

## Supplementary Materials

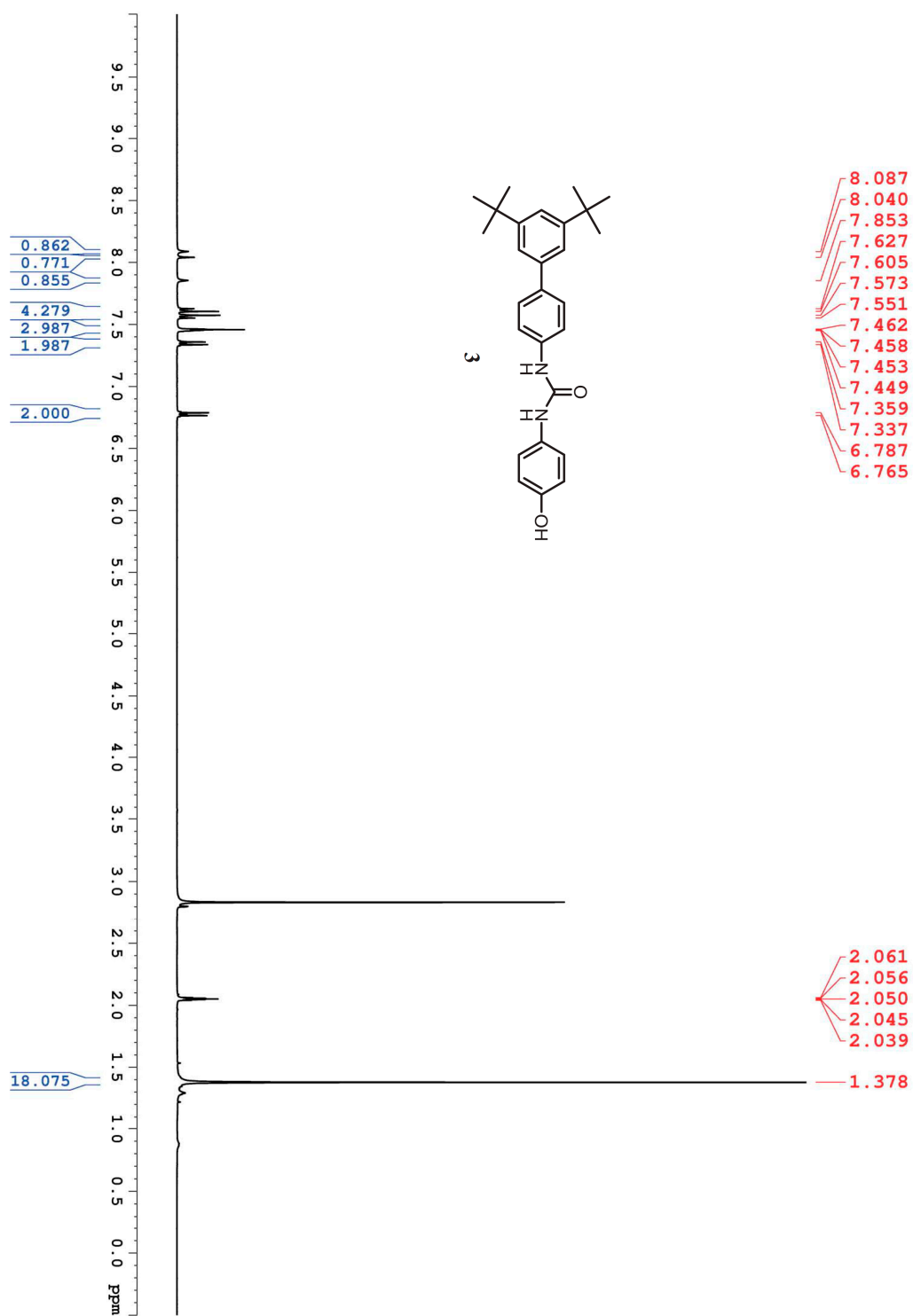
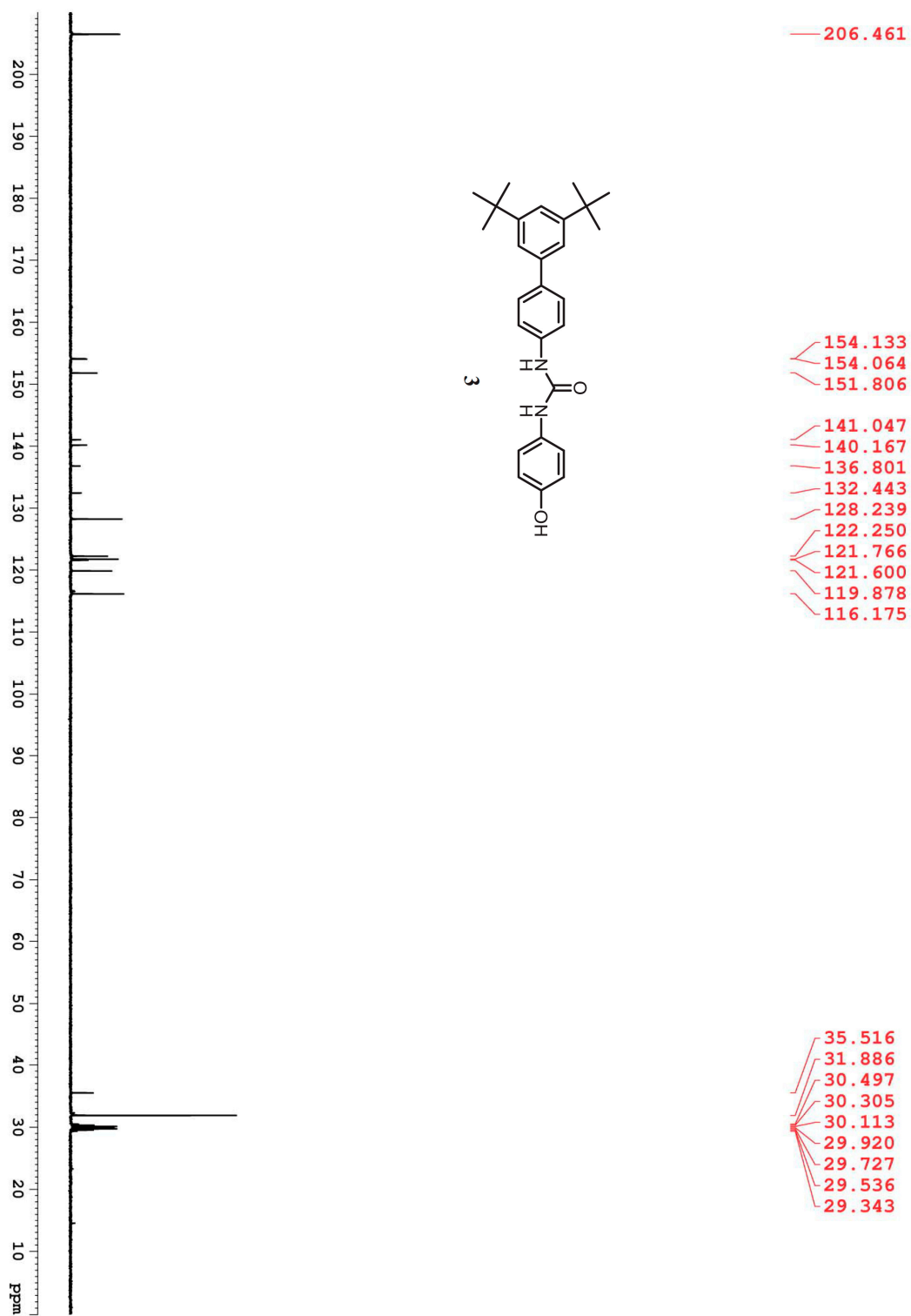
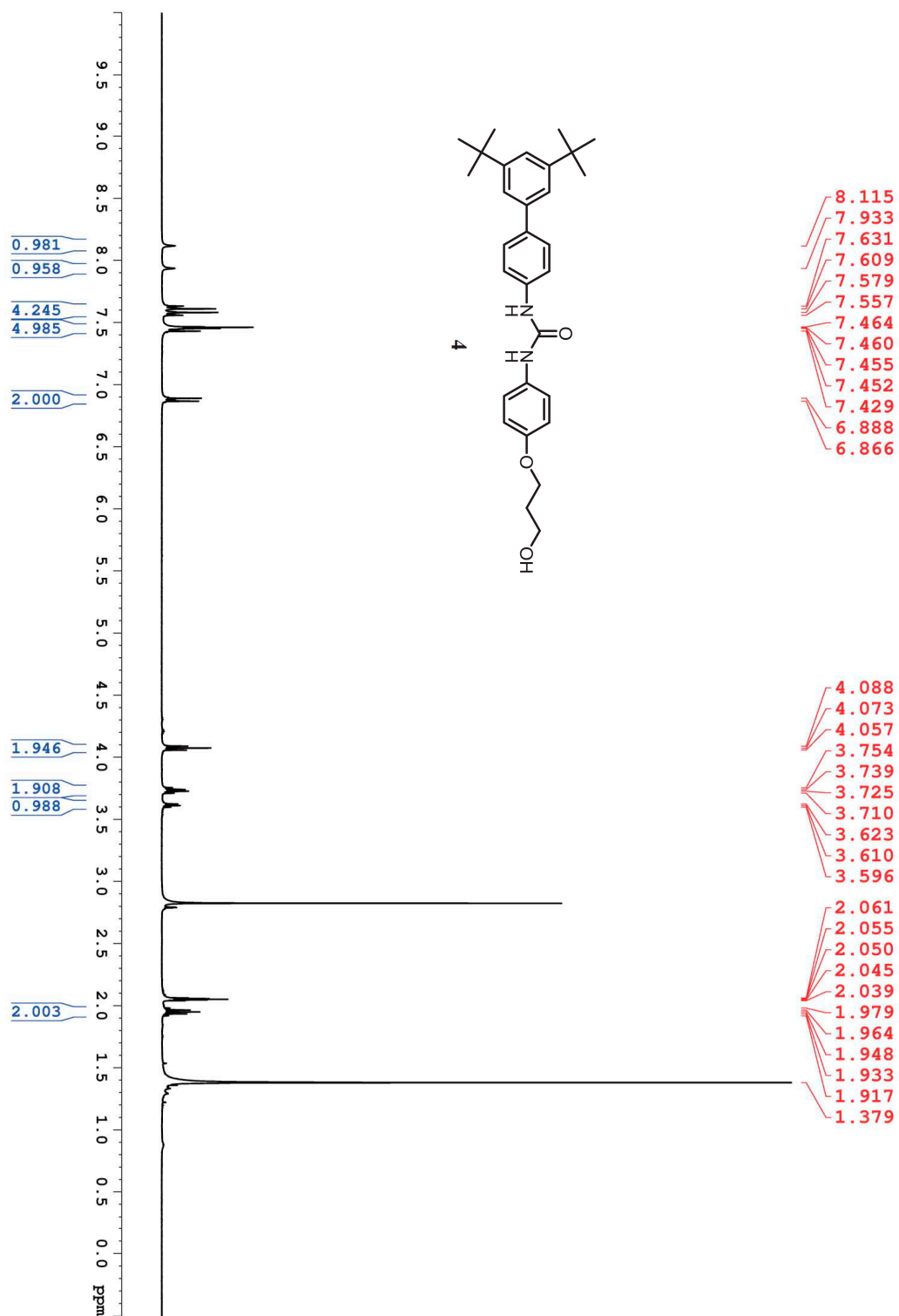


Figure S1. *Cont.*



**Figure S1.**  $^1\text{H}$  and  $^{13}\text{C}$ -NMR Spectra of the Urea **3**.

Figure S2. *Cont.*

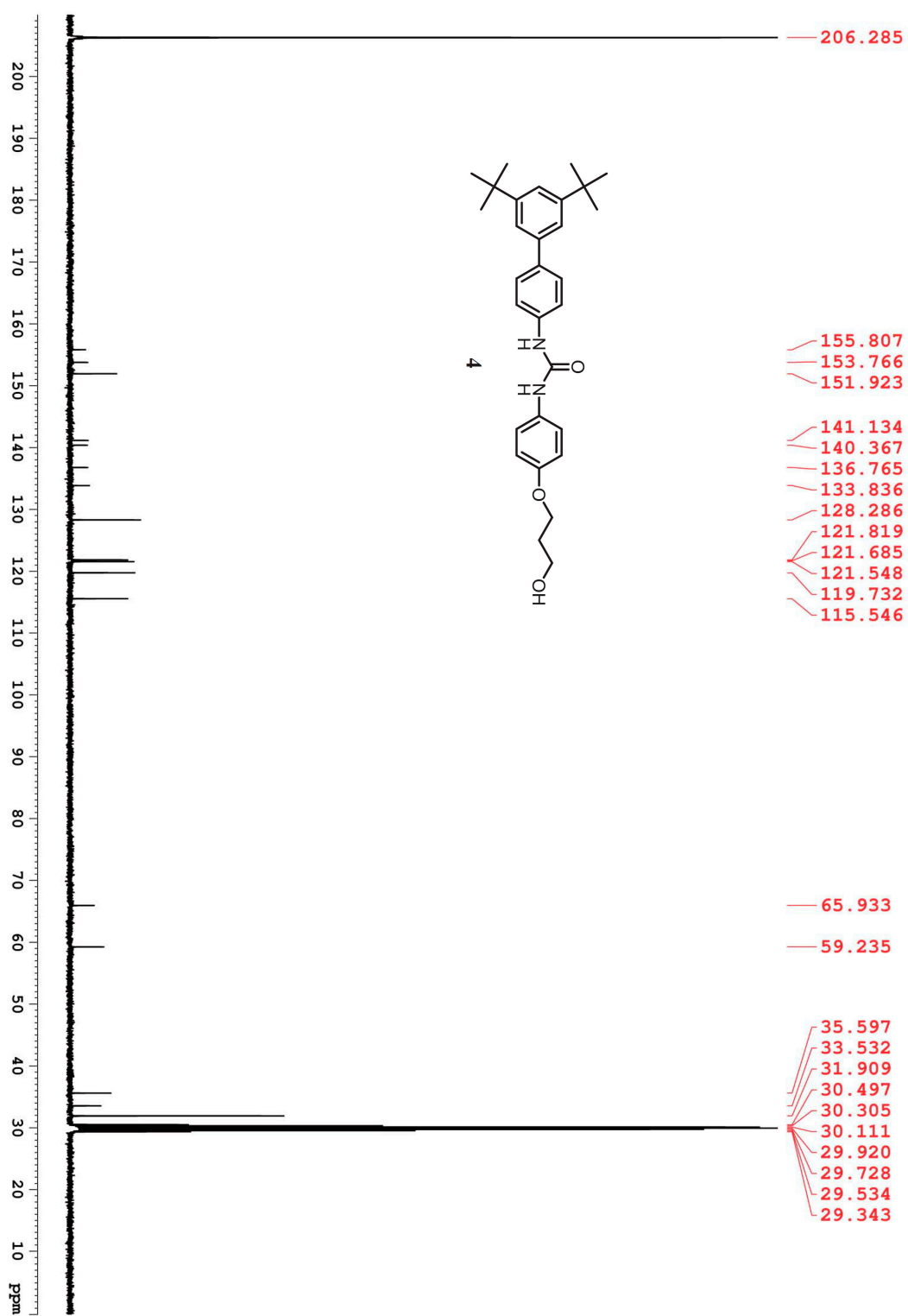
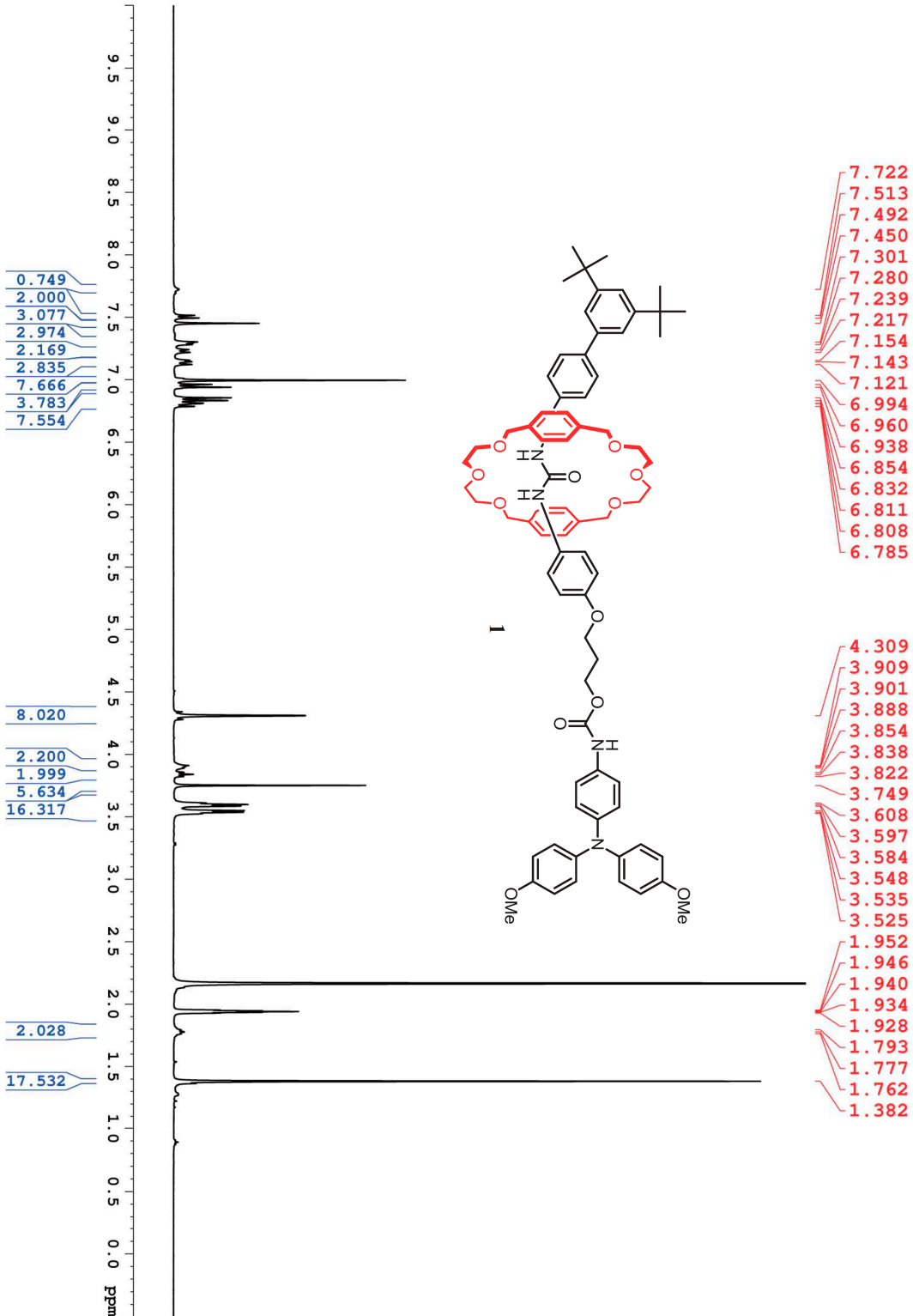
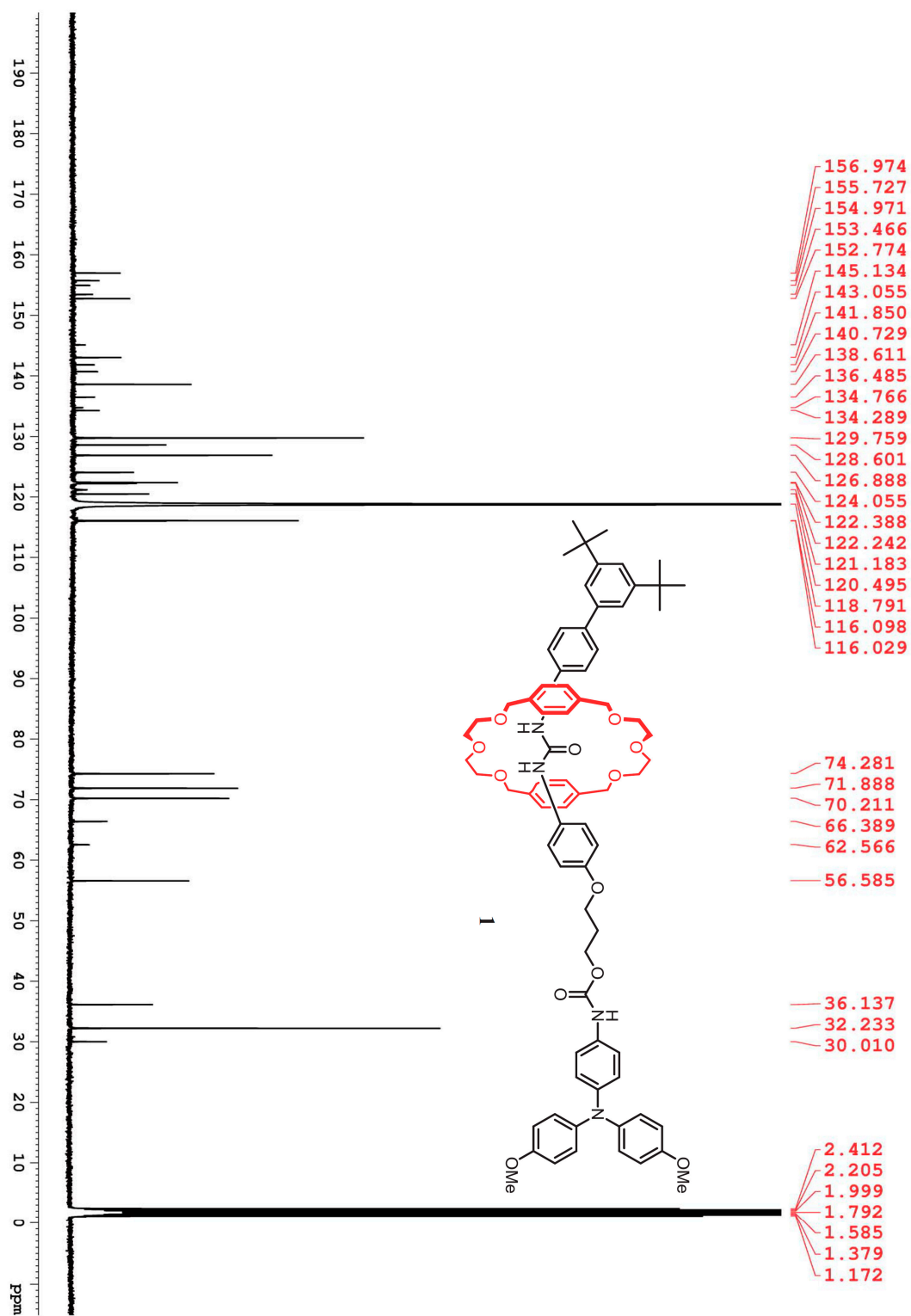


Figure S2.  $^1\text{H}$  and  $^{13}\text{C}$ -NMR Spectra of the Urea 4.

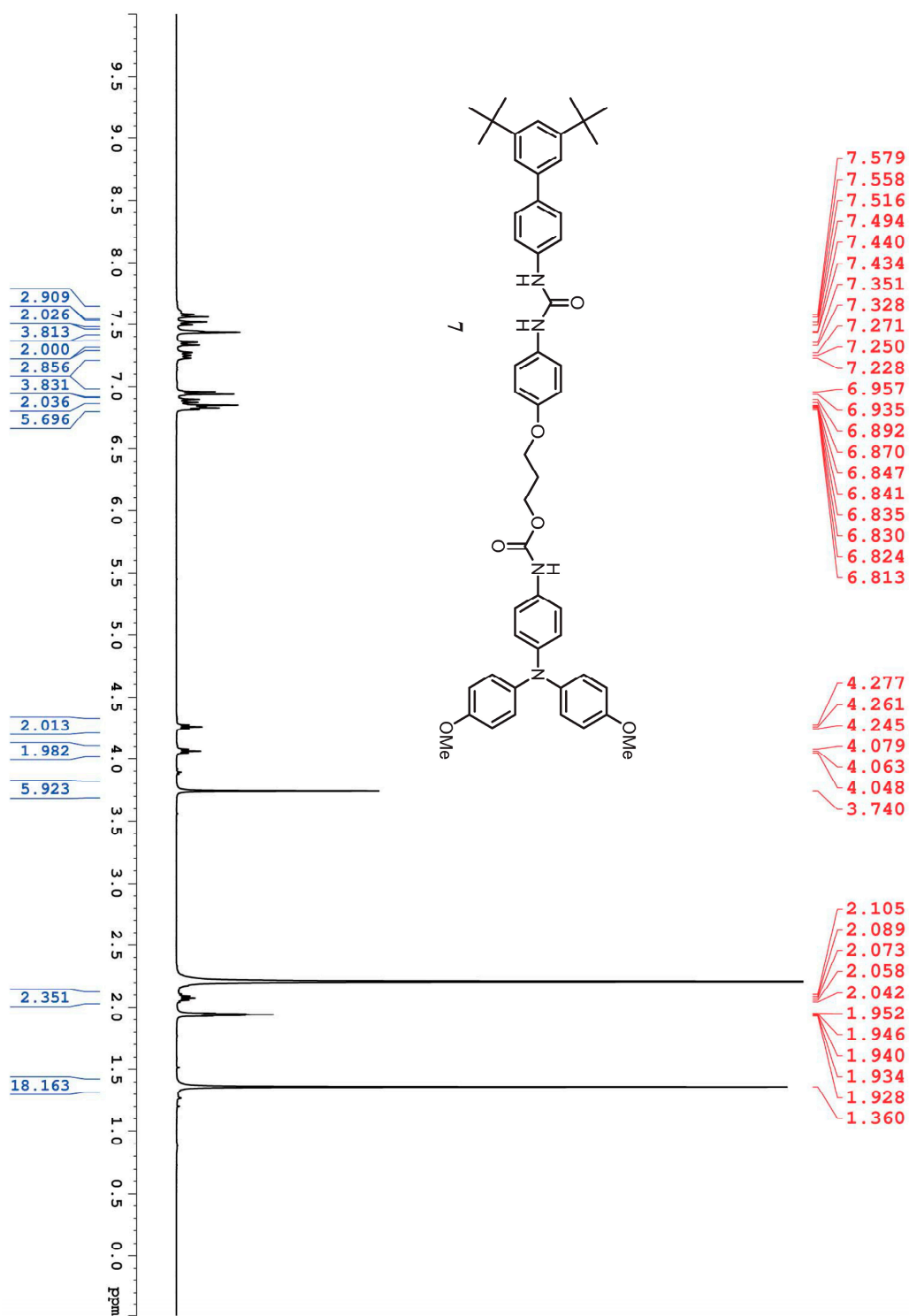




**Figure S3. *Cout.***



**Figure S3.** <sup>1</sup>H and <sup>13</sup>C-NMR Spectra of the [2]Rotaxane 1.

Figure S4. *Cont.*

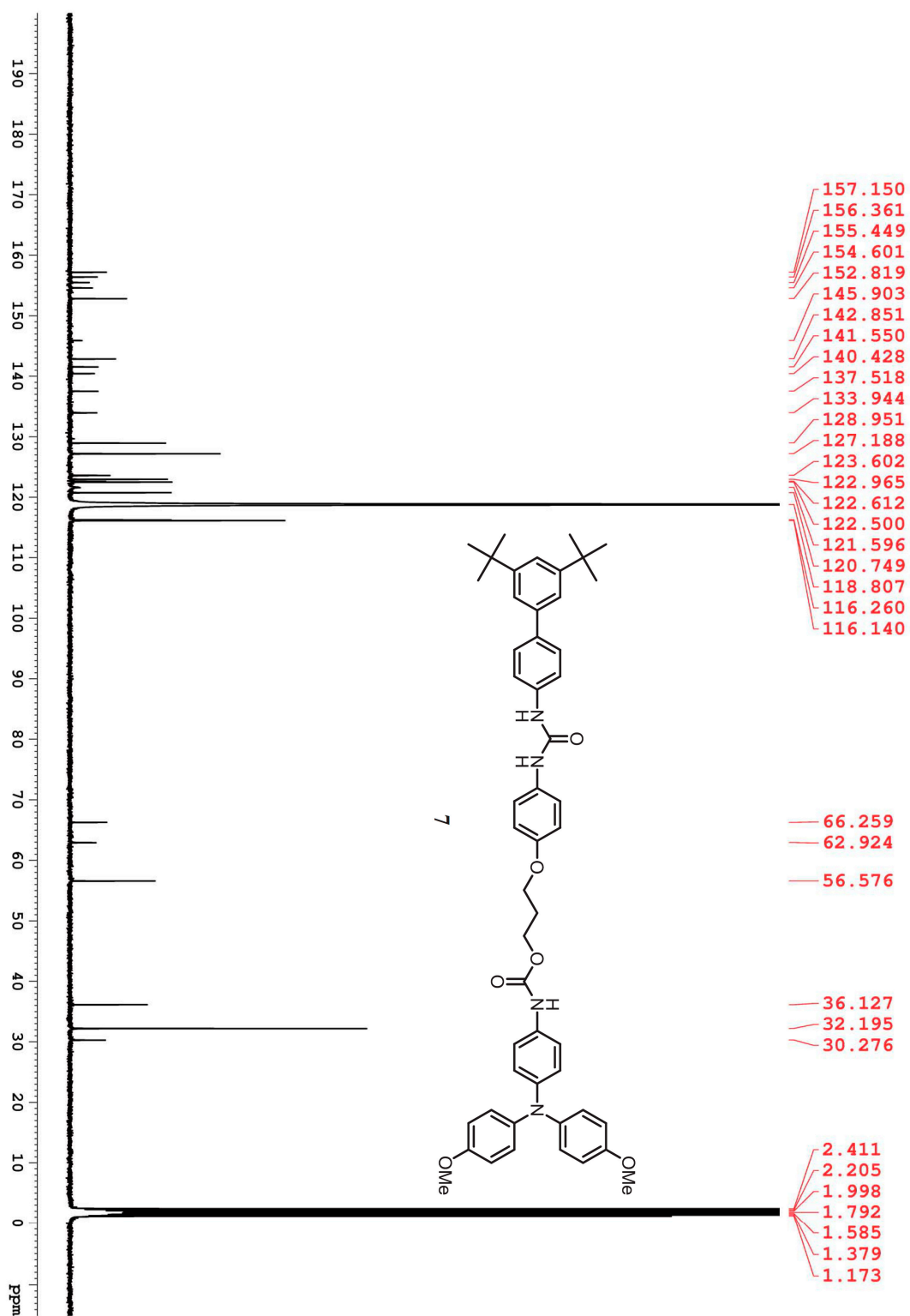
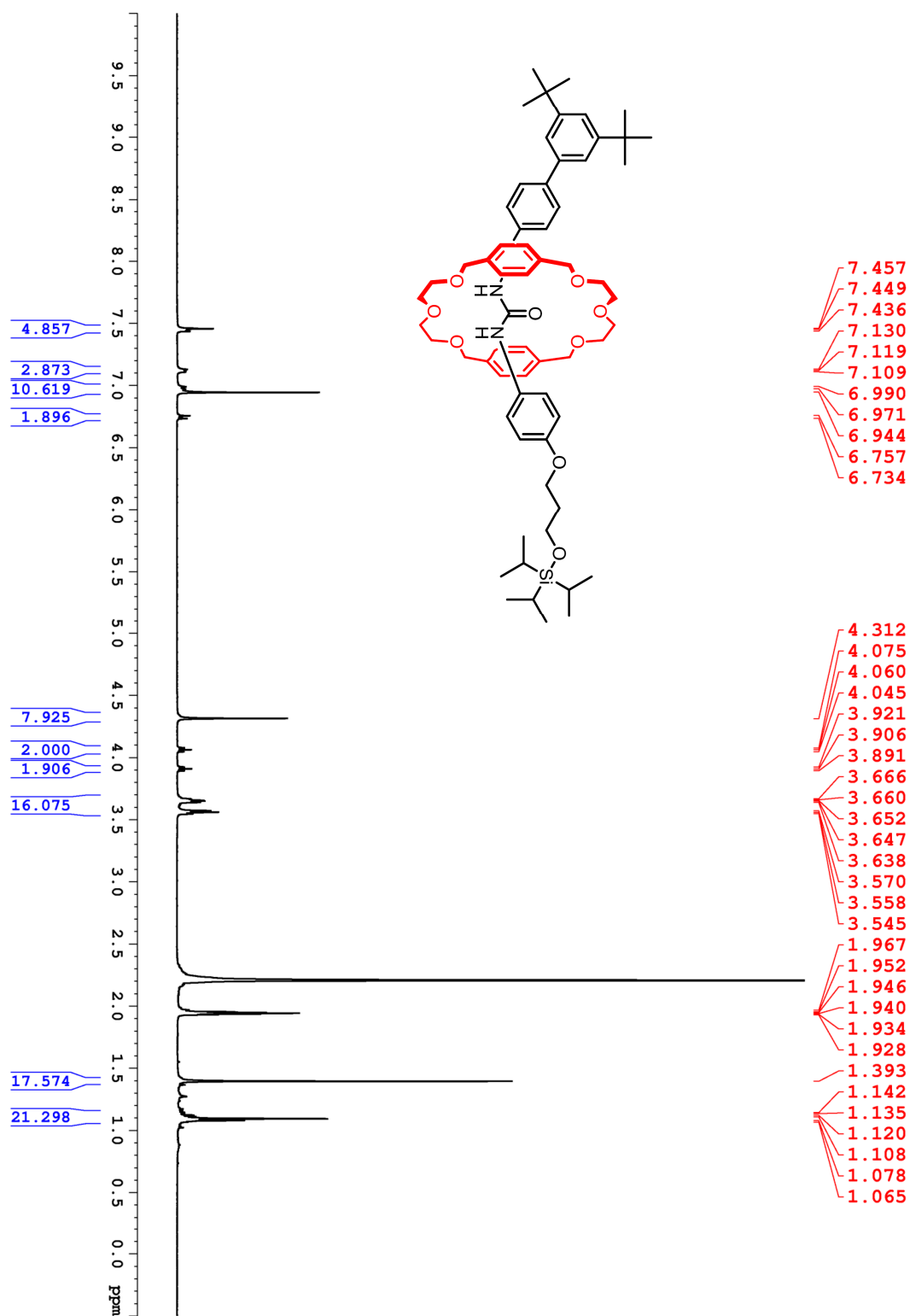


Figure S4.  $^1\text{H}$  and  $^{13}\text{C}$ -NMR Spectra of the Dumbbell 7.

Figure S5. *Cont.*

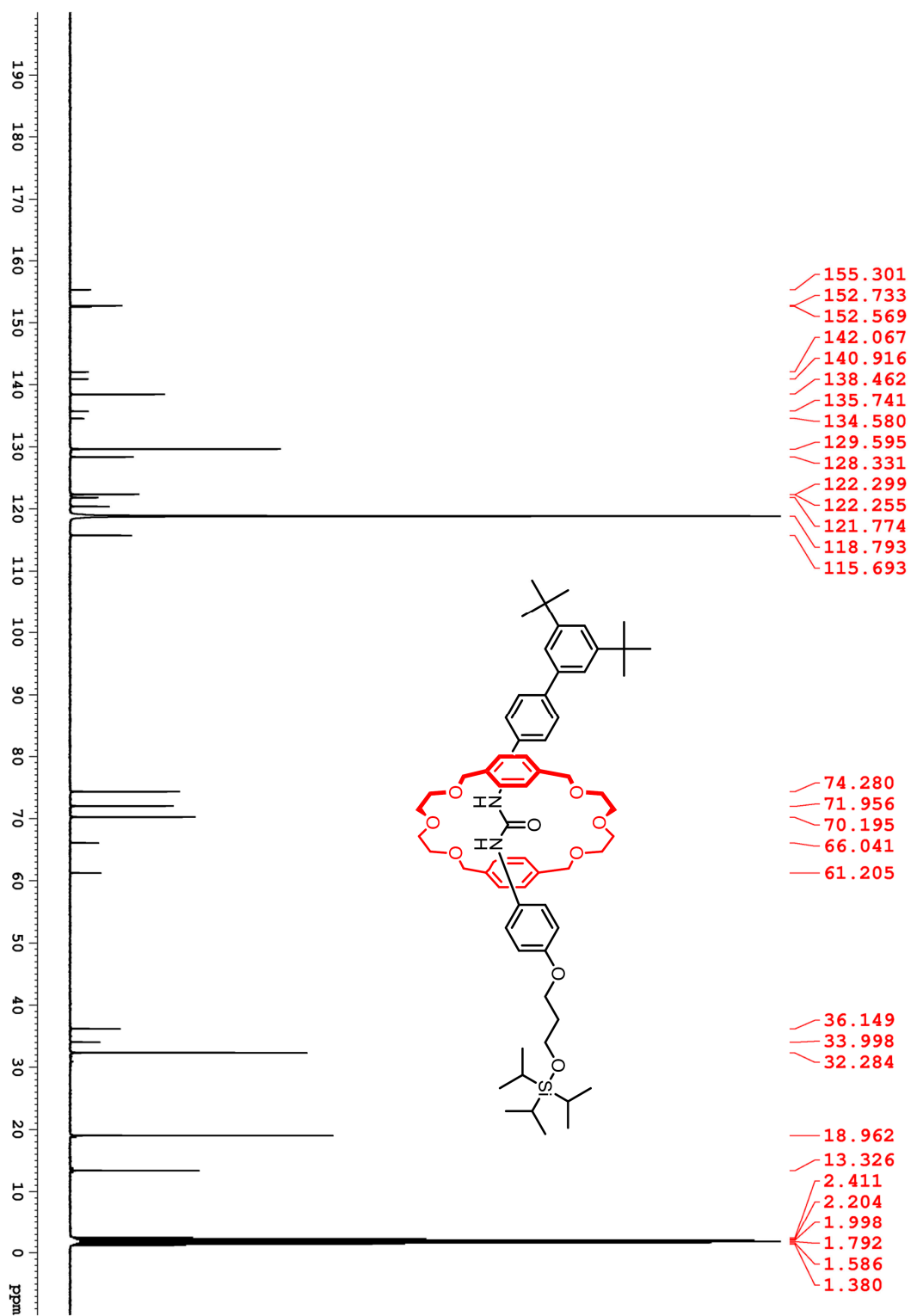
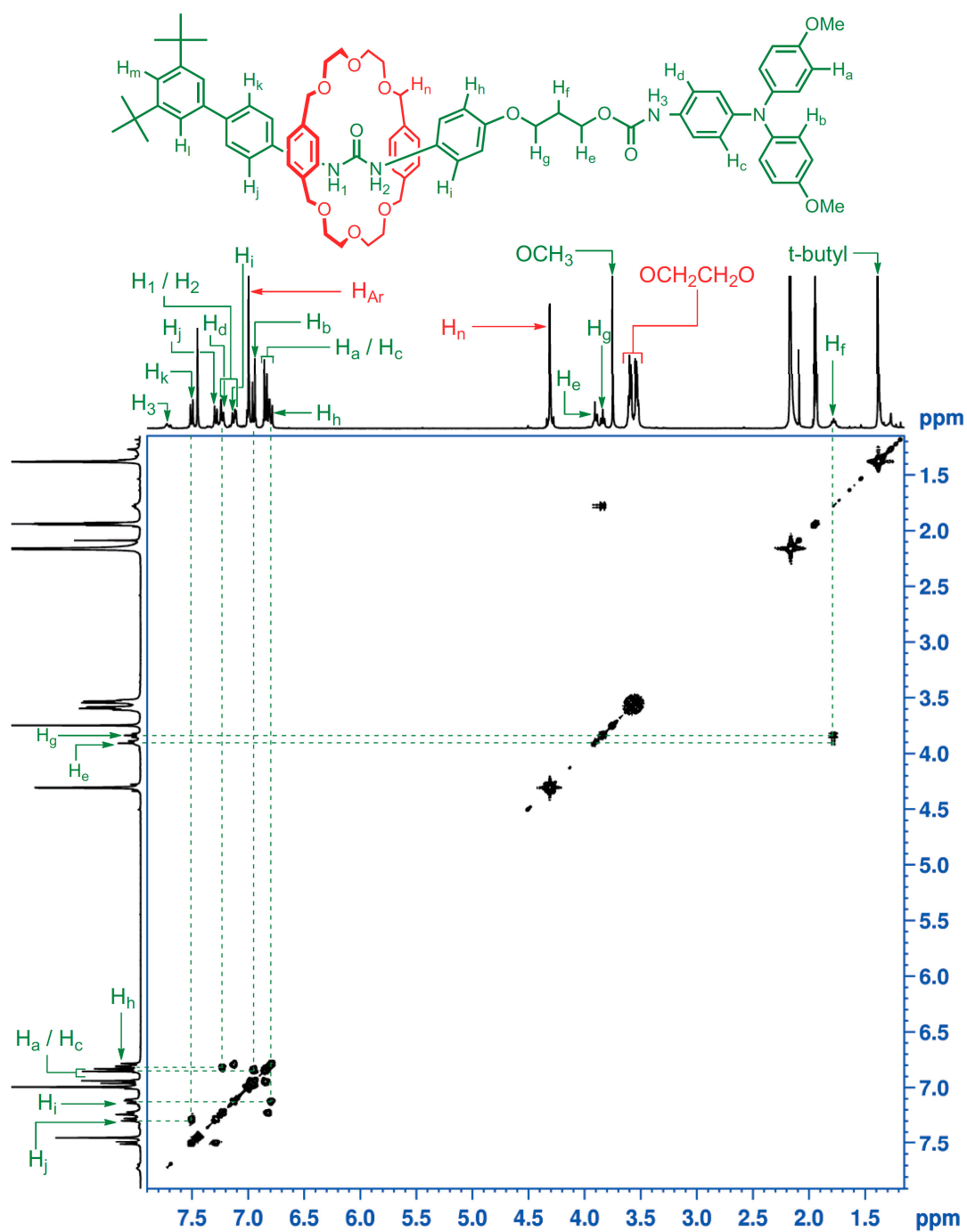
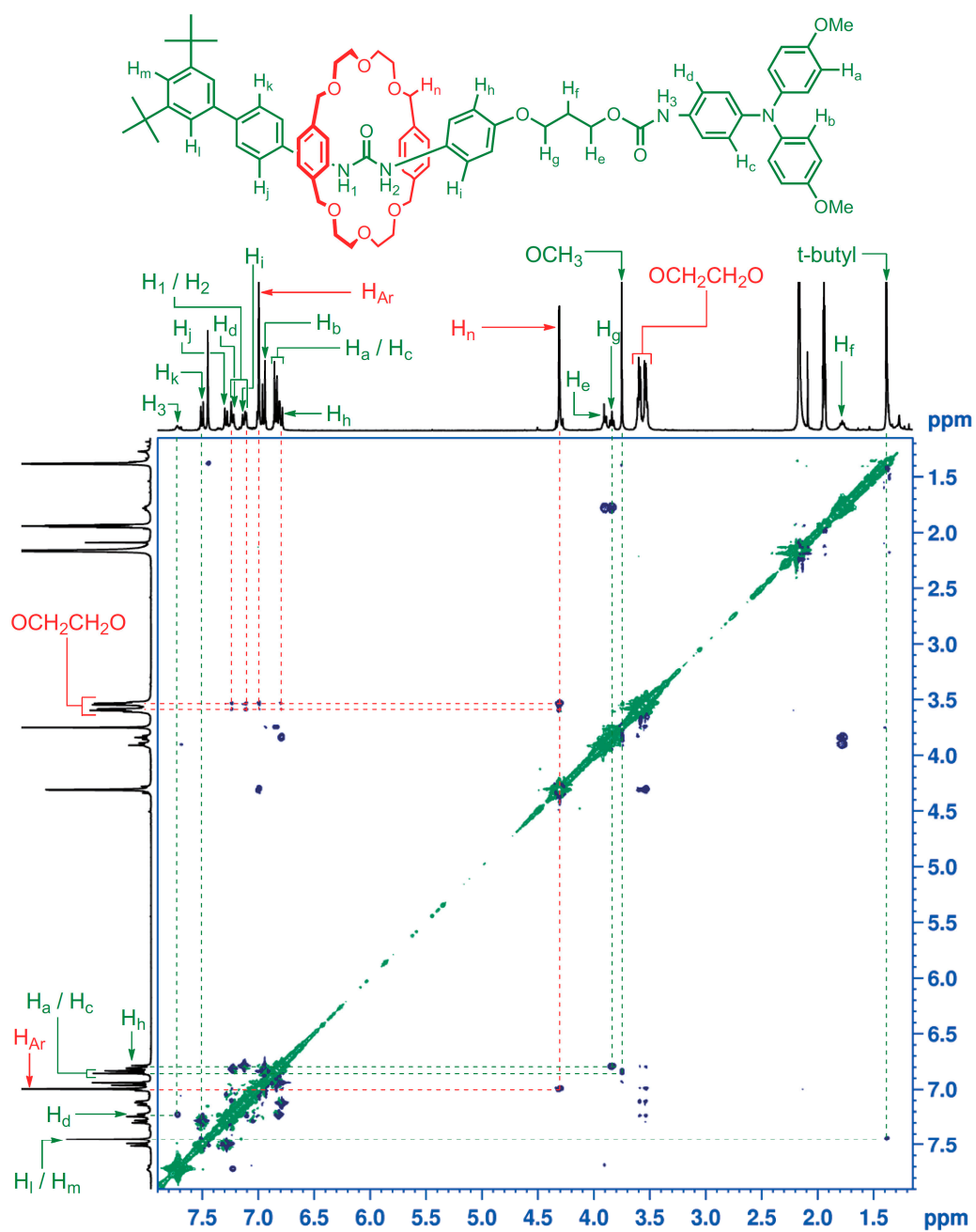


Figure S5.  $^1\text{H}$  and  $^{13}\text{C}$ -NMR Spectra of the [2]Rotaxane **8**.

COSY Spectrum (400 MHz, CD<sub>3</sub>CN, 298 K) of [2]rotaxane 1Figure S6. *Cont.*

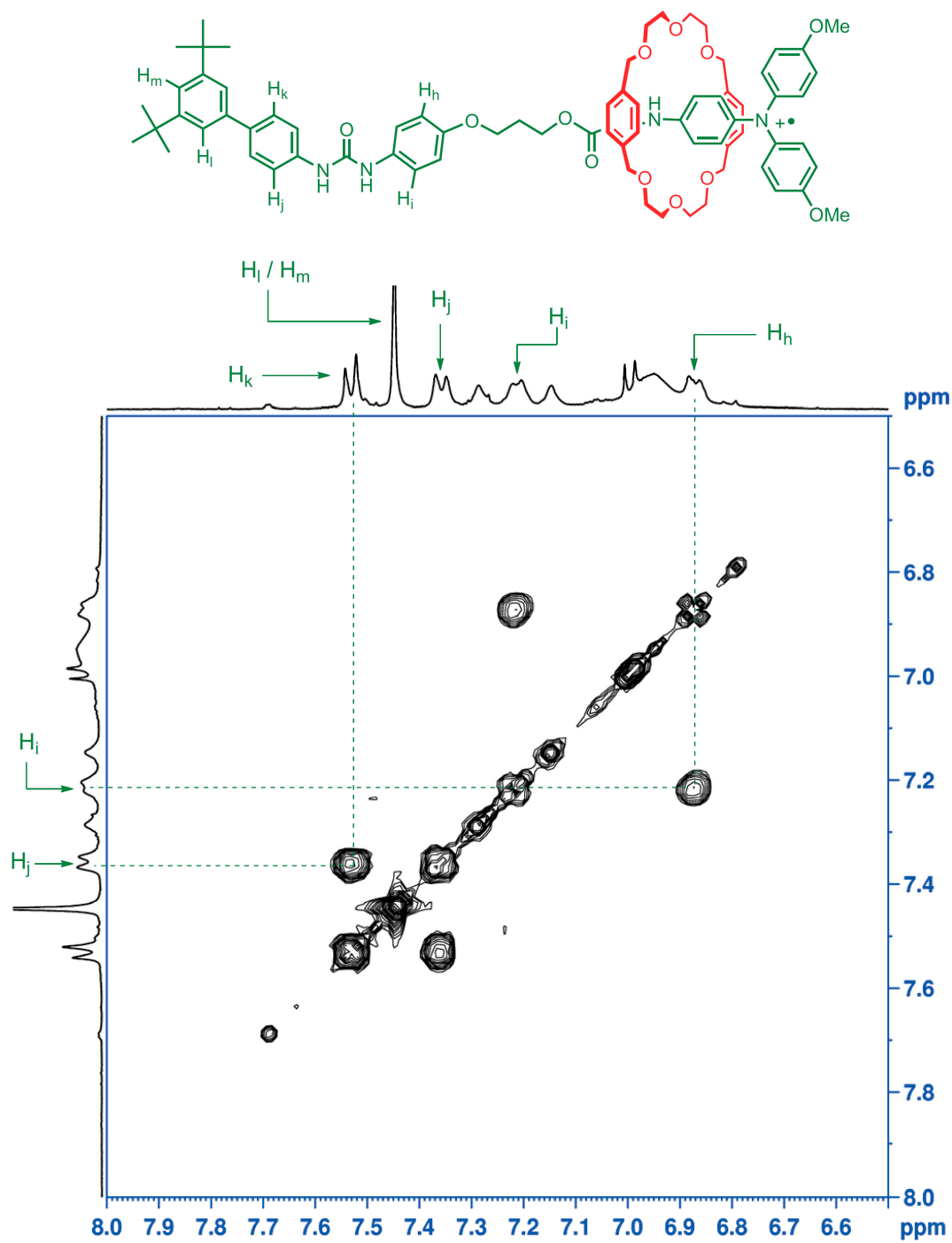
NOESY Spectrum (400 MHz, CD<sub>3</sub>CN, 298 K) of [2]rotaxane **1**



**Figure S6.** 2D COSY and NOSEY Spectra of the [2]Rotaxane **1**.



Partial COSY Spectrum (400 MHz, CD<sub>3</sub>CN, 298 K) of the equimolar mixture of [2]rotaxane **1** and NOBF<sub>4</sub> (6 mM)



**Figure S7.** Partial 2D COSY Spectra of the equimolar mixture of [2]Rotaxane **1** and NOBF<sub>4</sub> (6 mM).