Ramya Chandar Charles. M

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Research accomplishments:

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 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 SMYD and RPL and identification of hotspot residues primarily involved in the interaction. iii). Studying the role of Androgen receptor and Androgen binding protein in male contraception.

Technical expertise:

Bioinformatics Techniques:

- 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.
- Exposure and basic knowledge on NGS data analysis such as RNAseq, Chipseq and variant calling.

Computational skills (in bars-level of expertise):

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

Research appointments:

- Research scholar (August 2013 – July 2019, thesis submitted), 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 medallist 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

Publications from Ph.D., dissertation:

Published:

1. **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***, 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).

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.

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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3. **Prof. A. Dinakara Rao** (Mentor),
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