



**RÉPUBLIQUE
FRANÇAISE**

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WEBINAR: METAPATH

How to complete MSS composers for pesticides metabolism studies

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

Crop 1 Crop 2

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

Appendix 1



Test#	Number	Application Method	Application Rate	Number of Applications	Timing of Applications	PHI	Matrix	Experimental Descriptor	Remarks	Citation	RLTM	Test Crop	Soil Type
Summarize of all tested treatment group from metabolism study. Each line represents a treatment group													

Appendix 2



ID	Common Name / Code	Chemical Name	SMILES	Parent(s)	Expertise
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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.

Appendix 3

Summarize about the detection or not of compounds in treatment groups
Generated automatically once appendix 1 and 2 are fulfilled

Appendices

Crop 1 Crop 2

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

Appendix 1

To add new treatment group (raw)

To insert a treatment group (raw) between two existing ones (the new row is inserted below the selected one)

To remove a treatment group (raw)

To modify a treatment group (raw) (or double-clicking on a cell)



NEVER



PROBLEM fixed in last MSS version
MSS xml file into MetaPath database

Appendix 2

Similar functions but for compounds



TO BE NOTED: "Remove" or "delete" compounds function operational

Appendices

Crop 1 | Crop 2

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

Appendix 1

Appendix 1 fulfilled thanks to appendix 1 editor

Test#	Number	Application Method	Application Rate	Number of App	Timing of Applications	PHI	Matrix	Experiments	Remarks	Citation	RLTM	Test Crop	Soil Type
CN/PC_Foliar_Leaves_0DAT3		Foliar	150 g ai/ha	3	14 - 15 BBCH; 16 BBCH;	0 days	Leaves			Citation #1	[CN/PC-14C]-MTP_W29-31	Tomato/Fruiting vegetables	Acidic commercial growing

Appendix1 Editor

Test#

CN/PC_Foliar_Leaves_0DAT3 *

Number

PHI

0 days *

Application Method

Foliar

Application Rate

150 g ai/ha *

Number of Applications

3 *

Timing of Applications

14 - 15 BBCH; 16 BBCH; 53

Matrix

Leaves

Experimental Descriptor

Remarks

Citation

Citation #1

Radiolabeled Test Material

[CN/PC-14C]-MTP_W29



Test Crop (from Table 1)

"Tomato/Fruiting vegetables", "Solanum lycopersic"


Soil Type (from Table 2)

"Acidic commercial growing medium", "6.4,....."

Submit Cancel

Test# *	<p>→ Treatment group should be named briefly but unambiguously so that they can be easily distinguished</p> <ol style="list-style-type: none"> 1. first letters of the labelling (mandatory) 2. portion analysed (mandatory) 3. dose applied (optional) 4. PHI (optional) ... <p>→ Information separated from the next with an underscore (_)</p>
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

Appendices

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

Appendix 2

Appendix 2 fulfilled
thanks to appendix 2
editor

Common Name / Code

1 MTP_W-29-31
Common Name / Code

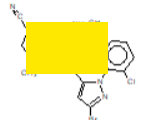
MTP_W-29-31

Chemical Name

MTP_W-29-31

Chemical Structure

Cc1cc(C#N)cc(C(=O)NC)C1NC(=O)C1=CC(Br)=NN1c1c(C)



Parent(s)

2 : IN-N7B69 (CNC(=O)c1cc(C#N)cc(CO)c1NC(=O)C1=CC(Br)=NN1c1c(C)ccn1)

3 : IN-DBC80 (OC(=O)C1=CC(Br)=NN1c1c(C)ccn1)

Click on Submit to validate
created compound

Expertise

None Tolerance Expression

Expertly specified Residue of Concern

Assumed by author(s)

Expert:

Decision:

Submit Cancel

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

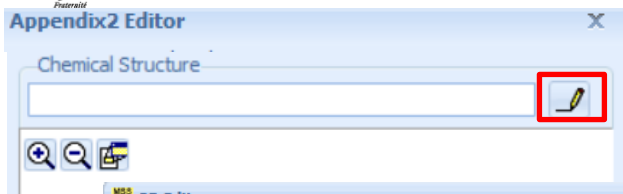
Tick the box(es) that correspond(s) to matrix(ces) in which the compound has been identified.

Expertise

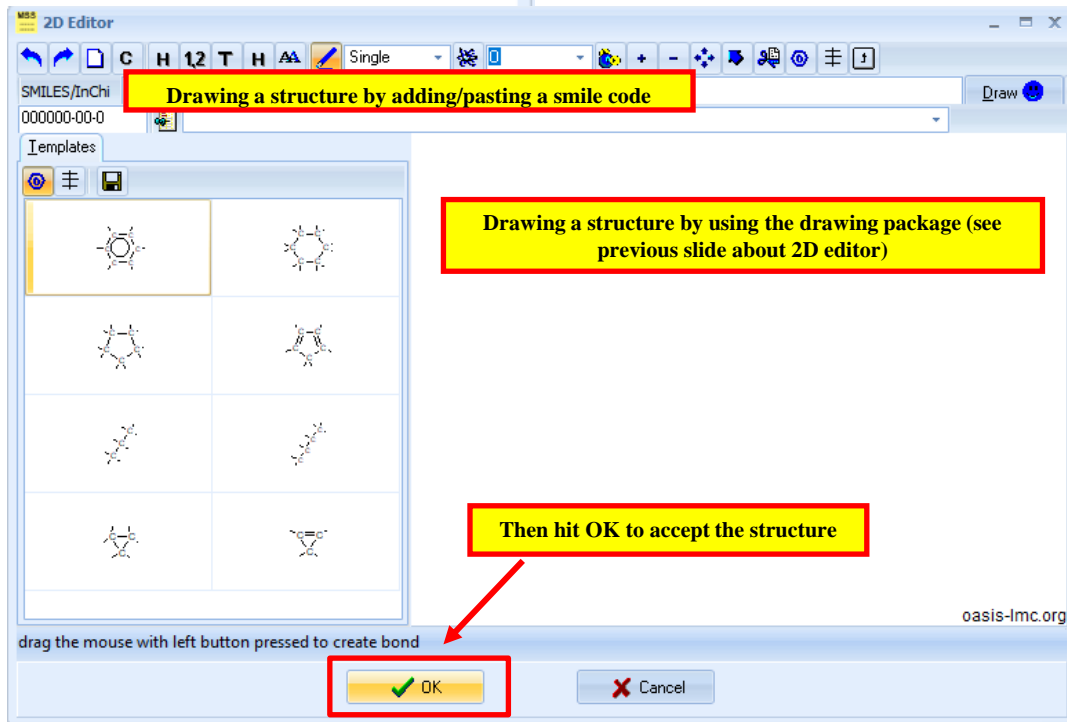
If **no issue** drawing the compound, select "**None**"
Select "**Expertly specified**" and "**Assumed by author(s)**" for
compounds that were not identified in the study but are assumed
intermediates between identified metabolites.

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



Click on this icon to insert a chemical structure



Drawing a structure by adding/pasting a smile code

Drawing a structure by using the drawing package (see previous slide about 2D editor)

Then hit OK to accept the structure

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 filled in automatically 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