Mgr Angelika Głębocka

Proton transfer equilibria in pyrazine-2-amidoxime studied by experimental and computational methods.

My research involved analyzing the structure and specifying the physicochemical properties of pyrazine-2-amidoxime. The structure of this compound was not previously investigated either by experimental or theoretical methods. This study is a complete structural analysis of the pyrazine derivative, pyrazine-2-amidoxime, made using computational and spectroscopic methods. I have studied fifteen possible pyrazine-2-amidoxime tautomeric forms together with their isomers and rotamers by the DFT method (B3LYP/6-311+G**). The result of the calculations are consistent with those obtained using IR spectroscopy. The second part of my research concerned the determination of acid-base equilibrium and pKa constant, by the quantum-chemical methods. These calculations were performed using three functionals (B3LYP, OLYP, M05-2X) in three different solvent models (CPCM, COSMO, SMD). The third part of the study involved defining the hydrophilic or lipophilic nature of pyrazine-2-amidoxime. The results I obtained for a single molecule confirmed poor water solubility while indicating the hydrophilic nature of the tested compound. However, my additional studies of tetrameric molecule showed its lipophilic nature.

The tested compound exhibits antifungal properties against *Candida albicans*, which is a pathogen that can cause severe illness in the human body. There is a constant need to look for preparations for use in the treatment and prevention of mycosis. The physicochemical properties of pyrazine-2-amidoxime investigated in this paper may be the basis for further research into the use of this compound in antifungal agents.

WYDZIAŁ CHEMII Pracownia Oddziaływań Międzycząsteczkowych
ul. Wita Stwosza 63, 80-308 Gdańsk
tel. (058) 523 50 56, email: angelika.glebocka@phdstud.ug.edu.pl