Journal of King Saud University – Science 33 (2021) 101313

Contents lists available at ScienceDirect

Journal of King Saud University – Science

journal homepage: www.sciencedirect.com

Original article

Molecular structure simulation of (*E*)-2-(butan-2-ylidene) hydrazinecarbothioamide using the DFT approach, and antioxidant potential assessment of its complexes

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ARTICLE INFO

Article history:
Received 15 November 2020
Revised 10 December 2020
Accepted 17 December 2020
Available online 24 December 2020

Keywords:
Gaussian
Optimization
Quantum
Mechanics
Thiosemicarbazone
Antioxidant

ABSTRACT

The molecular structure of (E)-2-(butan-2-ylidene)hydrazinecarbothiomide (2-butanone thiosemicarbazone) was validated by density functional theory (DFT) calculations. The characterization of the ligand was done using various spectroscopic techniques. Four transition metal complexes were prepared with the ligand and their antioxidant activity was tested. Molecular docking studies of the complexes were also performed against nicotinamide adenine dinucleotide phosphate (NADPH) and myeloperoxidase (MPO). Structure validation of the ligand was done in Gaussian 09 software. The geometry optimization was done at B3LYP/6-31G++(d,p) level. The ^{1}H and ^{13}C NMR chemical shifts, FT-IR vibrations and UV–visible transitions were validated with the help of theoretical calculations. The frontier molecular orbital analysis, molecular electrostatic potential (MEP) and global reactivity descriptors were calculated to predict the stability of the molecule. Non-linear optical (NLO) properties were assessed and compared with urea. Natural bond orbital (NBO) analysis was done to predict the stability of the ligand resulting from hyper conjugative interactions and electron delocalization. Molecular docking studies of the complexes were performed with iGEMDOCK 2.1 and AutoDock 4.2.6.Antioxidant potential was assessed by 2,2-diphenyl-1-picrylhydrazyl (DPPH) Assay. ^{1}H and ^{13}C correlation coefficients (R^2) were 0.9964 and 0.9974 respectively. In case of FT-IR, the correlation coefficient (R^2) was 0.9984. $[Fe(C_5H_{11}N_3S)_2(SO_4)]$ possessed maximum antioxidant potential followed by $[Cu(C_5H_{11}N_3S)_2(SO_4)]$. Molecular docking findings suggested that the Fe complex released the minimum binding energy. Computational structure validation is an important aspect in finding a lead moiety. The theoretical spectral findings correlated well with the experimental findings in the present study. The metal complexes showed appreciable antioxidant potential as predicted by the computational and experimental findings. The ligand possessed better NLO properties than urea.

1. Introduction

Through quantum mechanical simulations the structural characteristics of new materials can be easily and accurately predicted. The computational predictions can also validate the experimental findings. Owing to the fast and accurate predictions by automated softwares, computational chemistry has received considerable attention (Matulkova et al., 2008; Boo et al., 2008). Due to the remarkable growth in the field of computational resources, many theoretical algorithms have been proposed to calculate various properties of a compound using semi-empirical and DFT methods. The theoretical data can be easily compared with the experimental one (Brewerton, 2008; Ravna and Sager, 2008). DFT has become a major tool for structure prediction and understanding the mechanistic approach (Lipkowitz et al., 2009; Lorenc et al., 2008). Quantum studies enable to envisage the structure of a chemical entity with the help of computer aided softwares. With the added

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Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

https://doi.org/10.1016/j.jksus.2020.101313