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In silico and in vitro screening platform in search of new psychotropic agents

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It is almost two years since the first application of our multi-step virtual screening protocol to identify potential serotonin 5-HT7R antagonists. [1] It was based on two-dimensional (2D) pharmacophore similarity, physicochemical scalar descriptors, an ADME/Tox filter, three-dimensional (3D) pharmacophore searches and a docking protocol. Since then, the screening protocol was considerably expanded and automated. Its current status and directions of further development is discussed. Some case studies of the protocol application to search for ligands of other biological targets, such as 5-HT6 receptor or serotonin transporter, is presented.

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[1] Kurczab R, Nowak M, Chilmonczyk Z, Sylte I, Bojarski AJ. The development and validation of a novel virtual screening cascade protocol to identify potential serotonin 5-HT(7)R antagonists. Bioorg Med Chem Lett. 2010, 20, 2465-8.