

# Inclusion Complexes of 3,4-Ethylenedioxythiophene with Per-Modified $\beta$ - and $\gamma$ -Cyclodextrins

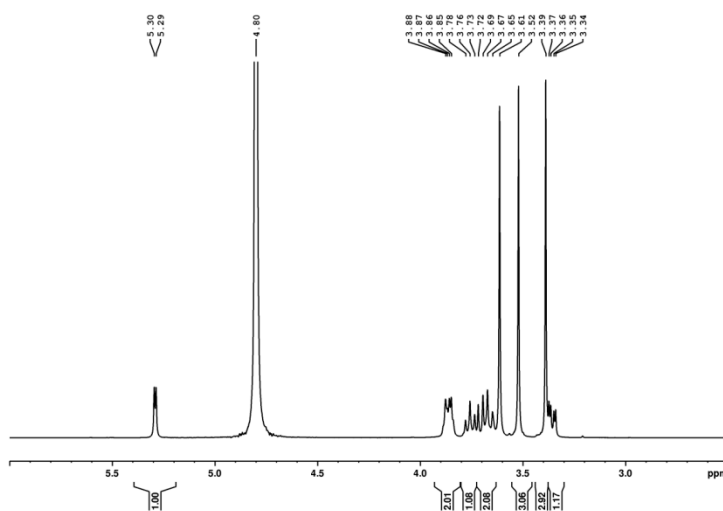
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## 1. Characterization data of compounds

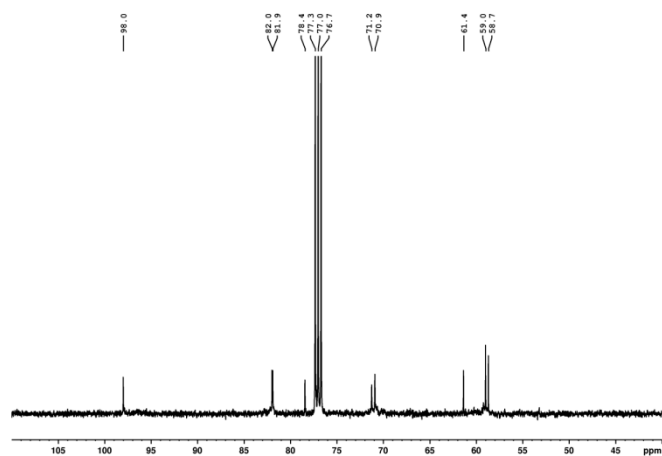
### 1.1. $^1\text{H}$ -NMR and $^{13}\text{C}$ -NMR of TMe- $\beta$ CD and TMe- $\gamma$ CD in $\text{D}_2\text{O}$



**Figure S1.**  $^1\text{H}$ -NMR spectrum of TMe- $\beta$ CD in  $\text{D}_2\text{O}$ .

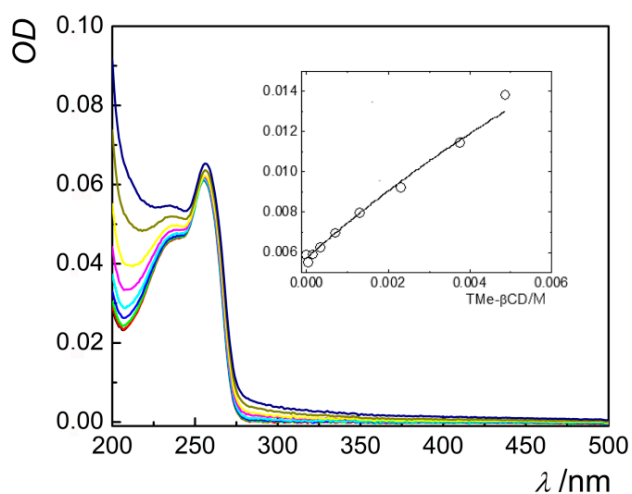
$^1\text{H}$ -NMR ( $\text{D}_2\text{O}$ , 400 MHz),  $\delta$  (ppm): 5.29 (d,  $J = 3.5$  Hz, 7H, H1), 3.88–3.85 (m, 14H, H5, H6a), 3.76 (t,  $J = 8.9$  Hz, 7H, H4), 3.72–3.65 (m, 14H, H3, H6b), 3.61 (s, 21H, C2- $\text{OCH}_3$ ), 3.52 (s, 21H, C3- $\text{OCH}_3$ ), 3.39 (s, 21H, C6- $\text{OCH}_3$ ), 3.36 (dd,  $J = 3.5$  Hz,  $J = 9.6$  Hz, 7H, H2).





**Figure S4.**  $^{13}\text{C}$ -NMR spectrum of TMe- $\gamma$ CD in  $\text{CDCl}_3$ .

$^{13}\text{C}$ -NMR ( $\text{CDCl}_3$ , 100 MHz),  $\delta$  (ppm): 98.0 (C1), 82.0 (C3), 81.9 (C2), 78.4 (C4), 71.2 (C6), 70.9 (C5), 61.4 (C2-OCH<sub>3</sub>), 59.0 (C6-OCH<sub>3</sub>), 58.7 (C3-OCH<sub>3</sub>).



**Figure S5.** Changes in the absorption spectra of the monomer EDOT upon addition of increasing amounts of TMe- $\beta$ CD in water. The fitted binding constant curve (according to a 1:1 host-guest complexation stoichiometry) is shown in the inset.

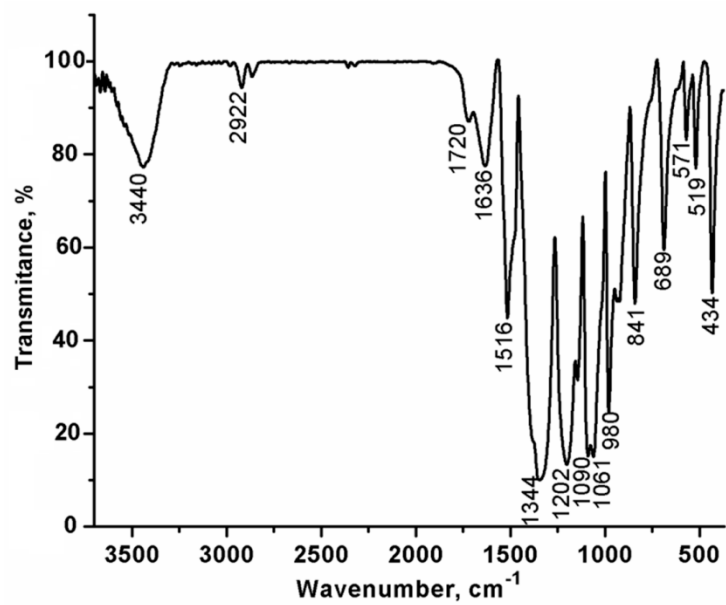


Figure S6. FT-IR spectrum of EDOT-TMe-βCD.

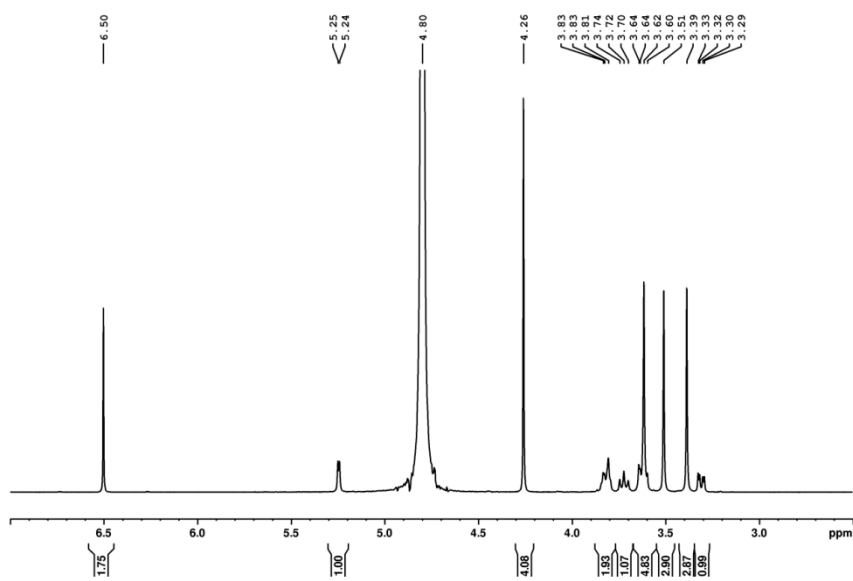
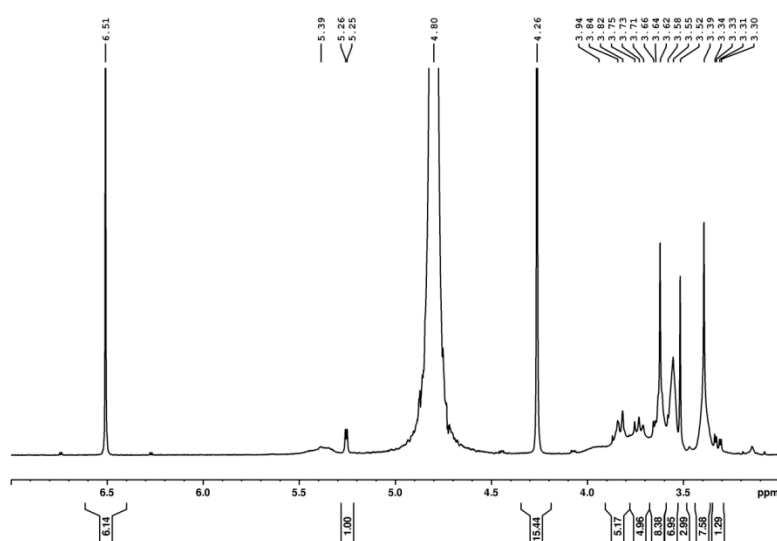
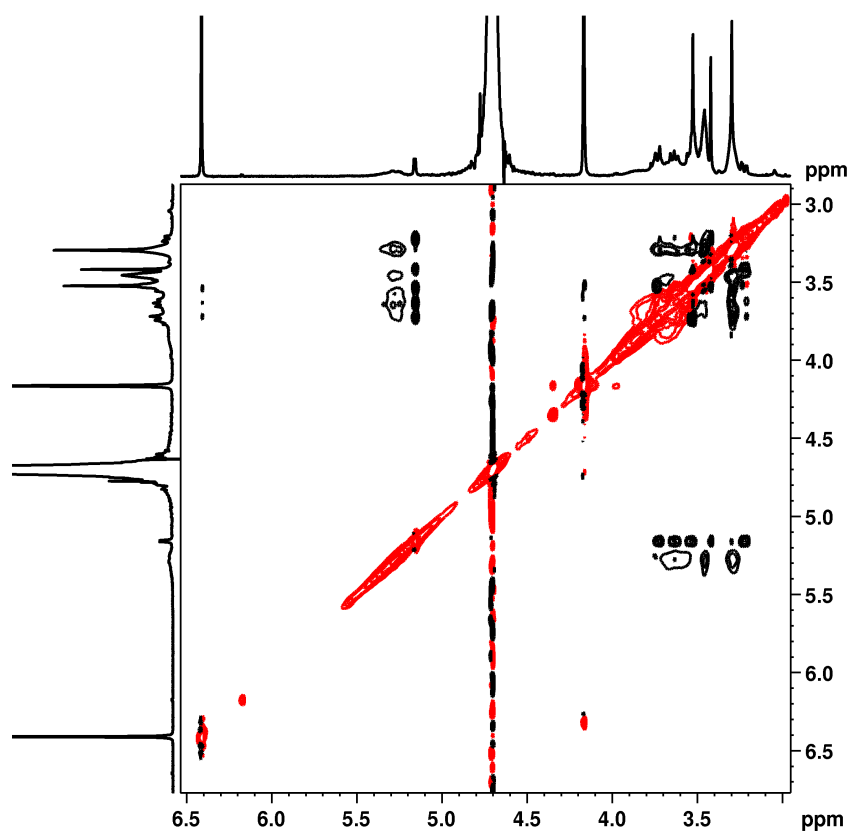


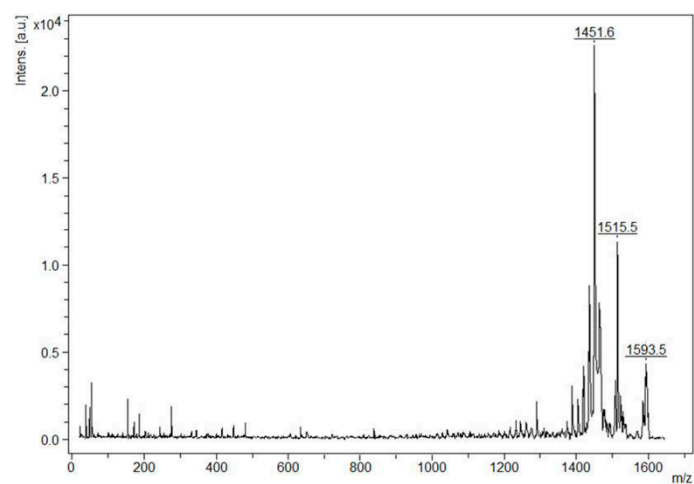
Figure S7. <sup>1</sup>H-NMR spectrum of EDOT-TMe-βCD in D<sub>2</sub>O.



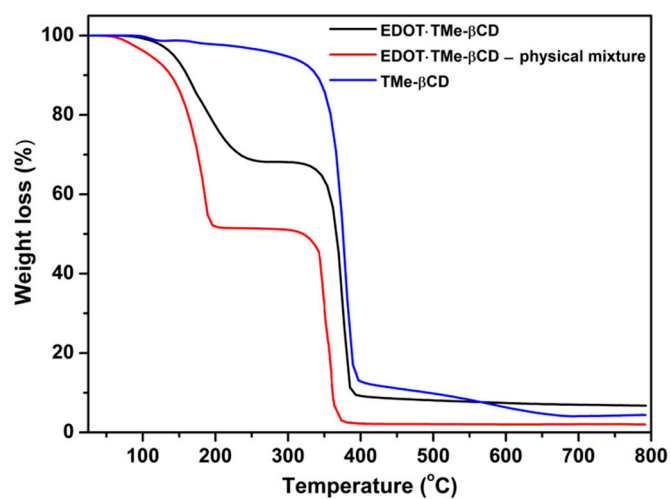
**Figure S8.**  $^1\text{H}$ -NMR spectrum of EDOT·TMe- $\gamma$ CD in  $\text{D}_2\text{O}$ .



**Figure S9.** H-H ROESY (400 MHz,  $\text{D}_2\text{O}$ ) spectrum for EDOT·TMe- $\gamma$ CD.



**Figure S10.** The positive-ion reflectron MALDI-TOF MS spectrum of the EDOT·TMe-βCD complex.



**Figure S11.** Thermograms of the EDOT·TMe-βCD inclusion complex (black line), physical mixture (red line) and TMe-βCD (blue line).