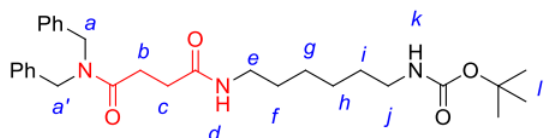


Files folders for the fair data of the published article

Mechanical bonding activation in rotaxane-based organocatalysts by *Jesús de María Pérez, Tainara Orlando, Aurelia Pastor, Marcos A. P. Martins, Mateo Alajarín, Alberto Martínez-Cuezva* and Jose Berna** published in *Org. Chem. Front.*, **2021**, DOI: [10.1039/D1QO00789K](https://doi.org/10.1039/D1QO00789K) - E-mail: amcuezva, ppberna@um.es

Compound S2a:



Fair data for compound S2a > NMR > 1H >

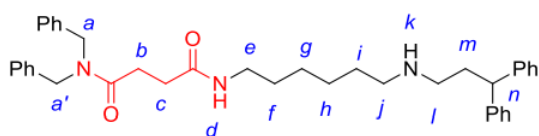
Fair data for compound S2a > NMR > 13C >

Fair data for compound S2a > NMR > COSY >

Fair data for compound S2a > NMR > DEPT >

Fair data for compound S2a > HRMS

Thread 1a:



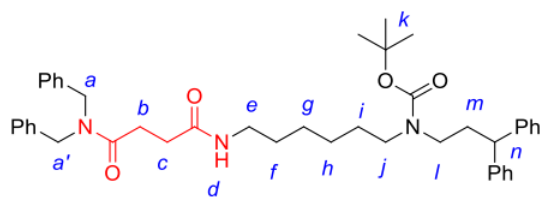
Fair data for compound 1a > NMR > 1H >

Fair data for compound 1a > NMR > 13C >

Fair data for compound 1a > NMR > DEPT >

Fair data for compound 1a > HRMS >

Thread **Boc1a**:



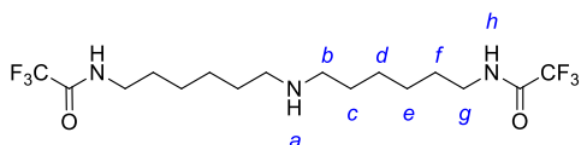
Fair data for compound **Boc1a** > NMR > ^1H >

Fair data for compound **Boc1a** > NMR > ^{13}C >

Fair data for compound **Boc1a** > NMR > DEPT >

Fair data for compound **Boc1a** > HRMS >

Compound **S2b**:

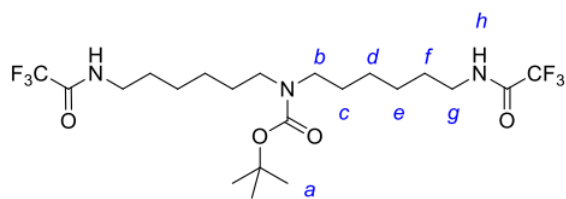


Fair data for compound **S2b** > NMR > ^1H >

Fair data for compound **S2b** > NMR > ^{13}C >

Fair data for compound **S2b** > NMR > ^{19}F >

Compound S3b:

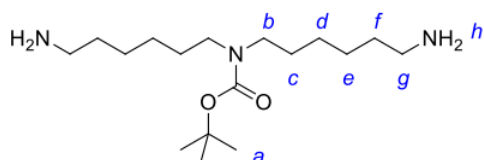


Fair data for compound **S3b** > NMR > 1H >

Fair data for compound **S3b** > NMR > 13C >

Fair data for compound **S3b** > NMR > 19F >

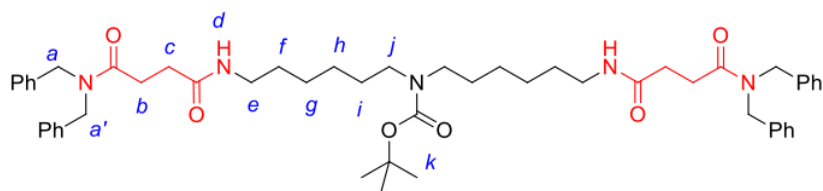
Compound S4b:



Fair data for compound **S4b** > NMR > 1H >

Fair data for compound **S4b** > NMR > 13C >

Thread Boc1b:

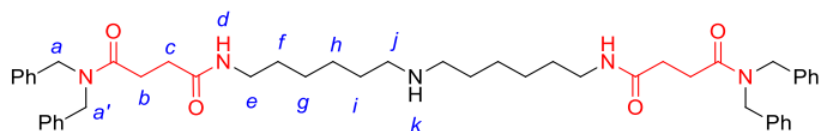


Fair data for Thread **Boc1b** > NMR > 1H >

Fair data for Thread **Boc1b** > NMR > 13C >

Fair data for Thread **Boc1b** > NMR > DEPT >

Thread 1b:



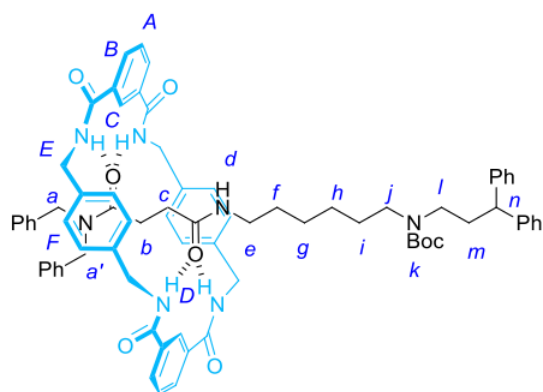
Fair data for Thread 1b > NMR > 1H >

Fair data for Thread 1b > NMR > 13C >

Fair data for Thread 1b > NMR > DEPT >

Fair data for Thread 1b > HRMS >

Rotaxane Boc2a:



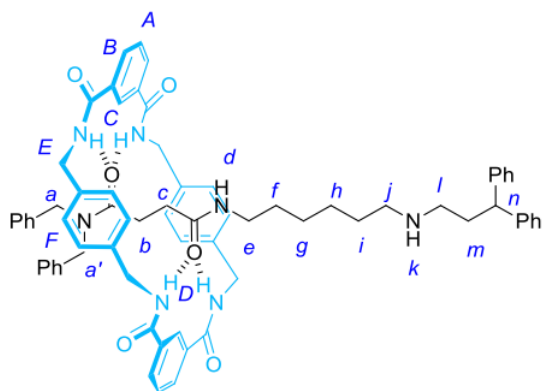
Fair data for Rotaxane Boc2a > NMR > 1H >

Fair data for Rotaxane Boc2a > NMR > 13C >

Fair data for Rotaxane Boc2a > NMR > DEPT >

Fair data for Rotaxane Boc2a > HRMS >

Rotaxane 2a:



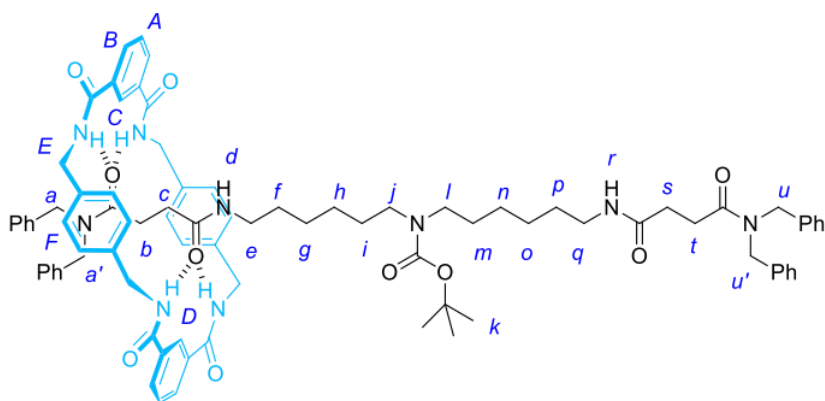
Fair data for Rotaxane 2a > NMR > 1H >

Fair data for Rotaxane 2a > NMR > 13C >

Fair data for Rotaxane 2a > NMR > DEPT >

Fair data for Rotaxane 2a > HRMS >

Rotaxane Boc2b:

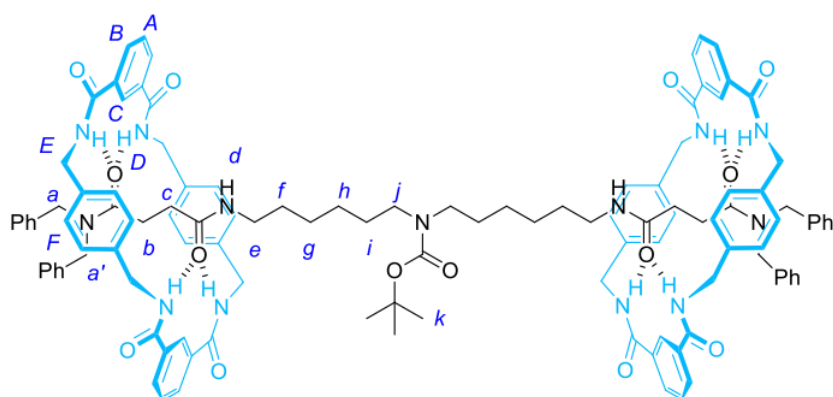


Fair data for Rotaxane Boc2b > NMR > 1H >

Fair data for Rotaxane Boc2b > NMR > 13C >

Fair data for Rotaxane Boc2b > NMR > DEPT >

Rotaxane **Boc3b**:

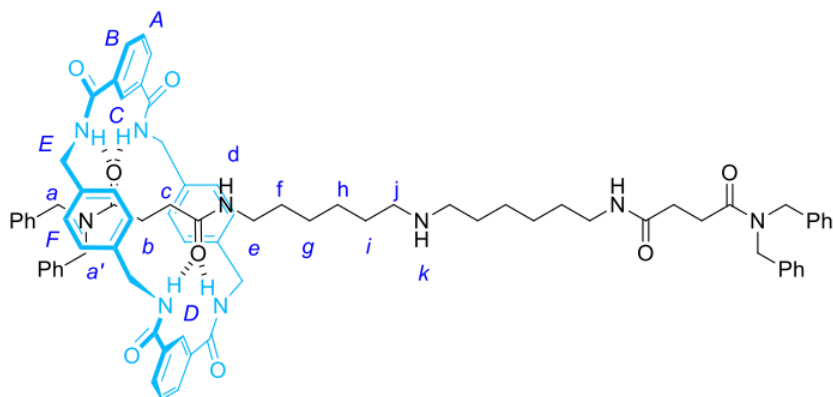


Fair data for Rotaxane **Boc3b** > NMR > ¹H >

Fair data for Rotaxane **Boc3b** > NMR > ¹³C >

Fair data for Rotaxane **Boc3b** > NMR > DEPT >

Rotaxane **2b**:



Fair data for Rotaxane **2b** > NMR > ¹H >

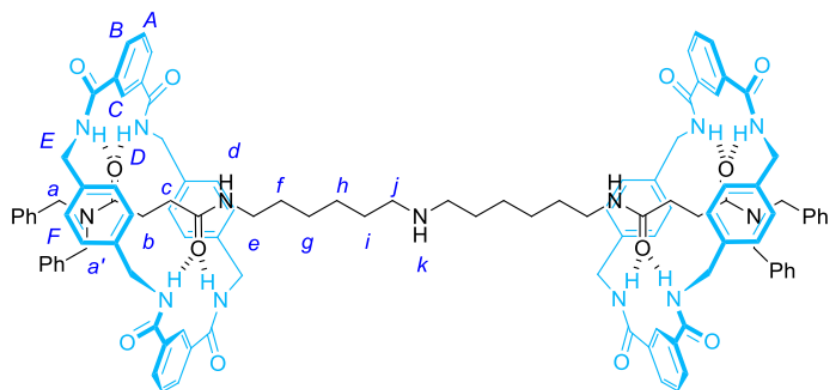
Fair data for Rotaxane **2b** > NMR > ¹³C >

Fair data for Rotaxane **2b** > NMR > DEPT >

Fair data for Rotaxane **2b** > NMR > COSY >

Fair data for Rotaxane **2b** > HRMS >

Rotaxane 3b:



Fair data for Rotaxane 3b > NMR > 1H >

Fair data for Rotaxane 3b > NMR > 13C >

Fair data for Rotaxane 3b > NMR > DEPT >