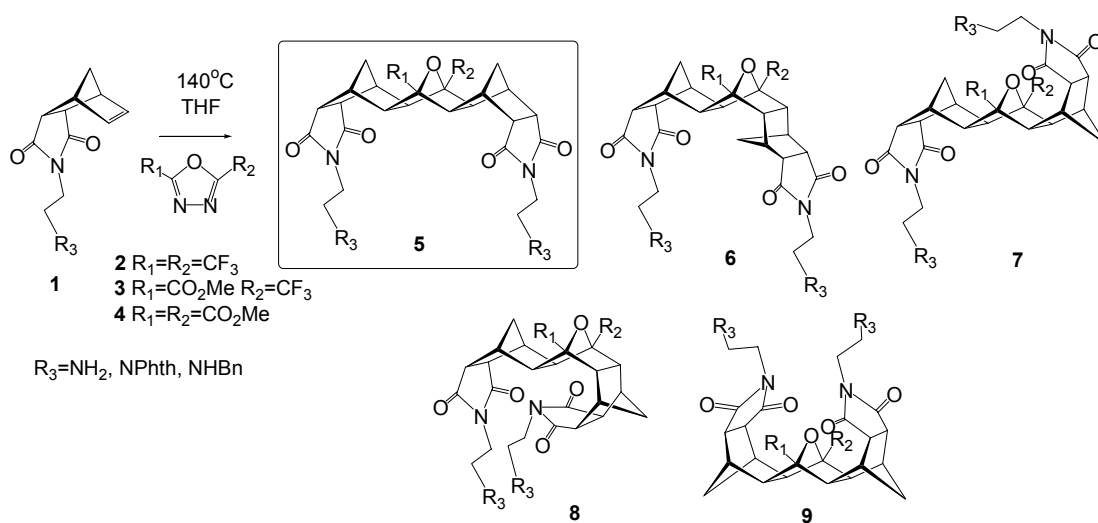


## Spectroscopic and Quantum-Chemical Assignments of Stereochemistry of Products Obtained by 1,3-dipolar Cycloaddition Reactions of Substituted 1,3,4-oxadiazoles With Norbornenes

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The 2-dimensional NMR spectroscopy (COSY, NOESY, ROESY, HMQC, HMBC) was employed to study the stereochemical outcomes of 1,3-dipolar cycloaddition reactions of substituted 1,3,4-oxadiazoles **2-4** with norbornenes [1]. In this reaction five possible products may be formed (**5-9**), while experimentally a single product has been isolated. In conjunction with spectroscopic assignments, density-functional quantum-chemical calculations (GIAO/DFT) were also performed for chemical shift calculations, specifically by GIAO/6-31+G\*//B3LYP/6-31G\* method [2]. Spectroscopic analysis and calculations have unequivocally proven that synthesized products possess linear (*exo,exo*-:*exo,exo*-) structures **5**.



[1] R.N. Warrener, D. Margetić, E.R.T. Tiekink, R.A. Russell, Synlett (1997) 196-198.

[2] T. Tsuji, M. Ohkita, H. Kawai, Bull. Chem. Soc. Jp. 75 (2002) 415-433.