

Predicted A2A structures with docked antagonist – January 19, 2009

The coordinate entries in this directory were submitted in response to the community-wide blind prediction experiment (GPCR Dock), in coordination with the release of the human adenosine A_{2A} receptor structure in October 2008. The coordinate entry mod3eml.pdb is for the experimentally determined structure of the receptor.

Depositors submitted up to 10 entries which they ranked with 1 being the “best” model. Each depositor was assigned an Accession ID and thus each entry is identified uniquely by its Accession ID and Rank Number. To facilitate analysis and to preserve anonymity during the evaluation process, we generated a random PDB-like idcode and assigned one to each coordinate entry. An excel spreadsheet is provided that gives the correspondence between the assigned PDB idcode and the Accession ID and Rank number. The spreadsheet contains rmsd's, number of correct contacts, and the combined z-score (see below for an explanation).

In February, 2009, we will be releasing a document containing descriptions provided by depositors on protocols that were used to generate and select these models. The document will contain a table of depositors and accession id numbers.

The coordinates in this directory were transformed from the submitted file as follows:

1. All atoms beyond 306 were removed
2. Protein C α atom superposition between model and crystal structure (3EML) was done using the align command in PyMOL (version 1.0r2, www.pymol.org). The matrix of transformation was then applied to all the atoms in the model including those for the antagonist.
3. Atom names for the antagonist were modified to be consistent with atom names used in the 3EML entry.

Z-Score:

The models were ranked by assigning a combined mixed z-score to each model. The combined z-score was calculated as the average of z-scores for ligand RMSD and number of correct contacts: $Z_{combined} = (-Z_{LigandRMSD} + Z_{N_CorrectContacts})/2$. The z-scores for ligand RMSD and number of correct contacts were computed in two passes as follows: i) assign a z-score to each model using the average and standard deviation values from all models, ii) re-compute the average and standard deviation excluding models with z-scores more than two standard deviations above (for ligand RMSD) and below (for number of correct contacts) the average, iii) re-assign a z-score to each model using the revised average and standard deviation values obtained in step ii.

Please send comments, suggestions, and/or questions to Professor Ray Stevens (stevens@scripps.edu)