

What is new in MetaPath ver.5.4.0 and MSS Composers ver.1.10

Modifications in MetaPath application

The following modifications in the MetaPath platform are introduced in the version 5.4.0:

- A new export functionality in MetaPath allowing all or some of the existing tables to be exported into one or more MS Excel files,
- An extended database structure which allows handling of generic (Markush) structures,
- Enhanced structure editor in MetaPath allowing generic structures to be used (for example, structures having a fragment which site of attachment is not specified),
- A functionality displaying all possible individual realizations of a generic structure,
- All types of searches are redesigned in order to handle generic structures,
- The visualization of search results is redesigned in order to display generic structures and their individual realizations.

Examples of newly developed functionalities are provided below.

The functionality for exporting tables is initiated via right-click on the maps tree (Fig.1).

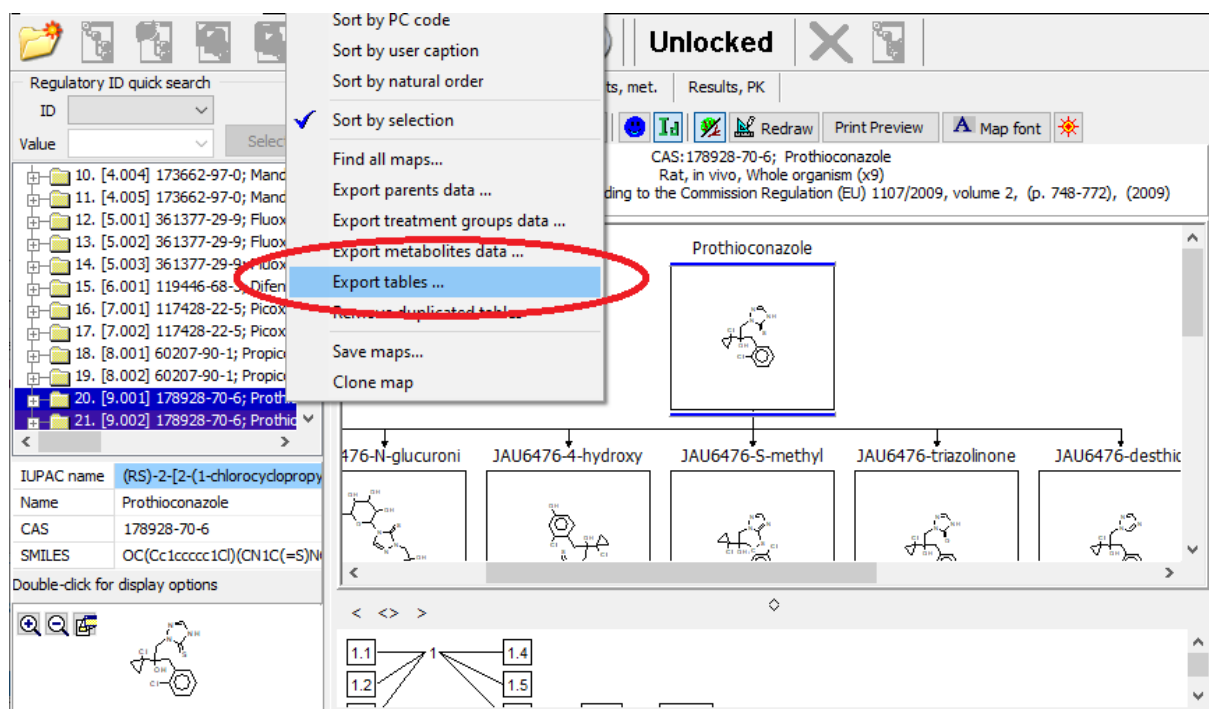


Fig.1 – Initiating tables export

Then the user is asked to select which types of tables to export (Fig.2).

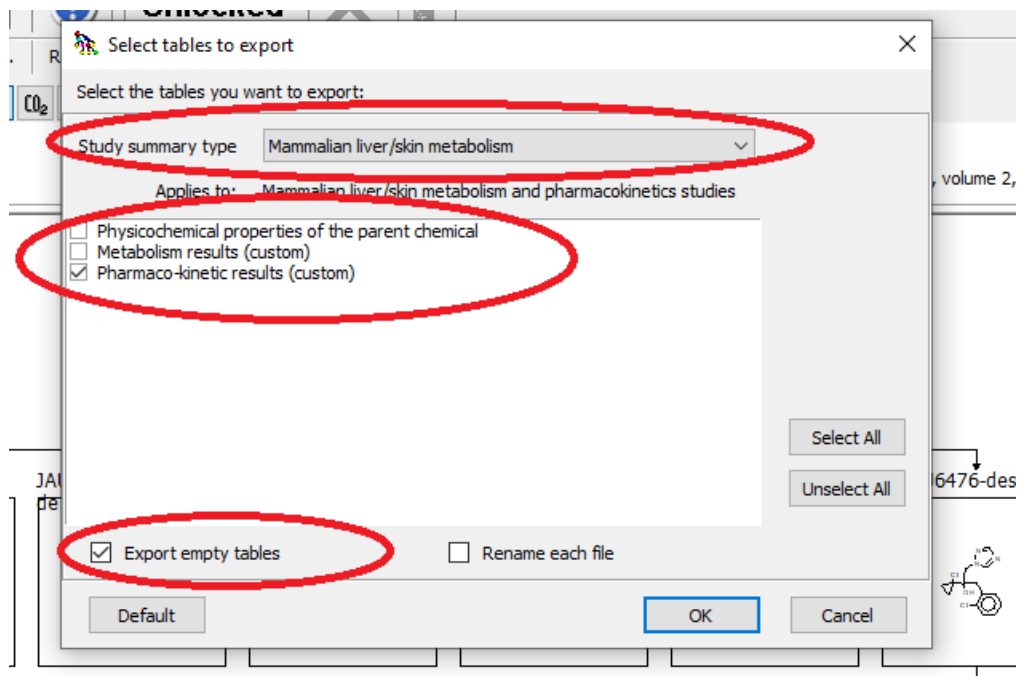


Fig. 2 – Specifying which tables to export

Once the export is completed the MS Excel files appear in the folder specified by the user – one file for each selected map (Fig.3).

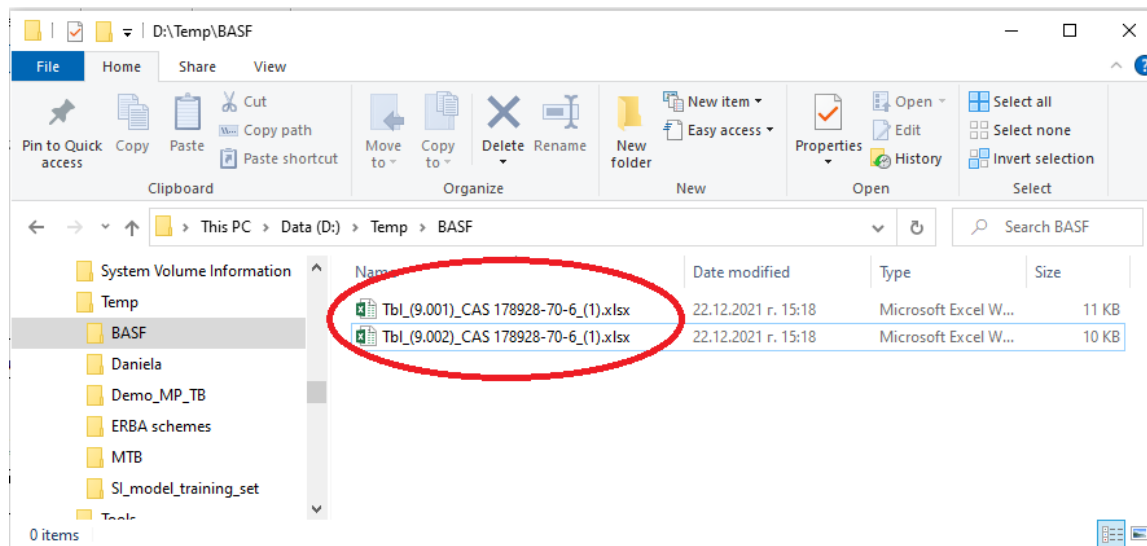


Fig.3 – MS Excel files containing the content of the selected tables

The structures editor introduces a new section “Common fragments” which allow entering generic (Markush) structures (Fig.4).

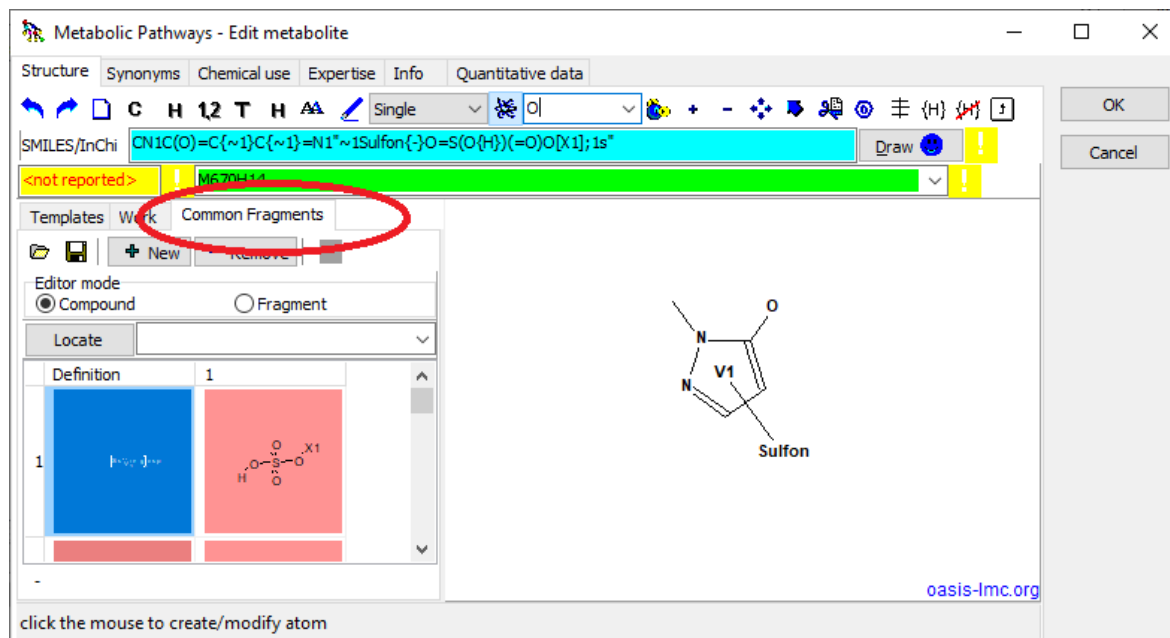


Fig.4 – The structures editor can define generic structures

Once a generic structure is displayed on the map, its individual realizations could be examined (Fig.5).

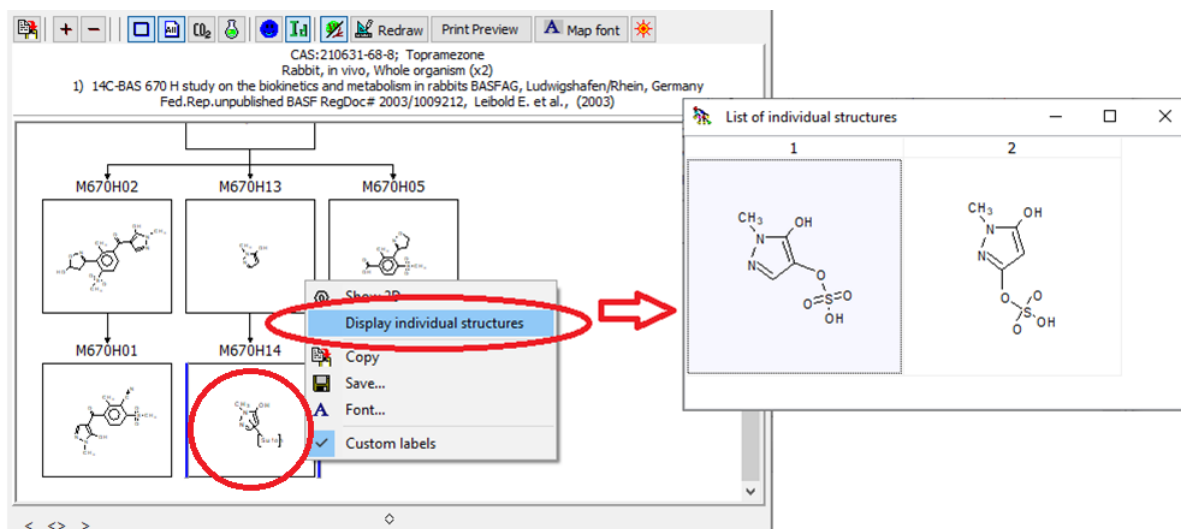


Fig.5 – Displaying the individual realizations of a generic structure

All different types of searches can handle generic structures, an example is shown below (Fig.6a, 6b).

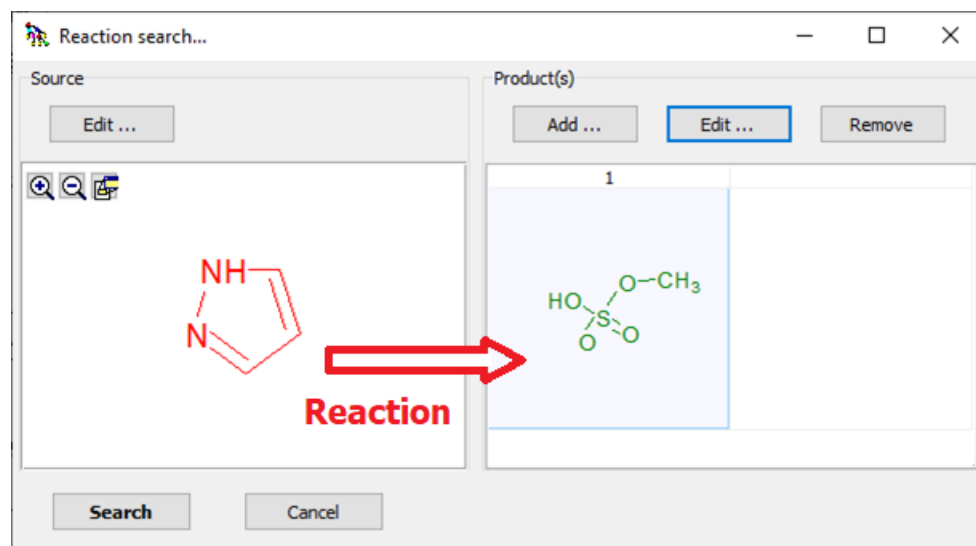


Fig.6a – A reaction search defined by the fragment which must be contained in the source (left, colored in red) and by the fragment which must be contained in the product (right, colored in green)

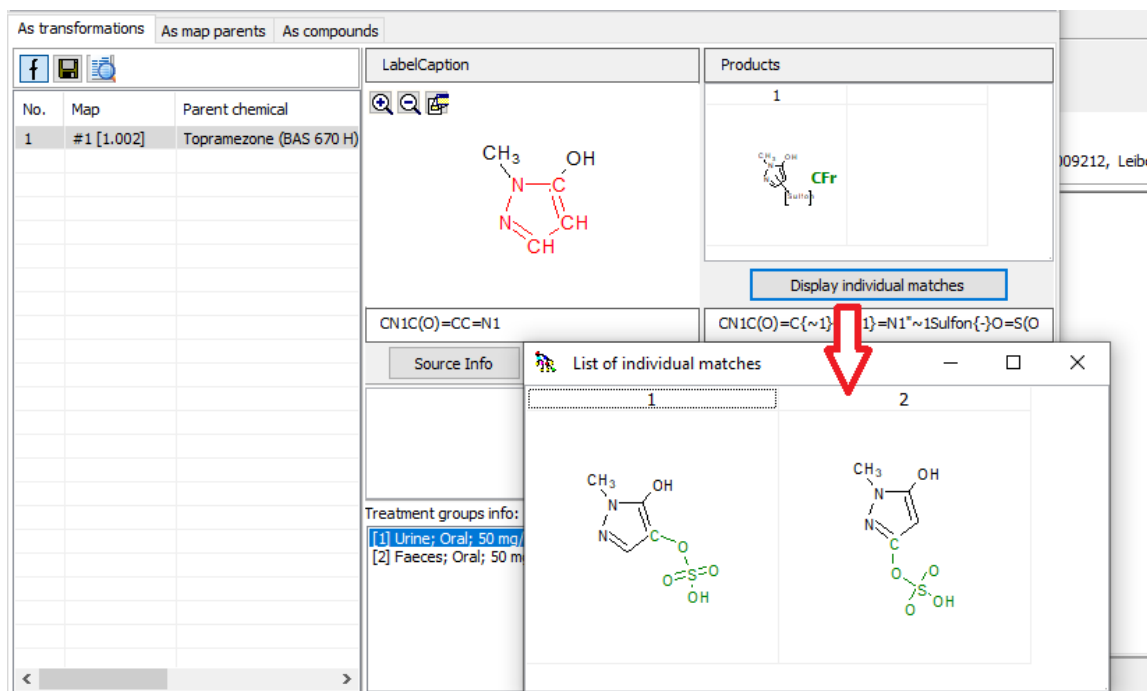


Fig.6b – The reaction search “captures” a generic structure appearing as a product and explains how its individual realizations meet the search criteria

Modifications in MSS Composers

The following modifications in the MSS Composers are introduced in the version 1.10:

- The structure editor in MSS Composers is enhanced to allow assigning generic structures (for example, structures having a fragment which site of attachment is not specified),
- A new functionality is added which displays all possible individual realizations of a generic structure.