Ramya Chandar Charles. M

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Centre for Bioinformatics,
Pondicherry University,
Puducherry-605014,
India.

Education

- Ph.D., in Bioinformatics, 2013-2020
  Pondicherry University.
- M.Sc., in Computational biology, 2011-2013
  CGPA - 7.92
  Pondicherry University.
- B.Sc., in Industrial microbiology 2007-2010
  CGPA - 7.85
  Madurai Kamaraj University.

Research accomplishments

Summary of Ph.D., research work

Title: ***"Computational Investigations of G9a Lysine Methyltransferase for the Design and Discovery of Novel Inhibitors"***

My doctoral research I have primarily focussed on structural evaluation, designing inhibitors and investigating the key perspectives involved in 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. Co-crystal structures of G9a and GLP (isoform of G9a) did not provide any structural clues for 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 some 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 SMYD and RPL and identification of hotspot residues primarily involved in the interaction.

iii). Studied the role of Androgen receptor and Androgen binding protein in male contraception.

iv). Performed SPR kinetics assay for protein – inhibitor and protein –peptide systems.

Technical expertise

Structural Bioinformatics

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

NGS Data Analysis

- Knowledge on NGS data analysis such as RNAseq, Chipseq, variant calling and, single cell data analysis.

Machine Learning

- Knowledge on machine learning and deep learning algorithms.

Computational skills (in bars-level of expertise)

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

Biophysical techniques

- Surface Plasmon resonance (SPR, Biacore 3000) to analyse bimolecular interactions

Research appointments

- Project Fellow — January 2015 - July 2015

  DST funded project, Pondicherry University

Teaching experience

- Monitored project dissertation work of postgraduate students of Bioinformatics/Computational biology
- Taught practical classes (Molecular modelling and Biomolecular simulations) for M.Tech., Computational biology/Bioinformatics students

Awards

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

National level Examination

- Qualified (GATE, specialization in Biotechnology) in 2014 conducted by IIT Madras

Peer Reviewed Publications

From Ph.D., dissertation

Published

1. **Ramya Chandar Charles, M.**, Arun Mahesh, Lin, S. Y., Hsieh, H. P., Arunkumar Dhayalan, Coumar, M.S., (2020). Identification of novel quinoline inhibitor for EHMT2/G9a through virtual screening. ***Biochimie***, 168, 220-230.
2. **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.
3. **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.

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).

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. (2020). Overcoming vincristine resistance in cancer: computational design and discovery of P-gp inhibiting piperine analogs. ***Chemical Biology & Drug Design***.

Manuscripts in preparation

- **Ramya Chandar Charles, M.**, Coumar, M.S., Mimicking substrate arginine (H3R8) in the design of G9a inhibitors: Insights from molecular dynamics simulations.

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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