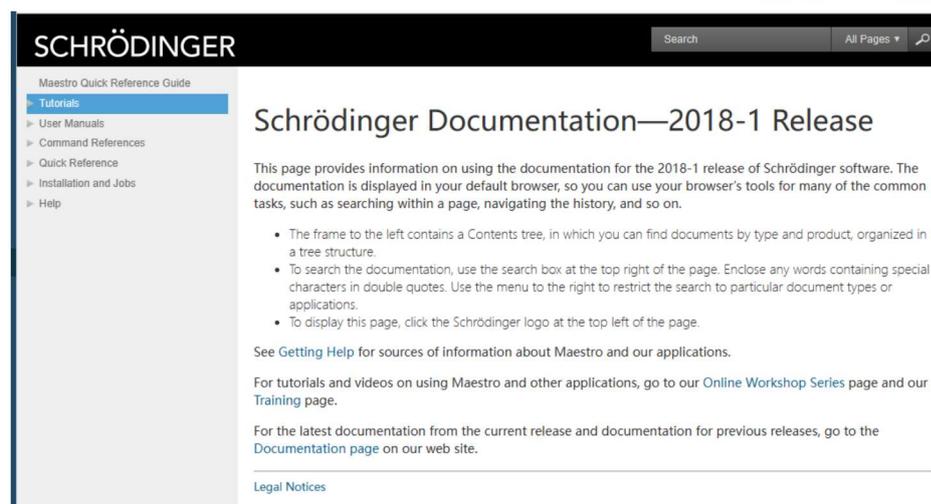
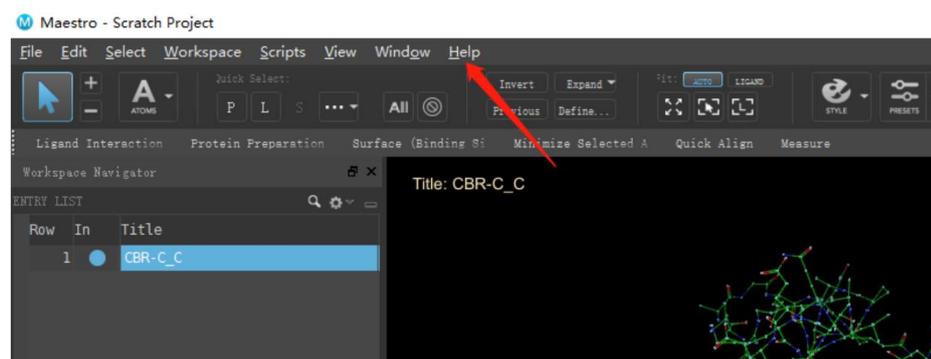


Schrödinger分子对接

0.官方文档与视频教程

0.1 官方文档

软件中点击Help, 可以跳转到薛定谔的官方教程文档



0.2 视频教程

钰沐涵的系列薛定谔分子对接教程

https://www.bilibili.com/video/BV1Cv411h72A/?spm_id_from=333.999.0.0&vd_source=...

1. 蛋白准备

1.1 导入蛋白质结构

File--import structure

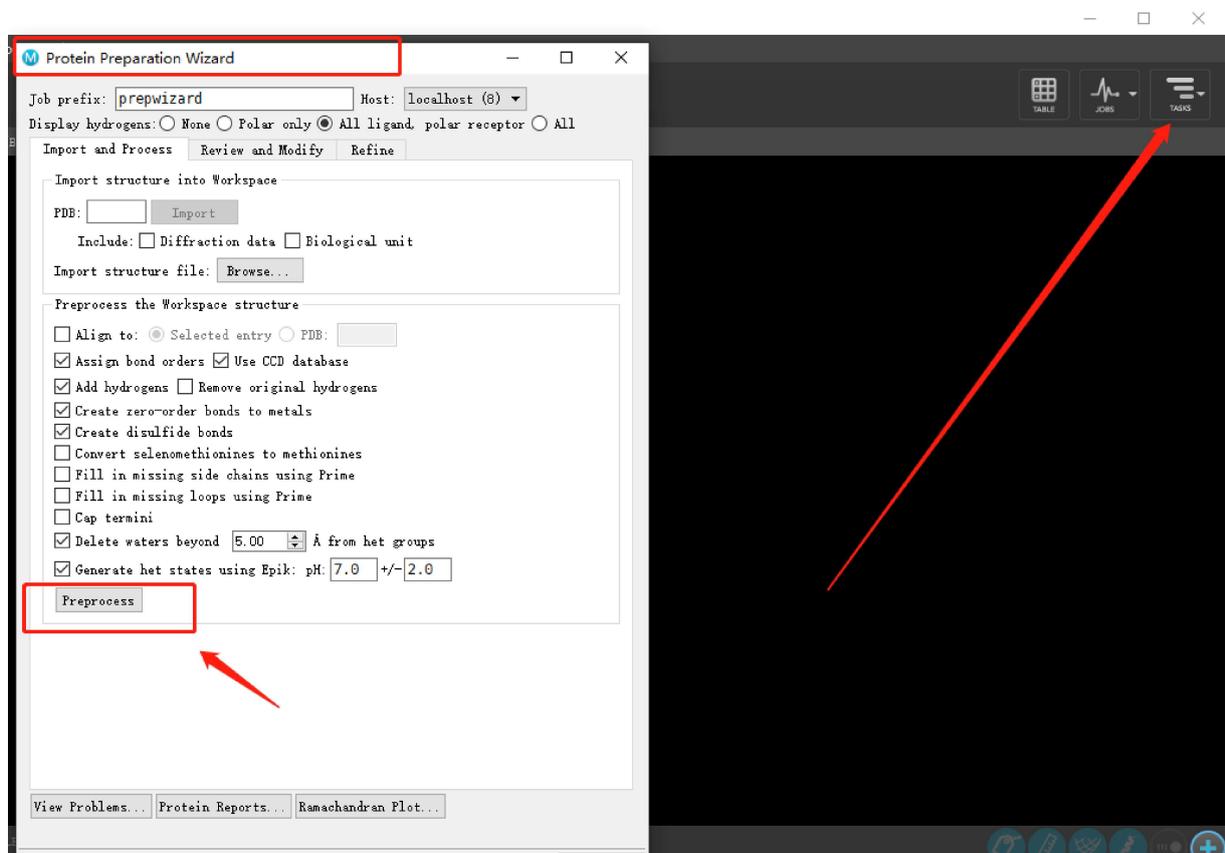
1.2 蛋白准备模块

选中Tasks--直接搜索'protein preparation'：

在'import and process'，勾选需要进行处理的操作，如最小化、填充缺失的侧链和/或loop等--点击process（开始处理）

在'review and modify'，对蛋白和配体（Hets）、水位置及电荷的校正。，删除不需要的部分，并生成电离、同分异构和金属离子结合状态等--点击generate states

在'refine'，进行结构优化，对蛋白进行加氢、去除多余水，以及能量最小化等操作--依次点击optimized, removed waters, minimize



Display hydrogens: none Total only All ligands polar receptor All

Import and Process Review and Modify Refine

Analyze Workspace

Fit on select Display selection only Pick

Select Hets/Waters within Å of selected chains

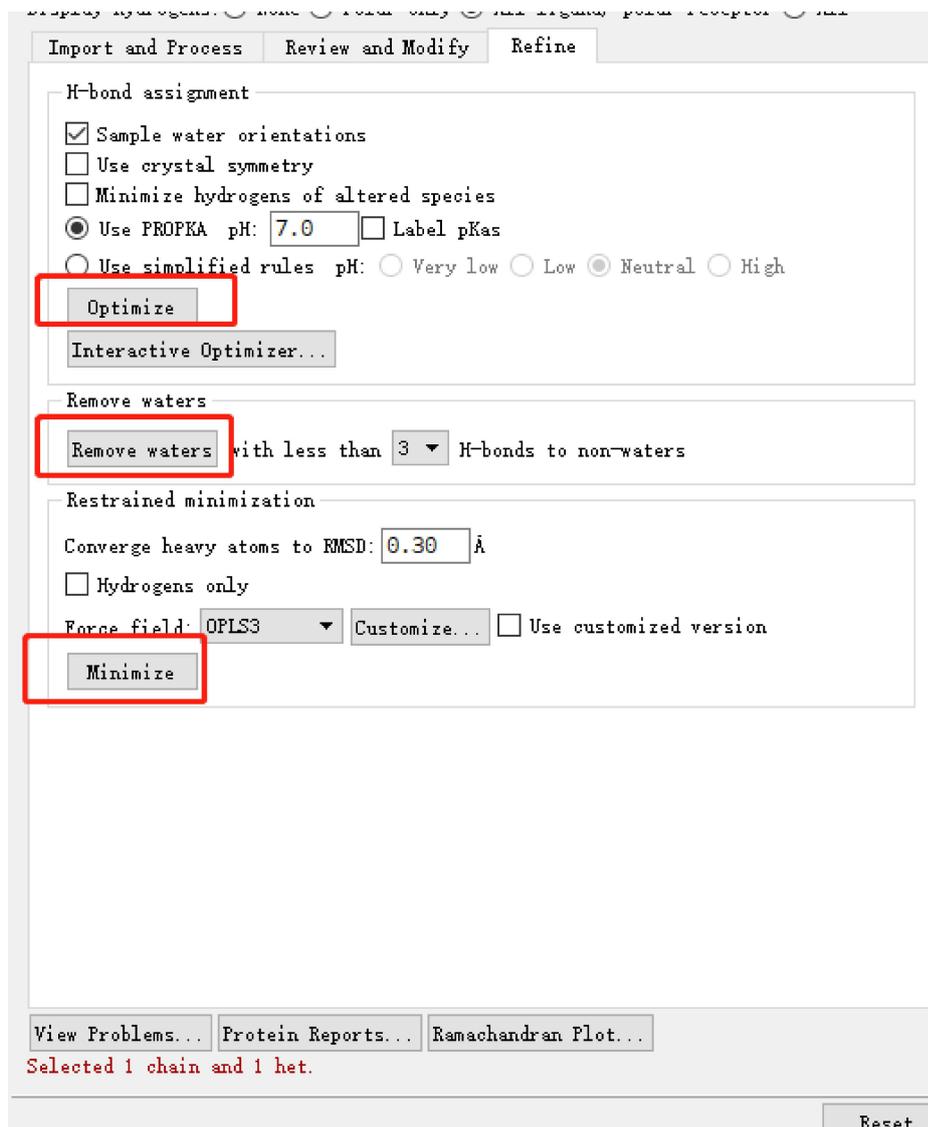
Select Lone Waters

Chain Name	Water No.	Chain	Residue No.
C			

Het No.	Het Name
1	C:DRG (1101)

 pH: +/-

Selected 1 chain and 1 het.



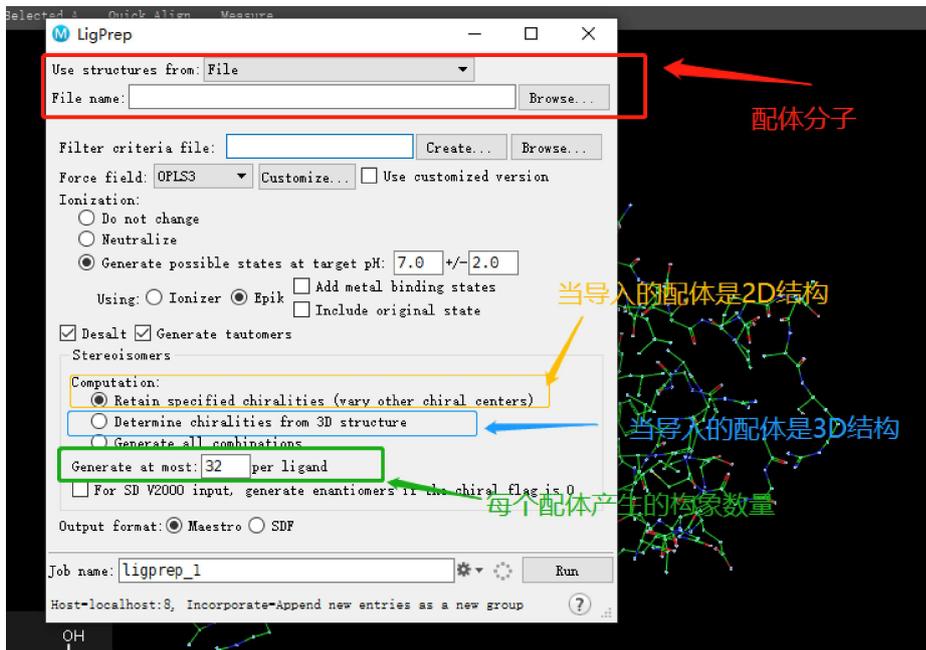
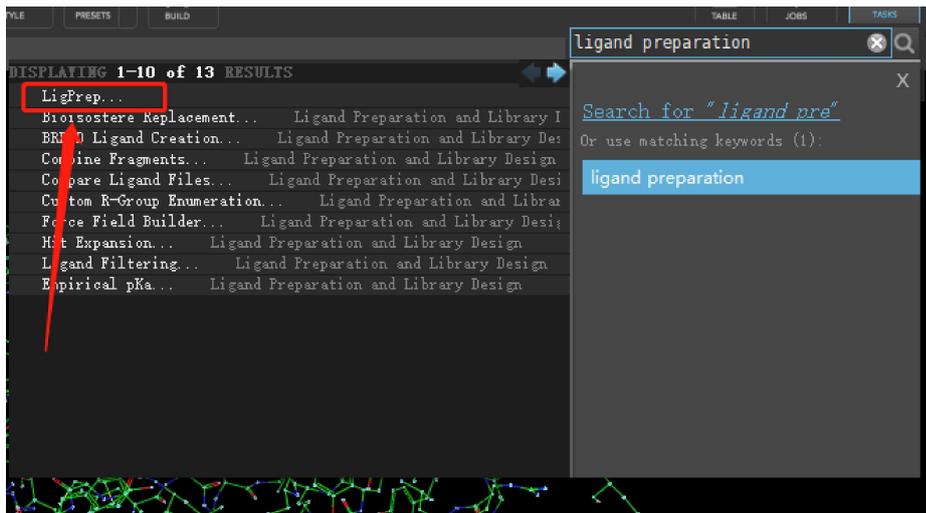
2. 配体准备

2.1 导入配体小分子

File--import structure --(全选)

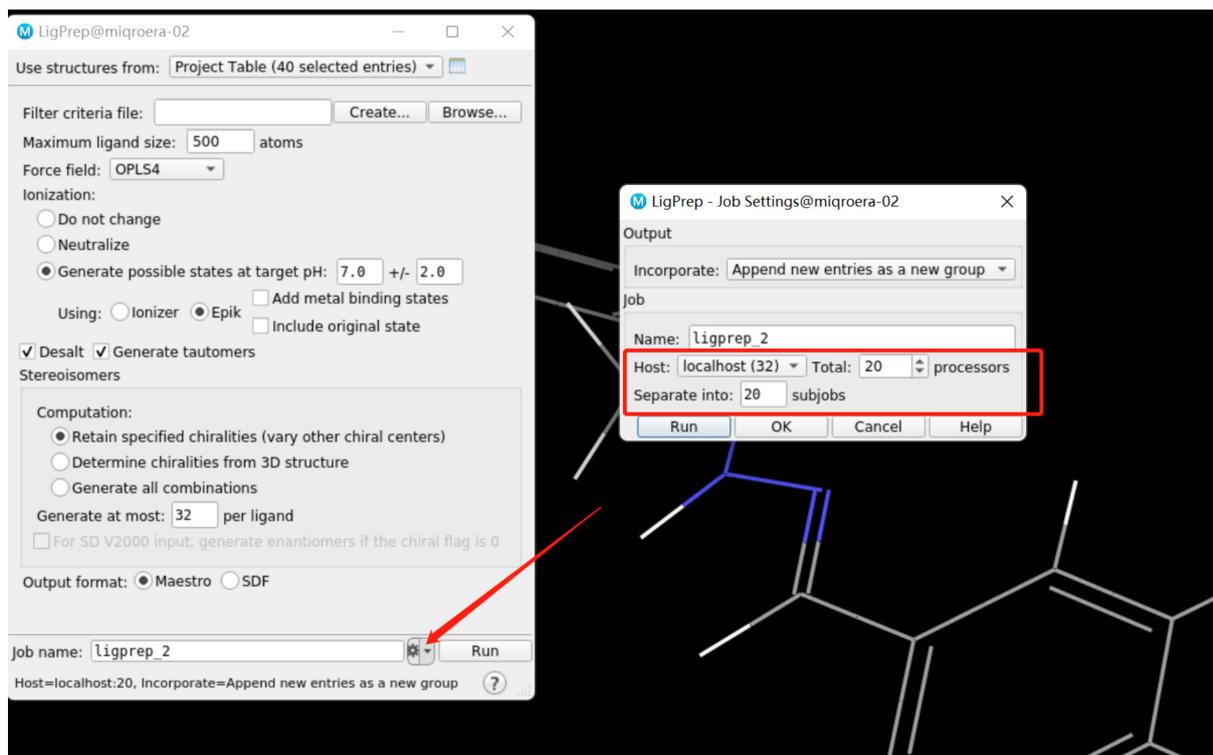
2.2 配体准备模块

Tasks--搜索'ligand preparation' -- LigPrep (一些设置具体见下图标注) -- run(job setting可以导出脚本write, 直接后台脚本运行bash xxx.sh)



2.3 运行脚本设置与运行

注意：一个小技巧，子任务数量=运行线程数，运行速度较快

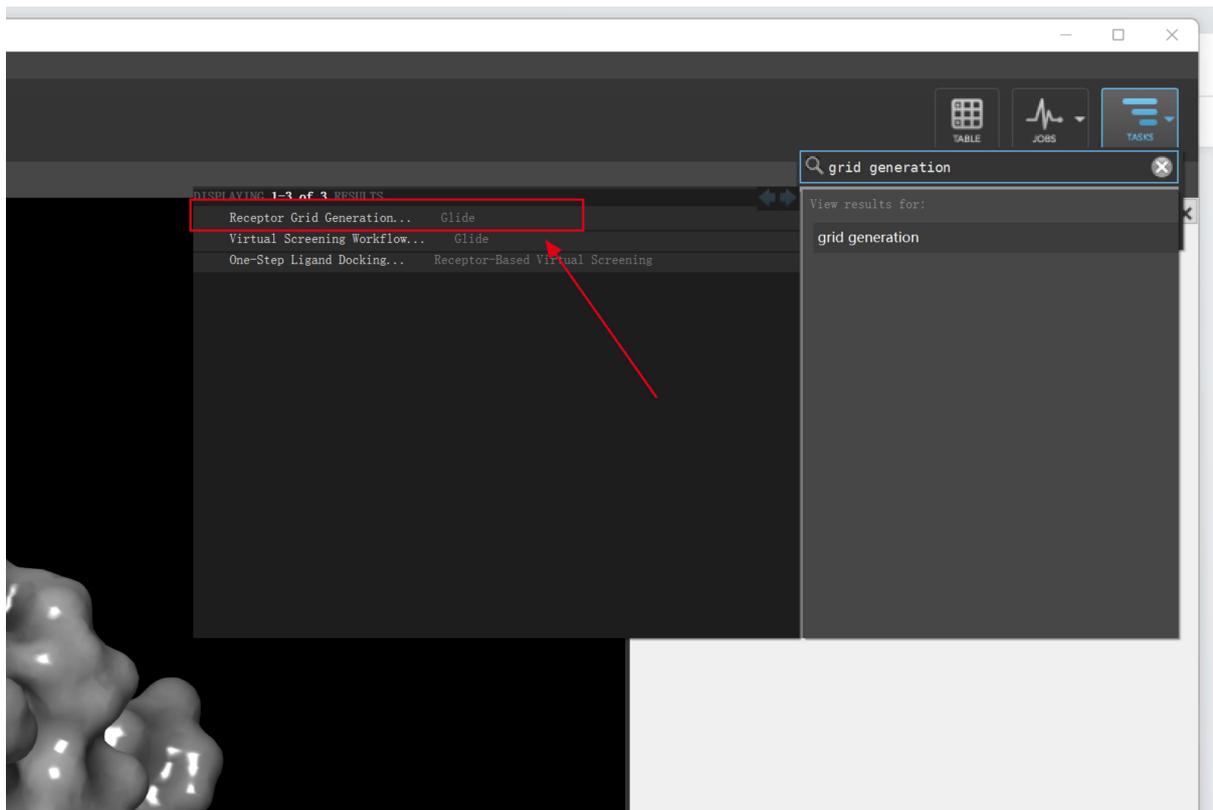


```
(base) laiguanxue@miquroera-02:~/my_project/RNF31/XP/ligprep_1$ ls
ligprep_1.inp  ligprep_1.maegz  ligprep_1.sh
(base) laiguanxue@miquroera-02:~/my_project/RNF31/XP/ligprep_1$ bash ligprep_1.sh
JobId: miquroera-02-0-64bdefc0
(base) laiguanxue@miquroera-02:~/my_project/RNF31/XP/ligprep_1$
```

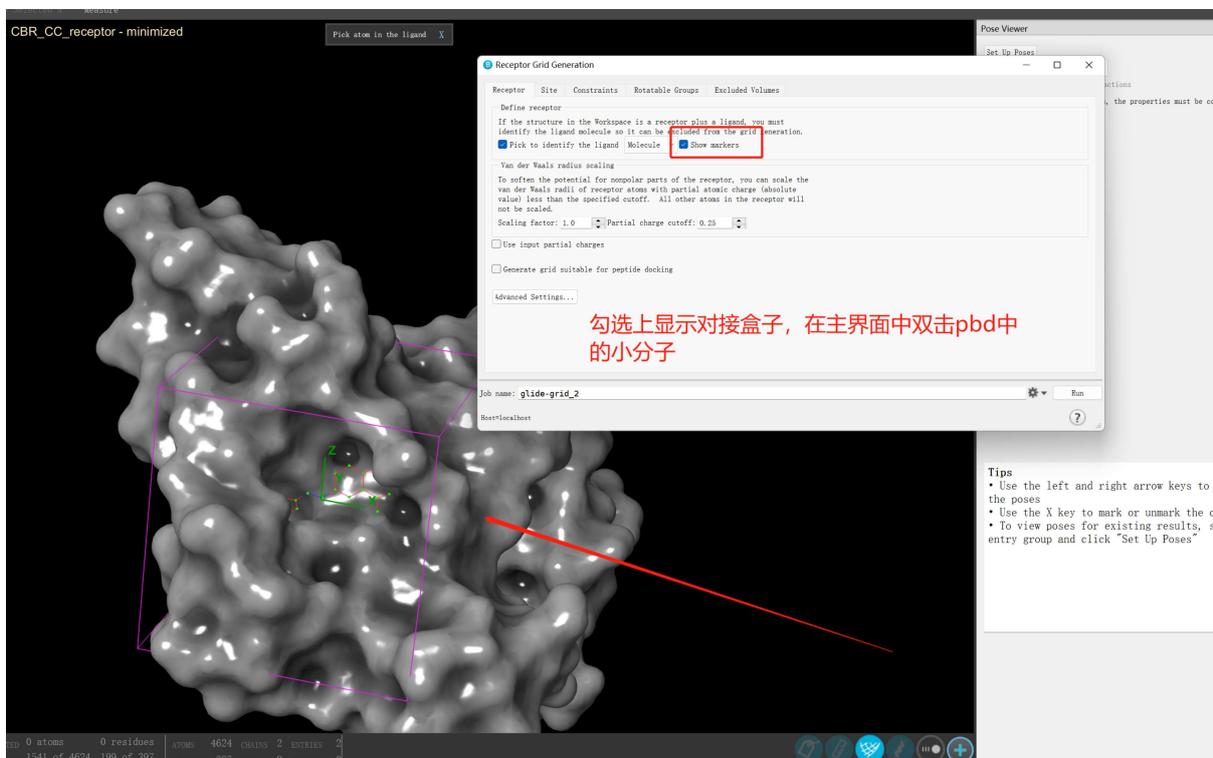
3. 对接盒子生成

3.1 对接盒子生成模块

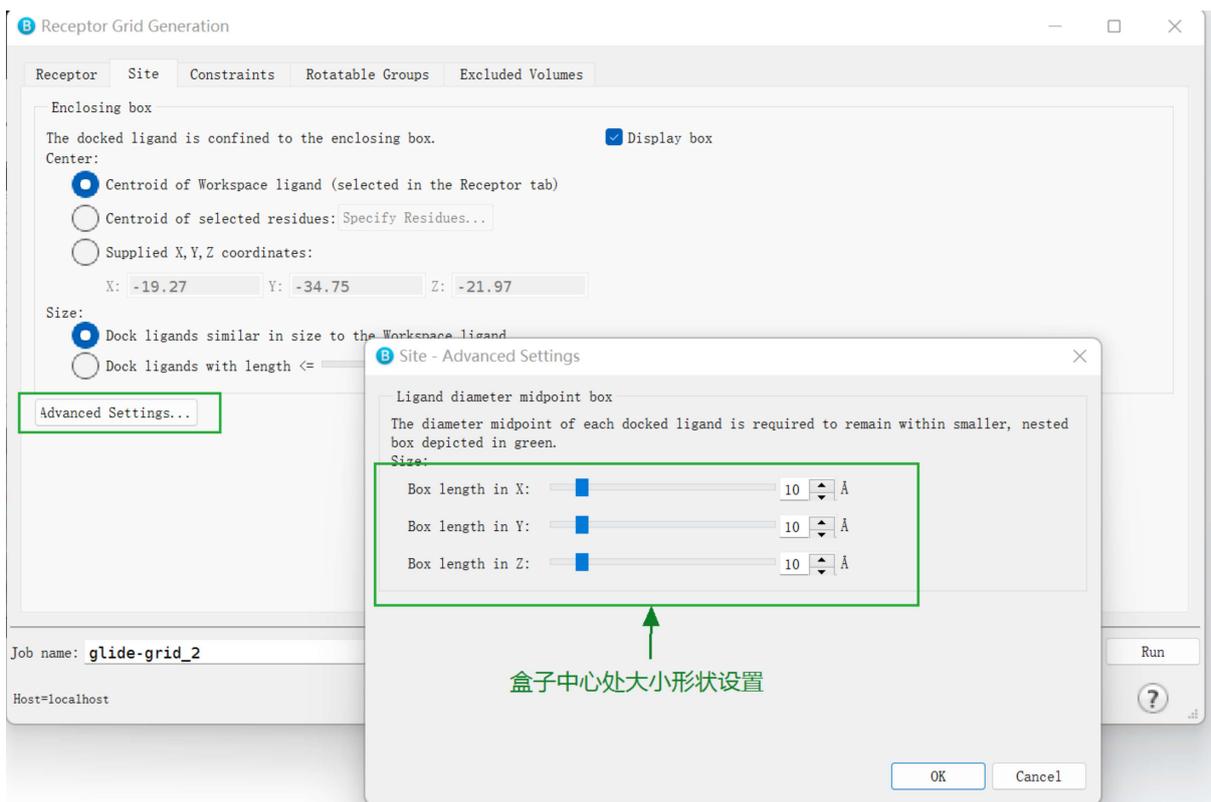
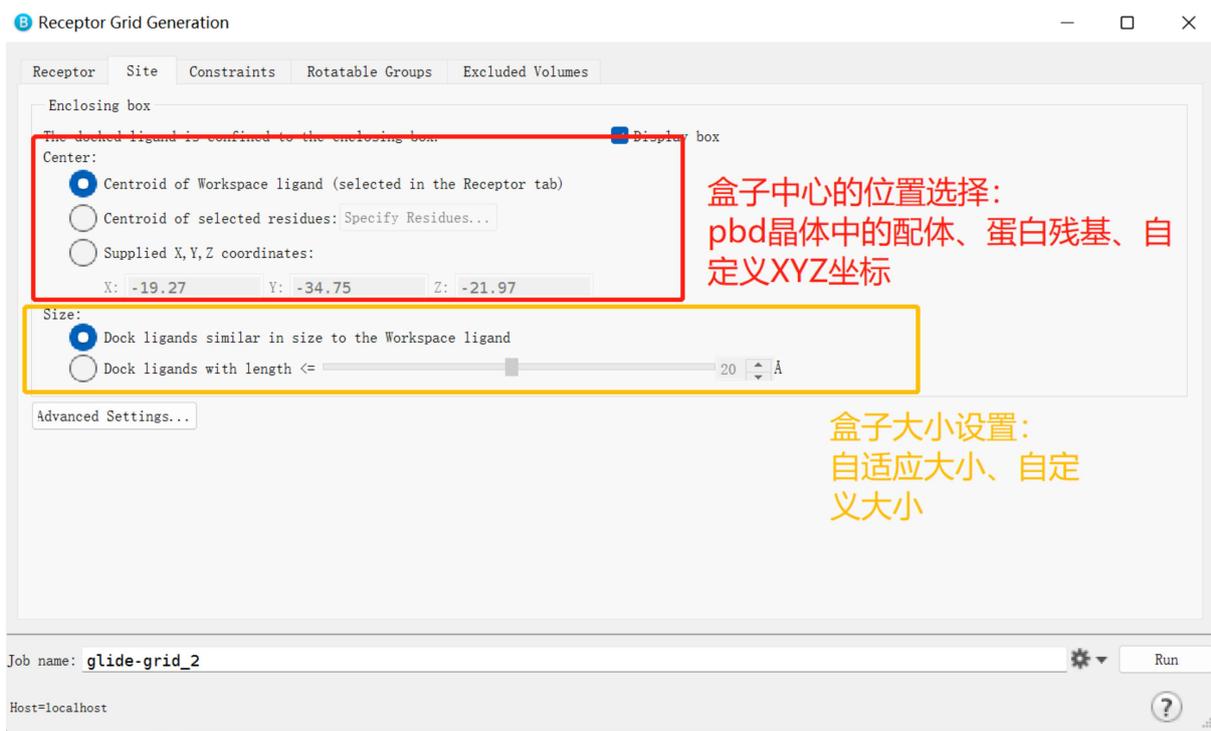
Tasks--搜索'grid generation'--receptors grid generation---设置完成之后, run运行



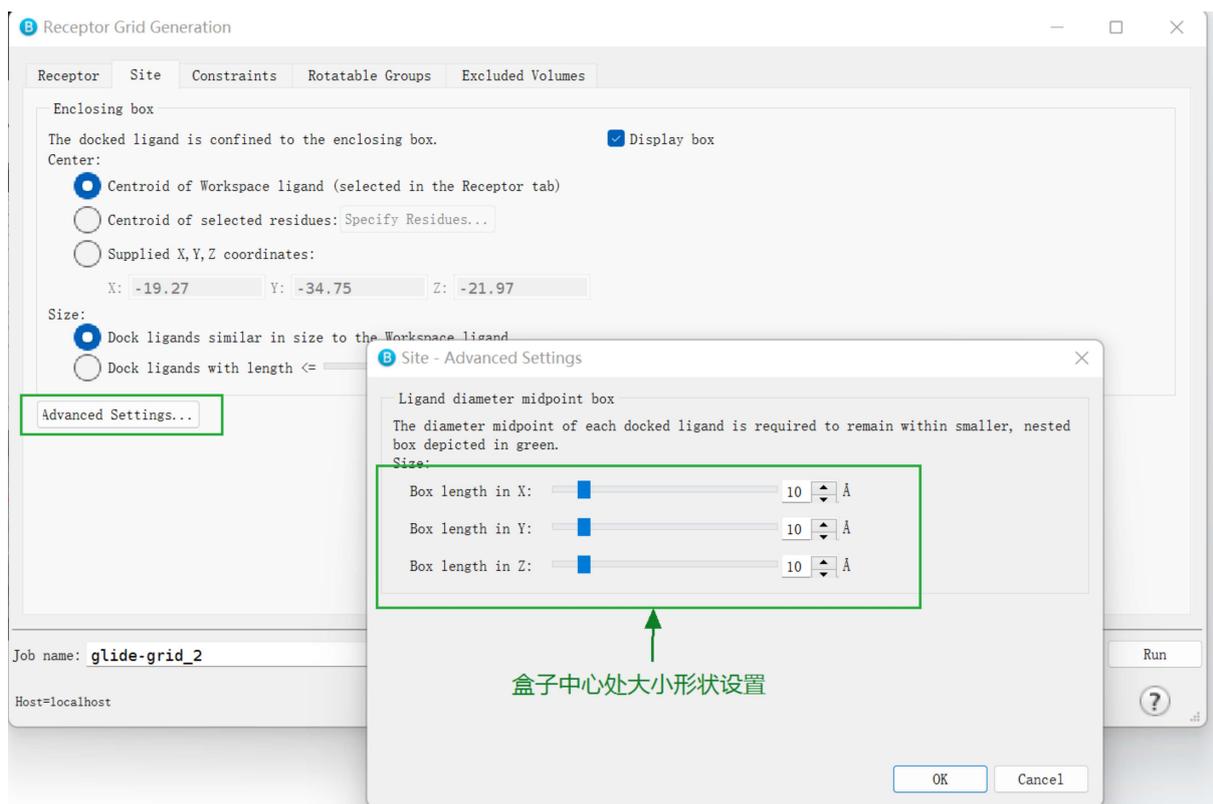
3.2 原pbd晶体中配体为盒子中心



3.3 自定义盒子



4. 对接



Tasks--ligand docking --receptor grid (含“grid”的.zip)

ligands (即配体准备的结果，一般含“out”的.maegz)

--settings --- HTVS(虚拟筛选，快速)

SP (标准对接)

XP (精对接)

---ligand sampling flexible -- run(job setting可以导出脚本，直接后台脚本运行)

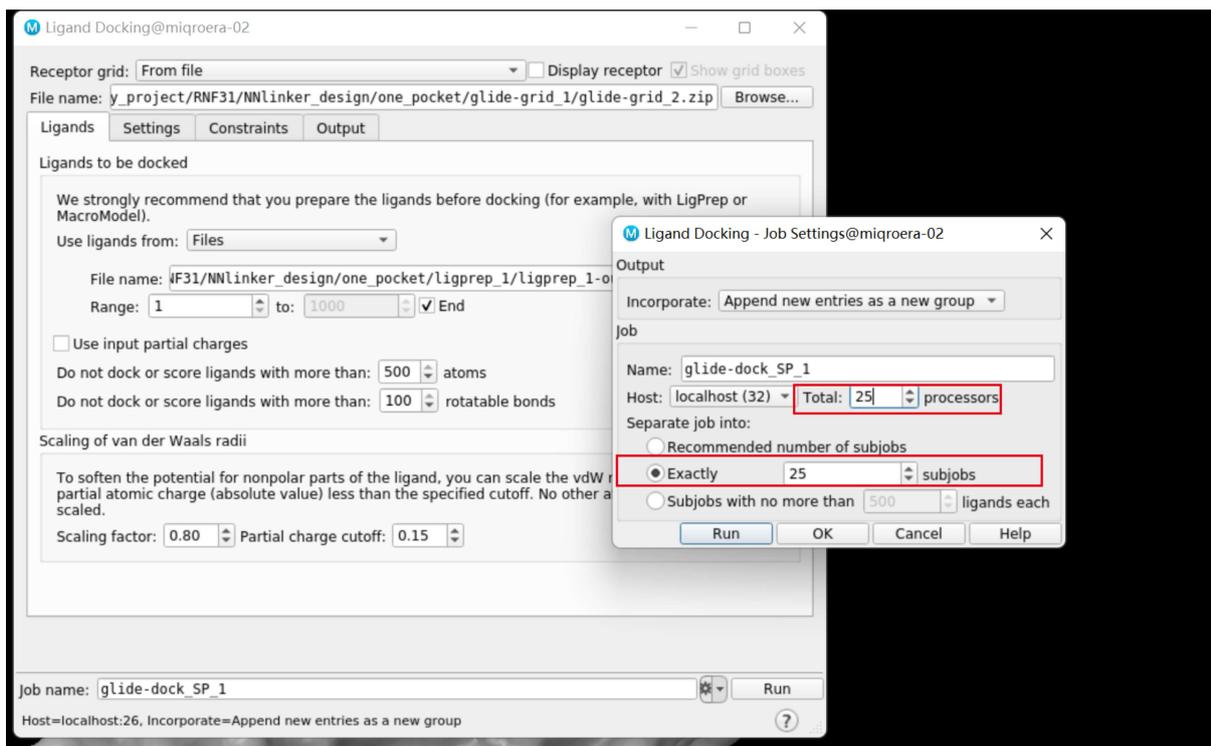
注意：一个小技巧，子任务数量=运行线程数，运行速度较快

之前生成的对接盒子

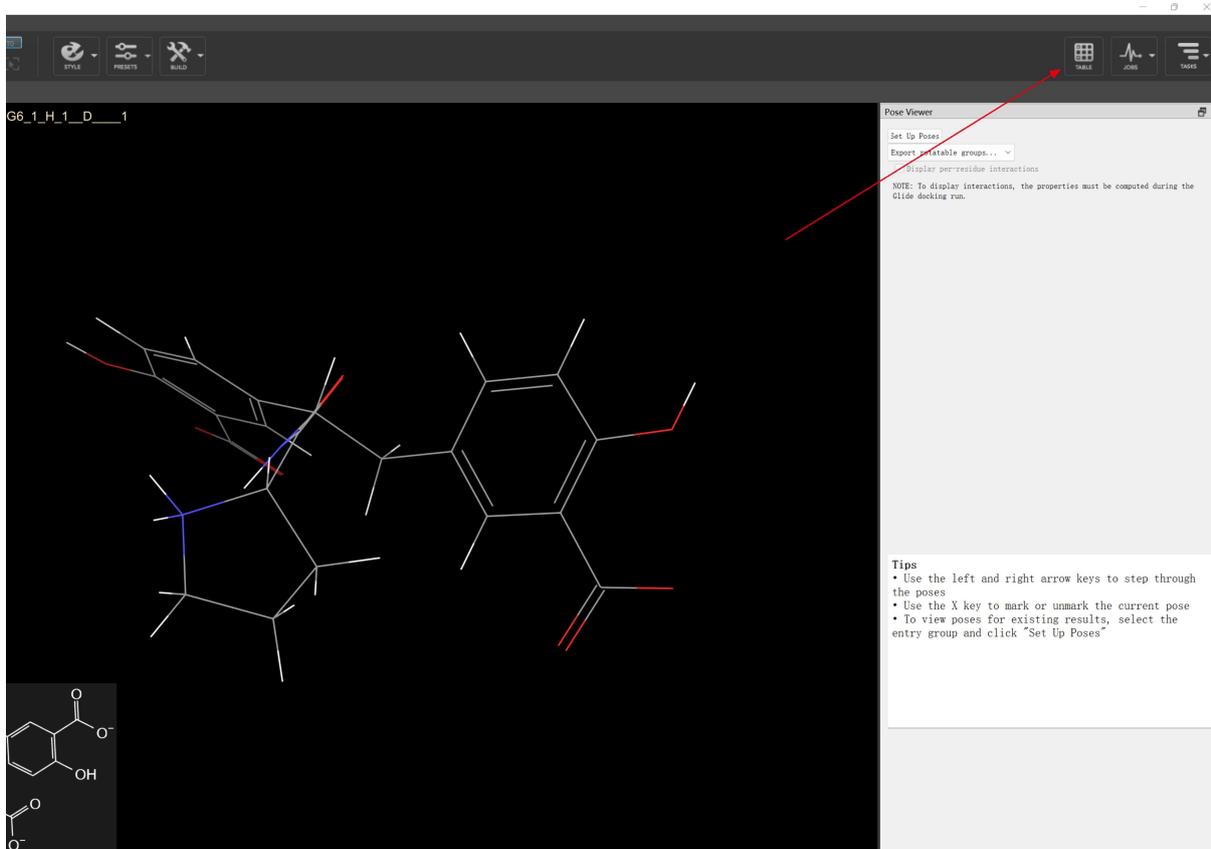
之前的准备完成的配体

对接模式选择

配体采样模式：刚体、柔性、半柔性



5. 对接结果查看和导出



Project Table --- NNIinker_onepocket.prj

File Table Data Select Window View

Import Export 2D Viewer Plot Sort Find/Replace Show Progs Color Rows Calculator

Columns Tree Show Show Family 2D Structure Hide Family

Row	In	Title	Stars	Entry ID	Date Added	Date Modified	PDB TITLE	PDB ID	Source Path	Source File	Source File Index	Prepared	Potential Energy-S-OPLSBIOSOLVEIT/HYDE_ATOM_SCORES (KJ)/BIOSOLVEIT
1		CBR-C_C	☆☆☆☆	3	18 7月 10.	18 7月 14:20			C:\Micro... CBR-C_C.p...		1		
2		C:\Micro\my project\RN31\redocking\CBR-C_C.pdb	☆☆☆☆	4	18 7月 10.	18 7月 10:25			C:\Micro... CBR-CC_LL...		1		
3		CBR_CC_receptor	☆☆☆☆	5	18 7月 10.	19 7月 10:53			C:\Micro... CBR-C_C.p...		1		
4		CBR_CC_receptor - preprocessed	☆☆☆☆	6	18 7月 10.	09:57			C:\Micro... CBR-C_C.p...		1		
5		CBR_CC_receptor - preprocessed	☆☆☆☆	7	18 7月 10.	18 7月 10:58			C:\Micro... CBR-C_C.p...		1		
6		CBR_CC_receptor - preprocessed	☆☆☆☆	8	18 7月 10.	18 7月 10:58			C:\Micro... CBR-C_C.p...		1		
7		CBR_CC_receptor - hbond-opt	☆☆☆☆	9	18 7月 10.	18 7月 10:59			C:\Micro... CBR-C_C.p...		1		
8		CBR_CC_receptor - removed waters	☆☆☆☆	10	18 7月 11.	18 7月 11:00			C:\Micro... CBR-C_C.p...		1		
9		CBR_CC_receptor - minimized	☆☆☆☆	11	18 7月 11.	18 7月 14:20			C:\Micro... CBR-C_C.p...		1		-391.167
gLite-dock_SP_1_pv (1325)													
1		choose (15)											
1335		DRG_A_214_3n1f_3RS_1_A_800_0_1	☆☆☆☆	1337	18 7月 22.	09:41			C:\Micro... glide-doc...		2		# Atom-ID: Total: Rec-Desolv: R...
1336		DRG_A_214_3oev_30E_1_K_213_MA_1	☆☆☆☆	1338	18 7月 22.	09:41			C:\Micro... glide-doc...		3		# Atom-ID: Total: Rec-Desolv: R...
1337		DRG_A_214_4x69_2CV_1_C_303_M_1	☆☆☆☆	1339	18 7月 22.	09:41			C:\Micro... glide-doc...		4		# Atom-ID: Total: Rec-Desolv: R...
1338		DRG_A_214_3ocb_X01_1_A_1_E_1	☆☆☆☆	1340	18 7月 22.	09:41			C:\Micro... glide-doc...		5		# Atom-ID: Total: Rec-Desolv: R...
1339		DRG_A_214_1f02_000_1_H_345_D_1	☆☆☆☆	1341	18 7月 22.	09:41			C:\Micro... glide-doc...		6		# Atom-ID: Total: Rec-Desolv: R...
1340		DRG_A_214_1hw_197_1_A_800_R_1	☆☆☆☆	1343	18 7月 22.	09:41			C:\Micro... glide-doc...		8		# Atom-ID: Total: Rec-Desolv: R...
1341		DRG_A_214_1p61_091_1_A_790_T_1	☆☆☆☆	1344	18 7月 22.	09:41			C:\Micro... glide-doc...		9		# Atom-ID: Total: Rec-Desolv: R...
1342		DRG_A_214_5p95_05W_1_D_403_T_1	☆☆☆☆	1345	18 7月 22.	09:41			C:\Micro... glide-doc...		10		# Atom-ID: Total: Rec-Desolv: R...
1343		DRG_A_214_440x_KAT_1_A_393_C_1	☆☆☆☆	1346	18 7月 22.	09:41			C:\Micro... glide-doc...		11		# Atom-ID: Total: Rec-Desolv: R...
1344		DRG_A_214_4m9_2E3_1_B_800_0_1	☆☆☆☆	1347	18 7月 22.	09:41			C:\Micro... glide-doc...		12		# Atom-ID: Total: Rec-Desolv: R...
1345		DRG_A_214_61js_09F_1_A_503_C_1	☆☆☆☆	1348	18 7月 22.	09:41			C:\Micro... glide-doc...		13		# Atom-ID: Total: Rec-Desolv: R...
1346		DRG_A_214_1sov_08X_1_A_500_F_1	☆☆☆☆	1349	18 7月 22.	09:41			C:\Micro... glide-doc...		14		# Atom-ID: Total: Rec-Desolv: R...
1347		DRG_A_214_5152_6MS_1_K_303_GA_1	☆☆☆☆	1350	18 7月 22.	09:41			C:\Micro... glide-doc...		15		# Atom-ID: Total: Rec-Desolv: R...
1348		DRG_A_214_5nh0_8X0_1_B_403_0_1	☆☆☆☆	1351	18 7月 22.	09:42			C:\Micro... glide-doc...		16		# Atom-ID: Total: Rec-Desolv: R...
1349		DRG_A_214_1dwe_006_1_H_1_D_1	☆☆☆☆	1352	18 7月 22.	11:16			C:\Micro... glide-doc...		17		# Atom-ID: Total: Rec-Desolv: R...

Export menu options:

- Include
- Fix in Workspace
- Lock (set non-editable)
- Split
- Duplicate
- Merge
- Delete
- Add to Shortcut Rows
- Set Stars
- Group...
- Move to
- Ungroup Groups
- Set Property...
- Copy Properties
- Paste Properties
- Group by Entry Property...
- Color Rows...
- Export
 - Structures...
 - Spreadsheet...

导出结构

导出对接打分, 计算的分子性质