Transforming data into knowledge for intelligent decision-making in early drug discovery

Paricharak, S.A.

List of Publications

Paricharak, S., Méndez-Lucio, O., Ravindranath, A. C., Bender, A., IJzerman, A. P., and Van Westen, G. J. P. Data-driven approaches used for compound library design, hit triage, and bioactivity modeling in high-throughput screening. *Submitted*

Paricharak, S., IJzerman, A. P., Jenkins, J. L., Bender, A., and Nigsch, F. (2016) Data-driven derivation of an "informer compound set" for improved selection of active compounds in high-throughput screening. *J. Chem. Inf. Model. DOI: 10.1021/acs.jcim.6b00244*.

Paricharak, S., IJzerman, A. P., Bender, A., and Nigsch, F. (2016) Analysis of iterative screening with stepwise compound selection based on Novartis in-house HTS data. *ACS Chem. Biol. 11*, 1255–1264.

Mohan, C. D., Srinivasa, V., Rangappa, S., Mervin, L., Mohan, S., Paricharak, S., Baday, S., Li, F., Shanmugam, M. K., Chinnathambi, A., Zayed, M. E., Alharbi, S. A., Bender, A., Sethi, G., Basappa, and Rangappa, K. S. (2016) Trisubstituted-imidazoles induce apoptosis in human breast cancer cells by targeting the oncogenic PI3K/Akt/mTOR signaling pathway. *PLoS One 11*, e0153155.

Kumar, K. H., Paricharak, S., Mohan, C. D., Bharathkumar, H., Nagabhushana, G. P., Rajashekar, D. K., Chandrappa, G. T., Bender, A., Basappa, and Rangappa, K. S. (2016) Nano-MoO3-mediated synthesis of bioactive thiazolidin-4-ones acting as anti-bacterial agents and their mode-of-action analysis using in silico target prediction, docking and similarity searching. *New J. Chem. 40*, 2189–2199.

Anusha, S., CP, B., Mohan, C. D., Mathai, J., Rangappa, S., Mohan, S., Chandra, Paricharak, S., Mervin, L., Fuchs, J. E., M, M., Bender, A., Basappa, and Rangappa, K. S. (2015) A nano-MgO and ionic liquid-catalyzed "green" synthesis protocol for the development of adamantyl-imidazolo-thiadiazoles as anti-tuberculosis agents targeting sterol 14α-demethylase (CYP51). *PLoS One 10*, e0139798.

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Neelgundmath, M., Dinesh, K. R., Mohan, C. D., Li, F., Dai, X., Siveen, K. S., Paricharak, S., Mason, D. J., Fuchs, J. E., Sethi, G., Bender, A., Rangappa, K. S., Kotresh, O., and Basappa. (2015) Novel synthetic coumarins that target NF-κB in hepatocellular carcinoma. *Bioorg. Med. Chem. Lett. 25*, 893–897.

Bharathkumar, H., Paricharak, S., Dinesh, K. R., Siveen, K. S., Fuchs, J. E., Rangappa, S., Mohan, C. D., Mohandas, N., Kumar, A. P., Sethi, G., Bender, A., Basappa, and Rangappa, K. S. (2014) Synthesis, biological evaluation and in silico and in vitro mode-of-action analysis of novel dihydropyrimidones targeting PPAR-γ. *R. Soc. Chem. Adv. 4*, 45143–45146.

Bharathkumar, H., Sundaram, M. S., Jagadish, S., Paricharak, S., Hemshekhar, M., Mason, D., Kemparaju, K., Girish, K. S., Basappa, Bender, A., and Rangappa, K. S. (2014) Novel benzoxazine-based aglycones block glucose uptake in vivo by inhibiting glycosidases. *PLoS One 9*, e102759.

Koutsoukas, A., Paricharak, S., Galloway, W. R. J. D., Spring, D. R., IJzerman, A. P., Glen, R. C., Marcus, D., and Bender, A. (2014) How diverse are diversity assessment methods? A comparative analysis and benchmarking of molecular descriptor space. *J. Chem. Inf. Model. 54*, 230–242.

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Curriculum Vitae

Shardul Paricharak was born in Willemstad, Curaçao, on 21st of July 1989. He went to high school at Radulphus College and graduated as the best VWO (highest level) student of Curaçao in 2007. He then moved to the Netherlands to pursue his undergraduate study Life Science & Technology at TU Delft and Leiden University, which he graduated *cum laude*. During this study, he spent one semester at Lund University (Sweden) to study bioinformatics and passed all courses with distinction. This exchange program sparked his interests in the computational side of biology and led him to pursue his undergraduate research internship at the Division of Medical Pharmacology at Leiden University, where he analyzed glucocorticoid signaling pathways in the brain using bioinformatics tools. He then gained some industrial experience during a summer job at Galapagos B.V. (The Netherlands), where he worked on developing proprietary software to design siRNA. Following this, he performed two graduate research internships in bioinformatics and cheminformatics at Utrecht University (The Netherlands) and the University of Cambridge (UK), respectively, where he worked on personalized genomics data analysis and kinase bioactivity modeling. He received the Fundatie van Renswoude grant and the Huygens Scholarship for academic excellence for his work at the University of Cambridge.

In 2012, Shardul obtained his master's degree in pharmaceutical sciences from Utrecht University, with a GPA score of 4.0. In the same year, he obtained an NWO Mosaic personal grant for a PhD at Leiden University and the University of Cambridge, during which he worked on cheminformatics data analyses and machine learning. He obtained Dr Hendrik Muller's Vaderlandsch Fonds scholarship and the Prins Bernhard Cultuurfonds Pieter Beijer scholarship in support of his PhD and fellowship at King's College (Cambridge) as an affiliate member, respectively. He gained some further industrial experience at Novartis in Switzerland, where he worked on applying computational methods to improve the efficiency of high-throughput screens. Shardul has presented his research at the 13th LCDS meeting: combining data science and drug discovery (Leiden, The Netherlands), the Big data in medicine conference (Cambridge, UK), the Cambridge Cheminformatics Meeting (Cambridge, UK), the Scandinavian Symposium on Chemometrics (Chia, Italy), the Towards New Therapeutics for Diseases of the Developing World conference, (Tres Cantos, Spain), and the 8th German Conference on Chemoinformatics (Goslar, Germany).

Acknowledgements

I feel incredibly fortunate to have had the opportunity to conduct research at three institutions across three countries during my PhD, collaborating with world-class scientists in both academia and the pharmaceutical industry. I would like to thank the Netherlands Organisation for Scientific Research (NWO), the Prins Bernhard cultuurfonds and Novartis for financial support. My supervisors Ad IJzerman, Andreas Bender and Florian Nigsch are thanked for invaluable scientific contributions, helpful advice and mentoring during my PhD.

My colleagues at the University of Cambridge, Leiden University and Novartis are thanked for insightful discussions, pleasant shared experiences, continuous support and friendship. In particular, I would like to thank Aakash Chavan Ravindranath, Oscar Méndez-Lucio, Richard Lewis, Alexios Koutsoukas, Basappa, Isidro Cortés-Ciriano and Gerard van Westen for fruitful collaborations. My students Richard Lewis, Oana Diaconescu and Chi Chung Lam are thanked for providing me the opportunity to develop my leadership skills.

From the personal side, I would like to thank my parents, Seema Paricharak and Atul Paricharak, and my brother Nakul Paricharak for unconditional support throughout my PhD, during both ups and downs. Finally, I would also like to thank my parents for striving hard to provide me the opportunity of pursuing academic education, which I value immensely and believe will tremendously benefit me in my future endeavors.