# Advanced Pharmacophores for Accurate Virtual Screening and Compound Profiling

Thierry Langer

University of Vienna, Department of Pharmaceutical Chemistry, Althanstrasse 14, 1090 Vienna, Austria

Prestwick Chemical SAS, 220 Blvd Gonthierd'Andernach, 67400 Strasbourg-Illkirch, France

## 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 LigandScout[2]technology developed by Inte:Ligand GmbH[3], 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

1. Langer T, Pharmacophores in Drug Research, Mol. Inf., 29, 470-475 (2010)
2.Wolber G, Langer T, LigandScout: 3D Pharmacophores Derived from Protein-Bound Ligands and their Use as Virtual Screening Filters, J. Chem. Inf. Model. 45, 160-169 (2005)
3. Inte:Ligand GmbH, Austria. http://www.inteligand.com