

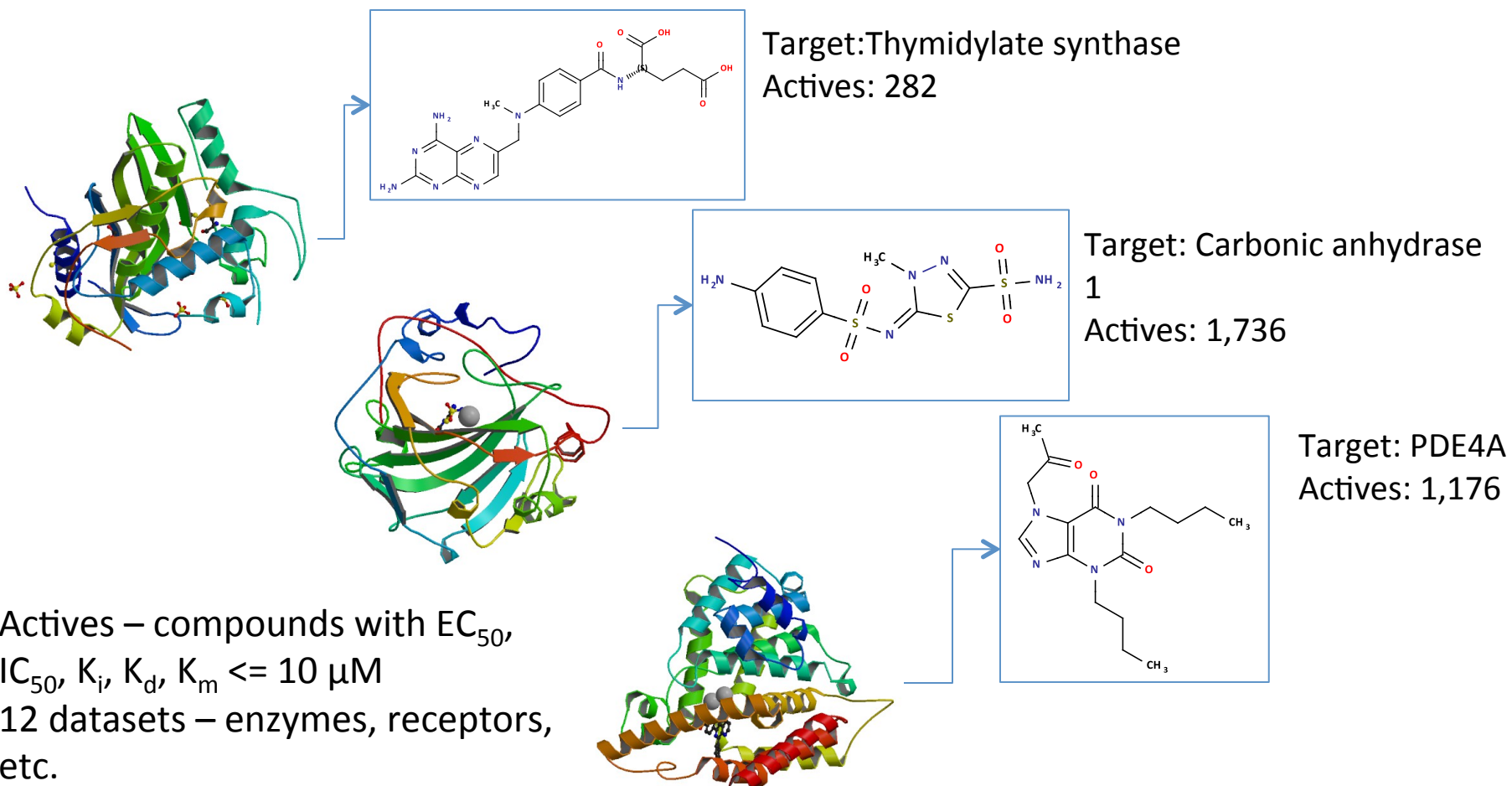
Screen3D: a new high-throughput flexible alignment method

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University of New Mexico



ChEMBLDb¹ datasets



1. www.ebi.ac.uk/chembl/db

Clean-up, 3D structure generation, and running Screen 3D

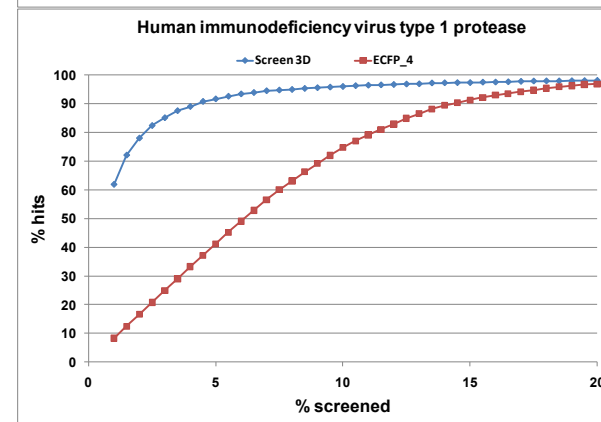
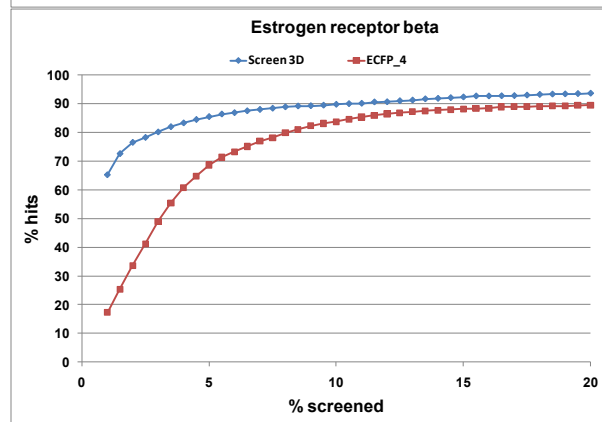
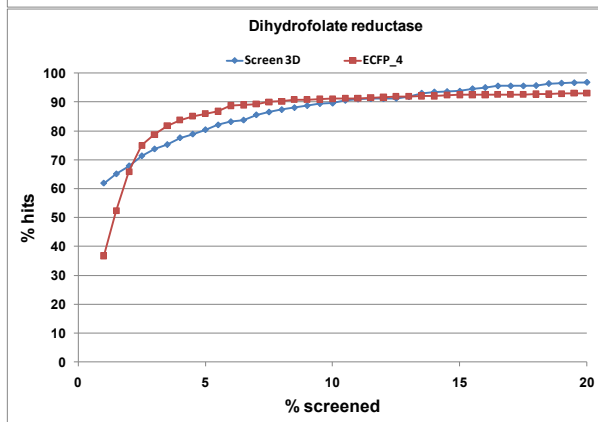
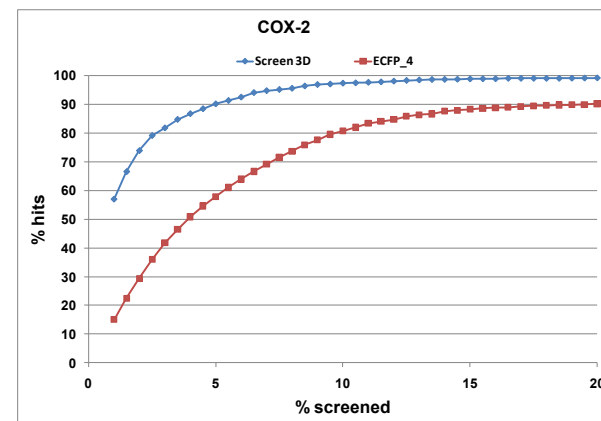
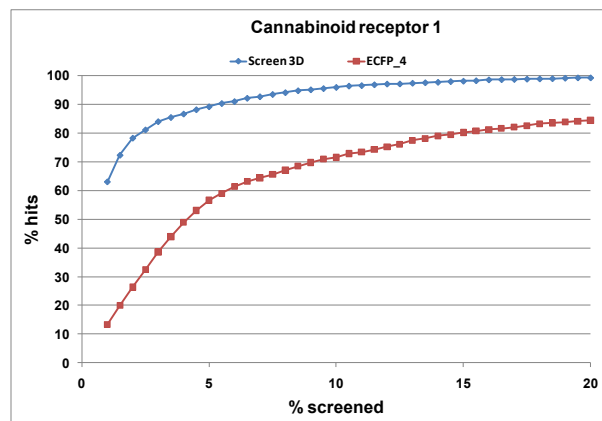
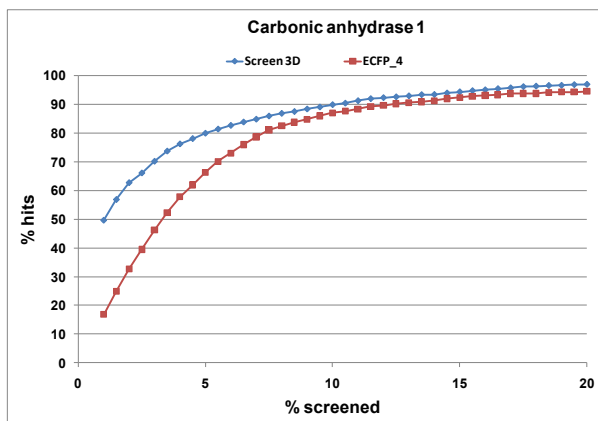
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molconvert -3:c3E[prehydrogenize] sdf chembl_clean.smi -o chembl_clean_3d.sdf
598,373 **595,713**

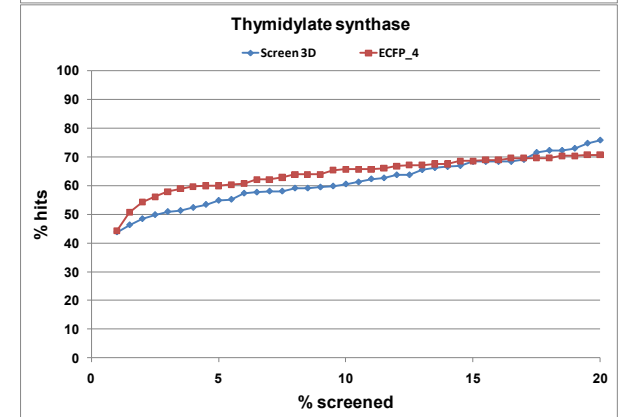
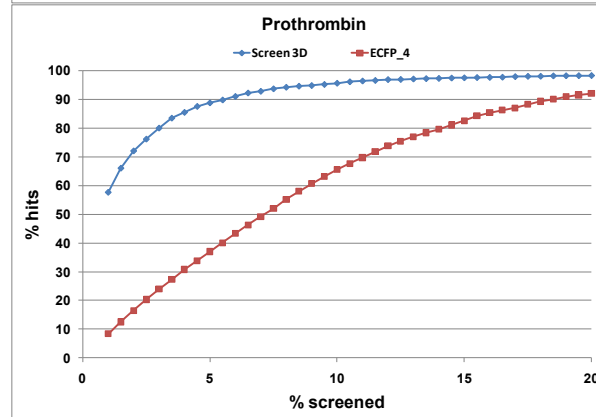
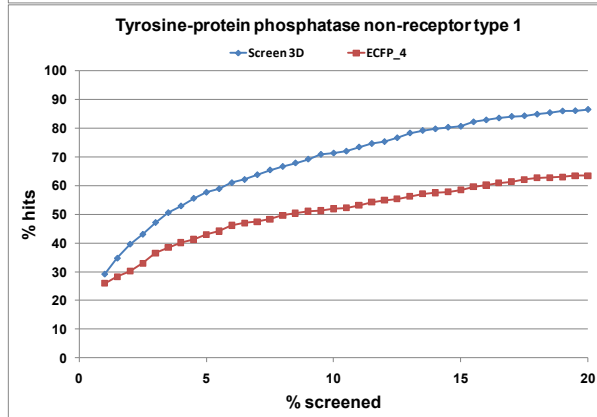
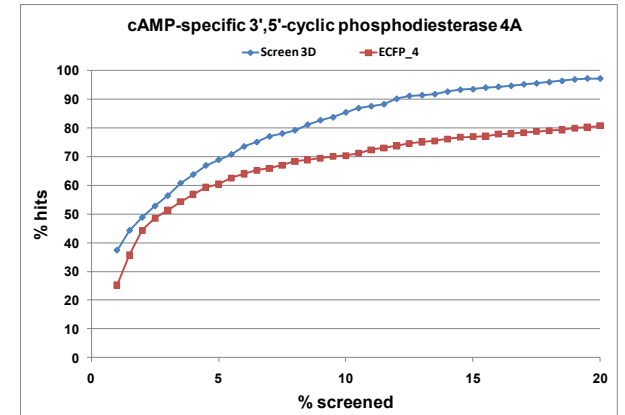
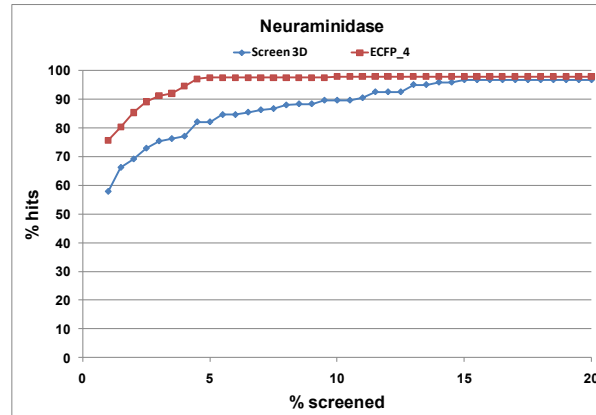
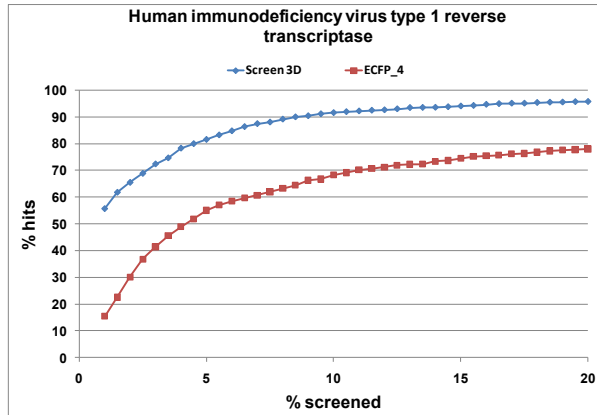
- Query molecules: random 1% of actives set
- Target molecules: rest of the actives set + random 30,000 decoys from database

- Prepare binary files (query/target): screen3d g target/query.sdf -F
- **Run Screen 3D: screen3d s -t targetF.ser -q queryF.ser**

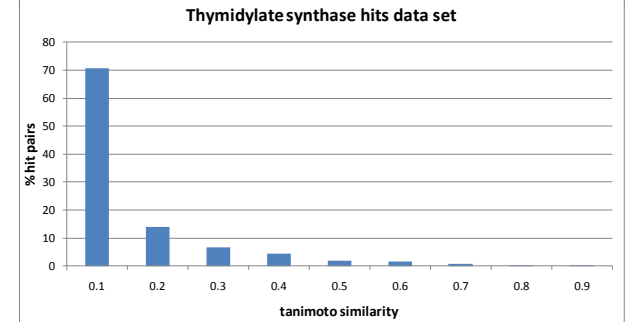
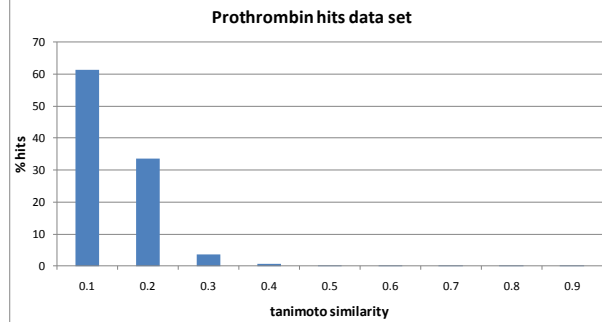
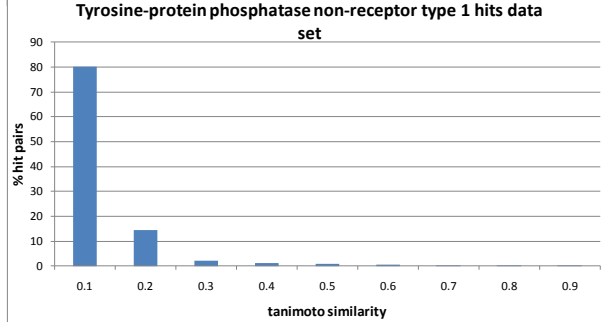
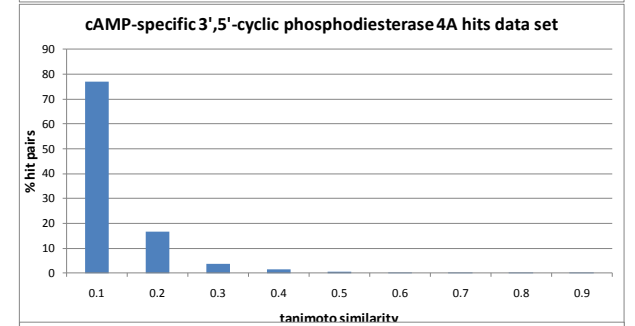
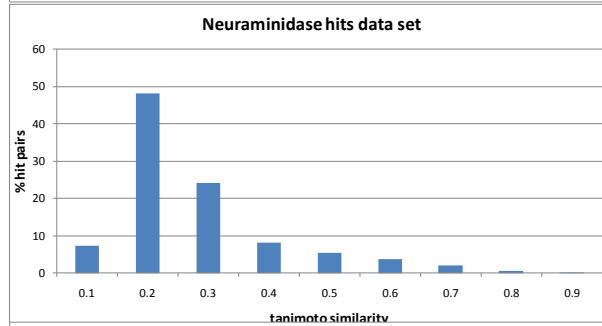
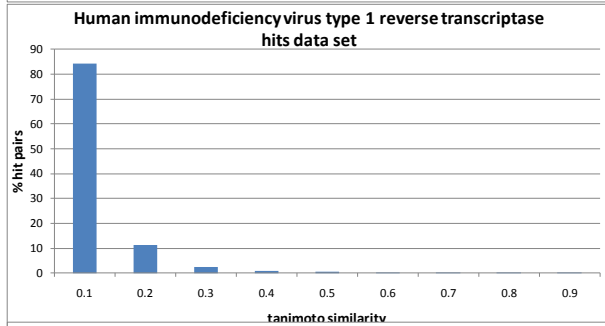
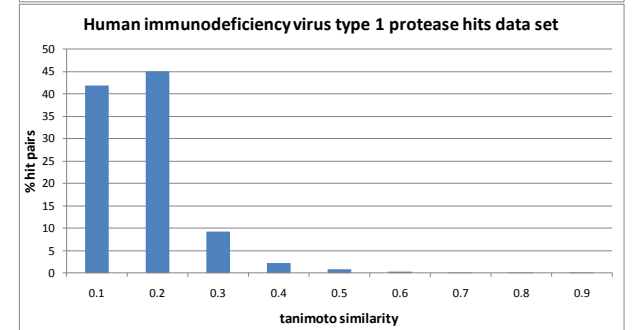
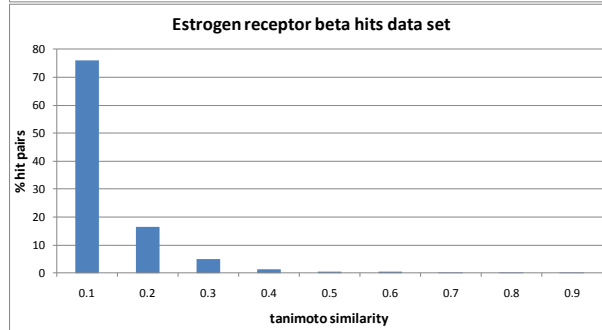
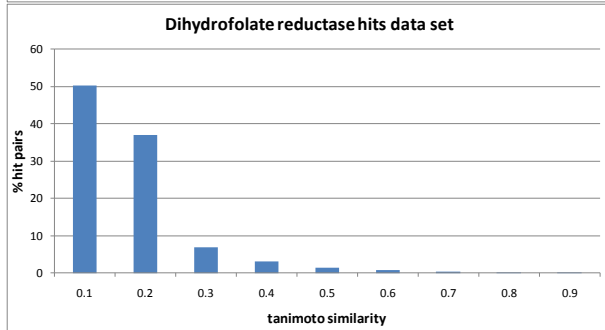
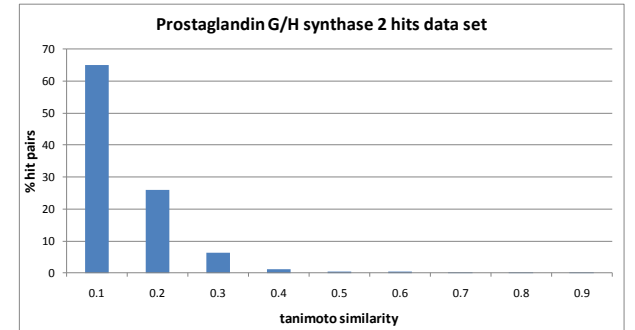
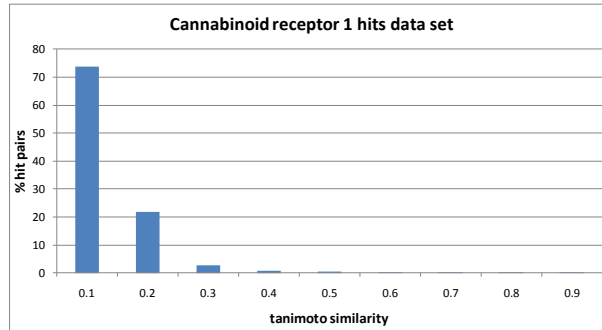
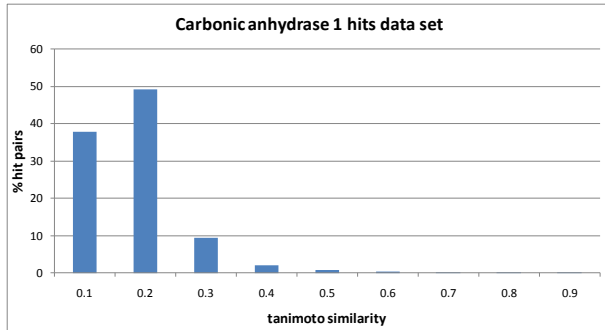
Hit recovery rates



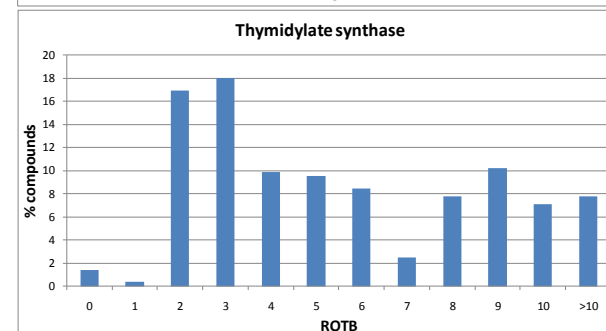
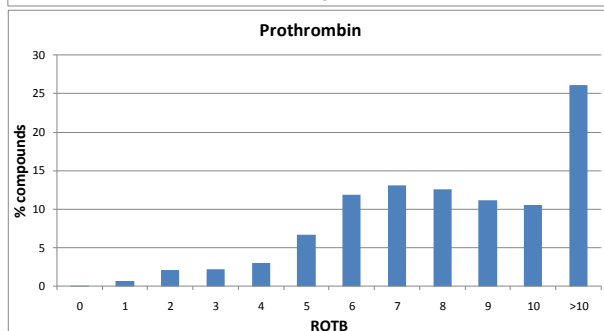
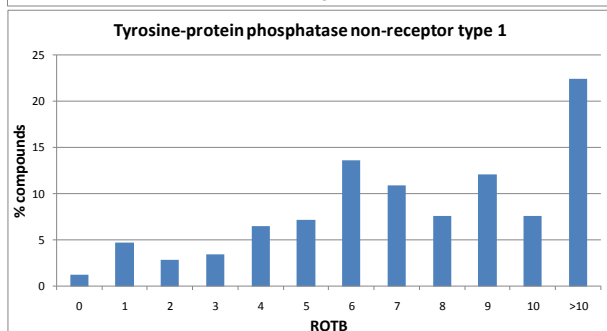
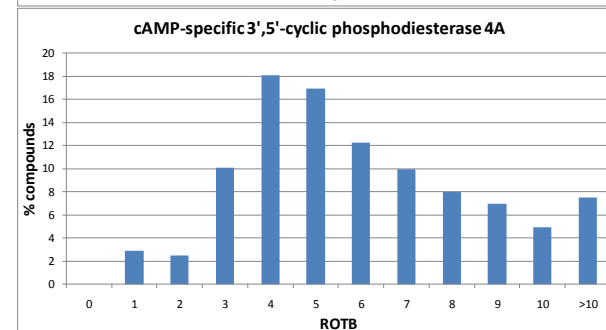
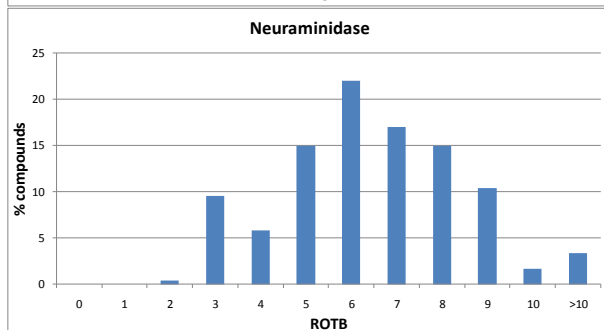
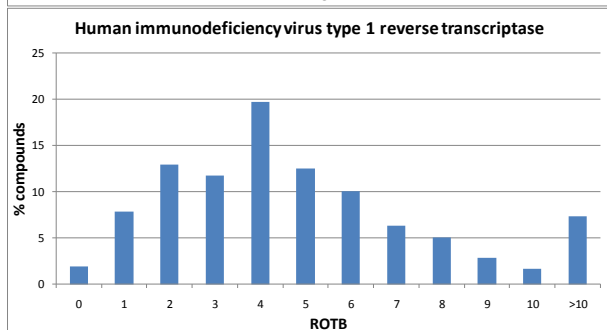
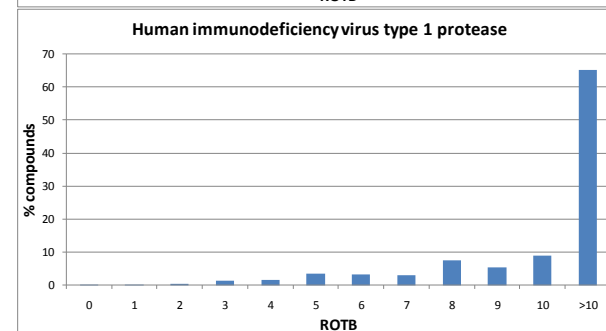
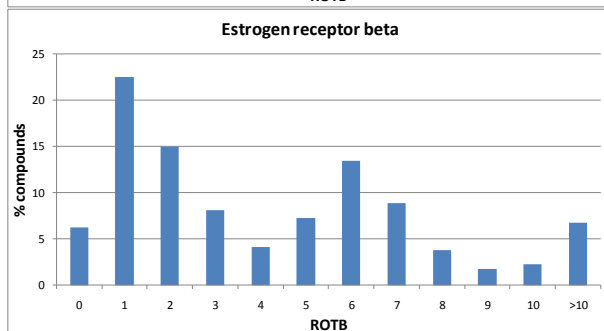
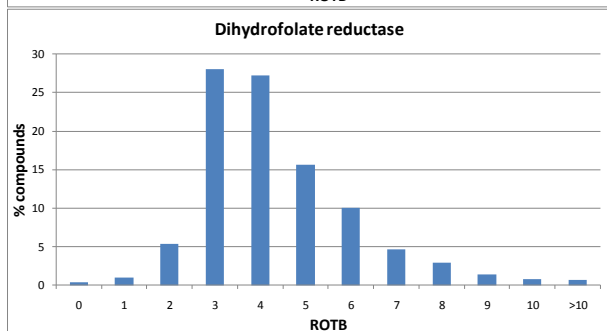
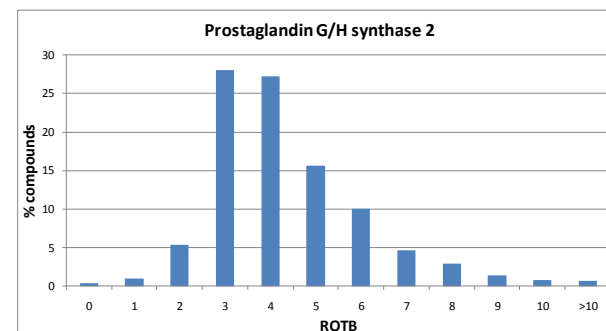
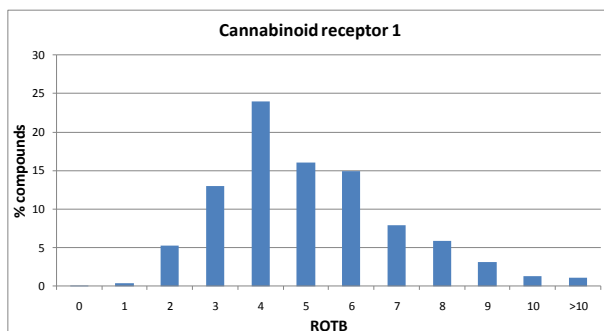
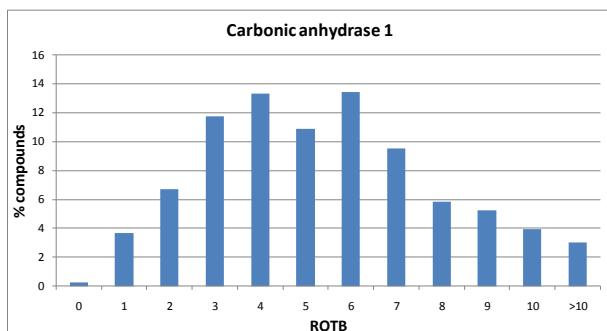
Hit recovery rates



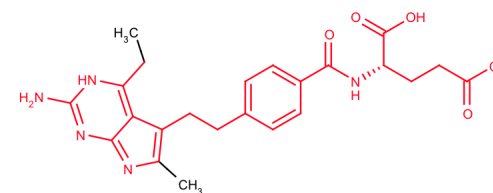
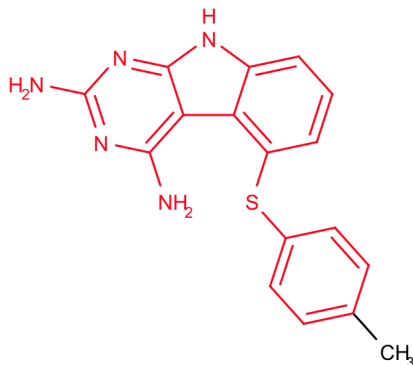
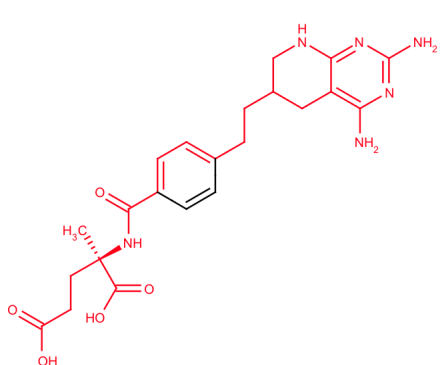
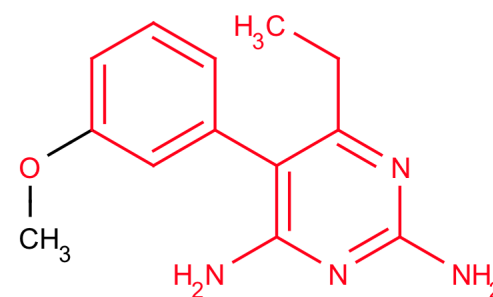
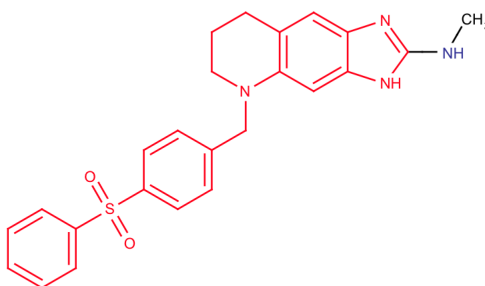
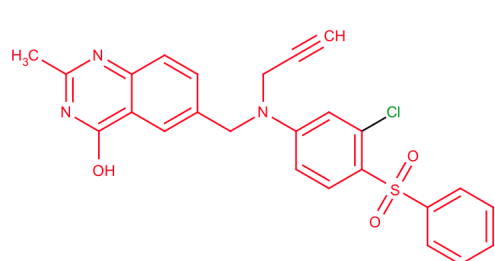
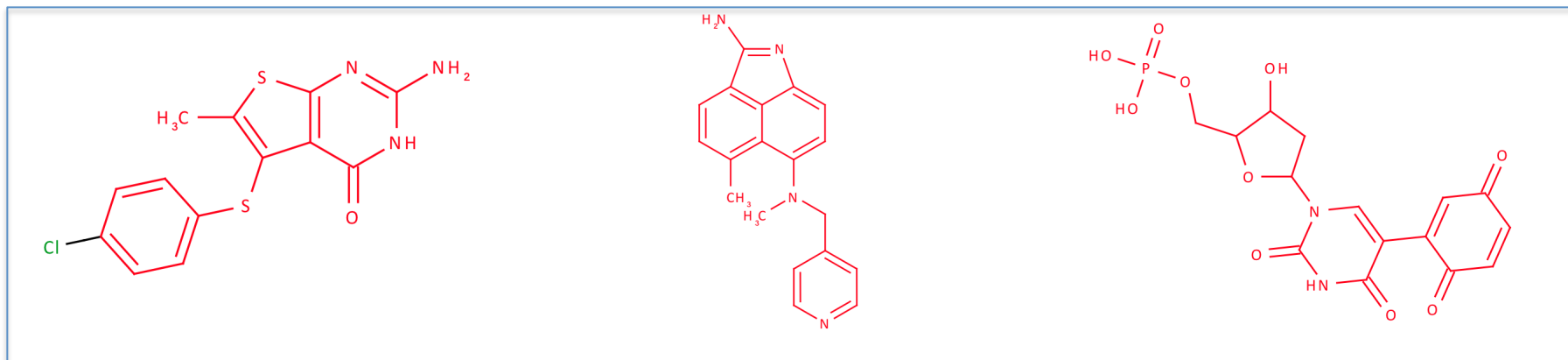
Tanimoto similarity

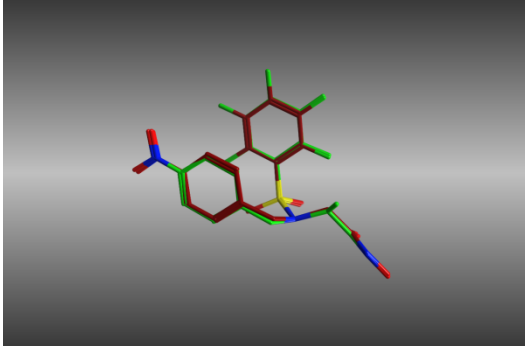


Rotatable bonds

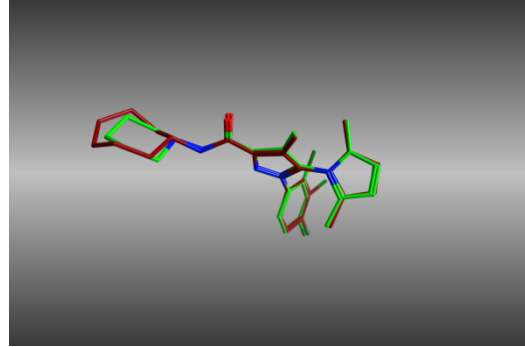


Thymidylate synthase sampling

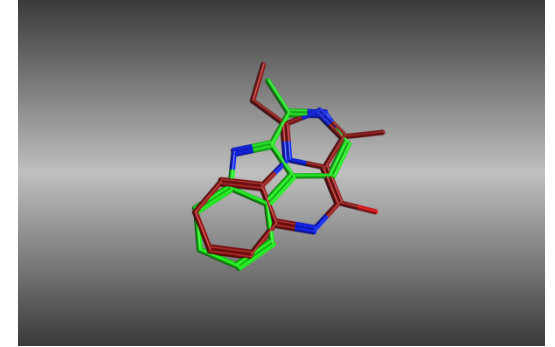




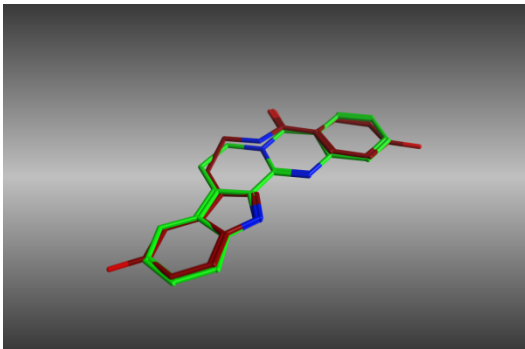
Carbonic anhydrase 1



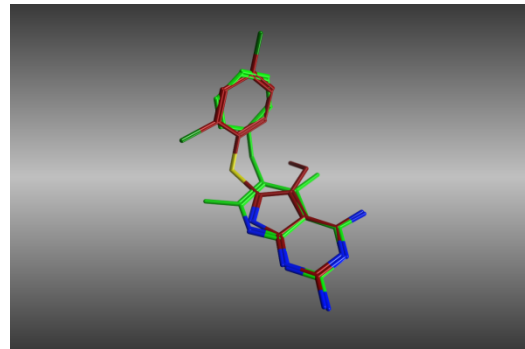
Cannabinoid receptor 1



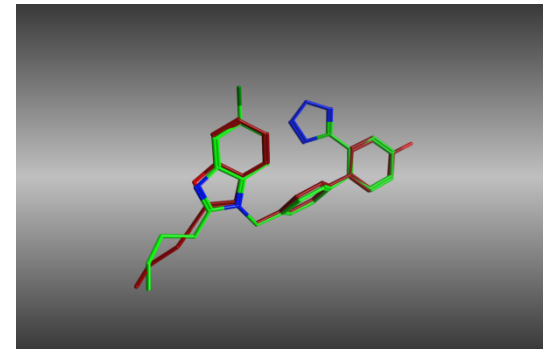
Phosphodiesterase 4A



Cyclooxygenase-2



Dihydrofolate reductase



Tyrosine phosphatase 1B

Conclusions

- New method to perform 3D shape/match virtual screening
- Good performance
- Good hit recall rates
- Integrated with other ChemAxon tools
- Questions?