

Experiment 18: 55% Completed--Has Been Halted  
NCI Diversity Set (1900) vs. 500 conformations from the first 5 ns of MD on the V82F/I84V drug-resistant "super-bug" of HIV protease. These results will be compared to those from Experiments 10, 11, and a future experiment, in order to help test and improve the methods and tools that can be used in drug design research against any target of interest.

This experiment involves faah3202-3702.

This experiment is now "on hold." It was halted before its completion, because an error was discovered in the code. The massive number of calculations that you perform for us helped us discover a serious error, and now we have made it much harder to accidentally mis-compile the code. In addition, we have now created new methods for checking the quality of the results. Thus, by helping us improve our code and our protocols, this little setback will help our research in the long-run, and it will help the research that over 4,000 other labs perform with the AutoDock code. We will repeat this experiment (or something very similar to it) with the WCG's new version of the AutoDock code, which is now up-and-running.

Experiment 17: 88% Completed--Has Been Halted  
Relaxed Complex Method of Several Compounds, Their Fragments & Several Derivatives versus the Exo site of snapshots from MD of the V82F/I84V drug-resistant "super-bug" of HIV protease (from 1D4S.pdb).

This experiment involves faah3145-3201.

This experiment is now "on hold." It was halted before its completion, because an error was discovered in the code. The massive number of calculations that you perform for us helped us discover a serious error, and now we have made it much harder to accidentally mis-compile the code. In addition, we have now created new methods for checking the quality of the results. Thus, by helping us improve our code and our protocols, this little setback will help our research in the long-run, and it will help the research that over 4,000 other labs perform with the AutoDock code. We will repeat this experiment (or something very similar to

it) with the WCG's new version of the AutoDock code, which is now up-and-running.

Experiment 16: 100% Completed

Relaxed Complex Method of Several Compounds, Their Fragments & Several Derivatives versus the Exo site of snapshots from MD of Wild Type 1KZK

Experiment 15: 100% completed

Relaxed Complex Method of the NCI Diversity Set versus the Exo site of snapshots from MD of Mutant 1D4S

Experiment 14: 100% Completed

Relaxed Complex Method of the NCI Diversity Set versus the Exo site of snapshots from MD of Wild Type 1KZK

Experiment 13: 100% Completed

Relaxed Complex Method of the 9 false negatives from the full NCI Diversity Set

Experiment 12: 100% completed

HIV protease cross-docking (i.e., this is a test of the new AutoDock code and the new scoring function). This experiment helps us test and improve the tools that we use in these calculations (and that thousands of other labs use in their drug design research against other diseases). This experiment involves faah2695-2714.

Experiment 11: 100% Completed

NCI Diversity Set (1900) vs. 500 conformations from the first 5 ns of MD on wild type HIV protease

Experiment 10: 100% Completed

This was Dr. Alex Perryman's first experiment on FAAH. The NCI Diversity Set of compounds was docked against 7 "interesting" snapshots of the V82F/I84V multi-drug-resistant "super bug" of

HIV protease. These snapshots were deemed "interesting," since they seemed to be very useful in Dr. Perryman's previous Relaxed Complex experiments. That is, these compounds displayed some of the lowest (i.e., best) Free Energies of Binding against the inhibitor JE-2147, and these 7 conformations helped resolve the compounds that bound well from those that did not bind (in previous computational experiments).

Experiment 9: 100% Completed

The "consensus" wild type crystal (2BPW.pdb) was used to screen Max Chang's version of the "DTP library of moderately-active compounds" from the NCI. For details on why this wild type protease is considered a "consensus wt," follow the link on the previous page to the FAAH paper published in the Journal of Chemical Information and Modelling.

Experiment 8b: 100% Completed

Drugs et al. vs. SCWRL-modeled mutants (no H<sub>2</sub>O) with flexible sidechains

Experiment 8a: 100% Completed

Drugs et al. vs. SCWRL-modeled mutants (no H<sub>2</sub>O) (rigid)

Experiment 7b2: 100% Completed

x2AZ8 vs ZINC Fragment Library (exo site)

Experiment 7b1: 100% Completed

x2AZ8 vs ZINC Fragment Library (active site)

Experiment 7a2: 100% Completed

x2BPW vs ZINC Fragment Library (exo site)

Experiment 7a1.1: 100% Completed

Fragment Library vs 2BPW (Active Site)

Experiment 6a, 6b, 6c, 6d: 100% Completed  
NCI vs. 1MEU, 2BPZ, 2BPW, & 2AZ8

Experiment 5: 100% completed  
BindingDB vs. HIV Protease, with and without Active Site Water  
Molecule

Experiment 4: 100% Completed  
NCI Diversity Set vs. HIV PR Monomer

Experiment 3: 100% completed  
Testing Sidechain Motion in HIV Protease Cross Dockings

Experiment 2: 100% Completed  
ChemBridge (500,000) vs. Wild Type HIV Protease (1)  
Top Hits from Stage 1 vs. Mutant HIV Protease Panel (270)  
NCI Diversity Set (1,900) vs. Monomeric HIV Protease (20)

Experiment 1b: 100% completed  
NCI Set (230,000) vs. Wild Type HIV Protease (1)

Experiment 1a: 100% Completed  
NCI Diversity Set (1,900) vs. Mutant HIV Protease Panel (270)