# Implementation of a soft grading system for chemistry in a Moodle plugin.

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## Summary

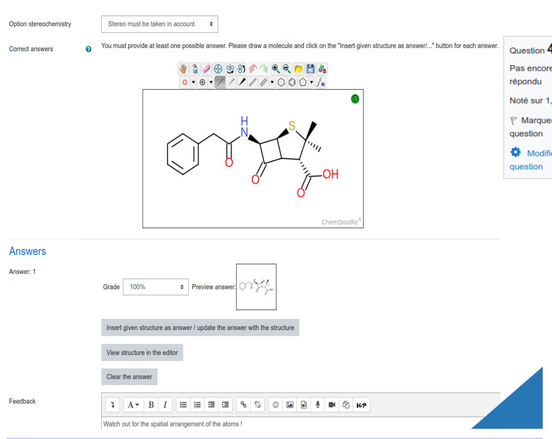
We propose a novel approach for grading chemical structures drawings for remote teaching, integrated to the Moodle platform. The platform uses a binary grading system, which often fails to give a nuanced evaluation of the answers. This is particularly true in the case of chemistry drawing, where most questions simply cannot be evaluated on a true/false basis. Specifically, a strict comparison of the candidate and the expected drawings is insufficient when some tolerance is deemed acceptable. To alleviate this constraint, the herein proposed grading workflow is based on computing the similarity between the chemical drawings. It is implemented as a Moodle plugin, using Chemdoodle engine for drawing structures, and communicating with a REST server to compute the similarity using ISIDA descriptors and Tanimoto coefficient.

## Developments

Presentation of two plugins:

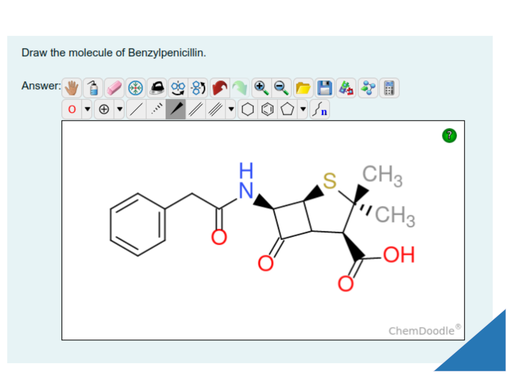
- Soft grading system for chemistry in a Moodle plugin: molsimilarity.
- Atto plugin to insert chemical drawings in any question on Moodle: molstructure.

## Front-end workflow



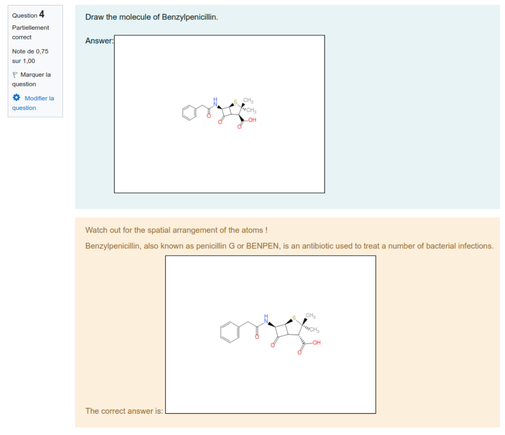

**1. Drafting the question**

- Intended answer
- Does the stereochemistry need to be taken in account
- Feedback




**2. Student's answer**

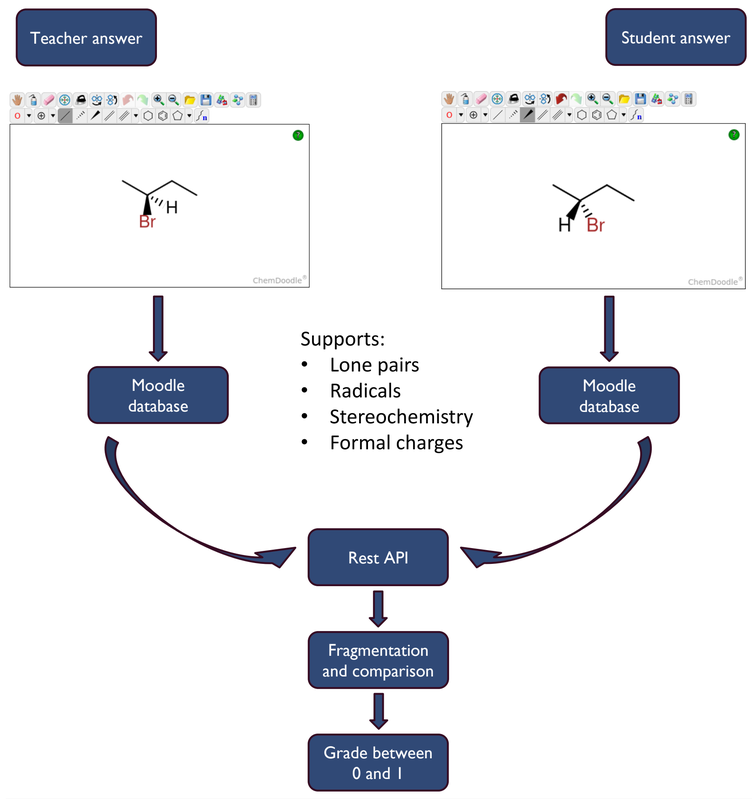
- Draws the answer




**3. Soft grading and feedback**

- Grade is shown to the user
- Both the student and teacher answers are shown
- If the grade is not correct, a special feedback is displayed

## Back-end workflow

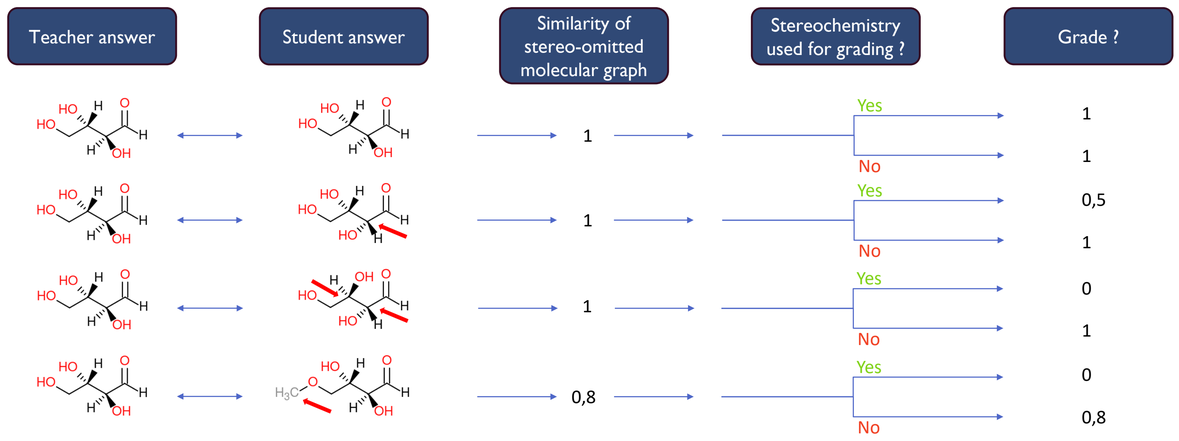



*Answer to be corrected: both student's and teacher's answers, and the stereochemistry parameters are sent to the Rest API which will fragment the molecules, compare them and send back the score to Moodle.*

## Possibilities in term of correction

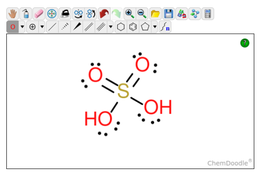
**Stereochemistry (R/S, Z/E)**

- Computed if both stereo-omitted molecular graphs are identical and the option is selected.
- Otherwise, the grade will be null.




**Lone pairs and radicals**

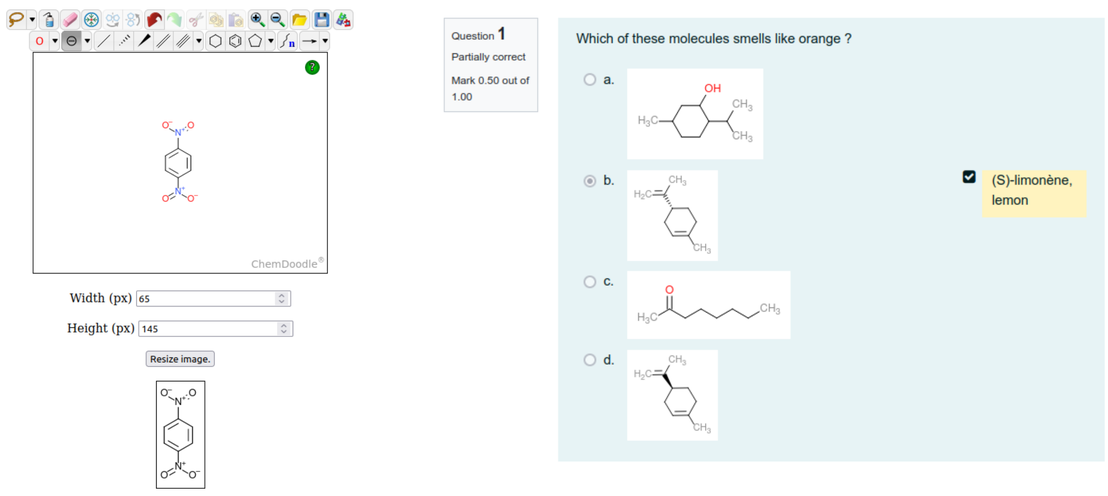
- Molecular descriptors sensitive to lone pairs and radicals.
- The score penalizes errors on radicals and lone pairs.




## Atto plugin

**Why the need for a new chemistry editor atto plugin ?**

- Insert chemical drawings in any type of question, E.g. multi choice questions
- 100% free tool and open source – no license
- Plug and play – no settings on the administrator side
- Live preview of the inserted drawing size




*Editing interface (left), and example of a multi choice question making use of the atto plugin (right).*

## Conclusions

- A new tool allowing teachers to ask several types of questions to be corrected automatically has been developed.
- The plugin is highly adaptable to any academic user; additionally, both embedding and similarity measures can be configured.
- The tool will be made available for the Moodle platform (developed under V3.9) on the Moodle plugin marketplace in 2022.
- A new tool allowing teachers to add chemical drawings in any question on Moodle has been developed. It will be made available on the Moodle plugin marketplace in 2022.

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