

## SUPPLEMENTARY MATERIAL

Analysis summary for 4-hydroxybenzoic acid-d<sub>4</sub>: <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD) δ 6.81 (residual signal), 7.87 (residual signal). <sup>2</sup>H NMR (61.4 MHz, CD<sub>3</sub>OD) δ 6.86 (br s), 7.91 (br s). <sup>13</sup>C{<sup>1</sup>H} NMR (101 MHz, CD<sub>3</sub>OD) δ 115.4–116.0 (m), 122.5–122.7 (m), 132.6 (t), 132.8 (s), 163.3 (s), 170.1 (s). <sup>13</sup>C{<sup>1</sup>H, <sup>2</sup>H, d1 = 20 s} NMR (101 MHz, CD<sub>3</sub>OD) δ 115.7 (s), 115.8 (s), 122.5 (s), 122.6 (s), 132.6 (s), 132.9 (s), 163.3 (s), 170.1 (s). MS (ESI<sup>-</sup>): 36.1%, d<sub>4</sub>; 42.6%, d<sub>3</sub>; 18.9%, d<sub>2</sub>; 2.4%, d<sub>1</sub>.

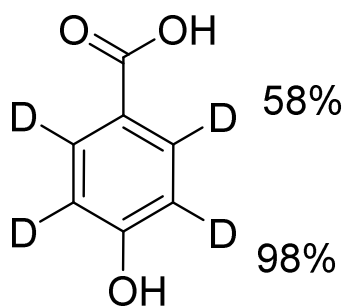


Figure S1. Site-specific deuteration of the prepared sample of 4-hydroxybenzoic acid-d<sub>4</sub>.

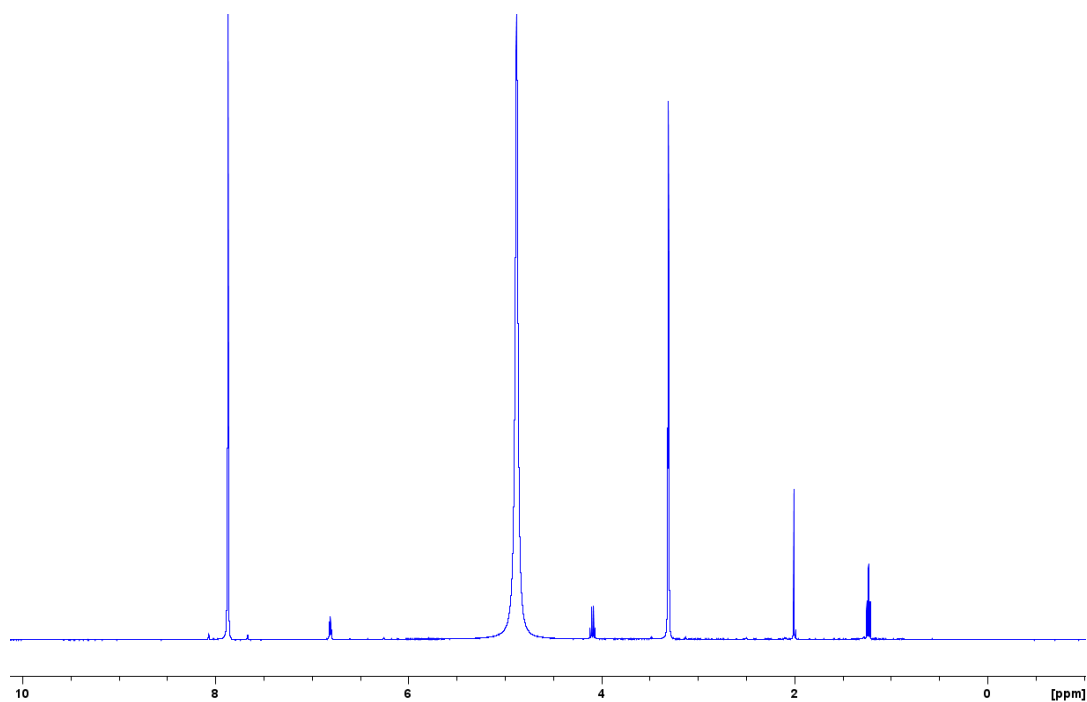


Figure S2. <sup>1</sup>H NMR (400 MHz, CD<sub>3</sub>OD) of deuterated 4-hydroxybenzoic acid-d<sub>4</sub>.

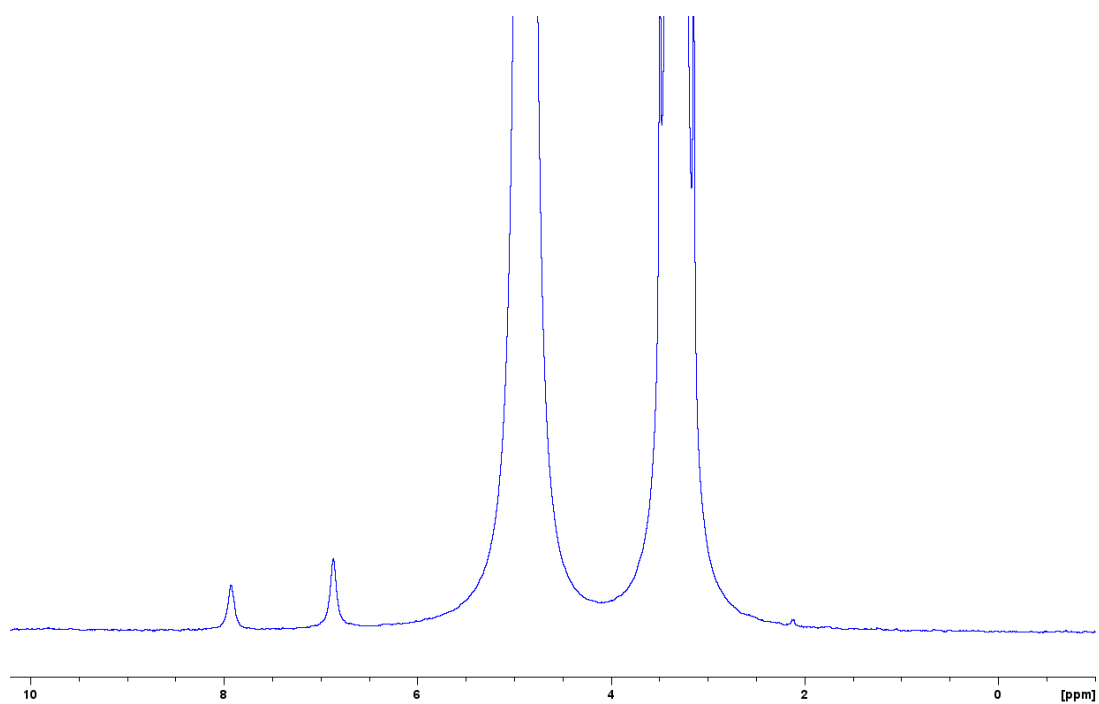


Figure S3.  $^2\text{H}$  NMR (61.4 MHz,  $\text{CD}_3\text{OD}$ ) of deuterated 4-hydroxybenzoic acid- $\text{d}_4$ .

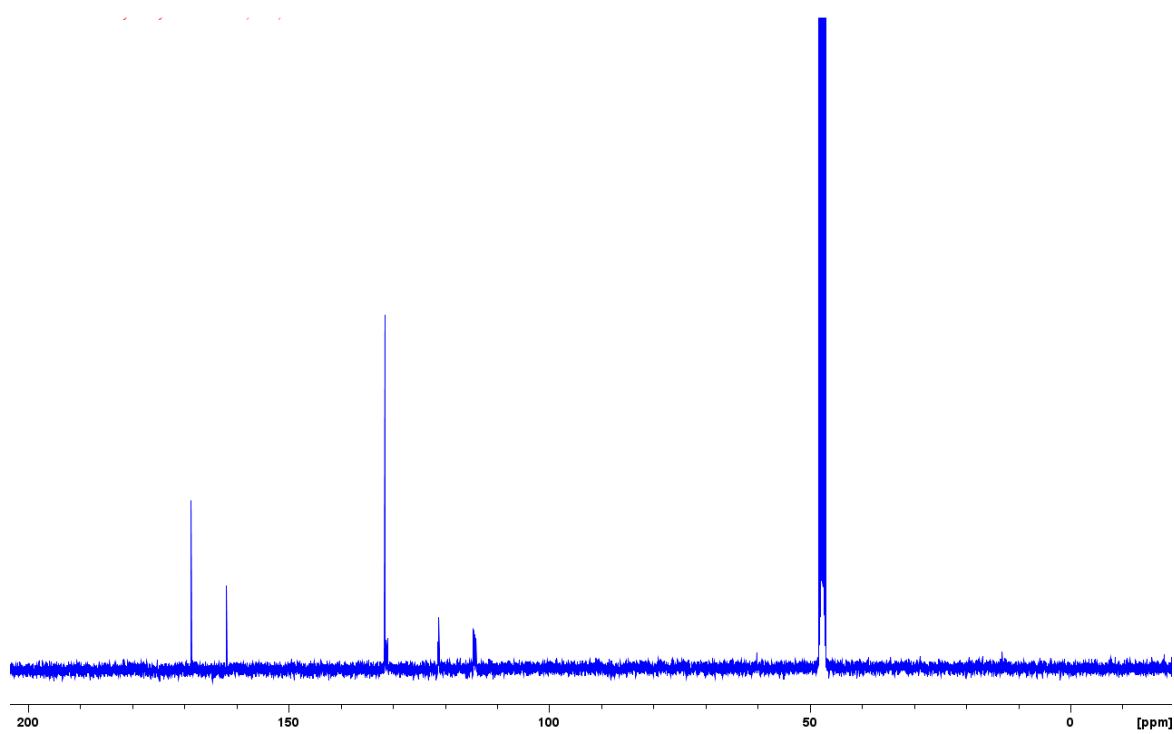


Figure S4.  $^{13}\text{C}\{^1\text{H}\}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ ) of deuterated 4-hydroxybenzoic acid- $\text{d}_4$ .

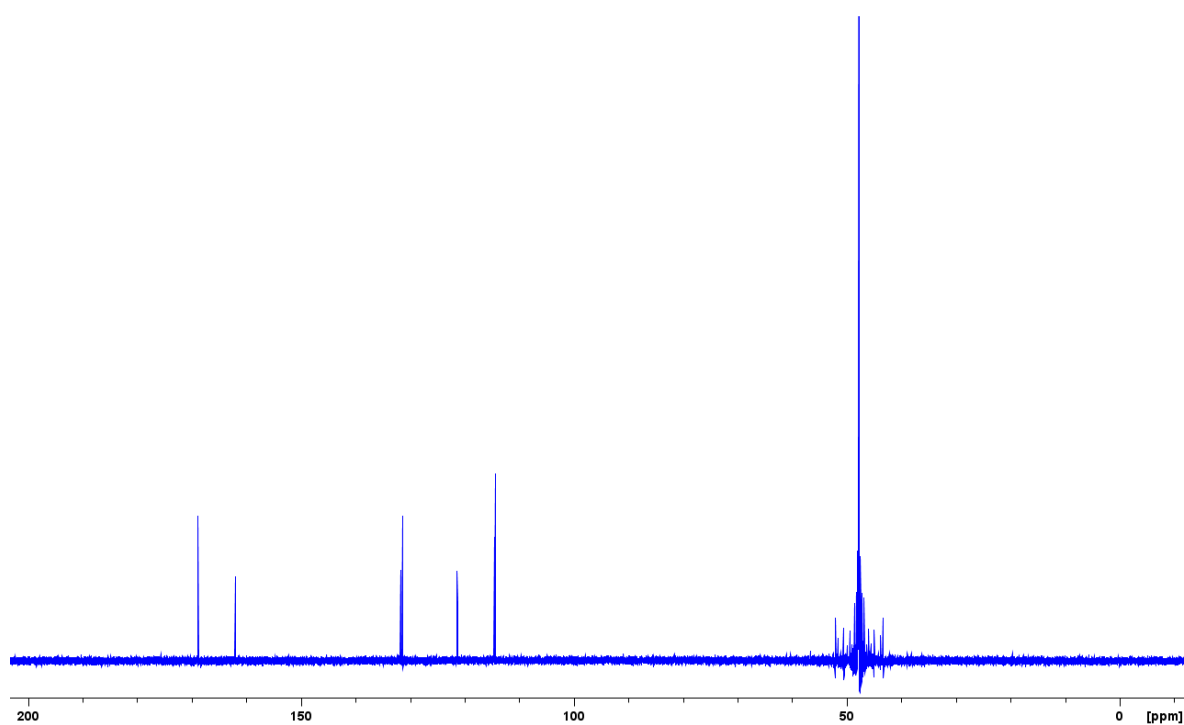


Figure S5.  $^{13}\text{C}\{^1\text{H}, ^2\text{H}\}$  NMR (101 MHz,  $\text{CD}_3\text{OD}$ ) of deuterated 4-hydroxybenzoic acid- $\text{d}_4$ .

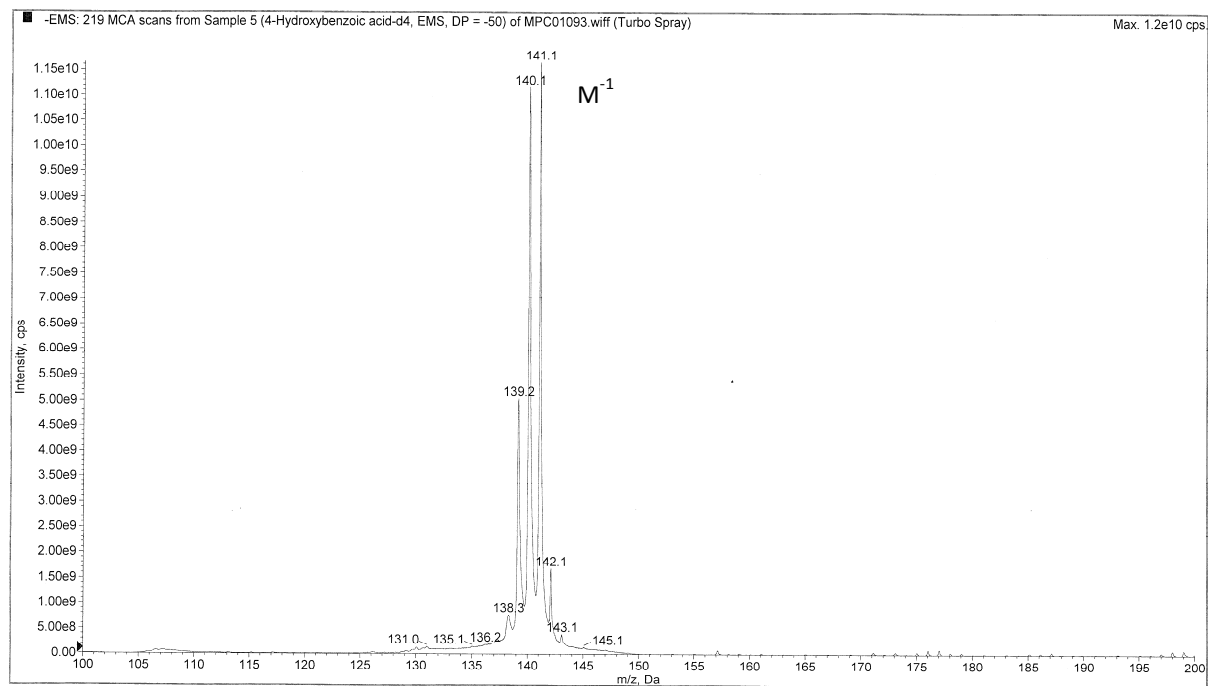


Figure S6. MS ESI  $m/z$  141 [ $\text{M}^{-1}$ ] (78% D).