

11 β -hydroxysteroid dehydrogenase type I (11 β -HSD1) target-focused library from Otava

Screening compounds for **drug discovery in endocrine and metabolic disorders treatment**

As a Director of Otava Ltd. I would like to offer you our new **11 β -hydroxysteroid dehydrogenase type I (11 β -HSD1) target-focused library (1,060 compounds)**. The library has been designed with flexible molecular docking. For the docking, we used crystal structure of human 11 β -HSD1 in complex with inhibitor and cofactor NADP (4C7K). The 11 β -HSD1 binding pocket in the crystal structure includes bound cofactor which has been preserved during the docking. The most important polar interactions between the cocrystallized ligand and 11 β -HSD1 in 4C7K include contacts with Ala172, Ser170 and Tyr183 residues. Presence of hydrogen bonds between docked ligands and these residues has been used as a selection criteria to retain the most promising compounds only. To filter molecular complexes obtained with the docking, a scoring cutoffs based on different scoring functions were used. Finally, the complexes selected with the H-bond and score filtering were subjected to visual analysis in order to discard ligands with improper binding mode.

This library **comprises drug-like compounds only** and provides an excellent basis for drug discovery in endocrine and metabolic disorders treatment

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Our price is **ONLY \$7.7** per 1mg (if more than 1,000 compounds are ordered)

Example price list in USD:

Num. of compounds ordered	1-20	21-50	51-100	101-500	501-1000	more than 1000
Price for 1mg	\$32.0	\$25.0	\$19.0	\$13.9	\$9.8	\$7.7

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

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