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FRANÇAISE**

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WEBINAR: METAPATH

How to complete MSS composers for pesticides metabolism studies

-

Plant metabolism studies

Let's start

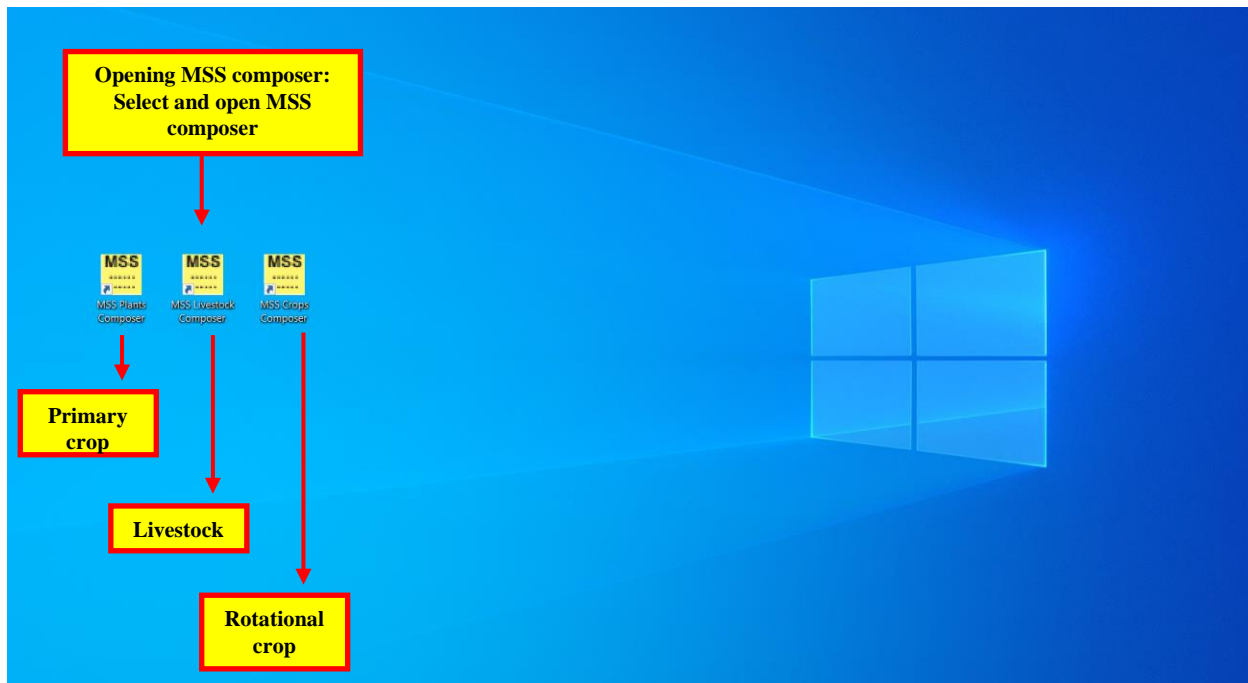
Monday 29 March

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 : Opening

Opening MSS



Opening MSS

The screenshot shows the MSS Composer interface. The top menu bar includes 'HOME' and 'OPTIONS'. Below the menu bar is a toolbar with buttons for 'New', 'Open', 'Save', and 'Render'. The 'Options' tab is highlighted. The main window displays a form for entering study information, including 'Study Title' and 'Reference Type'. A red bell icon is visible in the bottom left corner of the form.

Annotations:

- Spell Check feature found under the Options Tab**: Points to the 'OPTIONS' tab in the menu bar.
- To open a new file – will clear all fields**: Points to the 'New' button in the toolbar.
- Icon – to open a previously saved .XML file for editing or to continue work**: Points to the 'Open' button in the toolbar.
- Icon – used to save file or save file as from populated Composer as an .XML**: Points to the 'Save' button in the toolbar.
- Icon – used to generate a Study Summary in the form of a WORD document**: Points to the 'Render' button in the toolbar.

Warnings:

- WARNING:**
Save your file regularly because MSS xml files are not automatically saved when quitting the program
- WARNING:**
To enter decimal numbers, use the point "." (not the comma ",")
- WARNING:**
if you encounter an anomaly while coding on the MSS Composer, the anomaly will be passed on to other MSS xml files if these are opened at the same time

Opening MSS

The sequence of screenshots illustrates the process of opening the MSS (Microsoft Spelling) interface:

- Top Screenshot:** Shows the main application window with a menu bar (HOME, OPTIONS) and buttons for 'SpellCheck Options' and 'Manage Ids'. A red box highlights the 'SpellCheck Options' button.
- Second Screenshot:** The 'Spelling Options' dialog is open, showing the 'Spelling' tab. It contains sections for 'General options' (with checkboxes for showing errors, automatic correction, and flagging repeated words) and 'When checking spelling ignore:' (with checkboxes for uppercase, numbers, markup languages, internet addresses, and abbreviations).
- Third Screenshot:** The 'Spelling Options' dialog is open, showing the 'Language' tab. It includes 'Language settings' (a dropdown menu set to 'English') and 'Additional dictionaries' (a list of dictionaries with checkboxes, where 'Autocorrect.adu' is selected).
- Bottom Screenshot:** The 'Spelling Options' dialog is open, showing the 'Custom Dictionary' tab. It includes a section for 'Edit custom dictionary' (with a dropdown menu set to 'v.vallant.edu') and a section for 'Modify the contents of this custom dictionary' (with an 'Add' button and a list of words).

Opening MSS

MSS Composer (Plants) v.1.8

HOME OPTIONS

SpellCheck Options Manage Ids

SpellChecker Regulatory...

Crop 1 Crop 2

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

B.7.1 Metabolism, distribution and expression of residues in plants (Annex IIA 6.2.1)

References:

ADD DEL

Author(s): MRID
PMRA
Date: Other
Study Titles: PC Code
Reference Types: PARAM
Testing Laboratory:
Company Study Number:
Identifiers:

Test Material:

Identifiers:

Guidelines: EPA QCSPP Harmonized Test Guidelin
OECD Guideline 503 Metabolism in Liv

GLP:

Regulatory Identifiers

Add Update Delete

Identifier

Caption Agency
MRID US EPA

Description
Master Record Identification Number

☒ Show in Citations ☐ Show in General Info

OK Cancel

Add, update or delete Regulatory identifiers

Details on caption, agency and description

Opening MSS

MSS Composer (Plants) v1.8

HOME OPTIONS

New Open Save Render
Document

Cut Copy Paste
Clipboard

B U ABC
Format

Insert Symbol
Build Metabolic Map
Tools

Crop 1 Crop 2

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

B.7.1 Metabolism, distribution and expression of residues in plants (Annex IIA 6.2.1)

References:

ADD DEL

Citation #1

Author(s): MacAnom, X

Date: July 12 1998 **Pages:** 148

Study Title: The metabolism of [¹⁴C]MTP_WB-29-31 in tomatoes

Reference Type: IIA, 6.2.1/03

Testing Laboratory: XXX Laboratories, Somewhere

Company Study Number: Unknown-16985

Identifiers: EDIT

Test Material:

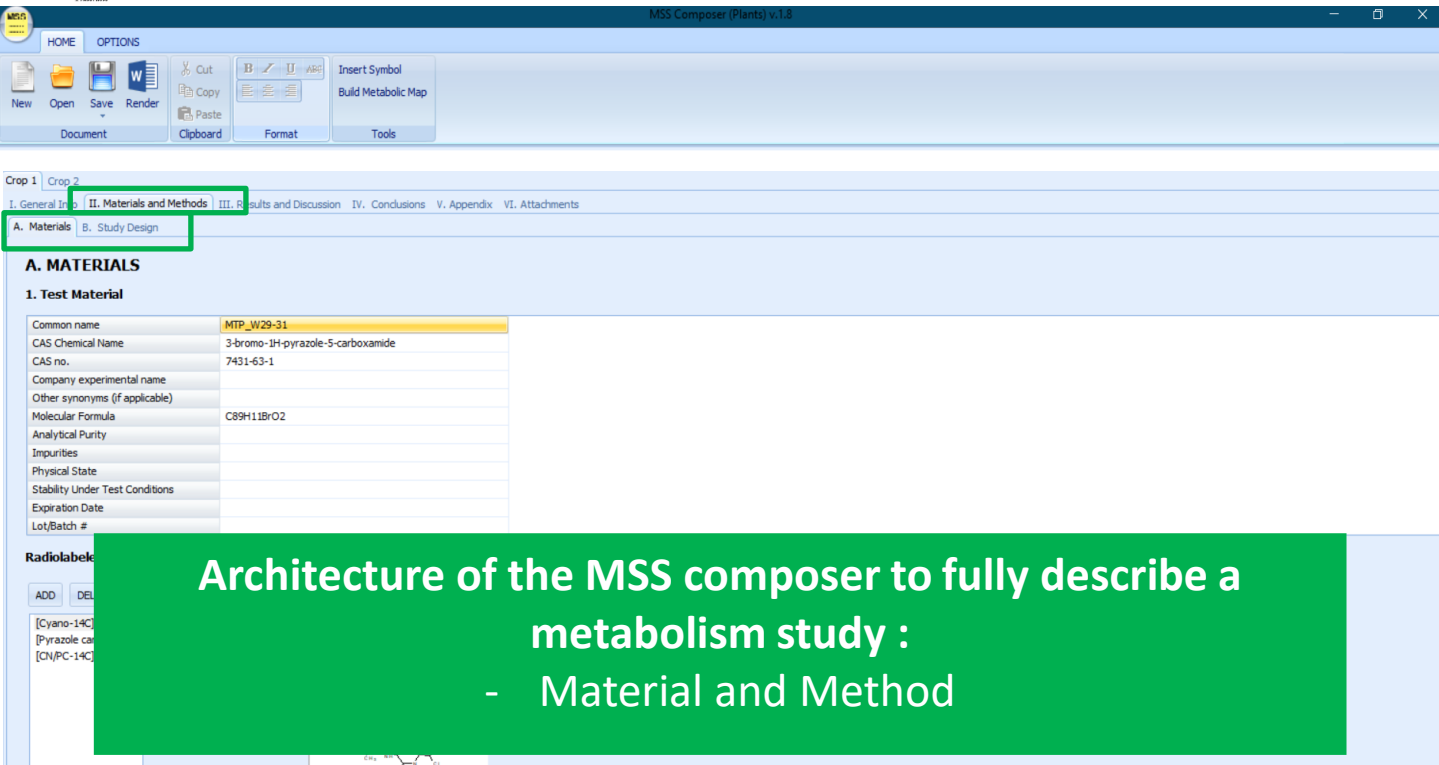
Identifiers:

Guidelines:

Architecture of the MSS composer to fully describe a metabolism study :

- General Information

Opening MSS



MSS Composer (Plants) v1.8

HOME OPTIONS

New Open Save Render Document Clipboard Format Tools

Crop 1 Crop 2

I. General Information 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	MTP_W29-31
CAS Chemical Name	3-bromo-1H-pyrazole-5-carboxamide
CAS no.	7431-63-1
Company experimental name	
Other synonyms (if applicable)	
Molecular Formula	C8H11BrO2
Analytical Purity	
Impurities	
Physical State	
Stability Under Test Conditions	
Expiration Date	
Lot/Batch #	

Radiolabels

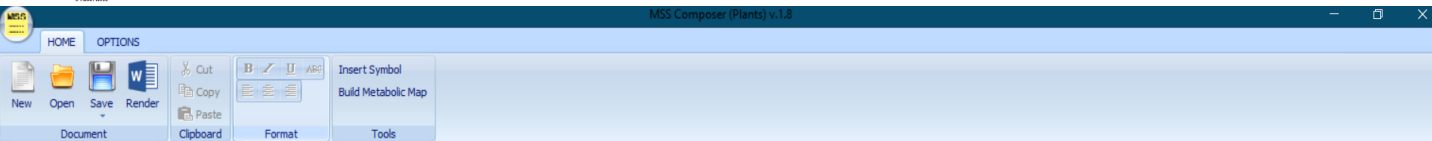
ADD DEL

[Cyano-14C]
[Pyrazole car
[CN/PC-14C]

Architecture of the MSS composer to fully describe a metabolism study :

- Material and Method

Opening MSS



Crop 1 Crop 2

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 Crop E. Proposed Metabolic Pathway

A. Total Radioactive Residues

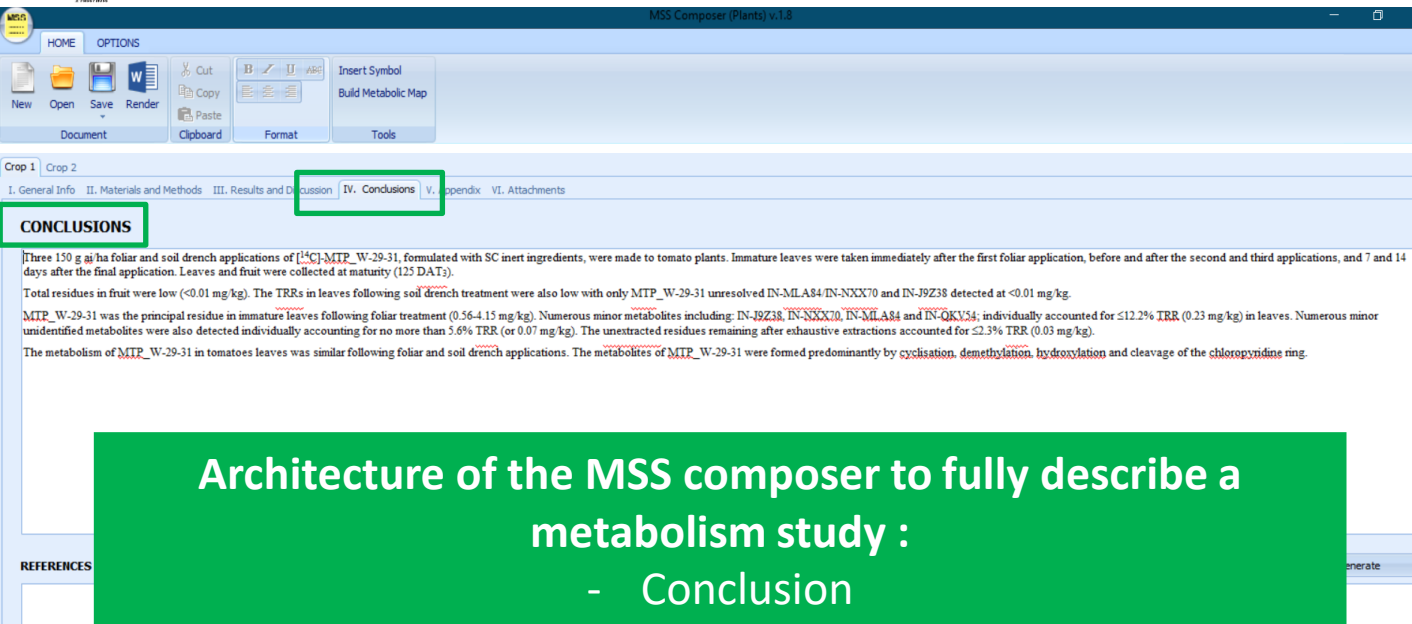
Extraction efficiency of radioactive residues from plant metabolism study using residue enforcement method

	Recovered equivalents (mg/kg)	Overall extraction efficiency (%)	Defined residue (mg/kg)	Defined residue extraction efficiency (%)
Enforcement method				
Extraction method used in study		100		100

Architecture of the MSS composer to fully describe a metabolism study :

- Results and discussion

Opening MSS



MSS Composer (Plants) v1.8

HOME OPTIONS

New Open Save Render

Document

Cut Copy Paste

Clipboard

Format

Insert Symbol

Build Metabolic Map

Tools

Crop 1 Crop 2

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

CONCLUSIONS

Three 150 g ai/ha foliar and soil drench applications of [¹⁴C]-MTP_W-29-31, formulated with SC inert ingredients, were made to tomato plants. Immature leaves were taken immediately after the first foliar application, before and after the second and third applications, and 7 and 14 days after the final application. Leaves and fruit were collected at maturity (125 DAT₂).

Total residues in fruit were low (<0.01 mg/kg). The TRRs in leaves following soil drench treatment were also low with only MTP_W-29-31 unresolved IN-MLA84/IN-NXX70 and IN-J9Z38 detected at <0.01 mg/kg.

MTP_W-29-31 was the principal residue in immature leaves following foliar treatment (0.56-4.15 mg/kg). Numerous minor metabolites including: IN-J9Z38, IN-NXX70, IN-MLA84 and IN-OKV54; individually accounted for ≤12.2% TRR (0.23 mg/kg) in leaves. Numerous minor unidentified metabolites were also detected individually accounting for no more than 5.6% TRR (or 0.07 mg/kg). The unextracted residues remaining after exhaustive extractions accounted for ≤2.3% TRR (0.03 mg/kg).

The metabolism of MTP_W-29-31 in tomatoes leaves was similar following foliar and soil drench applications. The metabolites of MTP_W-29-31 were formed predominantly by cyclization, demethylation, hydroxylation and cleavage of the chloropyridine ring.

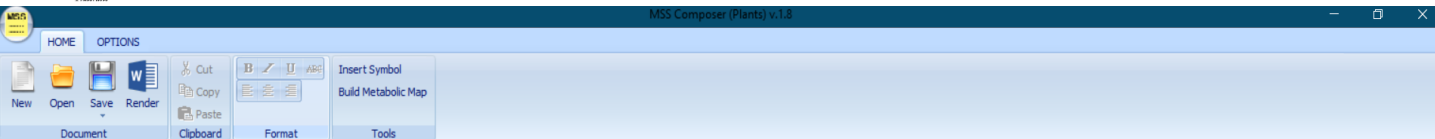
REFERENCES

generate

Architecture of the MSS composer to fully describe a metabolism study :

- Conclusion

Opening MSS



Crop 1 Crop 2

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

V. Appendix

Appendix 1



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 m
CN/PC_Foliar_Leaves_14 DAT3		Foliar	150 g ai/ha	3	14 - 15 BBCH; 16 BBCH; 14 day	Leaves				Citation #1	[CN/PC-14C]-MTP_W29-31	Tomato/Fruiting vegetables	Acidic commercial growing m
CN/PC_Foliar_Leaves_125 DAT3		Foliar	150 g ai/ha	3	14 - 15 BBCH; 16 BBCH; 125 da	Leaves				Citation #1	[CN/PC-14C]-MTP_W29-31	Tomato/Fruiting vegetables	Acidic commercial growing m

Appendix 2



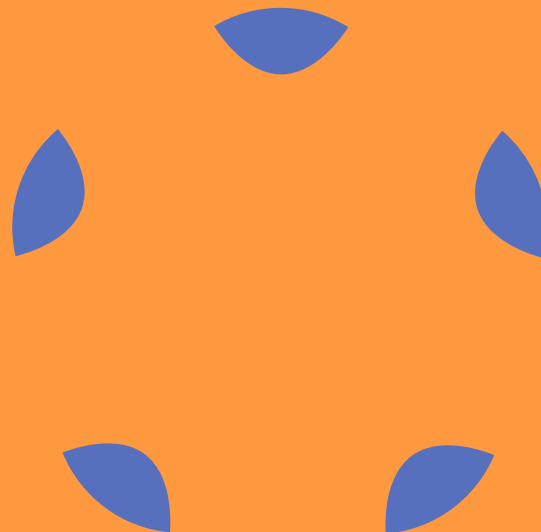
ID	Common Name / Code	Chemical Name	SMILES	Parent(s)	Expertise
1	MTP_W-29-31	MTP_W-29-31	Cc1cc(C#N)cc(C(=O)NC(=O)...		
2	IN-N7B69	IN-N7B69	CNC(=O)c1cc(C#N)cc(CO)C1NC(=...	1	
3	IN-D6C80	IN-D6C80	OC(=O)C1=CC(Br)=NN1c1c(C)cc...	1	

Architecture of the MSS composer to fully describe a metabolism study :

- Appendices

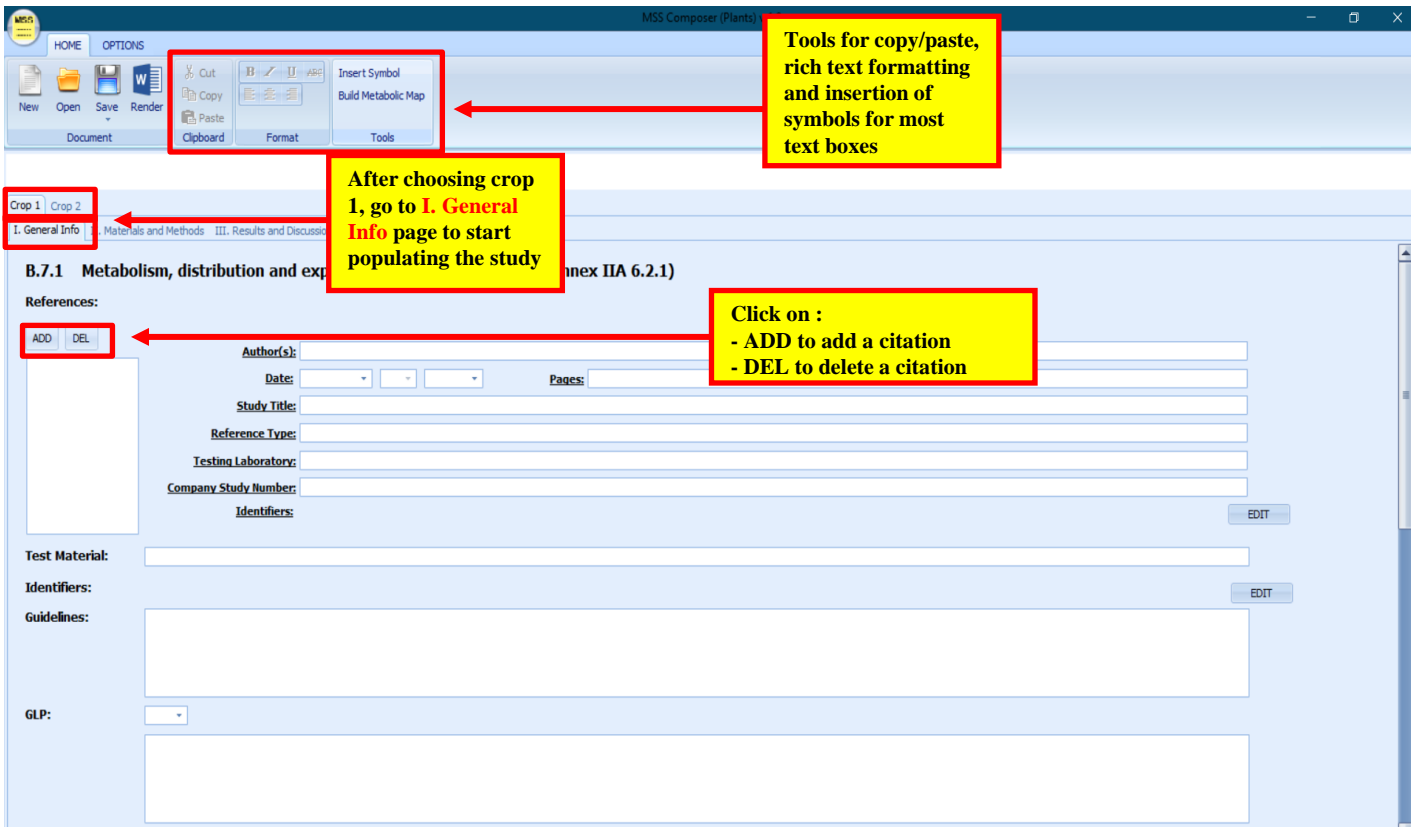
Plant MSS composer : Opening

Live Session



Plant MSS composer: General Info





General info

Filling in pertinent information by mouse-clicking within the boxed areas:

- Copying/pasting possible
- Limited number of characters

Crop 1 Crop 2

I. General Info II. Materials and Methods III. Results and Discussion

B.7.1 Metabolism, distribution and expression of residues in plants (Annex IIA 6.2.1)

References:

ADD DEL

Citation #1

Author(s): MacAnom, X

Date: July 12 1998

Pages: 148

Study Title: The metabolism of [14C]MTP_WB-29-31 in tomatoes

Reference Type: IIA, 6.2.1/03

Testing Laboratory: XXX Laboratories, Somewhere

Company Study Number: Unknown-16985

Identifiers: MRID:XX-YYY-ZZZZ;

EDIT

Regulatory Identifiers

Available Identifiers

MRID
PMRA
Other

Identifier

MRID

Agency

US EPA

Description

Master
Record
Identification
Number

Selected Identifiers

Identifier	Value
MRID:XX-YYY-ZZZZ	

>

To add a new Id

<

To delete one Id

OK

Cancel

All the identifiers currently available in the ID library with its properties (Caption, Agency, Description)

Add a new identifier entry : select it and click on the arrow pointing right (>). Then, fill in the value field directly in the text box
Delete an identifier: select it and click on the arrow pointing left (<)

General info

Crop 1 Crop 2

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

B.7.1 Metabolism, distribution and expression of residues in plants (Annex IIA 6.2.1)

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

Test Material:

Common name of active substance + company experimental name if available (in parentheses)

Identifiers:

EDIT

Guidelines:

Free text

Limited number of characters

GLP:

yes

Select Yes or No

Free text

Limited number of characters

Acceptability:

The study is considered scientifically acceptable.

Select Is or Is Not

Free text

Limited number of characters

Evaluators:

Evaluator Name

Evaluator Affiliation

Evaluator 1

Evaluator 2

Evaluator 3

Person/entity who prepares MSS composer

Person/entity who validates MSS composer

Entity who prepares MSS composer

Entity who validates MSS composer

BACKGROUND INFORMATION

Free text

Limited number of characters

Project, in co-operation between UK CRD as Rapporteur Member State for the EU and the Regulatory Authorities of the French ANSES (who are also co-evaluators) and the Australian APVMA. The evaluation of the MTP W29-31 dossier (hazard evaluation) was shared between these regulatory authorities.

General info

Crop 1 Crop 2

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

B.7.1 Metabolism, distribution and expression of residues in plants (Annex IIA 6.2.1)

Product Type:

Pesticide function : Free text + Limited number of characters

Product Use:

Use description: Free text + Limited number of characters

EXECUTIVE SUMMARY

Executive summary for metabolism study : Free text + Limited number of characters

en used during the study. Each was formulated with inert ingredients as a suspension concentrate (7 MBq/mg), as active ingredients for soil treatment. A mix of both these substances was used for foliar treatment (with a ratio of 1:1.003 regarding activity so that the specific activity is 0.59 MBq/mg). One to three 150 g ai/ha applications were made to tomatoes *via* foliar or soil drench application. Foliar applications were made to plants 3 weeks post-emergence (BBCH 14-15) and at 7 (BBCH 16) and 14 days (BBCH 53, 61) after the initial application. Soil drench applications were made 7 weeks post-emergence application (BBCH 19, 51) and 7 (BBCH 51) and 14 days (BBCH 55, 61) after the first application.

Plant MSS composer:

General Info

Live Session

Plant MSS composer : Opening – General info

QA Session