

**TOPBUILDER – MOLECULAR TOPOLOGY BUILDING
AND CHEMICAL DATABASE PROCESSING SOFTWARE**

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A useful extension for a popular docking and molecular dynamics software was developed and successfully integrated in database screening system. TOPBUILDER system controls integrated docking, quantum mechanics and MD simulation software to effectively predict activity of chemical substances in-silico.

TOPBUILDER algorithm uses semi-empirical calculation data obtained by GAMESS for explicit geometry optimization of the ligand and partial charge calculation. It allows generating molecular topology of each tested ligand using only structural data from the most popular molecular file formats. The topologies are optimally parameterized for individual characteristics of essential ligand and used as input for the MD simulation package GROMACS, flexible docking software DOCK and/or AutoDock.

The TOPBUILDER-based screening system successfully predicted CKII inhibitory activity of 4-aminoquinoline and 4-aminoquinazoline derivatives that was confirmed by in-vitro tests.