RÉPUBLIQUE FRANÇAISE
*Liberté*
*Égalité*
*Fraternité*

anses

efsa
European Food Safety Authority

# 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

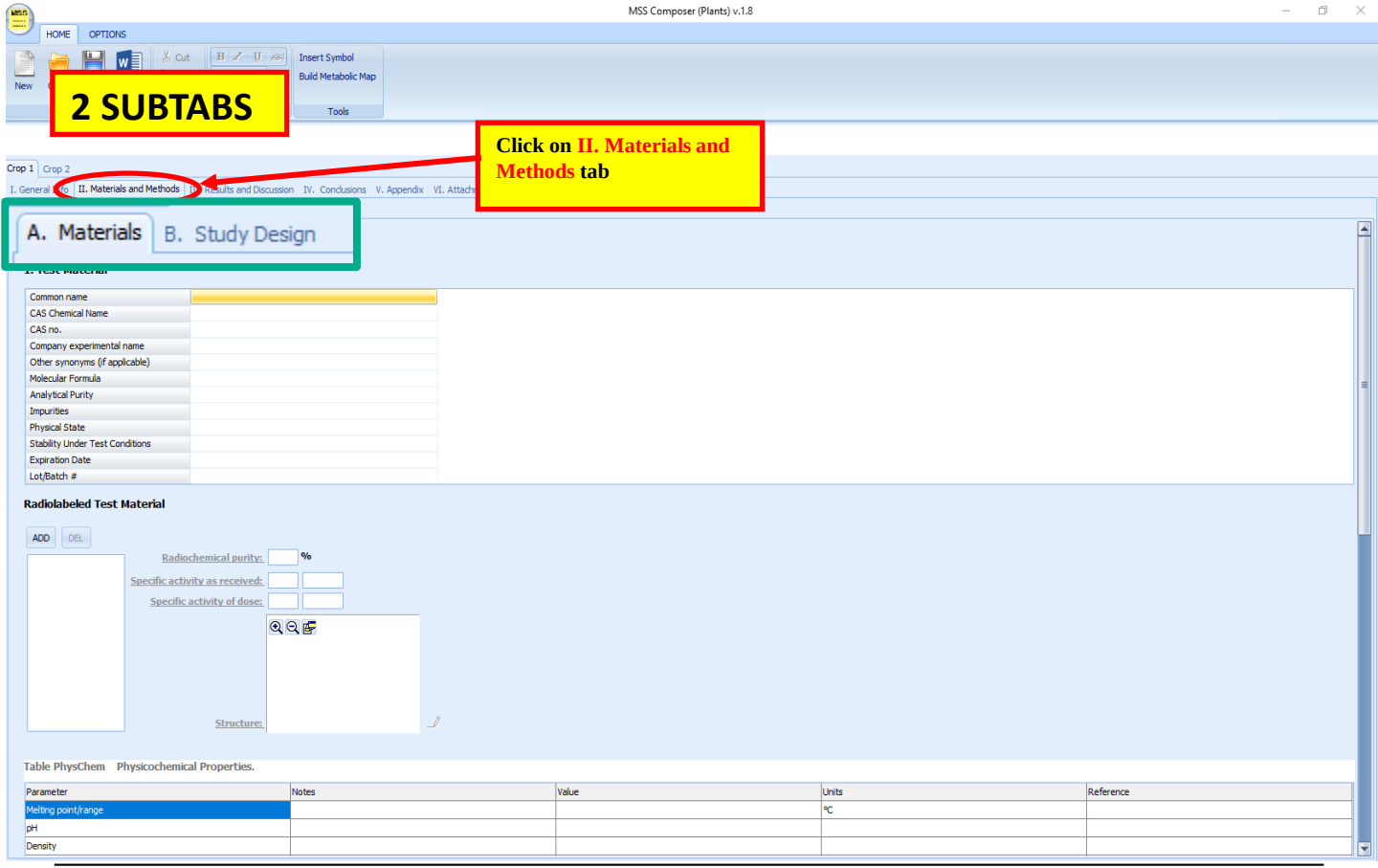
VIII. Attachment , Render & Conclusion

IX. Key points / Q&A

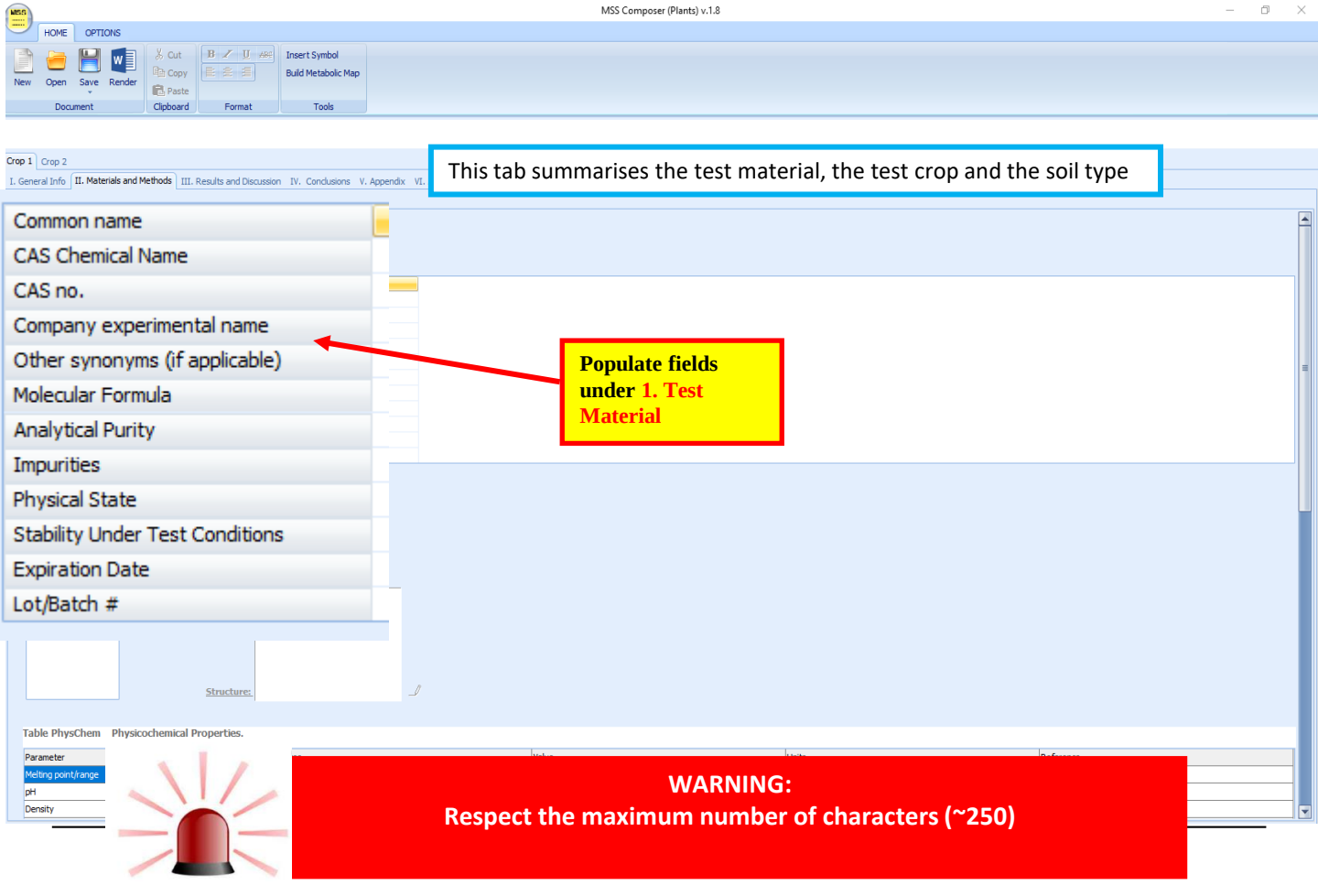
# IV. Materials & Methods

## Materials and study design

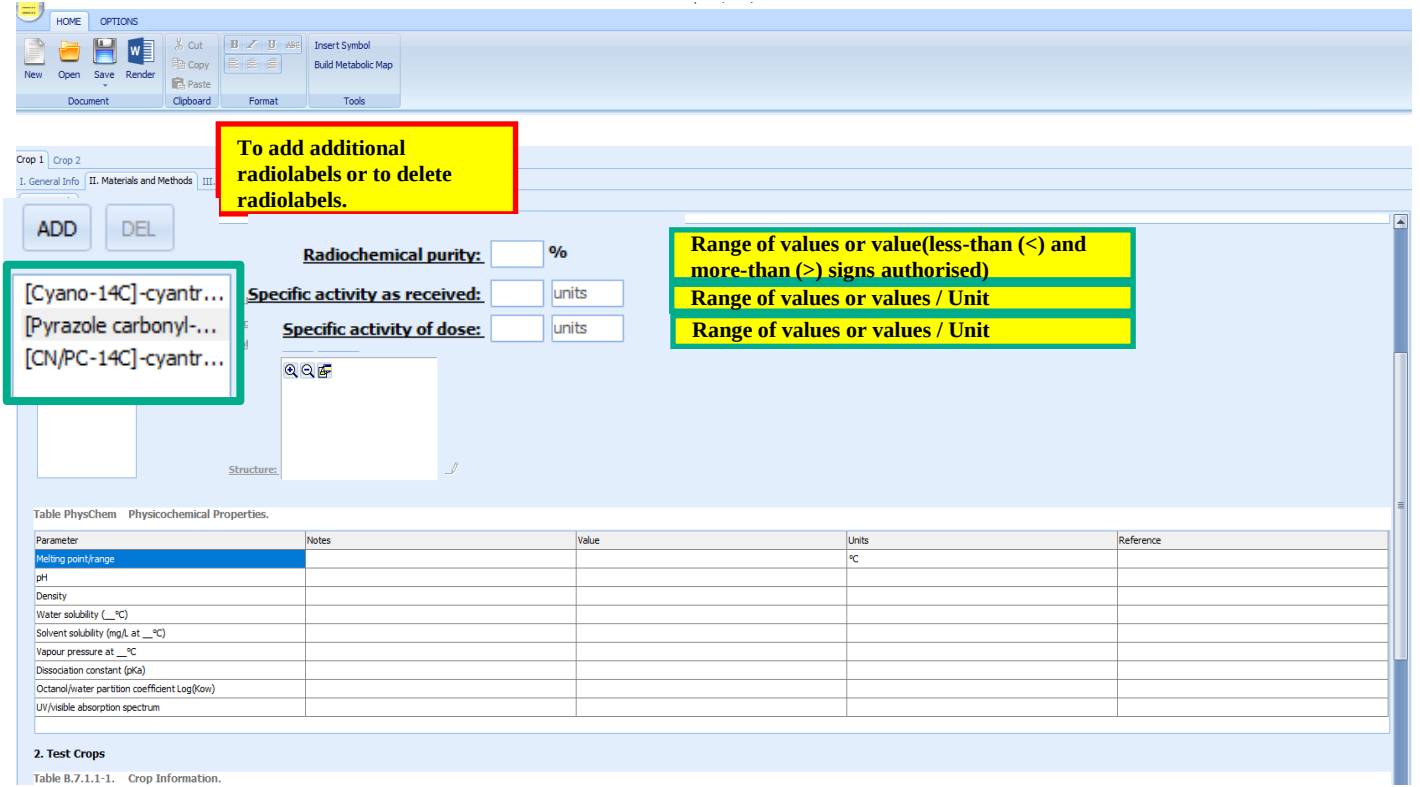
# II. Materials and methods



# II. Materials and methods- A- Materials



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



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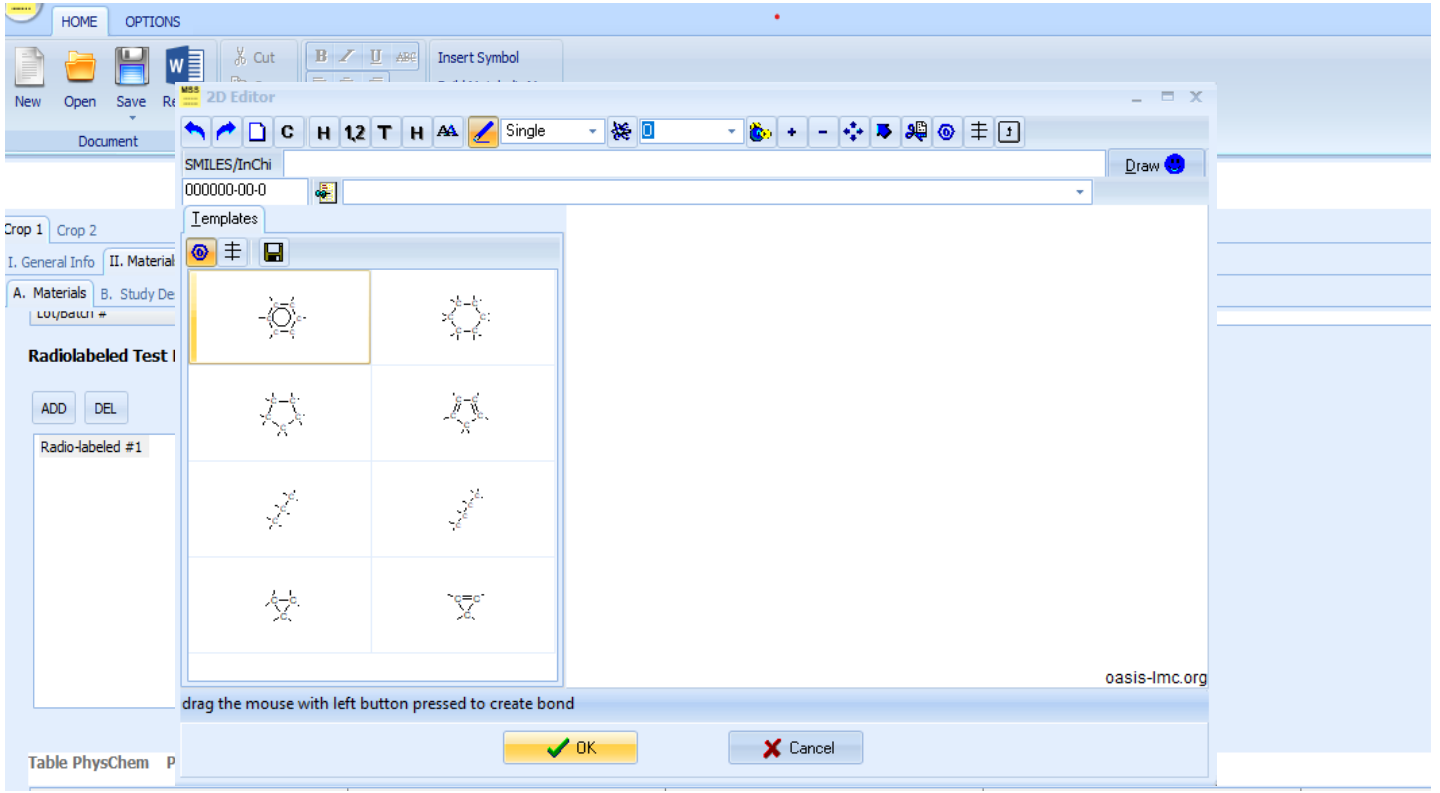
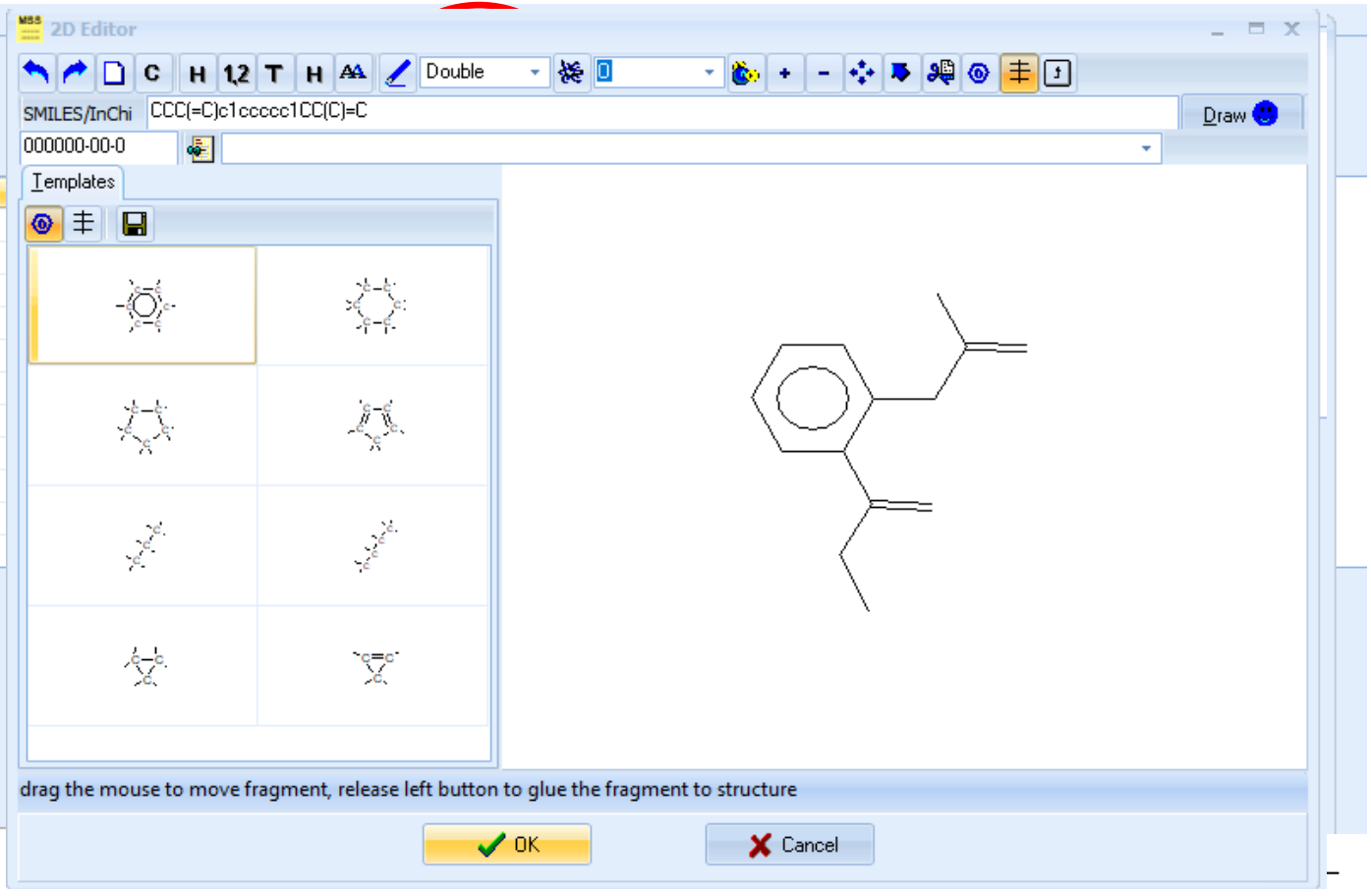
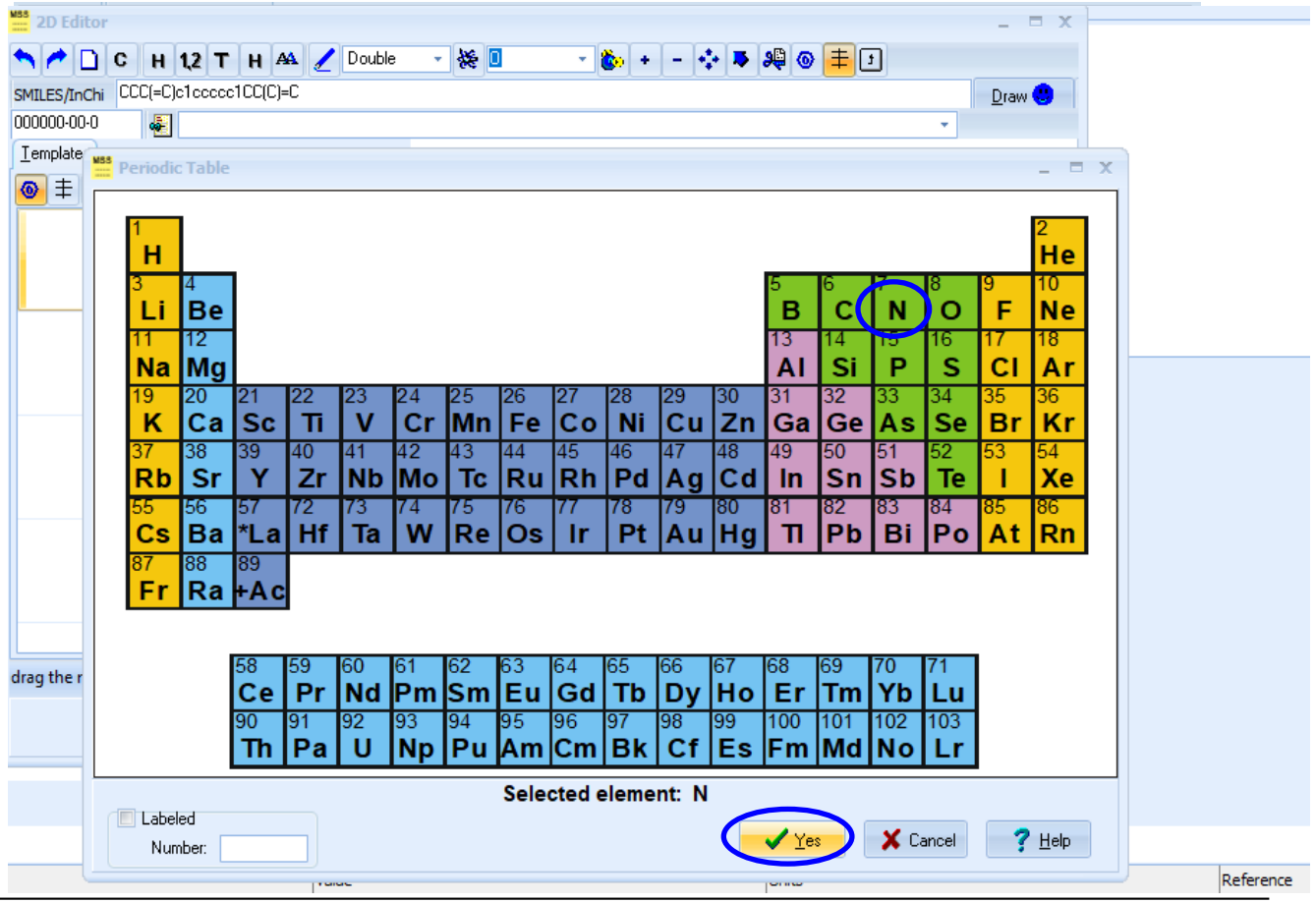


# Drawing tool: Using 2D Editor: draw the structure



# Drawing tool: Using 2D Editor: Modify the atom



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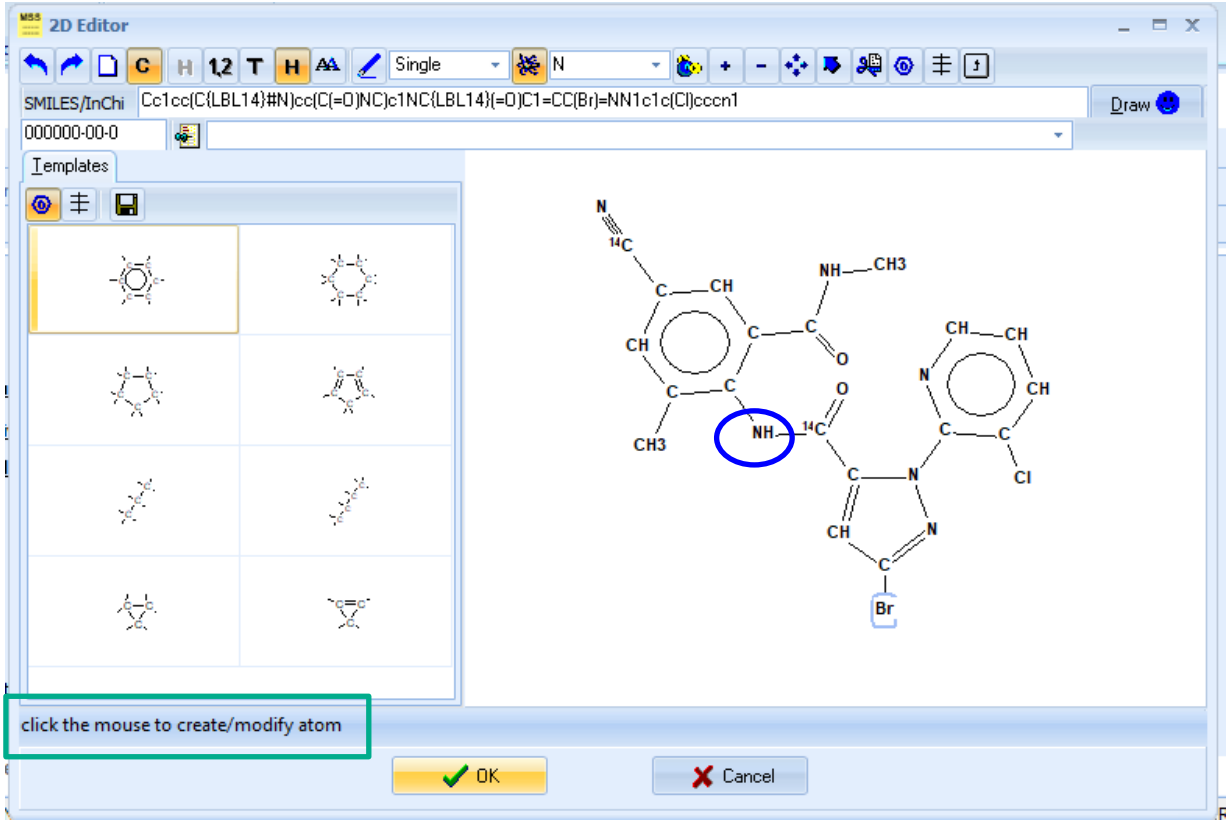
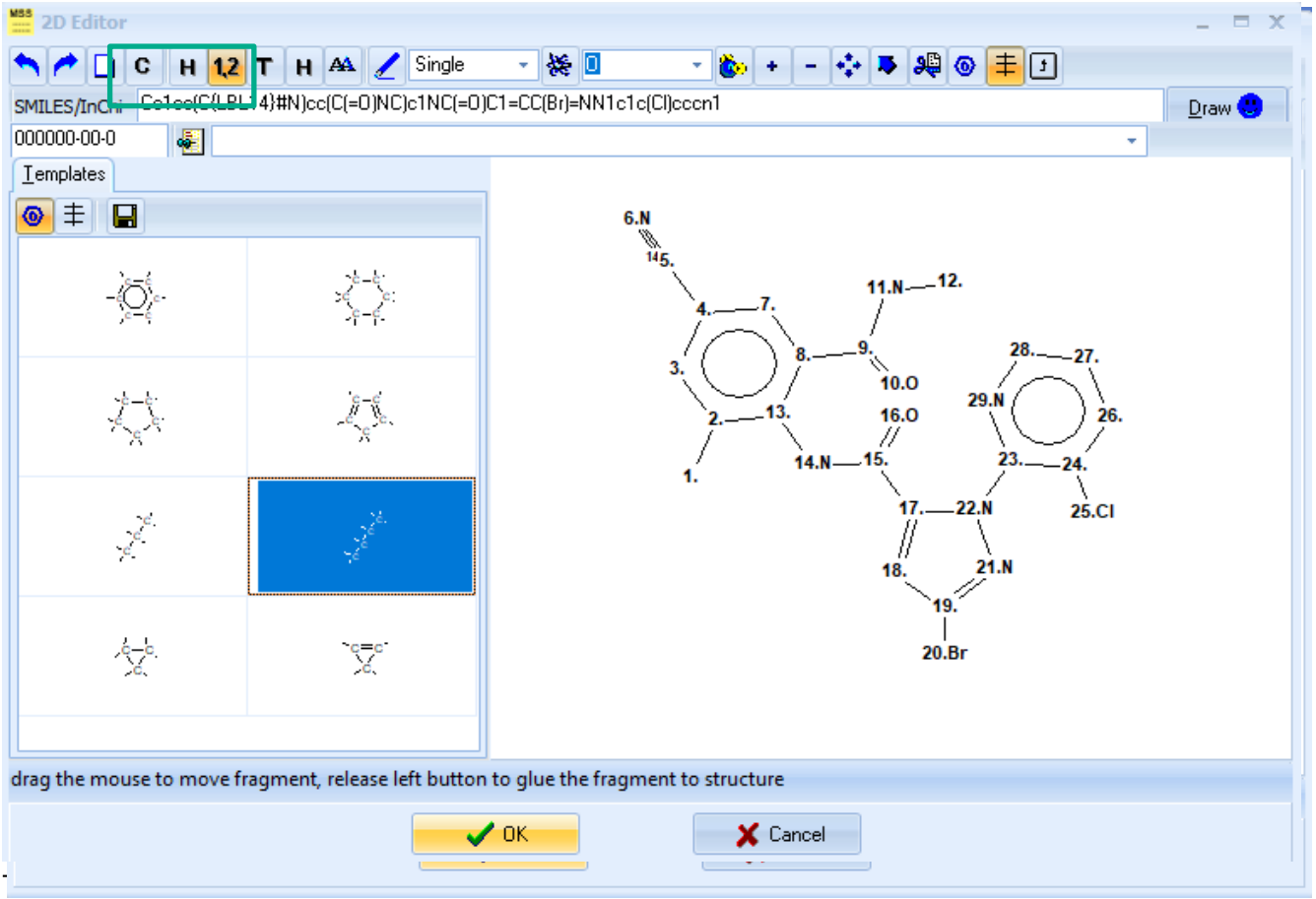


# Drawing tool: Using 2D Editor: main functions



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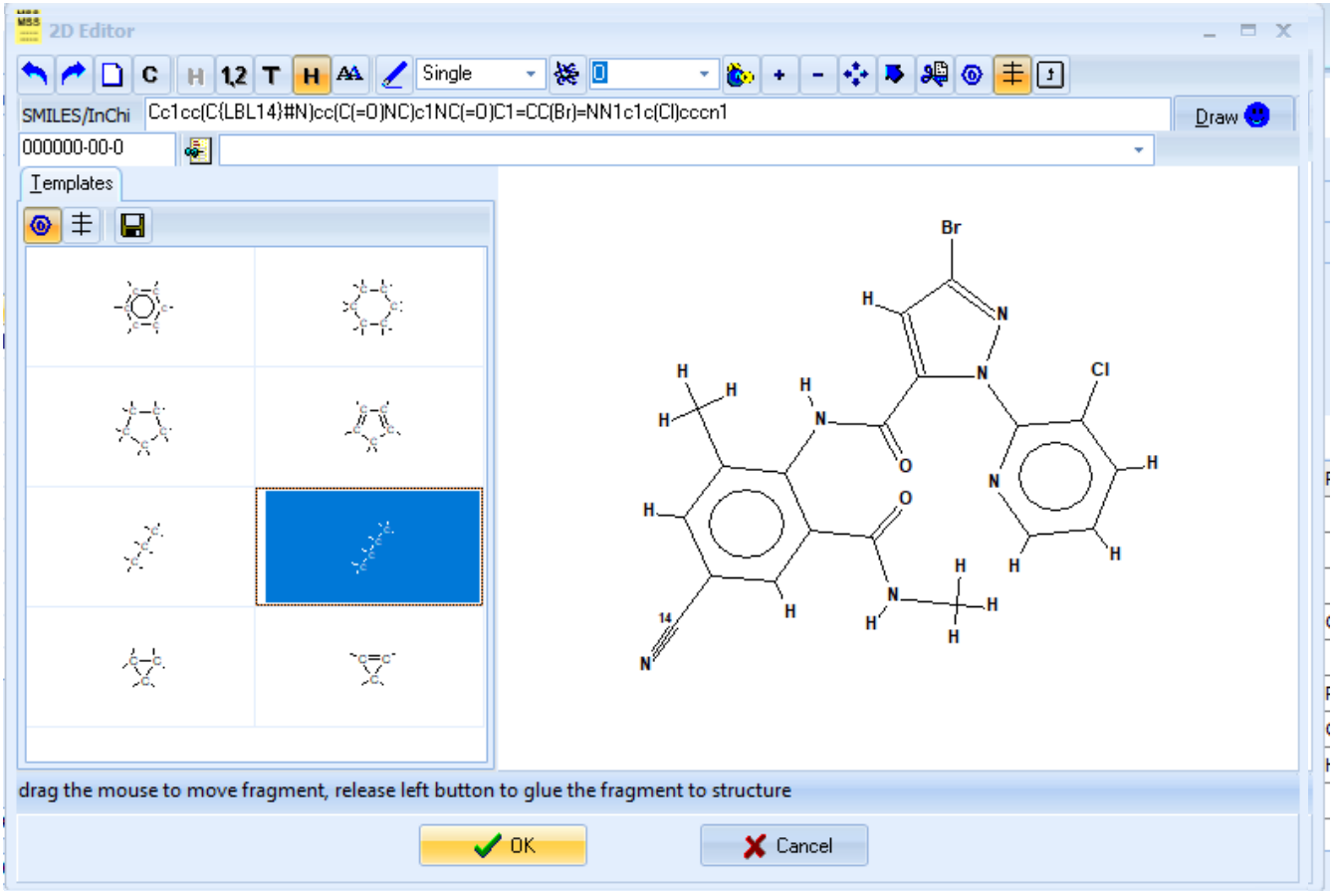
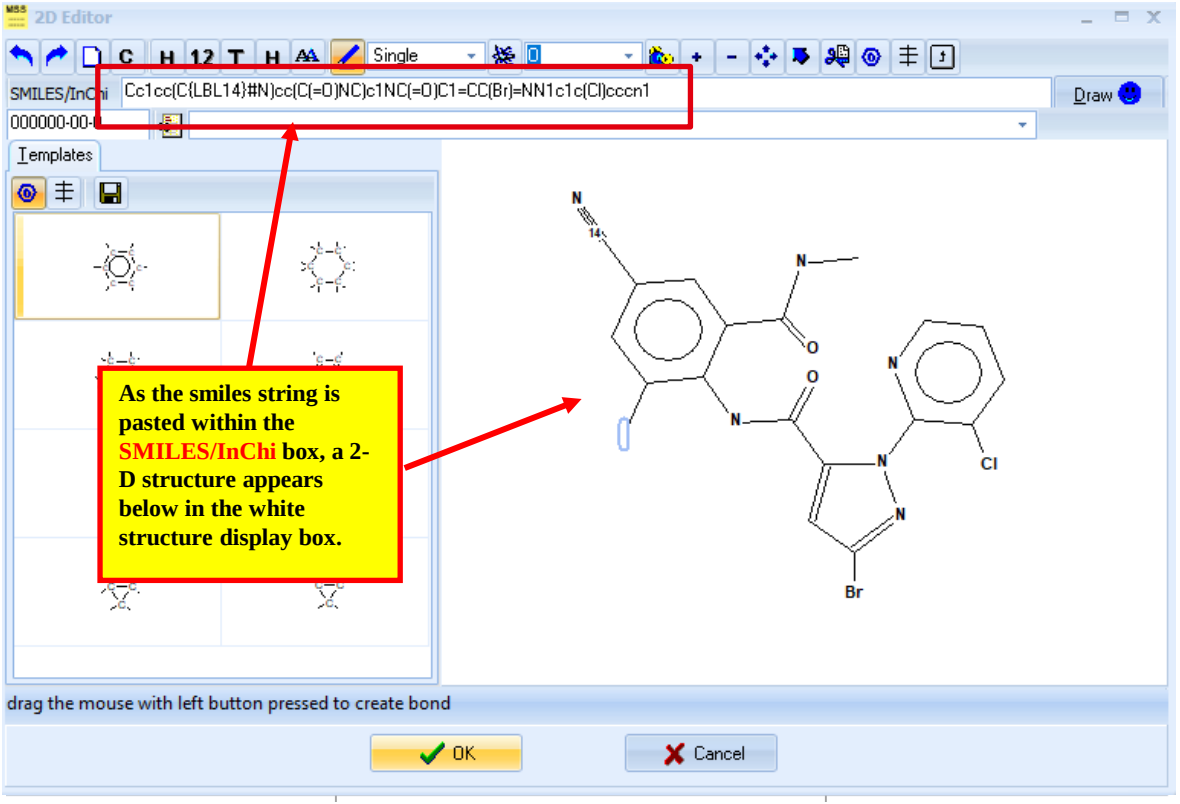


# Drawing tool: Using 2D Editor: using SMILES codes



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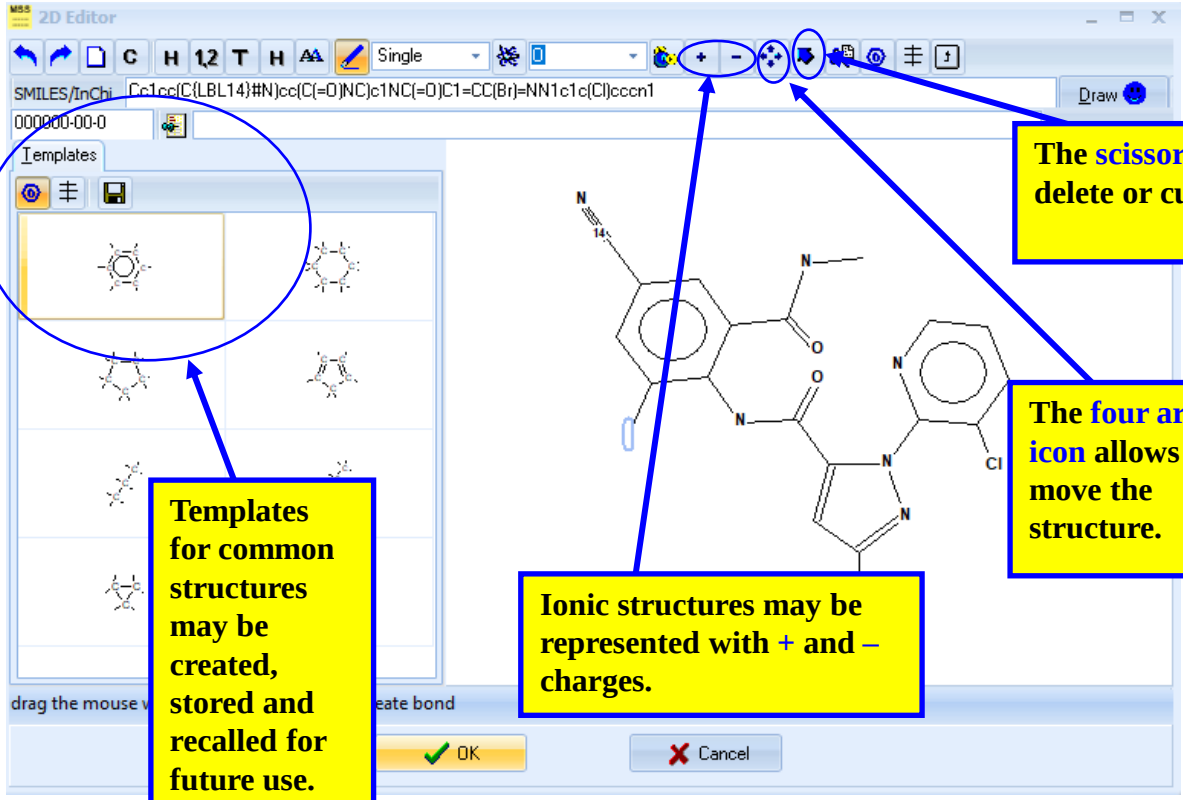
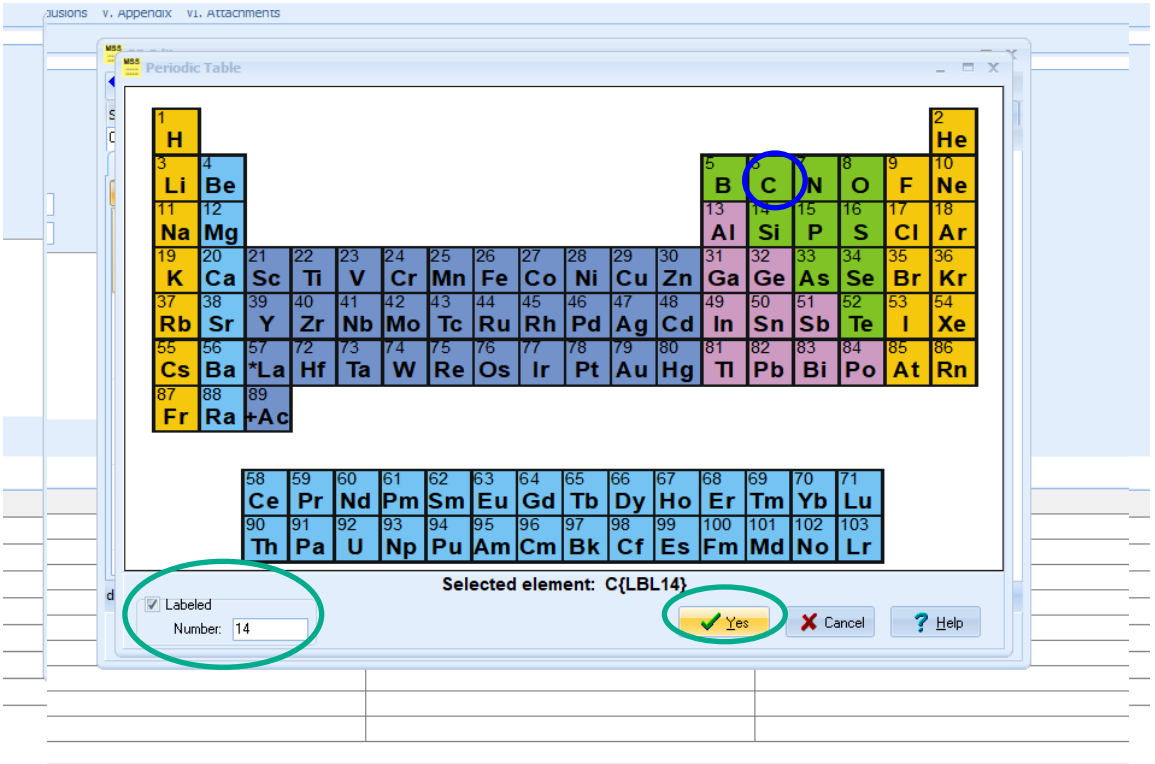


# Drawing tool: Using 2D Editor : Radio labeling of atoms



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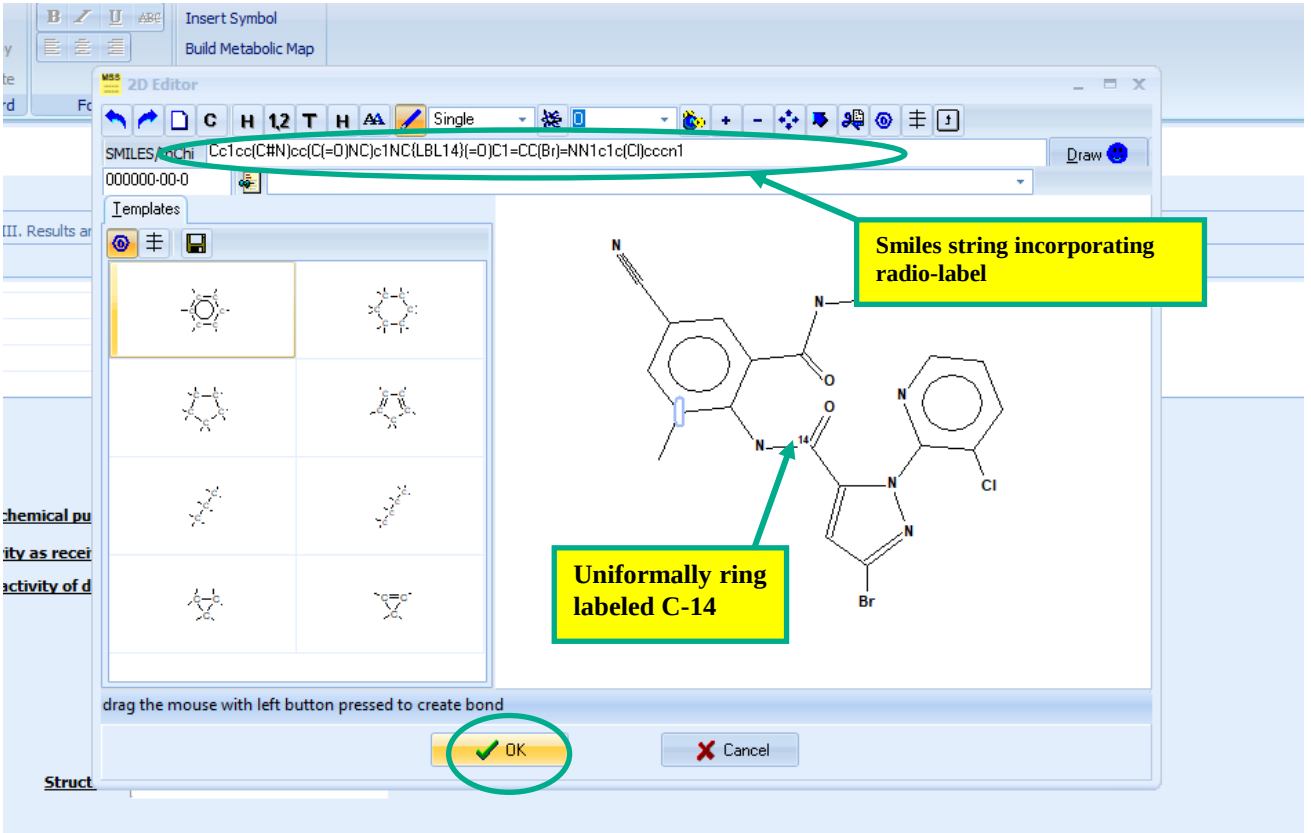

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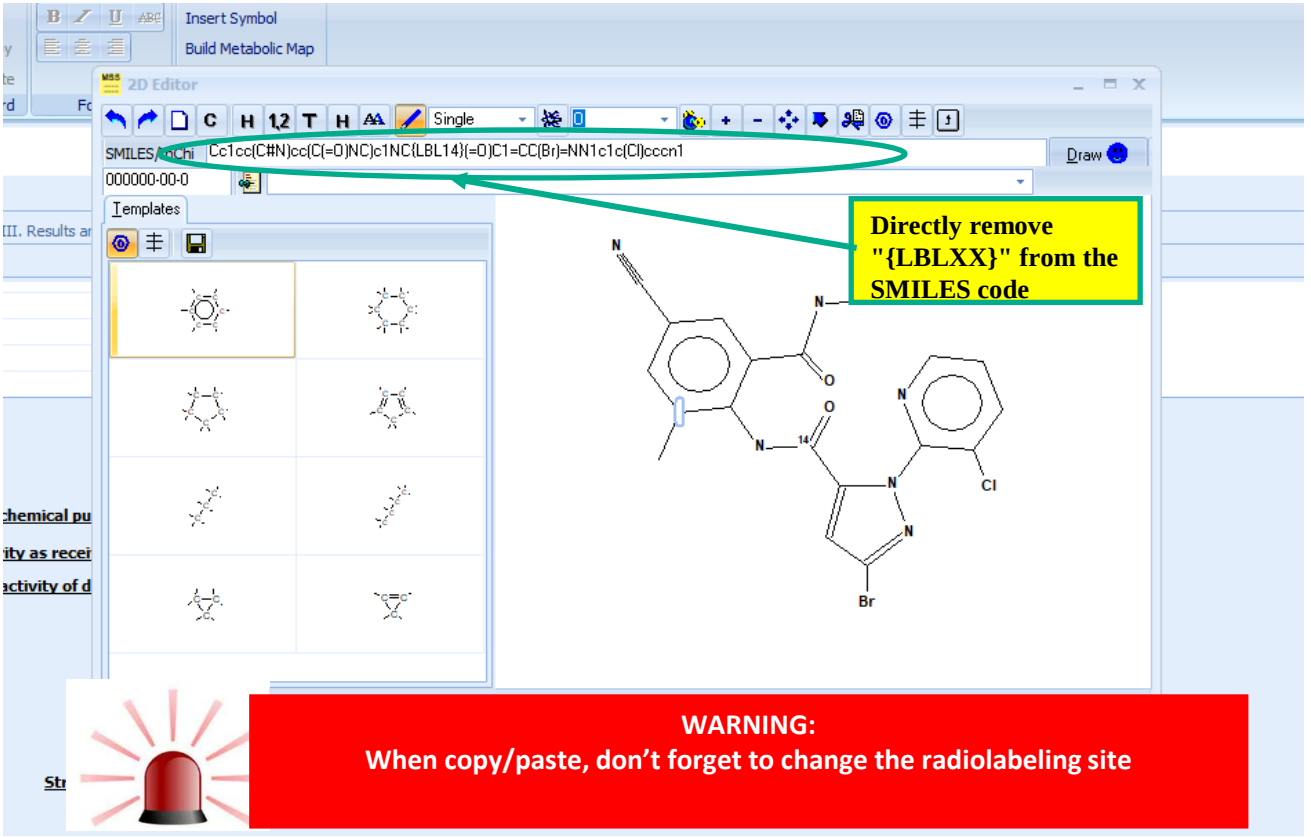
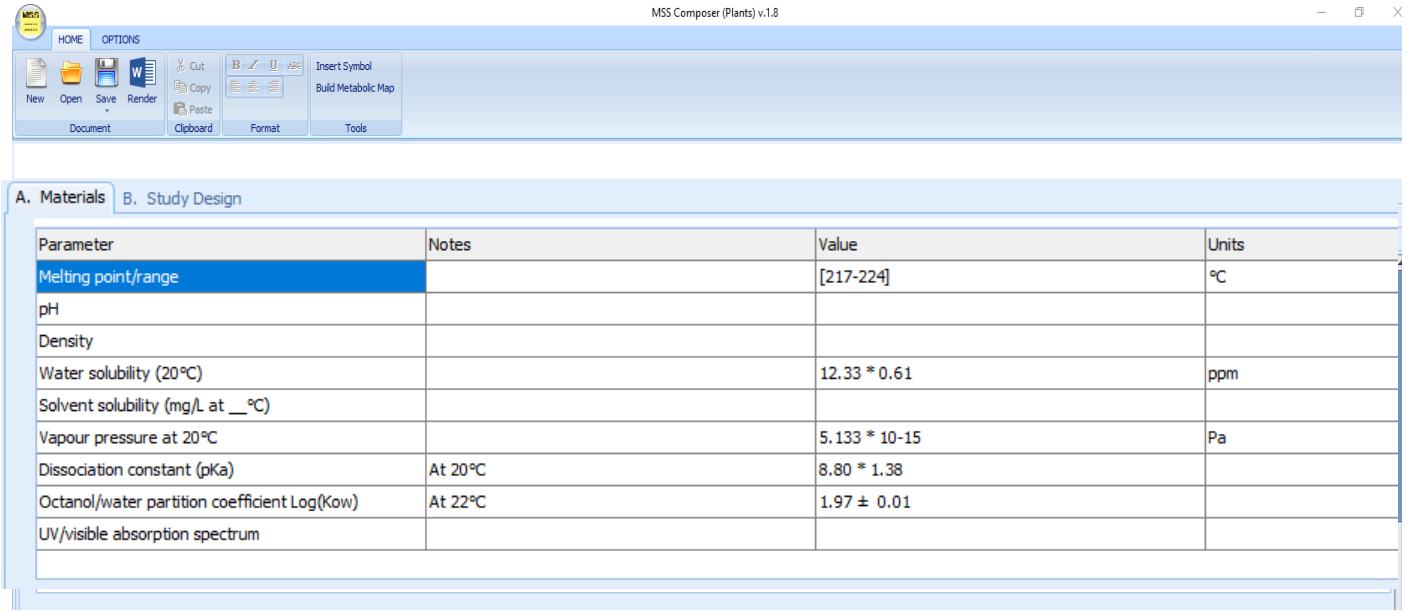
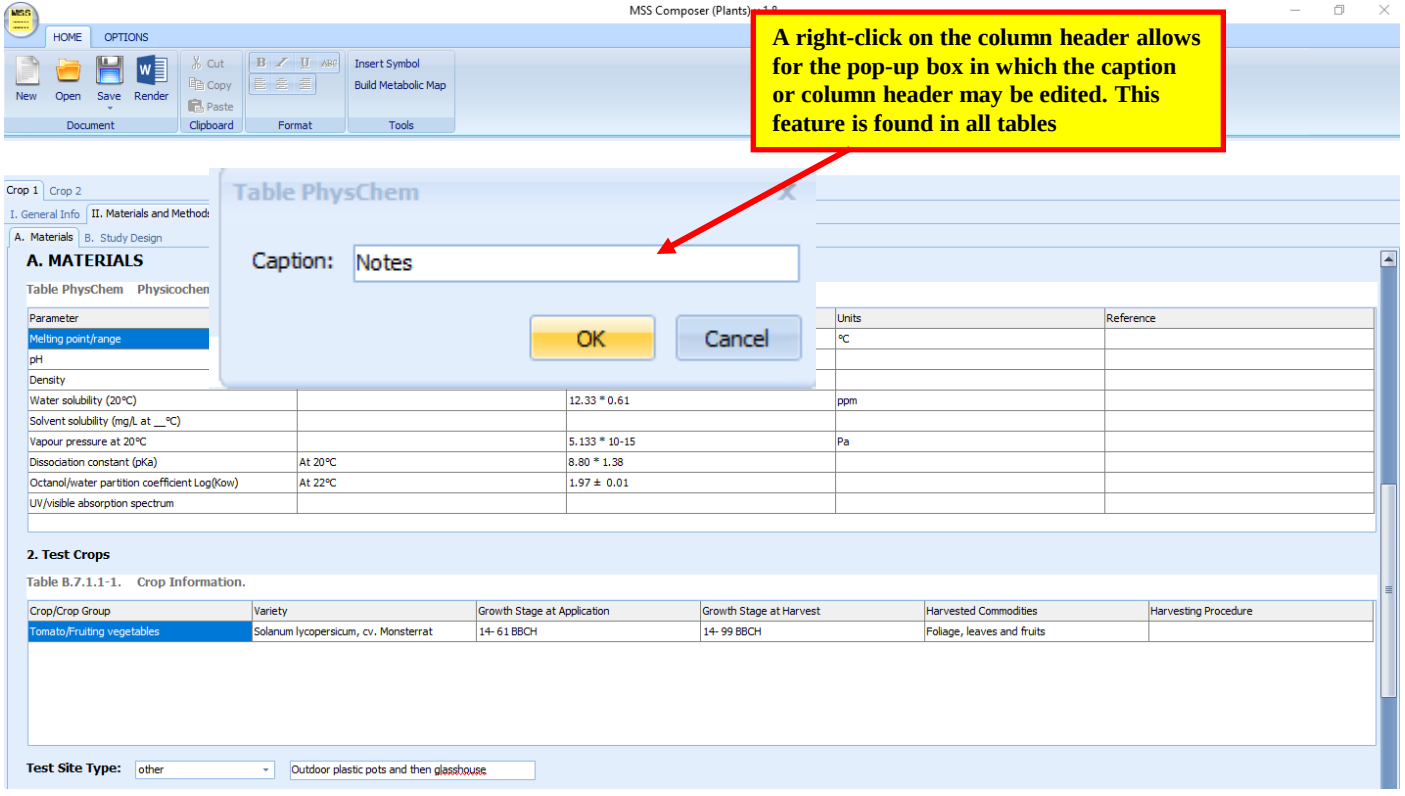


# II. Materials and methods- A- Materials- 1. Test Material- Physicochemical Properties




| 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



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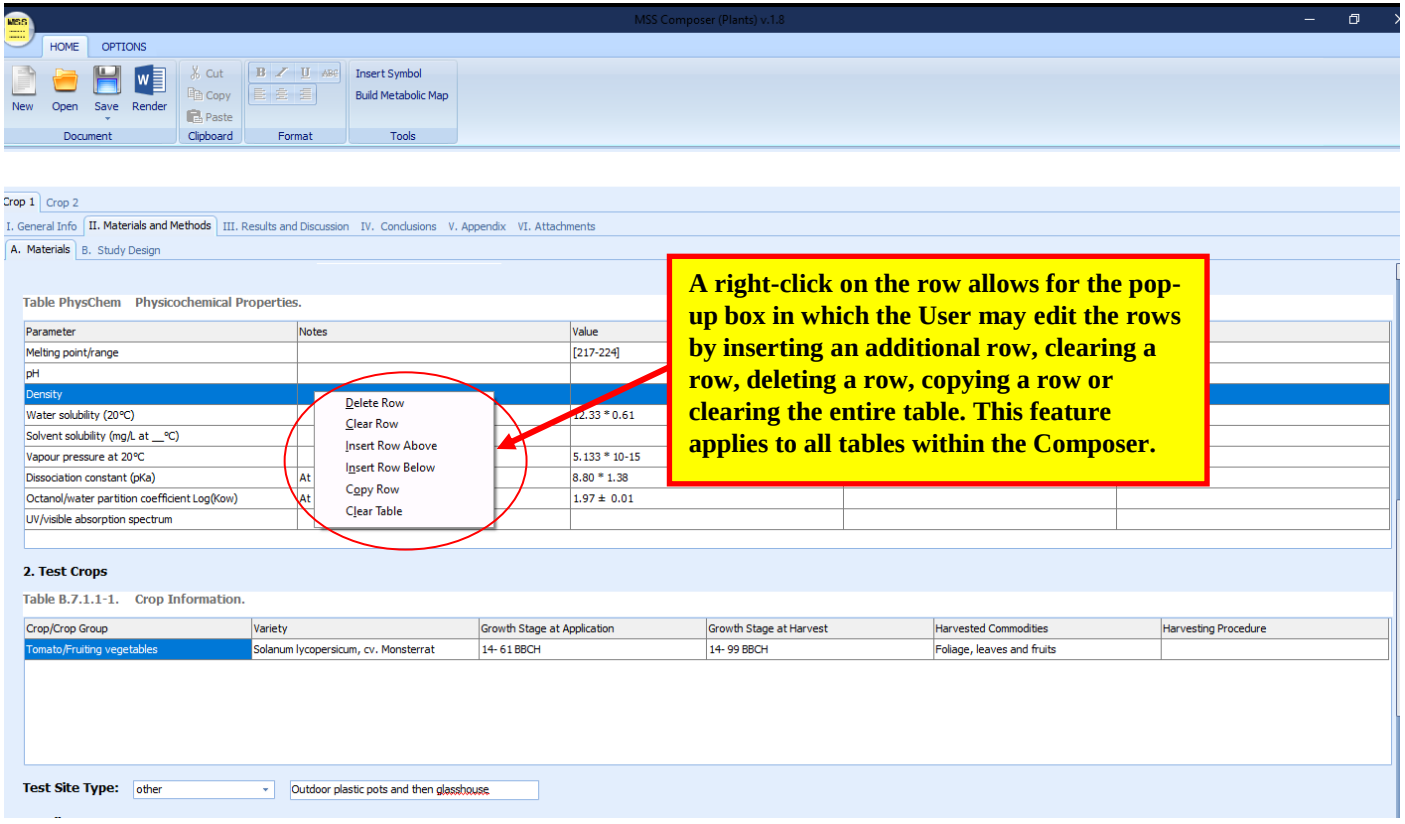
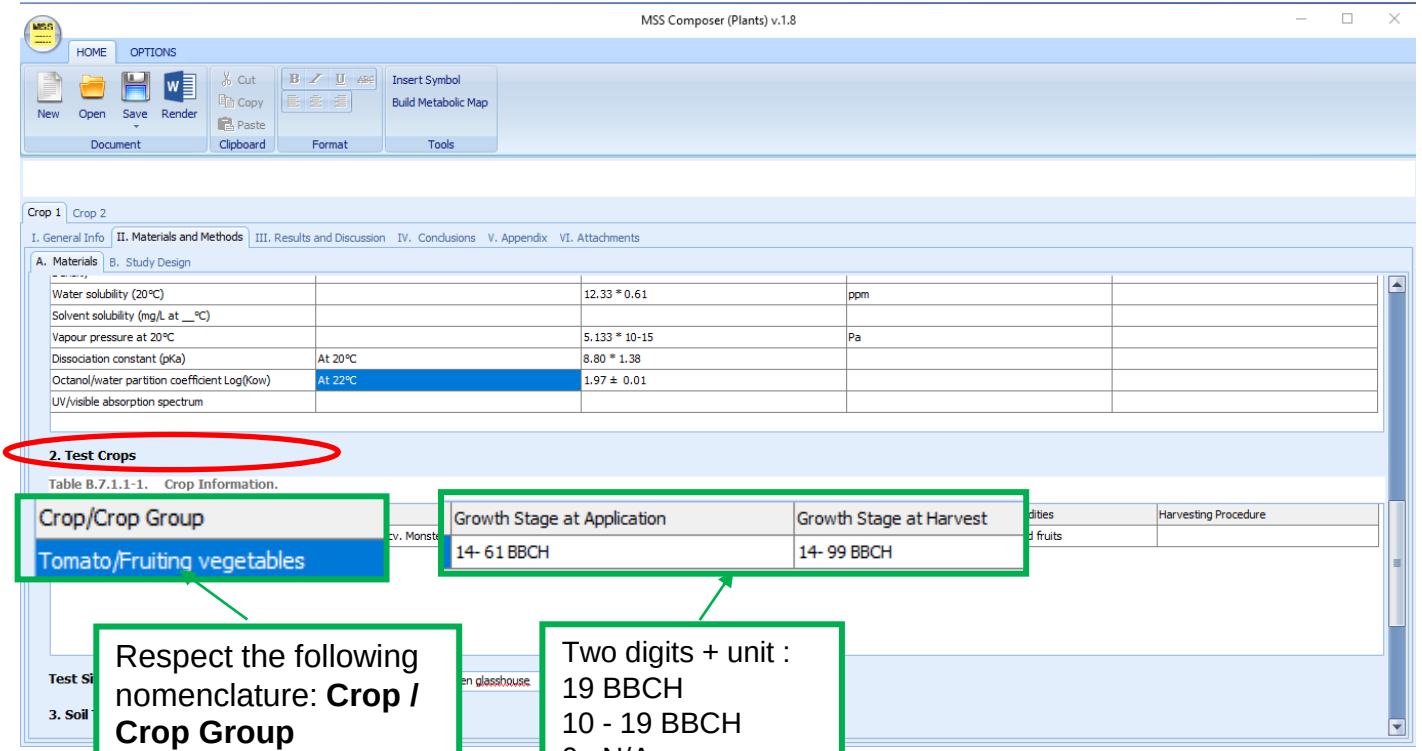
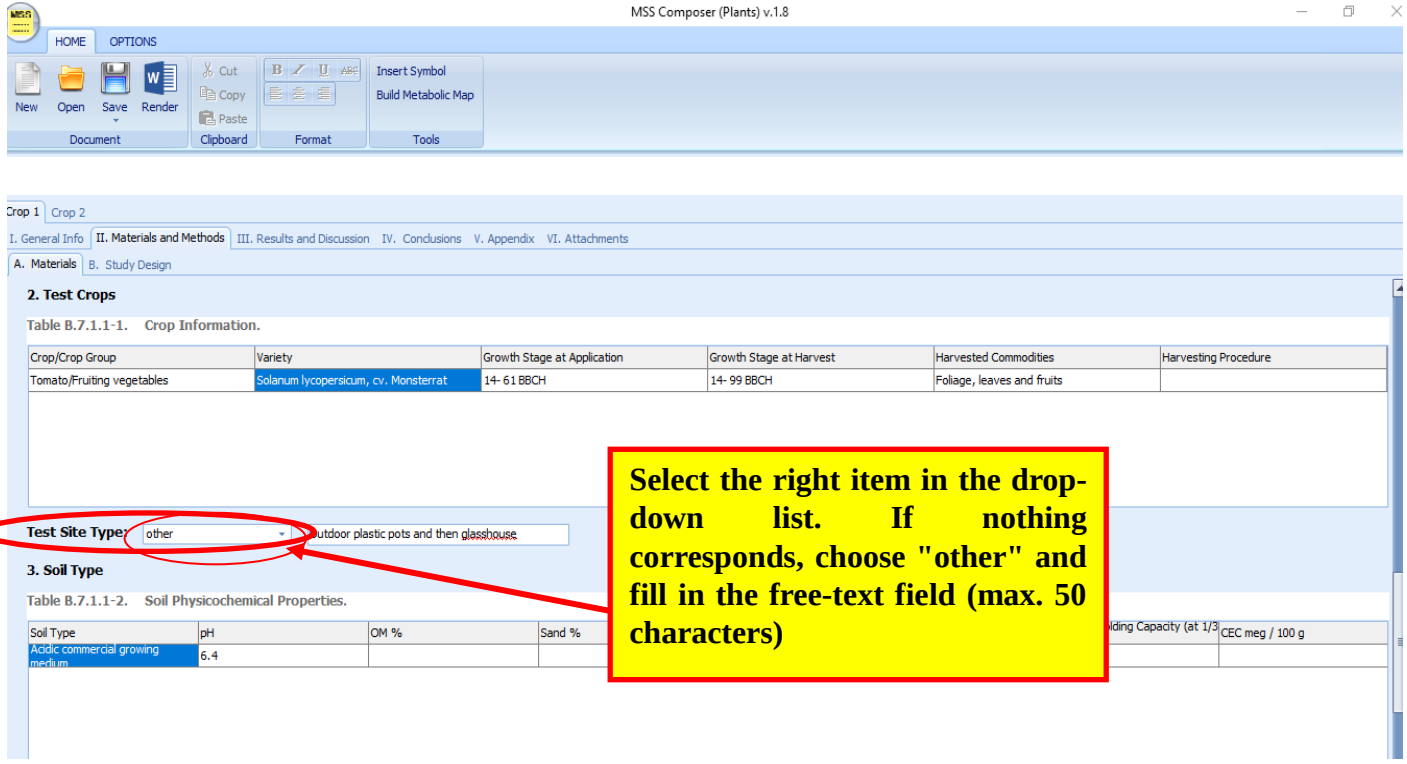


# II. Materials and methods- A- Materials- 2. Test Crops




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

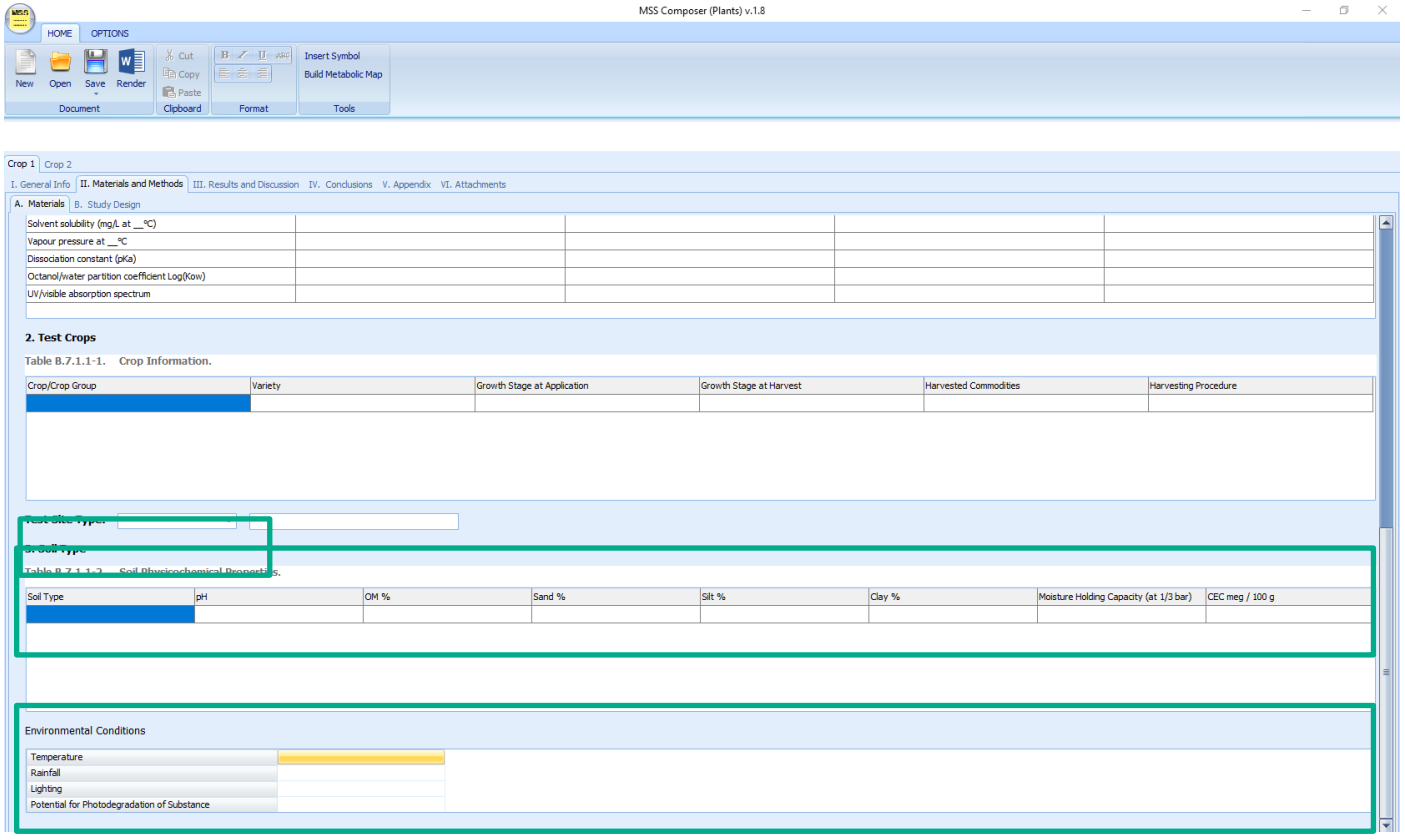
# II. Materials and methods- A- Materials- 2. Test Crops



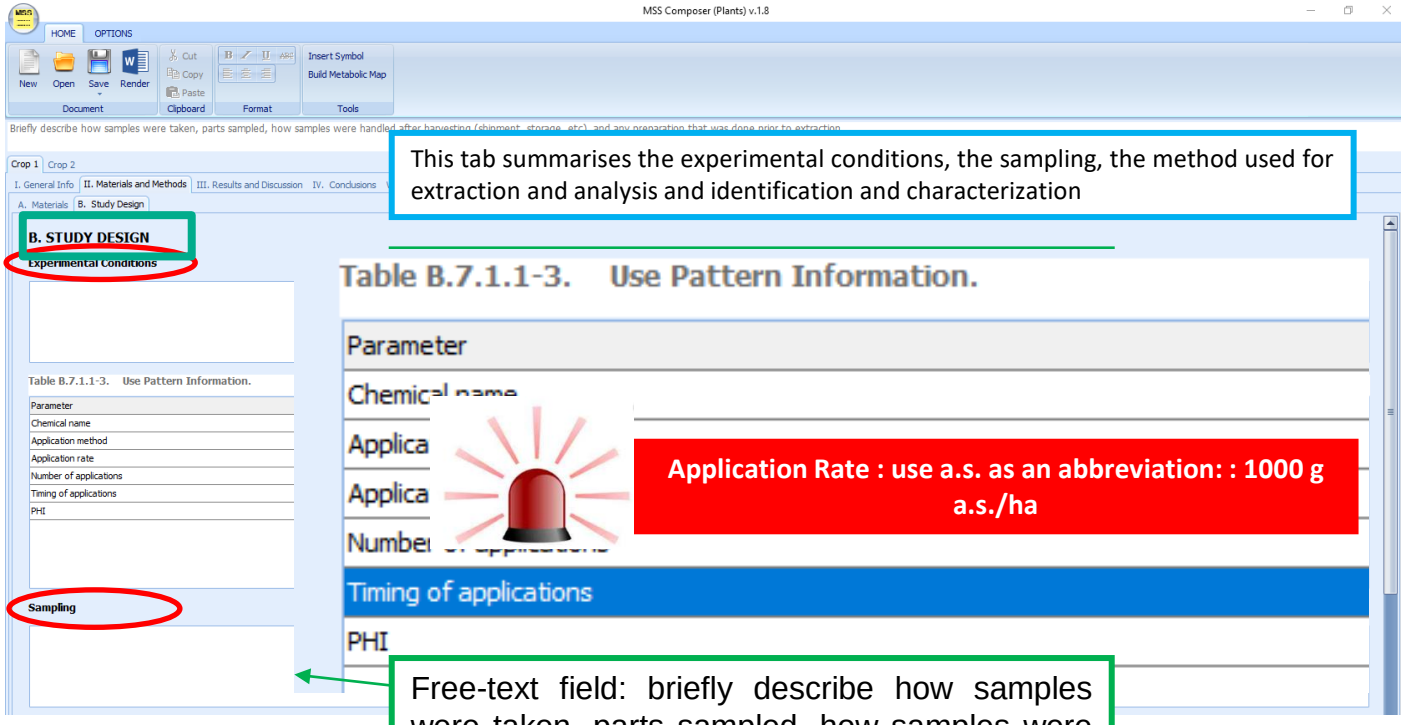

**Select the right item in the drop-down list. If nothing corresponds, choose "other" and fill in the free-text field (max. 50 characters)**

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



# II. Materials and methods- B- Study Design
# Experimental Conditions and Sampling

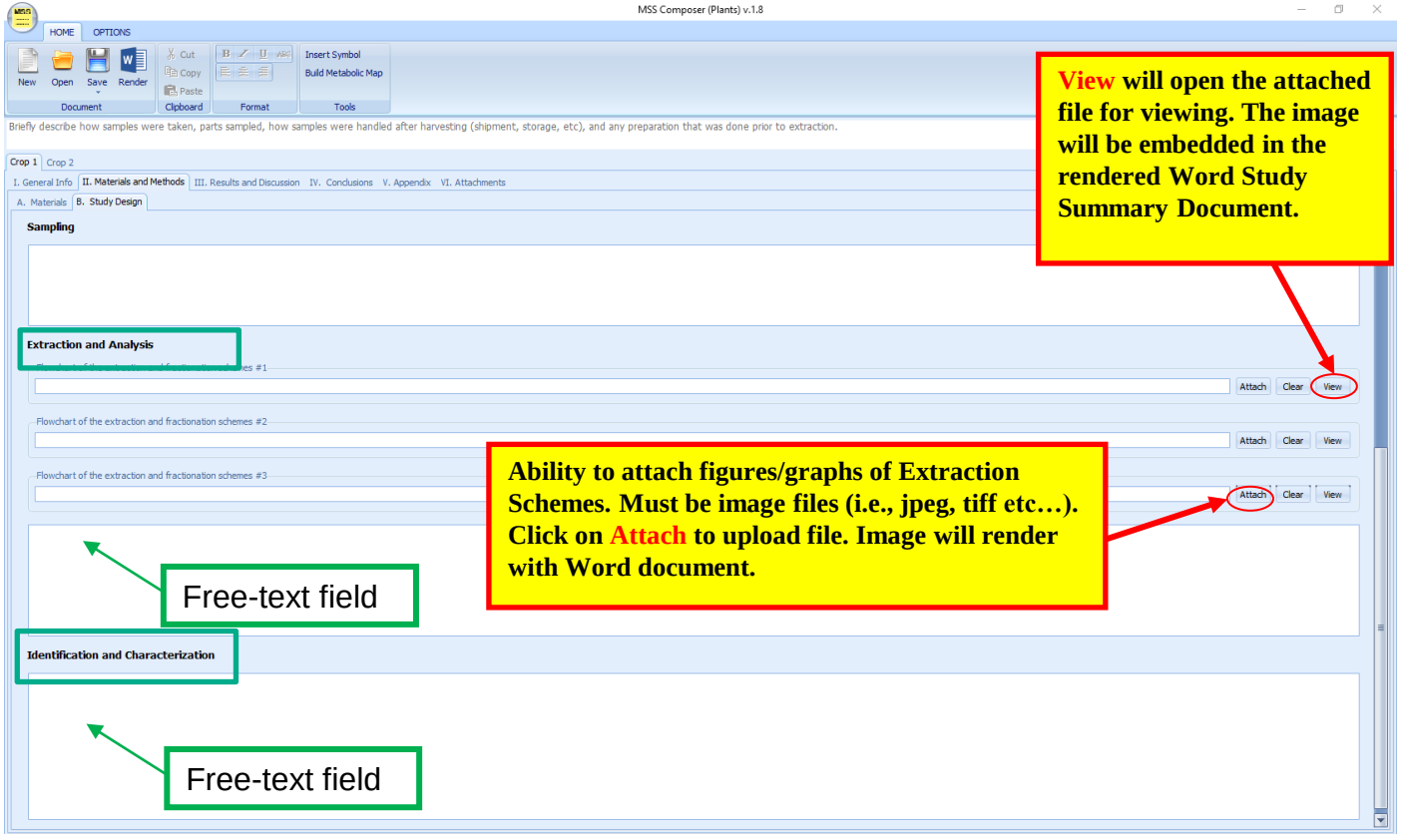



This tab summarises the experimental conditions, the sampling, the method used for extraction and analysis and identification and characterization

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

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; Identication and characterization



# IV. Materials & Methods

## Live session