Introduction to Schrodinger's Software



Yuk Sham / Feng Chen Center for Drug Design University of Minnesota MSI Fall Tutorial 2011

Outline

- Software
 - Usage

www.schrodinger.com



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http://www.schrodinger.com/CustomerLogon.php

Documentation



http://www.schrodinger.com/supportdocs/18/

Other presentations

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	Dr. Kathryn Loving Applications Scientist and Maest Manager, Schrödinger	tro Elements Product				

http://www.schrodinger.com/seminarprior/19/

On-line support

help@schrodinger.com

Software

CombiGlide – Combinatorial Library Design Glide – Ligand Docking Impact – Molecular Dynamics Simulation Induced Fit – Ligand Docking Jaguar – Quantum Mechanics Liaison – Predicts Binding Affinity LigPrep – 2D to 3D Ligand Conversion Tool

Software

- MacroModel Molecular Modeling
- <u>Maestro Graphical User Interface</u>
- Phase Pharmacophore Modeling
- Prime Protein Structure Prediction
- QikProp ADME Properties
- Qsite Reaction Mechanism (QM/MM)
- Strike Structural Activity Relationship

Running Maestro

module load schrodinger

maestro

Maestro



Maestro Pull-downs

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Maestro Pull-downs

Maestro		
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3 <u>Fog</u>	Rapid Torsion Scan QikProp	
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Atoms:0/0/0 Entries:0/0 Res:0 Chn:0 Mol:0 Chg:0		Jobs: 0/0
Commands:		
	P Fit	
middle=xy rotate, ctri+middle=2 rotate, right=xy translate, right click on a	atom=spot center, right click on atom/bond and hold=menu	1

You and Your Mouse

Left button click on atom to select atom. Hold down left button and drag to select a group of atoms

Hold down middle button and move the mouse to rotate

Hold down right button and move the mouse to translate

Hold down left and right buttons together and move the mouse to zoom



Aspirin or acetylsalicylic acid

Delete Atoms or Molecules

Maestro	×
Maestro Project Edit View Workspace Tools Applications Workflows Scripts Window Help	
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Commands:	
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Pick atom in residue to update half-bonds	1.

Molecular Representation

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middle=xy rotate; ctrl+middle=z	: rotate; right=xy translate; right click on atom=spot center; right click on atom/bond and hold=me

Workspace / Molecular Representation

Molecular Representation

Molecular Representation	
Settings Atoms Bonds Ribbons	
Default representation: Wire	
Set all to: Wire CPK Tube Ball & S	itick
-Rendering	
Scale wire width Min: 1.0 Max: 3.0	
Wire width (pixels).	2
CPK percentage:	85
Tube radius (Å).	0.16
Thin tube radius (Å):	0.08
Ball percentage:	16
Stick radius (Å):	0.12
Use simplified representation when moving	
Moving resolution:	13
Resting resolution:	13
Restore Defaults	

Workspace / Molecular Representation

Molecular Representation

CPK

Tube

Ball & Stick

Saving Project

Saving Project

Exporting Structures

Export Structures

Export		×
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File names are:	File name + entry name	
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Project / Export Structures

Format: Maestro

Save graphic information: on

Export

Other Formats

By Extension (*.*)

Maestro [uncompressed] (*.mae) Maestro [compressed] (*.maegz *.mae.gz) PDB (*.pdb *.ent) MOL2 (*.mol2) MDL SD [uncompressed] (*.sdf *.sd *.mol) MDL SD [compressed] (*.sdfgz *.sdf.gz) MacroModel (*.dat *.out) GAMESS Input (*.gamin) Gaussian Cartesian (*.cart)

And more

Coloring Atoms

Maestro	
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🔍 < 🏟 12345	
middle=xy rotate; ctrl+middle=z ro	otate; right=xy translate; right click on atom=spot center; right click on atom/bond and hold=me

Workspace / Atom Coloring

Coloring Atoms

🗶 Atom Coloring (coloratom)	🛛 🔀 Atom Coloring (coloratom)
Color Scheme Atom Color Legend for: Element	Color Scheme Atom Color
Color Element	Atom color
<pre>white Hydrogen (H) green Boron (B) gray Carbon (C) blue Nitrogen (N) red Oxygen (O) aquamarine Fluorine (F) orange Silicon (Si) maroon Phosphorus (P) yellow Sulfur (S) dark green Chlorine (Cl) Chain Name Flement Entry Entry (Carbons) Molecule Number (Carbons) Residue Charge Residue Property Residue Position Residue Type</pre>	
Apply current color scheme	Apply current color
Pick: Atoms - All Selection Previous	B Pick: Atoms All Selection Previous
Close He	elp Close Help

Workspace / Atom Bonding Coloring

Coloring Atoms

Minimize Structure Maestro Maestro Project Edit View Workspace Tools Applications Workflows Scripts Window Help Task View 10 R -Open Save As Import Export Table 2D Viewer Lig. Inf eate Entry Clear Save Image New Scene CombiGlide 讎 A 20 ConfGen Fix Rendering Material Undo/Redo Delete Sketcher Add H Transform Core Hopping Contacts Surfaces Select Project Edit View Workspace Style Saved Views Dis Desmond Labels Build Fragments Epik. <u>S</u> Glide 0 Impact Jaguar Liaison. ¢ LigPrep. [+| Current Energy 0 0 MCPRO+ Minimization. 0 Phase Coordinate Scan. 0 Prime Conformational Search. Co M S. PrimeX Redundant Conformer Elimination... ROS QikProp. Multiple Minimization. 0 QSite. Dynamics.. 8 Ś Semi-Empirical... MC/SD. SiteMap.. Embrace Minimization... D Strike Embrace Conformational Search. MINTA. Monitor Jobs. Start Job From File. Atoms:0/21/21 Entries: S/0/0 Res:3 Chn:1 Mol:1 Chg:0 Jobs: 0/0 0 12345 (iii) middle=xy rotate; ctrl+middle=z rotate; right=xy translate; right click on atom=spot center; right click on atom/bond and hold=me

Applications / MacroModel / Minimization

Minimize Structure

Minimization				
Use structures from: Workspace (included entry) 💌 Potential Constraints Substructure Mini				
Force field: OPLS_2005 Solvent: Water Electrostatic treatment: Constant dielectric Dielectric constant: 1.0 Charges from: Force field				
Cutoff: Extended Van der Waals: 8.0 Electrostatic: 20.0 H-bond: 4.0 Debugging Options:			Minimization - Start Output Incorporate: Append new entries as a new group Job Name: mmod mini	Compose
			Host: localhost (4)	Help
Start Write	Close	Help		

Applications / MacroModel / Minimization

Minimize Structure

Monitor		1		_ 🗆 🗙
Job ID	Name	Status	Errs	Start Time
vl7-0-4e85d092	mmod_mini	incorporated : finished	0	2011-09-30
Show: Jobs from this project only Monitor Pause Resum	Monitor frequency: 1	sec	n Un I	Postmortem 1
Details File		Delete		r ostnorteni
Files:	Job summary:			1
Nama		1		
mmod mini.log	Name: Program:	mmod_mini MacroModel		
mmod_min1.tmp	Exit Status:	finished		
mmod_mini-out.ou4	Status:	incorporated		
mmod_mini.inf	Status updated:	2011-09-30-09:22:10		
_mmod_mini-out.jwr	Job Directory:	/scratch/shamvy/mmod mini		
mmod_mini-out.ouX	Job Started:	2011-09-30-09:22:10		
mmod_mini.out.ou6	Job Ended:	2011-09-30-09:22	2:14	
mmod_mini-out.grd	JobId:	vl7-0-4e85d092		
mmod_mini-out.ou3	Sub JobId:	None		
mmod mini-out.ou2	Last updated:	Fri Sep 30 09:23:07 2011		
mmod mini-out.oul	· ·			
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			Close	Help

Minimize Structure

Monitor				
Job ID	Name	Status	Errs	Start Time
vl7-0-4e85d092	mmod_mini	incorporated : fin	nished O	2011-09-30
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Show: Jobs from this project only	Monitor frequency: 1	▼ sec		
Monitor Pause Resum	ie Stop Kill	Update Delete.	Clean Up	Postmortem
Details File				
File: /home/msi/shamyy/msitutoria	l/schrodinger/mmod_mini.log			
ITER= 340 MOVE(A)= 0.	022463 E(KJ/MOL)= -J	104.8531 Grad=	0.14/282/	
Iter= 360 Move(A)= 0.	031397 E(kJ/mol)= -]	104.8538 Grad=	0.1541197	
Iter= 380 Move(A)= 0.	067431 E(kJ/mol)= -]	104.8546 Grad=	0.9251309E-0	01
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Iter= 440 Move(A)= 0.	026208 E(kJ/mol)= -1	104.8562 Grad=	0.1134965	
Iter= 460 Move(A)= 0.	009121 E(kJ/mol)= -1	104.8565 Grad=	0.8531402E-0	01
Iter= 480 Move(A)= 0.	032498 E(KJ/mol) = -1	104.8570 Grad=	0./4135/2E-0	01
Iter= 500 Move(A)= 0.	036495 E(KJ/MOL) = -1	104.8574 Grad=	0.8/90289E-0	51
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э 	Pond = 2.023	34 KJ/mol		
П т		94 KJ/IIIOC こつ レコ/mol		
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Improper i	VDW = 26.96/	10 k1/mol		
Electro	$v_{Dm} = 20.004$	31 k1/mol		
Explicit Hydrogen	Ronds = 0.000	no ki/mol		
Cross	Terms = 0.000	00 kJ/mol		
Solva	tion = -47.7810	kJ/mol		
T.F. for cross-checking:	-105 3106 k1/mc			-
			Close	Help
Minimized Structure



Import PDB file

Minport 🕈											×
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Files of type: PDB (*	.pdb *.ent)							•		Cancel	

Project / Import Structures

Import PDB file





Protein Preparation Wizard				
Job prefix: prepwizard				
Display hydrogens: C None C Polar only C All				
Import and Process Review and Modify Refine	3			
Import structure into Workspace				
	>			
Import structure file: Browse				
2				
Preprocess the Workspace structure				
□ Align to:				
✓ Assign bond orders				
Add hydrogens 🗖 Remove original hydrogens				
✓ Create zero-order bonds to metals				
└ Create disulfide bonds				
Convert selenomethionines to methionines				
Fill in missing side chains using Prime				
Fill in missing loops using Prime				
Cap termini				
Delete waters beyond 5 Å from het groups				
Preprocess				
2				
3				
View Problems Protein Reports Ramachandran Plot				
ResetCI	ose	Help		



Protein Preparation Wizard				
Job prefix: prepwizard				
Display hydrogens: C None C Polar only C All				
Import and Process Review and Modify Refine	\searrow			
Import structure into Workspace				
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Import structure file: Browse				
Preprocess the Workspace structure				
Align to: Selected entry CPDB:				
☑ Assign bond orders				
Add hydrogens 🗖 Remove original hydrogens				
✓ Create zero-order bonds to metals				
🖵 Create disulfide bonds				
Convert selenomethionines to methionines				
Fill in missing side chains using Prime				
Fill in missing loops using Prime				
Cap termini				
Delete waters beyond 5 Å from het groups				
Preprocess				
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View Problems Protein Reports Ramachandran Plot				
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M Protein Preparation Wizard	Protein Preparation Wizard
Job prefix: prepwizard	Job prefix: prepwizard
Display hydrogens: C None C Polar only C All	Display hydrogens: C None C Polar only C All
Import and Process Review and Modify Refine	Import and Process Review and Modify Refine
Import structure into Workspace PDB: 1HVF Import structure file: Browse Preprocess the Workspace structure Align to: € Selected entry C PDB: Import ✓ Add hydrogens Remove original hydrogens ✓ Create zero-order bonds to metals C create disulfide bonds	Analyze Workspace Fit on select Display selection only Pick Delete Select Hets/Waters within 5.0 Å of selected chains Select Hets/Waters Within Chain Name Water No. A B
☐ Fill in missing side chains using Prime	
Fill in missing loops using Prime	Het No. Het Name
Cap termini	1 A:XK2 (263)
✓ Delete waters beyond 5 Å from het groups	
Preprocess	
	Generate States F Metal binding states pH: 7.0 +/- 4.0
	View Problems Protein Reports Remachandran Plot
View Problems Protein Reports Ramachandran Plot	
Reset Close Help	Reset Close Help

💐 Protein Preparation Wizard	Protein Preparation Wizard
Protein Preparation Wizard Job prefix: prepwizard Display hydrogens: None Poter Polar only Import and Process Review and Modif Refine Import structure into Workspace PDB: IMport structure file: Browse Preprocess the Workspace structure Align to: Selected entry PReprocess the Workspace structure Align to: Selected entry PDB: Vation orders Add hydrogens Remove original hydrogens Create zero-order bonds to metals Create zero-order bonds to metals Create disulfide bonds Convert selenomethionines to methionines Fill in missing loops using Prime Fill in missing loops using Prime Cap termini Delete waters beyond S Aftom het groups Preprocess View Problems Protein Reports Ramachandran Plot	Protein Preparation Wizard Job prefix: prepwizard Display hydrogens: None © Polar only © All Import and Process Review and Modify H-bond assignment Exhaustive sampling © Sample water orientations Minimize hydrogens of altered species Sample vater orientations Minimize hydrogens of altered species Sample result: Very low © Low © Neutral © High Optimize Interactive Optimizer Impref minimization ©.30 Å © Hydrogens only Excendent OPLS2005 ♥ Winimize. View Problems View Problems Protein Reports
Reset Close Help	Reset Close Help

Atom Labels

Atom Labels					
Update Existing Labels Clear All Labels Label Preferences Add labels Replace existing label C Append to existing label C Clear labels					
Label atoms All	Selection Previous Select				
All Selection Previous Select Reapply atom labels when Workspace changes Composition Color Hetatom Labels Atom properties: Entry properties:					
PDB atom name Occupancy PDB B Factor (Temperature) Residue name Residue number Chain name Maestro atom name Atom type (MacroModel) Grow name Atom number by molecule Atom number by molecule Atom number by entry Molecule number Molecule number Molecule number by entry constraint internal atom index pdb convert problem atomindex PDB serial segres index het pdb occupancy pdb tfactor	 Stars Title Entry ID Job Name Potential Energy-OPLS-2005 Stretch Energy-OPLS-2005 Bend Energy-OPLS-2005 Torsional Energy-OPLS-2005 Improper Torsional Energy-OPLS-2005 Electrostatic Energy-OPLS-2005 Electrostatic Energy-OPLS-2005 Minimization Converged-OPLS-2005 Minimization Converged-OPLS-2 RMS Derivative-OPLS-2005 prepared assigned bond orders added hydrogens treated metals converted selenomethionines deleted far waters PDB TITLE PDB ID PDB COVETION Table Order Alphabetica 				
	Close Help				

Workspace / Atom Labels



Display / Undisplay

Display/Undisplay Atoms		<u>∼ ⊡ ×</u>
Also display Pick: Molecules	All Selection	Previous Select
Undisplay Pick: Molecules	All Selection	Previous Select
Display only Pick: Molecules	All Selection	Previous Select
Also display:	Undisplay:	Display only:
Protein Backbone	Protein Backbone	Protein Backbone
Protein Side Chains	Protein Side Chains	Protein Side Chains
Waters	Waters	Waters
Nonpolar Hydrogens	Nonpolar Hydrogens	Nonpolar Hydrogens
Polar Hydrogens	Polar Hydrogens	Polar Hydrogens
		CloseHelp

Workspace / Display/Undisplay Atoms

Atom Selection

Atom Selection		
1	Display only	~
Atom Residue Molecule Chain	Entry Substructure Set	
Sequence Residue number Residue type 2 Classification Backbone/side chain Secondary structure PDB conversion status	Residue type: LYS MET PHE PRO SER THR TRP TYR VAL CSO XK2 3	dd 4 tract sect ate Markers matching:
ASL:	🔽 Show markers	
(res.ptype "XK2 ")		
	_	Proximity
	Clear I Invent I Braviava I Calaction I Atom Num I	Create Set
	Clear Invert Previous Selection Atom Num	Resilium
Matching 84 atoms	OK Cancel	Help

Atom Selection

Atom Selection	
1	Display only
Atom Residue Molecule Chain	Entry Substructure Set
Sequence Residue number Residue type 2 Classification Backbone/side chain Secondary structure PDB conversion status	Residue type: LYS MET PHE PRO SER THR TRP TYR VAL CSO XK2 3
ASL:	Show markers
(res.ptype "XK2 ")	Proximity Create Set
All Undo Redo C	Clear Invert Previous Selection Atom Num Res Num
Matching 84 atoms	4 OK Cancel Help

Display / Undisplay



Displaying Binding site

Atom Selection		
1	Display only	<i>b</i>
Atom Residue Molecule Chain	Entry Substructure Set	
Sequence Residue number Residue type 2 Classification Backbone/side chain Secondary structure PDB conversion status 3	Residue type: LYS MET PHE PRO SER THR TRP TYR VAL CSO XK2	Add 4 Subtract Intersect Update Markers Atoms matching: 84
ASL:	🔽 Shov	v markers
fillres within 6 ((res.ptype "XK	(2 "))	5 Proximity Create Set
All Undo Redo (Clear Invert Previous Selection	Atom Num Res Num
Matching 729 atoms	6 OK	Cancel Help

Selecting with "Proximity"



Displaying Binding site



Displaying Ribbons



Displaying Ribbons



Display Binding Site Surface



Workspace / Surface / Molecular Surface

Display Binding Site Surface

Atom Selection	2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 - 2 -	<u>.</u>		
	Atoms for surface display			3
Atom Residue Molecule Chain	Entry Substructure Set			
Sequence Residue number Residue type Classification Backbone/side chain Secondary structure PDB conversion status	Residue type: LYS MET PHE PRO SER THR TRP TYR VAL CSO XK2		A Sub Inter Upd Atoms 84	dd tract sect ate Markers matching:
ASL:		🔽 Sho	w markers	
(fillres within 4 ((res.ptype "X	K2 "))) AND NOT ((res.pt	ype "XK2	"))	Proximity Create Set
All Undo Redo C	Clear Invert Previous	Selection	Atom Num	Res Num
Matching 492 atoms		ок	Cancel	Help

Display Binding Site Surface



Manage Surfaces

					Surface Display Options
					Transparency: Front surface: 52 Adjust together Back surface: 52 Adjust together
Manana Surfaces					Color scheme:
V Limit Entry 6: 1HVR	Volume Name Surface Molecula	Name Comments ir Surf…	Surface Type Isova molecular s	lue Area 2490.2	Color ramp: Red_White_Blue Minimum: -0.3
Import Duplicate Delete	Split Limit Ex	port to Map. Display Option	s	L	Maximum: 0.3 Constant Color: Gray
Isovalue: Display at most: 10 Å?			Cl	ose Help	Negative color: Red C Map values from volume data:
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					Color ramp: Red_White_Blue
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Workspace / Surface / Manage Surfaces

Manage Surfaces



Detach Molecules



Detach Molecules



Delete Molecules

Details File			
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> Metabolism like	ely: benzylic-like H -> a	lcohol][
Principal Descrip	otors:	(Range 95% of Drugs)	
Solute	Molecular Weight =	= 606.763 (130.0 / 725.0)	
Solute	Dipole Moment (D) =	= 4.480 (1.0 / 12.5)	ч
Solute	Iotal SASA =	= 897.034 (300.0 /1000.0)	Ш
Solute	Hydrophobic SASA =	= 62.654 (0.0 / /50.0)	Ш
Solute	Hydrophilic SASA =	= 87.837 (7.0 / 330.0)	Ш
Solute	Carbon Pi SASA =	= 746.542 (0.0 / 450.0)*	Ш
Solute	Weakly Polar SASA =	= 0.000 (0.0 / 1/5.0)	Ш
Solute	Molecular Volume (A^3)=	= 1804.300 (500.0 /2000.0)	Ш
Solute	vdW Polar SA (PSA) =	63.320 (7.0 / 200.0)	Ш
Solute	No. of Rotatable Bonds=	= 10.000 (0.0 / 15.0)	Ш
Solute as Dor	nor - Hydrogen Bonds =	= 2.000 (0.0 / 6.0)	Ш
Solute as Acc	ceptor - Hydrogen Bonds =	= 5.400 (2.0 / 20.0)	11
Solute Globul	larity (Sphere = 1) =	- 0.799 (0.75 / 0.95)	
Solute Ioniza	ation Potential (eV) =	8.533 (7.9 / 10.5)	
Solute Electr	ron Affinity (ev) =	= 0.741 (-0.9 / 1.7)	
Predictions for H	Properties:		
QP Polarizabili	ty (Angstroms^3) =	= 66./63M (13.0 / /0.0)	
QP Log P for	hexadecane/gas =	= 21.152M (4.0 / 18.0)*	
QP Log P for	octanol/gas =	= 29.090M (8.0 / 35.0)	
QP Log P for	water/gas =	= 13.596M (4.0 / 45.0)	
QP Log P for	octanol/water =	= 8.481 (-2.0 / 6.5)*	
QP Log S for	aqueous solubility =	8.808 (- 6.5 / 0.5)*	
QP Log S - cont	formation independent =	11.009 (- 6.5 / 0.5)	
QP Log K hsa Se	erum Protein Binding =	= 1.986 (-1.5 / 1.5)*	
QP Log BB for	brain/blood =	-0.956 (-3.0 / 1.2)	
No. of Primary	Metabolites =	= 6 (1.0 / 8.0)	
Predicted CNS /	ACTIVITY (to ++) =		
HERG K+ Channel	L BLOCKAGE: LOG IL50 =	8.344 (concern below -5)	-1
Apparent Caco-2	<pre>2 Permeability (nm/sec) =</pre>	= 1455 (<25 poor, >500 great)	-1

Close

Delete Molecules

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Tools / Measurements / Distance

QikProp

Maestro	
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Atoms:0/48/84 Entries:1/7 Res:1 Chn:1 Mol:1 Chg:0	☐ Identify the 5 most similar drug molecules
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Applications / QikProp



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Princ	ipal Descrip	tors:			(F	Rand	ne 95% o	of Dru	as)		
S	Solute	Molecular	Weight	=	606.763	(]	130.0 /	725.0)		
s	Solute	Dipole Mon	nent (D)	=	4.480	(1.0 /	12.5)		
S	Solute	Total	SASA	=	897.034	(3	300.0 /1	1000.0)		
S	Solute	Hydrophobi	c SASA	=	62.654	(0.0 /	750.0)		
S	Solute	Hydrophili	.c SASA	=	87.837	(7.0 /	330.0			
5	Solute	Carbon Pi	SASA	=	746.542	(0.0 /	450.0)***		
S	Solute	Weakly Pol	ar SASA	=	0.000	(0.0 /	175.0)		
	Solute	Molecular	Volume (A	^3)=	1804.300	(5	00.0 /2	2000.0	0		
	solute	VOW Polar	SA (PSA)	=	10,000	ì	7.07	200.0	0		
	Solute as Don	NO. OF HV	Inden Bon	de –	2 000	ì	0.0 /	13.0	0		
	Solute as Acc	entor - Hyd	rogen Bon	ds =	5 400	è	20/	20.0))		
9	Solute Globul	arity (So	here = 1	=	0.799	è	0.75 /	0.95)		
9	Solute Ioniza	tion Potent	ial (eV)	=	8.533	(7.9 /	10.5)		
5	Solute Electr	on Affinity	(eV)	=	0.741	(-0.9 /	1.7)		
Predi	ctions for P	roperties:									
QP	Polarizabili	ty (Angstro	oms^3)	=	66.763M	(13.0 /	70.0)		
QP	log P for	hexadeca	ne/gas	=	21.152M	(4.0 /	18.0)*		
QP	log P for	octanol/	′gas	=	29.090M	(8.0 /	35.0)		
QP	log P for	water/ga	as	=	13.596M	(4.0 /	45.0)		
QP	log P for	octanol/	water .	=	8.481	(-2.0 /	6.5)*		
QP	log S for	aqueous so	lubility	=	-8.808	(-6.5 /	0.5)*		
QP ap	Log S - cont	ormation in	idependent	=	-11.009	(-6.5 /	0.5))+		
	log K nsa Se	rum Proteir		=	1.986	(-1.5 /	1.5	.) ↑		
	of Brimary	Motobolitor	.000	=	-0.956	ì	-3.0/	1.2	.)		
Dre	dicted CNS A	netabotites Activity (, to ++)	_		(1.0 /	0.0	·/		
HER	G K+ Channel	Blockage.	log IC50	_	- 8, 344	(oncern h	pelow	-5)		
App	arent Caco-2	2 Permeabili	tγ (nm/se	c) =	1455	(<2	25 poor,	, >500	great)		-
										Close	Help

Applications / QikProp



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Princ	ipal Descrip	tors:			(F	Rand	ne 95% o	of Dru	as)		
S	Solute	Molecular	Weight	=	606.763	(]	130.0 /	725.0)		
s	Solute	Dipole Mon	nent (D)	=	4.480	(1.0 /	12.5)		
S	Solute	Total	SASA	=	897.034	(3	300.0 /1	1000.0)		
S	Solute	Hydrophobi	c SASA	=	62.654	(0.0 /	750.0)		
S	Solute	Hydrophili	c SASA	=	87.837	(7.0 /	330.0			
5	Solute	Carbon Pi	SASA	=	746.542	(0.0 /	450.0)***		
S	Solute	Weakly Pol	ar SASA	=	0.000	(0.0 /	175.0)		
	Solute	Molecular	Volume (A	^3)=	1804.300	(5	00.0 /2	2000.0	0		
	solute	VOW Polar	SA (PSA)	=	10,000	ì	7.07	200.0	0		
	Solute as Don	NO. OF HV	Inden Bon	de –	2 000	ì	0.0 /	13.0	0		
	Solute as Don	entor - Hyd	rogen Bon	ds =	5 400	è	20/	20.0))		
9	Solute Globul	arity (So	here = 1	=	0.799	è	0.75 /	0.95)		
9	Solute Ioniza	tion Potent	ial (eV)	=	8.533	(7.9 /	10.5	.)		
5	Solute Electr	on Affinity	(eV)	=	0.741	(-0.9 /	1.7)		
Predi	ctions for P	roperties:									
QP	Polarizabili	ty (Angstro	oms^3)	=	66.763M	(13.0 /	70.0)		
QP	log P for	hexadeca	ne/gas	=	21.152M	(4.0 /	18.0)*		
QP	log P for	octanol/	′gas	=	29.090M	(8.0 /	35.0)		
QP	log P for	water/ga	as	=	13.596M	(4.0 /	45.0)		
QP	log P for	octanol/	water .	=	8.481	(-2.0 /	6.5)*		
QP	log S for	aqueous so	lubility	=	-8.808	(-6.5 /	0.5)*		
QP ap	Log S - cont	ormation in	idependent	=	-11.009	(-6.5 /	0.5))+		
	log K nsa Se	rum Proteir		=	1.986	(-1.5 /	1.5	.) ↑		
	of Brimary	Motobolitor	.000	=	-0.956	ì	-3.0/	1.2	.)		
Dre	dicted CNS A	netabotites Activity (, to ++)	_		(1.0 /	0.0	·/		
HER	G K+ Channel	Blockage.	log IC50	_	- 8, 344	(oncern h	pelow	-5)		
App	arent Caco-2	2 Permeabili	tγ (nm/se	c) =	1455	(<2	25 poor,	, >500	great)		-
										Close	Help

Applications / QikProp

Project Table

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	Close Help													
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Project / Show Table

Questions?