

A Multi-Step Synthesis Approach to a Functional [2]Rotaxane

Gustavo Henrique Weimer¹, Fellipe Freire Santos de Farias¹, Tainara Orlando², Paulo Roberto dos Santos Salbego³, and Marcos Antonio Pinto Martins^{1*}

1) Núcleo de Química de Heterociclos (NUQUIMHE), Department of Chemistry, Federal University of Santa Maria (UFSM), 97105-900, Santa Maria, RS, Brazil.

2) Academic Department of Chemistry, Federal Technological University of Paraná (UTFPR), Medianeira Campus, PR, Brazil.

3) Núcleo de Química de Heterociclos (NUQUIMHE), Department of Engineering and Environmental Technology (DETA), Federal University of Santa Maria (UFSM), 98400-000, Frederico Westphalen Campus, RS, Brazil.

*e-mail: martins.marcos@ufsm.br

Keywords: Molecular machines, rotaxanes, molecular dynamics

ABSTRACT

Mechanically Interlocked Molecules (MIMs) are characterized by the presence of mechanical bonds,¹ consisting of one or more components interconnected through their intrinsic topology.² Rotaxanes, a subclass of MIMs, typically comprise a linear molecule with bulky end groups (thread), and a cyclic molecule (macrocycle), connected by a mechanical bond.³ The controlled and reversible translational and rotational movements of the macrocycle in relation to the thread can classify these compounds as molecular machines.^{4,5} In this context, this study aims to present the synthesis of a [2]rotaxane molecule with two stations on the thread, enabling both rotational and translational movements. The synthesis of the target [2]rotaxane **1** involved several synthetic steps, including nucleophilic additions reactions, SN₂, [3+2] cycloaddition (CuAAC), multi component reactions applying the clipping methodology.

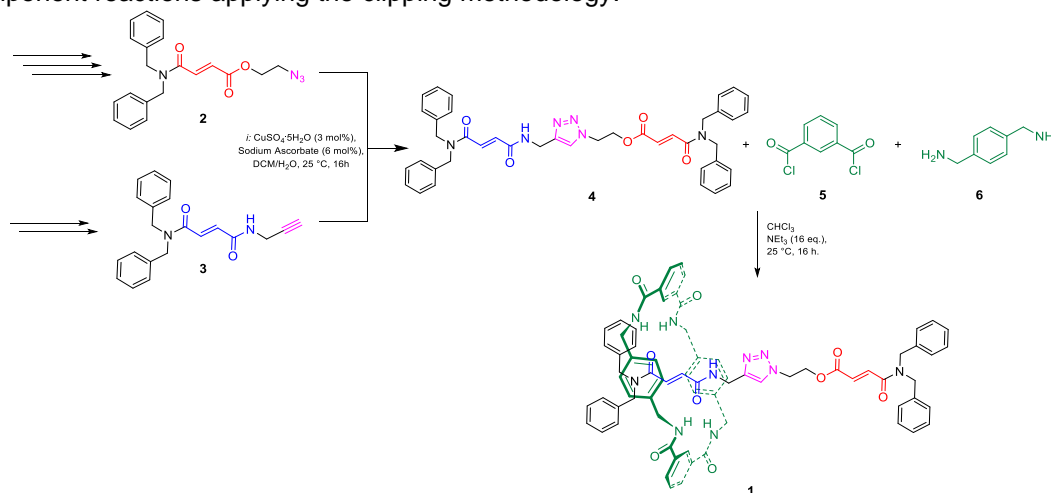


Figure 1. Reaction scheme for the synthesis of [2]rotaxane **1**.

ACKNOWLEDGEMENTS

The authors acknowledge the Fundação de Amparo à Pesquisa do Estado do Rio Grande do Sul (FAPERGS), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), and Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) for the financial support. The fellowship from CNPq (G.H.W.; M.A.P.M.) and CAPES (F.F.S.F) are also acknowledged.

REFERENCES

- (1) Stoddart, J. F. Mechanically Interlocked Molecules (MIMs)-Molecular Shuttles, Switches, and Machines (Nobel Lecture). *Angewandte Chemie International Edition* **2017**, *56* (37), 11094–11125. <https://doi.org/10.1002/anie.201703216>.
- (2) Leigh, D. A. Genesis of the Nanomachines: The 2016 Nobel Prize in Chemistry. *Angewandte Chemie International Edition* **2016**, *55* (47), 14506–14508. <https://doi.org/10.1002/anie.201609841>.
- (3) Farias, F.; Orlando, T.; Salbego, P.; Martins, M. ROTAXANOS – INTERAÇÕES INTERCOMPONENTES E MOVIMENTOS MOLECULARES. *Quim Nova* **2020**, *44* (1), 76–85. <https://doi.org/10.21577/0100-4042.20170623>.
- (4) Xue, M.; Yang, Y.; Chi, X.; Yan, X.; Huang, F. Development of Pseudorotaxanes and Rotaxanes: From Synthesis to Stimuli-Responsive Motions to Applications. *Chem Rev* **2015**, *115* (15), 7398–7501. <https://doi.org/10.1021/cr5005869>.
- (5) Farias, F. F. S.; Weimer, G. H.; Kunz, S. K.; Salbego, P. R. S.; Orlando, T.; Martins, M. A. P. The Rotational Movement in Solution of Fumaramide- vs. Succinamide [2]Rotaxanes: The Influence of Intercomponent Interactions. *J Mol Liq* **2023**, *385*, 122291. <https://doi.org/10.1016/j.molliq.2023.122291>.