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What is the difference between GlideScore and Emodel, and which should I use for ranking poses?

GlideScore is an empirical scoring function that approximates the ligand binding free energy. It has many terms, including force field (electrostatic, van der Waals) contributions and terms rewarding or penalizing interactions known to influence ligand binding. It has been optimized for docking accuracy, database enrichment, and binding affinity prediction. GlideScore should be used to rank poses of different ligands, for example in virtual screening. As it simulates a binding free energy, more negative values represent tighter binders. While the XP GlideScore shares many terms with the SP and HTVS GlideScore, they do have significant differences and have been optimized separately; as a result, these two GlideScores cannot be compared directly.

Emodel has a more significant weighting of the force field components (electrostatic and van der Waals energies), which makes it well-suited for comparing conformers, but much less so for comparing chemically-distinct species. Therefore, Glide uses Emodel to pick the ""best"" pose of a ligand (pose selection), and then ranks these best poses against one another with GlideScore. For Glide XP, the pose-selection procedure is a bit more complicated, though it still involves Emodel and GlideScore. Poses produced by Glide XP have an ""XP PoseRank"" property that shows how Glide XP has ranked the poses of a given ligand.

Glide sorts its results by GlideScore. This means that if you save multiple poses per ligand, the apparent ranking of poses for a given ligand (by GlideScore) will not reflect the actual ranking Glide used for pose selection. You should look at the value of Emodel or XP PoseRank properties to determine the ""best"" pose for a ligand.

There is a brief description of GlideScore in section 2.1 of the Glide User Manual. For more complete descriptions, please see the following papers:

- Friesner, R. A.; Banks, J. L.; Murphy, R. B.; Halgren, T. A.; Klicic, J. J.; Mainz, D. T.; Repasky, M. P.; Knoll, E. H.; Shaw, D. E.; Shelley, M.; Perry, J. K.; Francis, P.; Shenkin, P. S., ""Glide: A New Approach for Rapid, Accurate Docking and Scoring. 1. Method and Assessment of Docking Accuracy"", *J. Med. Chem.* **2004**, *47*, 1739-1749
- Friesner, R. A.; Murphy, R. B.; Repasky, M. P.; Frye, L. L.; Greenwood, J. R.; Halgren, T. A.; Sanschagrin, P. C.; Mainz, D. T., ""Extra Precision Glide: Docking and Scoring Incorporating a Model of Hydrophobic Enclosure for Protein-Ligand Complexes"", *J. Med. Chem.* **2006**, *49*, 6177-6196.

Most of the special XP rewards described in the latter paper have now been incorporated into the SP GlideScore.

The exact formula for Emodel is proprietary, but it is a combination of a version of the GlideScore, the internal ligand strain (Einternal), and the Coulomb and van der Waals energy.

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