

**Supporting Information
for
A switchable [2]rotaxane with two active alkenyl
groups**

Xiu-Li Zheng, Rong-Rong Tao, Rui-Rui Gu, Wen-Zhi Wang, Da-Hui Qu*

Address: Key Laboratory for Advanced Materials and Institute of Fine
Chemicals, School of Chemistry and Molecular Engineering, East China
University of Science and Technology, 130 Meilong Road, Shanghai, 200237,
China

Email: Da-Hui Qu* - dahui_qu@ecust.edu.cn

*Corresponding author

**^1H , ^{13}C NMR spectra and HRESI mass spectra of compounds
3, 4, 5, 8 and [2]rotaxane R1**

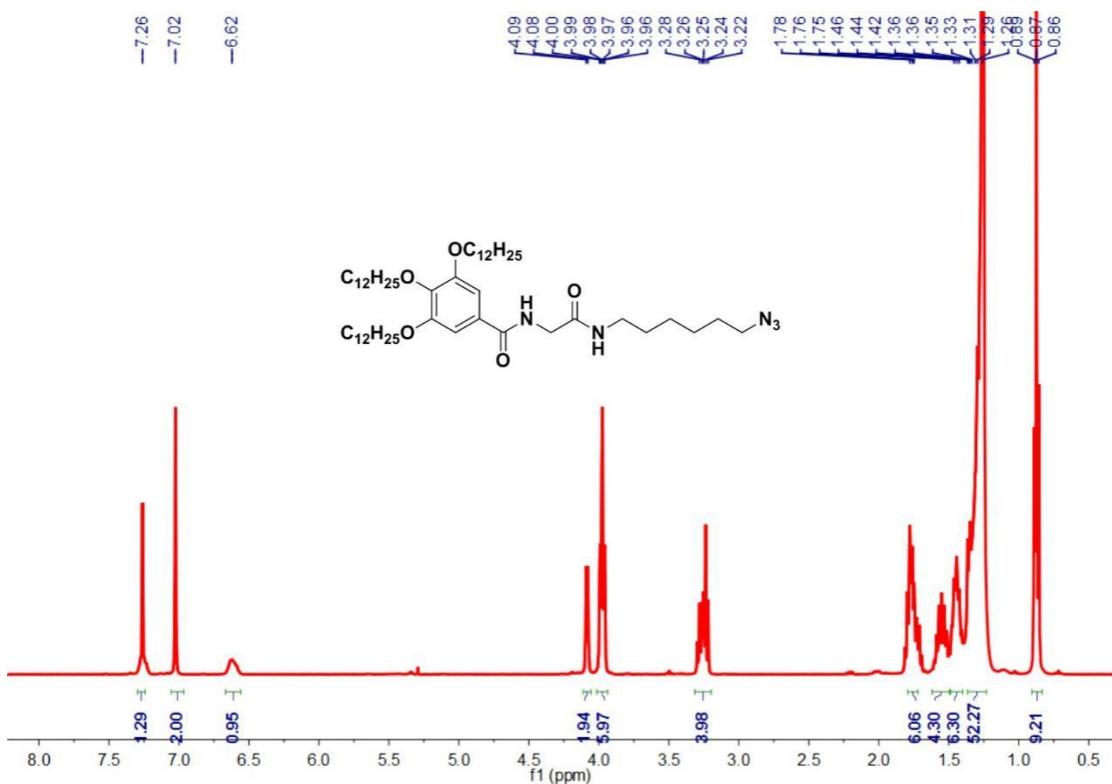


Figure S1: ¹H NMR spectrum of compound 8 (400 MHz, CDCl₃, 298 K).

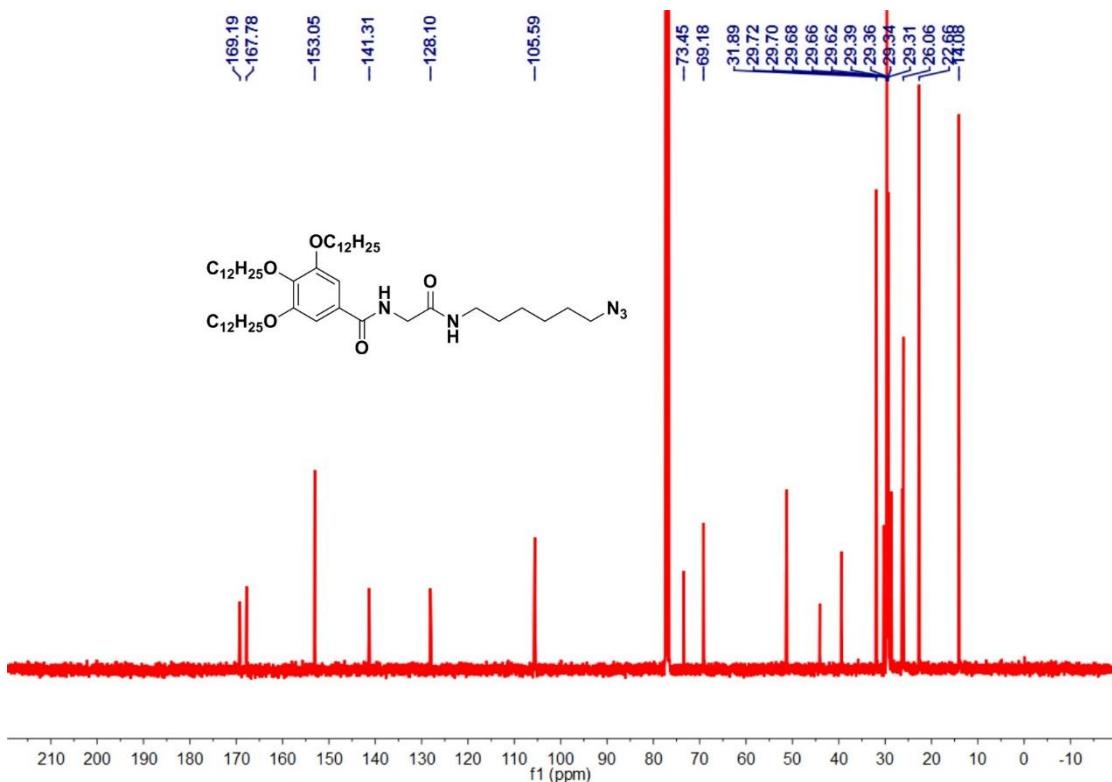


Figure S2: ¹³C NMR spectrum of compound 8 (100 MHz, CDCl₃, 298 K).

Single Mass Analysis

Tolerance = 30.0 PPM / DBE: min = -1.5, max = 100.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions
70 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-51 H: 0-94 N: 0-5 O: 0-5 K: 0-1

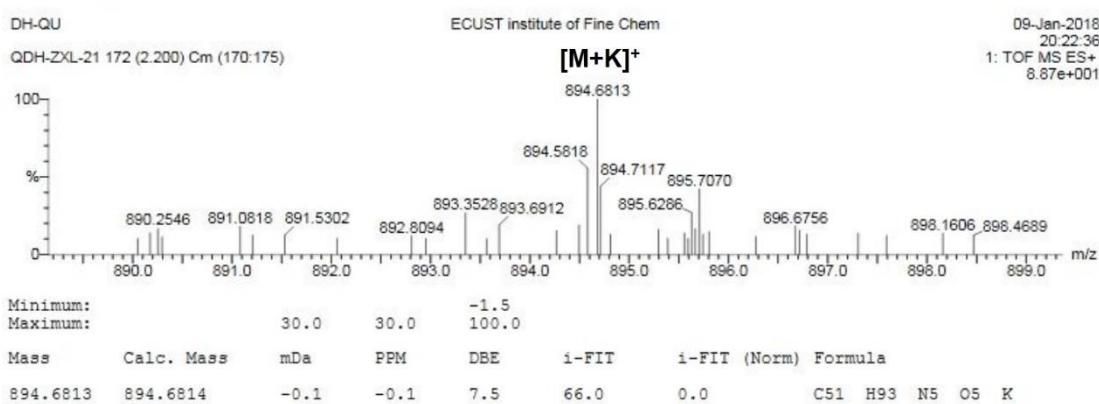


Figure S3: HRESI mass spectrum of compound 8.

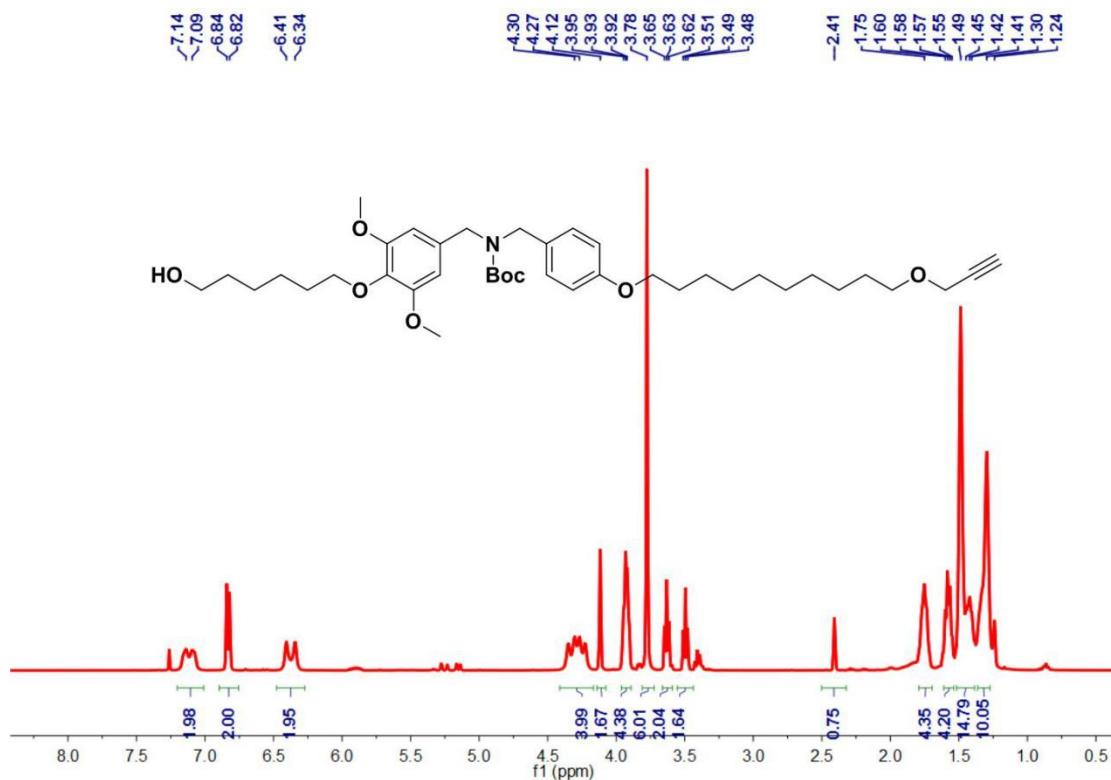


Figure S4: ^1H NMR spectrum of compound **3** (400 MHz, CDCl_3 , 298 K).

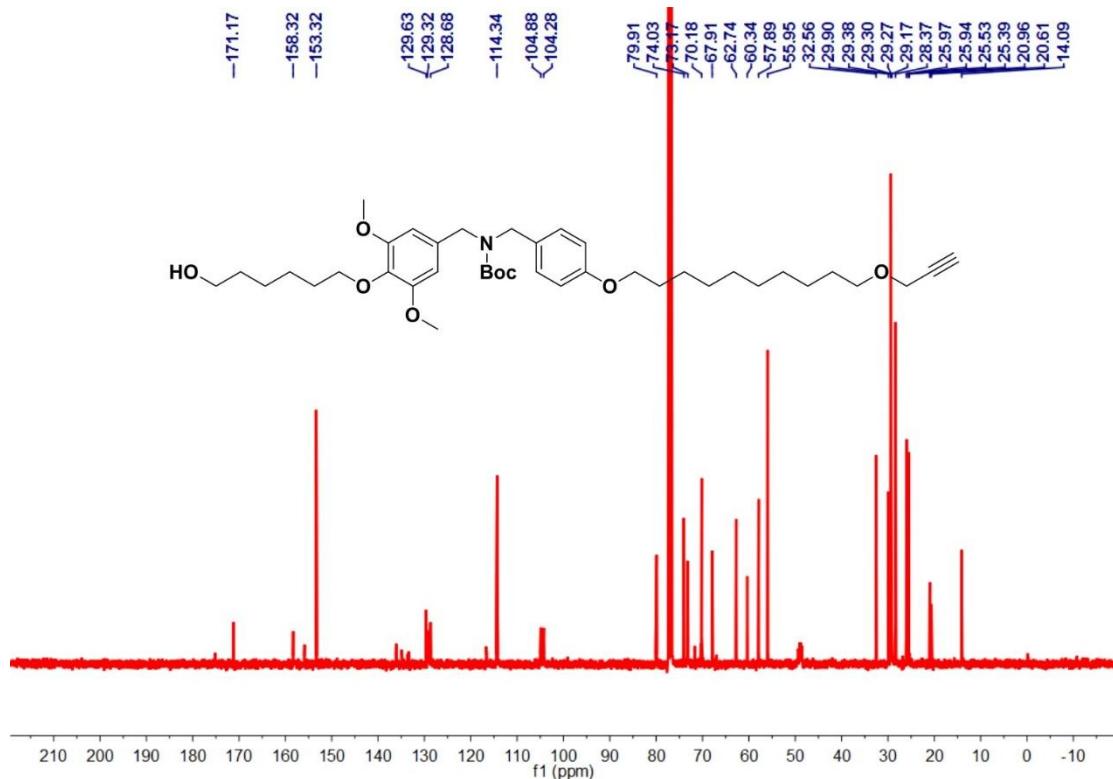


Figure S5: ^{13}C NMR spectrum of compound 3 (100 MHz, CDCl_3 , 298 K).

Single Mass Analysis

Tolerance = 30.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

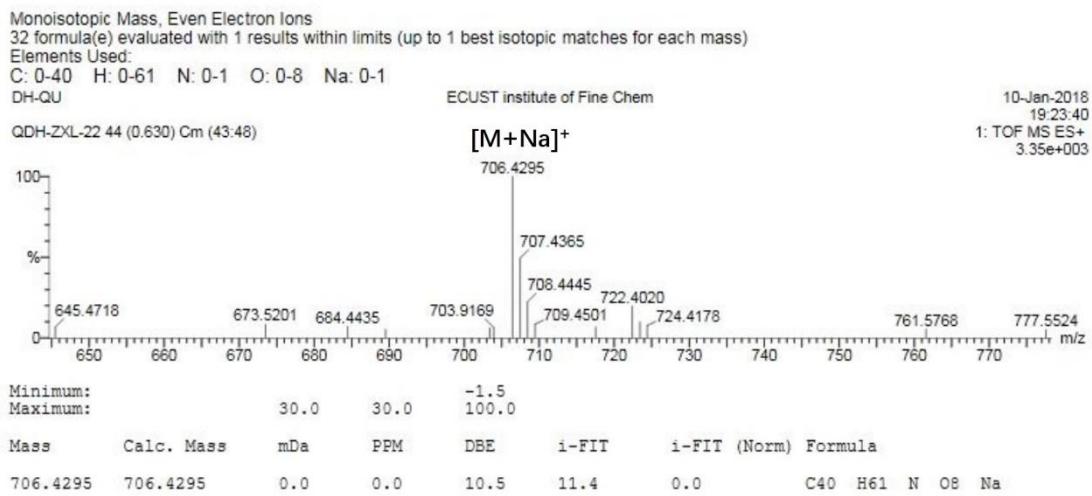


Figure S6: HRESI mass spectrum of compound 3.

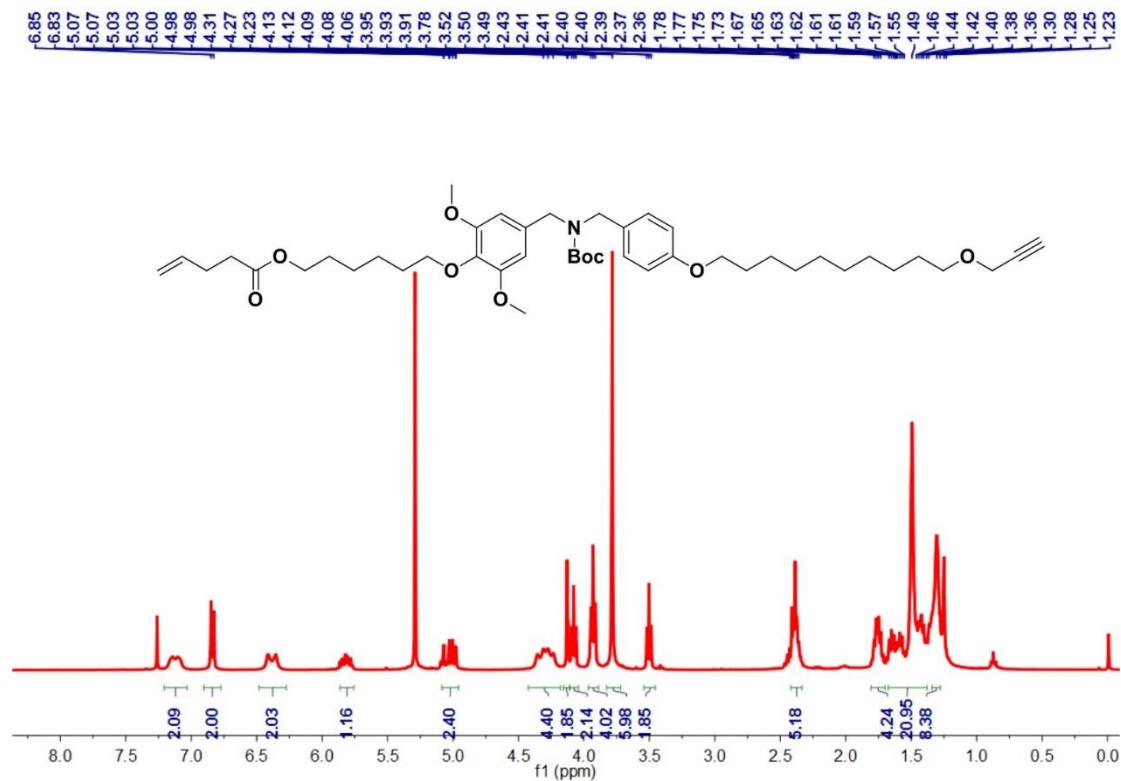


Figure S7: ^1H NMR spectrum of compound **4** (400 MHz, CDCl_3 , 298 K).

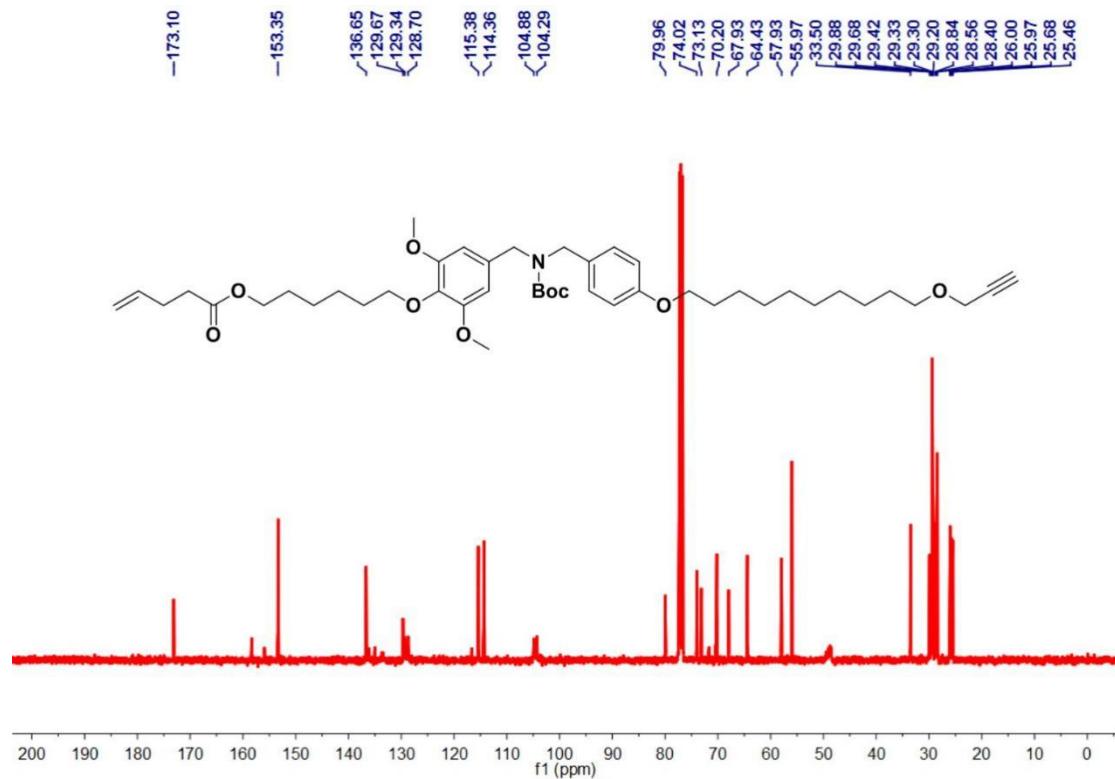


Figure S8: ^{13}C NMR spectrum of compound 4 (100 MHz, CDCl_3 , 298 K).

Single Mass Analysis

Tolerance = 30.0 PPM / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 2

Monoisotopic Mass, Even Electron Ions

35 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

C: 0-45 H: 0-68 N: 0-1 O: 0-9 Na: 0-1

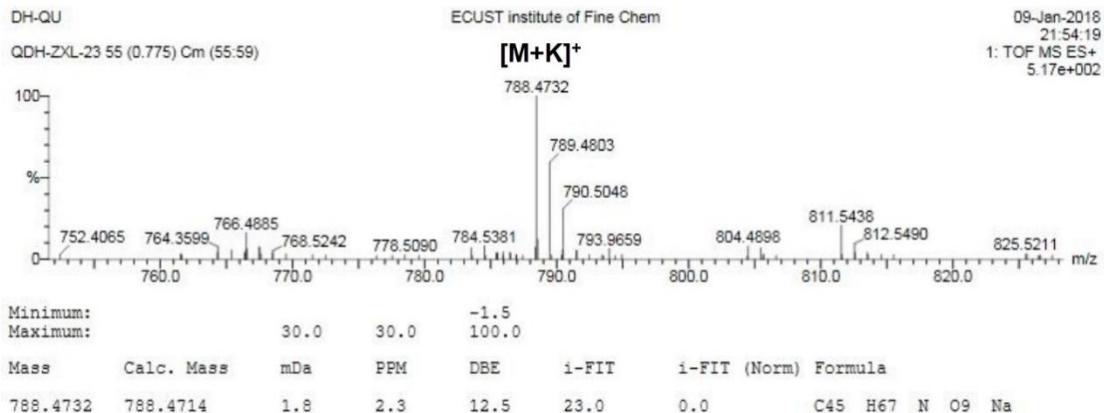


Figure S9: HRESI mass spectrum of compound 4.

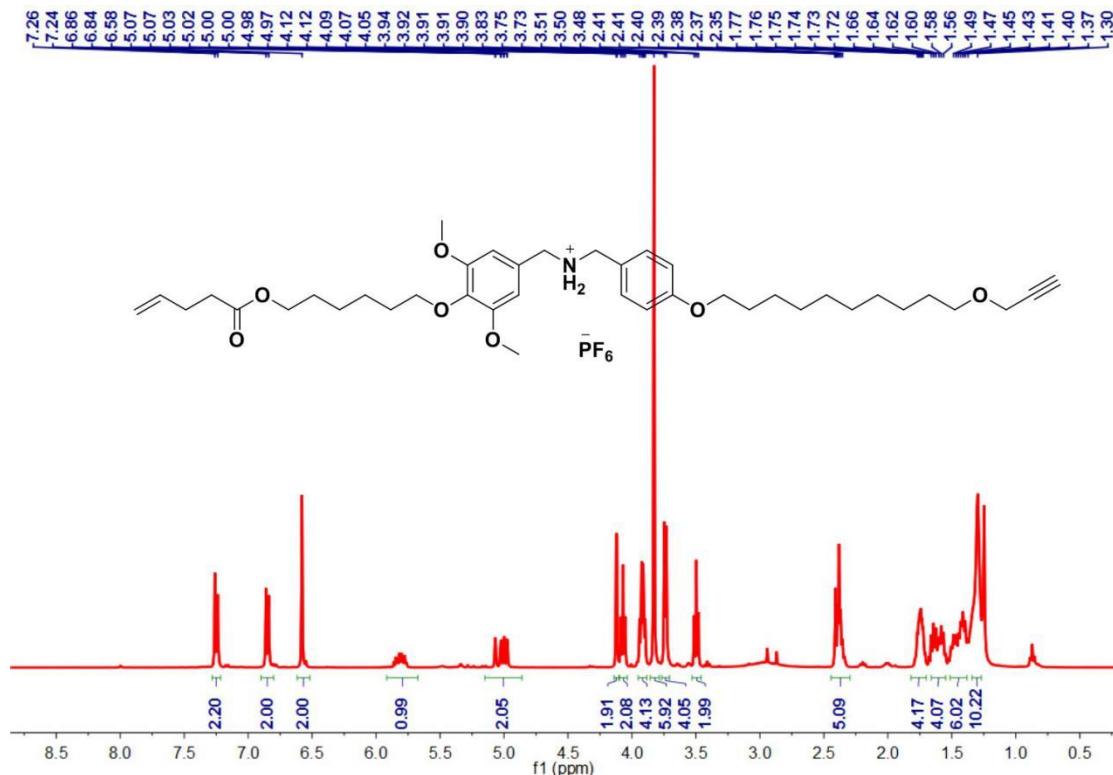


Figure S10: ^1H NMR spectrum of compound **5** (400 MHz, CDCl_3 , 298 K).

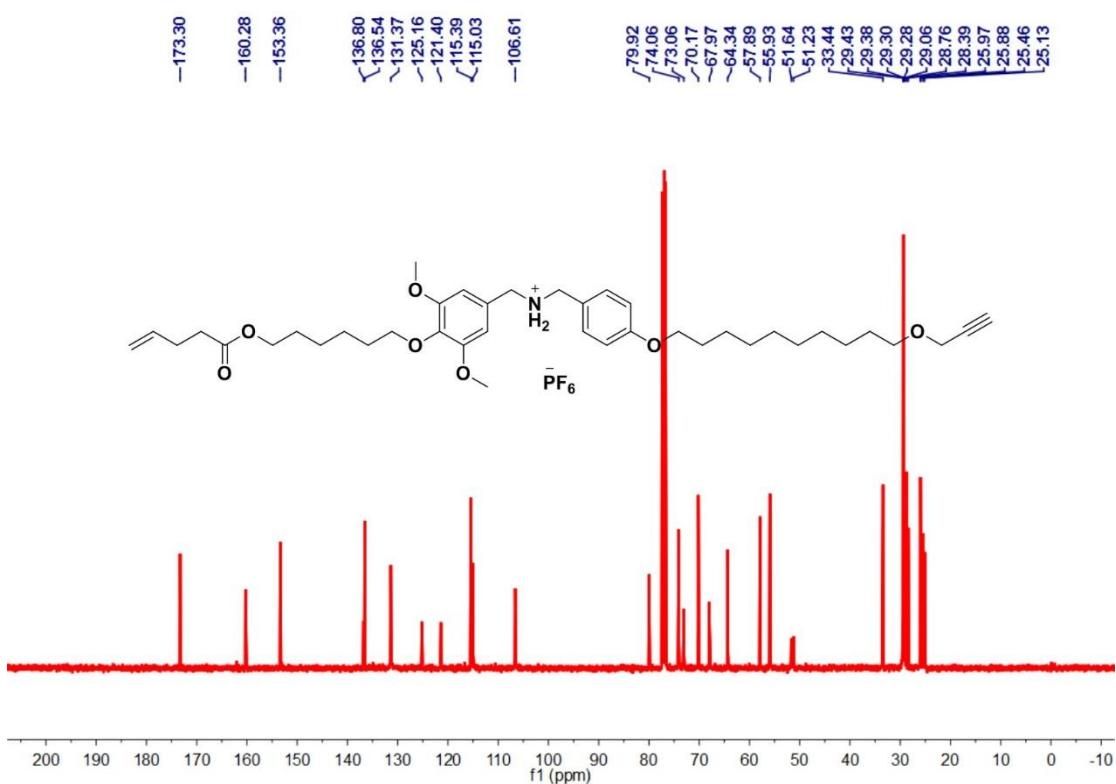


Figure S11: ^{13}C NMR spectrum of compound 5 (100 MHz, CDCl_3 , 298 K).

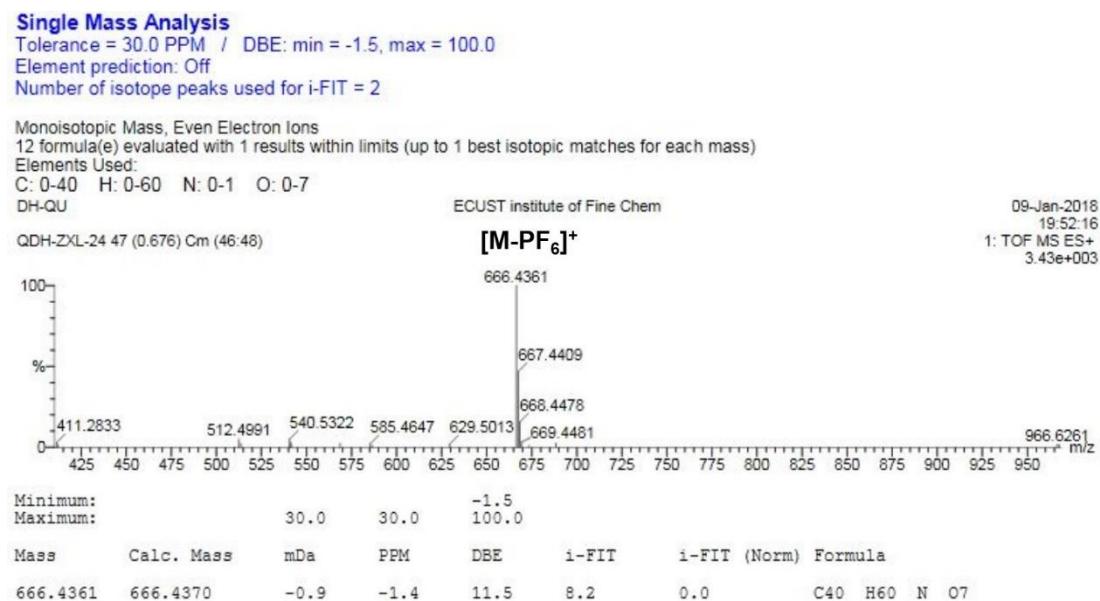


Figure S12: HRESI mass spectrum of compound 5.

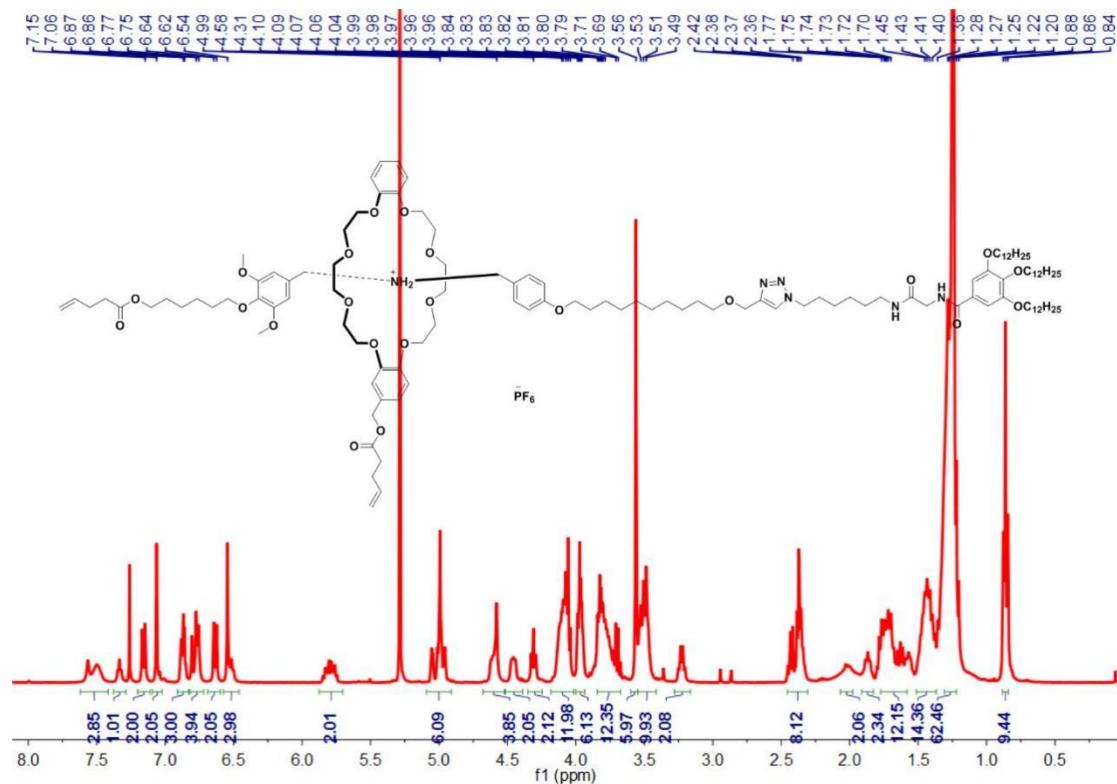


Figure S13: ^1H NMR spectrum of [2]rotaxane **R1** (400 MHz, CDCl_3 , 298 K).

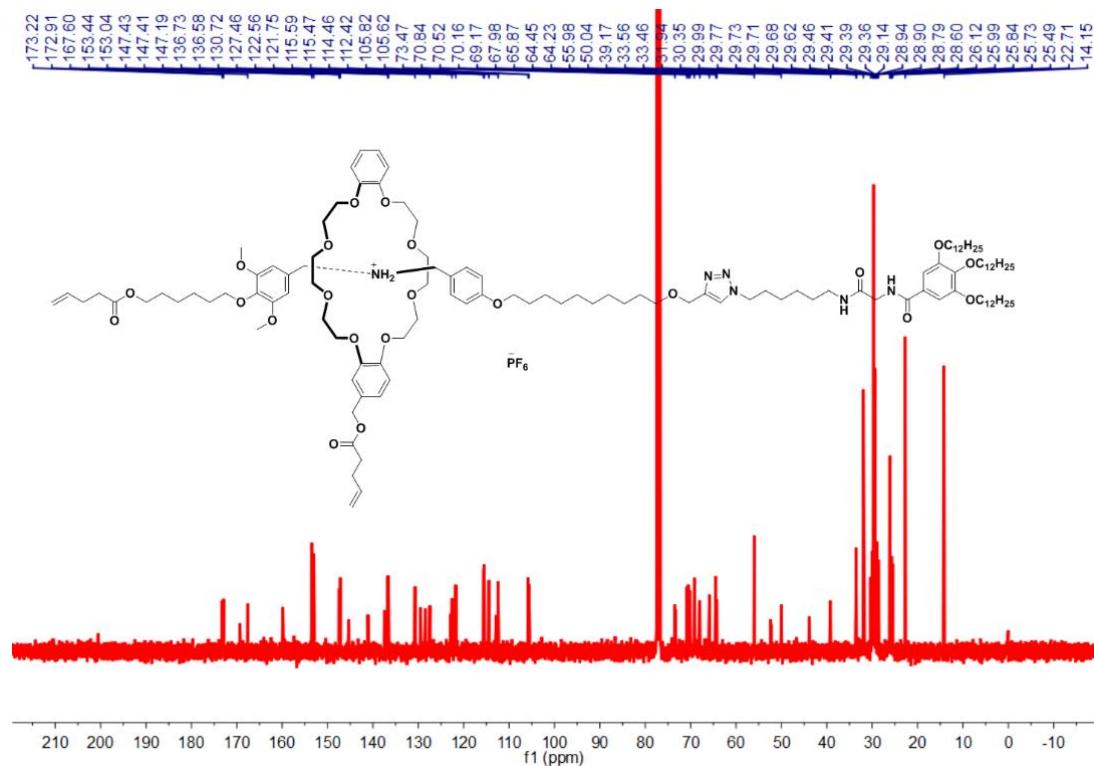


Figure S14: ^{13}C NMR spectrum of [2]rotaxane **R1** (100 MHz, CDCl_3 , 298 K).

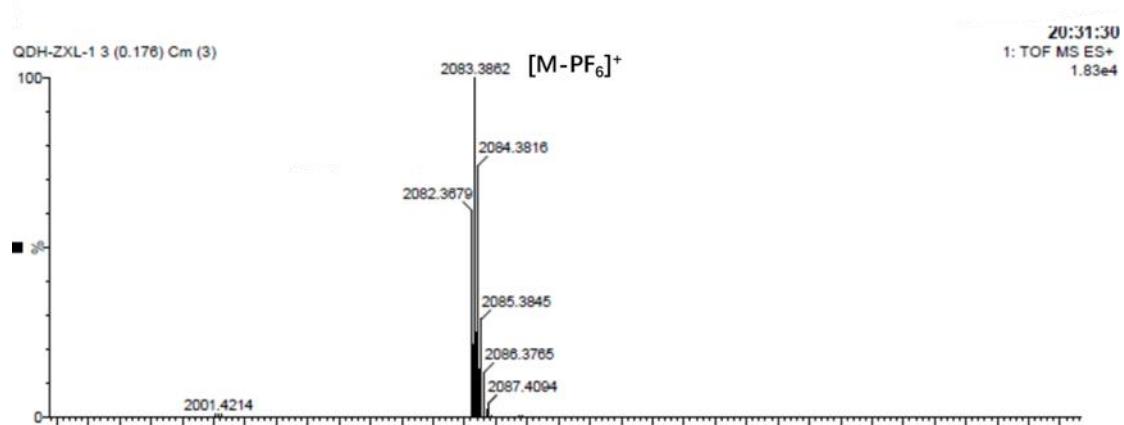


Figure S15: HRESI mass spectrum of [2]rotaxane **R1**.