
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 to continue.
- Accept the terms of the agreement clicking .
- Wait a few minutes while Anaconda installs.
- Once anaconda is installed, click .


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.

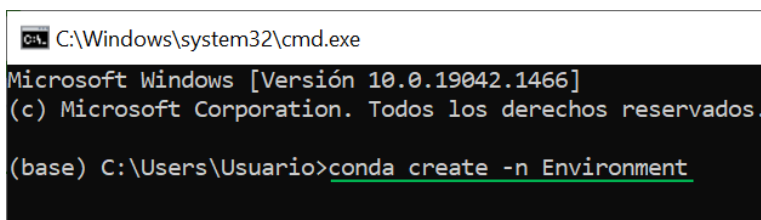
For more information about managing environment you can visit:

<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  to open the cmd terminal.
- In the cmd terminal enter the following line:

`"conda create -n Environment anaconda"`

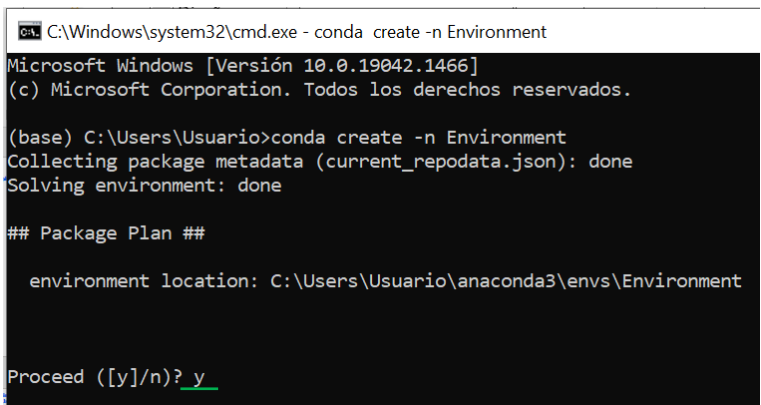
This command will create a new environment called "Environment" and install some Python libraries, making the installation more straightforward.



```
C:\Windows\system32\cmd.exe
Microsoft Windows [Versión 10.0.19042.1466]
(c) Microsoft Corporation. Todos los derechos reservados.

(base) C:\Users\Usuario>conda create -n Environment
```

- Press **y** to proceed.



```
C:\Windows\system32\cmd.exe - conda create -n Environment
Microsoft Windows [Versión 10.0.19042.1466]
(c) Microsoft Corporation. Todos los derechos reservados.

(base) C:\Users\Usuario>conda create -n Environment
Collecting package metadata (current_repodata.json): done
Solving environment: done

## Package Plan ##

   environment location: C:\Users\Usuario\anaconda3\envs\Environment

Proceed ([y]/n)? y
```

- To activate your virtual environment, type:
“activate Environment”

```
#
# To activate this environment, use
#
# $ conda activate Environment
#
# To deactivate an active environment, use
#
# $ conda deactivate
#

(base) C:\Users\Usuario>activate Environment

(Environment) C:\Users\Usuario>
```

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

- 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.

```
C:\Windows\system32\cmd.exe - python main.py

(Environment) C:\Users\Usuario>cd C:\Users\Usuario\Desktop\GUI (1)

(Environment) C:\Users\Usuario\Desktop\GUI>dir (2)
El volumen de la unidad C no tiene etiqueta.
El número de serie del volumen es: 86C0-4F87

Directorio de C:\Users\Usuario\Desktop\GUI

20/05/2022 10:15 a. m. <DIR> .
20/05/2022 10:15 a. m. <DIR> ..
02/05/2022 11:25 a. m.      8,196 .DS_Store
22/03/2022 01:35 p. m.    9,810 Analyte- Anti-RBD (Prostate Specific Antigen).xlsx
22/03/2022 01:36 p. m.   10,157 Analyte- H-IgG (Human Immunoglobuling G).xlsx
22/03/2022 01:36 p. m.   10,801 Analyte- PSA (Prostate Specific Antigen).xlsx
25/03/2022 01:54 p. m.   10,944 Datosprueba.xlsx
29/04/2022 11:06 a. m.   12,884 DatosRBD120min.xlsx
26/04/2022 02:14 p. m. <DIR> files
02/05/2022 01:53 p. m.    8,365 gui.ui (3)
02/05/2022 11:12 a. m.   15,899 main.py
26/04/2022 11:07 a. m.    8,736 no_data.xlsx
02/05/2022 02:00 p. m. <DIR> output
02/05/2022 12:17 p. m. <DIR> __MACOSX
          9 archivos          95,792 bytes
          5 dirs 208,657,231,872 bytes libres

(Environment) C:\Users\Usuario\Desktop\GUI>cd C:\Users\Usuario\Desktop\GUI

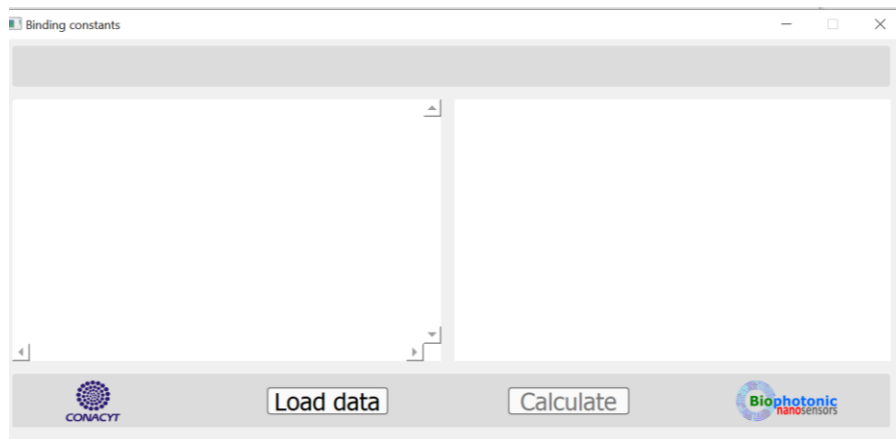
(Environment) C:\Users\Usuario\Desktop\GUI>python main.py (4)

(Environment) C:\Users\Usuario\Desktop\GUI>
```

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”

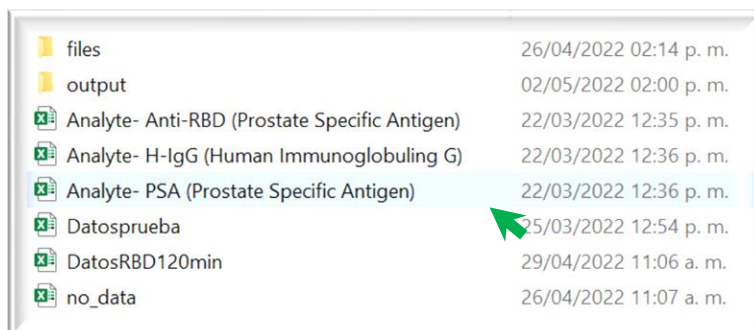
A pop-up window like the one shown below will appear.



Step 5

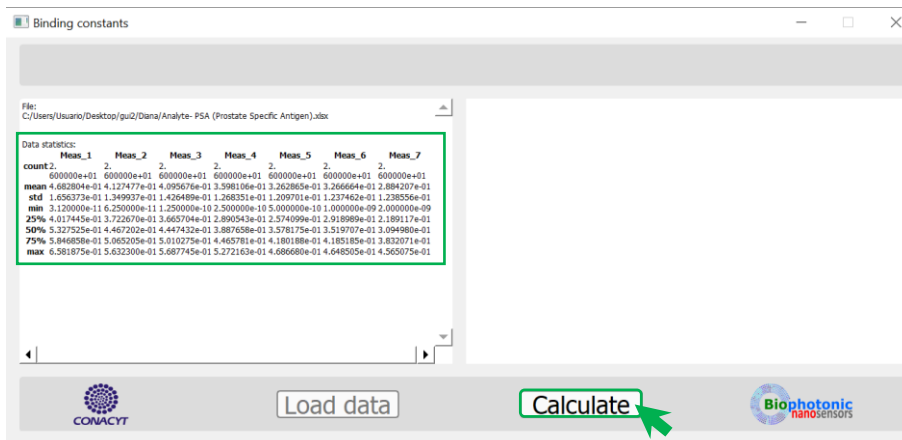
GUI Usage

- 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).

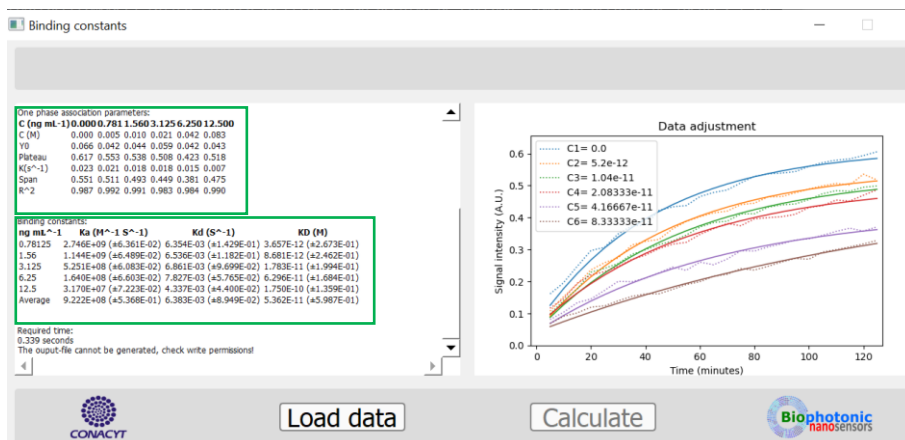
- To determine the one phase association parameter and binding constants, click on calculate button.



The following one phase association parameters are calculated:

- C (ng.mL⁻¹), Concentration.
- Y₀(a.u) is the Y value when X (time) is zero.
- Plateau is the Y value at infinite times, expressed in the same units as Y.
- K (s⁻¹) is the rate constant.
- Span is the difference between Y₀ and Plateau, expressed in the same units as your Y values.

Finally, the association rate Ka, the dissociation rate Kd, and the dissociation equilibrium constant KD are presented in inverse molarity and seconds (M⁻¹s⁻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.