

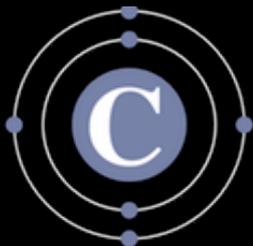


July 2010
v1.3

LabCalPlus - Quick Guide



LabCalPlus consist of 4 modules:



Molecular Weight Calculator for Elements

Calculation of molecular weights of chemical formulas



Molecular Weight Calculator for Amino Acids

Generation of amino acid sequences



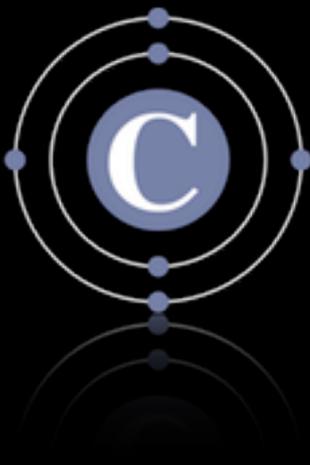
pH Calculator

pH calculation and titration



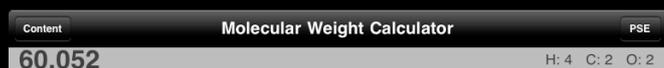
Molarity Calculator

Molarity, dilutions of stock concentration and conversions between amount and mass



Molecular Weight Calculator for Elements

Molecular Weight Calculator for Elements



Content Molecular Weight Calculator PSE
60.052 H: 4 C: 2 O: 2



CH₃COOH
(... ..) · [Grid] Enter Edit Mode |←| |→| [Trash]
3
3 | | | 32
H C N O Na
P S Cl
[Check] Atomic Weight Custom Element Browser

The molecular weight calculator for elements allows the determination of molecular weights of chemical formulas. Elements and optionally numerical suffixes can be entered. Parentheses are also supported. The corresponding molecular weight will be calculated and the elemental composition will be displayed.

Functionalities

- Choose up to 20 elements from the periodic system of elements
- Each formula can contain up to 30 terms (excluding numerical suffixes and parentheses)
- Numerical suffixes are between 2 and 999
- Sort elements by atomic weight or by custom order
- Formula editing (replacement or deletion of terms/ numerical suffixes)

Molecular Weight Calculator for Elements

Button to access periodic system of elements

Content Molecular Weight Calculator PSE

60.052 H: 4 C: 2 O: 2

Result

CH₃COOH

Chemical Formula

CH₃COOH

3

3 32

H	C	N	O	Na
P	S	Cl		

Selected Elements

Atomic Weight Custom Element Browser

Bottom Toolbar

Tools

Enclosing marks Spacer Switch between slider and NumPad Edit formula Delete last item Delete all

(...) . [NumPad] Enter Edit Mode | -+ | [Delete]

3

3 32

Select numeric suffix

Add numeric suffix

Bottom Toolbar

Sort selected elements Access and select elements

Atomic Weight Custom Element Browser

Enter a chemical formula

To enter a chemical formula tap on one of the selected elements. The corresponding term will appear in the upper part. Optionally a numerical suffix can be added by tapping the “Add numeric suffix” button. The molecular weight and elemental composition will be displayed above the formula.

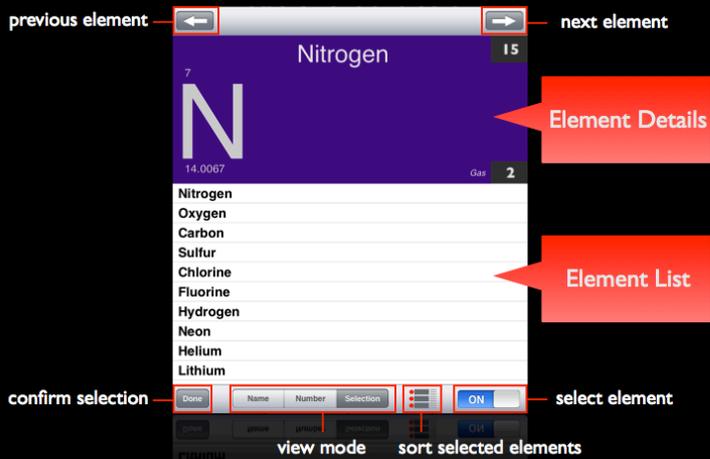
To delete the last entry tap the “Delete last item” button. To change a term tap “Enter Edit Mode”.

The formula will be highlighted. Select a term by tapping. The selected term will be highlighted. Tap the desired element from the selected elements or add a numeric suffix. When done tap “Leave Edit Mode”.

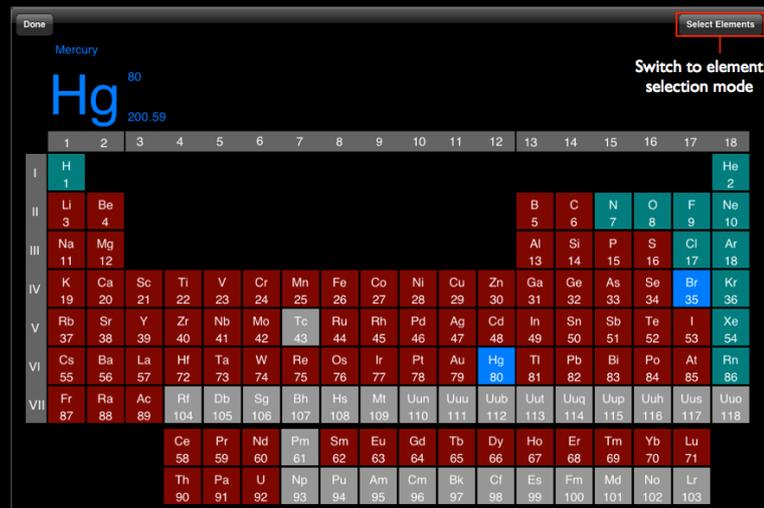
To add a parentheses tap the “open” enclosing mark button. Tap the desired elements. Then tap the “close” enclosing mark button and add a numerical suffix (mandatory).

Molecular Weight Calculator for Elements

Element Browser



Periodic system of elements



Selection of Elements

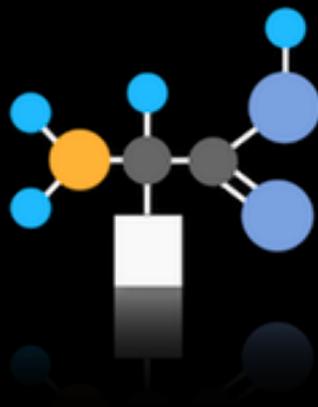
To select elements tap the “Element Browser” button or the “PSE” button.

Element Browser:

To add elements to the selection switch the view mode to “Name” or “Number”. Tap the desired element from the list. To select an element tap the “select element” switch (state: on). To deselect tap the “select element” switch (state: off). To view the selection switch the view mode to “Selection”. To rearrange the list tap the “sort selected elements” button, tap the handles at the right side of a row and move it to the desired location. Tap 2 “sort selected elements” again to exit the rearrangement mode. When finished tap “Done” to confirm the selection.

Periodic system of elements:

To reveal all elements turn the iPad into landscape mode (turn rotation lock off). Tap the “select elements” button. All non-selected elements will be displayed in light gray and selected elements in orange. To select or deselect an element tap the corresponding element. To confirm the selection tap the “Done” button.



Molecular Weight Calculator for Amino Acids

Molecular Weight Calculator for Amino Acids



The molecular weight calculator for amino acids allows the determination of molecular weights of amino acid sequences. Amino acid sequences can be generated and the corresponding average or monoisotopic mass will be calculated. Also post-translational modifications can be added. Additionally amino acid sequences from uniprot.org can be imported.

Functionalities

- Generation of amino acid sequences
- 20 common amino acids and 8 derivatives are supported
- Calculation of average or monoisotopic masses
- 18 post-translational modifications
- Amino acid sequence editing (deletion or substitution)
- Characteristics of each amino acid
- Animated chemical formula

Molecular Weight Calculator for Amino Acids

Animated Structure

Amino Acid Properties

Result

Amino Acid Sequence

Toolbar

Toolbar

- Delete sequence
- Load sequence from Uniprot
- Delete last amino acid
- Select monoisotopic or average mass
- Add or remove post-translational modification (H⁺)

Molecular Weight Calculator

To select the amino acid calculator switch the view to “Calculator”.

Molecular Weight Calculator:

To add amino acids tap an amino acid button. The corresponding one-letter code will appear in the upper part. The resulting molecular weight will be displayed on top.

Sequence Editing: Tap the a sequence part. A table will appear. To delete an amino acid tap “Edit”. For deletion use the standard build-in controls. To replace an amino acid tap the desired row. A new dialog will appear allowing the selection of an amino acid. Tap “select” and then “Done. To confirm the changes tap apply in the table view.

Post-translational modifications: Tap the corresponding button (H⁺) and add the desired modifications to the list.

Uniprot.org: Tap the UniProt-Button, enter the accession number and import the selected sequence.

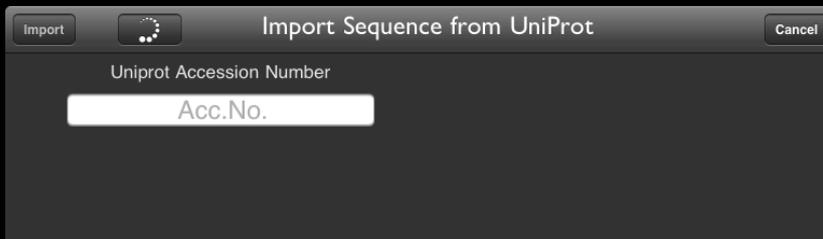
Molecular Weight Calculator for Amino Acids

Amino Acid Sequence Import from uniprot.org

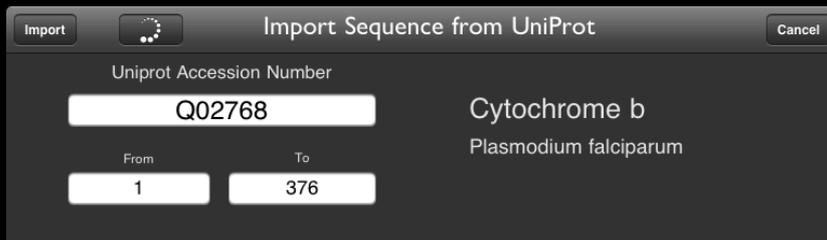
(internet connection required)



Tap the uniprot-button.

A dialog box titled "Import Sequence from UniProt" with "Import" and "Cancel" buttons. It contains a text input field labeled "Uniprot Accession Number" with the placeholder text "Acc.No." inside.

Enter an accession number. The sequence will be loaded.

A dialog box titled "Import Sequence from UniProt" with "Import" and "Cancel" buttons. It contains a text input field labeled "Uniprot Accession Number" with the value "Q02768". Below it are two smaller input fields labeled "From" (value "1") and "To" (value "376"). To the right of these fields, the text "Cytochrome b" and "Plasmodium falciparum" is displayed.

Select the range and tap import.

To determine an accession number

tap



376 AA Molecular Weight: 43377

```
ID CYB_PLAFA Reviewed; 376 AA.
AC Q02768;
DT 01-OCT-1996, integrated into UniProtKB/Swiss-Prot.
DT 01-OCT-1996, sequence version 1.
DT 15-JUN-2010, entry version 62.
DE RecName: Full=Cytochrome b;
DE AltName: Full=Ubiquinol-cytochrome-c reductase complex cytochrome b subunit;
DE AltName: Full=Cytochrome b-c1 complex subunit 3;
DE AltName: Full=Complex III subunit 3;
DE AltName: Full=Complex III subunit III;
GN Name=MT-CYB; Synonyms=COB, CYTB, MTCYB;
OS Plasmodium falciparum.
OG Mitochondrion.
OC Eukaryota; Alveolata; Apicomplexa; Aconoidasida; Haemosporida;
OC Plasmodium; Plasmodium (Laverania).
OX NCBI_TaxID=5833;
RN [1]
RP NUCLEOTIDE SEQUENCE [GENOMIC DNA].
RX MEDLINE=89040026; PubMed=3054536; DOI=10.1016/0166-6851(88)90098-9;
RA Suplick K., Akella R., Saul A.J., Vaidya A.;
RT "Molecular cloning and partial sequence of a 5.8 kilobase pair
RT repetitive DNA from Plasmodium falciparum.";
RL Mol. Biochem. Parasitol. 30:289-290(1988).
RN [2]
RP NUCLEOTIDE SEQUENCE [GENOMIC DNA].
RC STRAIN=Isolate Camp / Malaysia;
RX MEDLINE=93211452; PubMed=8459834; DOI=10.1016/0166-6851(93)90088-F;
RA Vaidya A.B., Lashgari M.S., Pologe L.G., Morrisey J.;
RT "Structural features of Plasmodium cytochrome b that may underlie
RT susceptibility to 8-aminoquinolines and hydroxynaphthoquinones.";
RL Mol. Biochem. Parasitol. 58:33-42(1993).
RN [3]
RP NUCLEOTIDE SEQUENCE [GENOMIC DNA] OF 26-376.
RX MEDLINE=92178987; PubMed=1542578; DOI=10.1093/nar/20.4.879;
```

The UniProt Consortium The Universal Protein Resource (UniProt) in 2010 Nucleic Acids Res. D142-D148 (2010).

The uniprot.org website will appear.
Search the desired protein, copy the
accession number, dismiss the
website and paste the accession
number into the search-field.



pH Calculator

pH Calculator

Content [c] ☰

Acid		Base	
123.000	mmol	4.000	mL
phosphoric acid	🔍	Strong	<input type="checkbox"/> OFF
+			

1.59



The pH calculator allows to determine the pH of solutions of acids and bases. Additionally the required molarity to achieve a desired pH can be calculated and visualized as a titration curve.

Functionalities

- Calculation of pH's based on molarity, volume and optionally pK.
- Animated result display
- Generation of solutions of acids and/or bases
- 28 pre-defined acids and bases
- Support of multiprotic acids
- Calculation of molarities to achieve desired pH's
- Display of titration curves

pH Calculator

The image shows two screenshots of the pH Calculator app interface. The left screenshot shows the main view with a large pH value of 1.59 and a graphical pH scale below it. The right screenshot shows the input form with various fields and buttons. Red callout boxes with white text point to specific features in both screenshots.

- Switch views:** Points to the menu icon (three horizontal lines) in the top right corner of the main view.
- Component Properties:** Points to the input fields for concentration (123.000 mmol) and volume (4.000 mL) in the main view.
- pH Value:** Points to the large digital display showing the pH value of 1.59.
- pH Scale:** Points to the graphical pH scale ranging from 0 to 14, with 'Acidity' on the left, 'Neutral' in the middle, and 'Basicity' on the right.
- Delete all:** Points to the trash can icon in the bottom right corner of the main view.
- Select acid or base:** Points to the 'Acid' and 'Base' tabs at the top of the input form.
- Enter concentration and volume:** Points to the input fields for concentration (123.000 mmol) and volume (4.000 mL) in the input form.
- Select strong acid or base:** Points to the 'Strong' toggle switch (currently OFF) in the input form.
- Add component to solution:** Points to the '+' button in the input form.
- Enter pK-value or select component from list:** Points to the text input field and the blue disclosure button (i) in the input form.

pH Calculation

pH Calculation for a single component : Select acid or base. Enter a molarity, volume and a pK value or turn the strong switch on. A pK value can also be chosen from a list by clicking the blue disclosure button.

Solution of acids and bases:

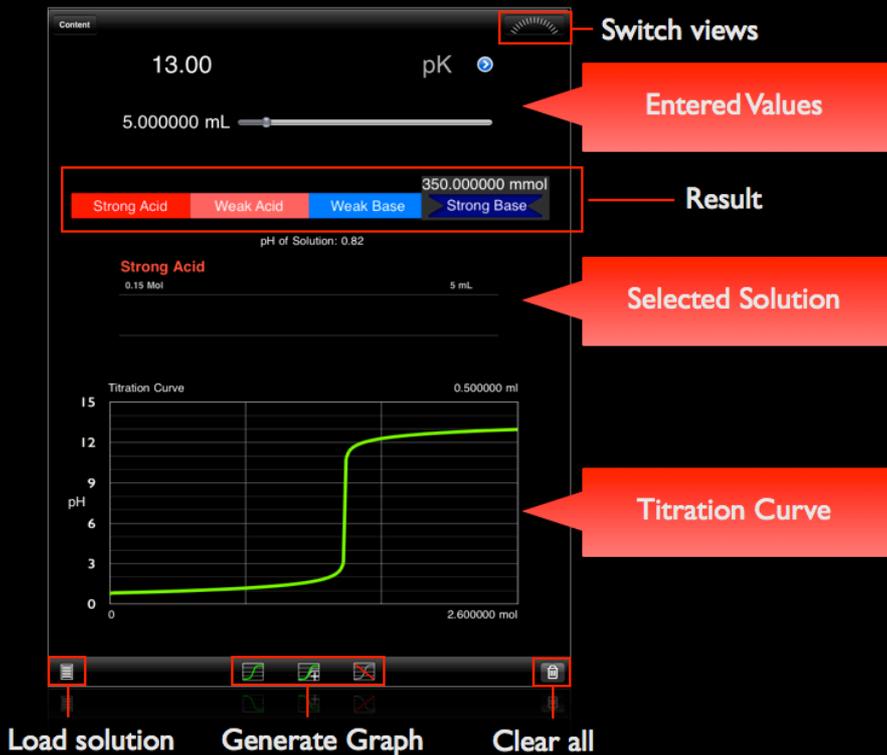
Enter the values for a single component. Tap the “Plus button”. Enter the values for the next component and tap the “Plus Button” again.

The graphical representation of the pH (Scale) is only visible if the device orientation is in portrait mode.

The pH of a solution is depicted above the components of the solution.

The pH value and the pointer position of the scale might either represent the pH of a single component or the pH of the solution.

pH Calculator



Titration

Molarity Calculation for a defined pH:

Enter the desired pH value. The corresponding molarity will be calculated. Optionally you can enter a pK-value.

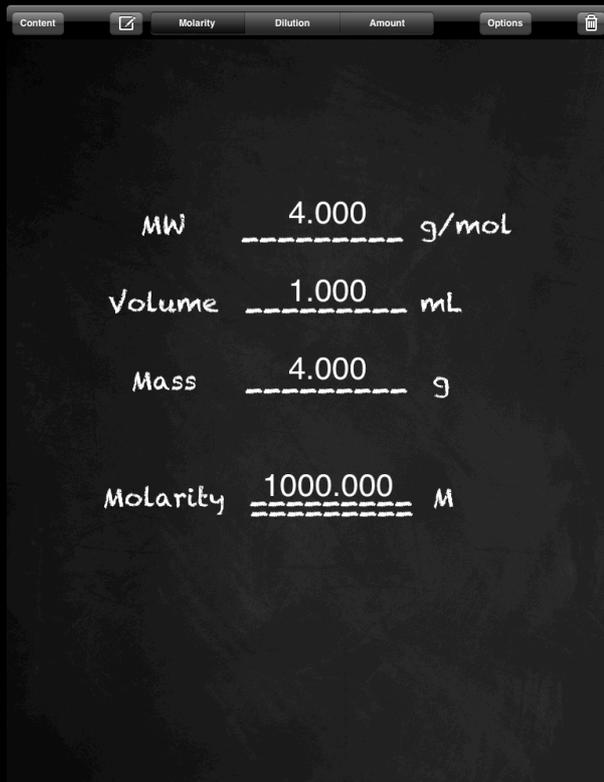
Titration Curve:

Load a solution generated with the pH calculator. Tap the "Generate Graph" button. A titration curve will be displayed. The x-axis refers to the molarity and the y-axis to the pH value. The generation of the curve may take a few seconds.



Molarity Calculator

Molarity calculator

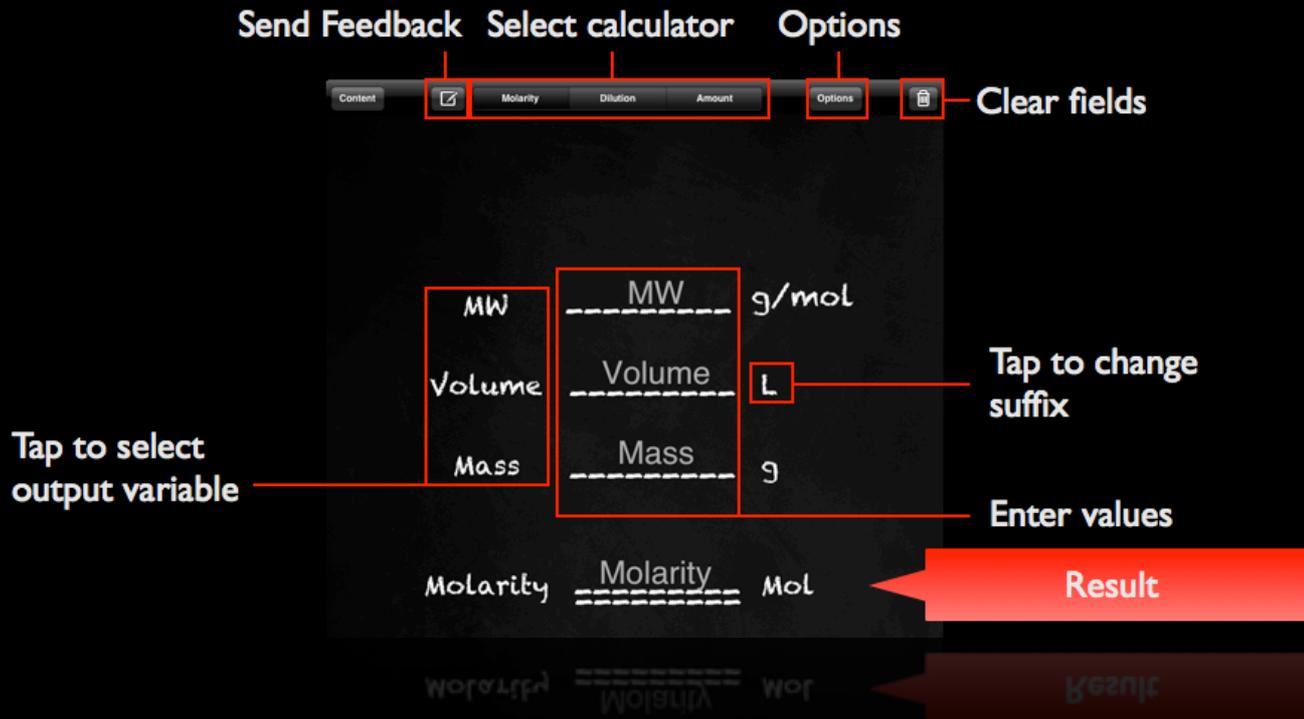


The molarity calculator allows to calculate molarities, to calculate dilutions of stock solutions and to convert between mass and amount.

Functionalities

- Calculation of molarities (or choose other output variables: MW, volume and mass)
- Output variable selection by tapping
- Unit prefix change by tapping
- Switch between mol/L and Dalton/kilo-Dalton
- Swipe to switch between calculators

Molarity Calculator



Calculators

Molarity Calculator:

Enter values for molecular weight (MW), volume and mass. The molarity will be calculated. To change the output variable tap MW, Volume or Mass. Tap to change the unit suffix.

Other Calculators:

To select a different calculator tap the corresponding buttons in the top toolbar or perform a swipe gesture.

Options:

- Clear before editing: The values of a given textfield will be cleared prior to editing.
- Save values on exit: Values will be saved. If deselected even switching to another module will clear all fields.
- Use Dalton/kDalton: Instead of mol/l Daltons will be used. Tap to switch between Dalton and kilo-Dalton.

For feedback, questions or suggestions please mail to :

sheep@isheepsoft.com

