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Efficient 3D pharmacophore alignment as a tool for structure-based modeling and scoring

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Chemical-feature based pharmacophore models have been established as state-of-the-art technique for bio-activity prediction. While in ligand-based drug design, chemical feature-based pharmacophore creation from a set of bio-active molecules is a frequently chosen approach, structure-based pharmacophores are still lacking the reputation to be an alternative or at least a supplement to docking techniques. Nevertheless, 3D pharmacophore screening bears the advantage of being much more efficient than unattended high-throughput docking and to transparently provide the user with all the information that is used by the screening algorithms to characterize the ligand-macromolecule interaction.

Our efficient, rigid 3D pharmacophore superpositioning technique [1] will be applied to a number of structure-based pharmacophores selected from a diverse set of targets. Molecule coordinates generated from geometric fitting of multi-conformational models of small organic molecules to structure-based pharmacophores are compared to docking poses and discussed in terms of scoring, conformational coverage, and eligibility for virtual screening.

References

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