

Observations on the Influence of Precursor Conformations on Macrocyclization Reactions - DTU Orbit (08/11/2017)

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Macrocycles hold great promise in drug discovery as an underutilized class of lead compounds. The low abundance of these molecules can, in part, be explained by the inherent difficulties in the synthesis of macrocycles and the lack of general methods for their rapid assembly. We have undertaken a research program aimed at developing methods for facile synthesis of macrocycles from simple precursors. The synthesis of two new cyclization precursors is described and the results of their reaction with thionyl chloride are presented and discussed. Whereas one acyclic diol smoothly underwent macrocyclization to afford a mixture of diastereomeric sulfites, subjection of the other precursor to identical reaction conditions resulted in the isolation of the linear dichloride. We hypothesize that there is a difference in the ability of the two molecules to adopt a conformation that is germane to macrocyclization, a proposition that is supported by conformational analyses using molecular mechanics.

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