

ATLaS: Assistant Toolkit for Laboratory Solutions

USER MANUEL

The main page of ATLaS contains five links in order to reach the calculation required during solution preparation. Five main modules are easily accessible from the home page (Figure 1).

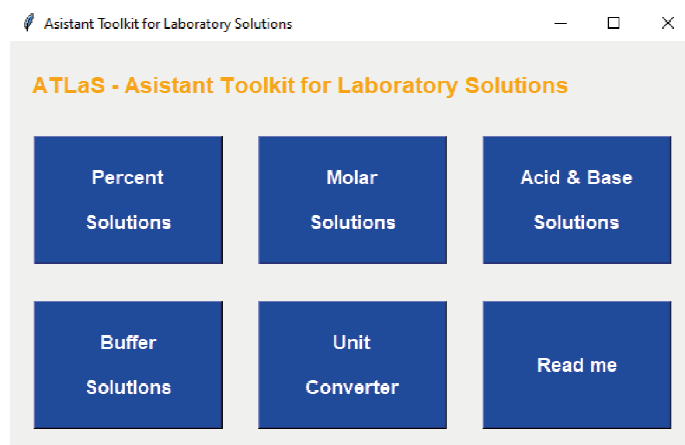


Figure 1. Main page of ATLaS

Figure 2 shows the "Percent Solutions" module. Each function is placed separately. In the first function, when the information is entered in the relevant places and the "Calculate" button is pressed, how the solution will be prepared is given as an output. The calculations required to prepare a 2.5% and 100 ml of solution by using a 10% solution are shown in the second function. In the third function, the molarity of 12% solution of NaOH was calculated. For this, the formula weight of NaOH (40 g / mol) was entered and the result is calculated as 3 M.

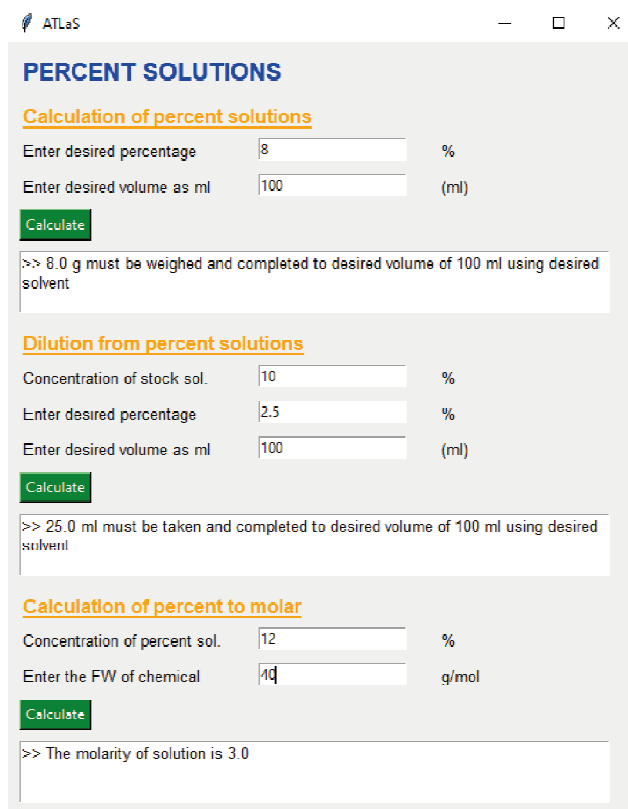
The image shows the "PERCENT SOLUTIONS" module in the ATLaS application. It has three distinct calculation sections, each with input fields, a "Calculate" button, and a text output area.
1. **Calculation of percent solutions**: Inputs are "Enter desired percentage" (8) and "Enter desired volume as ml" (100). The output is ">> 8.0 g must be weighed and completed to desired volume of 100 ml using desired solvent".
2. **Dilution from percent solutions**: Inputs are "Concentration of stock sol." (10), "Enter desired percentage" (2.5), and "Enter desired volume as ml" (100). The output is ">> 25.0 ml must be taken and completed to desired volume of 100 ml using desired solvent".
3. **Calculation of percent to molar**: Inputs are "Concentration of percent sol." (12) and "Enter the FW of chemical" (40). The output is ">> The molarity of solution is 3.0".

Figure 2. "Percent Solutions" window and demonstration of calculations

The second module makes molar calculations. Examples are given in Figure 3. In the first function of this module, the formula weight of NaOH 40 g / mol, 10 ml as the desired volume and 3 M as the desired molar concentration were entered to prepare the molar solution. In the second function, parameters were entered to prepare a 10 ml of 1 M solution from a 2.5 M stock solution. The results were shown after the "Calculate" button was pressed. In the third function, the calculation of the percentage of 2 M NaCl solution was shown in Figure 3.

MOLAR SOLUTIONS

Calculation of mass required for Molar solutions

Enter the FW of chemical: 40 g/mol

Enter the desired volume as ml: 10 (ml)

Enter desired concentration as M: 3 (M)

Calculate

>> 1.2 g must be weighed and completed to desired volume of 10 ml using desired solvent

Dilution of solution of known molarity

Enter Stock's concentration as M: 2.5 (M)

Enter desired volume as ml: 10 (ml)

Enter desired concentration as M: 1 (M)

Calculate

>> 4.0 ml must be taken and completed to desired volume of 10 ml using desired solvent

Molarity to Percent Calculation

Enter the FW of chemical: 58.44 (g/mole)

Enter molarity of solution as M: 2 (M)

Calculate

>> The concentration of the solution is 11.600%

Figure 3. "Molar Solutions" window and demonstration of calculations

There is a list box in the "Acid & Base Solution" module (Figure 4a). Chemicals in this list box are called from the MS Excel file in the program folder. This Excel file contains the names, formulas, formula weights and equivalents of the chemicals (Figure 4b). However, density and percentage weight values must be entered by the user. This is because these values may differ according to the brands of chemicals used in laboratories. When phosphoric acid is selected from the list and the necessary information is entered, the calculation result is given to the user as a prescription. If new chemicals are added by the researcher without deforming the format of the Excel file, the program will also calculate using up-to-date data.

ACID & BASE SOLUTIONS

Select acid or base

- Acetic Acid
- Ammonium Hydroxide
- Barium Hydroxide
- Calcium hydroxide
- Formic Acid
- Hydrobromic acid
- Hydrochloric Acid
- Hydrofluoric Acid
- Hydroiodic Acid
- Lithium hydroxide
- Nitric Acid
- Perchloric Acid
- Phosphoric Acid
- Potassium Hydroxide
- Sodium Hydroxide
- Sulfuric Acid

Phosphoric Acid

Formula: H3PO4

Formula weight: 98.0 g/mol

Equivalent: 3

Enter the density: 1.885 g/ml

Weight percentage: 85 % w/w

Enter desired volume as ml: 100 ml

Enter desired concentration as M: 3 M / N

Molarity Calculation

Normality Calculation

>> The concentration of your stock solution is 14.515 M.

>> Take 13.865 ml from 14.515 M solution

>> Slowly add 13.865 ml to 2% (10 ml pH7.0)

>> Then adjust the final volume to 100 ml.

	A	B	C	D
	Name	Formula	FW	Equivalent
1	Name	Formula	FW	Equivalent
2	Acetic Acid	CH3CO2H	60.05	1
3	Ammonium Hydroxide	NH4OH	35.05	1
4	Barium hydroxide	Ba(OH)2	171.34	2
5	Calcium hydroxide	Ca(OH)2	74.09	2
6	Formic Acid	HCOOH	46.03	1
7	Hydrobromic acid	HBr	80.91	1
8	Hydrochloric Acid	HCl	36.46	1
9	Hydrofluoric Acid	HF	20.01	1
10	Hydroiodic Acid	HI	127.91	1
11	Lithium hydroxide	LiOH	23.95	1
12	Nitric Acid	HNO3	63.01	1
13	Perchloric Acid	HClO4	100.46	1
14	Phosphoric Acid	H3PO4	98.0	3
15	Potassium Hydroxide	KOH	56.11	1
16	Sodium Hydroxide	NaOH	40.0	1
17	Sulfuric Acid	H2SO4	98.08	2

Figure 4. "Acid&Base Solutions" window (a) and MS Excel form of chemical list (b)

The "Buffer Solutions" module also calls its chemical information from the MS Excel file (Figure 5). If information is entered without distorting the format of the MS Excel file, the program will make calculations using the current data. As an example, Figure 5a shows the calculation for potassium phosphate monobasic.

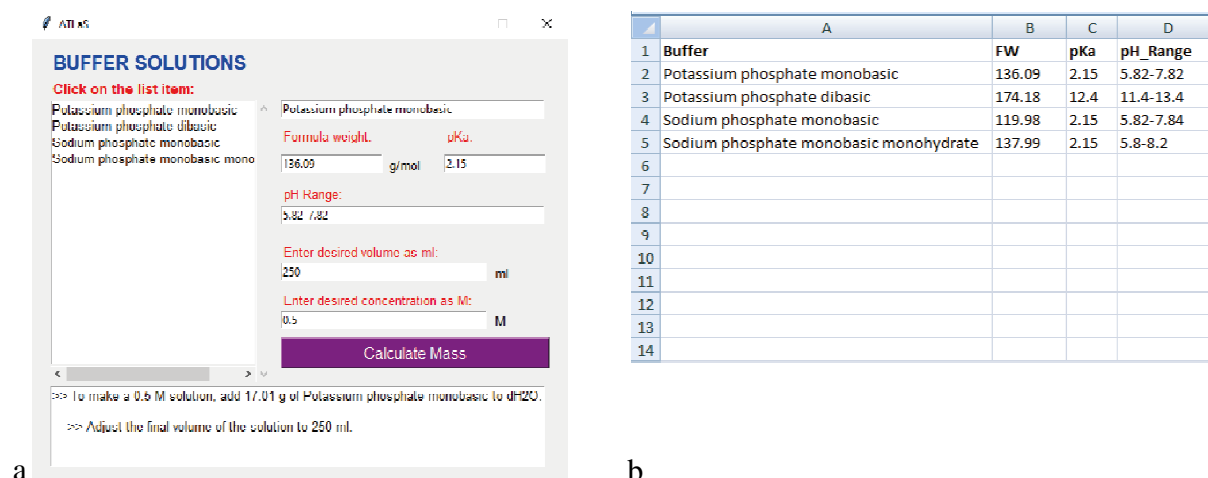


Figure 5. "Buffer Solutions" window (a) and MS Excel form of chemical list (b)

The "Unit Converter" module in ATLaS makes conversions in units of volume, mass and density. When the volume option is selected, microliter, milliliter and liter expressions appear on the radio buttons; when the mass option is selected, microgram, milligram and kilogram expressions appear; when the density option is selected, microgram / ml, milligram / ml and kilogram / L expressions appear. An example is given in Figure 6.

Figure 6 shows the 'Unit Converter' window in ATLaS. It has three sections: Volume, Mass, and Density. The Volume section is selected, showing three radio buttons: Microliter (selected), Milliliter, and Litre. Below the radio buttons are three input fields with their respective units: 100 microliter, 0.1 milliliter, and 0.0001 liter. At the bottom, there are two buttons: 'Clear the form >>' and 'Clear'.

Figure 6. "Unit Converter" window

Important warnings to be aware of when using the program:

- 1- For decimal numbers, a dot (eg 0.5) must be used.
- 2- Volume values should be entered in millilitres (ml).
- 3- Molar values must be entered as molar (M).

Citation: Comlekcioglu, U, Comlekcioglu, N, 2021. ATLaS: An assistant software for researchers to use in calculations for the preparation of solutions.