

Liberté Égalité Fraternité





WEBINAR: METAPATH

How to complete MSS composers for pesticides metabolism studies

1

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

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								This tab summarises th	e available sto	orage		
Crop 1								stability data				
							Appendix VI. Attachments	•				
A. Tot	al Radioac	tive Res	idues B.	Extraction, C	haracterization, and l	Distribution of Residue	C. Storage Stability of Residues D. Identity of Resid	dues in Crop E. Proposed Metabolic Pathway				
C.	Stora	ge St	ability	of Resi	dues							
Pla	nt sample	es were	stored fr	ozen (<i>ca</i> -20°	C) until they were t	aken for analysis. Fol	lowing analysis, all samples were retumed to storage	re at ca -20°C				
						-	a au au anna a			. Frozen storage did 1	not impact	
						sition remained unch	anged managed and	for narrative text to describe	U U	0.10 mg/kg) included i atoes.	N- J9Z 38,	
u u	esoiveu				·····		s unidentified components. The resules stabil	ity.		aloes.		
Tal	ole B.7.1	.1-6.	Summa	ry of Stor	age Conditions.							
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I. General Info II	. Materials and Me	ethods III. Results	and Discussion	IV. Conclusions V	Appendix VI. A	ttachments									
A. Total Radioactiv	ve Residues B. I	Extraction, Characte	erization, and Dis	tribution of Residues	C. Storage Stal	bility of Residues	D. Identity of Re	esidues in Crop	Proposed Meta	bolic Pathway					
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application, M TRR, respectiv NXX70 were hi TRR), decreas Attemps were	TP_W29-31 accouvely. IN-J9238, IN- ighest 7 days after sing to 5.8% TRR to made to further of the sing to 5.10 account of the single si	nted for 62.2% and HK7H19, IN-JCZ38, In the first application thereafter. Many of tharacterize IN-MLA Mary of Character	43.4% par IN-DBC80, IN-N7 n (11.5% \par her metabolites w 34 and IN-NXX70 ization and Id	B69, IN-MYX98, IN-J vere detected which o in selected immature lentification of F	SE76 and IN-QKVS did not correspond foliar extracts usi adioactive Res	54, were also ident d to known referen ing HPLC method. 1 sidues in Plant	tified with no single nee standards, nor The photodeorada Matrices Follo	e metabolite exce ne exceeding 5.6 the IN-NXX70 acco owing Applicat	6 TRR (0.07 mg/k unted for 12.2% tion of [CN/PC	g). The unextract TRR (0.23 ma/ka) -14C]-MTP_W	ed residue accou	nted for <2.3% T first application a labeled MTP_V	sponding to bod IRR (<003 mg/kg and was predomi	g.)\par nantly in the i0 g ai/ha	
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D.]	Identi	ty of Resid	lues in Cr	ор	istribution of Residue		Stability of Residue	D. Identity of	FResidues in Cro	P P Proposed M	etabolic Pathway					
MTF app TRR NXX TRR Atte	P_W29-31 blication, M R, respecti (70 were h R), decreas emps were	was the major co TP_W29-31 acco vely. IN-J9Z38, I ighest 7 days aft sing to 5.8% TRF made to further	omponent in leav unted for 62.29 N-K7H19, IN-JC ter the first appli thereafter. Mai characterize IN-	es, decreasing from 6 and 43.4% \par Z38, IN-DBC80, IN-1 cation (11.5% \par ny other metabolites -MLA84 and IN-NXX7	95.3% TRR immediat N7869, IN-MYX98, IN- swere detected which 10 in selected immatur Identification of	ely after the fir JSE76 and IN-0 did not corres e foliar extract	QKV54, were als pond to known r s using HPLC meaned	item a	nd con	itaining	oonding a table PC-14C]-MTP_W	with 7	colum	ns		
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	P_W29-31	95.3	2.429	61.1	1.132	86.5	4.154	- 0.2	1.377	43.4	0.562					
	K7H19		ND		ND		ND	1.2	0.025	1.4	0.019					
	JCZ38	_	Table B.7.1.1-	5.	×	0.2	0.010	1.0	0.022	TT 1		e*11 1		e 14		
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IN-I IN-I	MYX98 JSE76						0.016 ND ND	0.8	0.01. 0.023 ND		omatic e					
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A. To	tal Radioact	ive Residues B.	Extraction, Char	racterization, and	d Distribut	tion of Residues	C. Storage Stat	oility of Residues	D. Identity of Re	sidues in Crop	Proposed Metabo	olic Pathway					
[a T N T A	Cyano-14C] ITP_W29-31 pplication, M RR, respecti	TTP_W29-31 accord vely. IN-J9238, II highest 7 days aft sing to 5 8% TTP may .1-1 De	Pyrazole carbony mponent in leave unted for 62.2% N-K7H19, IN-JCZ er the first applic	yl-14C]-MTP_W29 es, decreasing fro and 43.4% \par 238, IN-DBC80, II 236, IN-DBC80, II	om 95.3% N-N7B69, ar ios were o in set lent	6 TRR immediate IN-MYX98, IN-3 detected which o lected immature	ly after the first ap SE76 and IN-QKV5 did not correspond foliar extracts usin tadioactive Res	4, were also ident to known referen D HPLC method. 1	ified with no single ce standards, non The photodeorada Matrices Follo	metabolite exceed e exceeding 5.6% te IN-NXX70 accou	ding 5.1% TRR. Co TRR (0.07 mg/kg) nted for 12.2% TF	. The unextracted RR (0.23 mg/kg) 7 L4C]-MTP_W29	ne unresolved radi residue accounte davs after the firs 9-31 Radiolabo	for 86.5% TRR. A oactivity correspon d for <2.3% TRR st application and s eled MTP_W29 trix 6	nding to both IN-1 (<003 mg/kg.)\pa vas predominanth -31 at 150 g	MLA84 an ar v in the	nd IN-
C	Compound					m	%TRR	ppm	%TRR	pom	%TRR	pom	%TRR	ppm	%TRR	ppm	
Ν	ITP_W29-31		sert Row Ab			1.132	86.5	4.154	62.2	1.377	43.4	0.562					
I	N-K7H19	_	ert Row Bel	low	N	ND		ND	1.2	0.025	1.4	0.019					
I	N-JCZ38	C <u>o</u>	py Row		C	0.019	0.2	0.010	1.0	0.022	2.8	0.036					
I	N-DBC80	CI.	ear Table		0	0.033	0.5	0.021	1.5	0.034		ND					
I	N-N7869	- C1			N	ND	0.3	0.016	0.8	0.019	2.9	0.037					
I	N-MYX98		ND		N	ND		ND	1.0	0.023	1.5	0.018					
I	N-JSE76		ND		N	ND		ND		ND	1.0	0.012					
I	N-HGW87		ND		N	ND	0.6	0.028		ND		ND					
I	N-QKV54		ND		N	ND	0.8	0.040	2.8	0.062	4.3	0.054					
Ē			la 222					0.440	1. e	0.447		0.074	1				

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(C A A A A A	yano-14C]- IP_W29-31 v plication, MI R, respectiv X70 were hi R), decreas temps were	was the major co TP_W29-31 accor vely. IN-J9Z38, II ighest 7 days aft ing to 5.8% TRR made to further	Pyrazole carbo mponent in lea unted for 62.2 v-K7H19, IN-2 er the first app thereafter. Mi characterize IN	nyl-14C]-MTP_W29-3 wes, decreasing from % and 43.4% \par CZ38, IN-DBC80, IN-1 alication (11.5% \par any other metabolite: -MLA84 and IN-NXX	N7B69, IN-MYX98, IN-J s were detected which (70 in selected immature	ly after the first applic SE76 and IN-QKV54, v did not correspond to foliar extracts using h	vere also iden known referei IPLC method.	% TRR seven days later. Seven days a tified with no single metabolite exceed nes standards, none exceeding 5.63 «On The photoderatabe IN-NXO7 as the photoderatabe IN-NXO7 as the thotogen set of the set of the set of the set of the the thotogen set of the set of the set of the set of the the set of the set of the set of the set of the set of the the set of the set of the set of the set of the set of the the set of the set of the set of the set of the set of the the set of the set of the the set of the	ng 5.1% TRR. Concentrations of th TRR (0.07 mg/kg). The unextracted ted for 12.2% TRR (0.23 mg/kg) 7 (e unresolved radioad residue accounted fi davs after the first a	ctivity correspo or <2.3% TRR polication and	nding to both IN (<003 mg/kg.)\ was predominar	N-MLA84 ar par htlv in the	
	ompound	Le	aves0DAT1	L	eaves7DAT1	Leaves7D	AT2	Leaves7DAT3	Leaves14DAT3	Matrix	6	1	Matrix 7	A
м	TP_W29-31 I-K7H19 I-JCZ38	%TRR 15.3	ppm 2.429 ND ND	%TRR 61.1 1.0	ppm 1.132 ND 0.019	NE	154 Us	e dot for decimals i			bm	%TRR	ppm	
	I-DBC80 I-N7B69		ND ND	1.9	0.033 ND		021 016		er of decimals					
	I-MYX98 I-JSE76		ND ND		ND ND	NE NE		'A, N/D, « - »						
I	I-HGW87		ND		ND		⁰²⁸ Co	py values of LOD or	LOO when repor	ted in				
	I-QKV54		ND		ND	0.8 0.0	040	• •		teu m				_
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Crop 1	Crop 2											
I. Gene	ral Info	II. Materia	als and Me	ethods III. F	Results and Discussion	IV. Conclusions V	Appendix VI. Attachments					

A. Total Radioactive Residues B. Extraction, Characterization, and Distribution of Residues C. Storage Stability of Residu

D. Identity of Residues in Crop

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 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% lpar

TRR, respectively. IN-J9238, 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-NX770 were highest 7 days after the first application (11.5% loar

TRR), decreasing to 5.8% TRR thereafter, Many other metabolites were detected which do 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). Van Attemos were made to further characterize IN-MA84 and IN-MOX70 in selected immature follar extracts using HPLC method. The obtolegeradate IN-MOX70 accounted for 12.2% TRR (0.23 mg/kg). Value accounted for selected immature follar extracts using HPLC method. The obtolegeradate IN-MOX70 accounted for 12.2% TRR (0.23 mg/kg). Value accounted for selected immature follar extracts using HPLC method. The obtolegeradate IN-MOX70 accounted for 12.2% TRR (0.23 mg/kg). Value accounted for 12.2% TRR (value accounted for 12.2% TRR (value

Compound	Leave	s0DAT1	Leaves	s7DAT1	Leave	7DAT2	Leave	s7DAT3	Leaves	14DAT3	Mat	rix 6	Mat	rix 7
Compound	%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-JCZ38		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-N7869		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		ND				
IN-QKV54	_	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 lessthan (<) 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