



**Mrs. Saumya Maria Jacob** M.Sc., Ph.D. (Thesis Submitted)

Assistant Professor

Specialization: Computational Chemistry

Thesis Title: A Computational Search for Non-Classical Organic Molecules

#### **PUBLICATIONS IN NATIONAL & INTERNATIONAL JOURNALS**

1. **Saumya M.J.**, Raghi K.R., Sherin D.R., Haridas K.R. and Manojkumar T.K. (2020). *Butterfly Methanes: Designing a Novel Class of anti-van't Hoff Carbons*. **ChemPhysChem**. Doi: <https://doi.org/10.1002/cphc.202000501>
2. Raghi K.R., Sherin D.R., **Saumya M.J.**, Arun P.S., Sobha V.N., and Manojkumar T.K. (2018). *Computational Study of Molecular Electrostatic Potential, Docking and Dynamics Simulations of Gallic Acid Derivatives as ABL Inhibitors*. **Computational Biology and Chemistry**, **74**, 239-246.
3. **Saumya M.J.**, Sherin D.R., Raghi K.R., and Manojkumar T.K. (2017). *Design of Novel Planar Tetracoordinate Carbon Molecules Containing Lithium*. **Journal of Chemistry and Chemical Sciences**, **7(12)**, 1129-1134.
4. Raghi K.R., **Saumya M.J.**, Sherin D.R., and Manojkumar T.K. (2017). *An In Silico Approach to Analyze the Novel Derivatives of Protocatechuic acid with Thiazazole as Effective Protein Kinase Inhibitors Against ABL in CML*. **Journal of Chemistry and Chemical Sciences**, **7(11)**, 1071-1078.

#### **PARTICIPATION/PRESENTATION IN SEMINARS/WORKSHOPS**

1. Attended two days national workshop on "Radio activity" organised by the Research Forum, School of Chemical Science, Kannur University in collaboration with Indian Association of Nuclear Chemists & Allied Scientists (Southern Regional Chapter) on 26- 27<sup>th</sup> November, 2015.
2. Attended one day national workshop on "Microscale Experiments in Chemistry" sponsored by Kerala State Council for Science, Technology and Environment and organised by Research Department of Chemistry, Pazhassi Raja NSS College, Mattannur on 05<sup>th</sup> December, 2015.
3. Attended Winter School on "Computational Chemistry" organized by UGC-NETworking resource

centre, School of Chemistry, University of Hyderabad from 8- 24<sup>th</sup> December, 2015.

4. Attended one month training visit programme and presented a project on "Computational Study on Planar Tetracoordinate Carbon" at UGC-Networking resource centre, School of Chemistry, University of Hyderabad from 15<sup>th</sup> February to 15<sup>th</sup> March 2016.
5. Presented a paper on the topic "Design of Neutral Planar Tetracoordinate Carbon Molecules by a Hybrid Approach" Proceedings of the International Conference on Emerging Frontiers in Chemical Sciences, Post Graduate and Research Department of Chemistry, Farook College, Calicut University, Calicut, Kerala, 23- 25<sup>th</sup> September, 2017.
6. Presented a paper on the topic "Theoretical design of a Non-classical Planar Tetracoordinate Carbon Molecule by using a Hybrid Approach", National Seminar on Advanced Materials, School of Chemical Sciences, University, Swami Anandatheertha Campus, Payyannur, Kerala. 15-16<sup>th</sup> March, 2018.
7. Attended a workshop on "Swayam Prabha DTH Channel" organised by the Educational Multimedia Research Centre (EMMRC) on 05<sup>th</sup> October, 2018 at the EMS seminar hall, University of Calicut.
8. Attended three days Science Academies Lecture Workshop on "Beyond the boundaries of Chemistry", Providence Women's College, Calicut from 29-31<sup>st</sup> October, 2018.
9. Presented a paper on the topic "An In-silico design of a Non-classical Planar Tetracoordinate Carbon Molecule by using a Hybrid Approach", National Seminar on Nascent and Sustainable Materials NSNSM-2018, Department of Chemistry and Department of Physics, Kannur University, Swami Anandatheertha Campus, Payyanur, Kerala, 28-30<sup>th</sup> November, 2018.
10. Convener of one day workshop on "Microscale Analysis" jointly organized by the Association of Chemistry Teachers, Kannur University and KMM Govt. Women's College, Kannur on 08<sup>th</sup> December, 2018.
11. Presented a paper on the topic "Theoretical design of double aromatic planar tetraco-ordinate carbon compound with a B2C ring", Two day National Seminar on Recent Advances in Chemistry, Department of Chemistry, Govt. Brennan College, Dharmadam, Thalassery, Kerala. 18-19<sup>th</sup> November, 2019.

#### **PARTICIPATION IN ORIENTATION, REFRESHER AND FACULTY DEVELOPMENT PROGRAMME**

1. Participated in the six days short term Faculty Development Programme "ERUDITION -2020" organised by PG Department of Chemistry, IQAC & Chemistry Alumni Association of Payyanur College in association with Kerala State Higher Education Council, from 23- 28<sup>th</sup> May, 2020.
2. Participated in the Faculty Development Programme on "Managing online classes and Co creating MOOCs:2.0" organised by Teaching learning centre, Ramanujan College, Delhi University during 18<sup>th</sup> May - 03<sup>rd</sup> June, 2020.