Electronic Supplementary Material (ESI) for Organic and Biomolecular Chemistry

Supplementary Information

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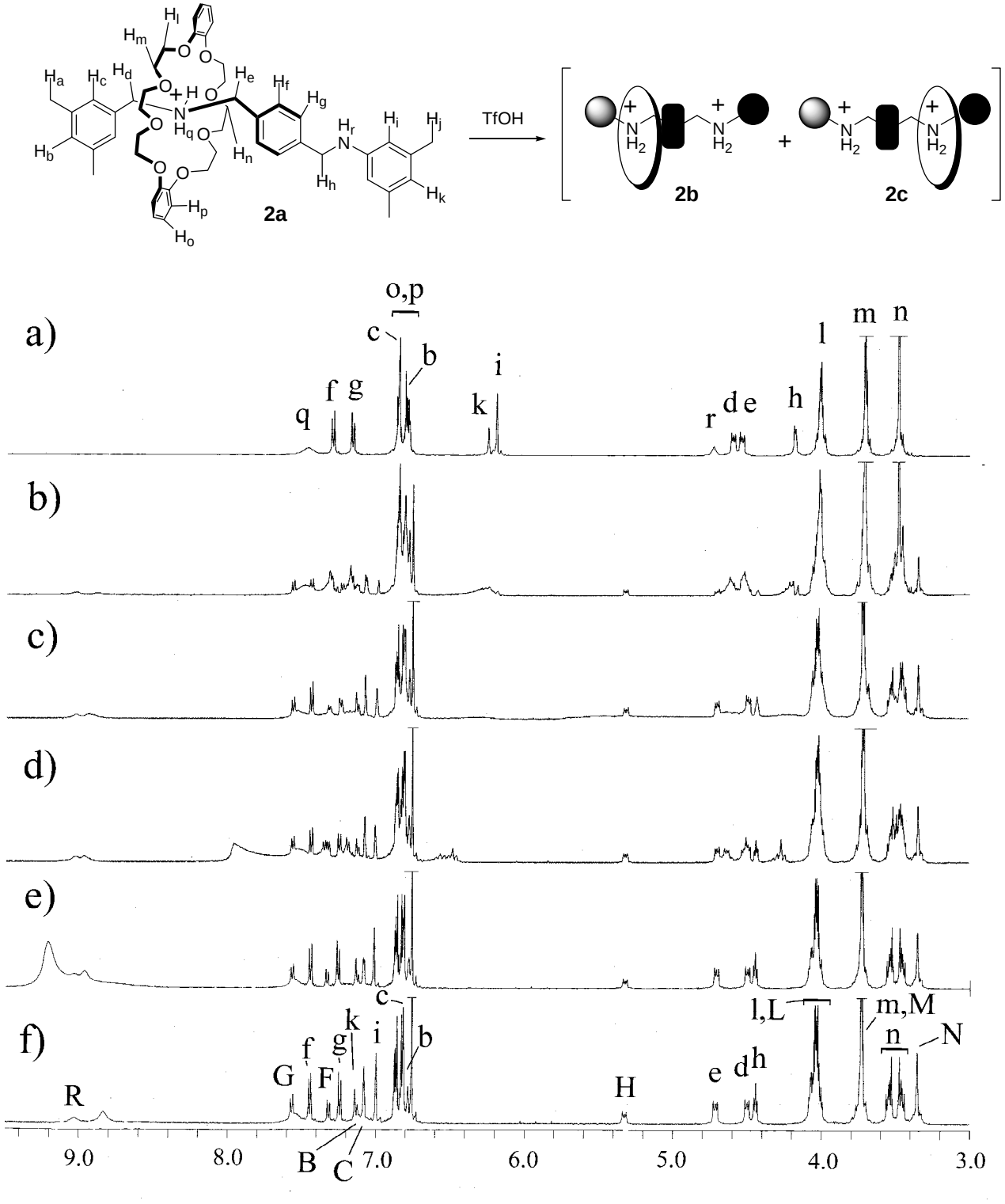
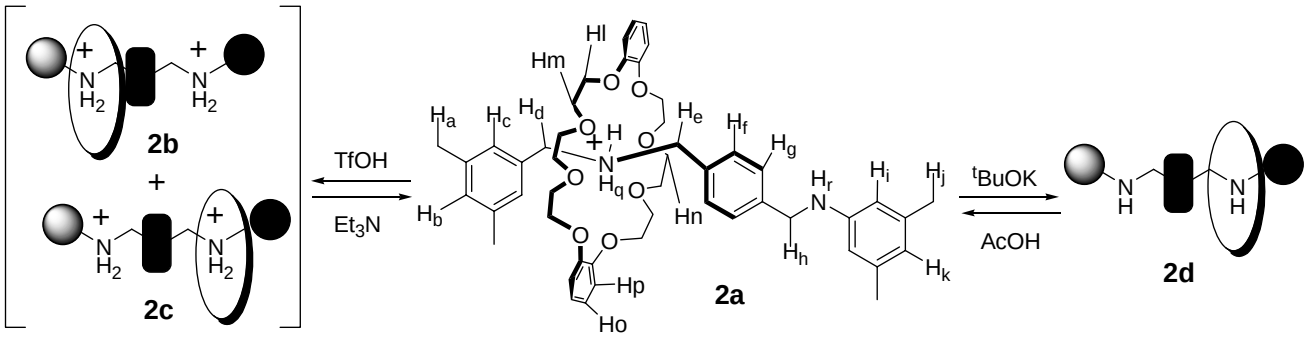


Figure S1 ^{1}H NMR spectra (500 MHz, CD_3CN) of the [2]rotaxanes **2a**–**c**. a) **2a** (X = HCO_3^-); b) **2a** + TfOH (0.31 eq); c) **2a** + TfOH (0.63 eq); d) **2a** + TfOH (1.25 eq); e) **2a** + TfOH (2.5 eq); f) **2a** + TfOH (5.0 eq). Capital letters represent the signals for **2a** and **2b**; lower-case letters for **2c**.



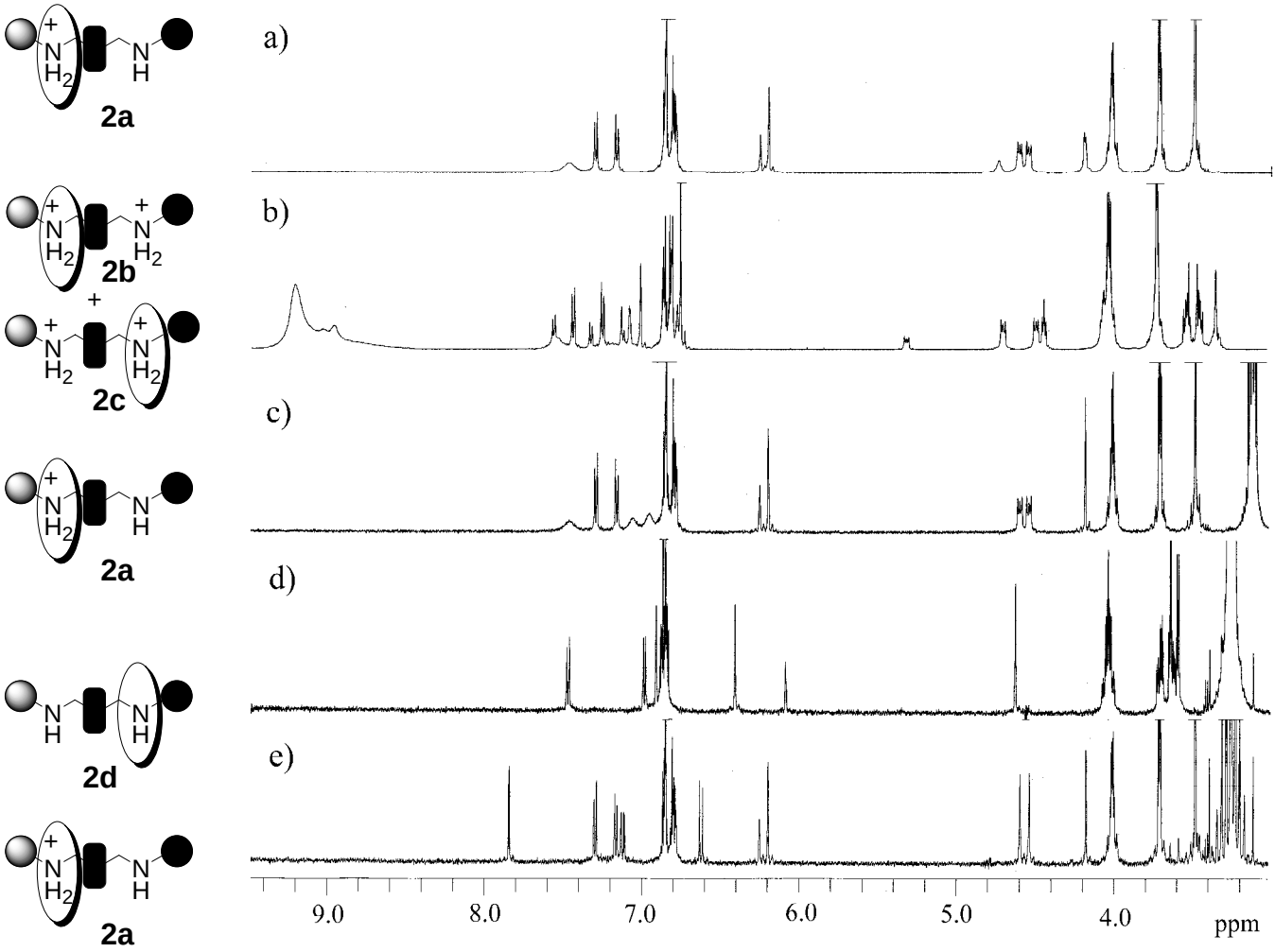


Figure S2 ^{1}H NMR spectra (500 MHz, CD_3CN) of the [2]rotaxane **2** in its three-state cycle. a) **2a** (X = HCO_3^-); b) sample in a) after the addition of TfOH (5 eq); c) sample in b) after the addition of Et_3N (5 eq); d) sample in c) after the addition of ^{t}BuONa (7 eq); e) sample in d) after the addition of 4-chloro-2-nitrophenol (5 eq).

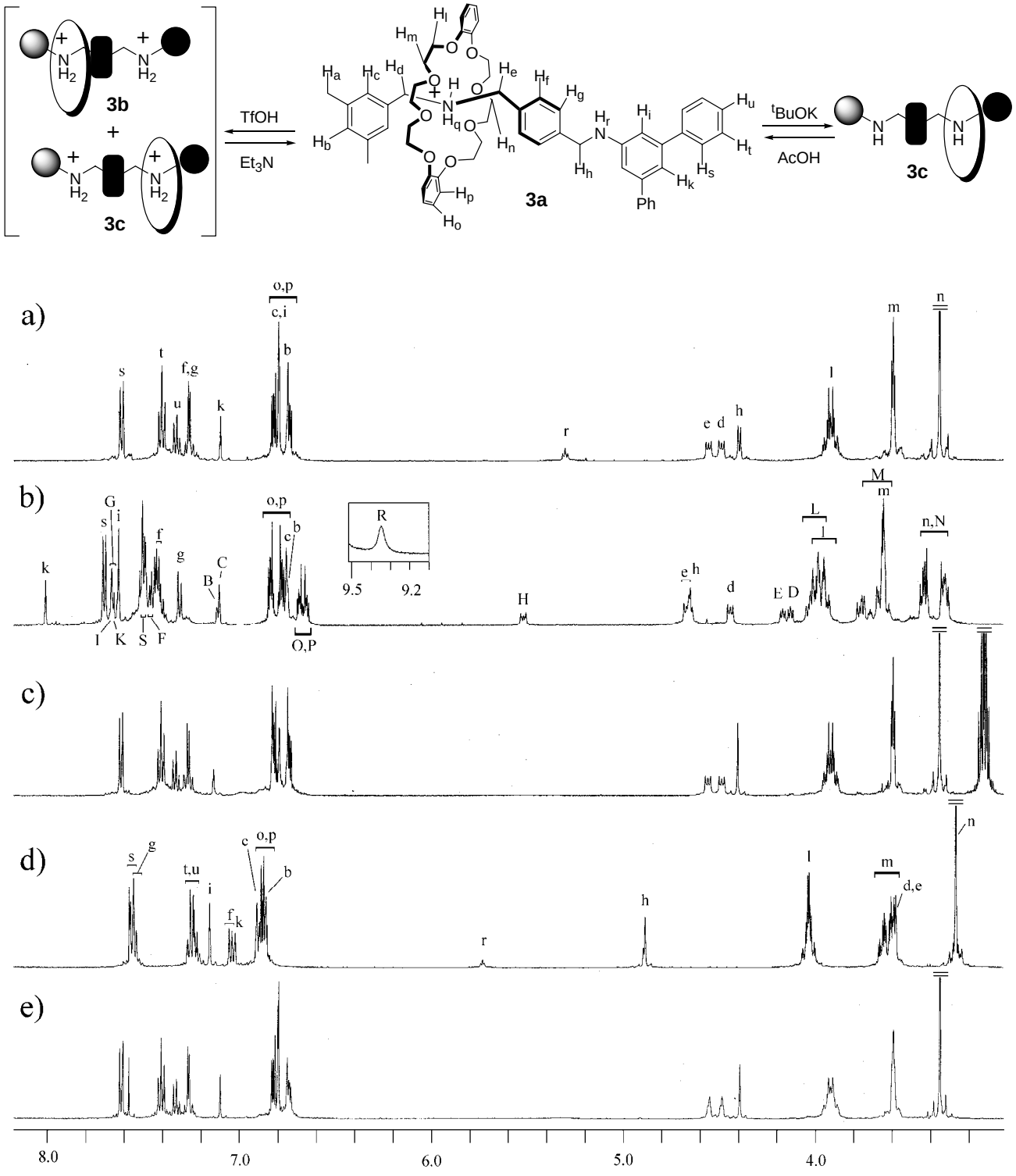


Figure S3. ^{1}H NMR spectra (500 MHz, CD_3CN) of the [2]rotaxane **3** in its three-state cycle. a) **3b** (X = PF_6^-); b) sample in a) after the addition of TfOH (5.0 eq); c) sample in b) after the addition of Et_3N (5.0 eq); d) sample in c) after the addition of ^{t}BuOK (2.0 eq); e) sample in d) after the addition of AcOH (3.0 eq).

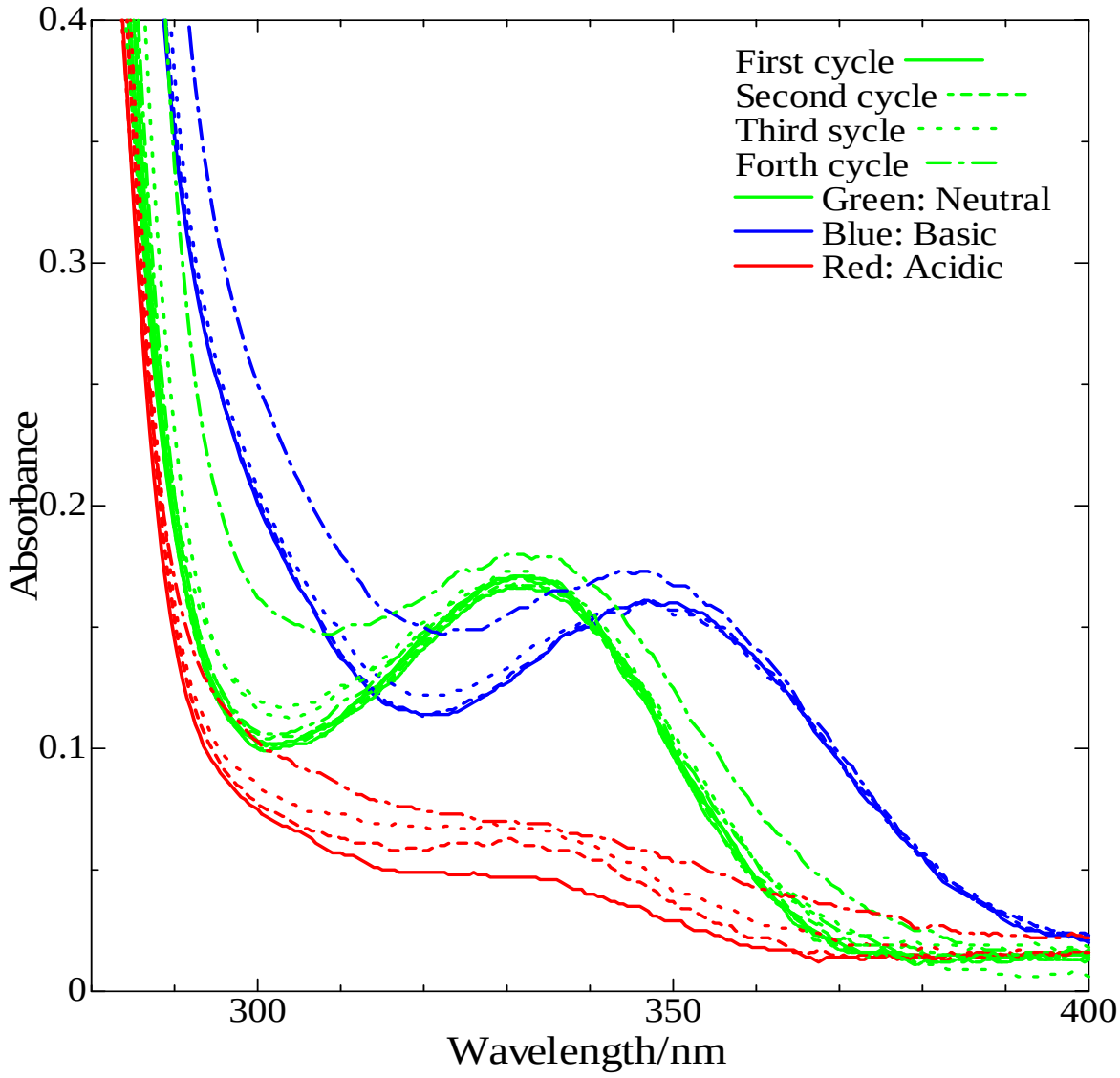
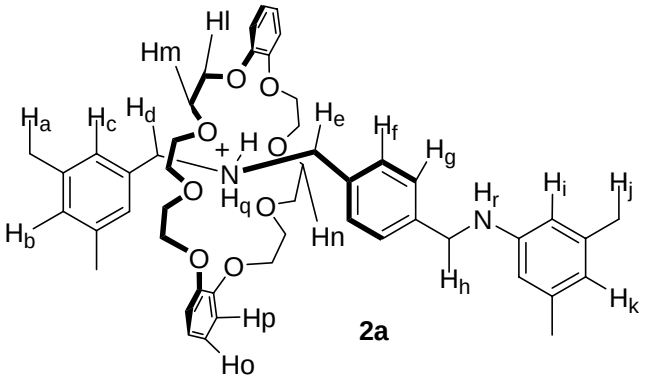


Figure S4. Absorption spectra of the [2]rotaxane **3** (40 μM) in CH_3CN/CH_3OH (9:1) at rt after sequential addition of ^tBuOK (process A), AcOH (process B), TfOH (process C), and Et_3N (process D).



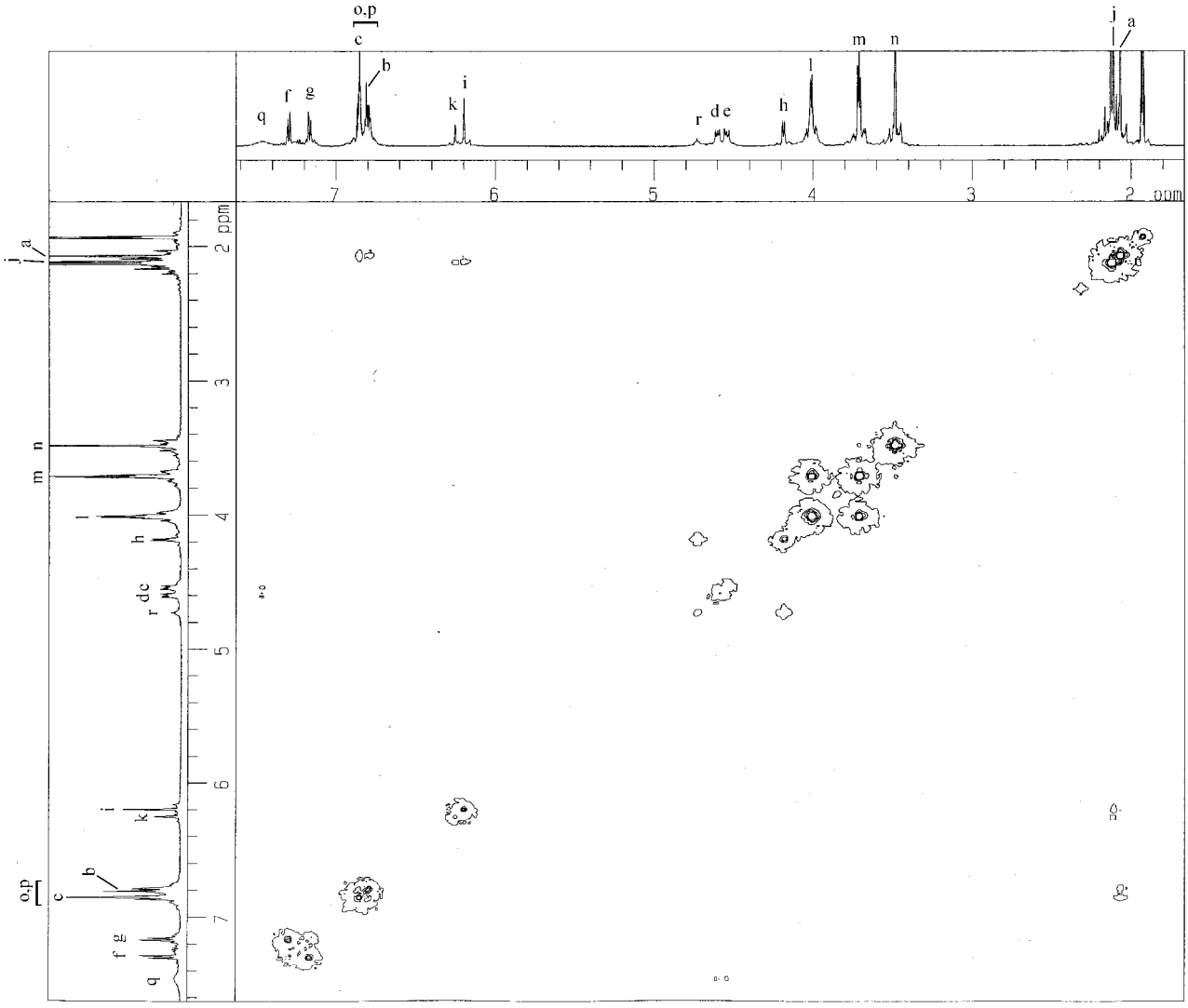


Figure S5. COSY spectrum (500 MHz, CD_3CN) of the [2]rotaxane **2a**.

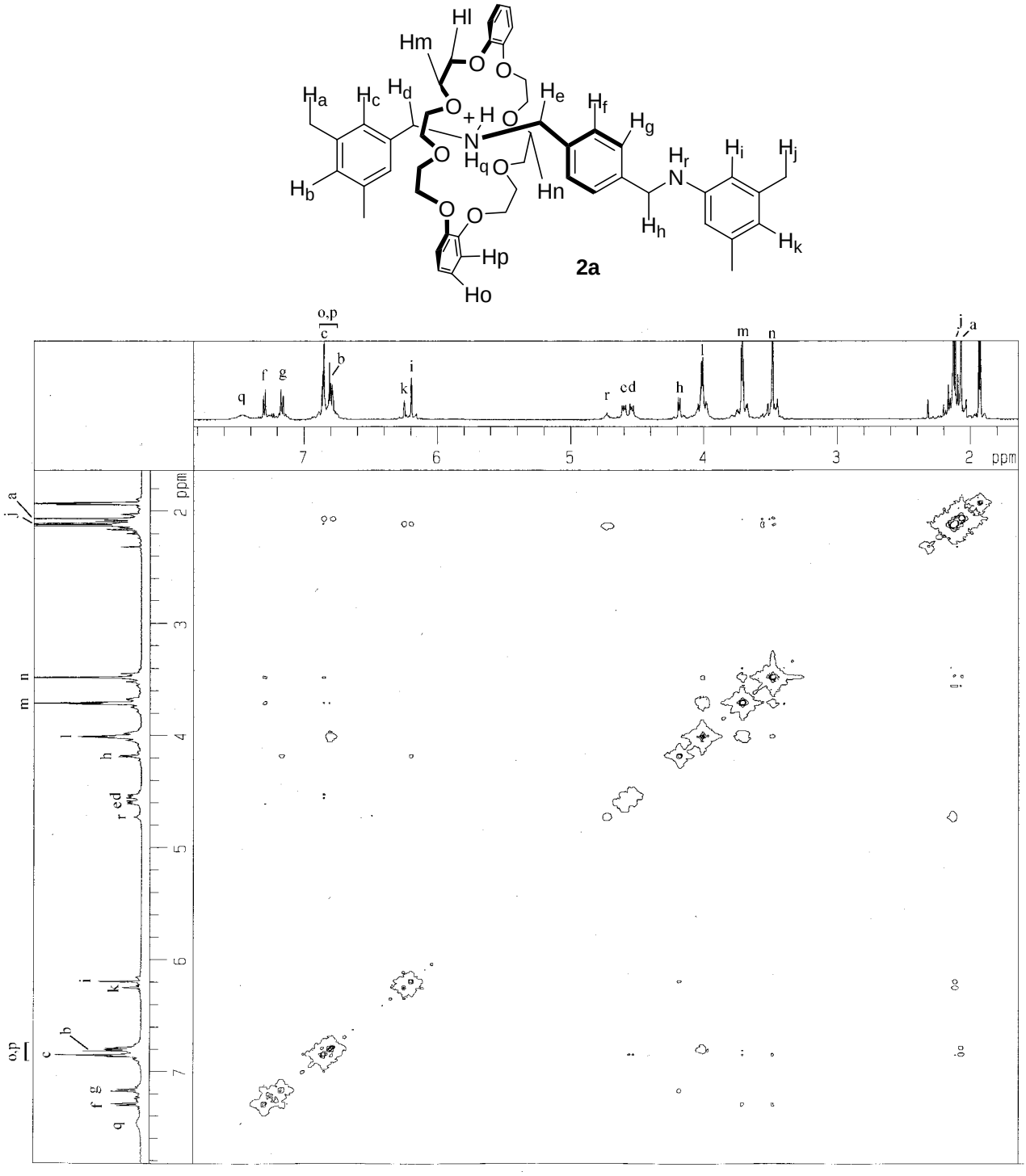


Figure S6. NOESY spectrum (500 MHz, CD_3CN) of the [2]rotaxane **2a**.

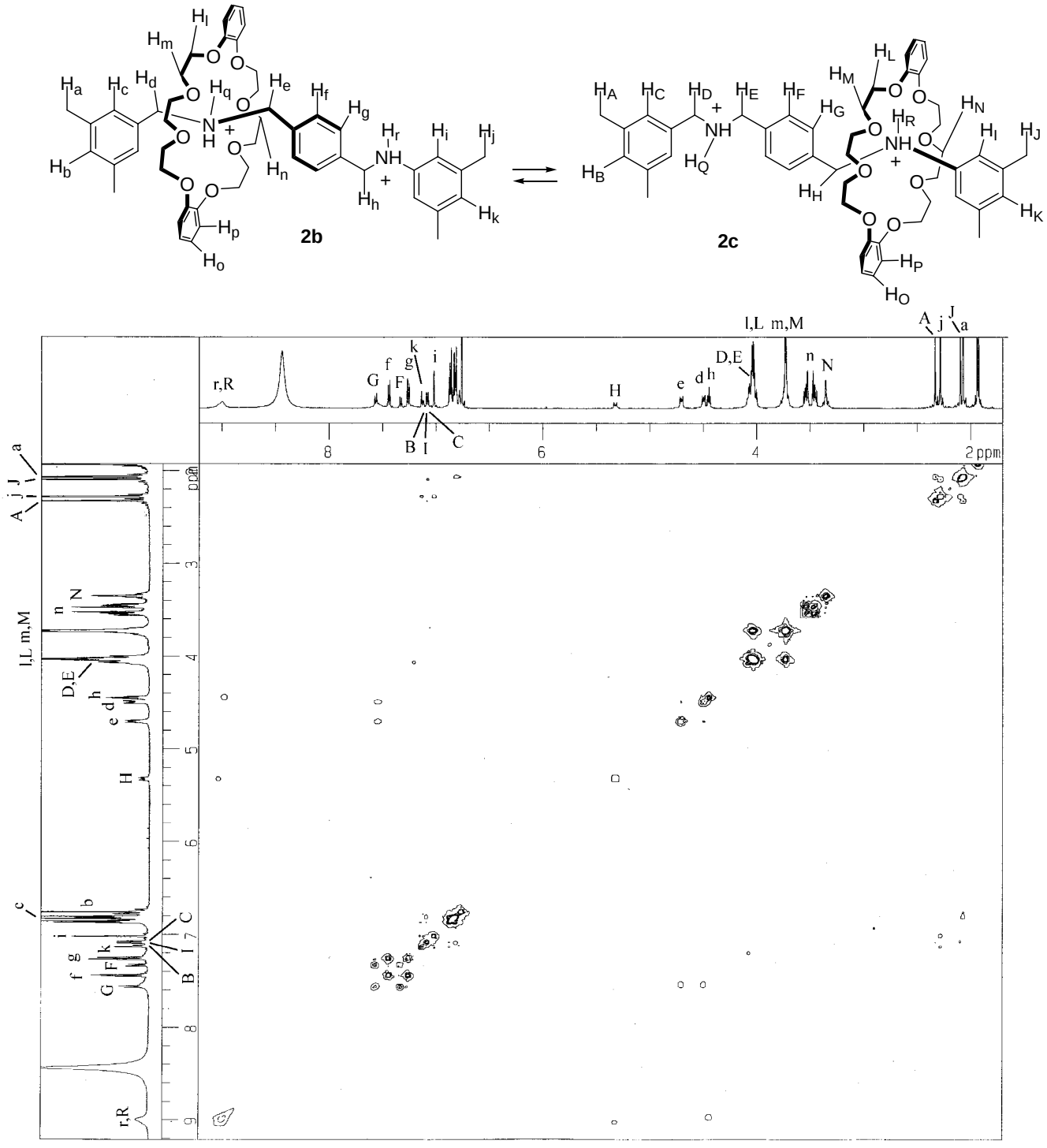
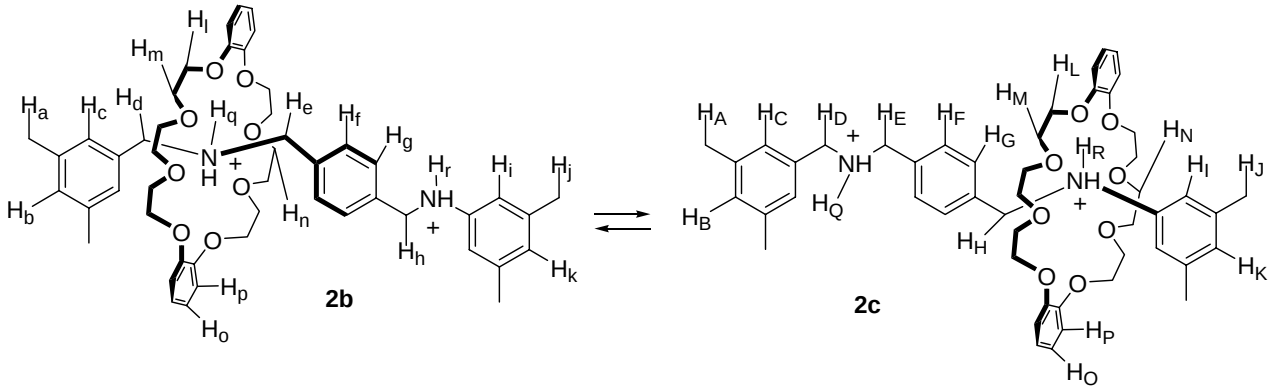


Figure S7. COSY spectrum (500 MHz, CD_3CN) of the [2]rotaxane **2a** in the presence of TfOH (5.0 eq). Lower-case letters: **2b**; capital letters: **2c**.



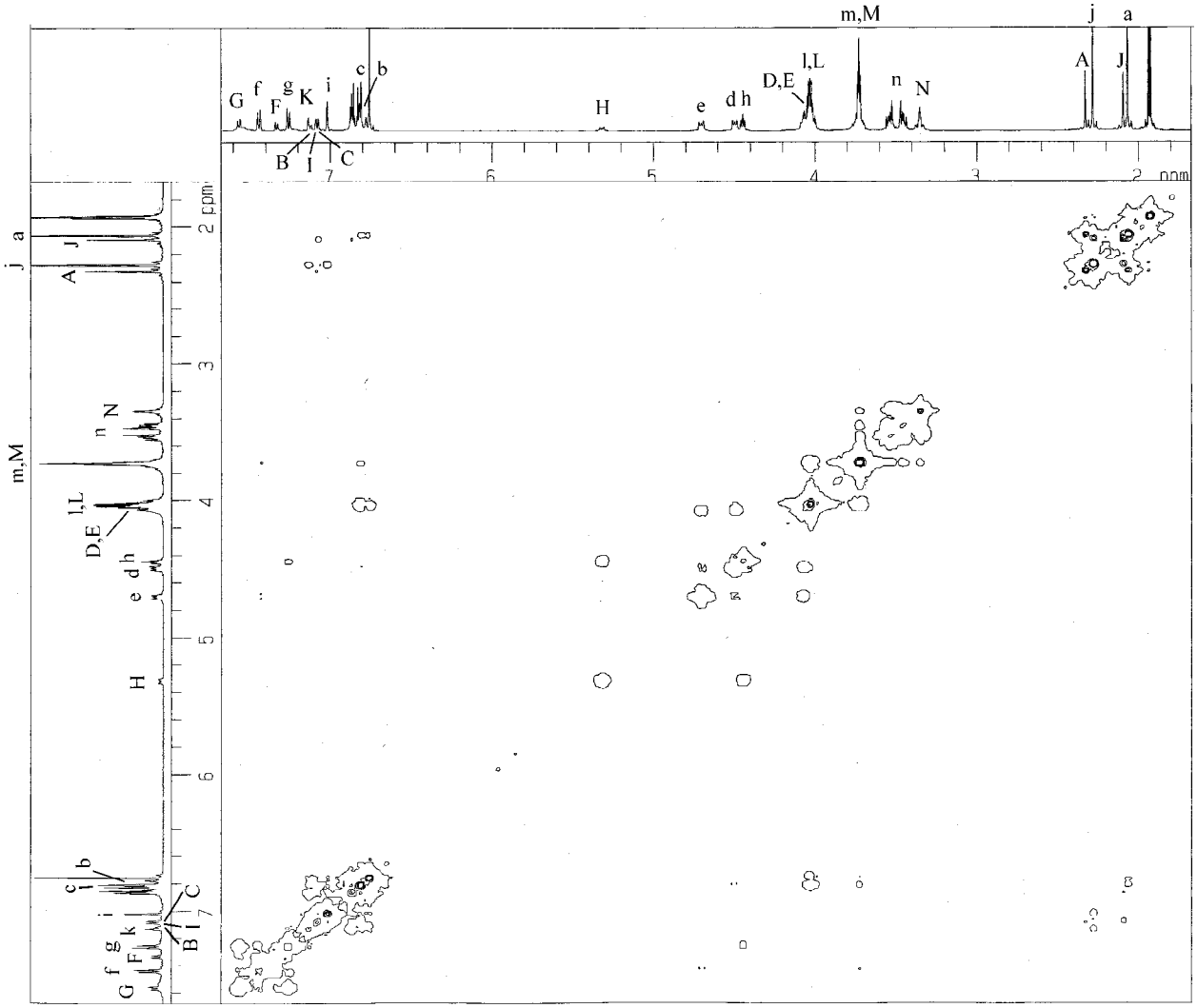
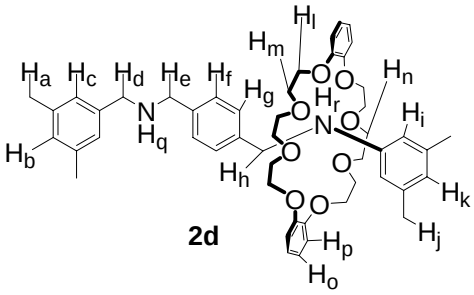


Figure S8. NOESY spectrum (500 MHz, CD_3CN) of the [2]rotaxane **2a** in the presence of TfOH (5.0 eq). Lower-case letters: **2b**; capital letters: **2c**.



2d

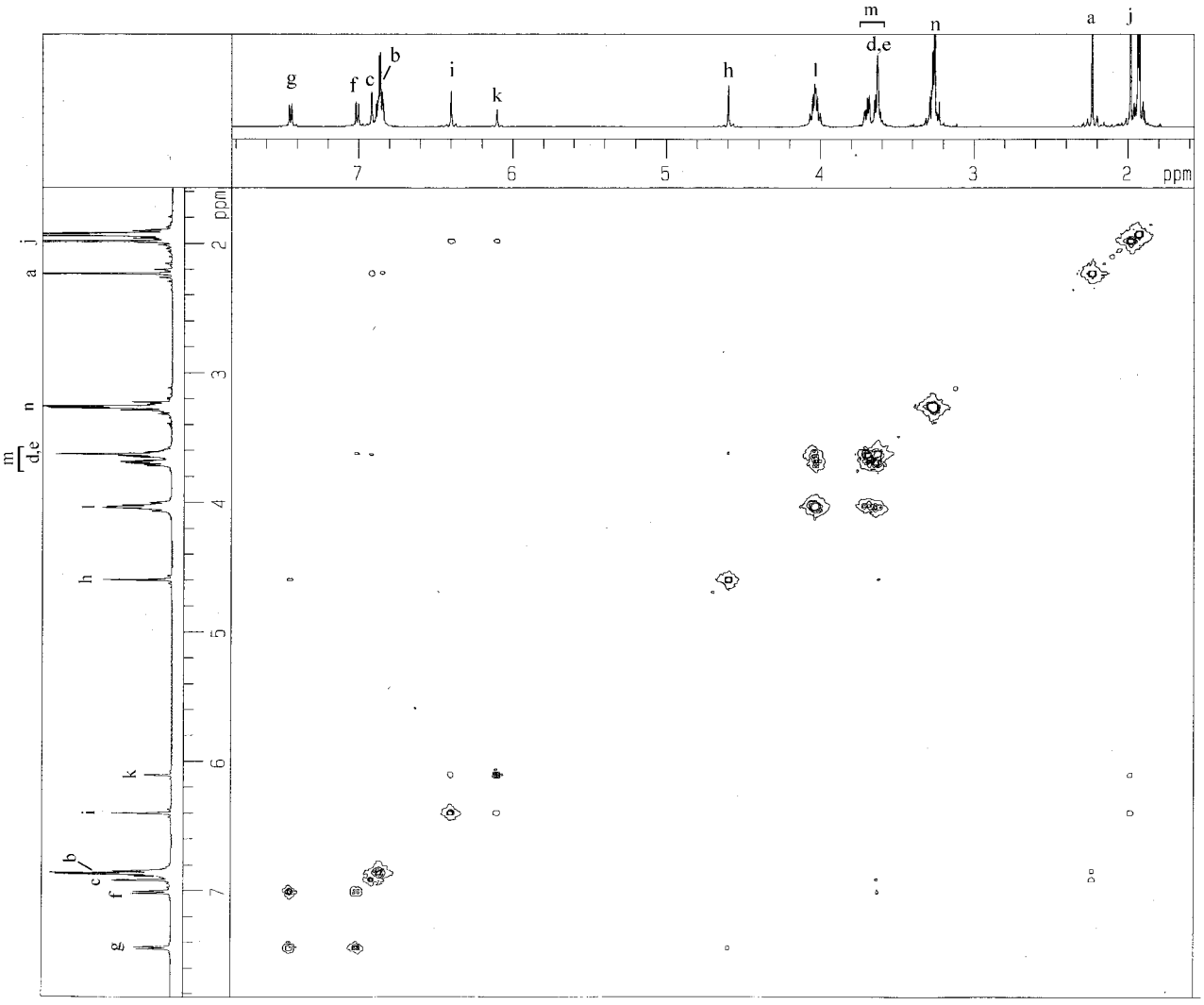
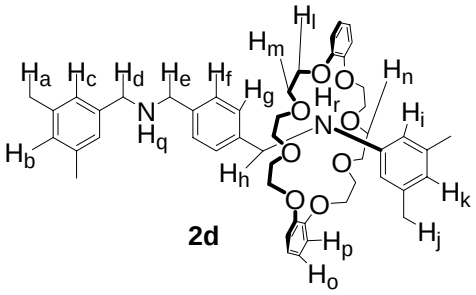


Figure S9. COSY spectrum (500 MHz, CD_3CN) of the [2]rotaxane **2a** in the presence of ^{t}BuONa (1.2 eq).



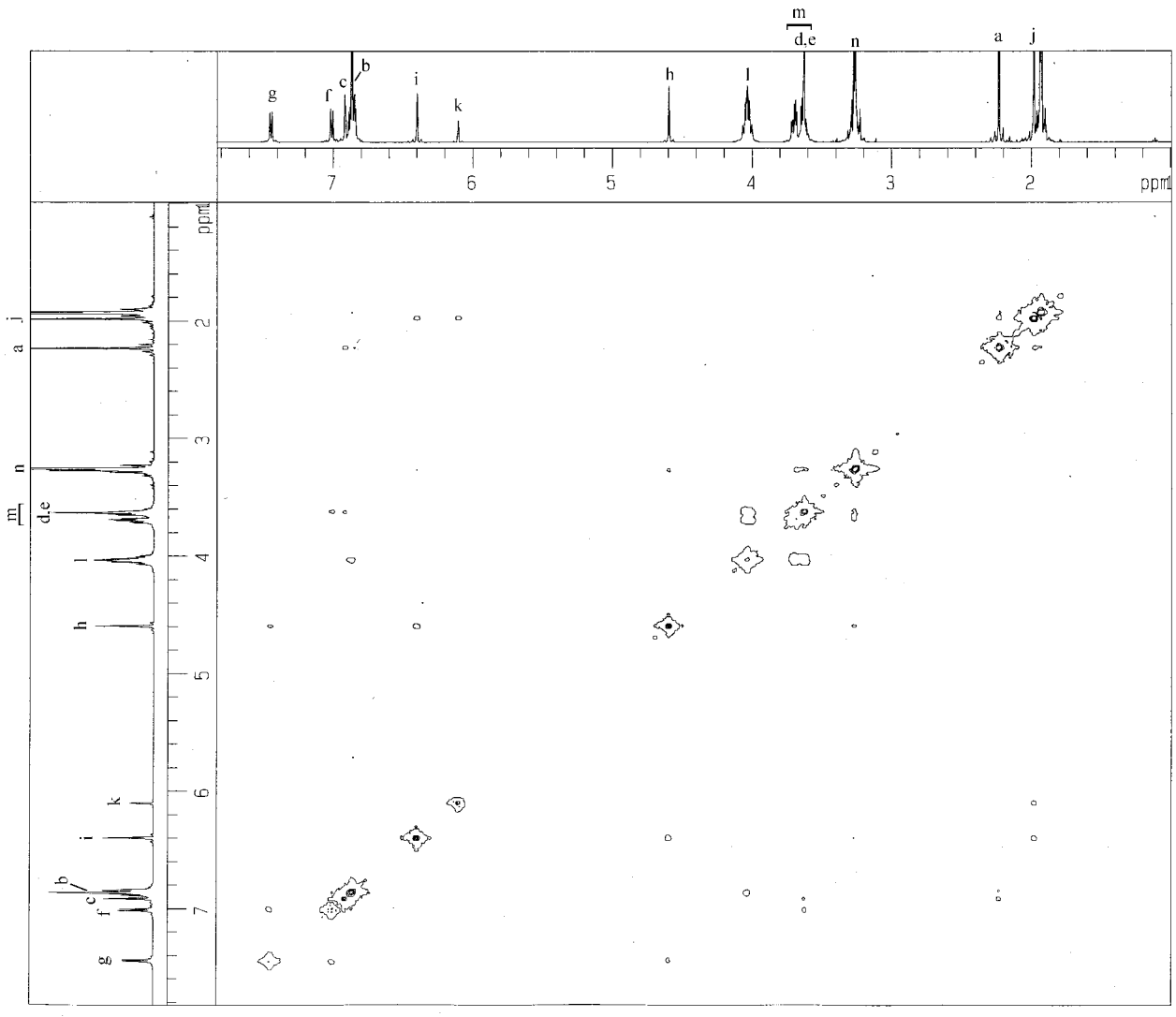


Figure S10. NOESY spectrum (500 MHz, CD_3CN) of the [2]rotaxane **2a** in the presence of ^{t}BuONa (1.2 eq).