

# Development and application of virtual screening protocol as a tool to support the process of finding new drugs

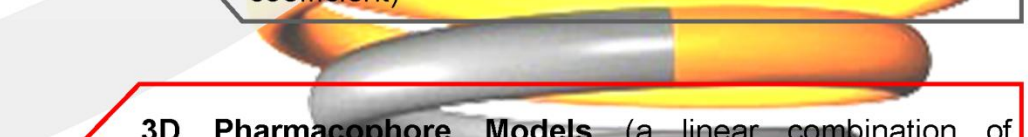
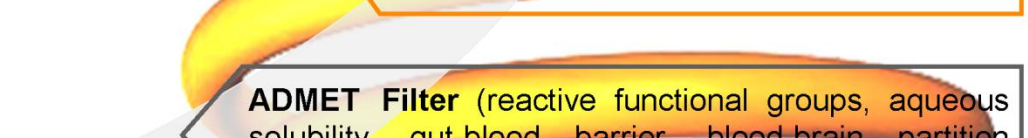
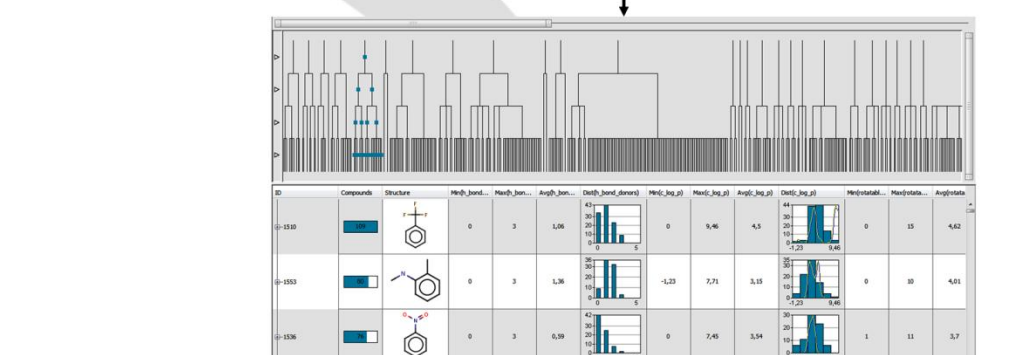
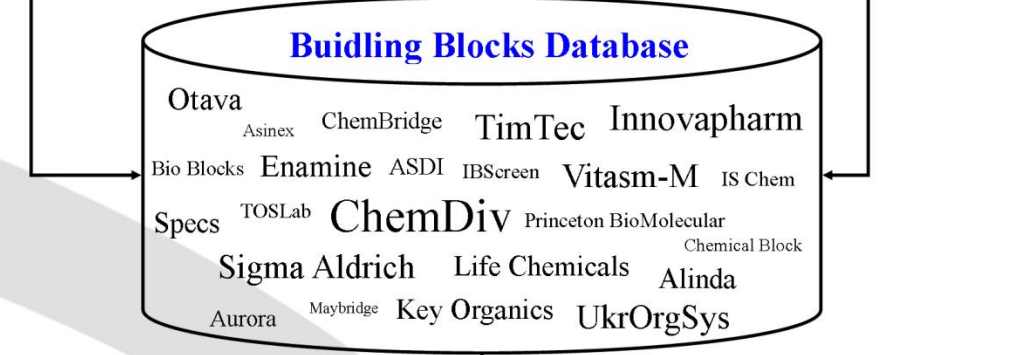
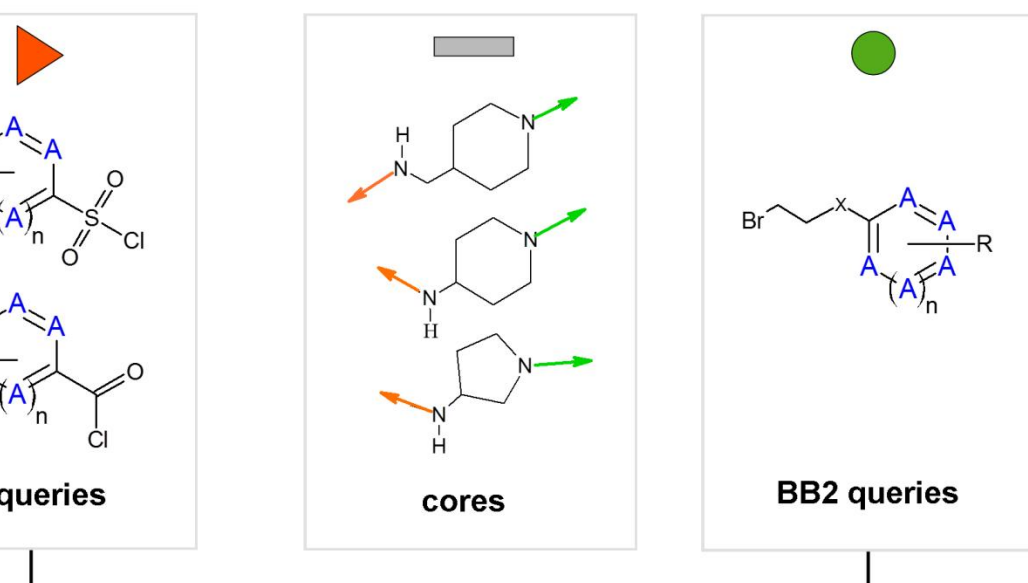
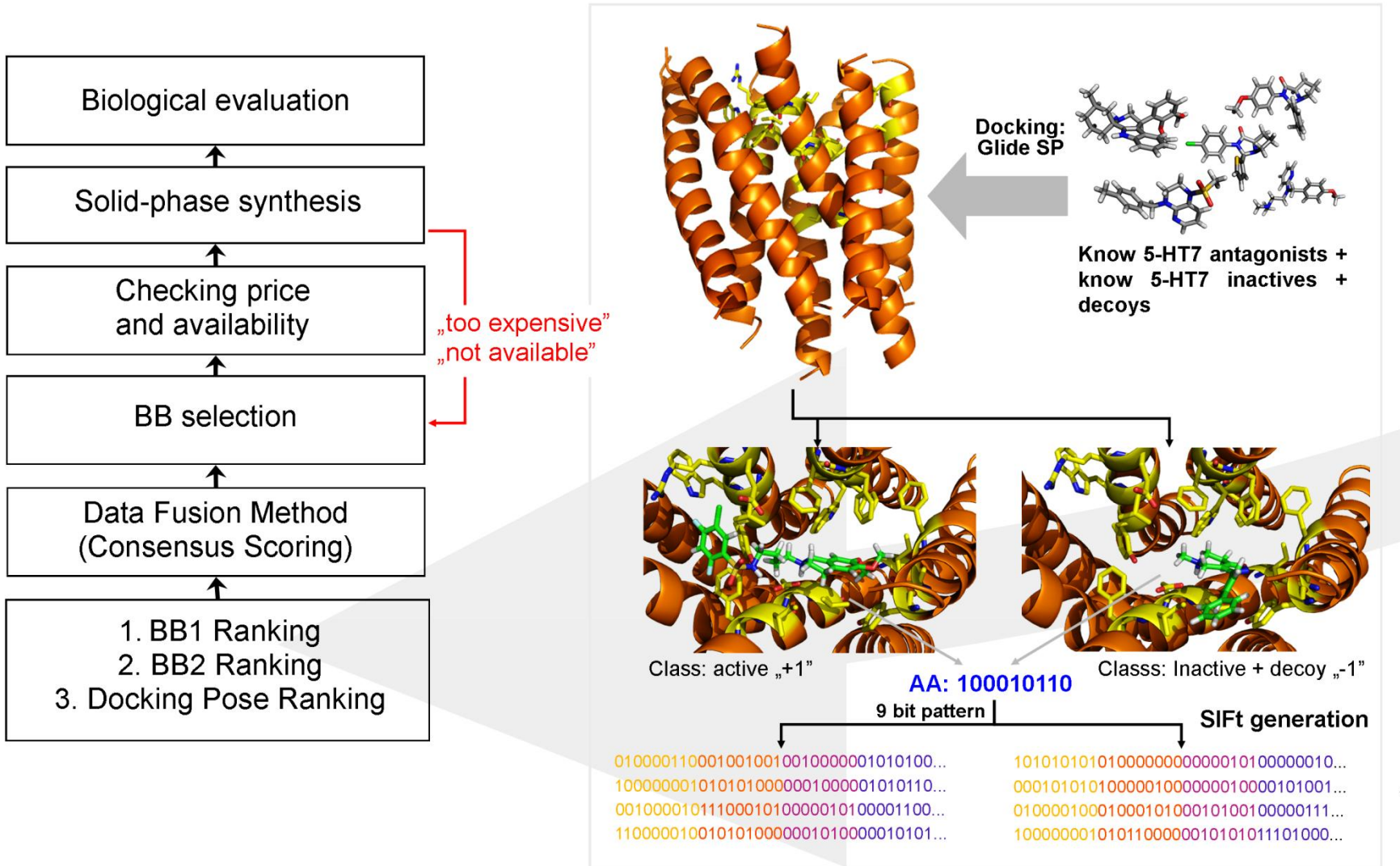
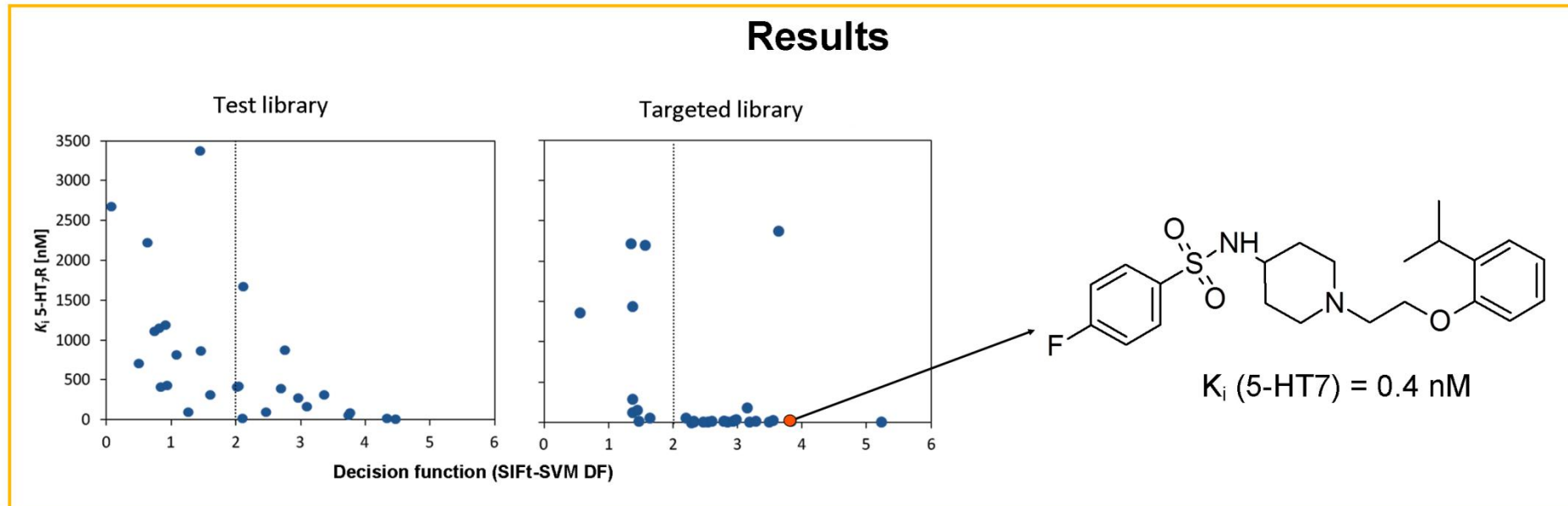
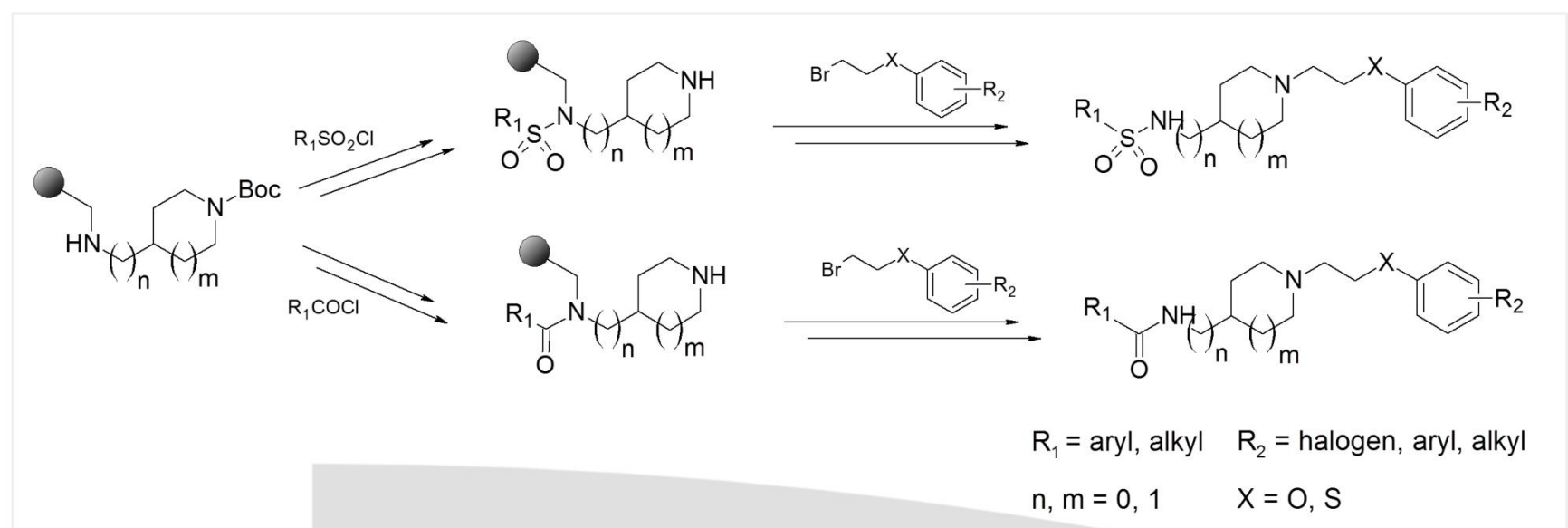


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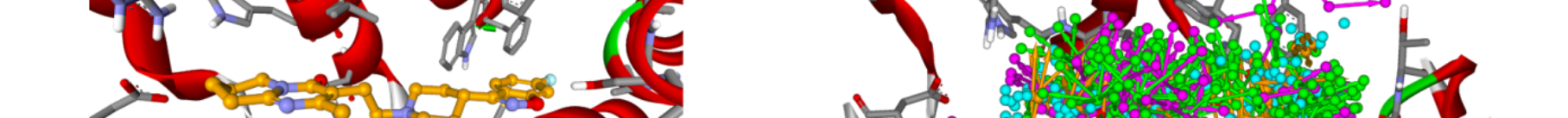
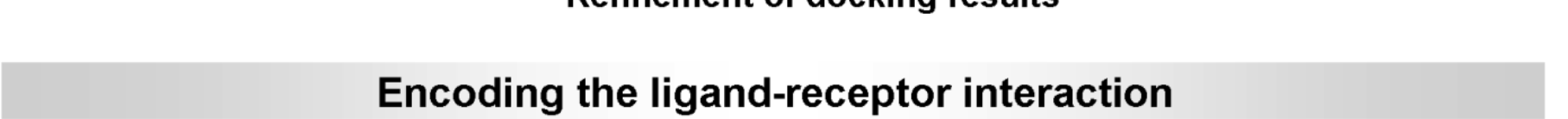
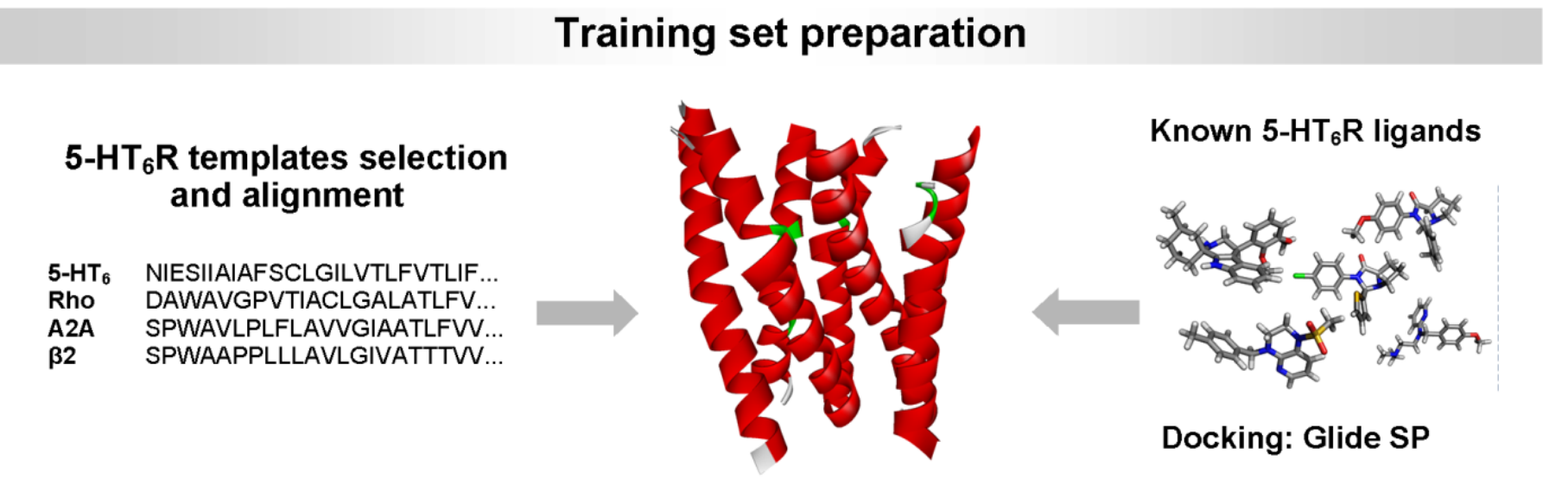


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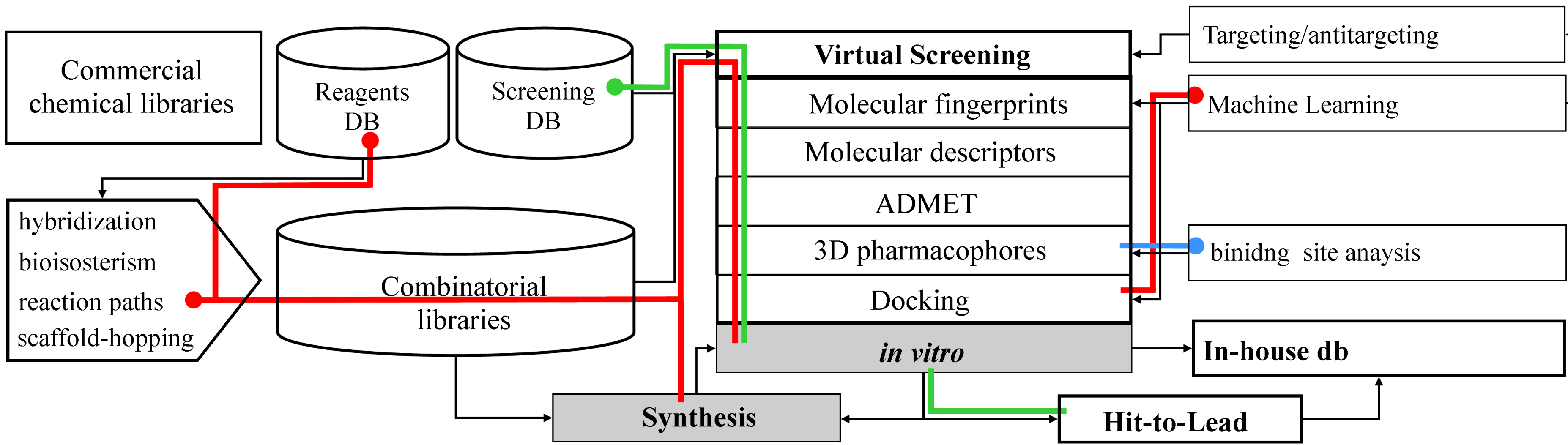
## Virtual Combinatorial Library Protocol<sup>1</sup>



## Receptor-based pharmacophore query definition<sup>3</sup>



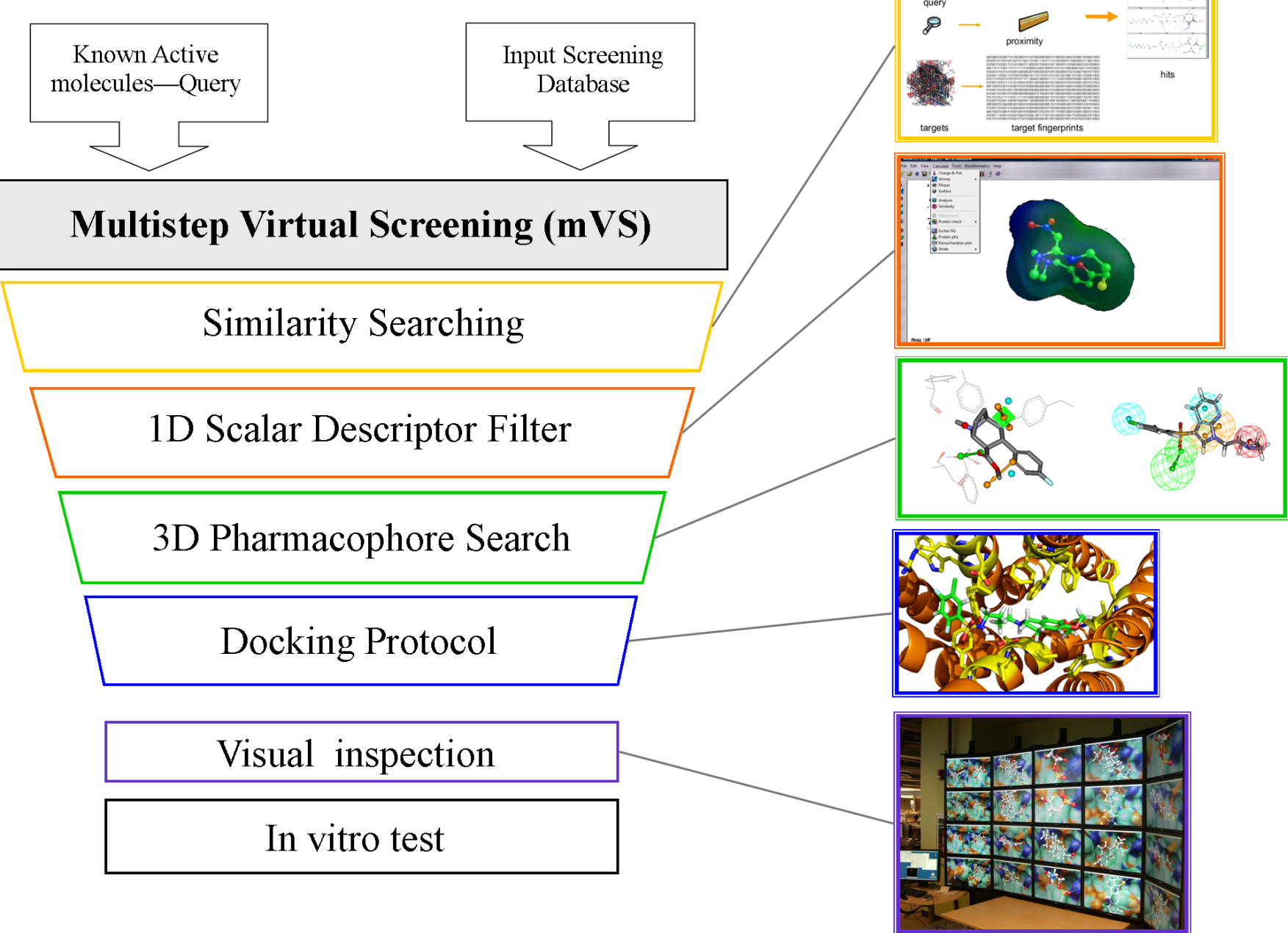
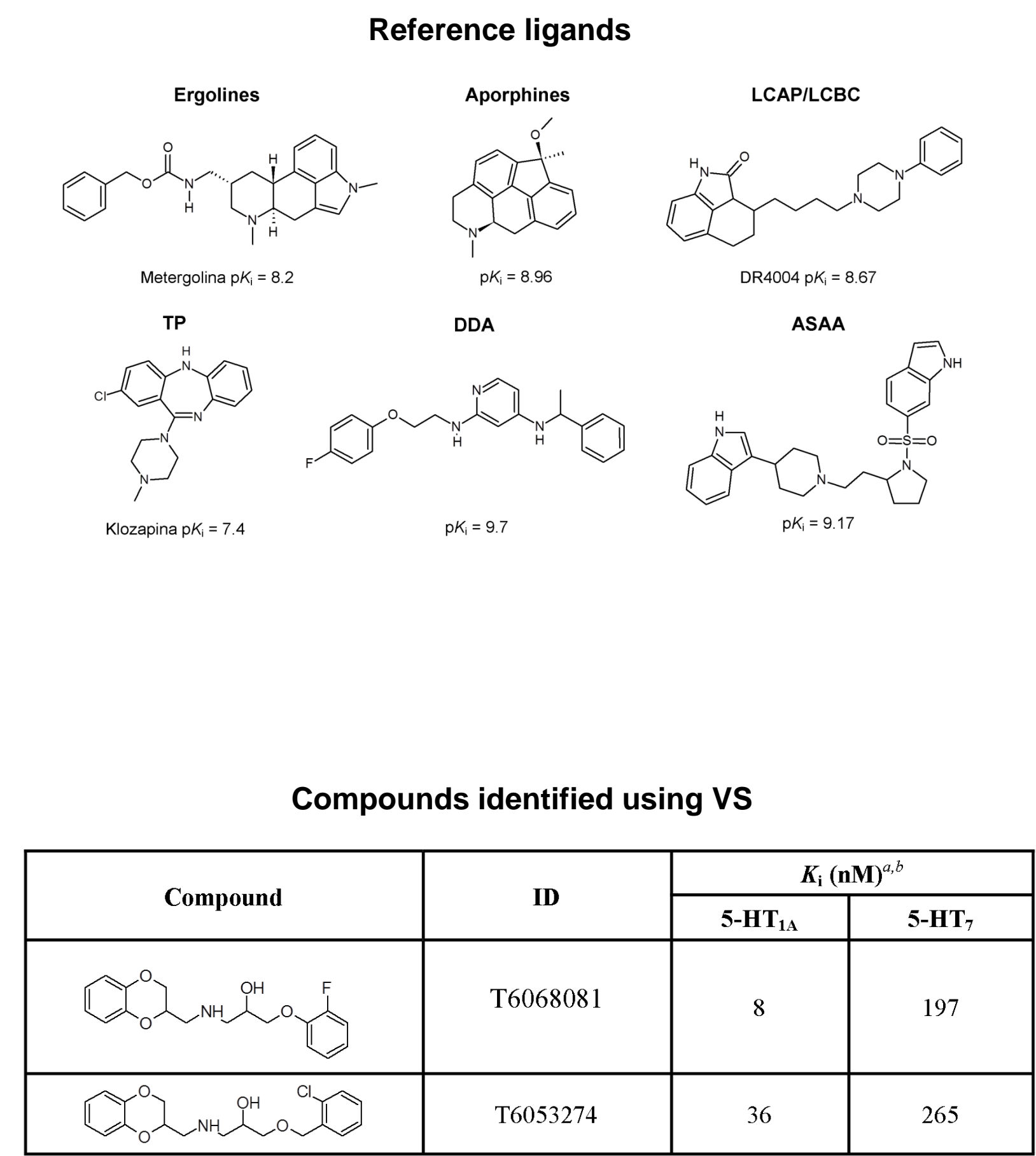
## Computer Aided-Drug Design Workflow



Presented research might be especially helpful for those who is aimed on developing a new material with desired properties (agricultural, material engineering, etc.).

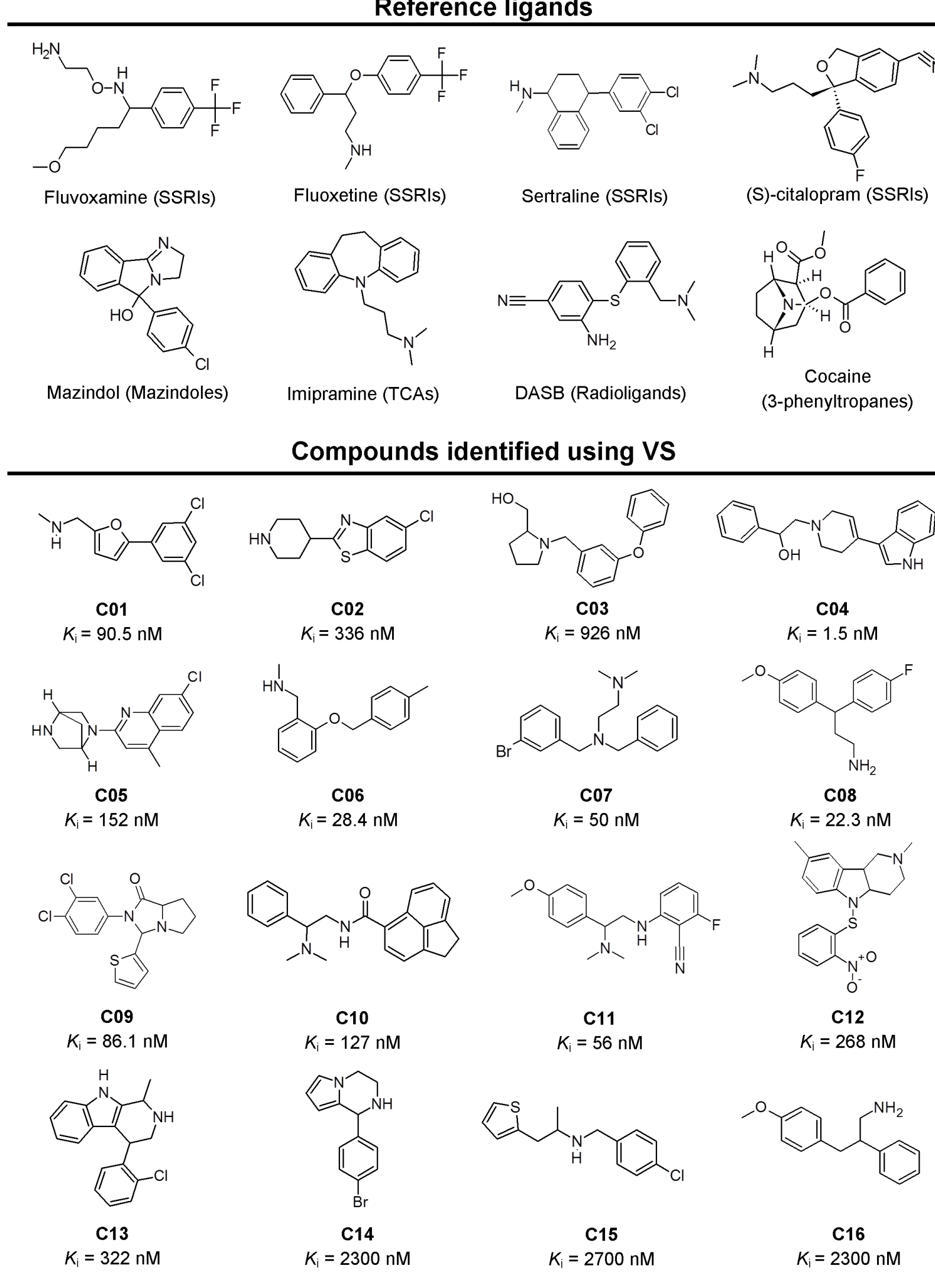
## Virtual Screening (VS) Protocol

### VS of 5-HT<sub>7</sub>R<sup>3</sup>



8% Hit rate 11.4%

### VS of SERT<sup>4</sup>



## References

[1] Zajdel P., Kurczab R., Grychowska K., Satala G., Bojarski A. J., 2012, *Eur. J. Med. Chem.*, 56: 348-360,  
[2] Kurczab R., Bojarski A. J., The new strategy in receptor-based pharmacophore query definition and its application to 5-HT<sub>7</sub>R, *J. Chem. Inf. Model.* 2013, 18, 3233-3243  
[3] Kurczab R., Nowak M., Chilmonczyk Z., Sylte I., Bojarski A. J., 2010, *Bioorg. & Med. Chem. Lett.*, 20: 2465-2468,  
[4] Gabrielsen M., Kurczab R., Siwek A., Wolak M., Ravna A., Kristiansen K., Kufareva I., Abagyan R., Nowak G., Chilmonczyk Z., Sylte I., Bojarski A. J., Identification of Novel Serotonin Transporter Compounds by Virtual Screening, *J. Chem. Inf. Model.*, 2014, 54, 933-943.