

## Supplementary Material

### Synthesis of mono-amino substituted $\gamma$ -CD: Host-guest complexation and *in vitro* cytotoxicity investigation

Figure S1:  $^1\text{H}$  NMR spectrum of  $\gamma$ -CD

Figure S2:  $^{13}\text{C}$ -NMR spectrum of  $\gamma$ -CD in  $\text{d}_6$ -DMSO

Figure S3:  $^{13}\text{C}$ - dept 135-NMR spectrum of  $\gamma$ -CD in  $\text{d}_6$ -DMSO

Figure S4:  $^1\text{H}$ - $^{15}\text{N}$ -HMBC spectrum of  $\gamma$ -CD-NHCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> (in 80%  $\text{d}_6$ -DMSO/ $\text{D}_2\text{O}$  at 25 °C)

Figure S5:  $^1\text{H}$ -NMR spectrum of  $\gamma$ -CD-NHCH<sub>2</sub>CH<sub>2</sub>OH in  $\text{D}_2\text{O}$  at 25 °C

Figure S6:  $^{13}\text{C}$ -NMR spectrum of  $\gamma$ -CD-NHCH<sub>2</sub>CH<sub>2</sub>OH in  $\text{d}_6$ -DMSO at 25 °C

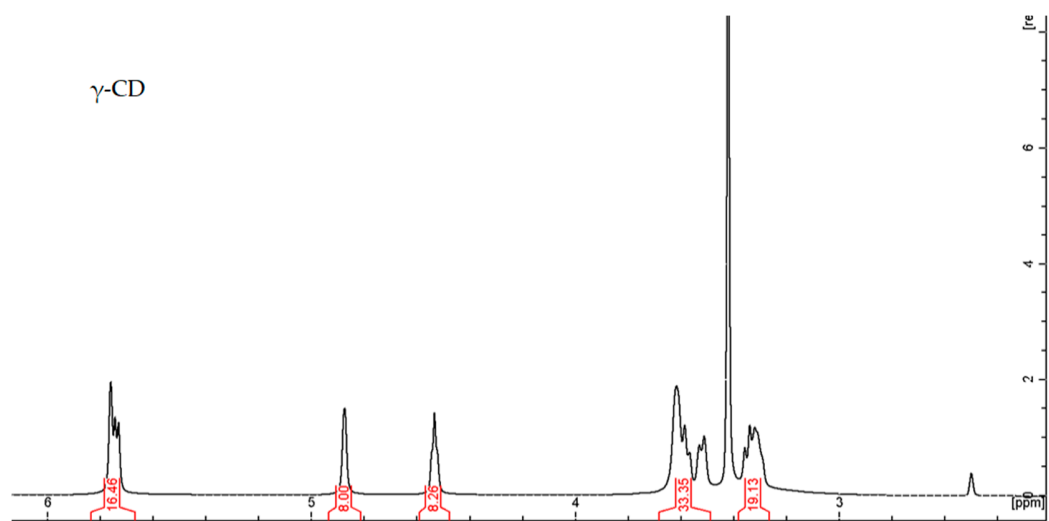


Figure S1:  $^1\text{H}$ -NMR spectrum of  $\gamma$ -CD in  $\text{d}_6$ -DMSO

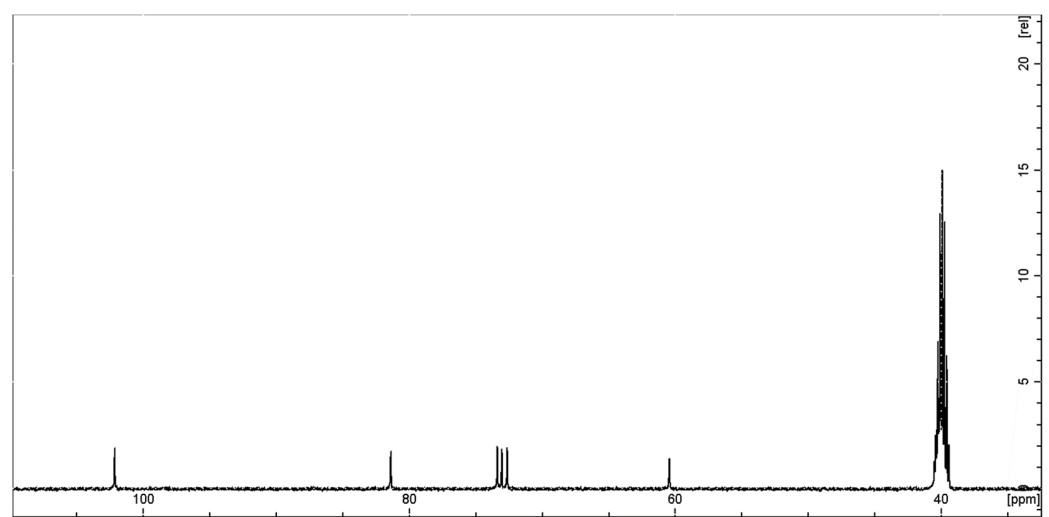


Figure S2:  $^{13}\text{C}$ -NMR spectrum of  $\gamma$ -CD in  $\text{d}_6$ -DMSO

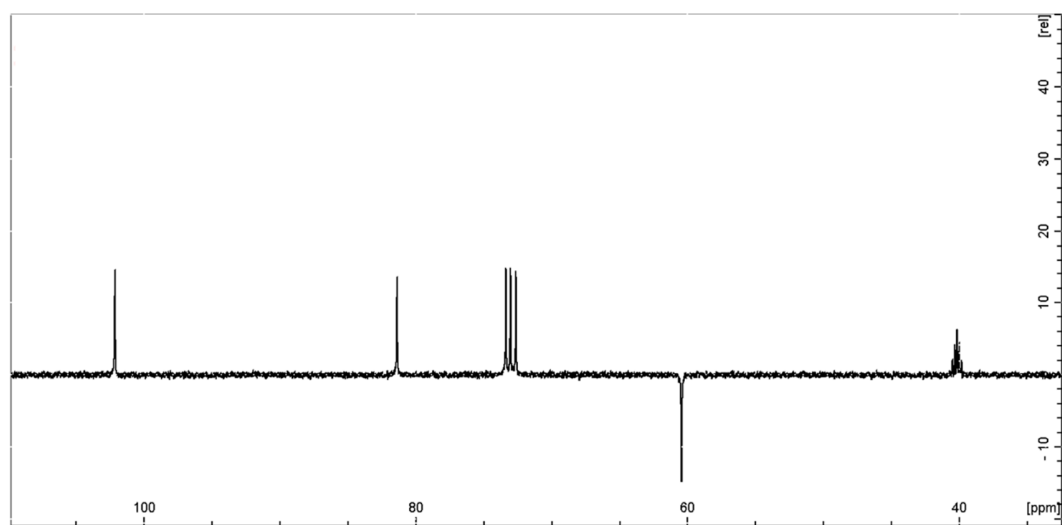


Figure S3:  $^{13}\text{C}$ -dept 135-NMR spectrum of  $\gamma$ -CD in  $\text{d}_6$ -DMSO

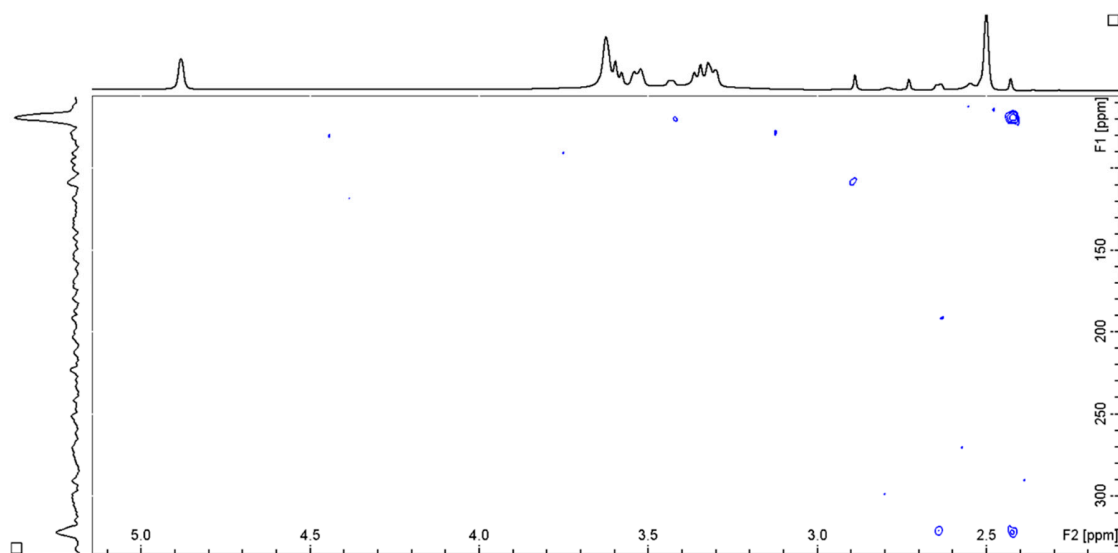


Figure S4:  $^1\text{H}$ - $^{15}\text{N}$ -HMBC spectrum of  $\gamma$ -CD- $\text{NHCH}_2\text{CH}_2\text{NH}_2$  (in 80%  $\text{d}_6$ -DMSO/ $\text{D}_2\text{O}$  at  $25^\circ\text{C}$ )

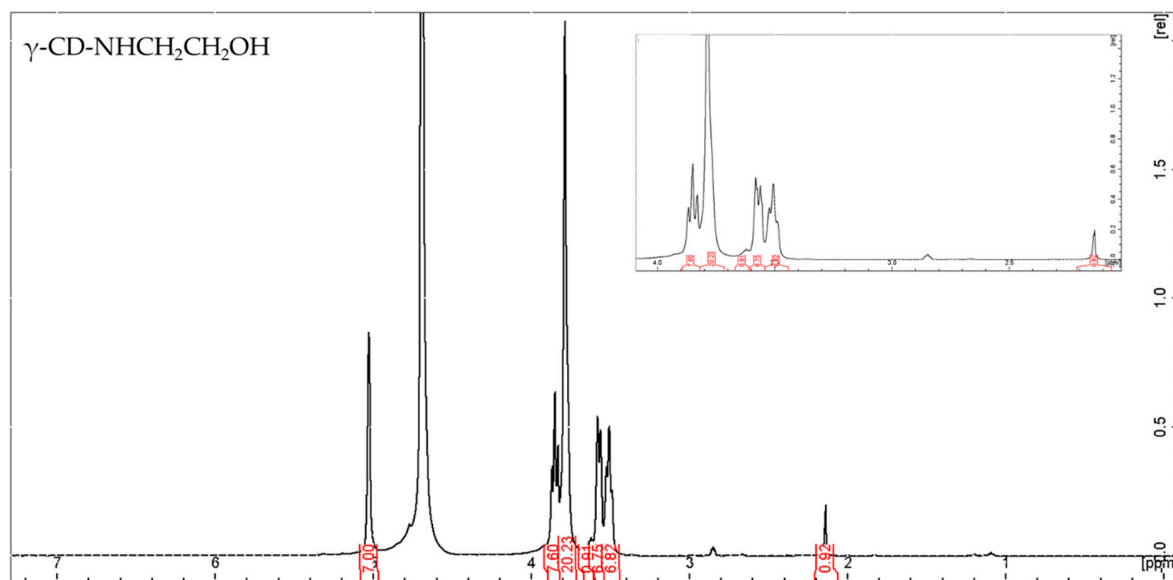


Figure S5: <sup>1</sup>H-NMR spectrum of  $\gamma$ -CD-NHCH<sub>2</sub>CH<sub>2</sub>OH in D<sub>2</sub>O at 25 °C

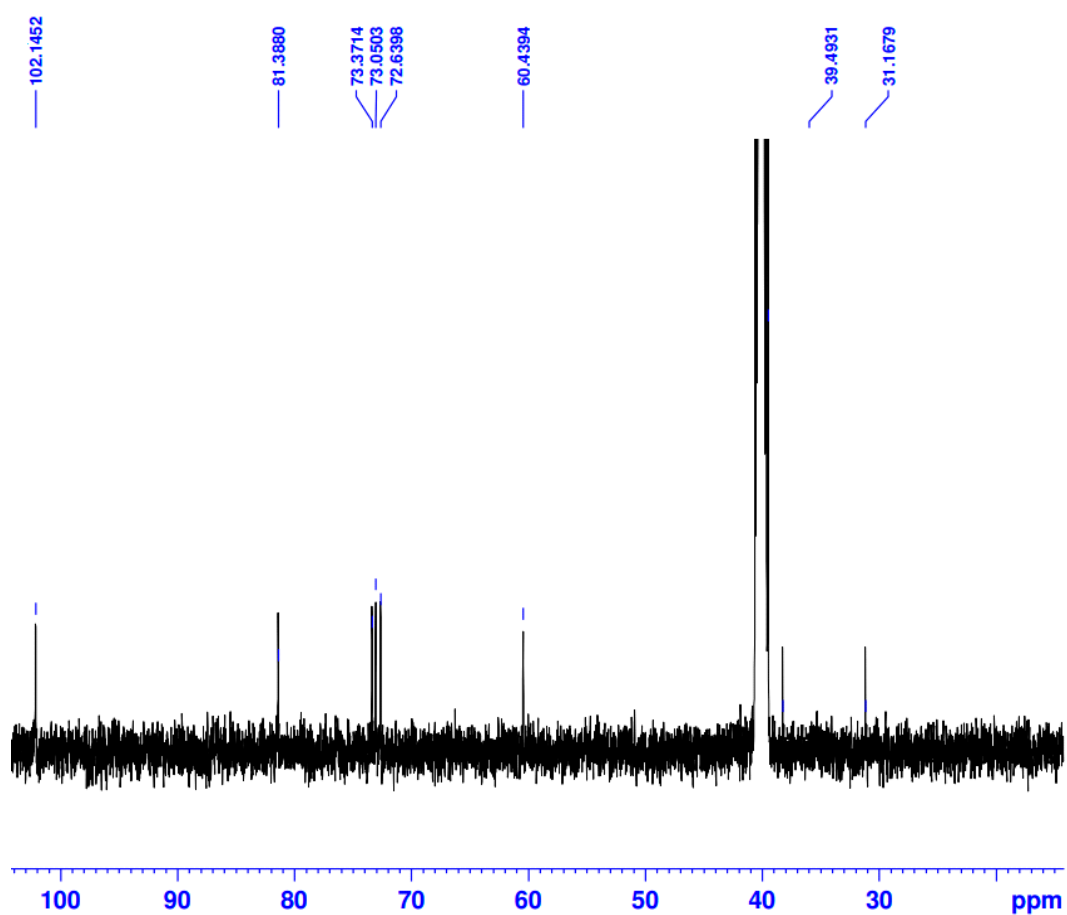


Figure S6: <sup>13</sup>C-NMR spectrum of  $\gamma$ -CD-NHCH<sub>2</sub>CH<sub>2</sub>OH in d<sub>6</sub>-DMSO at 25 °C