

High-yield preparation of [2]rotaxanes based on the bis(*m*-phenylene)-32-crown-10-based cryptand/paraquat derivative recognition motif

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Electronic Supplementary Information (5 pages)

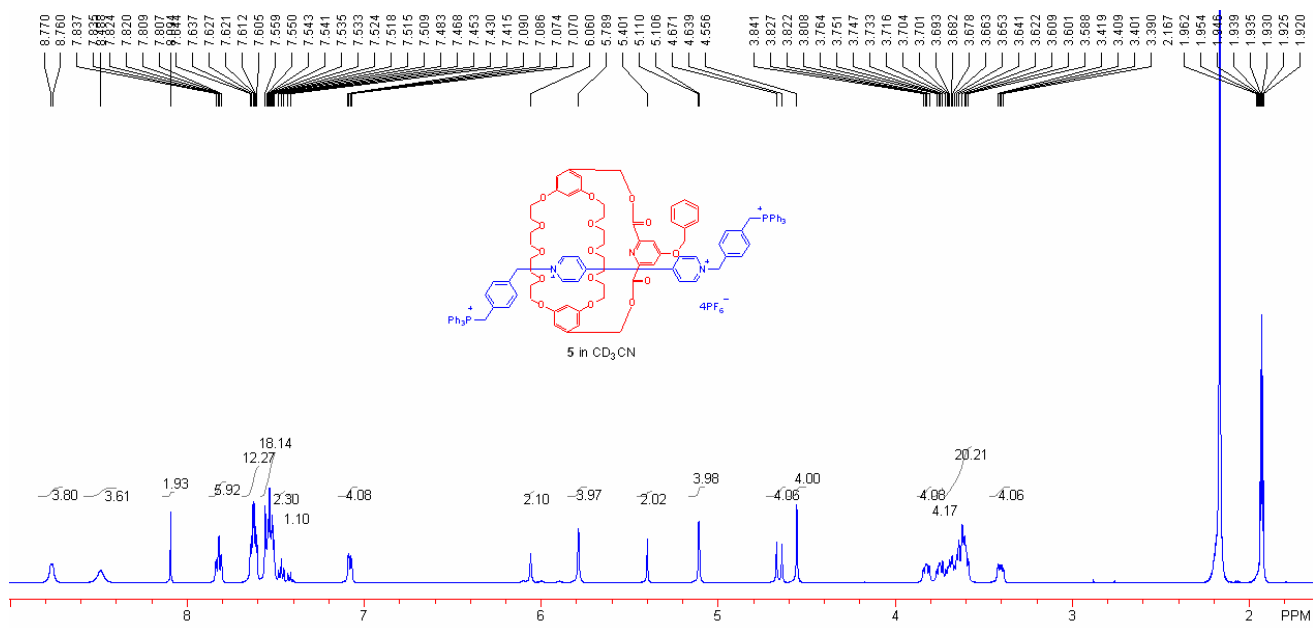


Fig. S1. ^1H NMR of **5** (500 MHz, CD_3CN , 22 °C).

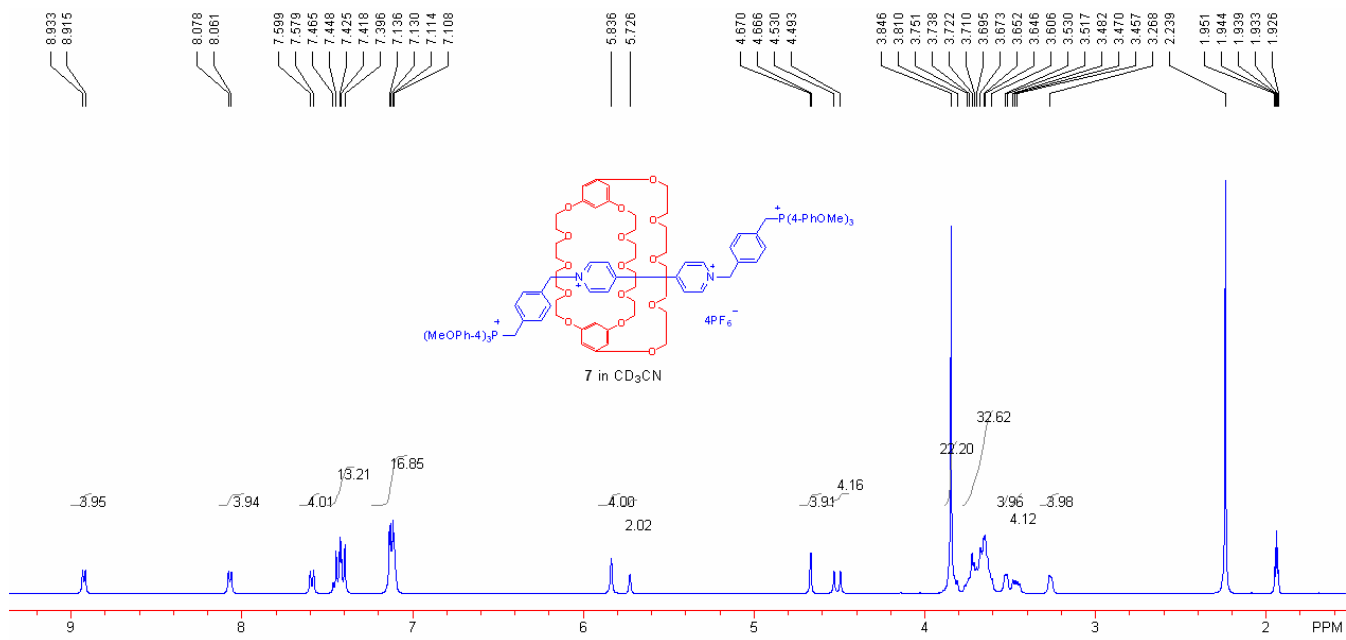


Fig. S2. ^1H NMR of **7** (400 MHz, CD_3CN , 22 °C).

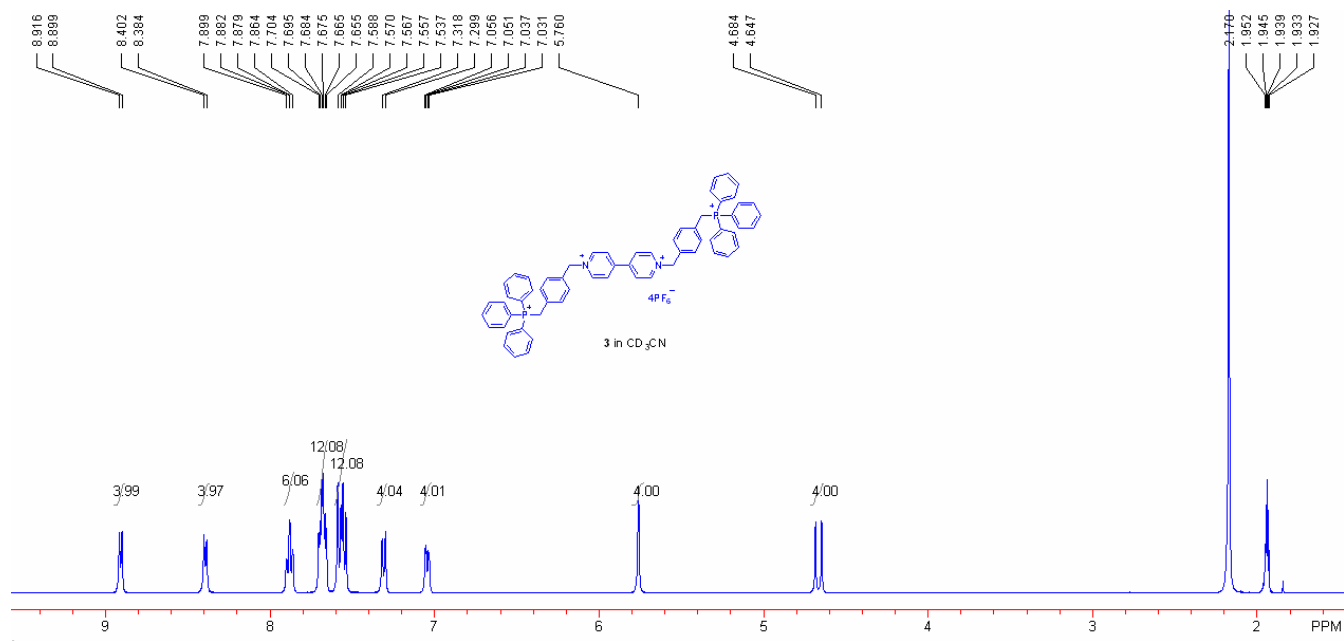


Fig. S3. ^1H NMR of **3** (400 MHz, CD_3CN , 22 °C).

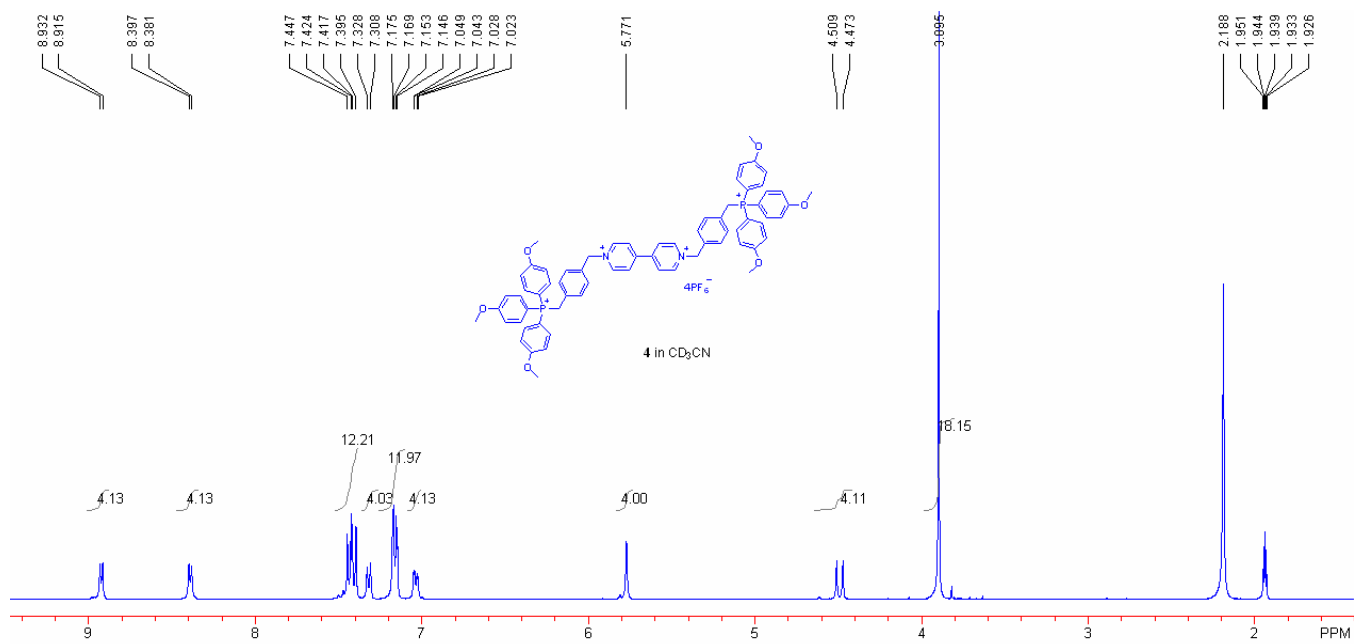


Fig. S4. ^1H NMR of **4** (400 MHz, CD_3CN , 22 °C).

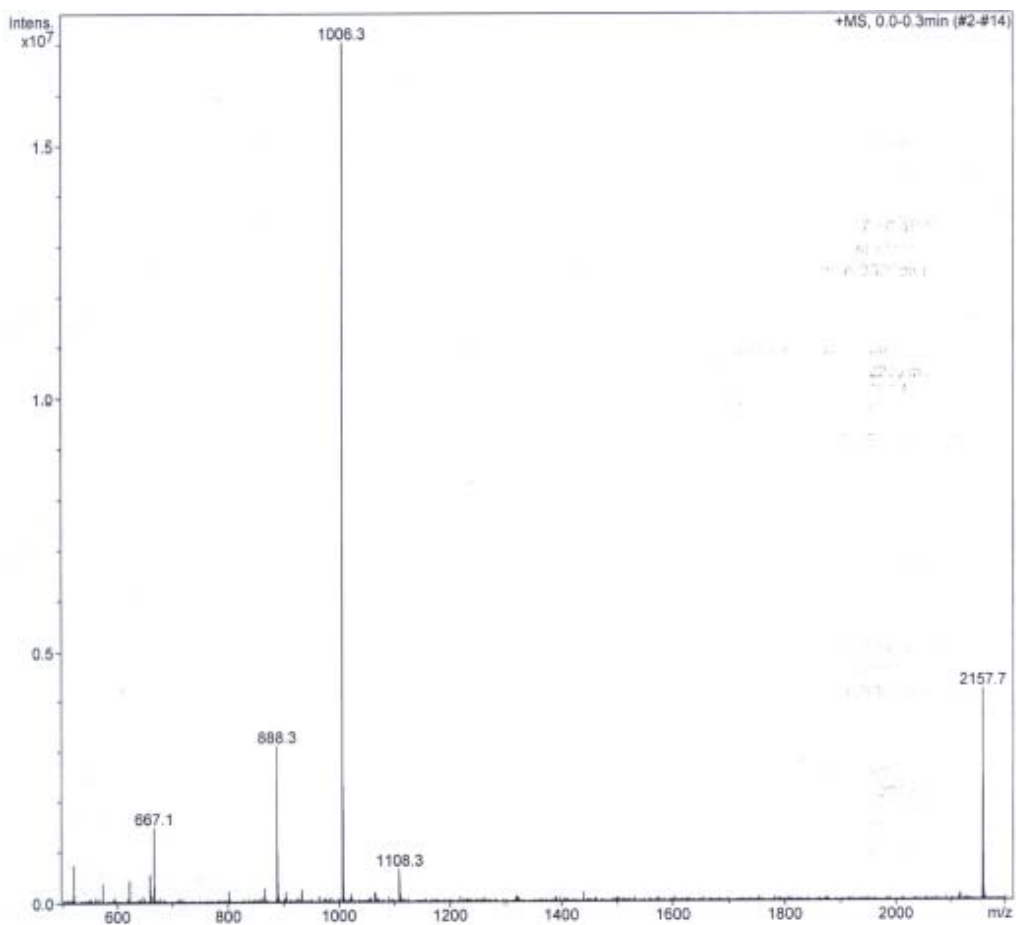


Fig. S5. Electrospray ionization mass spectrum (ESI) of [2]rotaxane **5** in acetonitrile/methanol. Assignment of main peaks: m/z 2157.7 (30%) $[\mathbf{5} - \text{PF}_6 + \text{H}]^+$, 1006.3 (100%) $[\mathbf{5} - 2\text{PF}_6]^{2+}$.

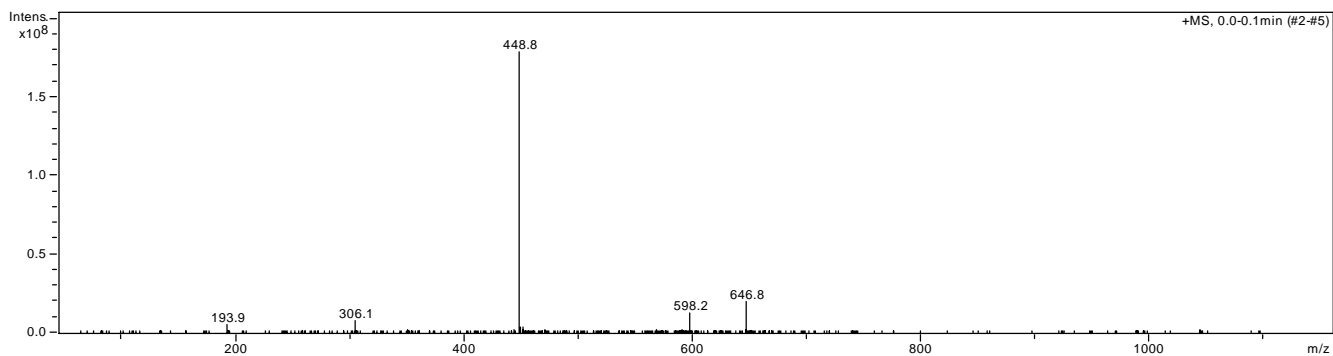


Fig. S6. Electrospray ionization mass spectrum (ESI) of [2]rotaxane **7** in acetonitrile/methanol. Assignment of main peaks: $m/z = 646.8$ (11%) $[\mathbf{7} - 3\text{PF}_6]^{3+}$, 598.2 (7%) $[\mathbf{7} - 3\text{PF}_6 - \text{HPF}_6]^{3+}$, 448.8 (100%) $[\mathbf{7} - 4\text{PF}_6]^{4+}$.

Isj103

LSJ-103 107 (1.987) Sb (1,40.00); Sm (SG, 2x3.00); Cm (90:115)

1: TOF MS ES+
4.45e4

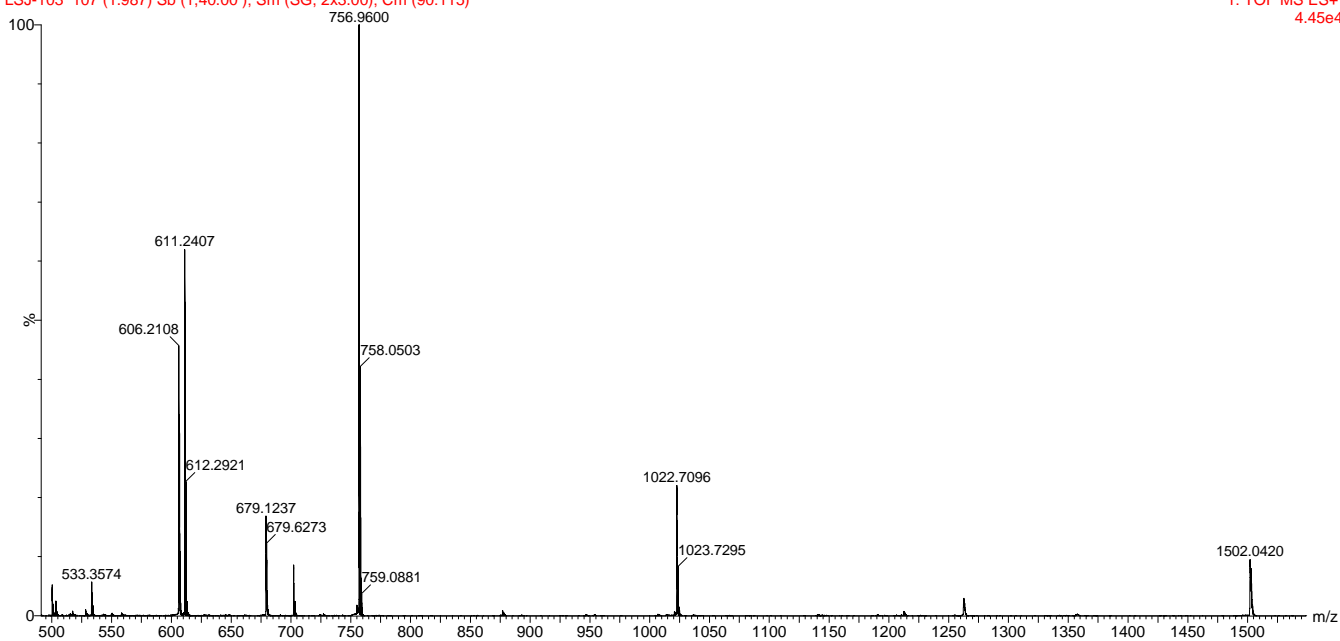


Fig. S7. Electrospray ionization mass spectrum (ESI) of dumbbell-shaped compound **4** in acetonitrile/methanol. Assignment of main peaks: m/z 1502.0 (25%) [**4** - HPF₆]⁺, 1022.7 (43%) [**4** - 2PF₆ - 2HPF₆ - 2OCH₃ + H₂O]⁺, 757.0 (100%) [**4** - 3PF₆ - (4-MeOPh)₃PCH₂PhCH₂]⁺, 679.1 (28%) [**4** - 2PF₆]²⁺, 611.2 (76%) [**4** - 3PF₆ - HPF₆ - (4-MeOPh)₃PCH₂PhCH₂]⁺, 606.2 (62%) [**4** - HPF₆ - 2PF₆]²⁺, 533.4 (9%) [**4** - 2HPF₆ - 2PF₆]²⁺.