HMG-CoA Reductase Targeted Library from OTAVA

Screening compounds for **cholesterol metabolism research**

OTAVA offers you our **HMG-CoA Reductase Targeted Library** **(823 compounds in total)** that was designed with combined receptor-based and ligand-based approach. For receptor-based approach, crystal structure of HMG-CoA reductase (PDB ID: 2R4F) was used. Ligand-based approach employed training set of known HMG-CoA reductase inhibitors taken from ChEMBL database. The input compounds (Otava's Drug-like Green Collection) have been ranged by physicochemical parameters of known HMG-CoA reductase inhibitors and then screened independently using molecular docking, receptor based pharmacophore search and 3D-QSAR ligand-based models. Obtained molecular docking complexes were filtered based on docking score cut-off and inspection of intermolecular hydrophobic contacts/ hydrogen bonds with key active site's residues. As a result, two subsets of compounds were created: the first subset comprises compounds obtained with molecular docking and pharmacophore method, and the second subset represents compounds resulted from molecular docking and 3d-QSAR method. Both subsets were visually inspected to avoid ligands with incorrect binding mode.

The library comprises drug-like compounds only.

Find out more...

All compounds are in stock.
The library is for prompt delivery, cherry-picking is available.

Feel free to contact me if you are interested to obtain this library or if you need more information.
I am looking forward to your reply.

Best regards,
Andriy Dmytrenko, MBA
Director of Business Development and Marketing

OTAVA Ltd.
Tel.: 1-416-549-8030
Fax: 1-866-881-9921 (Toll-free in US & Canada)
info@otavachemicals.com
north.america@otavachemicals.com