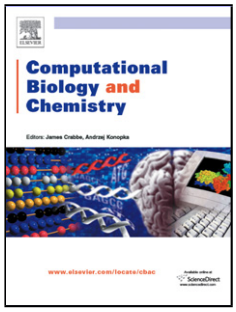

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Discovery of Natural Product Inhibitors of Phosphodiesterase 10A as Novel Therapeutic Drug for Schizophrenia Using a Multistep Virtual Screening

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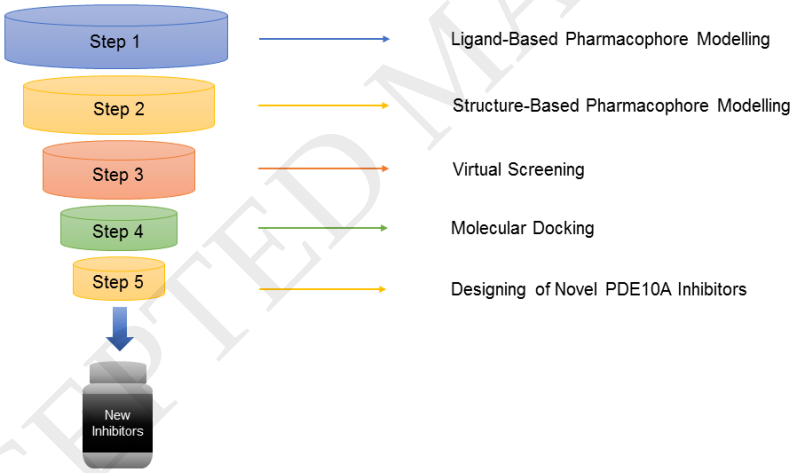
Graphical abstract

Multistep virtual screening protocol for discovering natural product inhibitors of PDE10A



Highlights

- Ligand and structure-based virtual screening of universal natural products database was performed.
- 3 of 37 compounds showed the highest affinity for phosphodiesterase 10A.
- UNPD216549 showed the lowest binding energy and has been chosen as starting point for designing of novel PDE10A inhibitors.

Abstract