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Notice for the PhD Viva Voce Examination

Ms Sheryl Cherian Parakkal (Registration Number: 2090196), PhD scholar at the School of Sciences, CHRIST (Deemed to be University), Bangalore will defend her PhD thesis at the public viva-voce examination on Wednesday, 12 June 2024 at 10.30 am in Room No. 044, Ground Floor, R & D Block, CHRIST (Deemed to be University), Bengaluru - 560029.

Title of the Thesis	:	**Computational Chemical Property Prediction and Anticancer Simulation of Heterocyclic Molecules**
Discipline	:	**Chemistry**
External Examiner (Outside Karnataka)	:	**Dr I Hubert Joe** Associate Professor Department of Nanoscience and Nanotechnology University of Kerala Kariavattom Thiruvananthapuram - 695581 Kerala
External Examiner (Within Karnataka)	:	**Dr Santosh L Gaonkar** Professor Department of Chemistry Manipal Institute of Technology Manipal - 576104 Karnataka
Supervisor	:	**Dr Riya Datta** Professor Department of Chemistry School of Sciences CHRIST (Deemed to be University) Bengaluru – 560029 Karnataka

The members of the Research Advisory Committee of the Scholar, the faculty members of the Department and the School, interested experts and research scholars of all the branches of research are cordially invited to attend this open viva-voce examination.

Registrar

Place: Bengaluru
Date: 03 June 2024

ABSTRACT

The Density Functional Theory (DFT) technique is popularly employed in establishing organic molecules' structural properties and reactivities. The DFT studies include energy minimisation (geometry optimisation), frontier molecular orbitals (FMO) analyses, theoretical UV spectral computation, natural bond orbital (NBO) evaluation, non-linear optical (NLO) studies, and molecular electrostatic potential (MEP) maps generation.

Topological analyses using Multiwfn 3.8 software are performed to evaluate the Pauli repulsion in atomic orbitals (as shown by ELF (Electron Localisation Function) maps), the areas of strong and weak pi-delocalisation in the molecules (as depicted in LOL (Localised Orbital Locator) maps) and the weak non-covalent intra-molecular interactions (as indicated in colour maps of RDG (Reduced Density Gradient)). Pharmacological evaluation is performed using SwissADME, ADMETLab 2.0, and PreADMET online tools. Molecular docking is performed using AutoDock Tools 1.5.6 with select anticancer target proteins to predict the bioactivity potential of the title molecules.

Keywords: DFT, Topology, ADMET, Docking, Anticancer action

Publications:

1. **S. C. Parakkal**, R. Datta, S. Muthu, A. Irfan, and A. Jeelani, "Computational investigation into structural, topological, electronic properties, and biological evaluation of spiro [1H-indole-3,2 -3H-1,3-benzothiazole]-2- one," Journal of Molecular Liquids, vol. 359, p. 119234, Aug. 2022, doi: 10.1016/j.molliq.2022.119234.
2. **S. Cherian Parakkal**, R. Datta, A. Saral, S. Muthu, A. Irfan, and A. Jeelani, "Solvent polarity, structural and electronic properties with different solvents and biological studies of 3,3,5-triphenylfuran-2(3H)-one-cancers of the blood cells," Journal of Molecular Liquids, vol. 368, p. 120674, Dec. 2022, doi: 10.1016/j.molliq.2022.120674.
3. **S. C. Parakkal**, R. Datta, S. Muthu, and A. A. Al-Saadi, "Structure of molecule, density gradient, orbital locator and reactivity of 5,6-dichloro-1-cyclopentyl-2-(methylsulfinyl)-1H-benzimidazole- potent inhibitor of map kinase," Journal of Molecular Structure, vol. 1289, p. 135794, Oct. 2023, doi: 10.1016/j.molstruc.2023.135794.
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5. **S. C. Parakkal**, S. Muthu, R. Datta, S. Kadaikunnan, and G. Abbas, "Solvent-solute polarity, electrophilic, steric effects, reactive sites, themodynamic quantities discussion and biological evaluation of lung cancer antiproliferative activities of spirobrassinin derivatives," Journal of Molecular Liquids, vol. 385, p. 122382, Sep. 2023, doi: 10.1016/j.molliq.2023.122382.
6. **S. C. Parakkal**, R. Datta, S. Muthu, N. S. Alharbi, and G. Abbas, "Solvent-solute interaction, thermodynamic behaviour, structural, chemical and anti-cancer biological properties of 3(2H)-furanone derivatives," Journal of Molecular Liquids, vol. 390, p. 123185, Nov. 2023, doi: 10.1016/j.molliq.2023.123185.
7. **S. Cherian Parakkal**, R. Datta, and D. Das, "DeepBBBP: High Accuracy BloodBrainBarrier Permeability Prediction with a Mixed Deep Learning Model," Molecular Informatics, p. 2100315, Apr. 2022, doi: 10.1002/minf.202100315.
8. W. Hammad, **S. C. Parakkal**, R. Datta, S. Muthu, N. S. Alharbi, and G. Abbas, "Computational studies into the chemical nature, thermal behaviour, solvent role, reactivity and biological evaluation of Rigidin E – A marine alkaloid with potent liver cancer inhibition," Journal of Molecular Liquids, vol. 392, p. 123514, Dec. 2023, doi: 10.1016/j.molliq.2023.123514.