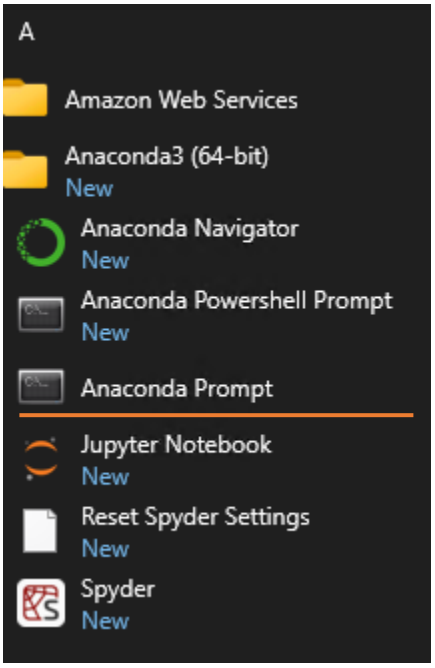
Installation Guide in Windows

1. Install Anaconda3 , please refer to the instructions in https://www.anaconda.com/download
2. Start Anaconda prompt from start Menu



3. Create Python 3.9 environment, and name it as “gpquest2.2” or any name you like

```
(base) C:\Users\Administrator>conda create --name gpquest2.2 python=3.9
```

4. Activate the conda python environment (gpquest2.2) and install gpquest package

```
(base) C:\Users\Administrator>conda activate gpquest2.2

(gpquest2.2) C:\Users\Administrator>cd Downloads\GPQuest

(gpquest2.2) C:\Users\Administrator\Downloads\GPQuest>pip install gpquest-2.1.2-cp39-cp39-win_amd64.whl
Processing c:\users\administrator\downloads\gpquest\gpquest-2.1.2-cp39-cp39-win_amd64.whl
Collecting matplotlib>=3.4.3 (from gpquest==2.1.2)
  Downloading matplotlib-3.8.2-cp39-cp39-win_amd64.whl.metadata (5.9 kB)
Collecting numpy>=1.21.2 (from gpquest==2.1.2)
  Downloading numpy-1.26.3-cp39-cp39-win_amd64.whl.metadata (61 kB)
     ---------------------------------------- 61.2/61.2 kB 1.1 MB/s eta 0:00:00
```

Usage of GPQuest2 in Windows

1. Type “gpquest -h” after successfully installing all dependency packages and gpquest in the python environment GPQuest 2.2. The Warning information about pandas package can be ignored.

```
(gpquest2.2) C:\Users\Administrator\Downloads\GPQuest>gpquest -h
C:\ProgramData\anaconda3\envs\gpquest2.2\Scripts\gpquest.exe\__main__.py:4: DeprecationWarning:
Pyarrow will become a required dependency of pandas in the next major release of pandas (pandas 3.0),
(to allow more performant data types, such as the Arrow string type, and better interoperability with other libraries)
but was not found to be installed on your system.
If this would cause problems for you,
please provide us feedback at https://github.com/pandas-dev/pandas/issues/54466


GPQuest is running...
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usage: gpquest [-h] [-i INPUT] -o OUTPUT [-d] [-p PARAMS] [-f]

ms_pycloud command line arguments

optional arguments:
  -h, --help            show this help message and exit
  -i INPUT, --input INPUT
                        Input FileName
  -o OUTPUT, --output OUTPUT
                        Output directory
  -d, --database        Prepare decoyed database
  -p PARAMS, --params PARAMS
                        GPQuest Parameters
  -f, --files           Prepare default parameter file
```

2. Run gpquest on HGI study sample file in the command line.
   gpquest -i C:\HGI\sample.mzML -o C:\HGI\out -p C:\HGI\gpquest_params.json
   Please replace the path name of the input file, output directory and parameter file using the absolute path name in your Windows system like below:

```
(gpquest2.2) C:\Users\Administrator\Downloads\GPQuest>gpquest -i C:\Users\Administrator\Downloads\MS-PyCloud\revision\M
SData\HGI\out\step1-mzml\A_glycopepnew_HCDETciDOTCIDpeptide.mzML -o C:\Users\Administrator\Downloads\MS-PyCloud\revisio
n\MSData\HGI\out2 -p C:\Users\Administrator\Downloads\MS-PyCloud\revision\MSData\HGI\out\configs\gpquest_params.json
```

   The sample parameter file (gpquest_param.json) ,protein .fasta file and glycan file can be found in the sample folder in the github repository. The details of the configuration in parameter file (gpquest_param.json) can be found in the document introduction_to_parameter_file.docx.