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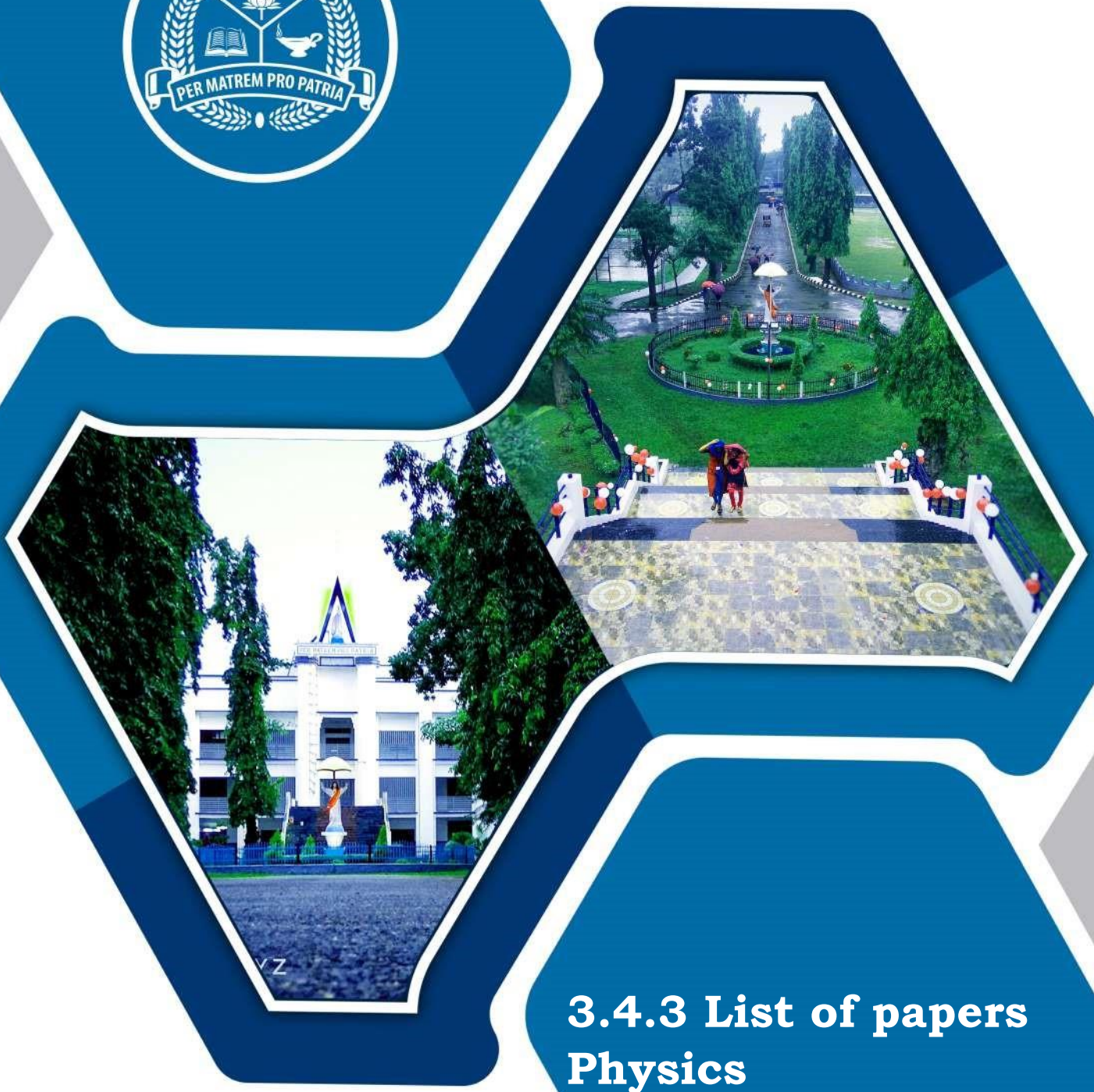

3.4.3 List of papers

Physics

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List of Research Papers in UGC CARE Listed Journals (2014-2019)

Department of Physics

Title of paper	Name of the author/s	Name of journal	Year of publication
FT-IR, molecular structure, HOMO-LUMO, MEP, NBO analysis and first order hyperpolarizability of Methyl 4,4â€³-difluoro-5â€²-methoxy-1,1â€²: 3â€²,1â€³-terphenyl-4â€²-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
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., **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
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
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

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	**Mary Y.S.,** 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
Vibrational spectra, molecular structure, NBO, HOMO-LUMO and first order hyperpoalarizability 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
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
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[5.2.1.02,6]dec-8-ene-3,5-dione	Renjith R., **Mary Y.S**., Panicker C.Y., Varghese H.T., PakosiÅ„ska-Parys M., Van Alsenoy C., Al-Saadi A.A.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
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	Chidan Kumar C.S., Yohannan Panicker C., Fun H.-K., **Sheena Mary Y.**, Harikumar B., Chandraju S., Quah C.K., Ooi C.W.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Molecular conformational analysis, vibrational spectra, NBO	**Sheena Mary Y.,** Raju	Spectrochimic	2014

analysis and first hyperpolarizability of (2E)-3-phenylprop-2-enoic anhydride based on density functional theory calculations	K., Panicker C.Y., Al-Saadi A.A., Thiemann T., Van Alsenoy C.	a Acta - Part A: Molecular and Biomolecular Spectroscopy	
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**.,** **Mary Y.S.**, Harikumar B., Chandraju S., Quah C.K., Ooi C.W.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Quantum mechanical and spectroscopic (FT-IR, FT-Raman, 1H NMR and UV) investigations of 2-(phenoxymethyl)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
Quantum mechanical and spectroscopic (FT-IR, FT-Raman, 1H NMR and UV) investigations of 5-nitro-2-phenylbenzoxazole	Bhagyasree J.B., V**arghese H.T.,** Panicker C.Y., Samuel J., Van Alsenoy C., Ertan-Bolelli T., Yildiz I.	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-dimethoxy-4-[3-(4-phenylpiperazin-1-yl)propyl]-4-azatricyclo[5.2.1.02,6]dec-8-ene-3,5- dione by density functional methods	Renjith R., **Mary Y.S.,** Panicker C.Y., **Varghese H.T.**, PakosiÅ„ska-Parys M., Van Alsenoy C., Manojkumar T.K.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Vibrational spectroscopic and computational study of 1,7,8,9-Tetrachloro-4- (4-bromo-butyl)-10,10-dimethoxy-4-aza-tricyclo[5.2.1.02,6] dec-8-ene-3,5-dione	Renjith R., **Mary Y.S.,** Panicker C.Y., **Varghese H.T.**, PakosiÅ„ska-Parys	Spectrochimica Acta - Part A: Molecular	2014

	M., Alsenoy C.V., Manojkumar T.K.	and Biomolecular Spectroscopy	
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.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
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., ProchÃ¡zkovÃ¡ M., Å evÄ Ãk R., Pazdera P.	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., **Mary Y.S.**, Panicker C.Y., **Varghese H.T.**, Yathirajan H.S., Byrappa K., Van Alsenoy C.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2014
Vibrational spectroscopic (FT-IR, FT-Raman, SERS) and quantum chemical calculations of 3-(10,10-dimethyl-anthracen-9-ylidene)-N,N,N- trimethylpropanaminiium chloride (Melitracenium 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.	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., **Jojo P.J.**, Van Alsenoy C., Kaur M., Siddegowda M.S., Yathirajan H.S., Nogueira	Spectrochimica Acta - Part A: Molecular and	2014

	H.I.S., Cruz S.M.A.	Biomolecular Spectroscopy	
Vibrational spectroscopic, 1H 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
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
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., **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
Vibrational spectroscopic and molecular docking study of (2E)-N-(4-chloro-2-oxo-1,2-dihydroquinolin-3-yl)-3-phenylprop-2-enamide	Ulahannan 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
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	**Mary Y.S.**, Panicker C.Y., Thiemann T., Al-Azani M., Al-Saadi A.A., Van Alsenoy C., Raju K., War J.A., Srivastava S.K.	Spectrochimica Acta - Part A: Molecular and Biomolecular	2015

		Spectroscopy	
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
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., **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
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
1-Alkyl-1-methylpiperazine-1,4-diium salts: Synthetic, acid-base, XRD-analytical, FT-IR, FT-Raman spectral and quantum chemical study	NÄ›meÄ kovÃ¡ D., **Mary Y.S.,** Panicker C.Y., **Varghese H.T.,** Van Alsenoy C., ProchÃ¡zkovÃ¡ M., Pazdera P., Al-Saadi A.A.	Journal of Molecular Structure	2015
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
Molecular structure, FT-IR, FT-Raman, NBO, HOMO and	Ulahannan R.T.,	Spectrochimic	2015

LUMO, MEP, NLO and molecular docking study of 2-[(E)-2-(2-bromophenyl)ethenyl]quinoline-6-carboxylic acid	Panicker C.Y., **Varghese H.T.**, Musiol R., Jampilek J., Van Alsenoy C., War J.A., Srivastava S.K.	a Acta - Part A: Molecular and Biomolecular Spectroscopy	
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., **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
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[5.2.1.02,6]dec-8-ene-3,5-dione	Resmi K.S., **Mary Y.S., Varghese H.T.,** Panicker C.Y., PakosiÅ„ska-Parys M., Alsenoy C.V.	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., **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
Vibrational spectra, HOMO, LUMO, NBO, MEP analysis and molecular docking study of 2,2-diphenyl-4-(piperidin-1-yl)butanamide	**Mary Y.S., Varghese H.T.,** Panicker C.Y., Girisha M., Sagar B.K., Yathirajan H.S., Al-Saadi A.A., Van Alsenoy C.	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	**Mary Y.S., Varghese H.T.**, Panicker C.Y., Thiemann T., Al-Saadi A.A., Popoola S.A., Van	Spectrochimica Acta - Part A: Molecular and	2015

	Alsenoy C., Al Jasem Y.	Biomolecular Spectroscopy	
Vibrational spectroscopic studies and molecular docking study of 2-[(E)-2-phenylethenyl]quinoline-5-carboxylic acid	Ulahannan 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
Vibrational spectroscopic and molecular docking study of 4-Methylphenylquinoline-2-carboxylate	Fazal E., 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
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.**, 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
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	Alzoman 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 C., War J.A.	Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy	2015
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

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
Infrared spectrum, structural and optical properties and molecular docking study of 3-(4-fluorophenyl)-5-phenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde	**Mary Y.S.,** 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
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., **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
Spectroscopic investigation (FT-IR, FT-Raman and SERS), vibrational assignments, HOMO-LUMO analysis and molecular docking study of Opipramol	**Mary Y.S.,** 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
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

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	**Mary Y.S.,** 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
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
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
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., **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
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
Conformational, NBO, NLO, HOMO-LUMO, NMR, electronic spectral study and molecular docking study of N,N-Dimethyl-	Resmi K.S., Haruna K., **Sheena Mary Y.**,	Journal of Molecular	2016

3-(10H-phenothiazin-10-yl)-1-propanamine	Yohannan Panicker C., Saleh T.A., Al-Saadi A.A., Van Alsenoy C.	Structure	
External dose measurements in the Eloor industrial area in the Ernakulam district of Kerala, India	Balakrishnan D., Umadevi A.G., Ben Byju S., **Sunil A.**, Abraham J.P., **Jojo P.J.**, Radhakrishnan S., Harikumar M.	International Journal of Radiation Research	2016
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., **Panicker C.Y**., El-Emam A.A., Salian V.V., Narayana B., Sarojini B.K., van Alsenoy C.	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.	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., **Sheena Mary Y., Yohannan Panicker C.**, Van Alsenoy C.	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., **Panicker C.Y.**, El-Emam A.A., Arisoy M., Temiz-Arpaci O., Van Alsenoy C.	Journal of Molecular Structure	2016
Evaluation of radionuclides transfer from soil-to-edible flora	Khandaker M.U., Mohd	Chemosphere	2016

and estimation of radiological dose to the Malaysian populace	Nasir N.L., Asaduzzaman K., Olatunji M.A., Amin Y.M., Kassim H.A., Bradley D.A., **Jojo P.J.**, 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., **Sheena Mary Y.,** Yohannan Panicker C., Abdel-Aziz A.A.-M., El-Sherbeny M.A., Van Alsenoy C.	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., **Mary Y.S.,** Panicker C.Y., Abdel-Aziz A.A.-M., Al-Suwaidan I.A., Van Alsenoy C.	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., **Mary Y.S**., Panicker C.Y., Attia M.I., El-Emam A.A., Alsenoy C.V.	Journal of Molecular Structure	2016
Vibrational spectroscopic & molecular docking studies of 2,6-dichlorobenzyl alcohol	Abraham M.M., Resmi K.S., Sheena Mary Y., YohannanPanicker C., Harikumar B.	Chemist	2016
Spectroscopic, single crystal XRD structure, DFT and molecular dynamics investigation of 1-(3-chloro-4-fluorophenyl)-3-[3-(trifluoromethyl)phenyl]thiourea	**Sheena Mary Y.**, Aswathy V.V., Panicker C.Y., Bielenica A., BrzÃ³zka P., Savczenko O., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C.	RSC Advances	2016
Spectroscopic analysis of 8-hydroxyquinoline-5-sulphonic acid and investigation of its reactive properties by DFT and	Sureshkumar B., **Sheena Mary Y.**, Panicker C.Y.,	Journal of Molecular	2017

molecular dynamics simulations	Resmi K.S., Suma S., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C.	Structure	
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., **Sheena Mary Y**., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Rao R.S., Suchetan P.A., Giri L., Pavithran R., Van Alsenoy C.	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	**Sarau Devi A**., Aswathy V.V.**, Sheena Mary** Y., Yohannan Panicker C., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Ravindran R., Van Alsenoy C.	Journal of Molecular Structure	2017
Investigation of reactive and spectroscopic properties of oxobutanoic acid derivative: Combined spectroscopic, DFT, MD and docking study	**Mary Y.S**., Mary Y.S., Panicker C.Y., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Narayana B., Sarojini B.K., Van Alsenoy C.	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., **Mary Y.S.**, Panicker C.Y., El-Emam A.A., Temiz-Arpaci O., Alsenoy C.V.	Journal of Molecular Structure	2017
Conformational, vibrational and DFT studies of a newly synthesized arylpiperazine-based drug and evaluation of its	Onawole A.T., Al-Ahmadi A.F.**, Mary Y.S**., Panicker	Journal of Molecular	2017

reactivity towards the human GABA receptor	C.Y., Ullah N., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C., Al-Saadi A.A.	Structure	
Comparison of thoron (220Rn) 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
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
Modification of benzoxazole derivative by bromine-spectroscopic, antibacterial and reactivity study using experimental and theoretical procedures	Aswathy V.V., Alper-Hayta S., Yalcin G.**, Mary Y.**S., Panicker C.Y., Jojo P.J., Kaynak-Onurdag F., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Yildiz I., Van Alsenoy C.	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	**Mary Y.S**., Al-Omary F.A.M., Mostafa G.A.E., El-Emam A.A., Manjula P.S., Sarojini B.K., Narayana B., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C.	Journal of Molecular Structure	2017
Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study	Murthy P.K., **Sheena Mary Y.**, Suneetha V., Panicker C.Y.,	Journal of Molecular Structure	2017

	ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Giri L., Suchetan P.A., Van Alsenoy C.		
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.**, Sheena M.Y**., 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., **Mary Y.S**., Panicker C.Y., Anto P.L., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Musiol R., Jampilek J., Van Alsenoy C.	Journal of Molecular Structure	2017
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	Joseph T.**, Varghese H.T**., Panicker C.Y., Viswanathan K., Dolezal M., Van Alsenoy C.	Arabian Journal of Chemistry	2017
Spectroscopic, DFT, molecular dynamics and molecular docking study of 1-butyl-2-(4-hydroxyphenyl)-4,5-dimethyl-imidazole 3-oxide	Benzon K.B., **Mary Y.S., Varghese H.**T., Panicker C.Y., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Pradhan K., Nanda A.K., Van Alsenoy C.	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	Aswathy V.V., **Mary Y.S., Jojo P.J**., Panicker C.Y., Bielenica A., ArmakoviÄ‡	Journal of Molecular Structure	2017

experimental and computational study	S., ArmakoviÄ‡ S.J., BrzÃ³zka P., Krukowski S., Van Alsenoy C.		
Synthesis, crystal structure analysis, spectral investigations, DFTÂ computations and molecular dynamics and docking study of 4-benzyl-5-oxomorpholine-3-carbamide, a potential bioactive agent	Murthy P.K., **Sheena Mary Y., Shyma Mary Y., Panicker C.Y., Suneetha V., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C., Suchetan P.A.**	Journal of Molecular Structure	2017
Spectroscopic and reactive properties of a newly synthesized quinazoline derivative: Combined experimental, DFT, molecular dynamics and docking study	El-Azab A.S., **Mary Y.S.,** Mary Y.S., Panicker C.Y., Abdel-Aziz A.A.-M., Mohamed M.A., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C.	Journal of Molecular Structure	2017
Newly synthesized dihydroquinazoline derivative from the aspect of combined spectroscopic and computational study	El-Azab A.S., **Mary Y.S.,** Mary Y.S., Panicker C.Y., Abdel-Aziz A.A.-M., El-Sherbeny M.A., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C.	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	**Sheena Mary Y.,** Al-Shehri M.M., Jalaja K., Al-Omary F.A.M., El-Emam A.A., Yohannan Panicker C., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J.,	Journal of Molecular Structure	2017

	Temiz-Arpaci O., Van Alsenoy C.		
Vibrational spectroscopic analysis of cyanopyrazine-2-carboxamide derivatives and investigation of their reactive properties by DFT calculations and molecular dynamics simulations	Beegum S., **Mary Y.S., Varghese H.T**., Panicker C.Y., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Zitko J., Dolezal M., Van Alsenoy C.	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-imidazol 3-oxide	Benzon K.B., **Sheena M.Y.,** Panicker C.Y., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Pradhan K., Nanda A.K., Van Alsenoy C.	Journal of Molecular Structure	2017
Vibrational spectroscopic investigations, molecular dynamic simulations and molecular docking studies of N'-diphenylmethylidene-5-methyl-1H-pyrazole-3-carbohydrazide	Pillai R.R., Menon V.V., **Mary Y.**S., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Panicker C.Y.	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.**, Mary Y.S**., Panicker C.Y., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Srivastava S.K., Van Alsenoy C.	Journal of Molecular Structure	2017
Vibrational spectroscopic analysis, molecular dynamics simulations and molecular docking study of 5-nitro-2-phenoxymethyl benzimidazole	Menon V.V., Foto E.**, Mary Y.S**., Karatas E., Panicker C.Y., Yalcin G., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C., Yildiz I.	Journal of Molecular Structure	2017
Spectroscopic characterization of 4-[2-(5-Ethylpyridin-2-	Jalaja K., **Mary Y.S.**,	Journal of	2017

yl)ethoxy]benzaldehyde oxime and investigation of its reactive properties by DFT calculations and molecular dynamics simulations	Panicker C.Y., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Sagar B.K., Girisha M., Yathirajan H.S., Van Alsenoy C.	Molecular Structure	
Reactive, spectroscopic and antimicrobial assessments of 5-[(4-methylphenyl) acetamido]-2-(4-tert-butylphenyl)benzoxazole: Combined experimental and computational study	**Mary Y.S.**, 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.	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.**, Mary Y.S**., Beegum S., Panicker C.Y., Al-Shehri M.M., El-Emam A.A., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C.	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.**, Mary Y.S**., Panicker C.Y., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Nagarajan S., Van Alsenoy C.	Journal of Molecular Structure	2017
Radiation dose to the populace in southern peninsular India through foodstuff	Jose R.M., **Jojo P.J.**	Nature Environment and Pollution Technology	2017
An assessment of ingestion dose to public from polonium -	Balakrishnan D., **Jojo**	Pollution	2017

210 and lead- 210 via dietary sources in an industrial area Eloor, Kerala, India	**P.J.,** Abraham J.P.	Research	
Quinoline derivatives as possible lead compounds for anti-malarial drugs: Spectroscopic, DFT and MD study	Sureshkumar B., **Mary Y.S.,** Panicker C.Y., Suma S., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C., Narayana B.	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., **Panakal John J.,** Bangaru D., Natarajan C., Sathiamurthy B.S., Mundiyanikal Thomas J., Mishra R.	Journal of Environmental and Public Health	2017
Synthesis, characterization and computational studies of semicarbazide derivative	Muthukkumar M., Bhuvaneswari T., Venkatesh G., Kamal C., Vennila P., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J**.,** **Sheena Mary Y**., Yohannan Panicker C.	Journal of Molecular Liquids	2018
Two novel imidazole derivatives â€“ Combined experimental and computational study	Smitha M., **Mary Y.S.**, Hossain M., Resmi K.S., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Pavithran R., Nanda A.K., Van Alsenoy C.	Journal of Molecular Structure	2018
Synthesis and spectroscopic study of three new oxadiazole derivatives with detailed computational evaluation of their reactivity and pharmaceutical potential	**Mary Y.S**., Miniyar P.B., Mary Y.S., Resmi K.S., Panicker C.Y., ArmakoviÄ‡ S.,	Journal of Molecular Structure	2018

	ArmakoviÄ‡ S.J., Thomas R., Sureshkumar B.		
Molecular structure, spectroscopic, dielectric and thermal study, nonlinear optical properties, natural bond orbital, HOMO-LUMO and molecular docking analysis of (C6Cl2O4)(C10H14N2F)2Â·2H2O	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
Molecular dynamic simulations, ALIE surface, Fukui functions geometrical, molecular docking and vibrational spectra studies of tetra chloro p and m-xylene	Venkatesh G., Kamal C., Vennila P., Govindaraju M., Mary Y.S., Armakovic S., Armakovic S.J., Kaya S., Panicker C.Y.	Journal of Molecular Structure	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., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C., Narayana B., Sobhana D.	Journal of Molecular Structure	2018
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
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.	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.	Journal of Molecular Structure	2018
Understanding reactivity of two newly synthetized 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.	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., **Mary Y.S.**, Resmi K.S., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Nanda A.K., Ranjan V.K., Vijayakumar G., Van Alsenoy C.	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., **Mary Y.S.**, Resmi K.S., Panicker C.Y., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C., Narayana B., Suma S.	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., **Mary Y.S.**, Abdel-Aziz A.A.M., Miniyar P.B., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J.	Journal of Molecular Structure	2018
Combined spectroscopic, DFT, TD-DFT and MD study of	Menon V.V., **Sheena**	Journal of	2018

newly synthesized thiourea derivative	**Mary** Y., Shyma Mary Y., Panicker C.Y., Bielenica A., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Van Alsenoy C.	Molecular Structure	
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., **Jojo P.J.**	Radiation Protection Dosimetry	2018
Adsorption properties of graphene towards the ephedrine â€“ A frequently used molecule in sport	ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., TomiÄ‡ B.T., Pillai R.R., **Panicker C.Y.**	Computational and Theoretical Chemistry	2018
A complete computational and spectroscopic study of 2-bromo-1, 4-dichlorobenzene â€“ A frequently used benzene derivative	Vennila P., Govindaraju M., Venkatesh G., Kamal C**., Mary Y.S**., Panicker C.Y., Kaya S., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J.	Journal of Molecular Structure	2018
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	**Mary S.Y.**, Al-Abdullah E.S., Aljohar H.I., Narayana B., Nayak P.S., Sarojini B.K., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Alsenoy C.V., El-Emam A.A.	Journal of the Serbian Chemical Society	2018
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
Retraction notice to â€œSynthesis, spectral characterisation, quantum mechanical analysis and light harvesting	Smitha M., **Mary Y.S**., Pradhan K., Brahman D.,	Journal of Molecular	2019

properties of two azoimidazole analoguesâ€ [J. Mol. Struct. 1197 (2019) 45â€“55](S0022286019306167)(10.1016/j.molstruc.2019.05.051)	Mary Y.S., Thomas R., Pavithran R., Alsenoy V.	Structure	
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
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
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.	ChemistrySelect	2019
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
DFT and molecular docking investigations of oxicam derivatives	**Mary Y.S.**, Mary Y.S., Resmi K.S., Thomas R.	Heliyon	2019
Conformational profile, vibrational assignments, NLO properties and molecular docking of biologically active herbicide1,1-dimethyl-3-phenylurea	Haruna K., Kumar V.S., **Sheena Mary Y**., Popoola S.A., Thomas R., Roxy M.S., Al-Saadi A.A.	Heliyon	2019
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
Synthesis, characterization and biological investigation of	Shafieyoon P.,	Journal of	2019

glycine-based sulfonamide derivative and its complex: Vibration assignment, HOMO â€“ LUMO analysis, MEP and molecular docking	Mehdipour E., **Mary Y.S.**	Molecular Structure	
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
Synthesis and spectroscopic study of two new pyrazole derivatives with detailed computational evaluation of their reactivity and pharmaceutical potential	Thomas R., **Mary Y.S**., Resmi K.S., Narayana B., Sarojini S.B.K., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Vijayakumar G., Alsenoy C.V., Mohan B.J.	Journal of Molecular Structure	2019
Dielectric spectroscopic studies in supercooled liquid and glassy states of Acemetacin, Brucine and Colchicine	Afzal A., Thayyil M.S., Sivaramakrishnan P.A., Sulaiman M.K., Hussan K.P.S., **Panicker C.Y.**, Ngai K.L.	Journal of Non-Crystalline Solids	2019
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.	Computational Biology and Chemistry	2019
Spectroscopic, antimicrobial and computational study of novel benzoxazole derivative	Beegum S., **Mary Y S**., Panicker C.Y., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Arisoy M., Temiz-Arpaci O., Van Alsenoy C.	Journal of Molecular Structure	2019
Cocrystals of pyrazinamide with p-toluenesulfonic and ferulic	Al-Otaibi J.S., **Sheena**	Journal of	2019

acids: DFT investigations and molecular docking studies	**Mary Y**., Shyma Mary Y., Panicker C.Y., Thomas R.	Molecular Structure	
Synthesis, conformational, characterization and reactivity study of 1,7-bis(4-bromophenyl)heptane-1,7-dione	Murthy P.K., Suneetha V., Smitha M., **Mary Y.**S., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Rao R.S., Suchetan P.A., Al-Saadi A.A., Pavithran R.	Journal of Molecular Structure	2019
Comparison of gamma dose levels assessed by various methods	Monica S., Visnu Prasad A.K., Soniya S.R., **Jojo P.J**.	Materials Today: Proceedings	2019
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
Theoretical Studies on the Structure and Various Physico-Chemical and Biological Properties of a Terphenyl Derivative with Immense Anti-Protozoan Activity	**Mary Y.S**., Mary Y.S., Thomas R., Narayana B., Samshuddin S., Sarojini B.K., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Pillai G.G.	Polycyclic Aromatic Compounds	2019
Synthesis, 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
Exploring the detailed spectroscopic characteristics, chemical and biological activity of two cyanopyrazine-2-carboxamide derivatives using experimental and theoretical tools	Beegum S., **Mary Y.S**., Mary Y.S., Thomas R., ArmakoviÄ‡ S., ArmakoviÄ‡ S.J., Zitko J., Dolezal M., Van	Spectrochimica Acta - Part A: Molecular and Biomolecular	2020

	Brzozka, O. Savczenko, S. Armakovic, SJ. Armakovic, C.Van Alsenoy		
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	Radiation Protection and Environment	2016

Head of the Department

FATIMA MATA NATIONAL COLLEGE
DEPARTMENT OF PHYSICS
KOLLAM

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Principal

PRINCIPAL
Fatima Mata National College
Kollam