OpenTitration V2. User Manual

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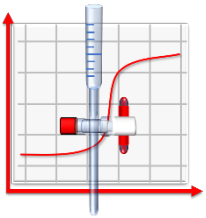
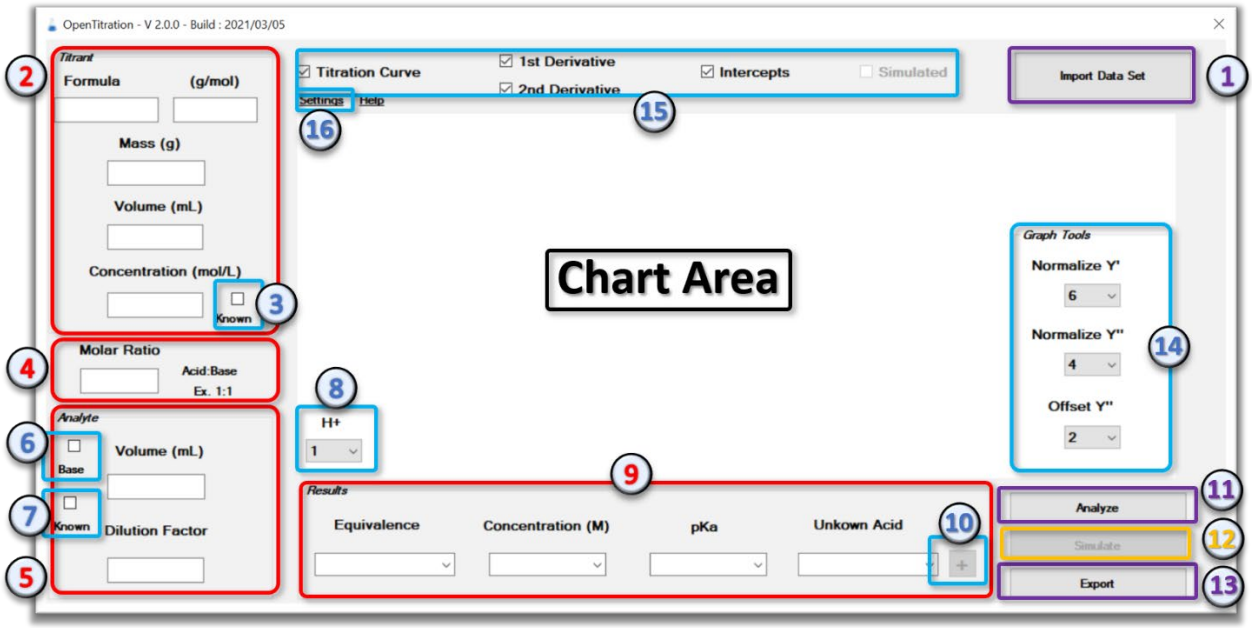


Getting Started:



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Read the import data section before getting started.

(1) Import Data

Imported data needs to be in the correct file format to be properly utilized by the program. That is a comma separated file, where **(volume(mL), PH)**. Each data entry needs to be on its own separate line (**figure 1**) and saved into a text file (.txt) using the windows notepad text editor.

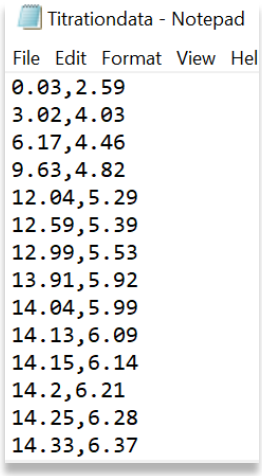

***Figure 1**. Data compiled in the proper file format*

Data can be automatically compiled into the proper format using excel. Simply input your data into the cells as illustrated (**figure 2**), where volumes are in the 'A' column and PH values are in the 'B' column. Do not include text labels for volume and PH in the respective rows as this will be rejected by the import wizard. Save the files as a comma separated file (.csv) and your data is ready to be opened by the application (**figure 3**).

	A	B
1	0.03	2.59
2	3.02	4.03
3	6.17	4.46
4	9.63	4.82
5	12.04	5.29
6	12.59	5.39
7	12.99	5.53
8	13.91	5.92
9	14.04	5.99
10	14.13	6.09
11	14.15	6.14
12	14.2	6.21
13	14.25	6.28
14	14.33	6.37
15	14.36	6.47
16	14.41	6.59
17	14.43	6.78
18	14.52	7.09
19	14.55	8.21
20	14.58	10.36
21	14.63	10.91

Figure 2. *Data format in excel*

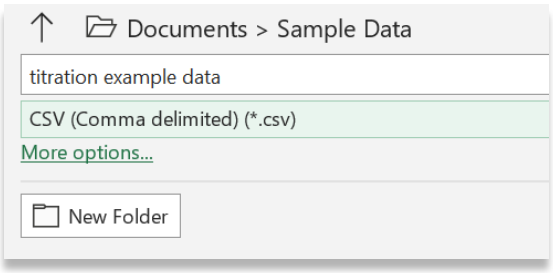

Figure 3. *Correct file type to save titration data*

Once your data is ready to be analyzed, press the import button and a prompt will open allowing you to select your data. By default, the file window looks for text files, but this file type can be changed if your data is in a (.csv) file. If you have done everything correctly your titration curve should be plotted on the chart window.

(2) Titrant Information

The titrant is the component in a titration that has a known concentration and is used to determine the equivalence point and molarity of the unknown solution. The formula entry will automatically compute the molar mass of the compound (**figure 4**). Currently brackets and chemical abbreviations for compounds are not supported.

To determine the molar concentration of your solution simply put in the mass and volume in addition to the formula. Pressing the analysis button will automatically compute the concentration. There is no need to manually compute the concentration, as this field will automatically be overwritten with the computation from the previous entries.

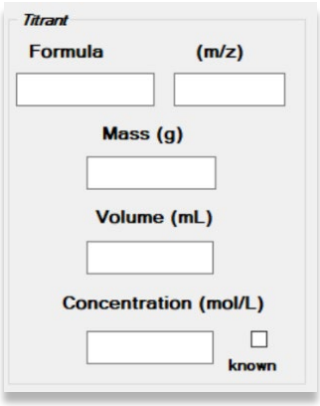

Figure 4. *Titrant controls and inputs*

The formula from the titrant is used to find a pKa value from an internal library. Since different compounds may have the same formula, a separate window may pop up asking the user to clarify which compound within the database has been used in the titration (**figure 5**). In the event that no acid or base matches the internal database, pKa values for that substance can be manually added in the settings window under 'Sim' (**see settings**).

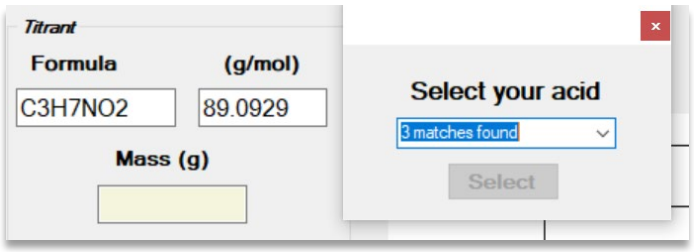

Figure 5. *Multiple Entries for Titrant Example*

(3) Known Concentration Toggle Switch

The known checkbox can be selected if the concentration of the titrant is already known. The mass and the volume will be omitted from the calculation, and their entry boxes will be closed to any data entry (**figure 6**). The mass of an inputted formula can be added optionally if that information is important to your export file. **Calculated concentration values will be automatically updated once the analysis has been completed if this toggle switch is selected.** Please note that values will only be updated if the moles of the titrant have been changed.

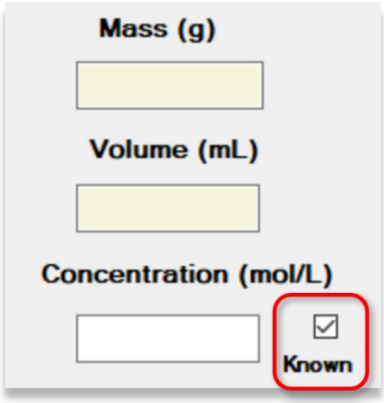

Figure 6. *Titrant controls with known concentration selected*

(4) Molar Ratio Entry

This field can be left blank as a 1:1 ratio will be added automatically. If you are dealing with a titration that requires a different ratio a particular format is required. That is the number of acid moles with a semicolon in between the number of base moles. Of example if you have 2 moles of acid (as in the case of H_2SO_4) to your base analyte your entry would be '**2:1**'.

(5) Analyte Information

As is often the case, the analyte is often diluted so multiple titrations can be performed on the same sample. To account for this simply put in the number of times your sample was diluted in the dilution factor field (**figure 7**). If no entry is done a default dilution factor of 1 is assigned to this field. To determine the overall concentration of the solution the volume of the analyte must be inputted into the volume field.

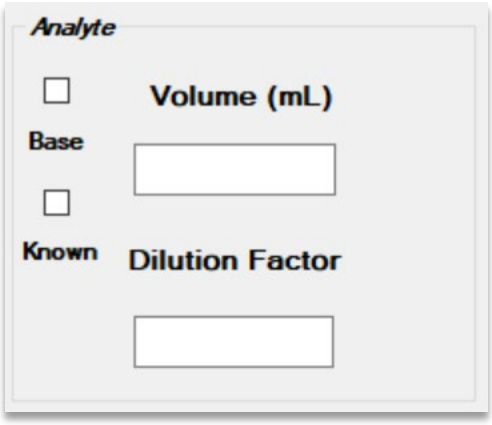

Figure 7: *Analyte information fields*

(6) Base Analysis Toggle Switch

By default, the application is set to analyze a solution with a basic titrant and acidic analyte. If the analysis is being done on a basic analyte, then the base checkbox must be selected. This application computes the equivalence point based on the derivative calculated from the data. An acid will abruptly increase when an equivalence is reached meaning there is a global maximum that can be obtained. A base analyte will decrease rapidly when approaching equivalency meaning a global minimum must be obtained. An incorrect selection will prevent this application from computing the value correctly.

(7) Known Acid Selector

Unlike the known concentration switch, the known acid selector allows the user to choose an acid from the internal acid library. Selecting this option will change the labels to the 'Known' acid which will also be reflected in all the exported files. Selecting the known acid selector checkbox will also allow for a custom acid to be added for recording and simulation purposes.

(8) Protonation State Selector

To accurately determine the unknown analyte and equivalences the correct protonation setting must be applied. Protonation states of the unknown are not automatically determined, and the largest peaks will ultimately be used for the calculations if the wrong setting is applied (**figure 8**). This selector must be used on acid analytes as well.

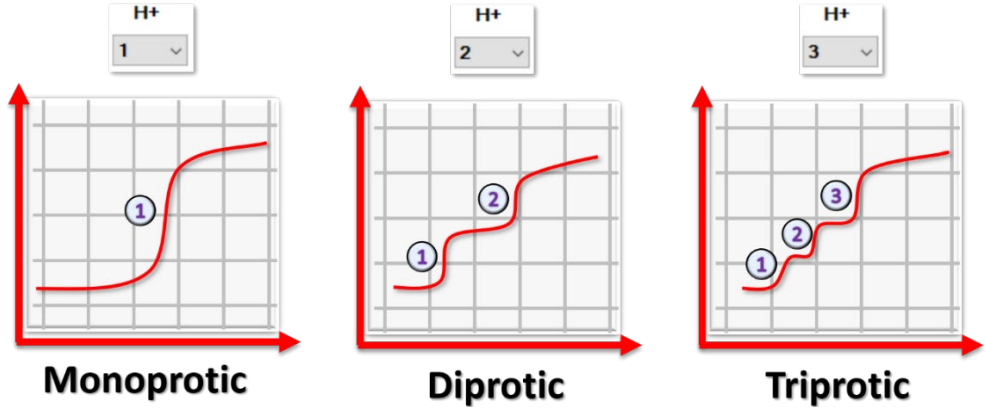

Figure 8. *Demonstration of different titration curves and recommended settings*

(9) Results

Results are tabulated upon use of the analyze button. Using the computed pKa data the unknown acid or base is determined from a library of acids and known pKa values. For bases the determined pKb values are converted to pKa values to be compared. The percentage match of also calculated to show how close your result is the actual value (**figure 9**). Multiple values for mono and diprotic analytes are logged into the combo boxes and are automatically output when the data is exported.

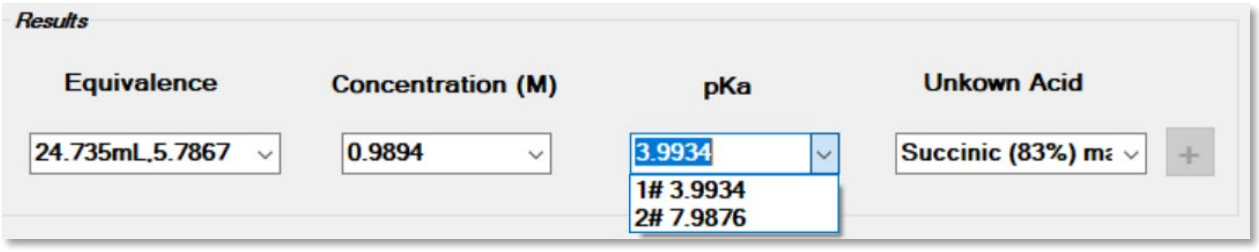

Figure 9*. Tabulated results of a diprotic acid analysis*

(10) Add Known Acid Utility

For the purposes of the simulation, a custom acid can be added as your analyte. To get started first select the acid selector switch. The add known acid utility button (seen as a plus sign beside the known acid combobox) will then be clickable (**figure 10**). Write the name of the acid and the pKa values of your custom acid. It is important that it is in the correct format, otherwise the utility will not accept those values. For example, if you have two pKa values being 3 and 4.5, simply write in the pKa Values field 3,4.5. That is the number of the first pKa separated by a comma followed by the pKa value. The value will automatically be inputed as your selected value. From there the custom acid will be accessible as the first item within the combobox. Adding a new acid will overwrite the old one in the current build of OpenTitration.

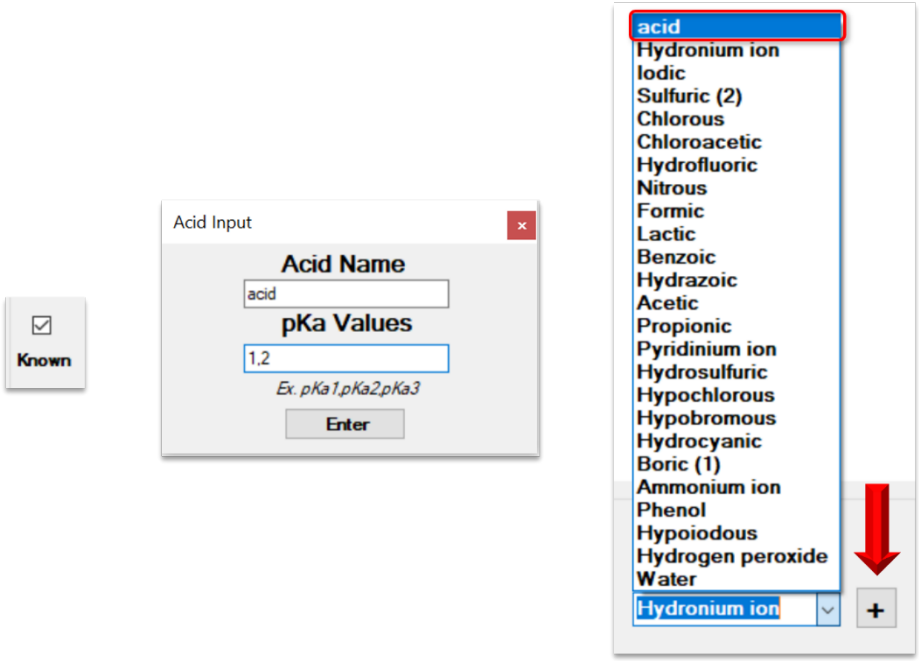

Figure 10: *Demonstration of the Known Acid Utility*

(11) Analyze

The analysis button uses all the settings and data input and initiates the computations on that information. It is not necessary to have the concentrations for the titrant to determine the pKa values. It is however necessary to determine the proper concentrations of your analyte. As the simulation functionality relies on the concentration determined from the analysis, it will not be accessible until the analysis has been completed.

(12) Simulation

Simulations can be run to compare user data with computationally generated data. This can be a useful tool when there are missing datapoints within user generated data or trying to determine whether a particular acid is a match for a certain unknown acid. The simulation framework was written in python and draws upon the internal python package within OpenTitration. Errors in data generation will open as a separate window when the simulation framework fails to generate that data. Simulation data created will be added to the export file for both PDF and TXT export formats.

(13) Export

The export button then allows you to output that information in three different file formats: 1) Text File (*.txt), 2) PDF (*.pdf) 3) Graphic Image (*.png). The PDF option outputs both the graph and all the compiled information into a single report. If you wish to manually compile the report, all computed information is more easily copied from the text file option. The graph itself can be exported separately to all the information by selecting the graphic image option (**figure 11**)

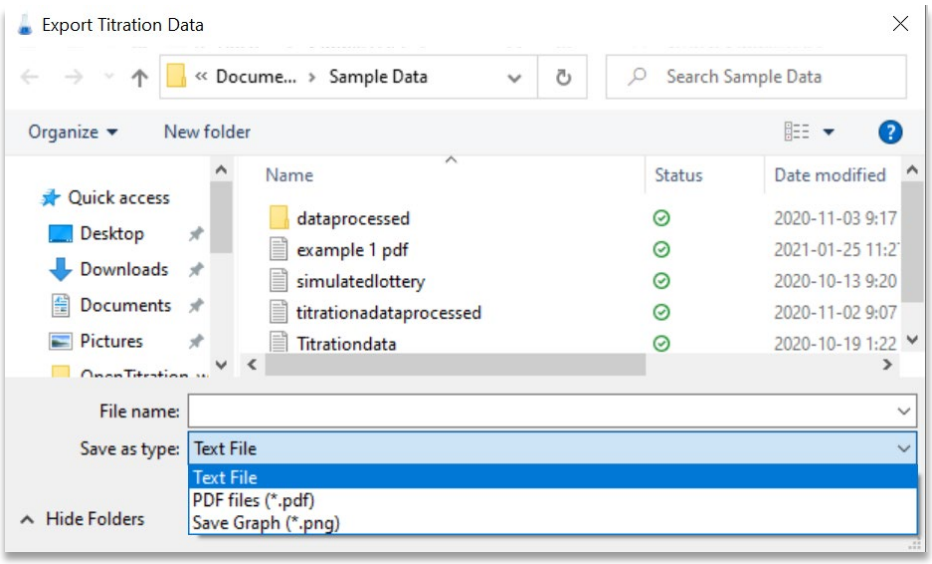

***Figure 11**. Exporting Titration Data*

(14) Graphing Tools

Graphing tools pertain to the visual presentation of the derivative and second derivative series on the graph. For a more convenient data visualization these series are normalized (**equation 1.**) before being plotted on the chart. The output values for the first and second derivatives are the values without normalization.

Equation 1: $$z_i = \frac{x_i - \min(x)}{\max(x) - \min(x)}$$

Figure 12: *Graphing Tools*

The normalized values are then multiplied by a factor. The default factor is 6 for Y' (z_i*6) and 4 for Y'' (z_i*4). This is simply to increase the size observed on the graph.

Due to the second derivative having a negative component an offset value is applied to keep it within the confines between 0-14 for the PH scale. This adds the selected value to every normalized value (z_i + offset).

(15) Chart Series Controls

You may not want to include the derivative and second derivative chart series on your graphs. You can remove these from the chart simply by toggling off the switch. The exported graphs will look exactly how they appear before they are exported. In addition, the ranges of the X and Y axis will automatically be recalculated whenever any of these switches are used.

(16) Settings

A wide array of text and chart options can be changed using the settings. There are also settings that allow you to change the font, size, margin and spacing options in the exported PDF files (figure 10). If you wish to preview these settings changes simply hit the apply button. If you found settings that you wish to apply to all data going forward hit the save button. All these settings will be automatically input whenever you reopen the application when the save button is applied. If you wish to return to the default buttons, simply hit the reset button.

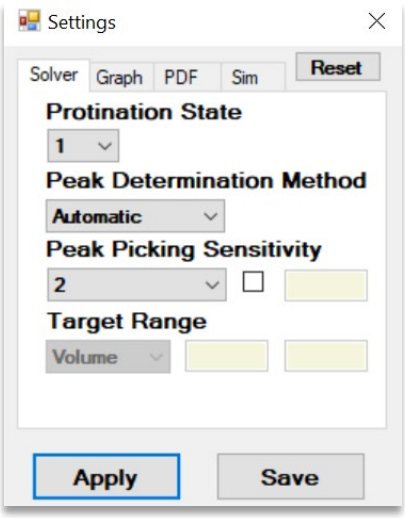

Figure 13. *Settings toolbox*

There are two types of solve methods available, 'automatic' and 'manual range'. Each has settings that can be adjusted for your data analysis needs.

Automatic:

Peak picking sensitivity is feature unique within the settings toolbox. There may be instances where the default settings will not find the peaks properly. The algorithm works by finding the largest peak in the derivative graph and computing the equivalence points from that. When you have multiple peaks due to multiple equivalence points the program first computes the largest peak, and then zeroes those values in a temporary derivative series (**figure 14**). The application then looks at the next global maximum and does the next set of computations based on that value. The peak picking sensitivity allows you to choose the number of values removed before and after the initial global maximum. This can be handy if there are many data points, or not a lot of data points in your titration curve. If you feel that the available range of peak picking selectivity is too small for your data set, you can check the box beside the selector to input your own custom peak picking selectivity.

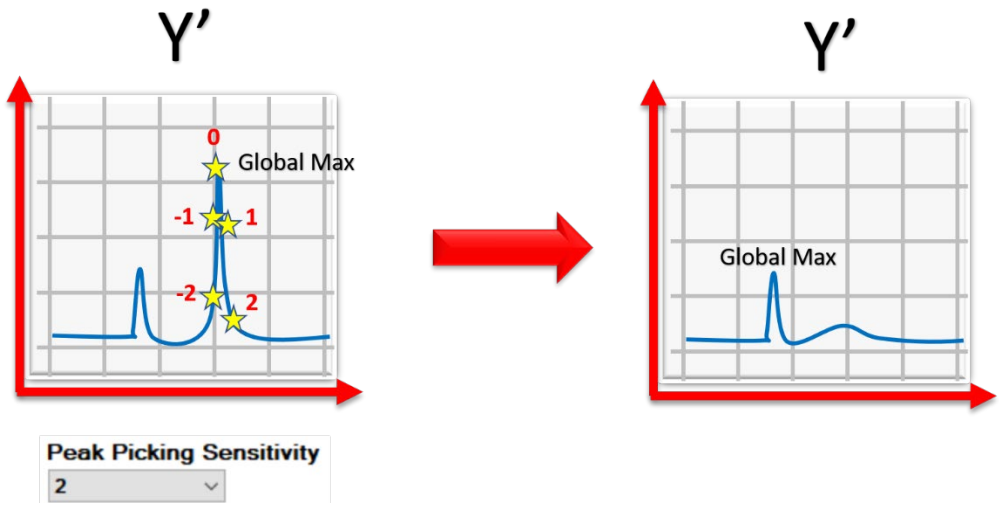

Figure 14. *Illustration of peak picking algorithm with a sensitivity value of 2*

Manual Range:

It is possible that the automatic peak picking option will not be sufficient for your analysis. For example, if there is a large difference in the size of the peaks, the automatic option will not be sufficient to capture it. In this case it will be prudent to select the 'Manual Range' option in the solver. To use this option, you will need to have more then one peak that you are trying to process. Simply select the 'Manual Range' option and input a value or values that are in between the two peaks. This can be done for both pH and volume. The solver will break both the graph into the sections between the value(s) that were selected (**figure 15.**)

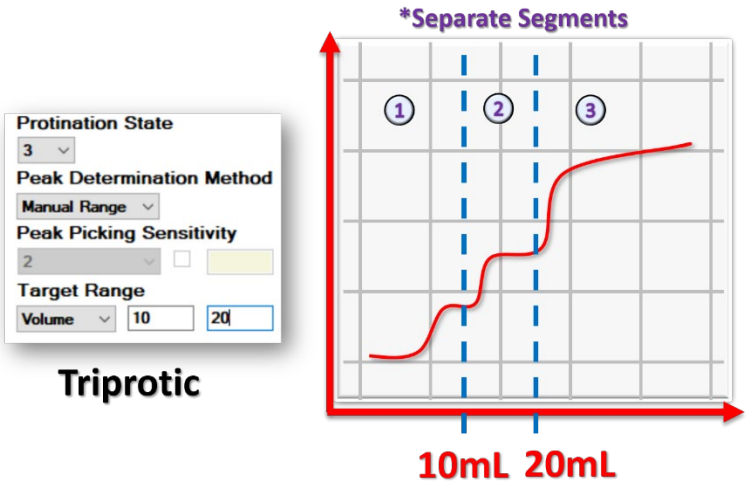

Figure 15. *Manual Entry Example for Triprotic Acid*

Simulator Settings (Sim):

The simulator settings window contains all the extra variables required for the simulation to run. Here the python directory can be redefined in required by clicking on the textbox with the directory pathway (**figure 16**). The interval in which the datapoints are generated can be modified by changing the data point resolution. Within this window the temperature in which the simulation is run at, as well as custom pKa values can be defined for titrants that are not contained within OpenTitrations internal database.

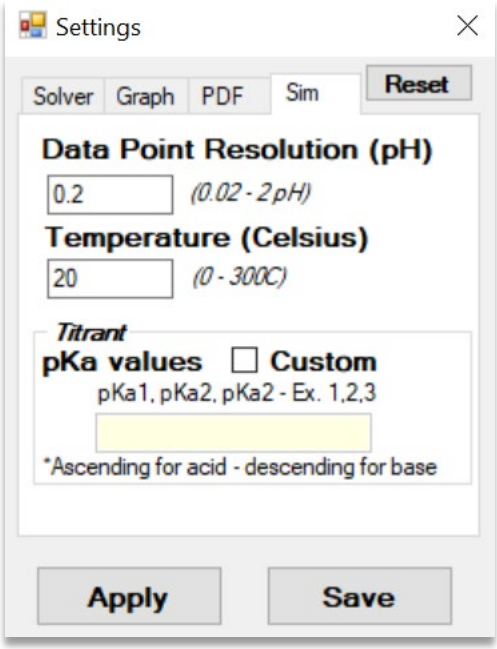

Figure 16. *Simulator Settings Window*