Expanding the small-molecule GDB with focused libraries of ligands for glutamate receptors

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We have recently reported the so-called Generated Database (GDB) [1] consists of 26.4 millions small organic molecules up to 11 C, N, O, F atoms. This database is an abundant source of numerous synthetically feasible small-molecule ligands for various drug targets. Herein we report the further expanding of the GDB database with the generated focused-libraries of aspartic acid and glutamic acid's analogs targeting the human glutamate receptors. Advanced molecular modeling and cheminformatic methods were also implemented to predict the bioactivity and to analyze the structure-activity relationships among compounds in those focused libraries *in silico*. The hit-list from virtual screening of the generated focused libraries offers a set of drug-like new structures which are very interesting in term of synthesis.

[1]. T. Fink, J.L. Reymond, *J. Chem. Info. Model.* **2007**, *47*, 342; T. Fink, H. Bruggesser, J.L. Reymond, *Angew. Chem. Int. Ed.* **2005**, *44*, 1504