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Supporting Information

for

Active-metal template clipping synthesis of novel [2]rotaxanes

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Copies of NMR and HRMS spectra

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Copies of NMR and mass spectra

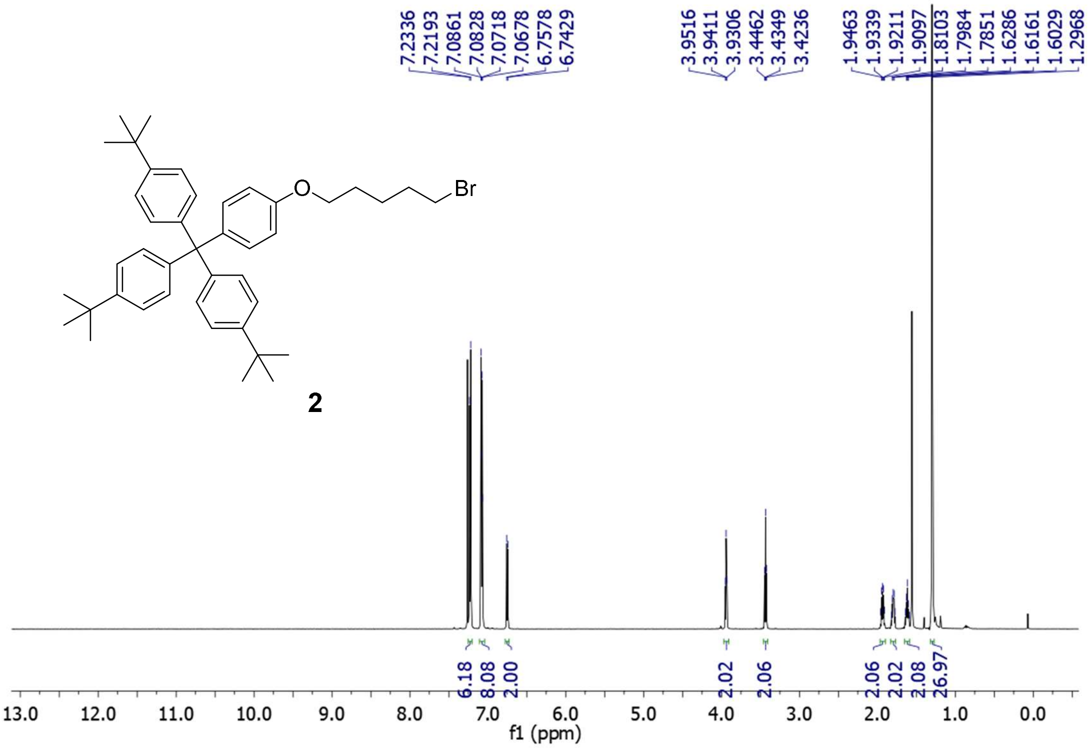


Figure S1: ^{1}H NMR (CDCl$_3$, 600 MHz) spectrum of compound **2**.

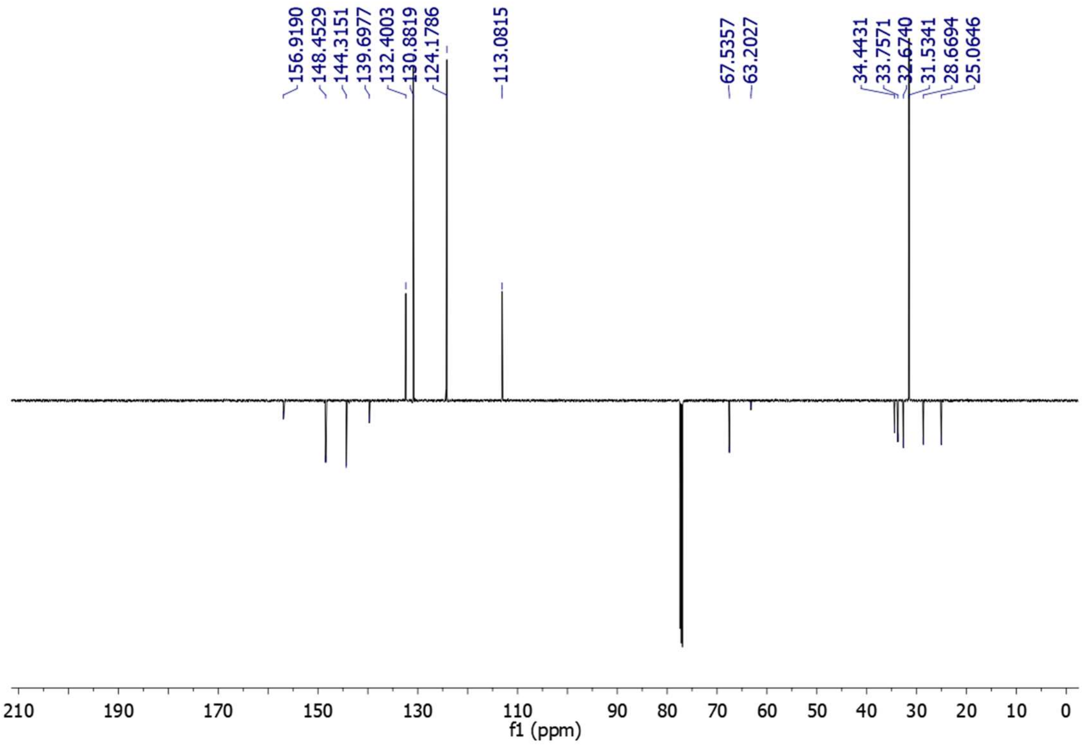
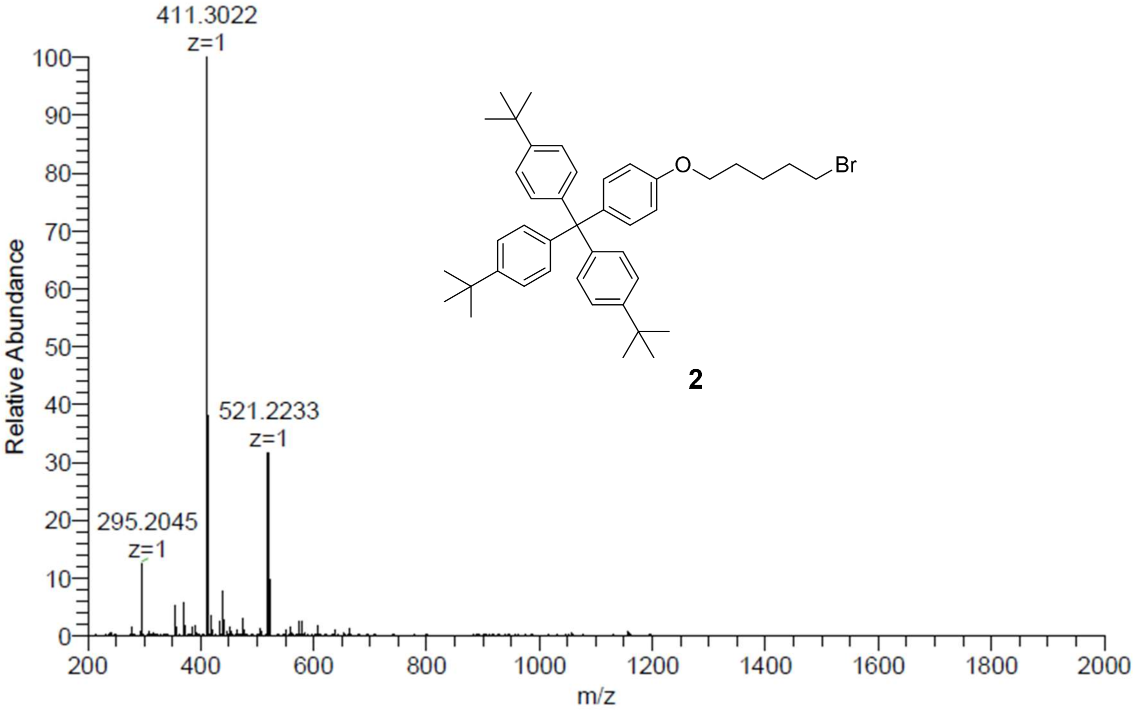
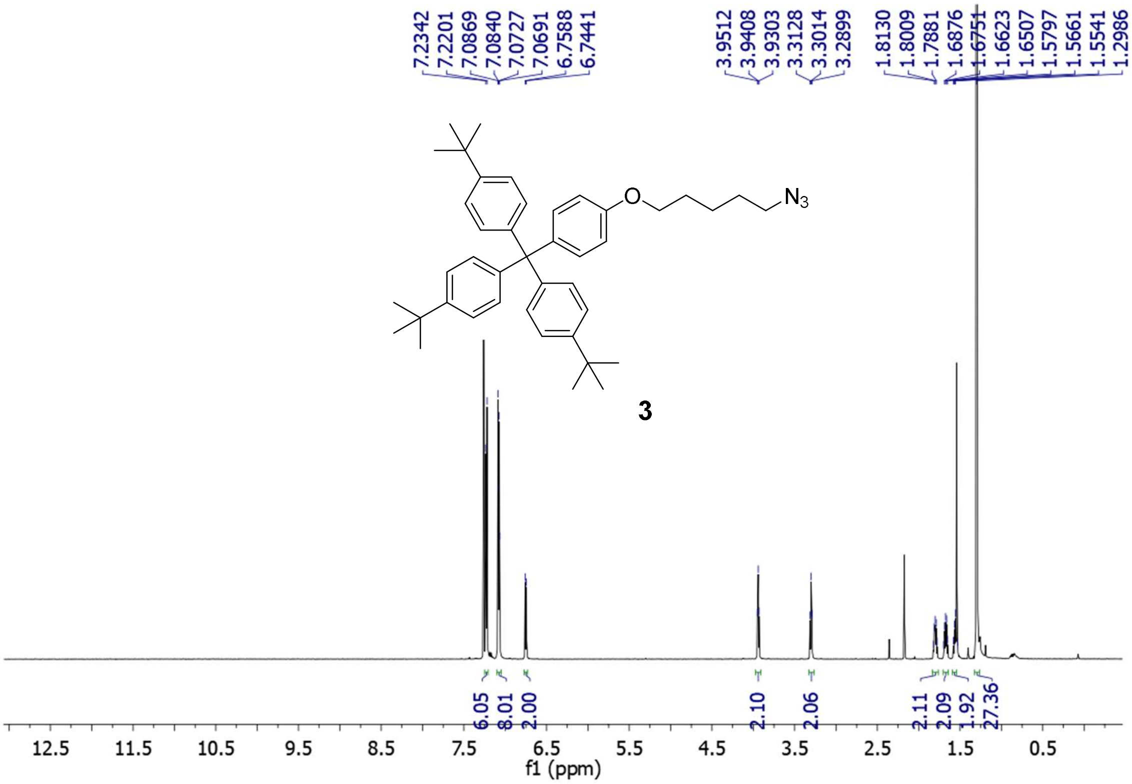


Figure S2: ^{13} C APT NMR (CDCl$_3$, 150 MHz) spectrum of compound **2**.



2

Figure S3: APCI(+)-HRMS spectrum of compound **2**.



3

Figure S4: ${}^{1}H$ NMR ($CDCl_3$, 600 MHz) spectrum of compound **3**.

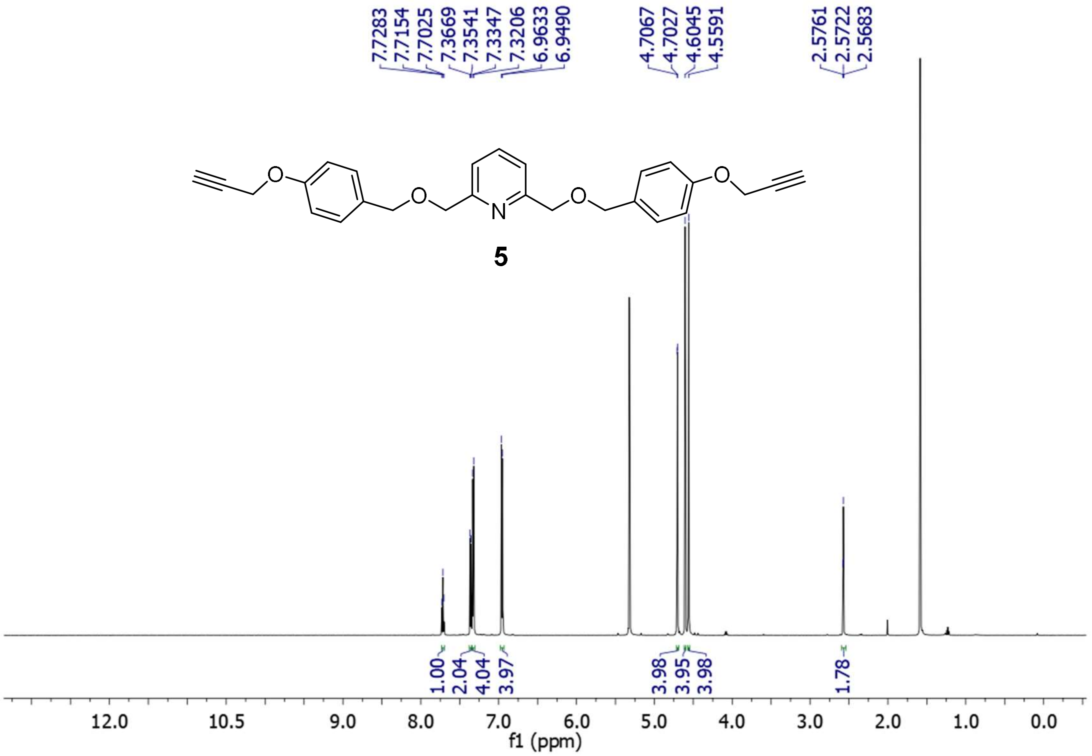


Figure S5: ^{1}H NMR (CD_2Cl_2, 600 MHz) spectrum of compound **5**.

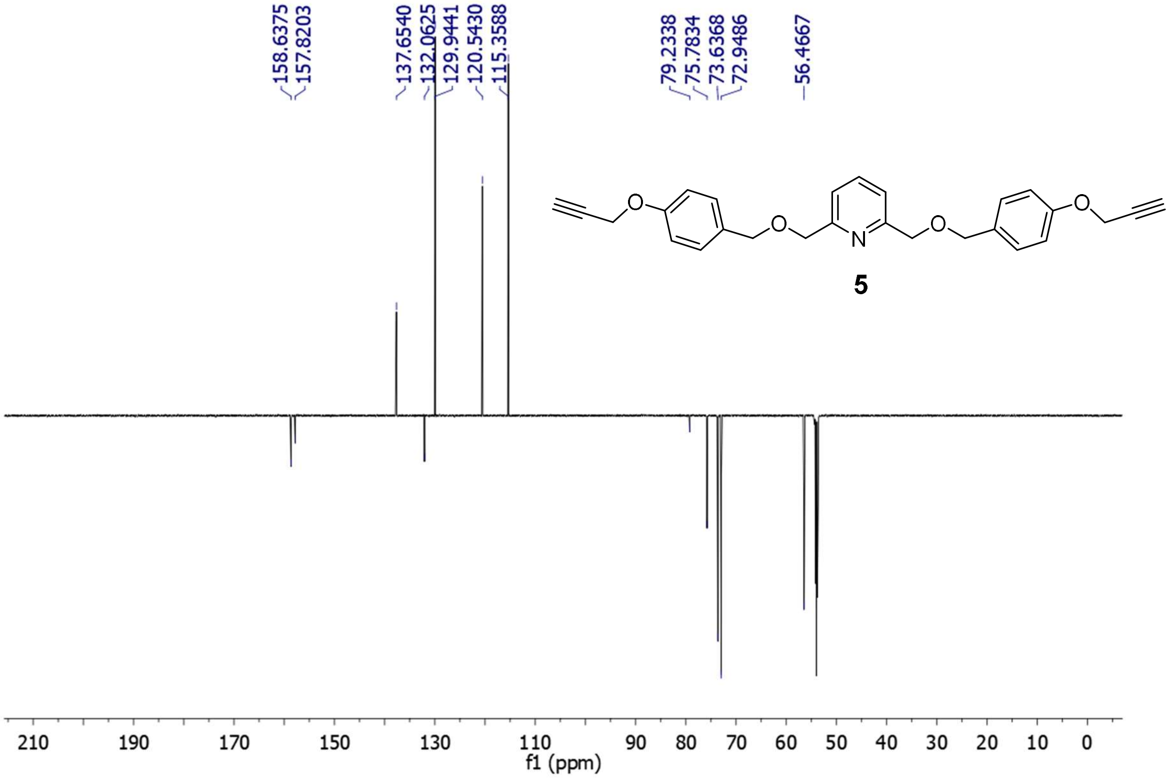


Figure S6: ^{13}C APT NMR (CD_2Cl_2, 150 MHz) spectrum of compound **5**.

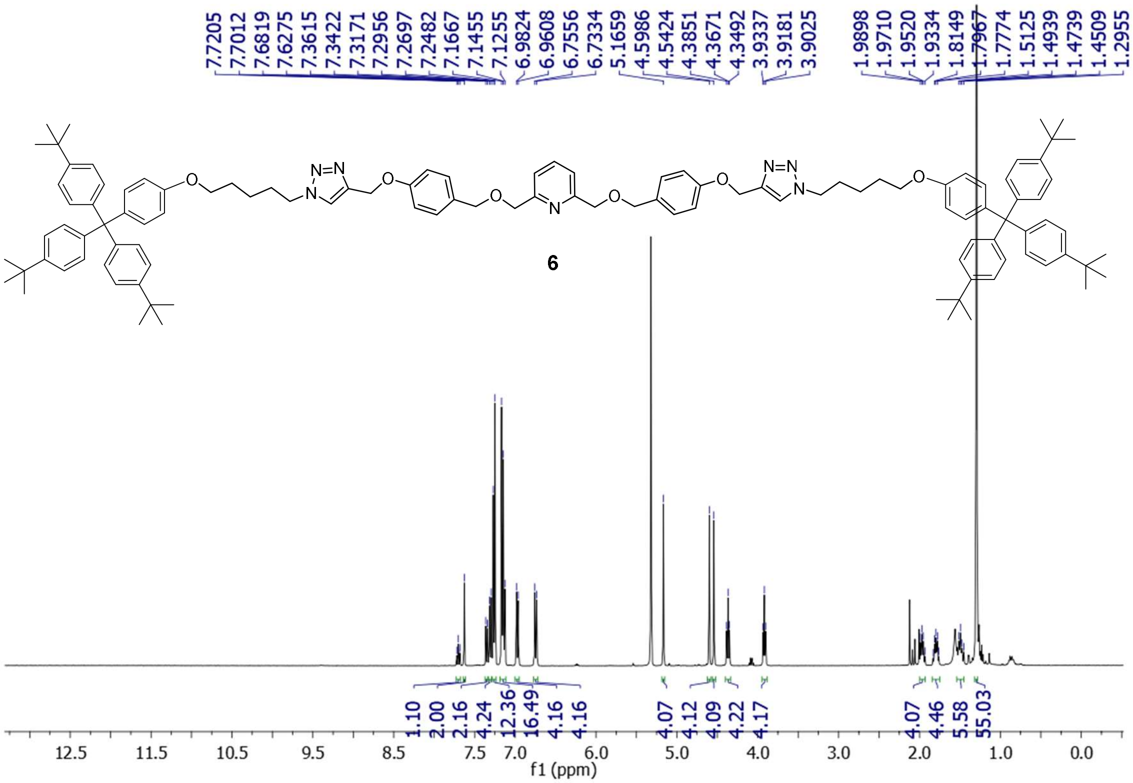


Figure S7: ^{1}H NMR (CD_2Cl_2, 400 MHz) spectrum of compound **6**.

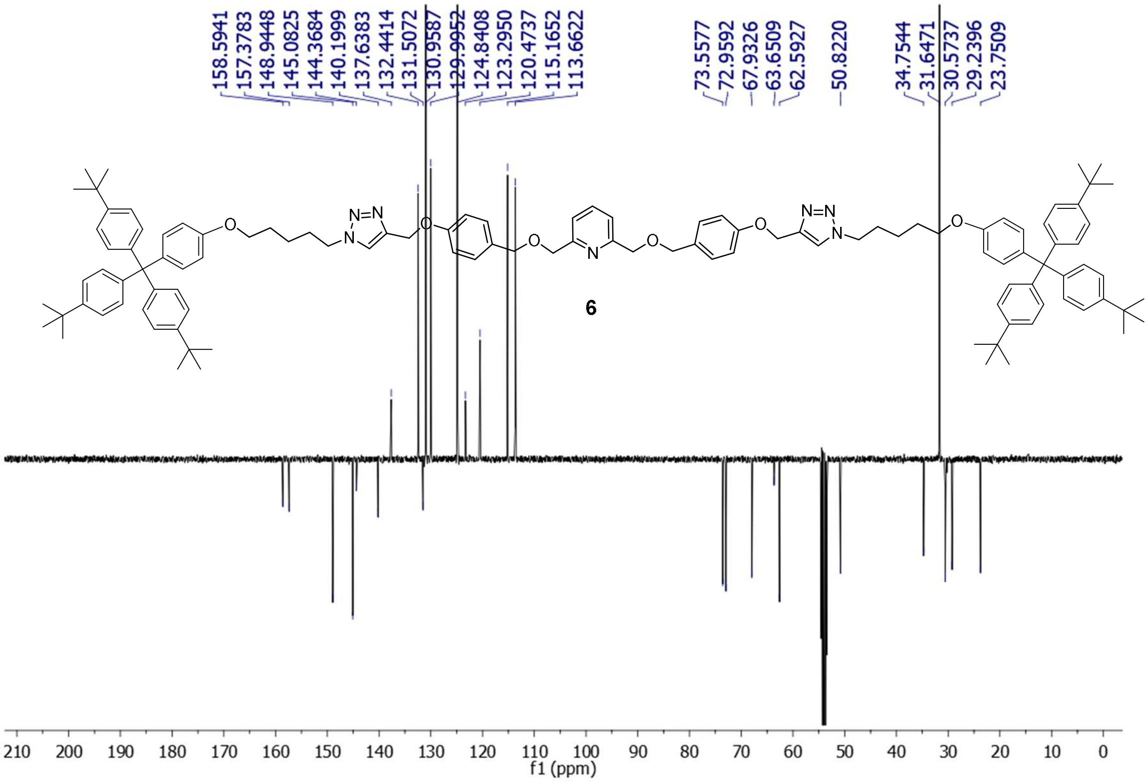


Figure S8: ^{13}C APT NMR (CD_2Cl_2, 100 MHz) spectrum of compound **6**.

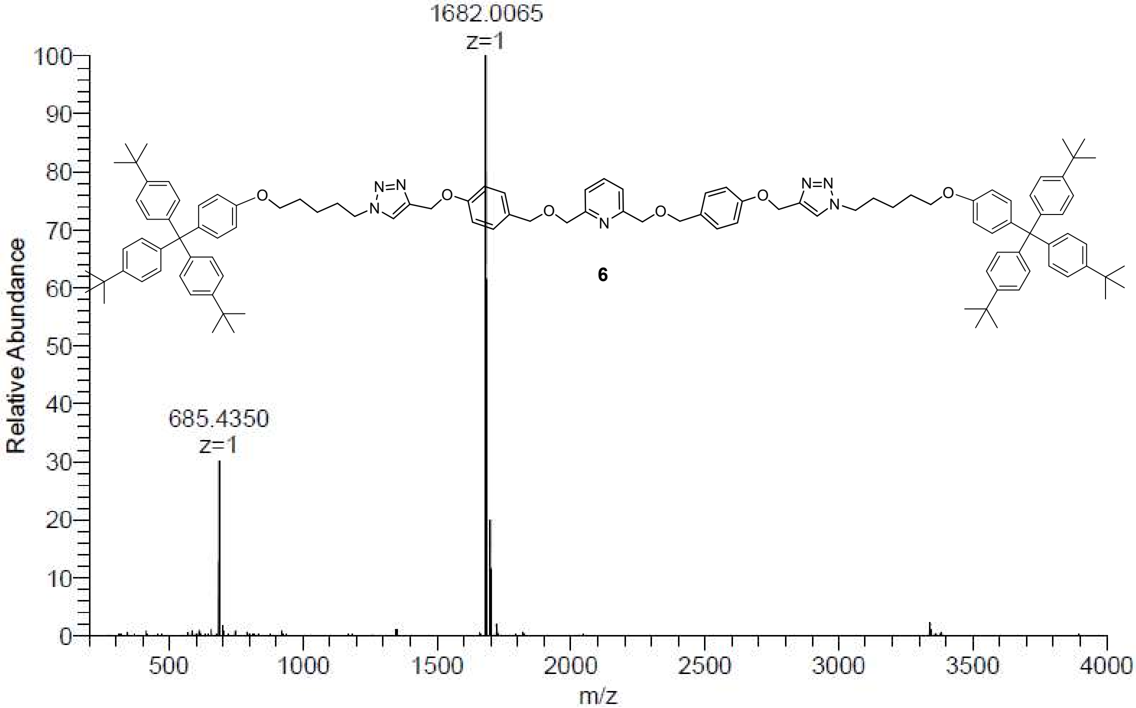


Figure S9: HRESI(+)-MS spectrum of compound **6**.

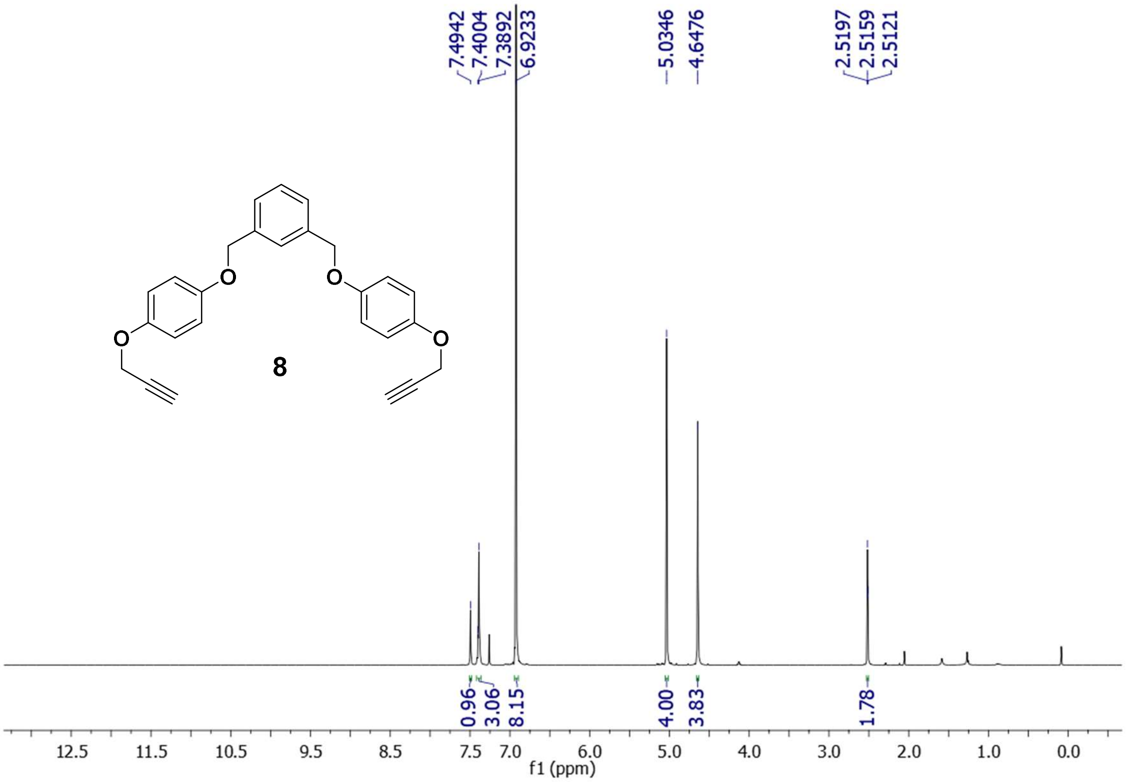


Figure S10: ^{1}H NMR (CDCl$_3$, 600 MHz) spectrum of compound **8**.

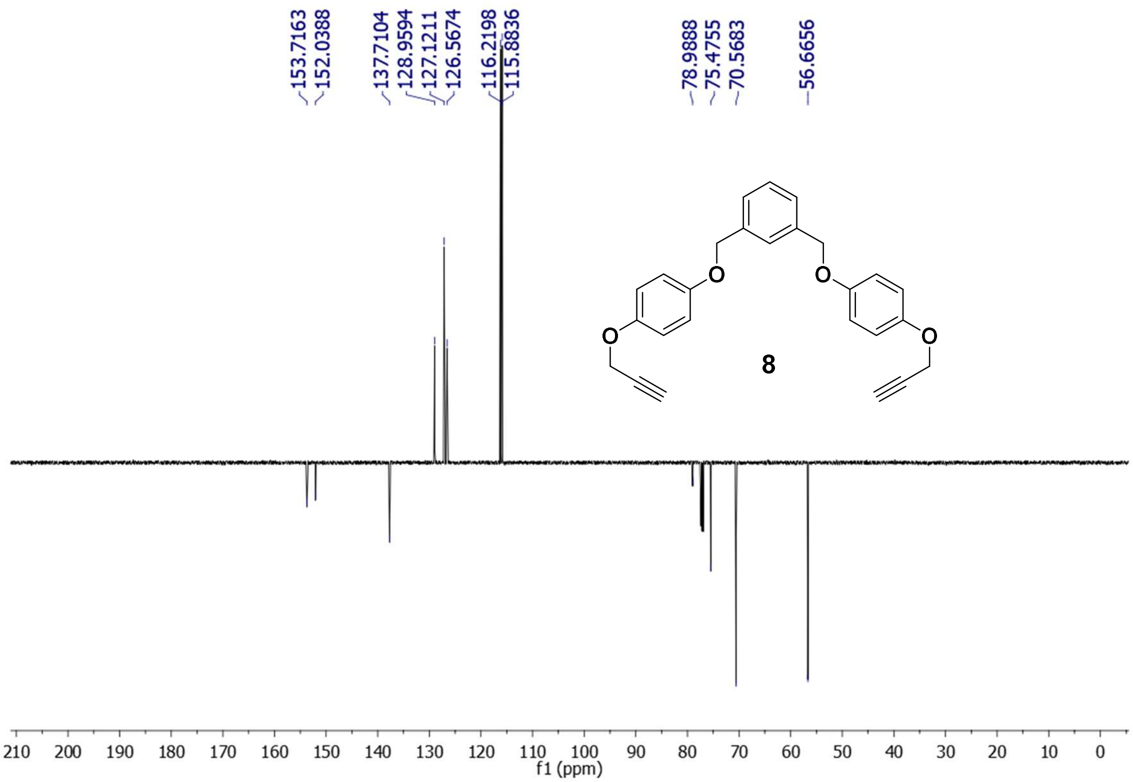


Figure S11: ^{13}C APT NMR ($CDCl_3$, 150 MHz) spectrum of compound **8**.

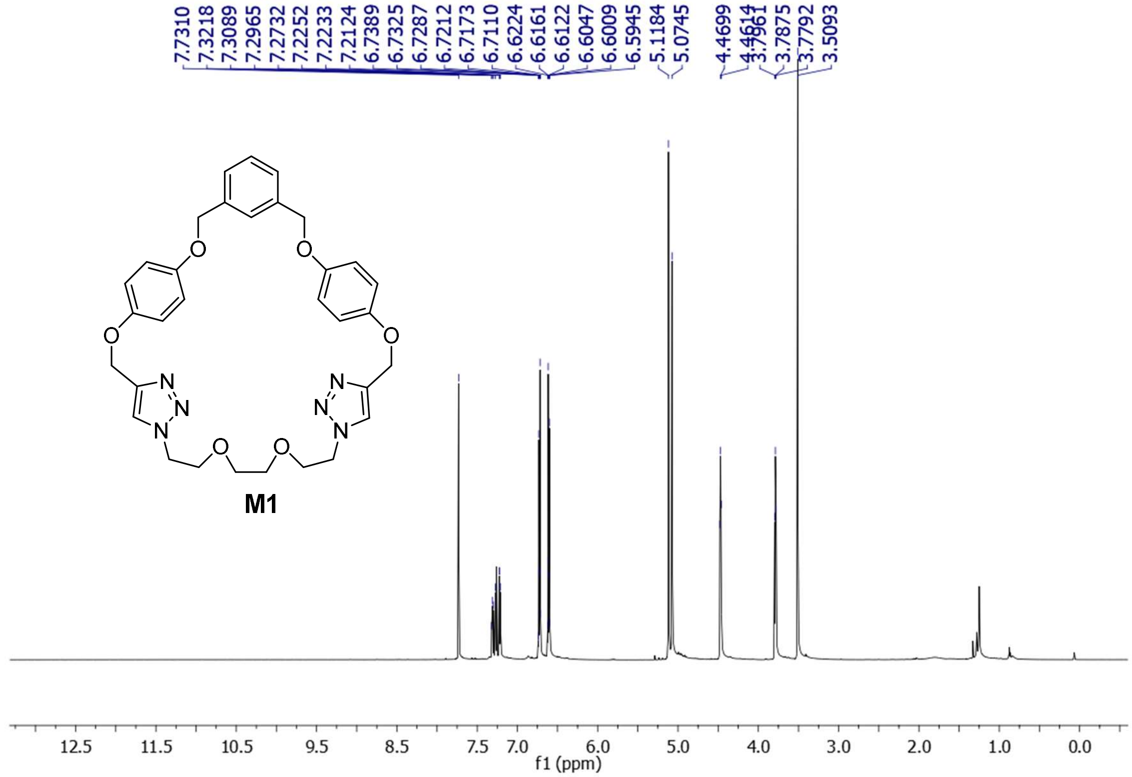


Figure S12: ^{1}H NMR ($CDCl_3$, 600 MHz) spectrum of compound **M1**.

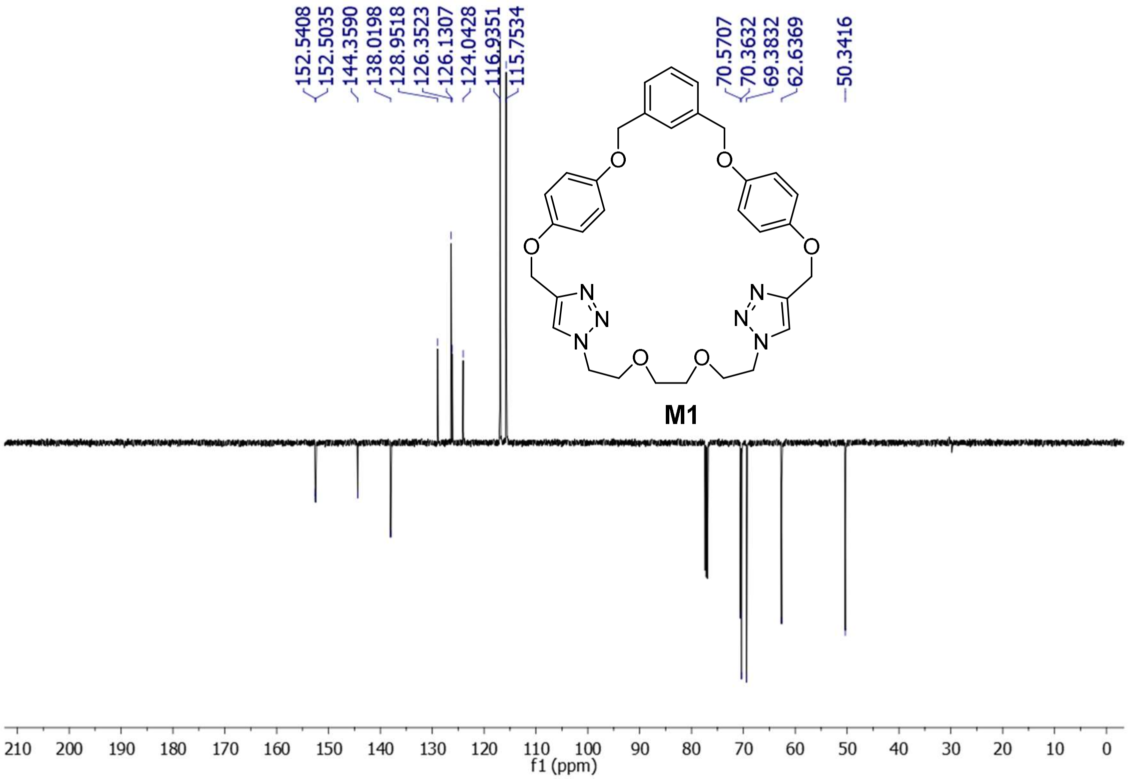


Figure S13: ^{13}C APT NMR ($CDCl_3$, 150 MHz) spectrum of compound **M1**.

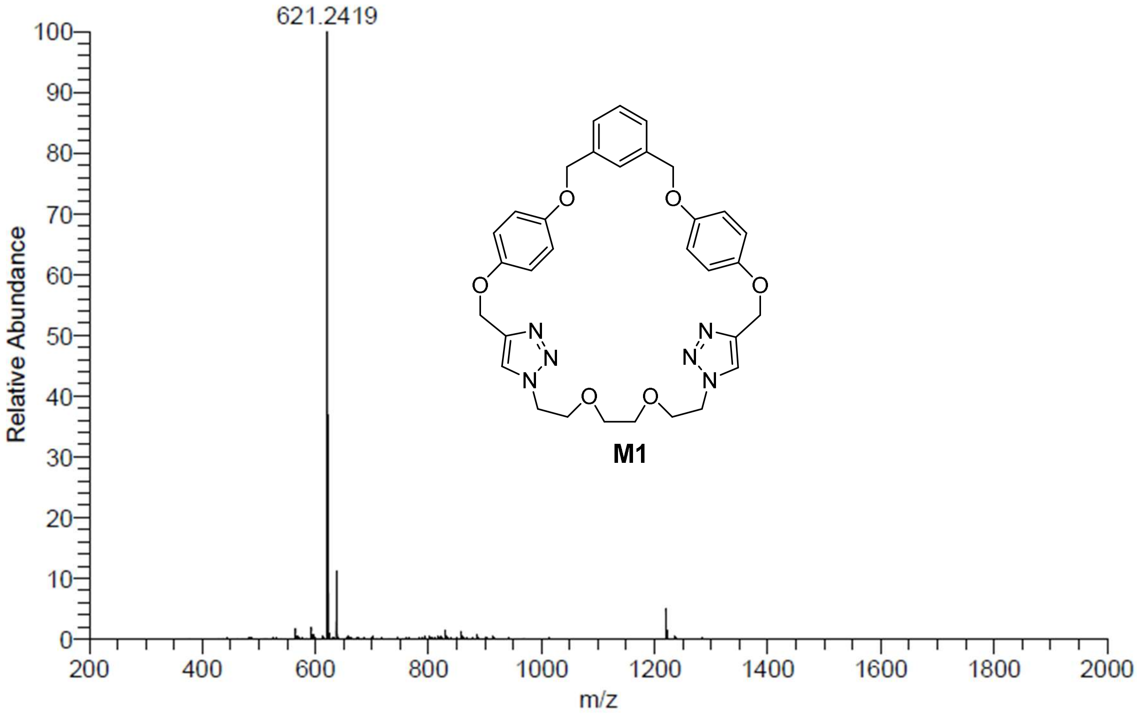


Figure S14: HRESI(+)-MS spectrum of compound **M1**.

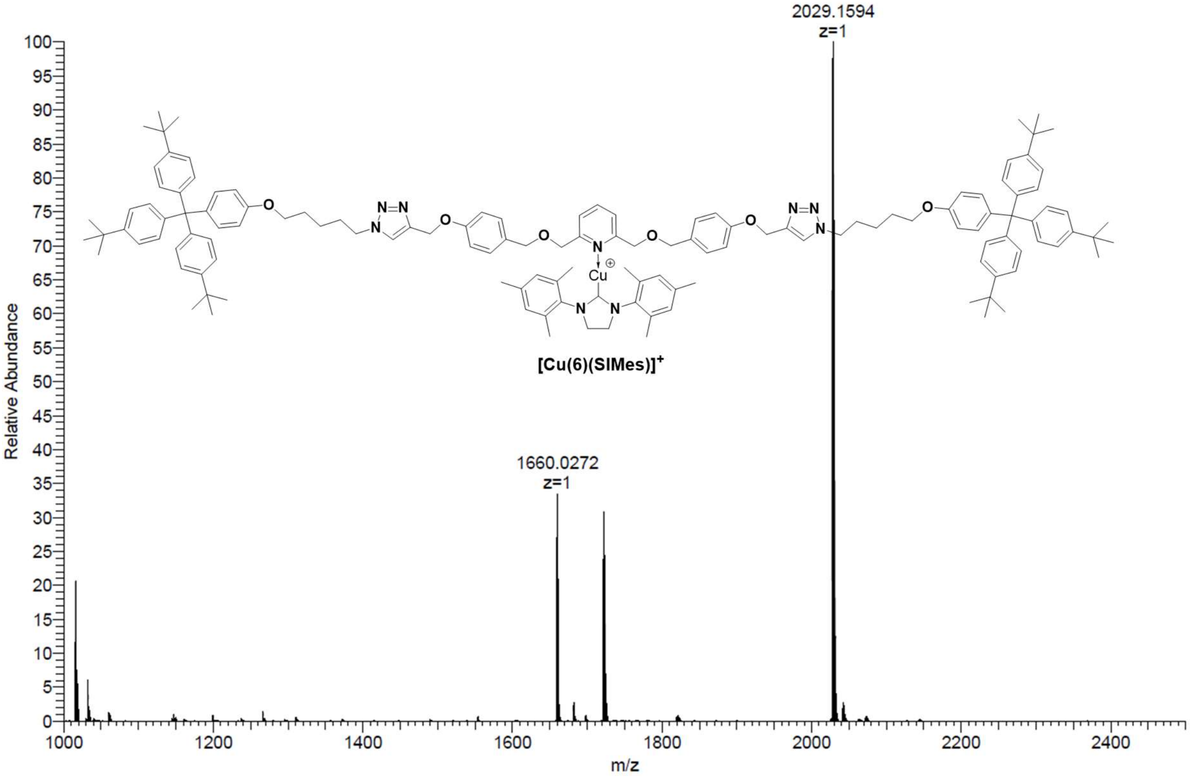


Figure S15: HRMS spectrum of the complex between axle **6** and **CuCl(SIMes)**.

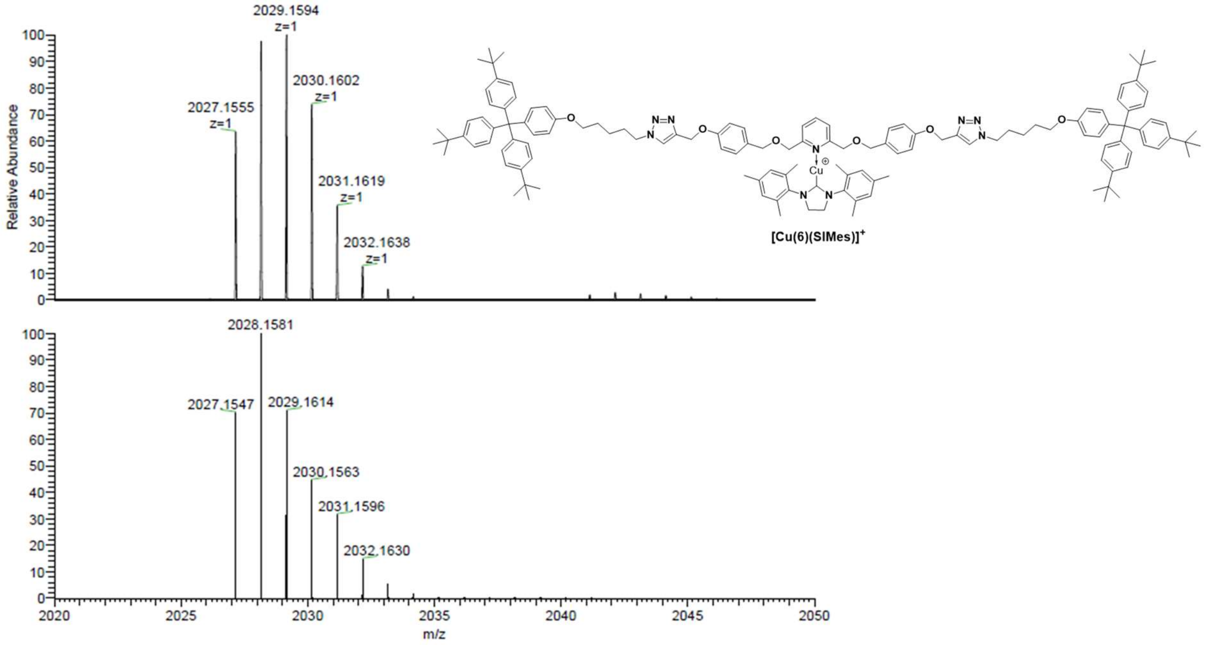


Figure S16: HRMS spectrum of the complex between axle **6** and **CuCl(SIMes**) [experimental (top) and calculated (bottom) isotopic patterns].

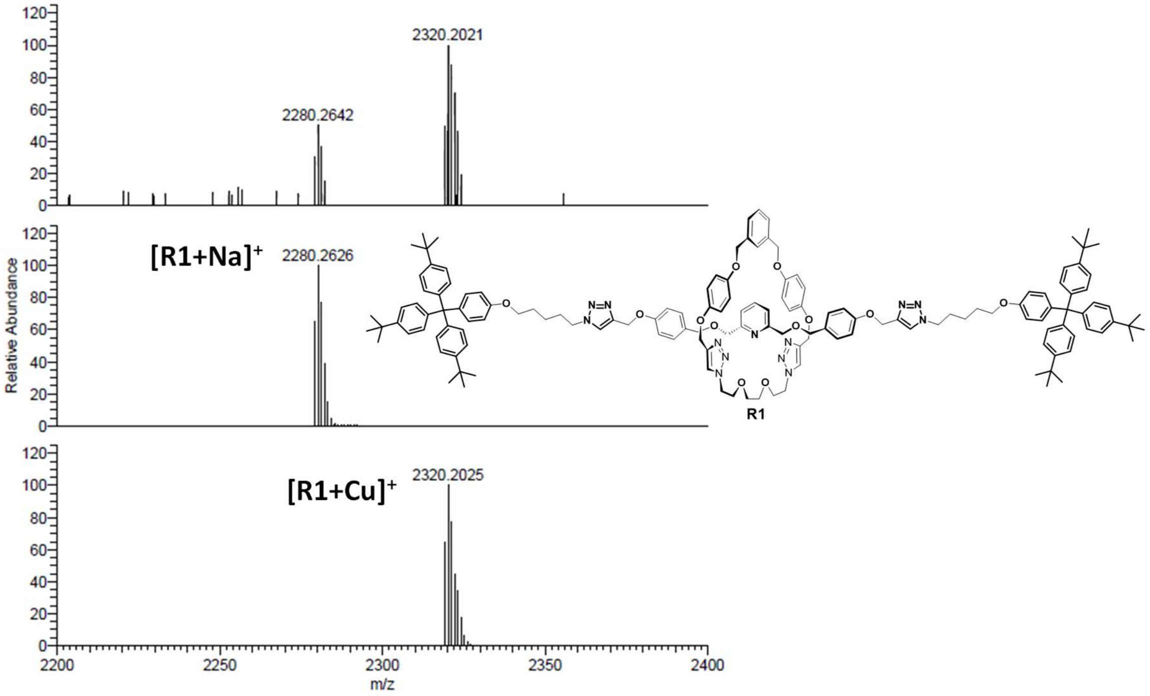


Figure S17: HRESI(+)-MS spectrum of the rotaxane **R1** [experimental (top) and calculated (bottom) isotopic patterns].

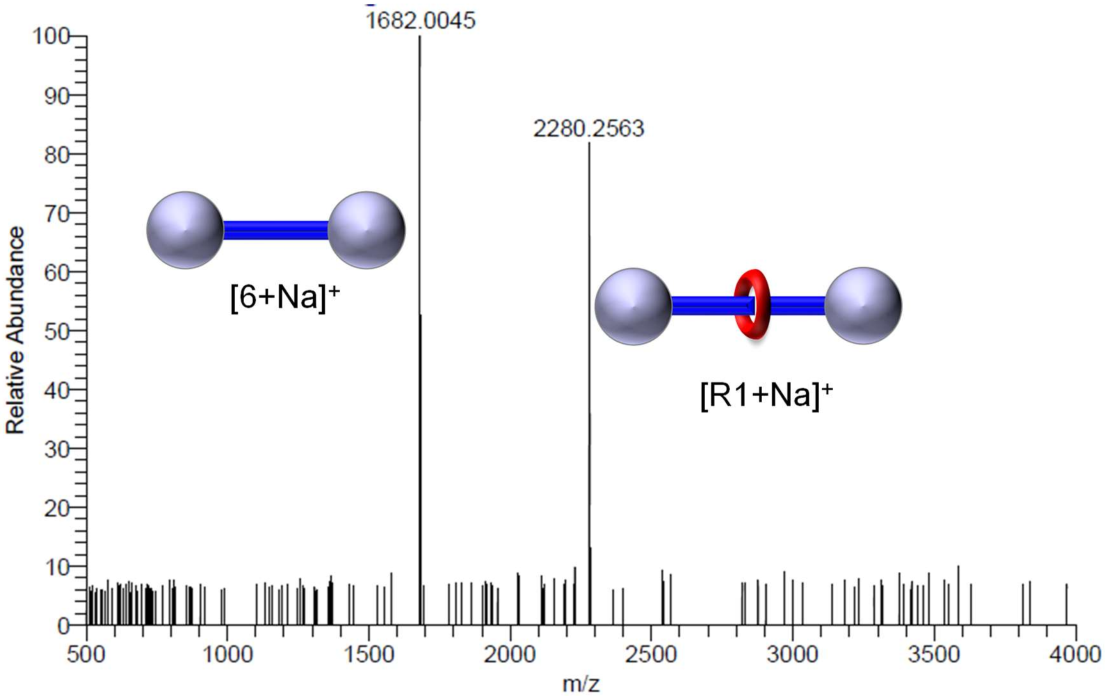


Figure S18: ESI(+)-MS^2 spectrum of rotaxane **R1**.

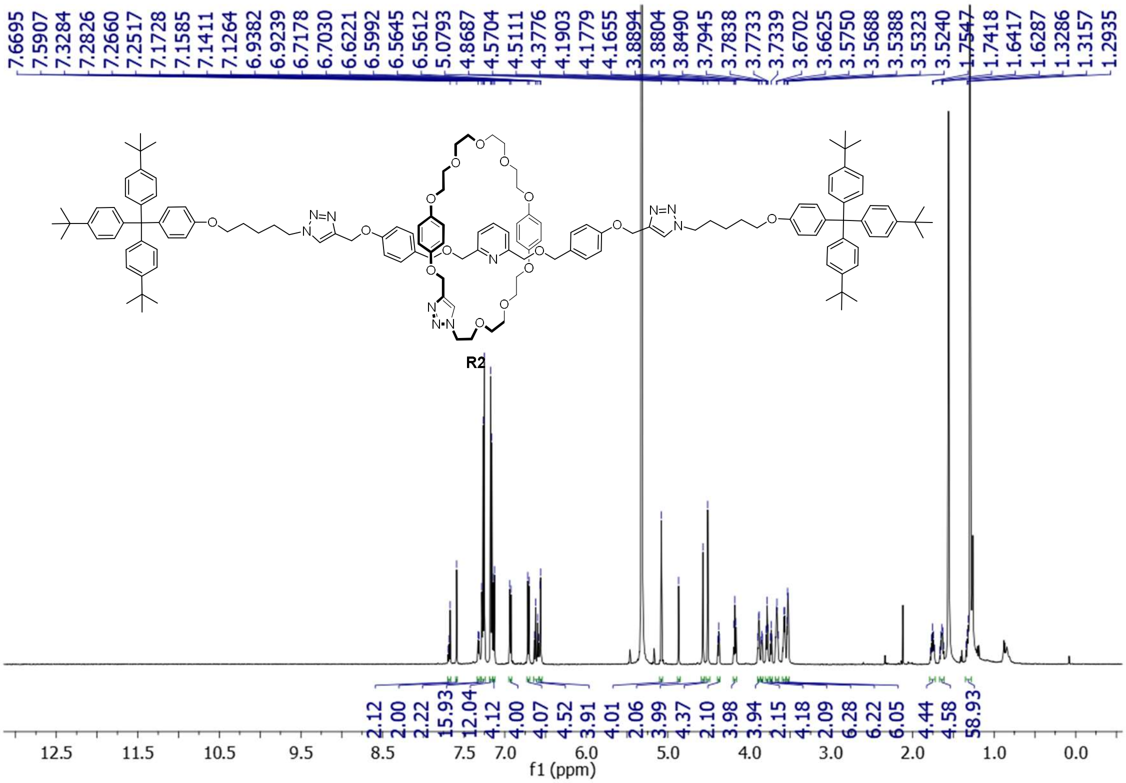


Figure S19: ^{1}H NMR (CD_2Cl_2, 600 MHz) spectrum of compound **R2**.

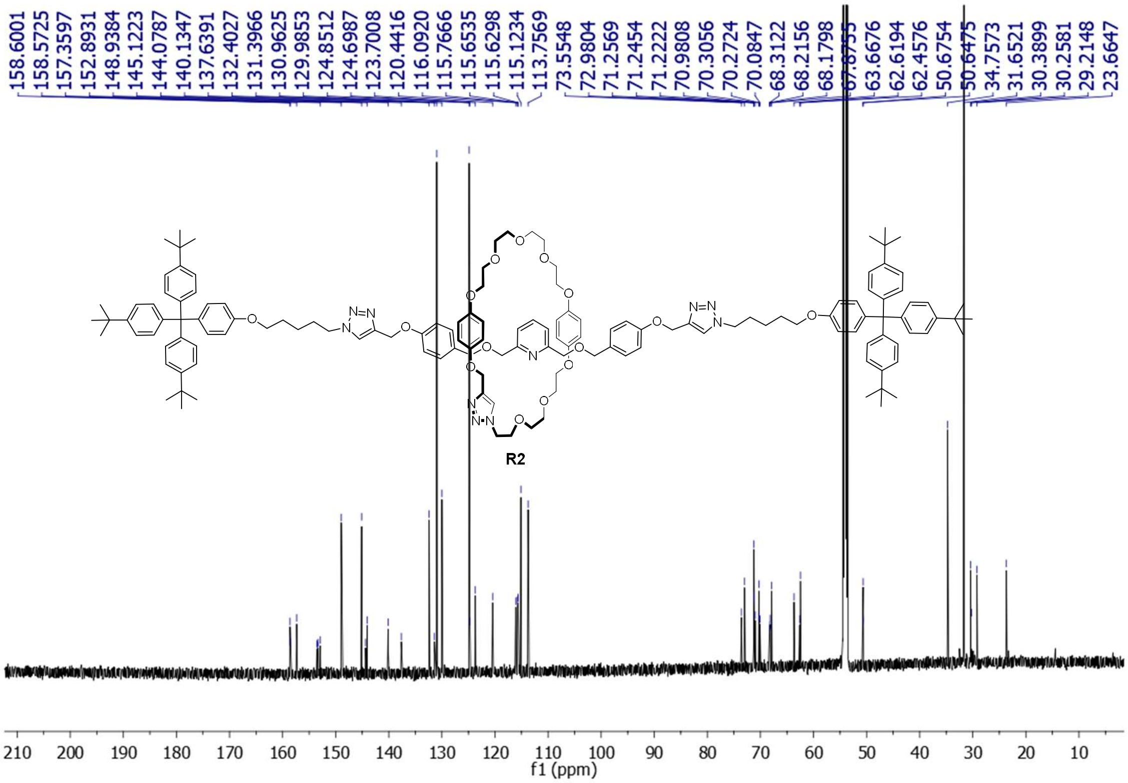


Figure S20: ^{13}C NMR (CD_2Cl_2, 150 MHz) spectrum of compound **R2**.

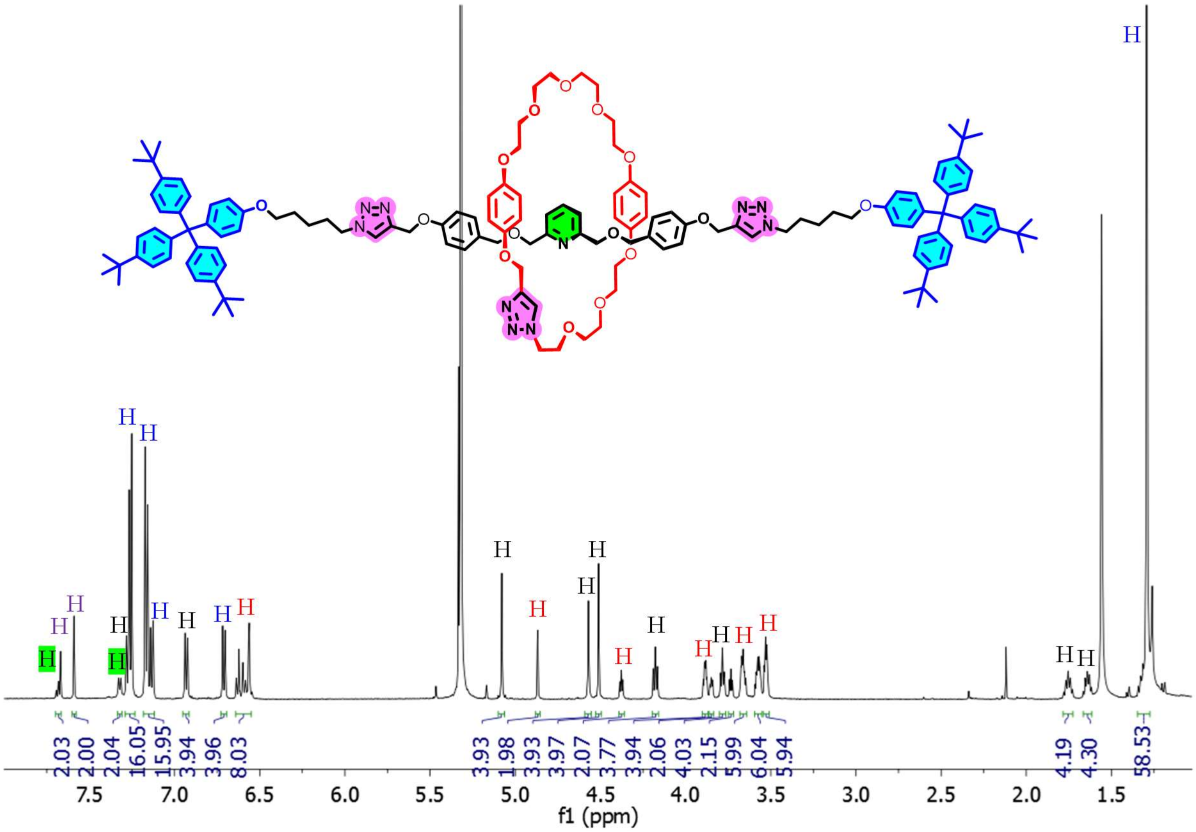


Figure S21: Zoom ^{1}H NMR (CD_2Cl_2, 600 MHz) spectrum of compound **R2**.

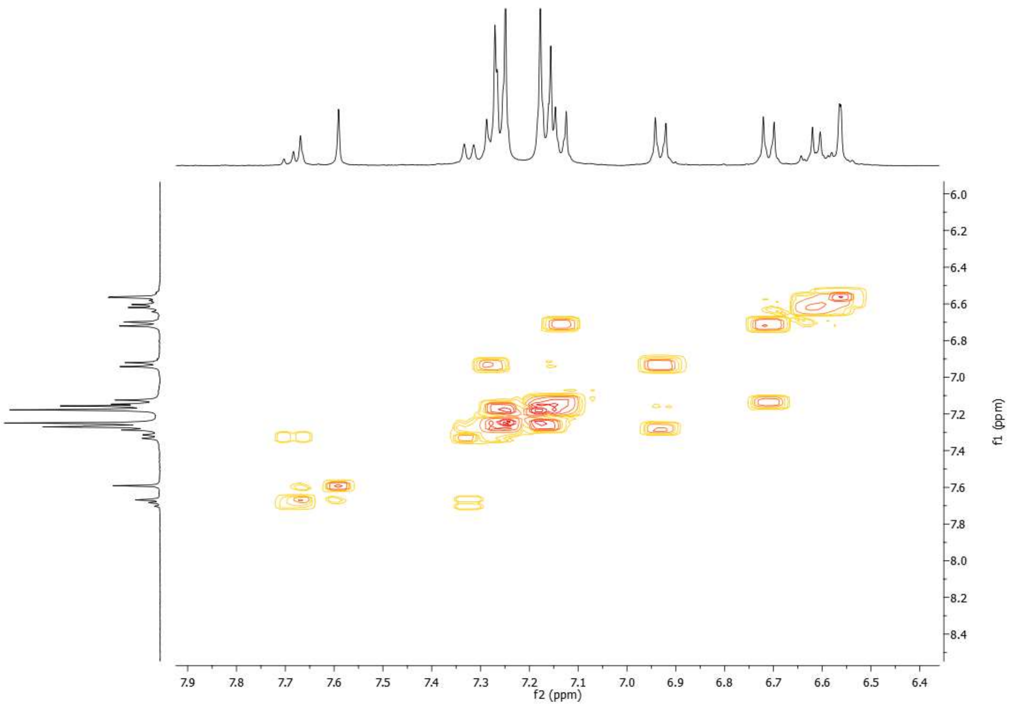


Figure S22: H,H-COSY NMR (CD_2Cl_2, 400 MHz) spectrum of compound **R2**: aromatic region.

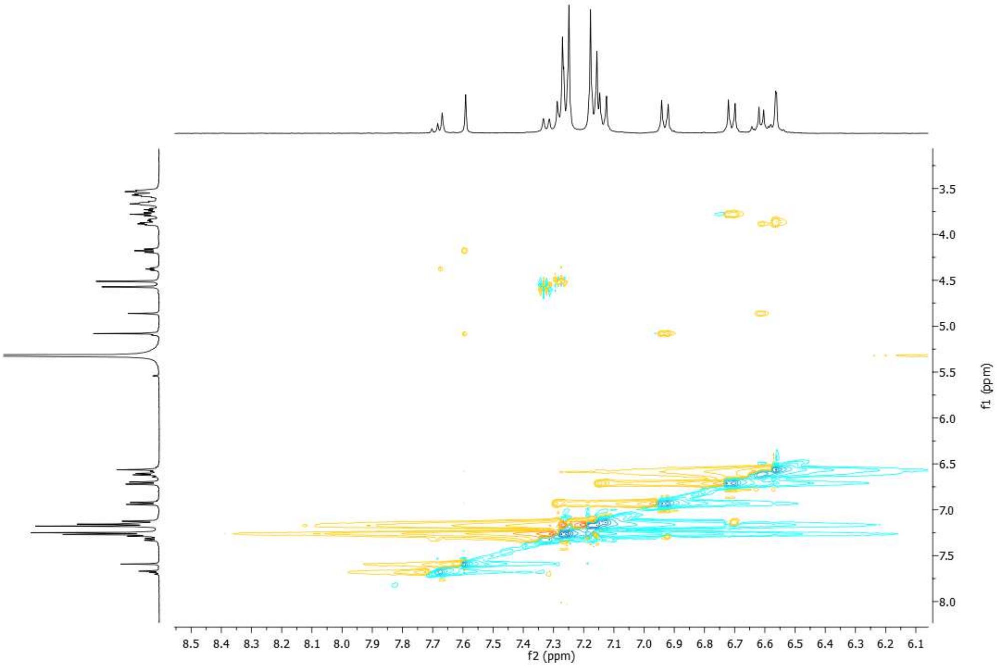


Figure S23: H,H-ROESY NMR (CD_2Cl_2, 400 MHz) spectrum of compound **R2**: aromatic region.

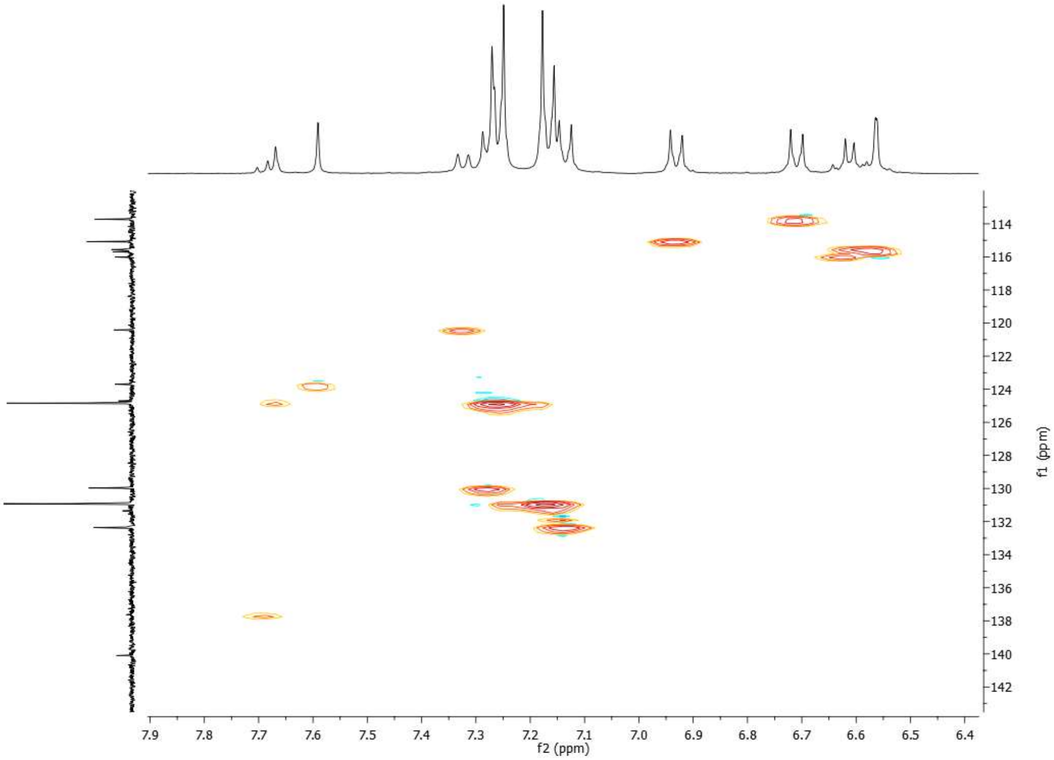


Figure S24: HSQC NMR (CD_2Cl_2, 400 MHz) spectrum of compound **R2**: aromatic region.

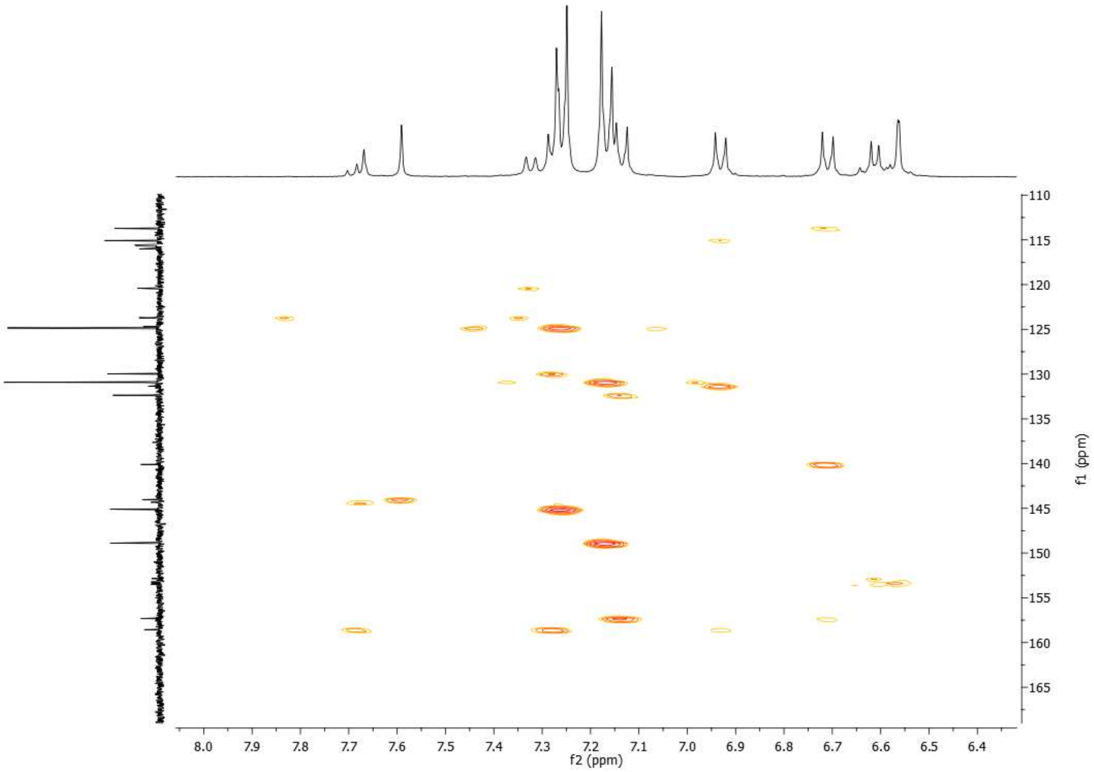


Figure S25: HMBC NMR (CD_2Cl_2, 400 MHz) spectrum of compound **R2**: aromatic region.

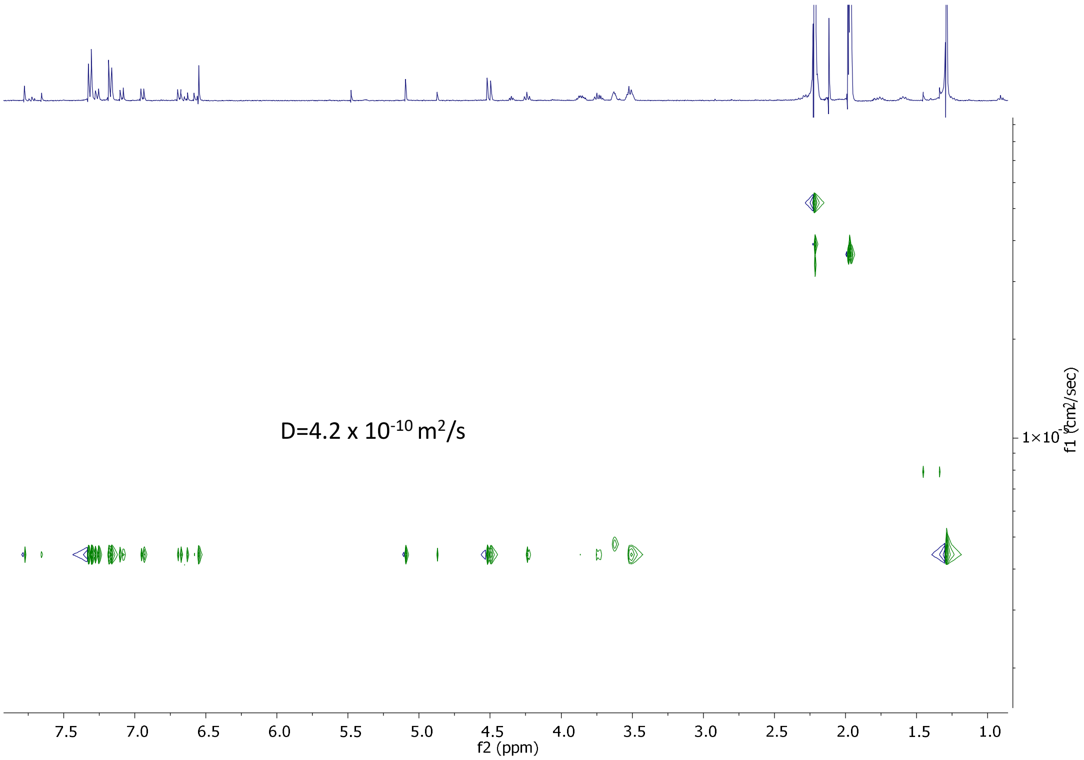


Figure S26: ^{1}H-DOSY NMR (MeCN-*d*$_3$, 400 MHz) spectrum of compound **R2**.

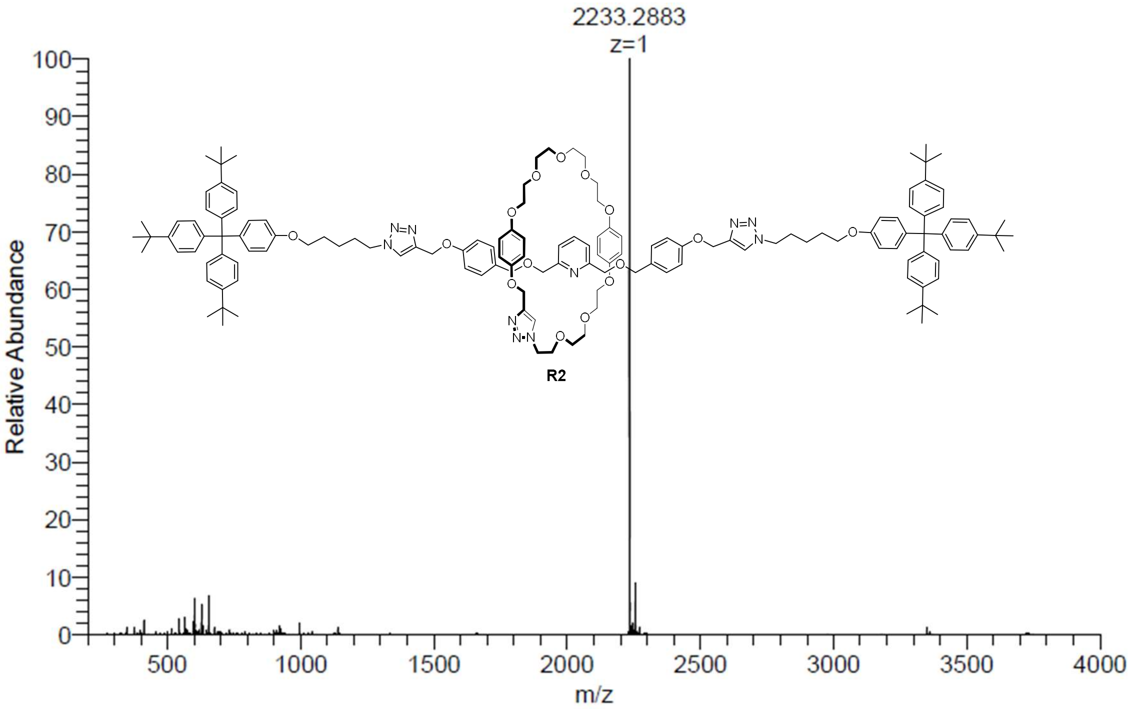


Figure S27: HRESI(+)-MS spectrum of compound **R2**.

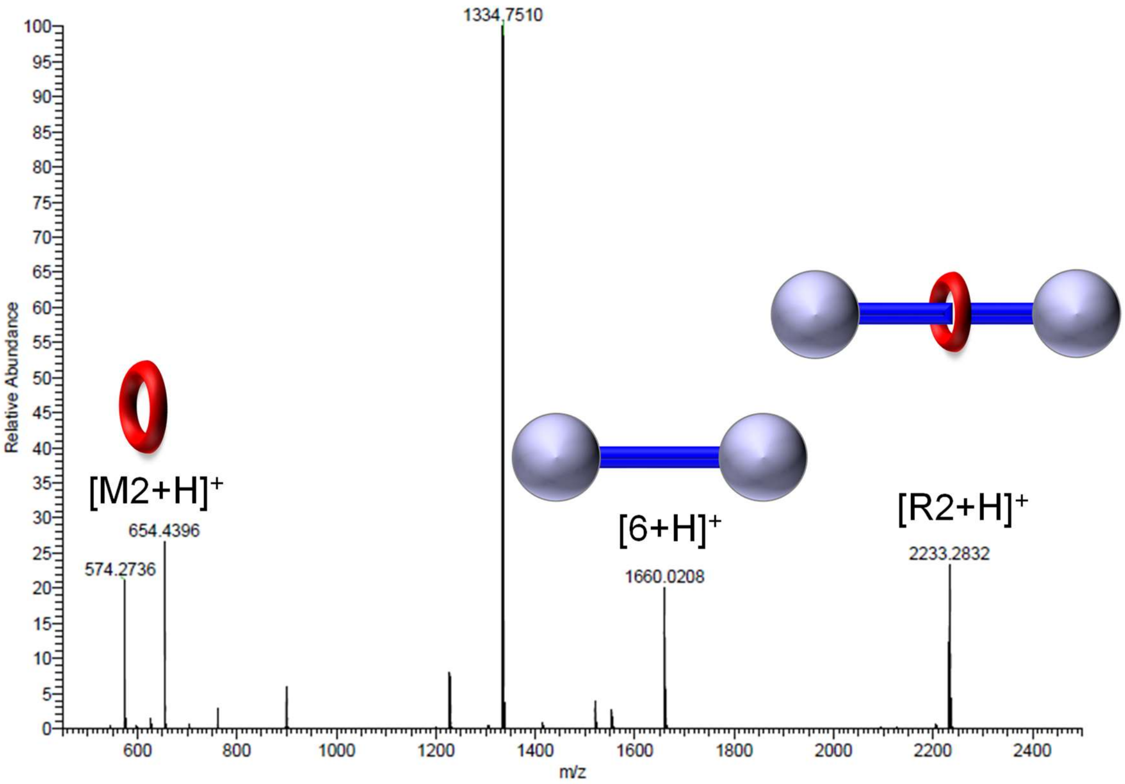


Figure S28: ESI(+)-MS^2 spectrum of rotaxane **R2**.