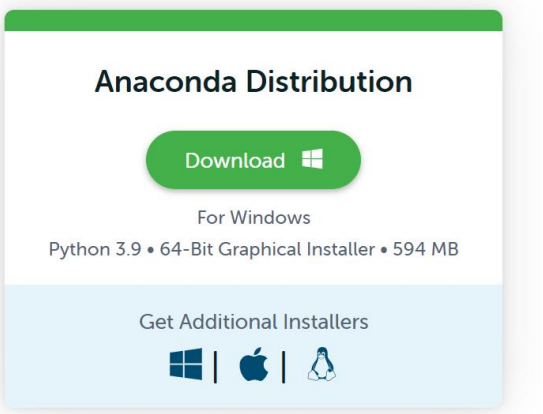
Installing Protein Kinetics Application

Step 1 Installing Anaconda

- In this example, we'll do the installation for Windows operative system: https://docs.anaconda.com/anaconda/install/windows/
- If you require a macOS installation please visit: https://docs.anaconda.com/anaconda/install/mac-os/
- Or a Linux installation: https://docs.anaconda.com/anaconda/install/linux/



- Download and run the .exe installer.
- Click Next > to continue.
- Accept the terms of the agreement clicking I Agree.
- Wait a few minutes while Anaconda installs.
- Once anaconda is installed, click Finish.

Step 2 Create virtual environments

The virtual environments in Anaconda allow us to isolate the programming environment in Python and work with specific versions of libraries or packages without affecting other virtual environments previously or later installed.

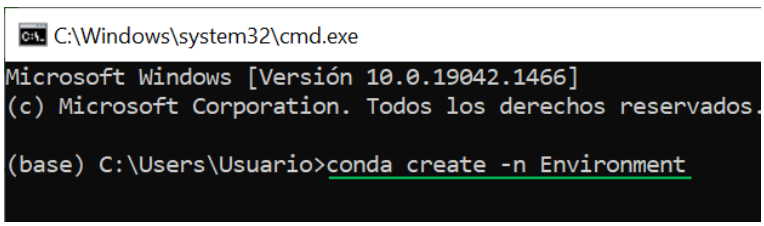
For more information about managing environment you can visit:

https://docs.conda.io/projects/conda/en/latest/user-guide/tasks/manage-environments.html

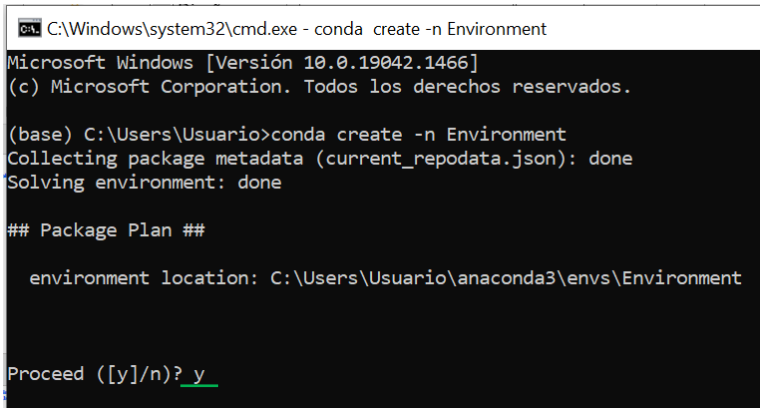
- Open Anaconda Navigator on your computer.
- Run CMD.exe Prompt clicking on Launch to open the cmd terminal.
- In the cmd terminal enter the following line:

"`conda create -n Environment anaconda`"

This command will create a new environment called "Environment" and install some Python libraries, making the installation more straightforward.

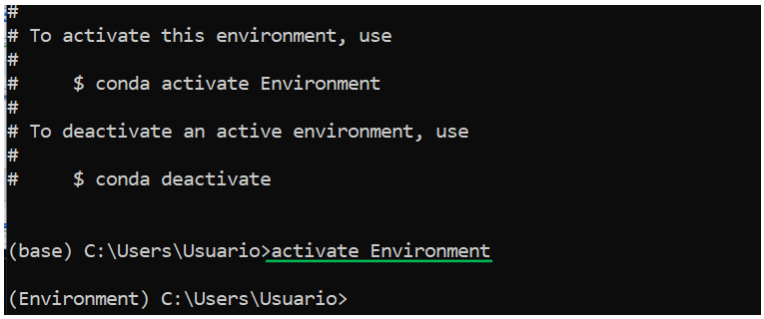


- Press **y** to proceed.



- To activate your virtual environment, type:

  “activate Environment”



It is necessary to activate your programming environment before installing the necessary libraries and before using this application.

Step 3 Add libraries

- The required libraries are:
  - ✓ Numpy
  - ✓ Scipy
  - ✓ Pandas
  - ✓ Sklearn
  - ✓ PyQt5
  - ✓ Matplotlib
  - ✓ Openpyxl
  - ✓ Prettytable

However, the Prettytable library was not installed in the previous step.

> Note: To install Prettytable package type:
>
> “conda install -c conda-forge prettytable”
>
> with Environment activated.
>
> Or visit this link:
>
> https://anaconda.org/conda-forge/prettytable
>
> To learn more about conda commands in the different operating systems you can visit:
>
> https://docs.conda.io/projects/conda/en/4.6.0/_downloads/52a95608c49671267e40c689e0bc00ca/conda-cheatsheet.pdf

Step 4 | Access the Protein Kinetics GUI file

- Navigate to the location of the Protein Kinetics GUI file.

Consider the following specific commands according to your operating system.

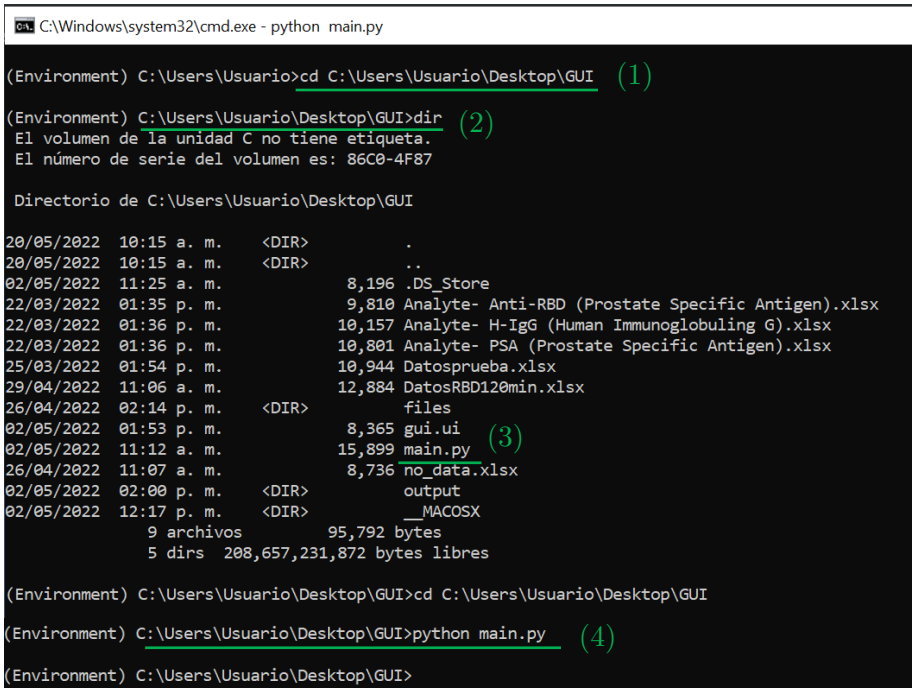
Windows :

- **dir**: list the contents of a particular directory
- **cd:** change to another directory.

Macintosh and **Linux :**

- **ls:** list the contents of a particular directory
- **cd:** change to another directory.

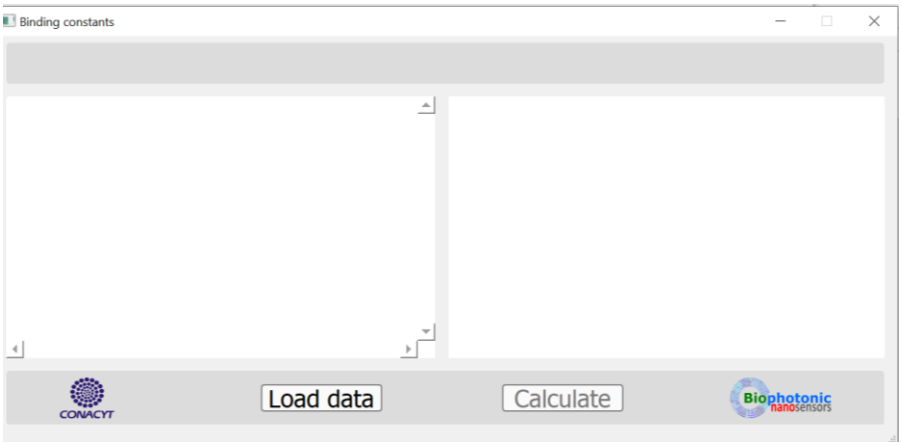
- The image below indicates the way you can employ the commands to find and run the GUI folder.



1. Write the command `cd` followed by the path of the GUI file.
2. Use `dir` to list the contents of the GUI file.
3. Identify the main.py file.
4. This file can be run by typing on the terminal:

"`python main.py`"

A pop-up window like the one shown below will appear.

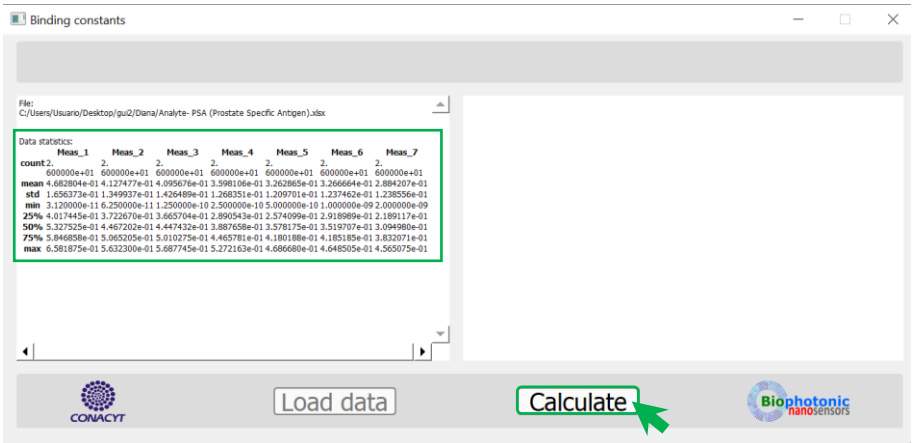


Step 5 GUI Usage

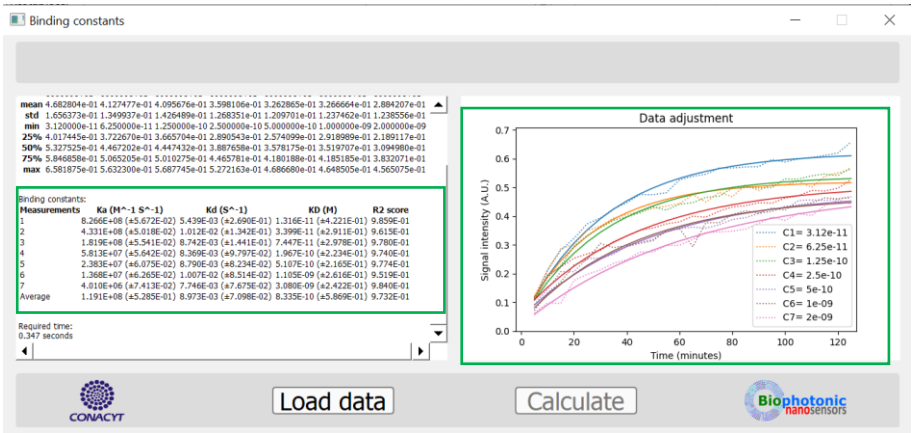
- To start, click in Load data.
- Select the file with the measurements to be analyzed.

Once the data has been loaded, data statistics will appear on the interface (see image below).

- To determine the binding constants, click on calculate button.



Finally, the association rate Ka, the dissociation rate Kd, and the dissociation equilibrium constant KD are presented in inverse molarity and seconds ($M^{-1}s^{-1}$), inverse seconds (s^{-1}), and molarity (M) units, respectively.



The graph shows the characteristic curves of phase association.

A .txt file is generated with the previously obtained information and a .png image with the signal calibration curves in the output folder.