Mangesh Damre, PhD
PostDoctoral Fellow
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Visa status: J1 Scholar Visa
GC & EAD are under process

Highly motivated Postdoctoral Researcher conducts Computational Chemistry research and participates in brainstorming topics that demonstrate experience with complex data analysis and high-performance computing. Dedicated, versatile computational chemist, author and co-author of international publications in peer-reviewed journals with extensive research experience in molecular modeling. Recent PhD in Neurobiology (Computational) with effective verbal and written communication skills to deliver excellent presentations and prepare written reports. Broad range of knowledge in advanced computational techniques. Develop and apply computational methods in the fields of biophysics, chemistry and other computationally intensive areas. Optimize and parallelize scientific programs for conventional clusters, supercomputers and GPU accelerated computers. Solve challenging problems in computational biophysics/ chemistry field through varied skills and interdisciplinary science knowledge.

SKILLS

Molecular Dynamics	GROMACS	AMBER
Coarse-grained Molecular Dynamics		Free Energy Calculations
Molecular Docking	Maestro Schrodinger	GLIDE
Forcefield Parameterization	MARTINI Forcefield	Membrane Simulations
Virtual Screening	Discovery Studio	Autodock
3D-QSAR	Sybyl-X	LBDD, SBDD
Homology Modelling	Modeller	SWISS-MODEL
Molecular Visualisers	VMD	Pymol
Scripting	Python + R	Bash
Toxicity	Derek Nexus	Toxtree
DMPK	Gastroplus	Chemoinformatics
Scientific Writing	LaTeX	
Illustrations	INKSCAPE	

WORK EXPERIENCE

PostDoctoral Reseracher February 2019 - Current

University Of Cincinnati – Cincinnati, OH, 45239, USA

- Conducted independent Computational Chemistry research and development to attain short and long-term objectives.
- Maintained accurate records of research findings and provided statistical analysis of data results.
- Drafted manuscripts and presented findings at major 3 National and International conferences.
- R package used to analyze raw data obtained from molecular dynamics simulations using Bio3D R package.
- Preparation of homology model of protein structure and perform molecular dynamics simulations at Ohio Supercomputer Center (OSC) cluster and at Pittsburgh Supercomputing Center (PSC) resources.
- Wrote several bash scripts to create all initial input files for GROMACS software to perform molecular dynamics simulations and to perform various analysis of obtained data from experiments.

Junior Research Fellow August 2013 - March 2014

NIPER, Mohali, 160062, India

- Built QSAR models to design new drug molecules.
- Supported and supervised students in Pharmacoinformatics research programs from brainstorming areas for potential research through publishing papers on completed projects.
- Edited papers for submission to prestigious journals, including GENE, Medicinal Chemistry Research, Bioorganic & medicinal chemistry letters, Current neurovascular research, Journal of Molecular Graphics and Modelling, Journal of Taiwan Institute of Chemical Engineers, PPAR Research, Journal of Molecular Structure, Current topics in Medicinal Chemistry, Arabian Journal of Chemistry, etc.

EDUCATION

Doctor of Philosophy, *SISSA, Trieste, 34136, Italy*, November 2014 - November 2018

- **Specialization** Computational Neurobiology
- **Thesis:** Computational studies on Membrane Proteins
- Wrote and implemented several bash scripts for successful development of a web-server **(MERMAID)** to perform molecular dynamics simulation and to analyze the results.

Master of Science, *NIPER, Mohali, 160062, India*, August 2011 - June 2013

- **Specialization** Pharmacoinformatics
- **Thesis:** Design and pharmacokinetic profiling of selective PPAR-alpha agonist: A molecular docking and MD simulation approach
- Graduated with 8.28 CGPA
- Member of DMPK (Drug Metabolism and Pharmacokinetics) committee

Bachelor of Pharmacy, *Government College of Pharmacy, Amaravati, India*, June 2007 - August 2011

ACCOMPLISHMENTS

- Collaborated with team of 6 in the development of *NSF* Funded project.
- Oral presentation in *American Physical Society (APS)*, 2020, Denver, Colorado
- Poster presentation in *Biophysical Society (BPS)*, 2018, SanFrancisco, California
- Best poster award winner in *The European Iron Club*, 2018, ETH Zürich
- Oral presentation in *Winter School Canazei, Applied bioinformatics*, 2018, Verona, Italy
- Best poster award winner in 5th *DMPK*, 2014, NIPER, Mohali, India
- **Developed web server : (MERMAID)** Martini Coarse Grained Membrane Protein Dynamics

GUEST REVIEWER

- Scientific Reports (SREP) Nature
- Computational and Structural Biotechnology Journal (CSBJ) elsevier
- Journal of Biomolecular Screening (JBS) SAGE Journals

PUBLICATIONS

- Google Scholar

1. **MANGESH DAMRE**, A. Dayananda, R. A. Varikoti, G. Stan, and R. I. Dima, "Factors underlying asymmetric dynamics of disaggregase and microtubule severing AAA+ machines," *bioRχiv*, nov 2020
2. **DAMRE, MANGESH**, R. A. Varikoti, and R. Dima, "Molecular dynamics study of katanin oligomeres: A mt-severing enzyme," *Bulletin of the American Physical Society*, vol. 65, 2020
3. **DAMRE, MANGESH**, A. Marchetto, and A. Giorgetti, "Mermaid: dedicated web server to prepare and run coarse-grained membrane protein dynamics," *Nucleic acids research*, vol. 47, no. W1, pp. W456–W461, 2019
4. **DAMRE, MANGESH Vitthalrao** *et al.*, "Computational studies on membrane proteins (bovine cnga1 & mouse tspo)," Ph.D. dissertation, SISSA, Trieste, Italy, 2018
5. J. Zeng, R. Guareschi, **DAMRE, MANGESH**, R. Cao, A. Kless, B. Neumaier, A. Bauer, A. Giorgetti, P. Carloni, and G. Rossetti, "Structural prediction of the dimeric form of the mammalian translocator membrane protein tspo: a key target for brain diagnostics," *International journal of molecular sciences*, vol. 19, no. 9, p. 2588, 2018
6. **DAMRE, MANGESH V**, A. Giorgetti, and V. Torre, "Gating mechanism investigation in homotetramer cnga1 ion channel by coarse-grained molecular dynamics simulation," *Biophysical Journal*, vol. 114, no. 3, p. 128a, 2018
7. M. V. DAMRE, "Design and pharmacokinetic profiling of selective ppar-α agonists: A molecular docking and md simulation approach," Ph.D. dissertation, National Institute of Pharmaceutical Education and Research, 2013
8. R. P. Gangwal, G. V. Dhoke, **DAMRE, MANGESH V**, V. Sharma, and A. T. Sangamwar, "Design of novel cytochrome bc1 inhibitors: A molecular modelling approach," *DMPK2013*, 2013
9. R. P. Gangwal, **DAMRE, MANGESH V**, and A. T. Sangamwar, "Overview and recent advances in qsar sudies," in *Chemometrics Applications and Research: QSAR in Medicinal Chemistry*. CRC Press, 2016, p. 1
10. N. Soumya, H. Tandan, **DAMRE, MANGESH V**, R. P. Gangwal, A. T. Sangamwar, and S. Singh, "Leucine-684: A conserved residue of an amp-acetyl coa synthetase (acecs) from leishmania donovani is involved in substrate recognition, catalysis and acetylation," *Gene*, vol. 580, no. 2, pp. 125–133, 2016
11. R. P. Gangwal, **DAMRE, MANGESH V**, N. R. Das, G. V. Dhoke, A. Bhadauriya, R. A. Varikoti, S. S. Sharma, and A. T. Sangamwar, "Structure based virtual screening to identify selective phosphodiesterase 4b inhibitors," *Journal of Molecular Graphics and Modelling*, vol. 57, pp. 89–98, 2015
12. R. P. Gangwal, **DAMRE, MANGESH V**, N. R. Das, S. S. Sharma, and A. T. Sangamwar, "Biological evaluation and structural insights for design of subtype-selective peroxisome proliferator activated receptor-α (ppar-α) agonists," *Bioorganic & medicinal chemistry letters*, vol. 25, no. 2, pp. 270–275, 2015
13. K. Khandelwal, R. P. Gangwal, U. Singh, R. Prajapati, **DAMRE, MANGESH V**, and A. T. Sangamwar, "Computational insights into the active site of human breast cancer resistance protein (bcrp/abcg2): a similarity search approach," *Medicinal Chemistry Research*, vol. 23, no. 11, pp. 4657–4668, 2014
14. D. Uppalapati, N. R. Das, R. P. Gangwal, **DAMRE, MANGESH V**, A. T. Sangamwar, and S. S. Sharma, "Neuroprotective potential of peroxisome proliferator activated receptor-α agonist in cognitive impairment in parkinson's disease: Behavioral, biochemical, and pbpk profile," *PPAR research*, vol. 2014, 2014
15. N. R Das, R. P Gangwal, **MANGESH, V DAMRE**, A. T Sangamwar, and S. S Sharma, "A ppar-β/δ agonist is neuroprotective and decreases cognitive impairment in a rodent model of parkinson's disease," *Current neurovascular research*, vol. 11, no. 2, pp. 114–124, 2014
16. R. P. Gangwal, N. R. Das, K. Thanki, **DAMRE, MANGESH V**, G. V. Dhoke, S. S. Sharma, S. Jain, and A. T. Sangamwar, "Identification of p38α map kinase inhibitors by pharmacophore based virtual screening," *Journal of Molecular Graphics and Modelling*, vol. 49, pp. 18–24, 2014
17. R. P. Gangwal, G. V. Dhoke, **DAMRE, MANGESH V**, K. Khandelwal, and A. T. Sangamwar, "Structure-based virtual screening and molecular dynamic simulation studies to identify novel cytochrome bc1 inhibitors as antimalarial agents," *Journal of Computational Medicine*, vol. 2013, 2013
18. **DAMRE, MANGESH V**, R. P. Gangwal, G. V. Dhoke, M. Lalit, D. Sharma, K. Khandelwal, and A. T. Sangamwar, "3d-qsar and molecular docking studies of amino-pyrimidine derivatives as pknb inhibitors," *Journal of the Taiwan Institute of Chemical Engineers*, vol. 45, no. 2, pp. 354–364, 2014
19. M. Lalit, R. P. Gangwal, G. V. Dhoke, **DAMRE, MANGESH V**, K. Khandelwal, and A. T. Sangamwar, "A combined pharmacophore modeling, 3d-qsar and molecular docking study of substituted bicyclo-[3.3. 0] oct-2-enes as liver receptor homolog-1 (lrh-1) agonists," *Journal of Molecular Structure*, vol. 1049, pp. 315–325, 2013
20. R. P. Gangwal, A. Bhadauriya, **DAMRE, MANGESH V**, G. V. Dhoke, and A. T. Sangamwar, "p38 mitogen-activated protein kinase inhibitors: a review on pharmacophore mapping and qsar studies," *Current topics in medicinal chemistry*, vol. 13, no. 9, pp. 1015–1035, 2013

21. A. Bhadauriya, G. V. Dhoke, R. P. Gangwal, **DAMRE, MANGESH V**, and A. T. Sangamwar, "Identification of dual acetyl-coa carboxylases 1 and 2 inhibitors by pharmacophore based virtual screening and molecular docking approach," *Molecular diversity*, vol. 17, no. 1, pp. 139–149, 2013

22. U. Singh, R. P. Gangwal, G. V. Dhoke, R. Prajapati, **DAMRE, MANGESH**, and A. T. Sangamwar, "3d-qsar and molecular docking analysis of (4-piperidinyl)-piperazines as acetyl-coa carboxylases inhibitors," *Arabian Journal of Chemistry*, 2012