



**RÉPUBLIQUE
FRANÇAISE**

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anses



European Food Safety Authority

WEBINAR: METAPATH

How to complete MSS composers for pesticides metabolism studies

-

Livestock metabolism studies

Let's start

Wednesday 30 March

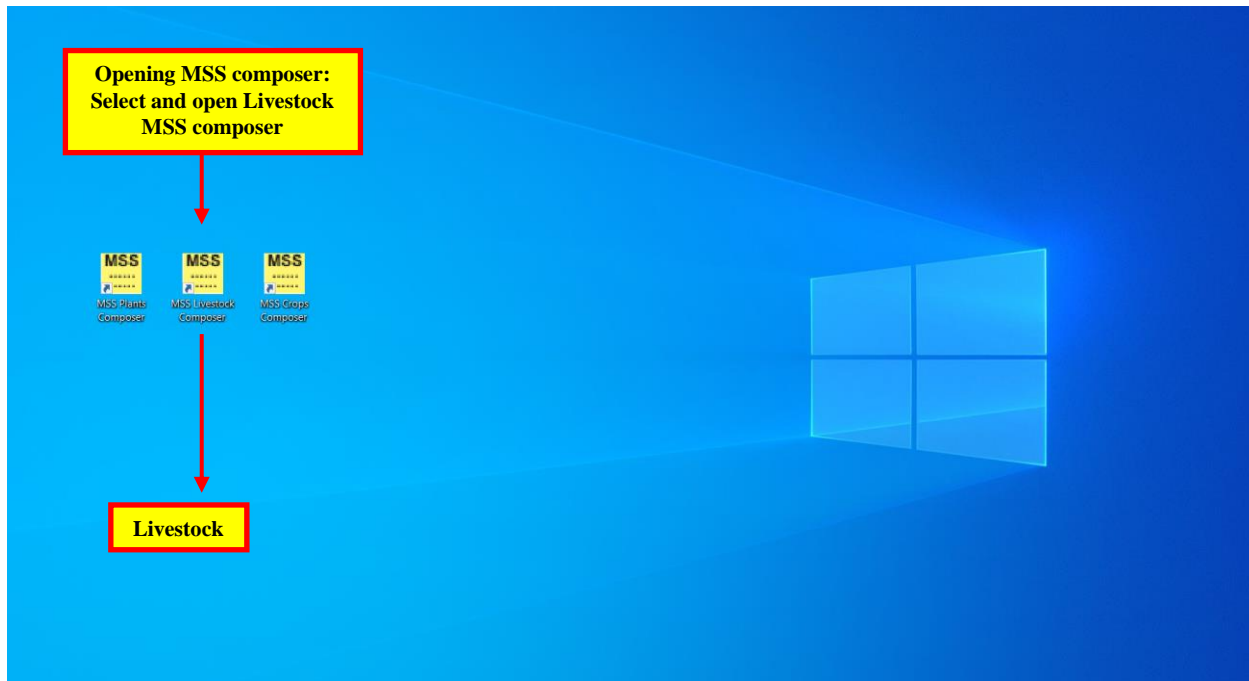
TIME	ITEM
09:30 – 09:35	Introduction
09:35 – 10:30	Livestock composer
10:30 – 10:45	Coffee Break
10:45 – 11:30	Crop composer / rotational
11:30 – 12:00	Q&A session and conclusion

Theory
Live Session
Summary KP
QA

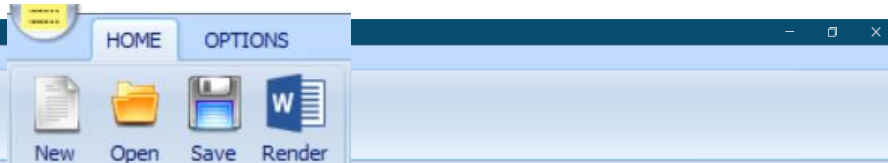
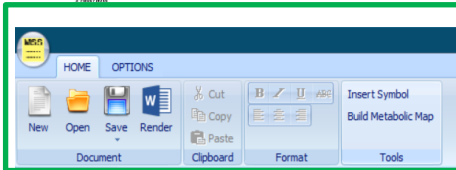


Livestock MSS composer : Opening

Opening MSS



Opening MSS




WARNING:
Be careful to encode the study in the right tab i.e. poultry, lactating ruminant or other animals depending on the animal(s) dosed in the study

In comparison with plant and rotational crops MSS composer :

- Same architecture and functions.
- Same manner to complete MSS composer

→ In the next slides, only specificities of livestock MSS composer are detailed



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

Livestock MSS composer :

General Info

General info

Poultry | Lactating Ruminants | Other Animals

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

B.7.2.1 Poultry

In comparison with plant and rotational crops MSS composer, same manner to fill in "General Info" section

References:

ADD DEL

Citation #1

Author(s):

Date:

Pages:

Study Title:

Reference Type:

Testing Laboratory:

Company Study Number:

Identifiers:

EDIT

Test Material:

Identifiers:

EDIT

Guidelines:

GLP:

Acceptability:

The study considered scientifically acceptable.

Evaluators:

Evaluator Name

Evaluator Affiliation

Evaluator 1

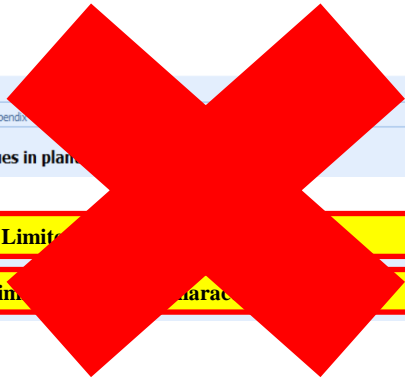
Evaluator 2

Evaluator 3

BACKGROUND INFORMATION

EXECUTIVE SUMMARY

General info



Crop 1 Crop 2

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

B.7.1 Metabolism, distribution and expression of residues in plants

Product Type:

Pesticide function : Free text + Limited

Product Use:

Intended Crops : Free text + Limited

Livestock MSS composer : Materials and Methods



Materials and Methods

Poultry | Lactating Ruminants | Other Animals

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

A. Materials | B. Study Design

A. MATERIALS

I. Test Material

Common name	
CAS Chemical Name	
CAS no.	
Company experimental name	
Other synonyms (if applicable)	
Molecular Formula	
Analytical Purity	
Impurities	
Physical State	
Stability Under Test Conditions	
Expiration Date	
Lot/Batch #	

Radiolabeled Test Material

Radiochemical purity: %

Specific activity as received:

Specific activity of dose:

Structure:

Table PhysChem Physicochemical Properties.

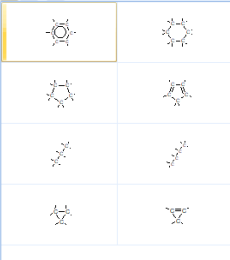
Parameter	Notes
Melting point/range	°C
pH	
Density	
Water solubility (___°C)	
Solvent solubility (mg/L at ___°C)	
Vapour pressure at ___°C	
Dissociation constant (pKa)	
Octanol/water partition coefficient Log(P _{ow})	
UV/visible absorption spectrum	

In comparison with plant and rotational crops MSS composer, same manner to fill in “Material and Method” section

2D Editor

SMILES/InChI
000000-00-0

Templates



drag the mouse with left button pressed to create bond

Materials and Methods

Poultry | Lactating Ruminants | Other Animals

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

A. Materials | B. Study Design

A. MATERIALS

2. Animals

Table B.7.2.1-1. General Test Animal Information.

General test animal information tab to be fulfilled !

Species	Breed	Age	Weight at Study Initiation (kg)	Health Status	Description of Housing/Holding Area
Hen					

Species

**Use only common name, not Latin name.
Limited number of characters**

Breed

Limited number of characters

Age

Value or range of value + unit



WARNING:
Must start with a figure. Figures need to be separated from the unit by a space character

Weight at Study Initiation (kg)

Value or range of value + unit



WARNING:
Only figures and colons entered in this field taken into consideration in METAPATH

Health Status

Free text

Description of Housing/Holding Area

Free text + limited number of characters

Materials and Methods

Poultry Lactating Ruminants Other Animals

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

A. Materials B. Study Design

B. STUDY DESIGN

Dose Regime

Number of Animals per Dose Group

Rationale for Selection of Dose Group

Analysis of Feed and Water

Table B.7.2.1-2. Test Animal Dietary Regime.

Composition of Diet	Feed consumption (kg/day)	Water	Acclimation period	Predosing
Limited number of characters	Value + unit	Limited number of characters	Value + unit	Select "Yes" or "No"



WARNING:
Must start with a figure.
Figures to be separated from the unit by a space character.
When encoding a range, hyphens have to be bounded by space characters

Materials and Methods

Poultry Lactating Ruminants Other Animals

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

A. Materials **B. Study Design**

Table B.7.2.1-3. Test Animal Dosing Regime.

Treatment Type	Treatment Level (mg/kg)	Vehicle	Parameters	Dosage Rate	Timing/Duration	Timing from final dose to sacrifice
Oral		capsule, feed, bolus, etc	Test material in vehicle			
Treatment Type	→ pre-filled by the software ("Oral"); can be changed if needed → if several lines to be created, respect the following nomenclature: abbreviation of the radiolabelled test material_oral .					
Treatment Level (mg/kg)	→ theoretical dose administered to animals → Specify the unit: mg/kg DM or mg/kg bw/day → if different treatment levels tested in the study, create a line for each treatment level					
Vehicle	→ pre-filled by the software ("capsule, feed, bolus, etc.") → select or write down the correct information					
Parameters	→ pre-filled by the software ("Test material in vehicle"); can be changed if needed					
Dosage Rate	→ experimental dose administered to animals → Specify the unit for sake of completeness: mg/kg DM or mg/kg bw/day. → if the administered dose not the same between the radiolabelled test materials, create a line for each radiolabel					
Timing/Duration	Value					
Timing from final dose to sacrifice	Value + unit					

Poultry Lactating Ruminants Other Animals

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

A. Materials **B. Study Design**

Sampling

Table B.7.2.1-4. Sample Collection Information.

Eggs Collected	Number of Eggs produced during normal production	Excreta and Cage Wash Collected	Interval From Last Dose to Sacrifice	Tissues Harvested and Analyzed
XXX daily		XXX daily	XXX hours	

[Eggs / Milk] Collected	Number of sampling per day
[Number of Eggs / Amount of milk / Amount of] produced during normal production	Value + unit
[Excreta / Urine, Feces] and Cage Wash Collected	Number of sampling per day
Interval From Last Dose to Sacrifice	Value + unit
Tissues Harvested and Analyzed	Free text + limited number of characters

Materials and Methods

Poultry Lactating Ruminants Other Animals

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

A. Materials B. Study Design

Sampling

Flowchart of the extraction and fractionation schemes #1

Attach

Clear

View

Attach Clear View

Flowchart of the extraction and fractionation schemes #2

Attach Clear View

Flowchart of the extraction and fractionation schemes #3

Attach Clear View

Attach, clear or view flowchart of the extraction and fractionation schemes

Extraction and Analysis

Free-text field: briefly describe the methods of extraction and analysis. If need be, files or diagrams can be attached.

Identification and Characterization

Free-text field: briefly describe the methods of identification and characterization

Livestock MSS composer :

General info – Material and method

Live Session



Livestock MSS composer : Results and discussion

Results and discussion

Poultry La **5 SUBTABS** Anal

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 Poultry E. Proposed Metabolic Pathway

A. Total Radioactive Residues

Extraction efficiency of radioactive residues from livestock 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

By mouse right clicking

On a line : different functions available for the 5 subtabs

- Delete Row
- Clear Row
- Insert Row Above
- Insert Row Below
- Copy Row
- Clear Table

On a column title: renaming available for the 5 subtabs

Overall extraction efficiency (%)

Caption: Overall extraction efficiency (%)

OK Cancel

Results and discussion

Poultry Lactating Ruminants Other Animals

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 Poultry E. Proposed Metabolic Pathway

A. Total Radioactive Residues

Extraction efficiency of radioactive residues from livestock 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

Fill in table if extraction efficiency data available

Quantitation

The overall ^{14}C -recoveries of the administered dose were quantified. **Fill in text Informations on the methods for determining TRR values** ed for 0.4-0.5% (0.20-0.26 mg/kg) while egg yolks contained 0.07% of the total administered dose. Abdominal fat, skin with fat and muscle each contained 0.17% of the total administered dose for either label, each equivalent 0.01 mg/kg. The data indicates good agreement between both radiolabels.

Table B.7.2.1-5. TRRs in Eggs, Tissue, and Excreta

Matrix	[Cyano- ^{14}C]-MTP_WB-29-31		[Pyrazole carbonyl- ^{14}C]-MTP_WB_29-31	
	% TRR	ppm	% TRR	ppm
Skin with fat	0.01	0.005	0.01	0.007
Eggs whites	0.54	0.259	0.40	0.203
Eggs yolks	0.07	0.092	0.07	0.087
Cagewash	3.83	NA	2.52	NA
Total recovery	101.4	NA	102.7	NA

Fill in table for TRR's in various matrices

Results and discussion

Poultry Lactating Ruminants Other Animals

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A. Total Radioactive Residues B. Extraction, Characterization, and Distribution of Residues C. Storage Stability of Residues D. Identity of Residues in Poultry E. Proposed Metabolic Pathway

A. Total Radioactive Residues

Select Did or Did not or left empty depending to results displayed in previous table


TRRs in eggs  did appear to have reached a plateau at the end of dosing (see Table B.7.2.1-6)

Table B.7.2.1-6. TRRs in Eggs as Function of Time.

Interval	[Cyano-14C]-MTP_WB-29-31			
	ppm	% of dose		
Day 1 AM	0.01	10		
Day 1 PM		15	0.02	15
Day 2 AM		15	0.02	15
Day 2 PM		15	0.02	15
Day 3 AM	0.02	15	0.02	15
Day 3 PM	0.02	15	0.02	15

Report respective results for radioactivity in eggs in function of time

WARNING:
Once "did" or "did not" has been selected, there is no way to come back to an empty field

Image Attachment

File attachment possible

Attach Clear View

General Health of Animals

Free-text field: describe general health of the animals during the study

Results and discussion

Poultry Lactating Ruminants Other Animals

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A. Total Radioactive Residues B. Extraction, Characterization, and Distribution of Residues C. Storage Stability of Residues D. Identity of Residues in Poultry E. Proposed Metabolic Pathway

B. Extraction, Characterization, and Distribution of Residues

Prefilled: Separate table/tab for each radiolabel – in this example there are two labels and 2 tables.

Cyano-14C]-MTP_WB-29-31 [Pyrazole carbonyl-14C]-MTP_WB_29-31

Free text for description of results (footnotes, abbreviations...)

Table B.7.2.1-7. Distribution of the Parent and the Metabolites in Poultry Matrices when Dosed with 14C-labeled MTP_WB-29-31.

Metabolite Fraction	Excreta		Egg white		Egg yolk		Liver - Aqueous ACN extract		Liver - Protease digest	
	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm
Total	100.0	0.137	100.0	0.137	100.0	0.137	100.0	0.137	100.0	0.137
Total extracted	8.09	0.052	8.09	0.052	8.09	0.052	8.09	0.052	8.09	0.052
Total characterized unknowns	8.22	-	7.75	0.021	23.62	0.025	7.58	0.010	22.33	0.042
Total characterized/identified	94.92	-	96.07	0.250	71.14	0.068	10.97	0.015	23.82	0.045
Total uncharacterized unknowns	5.08	-	3.25	-	26.46	-	89.03	-	76.17	-
Total uncharacterized/identified	5.08	-	3.25	-	26.46	-	89.03	-	76.17	-

This tab summarises the extraction, characterisation and distribution of the TRR among the different matrices

WARNING:

Pay attention to the number of column required to report all the data available in the study (one column per matrix). Knowing that each subtab contains a 7-column table, if you need 8 columns, you have to create a second radiolabelled test item to get the extra columns you need

WARNING:

You can rename columns but do not delete column headings: empty headings cause irreversible merger of columns

WARNING:

More-than (>) sign authorised but not less-than (<) sign! Using a less-than sign makes information disappear

Results and discussion

Poultry Lactating Ruminants Other Animals

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 Poultry E. Proposed Metabolic Pathway

C. Storage Stability of Residues

All samples were stored frozen (-20°C) for no more than 55 days before extraction and analyzed within 62 days after sampling. Storage stability analysis was not conducted for this study and was not required.

Free-text field: describe storage conditions, discuss if residues are stable during storage.

Table B.7.2.1-8. 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 or Months)
-------------------------	------------------------	--	--

Tab to summarize storage stability data in study and demonstrated storage stability

Results and discussion

Poultry Lactating Ruminants Other Animals

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 Poultry** E. Proposed Metabolic Pathway

D. Identity of Residues in Poultry

[Cyano-14C]-MTP_WB-29-31 [Pyrazole carbonyl-14C]-MTP_WB_29-31

Table B.7.2.1-9. Summary of Characterization and Identification of Radioactive Residues in Poultry Matrices Following Application of [Cyano-14C]-MTP_WB-29-31 Radiolabeled MTP_WB-29-31 at 1.07 mg/kg body weight/d

Compound	Excreta		Egg white		Egg yolk		Liver - Aqueous ACN extract		Liver - Protease digest	
	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm	%TRR	ppm
MTP_WB_29-31	76.56	-	32.48	0.084	10.28	0.009	ND	ND	ND	ND
IN-HGW87	1.20								ND	ND
IN-J9238	ND	ND	29.21	0.073	7.42	0.008	2.08	0.003	ND	ND
IN-MLA84										
IN-MYX98										
IN-Total uncharacterized										

This tab summarises the identification of compounds in tested matrices

WARNING:

Pay attention to the number of column required to report all the data available in the study (one column per matrix). Knowing that each subtab contains a 7-column table, if you need 8 columns, you have to create a second radiolabelled test item to get the extra columns you need



WARNING:

You can rename columns but do not delete column headings: empty headings cause irreversible merger of columns



WARNING:

More-than (>) sign authorised but not less-than (<) sign! Using a less-than sign makes information disappear



WARNING:

When filling header column, always start with the parent compound and carry on with identified metabolites



Results and discussion

HOME OPTIONS

New Open Save Render

Cut Copy Paste

B U ABC

Insert Symbol

Build Metabolic Map

Document Clipboard Format Tools

Poultry Lactating Ruminants Other Animals

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A. Total Radioactive Residues B. Extraction, Characterization, and Distribution of Residues C. Storage Stability of Residues D. Identity of Residues in Poultry

E. Proposed Metabolic Pathway

E. Proposed Metabolic Pathway

Metabolic map

Parent

WARNING:
Metabolic map can be built only once V. Appendix 2 has been filled in

Table B.7.2.1-10. Identification of Compounds from Metabolism Study (both proposed and found).

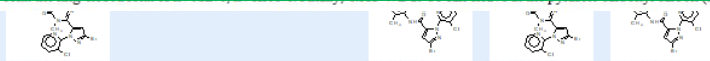
Common name/code	Chemical name	Chemical structure
MTP_WB_29-31	MTP_WB_29-31	<chem>Cc1cc(C#N)cc(C(=O)NC)c1NC(=O)C1=CC(Br)=NN1c1c(Cl)ccc1</chem>
IN-J9Z38	IN-J9Z38	<chem>Cc1cc(C#N)cc(C(=O)NC)c1NC(=O)C1=CC(Br)=NN1c1c(Cl)ccc1</chem>
IN-NBC94	IN-NBC94	<chem>Cc1cc(C#N)cc(C(=O)NC)c1NC(=O)C1=CC(Br)=NN1c1c(Cl)ccc1</chem>
IN-MLA84	IN-MLA84	<chem>Cc1cc(C#N)cc2c1N=C(C1=CC(Br)=NN1c1c(Cl)ccc1)NC2=O</chem>
IN-N7B69	IN-N7B69	<chem>CNC(=O)c1cc(C#N)cc(CO)c1NC(=O)C1=CC(Br)=NN1c1c(Cl)ccc1</chem>

Table about compounds identified automatically created and filled in from V. Appendix > Appendix 2

free-text field: briefly describe the metabolic pathway and reactions (oxidation, hydrolysis, etc.)

MTP_WB_29-31 is metabolized in hens by ... can then lose carbon dioxide after several ... IN-J9Z38 can also N-demethylate ... the ring-closed form of IN-JCZ38, which ca

to form IN-N7B69 and at the N-methyl g ... cyano group of IN-JCZ38 can then be hy ... Z38 can also undergo hydrolysis of its s ... of IN-N7B69) to form IN-DBC80.



Livestock MSS composer :

Conclusion and Appendices

Conclusions

Poultry Lactating Ruminants Other Animals

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

CONCLUSIONS

CONCLUSIONS

When hens were dosed orally with [¹⁴C]-MTP_WB-29-31 for 14 consecutive days, most of the dose was excreted (ca. 97-100%). Unchanged MTP_WB-29-31 was the major radioc from multiple metabolic reactions which included hydroxylation at the benzylic and N-methyl carbons; cyclization with and without subsequent N-demethylation; hydrolysis of th Minimal transfer of [¹⁴C]-MTP_WB-29-31 residue s of oral dosing. Eggs and tissues represent [CN-¹⁴C]-MTP_WB-29-31 respectively. Egg comp was characterized/identified in egg whites residue found in egg whites, lower levels were found in egg yolk. IN-MI A 84 and IN-MI A 84 being the principal m residues were minor accounting for ≤0.02 mg/kg. In liver, about 35-40% TRR was characterized/identified with most of the TRR remaining bound following solvent and protease ex digest from either label. TRR was low (less than 0.01 mg/kg) in muscle and fat.

Free-text field: briefly present the conclusions of the study

REFERENCES

McAnom G.. The metabo

Free-text field: cite references for other metabolism studies (if applicable); if available, include the EPA MRID# and PMRA# of both the study and the review.

Appendices

Poultry Lactating Ruminants Other Animals

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

Appendix 1

Summary of all treatment group from metabolism study. Each line represent a treatment group

Test#	Sex	Number	Dose Route	Dose (nominal)	mg/kg	single	14 days	Excreta	Parental Descriptor	Remarks	Citation	RLTM	Species	Diet	
CN_hen_Excreta	Female	5		10 mg/kg	mg/kg	single	14 days	Excreta			Citation #1	[Cyano-14C]-MTP_1	Hen	Layer pellets	
CN_hen_Egg_white	Female												C]-MTP_1	Hen	Layer pellets
CN_hen_Egg_yolk	Female												C]-MTP_1	Hen	Layer pellets

Appendix 2

Summary 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.

ID	Common Name / Code	Chemical Name	SMILES	Parent(s)	Expertise
1	MTP_WB_29-31	MTP_WB_29-31	Cc1cc(C#N)cc(C(=O)NC)c1NC(=O)		
2	IN-J9Z				
3	IN-NBC				
4	IN-MLA				
5	IN-N7B69	IN-N7B69	CNC(=O)c1cc(C#N)cc(CO)c1NC(=... 1		
6	IN-MYX98	IN-MYX98	Cc1cc(C#N)cc(C(=O)NCO)c1NC(=... 1		

Appendix 3

Summary about the detection or not of compounds in treatment group. Generated automatically once appendix 1 and 2 are fulfilled

	CN_hen_Ex	CN_hen_Ec	CN_hen_Ec	CN_hen_Liv	CN_hen_Liv	Py_hen_Ex	Py_hen_Eg	Py_hen_Eg	Py_hen_Liv	Py_hen_Liv
MTP_WB_29-31	linked	linked	linked	linked	linked	linked	linked	linked	linked	linked
IN-J9Z38	linked	linked	linked	linked	linked	linked	linked	linked	linked	linked

Appendices

Appendix 1

Appendix 1 fulfilled thanks to appendix 1 editor

Test#	Sex	Number	Dose Route	Dose (nominal)	Dose (measured)	Dose Type	Test Duration	Matrix	Experimental	Remarks	Citation	RLTM	Species	Diet	Dosing	Samples
CN_hen_	Female	5	oral	10 mg/kg				Liver - Ac			Citation #1	[Cyano-14C]-MTP	Hep	Layer pellets	Oral	Twice daily

Field	Requirement
Test#*	→ Matrices should be named briefly but unambiguously so that they can be easily distinguished 1. first letters of the labelling (mandatory) 2. animal species (mandatory) 3. tissue analysed (mandatory) 4. dose applied (optional) (...) → Every information separated from the next with an underscore (_)
Gender*	→ Select "Male", "Female" or "Not Reported"
Number	→ number of animals dosed with a given radiolabelled test material
Dose Route*	→ route of administration
Dose Nominal	→ theoretical dose administered to animals
Dose Measured*	→ experimental dose administered to animals
Matrix*	→ analysed tissue
Test Duration*	→ duration of the study

Appendix1 Editor

Test# *
CN_hen_Liver_ACNextract

Gender *
 Male Female Not Reported

Number Dose Route *
oral

Dose Nominal mg/kg Dose Measured *
10 mg/kg

Matrix *
Liver - Aqueous ACN e

Test Duration *
14 days

Experimental Descriptor

Appendices

Appendix 1 Appendix 1 fulfilled thanks to appendix 1 editor

Test#	Sex	Number	Dose Route	Dose (nominal)	Dose (measured)	Dose Type	Test Duration	Matrix	Experimental	Remarks	Citation	RLTM	Species	Diet	Dosing	Samples
CN1_hen_	Female	5	oral	10 mg/kg	10 mg/kg	multiple	14 days	Liver - Ac			Citation #1	[Cyano-14C]-MTP_	Hen	Layer pellets	Oral	Twice daily





Appendix1 Editor		
<p>Dose Type</p> <p>Single <input type="radio"/> Multiple <input checked="" type="radio"/></p> <p>on every: <input type="text"/> <input type="text"/></p> <p>for: <input type="text"/> <input type="text"/></p>	Dose Type	→ select "Single" or "Multiple" → clarify if available "on every for....."
<p>Remarks</p> <p><input type="text"/></p>	Remarks	→ free-text field. To explain terms and abbreviations
<p>Citation*</p> <p>Citation <input type="text"/> Radiolabeled Test Material <input type="text"/></p> <p>Citation #1 <input type="text"/> [Cyano-14C]-MTP_WB- <input type="text"/></p>	Citation*	→ select corresponding citation (according to the radiolabelled test material or the administered dose)
<p>Radiolabeled Test Material (RLTM)*</p> <p>Animal Information (from Table 1) <input type="text"/></p> <p>Hen, Warren, "25 weeks at dosing", "1.6 - 2.1 ", sati <input type="text"/></p>	Radiolabeled Test Material (RLTM)*	→ select corresponding radiolabelled test material
<p>Animal Information (from Table 1)*</p> <p>Dietary Regime (from Table 2) <input type="text"/></p> <p>Layer pellets, "0.128 - 0.213 kg/day for all 10 he <input type="text"/></p>	Animal Information (from Table 1)*	→ select corresponding to animal information
<p>Dietary Regime (from Table 2)*</p> <p>Dosing Regime (from Table 3) <input type="text"/></p> <p>Oral, "10 mg/kg DM diet", "Gelatin capsule", "Test m: <input type="text"/></p>	Dietary Regime (from Table 2)*	→ select corresponding animal's dietary regime during the study
<p>Dosing Regime (from Table 3)*</p> <p>Sampling Information (from Table 4) <input type="text"/></p> <p>Twice daily, "0.8 egg/day", "Once daily", "12 hours <input type="text"/></p>	Dosing Regime (from Table 3)*	→ select corresponding dosing regime (treatment)
<p>Submit <input type="button"/> <input type="button"/> Cancel</p>	Sampling Information (from Table 4)*	→ select corresponding sampling information

Click on Submit to validate created matrice

Appendices

Appendix 2

Appendix 2 fulfilled
thanks to appendix 2

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. <i>N.B.: The metabolic pathway is built based on the information encoded in this field.</i>
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)

Appendix2 Editor

Common Name / Code

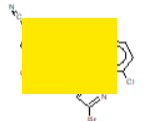
MTP_WB_29-31

Chemical Name

MTP_WB_29-31

Chemical Structure

Cc1cc(C#N)cc(C(=O)NC)c1NC(=O)C1=CC(Br)=NN1c1c(C)



Parent(s)

- 2 : IN-19238 (Cc1cc(C#N)cc2c1N=C(C1=CC(Br)=NN1c1c(C)ccc1)C2=CC(Br)=NN2c2c(C)cccn2)=Nc2c(CO)c2)
- 3 : IN-NBC94 (CN1C(C2=CC(Br)=NN2c2c(C)cccn2)=Nc2c(CO)c2)C1=CC(Br)=NN1c1c(C)ccc1)
- 4 : IN-MLA84 (Cc1cc(C#N)cc2c1N=C(C1=CC(Br)=NN1c1c(C)ccc1)C2=CC(Br)=NN2c2c(C)cccn2)=Nc2c(CO)c2)
- 5 : IN-N7B69 (CNC(=O)c1cc(Cc1cc(CO)c1NC(=O)C1=CC(Br)=NN1c1c(C)ccc1)C2=CC(Br)=NN2c2c(C)cccn2)=Nc2c(CO)c2)
- 6 : IN-N7B69 (CNC(=O)c1cc(Cc1cc(CO)c1NC(=O)C1=CC(Br)=NN1c1c(C)ccc1)C2=CC(Br)=NN2c2c(C)cccn2)=Nc2c(CO)c2)

Expertise

None Tolerance Expression

Expertly specified Residue of Concern

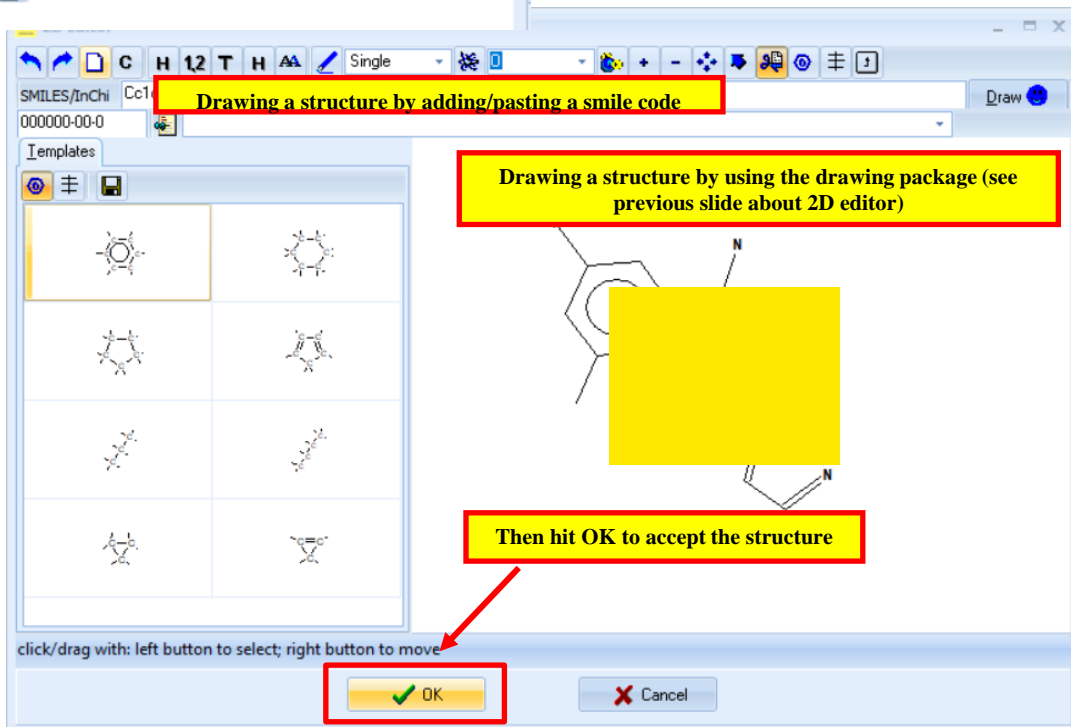
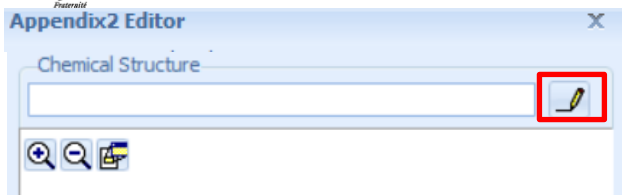
Assumed by author(s)

Expert:

Decision:

Click on Submit to validate
created compound

Appendices



Appendix 3

	CN_hen_Ex	CN_hen_Eg	CN_hen_Eg	CN_hen_Liv	CN_hen_Liv	Py_hen_Ex	Py_hen_Eg	Py_hen_Eg	Py_hen_Liv	Py_hen_Liv
MTP_WB_29-31	linked	linked	linked			linked	linked	linked		
IN-J9Z38		linked	linked		linked	linked	linked	linked		
IN-NBC94		linked	linked	linked			linked	linked		
IN-MLA84		linked	linked		linked	linked	linked	linked	linked	
IN-N7B69						linked				linked
IN-MYX98	linked	linked	linked	linked	linked	linked	linked	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.

Livestock MSS composer : Results and discussion - apendices

Live Session