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Supporting Information

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Helicate, Macrocycle or Catenate: Topological Control over Subcomponent Self-Assembly

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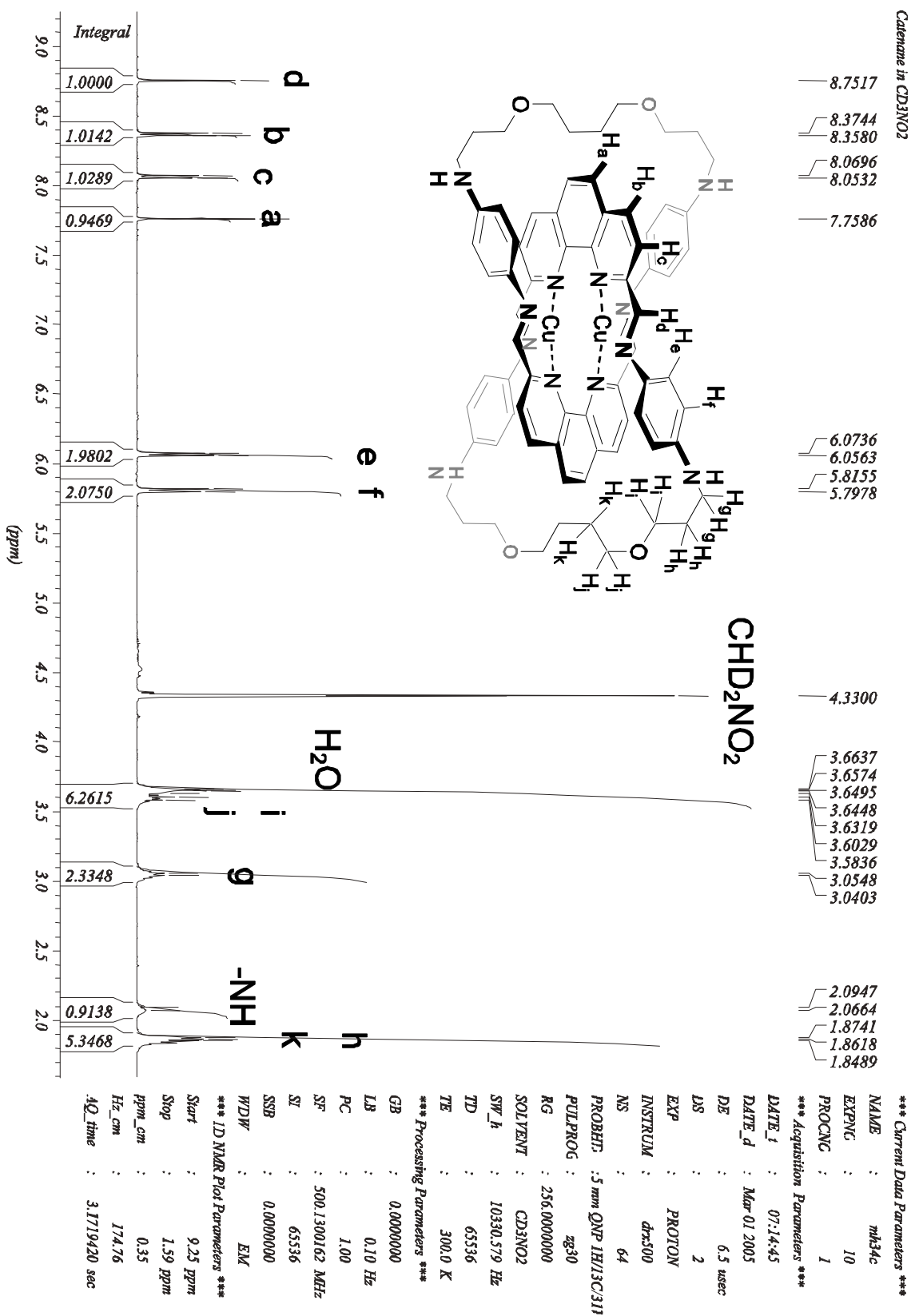


Figure S1. The proton NMR spectrum of catenate 4.

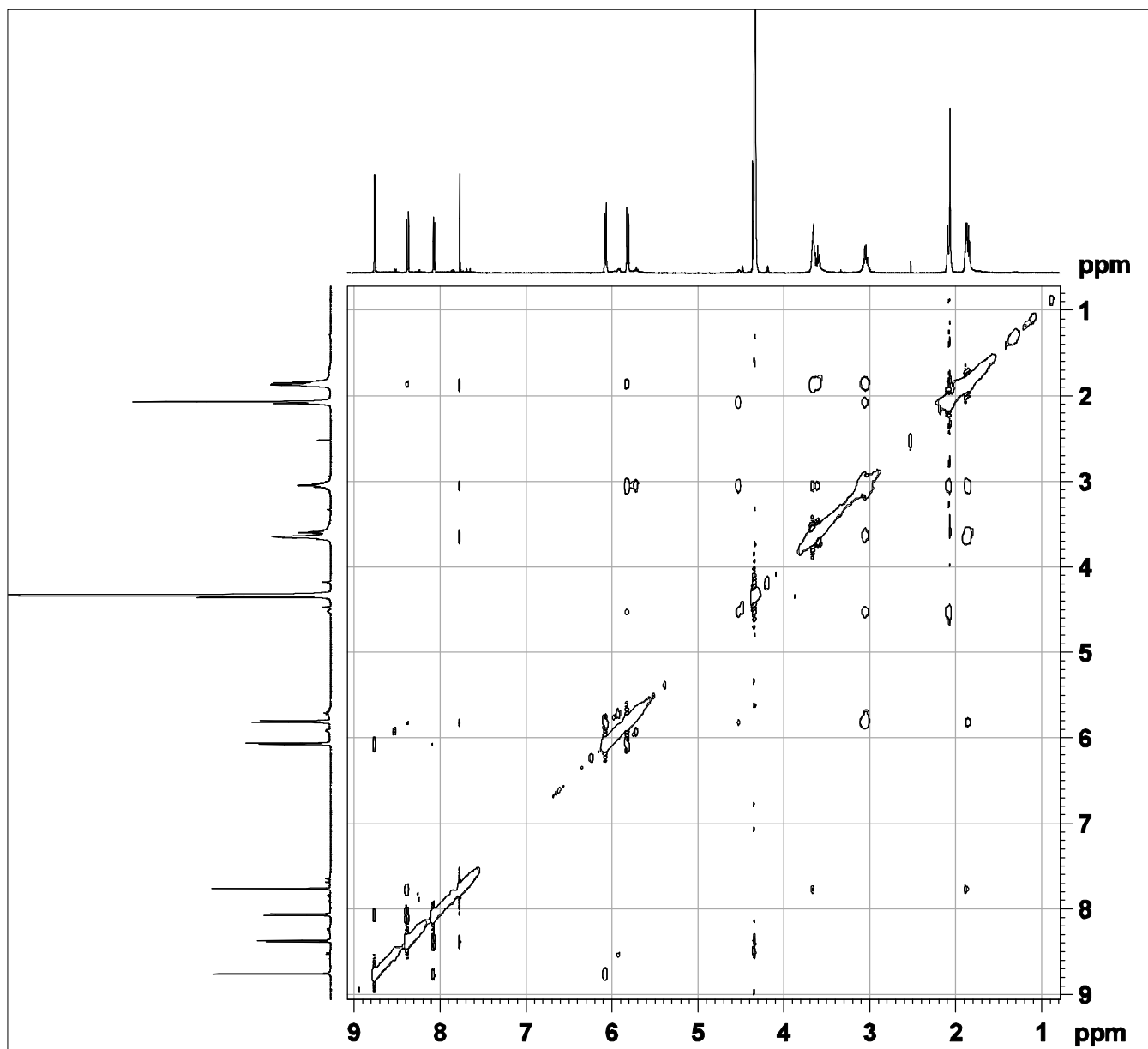


Figure S2. The ROESY NMR spectrum of catenate **4**.

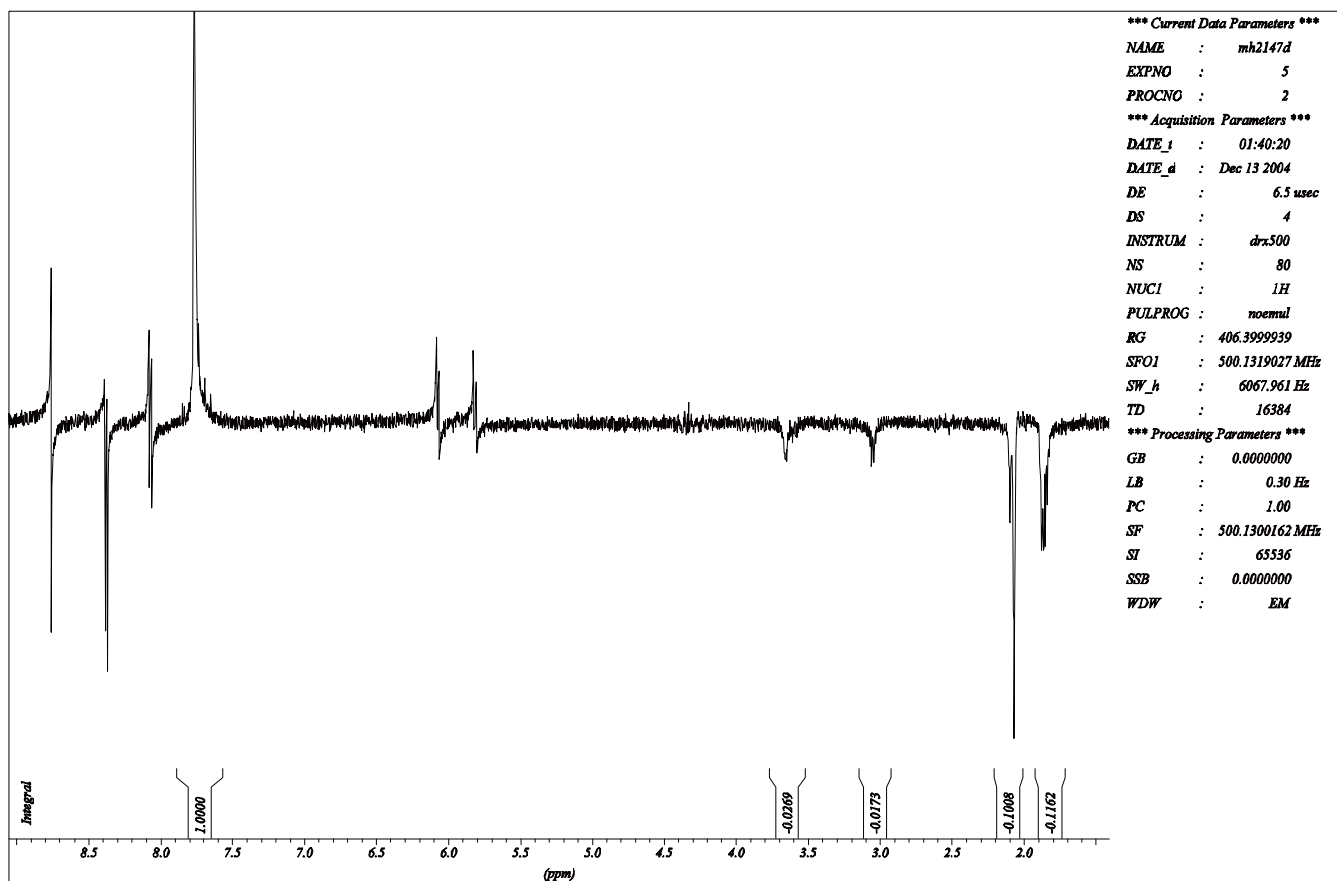


Figure S3. The 1d NOE difference NMR spectrum of catenate **4**, with irradiation of proton Ha.

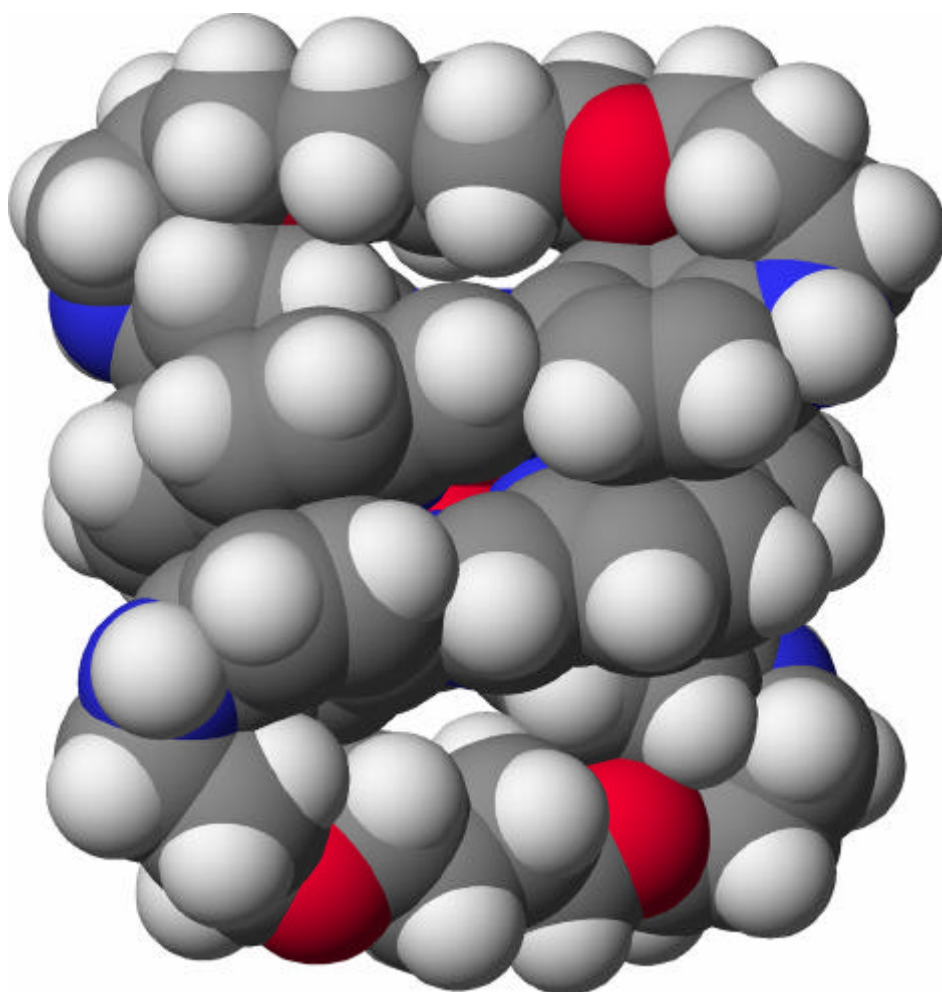


Figure S4. The MM2-minimized structure of a macrocyclic topological isomer of **4**, having a minimized energy of 335 kJ mol^{-1} greater than the catenate.

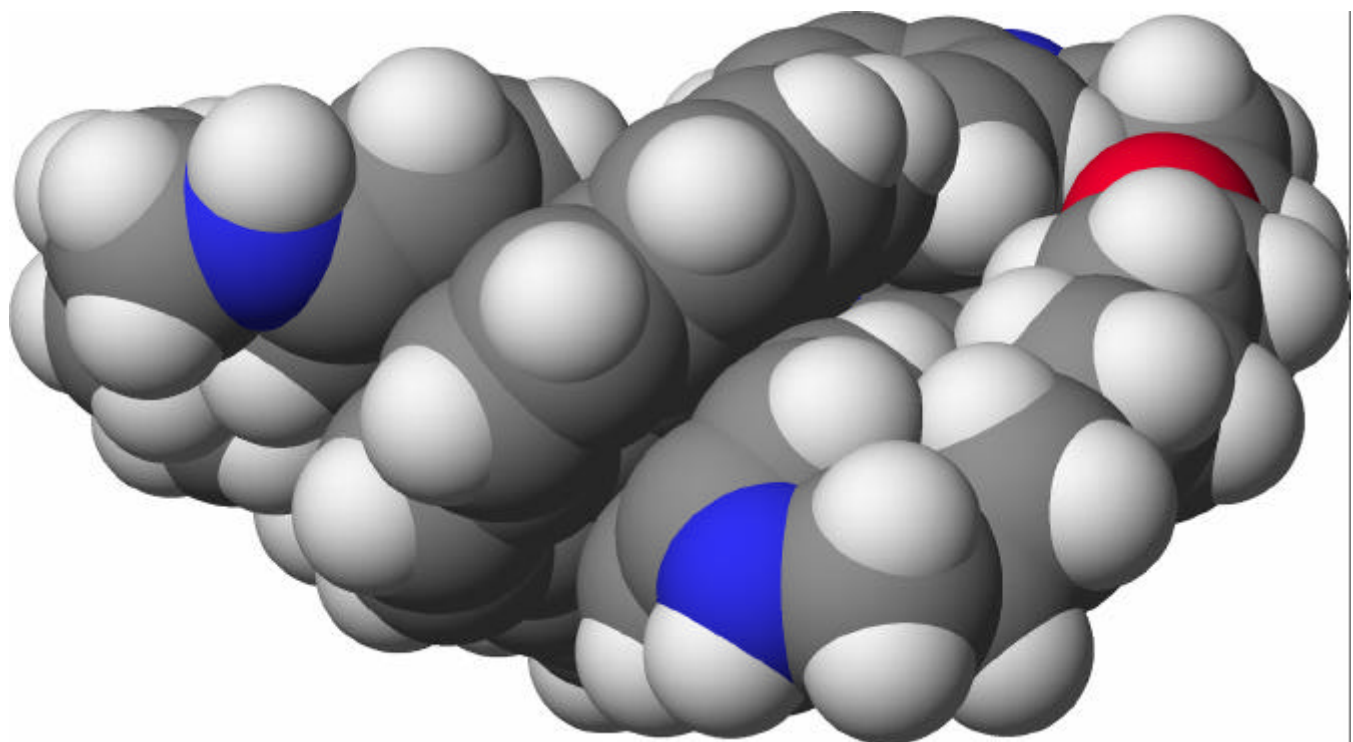


Figure S5. The MM2-minimized structure of the “crossed” macrocyclic topological isomer of **4**, having an MM2-minimized energy of 569 kJ mol^{-1} greater than the catenate.

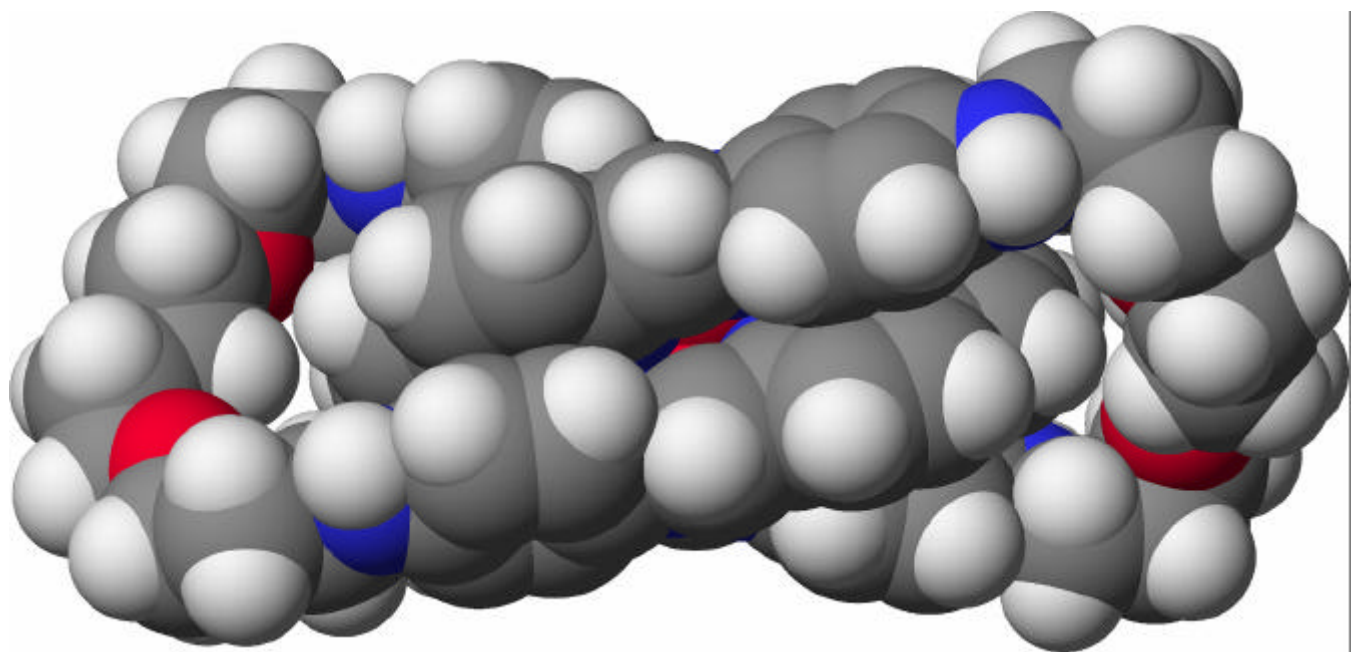


Figure S6. The MM2-minimized structure of **4**.

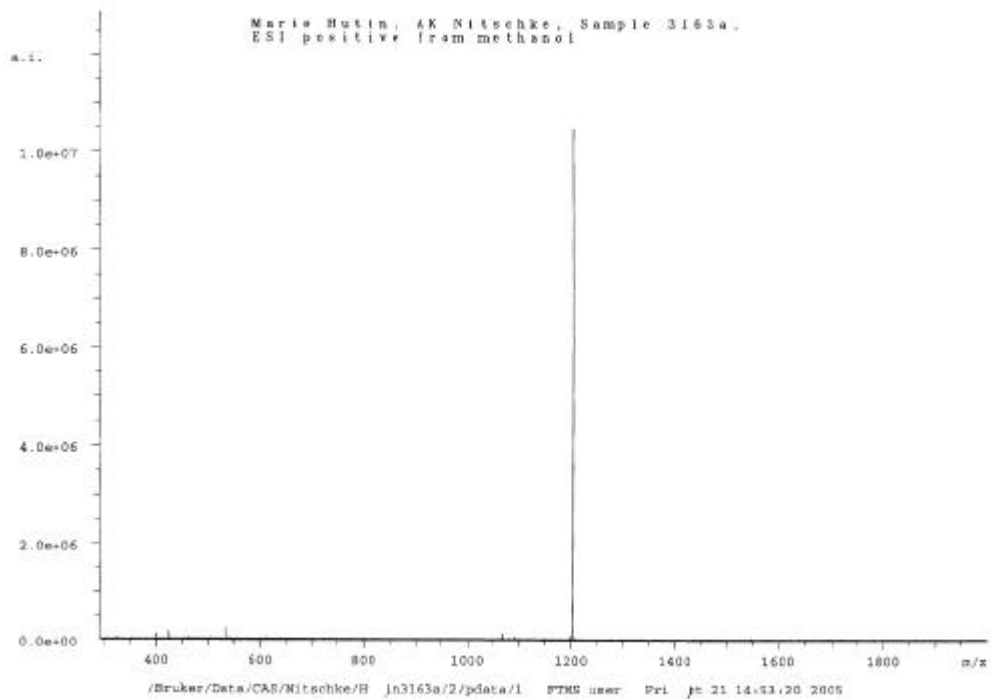


Figure S7. MS/MS spectrum of demetallated catenane **5**, consisting of the isolated first isotopic peak of $[5\cdot\text{Na}]^+$

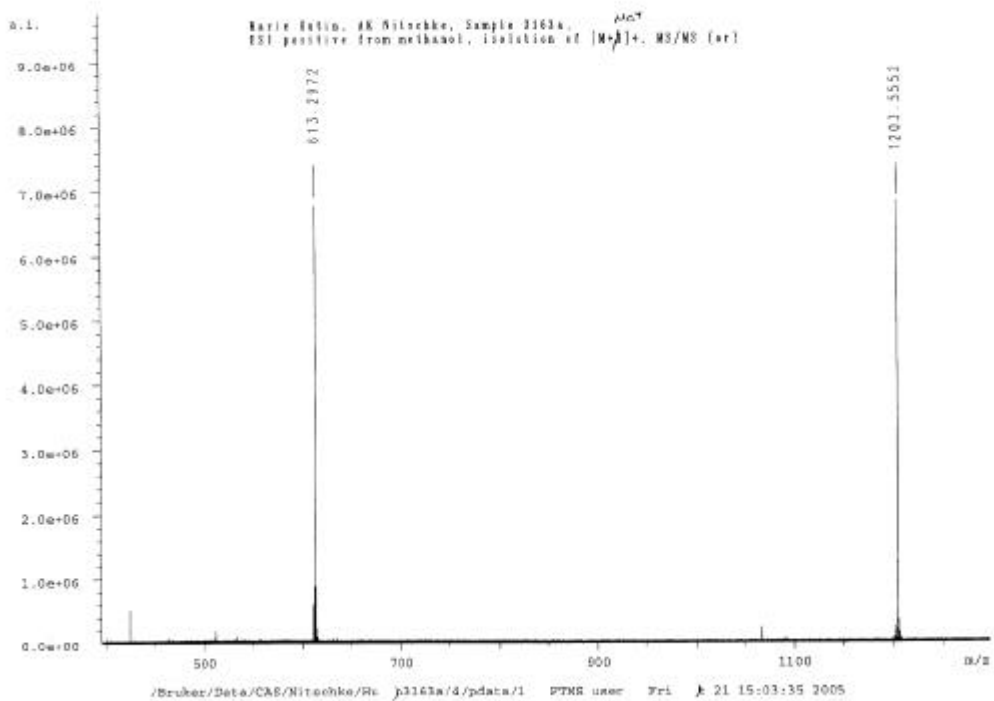


Figure S8. The symmetrical fragmentation of the isolated ion shown in Figure S7 with increasing acceleration voltage.