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POSTER PRESENTATION

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Brute-force pharmacophore assessment and scoring with Open3DQSAR

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During the last year we have developed Open3DQSAR, an open-source tool aimed at high-throughput 3D-QSAR model building and evaluation [1]. During development, high performance and ease of automation were defined as primary goals; the first was achieved by implementation of parallelized algorithms and the second by adopting a scriptable interface.

Molecular interaction fields of different kinds (namely, built-inMMFF94 or GAFF steric/electrostatic fields, GRID fields and QM electron density/ESP maps) can be seamlessly computed and combined in a 3D-QSAR model from within Open3DQSAR thanks to its interoperability with OpenBabel, Molecular Discovery GRID and most QM packages.

In the poster, we describe the recent integration in Open3DQSAR of existing open-source tools to

perform conformational analysis and molecular alignment, in order to automatically generate an exhaustive pool of pharmacophore hypotheses for a given dataset. Subsequently, such hypotheses are scored according to their ability to yield a predictive and robust 3D-QSAR model (Figure 1). We applied our brute-force pharmacophore assessment methodology on the benchmark datasets gathered by Sutherland et al. [2], to investigate whether the traditional alignment bottleneck in 3D-QSAR can be turned into a powerful instrument to challenge the goodness of a pharmacophore guess.

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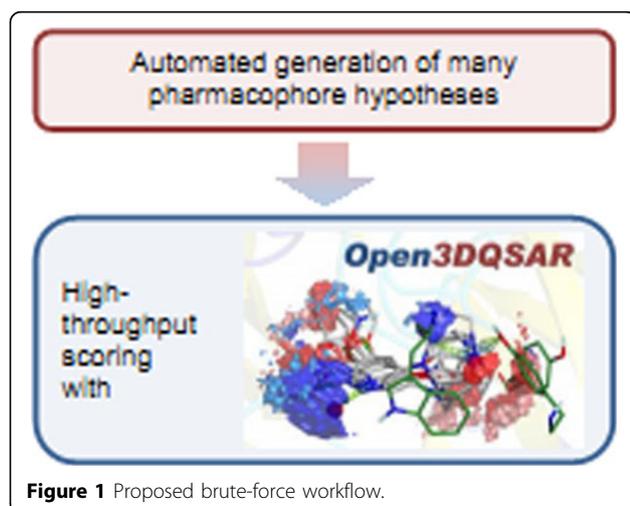


Figure 1 Proposed brute-force workflow.

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