

# FATIMA MATA NATIONAL COLLEGE

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3.2.4 List of research papers in  
UGC CARE listed journals

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**LIST OF PAPERS PUBLISHED IN UGC CARE LISTED JOURNALS (2014-2019)**

<b>Title of paper</b>	<b>Name of the author/s</b>	<b>Department</b>	<b>Name of journal</b>	<b>Year of publication</b>
Iron availability affects phosphate deficiency-mediated responses, and evidence of cross-talk with auxin and zinc in arabidopsis	Rai V., Sanagala R., <b>Sinilal B.</b> , Yadav S., Sarkar A.K., Dantu P.K., Jain A.	Botany	Plant and Cell Physiology	2014
FT-IR, molecular structure, HOMO-LUMO, MEP, NBO analysis and first order hyperpolarizability of Methyl 4,4-difluoro-5-methoxy-1,1,3-terphenyl-4-carboxylate	<b>Sheena Mary Y.</b> , Yohannan Panicker C., Narayana B., Samshuddin S., Sarojini B.K., Van Alsenoy C.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
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	Al-Abdullah E.S., <b>Mary Y.S.</b> , Panicker C.Y., El-Brollosy N.R., El-Emam A.A., Van Alsenoy C., Al-Saadi A.A.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
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.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
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	<b>Mary Y.S.</b> , Al-Tamimi A.-M.S., El-Brollosy N.R., El-Emam A.A., <b>Jojo</b>	Physics	Spectrochimica Acta - Part A: Molecular and	2014

	<b>P.J.</b> , Panicker C.Y., Alsenoy C.V.		Biomolecular Spectroscopy	
Sexual dimorphism in a benthic fish oxyurichthys tentacularis (Valenciennes, 1837), Gobiidae, Inhabiting Ashtamudi Estuary, Kerala, India	Mohan R., <b>Sherly W.E.</b>	Zoology	Journal of the Bombay Natural History Society	2014
Theoretical investigations on the molecular structure, vibrational spectral, HOMO-LUMO and NBO analysis of 9-[3-(Dimethylamino)propyl]-2-trifluoro- methyl-9H-thioxanthen-9-ol	<b>Mary Y.S.</b> , Panicker C.Y., Yamuna T.S., Siddegowda M.S., Yathirajan H.S., Al-Saadi A.A., Van Alsenoy C.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
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., <b>Mary Y.S., Varghese H.T.</b> , Panicker C.Y., Thiemann T., Van Alsenoy C.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
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	<b>Mary Y.S.</b> , Raju K., Panicker C.Y., Al-Saadi A.A., Thiemann T.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
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 <sup>2,6</sup> ]dec-8-ene-3,5-dione	Renjith R., <b>Mary Y.S.</b> , Panicker C.Y., Varghese H.T., Pakosińska-Parys M., Van Alsenoy C., Al-Saadi A.A.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Molecular structure, FT-IR, first order hyperpolarizability, NBO analysis, HOMO and	Chidan Kumar C.S., Yohannan Panicker	Physics	Spectrochimica Acta - Part	2014

LUMO analysis of 2-(4-chlorophenyl)-2-oxoethyl 3-methylbenzoate by HF and density functional methods	C., Fun H.-K., <b>Sheena Mary Y.</b> , Harikumar B., Chandraju S., Quah C.K., Ooi C.W.		A: Molecular and Biomolecular Spectroscopy	
Molecular conformational analysis, vibrational spectra, NBO analysis and first hyperpolarizability of (2E)-3-phenylprop-2-enoic anhydride based on density functional theory calculations	<b>Sheena Mary Y.</b> , Raju K., Panicker C.Y., Al-Saadi A.A., Thiemann T., Van Alsenoy C.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
FT-IR, molecular structure, first order hyperpolarizability, HOMO and LUMO analysis, MEP and NBO analysis of 2-(4-chlorophenyl)-2-oxoethyl 3-nitrobenzoate	Chidan Kumar C.S., Panicker C.Y., Fun H.-K., <b>Mary Y.S.</b> , Harikumar B., Chandraju S., Quah C.K., Ooi C.W.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Quantum mechanical and spectroscopic (FT-IR, FT-Raman, <sup>1</sup> H NMR and UV) investigations of 2-(phenoxyethyl)benzimidazole	<b>Mary Y.S., Jojo P.J.</b> , Panicker C.Y., Van Alsenoy C., Ataei S., Yildiz I.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Quantum mechanical and spectroscopic (FT-IR, FT-Raman, <sup>1</sup> H NMR and UV) investigations of 5-nitro-2-phenylbenzoxazole	Bhagyasree J.B., <b>Varghese H.T.</b> , Panicker C.Y., Samuel J., Van Alsenoy C., Ertan-Bolelli T., Yildiz I.	Physics	Journal of Molecular Structure	2014
Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 1,7,8,9-tetrachloro-10,10-	Renjith R., <b>Mary Y.S.</b> , Panicker C.Y., <b>Varghese H.T.</b> ,	Physics	Spectrochimica Acta - Part A: Molecular	2014

dimethoxy-4-[3-(4- phenylpiperazin-1-yl)propyl]-4-azatricyclo[5.2.1.0 <sup>2,6</sup> ]dec-8-ene-3,5- dione by density functional methods	PakosiÅ„ska-Parys M., Van Alsenoy C., Manojkumar T.K.		and Biomolecular Spectroscopy	
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 <sup>2,6</sup> ] dec-8-ene-3,5-dione	Renjith R., <b>Mary Y.S.</b> , Panicker C.Y., <b>Varghese H.T.</b> , PakosiÅ„ska-Parys M., Alsenoy C.V., Manojkumar T.K.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Theoretical investigations on the molecular structure, vibrational spectra, HOMO-LUMO and NBO analysis of 5-chloro-2-((4-chlorophenoxy)methyl)benzimidazole	<b>Mary Y.S., Jojo P.J.</b> , Panicker C.Y., Van Alsenoy C., Ataei S., Yildiz I.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Cerium(IV) tungstate as eco-friendly Bronsted acid catalyst	Apsara A.P., Anjali S.	Chemistry	Pollution Research	2014
Removal of Mercury(II) Ions from Aqueous Solutions using Chemically Modified Banana Stem: Kinetic and Equilibrium Modeling	<b>Mullassery M.D., Fernandez N.B.</b> , Anirudhan T.S.	Chemistry	Separation Science and Technology (Philadelphia)	2014
Acid-base properties, FT-IR, FT-Raman spectroscopy and computational study of 1-(pyrid-4-yl)piperazine	<b>Mary Y.S.</b> , Panicker C.Y., <b>Varghese H.T.</b> , Van Alsenoy C., ProchÅ¡zkovÅ¡ M., Å evÅ¡Åk R., Pazdera P.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Vibrational spectroscopic (FT-IR, FT-Raman) and quantum chemical calculations of 1-(5,5-dioxido-10H-phenothiazin-10-yl)ethanone	Kaur M., <b>Mary Y.S.</b> , Panicker C.Y., <b>Varghese H.T.</b> , Yathirajan H.S., Byrappa K., Van	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular	2014

	Alsenoy C.		Spectroscopy	
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)	<b>Mary Y.S., Jojo P.J.</b> , Van Alsenoy C., Kaur M., Siddegowda M.S., Yathirajan H.S., Nogueira H.I.S., Cruz S.M.A.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Vibrational spectroscopic studies (FT-IR, FT-Raman, SERS) and quantum chemical calculations on cyclobenzaprinium salicylate	Mary Y.S., <b>Jojo P.J.</b> , Van Alsenoy C., Kaur M., Siddegowda M.S., Yathirajan H.S., Nogueira H.I.S., Cruz S.M.A.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Vibrational spectroscopic, <sup>1</sup> H NMR and quantum chemical computational study of 4-hydroxy-2-oxo-1,2-dihydroquinoline-8-carboxylic acid	Ulahannan R.T., Panicker C.Y., <b>Varghese H.T.</b> , Van Alsenoy C., Musiol R., Jampilek J., Anto P.L.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
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., <b>Varghese H.T.</b> , Van Alsenoy C., Musiol R., Jampilek J., Anto P.L.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
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	Joseph T., <b>Varghese H.T.</b> , Panicker C.Y., Thiemann T., Viswanathan K.,	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular	2014

	Van Alsenoy C., Manojkumar T.K.		Spectroscopy	
Application of Social CRM towards information services of Academic Libraries in India : a MASTER approach	Prijith Jacob Thomas, Harish Babu	Library Science	IASLIC Bulletin	2014
Synergistic electrocatalytic effect of graphene / nickel hydroxide composite for the simultaneous electrochemical determination of ascorbic acid, dopamine and uric acid	Dr Mary Nancy T.E.	Chemistr y	Electrochimica Acta	2014
Removal of Mercury (II) ions from Aqueous Solutions Using Chemically Modified Banana Stem: Kinetic and equilibrium modeling.	Dr Manohar D. Mullassery & Dr. Noeline B. Fernandez	Chemistr y	Separation Science and Technology	2014
Macrobenthic polychaete distribution and abundance along the Arthunkal Coast of Kerala, south west coast of India: Relationships to environmental variables	Sinu J. Varghese and M.T.P. Miranda	Zoology	Journal of Aquatic Biology and Fisheries	2014
Culture of Fresh water Cladoceran <i>Daphnia Magna</i> and its application in fish Larviculture technology.	Vishnu Nair M S and Sherly Williams E	Zoology	Journal of Aquatic Biology and Fisheries.	2014
Ichthyofaunal diversity of Vattakayal-a part of Ashtamudi lake, Kollan district, Kerala, South India.	Seethal Lal S, Jaya D S and Sherly Williams E	Zoology	Journal of Aquatic biology and fisheries.	2014
“Self Narration and Incarceration in The Tale of My Exile”	Stancilaus S.	English	Journal of Literature and Aesthetics	2014
“Fiction as Critique of Civilization: A Study of J.M.G. Le Clezio’s Terra Amata and Desert”	Manoj S	English	Journal of Literature and Aesthetics	2014
Solar graphene modified glassy carbon electrode	Dr Mary Nancy T.E.	Chemistr	Journal of	2014

for the voltammetric resolution and detection of dopamine, ascorbic acid and uric acid		y	Electroanalytical Chemistry	
NiO.1CoO.9Fe <sub>2</sub> O <sub>4</sub> - based electrochemical sensor for the detection of paracetamol	Dr Mary Nancy T.E.	Chemistry	Journal of Solid State Electrochemistry	2014
AmartyaSen as a Universal Intellectual	Vincent B. Netto	English	Journal of Literature and Aesthetics	2015
Evaluation of radionuclides transfer from soil-to-edible flora and estimation of radiological dose to the Malaysian populace	Mayeen Khandaker, Noor Liyana Mohd Nasir, Khandoker Asaduzzaman, Michael Olatunji, Yusoff Mohd Amin, Hasan Abu Kassim, David Bradley, P. J. Jojo	Physics	Chemosphere 153, Pages 528-536, 2015(Impact factor: 3.8)	2015
Meiobenthic diversity and abundance along Arthunkal coast in Kerala, south west coast of India, 57(1):78-83.	Sinu J. Varghese and M.T.P. Miranda	Zoology	Journal of Marine Biological Association of India	2015
Macroinvertebrate communities in the bottom sediments in Arthungal, Kerala, South-west coast of India	Sinu J. Varghese and M.T.P. Miranda	Zoology	Nature, Environment and Pollution Technology	2015
“V. S. Ramachandran: A Neurological Understanding of the Brain, Consciousness and Self”	Manoj S	English	Journal of Literature and Aesthetics	2015
Vibrational spectroscopic and molecular docking	Ulahannan R.T.,	Physics	Spectrochimic	2015



study of (2E)-N-(4-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylprop-2-enamide	Panicker C.Y., <b>Varghese H.T.</b> , Musiol R., Jampilek J., Van Alsenoy C., War J.A., Al-Saadi A.A.		a Acta - Part A: Molecular and Biomolecular Spectroscopy	
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	<b>Mary Y.S.</b> , Panicker C.Y., Thiemann T., Al-Azani M., Al-Saadi A.A., Van Alsenoy C., Raju K., War J.A., Srivastava S.K.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
Macroinvertebrate communities in the bottom sediment of Arthunkal coast in Kerala, southwest coast of India	Varghese S.J., <b>Miranda M.T.P.</b>	Zoology	Nature Environment and Pollution Technology	2015
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., <b>Varghese H.T.</b> , Narayana B., Divya K., Sarojini B.K., War J.A., Van Alsenoy C., Fun H.K.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
Infrared spectrum, NBO, HOMO-LUMO, MEP and molecular docking studies (2E)-3-(3-nitrophenyl)-1-[4-piperidin-1-yl]prop-2-en-1-one	Panicker C.Y., <b>Varghese H.T.</b> , Nayak P.S., Narayana B., Sarojini B.K., Fun H.K., War J.A., Srivastava S.K., Van Alsenoy C.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015

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., <b>Sheena Mary Y., Tresa Varghese H.</b> , Yohannan Panicker C., Thiemann T., Shereef A., Al-Saadi A.A.	Physics	Journal of Physics and Chemistry of Solids	2015
1-Alkyl-1-methylpiperazine-1,4-dium salts: Synthetic, acid-base, XRD-analytical, FT-IR, FT-Raman spectral and quantum chemical study	Němečková D., <b>Mary Y.S., Varghese H.T.</b> , Van Alsenoy C., Procházková M., Pazdera P., Al-Saadi A.A.	Physics	Journal of Molecular Structure	2015
Spectroscopic and theoretical characterization of 2-(4-methoxyphenyl)-4,5-dimethyl-1H-imidazole 3-oxide	Benzon K.B., <b>Varghese H.T.</b> , Panicker C.Y., Pradhan K., Tiwary B.K., Nanda A.K., Alsenoy C.V.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
Synthesis, spectral, and magnetic studies of benzothiazolium tetrachlorocuprate salts: Crystal structure and semiconducting behavior of bis[2-(4-methoxyphenyl)benzothiazolium] tetrachlorocuprate(II)	<b>Sarau Devi A.</b> , Ravindran R., Fazil S., Minitha R.	Chemistry	Journal of Coordination Chemistry	2015
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	Ulahannan R.T., Panicker C.Y., <b>Varghese H.T.</b> , Musiol R., Jampilek J., Van Alsenoy C., War J.A., Srivastava S.K.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015

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	Panicker C.Y., <b>Varghese H.T.</b> , Manjula P.S., Sarojini B.K., Narayana B., War J.A., Srivastava S.K., Van Alsenoy C., Al-Saadi A.A.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
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 <sup>2,6</sup> ]dec-8-ene-3,5-dione	Resmi K.S., <b>Mary Y.S., Varghese H.T.</b> , Panicker C.Y., PakosiÅ„ska-Parys M., Alsenoy C.V.	Physics	Journal of Molecular Structure	2015
Spectroscopic investigation (FT-IR, FT-Raman), HOMO-LUMO, NBO analysis and molecular docking study of 4-chlorophenyl quinoline-2-carboxylate	Fazal E., Panicker C.Y., <b>Varghese H.T.</b> , Nagarajan S., Sudha B.S., War J.A., Srivastava S.K., Harikumar B., Anto P.L.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
Vibrational spectra, HOMO, LUMO, NBO, MEP analysis and molecular docking study of 2,2-diphenyl-4-(piperidin-1-yl)butanamide	<b>Mary Y.S., Varghese H.T.</b> , Panicker C.Y., Girisha M., Sagar B.K., Yathirajan H.S., Al-Saadi A.A., Van Alsenoy C.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
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	<b>Mary Y.S., Varghese H.T.</b> , Panicker C.Y., Thiemann T., Al- Saadi A.A., Popoola S.A., Van Alsenoy	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015

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Vibrational spectroscopic studies and molecular docking study of 2-[(E)-2-phenylethenyl]quinoline-5-carboxylic acid	Ulahannan R.T., Panicker C.Y., <b>Varghese H.T.</b> , Musiol R., Jampilek J., Alsenoy C.V., War J.A., Manojkumar T.K.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
Accumulation of heavy metals in the surface water of Asthamudi lake, Kollam, Kerala	Karim L.R., <b>Williams E.S.</b>	Zoology	Nature Environment and Pollution Technology	2015
Vibrational spectroscopic and molecular docking study of 4-Methylphenylquinoline-2-carboxylate	Fazal E., Panicker C.Y., <b>Varghese H.T.</b> , Nagarajan S., Sudha B.S., War J.A., Srivastava S.K., Harikumar B., Anto P.L.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
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	Al-Omary F.A.M., <b>Mary Y.S.</b> , Panicker C.Y., El-Emam A.A., Al-Swaidan I.A., Al-Saadi A.A., Van Alsenoy C.	Physics	Journal of Molecular Structure	2015
Removal of dyes using a composite cation exchanger-acrylamide cerium(IV) phosphomolybdate	<b>Apsara A.P.</b> , Beena B.	Chemistry	Indian Journal of Environmental Protection	2015
Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO, NBO, MEP analysis and molecular docking	Alzoman N.Z., <b>Mary Y.S.</b> , Panicker C.Y., Al-Swaidan I.A., El-	Physics	Spectrochimica Acta - Part A: Molecular	2015

study of 2-[(4-chlorobenzyl)sulfanyl]-4-(2-methylpropyl)-6-(phenylsulfanyl)-pyrimidine-5-carbonitrile, a potential chemotherapeutic agent	Emam A.A., Al-Deeb O.A., Al-Saadi A.A., Van Alsenoy C., War J.A.		and Biomolecular Spectroscopy	
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., <b>Varghese H.T.</b> , Panicker C.Y., Pradhan K., Tiwary B.K., Nanda A.K., Alsenoy C.V.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
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	<b>Sheena Mary Y.</b> , Yohannan Panicker C., Sapnakumari M., Narayana B., Sarojini B.K., Al-Saadi A.A., Van Alsenoy C., War J.A.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
Infrared spectrum, structural and optical properties and molecular docking study of 3-(4-fluorophenyl)-5-phenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde	<b>Mary Y.S.</b> , Panicker C.Y., Sapnakumari M., Narayana B., Sarojini B.K., Al-Saadi A.A., Van Alsenoy C., War J.A., Fun H.K.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
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	Bhagyasree J.B., <b>Varghese H.T.</b> , Panicker C.Y., Van Alsenoy C., Al-Saadi A.A., Dolezal M., Samuel J.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
Spectroscopic investigation (FT-IR, FT-Raman	<b>Mary Y.S.</b> , Panicker	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015

and SERS), vibrational assignments, HOMO-LUMO analysis and molecular docking study of Opi Pramol	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.		a Acta - Part A: Molecular and Biomolecular Spectroscopy	
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	<b>Mary Y.S.</b> , Panicker C.Y., Sapnakumari M., Narayana B., Sarojini B.K., Al-Saadi A.A., Van Alsenoy C., War J.A.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
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	<b>Mary Y.S.</b> , Panicker C.Y., Sapnakumari M., Narayana B., Sarojini B.K., Al-Saadi A.A., Van Alsenoy C., War J.A., Fun H.K.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
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	<b>Sheena Mary Y.</b> , Yohannan Panicker C., Anto P.L., Sapnakumari M., Narayana B., Sarojini B.K.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
Vibrational spectroscopic studies and molecular docking of 10,10-dimethylantrone	<b>Sheena Mary Y.</b> , Yamuna T.S., Yohannan Panicker C., Yathirajan H.S., Siddegowda M.S.,	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular	2015

	Al-Saadi A.A., Van Alsenoy C., War J.A.		Spectroscopy	
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	Haress N.G., Al-Omary F., El-Emam A.A., <b>Mary Y.S.</b> , Panicker C.Y., Al-Saadi A.A., War J.A., Van Alsenoy C.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
Adequacy study of 2-phenoxyethanol on hypselobarbus kurali as an anesthetic	Vishnu Nair M.S., <b>Sherly Williams E.</b>	Zoology	International Journal of Zoological Research	2015
Adsorptive removal of acid red from aqueous solutions by cationic surfactant-modified bentonite clay	<b>Mullassery M.D.</b> , <b>Fernandez N.B.</b> , Anirudhan T.S.	Chemistry	Desalination and Water Treatment	2015
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., <b>Sheena Mary Y.</b> , Yohannan Panicker C., Attia M.A., El-Emam A.A., Van Alsenoy C.	Physics	Journal of Molecular Structure	2016
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., <b>Sheena Mary Y.</b> , Yohannan Panicker C., Saleh T.A., Al-Saadi A.A., Van Alsenoy C.	Physics	Journal of Molecular Structure	2016
External dose measurements in the Eloor industrial area in the Ernakulam district of Kerala, India	Balakrishnan D., Umadevi A.G., Ben Byju S., <b>Sunil A.</b> ,	Physics	International Journal of Radiation	2016

	Abraham J.P., <b>Jojo P.J.</b> , Radhakrishnan S., Harikumar M.		Research	
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	Parveen S., Al-Alshaikh M.A., <b>Panicker C.Y.</b> , El-Emam A.A., Salian V.V., Narayana B., Sarojini B.K., van Alsenoy C.	Physics	Journal of Molecular Structure	2016
Spectroscopic, quantum chemical studies, Fukui functions, in vitro antiviral activity and molecular docking of 5-chloro-N-(3-nitrophenyl)pyrazine-2-carboxamide	Sebastian S.H.R., Al-Alshaikh M.A., El-Emam A.A., Panicker C.Y., Zitko J., Dolezal M., Vanalsenoy C.	Physics	Journal of Molecular Structure	2016
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., <b>Sheena Mary Y., Yohannan Panicker C.</b> , Van Alsenoy C.	Physics	Journal of Molecular Structure	2016
Synthesis, vibrational spectroscopic investigations, molecular docking, antibacterial and antimicrobial studies of 5-ethylsulphonyl-2-(p-aminophenyl)benzoxazole	Parveen S.S., Al-Alshaikh M.A., <b>Panicker C.Y.</b> , El-Emam A.A., Arisoy M., Temiz-Arpaci O., Van Alsenoy C.	Physics	Journal of Molecular Structure	2016
Evaluation of radionuclides transfer from soil-to-edible flora and estimation of radiological dose to	Khandaker M.U., Mohd Nasir N.L.,	Physics	Chemosphere	2016



the Malaysian populace	Asaduzzaman K., Olatunji M.A., Amin Y.M., Kassim H.A., Bradley D.A., <b>Jojo P.J.</b> , Alrefaed T.			
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., <b>Sheena Mary Y.</b> , Yohannan Panicker C., Abdel-Aziz A.A.-M., El-Sherbeny M.A., Van Alsenoy C.	Physics	Journal of Molecular Structure	2016
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., <b>Mary Y.S.</b> , Panicker C.Y., Abdel-Aziz A.A.-M., Al-Suwaidan I.A., Van Alsenoy C.	Physics	Journal of Molecular Structure	2016
Spectroscopic investigations and molecular docking study of 3-(1H-imidazol-1-yl)-1-phenylpropan-1-one, a potential precursor to bioactive agents	Al-Alshaikh M.A., <b>Mary Y.S.</b> , Panicker C.Y., Attia M.I., El-Emam A.A., Alsenoy C.V.	Physics	Journal of Molecular Structure	2016
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., <b>Williams E.S.</b>	Zoology	Journal of Environmental Science and Engineering	2016
Vibrational spectroscopic & molecular docking studies of 2,6-dichlorobenzyl alcohol	Abraham M.M., Resmi K.S., Sheena Mary Y., YohannanPanicker C., Harikumar B.	Physics	The Chemist (Journal of the American Institute of Chemists)	2016
Spectroscopic, single crystal XRD structure, DFT	<b>Sheena Mary Y.</b> ,	Physics	RSC Advances	2016

and molecular dynamics investigation of 1-(3-chloro-4-fluorophenyl)-3-[3-(trifluoromethyl)phenyl]thiourea	Aswathy V.V., Panicker C.Y., Bielenica A., Brzozka P., Savczenko O., Armaković S., Armaković S.J., Van Alsenoy C.			
Spectroscopic, single crystal XRD structure, DFT and molecular dynamics investigation of 1-(3-chloro-4-fluorophenyl)-3-[3-(trifluoromethyl)phenyl]thiourea	Y. Sheena Mary, V.V. Aswathy, C. Yohannan Panicker, A. Bielenica, P. Brzozka, O. Savczenko, S. Armaković, S.J. Armaković, C.Van Alsenoy	Physics	RSC Advances, Imp act Factor : 3.108	2016
Estimation of indoor and outdoor effective doses and lifetime cancer risk from gamma dose rates along the coastal regions of Kollam district, Kerala	S. Monica, A. K. Visnu Prasad, S. R. Soniya, P.J. Jojo	Physics	Radiation Protection and Environment 39,1,38-43 (2016) DOI: 10.4103/0972 -0464.185180 (Impact factor: 1.03)	2016
“The Politics of Culture: Hegemony and Resistance”	Manoj S	English	Journal of Literature and Aesthetics	2016
Spectroscopic analysis of 8-hydroxyquinoline-5-sulphonic acid and investigation of its reactive properties by DFT and molecular dynamics simulations	Sureshkumar B., <b>Sheena Mary Y.</b> , Panicker C.Y., Resmi K.S., Suma	Physics	Journal of Molecular Structure	2017

	S., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C.			
Supramolecular architecture of 5-bromo-7-methoxy-1-methyl-1H-benzoimidazole.3H2O: Synthesis, spectroscopic investigations, DFT computation, MD simulations and docking studies	Murthy P.K., Smitha M., <b>Sheena Mary Y.</b> , ArmakoviÄ S., ArmakoviÄ S.J., Rao R.S., Suchetan P.A., Giri L., Pavithran R., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
Synthesis, XRD single crystal structure analysis, vibrational spectral analysis, molecular dynamics and molecular docking studies of 2-(3-methoxy-4-hydroxyphenyl) benzothiazole	<b>Sarau Devi A.</b> , Aswathy V.V., <b>Sheena Mary Y.</b> , Yohannan Panicker C., ArmakoviÄ S., ArmakoviÄ S.J., Ravindran R., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
Investigation of reactive and spectroscopic properties of oxobutanoic acid derivative: Combined spectroscopic, DFT, MD and docking study	<b>Mary Y.S.</b> , Mary Y.S., Panicker C.Y., ArmakoviÄ S., ArmakoviÄ S.J., Narayana B., Sarojini B.K., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
Vibrational spectroscopic investigations and molecular docking studies of biologically active 2-[4-(4-phenylbutanamido)phenyl]-5-ethylsulphonyl-benzoxazole	Jalaja K., Al-Alshaikh M.A., <b>Mary Y.S.</b> , Panicker C.Y., El-Emam A.A., Temiz-Arpaci O., Alsenoy C.V.	Physics	Journal of Molecular Structure	2017

Conformational, vibrational and DFT studies of a newly synthesized arylpiperazine-based drug and evaluation of its reactivity towards the human GABA receptor	Onawole A.T., Al-Ahmadi A.F., <b>Mary Y.S.</b> , Panicker C.Y., Ullah N., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C., Al-Saadi A.A.	Physics	Journal of Molecular Structure	2017
Comparison of thoron ( <sup>220</sup> Rn) content and gamma radiation level in high background radiation area of Kollam district in Kerala, India	Midhun M., Mathew S., Rejith R.S., <b>Jojo P.J.</b> , Sahoo B.K.	Physics	Journal of Radioanalytical and Nuclear Chemistry	2017
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., <b>Yohannan Panicker C.</b> , Santhosh C., Patil A., Inamdar S.R.	Physics	Journal of Molecular Liquids	2017
Modification of benzoxazole derivative by bromine-spectroscopic, antibacterial and reactivity study using experimental and theoretical procedures	Aswathy V.V., Alper-Hayta S., Yalcin G., <b>Mary Y.S.</b> , Panicker C.Y., Jojo P.J., Kaynak-Onurdag F., ArmakoviÄ S., ArmakoviÄ S.J., Yildiz I., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
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	<b>Mary Y.S.</b> , Al-Omary F.A.M., Mostafa G.A.E., El-Emam A.A.,	Physics	Journal of Molecular Structure	2017

	Manjula P.S., Sarojini B.K., Narayana B., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C.			
Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study	Murthy P.K., <b>Sheena Mary Y.</b> , Suneetha V., Panicker C.Y., ArmakoviÄ S., ArmakoviÄ S.J., Giri L., Suchetan P.A., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
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	Ranjith P.K., Al- Abdullah E.S., Al- Omary F.A.M., El- Emam A.A., Anto P.L., <b>Sheena M.Y.</b> , ArmakoviÄ S., ArmakoviÄ S.J., Zitko J., Dolezal M., Van Alsenoy C.		Journal of Molecular Structure	2017
New quinolone derivative: Spectroscopic characterization and reactivity study by DFT and MD approaches	Ranjith P.K., <b>Mary Y.S.</b> , Panicker C.Y., Anto P.L., ArmakoviÄ S., ArmakoviÄ S.J., Musiol R., Jampilek J., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizability, NBO analysis, HOMO and	Joseph T., <b>Varghese H.T.</b> ,	Physics	Arabian Journal of	2017

LUMO analysis of N-[(4-(trifluoromethyl)phenyl)pyrazine-2-carboxamide by density functional methods	Panicker C.Y., Viswanathan K., Dolezal M., Van Alsenoy C.		Chemistry	
Spectroscopic, DFT, molecular dynamics and molecular docking study of 1-butyl-2-(4-hydroxyphenyl)-4,5-dimethyl-imidazole 3-oxide	Benzon K.B., <b>Mary Y.S., Varghese H.T.</b> , Panicker C.Y., ArmakoviÄ S., ArmakoviÄ S.J., Pradhan K., Nanda A.K., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
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	Aswathy V.V., <b>Mary Y.S., Jojo P.J.</b> , Panicker C.Y., Bielenica A., ArmakoviÄ S., ArmakoviÄ S.J., BrzÄzka P., Krukowski S., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
Synthesis, crystal structure analysis, spectral investigations, DFTÅ computations and molecular dynamics and docking study of 4-benzyl-5-oxomorpholine-3-carbamide, a potential bioactive agent	Murthy P.K., <b>Sheena Mary Y., Shyma Mary Y., Panicker C.Y., Suneetha V., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C., Suchetan P.A.</b>	Physics	Journal of Molecular Structure	2017
Spectroscopic and reactive properties of a newly synthesized quinazoline derivative: Combined experimental, DFT, molecular dynamics and	El-Azab A.S., <b>Mary Y.S.</b> , Mary Y.S., Panicker C.Y.,	Physics	Journal of Molecular Structure	2017

docking study	Abdel-Aziz A.A.-M., Mohamed M.A., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C.			
Newly synthesized dihydroquinazoline derivative from the aspect of combined spectroscopic and computational study	El-Azab A.S., <b>Mary Y.S.</b> , Mary Y.S., Panicker C.Y., Abdel-Aziz A.A.-M., El-Sherbeny M.A., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
Synthesis, vibrational spectroscopic investigations, molecular docking, antibacterial studies and molecular dynamics study of 5-[(4-nitrophenyl)acetamido]-2-(4-tert-butylphenyl)benzoxazole	<b>Sheena Mary Y.</b> , Al-Shehri M.M., Jalaja K., Al-Omary F.A.M., El-Emam A.A., Yohannan Panicker C., ArmakoviÄ S., ArmakoviÄ S.J., Temiz-Arpaci O., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
Vibrational spectroscopic analysis of cyanopyrazine-2-carboxamide derivatives and investigation of their reactive properties by DFT calculations and molecular dynamics simulations	Beegum S., <b>Mary Y.S.</b> , <b>Varghese H.T.</b> , Panicker C.Y., ArmakoviÄ S., ArmakoviÄ S.J., Zitko J., Dolezal M., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
Studies on the synthesis, spectroscopic analysis, molecular docking and DFT calculations on 1-hydroxy-2-(4-hydroxyphenyl)-4,5-dimethyl-	Benzon K.B., <b>Sheena M.Y.</b> , Panicker C.Y.,	Physics	Journal of Molecular Structure	2017

imidazol 3-oxide	ArmakoviÄ S., ArmakoviÄ S.J., Pradhan K., Nanda A.K., Van Alsenoy C.			
Vibrational spectroscopic investigations, molecular dynamic simulations and molecular docking studies of N'-diphenylmethyldene-5-methyl-1H-pyrazole-3-carbohydrazide	Pillai R.R., Menon V.V., <b>Mary Y.S.</b> , ArmakoviÄ S., ArmakoviÄ S.J., Panicker C.Y.	Physics	Journal of Molecular Structure	2017
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	War J.A., Jalaja K., <b>Mary Y.S.</b> , Panicker C.Y., ArmakoviÄ S., ArmakoviÄ S.J., Srivastava S.K., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
Vibrational spectroscopic analysis, molecular dynamics simulations and molecular docking study of 5-nitro-2-phenoxyethyl benzimidazole	Menon V.V., Foto E., <b>Mary Y.S.</b> , Karatas E., Panicker C.Y., Yalcin G., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C., Yildiz I.	Physics	Journal of Molecular Structure	2017
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	Jalaja K., <b>Mary Y.S.</b> , Panicker C.Y., ArmakoviÄ S., ArmakoviÄ S.J., Sagar B.K., Girisha M., Yathirajan H.S., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017



Reactive, spectroscopic and antimicrobial assessments of 5-[(4-methylphenyl) acetamido]-2-(4-tert-butylphenyl)benzoxazole: Combined experimental and computational study	<b>Mary Y.S.</b> , Alzoman N.Z., Menon V.V., Al-Abdullah E.S., El-Emam A.A., Panicker C.Y., Temiz-Arpaci O., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
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	Al-Omary F.A.M., <b>Mary Y.S.</b> , Beegum S., Panicker C.Y., Al-Shehri M.M., El-Emam A.A., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
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	Menon V.V., Fazal E., <b>Mary Y.S.</b> , Panicker C.Y., ArmakoviÄ S., ArmakoviÄ S.J., Nagarajan S., Van Alsenoy C.	Physics	Journal of Molecular Structure	2017
Radiation dose to the populace in southern peninsular India through foodstuff	Jose R.M., <b>Jojo P.J.</b>	Physics	Nature Environment and Pollution Technology	2017
Food and feeding of Hypselobarbus Kurali, a freshwater cyprinid endemic to Kallada River, Kollam, Kerala, India	<b>Williams S., Sarlin,</b> Sudhakaran V.N.M.	Zoology	International Journal of Zoological Research	2017

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., <b>Jojo P.J.</b> , Abraham J.P.	Physics	Pollution Research	2017
Quinoline derivatives as possible lead compounds for anti-malarial drugs: Spectroscopic, DFT and MD study	Sureshkumar B., <b>Mary Y.S.</b> , Panicker C.Y., Suma S., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C., Narayana B.	Physics	Arabian Journal of Chemistry	2017
Inhalation Dose and Source Term Studies in a Tribal Area of Wayanad, Kerala, India	Bhaskaran R., Damodaran R.C., Kumar V.A., <b>Panakal John J.</b> , Bangaru D., Natarajan C., Sathiamurthy B.S., Mundiyanikal Thomas J., Mishra R.	Physics	Journal of Environmental and Public Health	2017
Use of Koha in India: Problems and Prospects	Harish Babu,Prijith Jacob Thomas	Library Science	IASLIC Bulletin	2017
Synthesis, characterization and computational studies of semicarbazide derivative	Muthukkumar M., Bhuvaneswari T., Venkatesh G., Kamal C., Vennila P., ArmakoviÄ S., ArmakoviÄ S.J., <b>Sheena Mary Y.</b> , Yohannan Panicker C.	Physics	Journal of Molecular Liquids	2018
Two novel imidazole derivatives â€ Combined	Smitha M., <b>Mary</b>	Physics	Journal of	2018

experimental and computational study	<b>Y.S.</b> , Hossain M., Resmi K.S., Armakovi S., Armakovi S.J., Pavithran R., Nanda A.K., Van Alsenoy C.		Molecular Structure	
Synthesis and spectroscopic study of three new oxadiazole derivatives with detailed computational evaluation of their reactivity and pharmaceutical potential	<b>Mary Y.S.</b> , Miniyar P.B., Mary Y.S., Resmi K.S., Panicker C.Y., Armakovi S., Armakovi S.J., Thomas R., Sureshkumar B.	Physics	Journal of Molecular Structure	2018
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.	Chemistry	Sustainable Chemistry and Pharmacy	2018
Phylogenetic analysis and evolution of morphological characters in the genus Jasminum L. (Oleaceae) in India	Jeyarani J.N., Yohannan R., Vijayavalli D., Dwivedi M.D., Pandey A.K.	Botany	Journal of Genetics	2018
Molecular structure, spectroscopic, dielectric and thermal study, nonlinear optical properties, natural bond orbital, HOMO-LUMO and molecular docking analysis of (C <sub>6</sub> Cl <sub>2</sub> O <sub>4</sub> )(C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> F) <sub>2</sub> ·2H <sub>2</sub> O	Hosna S., Janzen D.E., Mary Y.S., Resmi K.S., Thomas R., Mohamed R., Wajda S.	Physics	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2018
Molecular dynamic simulations, ALIE surface, Fukui functions geometrical, molecular docking	Venkatesh G., Kamal C., Vennila	Physics	Journal of Molecular	2018

and vibrational spectra studies of tetra chloro p and m-xylene	P., Govindaraju M., Mary Y.S., Armakovic S., Armakovic S.J., Kaya S., Panicker C.Y.		Structure	
Dietary curcumin influences leptin, growth hormone and hepatic growth factors in Tilapia ( <i>Oreochromis mossambicus</i> )	Sruthi M.V., Nair A.B., Arun D., Thushara V.V., Sheeja C.C., Vijayasree A.S., Oommen O.V., Divya L.	Zoology	Aquaculture	2018
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.	Zoology	Journal of Applied Ichthyology	2018
Spectroscopic characterization of hydroxyquinoline derivatives with bromine and iodine atoms and theoretical investigation by DFT calculations, MD simulations and molecular docking studies	Sureshkumar B., Mary Y.S., Resmi K.S., Suma S., Armakovi S., Armakovi S.J., Van Alsenoy C., Narayana B., Sobhana D.	Physics	Journal of Molecular Structure	2018
A green approach for the synthesis of drug delivery system, mesoporous silica grafted acrylamide $\alpha$ - $\beta$ -cyclodextrin composite, for the controlled release of curcumin	Mullassery M.D., Fernandez N.B., Surya R., Thomas D.	Chemistry	Asian Journal of Pharmaceutical and Clinical Research	2018
Study on the structure, vibrational analysis and molecular docking of fluorophenyl derivatives using FT-IR and density functional theory	Al-Tamimi A.-M.S., Mary Y.S., Hassan H.M., Resmi K.S.,	Physics	Journal of Molecular Structure	2018

computations	El-Emam A.A., Narayana B., Sarojini B.K.			
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	Sureshkumar B., Sheena Mary Y., Suma S., ArmakoviÄ S., ArmakoviÄ S.J., Alsenoy C.V., Narayana B., Sasidharan B.P.	Physics	Journal of Molecular Structure	2018
Synthesis, spectroscopic analyses, chemical reactivity and molecular docking study and anti-tubercular activity of pyrazine and condensed oxadiazole derivatives	Al-Tamimi A.-M.S., Mary Y.S., Miniyar P.B., Al-Wahaibi L.H., El-Emam A.A., ArmakoviÄ S., ArmakoviÄ S.J.	Physics	Journal of Molecular Structure	2018
Understanding reactivity of two newly synthesized imidazole derivatives by spectroscopic characterization and computational study	Hossain M., Thomas R., Mary Y.S., K.S.Resmi, ArmakoviÄ S., ArmakoviÄ S.J., Nanda A.K., Vijayakumar G., Alsenoy C.V.	Physics	Journal of Molecular Structure	2018
Spectroscopic analysis and molecular docking of imidazole derivatives and investigation of its reactive properties by DFT and molecular dynamics simulations	Thomas R., Hossain M., <b>Mary Y.S.</b> , Resmi K.S., ArmakoviÄ S., ArmakoviÄ S.J., Nanda A.K., Ranjan V.K., Vijayakumar G., Van Alsenoy C.	Physics	Journal of Molecular Structure	2018

Spectroscopic analysis of 8-hydroxyquinoline derivatives and investigation of its reactive properties by DFT and molecular dynamics simulations	Sureshkumar B., <b>Mary Y.S.</b> , Resmi K.S., Panicker C.Y., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C., Narayana B., Suma S.	Physics	Journal of Molecular Structure	2018
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	El-Azab A.S., <b>Mary Y.S.</b> , Abdel-Aziz A.A.M., Miniyar P.B., ArmakoviÄ S., ArmakoviÄ S.J.	Physics	Journal of Molecular Structure	2018
Combined spectroscopic, DFT, TD-DFT and MD study of newly synthesized thiourea derivative	Menon V.V., <b>Sheena Mary Y.</b> , Shyma Mary Y., Panicker C.Y., Bielenica A., ArmakoviÄ S., ArmakoviÄ S.J., Van Alsenoy C.	Physics	Journal of Molecular Structure	2018
Characterization of biochars from a plant biomass and its effect on lead sorption capacity	<b>Fernandez N.B.</b> , <b>Mullassery M.D.</b> , Thomas D., Surya R., Jelen Das Y.	Chemistry	Desalination and Water Treatment	2018
Contribution of thoron and progeny towards inhalation dose in a thorium abundant beach environment	Visnuprasad A.K., Jaikrishnan G., Sahoo B.K., Pereira C.E., <b>Jojo P.J.</b>	Physics	Radiation Protection Dosimetry	2018
Adsorption properties of graphene towards the ephedrine – A frequently used molecule in sport	ArmakoviÄ S., ArmakoviÄ S.J., TomiÄ B.T., Pillai	Physics	Computational and Theoretical	2018

	R.R., <b>Panicker C.Y.</b>		Chemistry	
A complete computational and spectroscopic study of 2-bromo-1, 4-dichlorobenzene – A frequently used benzene derivative	Vennila P., Govindaraju M., Venkatesh G., Kamal C., <b>Mary Y.S.</b> , Panicker C.Y., Kaya S., ArmakoviÄ S., ArmakoviÄ S.J.	Physics	Journal of Molecular Structure	2018
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**Principal**