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Density functional theoretical study and DNA cleavage activity of 2,5-bis (cyclohexylamino)cyclohexa-2,5-diene-1,4-dione

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Herein is reported the density functional theoretical study and DNA cleavage activity of an aminobenzoquinone, 2,5-bis(cyclohexylamino)cyclohexa-2,5-diene-1,4-dione (BCBQ). Despite aminobenzoquinones being recognized for their biological activity, they remain relatively unexplored in theoretical studies. Single crystal X-ray analysis of BCBQ has already been reported. Detailed analysis of its structural parameters has elucidated the biological activity of such compounds, aiding the design of substituted ABQs for multiple uses.

Keywords: Aminobenzoquinones, DFT study, DNA cleavage activity

Biological electron transfer processes including cellular respiration and photosynthesis manifests the inevitable role played by *p*-benzoquinones and their amino derivatives[1,2]. They are widespread in many fungi which are the colour bearing pigments in them[3]. Use of Mitomycin as an anti-cancer and anti-bacterial agents is well demonstrated in the literature[4]. The anti-bacterial as well as the anti-fungal activity of aminobenzoquinones has been studied extensively which points their significance in pharmacology[5,6]. Benzoquinones and related compounds are effective redox reagents able to generate reactive oxygen species (ROS) which acts as electrophiles forming covalent bonds with tissue nucleophiles[7].

The vibrational spectra of amino naphthoquinones were studied by various research groups[8], however 2,5-diamino1,4-benzoquinones are less explored. This lead us to focus on the DFT study and DNA cleavage activity study of synthesized BCBQ.

Experimental Section

Materials

Cyclohexylamine and ethyl vanillin were of A R grade purchased from Merck and were used without any purification. Solvents used were purchased from Merck and used as received.

Synthesis of 2,5-bis(cyclohexylamino)cyclohexa-2,5-diene-1,4-dione

BCBQ was synthesized by the previously reported method[9]. Ethyl vanillin (10 mmol) and cyclohexylamine (20 mmol) were mixed in 20 mL methanol along with addition of a trace amount of glacial acetic acid and allowed for slow evaporation under open air at RT. Complete evaporation of methanol resulted in red needle shaped crystals of BCBQ. m.p.240-241°C. IR (KBr): 3270, 2852, 1640, 1562, 1091 cm^{-1}; UV-Vis λ_{max} (MeOH) nm: 306, 395, 453; ^1H NMR ($CDCl_3$): δ 1.18–1.42 (m, 10H), 1.59–1.69 (m, 3H), 1.74–1.83 (m, 4H), 1.94–2.02 (m, 4H), 3.26 (m, 2H), 5.33 (s, 2H), 6.59 (d, J ¼ 9 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ 24.5, 25.4,31.8, 51.3, 92.8, 150.2, 178.1; HR-ESI-MS: *m/z* Calcd for $C_{18}H_{27}N_2O_2$ $[M^+H^+]$: 303.2073. Obsd: 303.2078.

DFT study

The quantum chemical calculations have been carried out by DFT method using the Gaussian '09 software[10] by using B3LYP functional, employing 6-311 ++G(d,p) basis set which is the most effective level of theory available for the analysis of metallic systems[11]. The computed optimized geometry, IR and Raman spectra, Eigen vector distribution of vibrational modes, obtained using Gauss view 5.0 program[12] and PED[13] have been used for the comprehensive molecular structural and vibrational analysis. The calculated vibrational frequencies have been scaled, using standard scaling factor 0.9671 (Ref. 14).

In vitro DNA cleavage assay

Bacterial cultures were grown in LB medium with appropriate antibiotics at 37°C and kept overnight (O/N) with shaking. The O/N culture was transferred