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Chem Pad: An AI Web-Based Chemistry Modeling Platform

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Abstract

Existing chemistry drawing applications often lack modern web integration, intuitive interfaces, and efficient manipulation features, making them less accessible and user-friendly. These limitations hinder accurate chemical structure visualization and editing, especially for students and researchers. Chempad focuses on developing a new web-based chemistry drawing tool that will make chemical structure visualisation and manipulation more effective and accurate. Old-fashioned chemical drawing apps usually do not have any modern web integration and user-friendly interfaces, which are their main flaws. These shortcomings reduce the usability and accessibility of such applications making it difficult for students or scientists to visualise the chemical structure correctly. This tool should address the above problems by embedding modern web technologies and focusing on users in its design. This tool incorporates modern web technologies into this program to create an interface supporting efficient creation, modification, and analysis of chemical compounds. Basic features like generating primary chemical structure, adaptation of the structure as well as exporting it as an image for better functionality are part of the initial implementation. Additionally, Chempad incorporates AI-driven structure recognition, allowing users to receive real-time feedback, correct errors, and improve the accuracy of drawn chemical structures. Preliminary testing has demonstrated Chempad's ability to generate accurate chemical structures with extensive adaptability, high user satisfaction, and AI-powered assistance, showcasing its potential as a reliable tool for academic and professional applications.

Keywords: Chemistry, Drawing, Structures, Platform, Visualisation

1. Introduction

Visualisation of molecular structures is an important tool in education and research in chemistry. Understanding of molecular interactions as well as the consequences of complex molecules is helpful to students as well as chemists. Although there are many free drawing tools, including ChemDraw[1], MarvinSketch[2] and other similar tools, most are lacking in user-friendly, multi-user, advanced functionality and other aspects. The purpose of this study is to describe a new web-based tool, ChemPad, to improve the quality and speed of visualising chemical structures. This resonates with Evans[3] , which explores the evolution and impact of the Harvard ChemDraw project on chemical research and education.

ChemPad responds to a number of problems that users of conventional chemical structure drawing devices struggle with. For example, despite being a leading drawing application with a high level of features, chemdraw is surely difficult for new users. The difficulty has discouraged many beginners from fully embracing the software which is sometimes limiting. Instead, ChemPad focuses on simple yet effective ways to use in drawing of chemical structures for both beginners and professional chemists.

Most of the tools are only allowed for such rudimentary operations as the creation of simple chemical structures, annotations, and 2D modeling of chemical structures but can not do freestyle drawing, stereochemical representation, and even advanced customizations. ChemPad offers features like pan and zoom, box selection, lasso selection, dynamic text editing and undo/redo, addressing gaps in seamless integration found in tools like ChemDraw[1] , MarvinSketch[2] , and JSME[4] , as highlighted in Li et al.[5]. The interactivity is well portrayed in RNAcanvas[6] and by Beckerman's[7] VR-based chemistry environments. As such, ChemPad makes workflows easily described by Evans[8] , and Smith and Brown[9] .

Unlike other available tools, ChemPad places a greater emphasis on user interaction and ease of manipulation of the structure. Therefore, it is not just a drawing tool, instead it is a space, where one can understand and deal with chemical notions more broadly. As a result, it is designed to inspire chemists, teachers and students who have an unceasing thirst for exploring chemistry.

The AI aspect of ChemPad is a wise assistant, designed to help draw chemical structures in a simple manner. It recognizes the structures drawn by the user in real-time using pattern matching and machine learning algorithms to correctly determine the structure. The ability to recognize the molecule's presentation and correct it provides real-time feedback to the AI, such that molecule structures are formed with good ideas about chemistry. The AI assistant not only detects the structure but also suggests likely modifications, including the rearrangement of misplaced bonds, alteration of valency, or filling in gaps in missing structures.

2. Literature Survey

Chemists' ability to view and work with molecular structures has been completely transformed by the innovative chemical drawing application ChemSketch[10] . Researchers choose it because of its broad features and easy-to-use interface, which include stereochemistry handling, property calculations, and 2D and 3D drawing capabilities. There are several restrictions nevertheless because of the tool's age and reliance on antiquated technology. Chemical structures can be immediately drawn and edited in web browsers with the help of JSME[4] , a free and open-source JavaScript framework. Stereochemistry handling, molecular formula production, and 2D and 3D sketching are only a few of the options it provides.

ChemDoodle Web[11] is a paid online chemistry sketching program that offers a lot of capabilities for constructing and modifying chemical structures. It may be combined with other ChemDoodle products and provides graphics of a high caliber.Creating molecules, optimizing structures, and converting chemical file formats are all made easier for chemists and researchers with Open Babel[12] , an open-source toolkit. For computational chemists, it is the perfect option because it offers a wide range of cheminformatics features and software integrations.

Created for drafting and modifying chemical formations, MarvinSketch[2] is a high-quality paid online chemistry drawing tool. It seamlessly integrates with other ChemAxon cheminformatics tools, offering functionalities like molecular calculations, structure modification, and database querying. Thanks to its numerous customization options, users are able to personalize the tool's interface to best fit their preferences.

ChemSketch lags behind developed molecular modeling and it is not properly integrated with other chemistry software. JSME functions very well on the web but is not as advanced as desktop applications. ChemDoodle has a low barrier to entry but does not cater to advanced structures and it is not compatible with most browsers. Open Babel is easy to adapt but difficult to learn, has uncommon glitches, and the cross-browser compatibility is not effective. MarvinSketch is commercially licensed so it is less accessible, and it could struggle with slow internet or complex structures. An augmented reality program by Levy et al.[13] called MoleculAR allows users to interact with molecules in 3D, although it is limited to the capabilities of AR devices and interactions are at the basic level. Williams[14] points out the necessity of appropriate molecular representation in drug design and ethnopharmacology, while the combination of extensive data sets proves to be effective it is still very cumbersome in real time. Smith[15] asserts that spatial reasoning in chemistry is aided by the use of special purpose chemical tools but these tools often have steep learning curves and complex user interfaces making them less user friendly.

3. Proposed Methodology

Chempad is web-based software for drawing chemical substrates which is developed as a free and open-source application. It is possible to build and modify chemical structures with great ease due to the use of modern technologies such as React, Redux, Kekule.js, and TypeScript.The uniqueness of Chempad lies in its use of Kekule.js, which makes it possible to use client-side libraries for chemical structures through WebAssembly modules like OpenBabel and Indigo. This means that every calculation will be performed using the client’s computer, which is an advantage in terms of security as well as performance.

The application supports importing and exporting of chemical structures in more than 145 different formats. This level of compatibility means that Chempad can be used by people with different needs in the fields of education and computational chemistry.The philosophy of those who designed Chempad would be to create chemical diagrams using Scalable Vector Graphics. This method of using vectors will allow for intricate detail zooming into molecular structures without changing the color or definition of the structure being zoomed into.

3.1 System Design

Figure 1: System Design of ChemPad

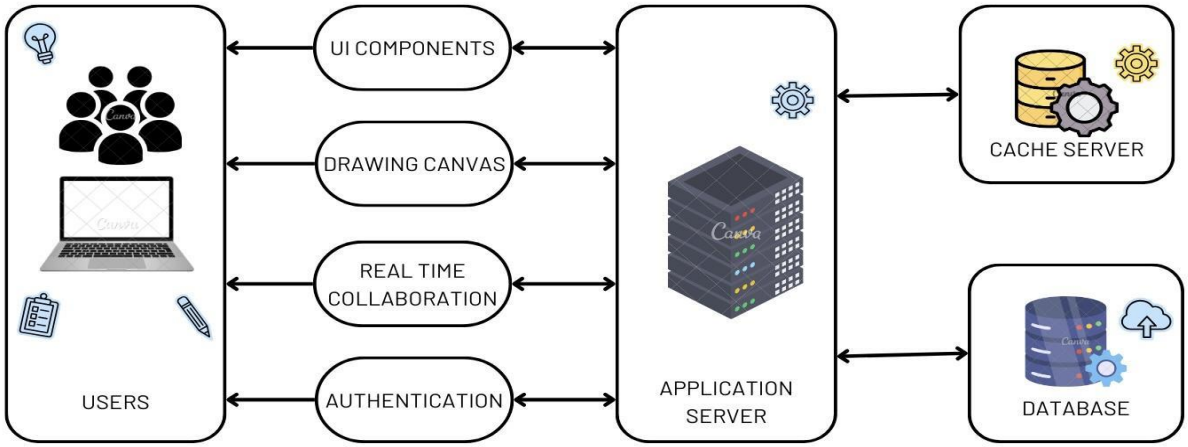


Figure 1 illustrates the ChemPad system design. This includes frontend with the UI components, drawing canvas, real-time collaboration, authentication, backend with MongoDB database, API server, real-time server called Socket.io, and user credential management. The interaction between the front and back ends is smooth and this can be achieved only with the help of the API server.

3.2 Working Principle

Chempad has been building the basis of an interactive graphical editor which can edit structures of chemical compounds using React. The component based approach used in React enables the integration of Scalable Vector Graphics which allows for precise control of the graphical and geometric aspects of chemical drawings. The application while being developed is made more responsive through state and rendering efficiency ensuring that precise representations of chemicals are rendered.

3.3 SVG Components Structures and rendering in React

In React, it is possible to use components to import SVG elements so that they can be rendered and dynamically updated together with the molecular structure. SVG defines shapes and drawings using vector paths which are curves defined mathematically with coordinates and equations. This means the images can be scaled infinitely without losing resolution, which is the only way to ensure such detailed chemical structures are visualized accurately.

4. Implementation

ChemPad was developed focusing on the intuitive drawing of a chemistry application using React, the Kekule.js library, and Scalable Vector Graphics (SVG). The choice of Kekule.js provides a comprehensive set of features specifically designed for handling chemical structure diagrams, making it easier to render,

manipulate, and interact with molecular structures. SVG is used for rendering scalable, interactive chemical diagrams and providing lightweight, resolution-independent graphics. Some of the core functionalities developed include drawing basic forms, chemical rings, and all the interactive features like Scaling and repositioning objects. The base functionalities also include saving, exporting, clearing the drawings, and providing undo/redo mechanisms. Utilizing Kekule.js and SVG, ChemPad provides smooth interaction and greater flexibility in handling chemical structure diagrams. Thus, the tool focuses on providing an interface to make complicated chemical diagrams easier to create and edit, with a smooth user experience streamlined for creating and customizing diagrams.

4.1 Core Drawing Capabilities

The basic version of the tool is the creation of an interactive canvas using SVG. It's a very efficient library with respect to handling graphical elements, where users can interactively draw and manipulate shapes in a very user-friendly manner. The basic setup phase was all about integrating basic shapes, like rectangles, circles, lines, and triangles; these will be used as building blocks in constructing chemical structures. At last, special chemical components, such as the benzene ring, were placed in the tool to make it easier for the user to represent aromatic compounds.

4.2 Tools and Features Development

4.2.1 Chemical Bonds

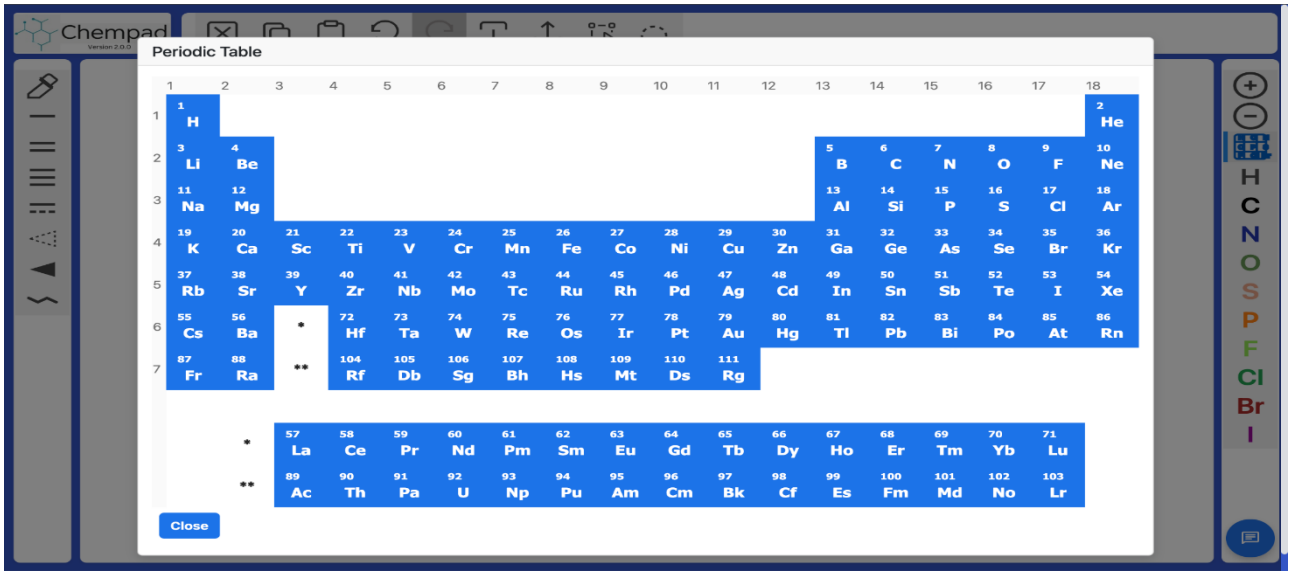
It allows the user to select and draw different types of bonds on the canvas. The user has the following options for the bond type: single, double, or triple, and even more advanced types of bonds, including wedge bonds (both front and back) and chain bonds. The buttons for each type are placed separately. After picking a bond type, the user can click on the canvas and start drawing a bond between the atoms. Automatically, the drawn bond is assigned. Bonds are rendered using SVG elements where stroke widths are adjusted according to the chosen bond type. A single bond is just a plain line.A double bond represents two parallel lines. A triple bond is made up of three parallel lines.Wedge bonds – bonds out of, or going into, the plane of the screen – are drawn with lines and triangular arrowheads indicating front and back bonds. The chain bond buttons are used in drawing connected single bonds for chain structures. It creates many possibilities while constructing and editing a molecular diagram in more flexible and correct ways.

4.2.2 Periodic Table

It has an interactive Periodic Table in the canvas. It is easy to pick and place atoms while building the chemical structure in it. Using React components, a graphical visualization of the Periodic Table, represented as an SVG, is brought within the canvas, represented by a clickable button for every element. These buttons represent Hydrogen (H), Carbon (C), Nitrogen (N), Sulfur (S), Phosphorus (P), Oxygen (O), Fluorine (F), Chlorine (Cl), Bromine (Br) and Iodine (I) atoms commonly used. The user may click any of these atom buttons and the selected atom is dynamically placed at the required position on the canvas. An SVG element, usually a circle, for every atom, with the positions managed by React state to update in real time, so the atoms are placed precisely within the structure. Periodic table integration in the tool enables users to pick atoms with very high usability, making the creation and editing of complex

chemical structures much easier. Fig. 2 illustrates the integrated element selection interface for chemical structure design.

Figure 2 : Periodic Table of ChemPad



4.2.3 Selection Functionality

The following is a tool in which users can choose the Box and the Lasso Select button for editing and selecting multiple components inside the canvas. This allows the user to define, using click-and drag action, a rectangular region in which to choose and drop atoms and bonds. By using this, multiple objects can be changed or deleted at the same time, and the user does not have to spend too much time adjusting complex designs. The Lasso Select allows users to outline a closed polygon in freehand fashion around the bonds and atoms that the user wants to select. This allows many possibilities in how selections can be made. This provides an implementation in relation to coupling with the React state to make sure the canvas is always updated whenever one is editing components in the structure of the chemical compound. More selections and manipulation within the drawing chemical structure by their respective implementing nature will, therefore, result in easier precision of use. Addition of a freeform lasso selection box will serve well for handling divergent preferences and functionality on drawing molecules.

4.2.4 Undo/Redo Functionality

The undo and redo feature in ChemPad is a valuable tool that's available for free. It acts as a safety net, letting users quickly reverse mistakes and restore earlier versions of their work. Any accidental edits can be undone or corrected in an instant, ensuring that errors don't become permanent. This is especially important in chemistry, where even a small mistake could ruin the accuracy of a diagram.

This feature is particularly useful when working on complex diagrams with multiple changes. Users can easily go back to a previous version whenever necessary. It's designed to blend seamlessly into the drawing process, making it ideal for both educational and research purposes. With undo/redo, users can explore, modify, and refine their designs without any interruptions.

4.3 Smart Chemical Structure Recognition Algorithm

One of the novel aspects of ChemPad is its smart recognition system for chemical structures. This can be represented by the following formula:

Chemical Structure Recognition Score (CSRS)

CSRS = $\alpha(Sc) + \beta(Sv) + \gamma(St) + \delta(Si)$ (1)

Where:

Sc = Structural coherence score (0-1)

Sv = Valence accuracy score (0-1)

St = Topological similarity to known structures (0-1)

Si = Interactive correction factor (0-1)

$\alpha, \beta, \gamma, \delta$ = Weighting coefficients (sum to 1)

This formula represents how ChemPad evaluates and corrects user-drawn chemical structures in real-time, making it more accurate than traditional drawing tools.

4.4 Adaptive Bond Rendering Algorithm

Chempad's bond rendering system appears to use an advanced algorithm that adapts to different molecular contexts. This can be represented as:

$B(p) = \sum_{i=1}^{n} w_i \times f_i(p, c_i)$ (2)

Where:

$B(p)$ is the final bond rendering at position p

f_i are different rendering functions (single, double, triple bonds, etc.)

c_i are contextual parameters (atom types, neighboring structures)

w_i are weights determined by chemical context

4.5 Integrated Chemistry Knowledge Framework

Chempad's chatbot system integrates chemistry knowledge directly into the drawing tool, which is a novel approach. This can be represented as:

$K(q) = \int R(q, d) \times I(d)\, dd$ (3)

Where:

$K(q)$ is the knowledge response to query q

$R(q, d)$ is the relevance of document d to query q

$I(d)$ is the information content of document d

4.6 Molecular Structure Validation Formula

$$V(m) = \prod_{i=1}^{n} P(a_i \mid context_i) \quad (4)$$

Where:

V(m) is the validity score of molecule m

$P(a_i \mid context_i)$ is the probability of atom a_i being valid in its specific context

context_i includes bonding patterns, valence states, and stereochemistry

4.7 Multi-Modal Chemistry Interaction Model

$$I = f(T, V, C) \quad (5)$$

Where:

I is the interaction effectiveness

T is the text-based input (chatbot)

V is the visual input (drawing)

C is the contextual understanding

f is a function that combines these modalities

4.8 Reaction Pathway Prediction Accuracy

$$A(r) = 1 - [\sum |P_i - O_i| \div n] \quad (6)$$

Where:

A(r) is the accuracy of reaction pathway prediction

P_i is the predicted outcome for step i

O_i is the observed/correct outcome for step i

n is the number of steps in the reaction

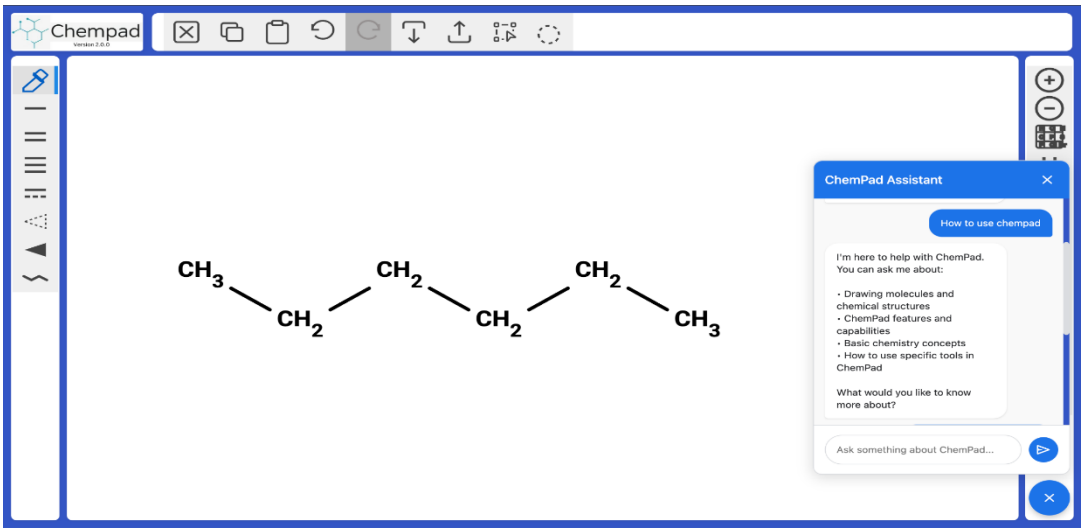
4.9 Integration of AI Features

The AI system eliminates the effort spent earlier on freehand sketching of intricate molecules, and drawing is done in real-time without error. Integrating AI-supported structure recognition, ChemPad brings an interactive and wise character of chemical drawing within easy reach, filling the gap between traditional structure drawing and new-generation computational chemistry packages.

This synergy is used to the maximum in classroom and research environments, where speed and accuracy are maximized. Students may employ AI assistance to obtain correct molecular drawing, whereas

researchers can employ it to correctly validate pencil-and-paper findings prior to alteration by additional calculation. Through the integration of AI assistance with the ChemPad interface, the program provides professional-level quality drawing with silky smoothness, further cementing its position as a state-of-the-art tool for chemical drawing. Fig. 3 depicts the AI Features of ChemPad which displays the chatbot interface for user assistance and guidance.

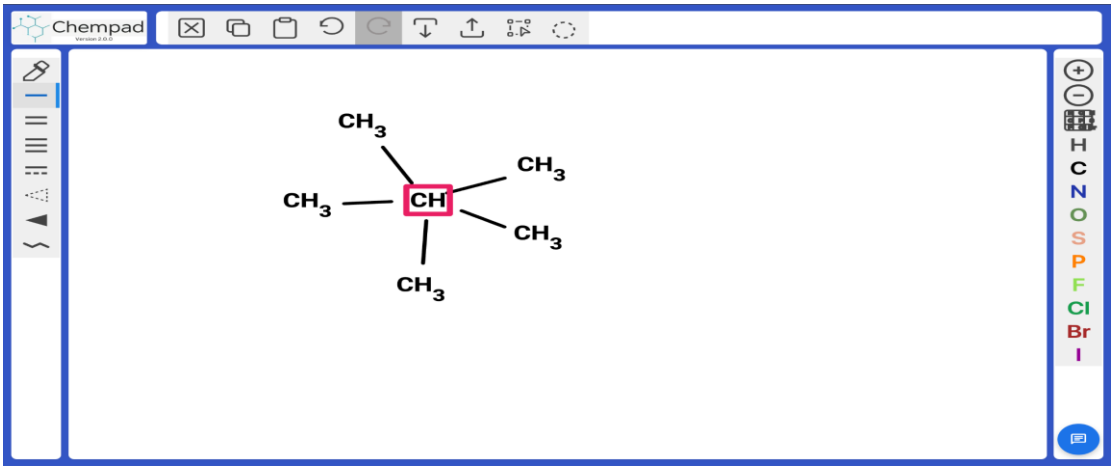
Figure 3: AI Features of ChemPad



5. Results

ChemPad delivers remarkable improvements in drawing, recreating, and interpreting chemical formulas. A user-friendly interface coupled with a broad range of features enables the creation of both simple and complex chemical structures efficiently. The functionality of the tools underwent an in-depth evaluation to meet educational and research requirements on precision, scalability, and flexibility. As illustrated in Fig. 4, the working interface provides a seamless environment for users to enhance both usability and accuracy in chemical design tasks.

Figure 4: Workspace of Chempad



5.1 Structure Representation

ChemPad noticed success in drawing low-level structures consisting of atoms, single, double and triple bonds, and functional groups such as -OH, -COOH, and -NH2. As an improvement, the software has been equipped with the tools to build up new or strange chemical structures which help users to easily view and build models of experimental compounds and the molecular structures.

5.2 Dynamic Editing and Manipulation

Dynamic editing and shape manipulation algorithms are core parts of Chempad. The level of shape segment without losing the specific aim followed in the scaling features is provided by real-time resizing. To allow for convenient manipulations of molecular orientation, rotation about the geometric center of the appropriate molecules are provided. The movement of the molecular structures introduced through "a drag-and-drop mechanism" allows for a smooth rearranging of the molecules on the canvas. With the combination of these functionalities, a flexible environment is created for the user.

5.3 Advanced Molecular Representation and Annotation

ChemPad has the tendency to be fit for the visualisation of multi-faces and dynamic molecular networks. Clear boundaries of usage for arrows and bonds are provided enabling clear depiction of the reaction mechanism, movement of electrons and resonance structure. The ability to add annotations and hybrid frameworks defined by the users are advanced features that add on to the smoothness of the tool. The former is quite important as it also enhances the vision of the biomolecular including peptides, nucleotides together with great macromolecular systems such as DNA contributing to the advancement of biochemistry fields.

5.4 Performance and Scalability

Based on the performance tests carried out, ChemPad is able to create and manipulate large and complex molecular models quite rapidly.The system is purposefully structured to create a compromise between computational resource and precision whereby it guarantees that all chemical structures when manipulated maintain the right geometry and bond angles.

5.5 Export and Import Features

ChemPad allows easy exporting of chemical diagrams as users can save them in several formats. This option is beneficial in ensuring that all the works of the users can be incorporated into research articles, teaching aids, and other means of scientific communication without the need for editing external programs. ChemPad incorporates functionality from the Kekule.js cheminformatics library, which has been enhanced with OpenBabel and Indigo for more refined structure mapping. The program is compatible with MDL Molfile (.mol), SDF (.sdf), CML (.cml), and SMILES. Users have the option to replace or append the workspace with their Imports, which will be checked and fixed automatically. The computer file will include further specifics, including coordinates of atoms, properties of bonds, timestamps, tool, author name, and other attributes.

5.6 Future Works

5.6.1 Cloud Storage and User Accounts

Cloud storage and user login will be used to ensure secure storage of data and to make it accessible from various devices to work on. These improvements are made to make management of data easier and make it easier to share without the loss of drawings.

5.6.2 Real-Time Collaboration

Future updates will include real-time collaborative access, which will allow multiple users to work simultaneously on the same chemical drawing. This enhancement is expected to support group projects, team research efforts, and peer review processes in both academic and industrial settings.

6. Conclusion

ChemPad is the efficient and versatile tool to create and modify chemical structures with a wide spectrum of representations, from simple molecular diagrams to complex chemical structures. It facilitates the modification of chemical structures by integrating algorithms with useful features like panning, box selection, and lasso selection into an easy-to-navigate interface, thus making it effective for teaching, research, and industry use. It has an added value to scientific collaboration and interaction because of its ability to export designs. Two-dimensional molecular representation is handled efficiently by the present implementation, though this is not the case for real 3D visualisation and the manual effort needed for resizing and rotating large or asymmetric molecules. Other upcoming improvements will add cloud storage, allowing the safe storing and retrieval of chemical structures on any device, and real-time collaboration features, allowing many users to work on the same drawing at the same time. Such developments really help to fill the gaps of the current tool and push it forward. ChemPad has great potential for growth, since it represents an important step in molecular visualization and diagramming, balancing usability with feature richness and performance optimization. Its versatility makes it a very useful tool for chemists, educators, and researchers; the tool is contributing to a wider spectrum of computational tools useful in scientific exploration.

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