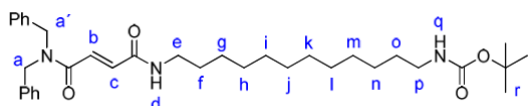


**Control of the assembly of a cyclic hetero[4]pseudorotaxane from a self-complementary [2]rotaxane**

by *Adrian Saura-Sanmartin, Tomas Nicolas-Garcia, Aurelia Pastor, David Quiñonero, Mateo Alajarin, Alberto Martinez-Cuezva and Jose Berna\** published in *Chemical Science*, **2023**, DOI: **10.1039D3SC00886J**; E-mail: [ppberna@um.es](mailto:ppberna@um.es)

**Compound S1**

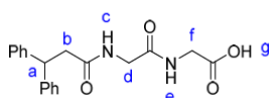


*Fair data for S1 > NMR > 1H >*

*Fair data for S1 > NMR > 13C >*

*Fair data for S1 > NMR > DEPT >*

**Compound S2**

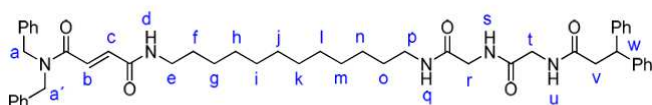


*Fair data for S2 > NMR > 1H >*

*Fair data for S2 > NMR > 13C >*

*Fair data for S2 > NMR > DEPT >*

**Thread 1**

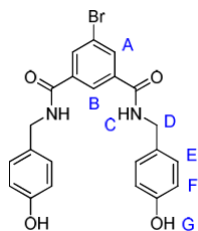


*Fair data for 1 > NMR > 1H >*

*Fair data for 1 > NMR > 13C >*

*Fair data for 1 > NMR > DEPT >*

### Compound S3

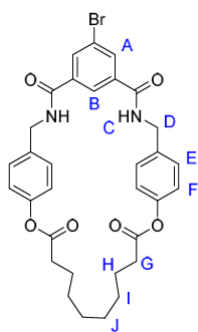


Fair data for S3 > NMR > 1H >

Fair data for S3 > NMR > 13C >

Fair data for S3 > NMR > DEPT >

### Macrocycle 3

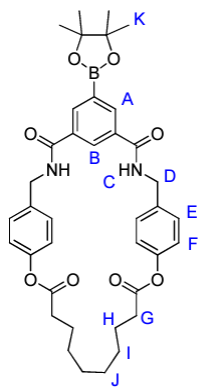


Fair data for 3 > NMR > 1H >

Fair data for 3 > NMR > 13C >

Fair data for 3 > NMR > DEPT >

### Macrocycle 4

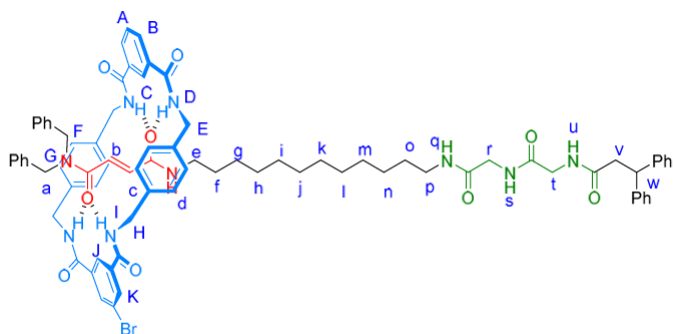


Fair data for 4 > NMR > 1H >

Fair data for 4 > NMR > 13C >

Fair data for 4 > NMR > DEPT >

### Rotaxane 2



Fair data for 2 > NMR > 1H >

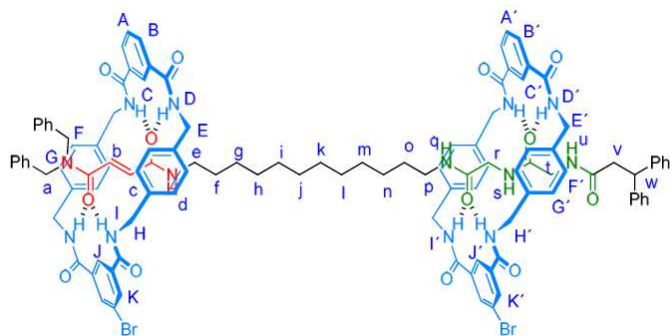
Fair data for 2 > NMR > 13C >

Fair data for 2 > NMR > DEPT >

Fair data for 2 > NMR > COSY >

Fair data for 2 > NMR > HMQC >

### [3]Rotaxane S4



*Fair data for S4 > NMR > 1H >*

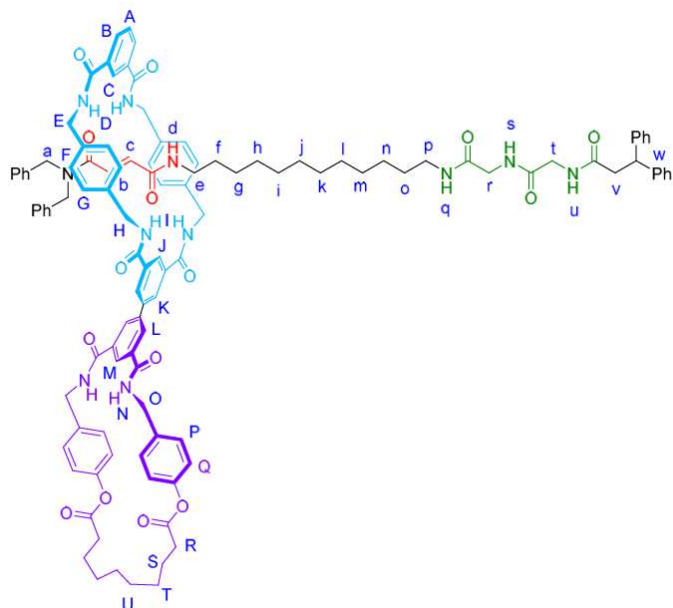
*Fair data for S4 > NMR > 13C >*

*Fair data for S4 > NMR > DEPT >*

*Fair data for S4 > NMR > COSY >*

*Fair data for S4 > NMR > HMQC >*

## Compound 5



Fair data for 5 > NMR > 1H >

Fair data for 5 > NMR > 13C >

Fair data for 5 > NMR > DEPT >

Fair data for 5 > NMR > COSY >

Fair data for 5 CD<sub>2</sub>Cl<sub>2</sub> > NMR > 1H >

Fair data for 5 CD<sub>2</sub>Cl<sub>2</sub> > NMR > COSY >

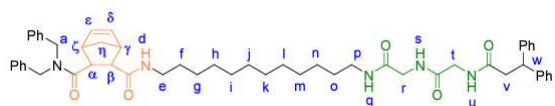
Fair data for 5 CD<sub>2</sub>Cl<sub>2</sub> > NMR > NOESY >

Fair data for 5 DMSO > NMR > 1H >

Fair data for 5 DMSO > NMR > COSY >

Fair data for 5 DMSO > NMR > NOESY >

### Thread Cp-1



Fair data for Cp-1 > NMR > 1H >

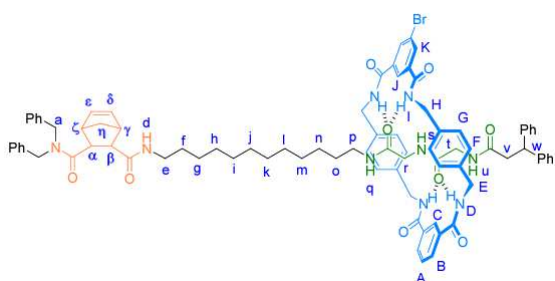
Fair data for Cp-1 > NMR > 13C >

Fair data for Cp-1 > NMR > DEPT >

Fair data for Cp-1 > NMR > COSY >

Fair data for Cp-1 > NMR > HMBC >

### Thread Cp-2



Fair data for Cp-2 > NMR > 1H >

Fair data for Cp-2 > NMR > 13C >

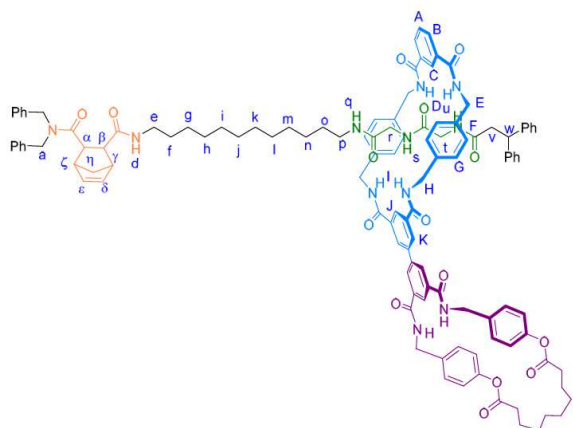
Fair data for Cp-2 > NMR > DEPT >

Fair data for Cp-2 > NMR > COSY >

Fair data for Cp-2 > NMR > HMBC >

Fair data for Cp-2 > NMR > HMQC >

## Cp-5



*Fair data for Cp-5 > NMR > 1H >*

*Fair data for Cp-5 > NMR > 13C >*

*Fair data for Cp-5 > NMR > DEPT >*

*Fair data for Cp-5 > NMR > COSY >*

*Fair data for Cp-5 > NMR > HMQC >*