LOUIS PLYER

New chemistry teaching tools for Moodle: Chemical substances, MolSimilarity, ReacSimilarity.

Supervisor: Dr Gilles Marcou

Moodle Advisor: Céline Perves

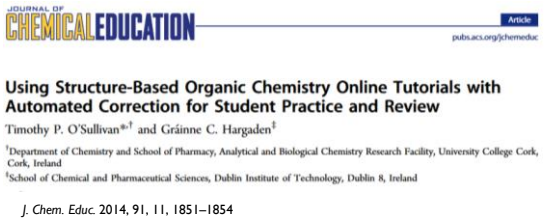
LMS and chemistry: different approaches

Quizz

Chatbot

Drawing structures, automatic correction

Uses drawing of structures



JOURNAL OF CHEMICAL EDUCATION — Article — pubs.acs.org/jchemeduc

Using Structure-Based Organic Chemistry Online Tutorials with Automated Correction for Student Practice and Review

Timothy P. O'Sullivan*[†] and Gráinne C. Hargaden[‡]

[†]Department of Chemistry and School of Pharmacy, Analytical and Biological Chemistry Research Facility, University College Cork, Cork, Ireland

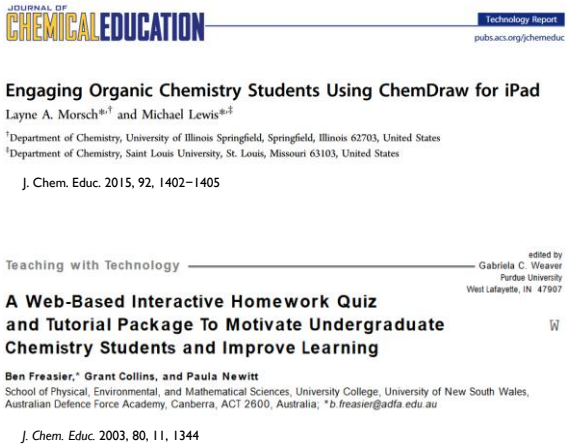
[‡]School of Chemical and Pharmaceutical Sciences, Dublin Institute of Technology, Dublin 8, Ireland

J. Chem. Educ. 2014, 91, 11, 1851−1854

OpenOChem: An LMS Agnostic Chemistry Quizzing Platform

Carl LeBlond (Indiana University of Pennsylvania)
Ehren Bucholtz (St. Louis College of Pharmacy)
Jennifer Muzyka (Centre College)

CCCE Newsletter. 2019, 04/29 - 05/01



JOURNAL OF CHEMICAL EDUCATION — Technology Report — pubs.acs.org/jchemeduc

Engaging Organic Chemistry Students Using ChemDraw for iPad

Layne A. Morsch*[,†] and Michael Lewis*[,‡]

[†]Department of Chemistry, University of Illinois Springfield, Springfield, Illinois 62703, United States

[‡]Department of Chemistry, Saint Louis University, St. Louis, Missouri 63103, United States

J. Chem. Educ. 2015, 92, 1402−1405

Teaching with Technology — edited by Gabriela C. Weaver, Purdue University, West Lafayette, IN 47907

A Web-Based Interactive Homework Quiz and Tutorial Package To Motivate Undergraduate Chemistry Students and Improve Learning

Ben Freasier,* Grant Collins, and Paula Newitt

School of Physical, Environmental, and Mathematical Sciences, University College, University of New South Wales, Australian Defence Force Academy, Canberra, ACT 2600, Australia; **b.freasier@adfa.edu.au*

J. Chem. Educ. 2003, 80, 11, 1344

JOURNAL OF CHEMICAL EDUCATION

pubs.acs.org/jchemeduc — Communication

Chemist Bot as a Helpful Personal Online Training Tool for the Final Chemistry Examination

Ekaterina Korsakova, Olga Sokolovskaya, Daria Minakova, Yulia Gavronskaya, Nadezhda Maksimenko, and Mikhail Kurushkin*

J. Chem. Educ. 2022, 99, 1110−1117

Developed plugins

Atto plugin to insert chemical drawings in any question and resources on Moodle:

Molstructure.

Soft grading system for chemistry in a Moodle plugin:

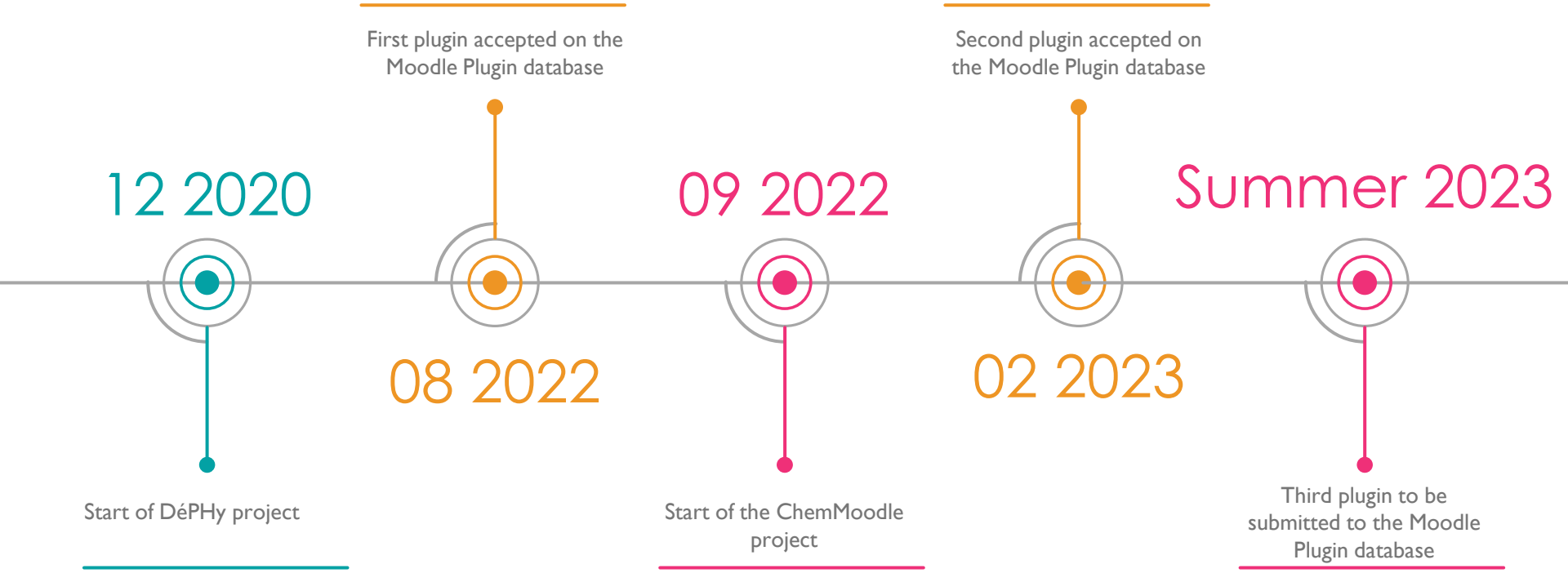
Molsimilarity[1]

Soft grading system for chemical reactions in a Moodle plugin:

Reacsimilarity

1. Plyer, L., Marcou, G., Perves, C., Schurhammer, R. & Varnek, A. Implementation of a soft grading system for chemistry in a Moodle plugin. J Cheminform 14, 72 (2022).

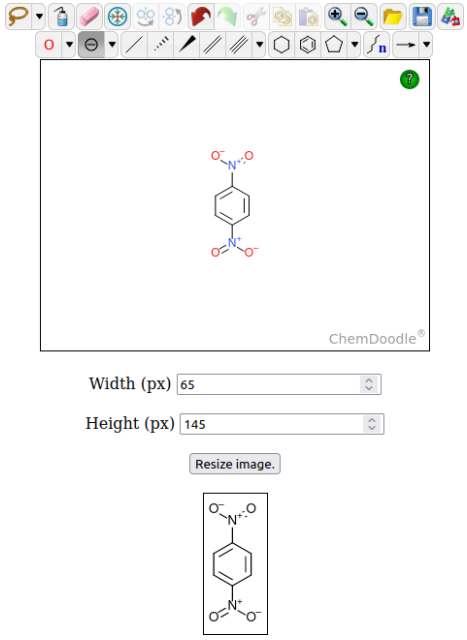
Projects timeline

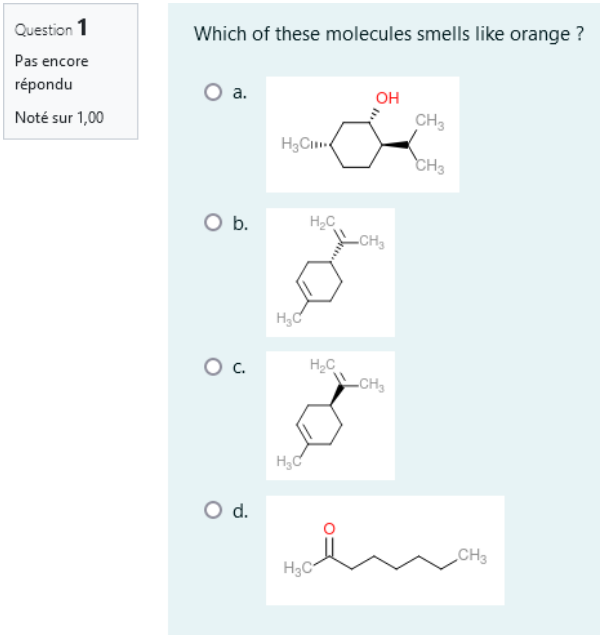


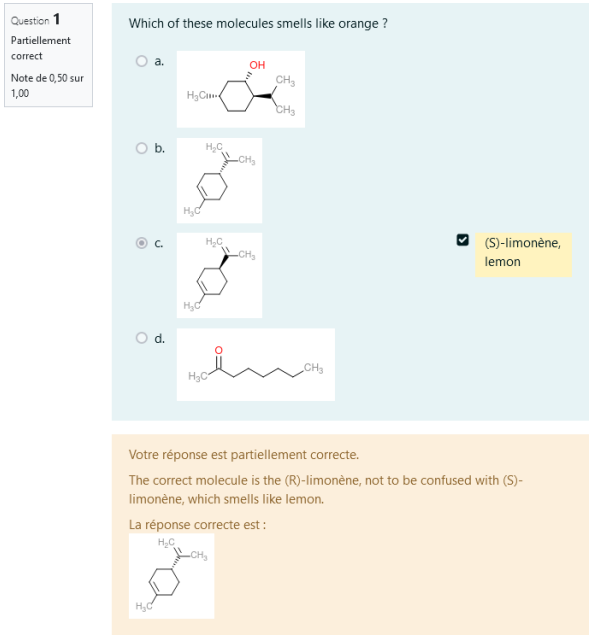
Atto plugin: molstructure

Why the need for a new chemistry editor atto plugin ?

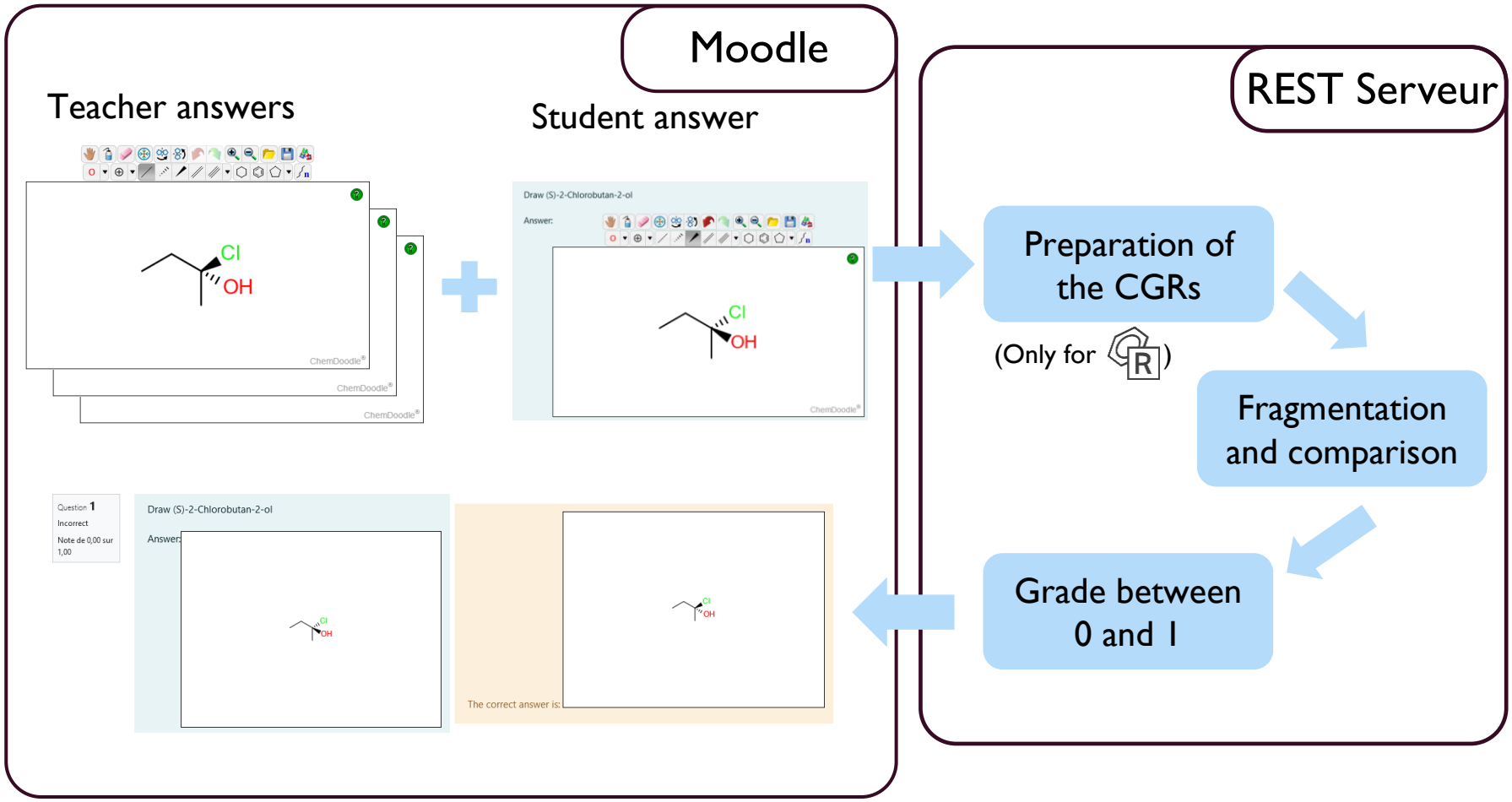
- 100% free tool and open source – no license
- Plug and play – no settings on the administrator side
- Live preview of the inserted drawing size
- Insert chemical drawings in any type of question, E.g., multi choice questions







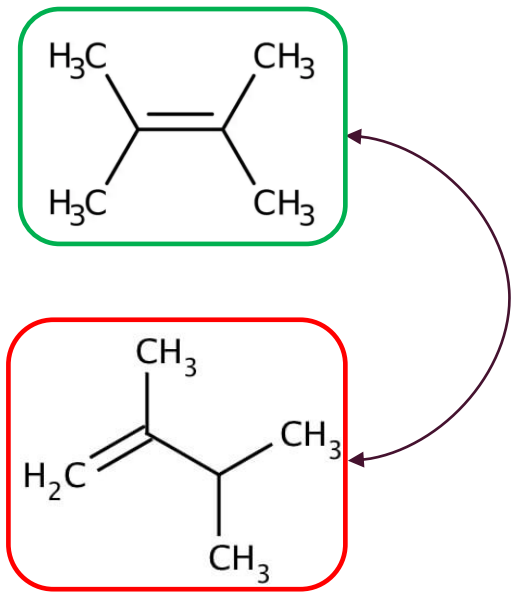
Workflow


Moodle
Teacher answers
Student answer
Cl
OH
ChemDoodle®
Draw (S)-2-Chlorobutan-2-ol
Answer:
Question 1
Incorrect
Note de 0,00 sur 1,00
The correct answer is:
REST Serveur
Preparation of the CGRs
(Only for R)
Fragmentation and comparison
Grade between 0 and 1

Soft grading through similarity (1)

Grade is proportional to the similarity

Example: Major product of 2,3-Dimethyl-2-butanol dehydration by H_2SO_4 ?



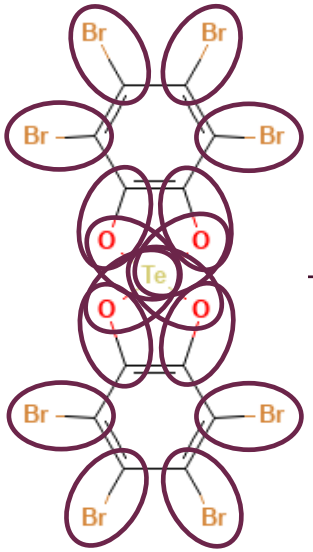
Grade computation

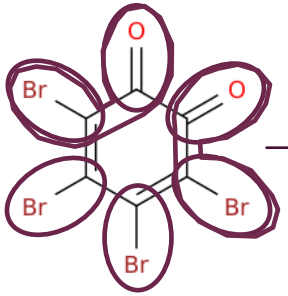
Good answer:
Other plugins: 1/1
Our plugin: 1/1

Wrong answer:
Other plugins: 0/1
Our plugin: 0,68/1*

* For the fragmentation scheme AB(2–4)FC_UR

Substructural molecular fragments (SMF)





ISIDA/Fragmentor SMF

C=O	C-O	C-Br	O-Te	Br-C-C=O	…
0	4	8	4	0	…
2	0	4	0	2	…

Molecules and reactions can be encoded by a descriptor vector[1]. It can be used for several applications from machine learning to description of a database.

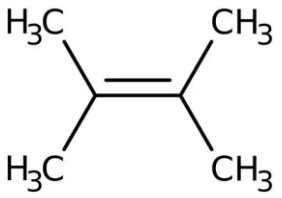
1. Varnek, A., Fourches, D., Hoonakker, F. & Solov'ev, V. P. Substructural fragments: an universal language to encode reactions, molecular and supramolecular structures. J Comput Aided Mol Des 19, 693–703 (2005).

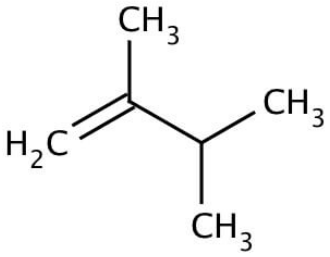
Soft grading through similarity (2)

Goal: Moving from binary to continuous notation
How ? → Tanimoto similarity

$$T_s = \frac{A \cap B}{A \cup B}$$

Example: Correction of the "incorrect" answer





SMF Computation*

C	C-C	C-C-C	C-C-C-C	C=C	C=C-C	C=C-C-C	C-C=C-C
6	4	2	0	1	4	0	4
6	4	4	2	1	2	2	0

$$\sum_i {A_i}^2 = 6^2 + 4^2 + 2^2 + 1 + 4^2 + 4^2 = 89$$

$$\sum_i {B_i}^2 = 6^2 + 4^2 + 4^2 + 2^2 + 1 + 2^2 + 2^2 = 81$$

$$\sum_i A_i B_i = 6^2 + 4^2 + (2 \times 4) + 1 + (4 \times 2) = 69$$

$$T_s = \frac{69}{89 + 81 - 69} = 0{,}68$$

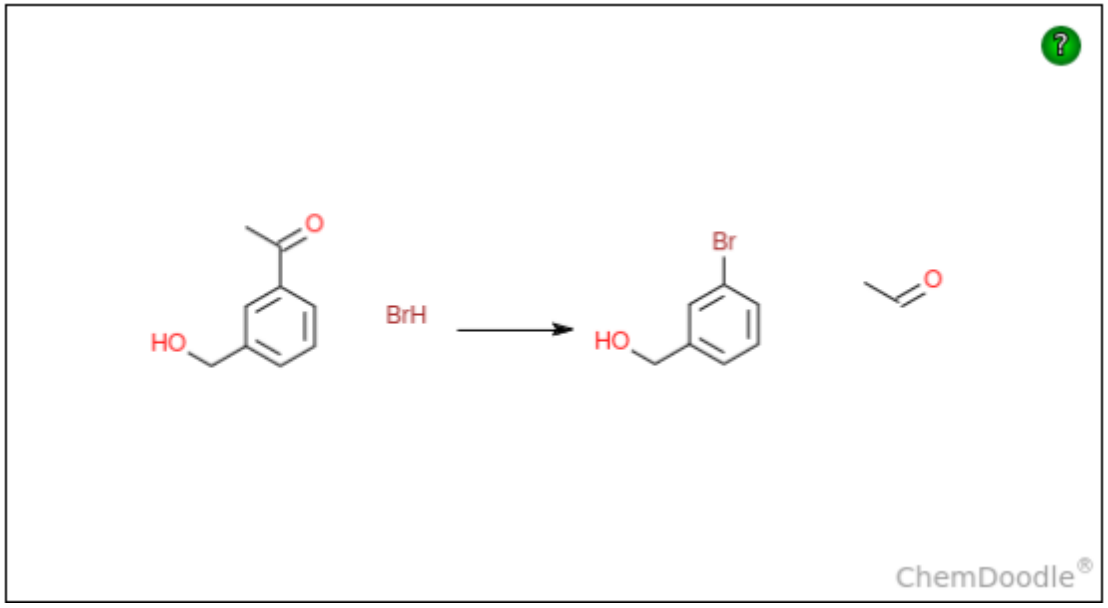
* For the fragmentation scheme AB(2–4)FC_UR

From molecules to reactions

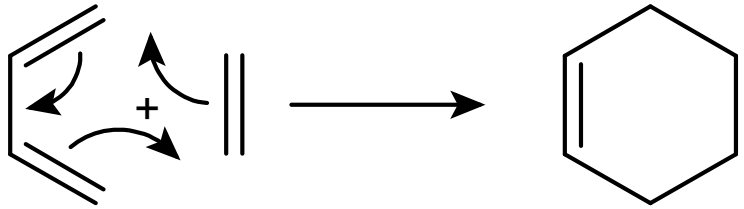
Other plugins: grading molecule by molecule

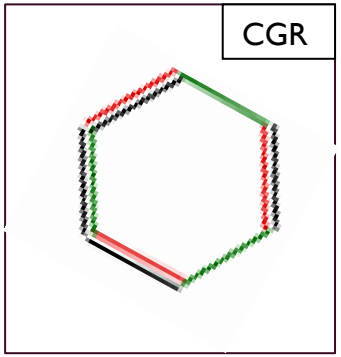
Issues: - Need to write molecules in same order

- Need to correct n object instead of one



Condensed graph of reaction (CGR)





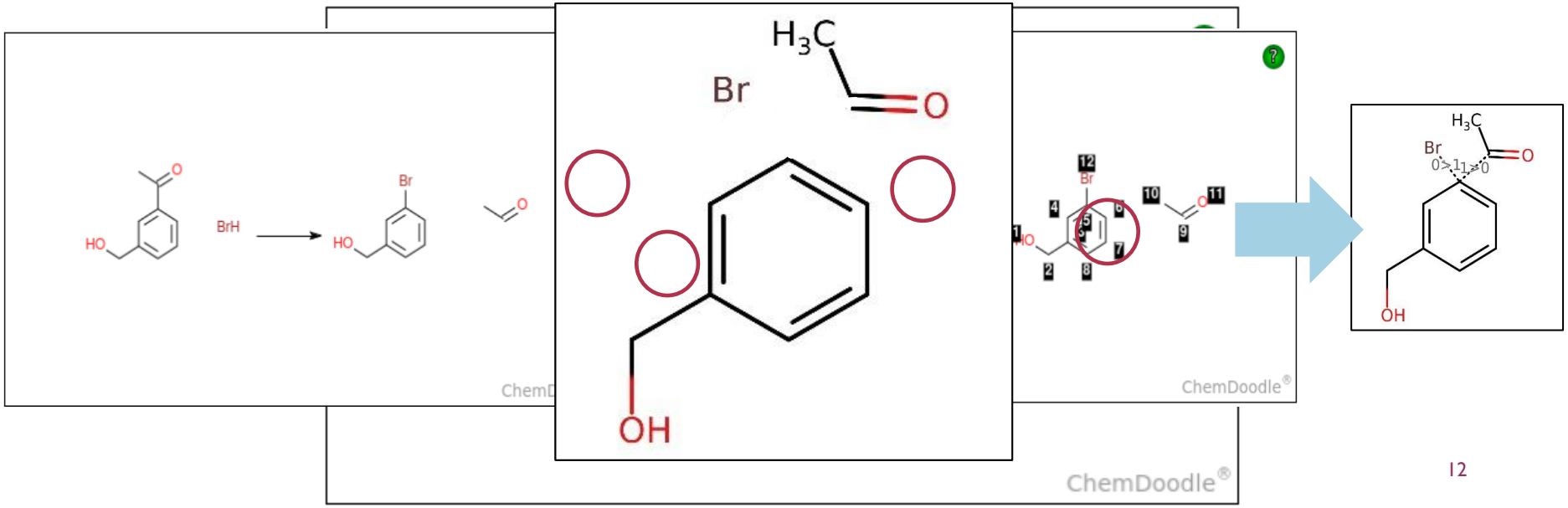
Example of a Diels-Alder reaction (left), with the associated Condensed Graph of Reaction[1] *(right). Green bonds are created one and red bonds are deleted one.*

A CGR can be considered as a pseudomolecule and chemoinformatic methods applied to it

1. Fujita, S. Description of organic reactions based on imaginary transition structures. 1. Introduction of new concepts. *J. Chem. Inf. Comput. Sci.* **26**, 205–212 (1986).

How to build a CGR

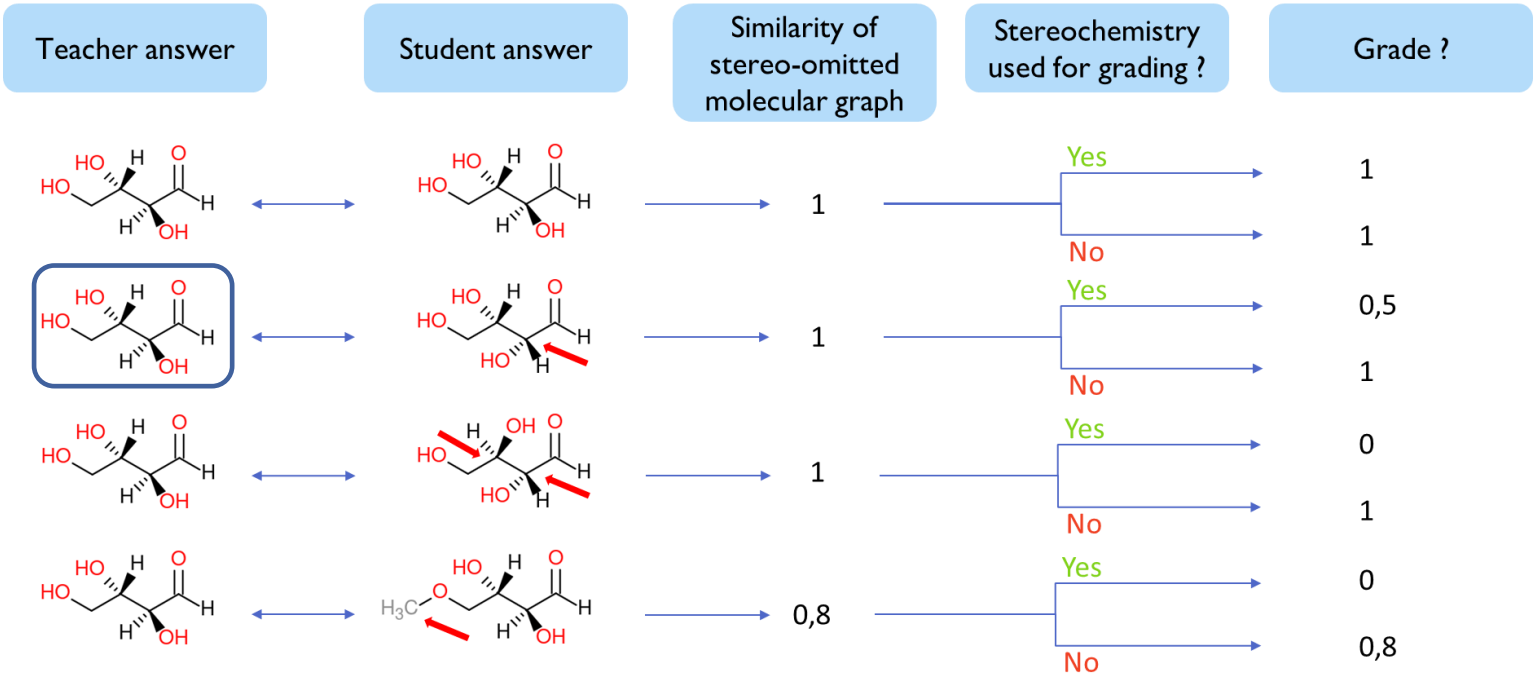
Atom mapping: needed to link the reactants and products graphs
It assigns a unique identifiers to the atoms of reactants and products
→ Find the environment of a product atom in the atoms of the reactants
→ Determine the changes in the graph
→ If the environment changed, dynamic bonds and/or atoms.



Possibilities in term of correction (1)

Stereochemistry (R/S, Z/E)

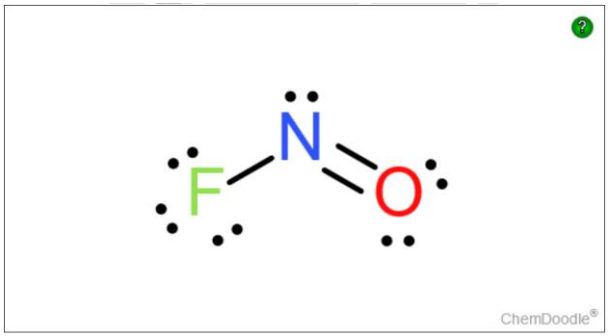
- Computed if both stereo-omitted molecular graphs are identical and the option is selected.



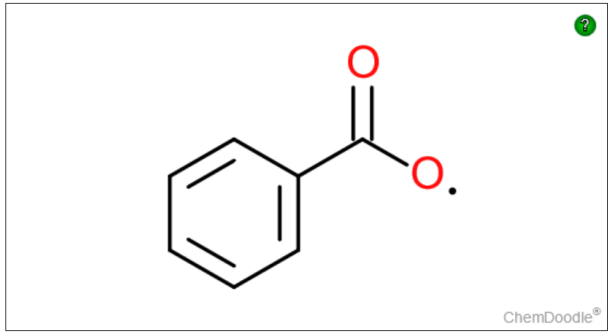
Possibilities in term of correction (2)

Lone pairs, radicals, and formal charges

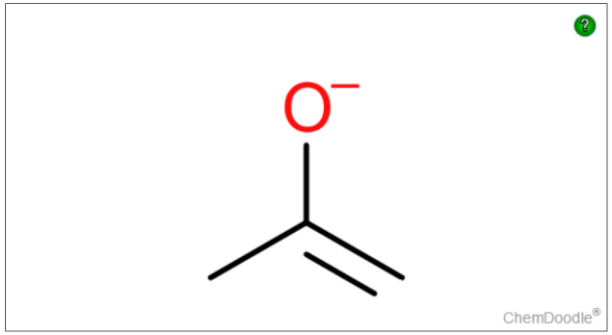
- Molecular descriptors sensitive to lone pairs, formal charges and radicals.
- The score penalizes errors on radicals and lone pairs.



Nitrosyl Fluoride

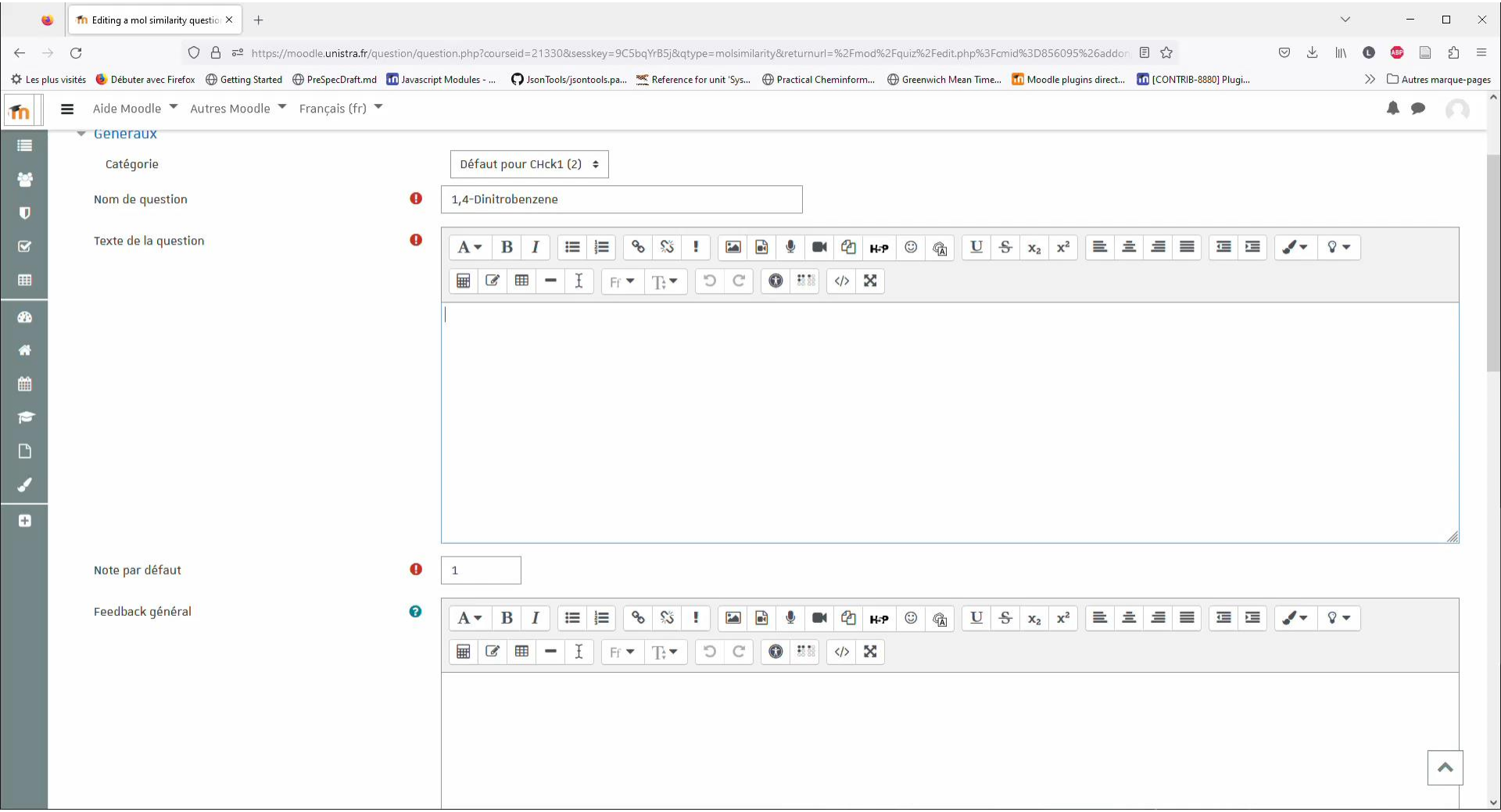


(Benzoyloxy) radical



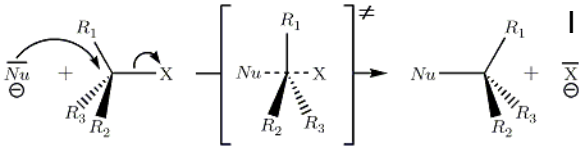
Propene-2-olate

Demo plugin molsimilarity

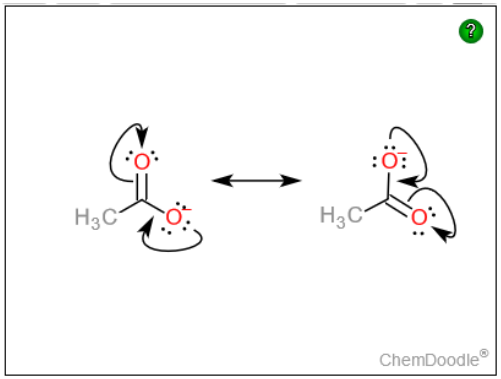


Perspectives

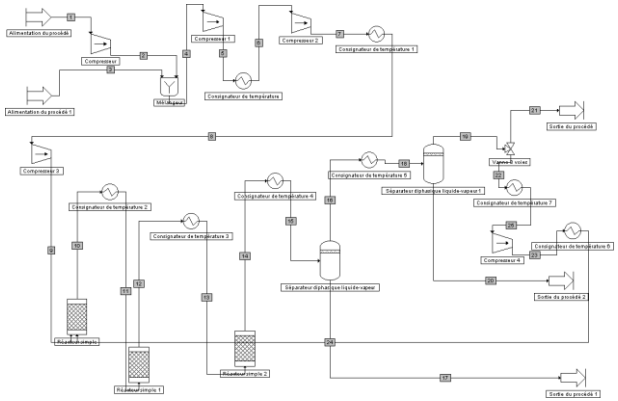
Several developments can be thought of :



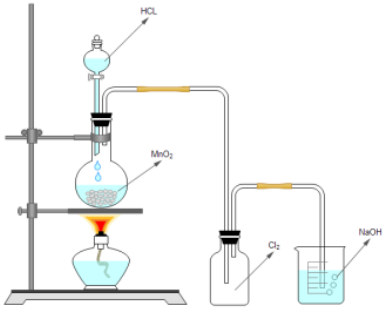
Stereochemistry for the reaction plugin



Drawing of mechanistic arrows → Plugin atto



Chemical engineering plugin



Chemical experimental setup plugin

Disseminate the plugins

- University
- Secondary

1. https://fr.wikipedia.org/wiki/Fichier:SN2.gif#/media/Fichier:SN2.gif

Thanks

Dr. Gilles Marcou

Pr. Alexandre VARNEK

Céline Perves

Link to the plugins

Grade calculation

- 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 ?

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

- 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