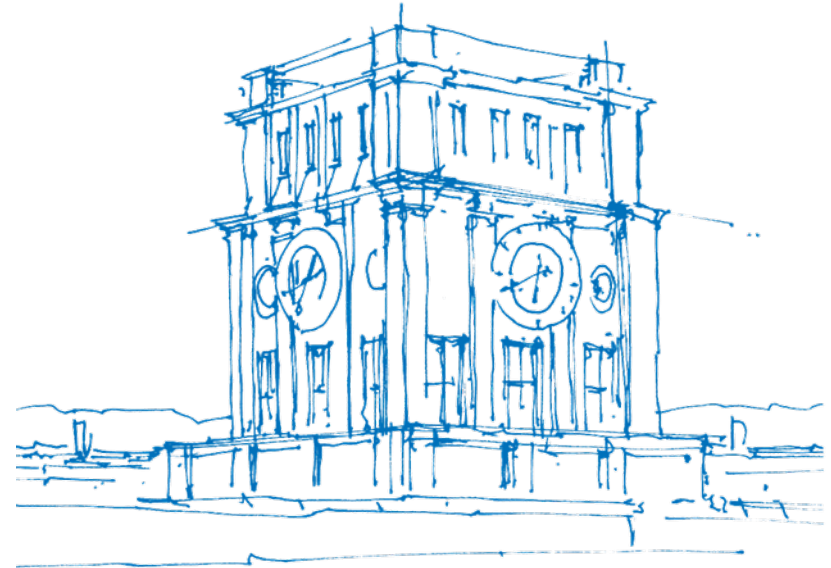


# Stoichiometry Plugin for eWorkbench Lab Books

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*TUM Uhrenturm*

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# PubChem

- Homepage: <https://pubchem.ncbi.nlm.nih.gov/>
  - the National Centre for Biotechnology Information (NCBI), a component of
  - the National Library of Medicine (NLM), a part of
  - the (US) National Institutes of Health (NIH)
- Database of chemical molecules and biological assays
- Over 111 million compounds
- Several public APIs to access the database
- API request volume limitations:
  - 5 requests per second
  - 400 requests per minute
  - 300 seconds runtime per minute
- (Plugin uses 2 requests per compound search)

# User Manual - Overview

## User Manual

Columns

Column Interactions

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Components

# Columns

Column	Input
Status	disabled
Type	drop-down
Search	text
Notes	text
Source	search/delete only
Highlight	hidden

Column	Input
Name	search/text
CAS	search/text
CID	search/text
SMILES	search/text
InChIKey	search/text
InChI	search/text

Column	Input	Unit	Precision
Amount	search/number	μmol/mmol/mol	3/4 sig.fig.
Eq	number	<none>	3/4 sig.fig.
EqRef	toggle	<none>	<none>
Molarity	number	M ( $\frac{\text{mol}}{\text{L}}$ )	2 digits
MW	search/number	$\frac{\text{g}}{\text{mol}}$	3 digits
Density	search/number	$\frac{\text{g}}{\text{cm}^3}$	3 digits
Mass	number	mg/g/kg	3/4 sig.fig.
Volume	number	μL/mL/L	3/4 sig.fig.

“number”: positive number | “sig.fig.”: significant figures | “digits”: digits after the decimal point

For columns with three units, the middle one is the input unit. The displayed unit will scale according to the size of the value.

# Column Interactions

Trigger	Target	Requires	Infos
Type	Type, Status		
Search	Status, SearchResult		[6]
SearchResult	Highlight		[6]
Amount	Eq		[1]
Amount	Mass	MW	
Amount	Volume	MW, Density/Molarity	[2]
Eq	Amount		[1]
EqRef	Eq		[3]
Molarity	Volume	Amount	
MW	Mass	Amount	
MW	Volume	Amount, Density	
Density	Volume	Amount, MW	[4]
Mass	Amount	MW	
Volume	Amount	Density	
Volume	Volume	Density	[5]

- 1 Reference Eq must have Amount set
- 2 Molarity takes precedence over Density
- 3 Reference Eq is always 1  
Other Eqs are scaled accordingly
- 4 Molarity must not be set
- 5 If Density is N/A then Volume is set to N/A,  
unless Molarity is set
- 6 SearchResult stands for these columns:
  - Name
  - CAS
  - CID
  - SMILES
  - InChIKey
  - InChI
  - MW
  - Density
  - Source

# Views and Precision

- Three view modes:
  - Minimal: Name, Amount, Eq, Mw, Mass, Volume
  - Standard: Status, Type, Search, EqRef, Molarity, CAS, Density, Notes, Source
  - Extended: CID, SMILES, InChIKey, InChI
  - *The views also contain the columns of all previous views*
- Two precision modes
  - Regular: 3 significant figures
  - High: 4 significant figures
  - *Affected columns: Amount, Eq, Mass, Volume*
- The modes can be cycled through with the respective buttons at the top

# Search Modes and Highlights

The search modes can be selected per row in the Type column. The Choices are:

- [auto]: (default) Automatically parse the search term for the correct search mode
- [locked]: Disables searching the database. **NB:** Does not disable editing the row
- CAS: CAS (Chemical Abstracts Service) registry number
- Name: Compound name. If multiple records match the name (e.g. glucose), only the first one is chosen
- CID: PubChem compound ID
- SMILES: SMILES (Simplified molecular-input lines-entry system)
- InChIKey: Fixed-length hashed InChI. Hash collisions *can* occur for different InChI values (but no hash collisions are known so far)
- InChI: IUPAC International Chemical Identifier

Search Highlights:

- Cells of search results are highlighted with a different background color.
- If these cells are edited they lose their highlight to signify that the value was entered manually



# Components

- Save Button:
  - Saves the current state of the plugin to the eWorkbench backend
  - A visual representations of the plugin is also saved as a preview image
- Load Button:
  - Loads the saved state from the eWorkbench backend
  - **NB:** This also overrides the current state. (“Reset Button”)
- Non-Commercial use:
  - This plugin uses the grid component Handsontable with a non-commercial licence
  - This allows for use including teaching and academic research, but excludes uses intended toward monetary compensation
  - Source: <https://handsontable.com/docs/11.0/license-key/#free-license>

# Live Demo

# Known Issues

- Plugin is too wide
  - *[Problem]*: eWorkbench sets a standard plugin (iFrame) size that cannot be changed, that hides the side scrollbar at the bottom in most user cases.
  - *[Solution]*: Solution is already being worked on by eWorkbench developers and said to be resolved in some upcoming update. Nothing can be done on the plugin side.
  - *[Workaround]*: If you don't have a way to side scroll (e.g. a touchpad or mouse with side scroll wheel) scroll to the bottom of the plugin to reveal the side scroll bar.
- [Potential issue]: Internal rate limits could not work
  - *[Current Implementation]*: Every plugin instance is rate limited to one request every 200ms (5 requests/s). Requests are done through the JavaScript fetch API.
  - *[Problem]*: It is unclear if the network setup of the eWorkbench or the TUM network could bundle all requests together and cause everyone collectively to hit that rate limit.
  - *[Previous Testing]*: A small scale test of 10 different plugin instances on one machine simultaneously sending search requests did not hit the PubChem request volume limitation.
  - *[Alternative Implementations]*: Should this case occur in production the rate limitation has to be adapted. Responses from Pubchem send status indicators for throttling control in their headers With JavaScript XHR Requests (instead of the fetch API which disallows reading custom response headers) one could adapt the rate limit dynamically depending on the current status. (<https://pubchemdocs.ncbi.nlm.nih.gov/dynamic-request-throttling>).

# Possible Extensions

- Connect to eWorkbench Rest API to allow it to interact outside of the plugin
  - Expose the currently entered compounds so that the eWorkbench search or other plugins could use these as search suggestions
  - Allow other plugins or other sources to suggest compounds to this plugin (e.g. through a new search mode)
  - Allow other plugins or other programs to automatically fill out rows or read arbitrary data
- Make it conform to the eWorkbench design
- Add animations, optional autosave, and save status
- Make it conform to the Web Content Accessibility Guidelines (W3 WAI WCAG AAA)

# Q&A Time