

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

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

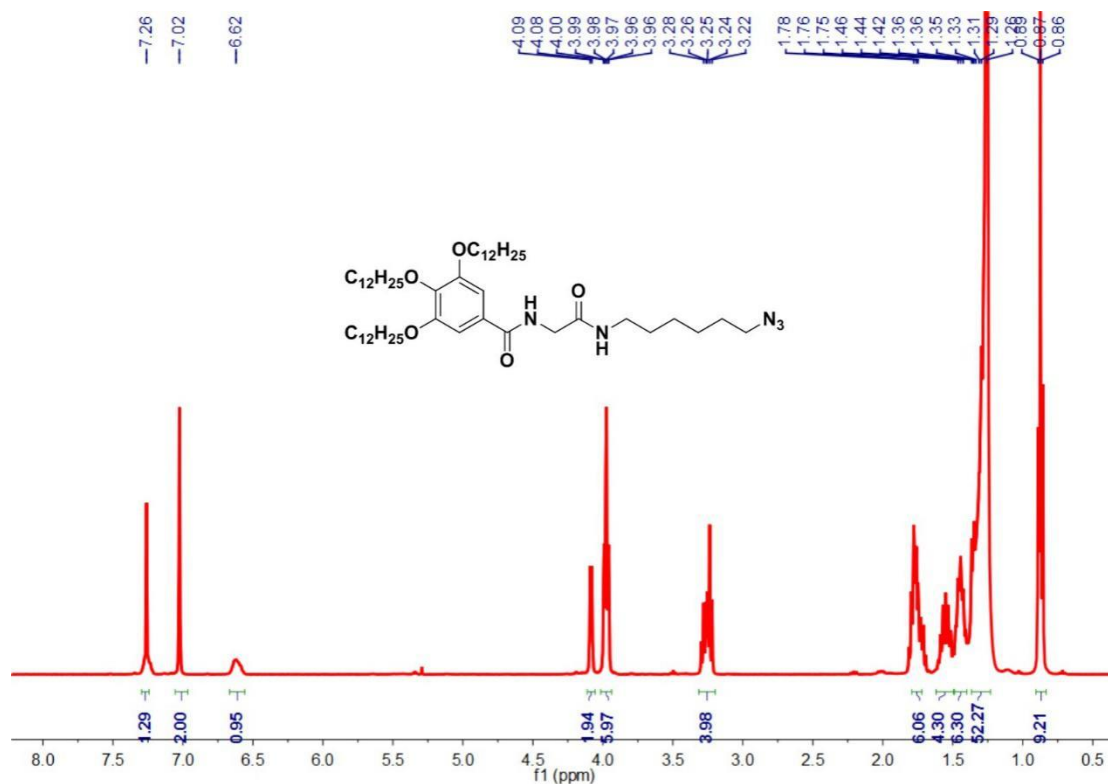


Figure S1: ¹H NMR spectrum of compound **8** (400 MHz, CDCl₃, 298 K).

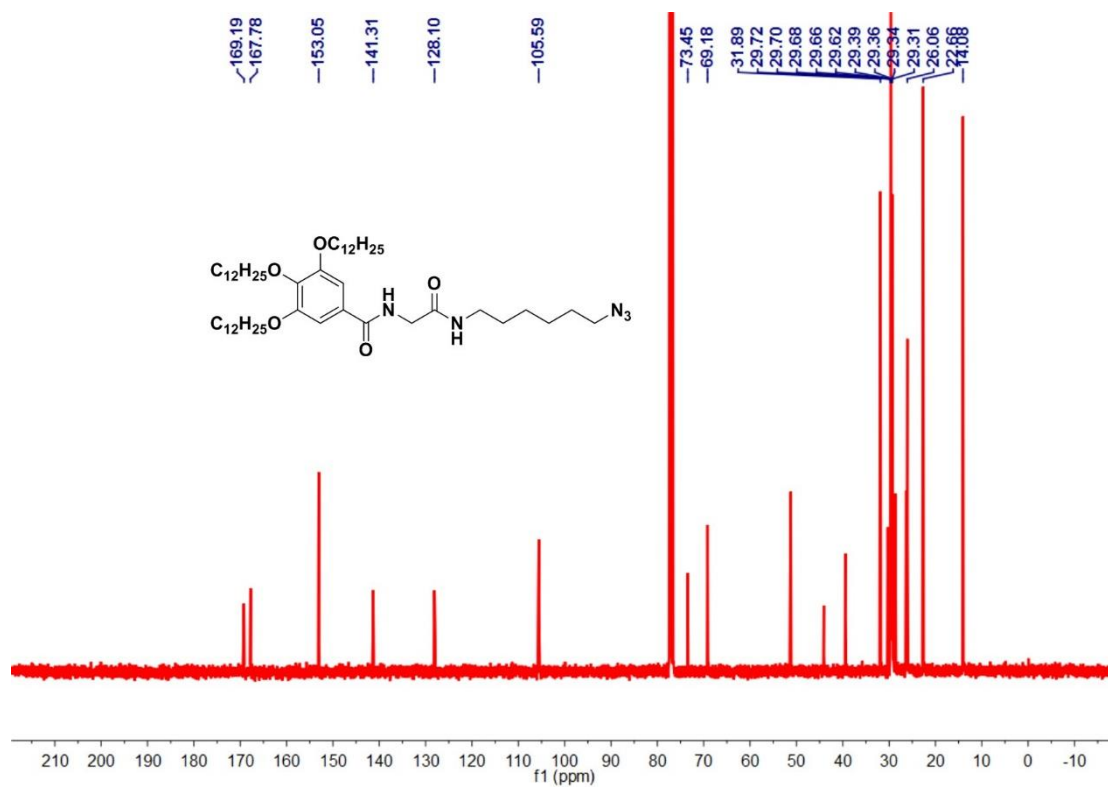


Figure S2: ¹³C NMR spectrum of compound **8** (100 MHz, CDCl₃, 298 K).

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

DH-QU

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09-Jan-2018

QDH-ZXL-21 172 (2.200) Cm (170-175)

20:22:36

1: TOF MS ES+

8.87e+001

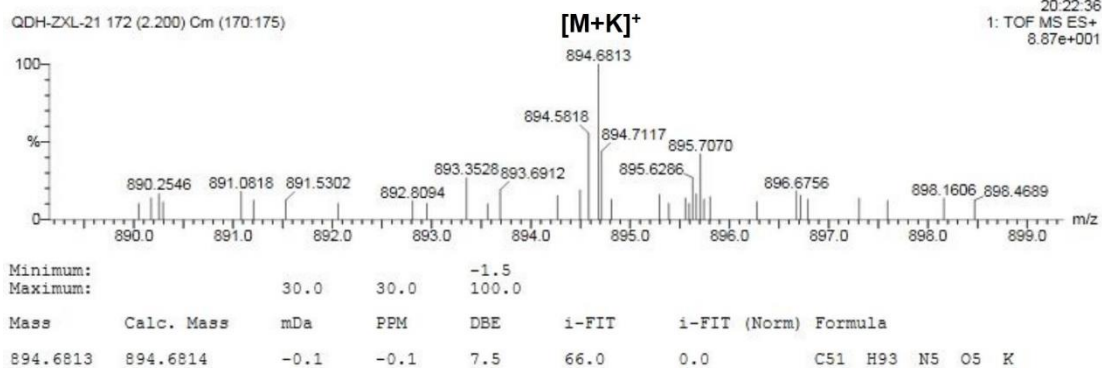


Figure S3: HRESI mass spectrum of compound 8.

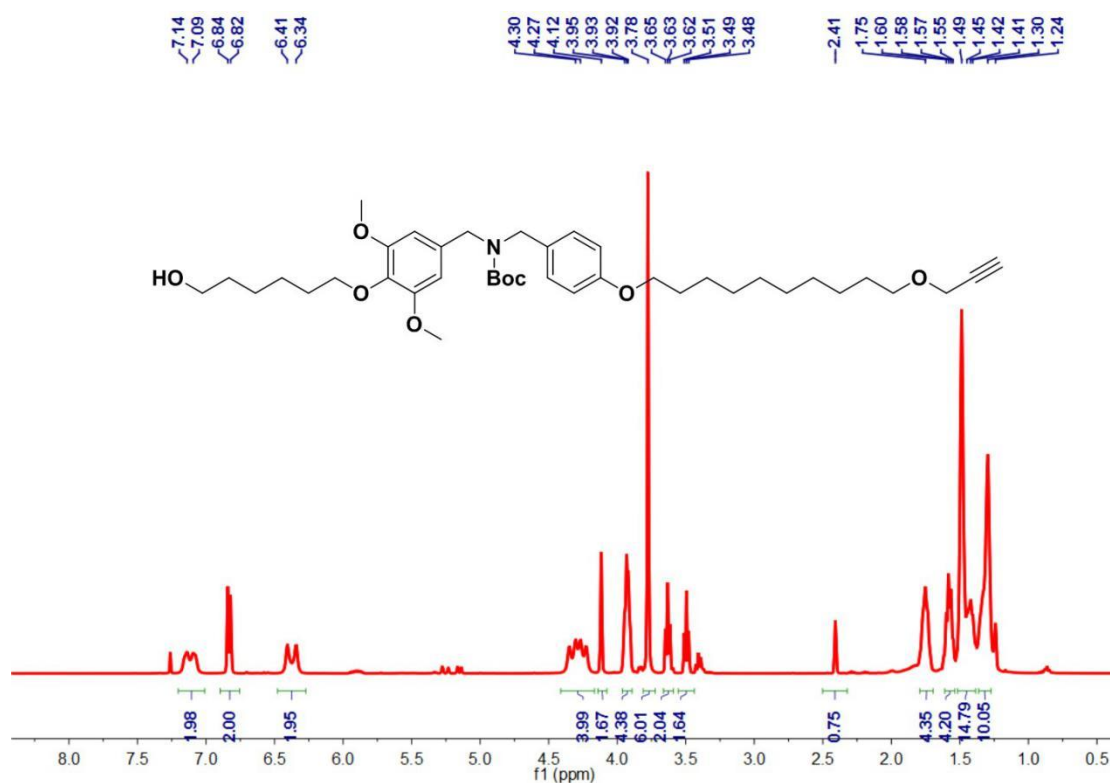


Figure S4: ^1H NMR spectrum of compound 3 (400 MHz, CDCl_3 , 298 K).

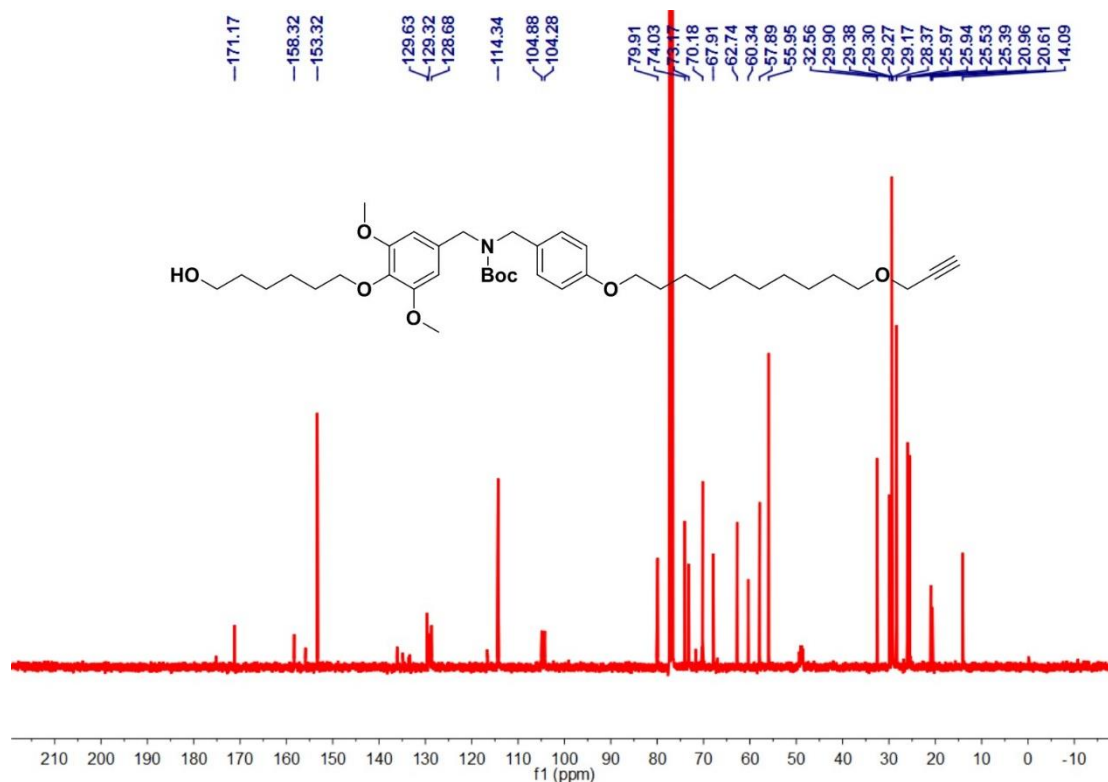


Figure S5: ^{13}C NMR spectrum of compound **3** (100 MHz, CDCl_3 , 298 K).

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

Monoisotopic Mass, Even Electron Ions

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

Elements Used:

C: 0-40 H: 0-61 N: 0-1 O: 0-8 Na: 0-1

DH-QU

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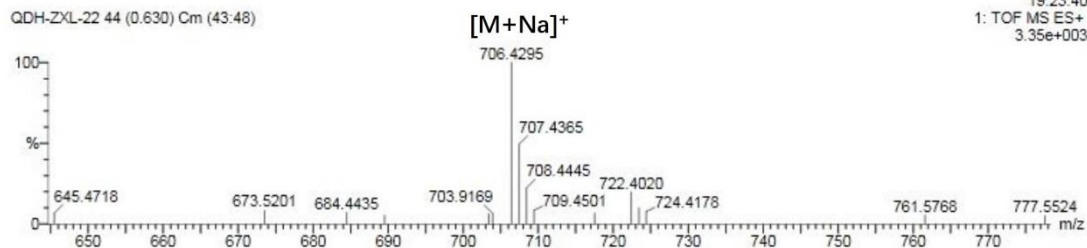
10-Jan-2018

19:23:40

1: TOF MS ES+

3.35e+003

QDH-ZXL-22 44 (0.630) Cm (43.48)



Minimum:

Maximum:

30.0

30.0

-1.5

100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
706.4295	706.4295	0.0	0.0	10.5	11.4	0.0	C40 H61 N 08 Na

Figure S6: HRESI mass spectrum of compound **3**.

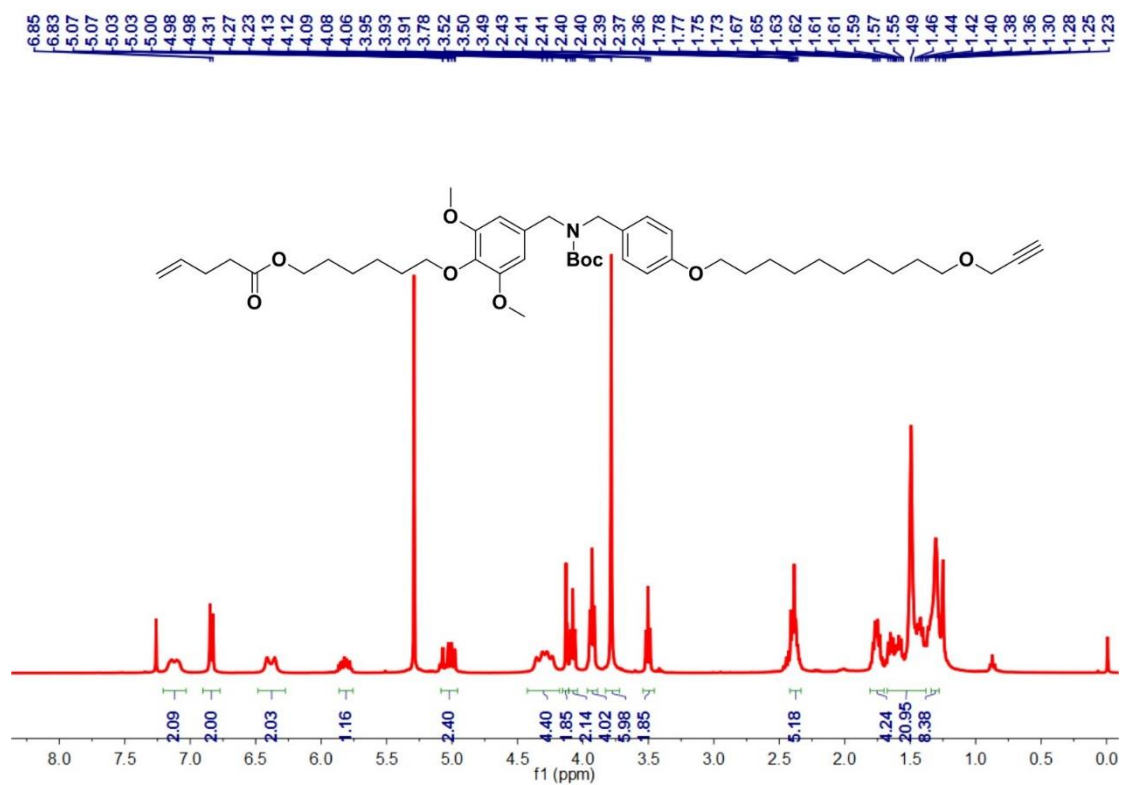


Figure S7: ¹H NMR spectrum of compound **4** (400 MHz, CDCl₃, 298 K).

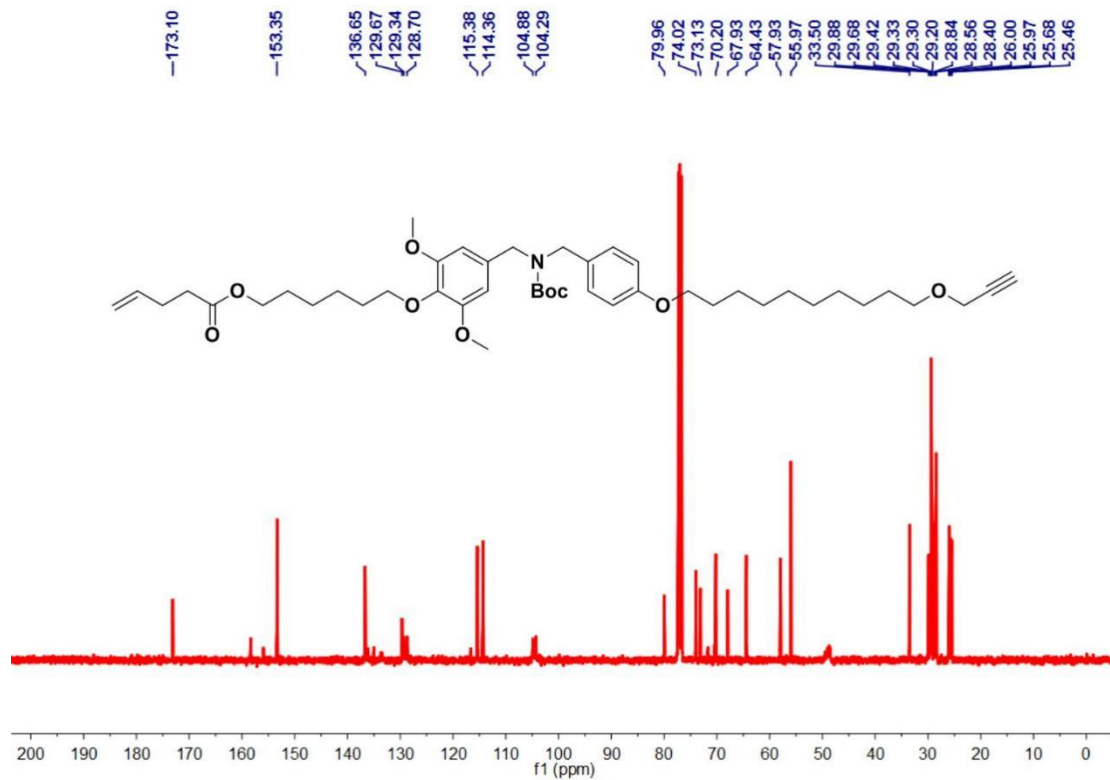


Figure S8: ¹³C NMR spectrum of compound **4** (100 MHz, CDCl₃, 298 K).

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

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

DH-QU

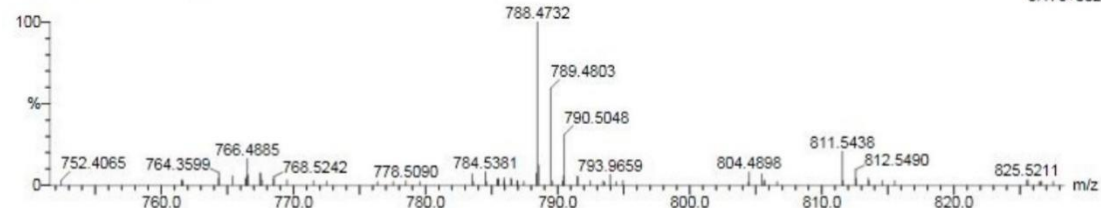
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09-Jan-2016

QDH-ZXL-23 55 (0.775) Cm (55.59)

[M+K]⁺

21:54:19
1: TOF MS ES+
5.17e+002



Minimum:

Maximum:

30.0

30.0

-1.5

100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
788.4732	788.4714	1.8	2.3	12.5	23.0	0.0	C45 H67 N O9 Na

Figure S9: HRESI mass spectrum of compound 4.

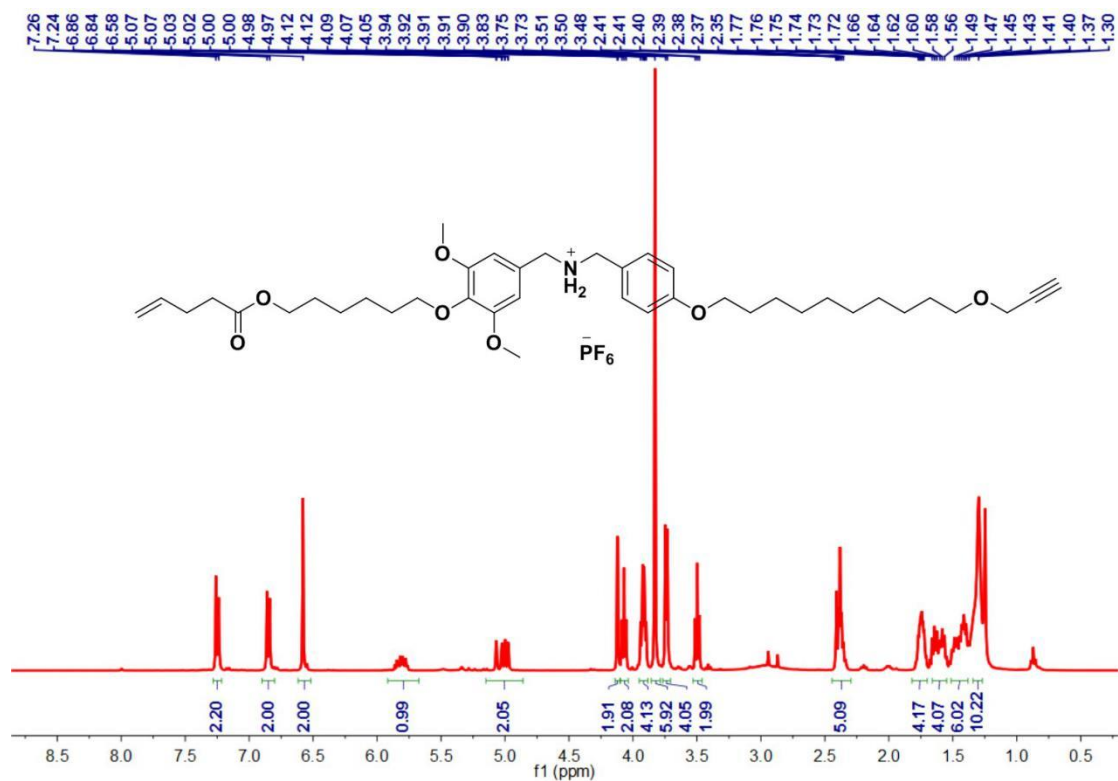


Figure S10: ¹H NMR spectrum of compound 5 (400 MHz, CDCl₃, 298 K).

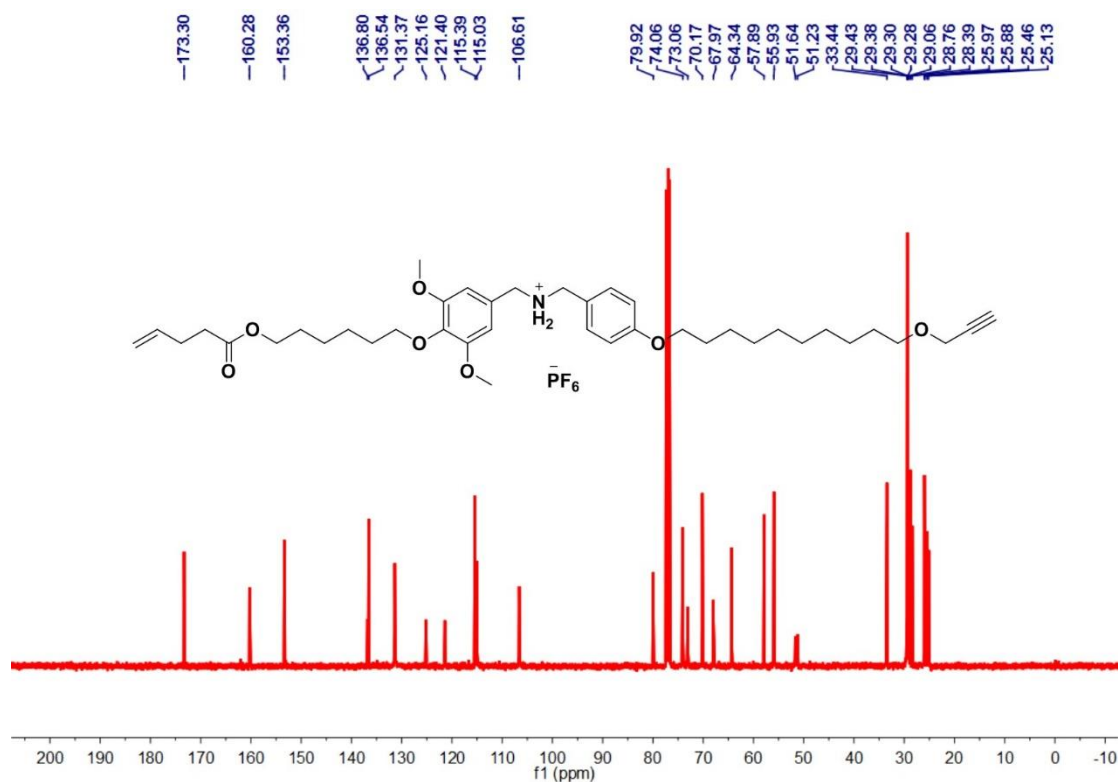


Figure S11: ^{13}C NMR spectrum of compound **5** (100 MHz, CDCl_3 , 298 K).

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

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

Elements Used:

C: 0-40 H: 0-60 N: 0-1 O: 0-7

DH-QU

QDH-ZXL-24 47 (0.676) Cm (46:48)

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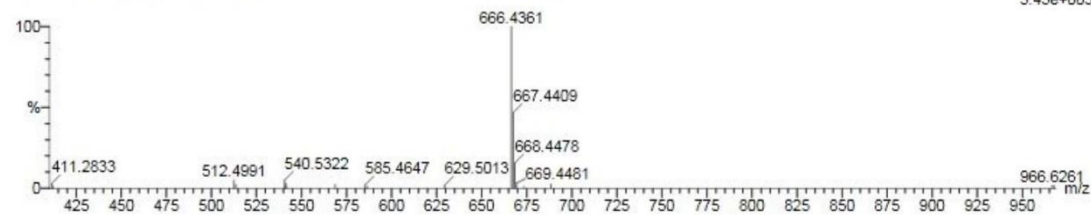
$[\text{M}-\text{PF}_6]^+$

09-Jan-2018

19:52:16

1: TOF MS ES+

3.43e+003



Minimum:

Maximum:

30.0

30.0

-1.5

100.0

Mass

Calc. Mass

mDa

PPM

DBE

i-FIT

i-FIT (Norm)

Formula

666.4361

666.4370

-0.9

-1.4

11.5

8.2

0.0

$\text{C}_{40}\text{H}_{60}\text{N}_7\text{O}_7$

Figure S12: HRESI mass spectrum of compound **5**.

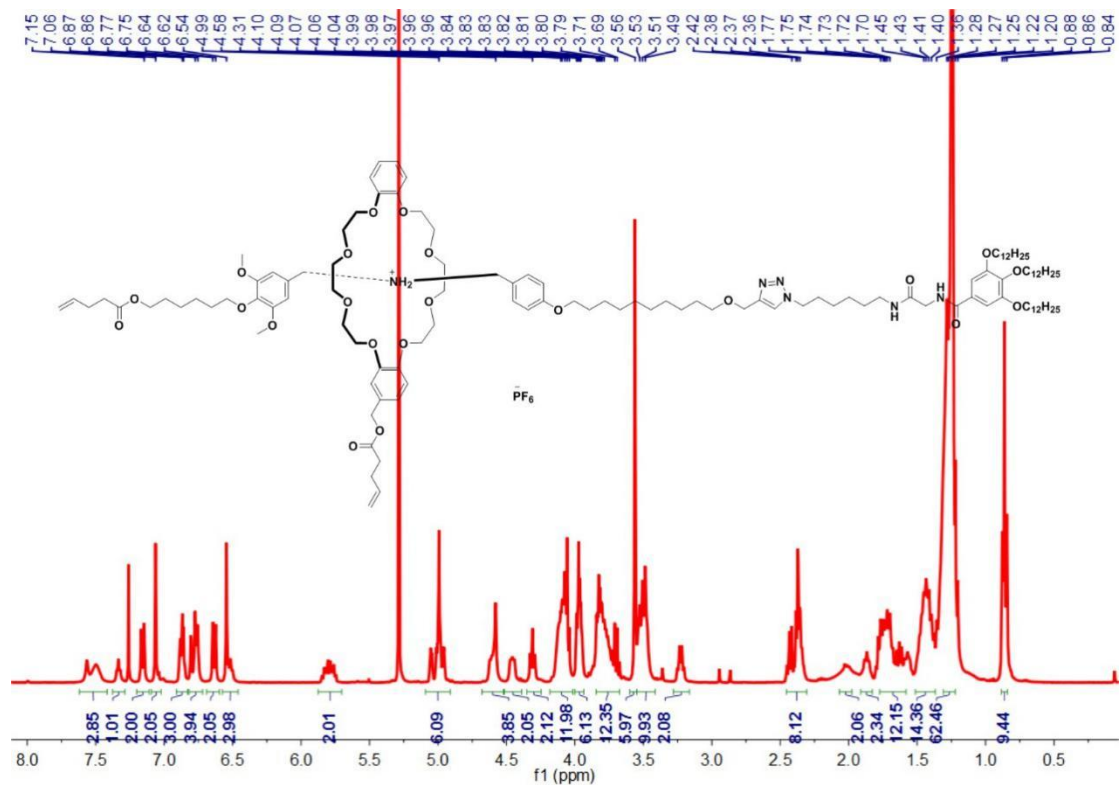


Figure S13: ^1H NMR spectrum of [2]rotaxane **R1** (400 MHz, CDCl_3 , 298 K).

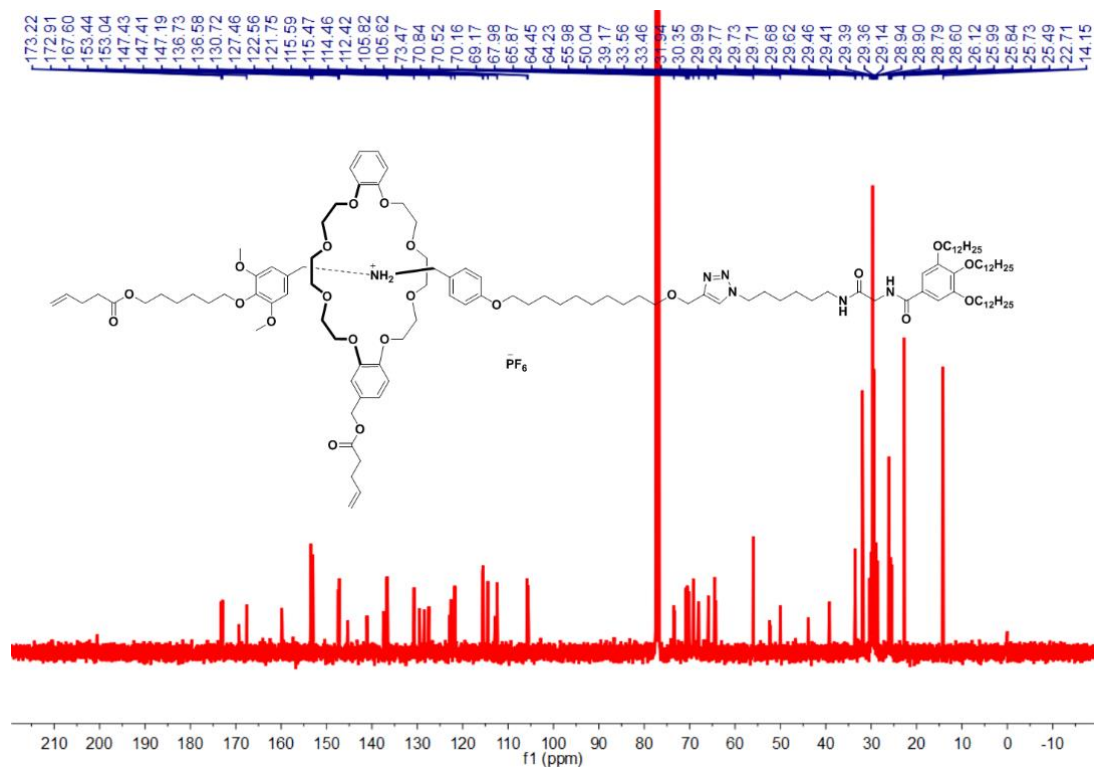


Figure S14: ^{13}C NMR spectrum of [2]rotaxane **R1** (100 MHz, CDCl_3 , 298 K).

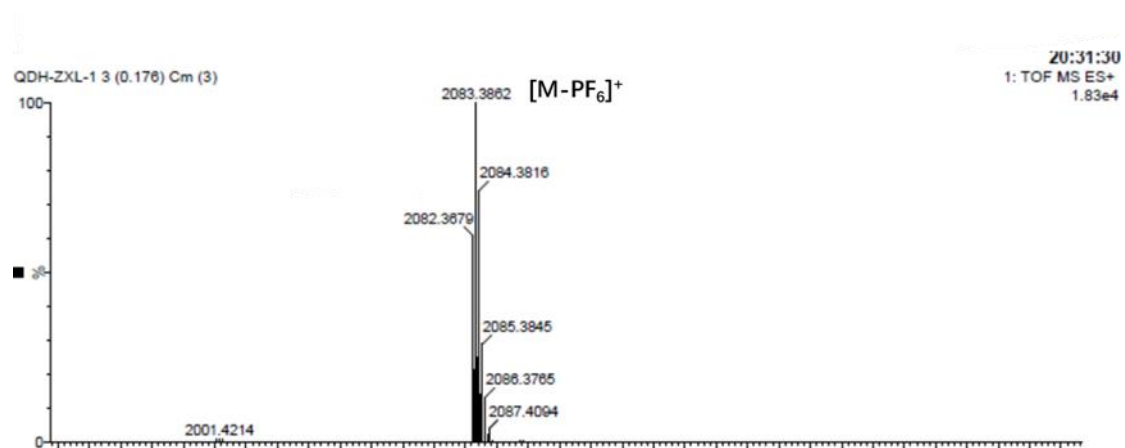


Figure S15: HRESI mass spectrum of [2]rotaxane R1.