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SYNSPACE: A DESIGN PLATFORM TO EXPAND SYNTHETICALLY-ENABLED SCAFFOLD AND LEAD ANALOGUE SPACE FOR MEDICINAL CHEMISTRY AND AI-ASSISTED DRUG DISCOVERY

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Despite significant advances in our understanding of the biological basis of diseases, pharmaceutical R&D is struggling to sustain the level of productivity and efficiency it reached in the second half of the 20th century. High failure rates and the increasing cost of drug discovery as well as extended research and development timelines hinder the development of medicines. Due to these challenges there has been an increasing need for substantial innovations in the pharmaceutical sector. It has been shown that if the selection of the synthetic targets in lead optimization cycles is supported by QSAR or deep learning methods, the number of compounds synthesized as well as the cycle time for each iteration can be significantly reduced. We have developed a rule-based artificial intelligence technology that can produce a large number of novel and synthetically-enabled lead analogues and scaffold hopping designs around lead structures. Since its introduction, the cloud-based SynSpace software has been found by multiple organizations to generate a larger number of relevant novel ideas around leads than medicinal chemist teams can do. Thus, SynSpace is a valuable addition to the medicinal chemistry toolbox. We have also been developing automated lead analysis tools that-in conjunction with SynSpace-can automatically carries out scaffold hopping and lead analogue idea generation and thereby offer large sets of novel and project specific lead-like structures to advanced AI platforms for selection. These platforms have the biggest impact on a number of key parameters in drug discovery: cycle time, number of discovery cycles, the number of compounds to be synthesized and coverage of IP space. Improvements in these factors can be converted into higher success rates and major resource savings towards a more economical and productive candidate development phase.

Biography

Gergely Makara has completed his PhD in medicinal chemistry at SUNY at Buffalo in 1996 and his postdoctoral studies in medicinal chemistry and molecular modelling with Garland Marshall at the Center for Molecular Design at Washington University at St. Louis in 1998. Since then he has spent 20 years in the pharmaceutical industry, most of it in leadership levels at Neogenesis Pharmaceuticals (Boston, USA), Merck & Co. (Rahway, USA), AMRI Hungary (Hungary), ComInnex (Hungary) and ChemPass (Hungary). His expertise includes organic synthesis, medicinal chemistry, fragment-based drug discovery, drug design, and cheminformatics. He has published more than 30 papers in reputed journals and has contributed to 10 patent applications.

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