Investigations of vibrational spectra and bioactivity of novel anticancer drug N-(6-ferrocenyl-2-naphthoyl)-gamma-amino butyric acid ethyl ester

Geethu Sudhi, S.R. Rajina, S.G. Praveen, T.S. Xavier, Peter T.M. Kenny, D. Jaiswal-Nagar, J. Binoy

PII:	S1386-1425(17)30439-0
DOI:	doi: 10.1016/j.saa.2017.05.056
Reference:	SAA 15198
To appear in:	*Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*
Received date:	31 December 2016
Revised date:	24 May 2017
Accepted date:	26 May 2017

Please cite this article as: Geethu Sudhi, S.R. Rajina, S.G. Praveen, T.S. Xavier, Peter T.M. Kenny, D. Jaiswal-Nagar, J. Binoy , Investigations of vibrational spectra and bioactivity of novel anticancer drug N-(6-ferrocenyl-2-naphthoyl)-gamma-amino butyric acid ethyl ester, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2017), doi: 10.1016/j.saa.2017.05.056

Investigations of Vibrational Spectra and Bioactivity Of Novel Anticancer Drug N-(6-Ferrocenyl-2-Naphthoyl)-Gamma-Amino Butyric Acid Ethyl Ester

Geethu Sudhi[1], S R Rajina[1], S G Praveen[2], T S Xavier[1], Peter T M Kenny[3], D. Jaiswal-Nagar[2], J Binoy[4,*]

[1]*Department of Physics, Research Scholar, University of Kerala, Govt College for Women, Thiruvananthapuram-695014. Kerala, India.*
[2]*School of Physics, Indian Institute of Science Education and Research, Thiruvananthapuram-695016, India.*
[3]*School of Chemical Sciences, Dublin City University, Glasnevin, Dublin 9, Ireland.*
[4]*Department of Physics, Govt College for Women, Thiruvananthapuram-695014. Kerala, India.*

*Corresponding Author: Email: binjohndas@yahoo.co.in , Tel: (+91)-9495413922

Abstract

The bioactivity of compounds is mainly dependent on molecular structure and the present work aims to explore the bonding features responsible for biological activity of novel anti cancer drug N-(6-ferrocenyl-2-naphthoyl)-gamma-amino butyric acid ethyl ester (FNGABEE). In the present study, we investigate the molecular structural properties of newly synthesized title compound through experimental and quantum chemical studies. The detailed vibrational analysis has been performed using FT IR and FT Raman spectrum, aided by DFT computed geometry, vibrational spectrum, eigen vector distribution and PED, at B3LYP/6-311++G(d,p) level. The resonance structure of naphthalene, different from that of benzene, revealed by molecular structure has been investigated using C-C and C=C stretching modes. The proton transfer in amide has been analyzed to obtain spectral distinction between different carbonyl and C-N groups which point to the reactive sites responsible for binding with DNA and bovine serum albumin (BSA). The spectral distinction between eclipsed and staggered form of ferrocene has been analyzed. The molecular docking of FNGABEE with BSA and DNA has been performed to find the strength of binding and the moieties responsible for the interactions. The experimental binding studies of FNGABEE with BSA and DNA has been performed using UV absorption spectroscopy and fluorometric assay, to find the nature and strength of binding.

Keywords: FT IR, FT Raman, DFT, Molecular docking, UV-Visible spectroscopy, Fluorescence spectroscopy

1 . Introduction

Ferrocene - based peptide compounds have recently aroused research interest for its ability to bind DNA, arresting cell reproduction and hence their derivatives are promising candidates in cancer research [1-5]. Since the functions and growth of cells are mainly controlled by the DNA, the interaction of drug with DNA play a crucial role in anticancer research and the