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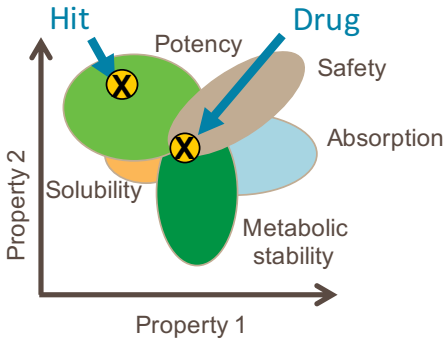
Dr. Pillai is one of the coordinator for Drug Discovery Hackathon 2020, Director and Founder of Zastra Innovations, Bengaluru, visiting Scientist at Nyro Research India and formerly a Marie Curie Research Fellow at Molcode Ltd., Estonia. He carried out his PhD at University of Florida with Prof. Katritzky and Prof. Karelson, University of Tartu. He holds 40 research papers in peer reviewed international journals, 1 US patent and co-authored a book chapter on mosquito repellents. His expertise are in the area of computational medicinal chemistry, mechanistic driven drug discovery and molecular modelling. Currently he has a PhD student working under him in the area of ageing and biomarkers. Apart from scientific positions he is reviewer to ACS, Wiley and Elseiver journals also a mentor at IIIT Kottayam, Govt of India's Niti Ayog ATL schools and research advisor to few academia.

Application of Machine Learning in Drug Discovery for Drug Candidate Selection

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Abstract

Computer aided design plays an important role in the phase of drug discovery and has considerably improved in the last decade with candidate selection and decision-making process. A successful, efficacious and safe drug must achieve a balance of many properties, including potency and appropriate physicochemical, absorption, distribution, metabolism, excretion and toxicity (ADMET) properties. Exploring the latest developments in methods that guide compound selection, which help to quickly target compounds with the best balance of properties for a drug discovery is objective. Predictive modelling of ADMET properties and how these models can be used to guide the design of improved compounds are trivial. Understanding of 3-dimensional (3D) structure-based design information can be linked with 2D SAR analysis is vital to meet the requirements of a drug, such as: (i) bind to biological target *invivo* (ii) pass through cell membrane or blood-brain barrier (iii) remain long enough to be effective (iv) eliminate from the body by metabolism, excretion, or other means. Use innovative, new methods to explore your complex data to find interpretable, multi-parameter scoring profiles, tailored to identify compounds for your drug discovery objective. The resulting scoring profiles will help you to quickly target compounds with a higher chance of success.



Reference

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