

# 3D Pharmacophore Perception and Screening Algorithms: Challenges and Pitfalls

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3D pharmacophores have become an established and consolidated method for in-silico drug discovery – mainly due to their ability to reflect the way of thinking of medicinal chemists in terms of hit identification, hit expansion and lead optimization. The simplicity and descriptive character of such a 3D pharmacophore model thus enables clear communication and rapid feedback cycles between modeling and synthesis teams. Despite the broad usage of the methodology, there are still several pitfalls and challenges for successful pharmacophore modeling – mainly related to the algorithmic challenge of flexibly fitting a molecule to a 3D pharmacophore model in a computationally efficient way. In this talk, several structure- and ligand-based 3D pharmacophore application studies will be presented and critically discussed in the context of virtual screening algorithms and overlay algorithms.