ScienceDirect

Journal of Molecular Structure
Volume 1123, 5 November 2016, Pages 180-190

Molecular docking and structural analysis of non-opioid analgesic drug acemetacin with halogen substitution: A DFT approach

D.R. Leenaraj, D. Manimaran, I. Hubert Joe

Centre for Molecular and Biophysics Research, Department of Physics, Mar Ivanios College, Thiruvananthapuram 695 015, Kerala, India

Received 12 March 2016, Revised 10 June 2016, Accepted 10 June 2016, Available online 14 June 2016, Version of Record 17 June 2016.

https://doi.org/10.1016/j.molstruc.2016.06.035

Abstract

Acemetacin is a non-opioid analgesic which belongs to the class, the non-steroidal anti-inflammatory drug. The bioactive conformer was identified through potential energy surface scan studies. Spectral features of acemetacin have been probed by the techniques of Fourier transform infrared, Raman and Nuclear magnetic resonance combined with density functional theory calculations at the B3LYP level with 6-311+G(d,p) basis set. The detailed interpretation of vibrational spectral assignments has been carried out on the basis of potential energy distribution method. Geometrical parameters reveal that the carbonyl substitution in between chlorophenyl and indole ring leads to a significant loss of planarity. The red-shifted C═O stretching wavenumber describe the conjugation between N and O atoms. The shifted C—H stretching wavenumbers of O—CH_3 and O—CH_2 groups depict the back-donation and induction effects. The substitution of halogen atoms on the title molecule influences the charge distribution and the geometrical parameters. Drug activity and binding affinity of halogen substitution in title molecule with target protein were undertaken by molecular docking study. This study enlightens the effects of bioefficiency due to the halogen substitution in the molecule.