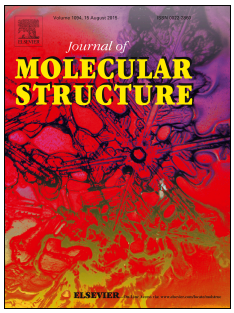
Accepted Manuscript



Vibrational (FT-IR and FT-Raman), electronic (UV–Vis), NMR (^{1}H and ^{13}C) spectra and molecular docking analyses of anticancer molecule 4-hydroxy-3-methoxycinnamaldehyde

K. Thirunavukkarasu, P. Rajkumar, S. Selvaraj, R. Suganya, M. Kesavan, S. Gunasekaran, S. Kumaresan

PII: S0022-2860(18)30822-6

DOI: 10.1016/j.molstruc.2018.07.003

Reference: MOLSTR 25408

To appear in: *Journal of Molecular Structure*

Received Date: 25 April 2018

Revised Date: 28 June 2018

Accepted Date: 2 July 2018

Please cite this article as: K. Thirunavukkarasu, P. Rajkumar, S. Selvaraj, R. Suganya, M. Kesavan, S. Gunasekaran, S. Kumaresan, Vibrational (FT-IR and FT-Raman), electronic (UV–Vis), NMR (^{1}H and ^{13}C) spectra and molecular docking analyses of anticancer molecule 4-hydroxy-3-methoxycinnamaldehyde, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.07.003.

GRAPHICAL ABSTRACT

In this work, a combined experimental and theoretical study on molecular structure, Vibrational spectra, HOMO- LUMO, Molecular docking study of 4-Hydroxy-3-methoxycinnamaldehyde