Supporting Information

In Trap Fragmentation and Optical Characterization of Rotaxanes

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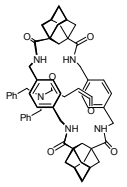
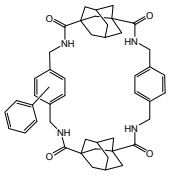
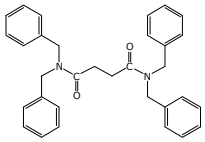
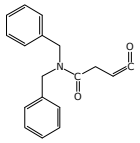
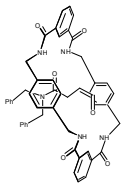
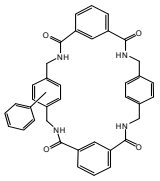
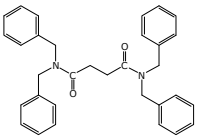
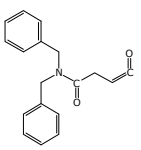
[molecule-H]$^+$	fragment	Chemical structure
Rotaxane 1 m/z= 1125.2	928.5	
	739.5	
	477.2	
	280.3	
Rotaxane 2 m/z= 1009.5	812.1	
	623.4	
	477.2	
	280.3	

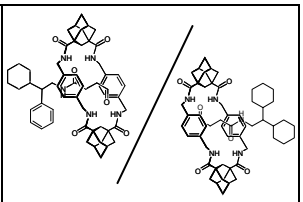
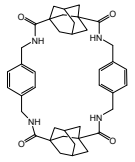
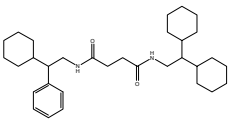
Rotaxane 3 m/z= 1143.8	940.6 / 934.9	
	649.4	
	495.4 (LID only)	

Figure S1: chemical structures of the fragmentation products of rotaxane **1**, rotaxane **2** and rotaxane **3**.

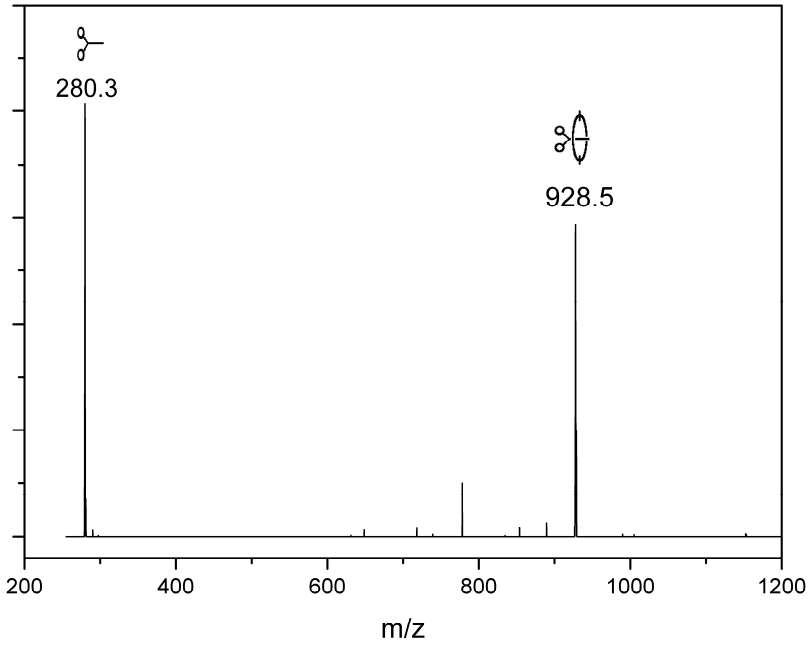


Figure S2: CID spectrum of the 928.5 fragment of rotaxane **1**

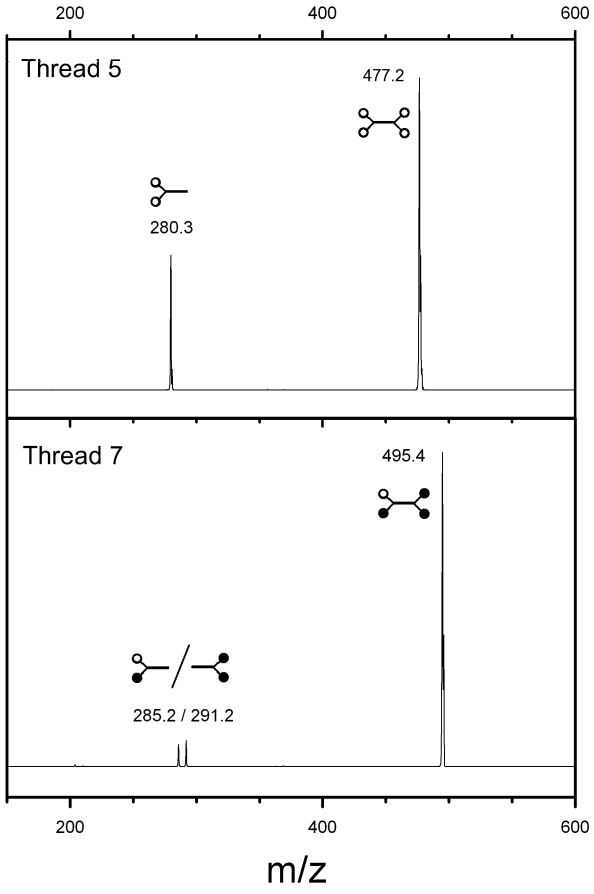


Figure S3: CID spectra of thread **5** and thread **7**.

Rotaxane **1**	Absorption maximum (nm)
Thread **5**	*≤ 220 nm*
Macrocycle **4**	*≤ 220 nm*
Rotaxane **1**	*≤ 220 nm*
Rotaxane **2**	
Thread **5**	*≤ 220 nm*
Macrocycle **6**	*228 nm*
Rotaxane **1**	*230 nm*
Rotaxane **3**	
Thread **5**	*≤ 220 nm*
Macrocycle **4**	*≤ 220 nm*
Rotaxane **3**	*≤ 220 nm*

Table S1: Absorption maxima for all three rotaxanes and their building blocks