

Sj Jenepha Mary

List of Publications by Year in descending order

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3
papers

36
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2682572

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| # | ARTICLE | IF | CITATIONS |
|---|--|-----|-----------|
| 1 | Quantum chemical insight into molecular structure, NBO analysis of the hydrogen-bonded interactions, spectroscopic (FTIR, Raman), drug likeness and molecular docking of the novel anti COVID-19 molecule 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(4-fluorophenyl)acetamide - dimer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 244, 118825. Molecular structure, NBO analysis of the hydrogen-bonded interactions, spectroscopic (FTIR, Raman), drug likeness and molecular docking of the novel anti COVID-19 molecule 2-[(4,6-diaminopyrimidin-2-yl)sulfanyl]-N-(4-fluorophenyl)acetamide - dimer. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 244, 118825. | 3.9 | 26 |
| 2 | (2E)-N-methyl-2-[(4-oxo-4H-chromen-3-yl)methylidene]-hydrazinecarbothioamide (Dimer) - quantum chemical approach. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 251, 119388. | 3.9 | 9 |
| 3 | Raman spectroscopic study of cinnamyl-1 diphenylmethyl-4 piperazine (Cinnarizine) at high pressure. <i>Journal of Molecular Structure</i> , 2022, 1253, 132214. | 3.6 | 1 |