MicroMap exploration with CellDesigner

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The aim of this tutorial is to guide you on **how to inspect the MicroMap with CellDesigner**. CellDesigner will require a fair bit of RAM to handle the MicroMap. We therefore suggest you use a computer with at least 16Gb of RAM. You can find an accompanying video walkthrough on YouTube.

Downloading resources

You can download the MicroMap CellDesigner .xml file from the Harvard Dataverse. We also provide an image-based .pdf version, i.e., you can explore it visually, but you cannot search species within. You may download the latest CellDesigner version from the CellDesigner website, which also contains plenty of technical documentation. In this tutorial, we shall focus on specifically exploring the MicroMap.

Inspecting the MicroMap .pdf version

For inspecting the .pdf, we suggest you right-click the file in your file explorer and choose ‘open with’ your internet browser. We found this to be the fastest way to explore the .pdf, as using a dedicated .pdf viewer, such as Adobe Acrobat, was noticeably slower.

Inspecting the MicroMap .xml with CellDesigner

General navigation

Open CellDesigner, then open the MicroMap .xml from within CellDesigner, by clicking on the ‘Open’ icon, or by using File>Open (**Figure 1**). Opening the MicroMap directly from your file explorer, e.g., by double-clicking, does not work – ensure you open the file from within CellDesigner. The MicroMap may take a moment to load, as indicated by the blue animation bar in the right bottom corner. The MicroMap is fully loaded when the animation stops and you can see a list of species in the list view. Most likely, the first view will be zoomed all the way into a white section at the top left corner.

To start exploring, you can grab one of the scroll handles and pan around the map (**Figure 1**). We suggest grabbing the handles directly for moving around the map – using your scroll wheel will likely be slower. You may zoom in and out of the MicroMap by clicking on the dedicated icons at the top (**Figure 1**). You will see an icon’s function by hovering over it.

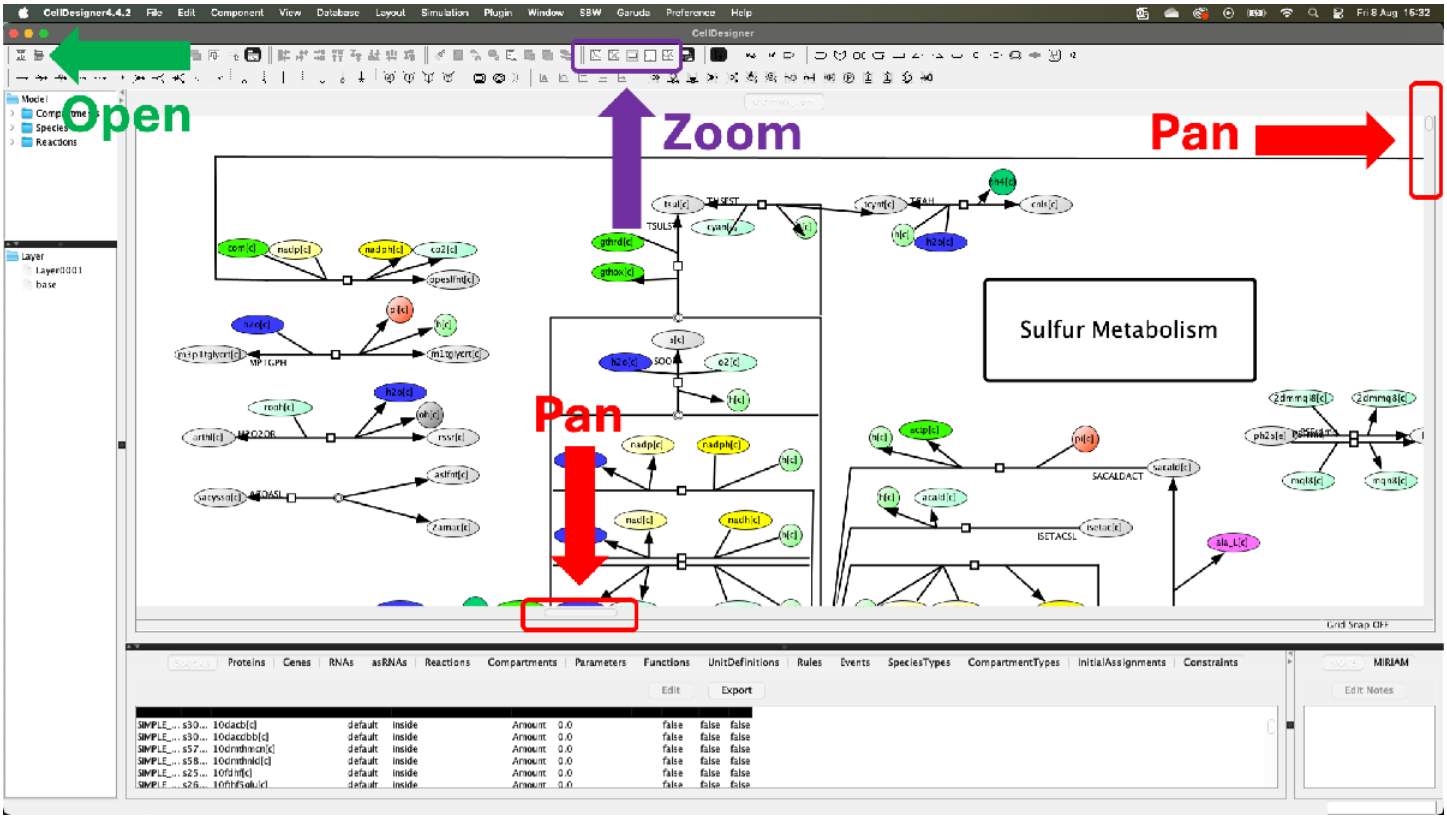

Figure 1: Overview of CellDesigner control functions to inspect the MicroMap. Open your .xml file from within CellDesigner. Use the Zoom icons to adjust your zoom levels. Pan by grabbing the scroll handles.

Metabolites

You can search for metabolites by using the ‘find species’ function (control + F, or Component > Find Species in the menu bar). A window will appear and allow you to select different search options (**Figure 2**). Please note that you will need to select ‘name’ to search for a VMH ID. CellDesigner IDs are arbitrarily assigned by CellDesigner, i.e., a VMH ID will correspond to a CellDesigner name, not CellDesigner ID! For example, for searching an exact match for cytosolic oxoglutaric acid, you shall enter akg[c] into a species name search, and select ‘equal’ in ‘pattern’. Your found metabolite will be highlighted with a pink bounding box, with any associated reactions highlighted in blue. Please note that several reactions can be linked to a single found metabolite. As a metabolite may occur several times throughout the map, you can navigate different search hits by clicking the ‘Next’ and ‘Prev’ buttons. The metabolite will be highlighted at the current zoom level. Therefore, please ensure to be at a reasonably zoomed-in level where you can easily spot the pink bounding box. If you still cannot spot your found metabolite, it may be barely off screen – you may need to scroll a wee bit to fully see it. You will get a ‘not matched’ popup window if your desired metabolite was not found.

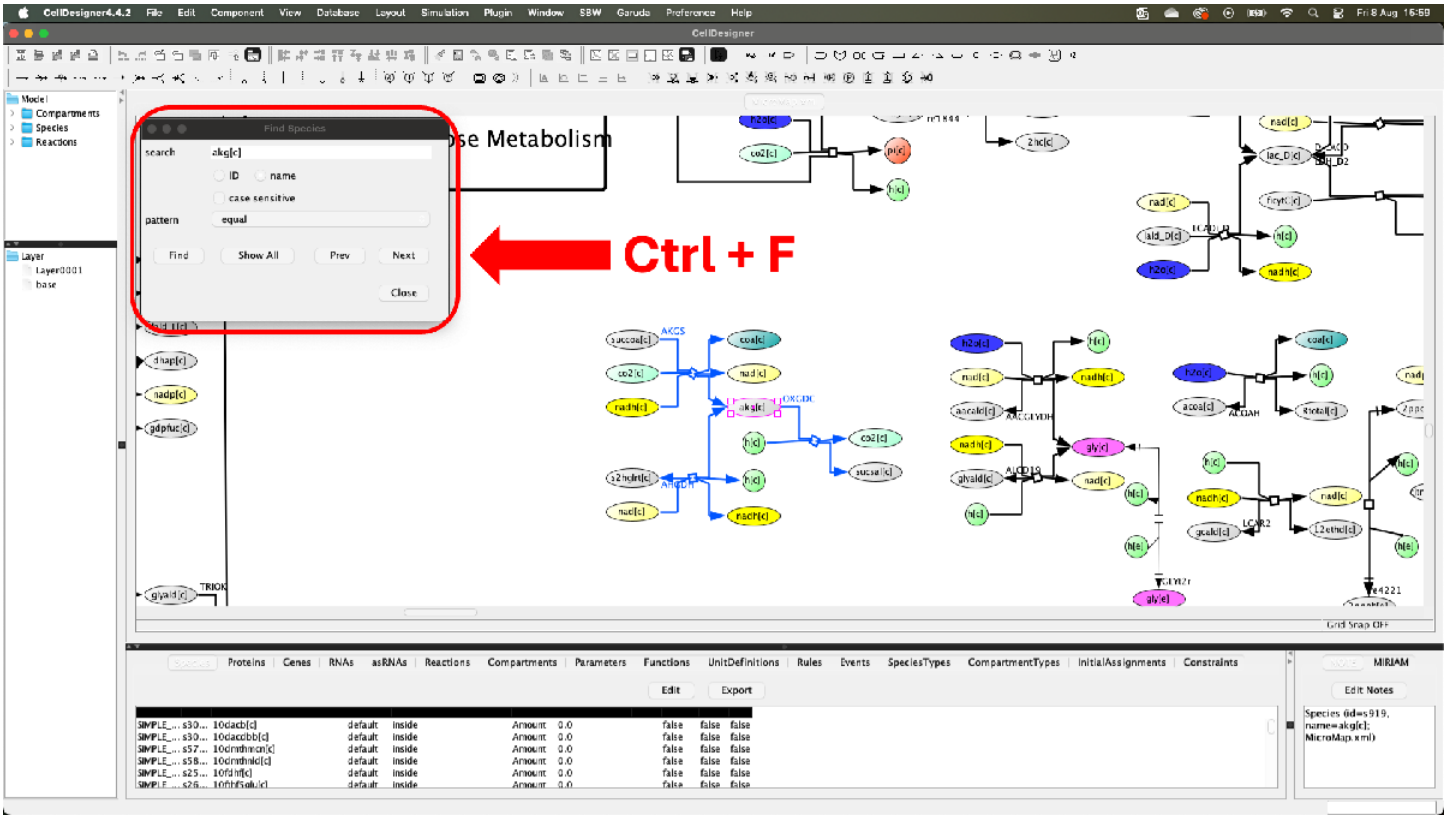

Figure 2: Overview of metabolite search. Open the ‘Find Species’ dialogue through Ctrl + F and search for VMH IDs by ensuring you have ‘name’ ticked in the search box. The found metabolites will be highlighted in a pink bounding box, with their associated reactions highlighted in blue. Cycle through the search hits by using the ‘Prev’ and ‘Next’ buttons.

Reactions

The most straightforward way to identify a given reaction within CellDesigner is to click on its reaction arrow. The selected reaction information, including its VMH ID (= CellDesigner name), will be displayed in the notes window, and the highlighted reaction will point to all the associated metabolites. This method is particularly helpful in areas where, due to CellDesigner layout constraints, several reaction arrows are close to each other, overlapping, or which span distantly distributed metabolites.

Reaction names are displayed next to their corresponding reaction arrow, where possible. However, due to naming constraints within CellDesigner, this was not possible for reaction IDs that start with a number, which, instead, show an automatically generated reaction label. This limitation is cosmetic only, as each reaction remains associated with its VMH ID, which will be displayed when clicking on the reaction arrow, as outlined above.

Unlike metabolites, however, reactions are not searchable. For finding a specific reaction, click on the ‘Reactions’ tab within the list window to display an alphabetically ordered list of all contained VMH reaction IDs, which will then allow you to find and select your reaction of interest (**Figure 3**). Clicking on the reaction ID will jump to the relevant section in the MicroMap and highlight the reaction of interest. As with searching for metabolites, the found reaction will be highlighted at the current zoom level. Therefore, please ensure to be at a reasonably zoomed-in display before clicking on your reaction of interest.

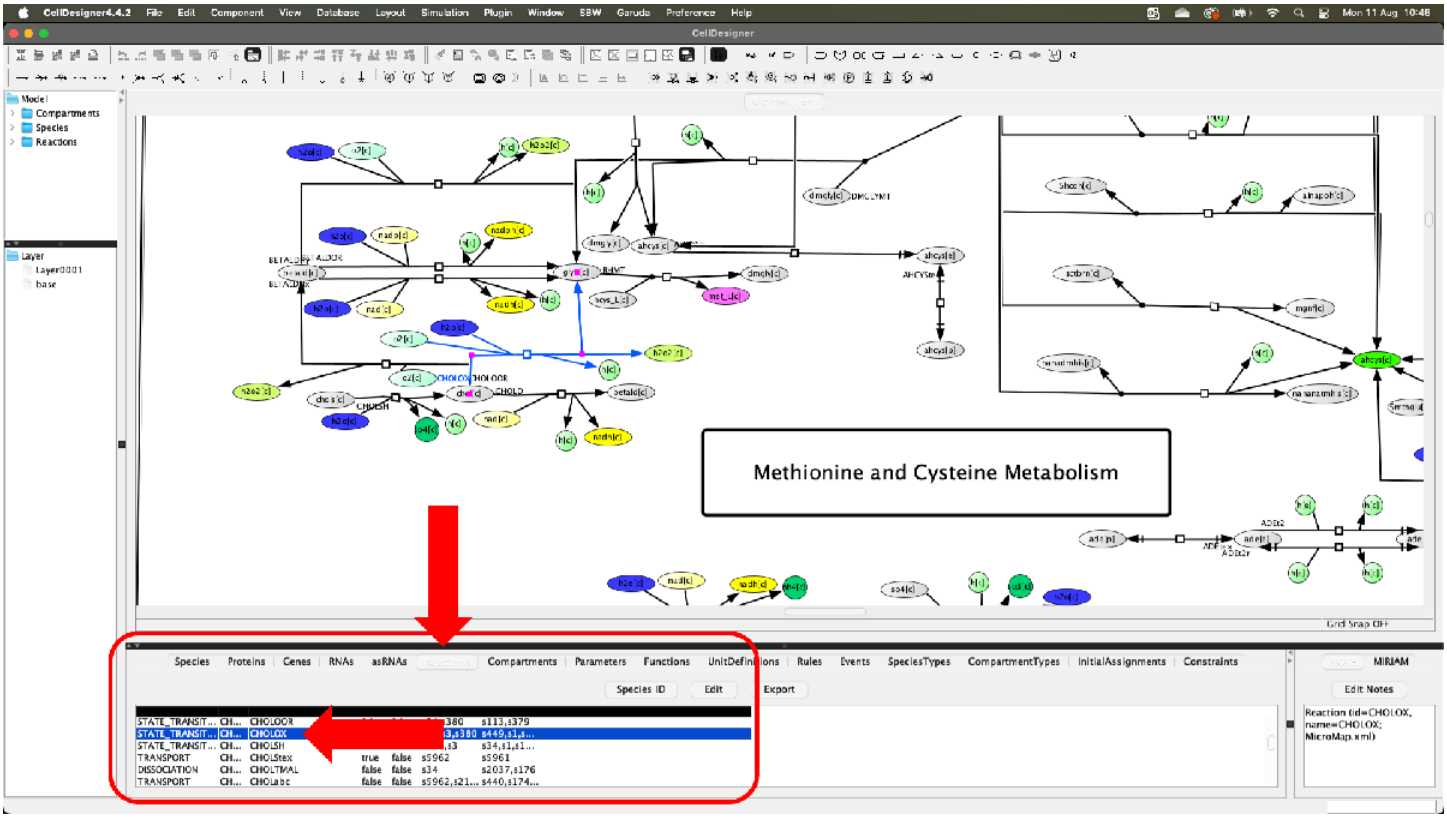

Figure 3: Overview of reaction search. Click on the ‘Reactions’ tab in the list view to access the alphabetically ordered reaction list. Select the reaction of interest, which will then appear highlighted on the map.

We encourage you to play around with the MicroMap and CellDesigner functionality to explore and identify the most suitable workflows for your use-case. For more information on CellDesigner and potential troubleshooting, please consult the ample CellDesigner documentation online.