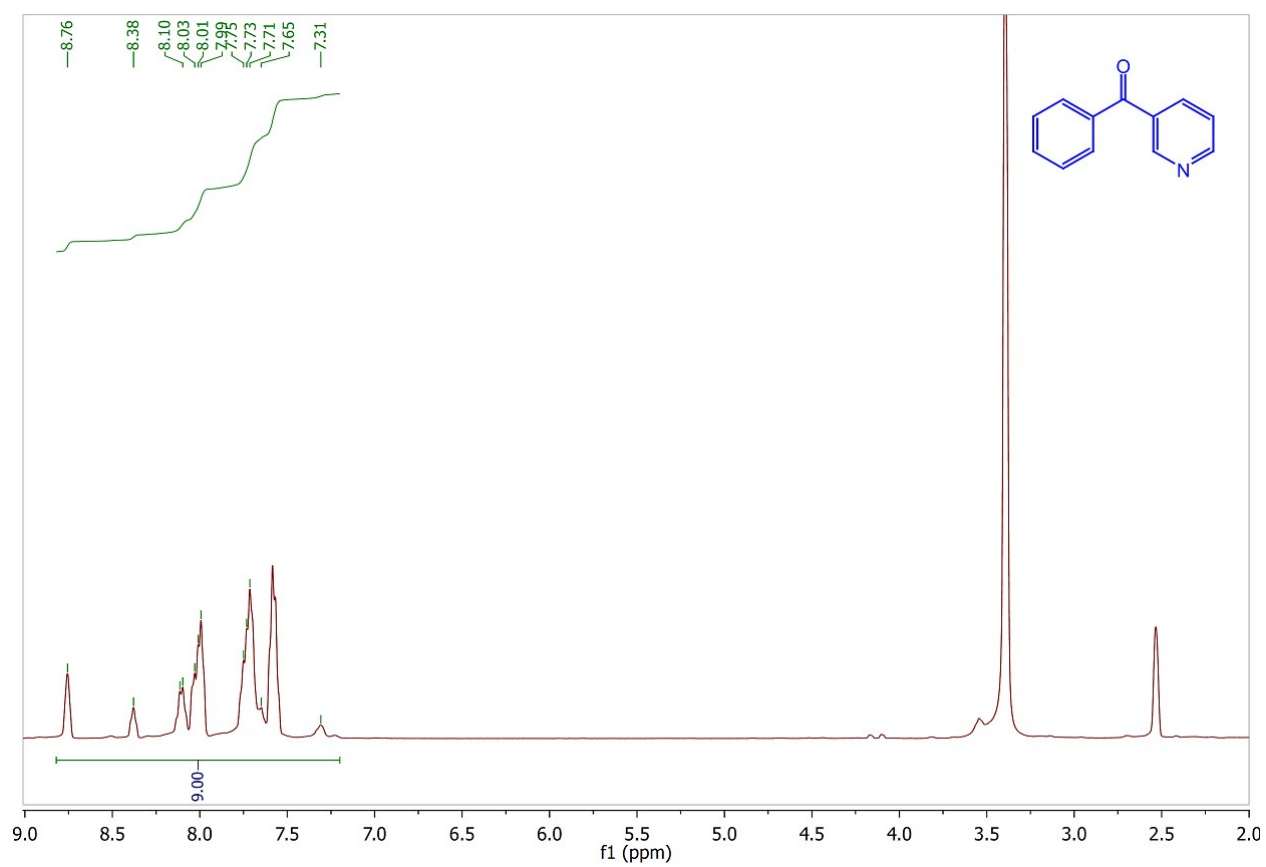
## 15. Benzophenone

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) = 7.85-7.64 (m, 4H), 7.63-7.50 (m,  $J=6\text{H}$ ).



## 16. Phenyl(pyridin-3-yl)methanone

$^1\text{H NMR}$  (400 MHz,  $d_6$ -DMSO):  $\delta$  (ppm) = 8.76- 7.31 (m, 9H).



## 17. 1-Tetralone

$^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  (ppm) = 8.03 (d,  $J=8$  Hz, 1H), 7.47-7.44 (m, 1H), 7.31- 7.23 (m, 2H), 7.49 (t,  $J=8$  Hz, 1H), 2.97-2.94 (m, 2H), 2.66-2.63 (m, 2H), 2.14-2.11 (m, 2H).

