

Taylor et al.

Parameters for Other Docking Programs

Autodock3.0

The following Autodock3.0 parameters were tried, but nearly all solutions failed to yield contacts between R* and transducin that were deemed important in previous mutational experiments. For all other parameters, the default values were used.

1. The rigidity of Gt_α(340-350) was varied, ranging from being completely flexible to completely rigid.
2. The following parameters were varied when the Lamarkian Genetic Algorithm was used: Population Size (100-250), Number of Energy Evaluations (250,000 – 1,500,000), Number of Generations (27,000 – 35,000), Elitism (1-5), Mutation Rate (0.02-0.08), Crossover Rate (0.8), Number of Runs (100-250).
3. The RMS for clustering was varied between 2 and 3 Å.

RosettaDock

A global run was done, with a total of 1000 to 9000 structures created. Both the receptor and the ligand were allowed to be flexible. Extra conformations for chi1, 3, and 4 angles were used.