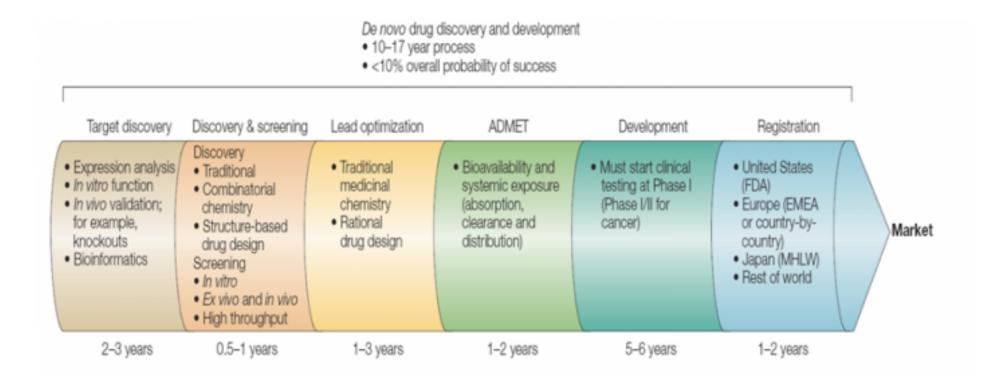
# Introduction to Maestro 11

Structure Visualization and Preparation

Jenny Chambers Ana Rojas

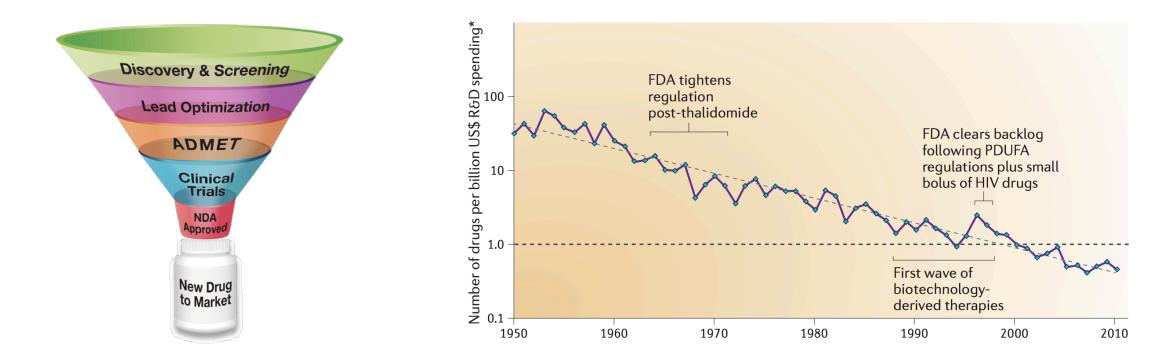
November 13<sup>th</sup>, 2017

# Background on the drug discovery pipeline





# Drug Discovery is Expensive and Slow



# Computer-aided drug design (CADD) can:

- Reduce the time and cost associated with preclinical development
- Inform the decision making process at each step

Scannell, J. W. et al. Nat. Rev. Drug Disc., **2012**, 11, 191-200. http://www.enzolifesciences.com/browse/drug-discovery/



# Structure-Based Drug Design is the Workhorse of CADD



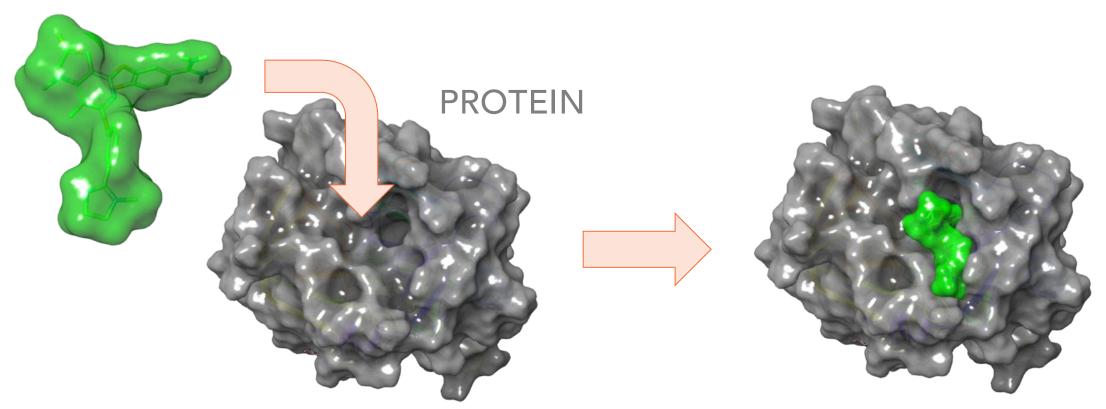
## With a structure you can:

- Predict druggability
- Identify ligand binding sites and hot spots
- Virtually screen for novel chemical matter
- Optimize potency of leads
- Reduce off-target effects



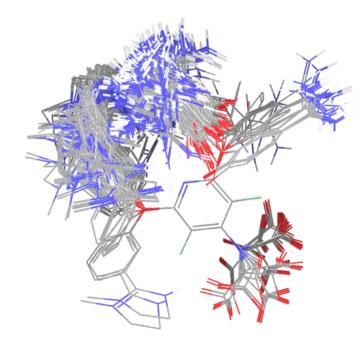
# Docking at its core is a shape matching problem

#### LIGAND





# Ligands are flexible, an docking determines best fit based on interatomic interactions

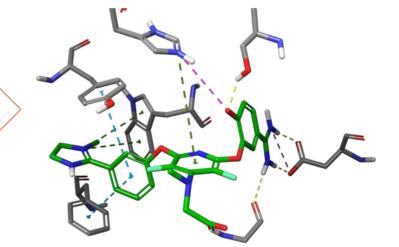


#### **Bonding Interactions**

- Bond length
- Bond angels
- Torsions

#### **Non-Bonding Interactions**

- van der Waal's interactions
- H-bonds
- Charge-Charge interactions
- pi-pi, pi-cation, etc.

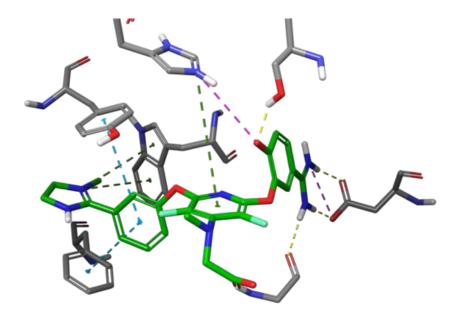


#### Limitations of Docking

- Entropy is not accounted for
- Protein flexibility is ignored
- Solvation is not accounted for



# A Docking Program Generates a...



#### 1) A Binding Pose

A model of the ordination of the ligand in the binding site of the receptor. Accuracy: RMSD ~1 Å to Co-crystal Structures

#### 2) Docking Score

A numerical value of the representing the quality of the pose. Often presented as binding energy.

Accuracy: Good for enrichment, High false positive rate, does not correlate with dGbinding



## How to create docking models with Glide:

Alternity president Hat seafor it	
Display hollingens Nove Polar only Q All Igand, polar receptor All	
Review and Modify Refine	
Import structure Into Workspace	
PDR Internet	
Include: Diffraction-data Biological unit	
Input structure file	
Proprocess the Workgasse structure	
Algette + belanced antry Film	
Araign hand orders 🙆 Use CCD database	
Add hydrogene Remove original hydrogene	
Chaile pare-order bonds to make     Chaile pare-order bonds to make     Chaile bonds     Chaile bonds     Chaile bonds     Chaile bonds     Chaile to bonds     C	
C Delate waters beyond \$00 1 Å from het groupe	
Conversion has states using Epik: pro: 7.8   +> 2.8	
Proprocess	

Receptor		ptor Grid Generation		
2010 Sec. 10		s Rotatable Groups	Excluded Volumes	
Define receptor				
If the structure in the W identify the ligand mole	lorkspace is a recepto cule so it can be exclu	r plus a ligand, you mu ided from the grid gene	st eration.	
Pick to identify the I	igand Molecule	Show markers		
Van der Waals radius so	aling			
To soften the potential van der Waals radii of n value) less than the spe not be scaled.	eceptor atoms with pa	rtial atomic charge (ab	solute	
Scaling factor: 1.0	C Partial charge cut	off: 0.25 C		
Use input partial charg	les			
Generate grid suitable	for peptide docking			
Advanced Settings				
	Lig	Prep	)	
		LigPrep		
Use structur	es from: File	E		
File name:			Browse	
Filter criter	la file:	Create	Browse	
	OPLS3e	Customize Use o	ustomized version	
Force field	Operation of the party of the p			
Ionization:	t change			

Computation

Dutput format: O Maestro SDF

 Retain specified chiralities (vary other chiral centers) Determine chiralities from 3D structure Denarate all combinations Generate at most: 32 per ligand

For SD V2000 input, generate enantiomers if the chiral flag is 0

d new entries as a new group

Ø\* 🔿 Run





# Glide Docking Workflow:

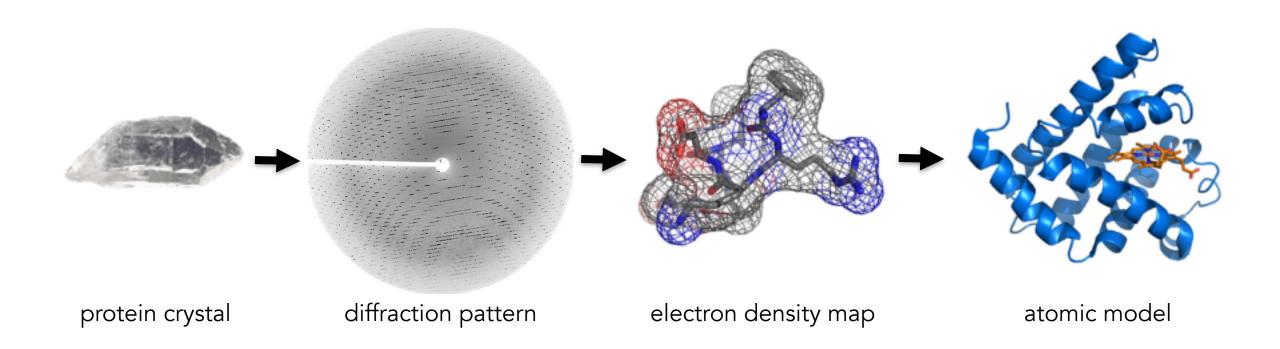
Delay between two in the one of a function to the one	C Protect Preparation Water      Align Price Preparation Water      Heg. Vectors ()
Note:     Othersine Adv       Incurs:     Othersine Adv       Incurs:     Othersine Adv       Incurs:     Othersine Adv       Incurs:     Incurs:       Incurs:	
mode:     Offwelline dati:     Beographical       Magnet distutione file:     Texators       Desting distore formation     Texators       Desting distore     Texators       Desting distors	Import structure into Workspace
Import shares for line and the second status           Mark to share and the second status	Re must
Approve the Workspace checks Approve the Management of the Management Approve the Management of the Management And Management Checks are sub-the foreign to make the Checks are sub-the foreign to make the Check are sub-the foreign to make the foreign to make the Check are sub-the foreign to make the foreign the Check are sub-the foreign to make the foreign the foreign the Check are sub-the foreign to make the foreign the fore	Include: Diffraction data Biological ant
Applies     • State       Representation     • The       Representation     • The    <	input stratue for Brone.
Anter hypergeners:      Anter hypergeners:     Anter hypergener	Proprocess the Workspace structure
Add hydrogens "Service employ hydrogens     Contract parts of period period     Contract period period by the service of	Alge to + beautes array that
Contra revision from the metals Contra revision from the metals Contra revision from the metal and the metals Contra revision from the metal and the metals Contra revision from the metals Contra revision from the metal of the metal instance Contra revision from the metal of the metal instance Contra revision from the metal of the metal instance Contra revision from the metals Contrevision from the metals Contra revision from the metals Contr	🔽 Assign bond orders 🛃 Like CCD database
Constraints resultable baseds Constraints resultable baseds Constraints resultable based based based Constraints resultable based b	D Abt hydrogens Remove original hydrogens
Demonstrate fact states using Epic. per: 7.4 [sc] 2.4	Crease straufice boote     Circuit execution to an execution to a set of the execution
	Delate waters beyond 5.00 1 A from het groupe
Preprinter	Generate net states using Epik: prt 7.8 v/- 2.8
	Preprocess

Dealing with crystal model limitations

Pecupitor Child Generation     Incode Volumes     Constraints Rotatable Groups Excluded Volumes     cooptor  Instant in the Workspace is a receptor plus a ligand, you must the ligand molecule so it can be accluded from they gind generation.     to identify the ligand Molecule
nucture in the Workspace is a receptor plus a figend, you must the figure molecule so it can be excluded from the grid generation. It deteritly the figure (Molecule ) (Show markers) Walar radius scaling on the potential for nonpolar parts of the receptor, you can scale the Walar and of receptor atoms with partial atomic fortunge (absolute scales). It deteritly the scale could be a scale of the receptor will exclude
the ligand molecule is in it can be excluded from the grid generation. to identify the ligand Molecule () () () () () () () () () () () () ()
to identify the ligand Molecule () how markers Waste radius scaling en the potential for nonpoint carts of the receptor, you can acide the Wask rate of experient atoms with partial atoms: charge (absolute ses than the specified cutoff: Al other atoms in the receptor will carded. Put partial charges ate grid suitable for peptide docking ed Settings
en the potential for nonpolar parts of the receptor, you can scale the Wasks rate of receptor atoms with partial atomic forange (absolute received. Tector; 1.0 C Partial charge cutoff; 0.25 C put partial charges ate grid suitable for peptide docking ad Settings
en the potential for nonpolar parts of the receptor, you can scale the Wasks rate of receptor atoms with partial atomic forange (absolute received. Tector; 1.0 C Partial charge cutoff; 0.25 C put partial charges ate grid suitable for peptide docking ad Settings
Waals radii of receptori atoms with partial atomic charge (absolute ses han the specified cutoff. Al other some in the receptor will called. factor: 1.0 C Partial charge cutoff: 0.25 C out partial charges ate grid suitable for poptide docking ed Settings
out partial charges alse grid suitable for peptide docking red Settings
ate grid suitable for peptide docking ed Settings
ed Settings
le-grid_2 0+⊙ R
LigProp
LigPrep
🗧 🗧 🔮 UlgPrep
Use structures from: File
🗧 🗧 🔮 UlgPrep
Use structures from: File
Ue shuches from: File Browse
Us structures from: File Browse File name Browse File offeria file: Create Browse Force find: OP.S32 Coutomize Use customized version Ionization
Costonizario:     Costoni
Constance     Constance
Constance     Constance
Us structures from File Browse Filter criteria file: Create Browse Force find: OP.S32 Customize Use customized version Ionization: Do not change Notatriate
Vie structures from: File Vie structures from: File Vie structures from: File Vie structures from: Vie cutomica Vie c
Utightee Ure structures from: File Ure structures from: File File name File name File collection File col
Castractures for: File     Castractures for: File     Castractures for: File     Castractures     Filer criteria file:     Castractures     Castractures     Castractures     Castractures     Castracture     Castractur
Classical devices from 2 structure     Constance
Constantiants     Constan

•••	🕹 Ligand Docking	
Receptor grid: From file	Display receptor 🖌 Show gri	d boxe
File name:	Brow	vse
Ligands Settings Core	Constraints Torsional Constraints Output	
Ligands to be docked		
We strongly recommend that you prepare MacroModel).	the ligands before docking (for example, with LigPrep or	
Use ligands from: Files		
File name:	Browse	
Range: 1 000	🗘 🗹 End	
Use input partial charges		
Do not dock or score ligands with more that		
Do not dock or score ligands with more that	an: 100 C rotatable bonds	
Scaling of van der Waals radii		
To soften the potential for nonpolar parts o	of the ligand, you can scale the vdW radii of ligand atoms wit than the specified cutoff. No other atoms in the ligand wil b	
Scaling factor: 0.80 0 Partial charge co	utoff: 0.15 0	
ocarring racios, orong o Partial criticage of	alan arta pa	
Job name: glide-dock_SP_2	Ø• ()	Ru

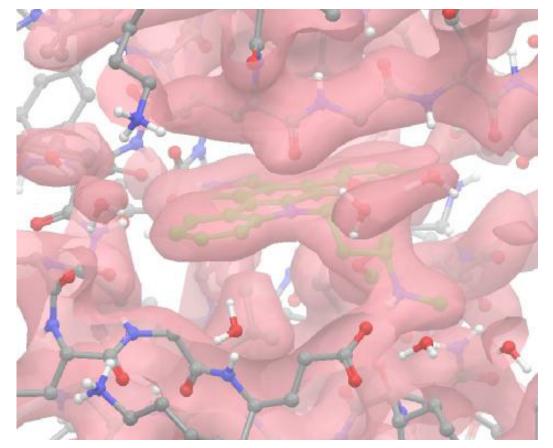
# Most SBDD Projects Utilize Crystal Structures



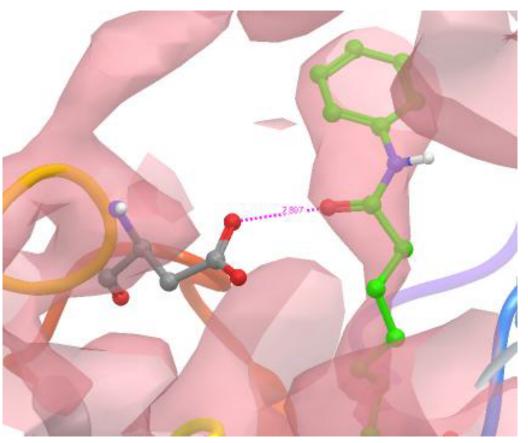


Adapted from: http://www.scistyle.com/

# Limitations to crystal structure models



In this case, the ligand density is relatively unambiguous.



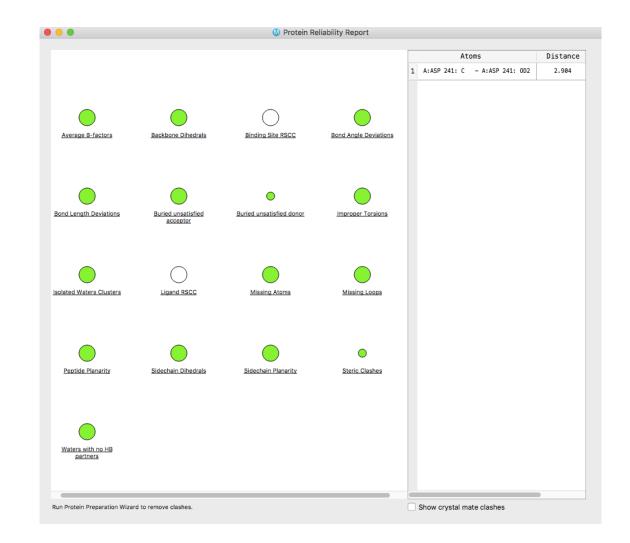
In this case the density is missing, which may result in misleading information.

# Good CADD Starts with Good Science: Minimizing model limitations

1. The quality of your structure matters

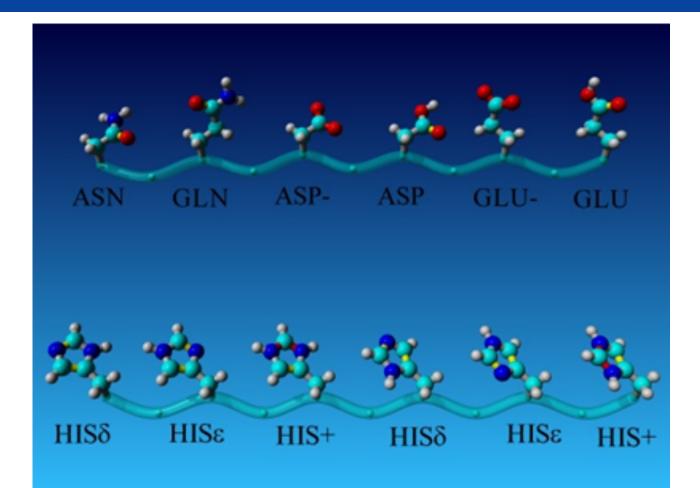
2. The conformational state of your structure matters

3. The design of your experiment matters





# Limitations of crystal structure models continued: Tautomeric states.



pH-dependent tautomeric and protonation states for His, Glu, and Asp

# Protein Preparation Wizard Augments Crystal Data

- Fix common problems
  - Protonation
  - Missing side chains
  - Missing loops
- Remove unwanted molecules
  - Counterions, artifacts of crystallography, waters
  - Biologically relevant?
- Optimize your model structure
  - Hydrogen-bond optimization
  - Restrained minimization

	🔘 Protein Preparation Wizard
Job prefix:	prepwizard Host: localhost (4)
Display hydi	rogens: 🔵 None 💿 Polar only 💿 All ligand, polar receptor 💿 All
	Import and Process Review and Modify Refine
Import st	ructure into Workspace
PDB:	Import
Inclue	de: Diffraction data Biological unit
inclus	
Import st	rructure file: Browse
Preproce	ss the Workspace structure
Align	to:      Selected entry      PDB:
🗹 Assig	n bond orders 🗹 Use CCD database
🔽 Add h	ydrogens Remove original hydrogens
_	e zero-order bonds to metals
	e disulfide bonds ert selenomethionines to methionines
	missing side chains using Prime
	missing loops using Prime ermini
Delet	e waters beyond 5.00 C Å from het groups
Conor	rate het states using Epik: pH: 7.0 +/- 2.0
Prepr	ocess
View Pro	blems Protein Reports Ramachandran Plot
Reset Par	rel



# Glide Docking Workflow:

## Model a protein for the computer

O Protein Preparation Waard	Wizard		Grid Ge	
All species (and an analysis) (and an an analysis) (and an analysis) (an an analysis) (an an analysis) (an an analysis) (an analysis) (an		Def If the Second To Second Second Cond Cond Cond Cond Cond Cond Cond C	Receptor Site Constraints R ne receptor se structure in the Workspace is a receptor plus titly the ligand molecule so it can be excluded fin	otatable Groups Excluded Vo a ligand, you must on the grid generation. Show markers eptor, you can scale the omic charge (absolute a in the receptor will
Van Hutern. Anger Baarte. Konschader Ret.	u ,	Jab name. Proj-hoanka	lide-grid_2 t.	
			LigP	
			Use structures from: File	
			File name:	Browse
			File name:	Create Browse

Ø+ 🔿 Run

Ø\* 🔿 Run

🗹 Desait 💟 Generate tautomers Sterecisomers Computation

Dutput format: O Maestro SDF

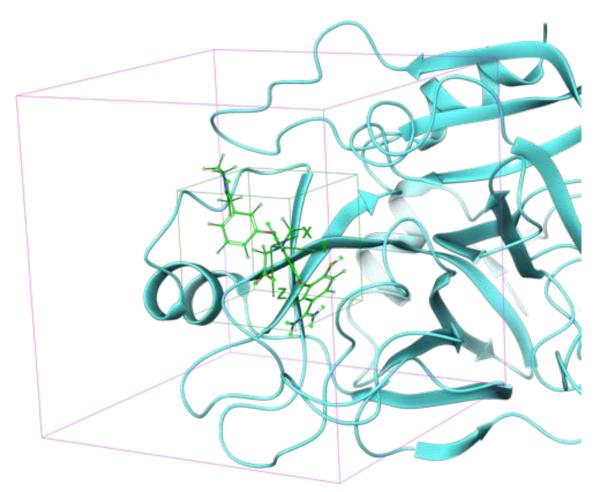
O Retain specified chiralities (vary other chiral centers) Determine chiralities from 3D structure Generate all combinations Generate at most: 32 per ligand

For SD V2000 input, generate enantiomers if the chiral flag is 0

I new entries as a new group

Igand Docking         Receptor grid:       From file         Image:       Image:         Ima
File name:       Browse         Ligands Settings Core Constraints Torsional Constraints Output         Ligands to be docked         We strongly recommend that you prepare the ligands before docking (for example, with LigPrep or MacroModel).         Use ligands from:         File name:         Browse         Range:       1         Use input partial charges         Do not dock or score ligands with more than:       500 ° atoms         Do not dock or score ligands with more than:       100 ° rotatable bonds         Scaling of van der Waals radii
Ligands Settings Core Constraints Torsional Constraints Output Ligands to be docked We strongly recommend that you prepare the ligands before docking (for example, with LigPrep or MacroModel). Use ligands from: Files File name: Browse Range: 1 to: 1000 C End Use input partial charges Do not dock or score ligands with more than: 500 C atoms Do not dock or score ligands with more than: 100 C rotatable bonds Scaling of van der Waals radii
Ligands to be docked We strongly recommend that you prepare the ligands before docking (for example, with LigPrep or MacroModel). Use ligands from: Files File name: Range: 1 0 to: 1000 C End Use input partial charges Do not dock or score ligands with more than: 500 C atoms Do not dock or score ligands with more than: 100 C rotatable bonds Scaling of van der Waals radii
We strongly recommend that you prepare the ligands before docking (for example, with LigPrep or MacroModel). Use ligands from: Files File name: Browse Range: 1 0 to: 1000 C End Use input partial charges Do not dock or score ligands with more than: 500 C atoms Do not dock or score ligands with more than: 100 C rotatable bonds Scaling of van der Waals radii
MacroModel). Use ligands from: Files File name: Browse Range: 1 0 to: 1000 0 End Use input partial charges Do not dock or score ligands with more than: 500 0 atoms Do not dock or score ligands with more than: 100 0 rotatable bonds Scaling of van der Waals radii
Use ligands from: Files  File name: Browse Range: 1 0 to: 1000 C End Use input partial charges Do not dock or score ligands with more than: 500 C atoms Do not dock or score ligands with more than: 100 C rotatable bonds Scaling of van der Waals radii
Range:       1       0       to:       1000       C       End         Use input partial charges       Do not dock or score ligands with more than:       500       0       atoms         Do not dock or score ligands with more than:       100       C       rotatable bonds         Scaling of van der Waals radii       Scaling of van der Waals radii       Scaling of van der Waals radii
Range:       1       0       to:       1000       C       End         Use input partial charges       Do not dock or score ligands with more than:       500       0       atoms         Do not dock or score ligands with more than:       100       C       rotatable bonds         Scaling of van der Waals radii       Scaling of van der Waals radii       Scaling of van der Waals radii
Use input partial charges Do not dock or score ligands with more than: 500 (2) atoms Do not dock or score ligands with more than: 100 (2) rotatable bonds Scaling of van der Waals radii
Do not dock or score ligands with more than: 500 © atoms Do not dock or score ligands with more than: 100 © rotatable bonds Scaling of van der Waals radii
Do not dock or score ligands with more than: 100 🔅 rotatable bonds Scaling of van der Waals radii
Scaling of van der Waals radii
To soften the potential for nonpolar parts of the ligand, you can scale the vdW radii of ligand atoms wi partial atomic charge (absolute value) less than the specified cutoff. No other atoms in the ligand will scaled.
Scaling factor: 0.80 0 Partial charge cutoff: 0.15 0

# What is the role of the grid?



- Protein represented as a series of grids
  - Site point grid (10Å<sup>3</sup> by default)
  - Chemscore grids
  - Adaptive Coulomb/vdW grids
- Grids precomputed once and applied for each ligand
- Ligand "center" must be found within inner box and all ligand atoms must be found within outer box
  - Inner box: 10Å3 by default
  - Outer box: (12Å+0.8\*ligand diameter)3 by default
- With energy-based grids ligand interaction energy for atom in a grid point evaluated using trilinear interpolation
- Want to use Goldilocks inner grid, i.e. smallest grid that will find desired poses



# Glide Docking Workflow:

<text></text>	<section-header></section-header>	State       Bible Docking         State       State         State       State
Ligand states are calculated in water, which may not adequately recapitulate active site		Use input partial charges         Do not dock or score ligands with more than:       500 °; rotatable bonds         Scaling of van der Waals radii       To soften the potential for nonpolar parts of the ligand, you can scale the vdW radii of ligand atoms with partial atoms charge (absolute value) less than the specified cutoff. No other atoms in the ligand will be scaled.         Scaling factor:       0.80 °; Partial charge cutoff:       0.15 °; Run         Job name:       glide-dock_SP_2       Run         Host-bob, incorporate-Append new entries as a new group       ?
		SCHRÖDINGER

# Required Inputs for Protein-Ligand Docking - Ligands

- Glide will only dock ligand states that are provided
- Recommendations for prepared ligand structures

-Use LigPrep to generate low energy ionization/tautomeric states for ligands

•Epik state penalties that estimate free energy required to generate ionization state in water with corrections for interaction with metal sites

-Typical expansion of compounds by ionization/tautomeric/stereo expansion is 2.5x

 Increase or decrease pH value and +/- range depending on target physiological location and project goals
 Methotrexate

bound to DHFR (1U72)

# State penalty=0.0 kcal/mol State penalty=1.43 kcal/mol SCHRÖDINGER.

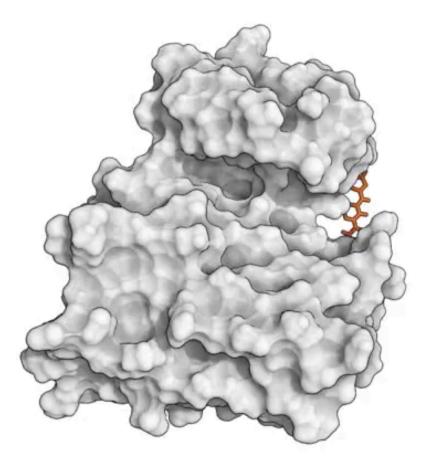
# Glide Docking Workflow:

Protein Prep Wizard	Grid Generation	
All purch TypesLarding       Not purchase the second of the	Receptor Critil Generation         Intervence       Bit       Constraints       Recatable Groups       Excluded Volumes         Under receptor       If the structure in the Workspace is a receptor glus a Signed, you must listentity the Signed molecule so is a necestor from the grig generation.       If the Signed molecule is an isome excluder from the grig generation.         Under Waals radius scaling       If the structure in the potential for nonpote parts of the receptor will build be about across in the receptor will be about the structure in the scaling.         Use input partial charges       If the input partial charges         Index structure is 10 scale across with partial across across the scale build be for peptide docking       Ren         Index readius grid scale across	Clipped Docking         Receptor grid: from file         @ Ligand Docking         Receptor grid: from file         @ Ligand Docking         Receptor grid: from file         @ Ligand Docking         @ Ligand Socking         @ Ligand Socking         @ Ligand Socking         @ Ligands to be docked         @ Wastrongloy recommend that you prepare the ligands before docking (for example, with LigPrep or Sacrohocole).         @ Ligands from: Files         @ Ligands from: Files
Not necessarily accounting for desolvation energies, entropy or protein dynamics	<pre>     Function     Function</pre>	Use input partial charges Do not dock or score ligands with more than: 500 $\bigcirc$ atoms Do not dock or score ligands with more than: 100 $\bigcirc$ rotatable bonds Scaling of van der Waals radii To soften the potential for nonpolar parts of the ligand, you can scale the vdW radii of ligand atoms with scalad. Scaling factor: 0.80 $\bigcirc$ Partial charge cutoff: 0.15 $\bigcirc$ Job name: glide-dock_SP_2 We $\bigcirc$ Run Host-bob, Icorporate-Append new entries as a new group ?

Ø\* 🔿 Ruh

d new entries as a new group.

Proteins are flexible which is a limitation in Glide based docking on its own... but when combined with molecular dynamics can be a powerful tool!

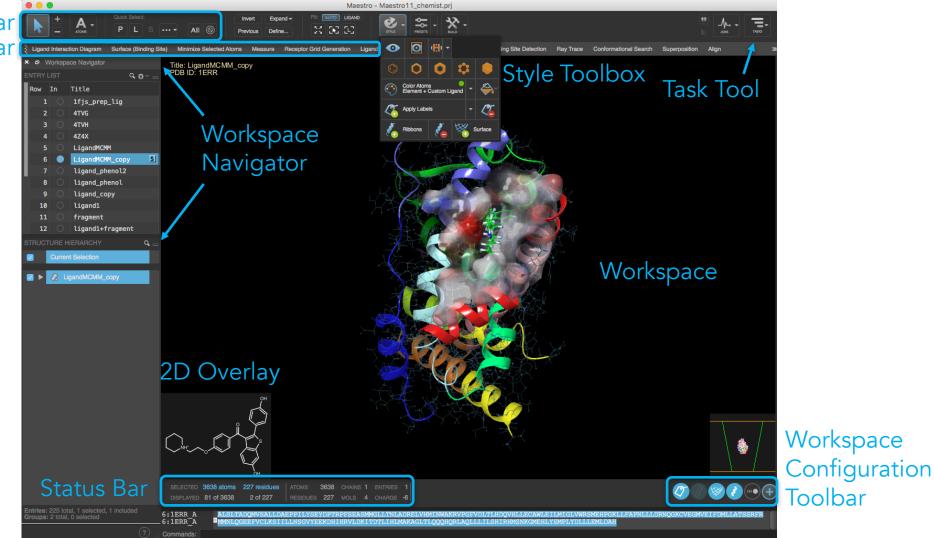




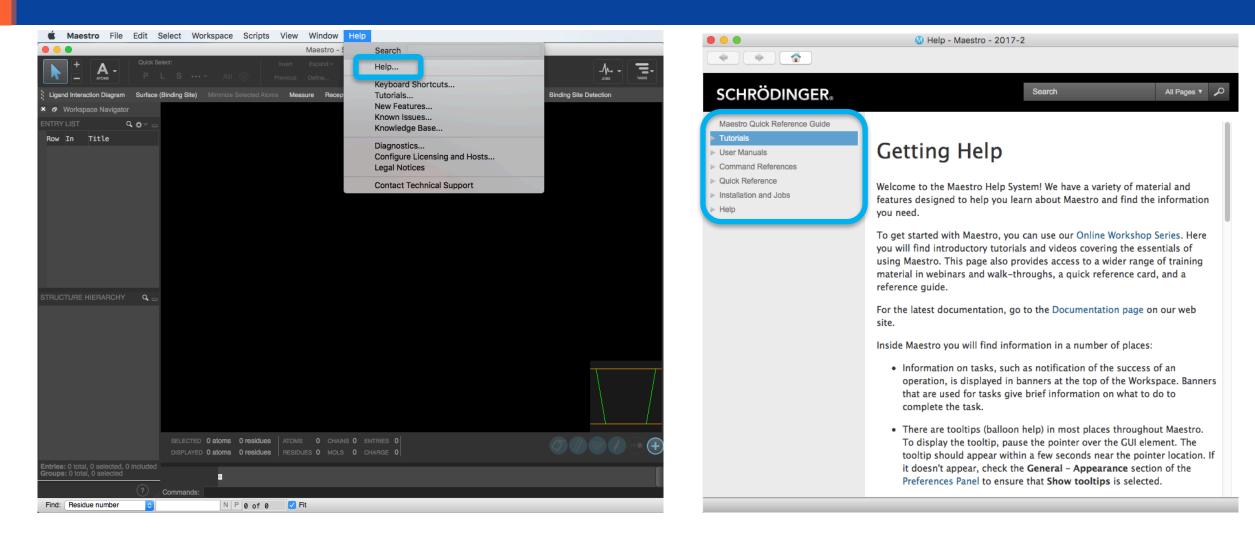


# The Maestro 11 Interface is User Friendly

Selection Toolbar Favorites Toolbar

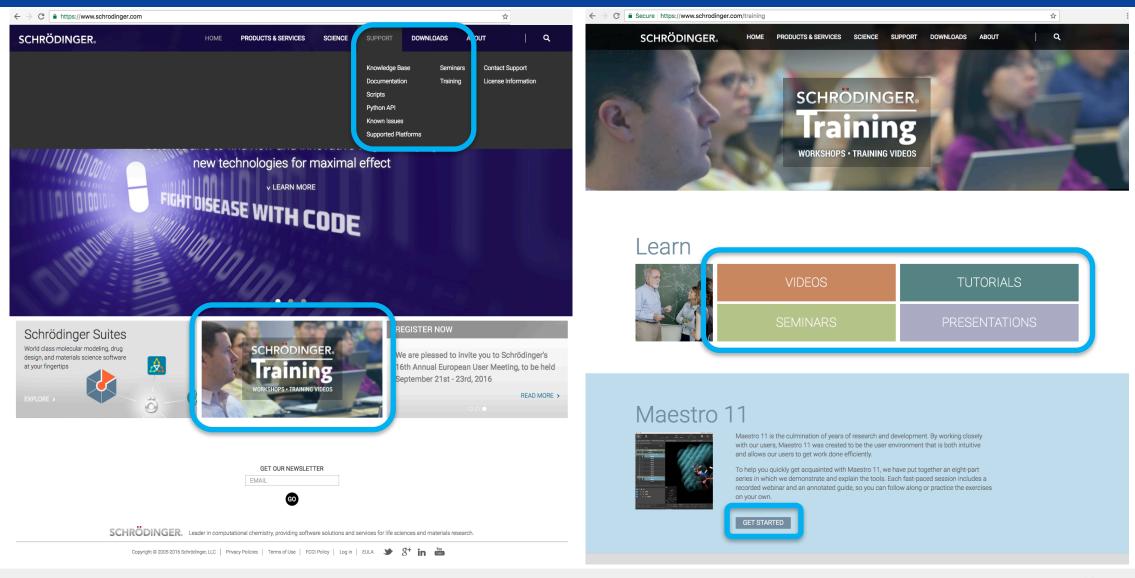


# The Help Menu Contains More Detail





# Learn More with the Training Portal



# Use Our List of Publications to Generate Ideas

$\leftarrow$ $\rightarrow$ C $[$ https://www.schrodinger.com			🖈 🌇 🛆 🖬 🕐 🗄	$\leftarrow$ $\rightarrow$ C $\blacksquare$ https://www.schrodinger.com/pub	olications				*	🖞 🖾 🚺 🕴 E
	Biologics Design DFT-based pKa Prediction	Catalysis and Chemical Reactivit	·	SCHRÖDINGER		RODUCTS & SERVICES S Publication	CIENCE SUPPORT	DOWNLOADS	ABOUT	Q
	Docking and Scoring Force Field Free Energy Methods (FEI Shape-based Screening Water Thermodynamics	Organic Electronics P)			Search			] Q		
	STOLTHAXITHALEHEOL ARN MORE			FILTER BY PRODUCT:		FILTER BY CATEGORY: Biologics Data Analysis and Visue LBDD Lead Optimization Materials Science	alization	Protein Str SBDD Target ID a Virtual Scr		
	••			Publications					Product(s) Referenced	Publication Year
Schrödinger Suites	64.6	REGISTER NOW		ö "Estimation of charge carrier mobility in amou Evansa, D.R.; Kwak, H.S.; Giesen, D.J.; Goldber			model"		Desmond, MS Jaguar	2016
World class molecular modeling, drug	ÖDINGER.	We are pleased to invite you to	-	"Towards understanding the unbound state of Foloppe, N.; Chen, I;, <i>Bioorg. Med. Chem., 20</i>		the intramolecular reorganizati	on energy upon binding"		Desmond, MacroModel	2016
at your fingertips	ining St TRAINING VIDEOS	16th Annual European User Me September 21st - 23rd, 2016	eeting, to be held	ö "Prediction of protein-ligand binding poses via Clark, A.J.; Tiwary, P.; Borrelli, K.; Feng, S.; Mille				s.jctc.6b00201	Induced Fit	2016
	ST THAINING VIDEUS		READ MORE >	ö "Simple Predictive Models of Passive Membri Leung, S. S. F., Sindhikara, D. J., and Jacobson			artition"		Membrane Permeability	2016
				OPLS3: A Force Field Providing Broad Covers Harder, E.; Damm, W.; Maple, J.; Wu, C.; Rebor R.; Friesner, R.A., J. Chem. Theory Comput., 2	ul, M.; Xiang, J.Y.; Wang, L.; Lupyan, D		aus, J.W.; Cerutti, D.S.; Krilov, C	8.; Jorgensen, W.L.; Abe	FEP+, OPLS3	2016
GFT OU	RNEWSLETTER			"Discovery and StructureActivity Relationship Dighe, S.N.; Deora,G.S.; Mora, E.; Nachon, F.; C					Glide, Phase	2016
EMAIL				<ul> <li>"Surface Oxide Characterization and Interface Cabrera, W.J.; Halls, M.D.; Povey, I.M.; Chabal,</li> </ul>			d by in Situ Infrared Spectrosco	ору"	MS Jaguar	2016
	60			"Determination of reactive properties of 1-but Armaković, S.; Armaković, S.J.; Vraneš, M.; To			ions"		MS Jaguar	2016
SCHRÖDINGER. Leader in computational chemistry, pro	widing software solutions and services for life	e sciences and materials research.		*Investigation of boron modified graphene na Armaković, S.; Armaković, S.J., Journal of Ph			and transport properties of gra	phene nanosheets*	MS Jaguar	2016
Copyright @ 2005-2016 Schrödinger, LLC   Privacy Policies   Terms of	of Use   FCOI Policy   Log in   EULA 🔰	9 <sup>+</sup> in 🐃		"Coordination compounds of a hydrazone de	rivative with Co(III), Ni(II), Cu(II) and 2	Zn(II): synthesis, characterizatio	on, reactivity assessment and I	piological evaluation*	MS Jaguar	2016

# Maestro 11 Useful Video Links

- Maestro 11 Quick Start Guide
  - <u>https://www.schrodinger.com/training/maestro11/home</u>
- Maestro 11 Short Videos
  - https://www.schrodinger.com/training/videos/maestro-11
- Maestro 11 Introductory Webinar Series
  - <u>https://www.schrodinger.com/seminars/archives/1238/introductory-series</u>
- Maestro 11 Advanced Webinar Series
  - <u>https://www.schrodinger.com/seminars/archives/1239/advanced</u>
- Protein Preparation Wizard
  - <u>https://www.schrodinger.com/training/videos/protein-preparation</u>
- Other Small-Molecule Drug Discovery Tools
  - <u>https://www.schrodinger.com/training/videos/small-molecule-drug-discovery</u>



# Other Education Resources are Available Online

- Knowledge Base: <u>https://www.schrodinger.com/kb/</u>
- Support Center: <u>https://www.schrodinger.com/supportcenter</u>
- Training Center: <u>https://www.schrodinger.com/training</u>
- Schrödinger Seminar Series: <u>https://www.schrodinger.com/seminars/current</u> <u>https://www.schrodinger.com/seminars/archives</u>
- Script Center: <u>https://www.schrodinger.com/scriptcenter/</u>



# Thanks for Joining Us!

Scientific and Technical Support help@schrodinger.com

Email us for more info at Training@schrodinger.com



