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Two Decades of Online Teaching: Trends, Challenges, and Future Directions

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Abstract: Over the past two decades, significant advancements in educational technology have revolutionized the field of chemical education. This publication presents our contributions using web-based tools that have been developed over this period, enabling chemistry students to engage with exercises that closely mirror real-world scenarios encountered in their future careers. These freely available online resources have facilitated the seamless integration of theoretical knowledge and practical applications, fostering critical thinking and problem-solving skills.

Keywords: e-Learning · Online teaching · Structural analysis

With a PhD in organic chemistry, ***Luc Patiny*** has always been interested in computer programming and has made significant contributions to the field of cheminformatics and chemical education. He has authored over 50 peer-reviewed publications and contributed to over 200 open-source projects. He is currently teaching and managing chemical information at EPFL, where he won the Crédit Suisse Best Teaching Award and is the Chief Scientific Officer at Zakodium. His pioneering work in using web technology to provide intuitive and useful tools for chemists has been invaluable in both education and research.

After a PhD in physical organic chemistry at the ETHZ, ***Régis Turin*** worked for several years in the private sector. He then became a chemistry teacher at the Lycée-collège des Creusets for a bit more than two decades, before retiring in 2021. He has always been interested in using software, applications, and web-based learning tools in his teaching activity, thereby collaborating with Luc Patiny on several projects. Besides other activities, he is now a teaching consultant to Zakodium.

1. Introduction

For the past 20 years, we have been striving to combine technology with teaching. Our main objectives were and still are to provide students with problem-solving exercises that are like those they will encounter in research and industry, as well as to provide the tools to test their hypotheses. Since the introduction of HTML, we have been using the web-browser as the primary interface for providing exercises. To ensure the best experience, our vision was to develop tools that should be directly accessible from the browser. Initially, we used Java Applets to create interactive applications in web pages, but this approach was discontinued after the introduction of the iPhone. We have since redeveloped over 200 scientific building blocks that process information in pure JavaScript. These building blocks are available on the *cheminfo*, *mljs*, *image-js* and *zakodium-oss* GitHub organizations. Our goal is to focus on teaching chemistry and providing students with the opportunity to progress at their own pace. To this end, auto-correction is essential. In effect, we have a large auditorium with students and teaching assistants to provide individualized assistance.

In this paper, we are presenting a suite of tools developed to facilitate learning in chemistry. These applications, which include interactive simulations, quizzes, and visualizations, are designed to make learning more engaging and effective, and to prepare students for the challenges they will face in the future. We believe that these tools are readily available for use in chemistry classes.

2. General Tools for Chemists

2.1 *gymnase.cheminfo.org*

Heavily used in the French-speaking part of Switzerland, this website has been designed for undergraduate students. It offers many innovative tools and exercises, some of which are presented here.

As a first example, acid-base titrations (Fig. 1), as well as more complex equilibria involving complexation and precipitation can be simulated. These webpages enable students to explore the mixing of inorganic chemicals and observe the concentrations at equilibrium. The system is pre-programmed with the majority of standard pK_a values and will automatically display the equations associated with a given equilibrium.

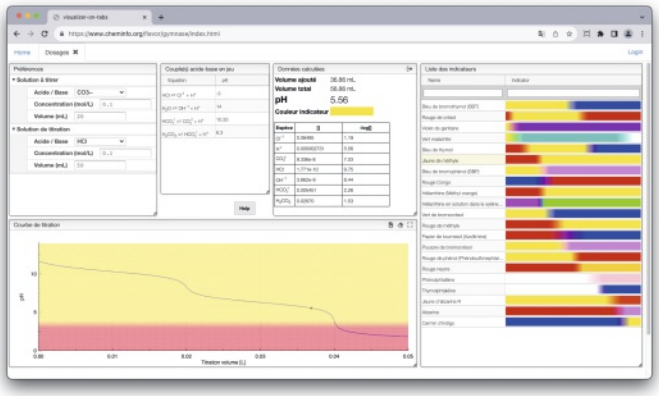

Fig. 1. Simulation of acid-base titration enhanced with the list of possible indicators.

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Exploring the 3D structure of organic compounds is of utmost importance for students to understand stereochemistry and mechanism of reactions. To facilitate the acquisition of this complex topic by autonomous learning, a web application has been designed that enables users to generate 3D models and conformations[1,2] from 2D models. Bond lengths, angles and distances[3] can also be measured, all within the browser (Fig. 2).

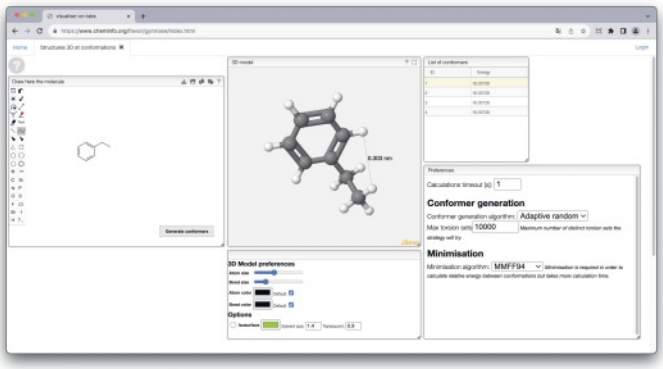

Fig. 2. Generation of 3D models and conformations from a 2D model.

Another tool allows the visualization of orbitals (Fig. 3), which is highly beneficial for explaining aromaticity and identifying the lone pair that may be part of the aromaticity, such as in the case of imidazole. This software can be used by teachers as well as by students for further review of orbital orientations.

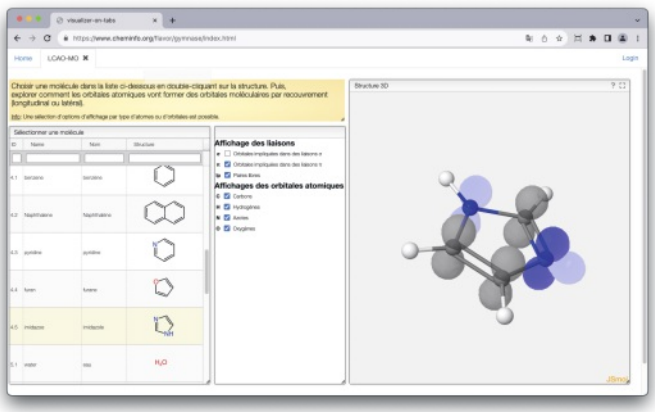

Fig. 3. Exploring orbitals and their orientations.

The determination of structural isomers related to a molecular formula is not only enjoyable, but also a critically important skill that holds significant value for structure elucidation. Students need to possess the ability to envision the various possible structural arrangements based on a given molecular formula. One of the proposed exercises not only facilitates the drawing of all potential structural isomers corresponding to a given molecular formula, but also provides the option to 'Give up', prompting the system to identify all the molecules that have been discovered and those that remain undiscovered (Fig. 4).

2.2 *wikipedia.cheminfo.org*

Wikipedia is a great tool to find encyclopedic information about nearly any topic. In this huge amount of data, the most relevant chemical structures are also described and are characterized by specific boxes that provide physical characteristics of

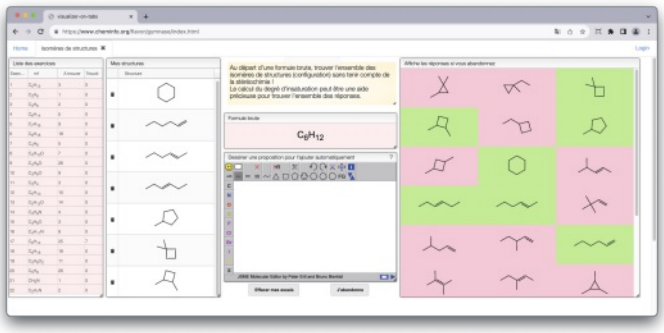

Fig. 4. Analyzing the structural isomers for a given molecular formula is a challenging exercise.

the compound as well as its structure. In 2015, we decided to scrap Wikipedia looking for chemical structure and to allow a substructure search of the described molecules instead.[4] This led to the creation of the website https://wikipedia.cheminfo.org that is, since then, nightly updated, thereby collecting newly published molecules and their associated characteristics (Fig. 5). One of the most remarkable features of this website is its scaffold search capability, allowing students to explore molecules by their substructure. This novel approach sparks curiosity and fosters a deeper understanding of the relationships between various chemical compounds.

In 2023, we completely redesigned and rebuilt this website to reflect new technologies and to make it available on mobile devices.

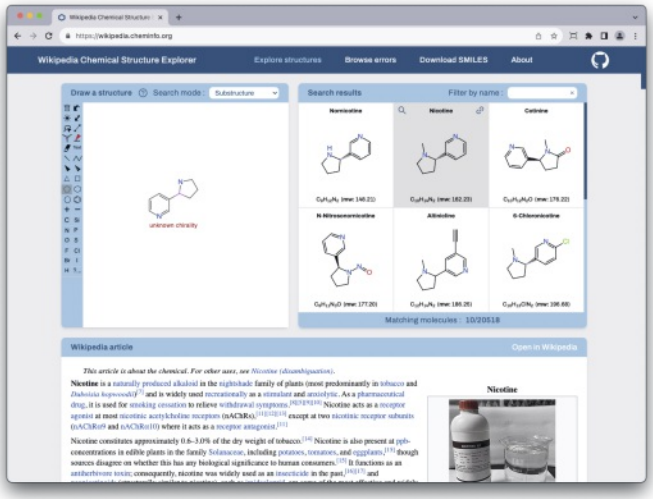

Fig. 5. Substructure and similarity searches of molecules present in Wikipedia.

3. Structural Analysis

The determination of an unknown compound's structure poses a challenging yet captivating task, akin to unraveling a complex criminal case. In this pursuit, disparate pieces of information gleaned from analytical techniques resemble the scattered traces left behind at a crime scene. Like a detective sifting through evidence to uncover the truth, students should meticulously analyze these fragments to construct a cohesive narrative regarding the compound's composition and structure.

In a typical workflow, students will attempt to determine the molecular formula through high resolution mass spectra. After calculating the double bond equivalent (DBE), they will then explore other data that can be found in mass fragments, infrared spectra, or NMR spectra. To ensure students have the necessary

skills to quickly assess all indices, we have created multiple websites that will initially focus on the various techniques.

3.1 *Mass Spectrometry: www.chemcalc.org*

Since 2001, ChemCalc[5] has enabled chemists to calculate molecular weight, monoisotopic mass and isotopic distribution (Fig. 6). By taking advantage of its features, students can gain a comprehensive understanding of theoretical mass spectra, which can be used to assess the presence or absence of certain elements with characteristic isotopes.

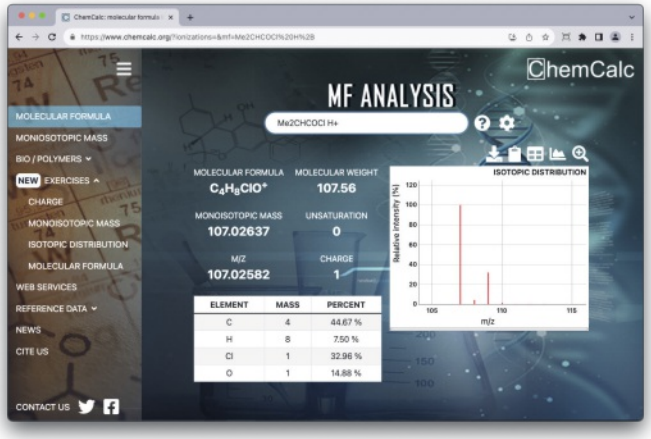

Fig. 6. ChemCalc enables the calculation of isotopic distributions from molecular formulas.

ChemCalc also enables the derivation of molecular formulas from monoisotopic mass, considering ionizations and the range of molecular formula to explore. This is the initial step in determining the potential molecular formula of an unknown product.

Recently, a new version of the website was developed, containing a section of exercises with an interesting feature: exercises are randomly generated, so that each student will solve a different series and as many exercises as he/she wishes (Fig. 7). The system provides immediate feedback, allowing students to work at their own pace, promoting autonomy and self-directed learning.

The determination of simple molecular formulas (up to 4 atoms among C, S, Cl and Br) from isotopic distributions is one of the most challenging exercises. Those exercises will demonstrate to students that the pattern is characteristic, and a great deal of information can be derived from the isotopic distribution (Fig. 7). An even more difficult problem is the elucidation of the molecular formula from a high-resolution mass spectrum. This exercise implies the calculation of the monoisotopic mass, accounting for experimental error (accuracy) and identifying which atoms are present, based on the isotopic distribution.

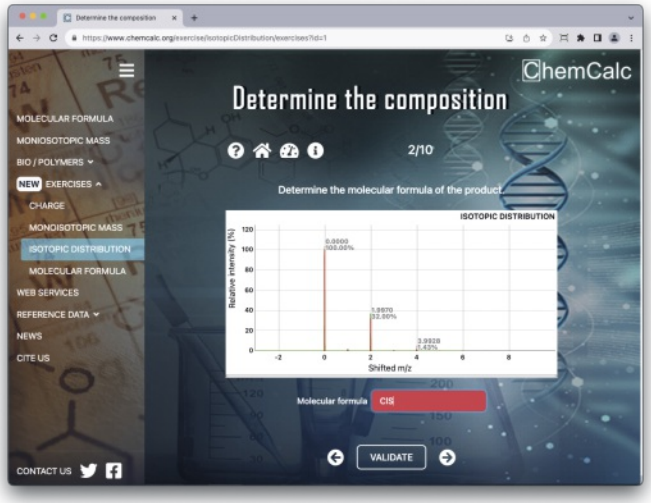

Fig. 7. A series of exercises to determine the molecular formula based on isotopic distribution.

3.2 *Nuclear Magnetic Resonance (NMR)*

The advent of www.nmrdb.org quickly became the top ranked website for nuclear magnetic resonance (NMR) spectra prediction. This dynamic website offers a novel and comprehensive approach to comprehend the intricate interplay between chemical structure and chemical shift as well as the multiplicity. By using sophisticated algorithms,[6,7] www.nmrdb.org enables users to predict NMR spectra, unraveling the subtle nuances of molecular interactions and providing invaluable insights into spectral analysis (Fig. 8). The predicted spectra will also take into account second-order effects[8] to provide a spectrum close to the reality.

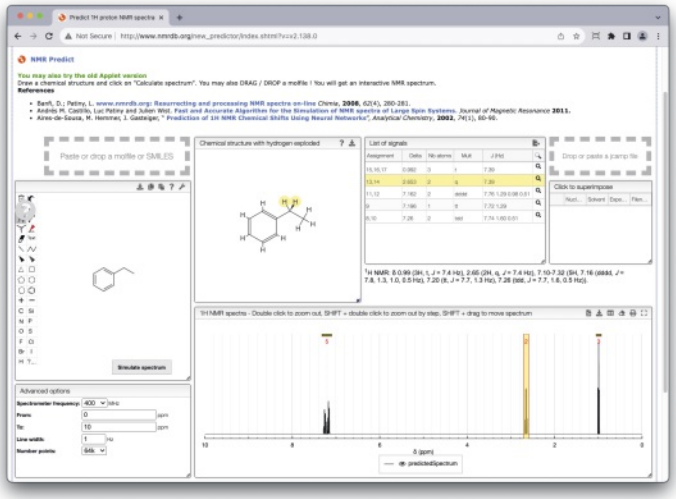

Fig. 8. Interactive prediction of ^{1}H NMR spectra

Furthermore, the platform provides a tool that enable interactive and accurate simulation of second order effects. This functionality can be used by teachers in classes, students, and professionals alike to explain complexities that are not immediately apparent (Fig. 9).

Fig. 9. Simulation of AA'XX' spin system

3.3 *Infrared Spectroscopy*

The energy corresponding to the vibrations of a molecule is observed in infrared spectroscopy. Surprisingly, there wasn't any easy-to-use tool that allowed students to draw a chemical structure and generate an interactive IR spectrum, where they could link a specific wavelength with the corresponding vibration (Fig. 10). Our aim in creating https://ir.cheminfo.org[9] was that users can not only generate spectra, but also superimpose simulations. For instance, teachers can use the vibration frequency of a carbonyl to explain inductive and mesomeric effects by examining the stretching frequency of the C=O double bond.

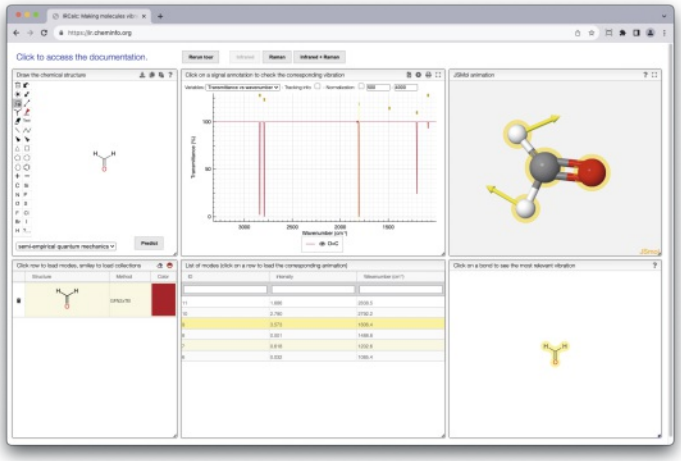

Fig. 10. https://ir.cheminfo.org for the interactive simulation of infrared spectra

4. Paving the Way to the Future

All the work accomplished during the last 20 years in creating small reusable libraries resulted in an incredible potential to develop more advanced applications and learning tools accessible from the browser. In this context, we are currently working on NMRium, a web application that finally allows everybody to process NMR spectra without the need to install software. This specific application reuses over 50 of our libraries proving the merits of our modular approach. NMRium is the ideal companion for practical laboratory work, during which students can receive data from their experiments *via* email (JCAMP-DX file[10,11] or zipped Bruker folder) and process directly on https://www.nmrium.org.[12] In addition to visualizing 1D and 2D spectra on this website, students will also be able to make the full processing of 1D spectra (line broadening, zero filling, Fourier transform, phase correction and baseline correction) as well as assigning signals to the corresponding structure (Fig. 11).

NMRium not only offers processing and assignment capabilities, but also provides students with a range of educational resources, such as tutorials, videos, and quizzes. These resources, which can be found in the 'Teaching' section, are designed to help students learn how to assign NMR spectra. The quizzes involve series of exercises in which students are given a molecular formula and must use the provided NMR spectra to elucidate the chemical structure (Fig. 12). We are more than willing to assist with the implementation of additional custom quizzes.

5. Conclusions

In conclusion, our research and contributions to innovative online platforms have demonstrated the immense potential of web-based e-learning in the field of chemistry. As technology continues to evolve, the shift towards web-based platforms offers numerous advantages that have the power to revolutionize the way students learn and engage with concepts relevant to chemistry.

Fig. 11. Utilizing a straightforward "drag and drop" method, 1D and 2D spectra can be superimposed.

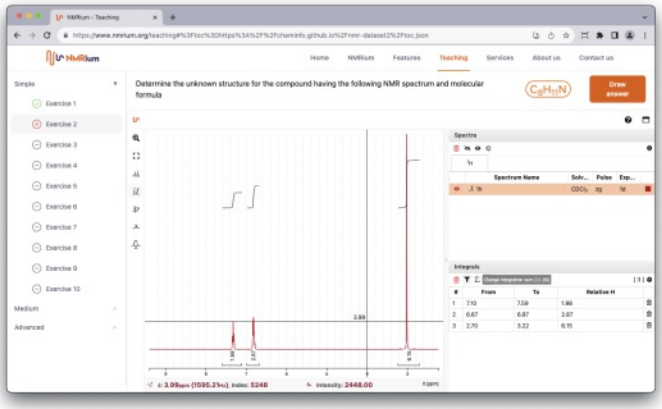

Fig. 12. Carrying out an exercise to elucidate the chemical structure of a compound using NMR spectra.

The future of chemical education lies in the seamless integration of online resources, where students can access a wealth of educational materials without the hassle of installing software or dealing with platform compatibility issues.

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