

# Supporting information for

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## Methane capture with $\alpha$ -cyclodextrins

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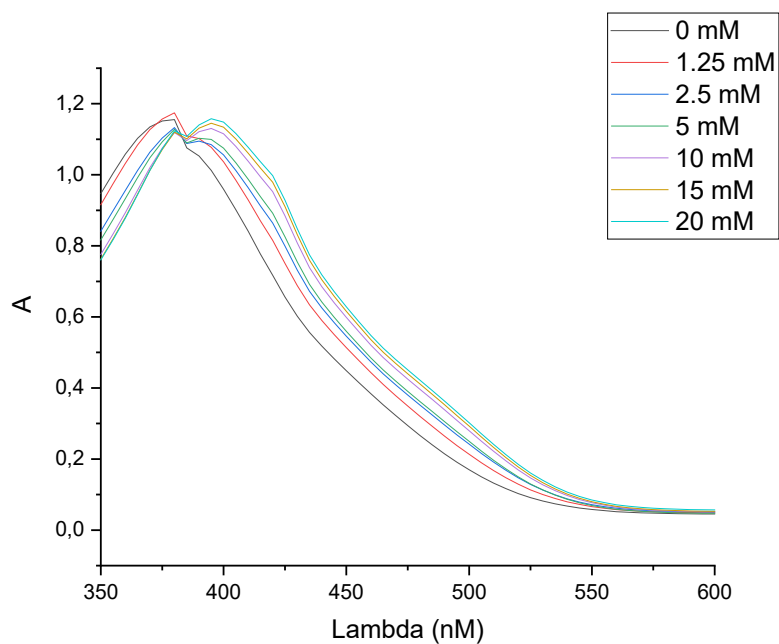


Figure S1. VIS spectra of **4** (40  $\mu\text{M}$ ) at pH 7 in the presence of increasing concentration of **1**.

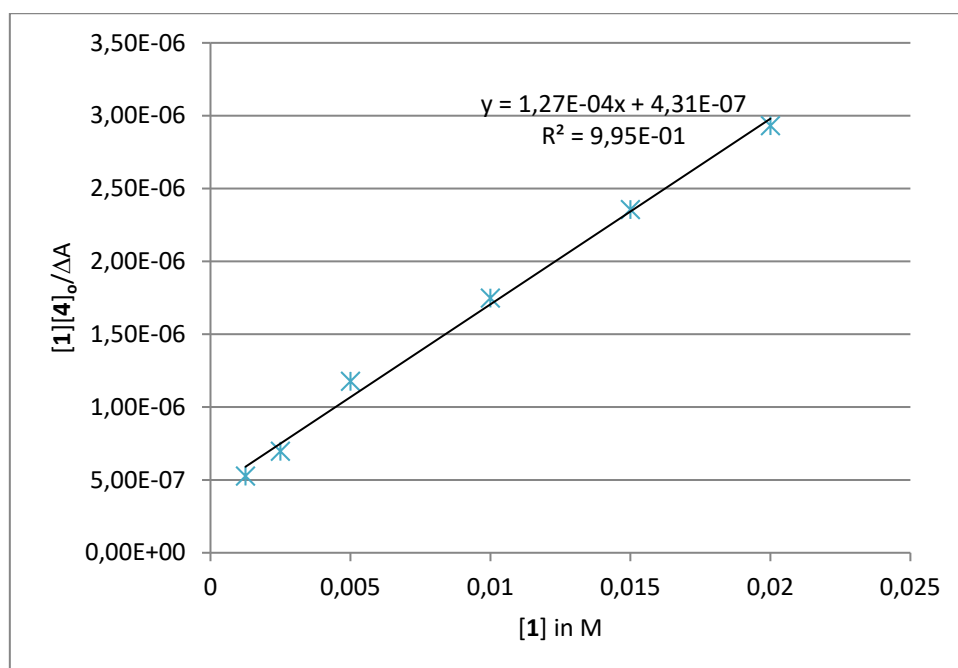
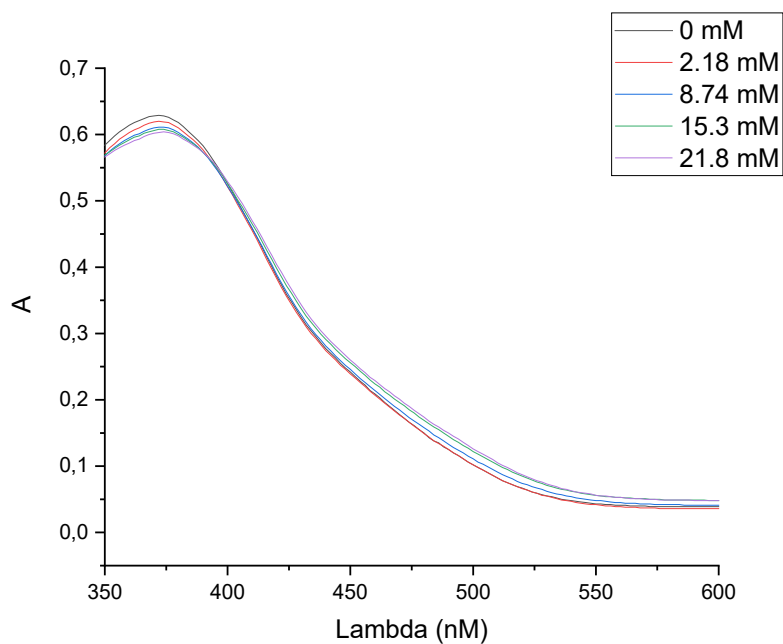
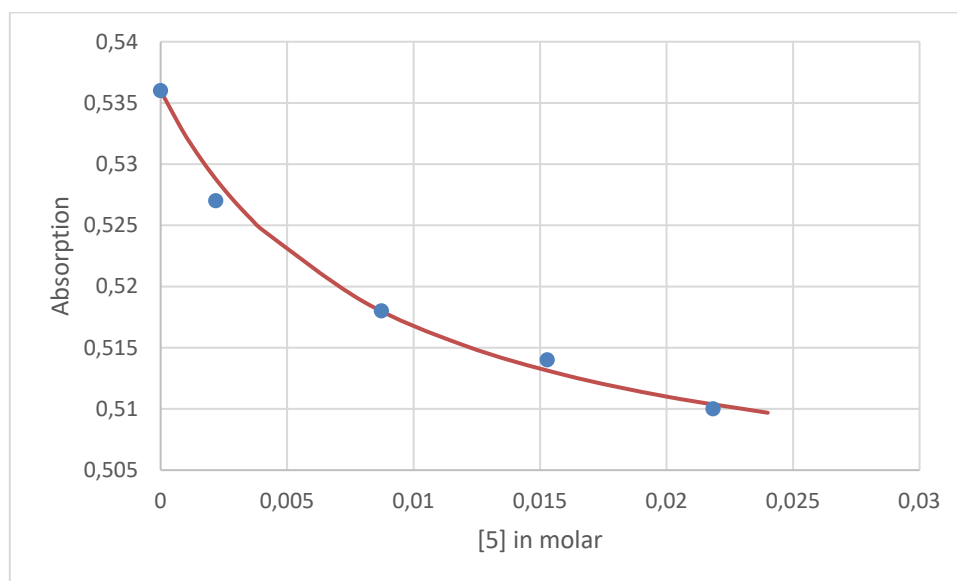


Figure S2. Benesi Hildebrand plot of **4** (40  $\mu\text{M}$ ) at pH 7 in the presence of increasing concentration of **1** at  $\lambda = 425 \text{ nm}$ . From slope ( $a = 1.27 \times 10^{-4}$ ) and intersection ( $b = 4.31 \times 10^{-7}$ )  $K_d$  is determined as  $b/a = 3.39 (\pm 0.41) \times 10^{-3} \text{ M}$



*Figure S3.* VIS spectra of **4** (40  $\mu$ M) at pH 7 in the presence of increasing concentration of **5**.



*Figure S4.* Non linear regression fit (red curve) of the absorption data (blue) of **4** (40  $\mu$ M) at pH 7 at  $\lambda = 370$  nm in the presence of increasing concentration of **5**. Fitting to the equation  $A = k_1/([5]+K_d) + k_2$  gave  $K_d = 8.62 (\pm 2.50) \times 10^{-3}$  M with a  $r^2 = 0.99$

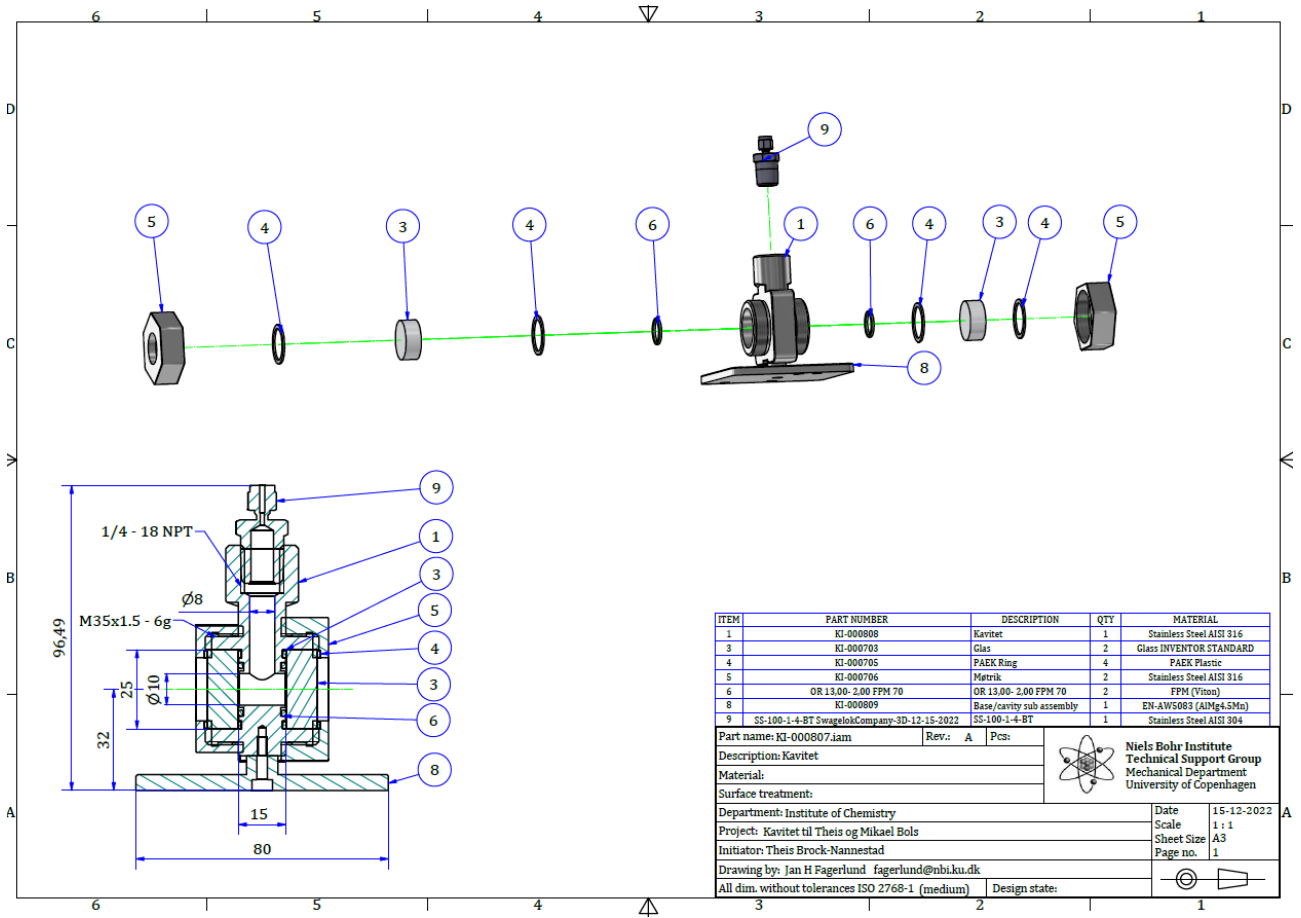
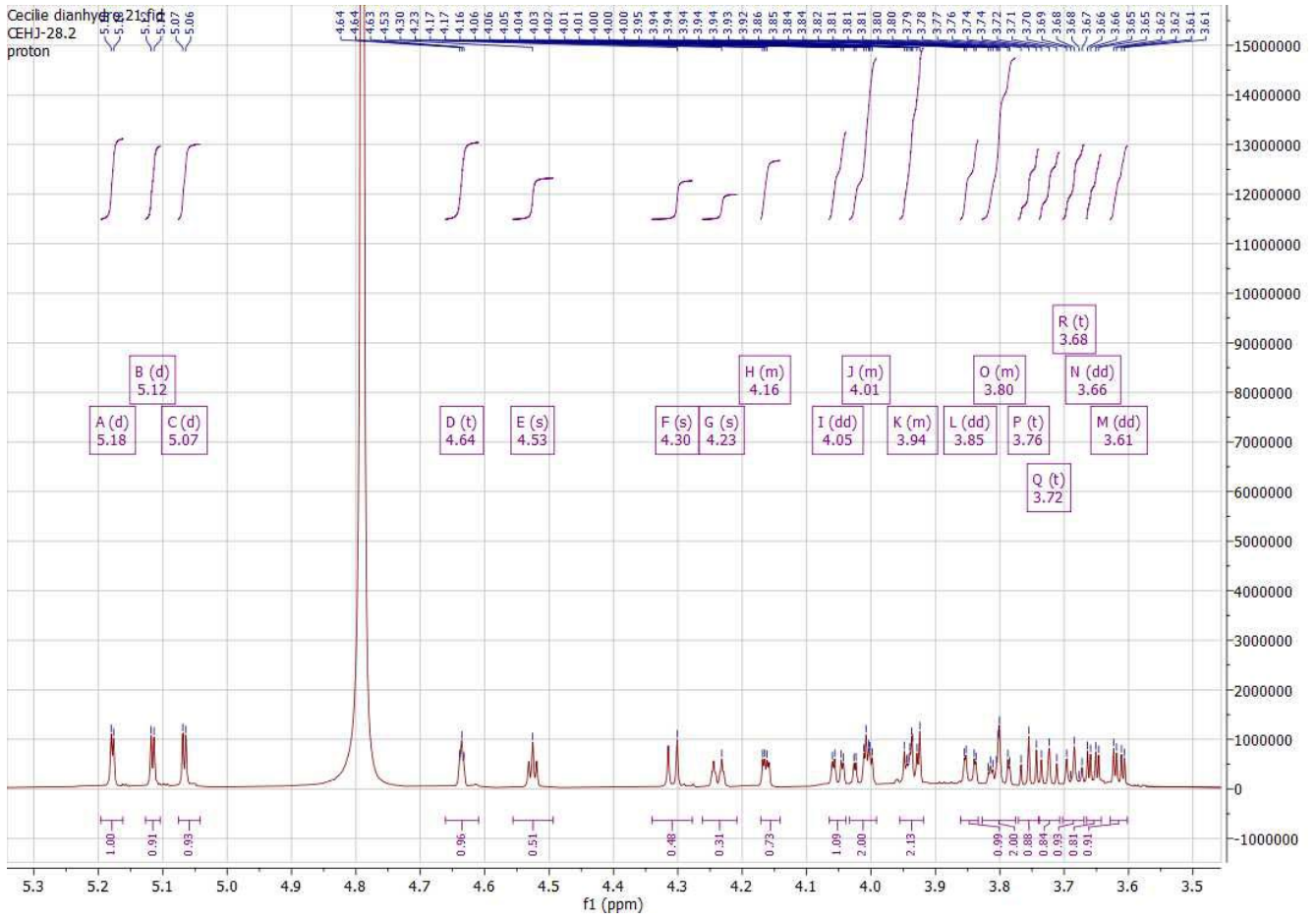
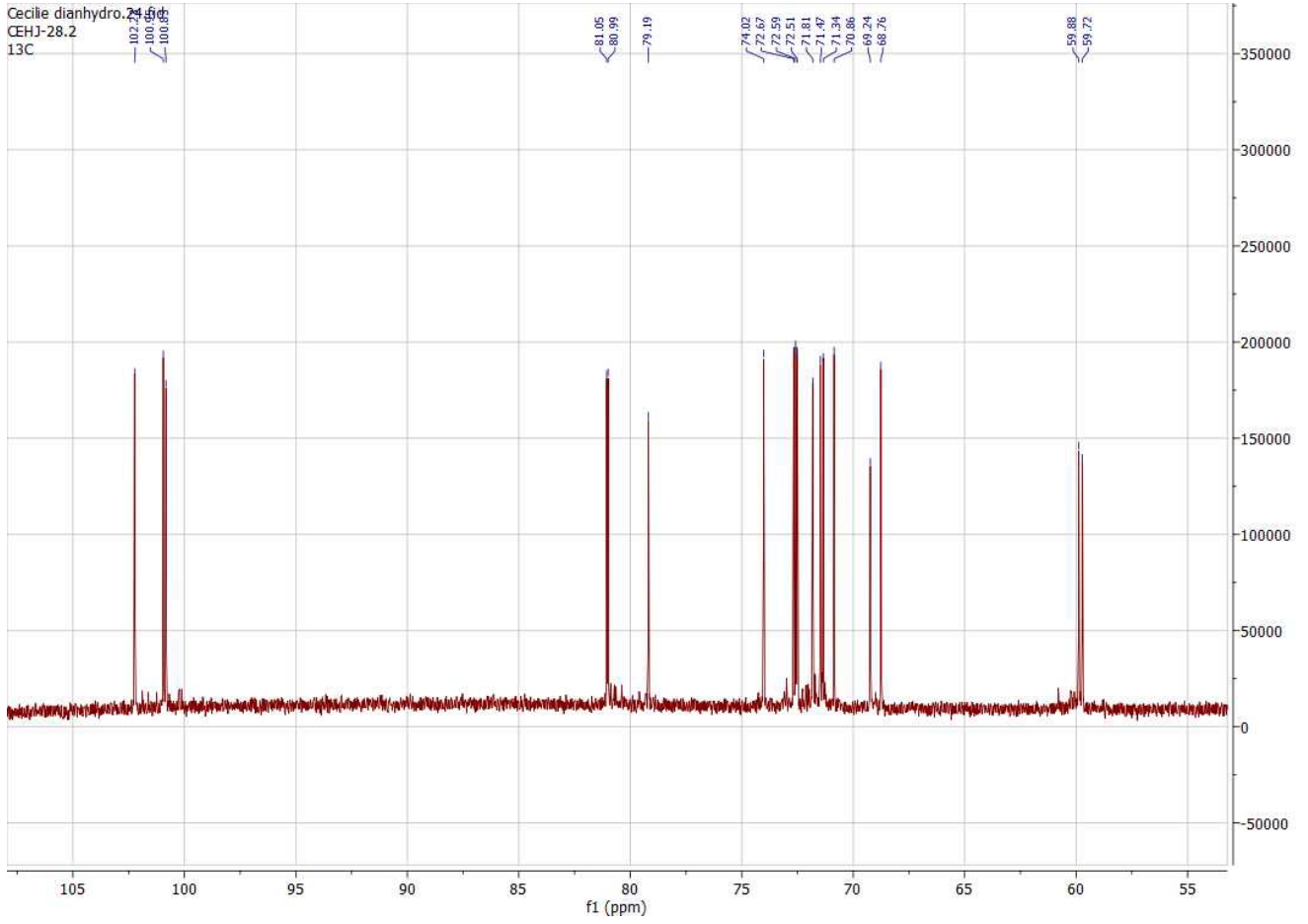


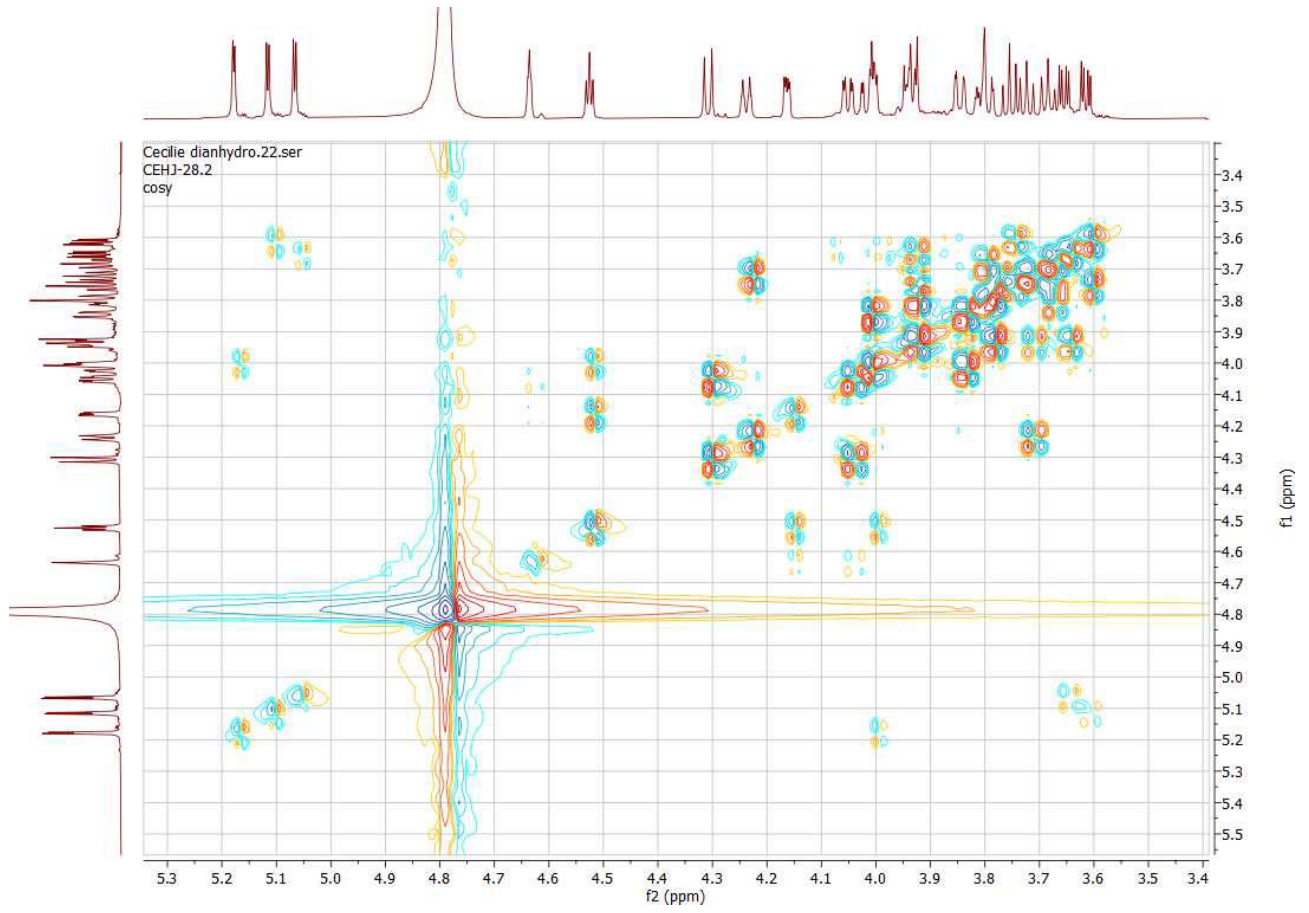
Figure S5. Specifications of pressure cell.

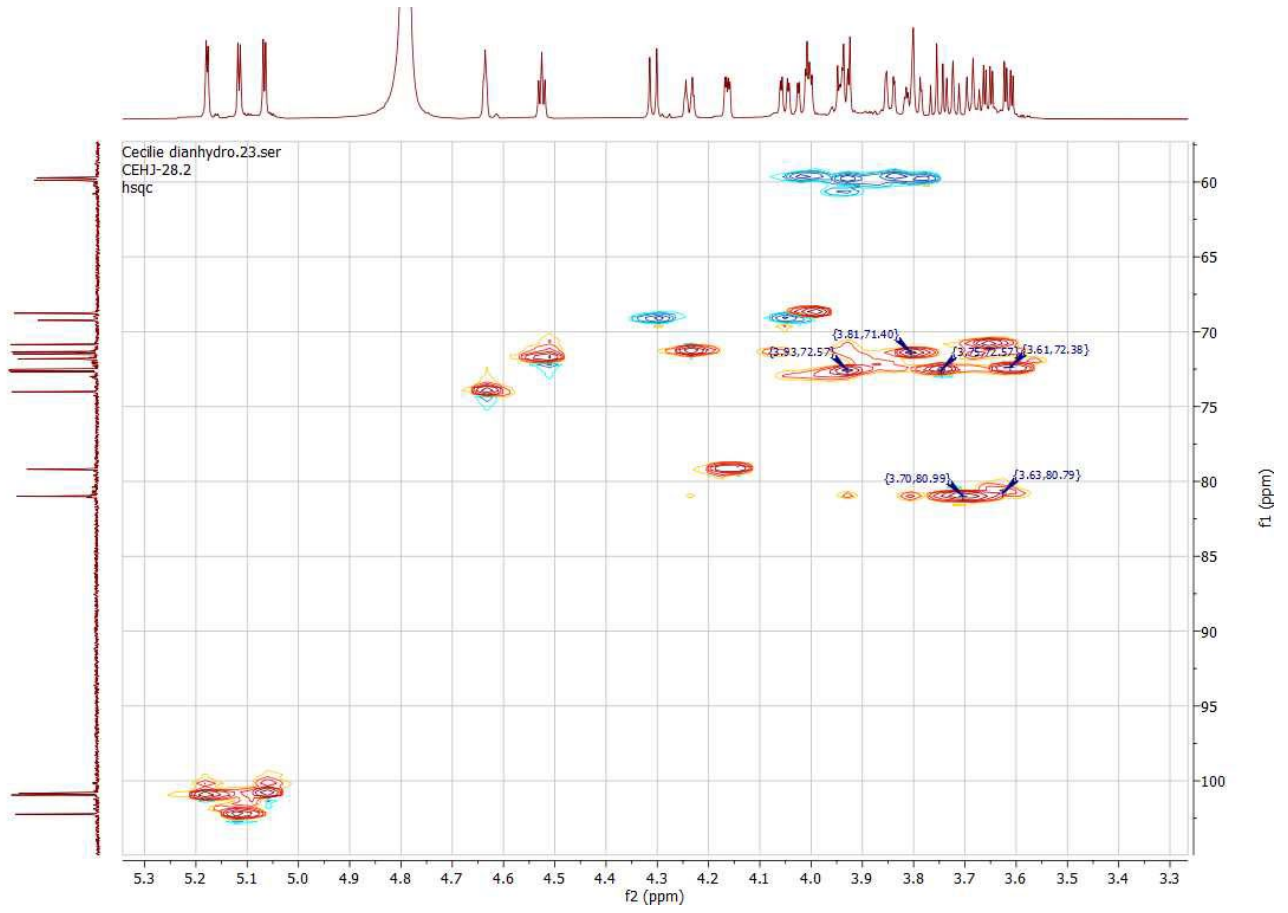
<sup>1</sup>H NMR (800 MHz; D<sub>2</sub>O) of 5



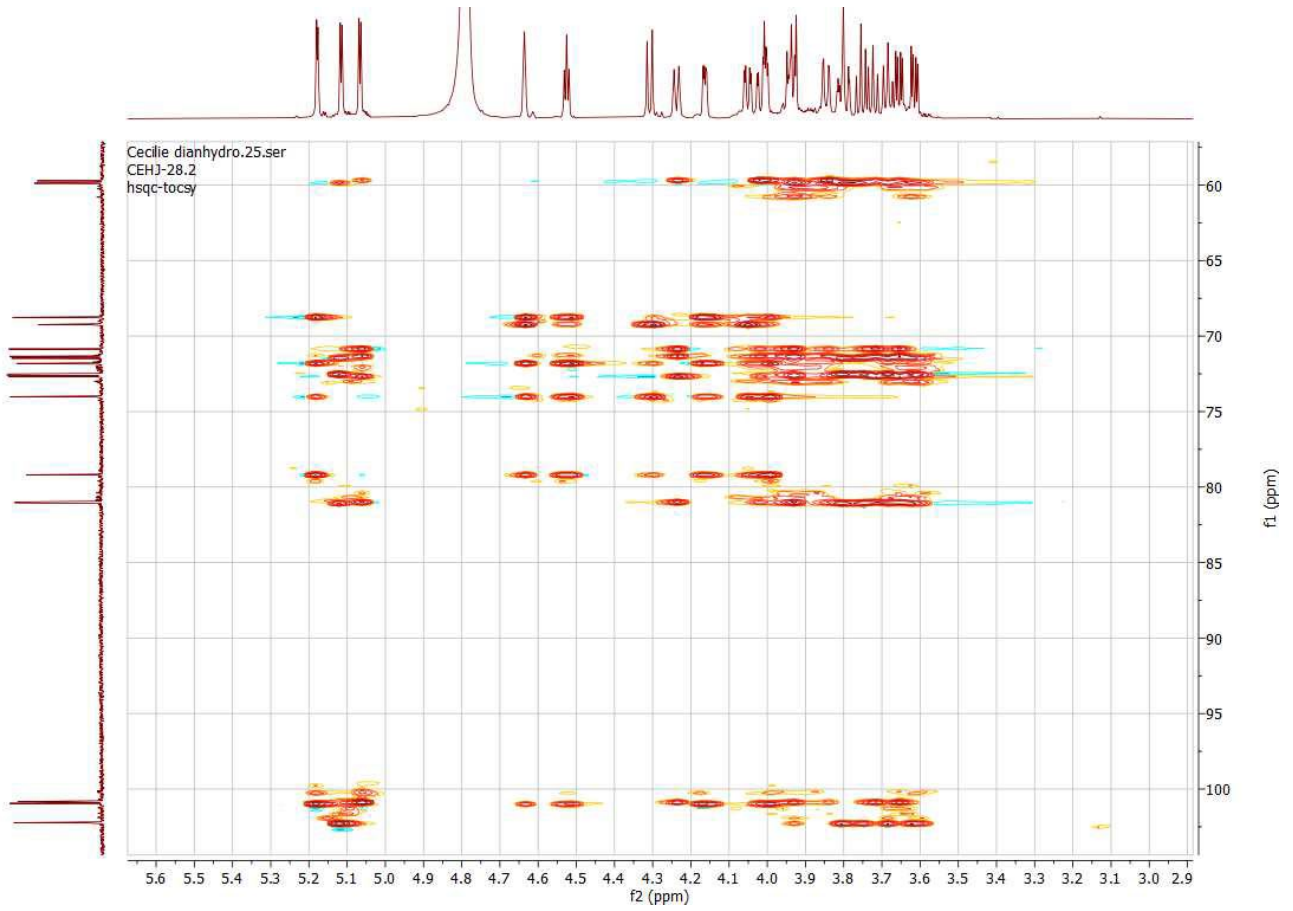
$^{13}\text{C}$  NMR (800 MHz;  $\text{D}_2\text{O}$ ) of **5**

Cosy (800 MHz; D<sub>2</sub>O) of 5



HSQC (800 MHz; D<sub>2</sub>O) of 5



HSQC-Tocsy (800 MHz; D<sub>2</sub>O) of 5

Roesy (800 MHz; D<sub>2</sub>O) of 5