



**RÉPUBLIQUE
FRANÇAISE**

*Liberté
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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

IV. Materials & Methods

Materials and study design



II. Materials and methods

HOME

OPTIONS

Insert Symbol

Build Metabolic Map

Tools

2 SUBTABS

Click on II. Materials and Methods tab

Crop 1

Crop 2

I. General

II. Materials and Methods

III. Results and Discussion

IV. Conclusions

V. Appendix

VI. Attachments

A. Materials

B. Study Design

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 #

ADD

DEL

Radiochemical purity: %

Specific activity as received:

Specific activity of doses:

Structures:

Table PhysChem Physicochemical Properties.

Parameter	Notes	Value	Units	Reference
Melting point/range			°C	
pH				
Density				

II. Materials and methods- A- Materials

MSS Composer (Plants) v.1.8

HOME

OPTIONS

New

Open

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Paste

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I

U

Format

Insert Symbol

Build Metabolic Map

Tools

Crop 1

Crop 2

I. General Info

II. Materials and Methods

III. Results and Discussion

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V. Appendix

VI.

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 #

Structures

Table PhysChem

Physicochemical Properties.

Parameter

Melting point/range

pH

Density

This tab summarises the test material, the test crop and the soil type

Populate fields under 1. Test Material

WARNING:

Respect the maximum number of characters (~250)

II. Materials and methods- A- Materials- 1. Test Material- Radiolabeled Test Material

HOME OPTIONS

New

Open

Save

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Document

Cut

Copy

Paste

Clipboard

Format

Tools

Insert Symbol

Build Metabolic Map

Crop 1

Crop 2

I. General Info

II. Materials and Methods

III.

ADD

DEL

To add additional radiolabels or to delete radiolabels.

Radiochemical purity:

%

Specific activity as received:

units

Specific activity of dose:

units

Range of values or value(less-than (<) and more-than (>) signs authorised)

Range of values or values / Unit

Range of values or values / Unit

[Cyano-14C]-cyantr...

[Pyrazole carbonyl]-...

[CN/PC-14C]-cyantr...

Structures:

Table PhysChem Physicochemical Properties.

Parameter	Notes	Value	Units	Reference
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(Pow)				
UV/visible absorption spectrum				

2. Test Crops

Table B.7.1.1-1. Crop Information.

II. Materials and methods- A- Materials- 1. Test Material- Radiolabeled Test Material

HOME OPTIONS

New Open Save Recent 2D Editor

Document

SMILES/InChI

000000-00-0

Templates

Crop 1 Crop 2

I. General Info II. Material

A. Materials B. Study Design

Radio-labeled Test Material

ADD DEL

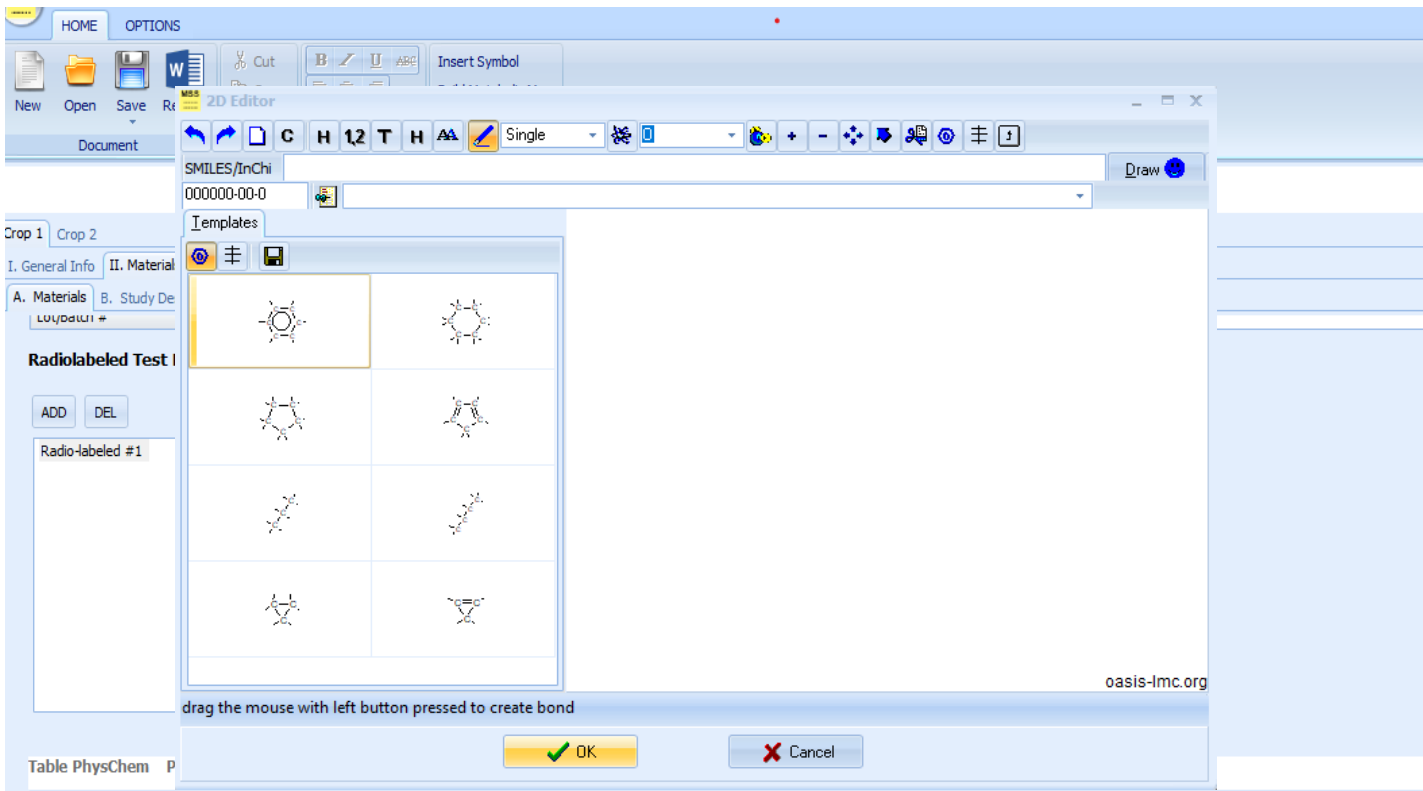
Radio-labeled #1

drag the mouse with left button pressed to create bond

oasis-lmc.org

Table PhysChem P

OK Cancel











Drawing tool: Using 2D Editor: draw the structure

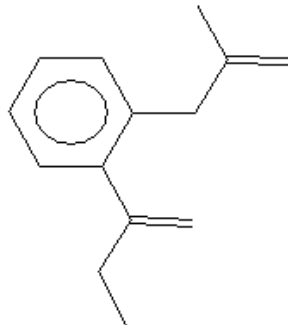
MS 2D Editor

SMILES/InChi CCC(=C)c1ccccc1CC(C)=C Draw

000000-00-0

Templates



drag the mouse to move fragment, release left button to glue the fragment to structure

OK Cancel

Drawing tool: Using 2D Editor: Modify the atom

2D Editor

SMILES/InChi: CCC(=C)c1ccccc1CC(C)=C Draw

000000-00-0

Template

Periodic Table

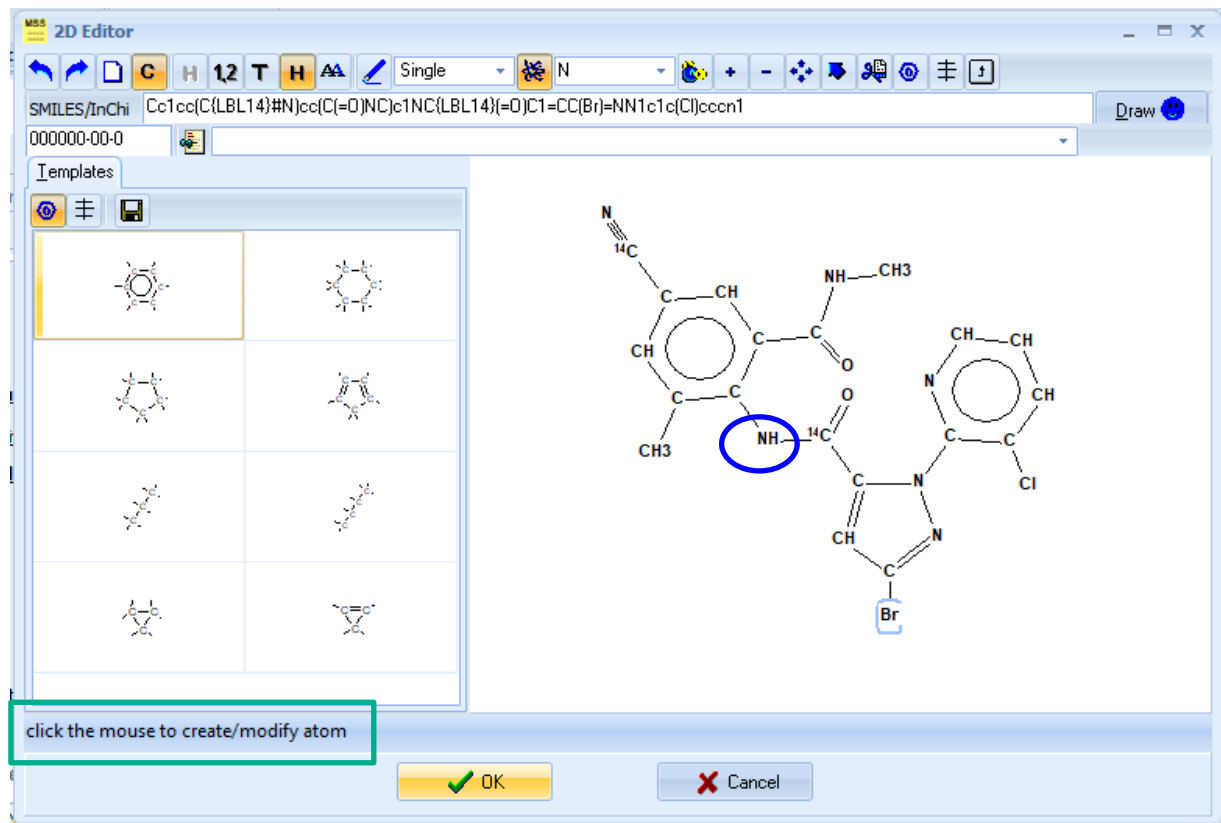
1 H																	2 He				
3 Li	4 Be															5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg															13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr				
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe				
55 Cs	56 Ba	57 *La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn				
87 Fr	88 Ra	89 *Ac																			

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Selected element: N

☐ Labeled
Number:

Drawing tool: Using 2D Editor: Modify the atom



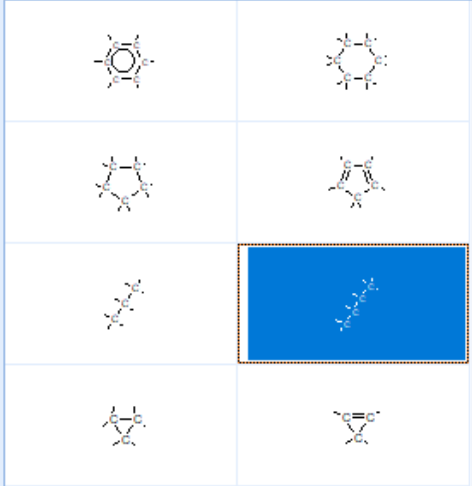
Drawing tool: Using 2D Editor: main functions

2D Editor

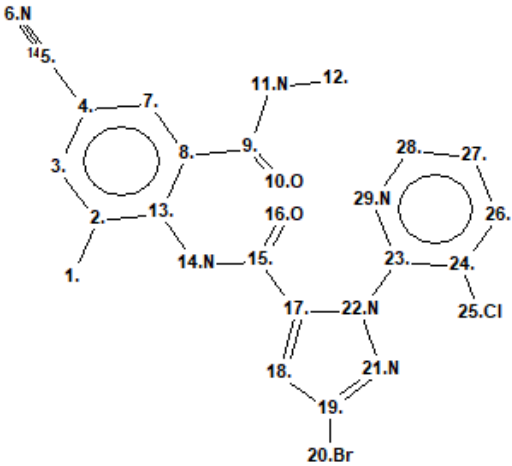
SMILES/InChI: Cc1cc(C(=O)Nc2cc(C(=O)Nc3cc(C(=O)N1C=CC(Br)=NN1c1c(Cl)cccn1)ccn1)ccn1)ccn1 Draw

000000-00-0

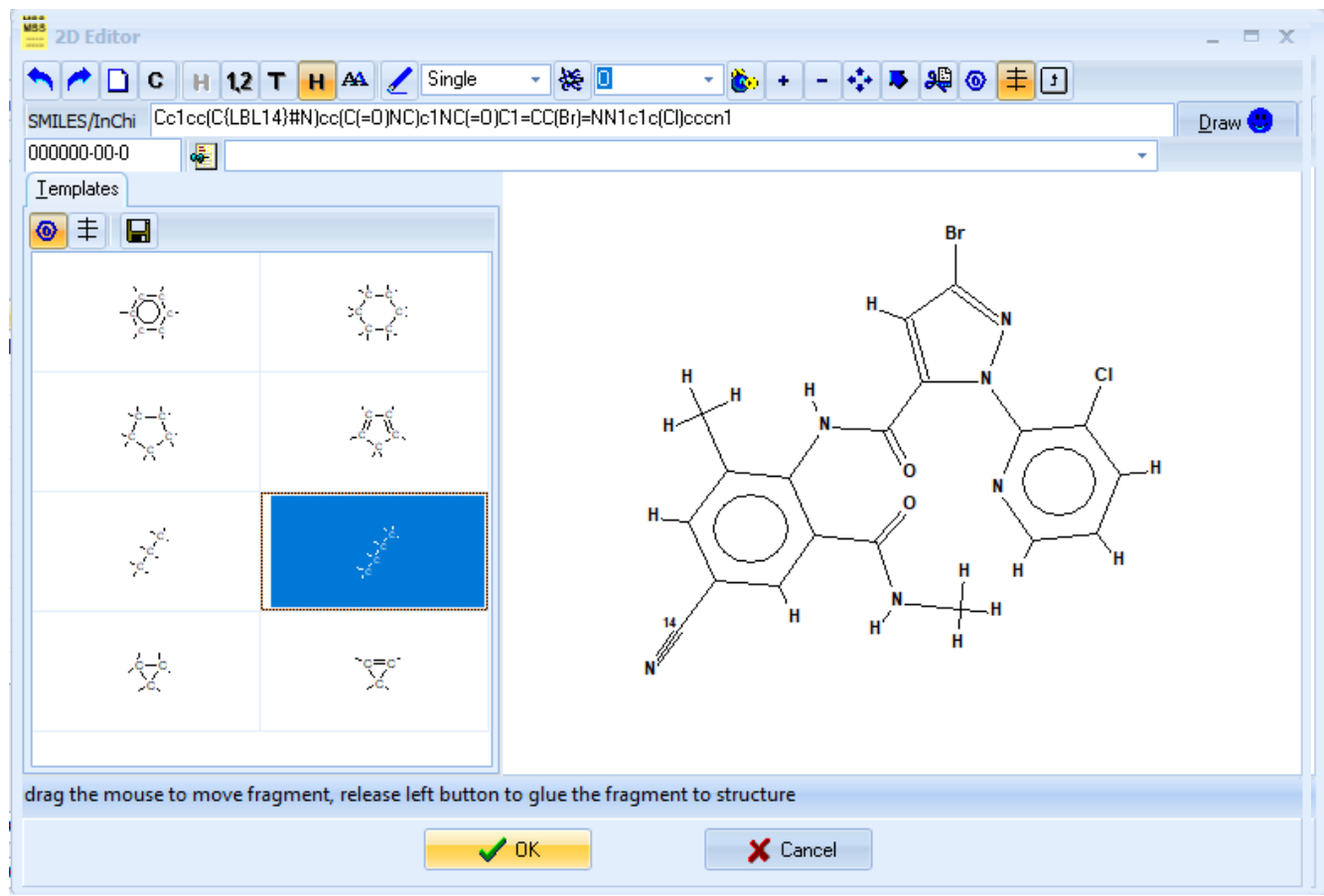
Templates



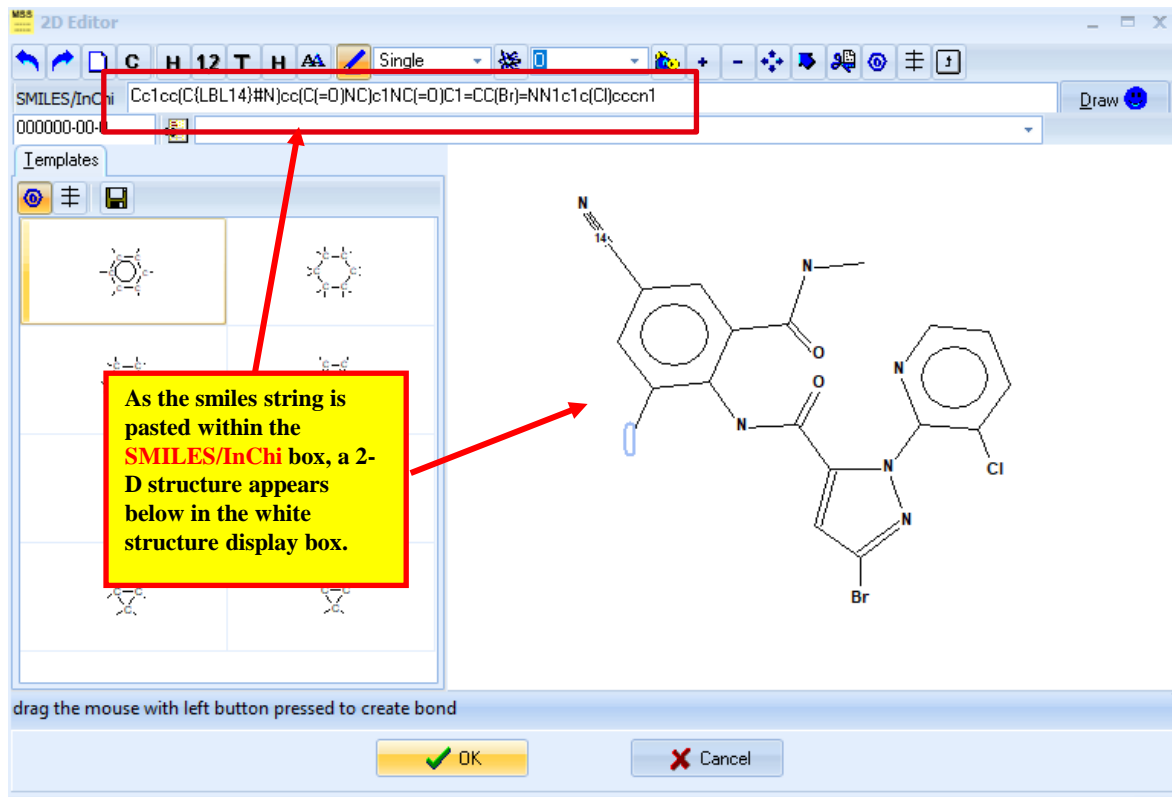
drag the mouse to move fragment, release left button to glue the fragment to structure



Drawing tool: Using 2D Editor: main functions



Drawing tool: Using 2D Editor: using SMILES codes



Drawing tool: Using 2D Editor: using SMILES codes

The screenshot shows the 2D Editor window with a toolbar at the top. The SMILES/InChi field contains the code: Cc1cc(C{LBL14}#N)cc(C(=O)NC(=O)C1=CC(Br)=NN1c1c(Cl)cccn1. The left sidebar shows a list of templates, with one highlighted by a blue circle and an arrow pointing to a yellow callout box. The main canvas displays a complex chemical structure, with a blue circle around a specific part of it and an arrow pointing to a yellow callout box. The bottom of the window has 'OK' and 'Cancel' buttons.

Templates for common structures may be created, stored and recalled for future use.

Ionic structures may be represented with + and - charges.

The four arrow icon allows you to move the structure.

The scissors icon is the delete or cut feature.

Drawing tool: Using 2D Editor : Radio labeling of atoms

usions V. Appenax V1. Attachments

MS Periodic Table

Periodic Table

1 H																	2 He						
3 Li	4 Be																	5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg																	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr						
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe						
55 Cs	56 Ba	57 *La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn						
87 Fr	88 Ra	89 *Ac																					

58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

Selected element: C(LBL14)

☒ Labeled
Number: 14

Drawing tool: Using 2D Editor : Radio labeling of atoms

The screenshot displays the 2D Editor window with the following components:

- Top Bar:** Includes icons for Bold (B), Italic (I), Underline (U), and ABC, along with buttons for "Insert Symbol" and "Build Metabolic Map".
- SMILES Input Field:** Contains the string Cc1cc(C#N)cc(C(=O)NC(LBL14)(=O)C1=CC(Br)=NN1c1c(C)cccn1. This field is highlighted with a green oval.
- Templates Panel:** Located on the left, it shows a grid of chemical structures for selection.
- Chemical Structure:** A complex molecule is shown in the center. A carbon atom in a ring is labeled with "14", indicated by a green arrow. A yellow box with the text "Uniformly ring labeled C-14" points to this label.
- SMILES String Label:** A yellow box with the text "Smiles string incorporating radio-label" points to the SMILES input field.
- Bottom Bar:** Contains the instruction "drag the mouse with left button pressed to create bond" and two buttons: "OK" (with a green checkmark icon) and "Cancel" (with a red X icon). The "OK" button is circled with a green oval.

Drawing tool: Using 2D Editor : Radio labeling of atoms

2D Editor

SMILES/InChI Cc1cc(C#N)cc(C(=O)NC(LBL14)(=O)C1=CC(Br)=NN1c1c(C)cccn1

000000-00-0

Templates

Directly remove "{LBLXX}" from the SMILES code

WARNING:
When copy/paste, don't forget to change the radiolabeling site

Str

The image shows a screenshot of a 2D chemical editor interface. At the top, there's a toolbar with various drawing tools. Below it, the SMILES/InChI input field contains a complex chemical formula: Cc1cc(C#N)cc(C(=O)NC(LBL14)(=O)C1=CC(Br)=NN1c1c(C)cccn1. A green oval highlights the "{LBL14}" part of the SMILES string. A yellow callout box with a green border points to this part, containing the text "Directly remove '{LBLXX}' from the SMILES code". Below the input field, there's a "Templates" section with a grid of chemical structures. To the right, a chemical structure is displayed, showing a complex molecule with a radiolabeling site marked with "14". A red banner at the bottom contains a warning icon (a bell) and the text "WARNING: When copy/paste, don't forget to change the radiolabeling site".

II. Materials and methods- A- Materials- 1. Test Material- Physicochemical Properties

MSS

MSS Composer (Plants) v.1.8

HOME

OPTIONS

New

Open

Save

Render

Cut

Copy

Paste

Insert Symbol

Build Metabolic Map

Document

Clipboard

Format

Tools

A. Materials

B. Study Design

Parameter	Notes	Value	Units
Melting point/range		[217-224]	°C
pH			
Density			
Water solubility (20°C)		12.33 * 0.61	ppm
Solvent solubility (mg/L at __°C)			
Vapour pressure at 20°C		5.133 * 10-15	Pa
Dissociation constant (pKa)	At 20°C	8.80 * 1.38	
Octanol/water partition coefficient Log(Kow)	At 22°C	1.97 ± 0.01	
UV/visible absorption spectrum			

II. Materials and methods- A- Materials- 1. Test Material- Physicochemical Properties

MSS Composer (Plants) 1.8

HOME OPTIONS

New Open Save Render Cut Copy Paste Clipboard Format Tools

Insert Symbol Build Metabolic Map

A right-click on the column header allows for the pop-up box in which the caption or column header may be edited. This feature is found in all tables

Crop 1 Crop 2

I. General Info II. Materials and Methods

A. Materials B. Study Design

A. MATERIALS

Table PhysChem Physicochem

Parameter

Melting point/range

pH

Density

Water solubility (20°C)

Solvent solubility (mg/L at ___°C)

Vapour pressure at 20°C

Dissociation constant (pKa)

Octanol/water partition coefficient Log(Kow)

UV/visible absorption spectrum

Table PhysChem

Caption: Notes

OK Cancel

Units	Reference
°C	
ppm	
Pa	

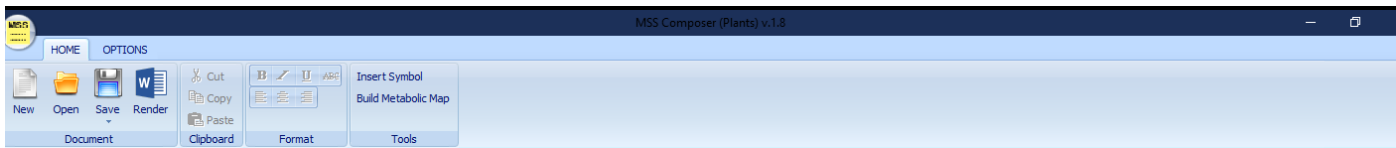
2. Test Crops

Table B.7.1.1-1. Crop Information.

Crop/Crop Group	Variety	Growth Stage at Application	Growth Stage at Harvest	Harvested Commodities	Harvesting Procedure
Tomato/Fruiting vegetables	Solanum lycopersicum, cv. Monsterrat	14- 61 BBCH	14- 99 BBCH	Foliage, leaves and fruits	

Test Site Type: other Outdoor plastic pots and then glasshouse

II. Materials and methods- A- Materials- 1. Test Material- Physicochemical Properties



Crop 1 Crop 2

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

A. Materials B. Study Design

Table PhysChem Physicochemical Properties.

Parameter	Notes	Value
Melting point/range		[217-224]
pH		
Density		
Water solubility (20°C)		12.33 * 0.61
Solvent solubility (mg/L at ____°C)		
Vapour pressure at 20°C		5.133 * 10 ⁻¹⁵
Dissociation constant (pKa)	At	8.80 * 1.38
Octanol/water partition coefficient Log(Kow)	At	1.97 ± 0.01
UV/visible absorption spectrum		

A right-click on the row allows for the pop-up box in which the User may edit the rows by inserting an additional row, clearing a row, deleting a row, copying a row or clearing the entire table. This feature applies to all tables within the Composer.

2. Test Crops

Table B.7.1.1-1. Crop Information.

Crop/Crop Group	Variety	Growth Stage at Application	Growth Stage at Harvest	Harvested Commodities	Harvesting Procedure
Tomato, Fruiting vegetables	Solanum lycopersicum, cv. Monsterrat	14- 61 BBCH	14- 99 BBCH	Foliage, leaves and fruits	

Test Site Type: other Outdoor plastic pots and then glasshouse

II. Materials and methods- A- Materials- 2. Test Crops

MSS Composer (Plants) v.1.8

HOME OPTIONS

New Open Save Render

Cut Copy Paste

Insert Symbol Build Metabolic Map

Document Clipboard Format Tools

Crop 1 Crop 2

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

A. Materials B. Study Design

Water solubility (20°C)		12.33 * 0.61	ppm
Solvent solubility (mg/L at ____°C)			
Vapour pressure at 20°C		5.133 * 10-15	Pa
Dissociation constant (pKa)	At 20°C	8.80 * 1.38	
Octanol/water partition coefficient Log(Kow)	At 22°C	1.97 ± 0.01	
UV/visible absorption spectrum			

2. Test Crops

Table B.7.1.1-1. Crop Information.

Crop/Crop Group	Growth Stage at Application	Growth Stage at Harvest	Identities	Harvesting Procedure
Tomato/Fruiting vegetables	14- 61 BBCH	14- 99 BBCH	ed fruits	

Test S
3. Soil
en glasshouse

Respect the following nomenclature: **Crop / Crop Group**

Two digits + unit :
19 BBCH
10 - 19 BBCH
0 : N/A



WARNING:
the information must start with a figure to appear once the MSS xml file imported into MetaPath.

II. Materials and methods- A- Materials- 2. Test Crops

MSS Composer (Plants) v.1.8

HOME OPTIONS

New Open Save Render Document Clipboard Format Tools

Crop 1 Crop 2

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

A. Materials B. Study Design

2. Test Crops

Table B.7.1.1-1. Crop Information.

Crop/Crop Group	Variety	Growth Stage at Application	Growth Stage at Harvest	Harvested Commodities	Harvesting Procedure
Tomato/Fruiting vegetables	Solanum lycopersicum, cv. Monsterrat	14- 61 BBCH	14- 99 BBCH	Foliage, leaves and fruits	

Test Site Type: other outdoor plastic pots and then glasshouse

3. Soil Type

Table B.7.1.1-2. Soil Physicochemical Properties.

Soil Type	pH	OM %	Sand %
Acidic commercial growing medium	6.4		

holding Capacity (at 1/3 CEC meg / 100 g

Select the right item in the drop-down list. If nothing corresponds, choose "other" and fill in the free-text field (max. 50 characters)

Please note that if another option than **"other"** is selected, the information displayed in the free-text field will not appear once the MSS xml file imported into MetaPath.

II. Materials and methods- A- Materials- 3. Soil type

MSU

HOME

OPTIONS

New

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Render

Cut

Copy

Paste

B

I

U

ABC

Insert Symbol

Build Metabolic Map

Document

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Tools

MSS Composer (Plants) v.1.8

Crop 1

Crop 2

I. General Info

II. Materials and Methods

III. Results and Discussion

IV. Conclusions

V. Appendix

VI. Attachments

A. Materials

B. Study Design

Solvent solubility (mg/L at ____°C)

Vapour pressure at ____°C

Dissociation constant (pKa)

Octanol/water partition coefficient Log(Kow)

UV/visible absorption spectrum

2. Test Crops

Table B.7.1.1-1. Crop Information.

Crop/Crop Group

Variety

Growth Stage at Application

Growth Stage at Harvest

Harvested Commodities

Harvesting Procedure

Test Site Type

Soil Type

Table B.7.1.1-2. Soil Physicochemical Properties.

Soil Type

pH

OM %

Sand %

Silt %

Clay %

Moisture Holding Capacity (at 1/3 bar)

CEC meq / 100 g

Environmental Conditions

Temperature

Rainfall

Lighting

Potential for Photodegradation of Substance

II. Materials and methods- B- Study Design

Experimental Conditions and Sampling

MSS Composer (Plants) v.1.8

HOME OPTIONS

New Open Save Render Cut Copy Paste Format Tools

Document Clipboard Format Tools

Insert Symbol Build Metabolic Map

Briefly describe how samples were taken, parts sampled, how samples were handled after harvesting (shipment, storage, etc.) and any preparation that was done prior to extraction

Crop 1 Crop 2

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

A. Materials B. Study Design

B. STUDY DESIGN

Experimental Conditions

Table B.7.1.1-3. Use Pattern Information.

Parameter
Chemical name
Application method
Application rate
Number of applications
Timing of applications
PHI

Application Rate : use a.s. as an abbreviation: : 1000 g a.s./ha

Sampling

Free-text field: briefly describe how samples were taken, parts sampled, how samples were handled after harvesting (shipment, storage, etc.), and any preparation that was done prior to extraction

II. Materials and methods- B- Study Design

Extraction and Analysis; Identification and characterization

MSS Composer (Plants) v.1.8

HOME OPTIONS

New Open Save Render Cut Copy Paste Format Tools

Document Clipboard Format Tools

Insert Symbol Build Metabolic Map

Briefly describe how samples were taken, parts sampled, how samples were handled after harvesting (shipment, storage, etc), and any preparation that was done prior to extraction.

Crop 1 Crop 2

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

A. Materials B. Study Design

Sampling

Extraction and Analysis

es #1

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

Free-text field

Identification and Characterization

Free-text field

View will open the attached file for viewing. The image will be embedded in the rendered Word Study Summary Document.

Ability to attach figures/graphs of Extraction Schemes. Must be image files (i.e., jpeg, tiff etc...). Click on **Attach to upload file. Image will render with Word document.**

IV. Materials & Methods

Live session