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Development of a new methods for virtual screening protocol

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Virtual screening (VS) is a very popular technique of selection of compounds with desired properties from, generally, large commercially/synthetically accessible chemical databases. Currently, a large variety of algorithms and software aiming at facilitating and automating the VS are available. However, due to increasing of computational power, the development of new VS tools is still required [1].

Herein we present the new algorithms and tools developed for VS, i.e. an approach for evaluation of docking results based on hybrid interaction fingerprint and machine learning methods and software for automatic generation of linear combination of pharmacophore models [2].

References

[1] Reddy AS, Pati SP, Kumar PP, Pradeep HN, Sastry GN, *Curr Protein Pept Sci.* 8(4) 2007, 329-51.
[2] Kurczab, R, Bojarski AJ, *J. Chem. Inf. Model*., 53 (2013), 3233–3243.