**4. Molecular docking**

Batch docking can be used for virtual screening, target fishing, result validation of network pharmacology studies, etc. Have fun docking!

1. Choose four directories for ligands (.pdbqt), receptors (.pdbqt), config files, and the docking results, respectively. **Note that all the files in *pdbqt* format in the selected directory will be considered as ligands/receptors. These directories should not be the same.** You can click “*Menu-Settings-New directory*” to create a new directory for a docking project.

**The config files should be named the same as the receptors**, e.g. *1r42.txt* for *1r42.pdbqt*, because the binding sites must be different for different receptors. We suggest using module 3 to get the config files. **If you want to use your own config file, remember to delete any ligand or receptor information in the config file**.

**Any “-” in the ligand name or receptor name will be replaced by “\_” as the result analysis after docking will use “-” to separate the ligand name and receptor name. If a receptor name is changed in this way, please correct the config file’s name so that it is the same as the receptor’s.**

1. Decide whether the docking results are analyzed automatically. The affinity scores for each docking will be summarized in an *Excel* file and the affinity HeatMap will be also plotted and displayed. The docking poses will be split into single pose files. If you don’t want to run the analysis automatically, or the result analysis failed, you can use module 5 to perform these analyses again.
2. If there are too many docking tasks in a batch docking project, the docking process can be artificially paused by closing the software. In another case, an unexpected accident killed the docking process. To continue an unfinished docking project, check the docking status “unfinished docking”. **Note that the four directories mentioned above should be the same as before**.
3. Select a docking algorithm or scoring function. Vinardo is reported to be a better scoring function with the same docking algorithm as Vina. QuickVina2 uses an improved algorithm to increase the docking speed. QuickVina-w is designed for blind docking. Vina-GPU can greatly accelerate docking by using GPU. Docking in 2 seconds is available on a personal computer. **If you want to use Vina-GPU, be sure to read the notes about Vina-GPU in “*Menu-About-FAQ*”**. QuickVina2, QuickVina-w and Vina-GPU have the same scoring function as Vina.

We recommend using the “Universal docking protocol with Vina” for batch docking tasks. This solution is universal for most protein-small molecule rigid receptor docking tasks, which achieves the best statistical results for re-docking and low docking costs on the CASF-2016 dataset. Using this protocol, only the docking box center is required in the config file. The box size will be automatically set to 4.5 times the ligand’s *R*g and the exhaustiveness parameter will be set to 16. For more information about the docking protocol, please see our research paper.

**4. 分子对接**

批量对接适用于虚拟筛选、反向钓靶、网络药理学结果验证等各种应用场景。Have fun docking!

1. 分别设置配体(.pdbqt)、受体(.pdbqt)、对接参数配置文件所在路径以及对接结果保存路径。**注意，路径中的所有pdbqt格式文件都会被识别为配体/受体。四个路径不能相同。**可以点击“*菜单栏-设置-新建路径*”来为您的对接项目创建一个新的工作路径。

**配置文件必须提前以受体名字命名以对应每个受体**，如1r42.pdbqt的配置文件名应为1r42.txt。因为不同受体的结合位点一定是不同的。建议使用本软件的模块3来生成配置文件，**如果您想使用自己的配置文件，记得删除配置文件中的任何配体和受体信息**。

**请注意，配体名称或受体名称中的任何"-"将被"\_"取代，原因是对接后的结果分析将使用"-"来分隔配体名称和受体名称。如果任何受体名称因此而改变，请相应更改配置文件的名称以对应每个受体**。

1. 决定是否自动进行结果分析。所有对接结果的亲和力分数将被汇总到一个Excel文件中，亲和力热图也将被绘制和显示。对接结果构象将被分割成单一的构象文件。如果不想自动分析或结果分析失败，可以使用模块5手动进行分析。
2. 若要进行大批量对接操作，对接进程可以被随时终止，直接关闭软件即可。或者是由于意外导致对接中断。可以通过勾选对接状态中“未完成的对接”来继续上次的对接任务，但**务必保证上述四个路径完全一致**。
3. 选择对接算法或打分函数。Vinardo被报道是一个更准确的打分函数，对接算法与Vina相同。QuickVina2使用一种改进的算法来提高对接速度。QuickVina-w用于盲对接准确性更佳。Vina-GPU可以通过使用GPU大大加速对接进程，2秒一次的对接在个人电脑上即可实现。**如果你想使用Vina-GPU，请务必阅读 "菜单栏-关于-FAQ "中关于Vina-GPU的使用注意事项**。QuickVina2、QuickVina-w和Vina-GPU具有与Vina相同的评分功能。

我们建议使用 "蛋白质-小分子半柔性对接通用方案"进行批量对接任务。这个方案对大多数蛋白质-小分子半柔性对接都是通用的，它在CASF-2016数据集上实现了最佳的重对接统计结果和尽可能低的对接成本。使用本方案，在参数配置文件中只需设置对接盒子中心。盒子的大小将被自动设置为配体回转半径的4.5倍，穷尽性参数exhaustiveness将被设置为16。关于本对接方案的更多信息，请参见我们的研究论文。