An application of chem- and bioinformatic methods in modern drug design process

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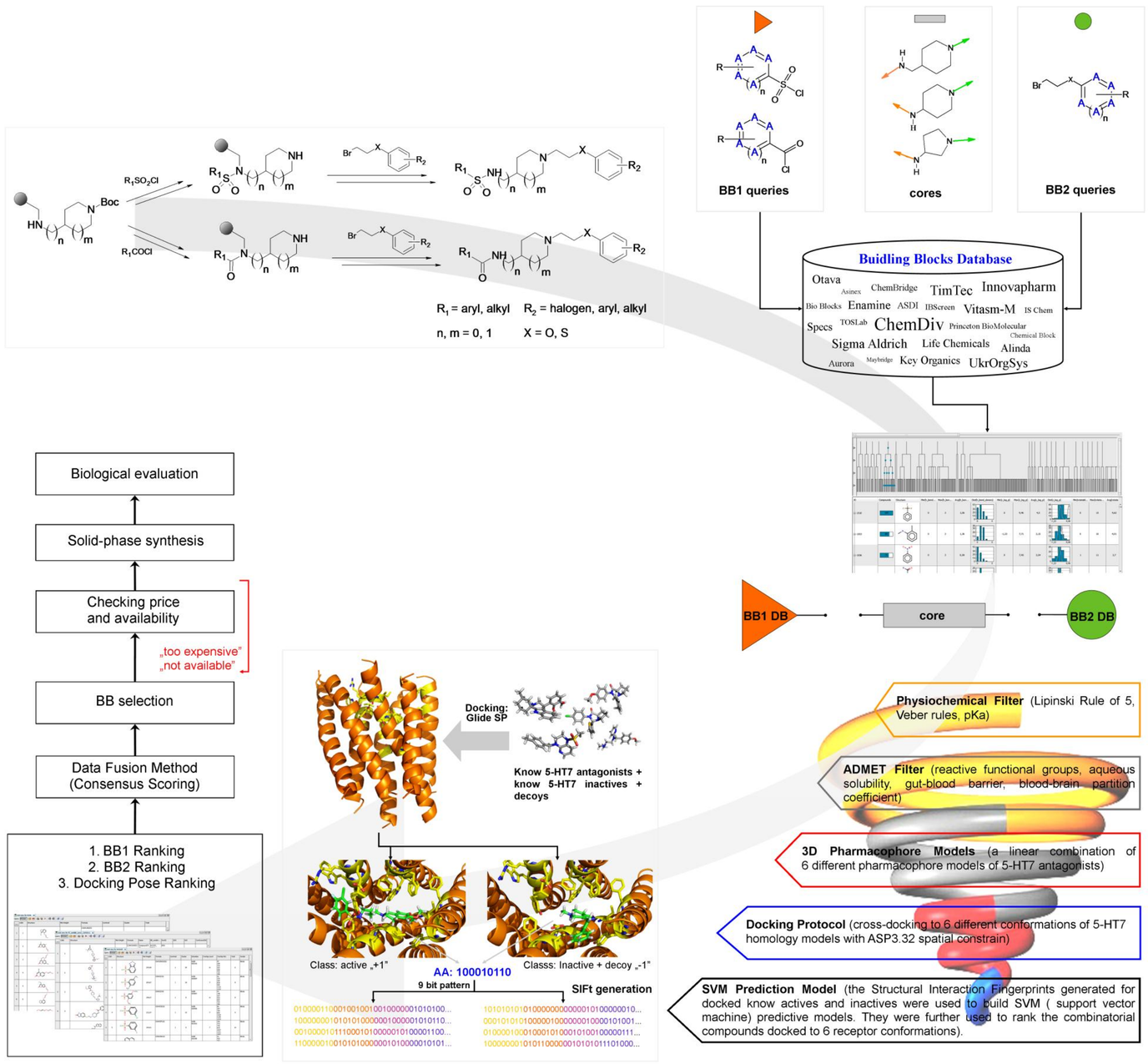
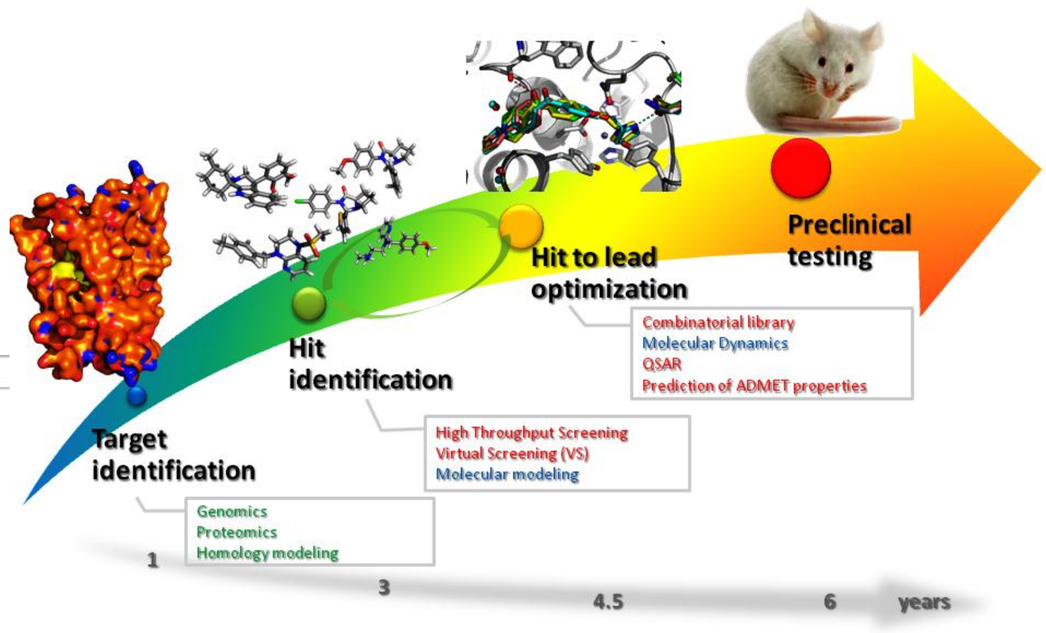
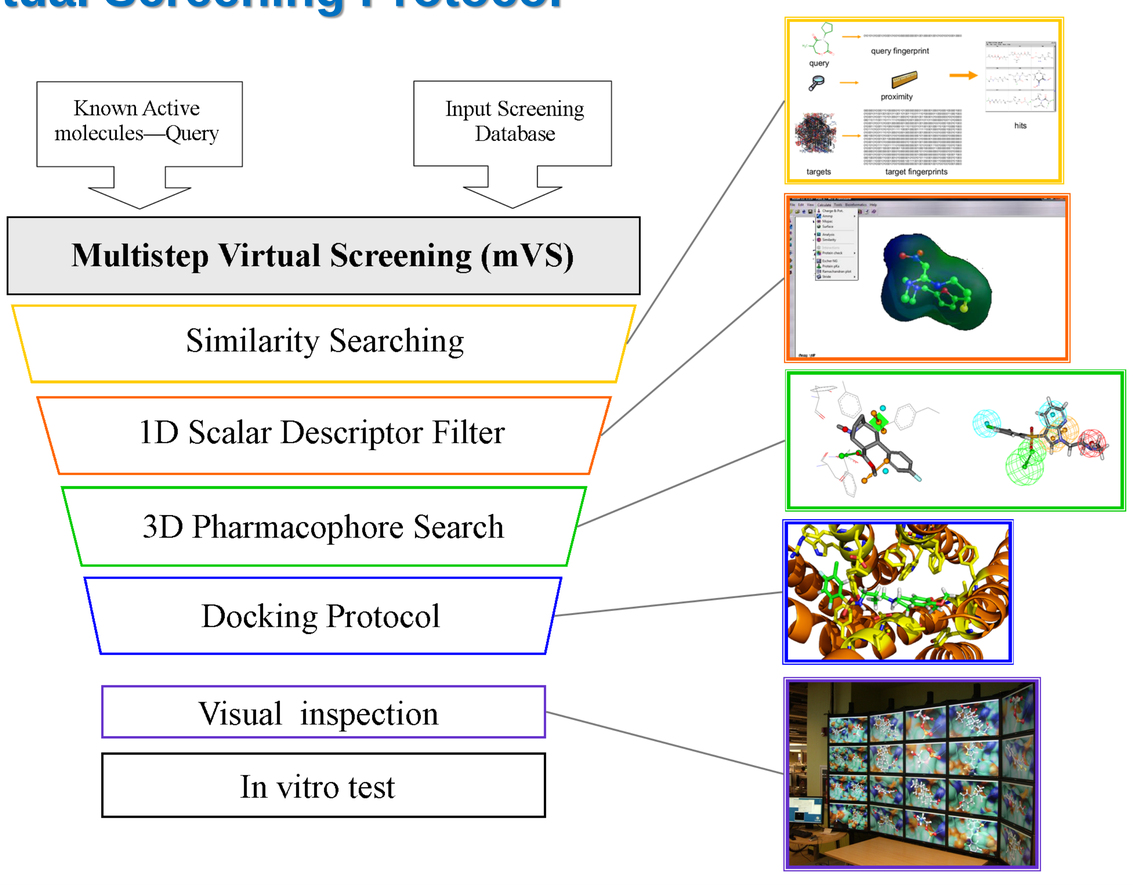
Virtual Combinatorial Library Protocol[1]

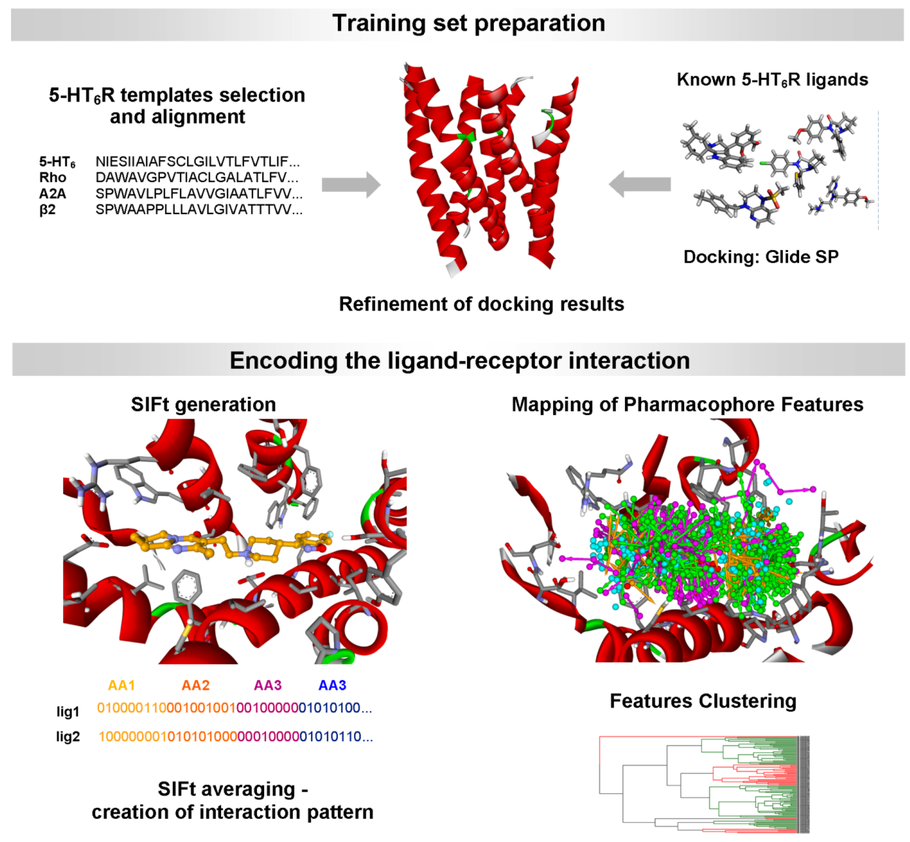




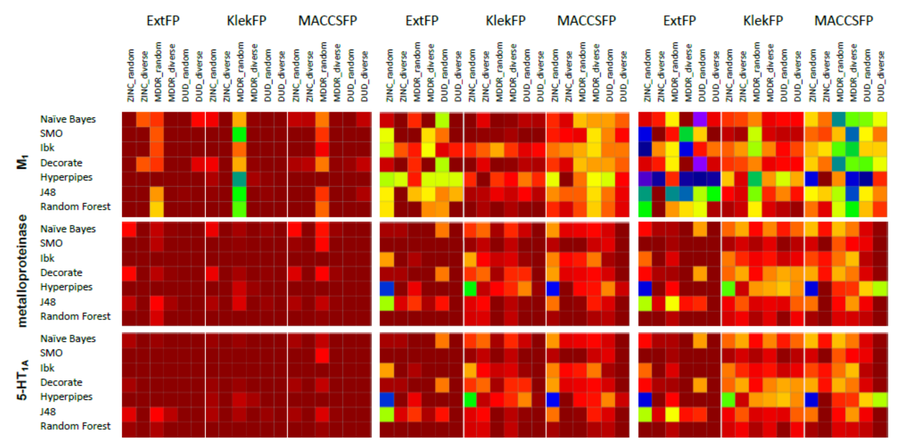
Virtual Screening Protocol[2]



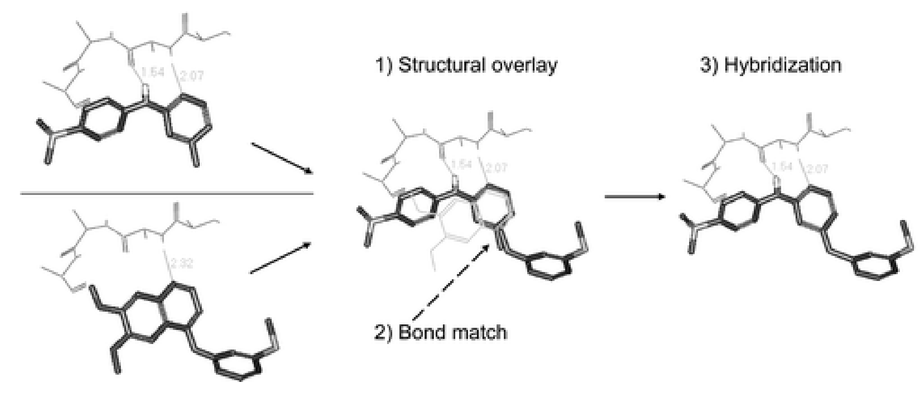
Receptor-based pharmacophore query definition[3]



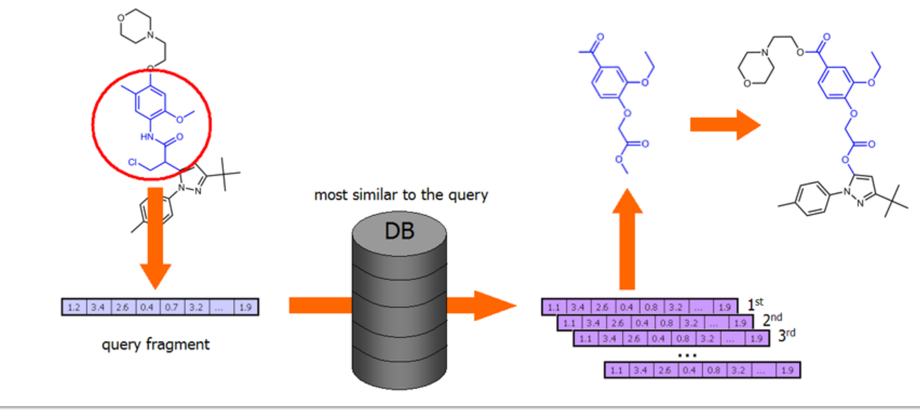
Machine Learning[4]



Hybridization of known ligands



Scaffold-hopping



References

[1] Zajdel P., Kurczab R., Grychowska K., Satała G., Bojarski A. J., 2012, *Eur. J. Med. Chem.,* 56: 348-360,

[2] Kurczab R., Nowak M., Chilmonczyk Z., Sylte I., Bojarski A. J., 2010, *Bioorg. & Med. Chem. Lett.*, 20: 2465-2468,

[3] Kurczab R., Bojarski A. J., The new strategy in receptor-based pharmacophore query definition and its application to 5-HT$_7$R, manuscript in preparation,

[4] Smusz S., Kurczab R., Bojarski A. J., The influence of the inactives subset generation on the performance of machine learning methods *J. Cheminformactics*, in revision.