Structure-based Screening

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Tags: *1_Drylab 3_Virtual Screening*
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{yes/no|:homology model usage:}

The library was subsequently docked in the **homology model of the {human muscle type nAChR|receptor} {human muscle type nAChR|receptor} (PDB-ID: {7EKT|PDB-ID})** using {DOCK 3.7|software}.

The binding site was prepared based on the ligand {acetylcholine| name of ligand}. To remove compounds with artificially enhanced scores due to known deficiencies of scoring functions, the top {2000|number of hits} hits were visually inspected based on their {overall docking score|scoring properties}, resulting in {15|number of virtual candidates} virtual candidates.