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WEBINAR: METAPATH

How to complete MSS composers for pesticides metabolism studies

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Let's start

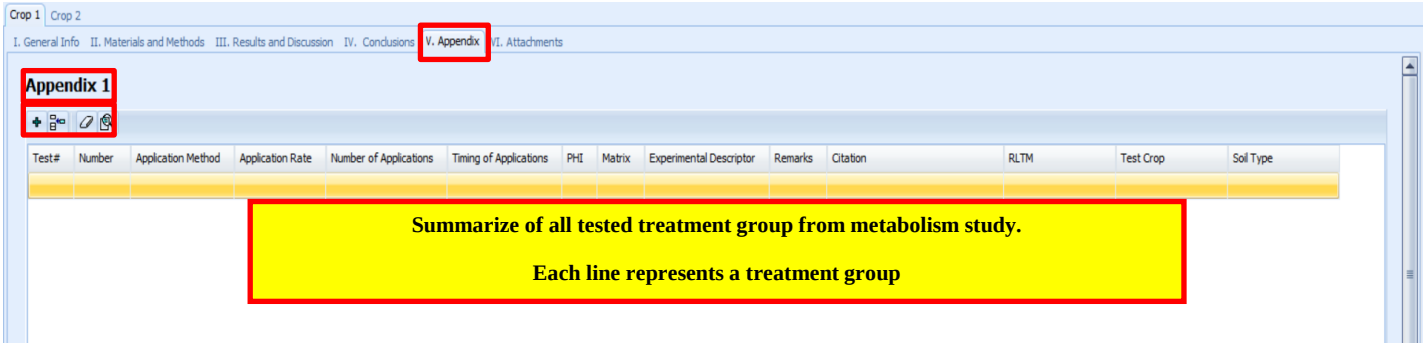
Monday 29 March

TIME	ITEM
09:30 – 09:45	Introduction & presentation of the project
09:45 – 10:00	Opening MSS
10:00 – 10:35	General Info tab
10:35 – 11:30	Materials
11:30 – 11:45	Coffee Break
11:45 – 12:30	Results tables part 1
12:30 – 14:00	Lunch Break
14:00 – 14:45	Results tables part 2
14:45 – 15:30	**Appendix**
15:30 – 15:45	Coffee break
15:45 – 16:15	Attachment / Render / Conclusion
16:15 – 17:00	Key points Q&A

Theory
Live Session
Summary KP
QA

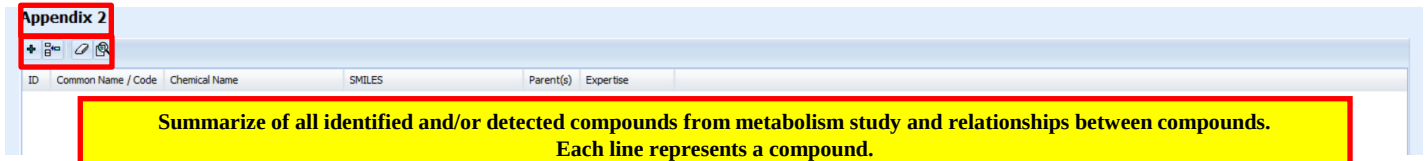
Plant MSS composer : Appendices

Appendices

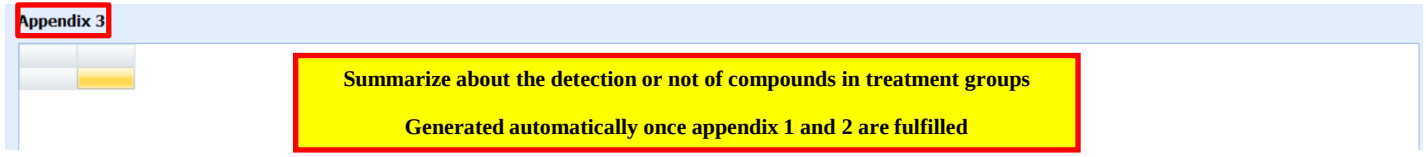


Summarize of all tested treatment group from metabolism study.

Each line represents a treatment group



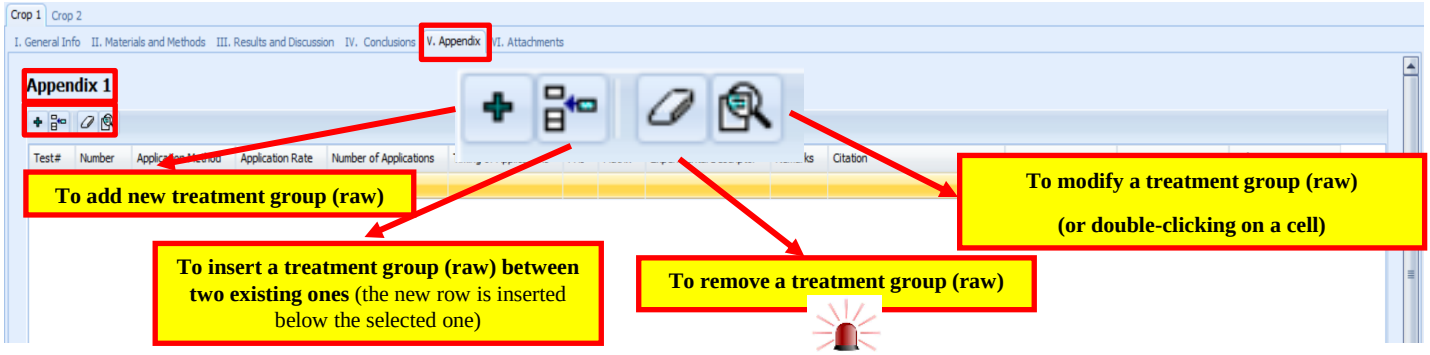
Summarize of all identified and/or detected compounds from metabolism study and relationships between compounds.
Each line represents a compound.
ALWAYS begin with parent compound and carry on with metabolites.



Summarize about the detection or not of compounds in treatment groups

Generated automatically once appendix 1 and 2 are fulfilled

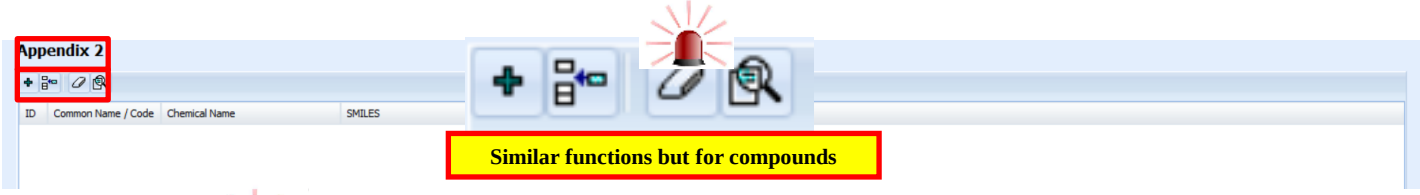
Appendices



NEVE

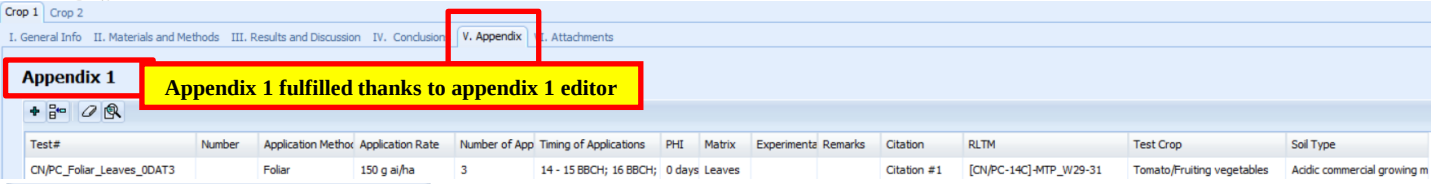
PROBLEM fixed in last MSS version

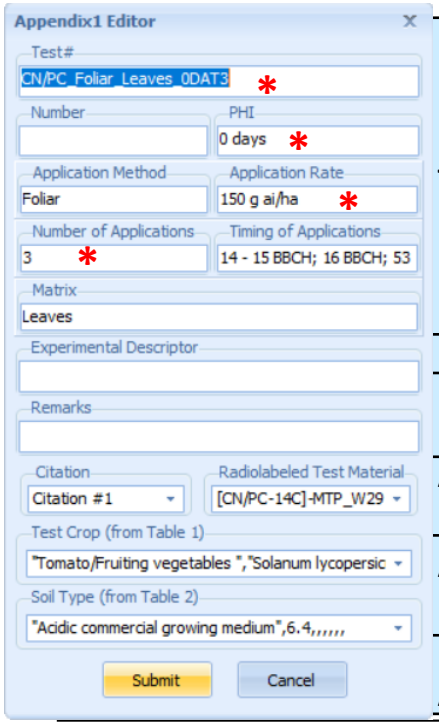
MSS xml file into MetaPath database



TO BE NOTED: “Remove” or “delete” compounds function operational

Appendices

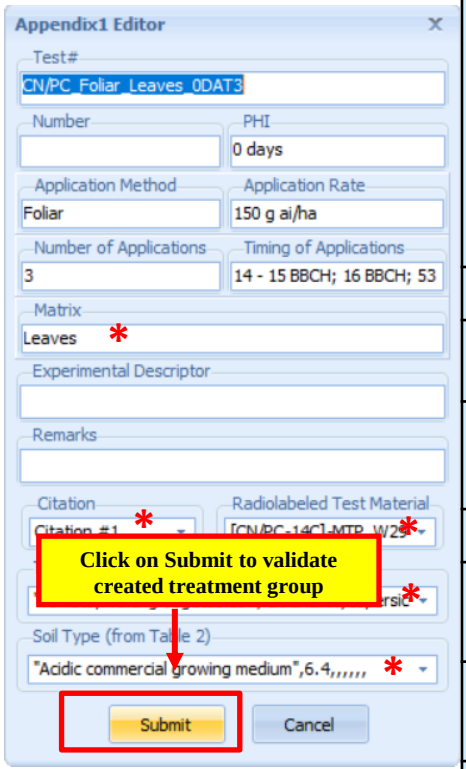




Test# *	→ Treatment group should be named briefly but unambiguously so that they can be easily distinguished 1. first letters of the labelling (mandatory) 2. portion analysed (mandatory) 3. dose applied (optional) 4. PHI (optional) … → Information separated from the next with an underscore (_)
Number	→ number of plants by radiolabelled test material
PHI *	The value must be separated from the unit by a space
Application Method	Type of application
Application Rate *	The dose rate must be separated from the unit by a space
Number of Applications *	Value

*: field must be filled in to allow importation of the MSS xml file into MetaPath

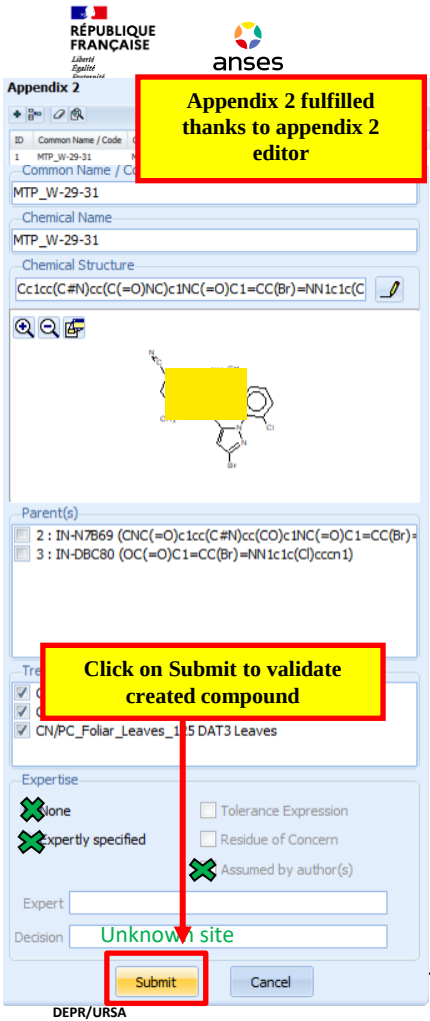
Appendices



Timing of Applications	Growth stage values or if no information, field with **0 : N/A or 0 : description of the stage** **For growth stage values :** hyphens to be bounded by space characters for a BBCH range (xx – yy BBCH) Information must start with figures followed by a space
Matrix *	Matrix name
Experimental Descriptor	
Remarks	Free-text field to explain terms and abbreviations or give some additional information
Citation *	Select corresponding citation, radiolabelled test material, test crop and soil type
Radiolabeled Test Material *	
Test Crop (from Table 1) *	
Soil type (from Table 2) *	

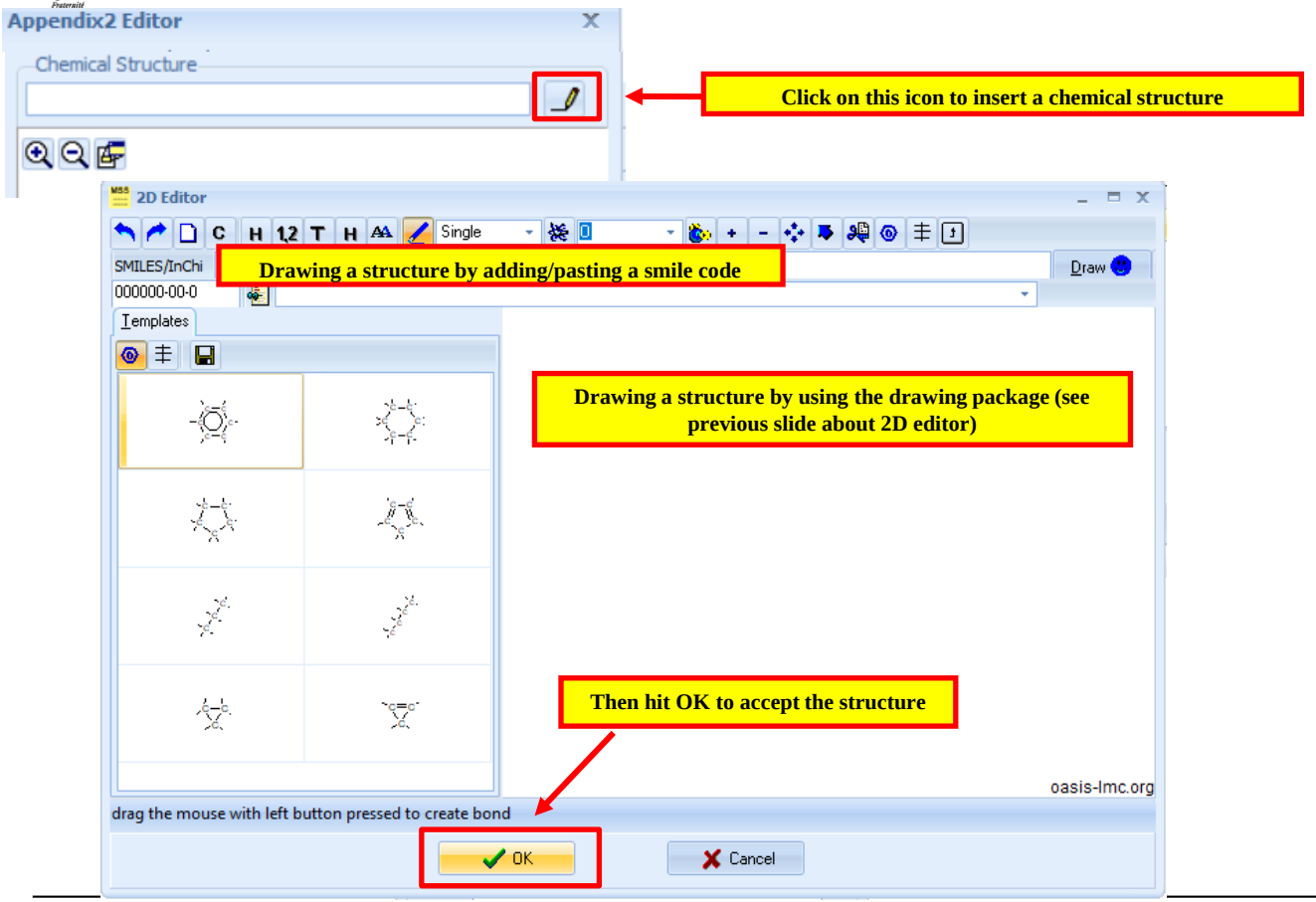
*: field must be filled in to allow importation of the MSS xml file into MetaPath

Appendices



Common Name/Code	**common name / company experimental name**
Chemical Name	**common name** (**company experimental name**) Do not write down the full chemical name of the molecules
Parents	Describe **relationship(s) between compounds** by ticking the box(es) that correspond(s) to **compound(s) from which the metabolite can be generated.** Relationships specified for all metabolites, except parent compound. *N.B.: The metabolic pathway is built based on the information encoded in this field.*
Treatment Groups	Tick the box(es) that correspond(s) to matrix(ces) in which the compound has been identified.
Expertise	If **no issue** drawing the compound , select "**None**" Select "**Expertly specified**" and "**Assumed by author(s)**" for compounds that were not identified in the study but are assumed intermediates between identified metabolites. In case of **uncertainties** while drawing a compound (e.g.: position of a chemical group not clearly determined), select **"Expertly specified**" and specify in the "**Decision**" field which assumptions were made when drawing the compound (e.g.: Unknown site of conjugation)

Appendices


Appendix2 Editor
Chemical Structure
Click on this icon to insert a chemical structure
2D Editor
Single
SMILES/InChi
Draw
000000-00-0
Drawing a structure by adding/pasting a smile code
Templates
Drawing a structure by using the drawing package (see previous slide about 2D editor)
Then hit OK to accept the structure
oasis-lmc.org
drag the mouse with left button pressed to create bond
OK
Cancel

Appendices

Appendix 3

	CN/PC_Foli	CN/PC_Foli	CN/PC_Foli
MTP_W-29-31	linked	linked	linked
IN-N7B69	linked	linked	linked
IN-DBC80	linked	linked	

This table is <u>filled in automatically</u> using the information available in Appendix 1 and 2.

You can link and unlink matrices and compounds by right-clicking in the cells. This can also be done by scrolling **but it is very sensitive**.

Recommendation:
we strongly recommend updating this table using the "Treatment group" fields of Appendix 2.

Plant MSS composer: Appendix

Live Session