Accepted Manuscript

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PII:	S1386-1425(18)30470-0
DOI:	doi:10.1016/j.saa.2018.05.074
Reference:	SAA 16108
To appear in:	*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*
Received date:	10 April 2018
Accepted date:	20 May 2018

Please cite this article as: Jaya Pandey, Preeti Prajapati, Anubha Srivastava, Poonam Tandon, Kirti Sinha, Alejandro P. Ayala, Arvind K. Bansal , Spectroscopic and molecular structure (monomeric and dimeric model) investigation of Febuxostat: A combined experimental and theoretical study. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Saa(2017), doi:10.1016/j.saa.2018.05.074

Spectroscopic and molecular structure (monomeric and dimeric model) investigation of Febuxostat: A combined experimental and theoretical study

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Abstract

Febuxostat (FXT) is a urate-lowering drug and xanthine oxidase inhibitor which is used for the treatment of hyperuricemia and gout caused by increased levels of uric acid in the blood (hyperuricemia). The present study aims to provide deeper knowledge of the structural, vibrational spectroscopic and physiochemical properties of FXT based on monomeric and dimeric model with the aid of combination of experimental and computational methods. The conformational analysis of form Q has been done to predict the possible structure of unknown form A. Vibrational spectra of form A and Q has been compared to get an idea of hydrogen bonding interactions of form A. A computational study of FXT has been executed at different level (B3LYP, M06-2X, WB97XD) of theory and 6-31 G (d, p) basis set for dimeric model to elucidate the nature of intermolecular hydrogen bond. The red shift observed in the stretching modes of OH, C=O groups and blue shift in stretching mode of C≡N group in experimental as well as in theoretical spectra explains the involvement of these groups in intermolecular hydrogen bonding. NBO analysis shows that change in electron density (ED) in the lone pair

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