















Schrodinger Chinese manual 薛定谔使用基本教程

薛定谔安装教程:

<http://library.shanghaitech.edu.cn/3986/list.htm>

Schrodinger图形界面工具

-  BioLuminate 3.7
-  Canvas
-  Configure Software
-  Diagnostics
-  Knime
-  Low Graphics Versions
-  Maestro 12.2
-  Maestro Elements 4.0
-  Manuals
-  Materials Science 3.6
-  Remote Login Configuration
-  Schrodinger Command Prompt
-  Schrodinger Power Shell
-  Uninstall

- Bioluminate 绘图及调用部分软件包（蛋白蛋白对接等）
- Maestro 最主要的计算生物学工具集
- Knime 自定义薛定谔workflow、pipeline
- Canvas 化学反应预测及化学反应数据库构建
- Configure 安装薛定谔license
- Diagnostics 当你需要联系薛定谔技术支持时，用这个来生成诊断信息



本地使用: 薛定谔安装教程:
<http://library.shanghaitech.edu.cn/3986/list.htm>

集群使用: 安装完成后, 需要修改安装目录下的schrodinger.host文件

```
(base) [baifang@hpc-login-gpu01 MS21]$ ls
aacg-v3.5      config      fep_binding_pose  impact-v9.0      ligand_strain    para_testapp     prime           run           tutorials
autots        consensus_nomology  fep_plus          installation_check  ligprep          pfam             prime_mmghsa   schrodinger.hosts  utilities
bioluminate   covalent_docking  fep_solubility   internal          lsbd             phase_build_qsar  primex         shape_screen     version.txt
bioluminate-v4.2  desmond        ffb_fep_plus     jaguar           machid           phase_database   psp-v6.3      shape_screen_gpu  vsw
blast         desmond-v6.5     gfxinfo          jaguar-v11.1     macromodel       phase_find_common  qikfit        sitemap
bmin          diagnostics      glide            jobcontrol       maestro          phase_fqsar      qikprop       ska
canvas        docs             glide-v9.0       jsc              maestro          phase_hypo_refine  qikprop-v6.7  ssp
canvas-v4.7    elements        hppmap           knime            maestro-v12.7   phase_qsar       qiksim        sta
combiglide-v6.0  epik            ifd              knime-v5.3      materials        phase_screen     qpld          structurebased_adme
confgen        epik-v5.5       ifcmd            licadmin         mmshare-v5.3    pipeline         qsite        testapp
confgenx       fep_absolute_binding  impact          licenses         mxmd             pldb-v5.3       queues        thirdparty
```

在Host文件中添加信息:

CPU队列

name: HPC_CPU
host: hpc-login-gpu01 (登录节点)
user: 用户名
queue: Torque
qargs: -q 队列名 -l nodes=1:ppn=%NPROC%
schrodinger: 自己的薛定谔安装路径
processors: 240
processors_per_node: 28
tmpdir: 自定义临时文件路径

GPU队列

name: HPC_GPU (名字可以随便起)
host: hpc-login-gpu01 (登录节点)
user: 用户名
queue: Torque
qargs: -q 队列名 -l nodes=1:ppn=%NPROC%:gpus=%NPROC%
schrodinger: 自己的薛定谔安装路径
processors: 16
processors_per_node: 4
tmpdir: 自定义临时文件路径
(显卡类型和数量要跟随你使用的GPU节点来更换)
gpgpu: 0, Tesla V100
gpgpu: 1, Tesla V100
gpgpu: 2, Tesla V100
gpgpu: 3, Tesla V100



```
# Guide for a description of the settings that can be made here.
#
##### NOTE #####
# The 'localhost' entry is special:
# * Settings in the 'localhost' entry are implicitly included in
#   every other host entry as well, so settings common to all entries
#   can be placed in the localhost entry.
# * The 'schrodinger:', 'host:' and 'queue:' fields may not be used in
#   the localhost entry.
#####
#
name: localhost
tmpdir: /public/hc[redacted]/tmp

# HPC CPU
name: HPC_CPU
host: hpc-login-gpu01
user: [redacted]
queue: Torque
qargs: -q s[redacted]u -l nodes=1:ppn=%NPROC%
schrodinger: /public/home/[redacted]esktop/Software/MS21
processors: 240
processors_per_node: 28
tmpdir: /public/hc[redacted]/tmp
#
name: HPC_CPU
host: HPC-login
user: [redacted]
queue: Torque
qargs: -q s[redacted]u -l nodes=1:ppn=%NPROC%
schrodinger: /public/home/[redacted]Software/MS21
processors: 240
processors_per_node: 28
tmpdir: /public/hc[redacted]/tmp

name: HPC_GPU
host: hpc-login-gpu01
user: [redacted]
queue: Torque
qargs: -q s[redacted] nodes=1:ppn=%NPROC%:gpus=%NPROC%:v100
schrodinger: /public/home/[redacted]Software/MS21
processors: 16
processors_per_node: 4
tmpdir: /public/hc[redacted]/tmp
gpgpu: 0, Tesla V100
gpgpu: 1, Tesla V100
gpgpu: 2, Tesla V100
gpgpu: 3, Tesla V100
```

最终示例Host文件:

队列名

用户名

登录节点

安装路径

当使用v100系列节点



Maestro基本界面

通过各种方式选择特定的一组原子或扩充选定的原子：**ASL expression**

Style: 调整所选中原子的展示方式，蛋白的cartoon形式

TABLE 展示每个entry的详细信息

TASK 面板，显示可用APP

Project名称: **Scrath Project**即临时Project

可控制鼠标点选后是增加选中还是取消选中

可控制鼠标点选选中的内容，**ATOM** 还是 **Residue**等

Project Table

这里会展示你workspace里的东西

在这里调整视角，整体视角、配体视角或选中的视角 (**focus**在什么上)

Build: 调整结构，画分子，修改键长键角，添加 **Fragment**等

Preset: 设置调整workspace时自动应用哪些设置，如自动**focus**到配体

Monitor 展示你每个job的信息

一系列你添加星号的app

动力学轨迹面板 (默认不调出)

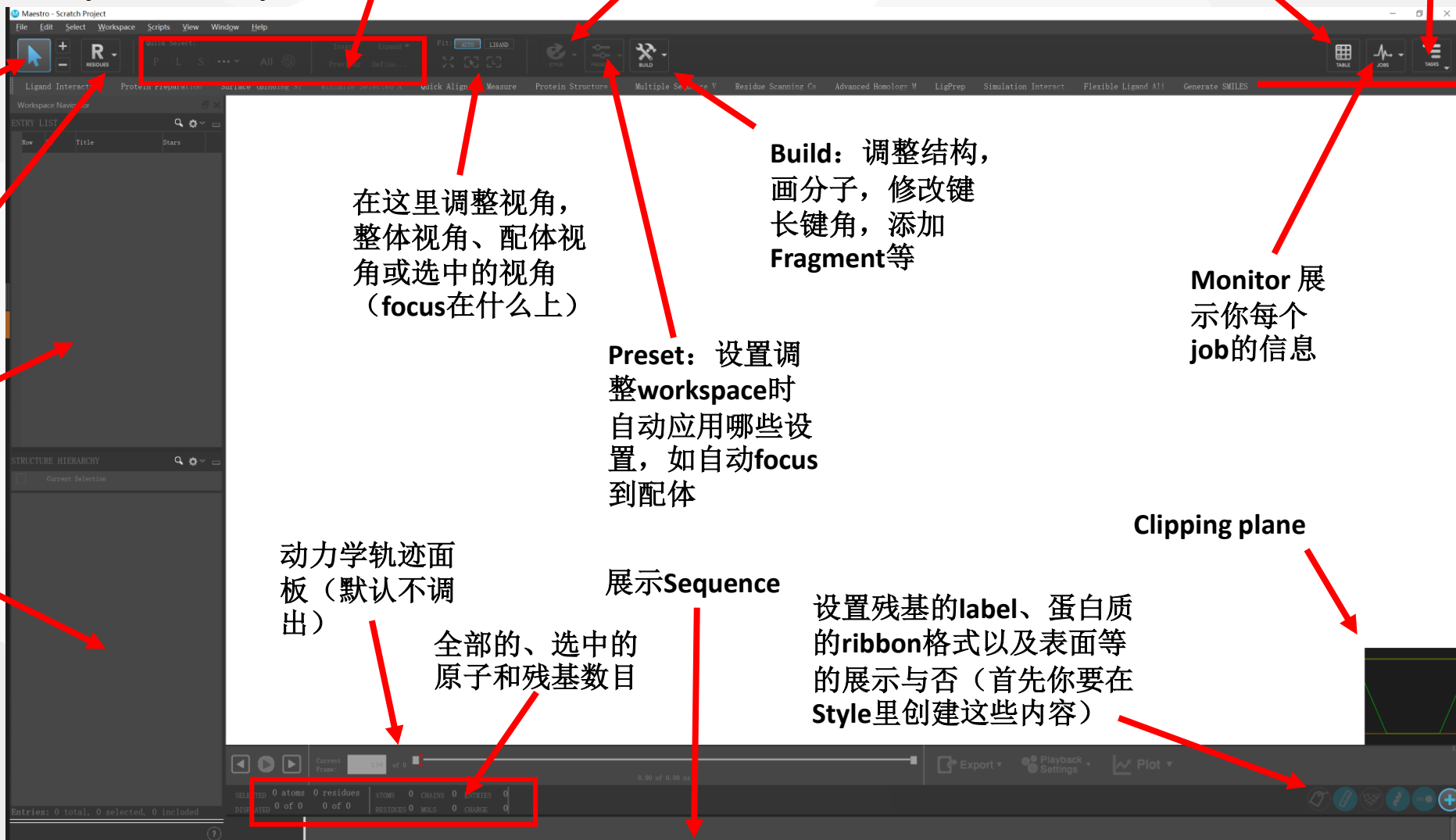
展示**Sequence**

设置残基的**label**、蛋白质的**ribbon**格式以及表面等的展示与否 (首先你要在**Style**里创建这些内容)

Clipping plane

设置整体设置，如是否展示左边的**Project table**、是否展示小分子**2D**结构等

全部的、选中的原子和残基数目



SELECTED	0 atoms	0 residues	ATOMS	0	CHAINS	0	ENTRIES	0
INCLUDED	0 of 0	0 of 0	RESIDUES	0	MOLE	0	CHANGE	0

Table: Project Table中不同Entry的详细信息

这些功能有时候会用到，比如sort，比如plot，比如2D viewer（概览选中的Entry的二维结构，在看一些小分子的共性的时候很有用），再比如Find（可以寻找一些特定Entry）

The screenshot shows the Project Table software interface. The main window displays a table with columns: Row, In, Title, Stars, Entry ID, Date Added, Date Modified, PDB TITLE, PDB ID, PDB RESOLUTION, PDB EXPDTA, PDB EXPDTA TEMPERATURE, PDB EXPDTA PH, Source Path, Source File, Source File Index, prepared, Job Name. A context menu is open over the table, listing options like Hide, Sort Selected (Ascending/Descending), Sort All (Ascending/Descending), Color By Property Value, Select By Property Value..., Deselect Duplicate Values, Change Case of Values, Fit To, Move To, Copy Property..., Edit Property, Delete Property, and Show Property in Workspace. A Property Tree panel on the right shows a search bar and a list of properties for the selected entry.

Row	In	Title	Stars	Entry ID	Date Added	Date Modified	PDB TITLE	PDB ID	PDB RESOLUTION	PDB EXPDTA	PDB EXPDTA TEMPERATURE	PDB EXPDTA PH	Source Path	Source File	Source File Index	prepared	Job Name
28		PDE6D (27) PDE6D-FL-5TB5	★★★★		14 5月 21:58	16 5月 17:36	CRYSTAL ...	5TB5	2.000	X-RAY DIF...	100.000		F:\Schrodin...	5tb5.pdb	1		
29		CRBN (17) 6UML	☆☆☆☆	29					3.580	EXPDTA				6uml.pdb	1		
30		4M91	☆☆☆☆						1.100					4m91.pdb	1		
31		4TZ4	☆☆☆☆	31					3.010					4tz4.pdb	1		
32		6H0G	☆☆☆☆	37					4.250	RAY DIF...				6h0g.pdb	1		
33		6H0G	★★★★	42					4.250	RAY DIF...				6h0g.pdb	1		
34		6H0F	☆☆☆☆	38					3.250	RAY DIF...				6h0f.pdb	1		
35		6H0F	★★★★	43					3.250	RAY DIF...				6h0f.pdb	1		
36		5HXB	★★★★	39					3.600	RAY DIF...				5hxb.pdb	1		
37		5FQD	★★★★	40					2.450	RAY DIF...				5fqd.pdb	1		
38		5V30	☆☆☆☆	41	14 5月 22:40	16 5月 15:55	CEREBLON...	5V30	3.200	RAY DIF...				5v30.pdb	1		
39		CRBN-PROTAC (7) 6BN7	☆☆☆☆	32	14 5月 22:40	15 5月 12:54	CRYSTAL ...	6BN7	3.500	RAY DIF...				6bn7.pdb	1		
40		6BN7 - preprocessed	☆☆☆☆	66	16 5月 17:36	16 5月 17:43								6bn7.pdb	1		
41		6BN7 - preprocessed	☆☆☆☆	44	15 5月 12:54	16 5月 17:43	CRYSTAL ...	6BN7	3.500	RAY DIF...				6bn7.pdb	1		
42		6BN9	☆☆☆☆	33	14 5月 22:40	16 5月 17:43	CRYSTAL ...	6BN9	4.380	RAY DIF...				6bn9.pdb	1		
43		6BN8	★★★★	34	14 5月 22:40	16 5月 17:14	CRYSTAL ...	6BN8	3.990	RAY DIF...				6bn8.pdb	1		
44		6BN8	★★★★	35	14 5月 22:40	16 5月 17:14	CRYSTAL ...	6BN8	6.340	RAY DIF...				6bn8.pdb	1		
45		6BOY	☆☆☆☆	36	14 5月 22:40	14 5月 23:07	CRYSTAL ...	6BOY	3.330	RAY DIF...				6bo.pdb	1		
46		SW7	☆☆☆☆	45	14 5月 22:40	16 5月 15:55	CEREBLON...	5V30	3.200					5v3.pdb	1		
47		Y70	☆☆☆☆	46	14 5月 22:40	16 5月 15:56	STRUCTUR...	6H0F	3.250	RAY DIF...				6h0.pdb	1		
48		L7Y	☆☆☆☆	47	14 5月 22:40	16 5月 15:56	STRUCTUR...	5FQD	2.450					5fqd.pdb	1		
49		prepwizard_4-out1 (9) SW7	☆☆☆☆	48	16 5月 15:59	16 5月 18:07	CEREBLON...	5V30	3.200	RAY DIF...				5v30.pdb	1		prepwi...
50		L7Y	☆☆☆☆	50	16 5月 15:59	16 5月 18:14	STRUCTUR...	5FQD	2.450	RAY DIF...				5fqd.pdb	1		prepwi...
51		L7Y-Z	☆☆☆☆	73	16 5月 18:12	16 5月 18:13											
52		Y70	☆☆☆☆	49	16 5月 15:59	16 5月 18:12	STRUCTUR...	6H0F	3.250	RAY DIF...				6h0f.pdb	1		prepwi...
53		134780	☆☆☆☆	70	16 5月 18:04	16 5月 18:12								Conformer3D...	1		
54		216326	☆☆☆☆	71	16 5月 18:04	16 5月 18:05								Conformer3D...	1		

Stars: 标记你的Entry, 这可能在manual screen一些计算结果的时候很有用

可对属性进行排序, 比如Docking Score

可用Copy Property将某项属性copy到Title从而设置为标题

所有Entry具有的所有属性, 一般可以查看薛定谔计算结果中不同app返回的不同属性, 如glide产生的Docking score

主界面Project Table---Workspace Navigator的使用

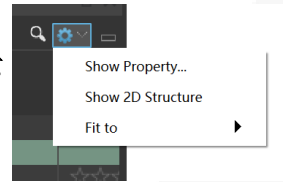


Row	In	Title	Stars
28		PDE6D (27)	
		PDE6D-FL-5TB5	★★★★
	1	CRBN (17)	
29		6UML	
30		4M91	
31		4TZ4	
32		6HOG	
33		6HOG	★★★★
34		6HOF	
35		6HOF	★★★★
36		5HXB	★★★★
37		5FQD	
38		5V30	
	1	CRBN-PROTAC (7)	
39		6BN7	
40		6BN7 - preprocessed	
41		6BN7 - preprocessed	
42		6BN9	

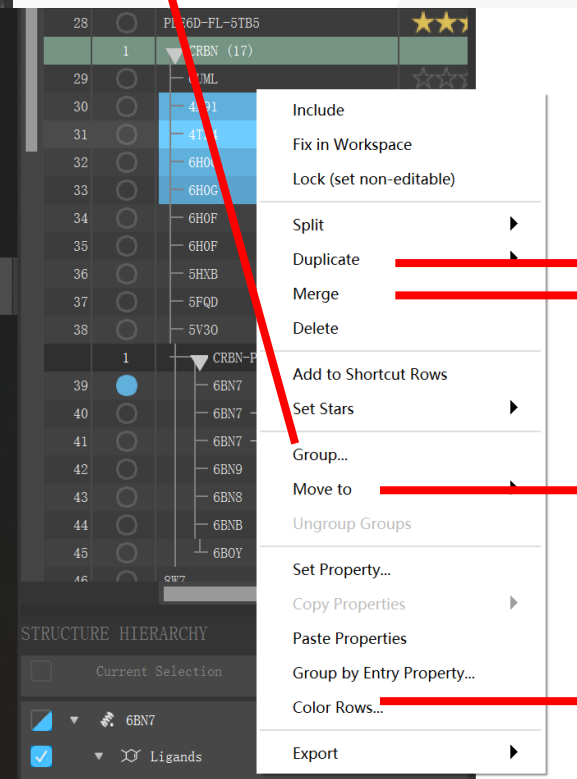
搜索Entry

可以调节显示的column

可以进行分组



双击可以将Entry锁定在workspace

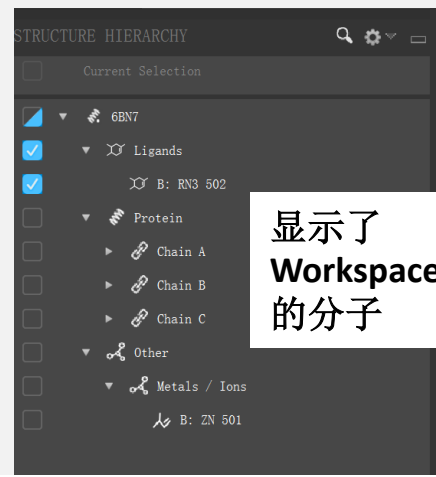


复制Entry

合并Entry (如将小分子和蛋白合并成一个复合物)

移动Entry

给Entry加特定颜色, 另一种标记法 (Stars比这个更简单些)



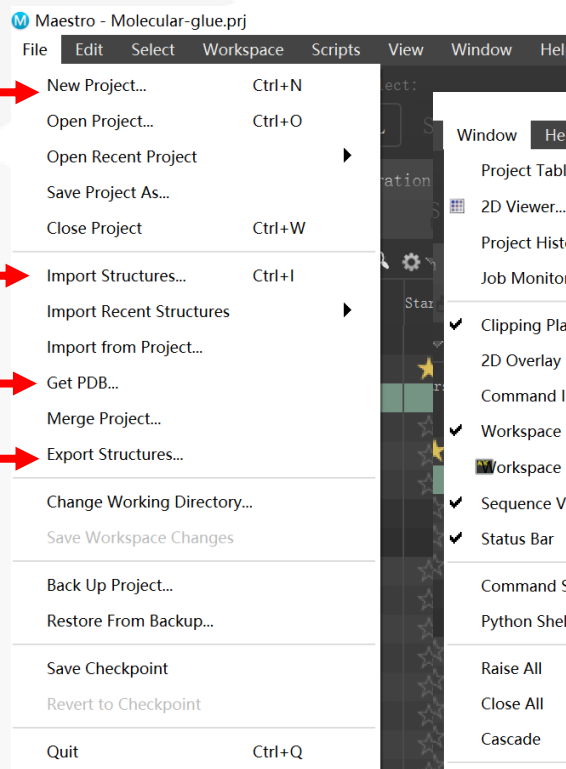
显示了Workspace中有的分子

显示了总Entry的数据, 选中以及include (在workspace中显示的) 的Entry的数目



主界面选项卡

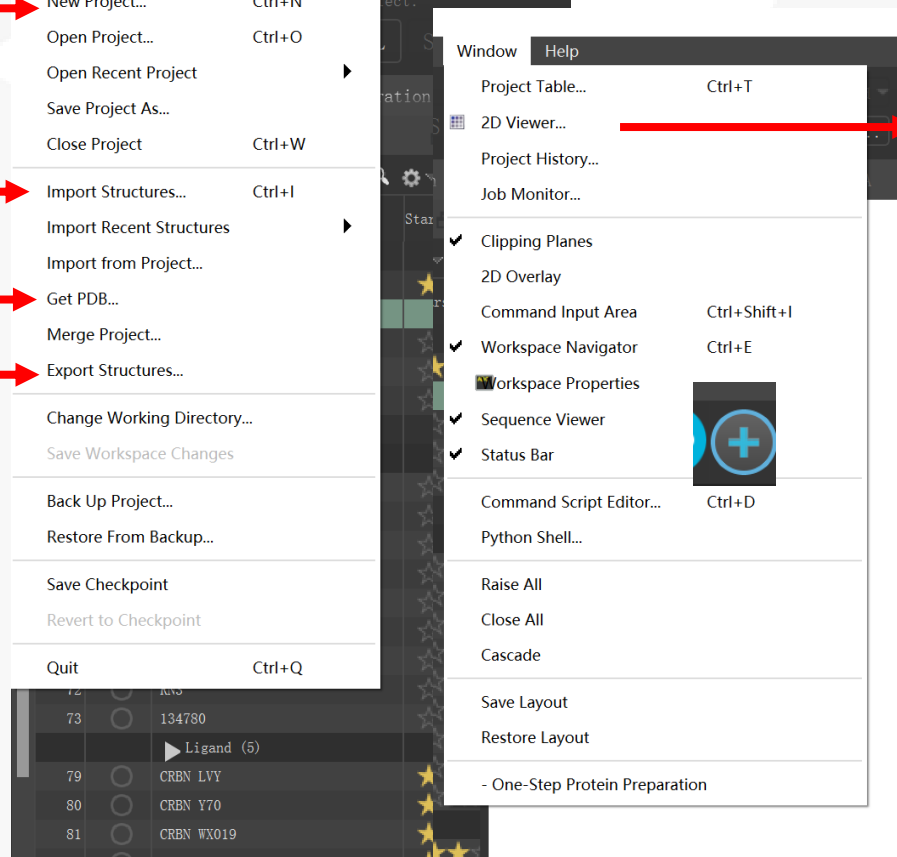
新Project建立



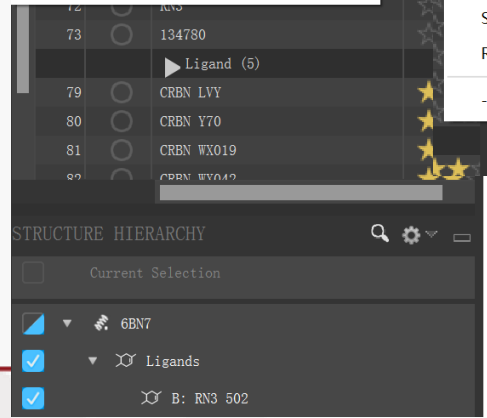
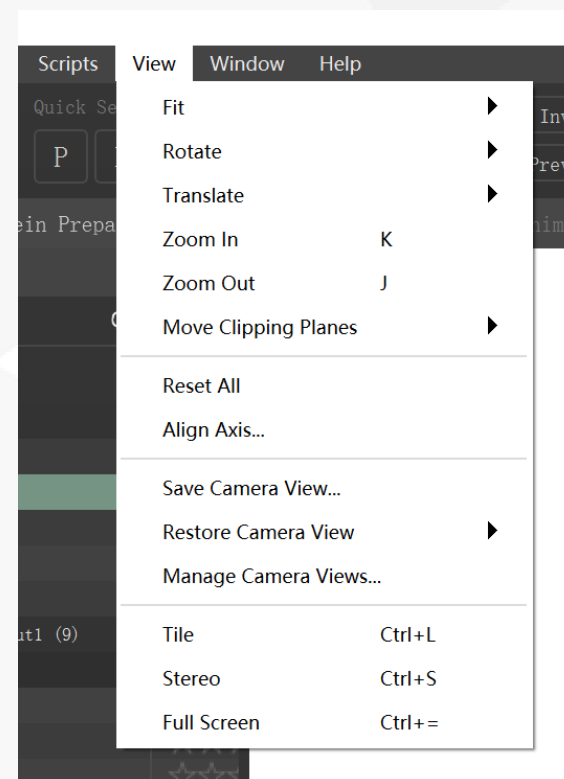
导入结构

获取PDB 需要PDB ID

导出结构



打开2D viewer看小分子分子式



工具栏



编辑Workspace
预设设置

启用预设

- Apply Custom Preset
- Edit Custom Preset...
- Reapply when Workspace changes

Maestro Default
BioLuminate Default

- Simple
- Simple (no solvent)
- Ball and Stick
- B Factor
- Technical
- Ligands
- Ligand Sites
- Pretty
- Pretty (with solvent)
- Publication
- Publication (with solvent)
- Protein Interface
- Antibody

复制当前Entry

给原子加减电荷

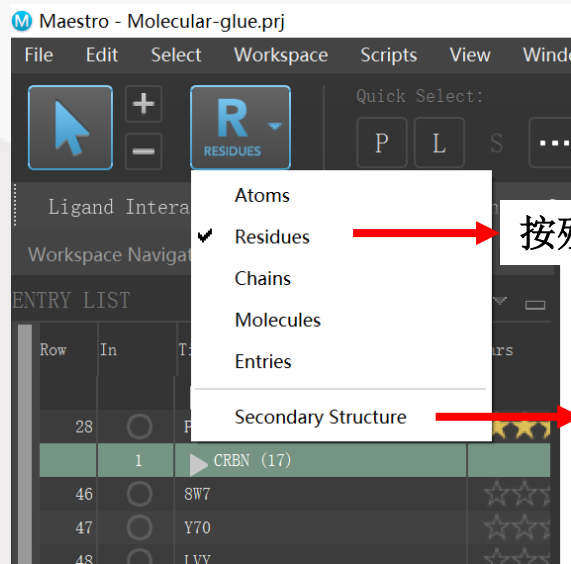


改换原子类型

移动或旋转选定的结构

按残基来选择

选择一段二级结构



Workspace中的分子操作

快速选择配体

反选

之前的选择

扩选

修改选中残基的属性，可以修改 Chain ID

突变成特定的残基

Focus选定的分子

可进行结构中原子、残基的逻辑选择

Atom Selection

Define atoms to select

Atom	Residue	Molecule	Chain	Entry	Substructure	Set
Sequence						
Residue number						
Residue type						
Classification						
Backbone/side chain						
Secondary structure						
PDB conversion status						

Residue number:

Examples:
≤ 12 or 3, 5-20, 34
Range in workspace:
1 - 1140

Atoms matching:
0

ASL:

Matching 0 atoms

GLN	GLU	GLY	HIS	ILE
LEU	LYS	MET	PHE	PRO
SER	THR	TRP	TYR	VAL
ASH	GLH	HID	HIE	HIP
LYN	MSE	PTR	SEP	TPO

Monitor: jobs监控面板

The Monitor application window displays a table of jobs with the following data:

Job ID	Name	Status	Start Time	Host
> DESKTOP-7CMMAHJ-0-5eb	m396-bb-sampling-residue_scan-1	incorporated : finished	2020-05-14-20:30:31	DESKTOP-7CMM
DESKTOP-7CMMAHJ-0-5eb	prepwizard_4	incorporated : finished	2020-05-16-15:59:17	DESKTOP-7CMM
> DESKTOP-7CMMAHJ-0-5eb	CRBN_MG	incorporated : finished	2020-05-16-21:19:39	DESKTOP-7CMM

Below the table, a tree view shows the sub-tasks for the selected job:

- DESKTOP-7CMMAHJ-0-5eb CRBN_MG
 - DESKTOP-7CMMAHJ-0- CRBN_MG-001
 - DESKTOP-7CMMAHJ-0- CRBN_MG-002
 - DESKTOP-7CMMAHJ-0- CRBN_MG-003
 - DESKTOP-7CMMAHJ-0- CRBN_MG-004
 - DESKTOP-7CMMAHJ-0- CRBN_MG-005

The interface includes a toolbar with buttons: Monitor, Pause, Resume, Stop, Kill, Delete, Postmortem... and a 'Details' panel with tabs for 'File' and 'Job summary'. The 'Log' file is selected in the 'Files' list.

选中对应的任务

点击查看子任务

监控任务

查看任务的log

The LigPrep window shows configuration options for a job. A red box highlights the gear icon in the bottom right corner, which opens the 'Job Settings' dialog.

任务设置选项卡

The 'LigPrep - Job Settings' dialog box has a 'Processors' table:

Host name	Processors	Use
localhost	12	12

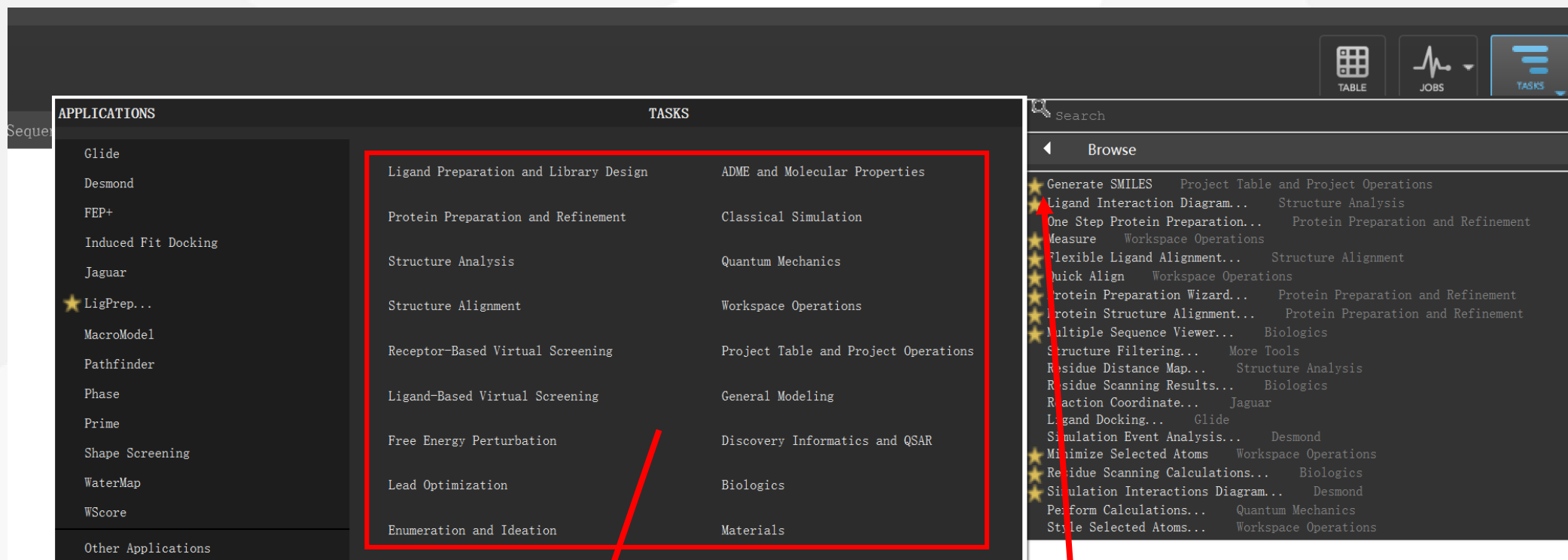
The 'Separate into' field is set to 1 subjobs. The 'Total to use' is 12.

调节要用的线程

设置分割的子任务数，一般要大于线程数

将做完的任务导入Project
必须在任务执行时选择 incorporate

TASK: Schrodinger的所有工具



众多不同用途的APP集合

加星号, 可将APP固定在主界面, 可以固定一些常用APP, 如Sequence viewer (看序列, 做多序列比对等)、Measure (测量原子之间的距离或二面角)、Ligand Interaction (可以画二维分子, 比Chemdraw好用) 以及Protein Structure alignment和Flexible Ligand Alignment



Schrodinger Ligand library设计



TASKS
← Ligand Preparation and Library Design

2D to 3D Conversion

- LigPrep... **经典配体准备**
- Generate Phase Database...

pKa Prediction

- Empirical pKa...
- Quantum-Mechanical...

Structure Building

- 2D Sketcher...

Databases

- Manage Phase Database...

Property Prediction

- Ligand-Based ADME/Tox Prediction...

Other

- Ligand Filtering...
- Compare Ligand Files...
- Force Field Builder...
- Enumeration

2D Workspace - Ligand Interacti...

File Edit **View**

Sync with 3D Ligand: B: RN3 5

展示相互作用 也可以只展示配体

可以调整view的角度和方向

LigPrep

Use structures from: File

File name: Browse...

Filter criteria file: Create... Browse...

Ionization:

- Do not change
- Neutralize
- Generate possible states at target pH: +/-

Using: Ionizer Epik Add metal binding states Include original state

Desalt Generate tautomers **一般不使用Generate Tautomer**

Stereoisomers **构型**

Computation:

- Retain specified chiralities (vary other chiral centers)
- Determine chiralities from 3D structure
- Generate all combinations

Generate at most: per ligand

For SD V2000 in **生成的构型数目** ers if the chiral flag is 0

Output format: Maestro SDF

Job name: Run

Host=localhost:12, Incorporate=Append new entries as a new group

TASKS
← Protein Preparation and Refinement

Protein Preparation

- Get PDB Structure...
- ★ Protein Preparation Wizard...
- One Step Protein Preparation...

Protein Alignment

- ★ Protein Structure Alignment...
- Binding Site Alignment...

Structure Building and Editing

- Protein Splicer...
- Mutate Residues...
- Build Peptide from Sequence...
- Generate Helices...
- Helix Manipulator...
- Structure Morpher... 变构
- Assign GPCR Generic Numbering...
- PDB Name Assignment
- Renumber Proteins by 3D Alignment...

Homology Modeling

- Homology Modeling...

Protein X-Ray Refinement

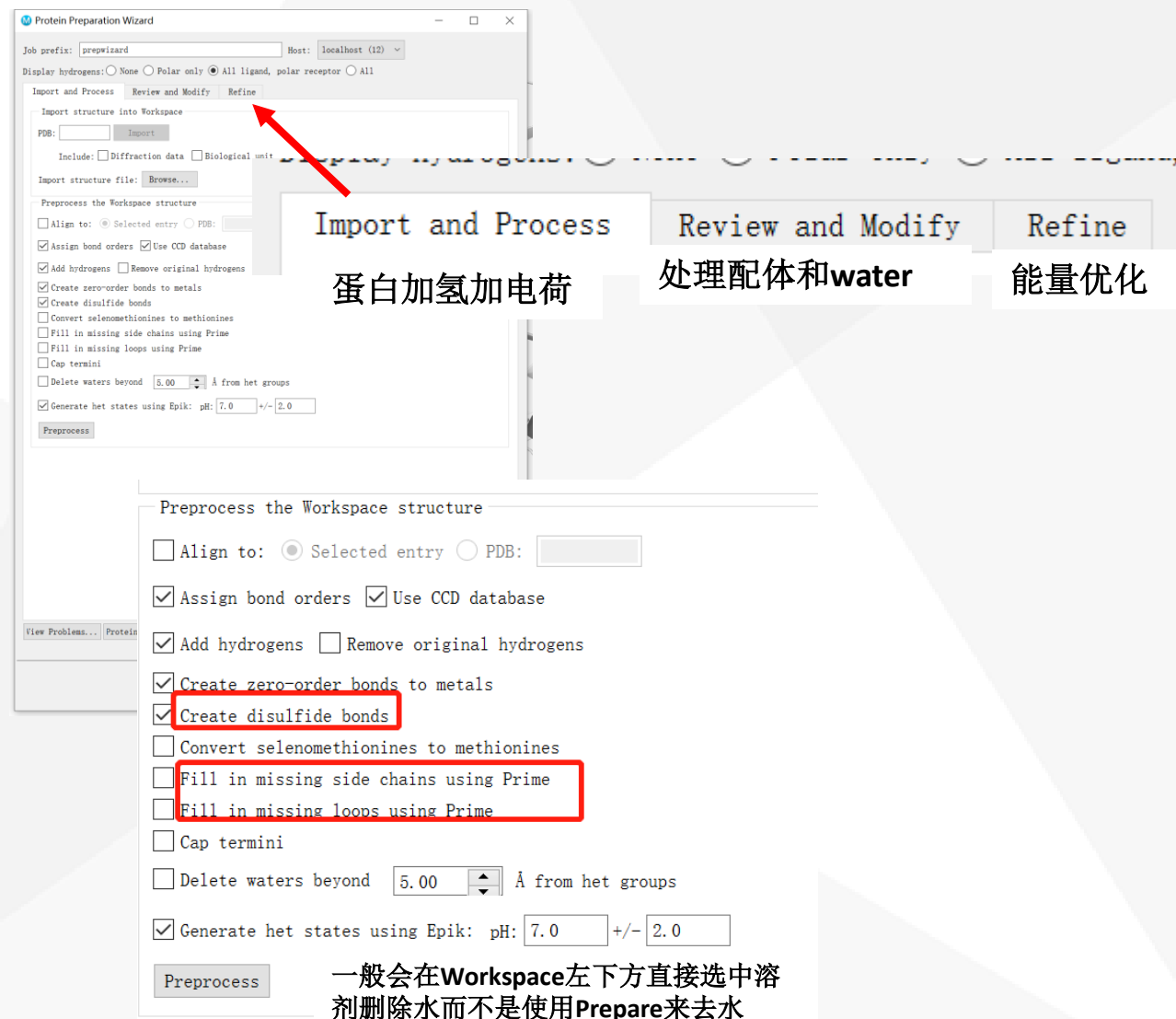
- Protein X-Ray Refinement...

Protein Refinement

- Calculate Energy...
- Minimize...
- Minimize as Rigid Body...
- Predict Side Chains...
- Refine Loops...
- Hybrid Monte Carlo...
- Refine Protein-Ligand Complex...

Sequence Editing

- ★ Multiple Sequence Viewer...



Protein Preparation Wizard

Job prefix: prepwizard Host: localhost (12)

Display hydrogens: None Polar only All ligand, polar receptor All

Import and Process Review and Modify Refine

Import structure into Workspace

PDB: Import

Include: Diffraction data Biological unit

Import structure file: Browse...

Preprocess the Workspace structure

Align to: Selected entry PDB:

Assign bond orders Use CCD database

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 Å from het groups

Generate het states using Epik: pH: +/-

Preprocess

Import and Process 蛋白加氢加电荷

Review and Modify 处理配体和water

Refine 能量优化

Preprocess 一般会在Workspace左下方直接选中溶剂删除水而不是使用Prepare来去水

TASKS
← Receptor-Based Virtual Screening

Docking Preparation

- Receptor Grid Generation...

Docking

- Ligand Docking...
- Virtual Screening Workflow...
- Covalent Docking...
- Induced Fit Docking...
- Binding Pose Metadynamics...

Other Docking Workflows

- QM-Polarized Ligand Docking...
- Cross Docking...
- One-Step Ligand Docking...
- Interactive Pose Prediction...

Docking Post Processing

- Pose Viewer...
- Select Top Poses...
- Filter Docked Poses...
- Pose Explorer...
- Visualize XP Interactions...
- Enrichment Calculator...
- Strain Energy Rescoring...

WScore

- Model Generation...
- Docking...
- Visualizer...

Fusion Methods

- Data Fusion...

Receptor Grid Generation

Receptor | Site | Constraints | Rotatable Groups | Excluded Volumes

Define receptor

If the structure in the Workspace is a receptor plus a ligand, you must identify the ligand molecule so it can be excluded from the grid generation.

Pick to identify the ligand Molecule Show markers

Van der Waals radius of

charge cutoff: 0.25

le docking

Job name: glide-grid_1

Host=localhost

Run

在这个盒子里加一些限制

在这个盒子里加一些限制

指定受体和受体上的配体结合位置
(本质上是指定一个配体可以在里面采样的盒子)

指定蛋白的哪些键是可以旋转的

Schrodinger 高级功能辅助分子对接



TASKS Receptor-Based Virtual Screening

Docking Preparation

Receptor Grid Generation...

Docking

Ligand Docking...

Virtual Screening Workflow...

Covalent Docking...

Induced Fit Docking...

Binding Pose Metadynamics...

Other Docking Workflows

QM-Polarized Ligand Docking...

Cross Docking...

One-Step Ligand Docking...

Interactive Pose Prediction...

其他特殊的对接方法

Docking Post Processing

Pose Viewer...

Select Top Poses...

可视化对接结果及筛选pose

Filter Docked Poses...

Pose Explorer...

Visualize XP Interactions...

Enrichment Calculator...

Strain Energy Rescoring...

WScore

Model Generation...

Docking...

Visualizer...

针对你的特定靶点来训练模型进行对接筛选

Fusion Methods

Data Fusion...

结合不同方法来搜索配体

TASKS General Modeling

Minimization

Force-Field...

Ligand-Receptor Complex...

Semiempirical NDDO...

MOPAC2016...

Ab Initio QM...

QM-MM...

通过构象搜索来寻找更合适的结合模式

Conformational Search

Bioactive Search...

Advanced Search...

Ligand-Receptor Complex...

Redundant Conformer Elimination...

Macrocycle Sampling...

Macrocycle Propensity...

TASKS Classical Simulation

Molecular Dynamics

System Setup...

Model System Regeneration...

Molecular Dynamics...

Simulated Annealing...

Binding Pose Metadynamics...

Metadynamics...

Metadynamics Analysis...

Replica Exchange...

Replica Exchange Review...

Molecular Dynamics Analysis

Simulation Quality Analysis...

Simulation Event Analysis...

Radial Distribution Function...

★ Simulation Interactions Diagram...

Desmond Trajectory Clustering...

通过分子动力学来寻找稳定结合模式