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- 1. T. Hannah Clara, **Johanan Christian Prasana**, D. Reuben Jonathan, B. K. Revathi, G. Usha, *E-1-(4-aminophenyl)-3-[4-(benzyloxy)phenyl]prop-2-en-one*, IUCrData, 1 (9), (2016) 161371.
- 2. Bharathy G., **Prasana Johanan Christian**, Muthu S., *Quantum Computational and Molecular docking studies of 2-{2-[(2,6-dichlorophenyl)amino]phenyl}acetic acid based on density functional theory*, Asian Journal of Research in Social Sciences and Humanities, 7 (2017) 395-427.
- 3. Christina Susan Abraham, **Johanan Christian Prasana**, S. Muthu, *Quantum mechanical*, *spectroscopic and docking studies of 2-Amino-3-bromo-5-nitropyridine by Density Functional Method*, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 181 (2017) 153–163.
- Jacob George, Johanan Christian Prasana, S. Muthu, Tintu K. Kuruvilla, Spectroscopic (FT-IR, FT Raman) and Quantum Mechanical Study on Isosorbide Mononitrate by Density Functional Theory, International Journal of Materials Science 12 (2) (2017) 302-320.
- 5. Fathima Rizwana B., **Johanan Christian Prasana**, S. Muthu, *Spectroscopic investigation (FT-IR, FT-Raman, UV, NMR), Computational analysis (DFT method) and Molecular docking studies on 2-[(acetyloxy) methyl]-4-(2-amino-9h-purin-9-yl)butyl acetate*, International Journal of Materials Science 12 (2) (2017) 196-216.
- 6. Tintu K Kuruvilla, **Johanan Christian Prasana**, S. Muthu, Jacob George Jacob George, *Quantum Mechanical Calculations and Spectroscopic (FT-IR, FT-Raman) Investigation on 1-cyclohexyl-1-phenyl-3-(piperidin-1-yl)propan-1-ol, by density functional method*, International Journal of Materials Science 12 (2) (2017) 282-301.
- 7. J. Christina Jebapriya, D. Reuben Jonathan, **Johanan Christian Prasana**, G. Usha, (2E)-2-[4-(Dimethylamino) benzylidene]-5-methylcyclohexanone, IUCrData, 2(12), (2017) 0171706.
- 8. Maha S. Almutairi, S. Muthu, **Johanan C. Prasana**, B. Chandralekha, Alwah R. Al-Ghamdi, Mohamed I. Attia, *Comprehensive spectroscopic (FT-IR, FT-Raman*,

- 1H and 13C NMR) identification and computational studies on 1-acetyl-1H-indole-2,3-dione, Open Chem., 15 (2017) 225–237.
- 9. P. Manjusha, **Johanan Christian Prasana**, S. Muthu, *Quantum mechanical calculations and spectroscopic investigations (FT-IR, FT Raman and UV-Visible) on*(6R,7R)-7-[(2Z)-2-(2-amino-1,3-thiazol-4-yl) [(carboxymethoxy)imino] acetmido]-3-ethenyl-o-oxo-5-thia-1-azabicyclo[4.2.0] octo-2-ene-2-carboxylic acid:a Pharmaceutical drug using Density Functional theory, International Journal of Advanced Research and Development, 3(3) (2018) 44-51.
- 10. G. Bharathy, Johanan Christian Prasana, S. Muthu, Molecular Conformational Analysis, Vibrational Spectra, NBO, HOMO–LUMO and Molecular docking of Modafinil Based on Density Functional Theory, International Journal of Current Research and Review, 10 (2018) 36-45.
- 11. Tintu K. Kuruvilla, **Johanan Christian Prasana**, S. Muthu, Jacob George, Vibrational spectroscopic (FT-IR, FT-Raman) and quantum mechanical study of 4-(2-chlorophenyl)-2-ethyl-9-methyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4] diazepine, Journal of Molecular Structure 1157 (2018) 519-529.
- 12. Christina Susan Abraham, **Johanan Christian Prasana**, S. Muthu, Fathima Rizwana B., M. Raja, *Quantum computational studies, spectroscopic (FT-IR, FT-Raman and UV-Vis) profiling, natural hybrid orbital and molecular docking analysis on 2,4 Dibromoaniline*, Journal of Molecular Structure 1160 (2018) 393-405.
- 13. Tintu K. Kuruvilla, **Johanan Christian Prasana**, S. Muthu, Jacob George, Sheril Ann Mathew, *Quantum mechanical and spectroscopic (FT-IR, FT-Raman) study, NBO analysis, HOMO-LUMO, first order hyperpolarizability and molecular docking study of methyl[(3R)-3-(2-methylphenoxy)-3-phenylpropyl]amine by density functional method, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 188 (2018) 382–393.*
- 14. B. Fathima Rizwana, Johanan Christian Prasana, Christina Susan Abraham, S. Muthu, Spectroscopic investigation, Hirshfeld surface analysis and molecular docking studies on anti viral drug Entecavir, Journal of Molecular Structure 1164 (2018) 447-458.
- 15. Jacob George, **Johanan Christian Prasana**, S. Muthu, Tintu K. Kuruvilla, S. Sevanthi, Rinnu Sara Saji, *Spectroscopic (FT-IR, FT Raman) and quantum mechanical study on N-(2,6-dimethylphenyl)-2-{4-[2-hydroxy-3-(2-thermoleculoscopic (FT-IR)]}.*

- *methoxyphenoxy)* propyl]piperazin-1-yl]acetamide,Journal of Molecular Structure, 1171 (2018) 268-278.
- 16. Christina Susan Abraham, S. Muthu, **Johanan Christian Prasana**, B. Fathima Rizwana, Stevan Armakovic, Sanja J. Armakovic, *Vibrational and electronic absorption spectroscopic profiling, natural hybrid orbital, charge transfer, electron localization function and molecular docking analysis on 3-amino-3-(2-nitrophenyl) propionic acid, Journal of Molecular Structure, 1171 (2018) 733-746.*
- 17. Christina Susan Abraham, S. Muthu, **Johanan Christian Prasana**, Sanja J. Armakovic, Stevan Armakovic, Fathima Rizwana B, Ben Geoffrey A.S., Spectroscopic profiling (FT-IR, FT-Raman, NMR and UV-Vis), autoxidation mechanism (H-BDE) and molecular docking investigation of 3-(4-chlorophenyl)-N,N-dimethyl-3-pyridin-2-ylpropan-1-amine by DFT/TD-DFT and molecular dynamics: a potential SSRI drug, Computational Biology and Chemistry, 77 (2018) 131-145.
- 18. Fathima Rizwana B., S. Muthu, **Johanan Christian Prasana**, Christina Susan Abraham, M. Raja, *Spectroscopic (FT-IR, FT-Raman) investigation, topology (ESP, ELF, LOL) analyses, charge transfer excitation and molecular docking (dengue, HCV) studies on ribavirin*, Chemical Data Collections 17-18 (2018) 236-250.
- 19. P. Horsley Solomon, **Johanan Christian Prasana**, *Analysis of Structural, Optical and Mechanical Property Analysis of Cadmium Sulphate Admixtured L-arginine: An optoelectronic material*, International journal of Research and analytical reviews, 5(4) (2018) 730-747.
- 20. P. Horsley Solomon, **Johanan Christian Prasana**, *Structural*, *Optical and Mechanical Property Analysis of Zinc Sulphate Admixtured L-arginine: A novel Optoelectronic material*, International journal for Research in Engineering Applications & Management, 4(8) (2018) 588-596.
- 21. Tintu K. Kuruvilla, **Johanan Christian Prasana**, S. Muthu, Jacob George, S. Sevvanthi, *Spectroscopic (FT-IR, FT-Raman), quantum mechanical and docking studies on methyl[(3S)-3-(naphthalen-1-yloxy)-3-(thiophen-2-yl) propyl] amine*, Journal of Molecular Structure, 1175 (2019) 163-174.
- 22. Fathima Rizwana B., **Johanan Christian Prasana**, S. Muthu, Christina Susan Abraham, *Molecular docking studies*, *charge transfer excitation and wave*

- function analyses (ESP, ELF, LOL) on valacyclovir: A potential antiviral drug, Computational Biology and Chemistry 78 (2019) 9-17.
- 23. P. Manjusha, **Johanan Christian Prasana**, S. Muthu, B. Fathima Rizwana, *A Computational and Spectroscopic interpretation (FTIR, FT-Raman, UV-Vis and NMR) with molecular docking studies on 3-carboxy-2- hydroxy- N, N, N-trimethyl- 1- propanaminium hydroxide: A pharmaceutical drug*, Chemical Data Collections, 20 (2019) 100-191.
- 24. Ben Geoffrey A.S., **Johanan Christian Prasana**, S. Muthu, Christina Susan Abraham, Host Antony David, *Spectroscopic and quantum/classical mechanics based computational studies to compare the ability of Andrographolide and its derivative to inhibit Nitric Oxide Synthase*, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 218 (2019) 374–387.
- 25. Christina Susan Abraham, S. Muthu, **Johanan Christian Prasana**, Stevan Armaković, Sanja J. Armaković, Fathima Rizwana B., Ben Geoffrey, Host Antony David R., *Computational evaluation of the reactivity and pharmaceutical potential of an organic amine: A DFT, molecular dynamics simulations and molecular docking approach*, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy 222 (2019) 117-188.
- 26. Tintu K. Kuruvilla,S. Muthu,Johanan Christian Prasana, Jacob George, Rinnu Sara Saji, Ben Geoffrey, Host Antony David R., *Molecular docking, Spectroscopic studies on 4- [2- (Dipropylamino) ethyl] 1,3 dihydro- 2H-indol- 2- one and QSAR study of a group of dopamine agonist by density functional method*, Spectrochemica Acta Part A: Molecular and Biomolecular Spectroscopy 222 (2019) 117-185.
- 27. Rinnu Sara Saji, Johanan Christian Prasana, S. Muthu, Jacob George, Tintu K. Kuruvilla, B.R. Raajaraman, *Spectroscopic and quantum computational study on naproxen sodium*, Spectrochemica Acta Part A: Molecular and Biomolecular Spectroscopy 222 (2019) 117-185.
- 28. B. Fathima Rizwana., **Johanan Christian Prasana**, S. Muthu, Christina Susan Abraham *Spectroscopic (FT-IR, FT-Raman, NMR) investigation on 2-[(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)methoxy]ethyl(2S)-2-amino-3-methylbutanoate by Density Functional Theory*, Materials Today: Proceedings 18 (2019) 1770–1782.

- 29. A.S. Ben Geoffrey, **Johanan Christian Prasana**, S. Muthu, Christina Susan Abraham, Host Antony David., *Structure–Activity relationship studies of two dietary flavonoids and their Nitric Oxide Synthase inhibition activity by spectroscopic and quantum/classical computational techniques*, Journal of Theoretical and Computational Chemistry, 18 (2019) 1950031.
- 30. Fathima Rizwana B., **Johanan Christian Prasana**, S. Muthu, Christina Susan Abraham, *Vibrational spectroscopy, reactive site analysis and molecular docking studies on 2-[(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)methoxy]-3-hydroxypropyl (2S)-2-amino-3-methylbutanoate*, Journal of Molecular Structure, 1202 (2020) 127274.
- 31. P. Manjusha, Johanan Christian Prasana, S. Muthu, BR. Raajaraman, *Density functional studies and spectroscopic analysis (FT-IR, FT Raman, UV- visible, and NMR) with molecular docking approach on an antifibrotic drug Pirfenidone*, Journal of Molecular structure, 1203 (2020) 12739.
- 32. Fathima Rizwana B., **Johanan Christian Prasana**, S. Muthu, Christina Susan Abraham, *Wavefunction analysis, charge transfer and molecular docking studies on Famciclovir and entecavir: Potential antiviral drugs*, Chemical Data Collections, 26(2020) 100353.
- 33. Jacob George, **Johanan Christian Prasana**, S. Muthu, Tintu K. Kuruvilla, Rinnu Sara Saji, *Evaluation of vibrational, electronic, reactivity and bioactivity of propafenone—A spectroscopic, DFT and molecular docking approach*, Chemical Data Collections, 26 (2020) 100360.
- 34. Muthu S., **Prasana J C.**, Bharathy G., *Vibrational Spectra*, *NBO*, *HOMO-LUMO and Molecular Docking of Diclofennac based on Density functional Theory*, Asian Journal of Research in Social Sciences and Humanities 7 (2017) 2249 -7315.
- 35. J. Christina Jebapriya, D. Reuben Jonathan S. Shahil Kirupavathy, R. Ragu, **Johanan Christian Prasana**, *Growth and characterization of a cyclohexanone based chalcone crystal* 2 (E)-(4-N,N-dimethylaminobenzylidene)-5-methylcyclohexanone for nonlinear optical applications, Optical Materials 107 (2020) 110035.
- 36. P. Manjusha, **Johanan Christian Prasana**, S. Muthu, B. Fathima Rizwana, Spectroscopic elucidation (FT-IR, FT-Raman and UV-visible) with NBO, NLO, ELF, LOL, drug likeness and molecular docking analysis on 1-

- (2ethylsulfonylethyl)-2-methyl-5-nitro-imidazole: An antiprotozoal agent, Computational Biology and Chemistry 88 (2020) 107330.
- 37. Ben Geoffrey A S, **Johanan Christian Prasana**, Muthu S, *Structure-Activity* relationship of Quercetin and its Tumor Necrosis Factor Alpha inhibition activity by computational and machine learning methods, Materials Today: Proceedings, https://doi.org/10.1016/j.matpr.2020.07.464, (In press)
- 38. Anuradha A, Rinnu Sara Saji, Mariam Varghese, Muthu S, **Johanan Christian Prasana**, *Vibrational Spectroscopic*, *DFT Studies and Molecular Docking on* (2R)-2-acetamido-N-benzyl-3-methoxy propanamide as an Antineuropathic Pain Drug, Materials Today: Proceedings, <a href="https://doi.org/10.1016/j.matpr.2020.07.465">https://doi.org/10.1016/j.matpr.2020.07.465</a>, (In press)
- 39. T. Hannah Clara, R. Ragu, D. Reuben Jonathan, **Johanan Christian Prasana**, Structural, optical, thermal, dielectric and Z-scan study on novel (2E)-1-(4-aminophenyl)-3-(4-benzyloxyphenyl)-prop-2-en-1-one(APBPP) chalcone crystal for nonlinear optical applications, Optical materials 109 (2020) 110331
- 40. J. Christina Jebapriya, Johanan Christian Prasana, S. Muthu, Fathima Rizwana B., Spectroscopic (FT-IR and FT-Raman), Quantum computational (DFT) and Molecular docking studies on 2(E)-(4-N,N-dimethylaminobenzylidene)-5-methylcyclohexanone, Materials Today: Proceedings. <a href="https://doi.org/10.1016/j.matpr.2020.08.221">https://doi.org/10.1016/j.matpr.2020.08.221</a>, (In press)
- 41. T. Hannah Clara, S. Muthu, **Johanan Christian Prasana**, Quantum mechanical, spectroscopic and docking studies of (2E)-1-(4-aminophenyl)-3-(4-benzyloxyphenyl)-prop-2-en-1one Chalcone derivative by Density functional Theory- A prospective respiratory drug, Materials Today: Proceedings, 2020, <a href="https://doi.org/10.1016/j.matpr.2020.08.804">https://doi.org/10.1016/j.matpr.2020.08.804</a>, (In press)