

# PyES User Manual

v1.0.0

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# 1 Introduction

PyES is a software for the computation of species concentration at equilibrium. This manual wants to be a quick start guide for the end user, allowing to get accustomed to the interface as possible. If interested in the math behind the calculations it would be more of interest to read [the paper](#).

This manual is organized as follows:

- Section 2 introduces some of the common terminology used throughout this document.
- Section 3 briefly guides through the installation process for the supported platforms.
- Section 4 presents the software interface and explains the meaning of the various input fields available to the user.
- Section 5 provides examples of the various work modes of the software.

## 2 Glossary

**Chemical System:** a closed chemical system which includes both liquid and solid phase.

**Species:** chemical entity present in the chemical system, it can be “soluble” (meaning it only resides in the liquid phase) or “precipitable” (it can precipitate leaving the liquid phase).

**Component:** subset of the species in the system that can be used to describe the rest through their stoichiometric coefficients. It is important to note that a component does not need to be a single atomic entity (i.e.  $\text{H}_3\text{PO}_4$  can be defined as  $3\times\text{H}^+ + 1\times\text{PO}_4^{3-}$ , a metallic complex of glycine and copper can be written as  $1\times\text{Cu} + 1\times\text{gly}$ )

**Analytical Concentration:** the “total concentration” of a component; that is the summed molar concentration of all the species containing said component multiplied by the corresponding stoichiometric coefficient.

**Background Ions:** chemical species that do not directly interact with the chemical system but affect the ionic strength of the solution.

## 3 Installation

In this a brief explanation on how to install PyES will be provided.

PyES is compatible with any X86-64 hardware. The following Operating System are officially supported.

- Windows 10+
- macOS 10.14+
- Ubuntu 20.04+

PyES might work on other systems but it is not guaranteed.

The various installers can be downloaded from the [release page](#) on GitHub.

### 3.1 Windows

1. Double click on the downloaded `.exe` installer
2. If prompted with the request of giving permissions to modify your system click “Yes”<sup>1</sup>.
3. Follow the instructions provided by the installer.

### 3.2 MacOS

1. Double click on the downloaded `.dmg` file
2. If the OS blocks the file from opening follow the [official instructions](#) to open unsigned applications<sup>1</sup>.
3. Follow the instructions provided by the installer.

### 3.3 Linux

1. Open a terminal
2. Execute `sudo apt install path_to_deb` where `path_to_deb` points to the downloaded `.deb` file on you system.

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<sup>1</sup>For the time being we are not able to sign our installers, this might prompt with some security alerts on Windows and macOS. Our software does not execute any code whose purpose is other then solving solution and precipitation equilibria. We encourage to audit our code on [GitHub](#)

## 4 User Interface

The main interface presented to the user after launching the software can be seen in Figure 1.

- 1 The title bar bears the path of the current project (or “New Project” if the current project has not been saved yet).
- 2 In the menu bar shortcuts for the most common operations are present (i.e. create/open a project, save the current project, launch a calculation, ...).
- 3 A brief explanation of the hovered field or button is displayed in the status bar at the bottom.

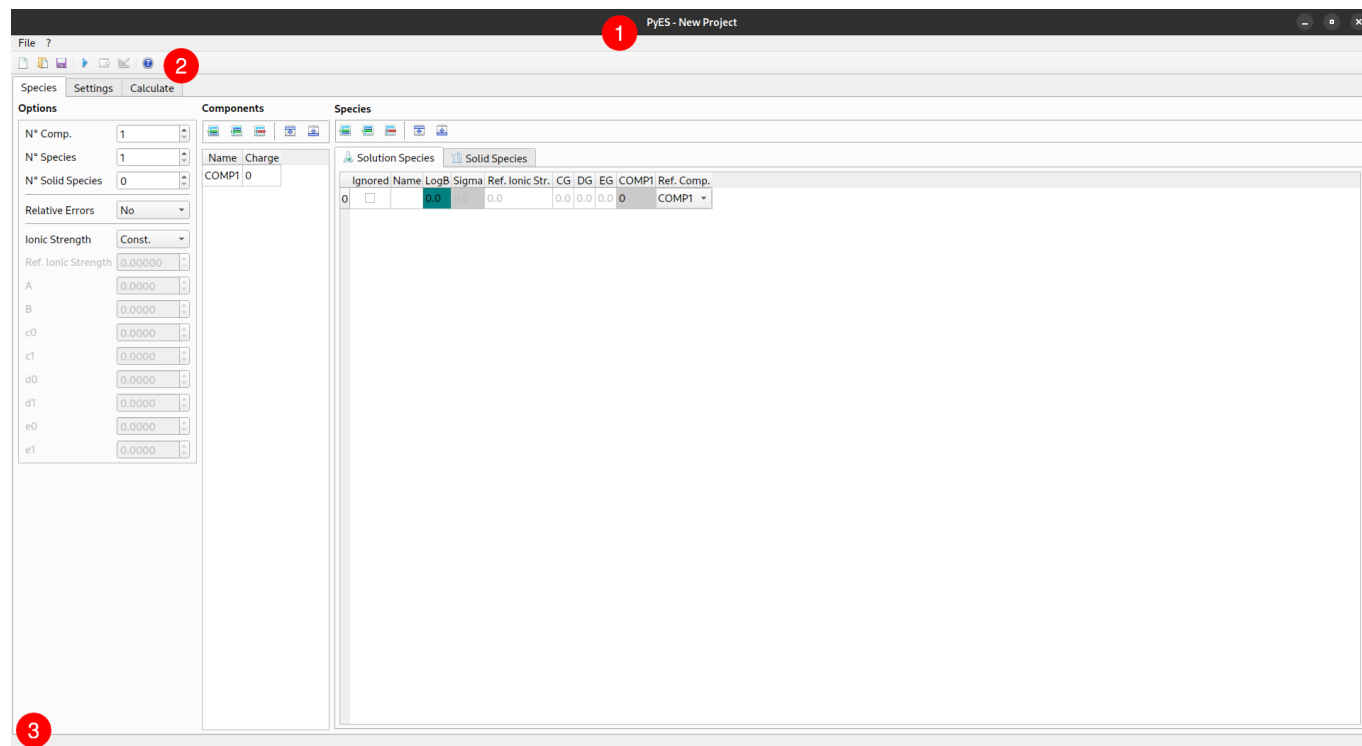


Figure 1: Main Window

The interface is organized in three main tabs, each representing a different step in the definition of the calculation parameters.

### 4.1 Species Tab

The “Species” tab (Figure 2) is the one shown by default to the user after opening the software for the first time. In this tab is where a qualitative description of the chemical system is input. In particular the interface presents the following input fields:

- 1 Number of components, soluble and precipitable species.
- 2 Computation of “Uncertainty Estimation” deriving from uncertainties of inputs and effect of ionic strength on stability constants.
- 3 Table for defining components names and charges.
- 4 Tables to input soluble and precipitable species.
- 5 Quick commands to move/insert/remove species and components from their corresponding tables.

Soluble and precipitable species tables are shown in details in Figure 3. They are very similar, requiring the user to provide the following information for each one of the species present:

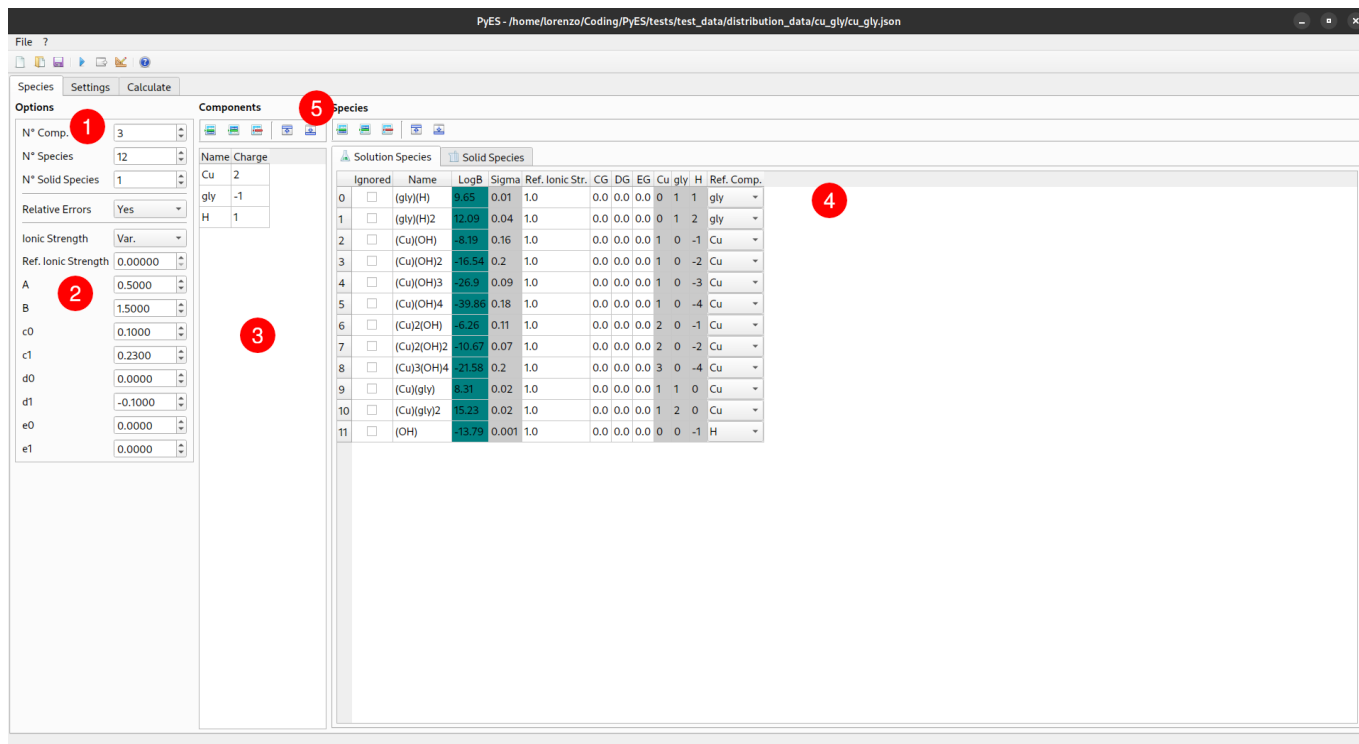


Figure 2: Species Tab

- ① Checkbox to exclude the corresponding species from the calculation (useful to test different systems assemblages without having to create a project for each one).
- ② Name of the species; this is not an editable space, the name is obtained from the stoichiometric coefficient of the species itself.
- ③ Depending on the type of species  $\log_{10}$  of stability constant/solubility product of the species.
- ④ Uncertainty on the stability constant/solubility product of the species, used for the propagation of uncertainty, only active when the corresponding option is selected in the “Species” tab.
- ⑤ Reference ionic strength and Debye-Hückel parameters for which the stability constant/solubility product of the species is defined; this can be left at zero, using the project-wise values defined in the “Species” tab.
- ⑥ Stoichiometric coefficients of components used to defined the species.
- ⑦ Component to use to compute the species concentration as a fraction of analytical concentration of the component.

## 4.2 Settings Tab

In the “Setting” tab the user can select the work mode for the calculation and provide the quantitative information of the system described in the “Species” tab.

Depending on the selected work mode different inputs are required from the user (Figure 5).

### 4.2.1 Titration Mode

- ① Table with the analytical concentration of the components in the titration vessel (C0) and in titrant solution (CT) in mol/L; uncertainty on this values can be provided too if “Uncertainty Estimation” has been selected in the “Species” tab.

Solution Species		Solid Species																	
Ignored	Name	LogB	Sigma	Ref. Ionic Str.	CG	DG	EG	Ca2+	Mg2+	PO4-3	C2O4-2	Cit3-	SO4-2	Na+	K+	NH4+	CO3-2	H	Comp. %
0	<input type="checkbox"/> (OH)	-14.0		0.0	0.0	0.0	0.0	0	0	0	0	0	0	0	0	0	0	-1	H
1	<input type="checkbox"/> (PO4-3)(H)	12.6		0.0	0.0	0.0	0.0	0	0	1	0	0	0	0	0	0	0	1	PO4-3
2	<input type="checkbox"/> (PO4-3)(H)2	19.3		0.0	0.0	0.0	0.0	0	0	1	0	0	0	0	0	0	0	2	PO4-3
3	<input type="checkbox"/> (PO4-3)(H)3	21.56		0.0	0.0	0.0	0.0	0	0	1	0	0	0	0	0	0	0	3	PO4-3

1

2

3

4

5

6

7

(a) Soluble

Solution Species		Solid Species																		
Ignored	Name	LogKs	Sigma	Ref. Ionic Str.	CGF	DGF	EGF	Ca2+	Mg2+	PO4-3	C2O4-2	Cit3-	SO4-2	Na+	K+	NH4+	CO3-2	H	Comp. %	
0	<input type="checkbox"/> (Ca2+) <sub>3</sub> (PO4-3) <sub>2</sub>	-24.69		0.0	0.0	0.0	0.0	3	0	2	0	0	0	0	0	0	0	0	Ca2+ ▾	
1	<input type="checkbox"/> (Ca2+)(CO3-2)	-8.48		0.0	0.0	0.0	0.0	1	0	0	0	0	0	0	0	0	1	0	Ca2+ ▾	
2	<input type="checkbox"/> (Ca2+)(PO4-3)(H)	-6.9		0.0	0.0	0.0	0.0	1	0	1	0	0	0	0	0	0	0	1	Ca2+ ▾	
3	<input type="checkbox"/> (Ca2+) <sub>5</sub> (PO4-3) <sub>3</sub> (OH)	-57.5		0.0	0.0	0.0	0.0	5	0	3	0	0	0	0	0	0	0	-1	Ca2+ ▾	

1

2

3

4

5

6

7

(b) Precipitable

Figure 3: Species Input Tables

- ② Volume of titration vessel, volume at first titration point (volume of titration vessel + volume of titrant added), volume of titrant added at each titration point, number of titration points.
- ③ If the effect of ionic strength has to be considered, as defined in the “Species” tab, the concentration of background ions in the titration vessel and in the titrant can be defined.

#### 4.2.2 Distribution Mode

- ① Table with the analytical concentration of the components (C0) in mol/L; uncertainty on this values can be provided too if “Uncertainty Estimation” has been selected in the “Species” tab.
- ② Component to use as the independent one, its initial, final and increment values; changing the component disables its row in the concentration tables since it will not be used for calculation purposes.
- ③ If the effect of ionic strength has to be considered, as defined in the “Species” tab, the concentration of background ions can be defined.

### 4.3 Calculate Tab

The “Calculation” tab (Figure 6) is reserved to calculation launching and reporting

- ① The text box in the center is where results and errors are reported in textual form to the user.
- ② Buttons dedicated to starting the calculation, exporting results and showing results in graphical form.
- ③ Toggle to allow writing a log file for debugging purposes.

### 4.4 Other Windows

After a successful calculation, using the dedicated buttons in the menu bar or the ones at the bottom of the calculation tab, it is possible to access other windows for the export and the graphical output of obtained results (Figure 7).

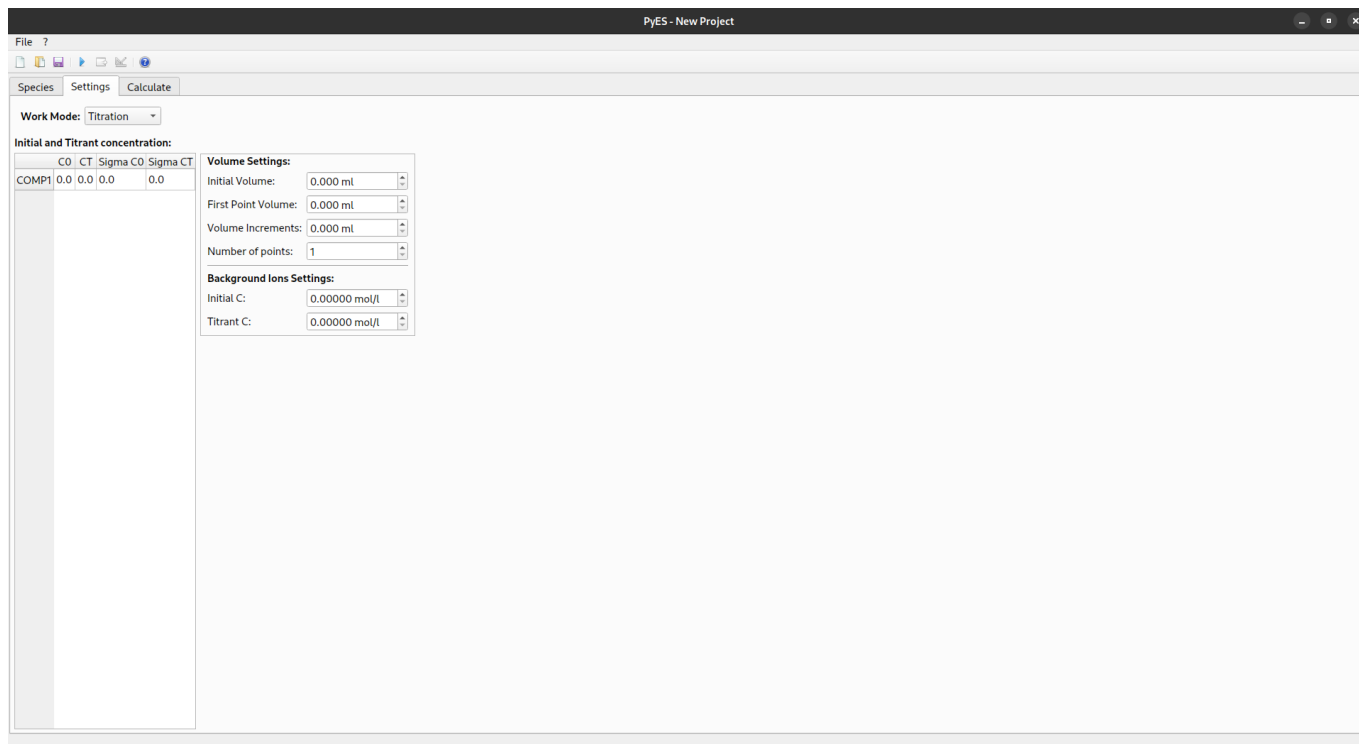
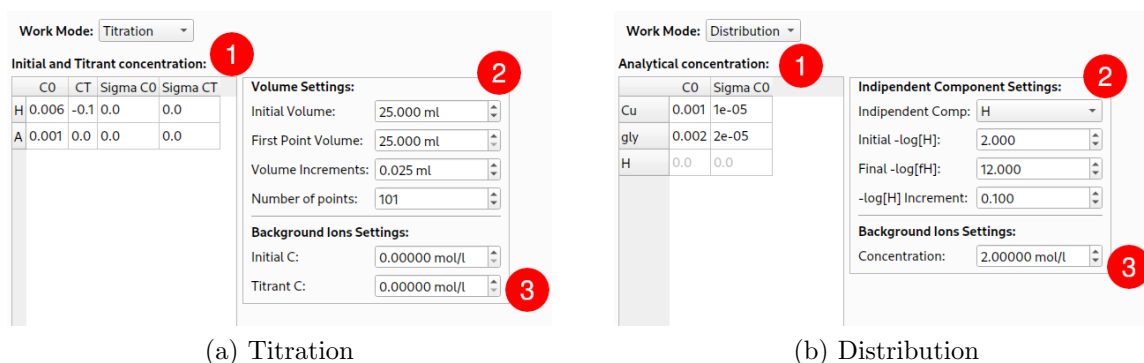


Figure 4: Settings Tab



(a) Titration

(b) Distribution

Figure 5: Different Work Mode Inputs

#### 4.4.1 Export Window

- ① The tabs allow to select if the results have to be exported as a single Excel spreadsheet or as multiple CSV files.
- ② Using the checkboxes it is possible to select only the desired results to be exported; some options may be grayed-out if the corresponding results have not being calculated (i.e. recalculated stability constants if the effect of ionic strength has not been considered).
- ③ The “Export” button let the user pick where to save the results.

#### 4.4.2 Plot Window

- ① The tabs allow to select the type of plot shown (concentration or percentages relative to components as defined in the tables in the “Species” tab).
- ② The plot itself; the legend can be moved by dragging it around with the mouse. right-clicking on the plot allow to change some options (i.e. axis scale, scaling, exporting as image, ...).
- ③ The table on the left lists all the soluble and precipitable species in two different tabs; tick-



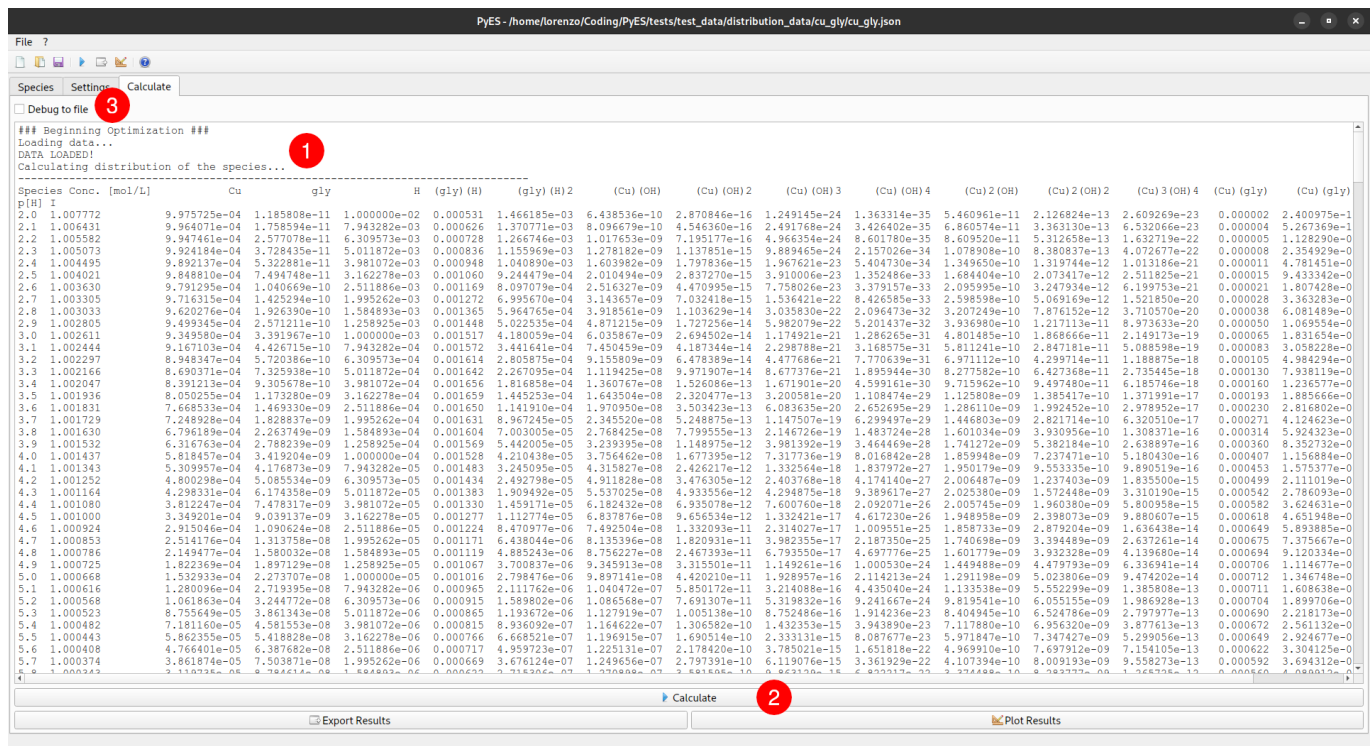


Figure 6: Calculate Tab

ing/untracking any species allow to display/hide them; clicking the colored square on the right of each species name it is possible to change the color used to plot it.

4 The buttons allow to select/deselect all the species and, clicking the “Filter” button, to select only the ones that contains a particular component; it is also possible, using the checkbox present to show the intervals of precipitation formation instead of the concentration of precipitates in the plot.



(a) Export

(b) Plot

Figure 7: Other Windows

## 5 Examples

In the following sections examples for the various work modes available in the software will be provided. The project files used can be found in the corresponding [‘test’ folders](#) in the official GitHub page.

### 5.1 Species Distribution (Cu-gly System)

The Cu-gly system as defined by IUPAC will be used to demonstrate the computation of species distributions.

1. Create a new PyES project.
2. Define a System of 3 components, 12 soluble species and 1 precipitable species.
3. Modify the components table to reflect the one shown in Table 1.
4. Modify the soluble species table to reflect the one shown in Table 2.
5. Modify the precipitable species table to reflect the one shown in Table 3.
6. In the “Settings” tab select “Distribution” as the “Work Mode”.
7. Select “H” as the independent component.
8. Define the range of  $-\log_{10} H$  from 2.0 to 12.0 with intervals of 0.100.
9. Modify the “Analytical concentration” table, setting C0 for Cu = 0.001 and gly = 0.002
10. In the “Calculate” tab press the “Calculate” button at the bottom.
11. Wait the pop-up reporting the termination of the calculation.
12. Access the results in textual form from the text box in the middle, in graphical form clicking the “Plot Results” button at the bottom, or export them clicking the “Export Results” button and following the instructions.

Name	Charge
Cu	2
gly	-1
H	1

Table 1: Components Table Cu-gly

### 5.2 Titration of Generic Hexaprotic Acid

The simulation of titration curves will be demonstrated through the definition of a generic system containing a single hexaprotic acid.

1. Create a new PyES project.
2. Define a System of 2 components, 7 soluble species and 0 precipitable species.
3. Modify the components table to reflect the one shown in Table 4.
4. Modify the soluble species table to reflect the one shown in Table 5.
5. In the “Settings” tab select “Titration” as the “Work Mode”.
6. Set the titration vessel and first point volumes to 25mL (that is, the first point of the titration will have 0mL of additional titrant added).

<b>LogB</b>	<b>Cu</b>	<b>gly</b>	<b>H</b>
9.65	0	1	1
12.09	0	1	2
-8.19	1	0	-1
-16.54	1	0	-2
-26.9	1	0	-3
-39.86	1	0	-4
-6.26	2	0	-1
-10.67	2	0	-2
-21.56	3	0	-4
8.31	1	1	0
15.23	1	2	0
-13.79	0	0	-1

Table 2: Soluble Species Table Cu-gly

<b>LogKs</b>	<b>Cu</b>	<b>gly</b>	<b>H</b>
8.91	1	0	-2

Table 3: Precipitable Species Table Cu-gly

7. Set the volume increments to 0.025mL and set the number of titration points to 101.
8. Modify the “Analytical concentration” table, setting C0 for H = 0.006 and A = 0.001
9. Modify the “Analytical concentration” table, setting CT for H = -0.1 (the titrant is basic) and leaving A to zero.
10. In the “Calculate” tab press the “Calculate” button at the bottom.
11. Wait the pop-up reporting the termination of the calculation.
12. Access the results in textual form from the textbox in the middle, in graphical form clicking the “Plot Results” button at the bottom, or export them clicking the “Export Results” button and following the instructions.

<b>Name</b>	<b>Charge</b>
A	-1
H	1

Table 4: Components Table Hexaprotic Acid

<b>LogB</b>	<b>Cu</b>	<b>H</b>
-13.77	0	-1
10.0	1	1
18.0	1	2
24.0	1	3
28.0	1	4
31.0	1	5
33.0	1	6

Table 5: Soluble Species Table Hexaprotic Acid