



< Back to results | < Previous 11 of 34 Next >

Download Print Save to PDF Save to list More... >

Heliyon • Open Access • Volume 7, Issue 4 • April 2021 • Article number e06593

Document type

Article • Gold Open Access • Green Open Access

Source type

Journal

ISSN

24058440

DOI

10.1016/j.heliyon.2021.e06593

View more

Crystallographic investigation, Hirshfeld surface analysis, NLO characterization and experimental spectral (UV and NMR) studies with DFT probe on(R)-9-(2-hydroxy propyl)adenine

Sharmila Tagore S.^a; Swaminathan J.^b; Manikandan D.^c; Gomathi S.^c; Sabarinathan N.^d; Ramalingam M.^e;

Sethuraman V.^c

Save all to author list

^a Department of Chemistry, M.R. Govt. Arts College, Mannargudi, Tamilnadu, India

^b Department of Chemistry, A.V.C. College of Engineering, Mayiladuthurai, Tamilnadu, India

^c Department of Chemistry, Periyar Maniammai Institute of Science and Technology, Vallam, Thanjavur, Tamilnadu, India

^d Department of Chemistry, Presidency College, Chennai, Tamilnadu, India

View additional affiliations

1 38th percentile
Citation in Scopus

0.14
FWCI

7
Views count

View all metrics >

View PDF Full text options Export

Abstract

Author keywords

Reaxys Chemistry database information

SciVal Topics

Metrics

Abstract

In this study, (R)-9-(2-hydroxy propyl)adenine (HPA) is the molecule of interest for investigation. The XRD from single crystal of HPA has been used to extract its structural features. Since HPA crystallised in a non-centro symmetric space group $P2_12_12_1$, its NLO property was studied and it was found to exhibit very good SHG activity. To explore the intermolecular interactions the generated Hirshfeld surface has been investigated along with 2D-fingerprint plots. The experimental electronic and NMR spectra taken in the UV-visible and radio frequency regions respectively for HPA have been corroborated in correlation with theoretical predictions at Density Function Theory using 6-311++g (d, p) basis set. The experimental XRD geometrical parameters, chemical shifts of ^{13}C and ^1H and λ_{max} values of HPA fit satisfactorily with the

Cited by 1 document

Spectroscopic and computational approach to study the interacting mechanism of drug-adenine complex

Sonia, C. , Devi, T.G. , Karlo, T. (2022) *Spectroscopy Letters*

View details of this citation

Inform me when this document is cited in Scopus:

Set citation alert >

Related research data

CCDC 1421496: Experimental Crystal Structure Determination

S, SharmilaTagore. , et al
Cambridge Crystallographic Data Centre

Data linking provided by
OpenAIRE's
Scholexplorer

Related documents

Synthesis and Biological Evaluation of Iodinated and Fluorinated 9-(2-Hydroxypropyl) and 9-(2-Hydroxyethoxy)methyl Purine Nucleoside Analogues

Prekupec, S. , Svedružić, D. , Gazivoda, T. (2003) *Journal of Medicinal Chemistry*

Crystallographic, spectral and computational studies on (S)-4-(4-aminobenzyl) oxazolidin-2-one

Manikandan, D. , Swaminathan, J. , Tagore, S.S. (2020) *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*

Vibrational assignment, HOMO - LUMO, first-hyperpolarizability and Mulliken's charge analysis of 2,7-dinitrofluorene

Arivazhagan, M. , Kumar, J.S. (2012) *Indian Journal of Pure and Applied Physics*

View all related documents based on references

Find more related documents in Scopus based on:

Authors > Keywords >