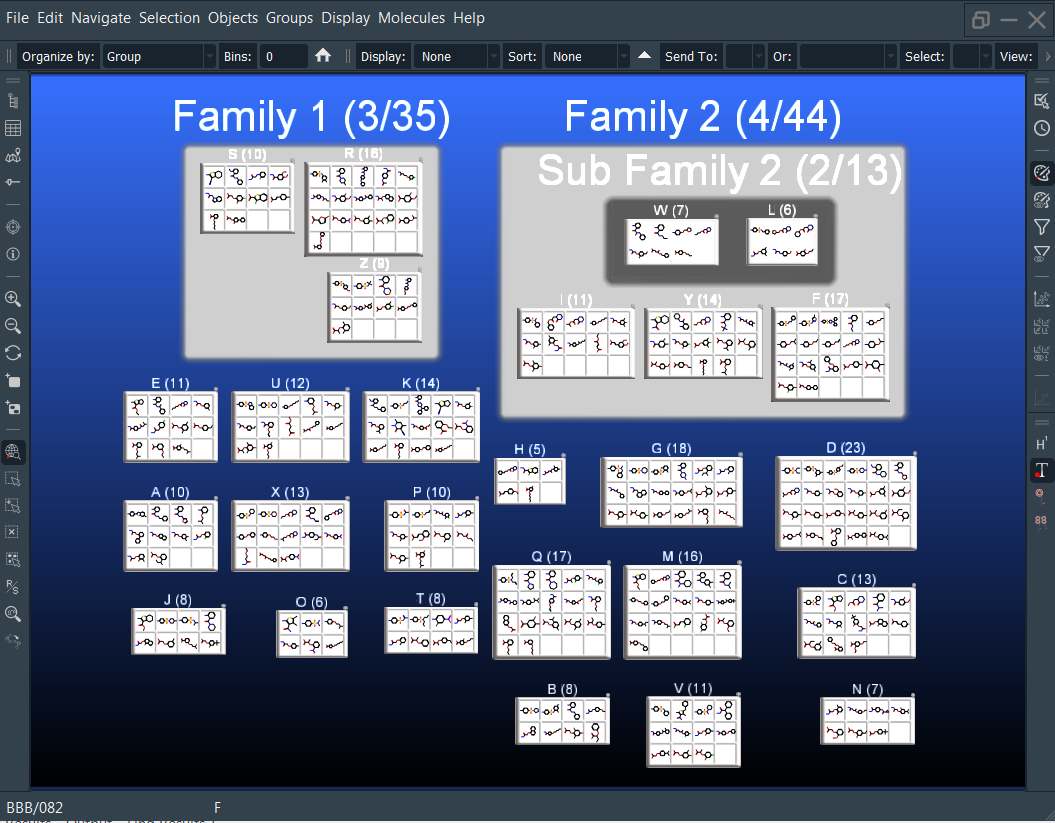
**What’s new in EyeMol 1.22**



**Highlights:**

* MCSS calculation per group.
* Murcko scaffolds highlight and grouping.
* 2D and 3D descriptors.
* Line plot and scatter plot in separate windows.
* Cosmetic: Dark theme and textured clusters.

**If you notice any bug please let us know at** [**contact@pikairos.com**](mailto:contact@pikairos.com)**.**

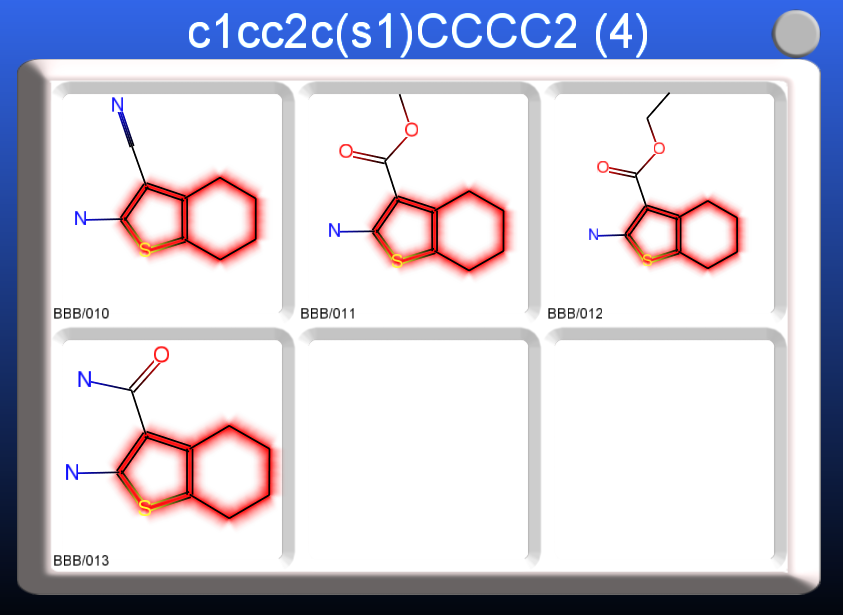
**If you are missing a functionality, please let us know at** [**contact@pikairos.com**](mailto:contact@pikairos.com)**.**

**Symbols:**

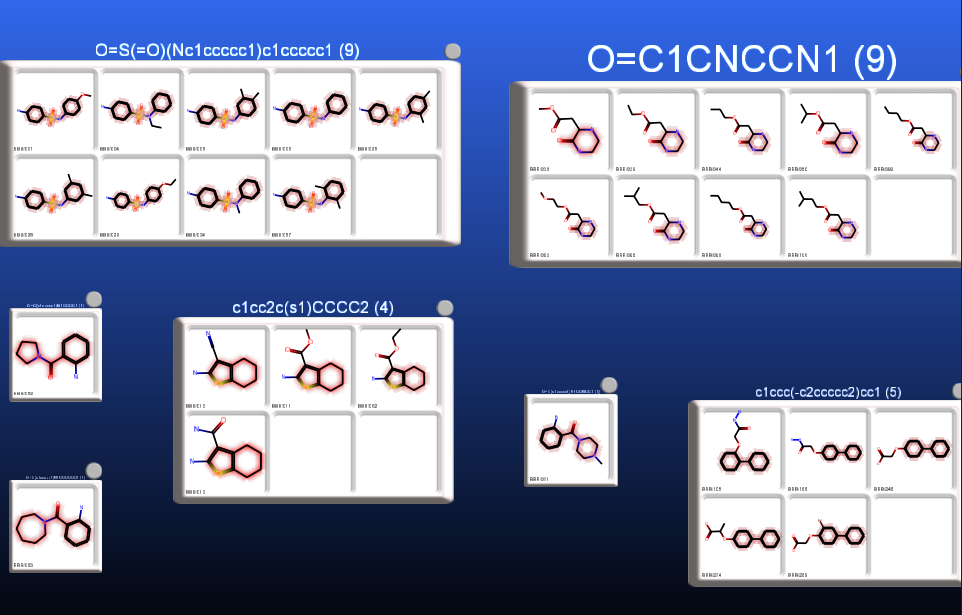
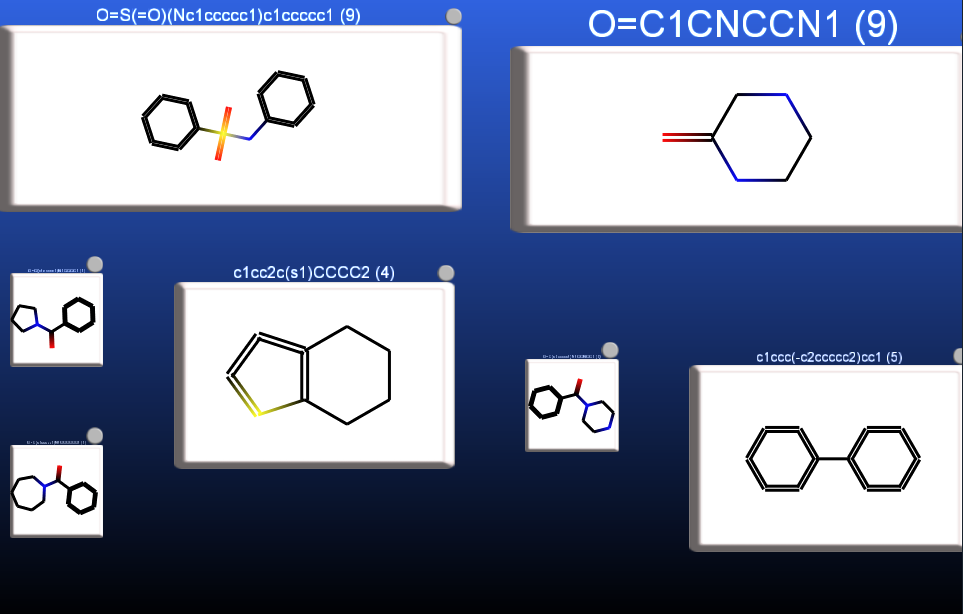
* +  : Mouse left click
  + http://cartographie.mairie-lille.fr/lille_polcom/img/mouseRight.png: Mouse right click
  + http://cartographie.mairie-lille.fr/lille_polcom/img/mouseMiddle.png: Mouse middle click
  +  : Drag the mouse while holding a button
  + : Alt key
  + : Control key
  + : Shift key
  + ←,→,↑,↓: Directional arrow keys

**MCSS calculation per group:**

* Start from menu Molecule/MCS or shortcut ’)’ or icon E:\seb\vc6\OPENGL\SEB\_x64\0Data\bigs\mcss.png .
* The calculation of the MCSS will be performed on a per group basis.
* Once a common scaffold is found for a group, all molecules of the group are aligned using this scaffold.
* Then the scaffold is highlighted on each molecule (the color of the highlight can be changed in the options).



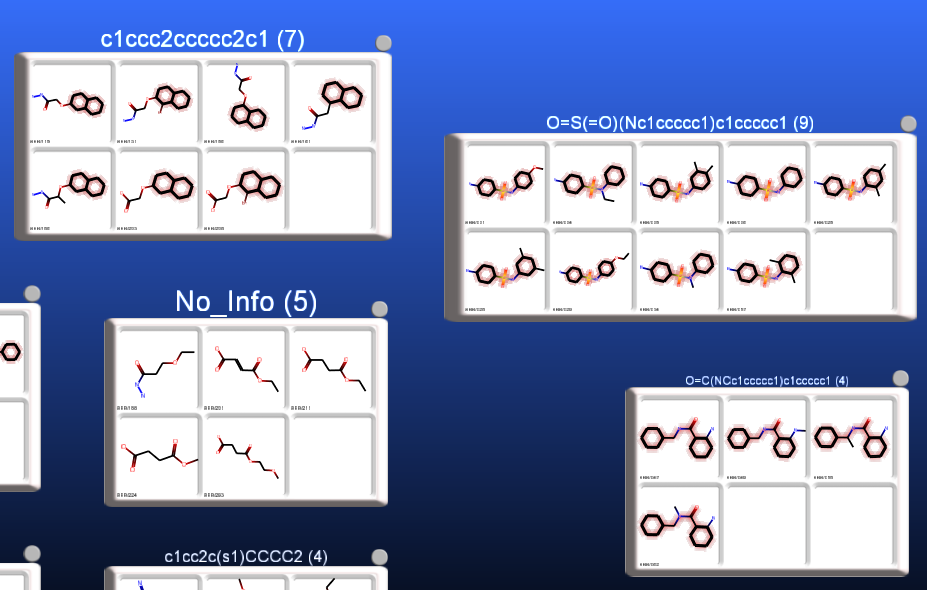
* Press and maintain the ‘<’ key to fill each group by the image of the common substructure.
  + Holding ‘<’ is similar but does not display scaffolds for single molecule groups.

* Temporarily hide the highlights using the menu Molecule/Hide scaffold or the icon

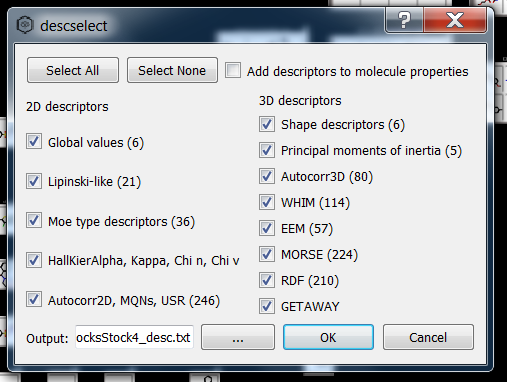
**Murcko scaffolds highlight and grouping:**

* Start from menu Molecule/Murcko or icon  .
* For each molecule in the dataset a Murcko scaffold is calculated.
  + A new property “ Murcko” is created and contains the SMILE of the scaffold.
  + The scaffold is highlighted on each molecule (highlight color can be changed in the options).
* Finally, molecules are grouped together according to their Murcko scaffold.



**2D and 3D descriptors:**

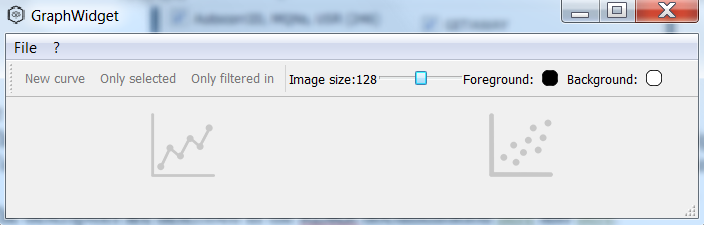
* Start from menu Molecule/Descriptors



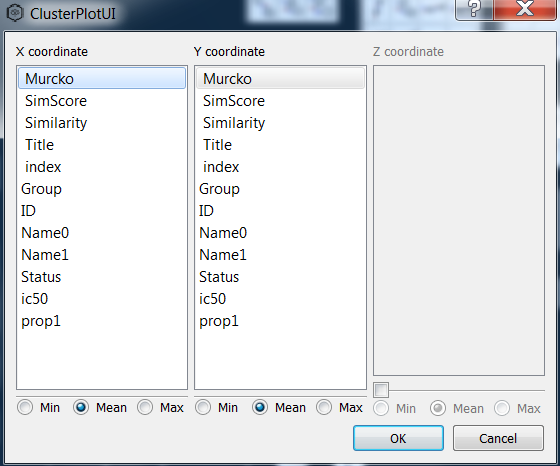
* Select the descriptors to compute
  + The number in parenthesis indicates the number of properties calculated per descriptor.
  + You can choose a text output file for the descriptors and/or to add them to the molecule list of properties.
    - Note that the total number of properties can add up to around a thousand.
  + The descriptors are described in the RDKit documentation [here](https://www.rdkit.org/docs/source/rdkit.Chem.rdMolDescriptors.html) and [here](https://www.rdkit.org/docs/source/rdkit.Chem.Descriptors3D.html).
    - Note that sometimes some descriptors fail for some molecules resulting in an application crash. It is therefore recommended to save your work before proceeding with the descriptor calculation.

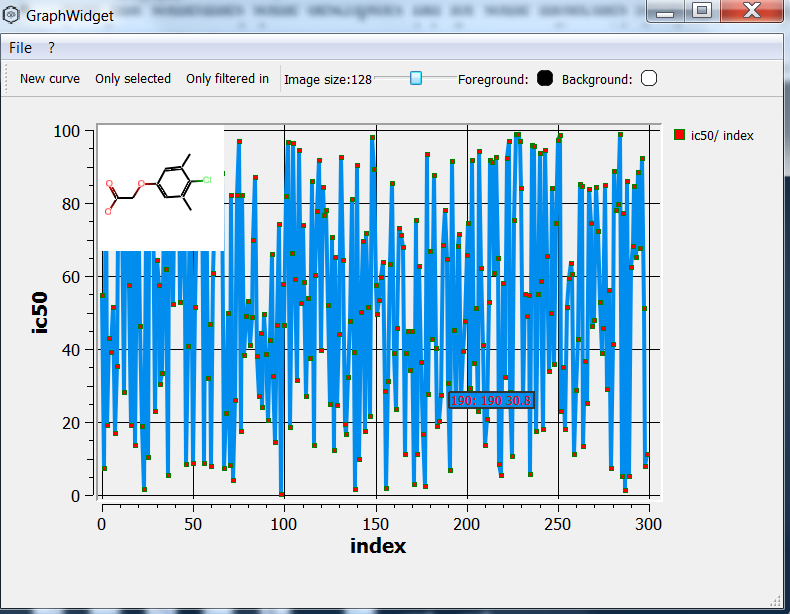
**Line plot and scatter plot in separate windows:**

* Start from menu Groups/Graph window or the icon 
* From the new window choose either a line plot or a scatter plot (more plot types coming soon).

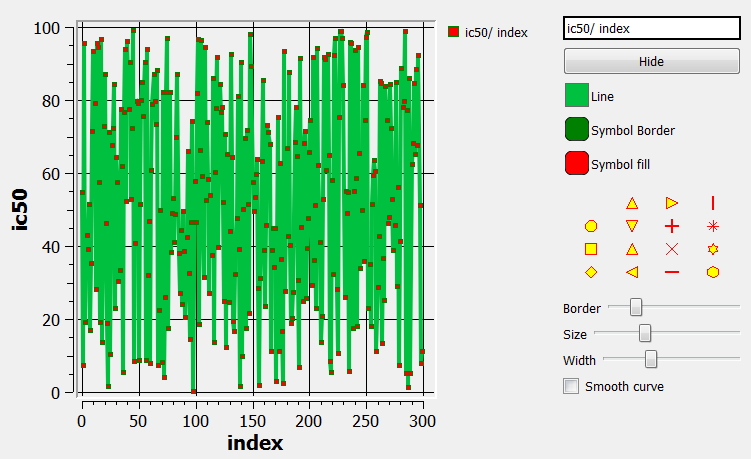


* Then select properties to use for x and y axis.





* When the mouse pointer is close to a point of the curve the coordinates and the image of the molecule are shown.
  + At the same time the pointed molecule becomes the active molecule in the main window.
  + http://cartographie.mairie-lille.fr/lille_polcom/img/mouseMiddle.png centers and zoom the main window on the pointed molecule.
  + The size and colors for the molecule image can be changed from the toolbar at the top of the graph window.
* Use the mouse wheel to zoom in and out.
  + Mouse wheel on an axis only zoom this axis.
* Use  to pan the view.
* Graph style and colors can be changed when clicking on the curve legend.
  + Click anywhere in the graph to close the customization panel



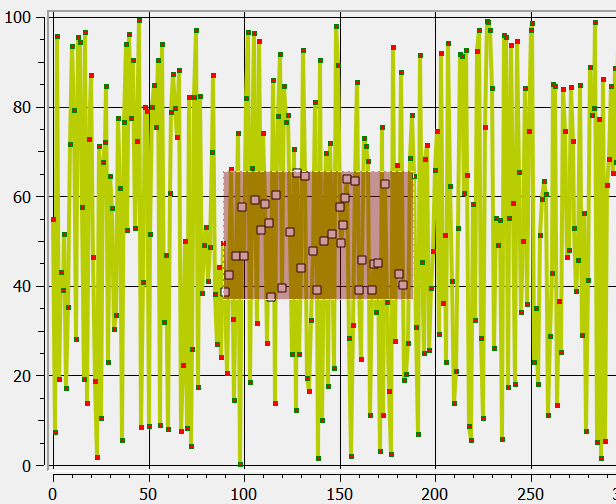
* Selections can be performed in three different ways
  +  on a point to select a single molecule.
    -  to add a single molecule to the current selection.



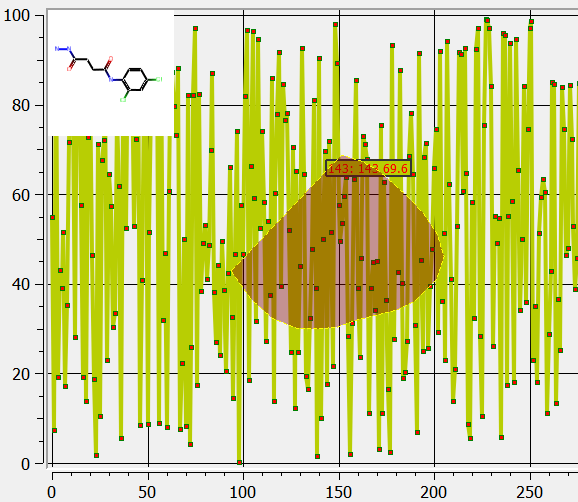
* +  to select a rectangular area.
    -  to add a new rectangular area to the current selection.



* + - The position of the rectangular area can be modified by  when the cursor is .
    - The size of the area can be changed by  when the cursor is , , or .



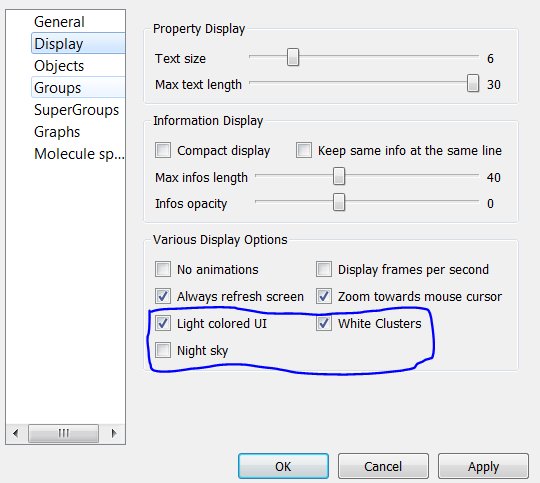
* +  to select a free form area.
    -  to add a new free form area to the current selection.



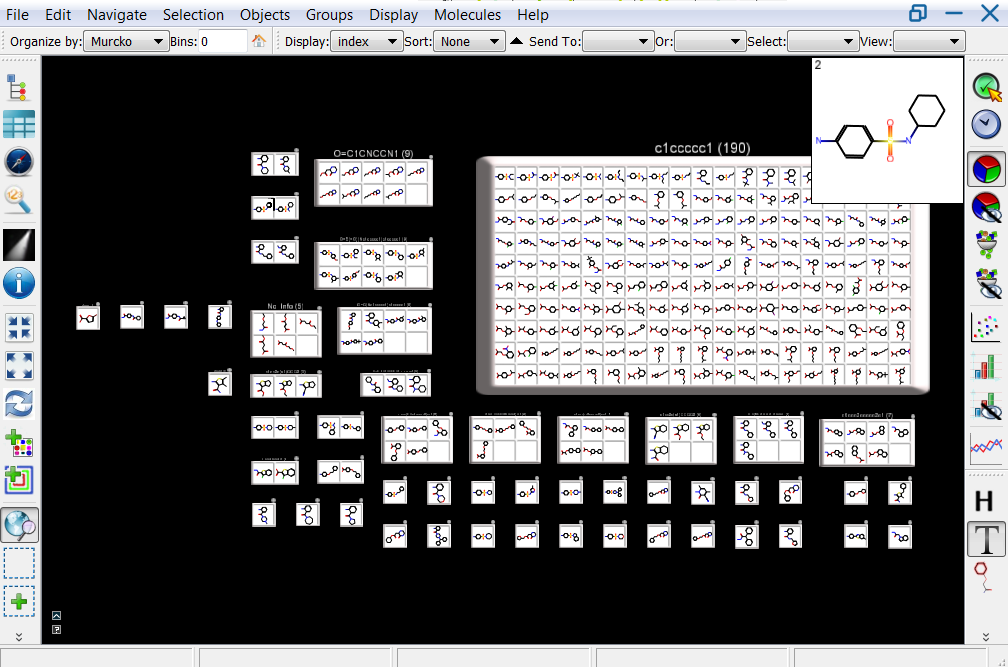
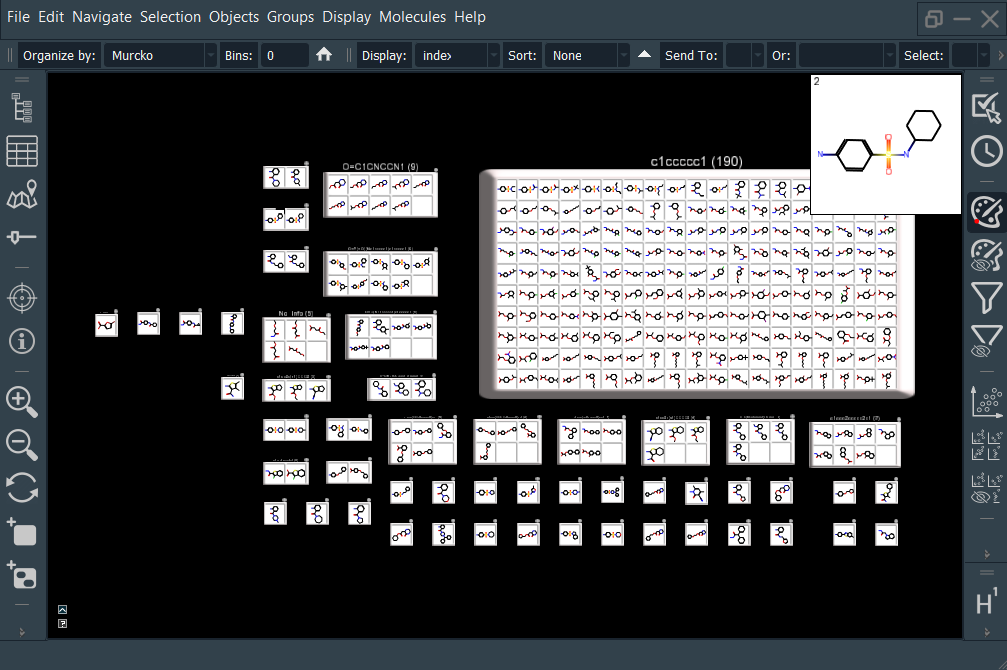
* Selection in the graph is reflected in the main window and reciprocally.
* The “Only selected” button will mask all unselected molecules from the graph.
* The “Only filtered in” button will mask all filtered out molecules from the graph.

**Cosmetic: Dark theme and textured clusters:**

* In the preference dialog (Menu/Preferences or shortcut meta + ’!’), in the display tab it is possible to change 2 interface parameters.



* The “Light colored UI” checkbox changes the interface between a light and a dark theme.

* The “Textured groups” changes the representation of the groups.

