

## Piyusha Pagare

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### Research Scholar

Memorial Sloan Kettering Cancer Center

Since August 2018

- P.I.: Dr. Gabriela Chiosis
- Project: Design, synthesis and the biological characterization of potent and selective GRP94 inhibitors.

### EDUCATION

#### **Ph.D., Medicinal Chemistry.**

May 2018

Virginia Commonwealth University

- Thesis research topic: Rational design of allosteric modulators of hemoglobin as dual acting antisickling agents for the treatment of sickle cell disease.
- Secondary project: Molecular mechanisms involved in the role of GRP170 as a nucleotide exchange factor.
- Advisors: Dr. Yan Zhang and Dr. Martin K. Safo

#### **MS, Organic Chemistry**

June 2012

Mumbai University

- Dissertation: p-TSA catalyzed microwave assisted synthesis of acridine derivatives using deep-eutectic solvents.
- Secondary project: Synthesis of gold nanoparticles.
- Advisor: Dr. Suhas Pednekar

#### **BS, Chemistry**

June 2009

Mumbai University

### RESEARCH SKILLS

- Chemistry: Synthetic organic chemistry, Multistep synthesis of small molecules, Structure based drug design, Microwave assisted reactions
- Structural Biology: Protein purification, X-ray crystallography
- Analytical Chemistry: Column chromatography, NMR, FT-IR, UV-Vis spectroscopy, HPLC
- Computational softwares: Crystal structure refinement (Phenix, CNS), Graphics programs (COOT, PyMOL, TOM), SYBYLX2.1.1, Homology modeling (Modeler), Docking (GOLD54), Scoring (HINT), Virtual screening (UNITY), Molecular dynamic simulations (NAMD, VMD), ChemDraw, Microsoft Office
- Database search engines: SciFinder, Reaxys

### PUBLICATIONS

1. **Pagare, P. P.**; Wang, H.; Wang, X. Y.; Zhang, Y. Understanding the role of glucose regulated protein 170 (GRP170) as a nucleotide exchange factor through molecular simulations. *J. Mol. Graph. Model.* **2018**, *85*, 160-170.
2. Deshpande, T.M.; **Pagare, P.P.**; Ghatge, M.S.; Chen, Q.; Musayev, F.N.; Venitz, J.; Zhang, Y.; Abdulmalik, O.; Safo, M.K. Rational modification of vanillin derivatives to stereospecifically destabilize sickle hemoglobin polymer formation. *Acta Cryst. D* **2018**, *74*, 956-94.
3. **Pagare, P. P.**; Ghatge, M.S.; Musayev, F.N.; Deshpande, T.M.; Chen, Q.; Braxton, C.; Kim, S.; Venitz, J.; Zhang, Y.; Abdulmalik, O.; Safo, M.K. Rational design of pyridyl derivatives of vanillin for the treatment of sickle cell disease. *Bioorg. Med. Chem.* **2018**, *26*, 2530-2538.
4. Xu, G.G.; **Pagare, P.P.**; Ghatge, M.S.; Safo, R.P.; Gazi, A.; Chen, Q.; David, T.; Alabbas, A.B.; Musayev, F.N.; Venitz, J.; Zhang, Y.; Safo, M.K.; Abdulmalik, O. Design, synthesis and biological evaluation of ester and ether derivatives of antisickling agent 5-HMF for the treatment of sickle cell disease. *Mol. Pharm.* **2017**, *14*, 3499-3511.
5. **Pagare, P.P.**; Zaidi, S.A.; Zhang, X.; Li, X.; Yu, X.; Wang, X.Y.; Zhang, Y. Understanding molecular interactions between scavenger receptor A and its natural product inhibitors through molecular modeling studies. *J. Mol. Graph. Model.* **2017**, *77*, 189-199.
6. Zheng, Y.; Li, X.; **Pagare, P.P.**; Yuan, Y.; Wang, X.Y.; Zhang, Y. Design, synthesis, and characterization of rhein analogs as novel inhibitors of scavenger receptor A. *Bioorg. Med. Chem. Lett.* **2017**, *27*, 72-76.

7. Ghatge, M.S.; Ahmed, M.H.; Omar, A.M.; **Pagare, P.P.**; Rosef, S.; Kellogg, G. E.; Abdulmalik, O.; Safo, M.K. Crystal structure of carbonmonoxy hemoglobin in R-state conformation. *J. Struct. Biol.* **2016**, *194*, 446-450.

### **PATENTS AND INVENTION DISCLOSURES**

- Safo MK, Zhang Y, Venitz J, Xu G, Pagare PP, Ghatge MS, Abdulmalik O. Derivatives of Pyridoxal (Vitamin B6) as Antisickling Agents, Invention Disclosure Filed 2015.

### **PRESENTATIONS**

1. **Piyusha P. Pagare**, Osheiza Abdulmalik, Martin Safo and Yan Zhang. "Aromatic aldehydes as allosteric modulators of hemoglobin for the treatment of sickle cell disease." Oral presentation at the Virginia Academy of Sciences (VAS) Annual Meeting, Richmond, VA, 2017.
2. **Martin K. Safo**, **Piyusha P. Pagare**, Mohini Ghatge, Guoyan Xu, Ronni P. Safo, Aheema Gazi, Qiukan Chen, Tanya David, Jurgen Venitz, Yan Zhang and Osheiza Abdulmalik. "Anti-sickling properties of novel structurally enhanced pyridyl derivatives of vanillin." Oral presentation at the 10<sup>th</sup> Annual Sickle Cell Disease Research and Educational Symposium and Scientific Meeting, Fort Lauderdale, FL, 2017.
3. **Piyusha P. Pagare**, Osheiza Abdulmalik, Martin Safo and Yan Zhang. "Design and development of a novel class of structurally enhanced allosteric modulators of hemoglobin for sickle cell disease treatment." Poster presented at the 253<sup>rd</sup> American Chemical Society national meeting and exposition, San Francisco, CA, 2017.
4. **Martin K. Safo**, Mohini Ghatge, Tanya David, Guoyan Xu, **Piyusha Pagare**, Tanvi Deshpande, Qiukan Chen, Yan Zhang, Jurgen Venitz and Osheiza Abdulmalik. "Development of allosteric effectors of hemoglobin to prevent hypoxia-induced sickle cell hemoglobin polymerization." Oral presentation at the 3<sup>rd</sup> Global Congress on Sickle Cell Disease, Bhubaneshwar, Odisha, India, 2017.
5. **Piyusha P. Pagare**, Osheiza Abdulmailk, Martin Safo and Yan Zhang. "Development of Allosteric Modulators of Hemoglobin for the Treatment of Sickle Cell Disease." Poster presented at the School of Pharmacy Research and Career day, Virginia Commonwealth University, Richmond, VA, 2016.
6. **Piyusha P. Pagare**, Martin Safo, Mohini Ghatge, Guoyan Xu, Ronni P. Safo, Aheema Gazi, Qiukan Chen, Tanya David, Jurgen Venitz, Yan Zhang, Osheiza Abdulmailk. "Antisickling Properties of a Novel Structurally Enhanced Class of Allosteric Hemoglobin Effectors." Oral presentation at the 10<sup>th</sup> Anniversary Conference of Academy for Sickle Cell and Thalassemia (ASCAT), Royal College of Physicians, London, United Kingdom, 2016.
7. **Piyusha P. Pagare**, Mohini Ghatge, Osheiza Abdulmalik, Martin Safo and Yan Zhang. "Development of Allosteric Modulators of hemoglobin for the Treatment of Sickle Cell Disease." Poster presented at the VCU 3D Summit, Virginia Commonwealth University, Richmond, VA, 2016.
8. **Piyusha P. Pagare**, Mostafa H. Ahmed and Yan Zhang. "Molecular Modeling Studies of Glucose Regulated Protein 170." Poster presented at the School of Pharmacy Research and Career day, Virginia Commonwealth University, Richmond, VA, 2015.
9. **Piyusha P. Pagare**. "Immune-modulating Strategies of GRP170 in Cancer-Immunotherapy." Oral presentation at the Department of Medicinal Chemistry, Virginia Commonwealth University, Richmond, VA, 2014.
10. **Piyusha P. Pagare**. "Application of  $\beta$ -arrestins as Surrogate Markers to Study GPCR Function." Oral presentation at the Department of Medicinal Chemistry, Virginia Commonwealth University, Richmond, VA, 2013.
11. **Piyusha P. Pagare** and Dhvani Nagodra. "Determination of Ion Concentration using polarography." Oral presentation at the Department of Bio-analytical Chemistry, Ramnarain Ruia College, Mumbai University, Mumbai, India, 2010.
12. **Piyusha P. Pagare** and Dhaniala Palani. "Chemistry of Optical Fibers." Oral presentation at NES Ratnam College for Inter-collegiate seminar competition, Mumbai University, 2008.
13. **Piyusha P. Pagare**. "Electro-analytical methods." Oral presentation at the Department of Chemistry, Ramnarain Ruia College, Mumbai University, Mumbai, India, 2007.

### **TEACHING EXPERIENCE**

- In-charge of Bruker 400MHz Nuclear Magnetic Resonance (NMR) 2014 - 2016
  - Hardware and software troubleshooting including changing probes
  - Regular liquid nitrogen and liquid helium fills
  - Training graduate students and post-docs
  - Managing accounting and billing for usage
- Teaching assistant, Virginia Commonwealth University 2013 - 2016

- MEDC670: Advanced Molecular Modeling Theory and Practice
- MEDC541: Survey of Molecular Modeling Methods
- MEDC524: Introduction to Bio-molecular 3D visualization (PyMOL)
- MEDC527: Basic Pharmacy Principles for Pharmacists
- PHAR523: Foundations I (Enzyme Kinetics)
- Lecturer, Ramnarain Ruia College, Mumbai University 2012 - 2013
  - Graduate organic chemistry and biochemistry courses covering the topics antibiotics, vitamins and biochemical pathways
- Lecturer, St. Xavier's College, Mumbai University 2012 - 2013
  - Undergraduate chemistry courses covering the topics alkenes, cycloalkanes, alkynes, aromaticity and stereochemistry
  - Undergraduate chemistry lab coordinator

### **HONORS AND AWARDS**

- Rector and Rorrer Dean's award runner-up (\$1,500) 2018
- J. Doyle Smith award recipient (\$250) 2018
- VCU graduate dissertation assistantship award (\$18,000) 2017 - 2018
- Best Student Oral Presentation award, Medical Sciences section, Virginia Academy of Sciences 2017
- Peter and Sian Byron, School of Pharmacy graduate student travel award (\$500) 2017
- Best poster, School of Pharmacy research and career day, Virginia Commonwealth University (\$200) 2016
- Graduate travel grant award, School of Pharmacy, Virginia Commonwealth University (\$500) 2016
- Scholarship holder, Honor Society of Phi Kappa Phi (\$650) 2015
- Best Student, Organic Chemistry Department, Ramnarain Ruia College 2012
- Sixth place, Indian Chemical Society Aptitude test 2010
- Best presentation, Inter-collegiate seminar competition, Mumbai University 2008
- First place, Inter-collegiate chemistry Olympiad, Mumbai University 2008
- Scholarship holder, Dr. A. P. Rao Foundation, Mumbai University 2007,2008

### **SERVICE**

- Virginia Junior's Academy of Sciences (VJAS) judge for 2018 VJAS research symposium 2018
- American Chemical Society Alpha-Chapter MEDI GSA Treasurer 2015 - 2016
- Ad-hoc reviewer for a manuscript submitted to the Journal of Molecular Graphics and Modeling 2015
- Organized and encouraged members of the MEDC GSA to attend health awareness walks (Juvenile Diabetes Research Foundation walk 10/2017, National Alliance on Mental Illness walk 10/2016, American Heart Association's Heart walk 10/2015, Walk to end Alzheimer's 10/2014) 2014-2017
- Invited by National Children's Science Congress to judge projects at Podar International School, New Horizon Scholar's School and Bhartiya Vidyapeeth High School, Mumbai 2011
- Department of Chemistry GSA IT-team, Ramnarain Ruia College 2008 - 2011
- Department of Life Sciences GSA Treasurer, Ramnarain Ruia College 2008

### **PROFESSIONAL DEVELOPMENT**

- Industrial training, Geochem Laboratories, Mumbai 2009
- Certificate course in Bio-analytical chemistry, Mumbai 2008
- Spectroscopy workshop, Ramnarain Ruia College, Mumbai 2008

### **PROFESSIONAL SOCIETIES AND AFFILIATIONS**

- American Chemical Society
- Virginia Academy of Sciences
- ACS Alpha-Chapter MEDI GSA
- Rho Chi Academic Honor Society in Pharmacy