

Employing substituted pyrazoles as stoppers in rotaxanes

Farias, Fellipe F. S.¹; Weimer, Gustavo H.¹ and Martins, Marcos A. P.^{1*}

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

*e-mail: marcos.nuquimhe@gmail.com

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ABSTRACT

[2]Rotaxanes consist of two main components: a linear 'thread' with bulky end groups called stoppers, and a cyclic component called 'macrocycle'.^{1,2} These molecules serve as excellent supramolecular models, displaying a range of interactions observable in both solution and solid states.^{3,4} Substituted pyrazoles can be synthesized as different regioisomers and their use as bulky groups may assist to recognize how intercomponent interactions reflect in the movements performed by rotaxanes.^{5,6} Based on our research group's expertise in pyrazoles synthesis, we propose the construction of novel threads and rotaxanes by exploring different regioisomers of pyrazoles as bulky groups. To synthesize the rotaxanes, several synthetic processes were used including acylation, allylic halogenation, nucleophilic substitution, cyclocondensation, organic reduction, nucleophilic addition and intramolecular cyclization. A multicomponent reaction was also employed to form a tetralactam macrocycle. Two rotaxanes (**1** and **2**) designed for this project are shown in Figure 1 as initial goals.

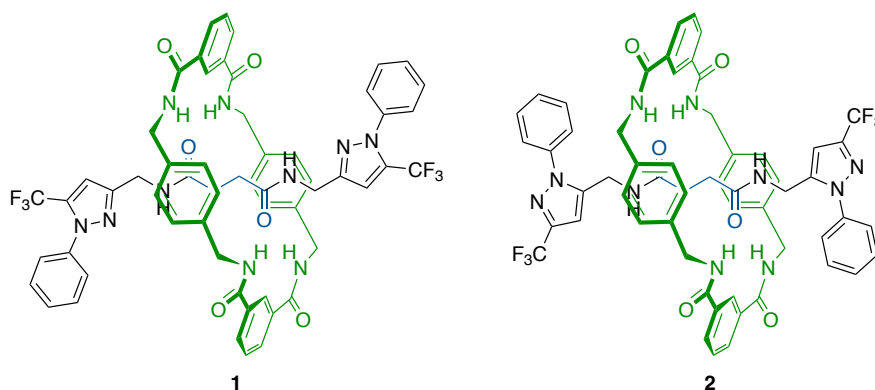


Figure 1. Rotaxanes **1** and **2** design for this study.

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