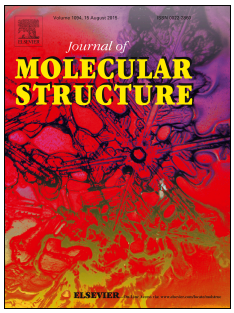
Accepted Manuscript



Vibrational spectroscopic (FT-IR, FT-Raman) and quantum mechanical study of 4-(2-chlorophenyl)-2-ethyl-9-methyl-6H-thieno[3,2-*f*] [1,2,4]triazolo[4,3-*a*][1,4] diazepine

Tintu K. Kuruvilla, Johanan Christian Prasana, S. Muthu, Jacob George

PII: S0022-2860(18)30001-2

DOI: 10.1016/j.molstruc.2018.01.001

Reference: MOLSTR 24723

To appear in: *Journal of Molecular Structure*

Received Date: 10 October 2017

Revised Date: 29 December 2017

Accepted Date: 2 January 2018

Please cite this article as: T.K. Kuruvilla, J.C. Prasana, S. Muthu, J. George, Vibrational spectroscopic (FT-IR, FT-Raman) and quantum mechanical study of 4-(2-chlorophenyl)-2-ethyl-9-methyl-6H-thieno[3,2-*f*] [1,2,4]triazolo[4,3-*a*][1,4] diazepine, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.01.001.

GRAPHICAL ABSTRACT

Experimental and theoretical calculations on the molecular structure, electronic and vibrational characteristics of 4-(2-chlorophenyl)-2-ethyl-9-methyl-6H-thieno[3,2-*f*] [1,2,4] triazolo [4,3-*a*][1,4] diazepine are presented .The theoretical calculations are obtained by DFT/B3LYP method with 6-311++G(d,p) as basis set. Molecular docking studies are performed and shows that the compound exhibit antidepressant property.