Mixology: a tool for calculating required masses and volumes for laboratory solutions [version 1; peer review: 1 approved]

Theo Sanderson

Francis Crick Institute, London, NW1 1AT, UK

Abstract
Laboratory work often requires making up solutions with defined concentrations of various components. Mixology is a tool we have created to simplify calculation of the masses and volumes required to obtain particular concentrations. It operates with many kinds of volumetric, mass and concentration units, including conversion between molarity- and mass-based concentrations using molecular masses retrieved from the Chemical Entities of Biological Interest (ChEBI) database. Mixology can be accessed at https://mixology.science.

Keywords
calculator, solutions, software, tool

This article is included in the The Francis Crick Institute gateway.
**Introduction**

Performing calculations to make up solutions is one of the first skills that a laboratory researcher learns. Despite efforts to facilitate sharing of laboratory protocols\(^1\), solutions are often described in publications only in terms of the molarities of their constituent parts, meaning that calculations are needed to determine the absolute amounts needed to make up some defined volume. These calculations can be surprisingly lengthy.

Suppose a researcher is implementing a new protocol, and needs to make a buffer containing, amongst other ingredients, “500 μg/ml sodium chloride”. She wants to make up 2 litres of the new buffer. On her bench she happens to already have a stock solution labelled “1.5 M NaCl”. What volume of stock solution does she need to add for the new buffer? One approach that she might follow to calculate this would be to:

1. Look up the molar mass of sodium chloride: 58.44g/mol
2. Convert the desired concentration, 500 μg/ml, to μg/L: 500μg/ml × 1000ml/L = 500000μg/L
3. Convert the desired concentration to g/L: 500000μg/L ÷ 1000000μg/g = 0.5g/L
4. Convert the desired concentration to mol/L (molarity): 0.5g/L ÷ 58.44g/mol = 0.0085M
5. Calculate the ratio of the two concentrations: 0.0085M ÷ 1.5M = 0.0056
6. Calculate the volume to add: 2L × 0.0056 = 0.0112L
7. Convert this volume to ml for pipetting: 0.0112L × 1000ml/L = 11.2ml

If her buffer contains five different such ingredients, she might need to perform a similar set of steps five times, requiring perhaps 35 individual steps. If an error occurs in just one of these, the final buffer will not be to the expected specification.

We decided to build a simple tool to perform calculations such as these (Figure 1). **Mixology** automates the retrieval of molecular masses, and the mathematical operations needed to calculate the required masses of reagent, or volumes of stock solutions, needed for desired final concentrations.

**Implementation**

Mixology provides a simple interface to record the specifications of a solution and calculate the required amount of each ingredient (Figure 1). A user first enters the volume of the solution they want to make, and a descriptive name. Then they add any number of components to the solution. For each component, they enter a desired final concentration. Concentrations can be entered in any of several unit forms:

- mass-based: g/ml, μg/ml, mg/l, % (w/v), etc.
- molarity-based: mol/l, nM, μM, mM, M, etc.
- volume-based: % (v/v), X
- other: units/ml, etc.

The user also enters the name of the chemical. Chemical names are autocompleted with known entities from the Chemical Entities of Biological Interest (ChEBI) database\(^2\). Where a known chemical is entered, its molecular mass is inferred from the ChEBI database. Alternatively a custom compound name can be entered, and a molecular mass (if needed) entered manually.

If the desired concentration is mass- or molarity-based, the user can select whether to weigh out the compound (mass units) or to measure out a volume of stock solution (with a mass- or molarity-based stock concentration). If the desired concentration is volumetric, a volume of stock solution (which can be 100% (v/v)) is required.

In either case, the user enters the units of mass or volume to weigh out, and Mixology automatically calculates the quantity of this unit required to make up the final volume at the desired concentration (Figure 2).

---

**Figure 1.** A screenshot of the Mixology interface, featuring the single compound solution described in the Introduction. The permalink for this recipe is https://mixology.science/?recipe=ngEh5UBDZx.
### Figure 2. A screenshot of the Mixology interface, with an example buffer demonstrating many of the different classes of interconversion of which Mixology is capable. The permalink for this recipe is https://mixology.science/?recipe=mN1j1sNSD5.

The user can add as many components as required, and also add notes, which might contain instructions such as “adjust pH to 7.2”. Finally they can create a ‘permalink’ pointing to their solution, creating a unique URL for the solution that can be saved and shared.

### Operation
The code behind Mixology is available in our [GitHub repository](https://github.com/). Mixology is developed with the Vue.js framework. This allows reactive behaviour in which all fields are updated in real time as others are changed. We use the vue-simple-suggest component\(^4\) to list available units and chemical entities from ChEBI. Mixology has been tested on recent versions of Chrome, Firefox and Safari.

All concentration terms are converted into a standard format consisting of some quantity (moles, grams, litres, activity units) per litre, facilitating downstream steps. Mol/l and g/l can be interconverted using the molecular mass, but these cannot be interconverted to the other unit types (volumetric and activity units).

Molecular masses, and compound names for autocompletion, are taken from ChEBI\(^2\). ChEBI entities are processed into JSON with a custom R notebook, available in our GitHub repository, using R and the tidyverse\(^5\).\(^6\). We take as input ChEBI’s three-star chemicals, which are those that have been curated. We exclude any name that is mapped to multiple distinct chemicals to avoid potential confusion. Sometimes multiple mass measurements are available for a chemical in ChEBI. Normally these are extremely similar, so we exclude only chemicals for which the standard deviation of masses is greater than 0.001.

Recipes can be saved using a “permalink” feature. This deposits a copy of the recipe in JSON format into an external Firebase database, with a unique identifier which can be used to retrieve it at the correct URL.

### Discussion
We have created a simple tool which we hope will be useful to laboratory scientists. In the day following Mixology’s release on Twitter, a user testing it identified an inconsistency with the calculations in a published protocol\(^7\). This turned out not to be a problem with the tool, but the use of an incorrect molar mass (hydrated vs. anhydrate) for calculations in the official protocol. This provides one example of how easily small mistakes can occur performing these operations manually.

Mixology has some limitations. It cannot currently perform any calculations which would require knowing the density of a substance (interconversion between mass and purely volumetric units). Additionally, it does not provide the facility to calculate quantities required to obtain a particular pH or osmolarity. We

<table>
<thead>
<tr>
<th>Component</th>
<th>Quantity</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1 % (v/v) Triton-X100</td>
<td>7.500 ml</td>
<td>of 10 % (v/v) stock</td>
</tr>
<tr>
<td>3 % (w/v) milk powder</td>
<td>22.50 g</td>
<td></td>
</tr>
<tr>
<td>10 mM Tris base (MW: 121.120)</td>
<td>908.5 mg</td>
<td></td>
</tr>
<tr>
<td>50 ug/ml sodium chloride (MW: 58.445)</td>
<td>641.7 ul</td>
<td>of 1 M stock</td>
</tr>
<tr>
<td>1 X ligation buffer</td>
<td>7.500 ml</td>
<td>of 100 X stock</td>
</tr>
<tr>
<td>25 mM sodium hydroxide (MW: 39.992)</td>
<td>749.9 mg</td>
<td></td>
</tr>
<tr>
<td>10 mg/ml carrot pulp</td>
<td>7.500 g</td>
<td></td>
</tr>
<tr>
<td>50 mM calcium chloride (MW: 110.983)</td>
<td>83.24 ml</td>
<td>of 5 % (w/v) stock</td>
</tr>
</tbody>
</table>

Dissolve in 600ml water. Then adjust pH to 7.2 with hydrochloric acid and make up to final volume.
welcome feature suggestions and pull requests in our GitHub repository.

We do not argue that the availability of a tool such as this replaces the need for scientists to know how to perform these types of calculations. However, we hope that by providing a streamlined tool that eases this process, Mixology can make one aspect of routine laboratory life simpler, and reduce errors.

Data availability
The ChEBI database can be downloaded at https://www.ebi.ac.uk/chebi/downloadsForward.do

Software availability
- Web tool available from: http://mixology.science
- Current source code available from: https://github.com/theosanderson/mixology
- Archived source code at time of publication: http://doi.org/10.5281/zenodo.4624415
- License: MIT

Acknowledgements
RRIDs used in this work: SCR_002088. An earlier version of this article can be found on bioRxiv (doi: 10.1101/2021.01.30.428948).

References
Open Peer Review

Current Peer Review Status: ✔

Joachim Goedhart
Molecular Cytology, Swammerdam Institute for Life Sciences, van Leeuwenhoek Centre for Advanced Microscopy, University of Amsterdam, Amsterdam, The Netherlands

The paper reports on a new, freely available and open-source web app 'Mixology' that simplifies the calculations necessary for preparing solutions that are used in labs. The advantages of using an app over manual calculations are clearly explained in the paper.

I have reviewed the manuscript and the app, but I haven't reviewed the source code (as the coding language that is used is outside my area of expertise).

Comments on the manuscript:
- The example calculation in the paper (11.2 ml) and the screenshot of the app (figure 1, 11.41 ml) show slightly different numbers (probably due to rounding at step 4). I'd recommend to make the numbers consistent.
- Using the same abbreviation for litre (uppercase L or lowercase l) improves consistency.
- The paper states "Concentrations can be entered in any of several unit forms", including µg/ml, but the app seems unable to accept the greek symbol 'mu' (see also comments below). If this is a limitation of the app, it should be highlighted in the paper.
- The bullet point "mass-based: g/ml, µg/ml, mg/l, % (w/v), etc." appears twice.

Comments on the webtool:
- The webtool can be used without reading the paper, suggesting that the user interface is intuitive.
- The automatic retrieval of molecular weights is elegant and works smoothly.
- The ability to generate a permalink is fantastic and will simplify the sharing of recipes.
The app didn't work for me on Safari (version 14.0, on Mac OS version 10.15.7) as I was unable to add compounds (for unclear reasons). It worked well on Firefox (version 88.0.1) and a mobile device.

I was able to reproduce a buffer that we use for imaging and the quantities that we normally use match with the results of the app. I was able to generate a permalink for the recipe (https://mixology.science/?recipe=MpW9AwsswL).

When I generate or retrieve the permalink, the decimal separator becomes a comma instead of a period. This turned out to be due to the language setting in Firefox (Dutch) and was solved by setting the language to English.

Accepting the micro (µ) sign in addition to the u would be an improvement.

The simplicity of the app is a strength, but one can easily think of features that could be added. Some improvements that I can think of:
1. Having grams as a default, instead of having to type it for each line
2. Showing the options of 'conc. unit' and 'mass unit' in a dropdown menu (or as tooltip)
3. Option to copy the permalink to the clipboard (or copy it to clipboard at the time it is generated). This can be another button 'copy permalink'.

Ultimately, the design of the app (and choice of which features to implement) should be the choice of the author(s).

The author invites readers to add suggestions to the Github repo and I would suggest to include the link to the repo immediately after that statement.

Does the author also accept comment requests through other channels (email, twitter) for readers not familiar with Github? If so, it would be helpful to indicate that.

**Is the rationale for developing the new software tool clearly explained?**
Yes

**Is the description of the software tool technically sound?**
Yes

**Are sufficient details of the code, methods and analysis (if applicable) provided to allow replication of the software development and its use by others?**
Yes

**Is sufficient information provided to allow interpretation of the expected output datasets and any results generated using the tool?**
Yes
Are the conclusions about the tool and its performance adequately supported by the findings presented in the article?
Yes

**Competing Interests:** No competing interests were disclosed.

**Reviewer Expertise:** Cell biology, Data visualization, Web apps.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.