

## Electronic Supplementary Information

### Cyclodextrin carriers of positively charged porphyrin sensitizers

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### ESI-mass spectra

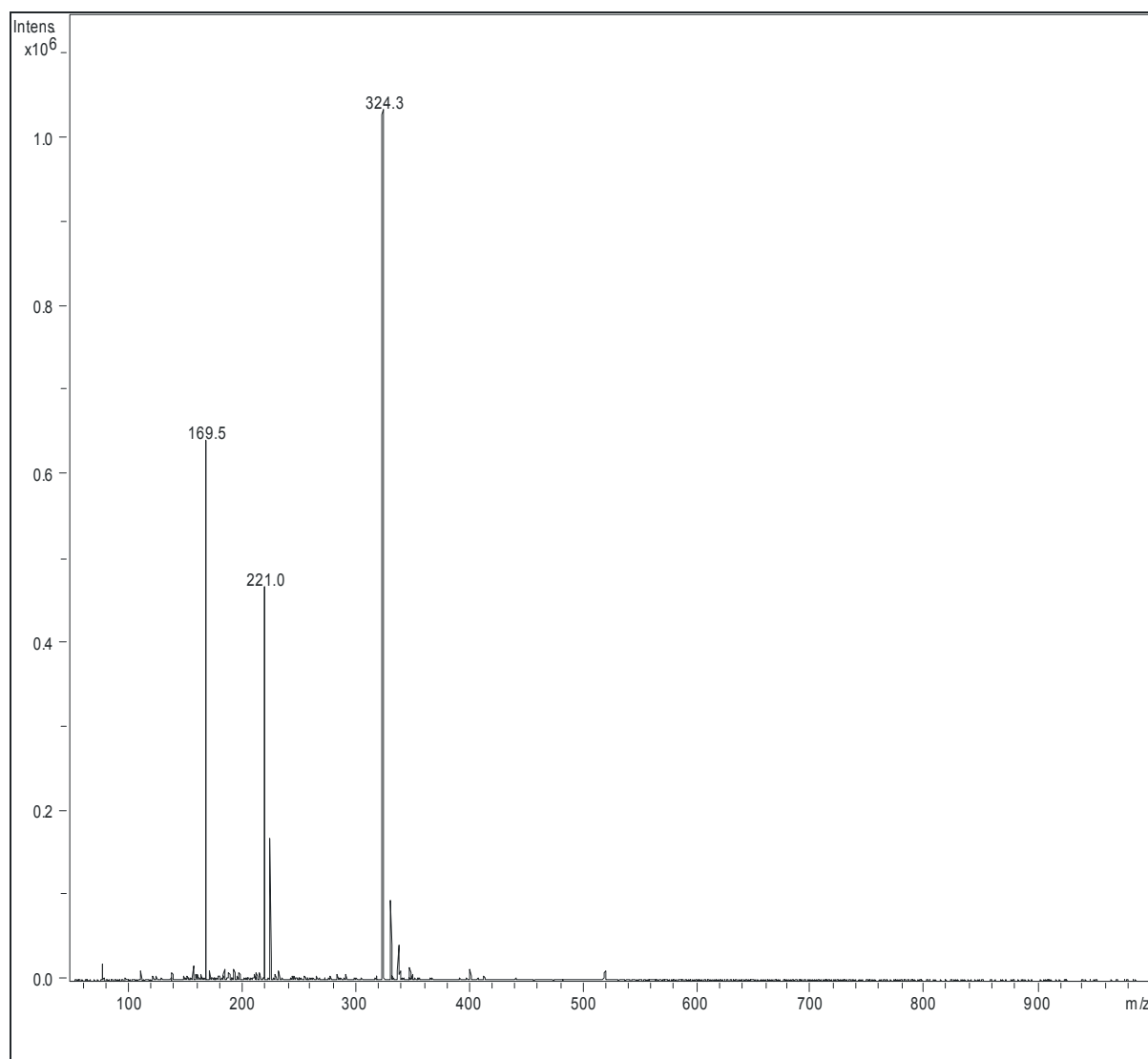


Figure S1.

ESI-MS of TMPyP/Cl shows fragments corresponding to  $M/z = 169.5$  (TMPyP)<sup>4+</sup>,  $221.0$  (TMPyP – CH<sub>3</sub>)<sup>3+</sup>,  $324.3$  (TMPyP – 2CH<sub>3</sub>)<sup>2+</sup>.

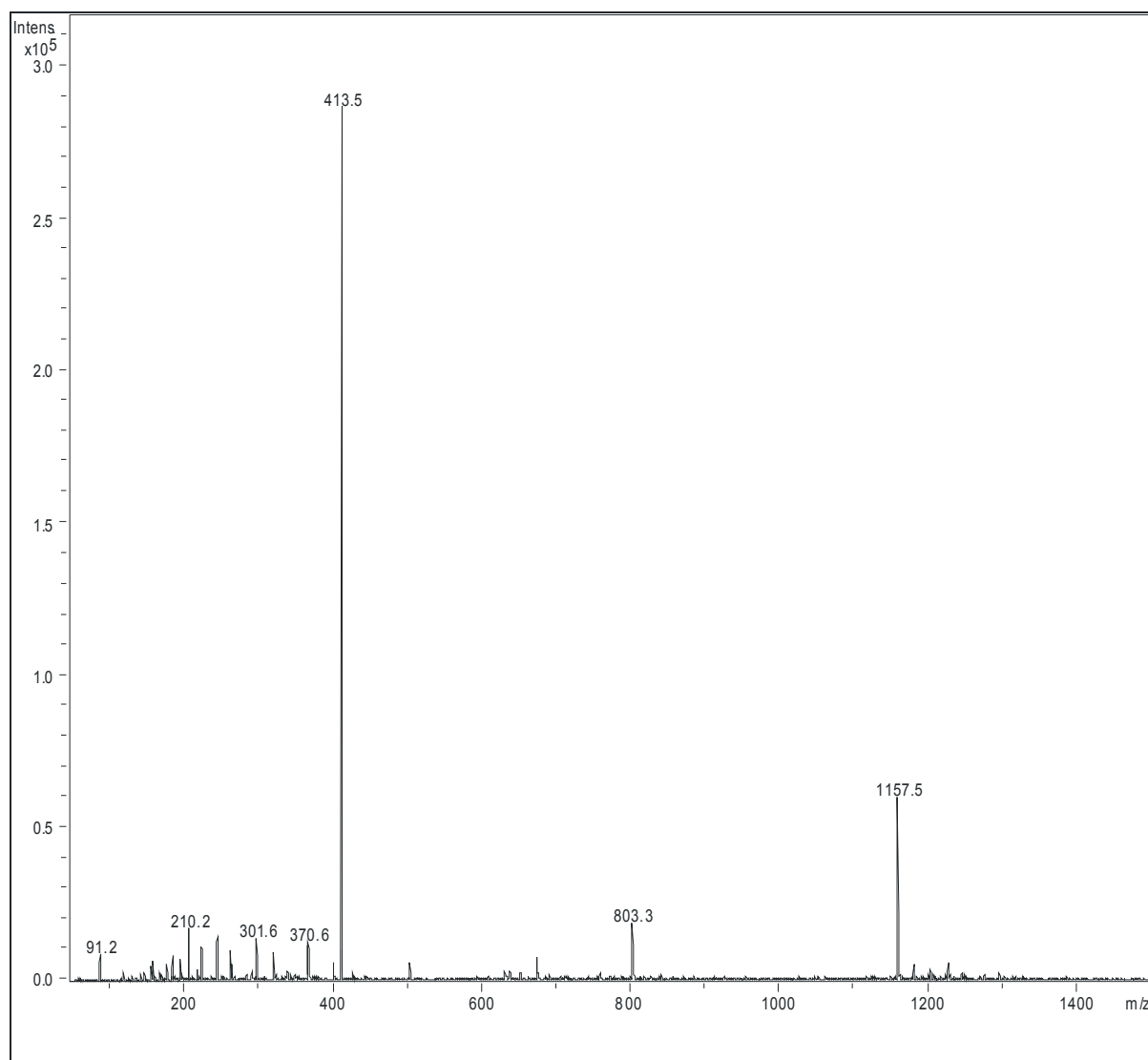


Figure S2.  
ESI-MS of  $\beta$ CD. Fragment  $M/z = 1157.5$  corresponds to  $(\beta\text{CD} + \text{Na})^+$ .

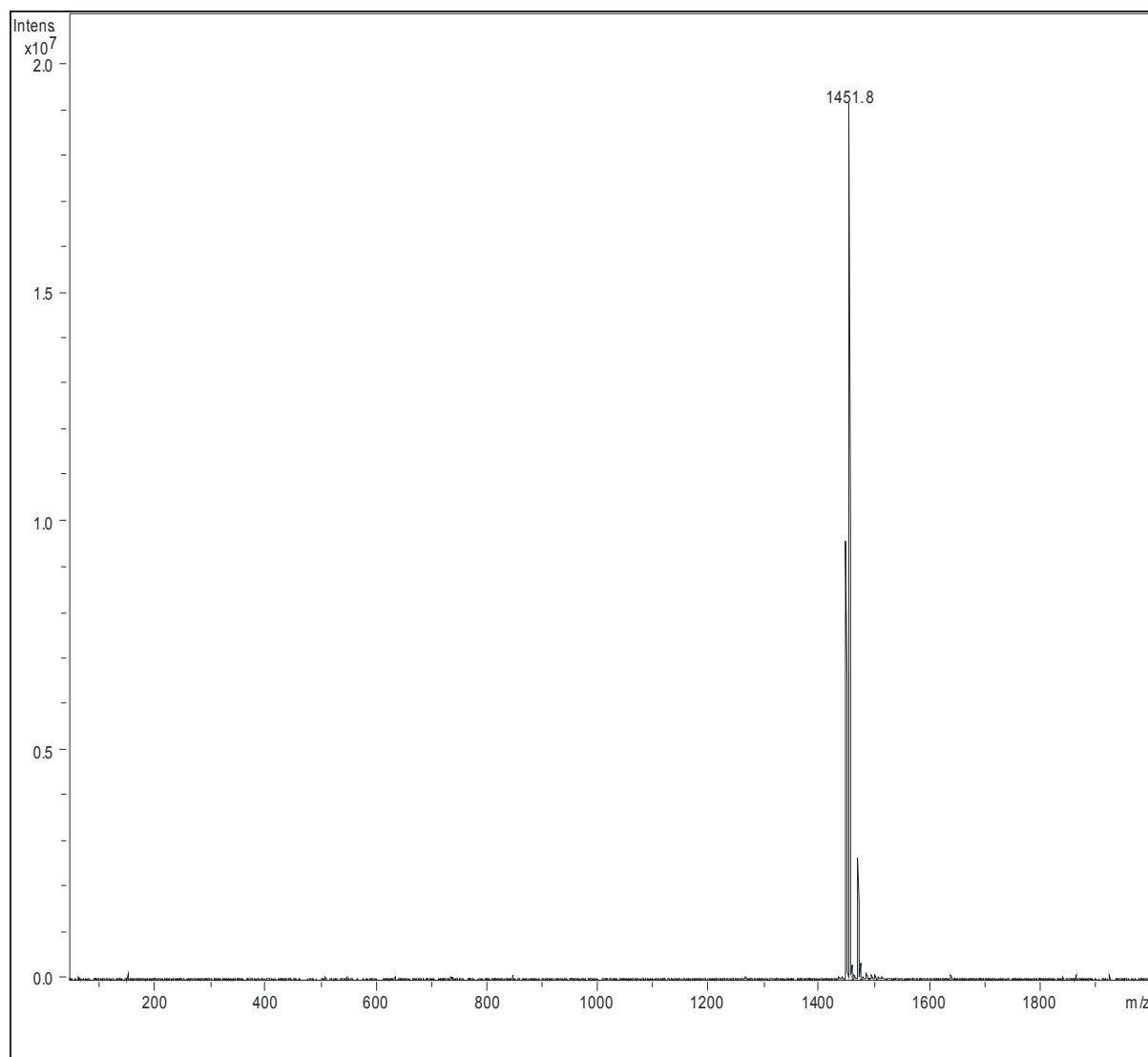


Figure S3.  
ESI-MS of triMe $\beta$ CD. Fragment  $M/z = 1451.8$  corresponds to  $(\text{triMe}\beta\text{CD} + \text{Na})^+$ .

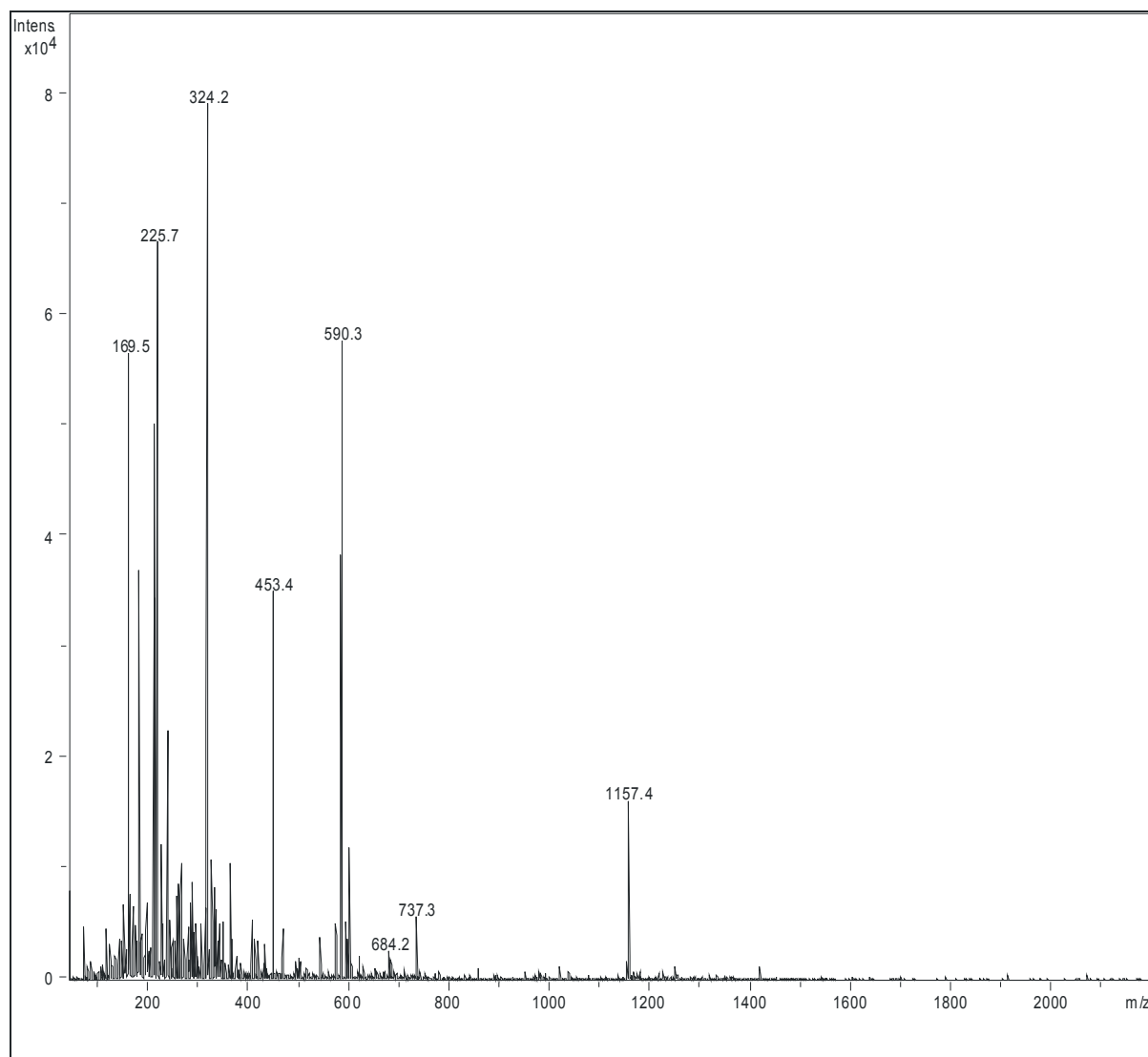


Figure S4.  
ESI-MS of supramolecular complex TMPyP- $\beta$ CD. Fragments correspond to  $M/z = 169.5$  (TMPyP)<sup>4+</sup>,  $324.2$  (TMPyP - 2CH<sub>3</sub>)<sup>2+</sup> and  $453.4$  (TMPyP +  $\beta$ CD)<sup>4+</sup>.

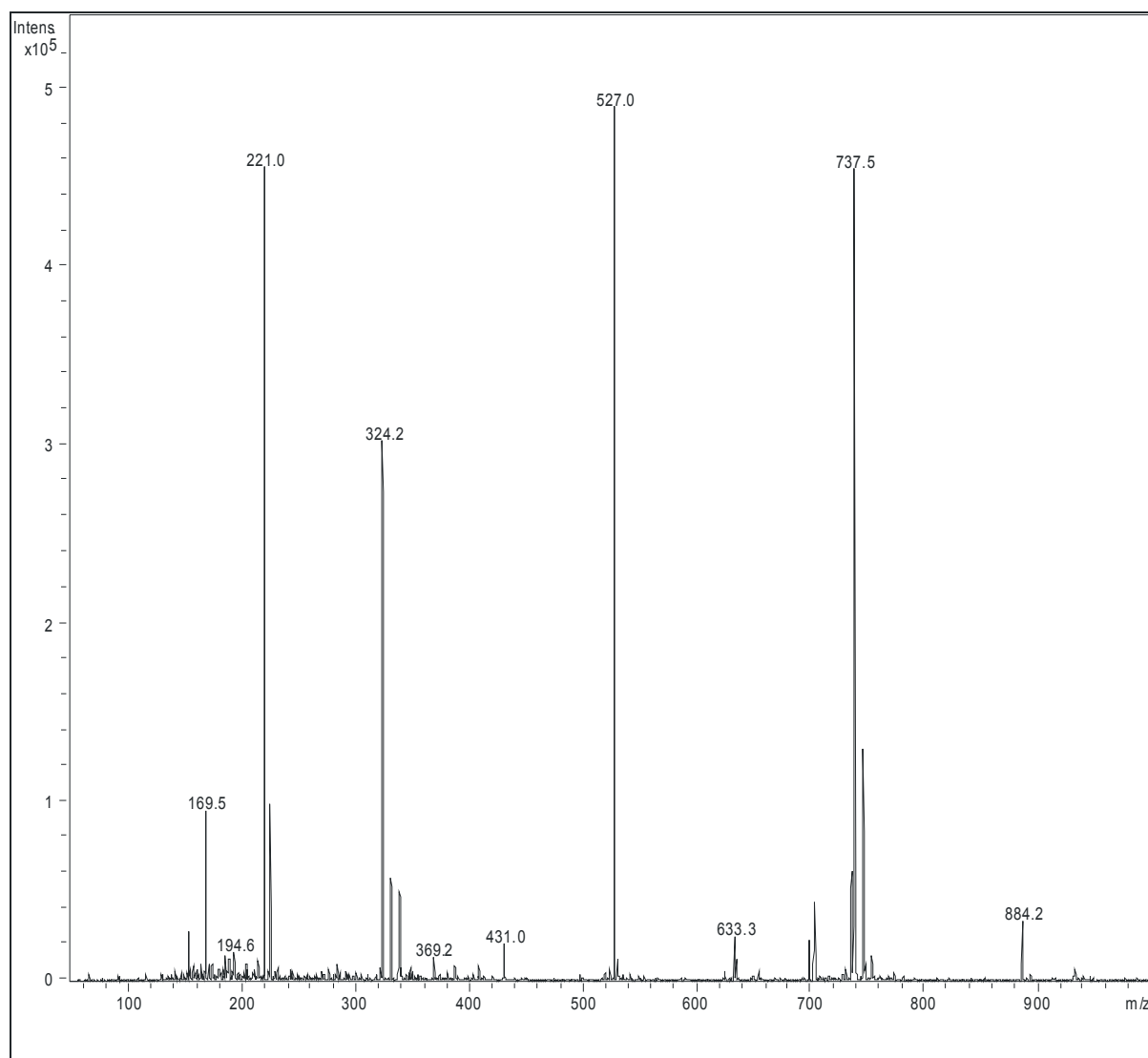


Figure S5.  
ESI-MS of supramolecular complex TMPyP-triMe $\beta$ CD. Fragments correspond to M/z = 169.5 (TMPyP)<sup>4+</sup>, 221.0 (TMPyP – CH<sub>3</sub>)<sup>3+</sup>, 324.2 (TMPyP – 2CH<sub>3</sub>)<sup>2+</sup> and 527.0 (TMPyP + triMe $\beta$ CD)<sup>4+</sup>.

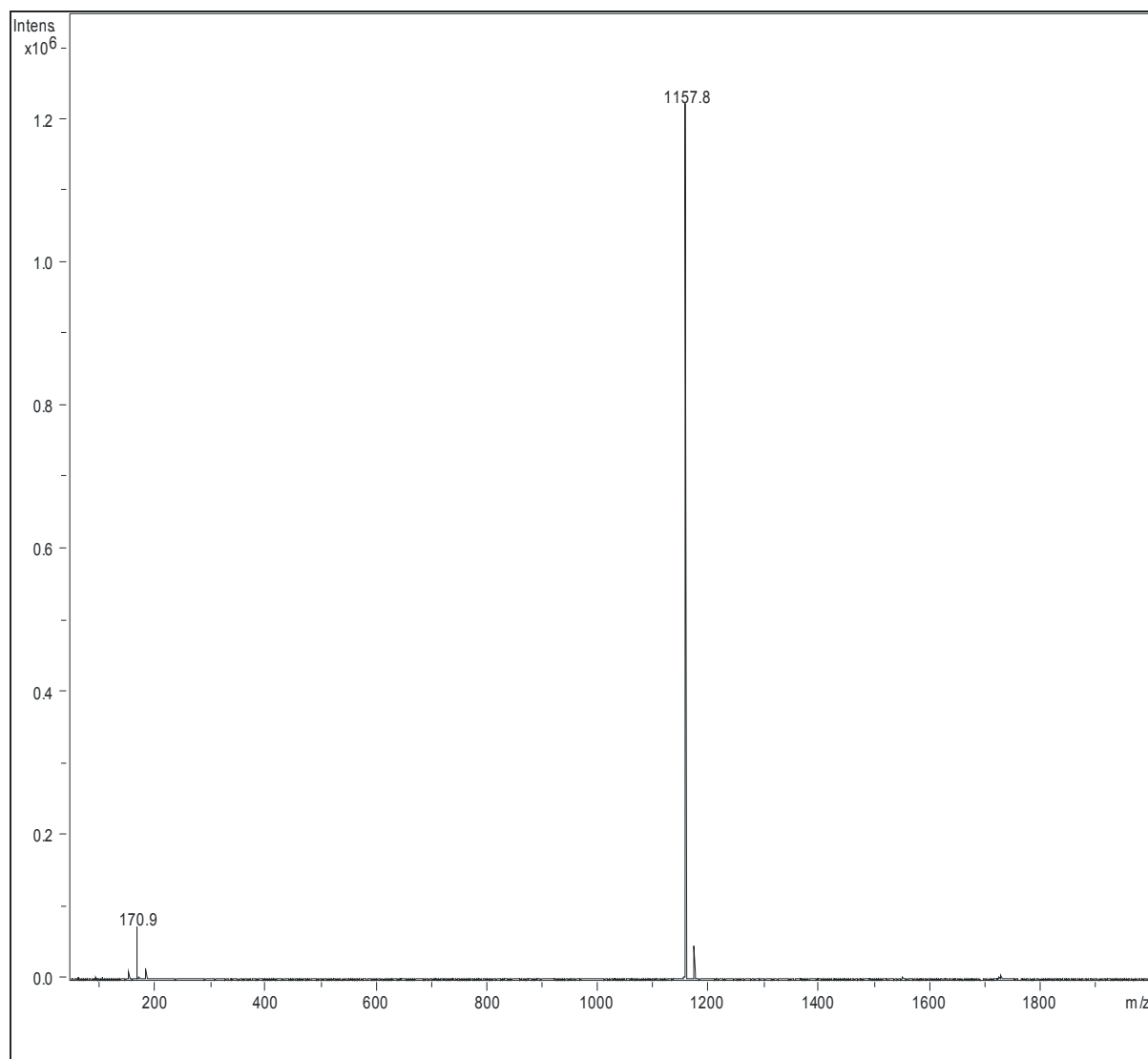


Figure S6.  
ESI-MS of supramolecular complex Tos- $\beta$ CD. Fragments correspond to  $M/z = 170.9$  (Tos),  
 $1157.8$  ( $\beta$ CD + Na)<sup>+</sup>.

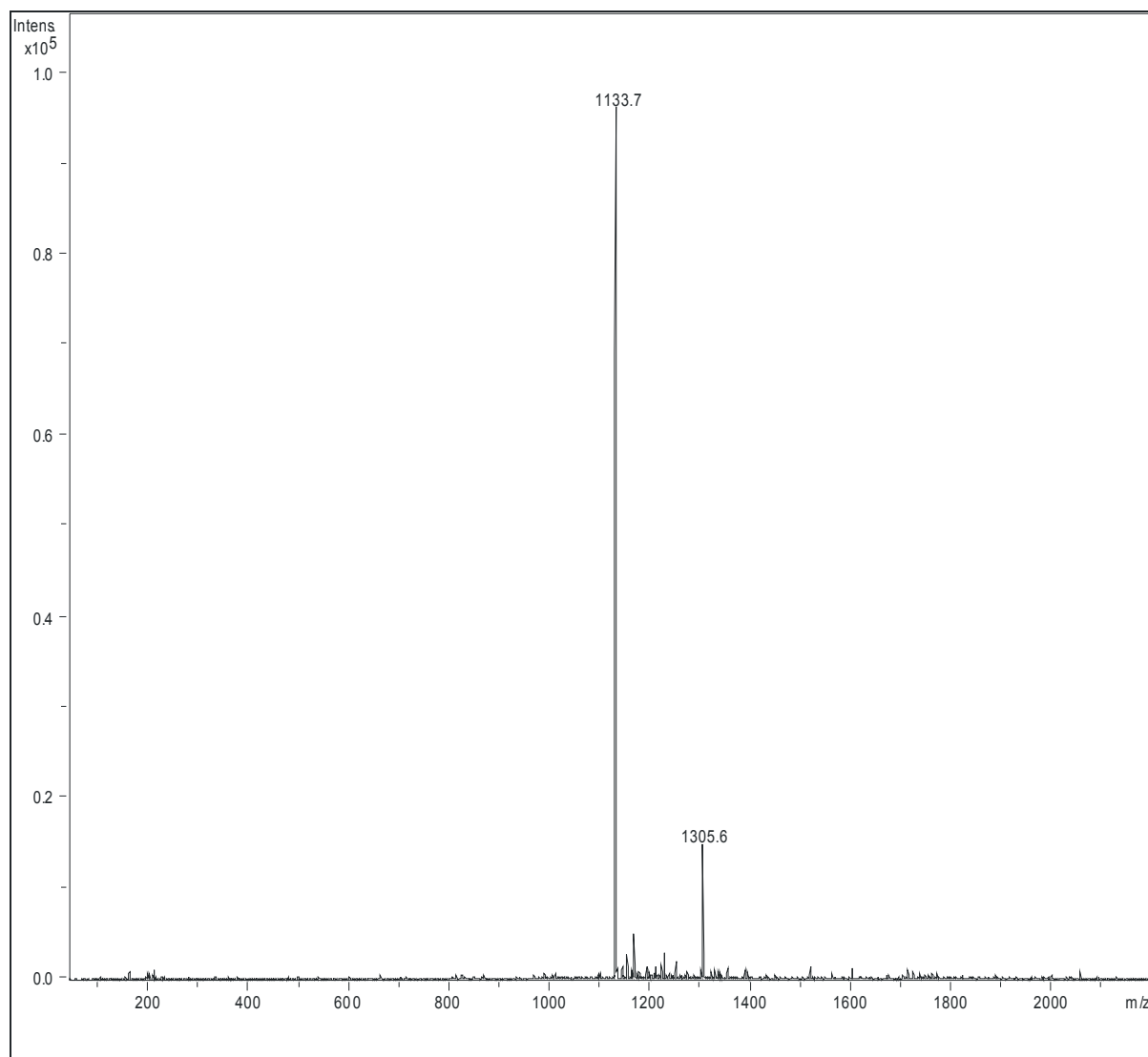


Figure S7.  
ESI-MS of supramolecular complex Tos- $\beta$ CD. Fragment corresponds to  $M/z = 1305.6$  (Tos +  $\beta$ CD)<sup>-</sup>.

## <sup>1</sup>H NMR spectra

Table S1.

<sup>1</sup>H NMR chemical shifts  $\delta_{\text{H}}$  (ppm) of triMe $\beta$ CD, TMPyP/Tos and corresponding supramolecular complex in D<sub>2</sub>O solution.

H	triMe $\beta$ CD	TMPyP/Tos	
		-	triMe $\beta$ CD
1	5.28	-	5.22
2	3.35	-	3.29
3	3.68	-	3.62
4	3.74	-	3.68
5	3.86	-	3.81
6	3.85	-	3.79
6'	3.66	-	3.62
Me-2	3.52	-	3.48
Me-3	3.62	-	3.54
Me-6	3.39	-	3.38
H-a	-	9.10	9.11
H-b	-	8.92	8.94
H-c	-	9.31	9.31
H-d	-	4.82	4.81
H-e	-	7.19	7.23
H-f	-	6.56	6.62
H-g	-	1.61	1.68