

## Vibrational Spectroscopic Investigation of Bioactive Aminoalcohols

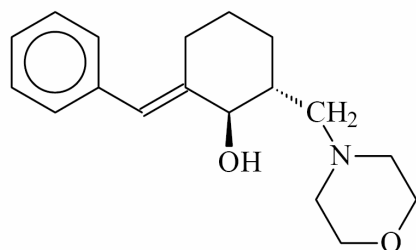
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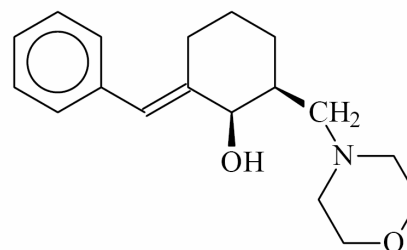
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As part of our continued interest in studying the infrared and Raman spectroscopic manifestations of *cis-trans* and conformational isomerism in bioactive polycyclic organic compounds, we have published our studies of isochromanone and coumarin derivatives [1-3]. The present work concerns with similar investigations of bioactive aminoalcohols obtained by reduction of cyclic Mannich ketones. The stereocomposition of the reaction mixtures is influenced by the type of reducing agent applied and the size of the central ring [4]. An increased preference for the *trans* isomer was attributed to a weak intramolecular hydrogen bond between the OH group and the N atom, as demonstrated by X-ray crystallography [4].



**MK-O23R *trans***  
(main product)



**MK-O23R *cis***  
(minor product)

The vibrational spectroscopic study consists of measurement of FT-IR and Raman spectra of the reaction products and subsequent DFT quantum mechanical calculations (prediction) of the vibrational spectra for the anticipated structural varieties of the synthesized molecules. Comparison of the measured and computed frequencies as well as the observed and simulated spectra is performed to resolve any uncertainties in identifying the reaction products.

The capabilities of vibrational frequency and normal mode calculations based on scaled quantum mechanical (SQM) force fields performed at the DFT/B3LYP/6-31G\* and higher levels of theory to predict the small spectral differences between the stereoisomers are tested in this work.

[1] G. Keresztury, S. Holly, T. Sundius, T. Lóránd: *Vibr. Spectrosc.*, 29 (2002) 53-9.

[2] G. Keresztury, S. Holly, K. István, T. Sundius, T. Lóránd, *J. Biochem. Biophys. Meth.* 61 (2004) 107-18.

[3] G. Keresztury, S. Holly, V. Komlósi, K. István, and T. Lóránd, *J. Biochem. Biophys. Meth.* 69/1-2 (2006) 163-177.

[4] T. Lóránd, E. Ósz, Gy. Kispál, G. Nagy, E. Weckert, D. Luebbert, A. Meents, B. Kocsis and L. Prókai, *ARKIVOC* (2004) (vii) 34-52.