

XEML DESIGNER

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XEML Designer Tutorial

1) Introduction

The Xeml Designer software was initially developed to invite biologists to share metadata collected during their experiments. The Xeml Lab Designer provides an interactive timeline visualisation that enables the intuitive design of experiments in terms of growth conditions and sampling strategy using related Ontologies (Xeo, EnvO, EO) while the corresponding metadata are automatically stored in the background in Xeml standardized format, ready for data mining. With these data on data, also known as "metadata", several statistical analyzes can be implemented to better understand the links between environmental and/or experimental conditions and metabolic profiles (e.g., in the context of plant development). Here, we present a new version of Xeml Designer able to work on Windows, Mac and Linux working system. Some functionalities are still in development like ISA export, And database connection.

2) Xeml Designer Main Window

Xeml Designer is composed of three different windows, each with his own role. The left Window represents the ontology view. It contains all ontology terms using to describe environmental variables. All environment ontologies are represented (XEO, EnvO, EO). The top right window shows the timeline of the experiment. Here is the main window of the Designer. From this window, you can add observation point, event, split story, samples, etc. Least but not last, the bottom right window displays genotype information.

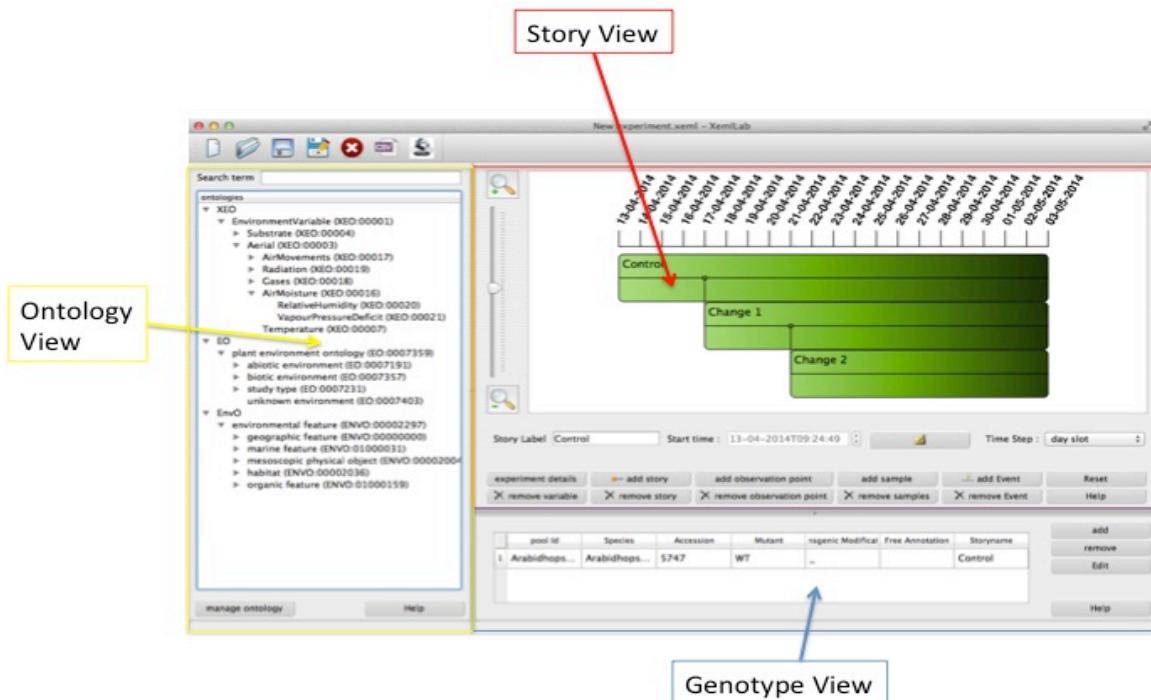


Figure 1: Main Window in Xeml Designer

3) Using XEML Document Editor

To check that you've correctly modified your XEML Document, Xeml Designer can display the document in a separate window

4) How to add stories?

There are two types of stories in Xeml Designer. First, we find the root Story. This kind of story establishes the initial conditions of your experiment. The experiment time is fixed by using experiment details and consequently, you can't move the root story in the scene. The other type of story is the Split Story. It contains generally a change in environmental conditions fixed in the root story.

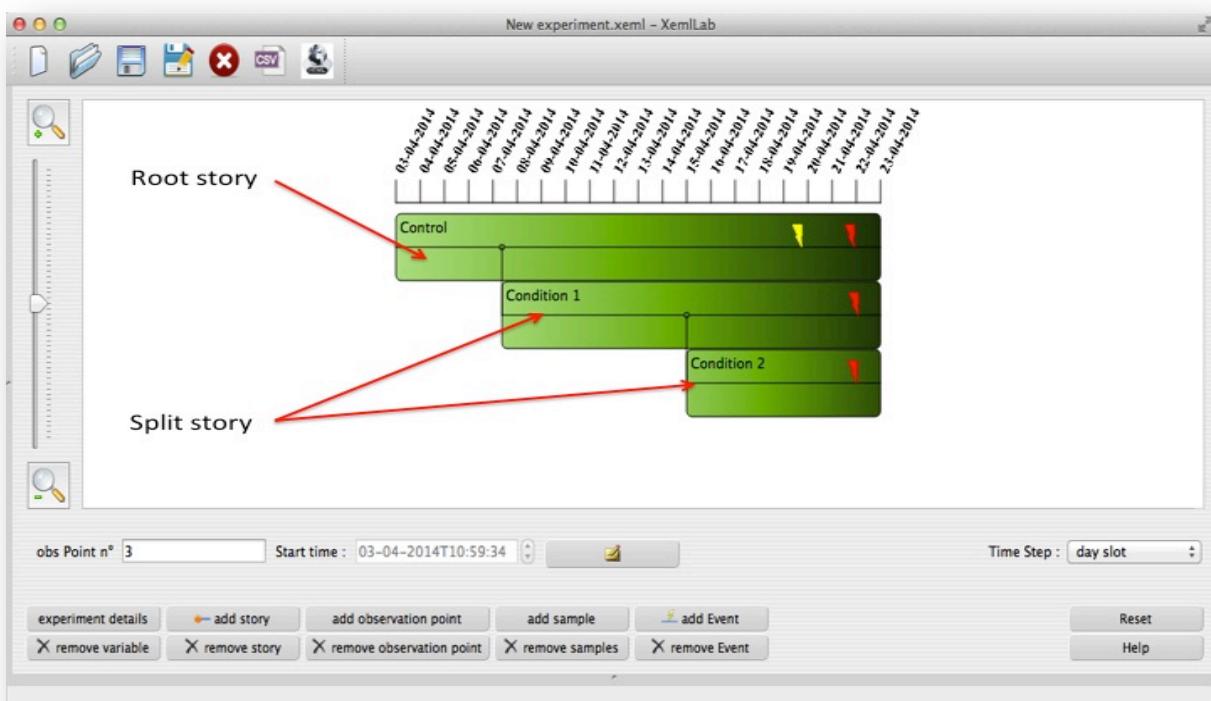


Figure 2: Story and Story split in Story view

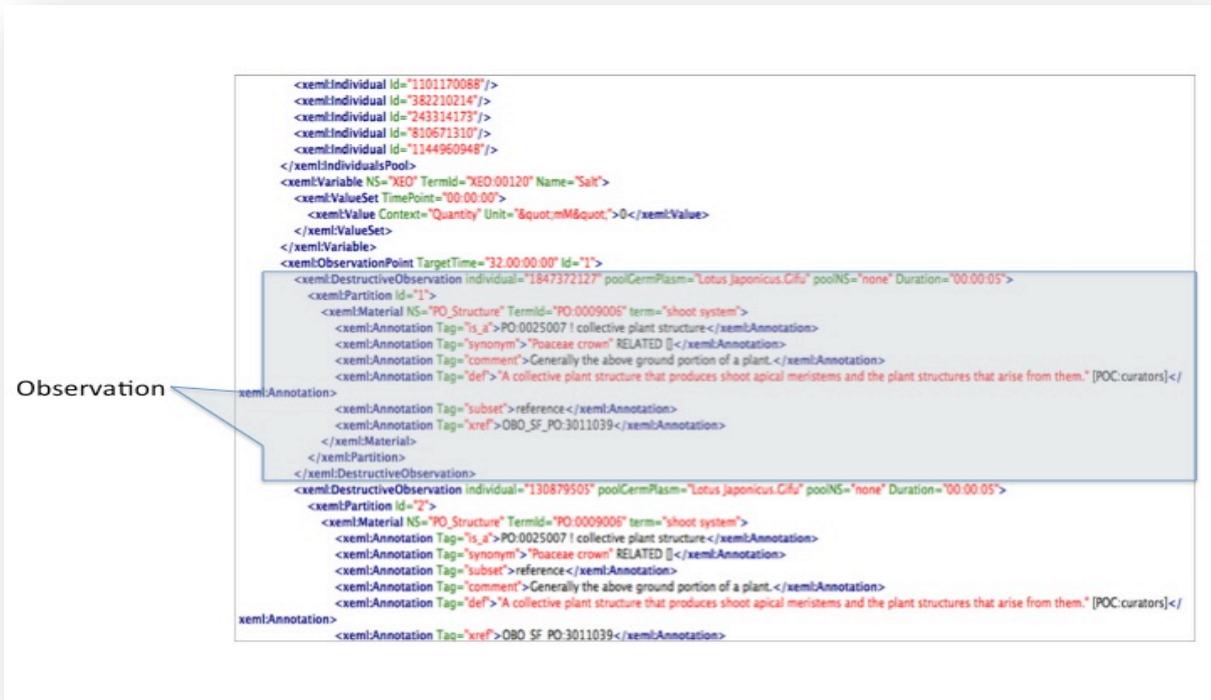
The story root also contains one or more pool of individuals used in the experiment. To add a new story, split or not, you just have to click on the add story button. By default the split checkbox is checked. If you want to add a root story, uncheck it.

5) How to add observation points?

The observation point describes a pool of observation point at a given time. To add an observation point, click on the add observation point button. A new red lightning is added to the scene. You need to have added and selected a story before adding an observation point. You can move the observation point to the right time location by left clicking on it and drag it

6) How to add observations?

An observation describes the development stage, the structure and the position of the plant or portion of the plant collected (individual). It can be a destructive observation if the plant or portion of the plant is destroyed after the collect. Several pieces of the plant can be sampled in the same observation. To an observation, corresponds an individual. An observation is automatically added during the Add sample wizard process. You can describe the duration of the observation in the Add sample wizard. Any observation added to the document is visible using the XEML code editor (Figure 3).



```

<xeml:Individual id="1011170088"/>
<xeml:Individual id="382210214"/>
<xeml:Individual id="243314173"/>
<xeml:Individual id="810671310"/>
<xeml:Individual id="1144960948"/>
</xeml:IndividualsPool>
<xeml:Variable NS="XEO" TermId="XEO_00120" Name="Salt">
  <xeml:ValueSet TimePoint="00:00:00">
    <xeml:Value Context="Quantity" Unit="&quot;mM&quot;>0</xeml:Value>
  </xeml:ValueSet>
</xeml:Variable>
<xeml:ObservationPoint TargetTime="32:00:00:00" Id="1">
  <xeml:DestructiveObservation individual="1847372127" poolGermPlasm="Lotus japonicus.Gifu" poolNS="none" Duration="00:00:05">
    <xeml:Partition id="1">
      <xeml:Material NS="PO_Structure" TermId="PO_0009005" term="shoot system">
        <xeml:Annotation Tag="is_a">PO_0025007 ! collective plant structure</xeml:Annotation>
        <xeml:Annotation Tag="synonym">Poaceae crown RELATED [<./xeml:Annotation>
        <xeml:Annotation Tag="comment">Generally the above ground portion of a plant.</xeml:Annotation>
        <xeml:Annotation Tag="def">"A collective plant structure that produces shoot apical meristems and the plant structures that arise from them." [POC.curators]</xeml:Annotation>
        <xeml:Annotation Tag="subset">reference</xeml:Annotation>
        <xeml:Annotation Tag="xref">OBO_SF_PO_3011039</xeml:Annotation>
      </xeml:Material>
    </xeml:Partition>
  </xeml:DestructiveObservation>
  <xeml:DestructiveObservation individual="130879505" poolGermPlasm="Lotus japonicus.Gifu" poolNS="none" Duration="00:00:05">
    <xeml:Partition id="2">
      <xeml:Material NS="PO_Structure" TermId="PO_0009005" term="shoot system">
        <xeml:Annotation Tag="is_a">PO_0025007 ! collective plant structure</xeml:Annotation>
        <xeml:Annotation Tag="synonym">Poaceae crown RELATED [<./xeml:Annotation>
        <xeml:Annotation Tag="subset">reference</xeml:Annotation>
        <xeml:Annotation Tag="comment">Generally the above ground portion of a plant.</xeml:Annotation>
        <xeml:Annotation Tag="def">"A collective plant structure that produces shoot apical meristems and the plant structures that arise from them." [POC.curators]</xeml:Annotation>
        <xeml:Annotation Tag="xref">OBO_SF PO_3011039</xeml:Annotation>
    </xeml:Material>
  </xeml:Partition>
</xeml:DestructiveObservation>

```

Figure 3: Xeml Document

7) How to add samples?

A sample is the part of the plant collected during the observation phase. It results from one or more individuals if the sample is pooled from multiple observations.

For more information about how to add samples, see the section called “Add sample wizard”. (Add screen shot)

8) How to add an environmental variable?

Xeml Designer has been made to allow biologist better describe their experiments, specifically in term of grow and environmental conditions. There are two different types of environmental variables, some are quantitative variables (temperature, relative humidity, etc....) while other are qualitative variables (type of Container (pot, micro plate, petri dish), substrates type). To add a variable using ontology tree (see section called ontology tree), you need to search the right term in the ontology tree then drag and drop it in the story scene. You need to have added a story and selected it before adding a term. When you dropped the term in the story scene, a window will appear to let you set the value for the variable. A variable has three different type of context to describe. Quantitative or qualitative (depending on the type of

variables) context is used to set the value of the variable. The response range context describes ... and free text context is use to add personal comment on the variable.

9) How to add events?

During the experiment time, some particular events could happen like a premature death of the plants. To describe this type of event, click on add event button and enter the description for your event. A new yellow lightning is added to the scene. You can position the event at any location (time) in the story. You need to have added and selected a story before adding an event.

10) How to load CSV files with environmental data?

The variables that you add in your experiment can be fixed before starting the experiment or measured during this one. If you have tons of measured data, it becomes obvious to automatize the process of adding variables. Here is the reason for what we integrate the Xeml Loader initially designed At the CBIB in Bordeaux for adding measured variable into Xeml Experiments. You can find more information on the csv wizard (part 17).

11) How to add a genotype?

A genotype describes individual type, species, and accession number. All genotypes added are visible in the table in Genotype view.

pool Id	Species	Accession	Mutant	nsgenic Modificat	Storyname
1 arabidopsis-tha...	arabidopsis-thaliana	654	WT	None	Control

Figure 4: genotype view and genotype table

To add a genotype, click on add genotype button (1).

Id	arabidopsis_thaliana.col_at0.Wt.None		Cancel
Species	arabidopsis_thaliana		OK
NCBI Taxonomy ID	1234	Add individuals	
Accession	col_at0		
Mutant	Wt		
Transgenic Modification	None		
Free Annotation			

Figure 5: Genotype edit form

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A window will appear where you can describe your genotype (species, NCBI taxon id, accession number, etc....) (Figure 5). The field “Id” is build with all other fields. You can also add annotations for each field you describe. For information about the “Add individuals” button, see Part 18.

pool Id	Species	Accession	Mutant	Nsgenic Modifical	Storyname	
1	arabidopsis-tha...	arabidopsis-thaliana	654	WT	None	Control

add
remove
Edit
Help

Figure 6: genotype selection

After that, click on ok to add your genotype. You can see in the genotype view that a new genotype has been added. To modify a genotype, select the entire raw in the genotype table corresponding to the genotype you want to edit use Edit button.

12) How to add individuals?

Users can add individuals (plants) in two manners. The first one is during the genotype registration process and the other is during the add samples process.

There are two ways for adding individuals (plants). The first one, the logical one, is to use “Add individual” button in the “Add genotype” window. In this window, when you click on the “Add individual” button, a wizard will appear. You have the choice between randomly create (in term of identifier) your individual or import individual id from a csv file. (See section individual wizard).

13) How to export to ISA-tab format?

You can export your XEML file to Isa tab format. The Isa tab format (Investigation Study, Assay) is a new structured format to describe different studies with their set of assays linked to the same investigation field. Open the file menu and click on export to ISA-Tab. This will create a directory with the name of your experiment and three files, one for investigation information, one for Study information and finally one for assay information. This part is still under development.

14) How to connect to databases (ex PLATO, GMD)?

This part is still in development.

15) How to display plot of environmental data?

To display plot parameters, just right click on the selected story, and select plot variables action. Not yet available.doc

16) How to change time scale?

To better dispose your Xeml component (stories, observation points and events), you can change the time scale by clicking on the time slot combo box and select a new range of time. Day is the default range.

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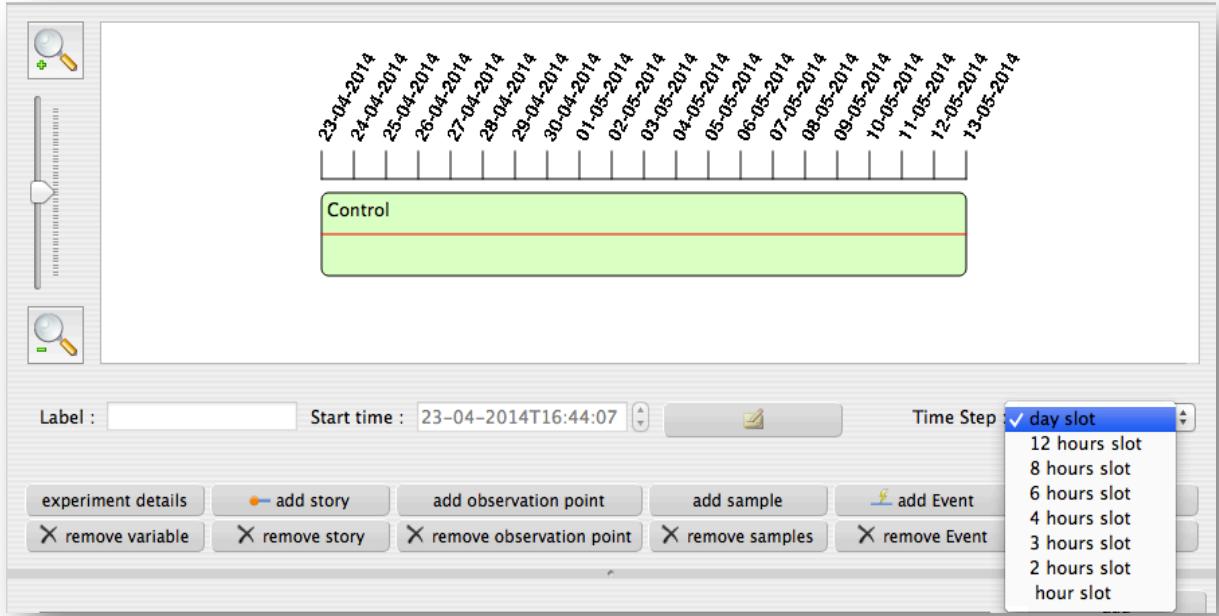


Figure 7: Daytime range

For example, if you choose a 2-hour slot, each day is decomposed into 12 x 2h ticks.

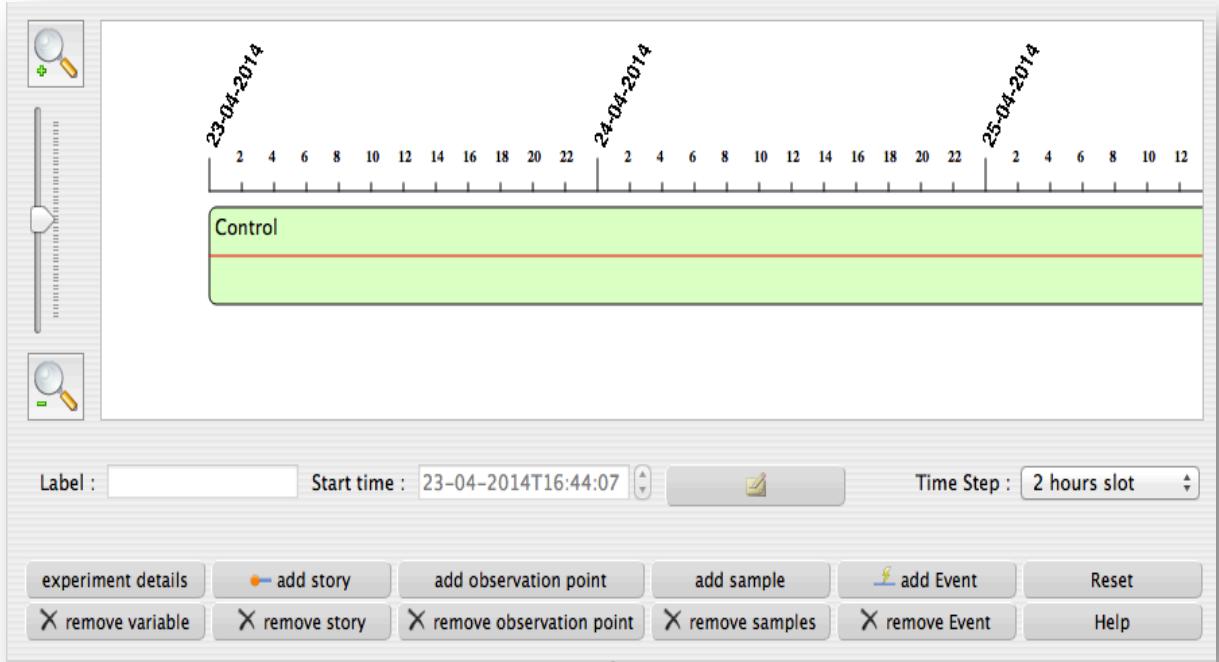


Figure 8: 2 hour-range

17) CSV wizard

In the new XEML Designer, you can separate environmental variable in two categories: the variable that you can keep fixed during the experiment like the type of substrate, the type of container used for plants and the variable that you can measure during the experiment like light

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intensity, temperature relative humidity and more. If you want to add lot of measured variables, it becomes soon a tedious and repetitive task. That is why we decided to incorporate XEML Loader into XEML Designer.

```

1 TIMESTAMP,RECORD,TempC_Avg(1),RH_Avg(1),Par_Avg(1),TempC_Avg(2),RH_Avg(2),Par_Avg(2)
2 23/08/2013 11:00,1684,27.84389,72.71555,245.0313,28.99555,57.09333,127.7816
3 23/08/2013 11:30,1685,29.53778,67.97222,237.3608,30.86889,51.18166,135.6936
4 23/08/2013 12:00,1686,29.80722,69.59999,180.744,31.185,50.74222,102.1066
5 23/08/2013 12:30,1687,28.76222,76.52055,294.9389,30.22611,52.01222,152.6835
6 23/08/2013 13:00,1688,29.88444,58.98444,287.1924,31.09222,48.26556,140.7297
7 23/08/2013 13:30,1689,28.85,59.435,333.4262,30.50.08055,168.5983
8 23/08/2013 14:00,1690,29.42889,58.22833,295.0823,30.08666,49.87333,136.0139
9 23/08/2013 14:30,1691,28.91611,63.98111,577.0943,29.70833,50.81166,195.7849
10 23/08/2013 15:00,1692,29.52278,63.00555,444.4605,29.99555,50.24611,221.3786
11 23/08/2013 15:30,1693,28.29111,61.48833,274.0936,29.725,49.52778,103.4702
12 23/08/2013 16:00,1694,26.32277,66.17722,147.0413,27.62778,54.48889,68.30059
13 23/08/2013 16:30,1695,25.54111,69.44166,119.3719,26.43722,57.91611,56.69787
14 23/08/2013 17:00,1696,24.945,69.40444,83.94543,25.74667,59.99666,40.71156
15 23/08/2013 17:30,1697,24.91,66.4111,76.36121,25.30167,60.60833,34.03071
16 23/08/2013 18:00,1698,25.09166,63.64777,57.1529,25.41389,59.35277,25.76032
17 23/08/2013 18:30,1699,24.59611,67.05833,4.912089,25.04111,61.85389,2.654678
18 23/08/2013 19:00,1700,23.84611,74.54111,0.8243235,24.505,66.75666,0.489393
19 23/08/2013 19:30,1701,23.20278,76.62055,0.00051995,23.80667,70.00166,0.02610001

```

Figure 9: Example of CSV file

The loader allows users to load their data in a fast and simple way. Figure 9 shows an example of well-formatted csv files. Before adding any data, you need to create the context of the experiment. If you want to add environmental data acquired at a certain date (for example from the 23th of August 2013 to the 24th October 2013, the story start date has to be set to a date anterior to the 23th of august 2013 and the same for the experiment end date.

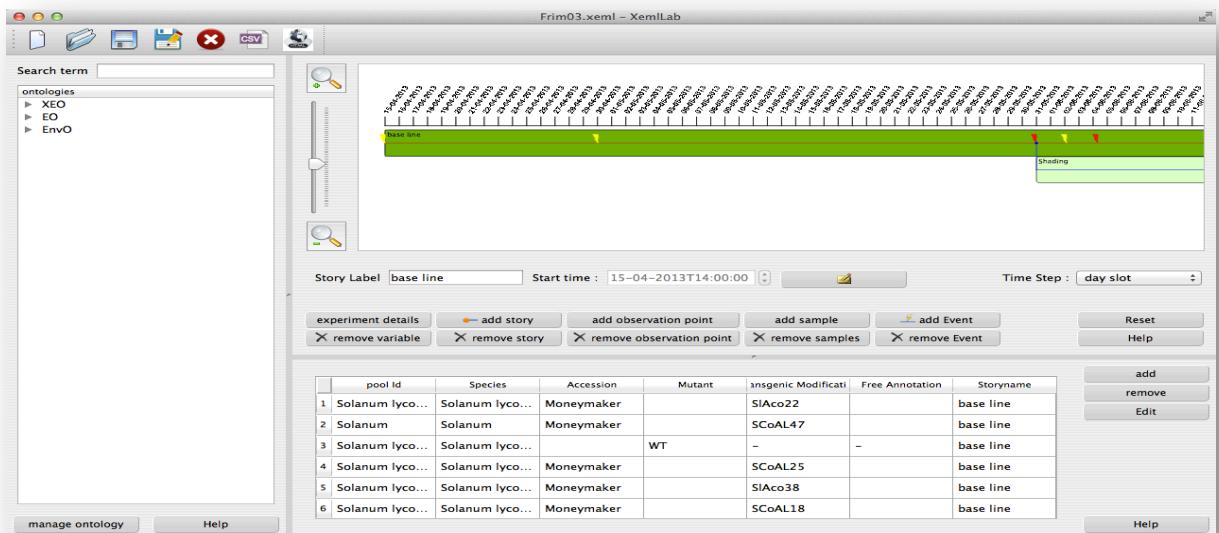


Figure 10: INRA experiment FRIM03 design

To add data to your current XEML Document, click on icon in the tool bar menu or select “load a csv file” in the file menu. The wizard will start. For demonstration we chose an INRA’s experiment started at 15/04/2013 and closed at 25/10/2013. It contains 6 pools of individuals, all derived from tomato species. The root story is called “Base line”. Notice that a split appears at 31 may 2013 called “Shading”

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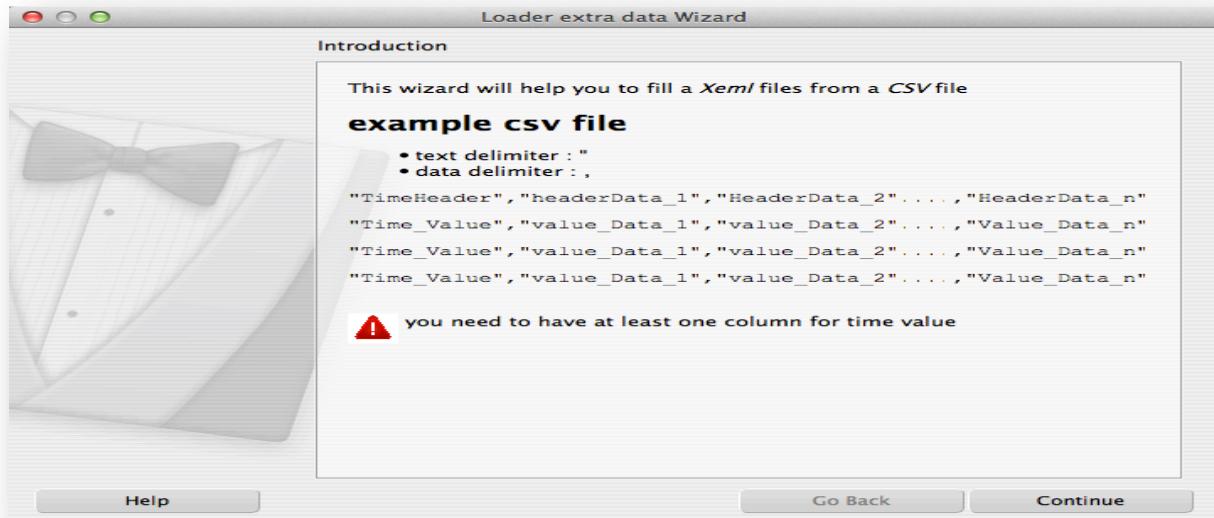


Figure 11: CSV Wizard introduction page

As explained for individual wizard (Part 18), search a file to load using browse button (1) and select the right delimiters (2), once done, click on load button (3).

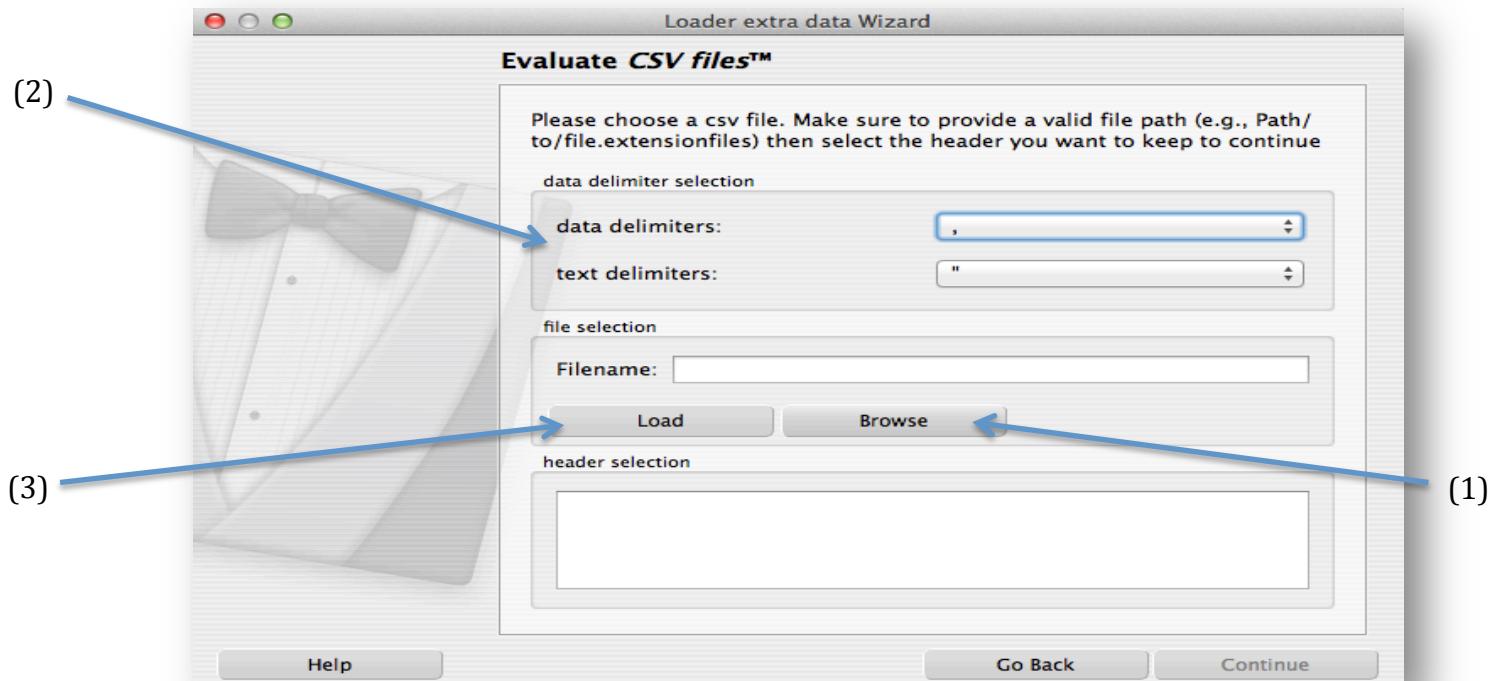


Figure 12: Load file and choose csv header

Now you can see all headers found in your csv files in the table header selection.

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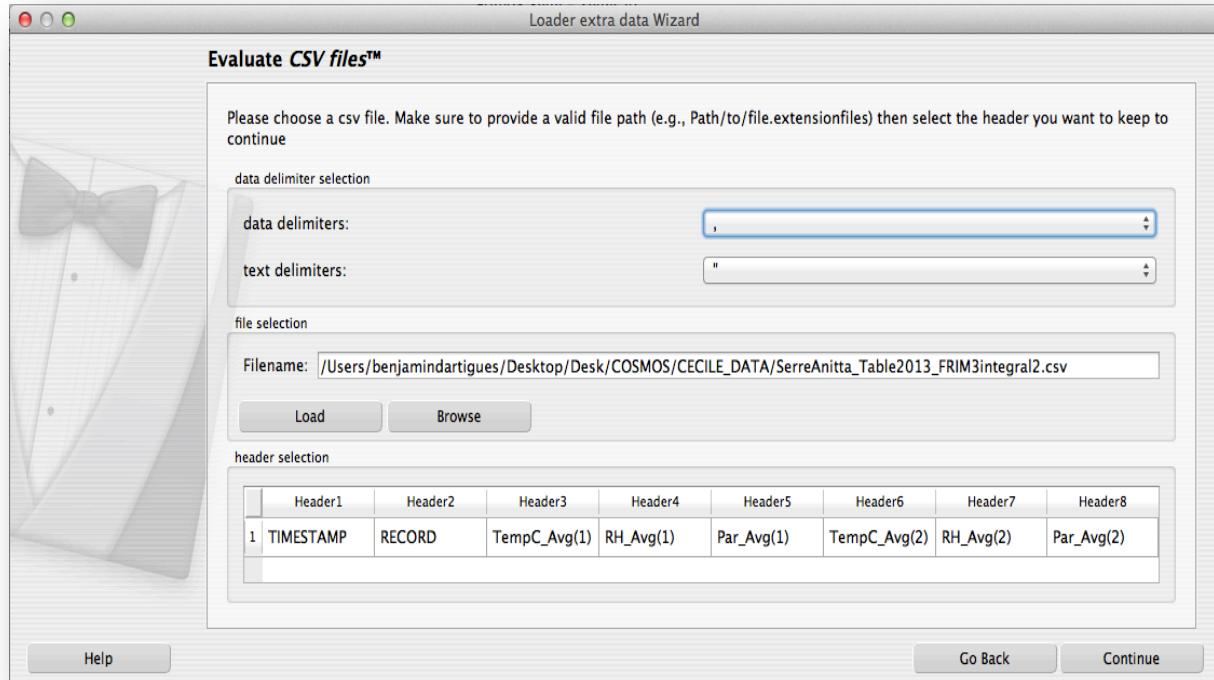


Figure 13: Header selection

Select the headers you want to keep by clicking on it (Figure 14) then click on continue.

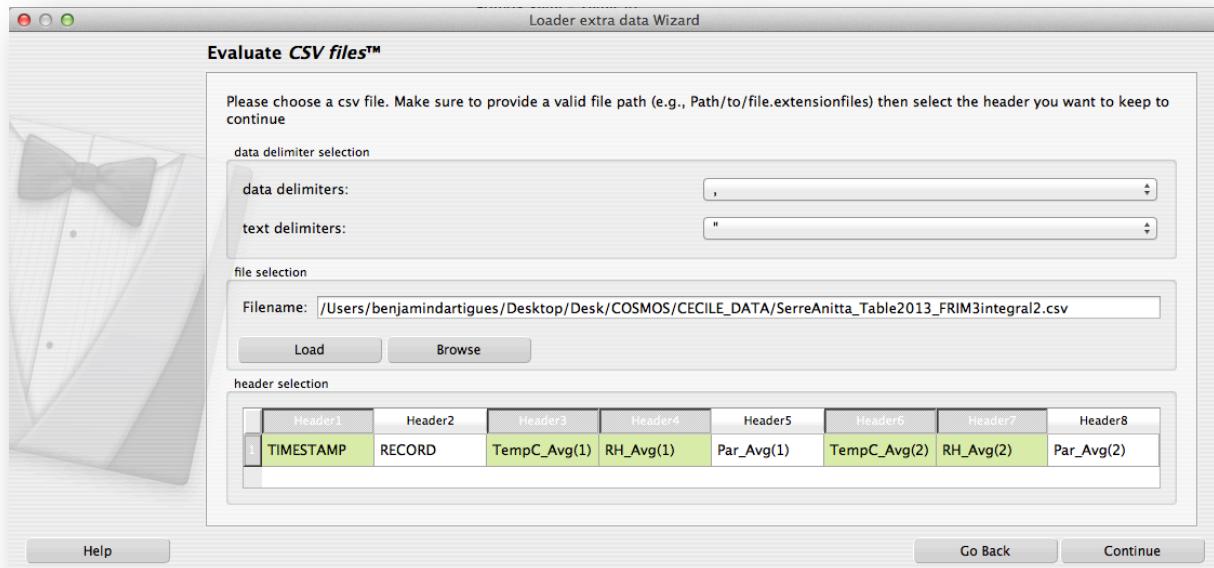


Figure 14: Header selection

Here we kept timestamp (mandatory if you want to date your measure), T°1, T° 2, RH1 (relative humidity) and RH2. Now, click on continue. A new table appears with headers you kept in the first column. The second and the third columns were respectively used to set the variable and the story while the last column is used to define which header is a time value

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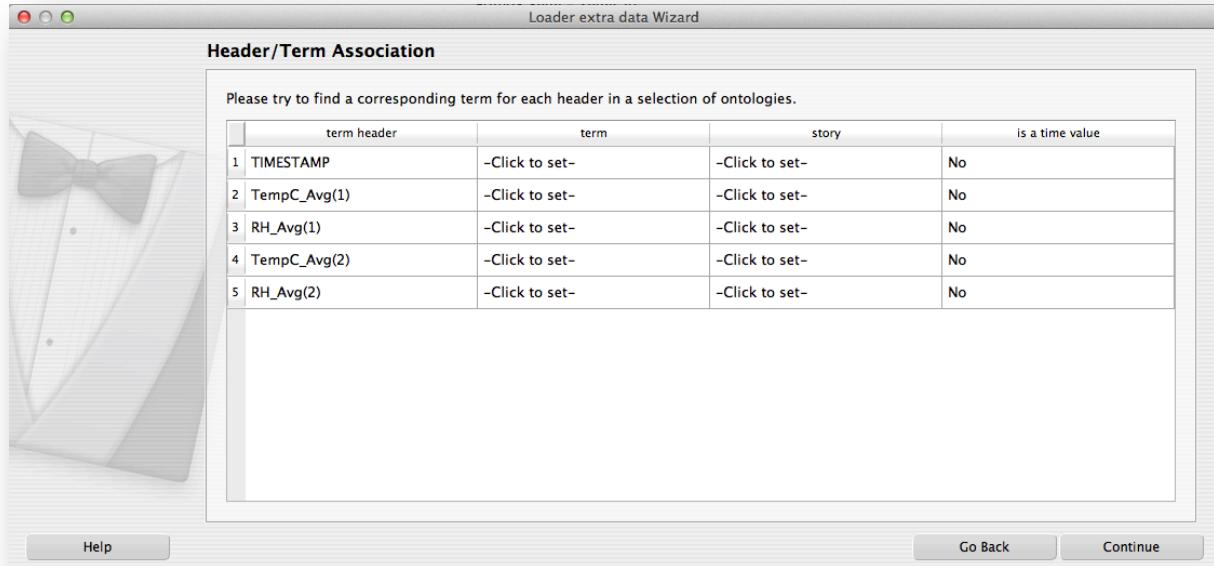


Figure 15:Header-Variable association

Click on the first row and the last column cell to set the time format. Choose expression similar to your time format. In our case, if you look on Figure 9, we have a format like dd/MM/yyyy hh:mm. you can find help on time format if you clicked on the help button.

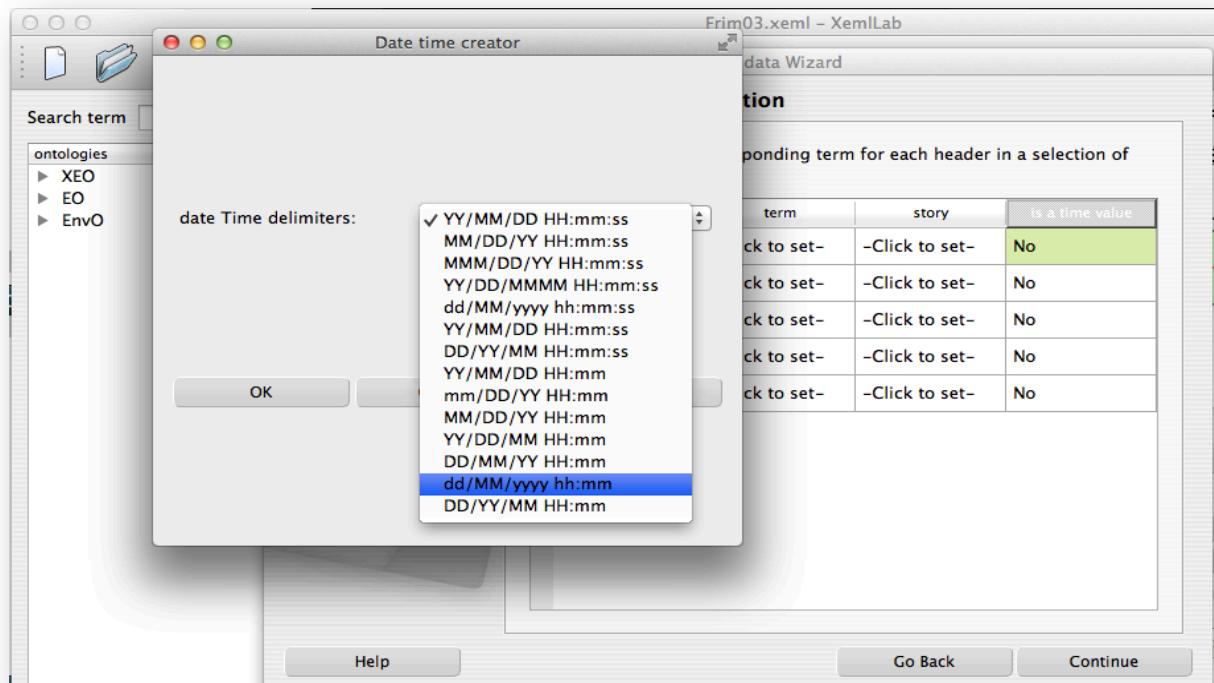


Figure 16: time format

Now that we set the time format, you can see that the first row is completed.

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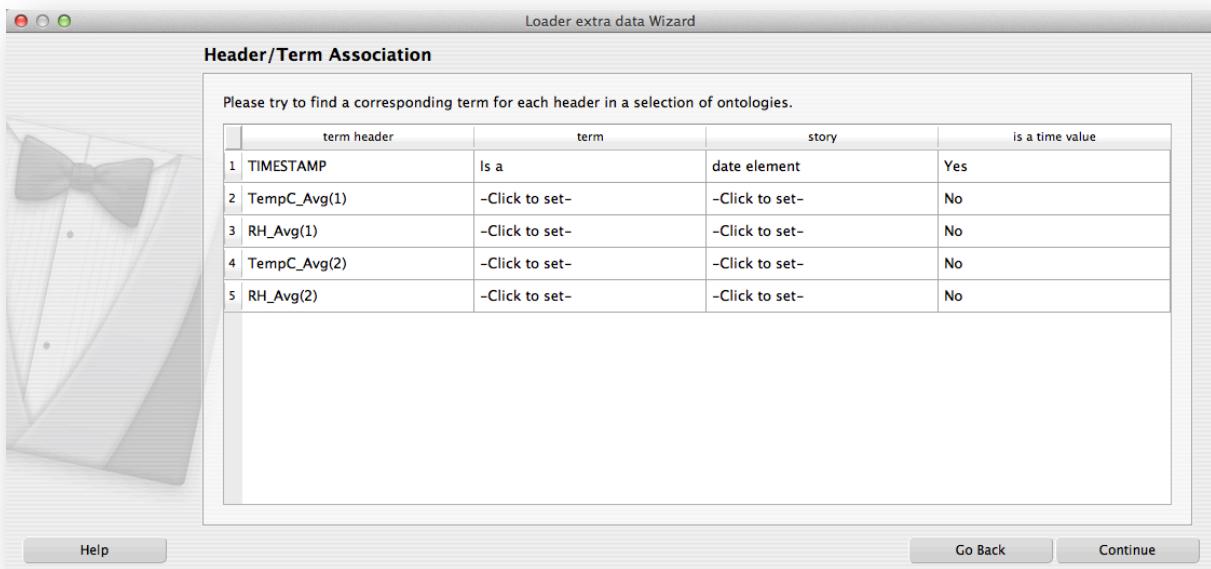


Figure 17: After time format setting

To define which variable you import and in which story the variable will be, click on next row (on term or story column has same effects) to open a new tab window.

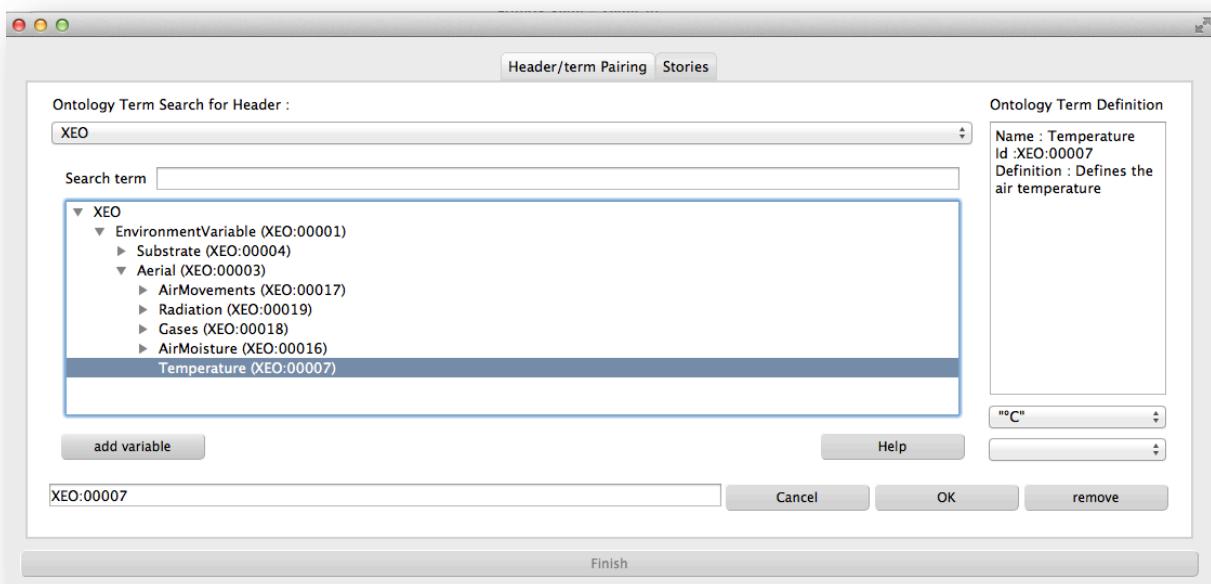


Figure 18 variable selections

On the header/term tab (Figure 18), you will find a tree containing all quantitative environmental variable available in XEO ontology. Here we want to define a temperature in the air, so we choose the term in the tree, select the right unity and click on ok button. The tab becomes unavailable. After that, we click on the stories tab (Figure 19) and here again we select the story by double clicking on the corresponding node. Then we clicked on OK button and the tab disappears. Click on Finish to add the variable.

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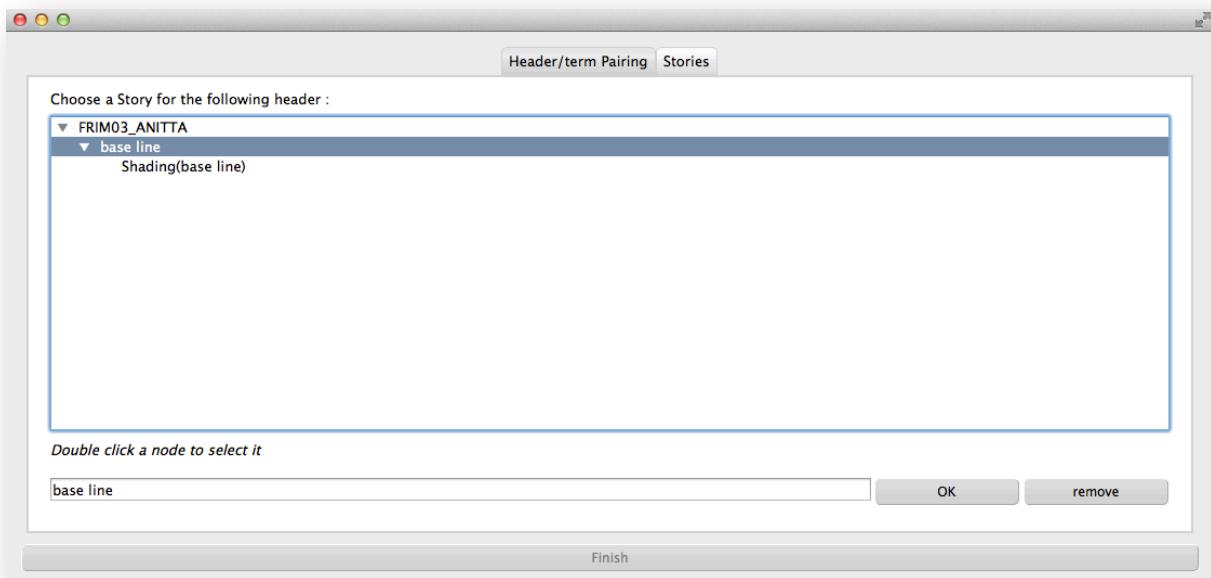


Figure 19 Story owner's variable selection

We repeat this step for each variable and we obtain the window showed in Figure 20

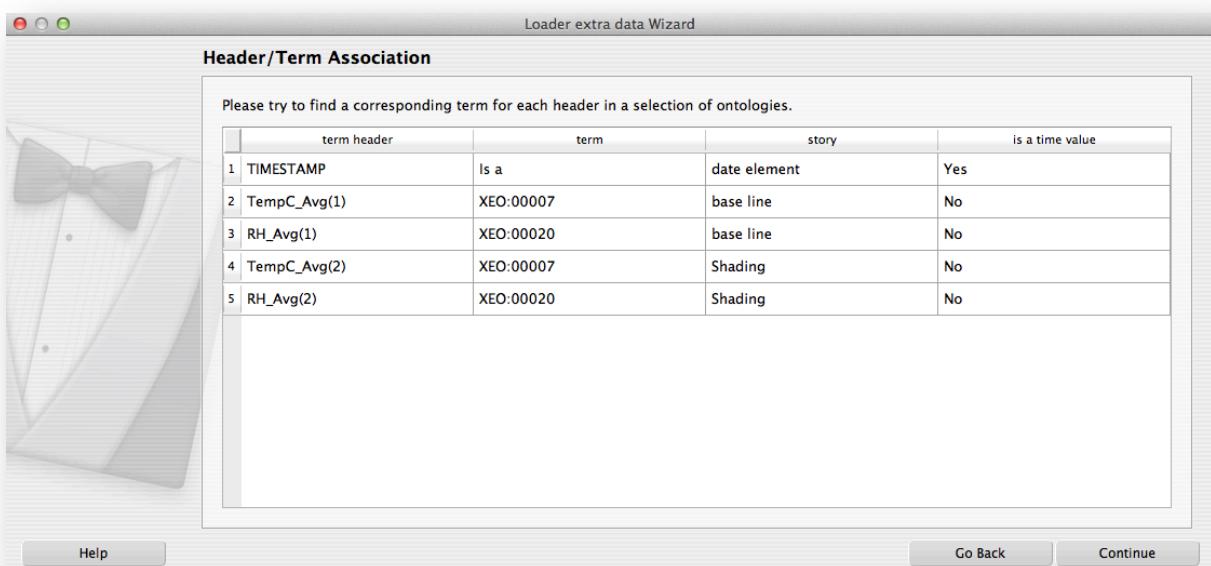


Figure 20: Complete description

Now Click on Continue button and if everything goes well, a window with a validation message will appear. Click on done to terminate the wizard.

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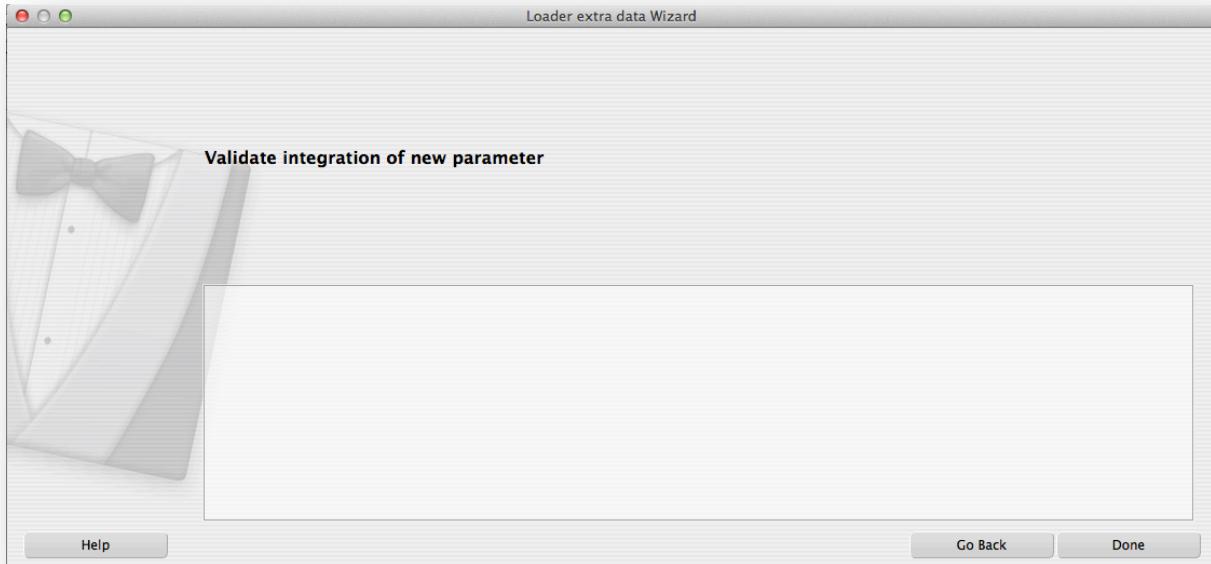


Figure 21 Wizard final Page

Now if you open your XEML Document using code editor, you will see all your variables added to the corresponding story.

```
</xeml:IndividualsPool>
<xeml:IndividualsPool GermPlasm="&#xa;Solanum lycopersicum L.Moneymaker .SCoAL47" NS="none">
  <xeml:Annotation Tag="FreeText">b-subunit of succinyl-coenzyme A ligase cloned in antisens orientation (Studart-Guimaraes et al., 2007)</xeml:Annotation>
  <xeml:Annotation Tag="NcbiTaxonomyId">4081</xeml:Annotation>
</xeml:IndividualsPool>
<xeml:IndividualsPool GermPlasm="Solanum lycopersicon L..WT.-.-" NS="none">
  <xeml:Annotation Tag="FreeText">Wild type</xeml:Annotation>
  <xeml:Annotation Tag="NcbiTaxonomyId">49274</xeml:Annotation>
</xeml:IndividualsPool>
<xeml:MeasuredVariable Name="Temperature" NS="XEO" TermId="XEO:00007">
  <xeml:ValueSet TimePoint="129.21:00:00">
    <xeml:Value Context="Quantity" Unit="°C">27.84389</xeml:Value>
  </xeml:ValueSet>
  <xeml:ValueSet TimePoint="129.21:30:00">
    <xeml:Value Context="Quantity" Unit="°C">29.53778</xeml:Value>
  </xeml:ValueSet>
  <xeml:ValueSet TimePoint="129.22:00:00">
    <xeml:Value Context="Quantity" Unit="°C">29.80722</xeml:Value>
  </xeml:ValueSet>
  <xeml:ValueSet TimePoint="129.22:30:00">
    <xeml:Value Context="Quantity" Unit="°C">28.76222</xeml:Value>
  </xeml:ValueSet>
  <xeml:ValueSet TimePoint="129.23:00:00">
    <xeml:Value Context="Quantity" Unit="°C">29.88444</xeml:Value>
  </xeml:ValueSet>
  <xeml:ValueSet TimePoint="129.23:30:00">
    <xeml:Value Context="Quantity" Unit="°C">28.85</xeml:Value>
  </xeml:ValueSet>
  <xeml:ValueSet TimePoint="130.00:00:00">
    <xeml:Value Context="Quantity" Unit="°C">29.42889</xeml:Value>
  </xeml:ValueSet>
  <xeml:ValueSet TimePoint="130.00:30:00">
    <xeml:Value Context="Quantity" Unit="°C">28.91611</xeml:Value>
  </xeml:ValueSet>
  <xeml:ValueSet TimePoint="130.01:00:00">
```

Figure 22 XEML Document Measured variables part.

18) Individual wizard

First, you need to describe a genotype and add it to a root story. Only root story can contain a genotype, split story inherits all the genotype described in the root story.

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To add a genotype, select a story and click on add genotype button in the bottom panel (genotype view). A window will appear (Figure below).

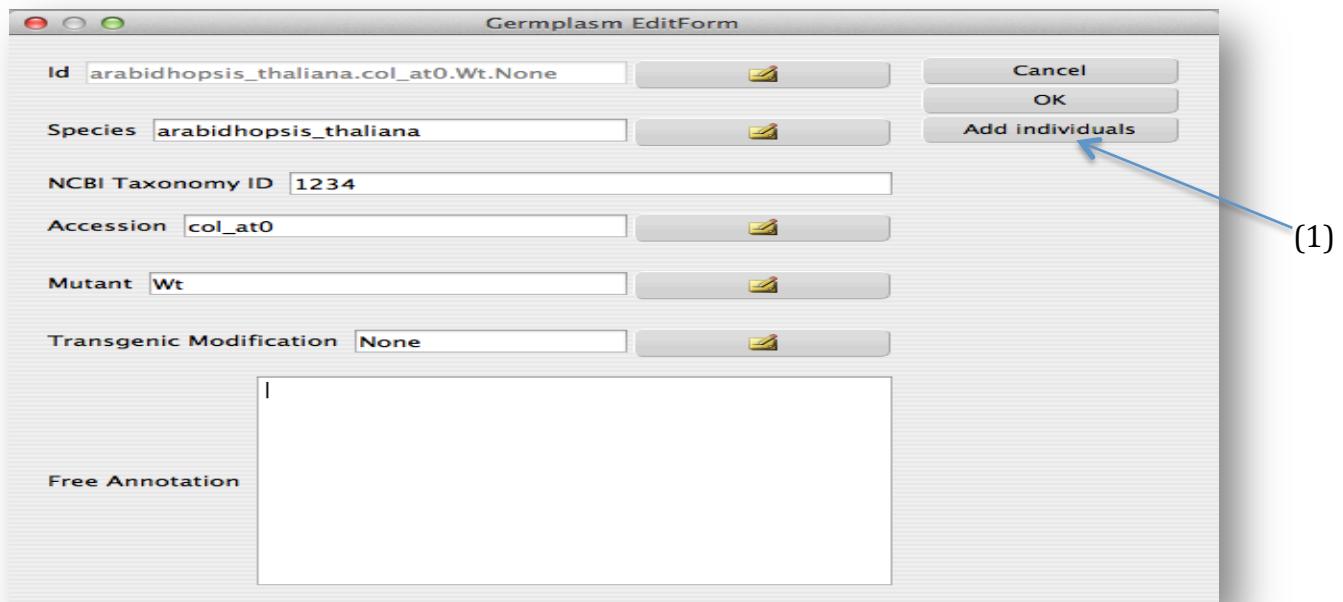


Figure 23: describe a new genotype window

You can describe your genotype before or after adding new individuals. But if you close the new genotype window, your individuals will not be added to the story. To add new individuals, click on the Add individual button (1) to open the wizard.

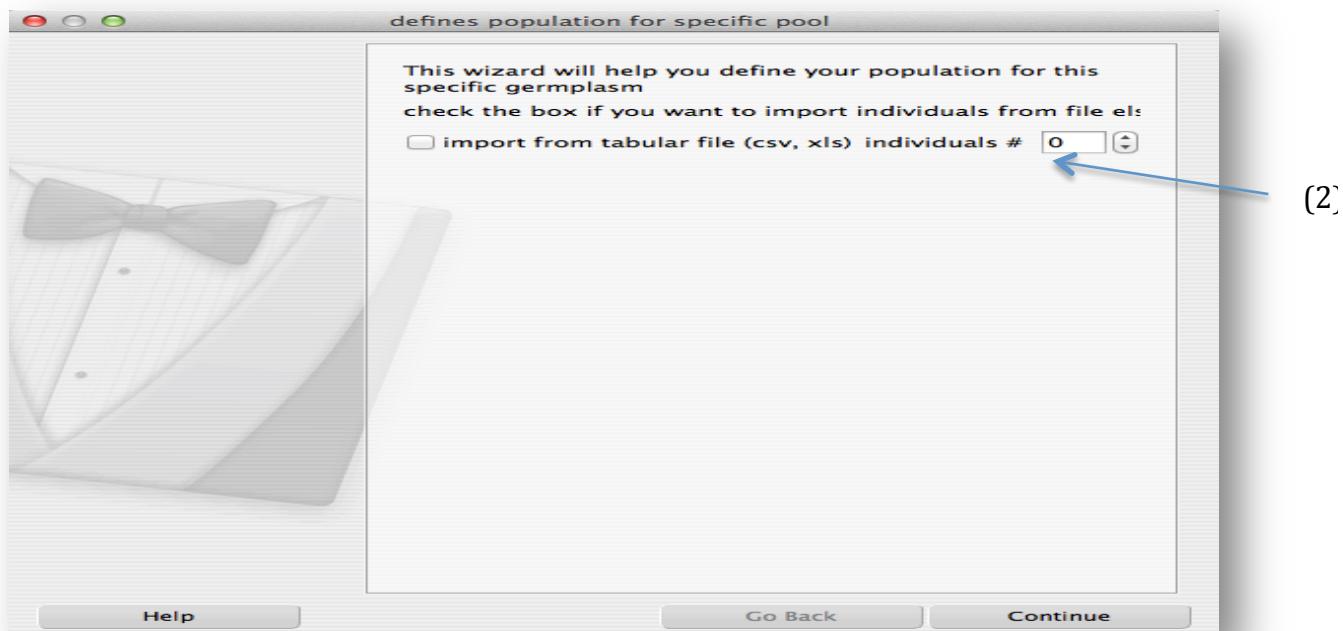


Figure 24: Individual wizard first page

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Here again you have two choices, either you can add individual with random id between 1 and 1000000000. To do this, select the right number of individuals in the spin box (2), for example 10, and click on continue button to go to the next page.

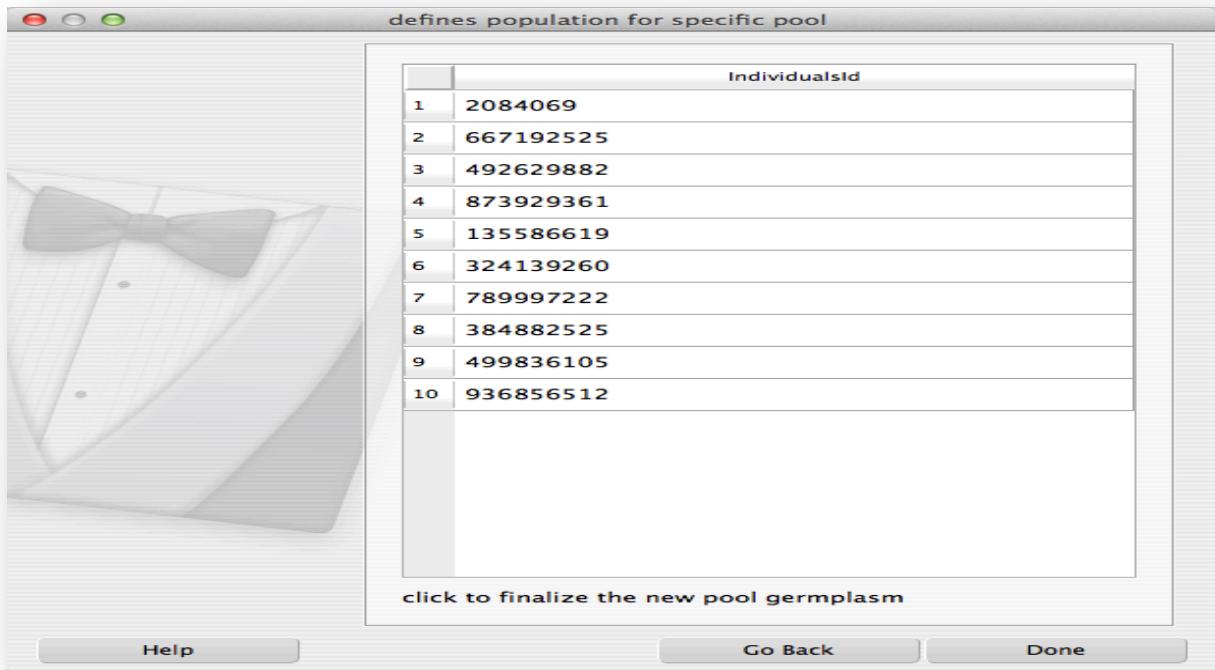


Figure 25: Second page individual wizard

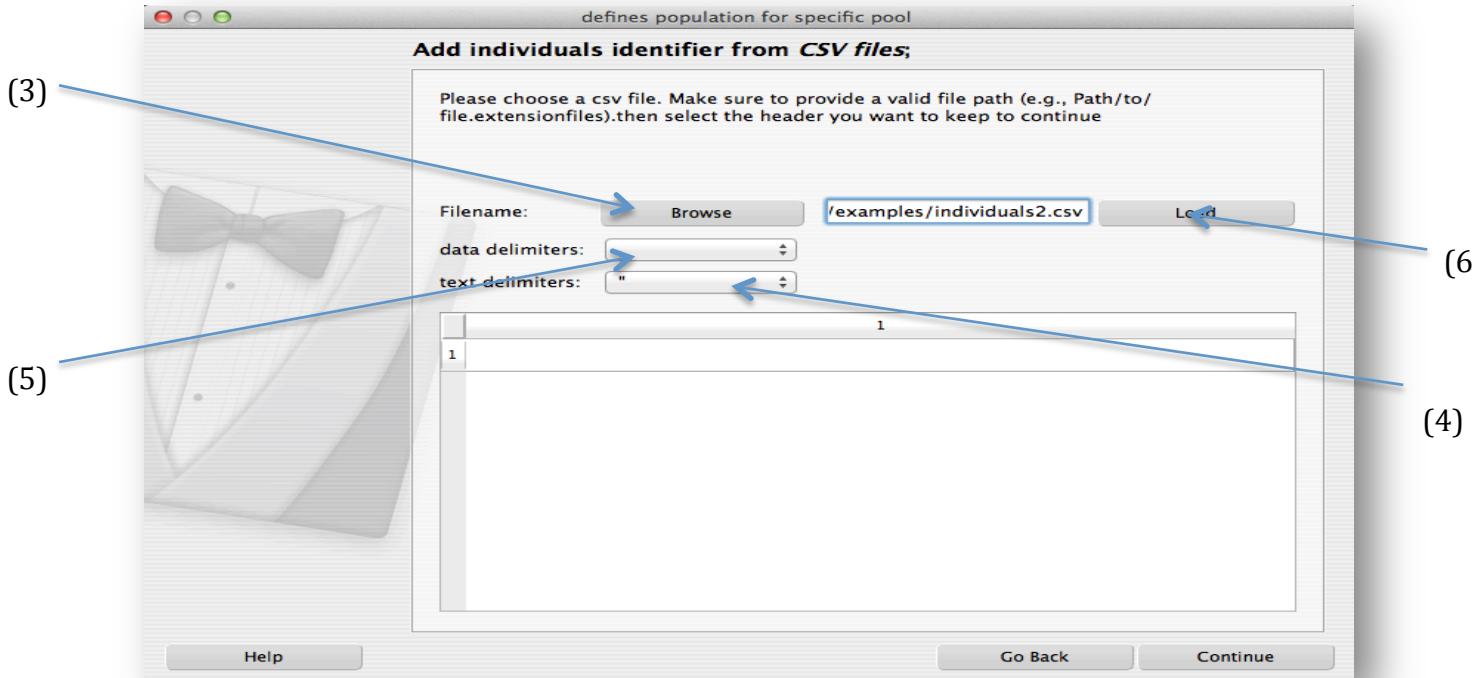


Figure 26: Wizard second for import id mode

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You can see that you generate 10 individual ids. Click on “done” to create the individuals and terminate the wizard. If you click on the checkbox “import from tabular file”, the wizard’s second page will differ. Here, you can select a csv file with id registered. Click on browse button (3) and select your file. Then choose the data (4) and text (5) delimiters. Here is an example of well-formatted csv file:

“Individuals Id”, “Individual age (dpa)”
“234635Z6T4Z”, “7”
“243Z4563565”, “7”

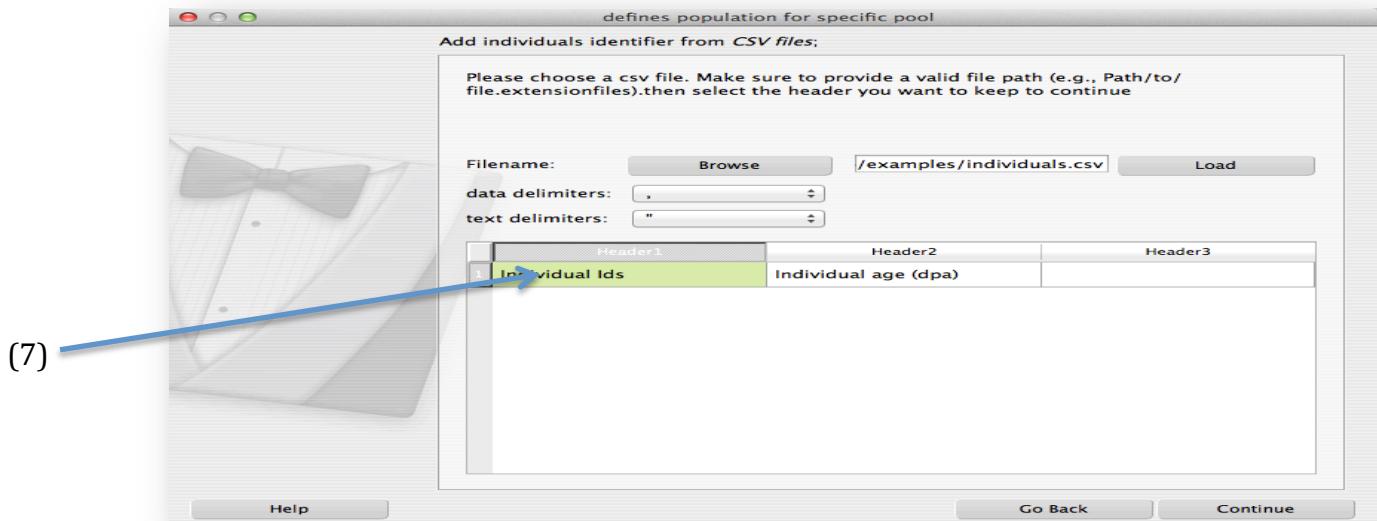


Figure 27: Wizard third page.

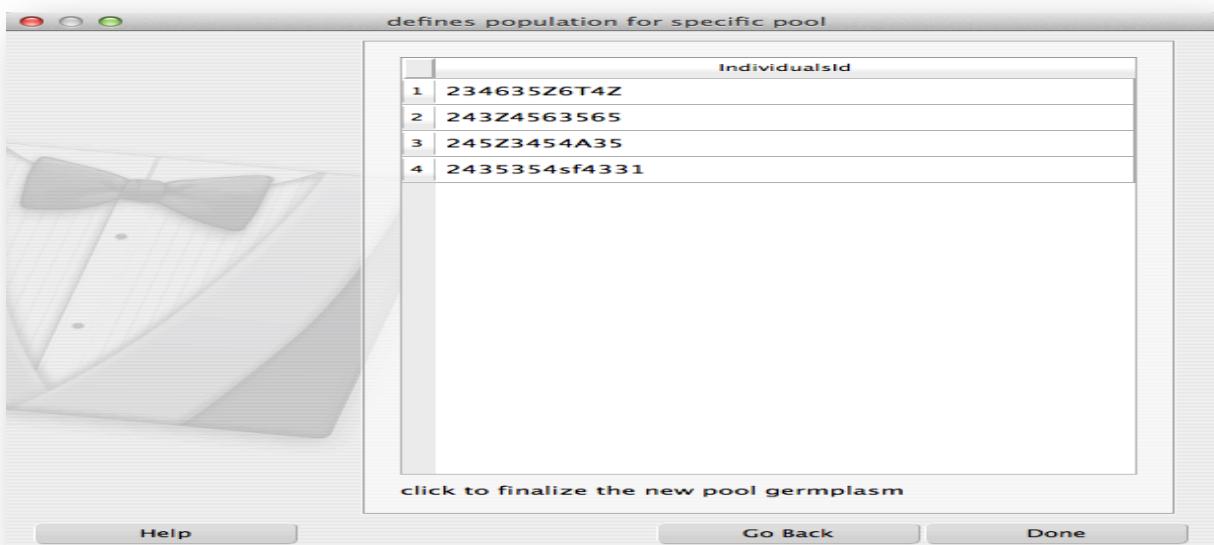


Figure 28: wizard last page

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Now click on the load button (6) and you will see the header label appear in the table. Click on the cell containing the label you want to keep (7), here individual Ids, and click on continue. You can see your ids have been imported and individuals ready to create (Figure 28). Now click on “done” to create individuals and terminate the wizard.

19) Sample Wizard

As we previously said, a sample is the part of the plant collected during the observation phase. It results from one or more individuals if the sample is pooled from multiple observations. To add new samples to an observation point, select the story that contains the observation point and click on add samples button. Select the observation point that you want by click on any cell of the OP row (1).

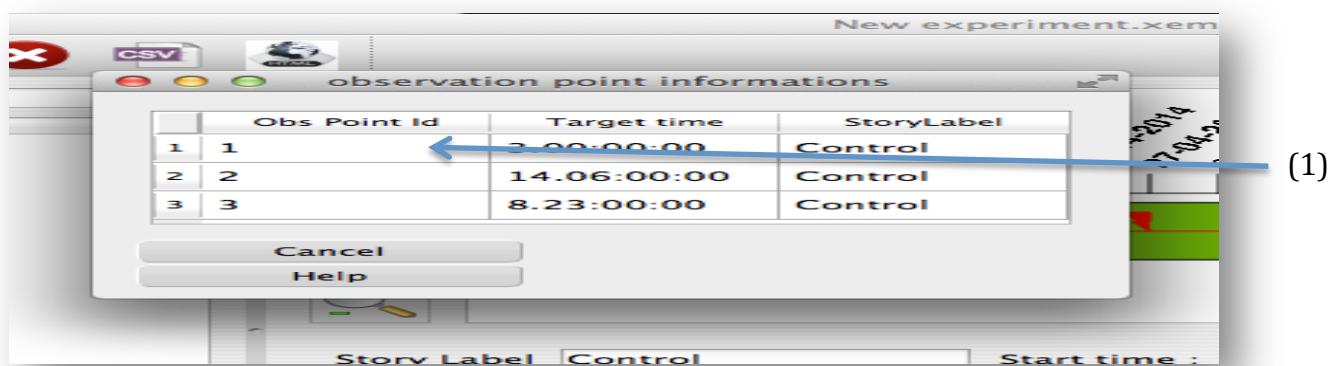


Figure 29: Observation point selection

Here we selected the observation point 1. Now you need to select one or more genotype (individuals pool) to observe. In our case, we only have one to select (2).

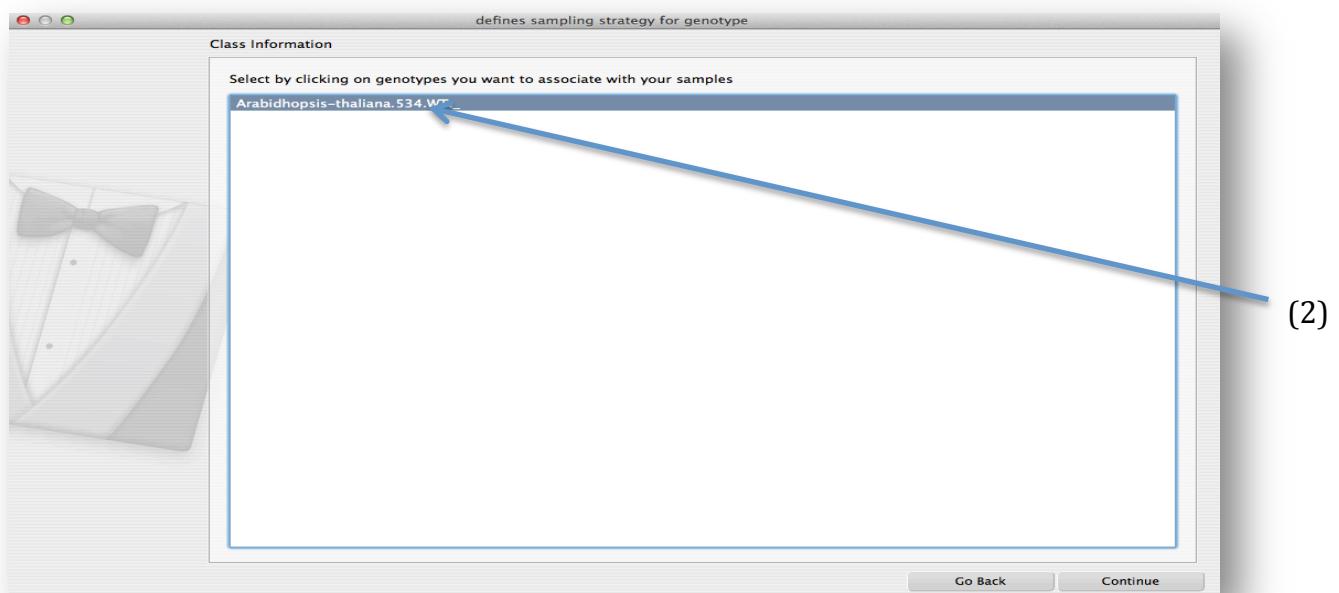


Figure 30: Genotype selection

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Once selected, click on Continue button and a new window will appear, this is the main window of the wizard. In the left panel, you see the Observations tree (3). The tree is empty here and you need to add individuals, cause you do not added before using the individual wizard (see previous chapter). On the top right, you will find a time box for observation duration. Just below, some optional checkboxes (4) that we will describe later, and at the bottom, a table with genotype selected and number of individuals by pool (5).

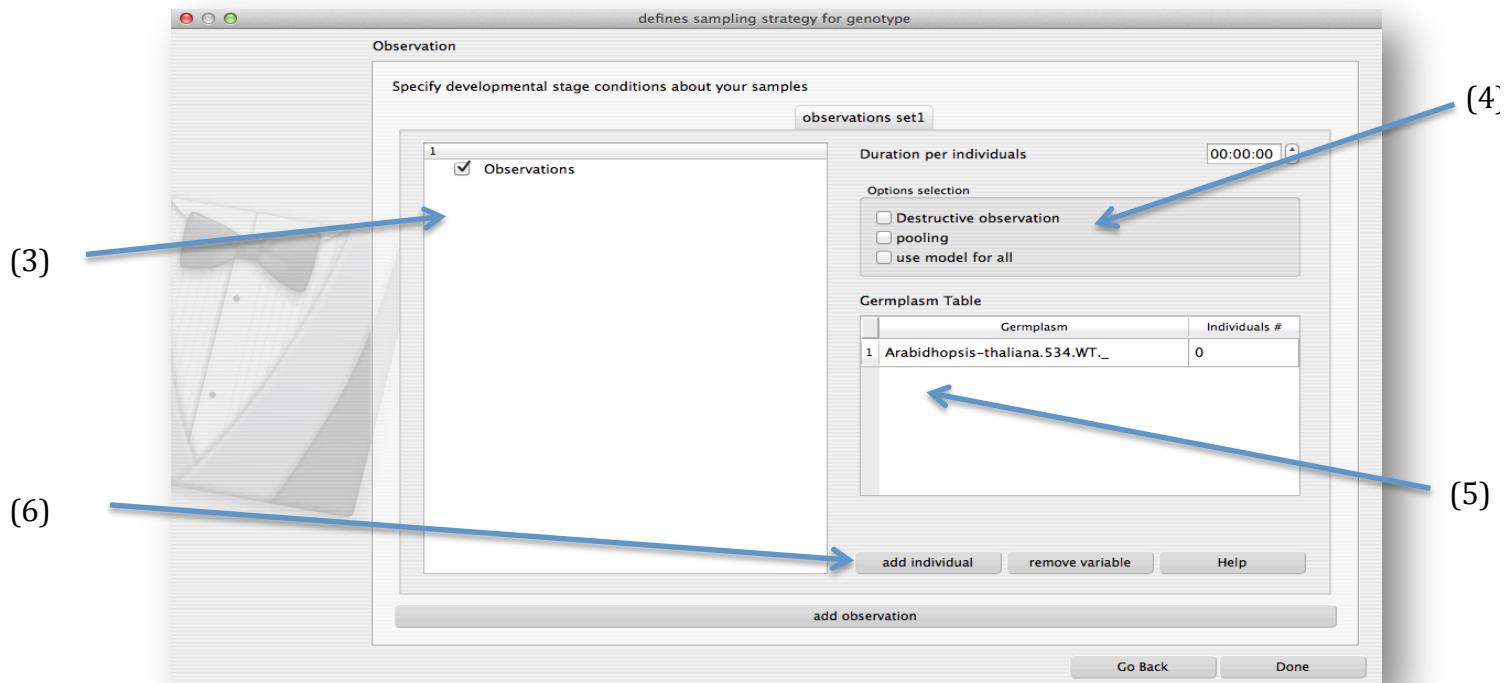


Figure 31: Sampling window

To add individual (this time with random id), click on add individual button (6). For this demonstration we added 5 individuals (Figure 32).

Use model for all:

Now, choose the individuals you want to observe by checking the box beside their names. An easiest way is to check only one individual and tick the “use model for all” checkbox (7). Now all individuals will be observed the same way (i.e. the same part of the plant at the same developmental stage).

Pool samples:

If you tick the “pooling” box (8), all part collected from all individuals will constitute only one sample. In other word, if you collected 5 leaves from 5 individuals without ticking the box, you will have five samples but with “pooling” box checked, you will only have one. A prerequisite for using “pooling” box is to have checked the “use model for all” box.

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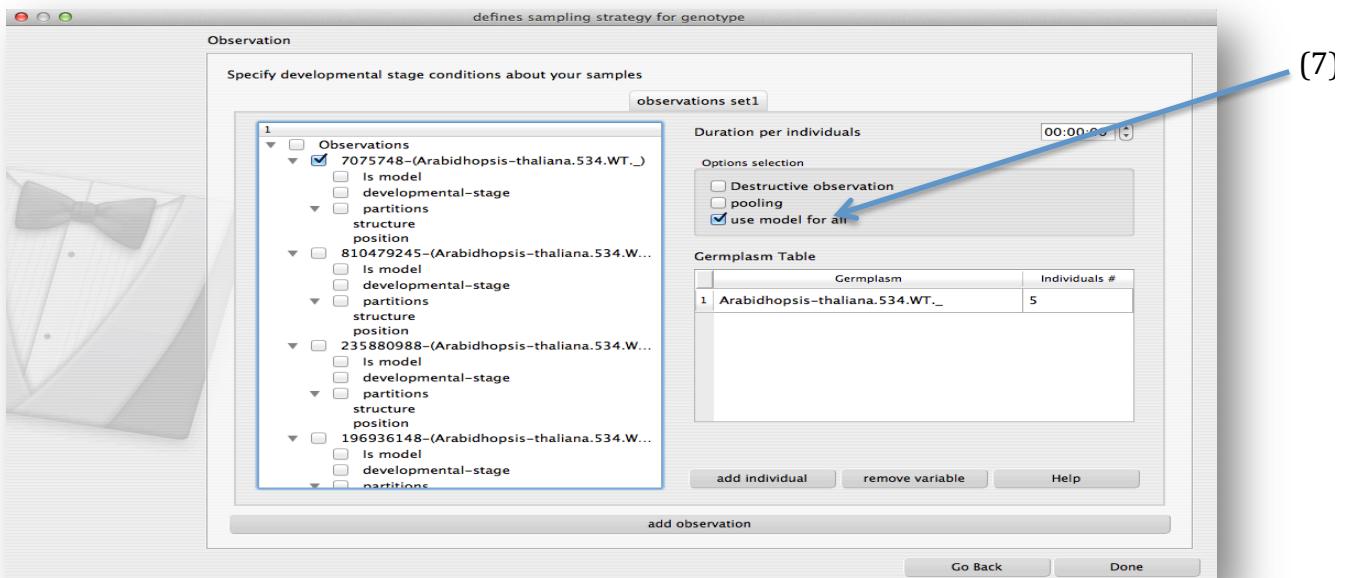


Figure 32: individual model selection

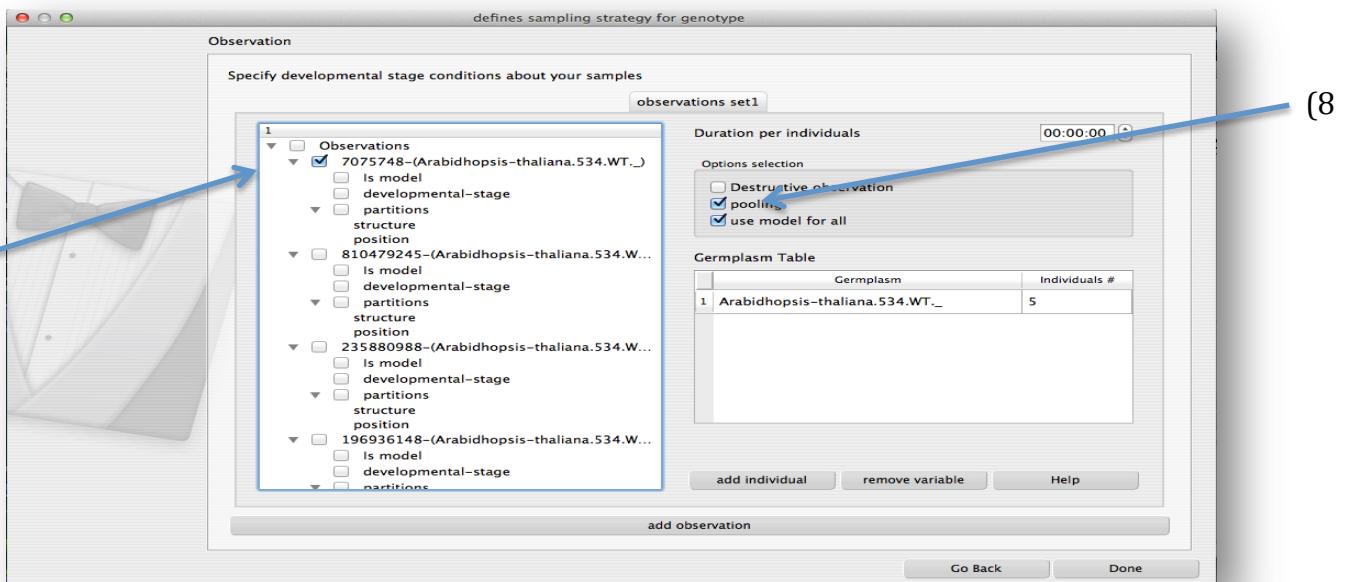


Figure 33: Sample description

Then, you have to describe a little bit your sample: What is the developmental stage of the plant or the organ, observed? Which structure to collect? Choose the developmental stage by double clicking on the developmental stage node of the individual defined as model plant you want to observe (9). A window will appear, containing once again a tree with all terms relative to developmental stage ontology.

Here we selected the fruit developmental stage (10).

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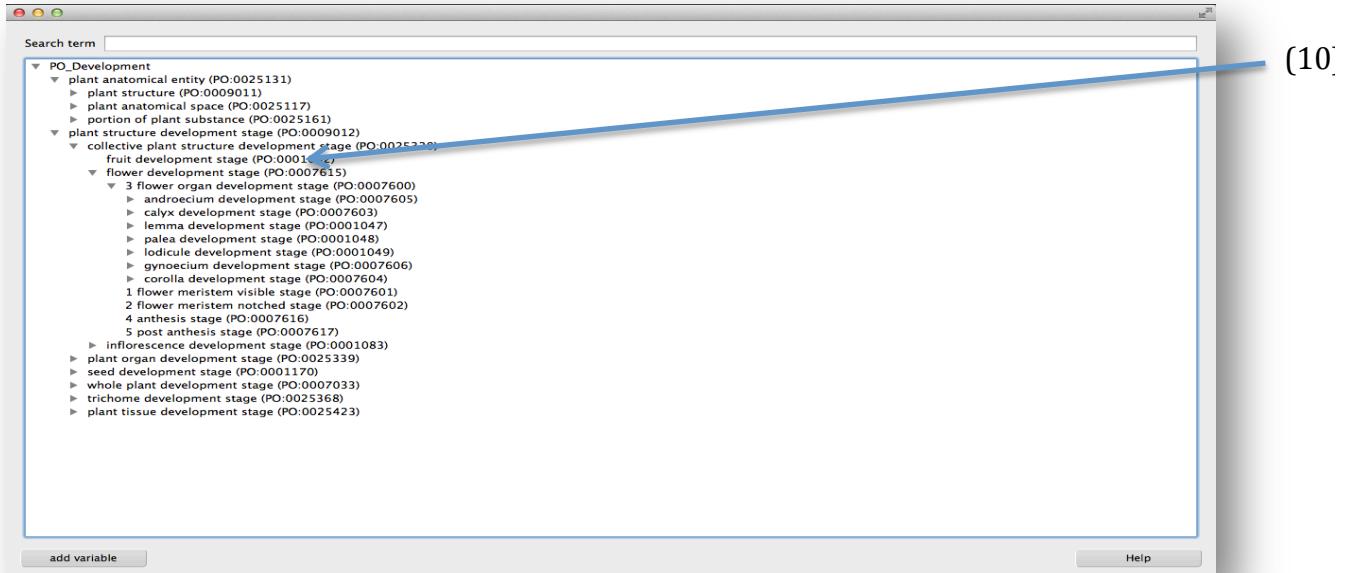


Figure 34: Developmental stage ontology tree

Now you can see that the variable has been added in the tree (11). We did the same for structural description (12).

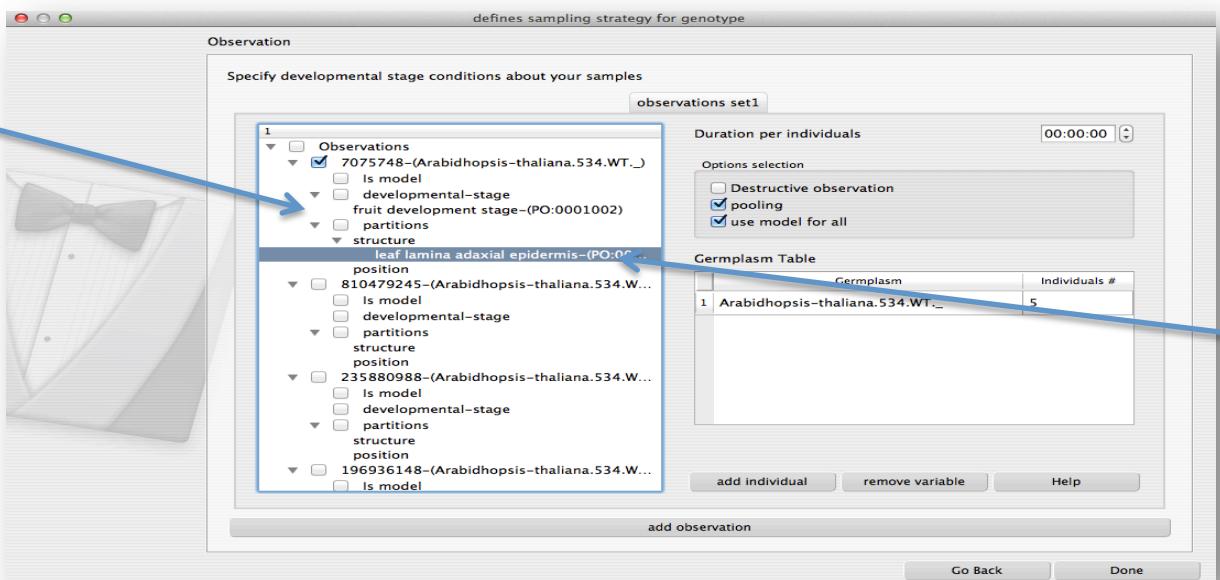


Figure 35: Sample structure selection

Now, we just have to precise the duration of each observation (13), we put 5 seconds for each. To finish click on done.

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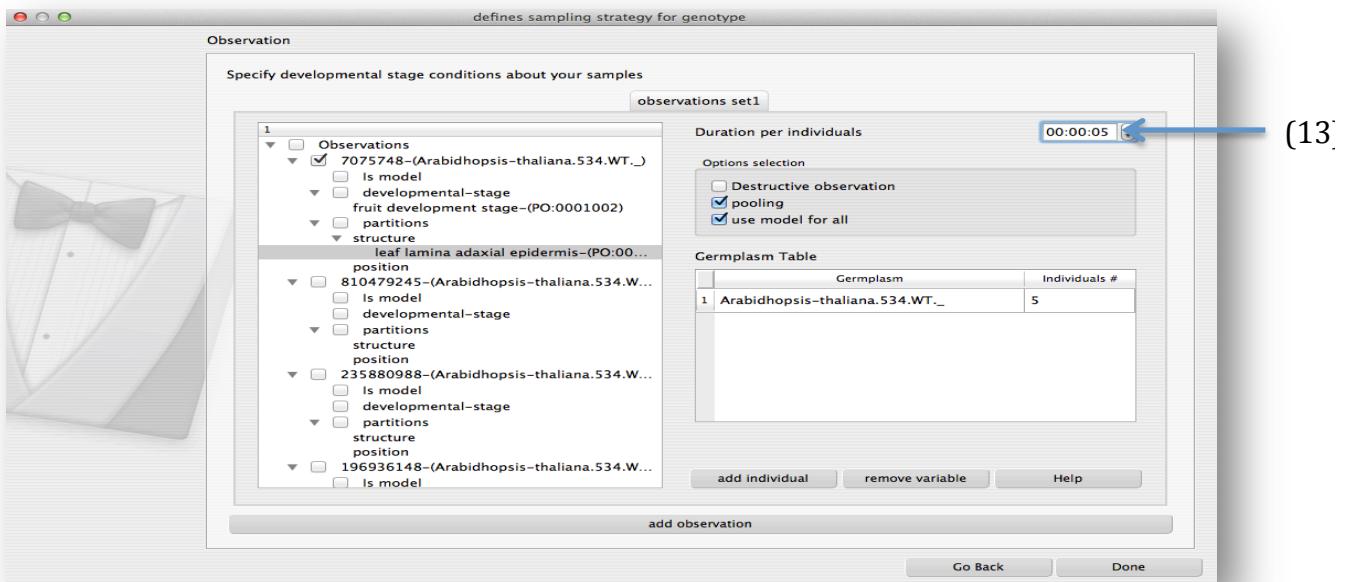


Figure 36: observation duration selection

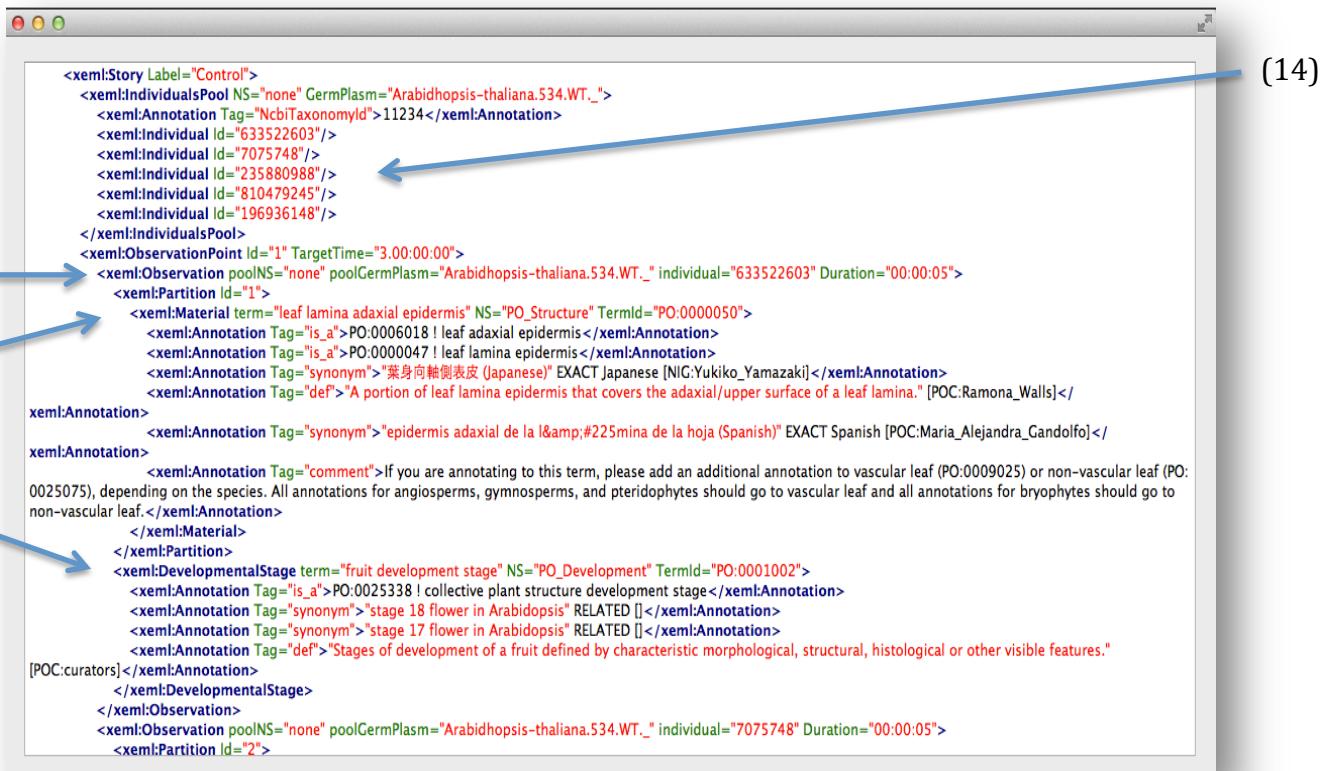


Figure 37: XEML Document observation part.

You can see in the Xeml document (Figure 37) that 5 individuals had been added to the corresponding individuals pool (14). Five observations (15) were also created with the developmental stage (17) and the structure (16) described during the wizard and added to the observation point 1. In our case, we have chosen pooling sample options and you can see at the

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end of the story in the XEML document that 1 sample had been added with 5 partition (Figure 38) corresponding to each partition of each observation.

```
</xeml:ObservationPoint>
<xeml:ObservationPoint id="2" TargetTime="14.06:00:00"/>
<xeml:ObservationPoint id="3" TargetTime="8.23:00:00"/>
<xeml:Sample id="1" Timeltermix="Min">
    <xeml:BioSource partition="1"/>
    <xeml:BioSource partition="2"/>
    <xeml:BioSource partition="3"/>
    <xeml:BioSource partition="4"/>
    <xeml:BioSource partition="5"/>
</xeml:Sample>
</xeml:Story>
</xeml:Experiment>
</xeml:XEMLDocument>
```

Figure 38: Xeml Document Sample part