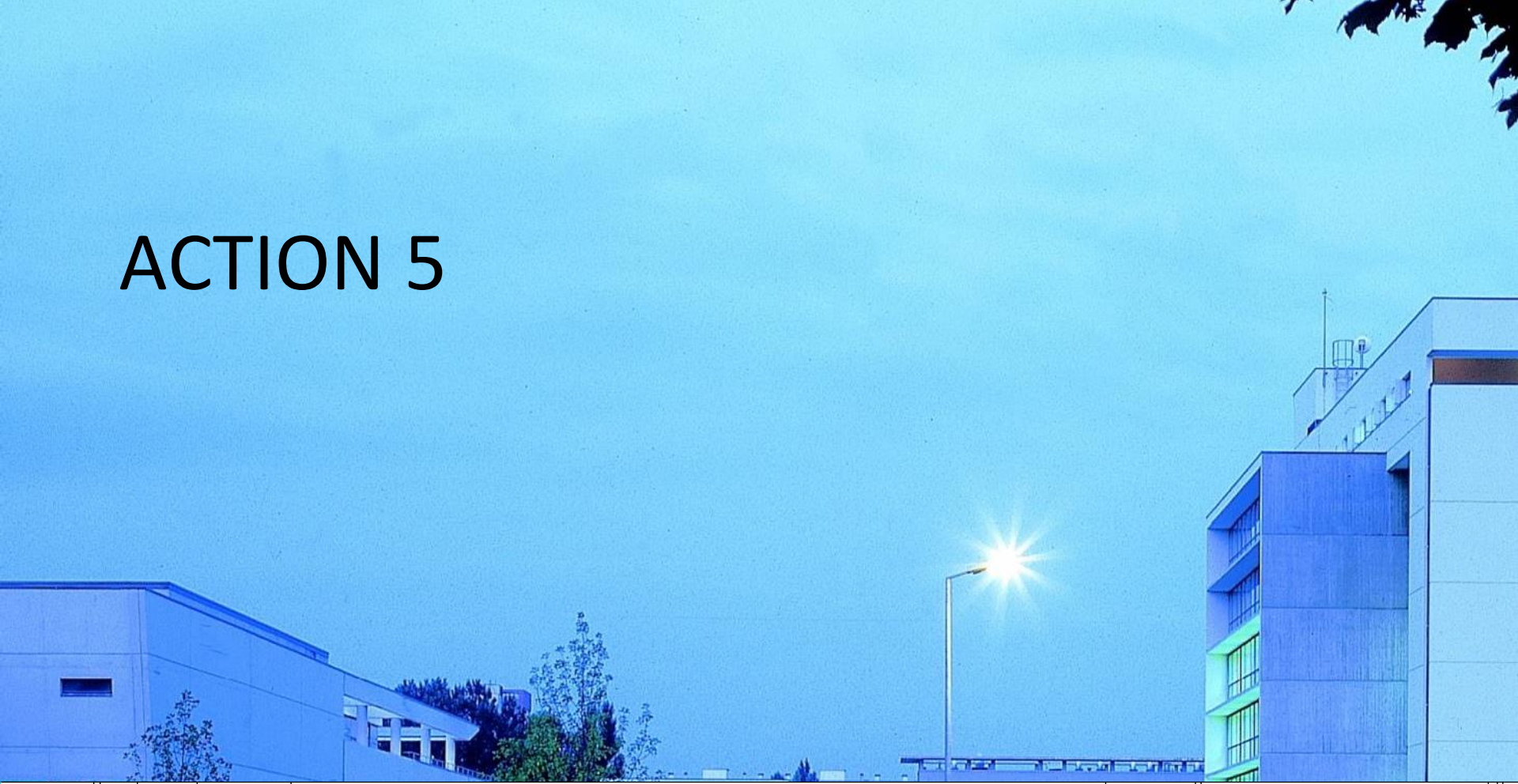
ACTION 5

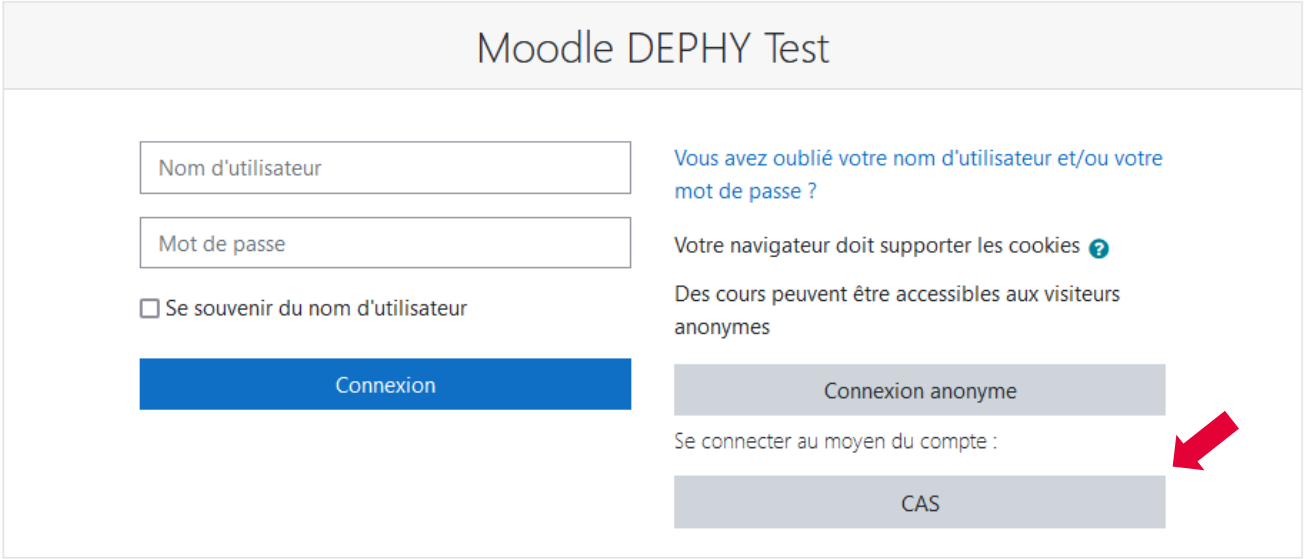


Action 5 - Développer la pratique virtuelle du dessin technique en chimie

CHM –Faculté de chimie, ECPM, Faculté de pharmacie, IUT Robert Schuman. **Intervenant: Ingénieur Chemo-informaticien CHM - Louis PLYER**

Démo plug in: Connection to the Moodle test platform

https://moodle-dephy.app.unistra.fr/



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Plugin Molsimilarity

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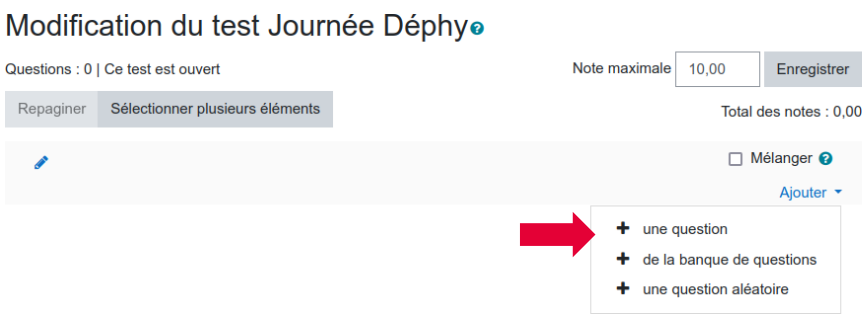
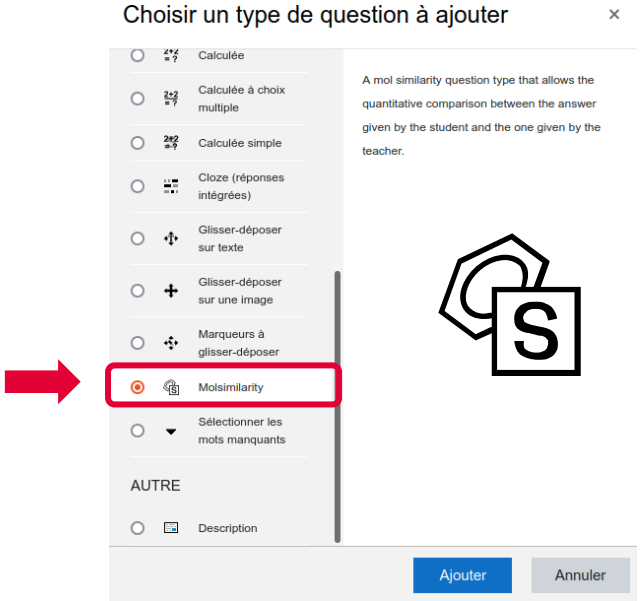
Plugin Molsimilarity : Creation of the question (1)





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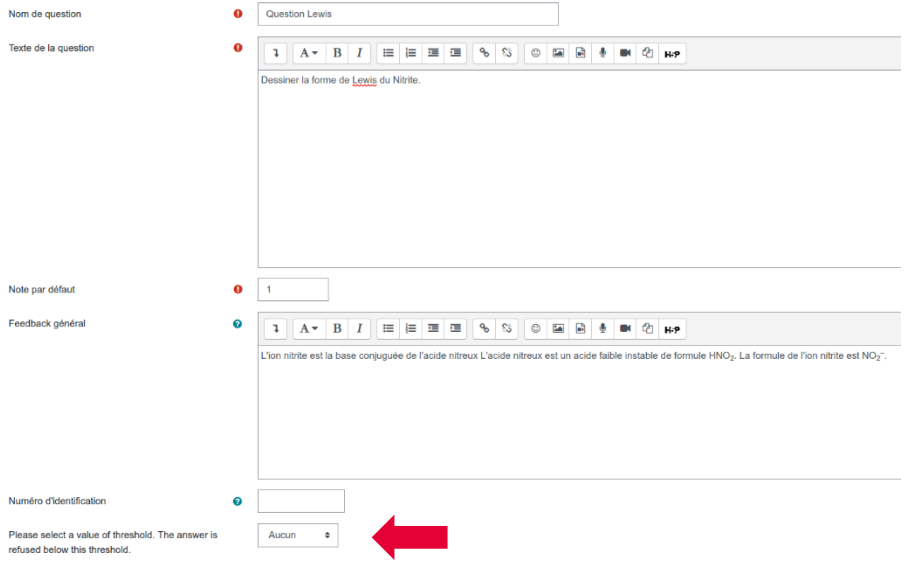
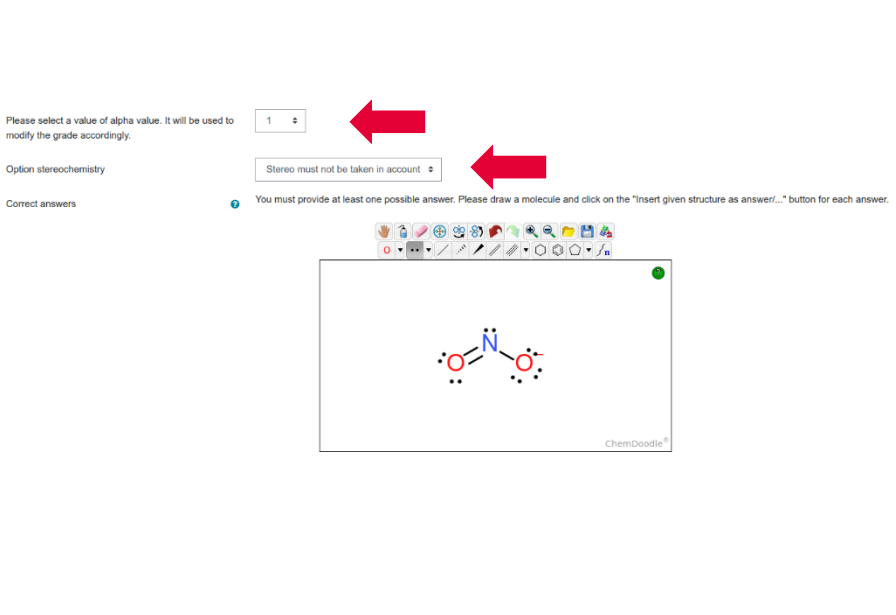
Plugin Molsimilarity : Creation of the question (2)





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Plugin Molsimilarity : Formulas

- Grade g_{rest} : Tanimoto similarity between the student's and teacher's structures, computed on the REST server.

- Stereochemistry analysis not requested ?

→ g_{rest} sent back to Moodle.

- Otherwise ?

→ $$g_{rest} = \begin{cases} \frac{\#Correct\ Stereo\ Center}{\#Total\ Stereo\ Center}, & if\ \ similarity\ score\ = 1 \\ 0, & if\ similarity\ score\ \neq 1 \end{cases}$$

- g_{rest} returned to the Moodle server, final grade g is calculated:

→ $$g = \begin{cases} (g_{rest})^{\alpha}, & if\ (g_{rest})^{\alpha}\ \geq t \\ 0, & otherwise \end{cases}$$

- t and α are user defined parameters.

- α parameter modulates teacher's exigency:
  - → α < 1 soft grading
  - → α > 1 severe grading

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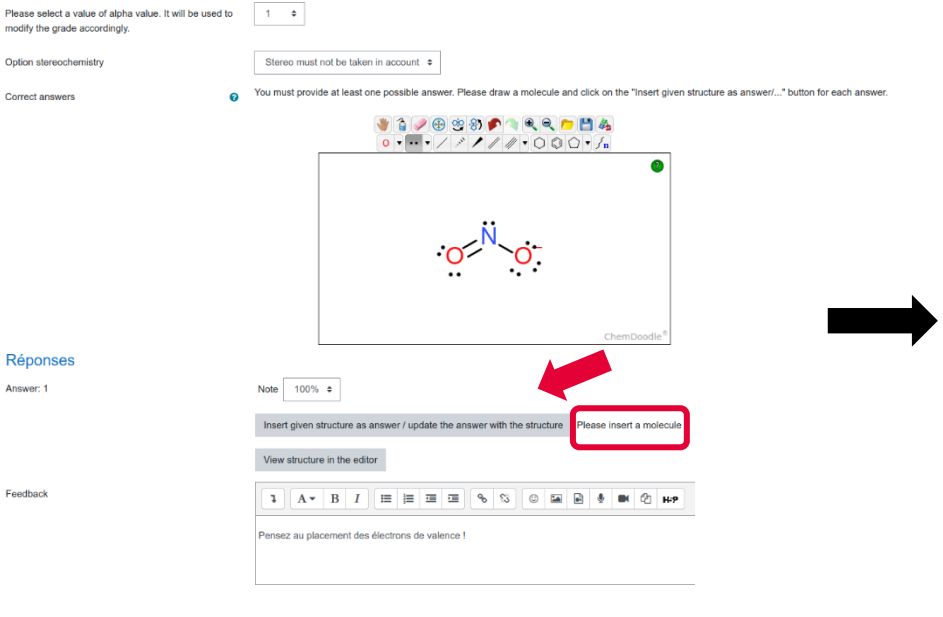
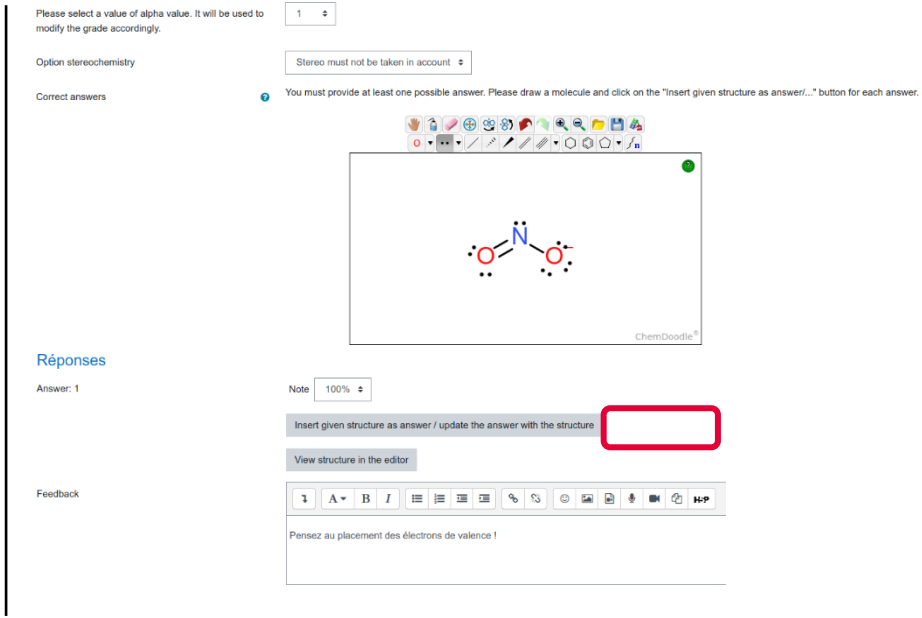
Plugin Molsimilarity : Creation of the question (3)





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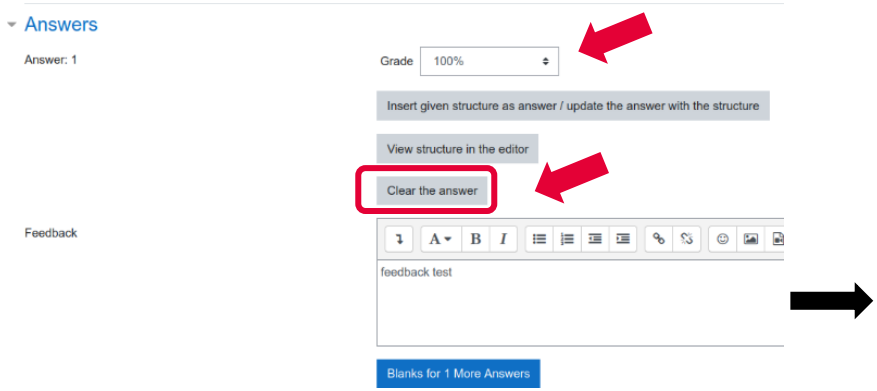
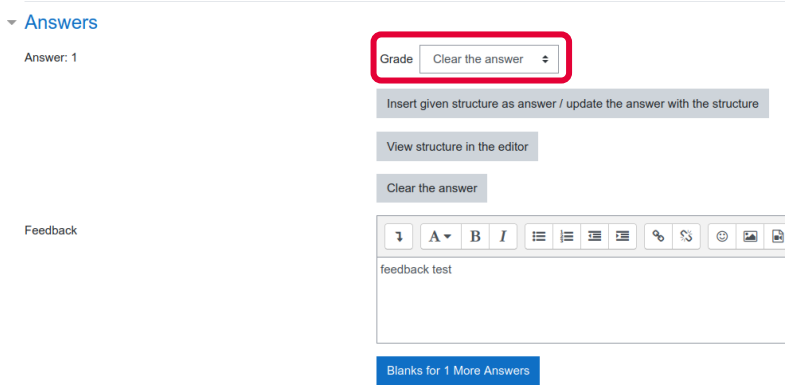
Plugin Molsimilarity : Deletion of an answer (4)





- Set the grade to « Clear the answer »
- Click on the « Clear the answer» button

- Click on the “save changes and continue editing” or “save changes” button

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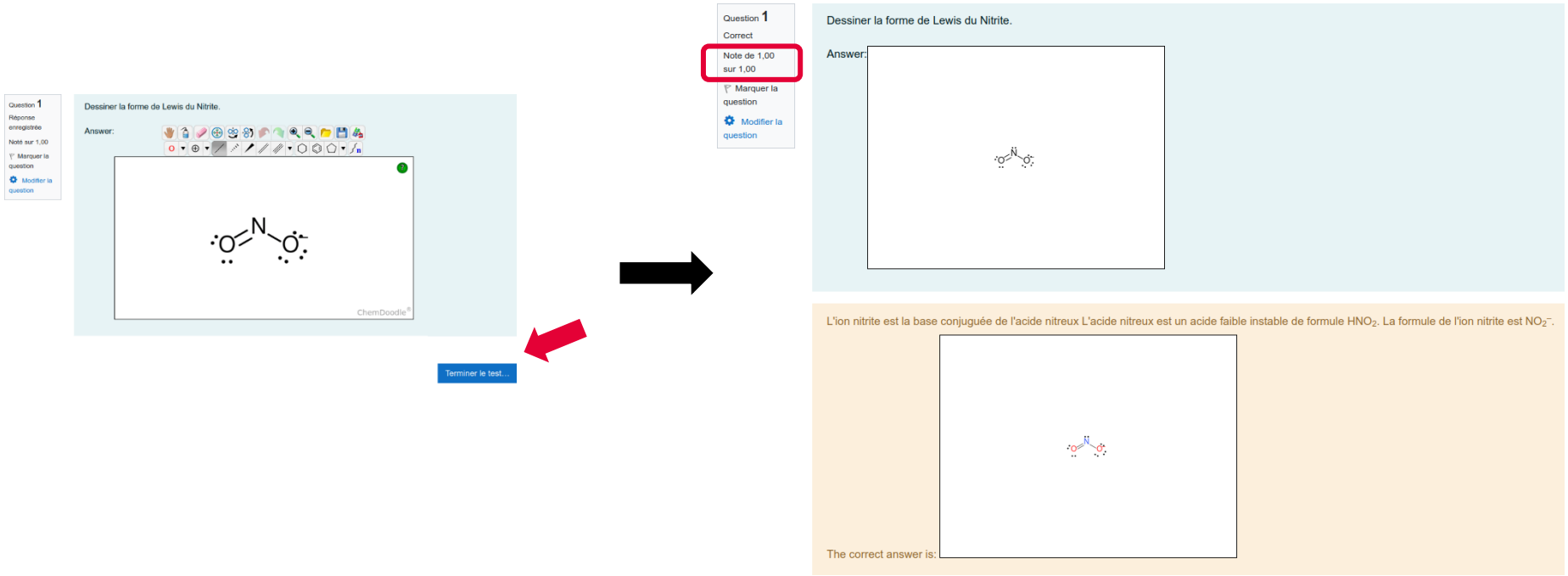
Plugin Molsimilarity : Student interface



Plugin Molsimilarity : Your turn

Possible types of question:

- Identify the major product of a reaction.
- Drawing a Lewis structure.
- Drawing a given configuration of a molecule (R/S, E/Z)
- Question with multiple good answers: ex “What is the structure of glucose ?”, where the answer can be one of three structures: open, furanose and pyranose.

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Plugin Molsimilarity : Stereochemistry

Stereocenters comparison using INCHI: impossible if the structures (without stereo labels) are not identical.

If the similarity score is not equal to 1, a g_{rest} = 0 is returned to Moodle.

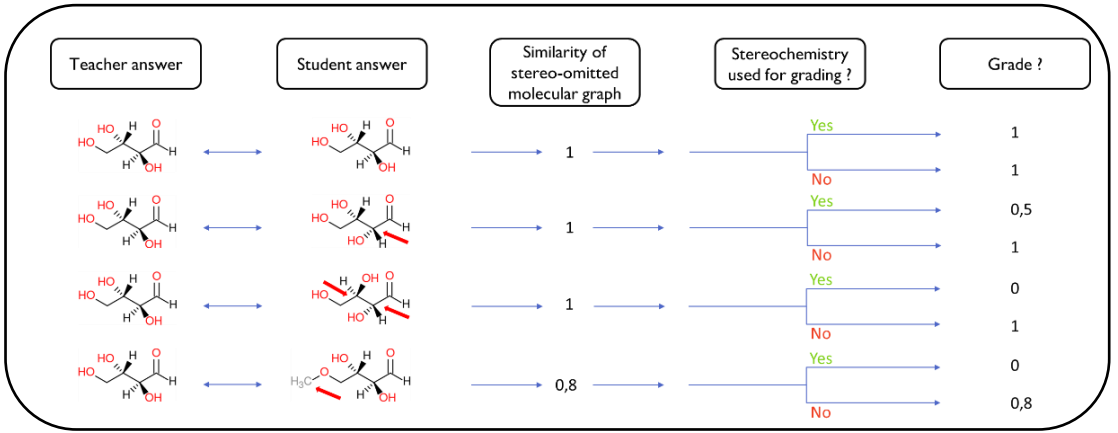
4th example: student has confused an alcohol function with an ether: the Tanimoto similarity score

student/teacher structures is 0.8.

Therefore:

→ g_{rest} = 0, if the stereochemistry is required

→ g_{rest} = 0.8 otherwise.



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Plugin Molstructure

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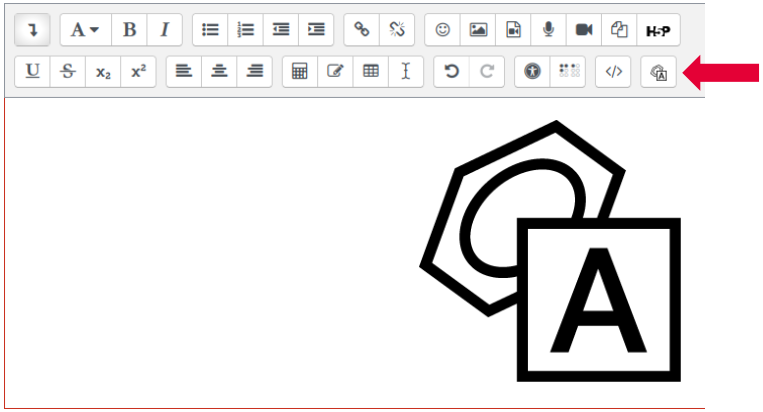
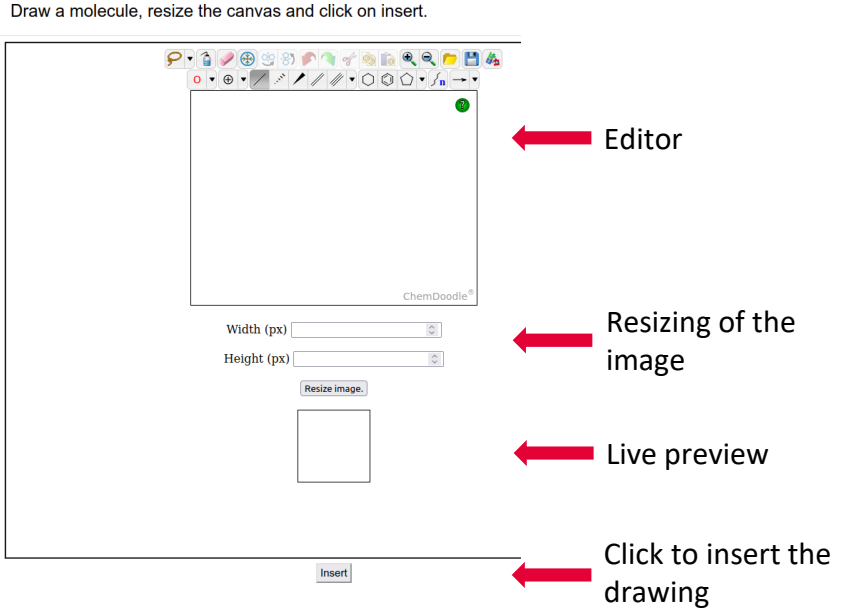
Plugin Molstructure : Where to find the Molstructure plugin / Interface

In any question, the plugin is available to add a picture of a molecule/reaction.





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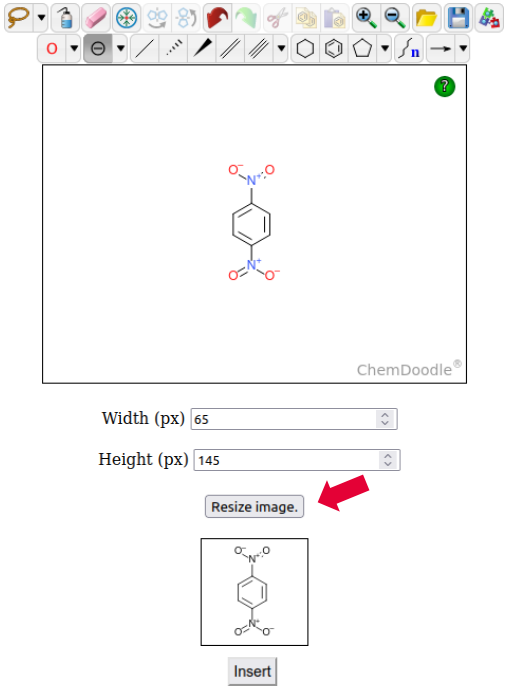
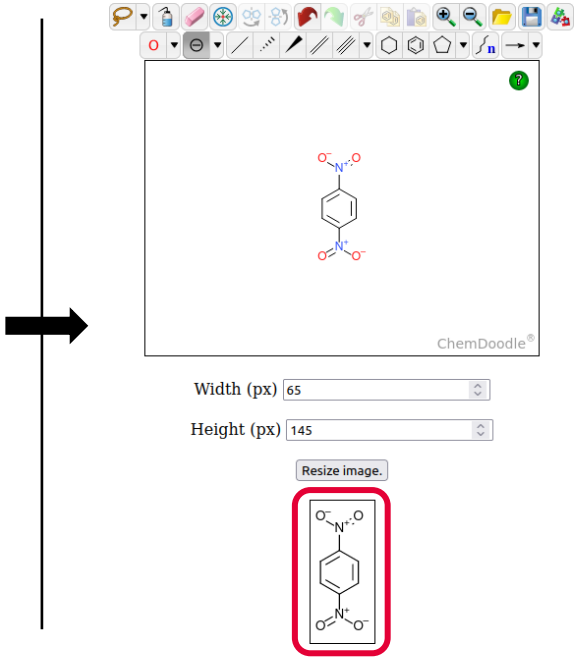
Plugin Molstructure: How to resize the image





To resize the image:

- Modify the values of Width and Height to fit the drawn compound.
- Click on the '*Resize image*' button.

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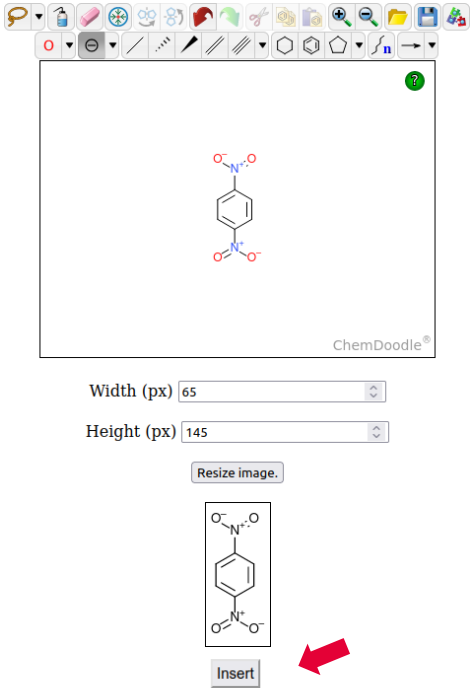
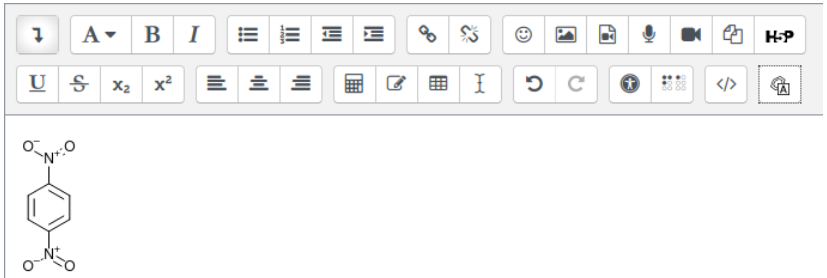
Plugin Molstructure: How to insert the image





To insert an image:

- Draw and resize the image as needed
- Click on the '*Insert*' button.