**1. Prepare receptors**

***1.1 Download proteins***

This module is used to automatically download protein structure files (*.pdb*) for docking from the RCSB PDB database. A protein index file (*.xlsx* or .*xls*) containing all the PDB IDs of the proteins to download is required. Click the "An example of index file" button to see how to prepare an *Excel* file.

1. Click "An example of index file" and follow this example to create your own *Excel* file and fill in all the PDB IDs of the proteins to download. Note that **each cell can only be filled with one PDB ID**. **Don’t fill in any other content**, such as line number, title, and so on.
2. Click "Select a protein index file" to select this *Excel* file.
3. Click "Choose saving directory" to set the directory where the protein structure files will be saved.
4. Click "Begin to download" and wait……

After the download task is complete, you can click "View download failure list" to see which proteins were not downloaded successfully (Blank content means that all the compounds were downloaded successfully).

***1.2 Prepare docking receptors***

This module is used to prepare original protein structure files and convert them into the *pdbqt* format which can be recognized by Vina and its derivatives.

**To use this module, please install MGLTools1.5.6 first. Note that any space or special character in the installation directory is forbidden. Otherwise, unknown BUGs may occur.** The installation package can be available from the MGLTools official website or our GitHub page: <https://github.com/DUTchecheche/BatchVinaGUI-v2.2.0/releases>.

1. Click "Choose MGLTools directory" button to set the installation directory of MGLTools, where the *python.exe* of MGLTools is located. (The Python interpreter is usually located in the first level folder of the installation directory.)
2. Click "Choose receptors directory" to set where the protein structure files are located (e.g. the saving directory in module 1.1). **Note that all the files in *pdb* format in this directory will be considered as docking receptors**.
3. Click "Choose saving directory" to set the directory where the docking receptors will be saved.
4. Check appropriate pre-processing steps according to the actual research purpose.
5. Select an appropriate protonation state for docking receptors.
6. Click "Begin to prepare" and wait……

**1. 准备受体**

***1.1下载蛋白质结构***

该模块用于自动地、批量化地从RCSB PDB数据库下载对接所需蛋白质结构(.*pdb*)。一个包含所有要下载的蛋白质的PDB ID的索引文件是必须的，格式为*.xlsx*或*.xls*。点击“索引文件示例”来查看如何准备一个Excel索引文件。

1. 点击“索引文件示例”，仿照该示例创建你自己的索引文件，将所有要下载的蛋白质的PDB ID填入其中，注意**每个单元格内只能填写一个PDB ID，不要填写其他如行号、标题等无关内容**。
2. 点击“选择蛋白质索引文件”来选中该Excel表格。
3. 点击“选择保存路径”来设定蛋白质结构文件的保存位置。
4. 点击“开始下载”并等待……

下载全部完成后，可以点击“查看下载失败列表”来查看哪些蛋白质下载失败了，显示空白说明全部下载成功。

***1.2准备对接受体***

该模块用于准备原始蛋白质结构文件并将其转化为Vina及其系列软件能够识别的*pdbqt*格式。

要使用此模块，请先安装MGLTools1.5.6。**请务必注意，MGLTools的安装目录中禁止出现空格、中文或特殊字符，否则会出现未知BUG**。安装包可以从MGLTools官网或者我们的GitHub页面获得<https://github.com/DUTchecheche/BatchVinaGUI-v2.2.0/releases>。

1. 点击“选择MGLTools安装路径”按钮，选定其安装路径，该路径下须含有MGLTools的python.exe(python解释器通常位于安装目录的一级文件夹下)。
2. 点击“选择受体所在路径”，设置蛋白质结构文件所在位置(例如模块1.1中的使用的结构保存路径)。**注意该目录下的所有*pdb*格式文件都会被视为对接受体。**
3. 点击“选择保存路径”设定准备后的对接受体保存位置。
4. 根据实际研究目的，勾选适宜的预处理步骤。
5. 为对接受体选择适宜的质子化状态。
6. 点击“开始转化”并等待……