

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).

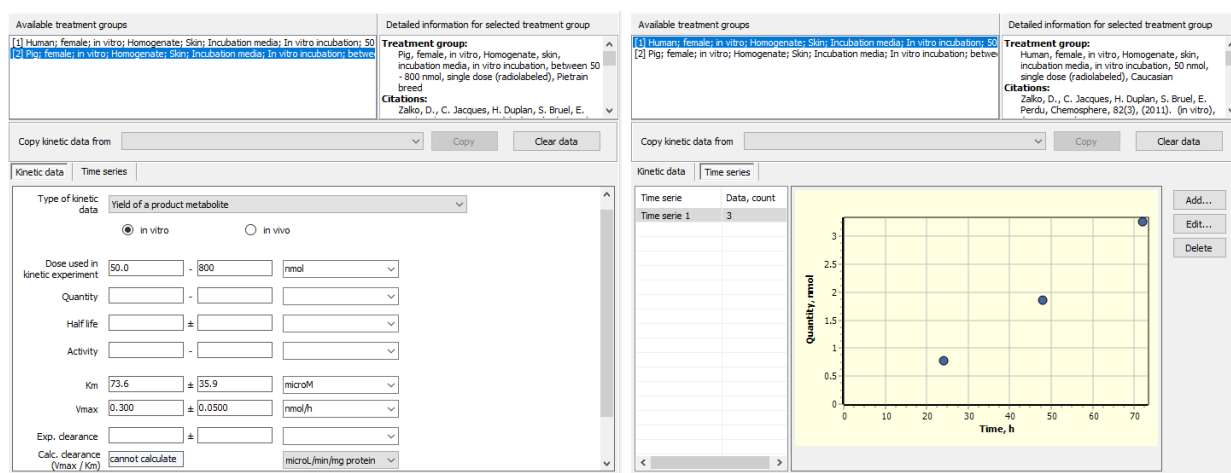


Fig.1 – Numerical values associated with treatment group #2 (pig) on the left, and a time series associated with treatment group #1 (human) on the right, for same chemical

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.

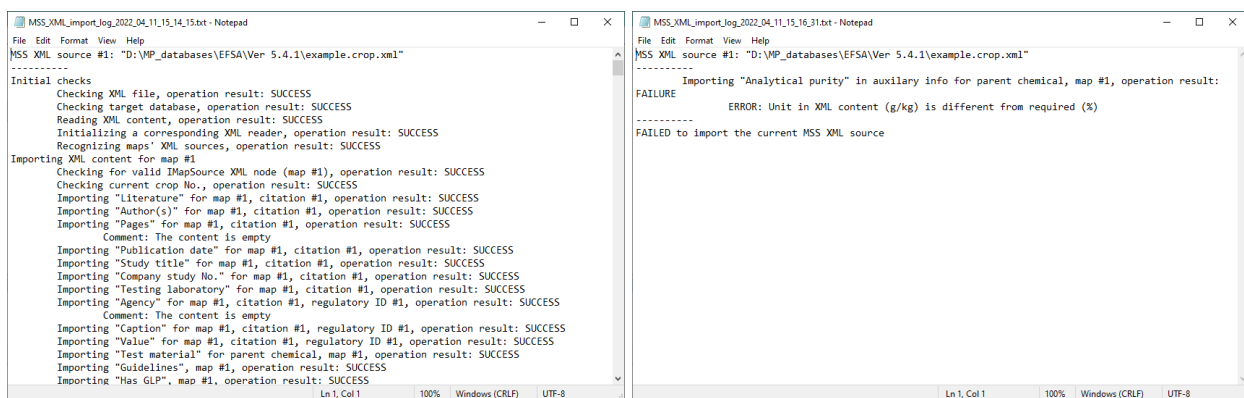


Fig.2 – Detailed log report for a MSS XML file containing information for each data field being imported (left) and short log report for the same file containing only import errors (right)

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).

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:

MSS Composer (Plants) v.1.11

HOME OPTIONS

New Open Save Render Cut Copy Paste Format Tools

Document Clipboard Insert Symbol Build Metabolic Map

Text, 250 chars

Crop 1 Crop 2

I. General Info II. Materials and Methods III. Results and Discussion IV. Conclusions V. Appendix VI. Attachments

A. Materials B. Study Design

A. MATERIALS

1. Test Material

Common name
IUPAC name
CAS Chemical Name
CAS no.
Company experimental name
Other synonyms (if applicable)
Molecular Formula
Analytical Purity
Impurities
Physical State
Stability Under Test Conditions
Expiration Date

Radiolabeled Test Material

ADD DEL

Radiochemical purity: %
Specific activity as received:

MSS Composer (Livestock) 1.11

HOME OPTIONS

New Open Save Render Cut Copy Paste Format Tools

Document Clipboard Insert Symbol Build Metabolic Map

Text, 5000 chars

Poultry Lactating Ruminants Other Animals

I. General Info II. Materials and Methods III. Results and Discussion IV. Conclusions V. Appendix VI. Attachments

A. Total Radioactive Residues B. Extraction, Characterization, and Distribution of Residues C. Storage Stability of Residues D. Identity of Residues in Poultry

B. Extraction, Characterization, and Distribution of Residues

Radio-labeled #1

Table B.7.2.1-7. Distribution of the Parent and the Metabolites in Poultry Matrices when Dosed with ¹⁴C-labeled .

Metabo	Excreta	Fat	Muscle	Liver	Eggs	Matrix 6	Matrix 7	Matrix 8	Matrix 9	Matrix 10
	%TRR ppm	%TRR ppm	%TRR ppm	%TRR ppm	%TRR ppm	%TRR ppm	%TRR ppm	%TRR ppm	%TRR ppm	%TRR ppm
Surface										
[Add a]										
[Under]										
Organic										
[Add a]										
[Under]										
Aqueous										
[Add a]										
[Under]										

The displayed information corresponds to any constraints 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.