

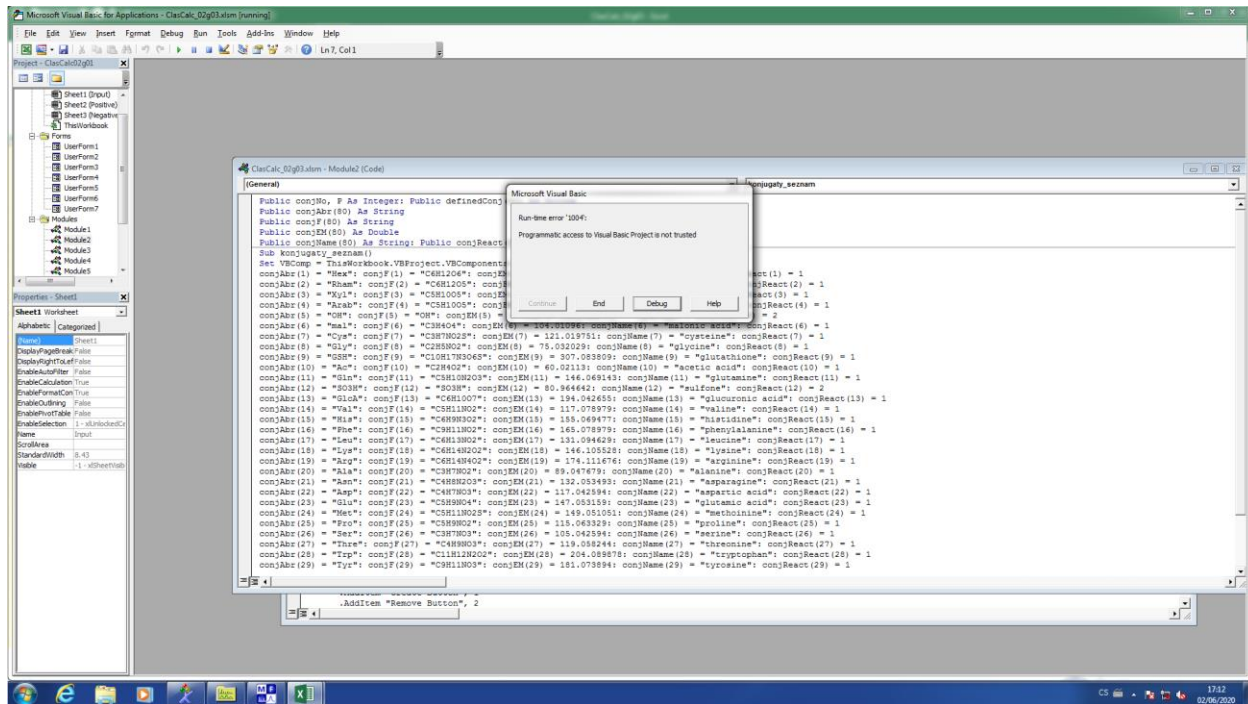
System Settings

- 1) Check, if you have set a dot as a decimal separator in your Windows system as well as in Microsoft Office.

If you have set a comma decimal separator, please change it to dot.

- 2) Allow the access to VBA Project for changes

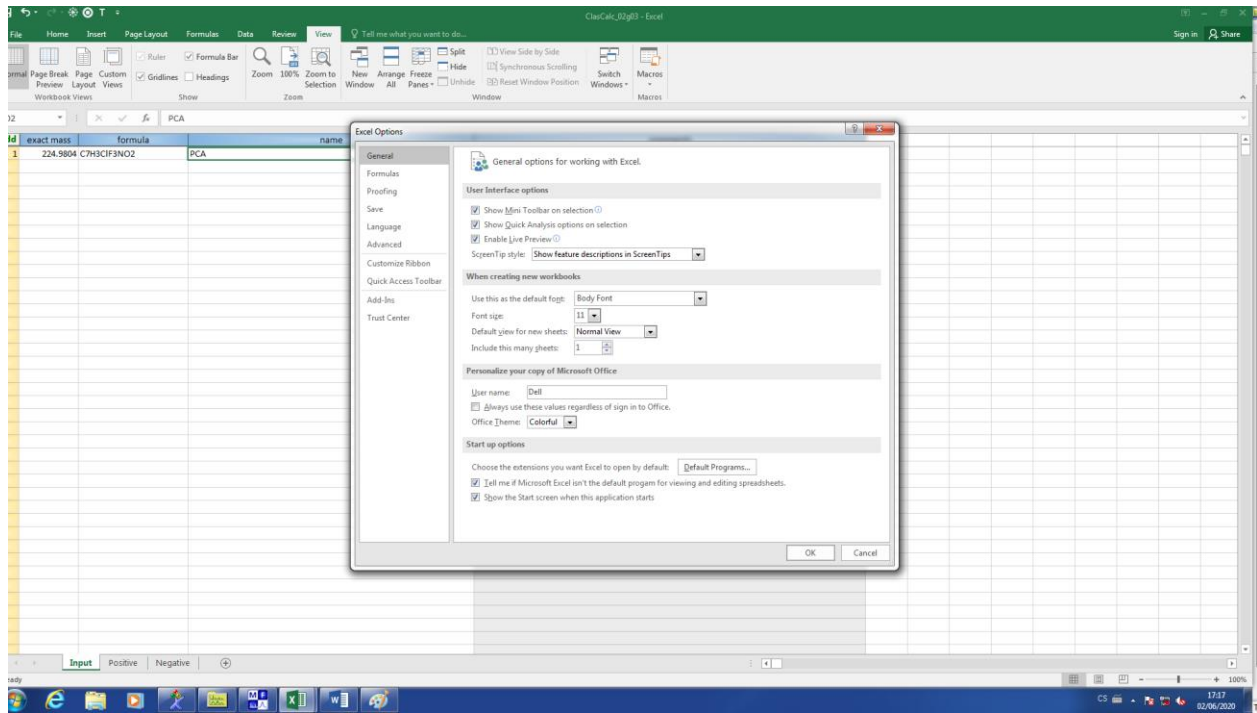
If the following message will appear, you have to allow programmatic access to VBA.



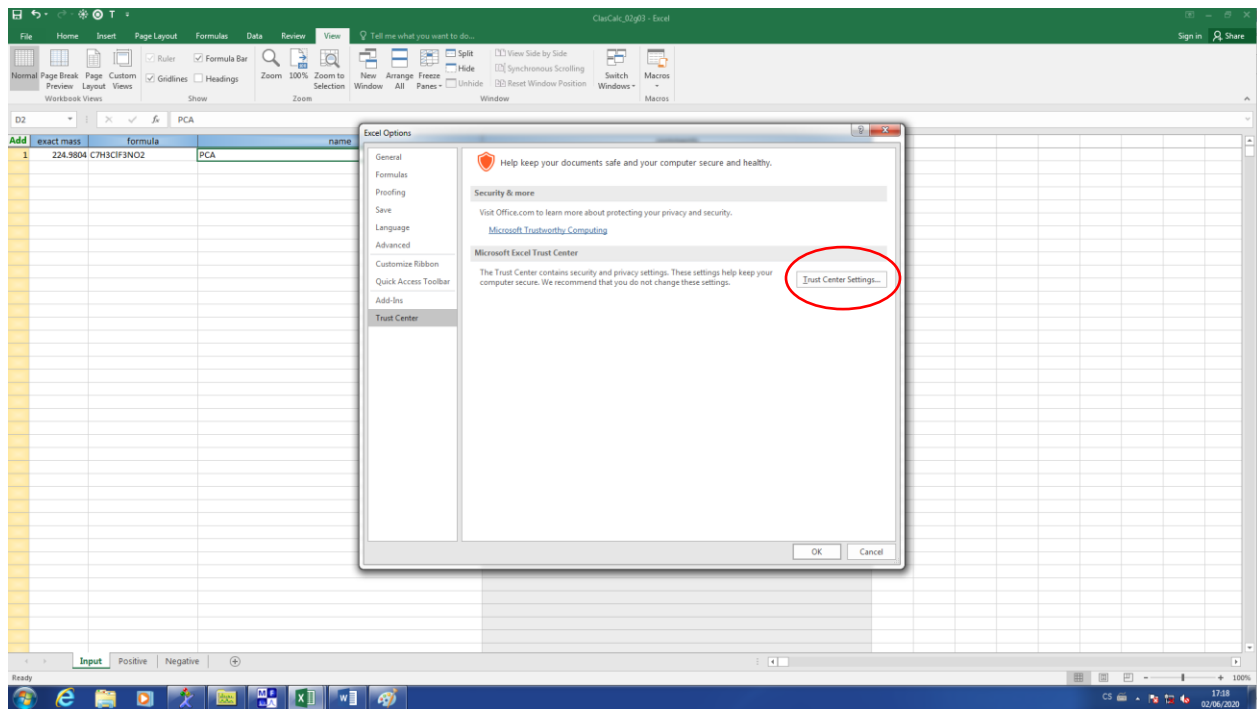
If you decided to continue, please take the following steps:

Click on **End** button.

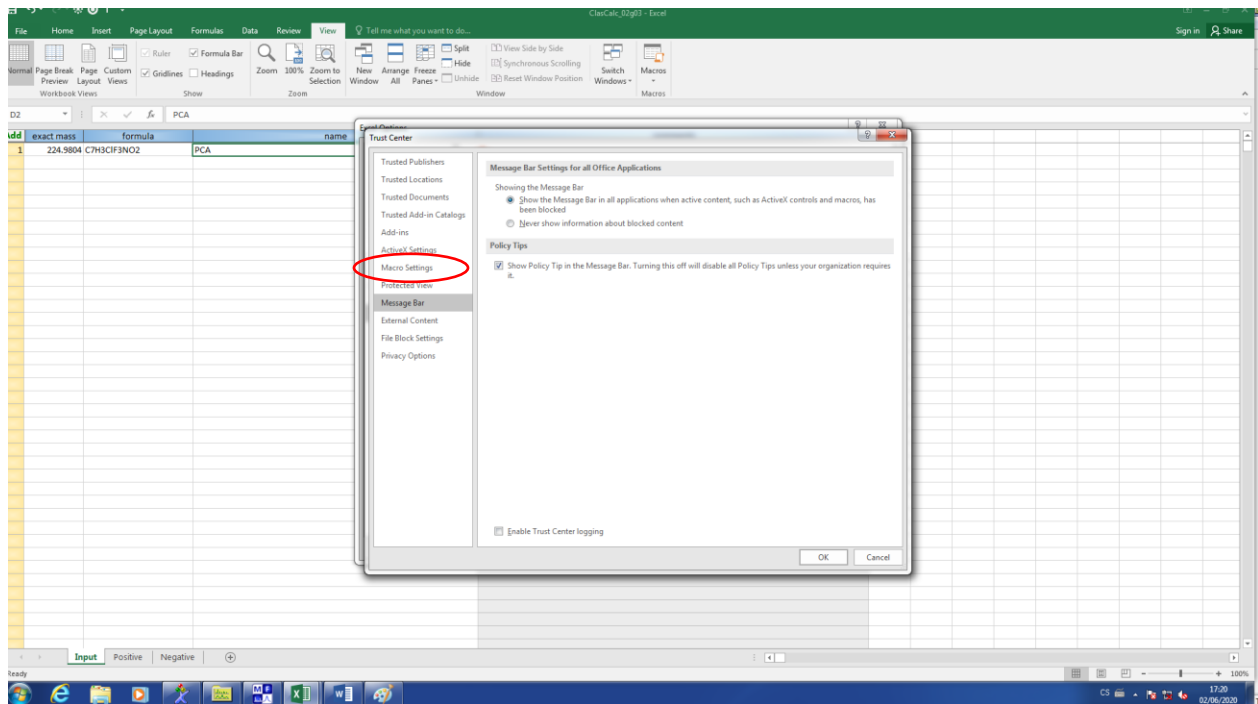
Go to File>Options>Trust Center



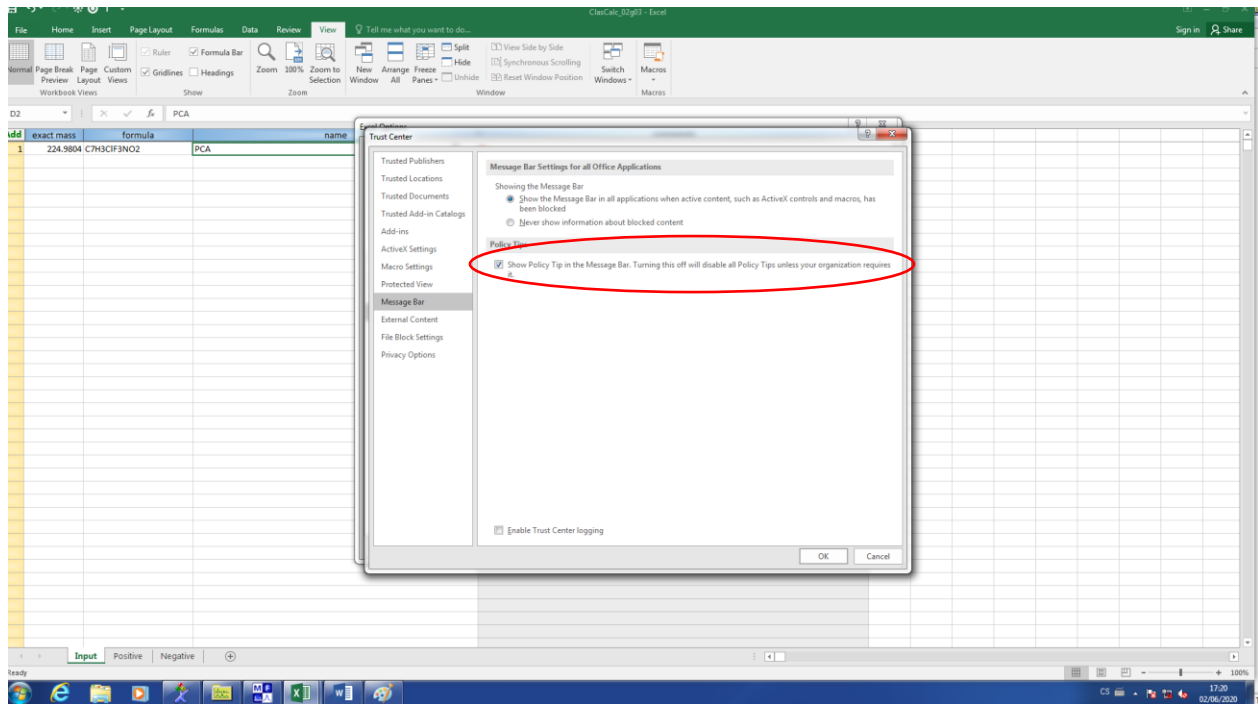
Click to Trust Center Settings...



In Macro Settings



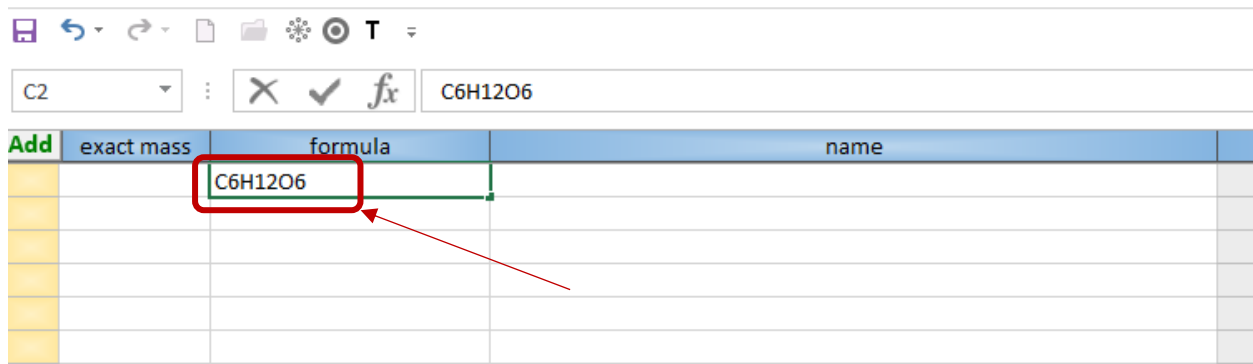
Check Trust Access to VBA Project Object Model



Getting start

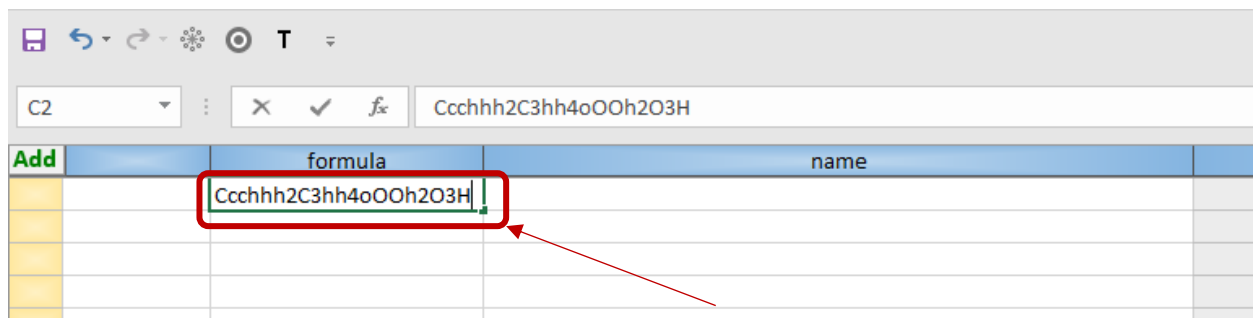
Fill in the molecular formulas (a) or exact mass (b) of searched compounds in the appropriate column. All other items ('Name', 'Comments') are optional.

(a) formula



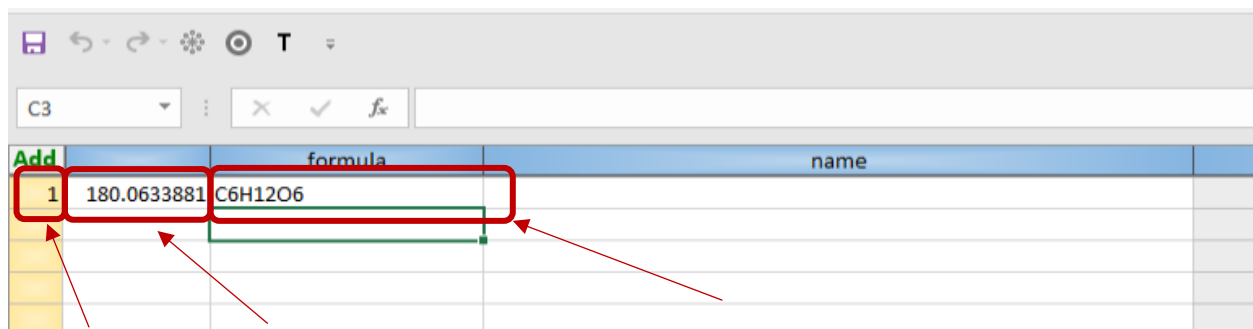
A screenshot of a spreadsheet interface. The active cell is C2, and the formula bar shows 'C6H12O6'. The spreadsheet has columns for 'exact mass', 'formula', and 'name'. The 'formula' column contains 'C6H12O6', which is highlighted with a red box. A red arrow points from the formula bar to the cell.

The format of the formula (number of the chemical element symbols, their order, font, upper or lower case...) can be arbitrary and it will be automatically corrected to the standard format according to Hill notation after leaving the cell (by **Enter** or cursor keys or mouse click).



A screenshot of a spreadsheet interface. The active cell is C2, and the formula bar shows 'Ccchhh2C3hh4oOOh2O3H'. The spreadsheet has columns for 'formula' and 'name'. The 'formula' column contains 'Ccchhh2C3hh4oOOh2O3H', which is highlighted with a red box. A red arrow points from the formula bar to the cell.

After leaving the cell, corresponding exact mass will be computed and issue number in the first yellow cell will show. Check if issue number column is visible. If not, the issue will not be processed. The issue number can be shown/hide by **Left Mouse Double Click** or **Enter**.



A screenshot of a spreadsheet interface. The active cell is C3, and the formula bar is empty. The spreadsheet has columns for 'exact mass', 'formula', and 'name'. The 'exact mass' column contains '180.0633881' and the 'formula' column contains 'C6H12O6'. Both cells are highlighted with a red box. A red arrow points from the formula bar to the 'formula' cell, and another red arrow points from the first yellow cell to the 'exact mass' cell.

Add	formula	name
1	180.0633881 C6H12O6	galactose

You can add the compound name to the appropriate column.

Add	formula	name
1	180.0633881 C6H12O6	galactose

Then continue by clicking to 'Add' button in the upper left corner.

In the following window you can select the type of the adduct(s), the polarity and optionally dimer ions.

Dialog box: Adduct selection

Polarity: Positive Negative Both Dimer

Positive adducts:

- H+
- H3O+
- Na+
- K+
- NH4+
- [MeOH+H]⁺
- [MeCN+H]⁺

Negative adducts/losses:

- H
- AcA-
- FA-
- Cl-

Defined adducts:

Buttons: Clear all, Library, Do

Footer: Input

The results will be shown on new sheets which will be added after **Do** button click.

The screenshot shows a software interface with a table. The table has three columns: 'formula', 'name', and 'comments'. The first row contains the value '180.0634' in the 'formula' column and 'galactose' in the 'name' column. Below the table, there is a navigation bar with buttons labeled 'Input', 'Positive', and 'Negative'. A red arrow points to the 'Positive' button, which is highlighted with a red box.

The Results are represented as a common Excel data.

The screenshot shows an Excel spreadsheet with the following data:

Name	Exact Mass	[M + H] ⁺	[M + H ₂ O] ⁺	[M + Na] ⁺	[M + K] ⁺	[M + NH ₄] ⁺	[M + CH ₃ OH] ⁺	[M + CH ₃ CNH] ⁺
galactose	180.0634	181.0712	199.0838	203.0532	219.0271	198.0978	213.0974	222.0978

The table arrangement can be simply changed by transposition via click on **T** button in Quick Access toolbar:

