# Ramya Chandar Charles. M

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**Research interest:**

My research interest lies on understating the regulatory and structural mechanisms involved in multi-layered epigenetic modifications involved in various biological processes. In specific, I would like to explore on "the co-dependence of various epigenetic modifications of DNA, RNA (also non-coding elements of RNA) and proteins involved in specific gene regulation".

**Research accomplishments:**

My doctoral research I have primarily focussed on designing inhibitors and investigating the selective inhibition of **G9a (EHMT2) lysine methyltransferse**. I have studied the structural details of G9a-H3 interactions and used the information for identification of novel quinoline based G9a inhibitor with improved inhibition profile lesser toxicity *in vitro* and *in vivo*. In addition, through the analysis of G9a-H3 peptide complexes, we have hypothesized a new strategy to mimic the arginine of substrate peptide in the inhibitor design. Computational profiling of the newly designed analogs showed 2-fold improved binding affinity towards G9a. G9a has a structural isoform GLP (has 80% sequence identity in their catalytic domains), which shares similar substrate and product specificities. G9a-inhibitor bound co-crystal structures did not provide any structural clues to their selectivity. We have used the inhibitor residence time, calculated using τRAMD simulations to correlate with the inhibitor's G9a/GLP selectivity.

Other than my doctoral research, I have contributed to many other research projects. To mention here, i). Identification of hotspot residues involved in the interaction of ASS1 with PRMT7 and Citrullinemia mutations that disrupt the interactions, ii). Mapping the interaction interface of SMYD2 and RPL21 and identification of hotspot residues primarily involved in the interaction.

**Research appointments:**

- Research scholar (August 2013 - present), Pondicherry University, India.
- Project Fellow in DST funded project (January 2015- July 2015), Pondicherry University, India.

**Educational background:**

- Thesis submitted (waiting for viva) for the degree of Ph.D., in Bioinformatics to Pondicherry University entitled **"***Computational Investigations of G9a Lysine Methyltransferase for the Design and Discovery of Novel Inhibitors"* (2013-2019)
- M.Sc., in Computational biology, from Pondicherry University, India. (7.92 CGPA, 2011-2013)
- B.Sc., in Industrial microbiology from Madurai Kamaraj University, Tamil Nadu, India. (7.85 CGPA, 2007-2015)

**Awards and Honours:**

- Gold medalist and best outgoing student of the year (2010) in under graduation.

**National level Examination:**

- Qualified Graduate aptitude test in Engineering (GATE, specialization in Biotechnology) in 2014 conducted by Indian Institute of Madras

**Technical expertise:**

**Bioinformatics Techniques:**

- Extensive working knowledge in analysis of Structural bioinformatics and cheminformatics.
- Experience in computational aided drug designing software's such as AutoDock, Discovery Studio and Schrodinger Maestro.
- Skilled in modelling and simulation, using molecular dynamics tools GROMACS, AMBER and NAMD.
- Exposure and basic knowledge on NGS data analysis.

**Computer skills (in bars-level of expertise):**

- Operating systems: Proficient in Linux/Unix, Windows environments.
- Programming languages: Java, C and C++

  Python, Perl

  SQL.

**Biophysical techniques:**

- Surface Plasmon resonance (Biacore, GE) to analyse bimolecular interactions

**Teaching experience:**

- Supervised project dissertation work of four postgraduate students as partial fulfilment of their degree in Bioinformatics/Computational biology, Pondicherry University.

- Conducted practical classes (Molecular modelling and bio molecular simulations) for M.Tech., computational biology students, Centre for Bioinformatics, Pondicherry University.

**Conferences presented:**

- Poster presented at 4th National conference on Recent trends in Industrial Pharmacology on 13th March 2015, at Mother Theresa Post graduate and Research Institute of Health Sciences,Pondicherry.
- Poster presented at 6th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 18th -21st February 2014, Alagappa University, Karaikudi, TN

**Workshops and short courses:**

- Two weeks Hands-on workshop on “Genomics in Healthcare and Translational Research” at IBAB, Bangalore conducted by Lakshmi Mittal South Asia Institute, Harvard University on December 10-23, 2017
- Short course on “Statistical methods in biological data analysis” offered by Prof. Saurabh Ghosh, Human Genetics Unit, Indian Statistical Institute, Kolkata at Pondicherry University on February 11-15, 2019
- Short course on “Drug Discovery-Role of Bioinformatics” offered by Prof. Naidu Subbarao, School of Computational and Integrative Sciences, Jawaharlal Nehru University, New Delhi at Pondicherry University on august 21-26, 2017
- Short course on development and application of molecular dynamics offered by Prof. Sourav Pal, Department of Chemistry, Indian institute of Technology-Bombay, at Pondicherry Universityon July 06-08, 2017
- Short course on Modelling Complex Biomolecular Systems and Processes Using Molecular Dynamics, offered by Professor U. Deva Priyakumar, Indian Institute of Information Technology-Hyderabad at Pondicherry University on Sep 06-10, 2016

**Publications from Ph.D., dissertation:**

**Published:**

1. **Charles, M. R. C.**, Dhayalan, A., Hsieh, H. P., & Coumar, M. S. (2019). Insights for the design of protein lysine methyltransferase G9a inhibitors. ***Future medicinal chemistry***, 11(09), 993-1014.
2. **Ramya Chandar Charles, M.**, Hsieh, H. P., & Selvaraj Coumar, M. (2018). Delineating the active site architecture of G9a lysine methyltransferase through substrate and inhibitor binding mode analysis: a molecular dynamics study. ***Journal of Biomolecular Structure and Dynamics***, 37(10), 2581–2592.

**Under revision:**

3. **Ramya Chandar Charles, M.**, Arun Mahesh, Lin, S. Y., Hsieh, H. P., Arunkumar Dhayalan, Coumar, M.S., (2019). Identification of novel quinoline inhibitor for EHMT2/G9a through virtual screening. ***Biochimie***, (minor revision).

**Other publications:**

**Published:**

4. Arya, H., Yadav, C. S., Lin, S. Y., Syed, S. B., **Charles, M. R. C.**, Kannadasan, S., ... & Coumar, M. S. (2019). Design of a potent anticancer lead inspired by natural products from traditional Indian medicine. ***Journal of Biomolecular Structure and Dynamics***, (published online) 1-19.

5. Sharma, A., Pallavi, B., Banerjee, R., **Charles, M.R.C**., Coumar, M.S., Chander, S., Sankaran, M. and Shukla, P., (2017). De novo Design and in-silico Studies of Coumarin Derivatives as Inhibitors of Cyclin Dependent Kinase-2. ***Journal of Pharmaceutical Chemistry***, *4*(4), pp.46-56.

6. Verma, M., **Charles, R.C.M**., Chakrapani, B., Coumar, M.S., Govindaraju, G., Rajavelu, A., Chavali, S. and Dhayalan, A., (2017). PRMT7 interacts with ASS1 and citrullinemia mutations disrupt the interaction. ***Journal of Molecular Biology***. 429(15), 2278-2289.

**7.** Chinta, G[#]., **Charles, M.R.C**.[#], Klopčič, I., Dolenc, M.S., Periyasamy, L. and Coumar, M.S., (2015). In Silico and in Vitro Investigation of the Piperine's Male Contraceptive Effect: Docking and Molecular Dynamics Simulation Studies in Androgen-Binding Protein and Androgen Receptor. ***Planta medica***, *81*(10), pp.804-812. ([#] sharing equal contribution).

**Under review:**

**8.** Syed, S. B., Lin, S. Y., Arya, H., Fu, I. H., Yeh, T. K., **Charles, M. R. C.**, Periyasamy, L., Hsieh, H. P., & Coumar, M. S. (2019). Overcoming vincristine resistance in cancer: computational design and discovery of P-gp inhibiting piperine analogs. ***Life sciences***.

**Manuscripts in preparation:**

- **Ramya Chandar Charles, M.**, Coumar, M.S., Structure based design of BIX-01294 and UNC0638 guanidine analogs as G9a inhibitors.

**Referees:**

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   Assistant Professor, Centre for Bioinformatics, Pondicherry University,
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3. **Prof. A. Dinakara Rao** (Mentor),
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