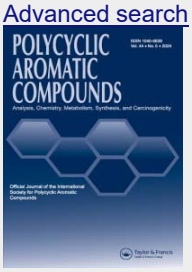

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Reactivity and Structural Investigation of Tetrahydroneoprzewaquinone A as an Anti-Inflammatory Agent: An Experimental and Molecular Modeling Perspective

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Received 12 May 2023, Accepted 06 Sep 2023, Published online: 20 Sep 2023

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Abstract

This intriguing study aimed to explore the reactivity and structural investigation of (3R,3′R)-2,2′,3,3′-tetrahydroneoprzewaquinone A (THNPQ A) as a potential anti-inflammatory agent. Substantially, the electronic properties were investigated using LanL2DZ, 6-311++G (d,p), and STO-3G basis sets, with electronegativity values of 7.9816, 6.3038, and 5.0166 eV, respectively. The natural bond orbital (NBO) analysis calculations of optimization energies revealed that LanL2DZ had the highest stabilization energy (526.65 kcal/mol) for the interaction between πC8-C9 and πC3-C4. Regarding nonlinear optical (NLO) properties, 6-311++G (d,p) exhibited the highest averaged polarizability and first-order hyperpolarizability values, while the polarizability anisotropies Δtotal followed the order 6-311++G (d,p) (65.2054 a.u.) > LanL2DZ (42.8782 a.u.) > STO-3G (29.9349 a.u.). Analysis of the density of states (DOS) and orbital contribution showed that 6-311++G (d,p) had the highest density peaks at both

the highest occupied molecular orbital (HOMO) (–0.5 a.u.) and the lowest unoccupied molecular orbital (LUMO) (0.00 a.u.). The condensed dual descriptors indicated minimal variations in the f_{A^-} and f_{A^+} values, with an increase in Δf_A, f_{A^-}, and f_{A^+} values following the order STO-3G > LanL2DZ > 6-311++G (d,p). The sites for potential nucleophilic attack were identified as O11, O12, O36, and O37, which exhibited the highest values with the STO-3G basis set. Empirical evidence from *in vitro* inhibition assays unequivocally validates the potent anti-inflammatory activity of THNPQ A. Particularly noteworthy is its exceptional binding affinity, surpassing that of diclofenac. By establishing conventional hydrogen bonds with the glycine of COX-I and histidine of COX-II, THNPQ A exhibits remarkable potential as an effective agent for combating inflammation. These findings boldly emphasize the promising therapeutic prospects of THNPQ A in the field of anti-inflammatory treatment, positioning it as a compelling candidate for further investigation and development.

Keywords:

- Anti-inflammatory
- DFT
- molecular docking
- *in silico*
- COX

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Acknowledgments

We acknowledge the Centre for High Performance Computing South Africa for providing the computational resources used in this work.

Author contributions

E.U. Ejiofor, E.C. Agwamba: conceptualization, design, supervision, and editing; I. Benjamin: analysis, writing, and manuscript final draft; E.F. Ahukwe and R.U. Ukpanukpong: analysis, writing, and manuscript review; K.T. Maxwell and I.U. Bassey: analysis, writing, and manuscript final draft; H. Louis: results analysis, writing, editing, and manuscript draft. A-L.E. Manicum: methodology, editing, and resources.

Disclosure statement

There are no financial conflicts to be declared by the authors.

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