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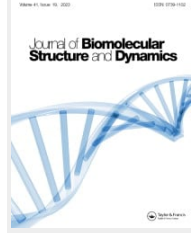
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Research Article

Anti-inflammatory biomolecular activity of chlorinated-phenyldiazenyl-naphthalene-2-sulfonic acid derivatives: perception from DFT, molecular docking, and molecular dynamic simulation

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- ## Abstract

In this study, two novel derivatives of naphthalene-2-sulfonic acid: 6-(((1S,5R)-3,5-dichloro-2,4,6-triazabicyclo [z3.1.0]hex-3-en-1-yl)amino)-5-((E)-phenyldiazenyl)naphthalene-2-sulfonic acid (DTPS1) and (E)-6-((4,6-dichloro-1,3,5-triazine2-yl)amino)-4-hydroxy-3-(phenyldiazenyl)naphthalene-2-sulfonic acid (DTPS2) have been synthesized and characterized using FT-IR, UV-vis, and NMR spectroscopic techniques. Applying density functional theory (DFT) at the B3LYP, APFD, PBEPBE, HCTH, TPSSTPSS, and ω B97XD/aug-cc-pVDZ level of theories for the electronic structural properties. In-vitro analysis, molecular docking, molecular dynamic (MD) simulation of the compounds was conducted to investigate the anti-inflammatory potential using COXs enzymes. Docking indicates binding affinity of -9.57 , -9.60 , -6.77 and -7.37 kcal/mol for DTPS1, DTPS2, Ibuprofen and Diclofenac which agrees with *in-vitro* assay. Results of MD simulation, indicates sulphonic group in DTPS1 has $> 30\%$ interaction with the hydroxyl and oxygen atoms in amino acid residues, but $> 35\%$ interaction with the DTPS2. It can be said that the DTPS1 and DTPS2 can induce inhibitory effect on COXs to halt biosynthesis of prostaglandins (PGs), a chief mediator of inflammation and pain in mammals.

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Keywords:

- [Anti-inflammation](#)
- [DFT](#)
- [in-vitro molecular docking](#)
- [MD simulation](#)
- [cyclooxygenases](#)

Author contributions

Ernest C. Agwamba: Project administration, analysis, writing, and editing. **Hitler Louis:** Conceptualization, design, supervision, writing, and editing. **Akaninyene D. Udoikono:** Results analysis, writing, editing, and manuscript first draft. **Innocent Benjamin:** Analysis, writing and manuscript final draft. **Eze F. Ahuekwe:** Resources, analysis, writing, and editing. **Kelechi Chukwuemeka and Emmanuel U. Ejiofor:** Analysis, writing, and editing. validation, writing and editing. **Adeyinka S. Adeyemi and Iqrar Ahmad:** Methodology, **Harun Patel, Amanda-Lee Manicum, and Moses M. Edim:** analysis and discussion of molecular dynamics

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Ethics approval and consent to participate

Not applicable.

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Availability of data and material

All data are contained within the manuscript and manuscript supporting information document (ESI).

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