crystals

MDPI

Article

Isolation, Identification, Spectral Studies and X-ray Crystal Structures of Two Compounds from *Bixa orellana*, DFT Calculations and DNA Binding Studies

Mehtab Parveen [1,*], Mohammad Azeem [1], Afroz Aslam [1], Mohammad Azam [2,*], Sharmin Siddiqui [3], Mohammad Tabish [3], Ali Mohammad Malla [1,4], Kim Min [5], Vitor Hugo Rodrigues [6], Saud I. Al-Resayes [2] and Mahboob Alam [5,*]

[1] Division of Organic Synthesis, Department of Chemistry, Aligarh Muslim University, Aligarh 202002, India; azam23961@gmail.com (M.A.); afrozaslam10@gmail.com (A.A.); haiderchem09@gmail.com (A.M.M.)
[2] Department of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh 11451, Saudi Arabia; sresayes@ksu.edu.sa
[3] Department of Biochemistry, Aligarh Muslim University, Aligarh 202002, India; sharminbcb@gmail.com (S.S.); tabish.biochem@gmail.com (M.T.)
[4] Government Degree College, Beerwah, Budgam, Kashmir 193411, India
[5] Department of Safety Engineering, Dongguk University, 123 Dongdae-ro, Gyeongju 780714, Gyeongbuk, Korea; kimmin@dongguk.ac.kr
[6] CFisUC, Department of Physics, University of Coimbra, 3004-516 Coimbra, Portugal; vhugo@uc.pt
* Correspondence: mehtab.organic2009@gmail.com (M.P.); mhashim@ksu.edu.sa (M.A.); mahboobchem@gmail.com (M.A.)

Abstract: 4,6-Diacetylresorcinol (**1**) and 3-*O*-methylellagic acid dihydrate (**2**), both biologically significant compounds, were extracted from *Bixa orellana* and studied using IR, ^{1}H, and ^{13}C NMR, and UV-vis spectroscopic techniques. X-ray crystallographic techniques were also used to establish the molecular structure of the isolated compounds **1** and **2**. Geometric parameters, vibrational frequencies, and gauge including atomic orbital (GIAO) ^{1}H and ^{13}C NMR of **1** and **2** in the ground state were computed by the density functional theory (DFT) using B3LYP/6-311G(d,p) basis set backing up experimental studies and established the correct structure of isolated compounds. The parameters obtained from the combined DFT, and X-ray diffraction studies are mutually agreed to establish correct structures of **1** and **2**. In addition, an electrostatic potential map and HOMO−LUMO energy gap were made using the DFT calculation to determine the distribution of energy and the chemical reactivity region of the isolated compounds. The current study also provides further insights into the interaction of compound **2** with ct-DNA using numerous biophysical and *in silico* techniques. Moreover, *in silico* studies indicate that compound **2** binds to the DNA in the minor groove. Lipinski's rule of five revealed a higher tendency of compound **2** towards drug-likeness. The bioavailability and synthetic accessibility score for compound **2** was found to be 0.55 and 3.21, suggesting that compound **2** could serve as an effective therapeutic candidate.

Keywords: *Bixa orellana* (Family: Bixaceae); 4,6-diacetylresorcinol; 3-*O*-methylellagic acid dihydrate; X-ray diffraction; DFT; NMR; frontier molecular orbitals

Citation: Parveen, M.; Azeem, M.; Aslam, A.; Azam, M.; Siddiqui, S.; Tabish, M.; Malla, A.M.; Min, K.; Rodrigues, V.H.; Al-Resayes, S.I.; et al. Isolation, Identification, Spectral Studies and X-ray Crystal Structures of Two Compounds from *Bixa orellana*, DFT Calculations and DNA Binding Studies. *Crystals* **2022**, *12*, 380. https://doi.org/10.3390/cryst12030380

Academic Editors: Radu Claudiu Fierascu, Florentina Monica Raduly and Dinadayalane Tandabany

Received: 10 February 2022
Accepted: 7 March 2022
Published: 11 March 2022

1. Introduction

The Bixaceae family includes *Bixa orellana* L., also known as annatto. It is a Central and South American shrub that grows 3–6 m tall and is one of the oldest plants to produce natural colors. Originally, the herb was used as body paint, a treatment for heartburn, an insect repellant, a sunscreen, and to fight off evil. It was named after *Francisco de Orellana*, a Spanish conquistador [1]. Constipation, fevers, heartburn, asthma, scabies, ulcers, diarrhea, stomach upset, skin diseases, measles, anecdotal treatment of diabetes, allergy, leprosy, infectious diseases, burns, measles, gonorrhea, diarrhea, asthma, angina,