Mangesh Damre

PostDoctoral Researcher | Bioinformatician

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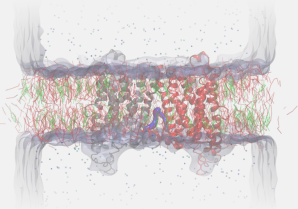


About Me

I am PostDoctoral researcher in Department of Chemistry in Univeresity of Cincinnati (Ohio, USA). I have completed my Ph.D. (11/2014-11/2018) from SISSA institute (Trieste, Italy) in Neurobiology department. My Ph.D. research was mainly focused on the homology model development of ion channels, membrane proteins, and their investigation through coarse-grained molecular dynamics along with the development of coarse-grained force field parameters for the small molecules. I completed my MS (08/2011-06/2013) in PharmacoInformatics discipline from NIPER (Mohali, India). During MS, I dealt with different techniques like Homology Modelling, PKPD modeling, Molecular Dynamics, Molecular Docking, Pharmacophore generation, Virtual Screening and 3D QSAR studies. Working in a good scientific environment on various projects benefit me to add international publications in my research profile.

SKILLS

Core Competencies

- Pharmacoinformatics
- Bioinformatcs
- Homology modeling
- Molecular Dynamics
- Coarse-grained MD
- Illustartion creation
- WEB designing

Tools

- Gromacs
- Modeller
- Latex
- Bash Script
- GNUPLOT
- VMD
- PYMOL
- INKSCAPE
- HTML & PHP

CONFERENCES

2018-02 | Poster Presentation in Biophysical Society, 62nd Annual meeting 2018, SanFrancisco
www.linkinghub.elsevier.com/retrieve/pii/S0006349517319604

2018-02 | Poster presentation in The European Iron Club 2018, ETH Zürich
IronGenes : a webserver for rare genetic disorders of Iron metabolism
http://www.ironclub2018.ethz.ch/

2018-01 | Oral Presentation in Winter School Canazei 2018, Applied Bioinformatics, Verona (Italy)
https://www.winterschoolbiotech2018.com/

2014-03 | Poster Presentation in 5th International DMPK (Drug Metabolism and Pharmacokinetics) Symposium.

ACHIEVEMENTS

2018-02 | The Crichton Prize winner for Best Poster in The Iron Club 2018, ETH Zürich

2014-03 | Best Poster Award Winner in 5th International DMPK (Drug Metabolism and Pharmacokinetics) Symposium.

LANGUAGES

- HINDI/ MARATHI — Native
- ENGLISH — Advanced Level
- SANSKRIT — Basic Level

EXPERIENCE

PostDoctoral Researcher | 2019/02 - Present
A&S-Chemistry, CROSLEY, 301 Clifton Ct, Cincinnati OH 45221-0172
* Modeling and simulation of biological macromolecules.

Bioinformatician | 2014/11 -2018/11
SISSA, Via Bonomea 265, 34136, Trieste, Italy 34136 (Trieste, Italy)
* Modeling and simulation of CNGA1 ion channel

Visiting PhD Student | 2016/12 -2018/11
University of Verona, Department of Biotechnology, Ca' Vignal 1, Strada Le Grazie, 15 I-37134 Verona
* Bioinformatics and simulation studies of membrane proteins

Junior Research Fellow | 2013/08 - 2014/03
NIPER, National Institute of Pharmaceutical Education and Research, S.A.S. Nagar, Mohali. Panjab. 160062

EDUCATION

PhD student | 2014/11 -2018/11
SISSA, Via Bonomea 265, 34136, Trieste, Italy
* Modeling and simulation of CNGA1 ion channel

MS Scholar (Pharmacoinformatics) | 2011/08 -2013/06
NIPER, National Institute of Pharmaceutical Education and Research, S.A.S. Nagar, Mohali. Panjab. 160062

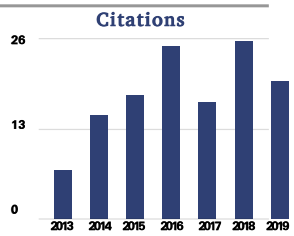
Bachelor of pharmacy | 2007/06 -2011/08
Government College of Pharmacy Amravati, Maharashtra. 444601

METRICS

18 Articles | 1 Chapter | 8 h-index

Google Scholar

2 Articles under preparation



WEB SERVERS UNDER DEVELOPMENT

- IronGenes | Genes and Proteins of iron related genetic diseases server designed by University of Verona.
- MERMAID | Martini Coarse Grained Membrane Protein Dynamics

REFERENCES

Prof. Ruxandra Dima
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Prof. Alejandro Giorgetti
@ alejandro.giorgetti@univr.it +39 045 802 7982
University of Verona, Department of Biotechnology, Ca' Vignal 1
Strada Le Grazie, 15 I-37134 Verona, Italy

INTERESTS

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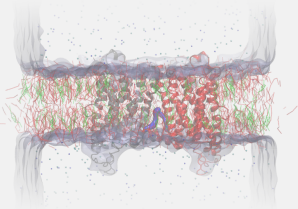

Publications under preparation

- Gating Mechanism Investigation in Homotetramer CNGA1 Ion Channel by Coarse-Grained Molecular Dynamics Simulation
  MV Damre, A Giorgetti, V Torre
- IronGenes : Genes and Proteins of iron related genetic diseases server
  MV Damre, A Marchetto, A Giorgetti
- Molecular insight of CB1 receptor by Coarse-grained molecular dynamics simulation
  MV Damre, A Tocci, A Giorgetti, E Dainese

Publications

2019-05 **(IF : 11.56)**
MERMAID web server : Martini coarsE gRained MembrAne proteIn Dynamics
MV Damre, et. al. Nucleic Acids Research, 2019

2018-08 **(IF : 3.687)**
Structural prediction of the physiologically relevant form of mammalian TSPO - a key target for brain diagnosticss
MV Damre, et. al, Int. J. Mol. Sci. 2018, 19(9), 2588

2016-04 **(IF : 2.498)**
Leucine-684: A conserved residue of an AMP-acetyl CoA synthetase (AceCS) from Leishmania donovani is involved in substrate recognition, catalysis and acetylation
N Soumya, H Tandan, **MV Damre**, RP Gangwal, AT Sangamwar, S Singh *Gene* 580 (2), 125-133

2016-03
Overview and recent advances in QSAR studies
RP Gangwal, **MV Damre**, AT Sangamwar
Chemometrics Applications and Research: QSAR in Medicinal Chemistry, 1

2015-04 **(IF : 1.885)**
Structure based virtual screening to identify selective phosphodiesterase 4B inhibitors RP Gangwal, **MV Damre**, NR Das, GV Dhoke, A Bhadauriya, RA Varikoti,
Journal of Molecular Graphics and Modelling 57, 89-98

2015-01 **(IF : 2.442)**
Biological evaluation and structural insights for design of subtypeselective peroxisome proliferator activated receptor-α (PPAR-α) agonists RP Gangwal, **MV Damre**, NR Das, SS Sharma, AT Sangamwar *Bioorganic & medicinal chemistry letters* 25 (2), 270-275

2014-11 **(IF : 1.607)**
Computational insights into the active site of human breast cancer resistance protein (BCRP/ABCG2): a similarity search approach K Khandelwal, RP Gangwal, U Singh, R Prajapati, **MV Damre**, *Medicinal Chemistry Research* 23 (11), 4657-4668

2014-05 **(IF : 2.051)**
A PPAR-β/δ agonist is neuroprotective and decreases cognitive impairment in a rodent model of Parkinson's disease NR Das, RP Gangwal, **MV Damre**, AT Sangamwar, SS Sharma
Current neurovascular research 11 (2), 114-124

2014-04 **(IF : 1.885)**
Identification of p38α MAP kinase inhibitors by pharmacophore based virtual screening
RP Gangwal, NR Das, K Thanki, **MV Damre**, GV Dhoke, SS Sharma,
Journal of Molecular Graphics and Modelling 49, 18-24

2014-03 **(IF : 3.849)**
3D-QSAR and molecular docking studies of amino-pyrimidine derivatives as PknB inhibitors **MV Damre**, RP Gangwal, GV Dhoke, M Lalit, D Sharma, K Khandelwal,
Journal of the Taiwan Institute of Chemical Engineers 45 (2), 354-364

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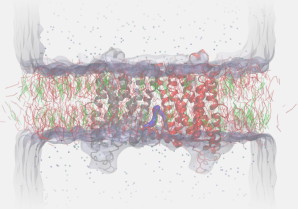

Publications

2014-02 **(IF : 3.386)** Neuroprotective potential of peroxisome proliferator activated receptor-α agonist in cognitive impairment in Parkinson's disease: Behavioral, biochemical, and PBPK profile D Uppalapati, NR Das, RP Gangwal, **MV Damre**, AT Sangamwar, *PPAR research* 2014

2013-10 **(IF : 2.011)** 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 M Lalit, RP Gangwal, GV Dhoke, **MV Damre**, K Khandelwal, *Journal of Molecular Structure* 1049, 315-325

2013-08 Structure-Based Virtual Screening and Molecular Dynamic Simulation Studies to Identify Novel Cytochrome bc1 Inhibitors as Antimalarial Agents RP Gangwal, GV Dhoke, **MV Damre**, K Khandelwal, AT Sangamwar *Journal of Computational Medicine* 2013

2013-05 **(IF : 3.374)** p38 Mitogen-activated protein kinase inhibitors: a review on pharmacophore mapping and QSAR studies RP Gangwal, A Bhadauriya, **MV Damre**, GV Dhoke, AT Sangamwar *Current topics in medicinal chemistry* 13 (9), 1015-1035

2013-02 **(IF : 2.229)** Identification of dual Acetyl-CoA carboxylases 1 and 2 inhibitors by pharmacophore based virtual screening and molecular docking approach A Bhadauriya, GV Dhoke, RP Gangwal, **MV Damre**, AT sangamwar *Journal of Computational Medicine* 17 (1), 139-149

2012-11 **(IF : 4.008)** 3D-QSAR and Molecular Docking Analysis of (4-Piperidinyl)-Piperazines as Acetyl-CoA Carboxylases Inhibitors U Singh, RP Gangwal, GV Dhoke, R Prajapati, **M Damre,** AT Sangamwar *Arabian Journal of Chemistry* 2012

Guest Reviewer

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