Mangesh Damre, **PhD**

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SUMMARY

- Strong technical skills including 10+ years of hands-on experience in Computational Chemistry, Chemoinformatics, Molecular Dynamics, Molecular Docking, Homology Modelling, Free Energy Calculations, 3D-QSAR, Virtual screening.
- Proven ability to design, execute, analyze, interpret, and document results of experiments as demonstrated by a 16 publication record.
- Excellent in science communication and technical writing skills.
- Ability to achieve research targets by managing multiple projects simultaneously.
- Proven ability to work in a multidisciplinary team in highly collaborative environments.
- Extensive experience in supervising, mentoring, and training lab personnel.

WORK EXPERIENCE

Molecular Dynamics Expert | as a Postdoctoral Associate 02/2019-05/2021

- Expanded the use of Molecular dynamics techniques to study protein conformational changes.
- Perform the homology modelling to construct an atomic-resolution model of the "target" protein from its amino acid sequence and an experimental three-dimensional structure of a related homologous protein (the "template").
- Participated in a collaborative research team involved in the development of the project.
- Provided technical assistance as subject matter expert in computational chemistry.
- Published 1first-author paper and 2 first-author publications in preparation.
- Mentored and trained more than 5 graduate and undergraduate students.

Homology modelling expert | as a Doctoral student 11/2014-11/2018

- Develop web server to perform Coarse-grained molecular dynamics (MERMAID).
- Perform homology modeling and molecular dynamics of membrane proteins.
- Published 2 first-author research publications.

Computational Chemist | as a Junior Research Fellow 08/2013-03/2014

- Worked on Computer Aided Drug Design projects in a multidisciplinary collaborative environment.

CADD Expert | as a Master's student 08/2011-06/2013

- Developed 3D-QSAR models for the development of protein kinase inhibitors as new potential anti-tubercular agents.
- Perform molecular dynamics simulations to study structural insights for design of subtype-selective peroxisome proliferator activated receptor-α (PPAR-α) agonists.
- Collaborate in multiple cross-disciplinary projects, which results in 13 research publications with 1 first author, 2 second author and 1 book chapter.

EDUCATION

PhD in Computational Neurobiology | from SISSA, Trieste, ITALY 2014-2018

MS in Pharmacoinformatics | from NIPER, Mohali, INDIA 2011-2013

Bachelor in Pharmacy | from GCOPA, Amaravati, MH, INDIA 2007-2011

SKILLS

Molecular Dynamics	**Coarse-grained MD**	**Molecular Docking**
Virtual Screening	**3D-QSAR**	**Homology Modelling**
Membrane Simulations	**Martini Forcefield**	**LBDD, SBDD**
GROMACS	**AMBER**	**Discovery Studio**
Maestro	**Modeller**	**GastroPlus**
LATEX	**Chemoinformatics**	**Python, Scripting**
Toxicity prediction	**Toxtree**	**Derek Nexus**
Forcefield parameterization	**Free Energy Calculation**	**Autodock**
Glide	**Scientific Writing**	**R, BASH, Tableau**

ACCOMPLISHMENTS

- 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 Z¨urich
- 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(Old) and MERMAID(New) Martini coarsE gRained MembrAne proteIn Dynamics. Tutorial Link: Youtube
- Quality assurance, Software testing and Website development: DruLiTo (Drug Likeness Tool)

Guest Reviewer

- Scientific Reports (SERP)
- Computational and Structural Biotechnology Journal (CSBJ) Elsevier
- Journal of Biomolecular Screening (JBS) SAGE Journals

Publications

- Google Scholar

1. DAMRE, MANGESH V, A. Dayananda, R. A. Varikoti, G. Stan, and R. I. Dima, ``Factors underlying asymmetric pore dynamics of disaggregase and microtubule severing aaa+ machines," Biophysical Journal, 2021
2. DAMRE, MANGESH V, 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 V, 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 V 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 V, 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, DAMRE, MANGESH V, 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 V, and A. T. Sangamwar, ``3d-qsar and molecular docking analysis of (4-piperidinyl)-piperazines as acetyl-coa carboxylases inhibitors," Arabian Journal of Chemistry, 2012