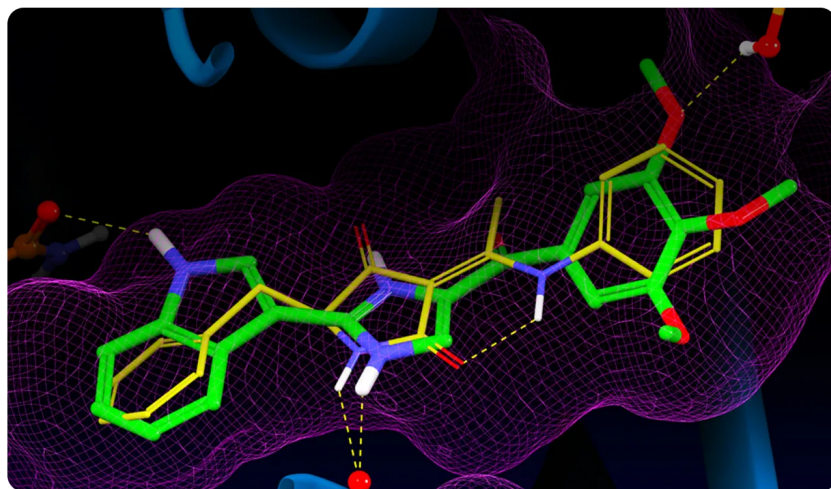


Docking and scoring



Virtual screening has proven to be a very successful approach for finding ligand hits and assisting lead optimization in structure-based drug discovery projects. By docking a large library of compounds into one or more high-resolution structures of the target receptor, fewer compounds typically need to be experimentally screened to identify prospective lead optimization candidates. Beyond identifying small molecules likely to bind well to a protein target, docking methods are used in a variety of context such as polypeptide and macrocycle pose prediction, predicting protein-ligand complex geometries, and preparing congeneric series for binding affinity prediction with methods such as Free Energy Perturbation or MM-GBSA. Moving beyond the rigid receptor approximation common in structure-based virtual screening, the Induced Fit docking protocol predicts the effect of ligand docking on protein structure.

Rigid Receptor Docking with Glide

Glide Docking and Scoring Methodology

The Glide HTVS, SP and XP docking methodologies have previously been described in detail.¹⁻³ Glide HTVS and SP use a series of hierarchical filters to search for possible locations of the ligand in the binding-site region of a receptor. The shape and properties of the receptor are represented on a grid by different sets of fields that provide progressively more accurate scoring of the ligand pose. Exhaustive enumeration of ligand torsions generates a collection of ligand conformations that are examined during the docking process. Given these ligand conformations, initial screens are deterministically performed over the entire phase space available to the ligand to locate promising ligand poses. From poses selected by initial screening, the ligand is refined in torsional space in the field of the receptor using OPLS3⁴ (Glide SP & XP) or OPLS2005 (GLIDE HTVS) with a distance-dependent dielectric model. Finally, a small number of poses are minimized within the field of the receptor with full ligand flexibility (post-docking minimization or PDM). This process is referred to as the docking funnel as illustrated in Figure 1.

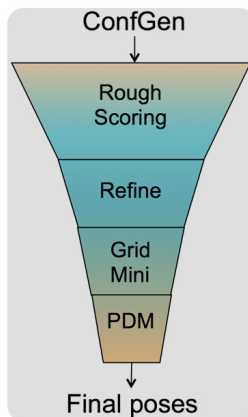


Figure 1: Glide HTVS and SP docking funnel.

Glide HTVS can dock compounds at a rate of about 2 seconds/compound and trades sampling breath for higher speeds. Glide SP performs exhaustive sampling and is the recommended balance between speed and accuracy, requiring about 10 seconds/compound. Glide XP employs an anchor-and-grow sampling approach and a different functional form for GlideScore. It can dock compounds at a rate of about 2 minutes/compound. These three docking modes provide an array of options in the balance of speed vs. accuracy for most situations.

Glide uses the Emodel¹ scoring function to select between protein-ligand complexes of a given ligand and the GlideScore² function to rank-order compounds to separate compounds that bind strongly (actives) from those that don't (inactives). The Emodel scoring function is primarily defined by the protein-ligand coulomb-vdW energy with a small contribution from GlideScore. GlideScore is an empirical scoring function designed to maximize separation of compounds with strong binding affinity from those with little to no binding ability. As an empirical scoring function it is comprised of terms that account for the physics of the binding process including a lipophilic-lipophilic term, hydrogen bond terms, a rotatable bond penalty, and contributions from protein-ligand coulomb-vdW energies. In addition to these terms, GlideScore includes terms to account for hydrophobic enclosure³, which is the displacement of water molecules by a ligand from areas with many proximal lipophilic protein atoms. Particularly beneficial to binding is the formation of one or more protein-ligand hydrogen bonds within regions of hydrophobic enclosure as illustrated in Figures 2 and 3.

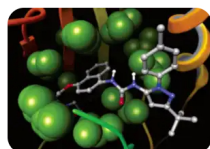


Figure 2: Boehringer active for 1kv2 bound to human p38 map kinase. The naphthyl group receives a hydrophobic enclosure packing reward.

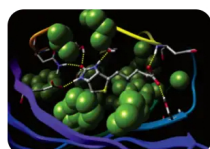


Figure 3: Biotin bound to streptavidin. The identification of a triplet of correlated hydrogen bonds in the ring in a hydrophobically enclosed region, and the three hydrogen bonds to the ligand carbonyl within that ring each significantly contributes to a very favorable GlideScore for this tightly bound complex ($\Delta G_{exp} = -18.3$ kcal/mol).

Glide Docking Accuracy and Enrichment Performance

The first Glide article¹ is the 2nd most cited paper ever in the Journal of Medicinal Chemistry (as of Feb. 2016) with many references citing its application in drug discovery projects. Glide's ability to consistently identify hits for lead optimization and guide understanding of the key interactions and desolvation effects impacting protein-ligand binding have helped drive its widespread adoption. A pre-requisite to obtaining the highest-quality docking results is to use protein and ligand structures prepared using best-practices methods by the Protein Preparation Wizard and LigPrep. As part of an unbiased comparison of docking methods, we have evaluated Glide SP for binding mode prediction using the Astex⁵ set of self-docking tests, and enrichment in a virtual screening context using the DUD dataset⁶. The datasets, evaluation metrics, and experiments performed were prescribed by conditions of the Docking and Scoring Symposium at the 241st ACS Meeting in Anaheim.⁷

In these retrospective experiments, Glide SP reproduces crystal complex geometries in 85% of Astex cases with < 2.5 Å RMSD as shown in Figure 4. Glide is also effective in enriching screened databases in known actives, beating random selection in 97% of DUD targets and giving an average AUC of 0.80 across all 39 target systems. Early enrichment performance shows on average 12%, 25%, and 34% of known actives are recovered in screening the top-ranked 0.1%, 1%, and 2% of recovered decoys. This enrichment is particularly impressive given the structural similarity between active and decoy ligands in the DUD dataset⁸ and that docking a ligand with SP Glide takes only about 10 seconds using modern hardware.

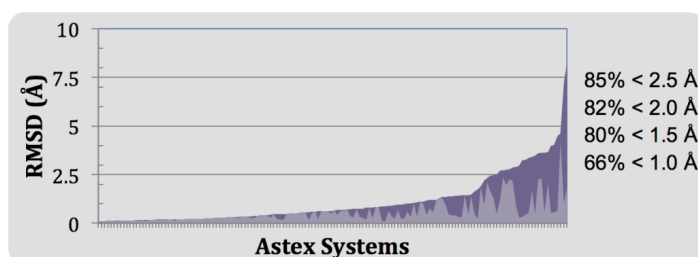


Figure 4: Plots of Glide SP RMSDs from Astex docking experiments for the top-ranked Emodel pose (blue) and lowest-RMSD refined pose (light blue-grey). The percentage of top-ranked Emodel poses that meet different RMSD cutoffs is shown.

	ROC(0.1%)	ROC(1%)	ROC(2%)	AUC
Best-Practices Structures				

Average	0.12	0.25	0.34	0.80
Median	0.06	0.19	0.27	0.14
Std. Dev.	0.17	0.22	0.24	0.14
Maximum	0.82	0.88	0.88	0.98

Table 1: Early and complete Glide SP enrichment results using best-practices prepared structures for the DUD dataset of 40 systems.

Using Glide to “Stay Close to Experiment”

Glide’s wide range of constraints enable one to “stay close to experiment” which has been reported as a common theme in pharmaceutical projects at Roche that were positively impacted by computational chemistry.⁹ Hydrogen bond constraints require formation of a hydrogen bond to particular functional groups on the receptor, positional constraints can enforce docked poses to place particular chemistry in a volume of space relative to the receptor, metal constraints enforce coordination geometries. Core constraints are particularly valuable for enforcing expected binding modes of congeneric series in preparing docked poses for binding affinity prediction via MM-GBSA or Free Energy Perturbation.

Docking Macrocycle

Efficient sampling of ring conformations is essential to reproduce experimental binding modes in docking experiments, particularly for macrocycles where there can be hundreds of low energy conformations. Glide relies on an extensive database of ring conformations to sample low-energy states and otherwise does not sample macrocycle ring systems. Generating ring templates for macrocycles considerably improves native pose prediction.

A representative example is the macrocycle from 2QKZ shown in this figure where the native ligand buries the macrocycle ring into a mostly enclosed pocket. To bind in this pocket requires a particular ring conformation that forms key interactions to a ligand carbonyl and protonated amine moieties. Using ring templates for this macrocycle the docked pose has a low RMSD of 0.22 Å. Without the macrocycle ring templates, even with a visually similar ring conformation of RMSD 0.71 Å for macrocycle ring atoms, Glide positions the ring outside the pocket leading to a very large RMSD of 10.23 Å.

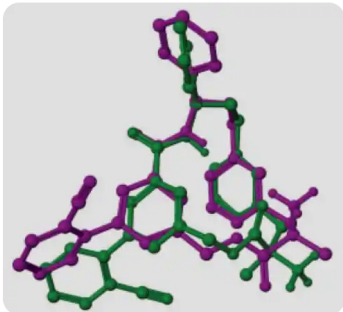


Figure 5: A computed macrocycle conformation (purple) of 2QKZ overlaid with the crystal structure (green).

Docking Polypeptides

The increased use of peptides and peptidomimetics as drugs has created a need for the accurate prediction of binding complex geometries of polypeptides to receptors. The Glide SP-peptide mode¹⁰ was developed to address this need as default application of Glide to such ligands results in a successful docking for 24% of the peptides in a benchmark set. To improve binding mode prediction, the Glide sampling algorithm was modified by systematically changing all parameters that control how peptide conformations make it through the Glide funnel. Applying the optimal combination of these parameters increased pose prediction accuracy to 41%. In addition, we leveraged the previously reported sensitivity of Glide to input conformations¹¹ and increased sampling by running multiple independent Glide jobs and pooling the results. This increased accuracy of pose prediction to 53%. Finally, by applying MM-GBSA scoring to each of the predicted poses, further boosting the accuracy to 58%. This approaches accuracy of brute-force methods like FlexPepDock (63% for this dataset) at a fraction of the computational cost (24 CPU hours for the Glide protocol).

		Prediction Accuracy			Peptide Structural Properties			
		Number of good poses (< 2 Å RMSD) in ensemble of poses (up to 1000)	Lowest iRMSD in ensemble	Lowest iRMSD of 10 top scoring poses (backbone/Heavy atom)	Residues	Normalized Extendedness	Charged Side Chains	Solvated Charged Side Chains
A	1N7F	67	1.22	1.96/2.42	8	0.91	1	1
	1NLN	144	0.41	0.41/1.41	11	0.92	4	0
	1NVR	154	0.8	0.63/0.92	5	0.94	0	0
	1TW6	262	0.34	0.34/0.34	4	0.79	0	0
	2FNT	4	1.31	1.31/2.09	7	0.9	1	0
B	3D1E	170	0.39	0.85/0.76	6	0.86	0	0
	1AWR	172	0.94	1.12/3.27	6	0.85	0	0
	1ER8	2	1.77	1.78/2.33	8	0.78	0	0
	1SSH	125	0.48	0.75/0.74	11	0.91	1	0
	1W9E	9	0.3	1.65/2.94	5	0.87	1	1
	2P1K	3	1.08	2.43/2.72	11	0.9	2	1

	2VJ0	4	1.79	1.79/1.40	7	0.63	1	0
C	2J6F	11	1.32	10.74/12.86	8	0.88	4	2
	2OPV	2	1.94	2.05/2.49	10	0.88	0	0
D	1QKZ	2	1.74	7.40/8.03	10	0.41	1	1
	1RXZ	0	3.57	4.77/6.57	11	0.75	3	3
	1Z9O	0	3.65	5.45/5.34	9	0.91	4	4
	2C3I	0	2.96	4.00/3.77	8	0.67	5	1
	2FGR	0	4.52	4.91/5.11	8	0.54	1	1
		< 2 Å iRMSD	15	11/6				
		< 3 Å iRMSD	16	13/12				

Table 2: Results of peptide docking using Glide. Peptides were docked against the holo structure. Results are grouped into categories reflecting docking accuracy. Category A peptides can be easily and reliably docked. Category B peptides have predictions where the flexible termini are different from the crystal structures. Category C (poly-proline) and D (miscellaneous structures) peptides are predicted with poor accuracy. For each of the 19 test cases, 10 Glide runs produced up to 1000 total poses (maximum of 100 from each run) and the number of poses with iRMSD < 2.0 Å in the entire ensemble is shown in the third column. We also measured both the lowest iRMSD in the entire ensemble (fourth column) and in the top 10 ranked structures (fifth column). The last 4 columns list structural properties of the studied peptides, revealing that docked peptide accuracy is typically higher when the peptides are short, extended, and have a small number of ionizable side-chains typically have better accuracy.

Which Peptides are Handled Best?

Glide can dock ligands with up to 300 atoms and 50 rotatable bonds. Since many peptide ligands may exceed these limits, this effectively limits docking application to peptides of around 11 residues or less. In some cases, it is necessary to freeze the amide bonds in their trans configuration to dock peptides of longer lengths. Strong correlations are found between structural features of peptides and their ability to be docked accurately. For example, we found that reduced peptide length, increased extendedness, and small number of ionizable groups increased the probability that a peptide was docked correctly. In addition, we noted a strong correlation between the quality of prediction for segments of the peptides with low B-factors, while the high B-factor (typically the N- and/or C- termini) would have significant deviation from the crystal structure, suggesting that these terminal predictions might actually be accessible states in solution.

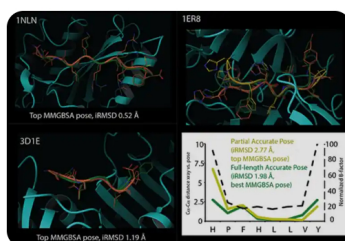


Figure 6: Prediction of protein-peptide complexes using the peptide-customized version of Glide. Predicted complexes on the left (green) for INLN and 3DIE compare very favorably to the experimental X-ray structures (orange). The top-ranked prediction for TERB (top right, yellow) is less accurate when considering the whole peptide. However, the high RMSD is caused mainly by segments of the peptide that have high b-factors (bottom right). In addition, a lower-scoring prediction for this peptide (green) does have low RMSD across all the segments. It is possible that both conformations of the peptide represent accessible states.

Induced Fit Docking

The active site geometry of a protein complex depends heavily upon conformational changes induced by the bound ligand. However, resolving the crystallographic structure of a protein-ligand complex requires a substantial investment of time, and is frequently infeasible or impossible. Schrödinger's Induced Fit (IFD) protocol solves this problem by using Glide and Prime to exhaustively consider possible binding modes and the associated conformational changes within receptor active sites. The unique procedure allows chemists to quickly predict active site geometries with minimal expense, even for systems as challenging as hERG homology models.

The Induced Fit protocol begins by docking the active ligand with Glide. In order to generate a diverse ensemble of ligand poses, the procedure uses reduced van der Waals radii and an increased Coulomb-vdW cutoff, and can temporarily remove highly flexible side chains during the docking step. For each pose, a Prime structure prediction is then used to accommodate the ligand by reorienting nearby side chains. These residues and the ligand are then minimized. Finally, each ligand is re docked into its corresponding low energy protein structures and the resulting complexes are ranked according to a scoring function combining GlideScore and Prime energies.

The Induced Fit methodology has been thoroughly refined in real-world research applications, and is readily used by novice and expert modelers alike. As shown in Table 3 binding pose prediction of Induced Fit for a range of targets where protein conformational changes are necessary for binding is very good. In addition to default settings suitable for a wide range of systems, the Induced Fit interface features advanced options that can be customized to solve more challenging cases. Calculations can be completed in a matter of hours on a desktop machine, or in as few as 30 minutes when distributed across multiple processors.

RMSD of Top-Ranked Poses Returned by Induced Fit

Target	Receptor	PDB source of ligand structure	Docking RMSD before Induced Fit (Å)	Ligand RMSD after Induced, Fit (Å)
Aldose reductase	2acr	1ah3	6.5	0.9

Antibody DB3	1dba	1dbb	7.6	0.3
CDK2	1buh	1dm2	6.4	1.1
CDK2	1dm2	1aq1	6.2	0.8
CDK2	1aq1	1dm2	0.6	0.8
COX-2	3pgh	1cx2	11.1	1
COX-2	1cx2	3pgh	6.6	1.0 (0.51)
Estrogen receptor	1err	3ert	5.3	1
Estrogen receptor	3ert	1err	2.3	1.4 (1.02)
Factor Xa	1ksn	1xka	9.3	1.5
Factor Xa2	1xka	1ksn	5.3	1.5
HIV-RT	1rth	1c1c	2.5	1.3
HIV-RT	1c1c	1rth	12	2.5
Neuraminidase	1nsc	1a4q	3.9	0.8
Neuraminidase	1a4q	1nsc	1	1.7
PPAR – gamma	1fm9	2prg	9.1	1.8 (0.43)
PPAR – gamma	2prg	1fm9	9.8	3.0 (1.54)
Thermolysin	1kr6	1kjo	1.1	1.3
Thermolysin	1kjo	1kr6	3.5	3.2 (1.65)
Thymidine Kinase	1kim	1ki4	4.7	0.4
Thymidine Kinase	1ki4	1kim	0.5	1.2

RMSD of Top-Ranked Poses Returned by Induced Fit:3 RMSD excluding 10 atoms in the partially solvent exposed methyl-2-pyridinylamino tail of the ligand that has atoms with very high B-factors (>60 Å²)
4 RMSD excluding 13 atoms in the partially solvent exposed methyl/phenyloxazole tail of the ligand
5 RMSD excluding 6 atoms in the symmetric di-carboxylate that are flipped 180° in the IFD structure
The Receptor column lists the rigid receptors into which the ligands of other co-crystallized structures are inducing conformational changes. Prior to treatment with Induced Fit, docking results to the rigid receptor return either no poses or high RMSDs. Ligand poses improve dramatically as Induced Fit accurately predicts the active site geometry.

Covalent Ligand Docking

In recent years, there has been a growing interest in the design of drugs forming a covalent bond with the target protein, with nearly 30% of the marketed drugs targeting enzymes known to act by covalent inhibition¹². Covalent interaction with the target protein has the benefit of prolonged duration of the biological effect and potential for improved selectivity. Examples of proteins that have been targeted by covalent drugs include serine penicillin-binding proteins (PBPs) which bind to β lactams and β-lactone antibiotics, cysteine proteases such as Cathepsin B, K, and S, which are covalently modified by vinyl sulfones, epoxides, isothiazolones, and ketoamides, as well as other chemical groups, and hepatitis C virus (HCV) protease, which covalently binds the ketoamide groups of boceprevir and telaprevir.

To address this need a covalent docking protocol, CovDock^{13, 14} was developed that yields good accuracy in binding mode prediction and has automatic detection of reactive atoms using SMARTS patterns. Using a workflow that combines Glide docking and Prime optimization, the CovDock-VS (virtual screening) and CovDock-LO (lead optimization) modes enable application of covalent docking in large-scale virtual screening or lead optimization projects, respectively. The workflow for these two approaches is shown in Figure 7. Thanks largely to reduced sampling, the CovDock-VS mode is 10 to 40 times faster than CovDock-LO mode.

Docking accuracy for CovDock is good with an average RMSD of 1.9Å for CovDock-VS and 1.5 Å for CovDock-LO in a retrospective

native docking experiment with results shown in Table 4. In combination with interaction filters (in these cases, H-bond constraints), CovDock-VS has also demonstrated excellent enrichment in retrospective experiments as shown in Table 5. In a recent test it has been shown to retrieve 71%, 72%, and 77% of the known actives for Cathepsin K, HCV NS3 protease, and EGFR within 5% of a decoy library, respectively. Even in cases where interaction filters could not be used, as for XPO1, CovDock-VS was still able to retrieve 95% of known actives within the top 30% of decoy compounds, with 33% of known compounds found in the top 1% of decoys.

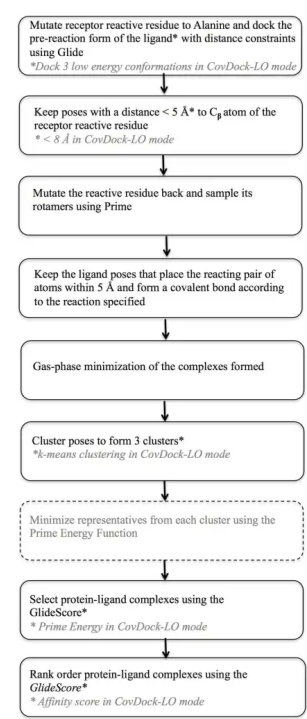


Figure 7: CovDock workflow utilizing Glide and Prime to dock and score covalently bound ligands.

		CovDock-VS	CovDock-LO
Cathepsin K actives			
	1YT7-ligand ^c	2.68	0.68
	2BDL-ligand	2.48	2.89 ^a
	1TU6-ligand	1.43	3.18
HCV NS3 protease actives			
	3KNX-ligand	2.89 ^a	2.45
	2GVF-ligand	1.66	1.51
	3LON-ligand	6.69 ^a	1.81
	2OC7-ligand	1.38	1.12
	2F9U-ligand [#]	1.19	1.30
	2OBO-ligand	1.29	0.98
	2OC8-ligand	1.55	1.04

	2A4Q-ligand	2.51	2.28
	2OC0-ligand	3.03	0.88
	3LOX-ligand	2.07	1.72
	2OC1-ligand	3.75 ^a	3.14
EGFR actives			
	4I24-ligand (Dacomitinib)	1.46	0.85
	4G5J-ligand (Afatinib)	1.81	0.86
	3IKA-ligand (WZ4002)	2.53 ^a	1.67
	2JIV-ligand (Neratinib)	6.54 ^a	2.41 ^a
	2J5F-ligand (34-JAB)	1.57	1.20
XPO1 actives			
	4GMX-ligand (KPT-185) ^c	2.19 ^b	0.67
	KPT-276 (not submitted to PDB) ^c	2.54 ^a	1.07
Mean		1.87	1.50

Table 4: Docking accuracy results from CovDock-VS and CovDock-LO.^aRMSDs for poses with lowest GlideScore are reported for ligands that did not satisfy the postdocking H-bond filters. These are excluded from the mean RMSD calculations. ^bFlip of -OMe and -CF3 groups. ^cSelf-docking of the cocrystal ligands to the protein structures used in VS.

	EF1%	EF10%	BEDROC ($\alpha = 20$)
HCV NS3 protease	52	7	0.70
Cathepsin K	9	8	0.48
EGFR	46	8	0.65
XPO1	33	7	0.52

Table 5:Early enrichment results from CovDock-VS in combination with H-bond constraints as interaction filters.

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