What's new in MetaPath v. 5.4.2 and MSS Composers v. 1.14

Modifications in the MetaPath application

The following modifications take place in MetaPath platform version 5.4.2:

- Some textual fields are expanded to allow content up to 50,000 characters,
- Resolved is a bug in DER XML import appearing when the number of rows in Table 8 is bigger than metabolites in Appendix 2.

The expanded textual fields are as follows:

- *Section "Study summary"* - "Background information", "Executive summary"
- *Section "Study design"* - "Experimental details", "Sampling", "Extraction and analysis", "Identification and characterization"
- *Section "Results"* - "Quantitation", "Storage stability", "Proposed metabolic pathway"
- *Section "Results" (for any radiolabel)* - "Extraction, characterization and distribution of residues", "Identification of residues"

Modifications in the MSS Composers Suite

The updated **MSS Composers** package includes:

- MSS Livestock Composer 1.14*
- MSS Plants Composer 1.14*
- MSS Crops Composer 1.14*
- DocBuilder 1.14

The Composers in this package display v.1.13 in their title bar. The correct version number (1.14) is shown in the file details of each Composer executable (.exe file).
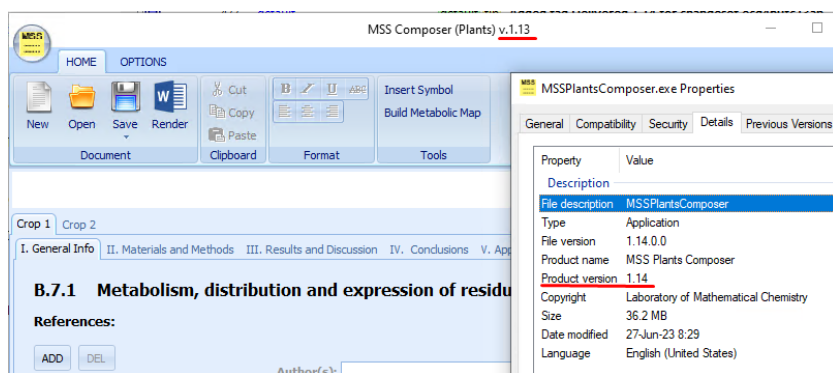
1. New Features:

1.1 Copy/paste function in selected tables across all MSS Composers

As of this version, users can copy a table from an Excel spreadsheet and paste it into a MSS Composer table. The paste option is available in the context menu of all compatible tables and is only enabled when there is an actual Excel table copied into the clipboard.
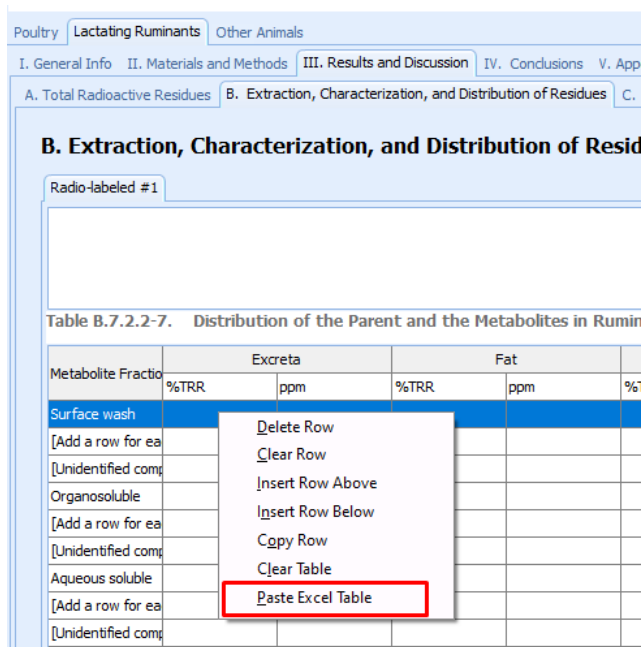
1.2 Batch loading .mol files and SMILES codes (import of Appendix 2)

This feature allows users to easily load a lot of structures into Appendix2 and avoid the need for manually drawing/entering each one. For this purpose, there is a new button in the Appendix 2 toolbar that brings up the Structure Loader dialog. In it, users have the option to import all structures from a single .smi file OR to batch import multiple .mol files. In both cases users have control on the mapping of the source information to the Appendix 2 columns - Common Name, Chemical Name and SMILES. Once the chemical information is imported, users can then manually edit the relations between the imported structures.
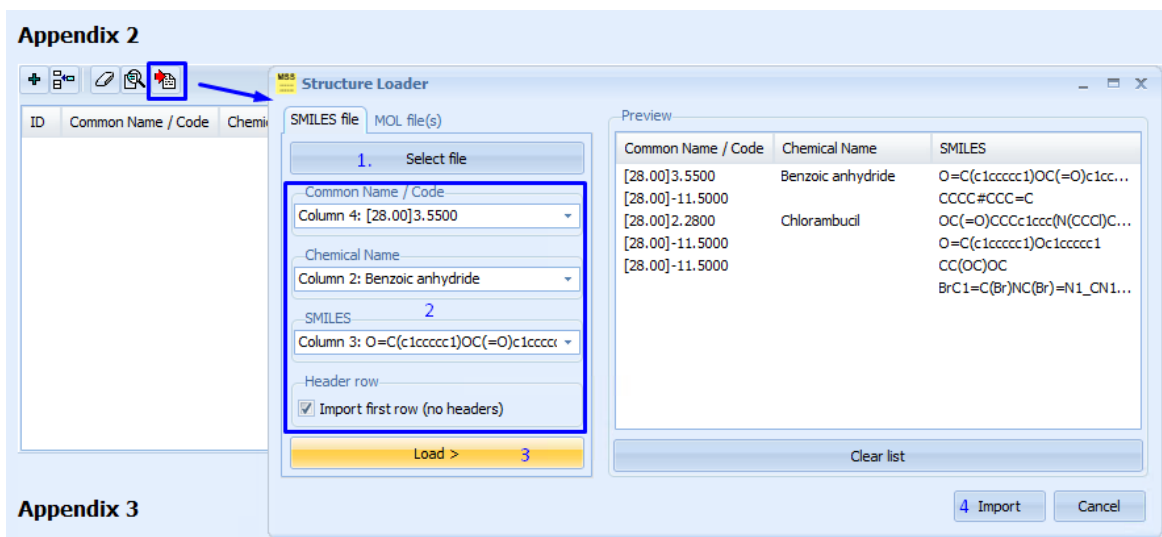
2. Improvements and bugfixes:

2.1 Tables in section III. Results and Discussions have been tested and confirmed to handle properly text containing the "less than" (<) character. XML files were properly saved and loaded and then imported into MetaPath.

2.2 The Word rendering has been improved following submitted requests. 2D structures appear bigger and clearer. Reported missing information is now rendered. Data in Appendix1 and Appendix2 is now complete. Metabolite tables are now rendered for Plants and Crops (not just in Livestock).

2.3 All Composer free text fields are unrestricted in terms of character length. The necessary changes have been made in the MetaPath database (described in the previous section) to allow up to 50000 characters in selected fields.

2.4 The table in section III A (Extraction efficiency) was flagged as not fixed and allows the insertion of multiple rows.

2.5 Several issues identified during the internal testing and related to missing information in the rendered Word document were also addressed.

2.6 Corrected instructional text indicating field restrictions for some text fields.

What's new in MetaPath v. 5.4.1 and MSS Composers v. 1.12

Modifications in the MetaPath application

The following modifications take place in MetaPath platform version 5.4.1:

- The kinetic data layer, previously developed for private use, was transferred to the public version; these changes cover both data entry and search functionalities,
- The MSS XML import was redesigned in order to provide more useful information about the fields from MSS Composers which were imported and the ones which failed, along with the errors that occurred,
- MSS XML import was updated, so the user comments for tables "III B. Extraction, Characterization, and Distribution of Residues" and "III D. Identity of Residues" to be saved as footnotes in the corresponding MetaPath tables,
- Display options for maps tree captions are expanded with data from plant/crop studies.

Examples of newly developed functionalities are provided below.

The kinetic data includes two types of information – numerical values (like half-life, clearance, Vmax, etc.) and time series (various values presented as function of time). Both are assigned to chemicals, but the specifics of the experiments in which they were measured are also taken into account. In this respect one chemical may have different sets of kinetic data for the different experiments (Fig.1).
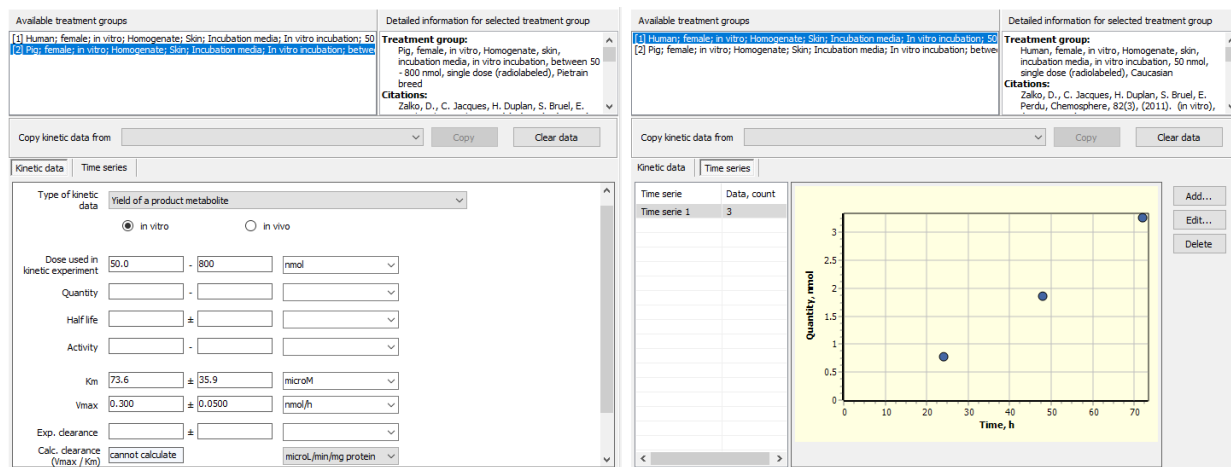

Fig.1 – Numerical values associated with treatment group #2 (pig) on the left, and a time serie associated with treatment group #1 (human) on the right, for same chemical

The MSS XML import is modified to provide detailed information for each data field being imported. In addition, the import doesn't stop after certain errors, but continues till the end of the last file in order to check the content of the any data field intended to be imported.

After the import procedure is completed, a short message appears informing about the count of successfully imported XML files and the count of failed XML files. At this stage the user can choose:

- to get a detailed log report including information about each XML file and each data field being imported,
- to get a short log report containing only data fields that failed during the import (i.e. only import errors),
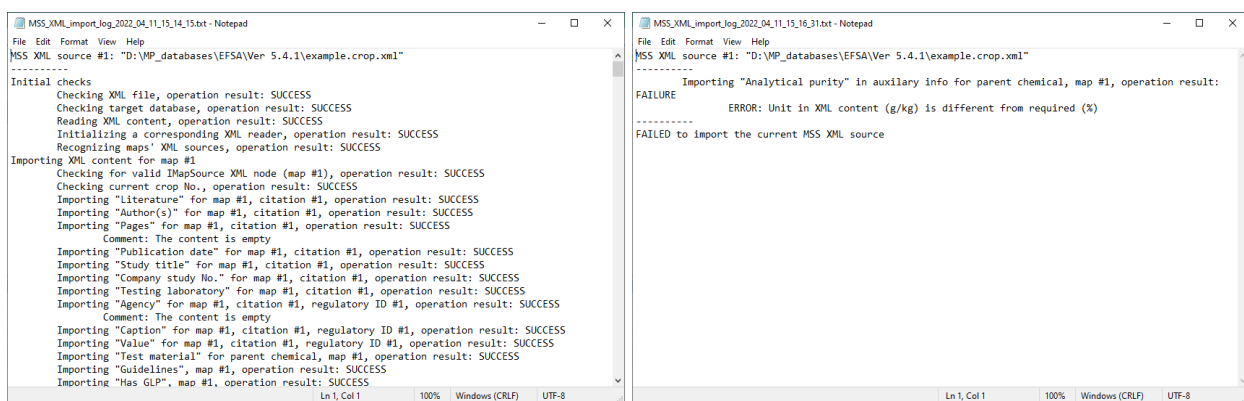- to skip the log reports.

Fig.2 – Detailed log report for a MSS XML file containing information for each data field being imported (left) and short log report for the same file containing only import errors (right)

The user comments for tables "III B. Extraction, Characterization, and Distribution of Residues" and "III D. Identity of Residues" from section "III. Results and Discussion" are saved as footnotes in the corresponding tables (Fig.3).

Distribution of the Parent and the Metabolites in Plant Matrices when Dosed with 14C-labeled Penconazole .

Metabolite Fraction	Leaves 7 DALA		Fruits 7 DALA		Foliage 40 DALA		Green tomatoes 40 DALA		Mature tomatoe
	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR
Total residues	-	2.7	-	0.034	-	0.424	-	0.001	-
Penconazole	-	0.22	-	0.005	-	LOD 0.001	-	LOD 0.001	-
Surface radioactivity	-	-	13.7	-	-	-	17.9	-	2.4
Penetrated radioactivity									
- extractable	99	-	84.1	-	103	-	82.1 (a)	-	97.5
- non-extractable	3.6	-	0.9	-	3.3	-	-	-	1.9
Total	103	-	98.7	-	107	-	100	-	102

- = not analysed
(a) extracable and non-extractable summarized
(b) results based on crude MeOH/water extract

Fig.3 – User comments saved as footnotes in the corresponding table

The display options for maps tree captions were expanded with data from plant/crop studies (Fig.4).
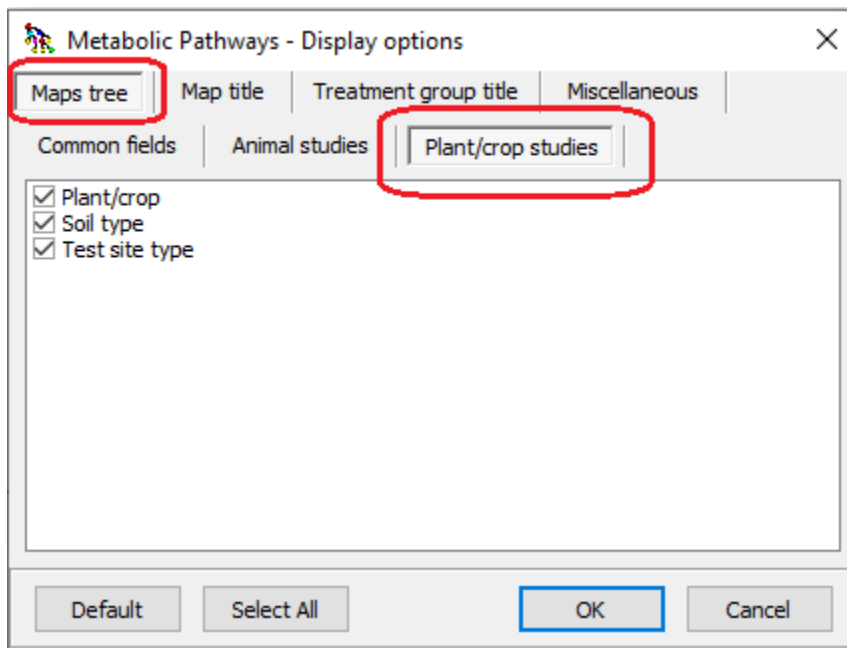

Fig.4 – Display options for maps tree captions – section for data from plant/crop studies

Modifications in the MSS Composers Suite

The updated **MSS Composers** package includes:

- MSS Livestock Composer 1.12
- MSS Plants Composer 1.12
- MSS Crops Composer 1.12
- DocBuilder 1.11

The following modifications in the above components have been made:

1. Fixed saving/loading of text for Experimental Conditions in section Materials and Methods → Study Design (Plants and Crops composers)
2. Restored field for Quantitation in section Results and Discussion → A. Total Radioactive Residues for Ruminants and Other (Livestock composer)
3. Added field restrictions labeling for all directly editable fields (all composers, details below)
4. Extended the predefined number of columns per radiolabel in tables in sections Results and Discussion → B and Results and Discussion D (all composers)
5. Replaced the 3 fixed flowchart attachment modules in section Materials and Methods → Study Design → Extraction and Analysis with a module for attaching multiple images
6. Fixed an issue that prevented the display of the currently loaded document in the document title (Plants and Crops composers)

Field restrictions labeling:

To inform users about the expected format of the entered data, a new feature has been implemented. Clicking in a text field (single line, multi line or table cell) triggers a notification mechanism which displays any restrictions (imposed by the underlying database format in MetaPath) for the current control. The information is displayed in a notification bar above the data entry sections.

Examples:
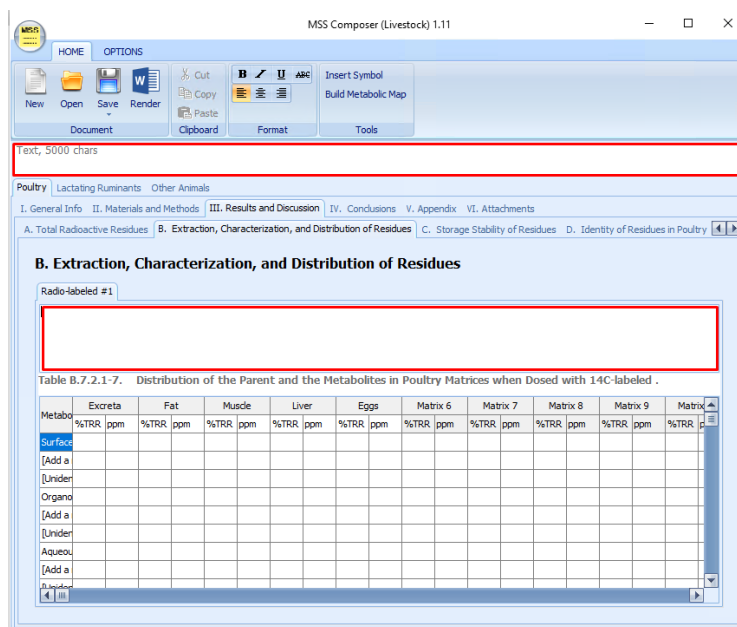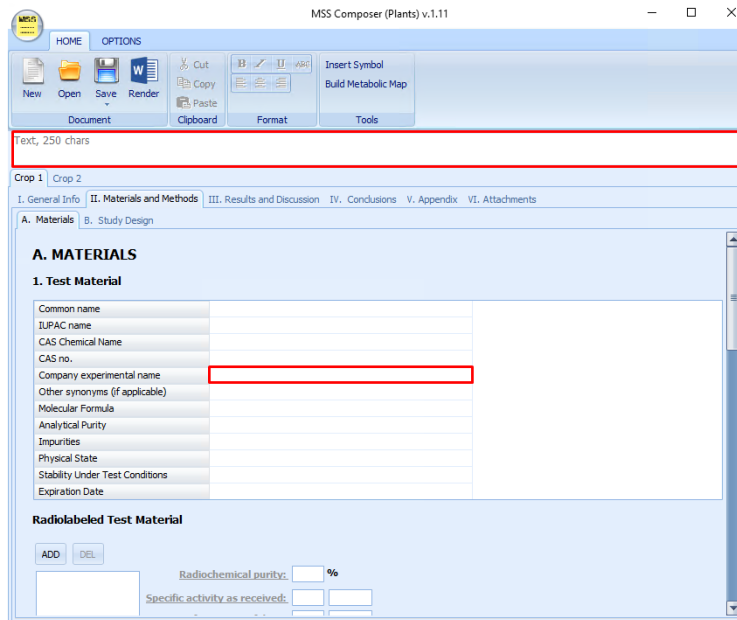
The displayed information corresponds to any constrains imposed by the MetaPath database. User input in the Composers is not limited and users can enter data that does not conform to the specifications. Files that contain such data can still be saved/load in the Composers and can be used for Word Document rendering.

XML schemas:

In order to implement the requested ability to attach multiple flowcharts in section Materials and Methods → Study Design → Extraction and Analysis (p. 5 above), the XML schemas for both Livestock and Plants/Crops had to be updated. The updated consists of:

Added a new element under Materials and Methods → Study Design → Extraction and Analysis called Flowcharts with the following structure:

```
<xs:element name="Flowcharts" type="TAttachment" minOccurs="0" maxOccurs="unbounded"/>
```

Existing elements (Flowchart, Flowchart2, Flowchart3) have been kept in order to ensure backwards compatibility.