

FATIMA MATA NATIONAL COLLEGE

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3.4.5 List Citation Index

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Title of the paper	Name of the author	Title of the journal	Year of publication	Web of Science	Scopus	Indian Citation Index	Citation Index	Number of citations excluding self citations
ynthesis, spectral properties, chemical descriptors and light harvesting studies of a new bioactive azo imidazole compound	Kumar V.S., Mary Y.S., Pradhan K., Brahman D., Mary Y.S., Thomas R., Roxy M.S., Alsenoy C.V.	Journal of Molecular Structure	2020	1	2		0.016453	0
Exploring the detailed spectroscopic characteristics, chemical and biological activity of two cyanopyrazine-2-carboxamide derivatives using experimental and theoretical tools	Mary Y.S., Mary Y.S., Thomas R., Armakovic S., Armakovic S.J., Zitko J., Dolezal M., Van Alsenoy C.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2020	1	4		0.027422	0

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Effects of mobile phone radiation on certain hematological parameters	B., Sheena Mary Y., Khandaker M.U., Bradley D.A., Chew M.T., Jojo P.J.	Radiation Physics and Chemistry	2020		0		0	0
Quantum mechanical and photovoltaic studies on the cocrystals of hydrochlorothiazide with isonazid and malonamide	Al-Otaibi J.S., Mary Y.S., Mary Y.S., Thomas R.	Journal of Molecular Structure	2019	0	1		0.005484	0
Synthesis, spectral characterisation, quantum mechanical analysis and light harvesting properties of two azoimidazole analogues	Smitha M., Mary Y.S., Pradhan K., Brahman D., Mary Y.S., Thomas R., Pavithran R., Alsenoy C.V.	Journal of Molecular Structure	2019	1	0		0.005484	0
Fabrication of innocuous gold nanoparticles using plant cells in culture	Bhaskaran S., Sharma N., Tiwari P., Singh S.R., Sahi S.V.	Scientific Reports	2019	0	0		0	0
Detailed quantum mechanical, molecular docking, QSAR prediction, photovoltaic light harvesting efficiency analysis of benzil and its halogenated analogues	Mary Y.S., Mary Y.S., Resmi K.S., Kumar V.S., Thomas R., Sureshkumar B.	Heliyon	2019		0		0	0

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A novel voltammetric sensor for morphine detection based on electrochemically synthesized poly (p-aminobenzenesulfonicacid)/reduced graphene oxide composite	Abraham P., Renjini S., Mary T.E.N., Kumary V.A., Chithra P.G.	AIP Conference Proceedings	2019		0		0	0
Anti-Cancerous Brucine and Colchicine: Experimental and Theoretical Characterization	Afzal A., Thayyil M.S., Shariq M., Mary Y.S., Resmi K.S., Thomas R., Islam N., Abinu A.J.	Chemistry Select	2019	0	0		0	0
A novel heterogeneous catalyst based on reduced graphene oxide supported copper coordinated amino acid " A platform for morphine sensing	Abraham P., S R., Swamy B.E.K., Nancy T.E.M., Sreevalsan A.	Journal of Electroanalytical Chemistry	2019		0		0	0
Synthesis and characterization of a clay-alginate nanocomposite for the controlled release of 5-Flurouracil	Surya R., Mullassery M.D., Fernandez N.B., Thomas D.	Journal of Science: Advanced Materials and Devices	2019		0		0	0
Comparison of results from indoor radon measurements using active and passive methods with those from mathematical modeling	Visnuprasad A.K., Reby Roy K.E., Jojo P.J., Sahoo B.K.	Radiation and Environmental Biophysics	2019	0	0		0	0

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DFT and molecular docking investigations of oxicam derivatives	Mary Y.S., Mary Y.S., Resmi K.S., Thomas R.	Heliyon	2019				0	0	0	
Conformational profile, vibrational assignments, NLO properties and molecular docking of biologically active herbicide 1,1-dimethyl-3-phenylurea	Kumar V.S., Sheena Mary Y., Popoola S.A., Thomas R., Roxy M.S., Al-Saadi A.A.	Heliyon	2019				3	0.016453	0	
Activity concentrations of radionuclides in soil samples along the coastal areas of Kerala, India and the assessment of radiation hazard indices	Ramsiya M., Joseph A., Eappen K.P., Visnuprasad A.K.	Journal of Radioanalytical and Nuclear Chemistry	2019				0	1	0.005484	1
Synthesis and spectroscopic study of two new pyrazole derivatives with detailed computational evaluation of their reactivity and pharmaceutical potential	Mary Y.S., Resmi K.S., Narayana B., Sarojini S.B.K., Armakovic S., Armakovic S.J., Vijayakumar G., Alsenoy C.V., Mohan B.J.	Journal of Molecular Structure	2019				4	6	0.054845	0

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Two neoteric pyrazole compounds as potential anti-cancer agents: Synthesis, electronic structure, physico-chemical properties and docking analysis	Thomas R., Mary Y.S., Resmi K.S., Narayana B., Sarojini B.K., Vijayakumar G., Van Alsenoy C.	Journal of Molecular Structure	2019	4	7	0.060329	0
Synthesis, characterization and biological investigation of glycine-based sulfonamide derivative and its complex: Vibration assignment, HOMO & LUMO analysis, MEP and molecular docking	Shafieyoon P., Mehdipour E., Mary Y.S.	Journal of Molecular Structure	2019	5	6	0.060329	5
Dielectric spectroscopic studies in supercooled liquid and glassy states of Acemetacin, Brucine and Colchicine	Thayyil M.S., Sivaramakris hnan P.A., Sulaiman M.K., Hussan K.P.S., Panicker C.Y., Ngai	Journal of Non- Crystalline Solids	2019	2	2	0.021938	0
Single crystal XRD, DFT investigations and molecular docking study of 2- ((1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)amino)naphthalene-1,4-dione as a potential anti-cancer lead molecule	P.R. K.R., Mary Y.S., Fernandez A., S A.P., Mary Y.S., Thomas R.	Computati onal Biology and Chemistry	2019	6	9	0.082267	2

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Spectroscopic, antimicrobial and computational study of novel benzoxazole derivative	Mary Y S., Panicker C.Y., Armakovic S., Armakovic S.J., Arisoy M., Temiz- Arpaci O., Van Alsenoy	Journal of Molecular Structure	2019	0	1	0.005484	1
Cocrystals of pyrazinamide with p-toluenesulfonic and ferulic acids: DFT investigations and molecular docking studies	J.S., Sheena Mary Y., Shyma Mary Y., Panicker C.Y., Thomas R.	Journal of Molecular Structure	2019	2	4	0.032907	1
Synthesis, conformational, characterization and reactivity study of 1,7-bis(4-bromophenyl)heptane-1,7-dione	Suneetha V., Smitha M., Mary Y.S., Armakovic S., Armakovic S.J., Rao R.S., Suchetan P.A., Al- Saadi A.A.,	Journal of Molecular Structure	2019	0	1	0.005484	1
Electrochemical synthesis of thin-layered graphene oxide-poly(CTAB) composite for detection of morphine	Abraham P., Renjini S., Nancy T.E.M., Kumary V.A.	Journal of Applied Electroche mistry	2019		0	0	0

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Hybrid and bioactive cocrystals of pyrazinamide with hydroxybenzoic acids: Detailed study of structure, spectroscopic characteristics, other potential applications and noncovalent interactions using SAPT	Al-Otaibi J.S., Mary Y.S., Armakovic S., Thomas R.	Journal of Molecular Structure	2019		0		0	0
Spectral characterization, thermochemical studies, periodic SAPT calculations and detailed quantum mechanical profiling various physico-chemical properties of 3,4-dichlorodiuron	Kumar V.S., Armakovic S.J., Armakovic S., Mary Y.S., Thomas R., Popoola S.A., Almohammed A.R., Roxy M.S., Al-Saadi A.A.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2019		0		0	0
Quantum Mechanical Studies of Three Aromatic Halogen-Substituted Bioactive Sulfonamidobenzoxazole Compounds with Potential Light Harvesting Properties	Sheena Mary Y., Ertan-Bolelli T., Thomas R., Krishnan A.R., Bolelli K., Kasap E.N., Onkol T., Yildiz I.	Polycyclic Aromatic Compounds	2019	0	0		0	0
Comparison of gamma dose levels assessed by various methods	Visnu Prasad A.K., Soniya S.R., Jojo P.J.	Materials Today: Proceedings	2019		0		0	0

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Evaluating Genetic Diversity Within Genus Jasminum L. (Oleaceae) Using Intersimple Sequence Repeats (ISSR) Marker	Yohanan R., Jeyarani N.J., Devipriya V., Rather S.A., Kasana S., Thakur J., Dwivedi M.D., Pandey A.K.	Proceedings of the National Academy of Sciences India Section B - Biological Sciences	2019		0		0	0
Theoretical Studies on the Structure and Various Physico-Chemical and Biological Properties of a Terphenyl Derivative with Immense Anti-Protozoan Activity	Mary Y.S., Thomas R., Narayana B., Samshuddin S., Sarojini B.K., Armakovic S., Armakovic S.J., Pillai G.G.	Polycyclic Aromatic Compounds	2019	2	4		0.032907	0

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Synthesis, characterization and computational studies of semicarbazide derivative	ar M., Bhuvaneswa ri T., Venkatesh G., Kamal C., Vennila P., Armakovic S., Armakovic S.J., Sheena Mary Y., Yohannan	Journal of Molecular Liquids	2018	3	2	0.027422	1
Synthesis and spectroscopic study of three new oxadiazole derivatives with detailed computational evaluation of their reactivity and pharmaceutical potential	Miniyar P.B., Mary Y.S., Resmi K.S., Panicker C.Y., Armakovic S., Armakovic S.J., Thomas R., Sureshkuma	Journal of Molecular Structure	2018	6	9	0.082267	3
Two novel imidazole derivatives “ Combined experimental and computational study	Mary Y.S., Hossain M., Resmi K.S., Armakovic S., Armakovic S.J., Pavithran R., Nanda A.K., Van Alsenoy C.	Journal of Molecular Structure	2018	1	1	0.010969	1

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Phylogenetic analysis and evolution of morphological characters in the genus <i>Jasminum</i> L. (Oleaceae) in India	J.N., Yohannan R., Vijayavalli D., Dwivedi	Journal of Genetics	2018	0	1	0.005484	0
Microwave- assisted green synthesis of acrylamide cyclodextrin-grafted silylated bentonite for the controlled delivery of tetracycline hydrochloride	Mullassery M.D., Fernandez N.B., Surya R., Thomas D.	Sustainable Chemistry and Pharmacy	2018	3	3	0.032907	2
Molecular dynamic simulations, ALIE surface, Fukui functions geometrical, molecular docking and vibrational spectra studies of tetra chloro p and m-xylene	G., Kamal C., Vennila P., Govindaraju M., Mary Y.S., Armakovic S., Armakovic S.J., Kaya S.,	Journal of Molecular Structure	2018	5	6	0.060329	1
Molecular structure, spectroscopic, dielectric and thermal study, nonlinear optical properties, natural bond orbital, HOMO-LUMO and molecular docking analysis of (C ₆ Cl ₂ O ₄) (C ₁₀ H ₁₄ N ₂ F ₂ ·2H ₂ O)	Hosna S., Janzen D.E., Mary Y.S., Resmi K.S., Thomas R., Mohamed R., Wajda S.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2018	2	4	0.032907	1

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Dietary curcumin influences leptin, growth hormone and hepatic growth factors in Tilapia (<i>Oreochromis mossambicus</i>)	Nair A.B., Arun D., Thushara V.V., Sheeja C.C., Vijayasree A.S., Oommen O.V., Divya	Aquacultur e	2018	4	4		0.043876	4
Reproductive biology of a Gobiid fish <i>Oxyurichthys tentacularis</i> (Valenciennes, 1837) inhabiting Ashtamudi Lake, S. India	Remya Mohan S., Harikrishnan M., Sherly Williams E.	Journal of Applied Ichthyology	2018	1	1		0.010969	0
Spectroscopic characterization of hydroxyquinoline derivatives with bromine and iodine atoms and theoretical investigation by DFT calculations, MD simulations and molecular docking studies	r B., Mary Y.S., Resmi K.S., Suma S., Armakovic S., Armakovic S.J., Van Alsenoy C., Narayana B.,	Journal of Molecular Structure	2018	0	0		0	0
A green approach for the synthesis of drug delivery system, mesoporous silica grafted acrylamide β -cyclodextrin composite, for the controlled release of curcumin	Mullassery M.D., Fernandez N.B., Surya R., Thomas D.	Asian Journal of Pharmaceu tical and Clinical Research	2018		0		0	0

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Synthesis, spectroscopic analyses, chemical reactivity and molecular docking study and anti-tubercular activity of pyrazine and condensed oxadiazole derivatives	M.S., Mary Y.S., Miniyar P.B., Al- Wahaibi L.H., El- Emam A.A., Armakovic S., Armakovic	Journal of Molecular Structure	2018	5	6	0.060329	3
Spectroscopic characterization of 8-hydroxy-5-nitroquinoline and 5-chloro-8-hydroxy quinoline and investigation of its reactive properties by DFT calculations and molecular dynamics simulations	r B., Sheena Mary Y., Suma S., Armakovic S., Armakovic S.J., Alsenoy C.V., Narayana B., Sasidharan B.P.	Journal of Molecular Structure	2018	2	2	0.021938	2
Study on the structure, vibrational analysis and molecular docking of fluorophenyl derivatives using FT-IR and density functional theory computations	Al-Tamimi A.- M.S., Mary Y.S., Hassan H.M., Resmi K.S., El- Emam A.A., Narayana B., Sarojini B.K.	Journal of Molecular Structure	2018	2	2	0.021938	2

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Understanding reactivity of two newly synthesized imidazole derivatives by spectroscopic characterization and computational study	Thomas R., Mary Y.S., K.S.Resmi, Armakovic S., Armakovic S.J., Nanda A.K., Vijayakumar G., Alsenoy C.V.	Journal of Molecular Structure	2018	7	10		0.093236	1
Spectroscopic analysis and molecular docking of imidazole derivatives and investigation of its reactive properties by DFT and molecular dynamics simulations	Hossain M., Mary Y.S., Resmi K.S., Armakovic S., Armakovic S.J., Nanda A.K., Ranjan V.K., Vijayakumar G., Van Alsenoy C.	Journal of Molecular Structure	2018	4	3		0.038391	2
Synthesis, spectroscopic analyses (FT-IR and NMR), vibrational study, chemical reactivity and molecular docking study and anti-tubercular activity of condensed oxadiazole and pyrazine derivatives	Mary Y.S., Abdel-Aziz A.A.M., Muniyar P.B., Armakovic S., Armakovic S.J.	Journal of Molecular Structure	2018	5	5		0.054845	4

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Spectroscopic analysis of 8-hydroxyquinoline derivatives and investigation of its reactive properties by DFT and molecular dynamics simulations	r B., Mary Y.S., Resmi K.S., Panicker C.Y., Armakovic S., Armakovic S.J., Van Alsenoy C.,	Journal of Molecular Structure	2018	3	9	0.065814	2
Combined spectroscopic, DFT, TD-DFT and MD study of newly synthesized thiourea derivative	Sheena Mary Y., Shyma Mary Y., Panicker C.Y., Bielenica A., Armakovic S., Armakovic S.J., Van	Journal of Molecular Structure	2018	4	4	0.043876	4
Characterization of biochars from a plant biomass and its effect on lead sorption capacity	N.B., Mullassery M.D., Thomas D., Surya R., Jelen Das Y.	Desalination and Water Treatment	2018	0	0	0	0
Contribution of thoron and progeny towards inhalation dose in a thorium abundant beach environment	A.K., Jaikrishnan G., Sahoo B.K., Pereira C.E., Jojo P.J.	Radiation Protection Dosimetry	2018	1	2	0.016453	2

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Adsorption properties of graphene towards the ephedrine " A frequently used molecule in sport	Armakovic S., Armakovic S.J., Tomic B.T., Pillai R.R., Panicker C.Y.	Computational and Theoretical Chemistry	2018	4	5	0.04936	4
A complete computational and spectroscopic study of 2-bromo-1, 4-dichlorobenzene " A frequently used benzene derivative	Govindaraju M., Venkatesh G., Kamal C., Mary Y.S., Panicker C.Y., Kaya S., Armakovic S., Armakovic	Journal of Molecular Structure	2018	7	8	0.082267	2
4-[(4-acetylphenyl)amino]-2-methylidene-4-oxobutanoic acid, a newly synthesized amide with hydrophilic and hydrophobic segments: Spectroscopic characterization and investigation of its reactive properties	Abdullah E.S., Aljohar H.I., Narayana B., Nayak P.S., Sarojini B.K., Armakovic S., Armakovic S.J., Alsenoy C.V., El-	Journal of the Serbian Chemical Society	2018	1	1	0.010969	1

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Phylogenetic analysis and evolution of morphological characters in the genus <i>Jasminum</i> L. (Oleaceae) in India	Jeyarani J Nirmala, Yohannan Regy, Vijayavalli Devipriya, Dwivedi D Mayank, Pandey K Arun	JOURNAL OF GENETICS	2018			0	0	0
Strategic human resource management: An overview	John Ancy, Kalarani T G	INTERNATIONAL JOURNAL OF MANAGEMENT STUDIES	2018			0	0	0
: A fixed point theorem in complex valued B - Metric space using contractive mappings	Lekshmi S, Dersanambika K S	BULLETIN OF PURE AND APPLIED SCIENCES SEC. E - MATHEMATICS & STATISTICS	2018			0	0	0

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Seasonal and positional variations in the rate of nacre coating in Indian pearl oyster <i>Pinctada fucata</i> (Gould, 1850)	Rinju R Mary, Anil M K, Williams E Sherly	JOURNAL OF THE MARINE BIOLOGIC AL ASSOCIATI ON OF INDIA	2018				0	0	0
Spectroscopic analysis of 8-hydroxyquinoline-5-sulphonic acid and investigation of its reactive properties by DFT and molecular dynamics simulations	r B., Sheena Mary Y., Panicker C.Y., Resmi K.S., Suma S., Armakovic S., Armakovic S.J., Van	Journal of Molecular Structure	2017	11	11		0.120658		1
Supramolecular architecture of 5-bromo-7-methoxy-1-methyl-1H-benzoimidazole. $3H \cdot 2O$: Synthesis, spectroscopic investigations, DFT computation, MD simulations and docking studies	Smitha M., Sheena Mary Y., Armakovic S., Armakovic S.J., Rao R.S., Suchetan P.A., Giri L., Pavithran R.,	Journal of Molecular Structure	2017	1	1		0.010969		0

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Synthesis, XRD single crystal structure analysis, vibrational spectral analysis, molecular dynamics and molecular docking studies of 2-(3-methoxy-4-hydroxyphenyl) benzothiazole	A., Aswathy V.V., Sheena Mary Y., Yohannan Panicker C., Armakovic S., Armakovic S.J., Ravindran R., Van	Journal of Molecular Structure	2017	3	4	0.038391	2
Investigation of reactive and spectroscopic properties of oxobutanoic acid derivative: Combined spectroscopic, DFT, MD and docking study	Mary Y.S., Panicker C.Y., Armakovic S., Armakovic S.J., Narayana B., Sarojini B.K., Van Alsenoy	Journal of Molecular Structure	2017	1	2	0.016453	0
Vibrational spectroscopic investigations and molecular docking studies of biologically active 2-[4-(4-phenylbutanamido)phenyl]-5-ethylsulphonyl-benzoxazole	Alshaikh M.A., Mary Y.S., Panicker C.Y., El- Emam A.A., Temiz-Arpaci O., Alsenoy C.V.	Journal of Molecular Structure	2017	5	5	0.054845	0

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Conformational, vibrational and DFT studies of a newly synthesized arylpiperazine-based drug and evaluation of its reactivity towards the human GABA receptor	A.T., Al-Ahmadi A.F., Mary Y.S., Panicker C.Y., Ullah N., Armakovic S., Armakovic S.J., Van	Journal of Molecular Structure	2017	2	2	0.021938	1
A combined experimental and computational investigation of solvatochromism of nonpolar laser dyes: Evaluation of ground and singlet excited-state dipole moments	Pujar G.H., Wari M.N., Steffi B., Varsha H., Kavita B., Yohannan Panicker C., Santhosh C., Patil A., Inamdar S.R.	Journal of Molecular Liquids	2017	4	4	0.043876	1
Comparison of thoron (Rn-220) content and gamma radiation level in high background radiation area of Kollam district in Kerala, India	Midhun M., Mathew S., Rejith R.S., Jojo P.J., Sahoo B.K.	Journal of Radioanalytical and Nuclear Chemistry	2017	1	1	0.010969	1

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Insight into the reactive properties of newly synthesized 1,2,4-triazole derivative by combined experimental (FT-IR and FR-Raman) and theoretical (DFT and MD) study	Omary F.A.M., Mostafa G.A.E., El-Emam A.A., Manjula P.S., Sarojini B.K., Narayana B., Armakovic S., Armakovic S.J., Van	Journal of Molecular Structure	2017	1	1		0.010969	1
Modification of benzoxazole derivative by bromine-spectroscopic, antibacterial and reactivity study using experimental and theoretical procedures	V.V., Alper-Hayta S., Yalcin G., Mary Y.S., Panicker C.Y., Jojo P.J., Kaynak-Onurdag F., Armakovic S., Armakovic S.J., Yildiz I., Van Alsenoy	Journal of Molecular Structure	2017	11	11		0.120658	5

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Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study	Sheena Mary Y., Suneetha V., Panicker C.Y., Armakovic S., Armakovic S.J., Giri L., Suchetan P.A., Van Alsenoy C.	Journal of Molecular Structure	2017	4	5		0.04936	3
FT-IR and FT-Raman characterization and investigation of reactive properties of N-(3-iodo-4-methylphenyl)pyrazine-2-carboxamide by molecular dynamics simulations and DFT calculations	Al-Abdullah E.S., Al-Omary F.A.M., El-Emam A.A., Anto P.L., Sheena M.Y., Armakovic S., Armakovic S.J., Zitko J., Dolezal M., Van Alsenoy	Journal of Molecular Structure	2017	8	9		0.093236	3
New quinolone derivative: Spectroscopic characterization and reactivity study by DFT and MD approaches	Mary Y.S., Panicker C.Y., Anto P.L., Armakovic S., Armakovic S.J., Musiol R., Jampilek J., Van	Journal of Molecular Structure	2017		4		0.021938	3

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Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of N-[(4-(trifluoromethyl)phenyl)pyrazine-2-carboxamide by density functional methods	Varghese H.T., Panicker C.Y., Viswanathan K., Dolezal M., Van Alsenoy C.	Arabian Journal of Chemistry	2017	12	14	0.142596	13
Spectroscopic and reactive properties of a newly synthesized quinazoline derivative: Combined experimental, DFT, molecular dynamics and docking study	Mary Y.S., Mary Y.S., Panicker C.Y., Abdel-Aziz A.A.-M., Mohamed M.A., Armakovic S., Armakovic S.J., Van Alsenoy C.	Journal of Molecular Structure	2017	2	2	0.021938	0
Newly synthesized dihydroquinazoline derivative from the aspect of combined spectroscopic and computational study	Mary Y.S., Mary Y.S., Panicker C.Y., Abdel-Aziz A.A.-M., El-Sherbeny M.A., Armakovic S., Armakovic S.J., Van Alsenoy C.	Journal of Molecular Structure	2017	2	2	0.021938	0

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Investigation of spectroscopic, reactive, transport and docking properties of 1-(3,4-dichlorophenyl)-3-[3-(trifluoromethyl)phenyl]thiourea (ANF-6): Combined experimental and computational study	V.V., Mary Y.S., Jojo P.J., Panicker C.Y., Bielenica A., Armakovic S., Armakovic S.J., Brzozka P.,	Journal of Molecular Structure	2017	6	7	0.071298	3
Spectroscopic, DFT, molecular dynamics and molecular docking study of 1-butyl-2-(4-hydroxyphenyl)-4,5-dimethyl-imidazole 3-oxide	Mary Y.S., Varghese H.T., Panicker C.Y., Armakovic S., Armakovic S.J., Pradhan K., Nanda A.K.,	Journal of Molecular Structure	2017	6	7	0.071298	6
Synthesis, crystal structure analysis, spectral investigations, DFTÀ computations and molecular dynamics and docking study of 4-benzyl-5-oxomorpholine-3-carbamide, a potential bioactive agent	Sheena Mary Y., Shyma Mary Y., Panicker C.Y., Suneetha V., Armakovic S., Armakovic S.J., Van Alsenoy C.,	Journal of Molecular Structure	2017	3	5	0.043876	2

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Synthesis, vibrational spectroscopic investigations, molecular docking, antibacterial studies and molecular dynamics study of 5-[(4-nitrophenyl)acetamido]-2-(4-tert-butylphenyl)benzoxazole	Y., Al-Shehri M.M., Jalaja K., Al-Omary F.A.M., El-Emam A.A., Yohannan Panicker C., Armakovic S., Armakovic S.J., Temiz-Arpaci O., Van Alsenoy C.	Journal of Molecular Structure	2017	2	3	0.027422	3
Vibrational spectroscopic analysis of cyanopyrazine-2-carboxamide derivatives and investigation of their reactive properties by DFT calculations and molecular dynamics simulations	Mary Y.S., Varghese H.T., Panicker C.Y., Armakovic S., Armakovic S.J., Zitko J., Dolezal M., Van Alsenoy	Journal of Molecular Structure	2017	5	6	0.060329	2
Studies on the synthesis, spectroscopic analysis, molecular docking and DFT calculations on 1-hydroxy-2-(4-hydroxyphenyl)-4,5-dimethyl-imidazol 3-oxide	Sheena M.Y., Panicker C.Y., Armakovic S., Armakovic S.J., Pradhan K., Nanda A.K.,	Journal of Molecular Structure	2017		1	0.005484	1

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Vibrational spectroscopic investigations, molecular dynamic simulations and molecular docking studies of N'-diphenylmethylidene-5-methyl-1H-pyrazole-3-carbohydrazide	Menon V.V., Mary Y.S., Armakovic S., Armakovic S.J., Panicker C.Y.	Journal of Molecular Structure	2017	4	5	0.04936	4
Vibrational spectroscopic analysis, molecular dynamics simulations and molecular docking study of 5-nitro-2-phenoxyethyl benzimidazole	Foto E., Mary Y.S., Karatas E., Panicker C.Y., Yalcin G., Armakovic S., Armakovic S.J., Van Alsenoy C.,	Journal of Molecular Structure	2017		5	0.027422	1
Spectroscopic characterization of 1-[3-(1H-imidazol-1-yl)propyl]-3-phenylthiourea and assessment of reactive and optoelectronic properties employing DFT calculations and molecular dynamics simulations	Jalaja K., Mary Y.S., Panicker C.Y., Armakovic S., Armakovic S.J., Srivastava S.K., Van	Journal of Molecular Structure	2017		22	0.120658	4

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Reactive, spectroscopic and antimicrobial assessments of 5-[(4-methylphenyl) acetamido]-2-(4-tert-butylphenyl)benzoxazole: Combined experimental and computational study	Alzoman N.Z., Menon V.V., Al-Abdullah E.S., El-Emam A.A., Panicker C.Y., Temiz-Arpaci O., Armakovic S., Armakovic	Journal of Molecular Structure	2017			7	0.038391	4
Spectroscopic characterization of 4-[2-(5-Ethylpyridin-2-yl)ethoxy]benzaldehyde oxime and investigation of its reactive properties by DFT calculations and molecular dynamics simulations	Mary Y.S., Panicker C.Y., Armakovic S., Armakovic S.J., Sagar B.K., Girisha M., Yathirajan	Journal of Molecular Structure	2017			8	0.043876	4
Molecular conformational analysis, reactivity, vibrational spectral analysis and molecular dynamics and docking studies of 6-chloro-5-isopropylpyrimidine-2,4(1H,3H)-dione, a potential precursor to bioactive agent	F.A.M., Mary Y.S., Beegum S., Panicker C.Y., Al-Shehri M.M., El-Emam A.A., Armakovic S., Armakovic S.J., Van	Journal of Molecular Structure	2017			1	0.005484	0

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FT-IR, FT-Raman and NMR characterization of 2-isopropyl-5-methylcyclohexyl quinoline-2-carboxylate and investigation of its reactive and optoelectronic properties by molecular dynamics simulations and DFT calculations	Fazal E., Mary Y.S., Panicker C.Y., Armakovic S., Armakovic S.J., Nagarajan S., Van Alsenoy	Journal of Molecular Structure	2017		22		0.120658	8
An assessment of ingestion dose to public from polonium -210 and lead- 210 via dietary sources in an industrial area Eloor, Kerala, India	Balakrishnan D., Jojo P.J., Abraham J.P.	Pollution Research	2017		0		0	0
Radiation dose to the populace in southern peninsular India through foodstuff	Jose R.M., Jojo P.J.	Nature Environment and Pollution Technology	2017		0		0	0
Food and feeding of Hypselobarbus Kurali, a freshwater cyprinid endemic to Kallada River, Kollam, Kerala, India	Williams S., Sarlin, Sudhakaran V.N.M.	International Journal of Zoological Research	2017		0		0	0
Biochemical analysis of a few marine macroalgae from the Kollam Coast of India	Shashidharan A., Plomindas S.N.	International Journal on Algae	2017		0		0	0

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Quinoline derivatives as possible lead compounds for anti-malarial drugs: Spectroscopic, DFT and MD study	r B., Mary Y.S., Panicker C.Y., Suma S., Armakovic S., Armakovic S.J., Van	Arabian Journal of Chemistry	2017		21		0.115174	3
Estimation of Indoor Radon and Thoron in dwellings of Palakkad, Kerala, India using solid state nuclear track detectors	Ramsiya M., Joseph A., Jojo P.J.	Journal of Radiation Research and Applied Sciences	2017	2	Nil		#VALUE!	
An assessment of ingestion dose to public from polonium-210 and lead-210 via dietary sources in an industrial area Eloor, Kerala, India	Balakrishnan Dhanya, Jose PJ , Jojcfand, Abraham P	POLLUTION RESEARCH	2017				0	0
Radiation dose to the populace in Southern peninsular India through foodstuff	Jose Reebea Maria, Jojo PJ	: NATURE ENVIRONMENT & POLLUTION TECHNOLOGY	2017				0	0

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Sway on FDI in India: Some rudimentary corroborations	Joseph James V, Sajeeve V P, Periera Catherine E	INTERNATIONAL JOURNAL OF RESEARCH IN COMMERCE, ECONOMICS & MANAGEMENT	2017				0	0	0
Measurement of radium content and radon exhalation rates in soil samples along the coastal regions of Karunagapally, Kollam district, Kerala	Monica S, Soniya S R, Prasad A K Visnu, Jojo P J	INDIAN JOURNAL OF SCIENTIFIC RESEARCH	2017				1	0.001219	1
Estimation of radiation exposure in environmental soil samples from Thirumullavaram coastal region, Kerala	Soniya S R, Monica S, Jojo P J	INDIAN JOURNAL OF SCIENTIFIC RESEARCH	2017				0	0	0

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Assessing multiple stressors on macrofaunal benthic communities along the coastal ecosystem of Southern Kerala	Mumthas Y, Miranda M T P	JOURNAL OF THE MARINE BIOLOGICAL ASSOCIATION OF INDIA	2017				0	0	0
Vibrational spectroscopic studies, Fukui functions, HOMO-LUMO, NLO, NBO analysis and molecular docking study of (E)-1-(1,3-benzodioxol-5-yl)-4,4-dimethylpent-1-en-3-one, a potential precursor to bioactive agents	Al-Wabli R.I., Resmi K.S., Sheena Mary Y., Yohannan Panicker C., Attia M.A., El-Emam A.A., Van Alsenoy C.	Journal of Molecular Structure	2016			8		0.043876	5
Conformational, NBO, NLO, HOMO-LUMO, NMR, electronic spectral study and molecular docking study of N,N-Dimethyl-3-(10H-phenothiazin-10-yl)-1-propanamine	Resmi K.S., Haruna K., Sheena Mary Y., Yohannan Panicker C., Saleh T.A., Al-Saadi A.A., Van Alsenoy C.	Journal of Molecular Structure	2016			5		0.027422	1

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External dose measurements in the Eloor industrial area in the Ernakulam district of Kerala, India	D., Umadevi A.G., Ben Byju S., Sunil A., Abraham J.P., Jojo P.J., Radhakrishn an S.,	Internation al Journal of Radiation Research	2016		0		0	0
Spectroscopic investigations and molecular docking study of (2E)-1-(4-Chlorophenyl)-3-[4-(propan-2-yl)phenyl]prop-2-en-1-one using quantum chemical calculations	Al-Alshaikh M.A., Panicker C.Y., El- Emam A.A., Salian V.V., Narayana B., Sarojini B.K., van Alsenoy C.	Journal of Molecular Structure	2016		10		0.054845	5
Spectroscopic analysis (FT-IR, FT-Raman and NMR) and molecular docking study of ethyl 2-(4-oxo-3-phenethyl-3,4-dihydroquinazolin-2-ylthio)-acetate	El-Azab A.S., Jalaja K., Abdel-Aziz A.A.-M., Al- Obaid A.M., Sheena Mary Y., Yohannan Panicker C., Van Alsenoy C.	Journal of Molecular Structure	2016		8		0.043876	2

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Spectroscopic, quantum chemical studies, Fukui functions, in vitro antiviral activity and molecular docking of 5-chloro-N-(3-nitrophenyl)pyrazine-2-carboxamide	S.H.R., Al-Alshaikh M.A., El-Emam A.A., Panicker C.Y., Zitko J., Dolezal M., Vanalsenoy	Journal of Molecular Structure	2016		26		0.142596	13
Synthesis, vibrational spectroscopic investigations, molecular docking, antibacterial and antimicrobial studies of 5-ethylsulphonyl-2-(p-aminophenyl)benzoxazole	Al-Alshaikh M.A., Panicker C.Y., El-Emam A.A., Arisoy M., Temiz-Arpaci O., Van Alsenoy C.	Journal of Molecular Structure	2016		7		0.038391	0
Evaluation of radionuclides transfer from soil-to-edible flora and estimation of radiological dose to the Malaysian populace	M.U., Mohd Nasir N.L., Asaduzzaman K., Olatunji M.A., Amin Y.M., Kassim H.A., Bradley D.A., Jojo P.J., Alrefaed T.	Chemosphere	2016		17		0.093236	5

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DFT and experimental (FT-IR and FT-Raman) investigation of vibrational spectroscopy and molecular docking studies of 2-(4-oxo-3-phenethyl-3,4-dihydroquinazolin-2-ylthio)-N-(3,4,5-trimethoxyphenyl) acetamide	El-Azab A.S., Sheena Mary Y., Yohannan Panicker C., Abdel-Aziz A.A.-M., El- Sherbeny M.A., Van Alsenoy C.	Journal of Molecular Structure	2016				22	0.120658	13
FT-IR, FT-Raman and molecular docking study of ethyl 4-(2-(4-oxo-3-phenethyl-3,4-dihydroquinazolin-2-ylthio)acetamido)benzoate	El-Azab A.S., Mary Y.S., Panicker C.Y., Abdel- Aziz A.A.-M., Al-Suwaidan I.A., Van Alsenoy C.	Journal of Molecular Structure	2016				6	0.032907	5
Spectroscopic investigations and molecular docking study of 3-(1H-imidazol-1-yl)-1-phenylpropan-1-one, a potential precursor to bioactive agents	M.A., Mary Y.S., Panicker C.Y., Attia M.I., El- Emam A.A., Alsenoy C.V.	Journal of Molecular Structure	2016				3	0.016453	3
Assessment of pollution status of vattakkayal, a part of ashtamudi lake - Ramsar site in Kerala (India) ' Using multivariate statistical analysis	Lal S.S., Jaya D.S., Williams E.S.	Journal of Environme ntal Science and Engineerin g	2016				0	0	0

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Vibrational spectroscopic & molecular docking studies of 2,6-dichlorobenzyl alcohol	M.M., Resmi K.S., Sheena Mary Y., Yohannan Panicker C., Harikumar B.	Chemist	2016				0	0	0
Spectroscopic, single crystal XRD structure, DFT and molecular dynamics investigation of 1-(3-chloro-4-fluorophenyl)-3-[3-(trifluoromethyl)phenyl]thiourea	Y., Aswathy V.V., Panicker C.Y., Bielenica A., Brzozka P., Savczenko O., Armakovic S., Armakovic	RSC Advances	2016				25	0.137112	3
History handcuffed: The personal and the political in Jhumpa Lahiri's The lowland	Marshal R	THE CRITERION: AN INTERNATIONAL JOURNAL IN ENGLISH	2016				0	0	0

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Assessment of pollution status of vattakkayal, a part of ashtamudi lake - Ramsar site in Kerala (India) using multivariate statistical analysis	Lal S Seethal, Jaya D S, Williams E Sherly	JOURNAL OF ENVIRONMENTAL SCIENCE & ENGINEERING	2016				0	0	0
A study on women entrepreneurs in micro enterprises	Jency S, Siniya A	INTERNATIONAL JOURNAL OF RESEARCH IN COMMERCE & MANAGEMENT	2016				2	0.002438	2
Antimicrobial potential of theepiphytic bacteria of marine alga, Gelidium pusillum	Naziya, Gayathri Lakshmi, Miranda Mary Teresa P , Parvathy G, Laxmisaxena Vija Y	JOURNAL OF APPLIED ZOOLOGICAL RESEARCHES	2016				0	0	0

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Vibrational spectroscopic and molecular docking study of (2E)-N-(4-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylprop-2-enamide	R.T., Panicker C.Y., Varghese H.T., Musiol R., Jampilek J., Van Alsenoy C., War J.A., Al-Saadi A.A.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015		13		0.071298	2
Molecular conformational analysis, vibrational spectra, NBO, NLO analysis and molecular docking study of bis[(E)-anthranyl-9-acrylic]anhydride based on density functional theory calculations	Panicker C.Y., Thiemann T., Al-Azani M., Al-Saadi A.A., Van Alsenoy C., Raju K., War J.A., Srivastava	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015		9		0.04936	7
Macroinvertebrate communities in the bottom sediment of Arthunkal coast in Kerala, southwest coast of India	Varghese S.J., Miranda M.T.P.	Nature Environment and Pollution Technology	2015		0		0	0

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FT-IR, NBO, HOMO-LUMO, MEP analysis and molecular docking study of Methyl N-({2-(2-methoxyacetamido)-4-(phenylsulfanyl)phenyl}amino){(methoxycarbonyl)imino}methyl)carbamate	Panicker C.Y., Varghese H.T., Narayana B., Divya K., Sarojini B.K., War J.A., Van Alsenoy C., Fun H.K.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				11	0.060329	8
Infrared spectrum, NBO, HOMO-LUMO, MEP and molecular docking studies (2E)-3-(3-nitrophenyl)-1-[4-piperidin-1-yl]prop-2-en-1-one	C.Y., Varghese H.T., Nayak P.S., Narayana B., Sarojini B.K., Fun H.K., War J.A., Srivastava S.K., Van Alsenoy C.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				17	0.093236	9
Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO analysis and molecular docking study of 1-hydroxy-4,5,8-tris(4-methoxyphenyl) anthraquinone	Renjith R., Sheena Mary Y., Tresa Varghese H., Yohannan Panicker C., Thiemann T., Shereef A., Al-Saadi A.A.	Journal of Physics and Chemistry of Solids	2015				6	0.032907	4

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1-Alkyl-1-methylpiperazine-1,4-dium salts: Synthetic, acid-base, XRD-analytical, FT-IR, FT-Raman spectral and quantum chemical study	D., Mary Y.S., Panicker C.Y., Varghese H.T., Van Alsenoy C., Prochazkova M., Pazdera P., Al-Saadi	Journal of Molecular Structure	2015			5	0.027422	3
Spectroscopic and theoretical characterization of 2-(4-methoxyphenyl)-4,5-dimethyl-1H-imidazole 3-oxide	Benzon K.B., Varghese H.T., Panicker C.Y., Pradhan K., Tiwary B.K., Nanda A.K., Alsenoy C.V.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015			20	0.109689	9
Synthesis, spectral, and magnetic studies of benzothiazolium tetrachlorocuprate salts: Crystal structure and semiconducting behavior of bis[2-(4-methoxyphenyl)benzothiazolium] tetrachlorocuprate(II)	Sarau Devi A., Ravindran R., Fazil S., Minitha R.	Journal of Coordination Chemistry	2015			1	0.005484	1

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Molecular structure, FT-IR, FT-Raman, NBO, HOMO and LUMO, MEP, NLO and molecular docking study of 2-[(E)-2-(2-bromophenyl)ethenyl]quinoline-6-carboxylic acid	R.T., Panicker C.Y., Varghese H.T., Musiol R., Jampilek J., Van Alsenoy C., War J.A., Srivastava S.K.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				22	0.120658	15
FT-IR, HOMO-LUMO, NBO, MEP analysis and molecular docking study of 3-Methyl-4-[(E)-[4-(methylsulfanyl)-benzylidene]amino]1H-1,2,4-triazole-5(4H)-thione	C.Y., Varghese H.T., Manjula P.S., Sarojini B.K., Narayana B., War J.A., Srivastava S.K., Van Alsenoy C., Al-Saadi A.A.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				15	0.082267	11
Spectral investigations, DFT computations and molecular docking studies of 1,7,8,9-tetrachloro-10,10-dimethoxy-4-[[3-[4-(2-methylphenyl)piperazin-1-yl]propyl]-4-azatricyclo[5.2.1.0 ^{2,6}]dec-8-ene-3,5-dione	Mary Y.S., Varghese H.T., Panicker C.Y., Pakosinska- Parys M., Alsenoy C.V.	Journal of Molecular Structure	2015				5	0.027422	1

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Spectroscopic investigation (FT-IR, FT-Raman), HOMO-LUMO, NBO analysis and molecular docking study of 4-chlorophenyl quinoline-2-carboxylate	Panicker C.Y., Varghese H.T., Nagarajan S., Sudha B.S., War J.A., Srivastava S.K., Harikumar B., Anto P.L.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				12	0.065814	10
Vibrational spectra, HOMO, LUMO, NBO, MEP analysis and molecular docking study of 2,2-diphenyl-4-(piperidin-1-yl)butanamide	Varghese H.T., Panicker C.Y., Girisha M., Sagar B.K., Yathirajan H.S., Al-Saadi A.A., Van Alsenoy	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				16	0.087751	5
Molecular conformational analysis, vibrational spectra, NBO, NLO, HOMO-LUMO and molecular docking studies of ethyl 3-(E)-(anthracen-9-yl)prop-2-enoate based on density functional theory calculations	Varghese H.T., Panicker C.Y., Thiemann T., Al-Saadi A.A., Popoola S.A., Van Alsenoy C., Al Jasem Y.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				10	0.054845	8

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Vibrational spectroscopic studies and molecular docking study of 2-[(E)-2-phenylethenyl]quinoline-5-carboxylic acid	R.T., Panicker C.Y., Varghese H.T., Musiol R., Jampilek J., Alsenoy C.V., War J.A., Manojkumar T.K.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				12	0.065814	8
Accumulation of heavy metals in the surface water of Asthamudi lake, Kollam, Kerala	Karim L.R., Williams E.S.	Nature Environment and Pollution Technology	2015				3	0.016453	3
Vibrational spectroscopic and molecular docking study of 4-Methylphenylquinoline-2-carboxylate	Panicker C.Y., Varghese H.T., Nagarajan S., Sudha B.S., War J.A., Srivastava S.K., Harikumar B., Anto P.L.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				2	0.010969	0

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Spectroscopic investigations, NBO, HOMO-LUMO, NLO analysis and molecular docking of 5-(adamantan-1-yl)-3-anilinomethyl-2,3-dihydro-1,3,4-oxadiazole-2-thione, a potential bioactive agent	F.A.M., Mary Y.S., Panicker C.Y., El-Emam A.A., Al-Swaidan I.A., Al-Saadi A.A., Van Alsenoy C.	Journal of Molecular Structure	2015		26		0.142596	12
Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO, NBO, MEP analysis and molecular docking study of 2-[(4-chlorobenzyl)sulfanyl]-4-(2-methylpropyl)-6-(phenylsulfanyl)-pyrimidine-5-carbonitrile, a potential chemotherapeutic agent	N.Z., Mary Y.S., Panicker C.Y., Al-Swaidan I.A., El-Emam A.A., Al-Deeb O.A., Al-Saadi A.A., Van Alsenoy	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015		7		0.038391	3
Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO, NBO, MEP analysis and molecular docking study of 2-(4-hydroxyphenyl)-4,5-dimethyl-1H-imidazole 3-oxide	Benzon K.B., Varghese H.T., Panicker C.Y., Pradhan K., Tiwary B.K., Nanda A.K., Alsenoy C.V.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015		14		0.076782	5

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Infrared spectrum, structural and optical properties and molecular docking study of 3-(4-fluorophenyl)-5-phenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde	Panicker C.Y., Sapnakumari M., Narayana B., Sarojini B.K., Al-Saadi A.A., Van Alsenoy C., War J.A., Fun H.K.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015		14		0.076782	8
Molecular structure, FT-IR, vibrational assignments, HOMO-LUMO, MEP, NBO analysis and molecular docking study of ethyl-6-(4-chlorophenyl)-4-(4-fluorophenyl)-2-oxocyclohex-3-ene-1-carboxylate	Sheena Mary Y., Yohannan Panicker C., Sapnakumari M., Narayana B., Sarojini B.K., Al-Saadi A.A., Van Alsenoy C., War J.A.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015		3		0.016453	0
Spectroscopic investigation (FT-IR, FT-Raman and SERS), vibrational assignments, HOMO-LUMO analysis and molecular docking study of Opipramol	Panicker C.Y., Kavitha C.N., Yathirajan H.S., Siddegowda M.S., Cruz S.M.A., Nogueira H.I.S., Al-Saadi A.A., Van Alsenoy C., War J.A.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015		5		0.027422	4

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Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 5-tert-Butyl-6-chloro-N-[(4-(trifluoromethyl)phenyl)pyrazine-2-carboxamide	J.B., Varghese H.T., Panicker C.Y., Van Alsenoy C., Al-Saadi A.A., Dolezal M., Samuel J.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015		10		0.054845	10
FT-IR, NBO, HOMO-LUMO, MEP analysis and molecular docking study of 1-[3-(4-Fluorophenyl)-5-phenyl-4,5-dihydro-1H-pyrazol-1-yl]ethanone	Mary Y.S., Panicker C.Y., Sapnakumari M., Narayana B., Sarojini B.K., Al-Saadi A.A., Van Alsenoy C., War J.A.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015		12		0.065814	2
Molecular structure, FT-IR, vibrational assignments, HOMO-LUMO analysis and molecular docking study of 1-[5-(4-Bromophenyl)-3-(4-fluorophenyl)-4,5-dihydro-1H-pyrazol-1-yl]ethanone	Panicker C.Y., Sapnakumari M., Narayana B., Sarojini B.K., Al-Saadi A.A., Van Alsenoy C., War J.A., Fun H.K.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015		18		0.09872	5

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Vibrational spectroscopic studies and molecular docking of 10,10-dimethylanthrone	Sheena Mary Y., Yamuna T.S., Yohannan Panicker C., Yathirajan H.S., Siddegowda M.S., Al-Saadi A.A., Van Alsenoy C., War J.A.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				0.016453	2
Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO analysis and molecular docking study of 2-(Adamantan-1-yl)-5-(4-nitrophenyl)-1,3,4-oxadiazole	Al-Omary F., El-Emam A.A., Mary Y.S., Panicker C.Y., Al-Saadi A.A., War J.A., Van Alsenoy C.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				0.120658	7
Molecular structure, FT-IR, NBO, HOMO and LUMO, MEP and first order hyperpolarizability of (2E)-1-(2,4-Dichlorophenyl)-3-(3,4,5-trimethoxyphenyl) prop-2-en-1-one by HF and density functional methods	Sheena Mary Y., Yohannan Panicker C., Anto P.L., Sapnakumari M., Narayana B., Sarojini B.K.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015				0.093236	11

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Relationships between the hydrochemical characteristics, phytoplankton chlorophyll and phaeophytin in the Southwest coast of India	Jose J.J., Lipton A.P., Udayakumar P., Rajesh B.R., Alex L., Chandran A.	Journal of Environmental Science and Engineering	2015		0		0	0
Adsorptive removal of acid red from aqueous solutions by cationic surfactant-modified bentonite clay	Mullassery M.D., Fernandez N.B., Anirudhan T.S.	Desalination and Water Treatment	2015		5		0.027422	5
Adequacy study of 2-phenoxyethanol on hypselobarbus kurali as an anesthetic	Vishnu Nair M.S., Sherly Williams E.	International Journal of Zoological Research	2015		0		0	0
Macroinvertebrate communities in the bottom sediment of Arthunkal coast in Kerala, Southwest coast of India	Varghese Sinu J, Miranda M T P	NATURE ENVIRONMENT & POLLUTION TECHNOLOGY	2015				0	0

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Macrobenthic invertebrates as coastal ecological bioindicators of environmental health	Miranda Mary Teresa P, Rajesh B R, Sreelekshmy S G, Udayakumar P, Jose J Jean	JOURNAL OF ENVIRONMENTAL SCIENCE & ENGINEERING	2015				0	0	0
Accumulation of heavy metals in the surface water of Asthamudi Lake, Kollam, Kerala	Karim L Razeena, Williams E Sherly	NATURE ENVIRONMENT & POLLUTION	2015				1	0.001219	1
: Removal of dyes using a composite cation exchanger - Acrylamide cerium(IV) phosphomolybdate	Apsara A P, Beena B	INDIAN JOURNAL OF ENVIRONMENTAL PROTECTION	2015				0	0	0
: Dietary overlapping between introduced species and the native fish species Etroplus suratensis in Vellayani Freshwater Lake, Kerala	Reenamole G R, Ambili T, D'Cruz F George	JOURNAL OF ECOBIOLOGY	2015				0	0	0
Sediment texture and benthic ecology of Upper Ckittar River, Kerala	: Ambili T, Reenamole G R, D'Cruz F George	JOURNAL OF ECOBIOLOGY	2015				0	0	0

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Relationship between the hydrochemical characteristics, phytoplankton chlorophyll and phaeophytin in the south west coast of India	Jean Jose J, Lipton A P, Udayakumar P, Rajesh B R , Lincy Alex, Chandran A	JOURNAL OF ENVIRONMENTAL SCIENCE & ENGINEERING	Jan-15			0	0	0
Meiobenthic diversity and abundance along Arthunkal coast in Kerala, southwest coast of India	Varghese Sinu J, Miranda M T P	JOURNAL OF THE MARINE BIOLOGICAL ASSOCIATION OF INDIA	2015			0	0	0
Iron availability affects phosphate deficiency-mediated responses, and evidence of cross-talk with auxin and zinc in arabidopsis	Rai V., Sanagala R., Sinilal B., Yadav S., Sarkar A.K., Dantu P.K., Jain A.	Plant and Cell Physiology	2014		26		0.142596	20

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Theoretical investigations on the molecular structure, vibrational spectra, HOMO-LUMO analyses and NBO study of 1-[(Cyclopropylmethoxy)methyl]-5-ethyl-6-(4-methylbenzyl)-1,2,3,4-tetrahydropyrimidine-2,4-dione	E.S., Mary Y.S., Panicker C.Y., El-Brollosy N.R., El-Emam A.A., Van Alsenoy C., Al-Saadi A.A.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014				12	0.065814	7
Vibrational spectra, NBO analysis, HOMO-LUMO and first hyperpolarizability of 2-[(2-Methylprop-2-en-1-yl)oxy]methyl-6-phenyl-2,3,4,5-tetrahydro-1,2,4-triazine-3,5-dione, a potential chemotherapeutic agent based on density functional theory calculations	Mary Y.S., El-Brollosy N.R., El-Emam A.A., Al-Deeb O.A., Jojo P.J., Panicker C.Y., Van Alsenoy C.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014				10	0.054845	4
Molecular structure and vibrational spectra of 2-Ethoxymethyl-6-ethyl-2,3,4,5-tetrahydro-1,2,4-triazine-3,5-dione, a potential chemotherapeutic agent, by density functional methods	Mary Y.S., Al-Tamimi A.-M.S., El-Brollosy N.R., El-Emam A.A., Jojo P.J., Panicker C.Y., Alsenoy C.V.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014				2	0.010969	2

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FT-IR, molecular structure, HOMO-LUMO, MEP, NBO analysis and first order hyperpolarizability of Methyl 4,4-difluoro-5-methoxy-1,1-dimethyl-3-terphenyl-4-carboxylate	Sheena Mary Y., Yohannan Panicker C., Narayana B., Samshuddin S., Sarojini B.K., Van Alsenoy C.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		10		0.054845	5
Sexual dimorphism in a benthic fish oxyurichthys tentacularis (Valenciennes, 1837), Gobiidae, Inhabiting Ashtamudi Estuary, Kerala, India	Mohan R., Sherly W.E.	Journal of the Bombay Natural History Society	2014		0		0	0
Theoretical investigations on the molecular structure, vibrational spectral, HOMO-LUMO and NBO analysis of 9-[3-(Dimethylamino)propyl]-2-trifluoromethyl-9H-thioxanthen-9-ol	Panicker C.Y., Yamuna T.S., Siddegowda M.S., Yathirajan H.S., Al-Saadi A.A., Van Alsenoy C.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		22		0.120658	5

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Molecular conformational analysis, vibrational spectra, NBO analysis and first hyperpolarizability of (2E)-3-(3-chlorophenyl)prop-2-enoic anhydride based on density functional theory calculations	Mary Y.S., Raju K., Panicker C.Y., Al-Saadi A.A., Thiemann T.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		19		0.104205	5
Vibrational spectra, molecular structure, NBO, HOMO-LUMO and first order hyperpolarizability analysis of 1,4-bis(4-formylphenyl)anthraquinone by density functional theory	Renjith R., Mary Y.S., Varghese H.T., Panicker C.Y., Thiemann T., Van Alsenoy C.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		7		0.038391	5
Spectroscopic (FT-IR, FT-Raman) investigations and quantum chemical calculations of 1,7,8,9-tetrachloro-10,10-dimethoxy-4-{3-[4-(3-methoxyphenyl) piperazin-1-yl]propyl}-4-azatricyclo[5.2.1.0 ^{2,6}]dec-8-ene-3,5-dione	Mary Y.S., Panicker C.Y., Varghese H.T., Pakosinska-Parys M., Van Alsenoy C., Al-Saadi A.A.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		10		0.054845	1

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Molecular conformational analysis, vibrational spectra, NBO analysis and first hyperpolarizability of (2E)-3-phenylprop-2-enoic anhydride based on density functional theory calculations	Sheena Mary Y., Raju K., Panicker C.Y., Al-Saadi A.A., Thiemann T., Van Alsenoy C.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		14		0.076782	4
Molecular structure, FT-IR, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 2-(4-chlorophenyl)-2-oxoethyl 3-methylbenzoate by HF and density functional methods	Kumar C.S., Yohannan Panicker C., Fun H.-K., Sheena Mary Y., Harikumar B., Chandraju S., Quah	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		10		0.054845	7
FT-IR, molecular structure, first order hyperpolarizability, HOMO and LUMO analysis, MEP and NBO analysis of 2-(4-chlorophenyl)-2-oxoethyl 3-nitrobenzoate	Kumar C.S., Panicker C.Y., Fun H.-K., Mary Y.S., Harikumar B., Chandraju S., Quah C.K., Ooi	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		21		0.115174	10

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Quantum mechanical and spectroscopic (FT-IR, FT-Raman, ¹ H NMR and UV) investigations of 2-(phenoxy-methyl)benzimidazole	Mary Y.S., Jojo P.J., Panicker C.Y., Van Alsenoy C., Ataei S., Yildiz I.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		8		0.043876	4
Quantum mechanical and spectroscopic (FT-IR, FT-Raman, ¹ H NMR and UV) investigations of 5-nitro-2-phenylbenzoxazole	J.B., Varghese H.T., Panicker C.Y., Samuel J., Van Alsenoy C., Ertan-Bolelli T., Yildiz I.	Journal of Molecular Structure	2014		6		0.032907	5
Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 1,7,8,9-tetrachloro-10,10-dimethoxy-4-[3-(4-phenylpiperazin-1-yl)propyl]-4-azatricyclo[5.2.1.0 ^{2,6}]-dec-8-ene-3,5-dione by density functional methods	Mary Y.S., Panicker C.Y., Varghese H.T., Pakosinska-Parys M., Van Alsenoy C., Manojkumar	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		6		0.032907	4

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Vibrational spectroscopic and computational study of 1,7,8,9-Tetrachloro-4- (4-bromo-butyl)-10,10-dimethoxy-4-aza-tricyclo[5.2.1.0 ^{2,6}]dec-8-ene-3,5-dione	Mary Y.S., Panicker C.Y., Varghese H.T., Pakosinska- Parys M., Alsenoy C.V., Manojkumar T.K.	Spectrochi mica Acta - Part A: Molecular and Biomolecul ar Spectrosco py	2014				7	0.038391	0
Theoretical investigations on the molecular structure, vibrational spectra, HOMO-LUMO and NBO analysis of 5-chloro-2-((4-chlorophenoxy)methyl)benzimidazole	Mary Y.S., Jojo P.J., Panicker C.Y., Van Alsenoy C., Ataei S., Yildiz I.	Spectrochi mica Acta - Part A: Molecular and Biomolecul ar Spectrosco py	2014				19	0.104205	12
Removal of Mercury(II) Ions from Aqueous Solutions using Chemically Modified Banana Stem: Kinetic and Equilibrium Modeling	Mullassery M.D., Fernandez N.B., Anirudhan T.S.	Separation Science and Technology (Philadelph ia)	2014				3	0.016453	3

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Acid-base properties, FT-IR, FT-Raman spectroscopy and computational study of 1-(pyrid-4-yl)piperazine	Mary Y.S., Panicker C.Y., Varghese H.T., Van Alsenoy C., Prochazkova M., Sevcik R., Pazdera P.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		4		0.021938	3
Vibrational spectroscopic, ¹ H NMR and quantum chemical computational study of 4-hydroxy-2-oxo-1,2-dihydroquinoline-8-carboxylic acid	Ulahannan R.T., Panicker C.Y., Varghese H.T., Van Alsenoy C., Musiol R., Jampilek J., Anto P.L.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		15		0.082267	5
Spectroscopic (FT-IR, FT-Raman) investigations and quantum chemical calculations of 4-hydroxy-2-oxo-1,2-dihydroquinoline-7-carboxylic acid	Ulahannan R.T., Panicker C.Y., Varghese H.T., Van Alsenoy C., Musiol R., Jampilek J., Anto P.L.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		13		0.071298	5

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Vibrational spectroscopic (FT-IR, FT-Raman, SERS) and quantum chemical calculations of 3-(10,10-dimethyl-anthracen-9-ylidene)-N,N,N- trimethylpropanaminium chloride (Melitraceniium chloride)	Mary Y.S., Jojo P.J., Van Alsenoy C., Kaur M., Siddegowda M.S., Yathirajan H.S., Nogueira H.I.S., Cruz S.M.A.	Spectrochi mica Acta - Part A: Molecular and Biomolecul ar Spectrosco py	2014				17	0.093236	12
Vibrational spectroscopic studies (FT-IR, FT-Raman, SERS) and quantum chemical calculations on cyclobenzaprinium salicylate	Mary Y.S., Jojo P.J., Van Alsenoy C., Kaur M., Siddegowda M.S., Yathirajan H.S., Nogueira H.I.S., Cruz S.M.A.	Spectrochi mica Acta - Part A: Molecular and Biomolecul ar Spectrosco py	2014				20	0.109689	9
Vibrational spectroscopic (FT-IR, FT-Raman) and quantum chemical calculations of 1-(5,5-dioxido-10H-phenothiazin-10-yl)ethanone	Mary Y.S., Panicker C.Y., Varghese H.T., Yathirajan H.S., Byrappa K., Van Alsenoy C.	Spectrochi mica Acta - Part A: Molecular and Biomolecul ar Spectrosco py	2014				8	0.043876	4

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Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 2,4-bis(2-methoxyphenyl)-1-phenylanthracene- 9,10-dione by ab initio HF and density functional methods	Varghese H.T., Panicker C.Y., Thiemann T., Viswanathan K., Van Alsenoy C., Manojkumar T.K.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014		40		0.219378	15
Taxonomic notes on Hypselobarbus sp. distributed along the Southern Western Ghats	Williams Sherly , Jose E J Jean, Nair M S Vishnu, Vijayalakshmi P V, Razeenakari m L	JOURNAL OF THE INLAND FISHERIES SOCIETY OF INDIA	Dec-14				0	0
Cerium(IV) tungstate as eco-friendly Bronsted acid catalyst	Apsara A P , Anjali S	POLLUTION RESEARCH	2014				1	0.001219