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WEBINAR: METAPATH

How to complete MSS composers for pesticides metabolism studies

1ST DAY WEBINAR PROGRAM

I. Introduction & presentation of the project

II. Opening MSS

III. General Info tab

IV. Materials & Methods

Coffee break

V. Results tables (part 1)

Lunch break (until 14 h)

VI. Results tables (part 2)

VII. Appendixes

Coffee break

VIII. Attachment , Render & Conclusion

IX. Key points / Q&A

VI. Results and discussion (part 2)

Storage stability of residues and Identity of Residues in crops

III. Results and Discussion- C. Storage Stability of Residues

MSS Composer (Plants) v.1.8

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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

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

C. Storage Stability of Residues

Plant samples were stored frozen (ca -20°C) until they were taken for analysis. Following analysis, all samples were returned to storage at ca -20°C. To assess if storage at -20°C resulted in degradation of radioactive residues, a sub-sample of stored tissue (7 DATs, for the extractability of... and its metabolites. The residue composition remained unchanged... as the... unresolved IN-MLA84/IN-NXXX70, IN-K7H19, IN-DBC80, IN-QKV54 and numerous unidentified components. The result...

Frozen storage did not impact... (0.10 mg/kg) included IN-19Z38, atoes.

Box for narrative text to describe storage stability.

Table B.7.1.1-6. Summary of Storage Conditions.

Matrix (RAC or Extract)	Storage Temperature °C	Actual Storage Duration (Days or Months)	Interval of Demonstrated Storage Stability (specify crop/matrix if different) (days/months)
Leaf tissue	-20°C	392 days	392 days

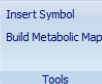
Population of table with the same editing features of other tables found within the Composer.

III. Results and Discussion- D. Identity of Residues in Crops

MSS Composer (Plants) v.1.8



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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

D. Identity of Residues in Crop

[Cyano-14C]-MTP_W29-31 [Pyrazole carbonyl-14C]-MTP_W29-31 [CN/PC-14C]-MTP_W29-31

MTP_W29-31 was the major component in leaves, decreasing from 95.3% TRR immediately after the first application to 61.1% TRR seven days later. Seven days after application, MTP_W29-31 accounted for 62.2% and 43.4% of the total TRR, respectively. IN-J9Z38, IN-K7H19, IN-JCZ38, IN-DBC80, IN-N7B69, IN-MYX98, IN-JSE76 and IN-QKV54, were also identified with no single metabolite exceeding 5.6% TRR. The concentrations of the unresolved radioactivity corresponding to both IN-PCA84 and IN-NOX70 were highest 7 days after the first application (11.5% of the total TRR), decreasing to 5.8% TRR thereafter. Many other metabolites were detected which did not correspond to known reference standards, none exceeding 5.6% TRR (0.07 mg/kg). The unextracted residue accounted for <2.3% TRR (<003 mg/kg.) per application. Attempts were made to further characterize IN-HLA84 and IN-NOX70 in selected immature foliar extracts using HPLC method. The photodegradeate IN-NOX70 accounted for 12.2% TRR (0.23 mg/kg.) 7 days after the first application and was predominantly in the Table B.7.1.1-7. Summary of Characterization and Identification of Radioactive Residues in Plant Matrices Following Application of [CN/PC-14C]-MTP_W29-31 at 150 g ai/ha

Box for narrative text to describe identification and quantification of residues.

Table to be populated with list of compounds identified in the metabolism study

Compound	Leaves0DAT1		Leaves7DAT1		Leaves7DAT2		Leaves7DAT3		Leaves14DAT3		Matrix 6		Matrix 7	
	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm
MTP_W29-31	95.3	2,429							43.4	0.562				
IN-K7H19		ND							1.4	0.019				
IN-JCZ38		ND							2.8	0.036				
IN-DBC80		ND								ND				
IN-N7B69		ND							2.9	0.037				
IN-MYX98		ND		ND		ND	1.0	0.023	1.5	0.018				
IN-JSE76		ND		ND		ND		ND	1.0	0.012				
IN-HGW87		ND		ND	0.6	0.028		ND		ND				
IN-QKV54		ND		ND	0.8	0.040	2.8	0.062	4.3	0.054				

III. Results and Discussion- D. Identity of Residues in Crops

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D. Identity of Residues in Crop

[Cyano-14C]-MTP_W29-31 [Pyrazole carbonyl-14C]-MTP_W29-31 [CN/PC-14C]-MTP_W29-31

MTP_W29-31 was the major component in leaves, decreasing from 95.3% TRR immediately after the first application to 43.4% TRR after 7 days. IN-K7H19, IN-JC238, IN-DBC80, IN-N7B69, IN-MYX98, IN-JSE76 and IN-QKV54, were also detected in leaves, with IN-K7H19, IN-JC238, IN-DBC80, IN-N7B69, IN-MYX98, IN-JSE76 and IN-QKV54, being the most abundant. IN-N7B69 was the most abundant metabolite in roots, decreasing from 11.5% TRR immediately after the first application to 5.8% TRR after 7 days. Many other metabolites were detected which did not correspond to known metabolites. IN-MLA84 and IN-NX070 in selected immature foliar extracts using HPLC method. The chromatograms of IN-NX070 and IN-MLA84 are shown in Figure 7. The first application was made on 15/04/2010 and was repeated on 22/04/2010. Table B.7.1.1-7. Summary of Characterization and Identification of Radioactive Residues in Plant Matrices Following Application of [CN/PC-14C]-MTP_W29-31 Radiolabeled MTP_W29-31 at 150 g ai/ha

Compound	Leaves0DAT1		Leaves7DAT1		Leaves7DAT2		Leaves7DAT3		Leaves14DAT3		Matrix 6		Matrix 7	
	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm
MTP_W29-31	95.3	2,429	61.1	1,132	86.5	4,154	8.2	1,377	43.4	0,562				
IN-K7H19	ND		ND		ND		1.2	0.025	1.4	0.019				
IN-JC238					0.2	0.010	1.0	0.022						
IN-DBC80					0.5	0.021	1.5	0.034						
IN-N7B69					0.3	0.016	0.8	0.019						
IN-MYX98					ND		1.0	0.023						
IN-JSE76					ND		ND							
IN-HGW87	ND		ND		0.6	0.028	ND		ND					
IN-QKV54	ND		ND		0.8	0.040	2.8	0.062	4.3	0.054				

Table B.7.1.1-5.

Caption: Leaves14DAT3

Right-click to rename, clear, delete or add row

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III. Results and Discussion- D. Identity of Residues in Crops

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MTP_W29-31 was the major component in leaves, decreasing from 95.3% TRR immediately after the first application to 61.1% TRR seven days later. Seven days after the second application, MTP_W29-31 accounted for 86.5% TRR. At 7 and 14 days after the final application, MTP_W29-31 accounted for 62.2% and 43.4% par TRR, respectively. IN-JC238, IN-K7H19, IN-JC238, IN-DBC80, IN-N7B69, IN-MYX98, IN-JSE76 and IN-QKV54, were also identified with no single metabolite exceeding 5.1% TRR. Concentrations of the unresolved radioactivity corresponding to both IN-MLA84 and IN-NOX70 were highest 7 days after the first application (11.5% par TRR), decreasing to 5.8% TRR thereafter. Many other metabolites were detected which did not correspond to known reference standards, none exceeding 5.6% TRR (0.07 mg/kg). The unextracted residue accounted for <2.3% TRR (<0.03 mg/kg.) par Attemus were ma in selected immature foliar extracts using HPLC method. The photodegrade IN-NOX70 accounted for 12.2% TRR (0.23 mg/kg) 7 days after the first application and was predominantly in the identification of Radioactive Residues in Plant Matrices Following Application of [CN/PC-14C]-MTP_W29-31 Radiolabeled MTP_W29-31 at 150 g ai/ha

Compound	Leaves7DAT1		Leaves7DAT2		Leaves7DAT3		Leaves14DAT3		Matrix 6		Matrix 7	
	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR
MTP_W29-31	1.132	86.5	4.154	62.2	1.377	43.4	0.562					
IN-K7H19	ND		ND	1.2	0.025	1.4	0.019					
IN-JC238	0.019	0.2	0.010	1.0	0.022	2.8	0.036					
IN-DBC80	0.033	0.5	0.021	1.5	0.034		ND					
IN-N7B69	ND	0.3	0.016	0.8	0.019	2.9	0.037					
IN-MYX98	ND		ND	1.0	0.023	1.5	0.018					
IN-JSE76	ND		ND		ND	1.0	0.012					
IN-HGW87	ND		ND	0.6	0.028		ND					
IN-QKV54	ND	0.8	0.040	2.8	0.062	4.3	0.054					

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III. Results and Discussion- D. Identity of Residues in Crops

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Compound	Leaves0DAT1		Leaves7DAT1		Leaves7DAT2		Leaves7DAT3		Leaves14DAT3		Matrix 6		Matrix 7	
	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm
MTP_W29-31	5.3	2,429	61.1	1,132	86.5	4,154								
IN-K7H19		ND		ND		ND								
IN-JCZ38		ND	1.0	0.019	0.2	0.010								
IN-DBC80		ND	1.9	0.033	0.5	0.021								
IN-N7B69		ND		ND	0.3	0.016								
IN-MYX98		ND		ND		ND								
IN-JSE76		ND		ND		ND								
IN-HGW87		ND		ND	0.6	0.028								
IN-QKV54		ND		ND	0.8	0.040								

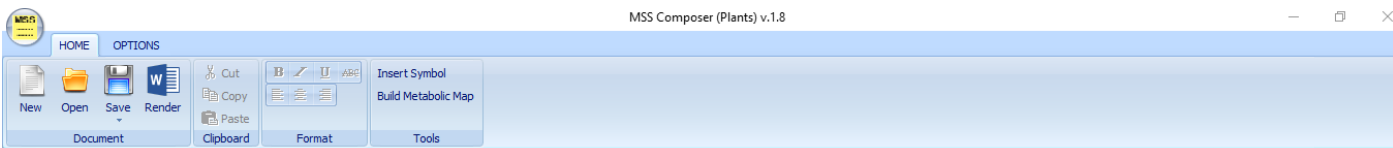
Use dot for decimals instead of coma

Harmonise the number of decimals

N/A, N/D, « - »

Copy values of LOD or LOQ when reported in the report: ex: LOD 0,01

III. Results and Discussion- D. Identity of Residues in Crops



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Compound	Leaves0DAT1		Leaves7DAT1		Leaves7DAT2		Leaves7DAT3		Leaves14DAT3		Matrix 6		Matrix 7	
	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm
MTP_W29-31	95.3	2,429	61.1	1,132	86.5	4,154	62.2	1,377	43.4	0,562				
IN-K7H19		ND		ND		ND	1.2	0.025	1.4	0.019				
IN-JC238		ND	1.0	0.019	0.2	0.010	1.0	0.022	2.8	0.036				
IN-DBC80		ND	1.9	0.033	0.5	0.021	1.5	0.034		ND				
IN-N7B69		ND		ND	0.3	0.016	0.8	0.019	2.9	0.037				
IN-MYX98		ND		ND		ND	1.0	0.023	1.5	0.018				
IN-JSE76		ND		ND		ND		ND	1.0	0.012				
IN-HGW87		ND		ND	0.6	0.028				ND				
IN-QK/54		ND		ND	0.8	0.040	2.8	0.062	4.3	0.054				

WARNINGS:

- Always start with the parent compound and carry on with identified metabolites
- Rename columns but don't delete column headings: empty headings cause irreversible merger of columns
- Characterization, and Distribution of Residues, more-than (>) sign authorised but not less-than (<) sign! Using a less-than sign makes information disappear



III. Results and discussion (part 2)

Storage stability of residues and Identity of Residues in crops

Live session