Advanced Pharmacophores for Accurate Virtual Screening and Compound Profiling

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Summary
Prof. Langer will showcase the results of a recent research project using pharmacophore-based in silico fragment screening for the discovery of novel attractive starting points for a medicinal chemistry hit to lead optimization program.

Abstract
Pharmacophore-based virtual screening and activity profiling has become one of the most popular in silico techniques for supporting medicinal chemists in their hit finding, hit expansion, hit to lead, and lead optimization programs.¹

In his presentation, Prof. Langer will showcase recent results obtained when combining fragment-based in silico screening with traditional medicinal chemistry. Using structure-based pharmacophore models generated with the LigandScout² technology developed by Inte:Ligand GmbH³, a customized fragment library was screened. Fragment hits were combined and molecules obtained were prioritized according i) to best fitting the interactions in the binding site, ii) chemical tractability, and iii) novelty. Within a time period of 3 months, starting from scratch, novel compounds were obtained exhibiting low micromolar affinity to the target protein, followed by hit to lead expansion and lead optimization.

References