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3D pharmacophore alignments: does improved geometric accuracy affect virtual screening performance?

Gerhard Wolber[1*], T Seidel[2], F Bendix[2]

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Virtual screening using three-dimensional arrangements of chemical features (3D pharmacophores) has become an important method in computer-aided drug design. Although frequently used, considerable differences exist in the interpretation of these chemical features and their corresponding 3D overlay algorithms. We have recently developed an efficient and accurate 3D alignment algorithm based on a pattern recognition technique [1]. In the presented work, we extend this algorithm to be used for high-performance virtual database screening and investigate, whether applying this geometrically more accurate 3D alignment algorithm improves virtual screening results over conventional incremental n-point distance matching approaches.

Author details
[1]University of Innsbruck, Institute of Pharmacy, Dept. Pharmaceutical Chemistry, Innrain 52, 6020 Innsbruck, Austria. [2]Inte:Ligand GmbH, Mariahilferstrasse 74B/11, A-1070 Vienna, Austria.

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* Correspondence: gerhard.wolber@uibk.ac.at
[1]University of Innsbruck, Institute of Pharmacy, Dept. Pharmaceutical Chemistry, Innrain 52, 6020 Innsbruck, Austria