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CHEMDRAW: ENHANCING CHEMICAL COMMUNICATION & ANALYSIS

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ABSTRACT:

The application of modern computer software in chemistry education establishes the groundwork for increased interest in chemistry among students and researchers, as well as for the transmission and consolidation of knowledge. Chemical computer programs are used to draw both simple and complex chemical compounds, as well as to calculate complex chemical equations and processes. This makes it possible to understand complicated systems biologically. This review covers widely used, mostly free tools that may be used for locating, categorizing, and displaying characteristics of various materials as well as for learning chemistry. Structured interpretation algorithms and strategies designed to aid in the description of unknown substances are also analysed and discussed in this work.

Keywords: Chemdraw Software, Cambridge soft, ACD, Chemical Drawing Software

INTRODUCTION:

ChemDraw software is the go-to drawing tool for researchers to illustrate chemicals for publications, presentations, and chemical database inquiries. Most academic institutions utilize the software for chemical drawings rather than as a teaching tool.

ChemDraw is a desktop application that helps scientists and biologists sketch and analyse chemical structures. This well-liked program allows users to compute and create three-dimensional models of biological materials and small molecules. Chemical structure and formula data can also be worked with in ChemDraw to create figures for publications.

ChemDraw features two products:

CHEMDRAW PROFESSIONAL:

ChemDraw Professional includes options for atom, bond, and ring colouring, as well as name-to-structure and structure-to-name operations, and 1H and 13C NMR predictions.

CHEMDRAW STANDARD:

The **ChemDraw Standard** includes all of the fundamental elements of chemical structure, such as rings, bonds, chains, and atoms.

APPLICATION OF CHEMDRAW:

Chemical and biological structures, including three-dimensional ones, can be drawn by users of the scientific communication package ChemDraw. It may be used for a variety of activities, including:

- Drawing: Produce reactions and structures in chemistry and biology, as well as accurate three-dimensional molecular conformations.
- Converting: Convert chemical names and structures to IUPAC names and vice versa.
- Calculating: Determine chemical characteristics and molecular weights.
- Predicting: Ascertain characteristics, spectra, and shifts in 1-H and 13-C NMR.

- Looking for literature on chemicals and reactions? Try searching SciFinder Scholar for references.
- Presenting: Coordinate, record, and communicate chemical research; access safety data from regulatory bodies and locate chemical suppliers.

Chem Office + Cloud, a new version of the software, has been released. This is a powerful all-in-one solution that will make things easier for you. Accelerate the rate of chemical interaction and change. Chemical drawings include chemical information that can be communicated.

ChemDraw software is now available in the following versions:

CHEMDRAW PRIME:

"ChemDraw Prime" is a full-featured entry-level structure drawing program that gives researchers everything they need to quickly and efficiently create chemically intelligent, "publication-ready chemical" structures and reactions, laboratory notes, and experiment write-ups. In addition to a full range of chemical structure essentials, ChemDraw Prime includes property calculators, chemical and lab equipment templates, and handy TLC and "Gel Electrophoresis Plate design tools".

CHEMDRAW PROFESSIONAL:

The features of "ChemDraw Prime" are all present in "ChemDraw Professional," along with additional tools for retrosynthesis, ChemDraw Cloud, Bio Draw, NMR prediction, enhanced name to structure, and even interface with chemical databases like as SciFinder. ChemDraw Professional also connects with ChemDraw for Excel, Chem Finder Standard, Chem Script, and ChemDraw 3D to organize and manage structural data.

CHEM OFFICE PROFESSIONAL:

The most complete and intelligently scientific research productivity tool available on the market is Chem Office Professional. Building on the strengths of ChemDraw Prime and Professional, it provides chemists and biologists with powerful features to manage their work, visualize their results, and gain a deeper comprehension of their discoveries.

Comprising the following applications, Chem Office:

- By utilizing Excel's analytical, sorting, and organizing features, ChemDraw for "Excel adds chemical intelligence" to "Microsoft Excel spreadsheets" allows scientists to investigate structure-activity correlations and further modify and enhance sets of chemicals and data.
- Chem3D creates three-dimensional representations of molecules so researchers can study their structure and properties to optimize their activity or selectivity.
- NMR and IR spectrum predicting tools are available in ChemDraw and Chem3D.
- The "chemically intelligent personal database system," or "ChemFinder," is used by scientists to organize their compounds, seek up structures, and connect biological aspects to structures.

CHEMDRAW DIRECT:

Chemicalization-requiring "internal applications" and web browsers can both use "ChemDraw Direct." A compact software called "ChemDraw Direct" has all of the main functions of the ChemDraw series, such as the well-known drawing features, advanced name-to-structure and structure-to-name capabilities, hotkeys and shortcuts, structure templates, and structure query tools.

ACD/CHEMSKETCH:

It (ACD/ChemSketch) is a great tool for sharing scientific and chemical data, with a large feature set and a powerful structural editor. Create molecular structures by drawing them, importing them from InChI or SMILES strings, or copying and pasting them from ChemDraw. Easily and quickly add well-known compounds. Included are pre-drawn templates for various substances such as sugars, steroids, aromatics, and amino acids. With this dictionary, you may quickly design complex chemical schemas and reactions, including biotransformation maps, by browsing through more than 170,000 systematic and commercial names. Numerous liquid parameters, including molar refractivity, molar volume, index of refraction, surface tension, density, and dielectric constant, can be found using ChemSketch. These computations are done using topological and group additive methods. Chem drawing can be downloaded for free for educational use.

CHIRYS DRAW:

Chirys Draw makes it simple to use just your fingertips to design complex chemical structures and reaction schemes. When you employ a simple circular gesture, designing even complex multi-loop loops becomes enjoyable and simple. Adding more than one workgroup or two connections at once is simple. Chirys Sketch

expedites scientists' drawing and communication skills. Users can compute features and use the "glowing molecule" display to emphasize key attributes once the structure has been sketched. Resonance and balance, complicated fused and spiro looping systems, single pairs, sketching reactions and interaction diagrams with reaction conditions, and making multi-line text annotations with lines and colours are some of the other capabilities. Compute is done using the Asteris cloud server from Amazon Web Services.

KINGDRAW:

This complex chemical structure formula editor for iOS and Android is called KingDraw, and it was created with scientists, academics, and students in mind. The current version gives one ID and one-click sync for multi-terminal synchronization on PC, tablet, and mobile phone to satisfy the demands of sketching in many scenarios. It also offers intelligent gesture drawing, cleaning, 3D modelling, name and structure conversion, structure searching, chemical property analysis, and built-in groups.

A file format converter called KingDraw works with ChemDraw and other important chemical structure drawing programs. It can save files in a variety of formats, including as mol, cdx, and SMILES, and supports a number of drawing standards, including ACS 1996. Among the chemical properties are formulas, elemental analysis, m/z, exact mass, decimals, and molecular weight. All features that are accessible for the phone, tablet, and PC versions are always free. Spraying KingDraw will capture every notion for you. Finally, using the KingDraw cloud account, users will build an all-platform chemical structure system.

REVIEW LITERATURE:

Emam M Hasan at el., investigating bioactive chemical compounds using traditional synthesis and testing methods still has a number of drawbacks. Among these disadvantages are that it takes a lot of time, money, and resources to process, among other things. Through the creation of several software applications, chemistry computation may offer a window of opportunity to address these difficulties. Additionally, in some circumstances like the COVID-19 pandemic these tools can facilitate working from home. Consequently, there is now a great deal of interest in the development projects for chemical assistance, and they are the topic of various scientific papers. In conclusion, the creation of a long-lasting, trustworthy, and expandable molecular simulation tool necessitates the collaboration of a multidisciplinary team consisting of domain scientists, computer programmers, and applied mathematicians. Initiatives aimed at creating chemical support could serve as a neutral, home base for collaboration and communication between various modelling communities in order to tackle new challenges in scientific victory series that fall outside the current domain of more specialized communities.

According to Wei Yu, Lifei Chen, chemistry professors are currently facing both new opportunities and challenges due to the recent and rapid advancements in computer software. The diverse individual and psycho-emotional capacities of students (interests, work, beliefs, talents, and emotional growth) complement each other when they use a computer to learn chemistry, leading to positive results. When chemistry classrooms are set up with computers in mind, students' creativity and unique interest in the natural sciences are encouraged. Additionally, it encourages creativity in research projects. In this publication, we provided basic instructions and some useful examples for a few chemical software applications. We anticipate that this will aid in the teaching of chemistry.

According to Jamal Raiyn, Anwar Rayan, it is beneficial, we concluded, to incorporate modelling tools like the CHEMDRAW program into chemistry instruction. Significant progress has been made in the average score, which went from 5.7 before CHEMDRAW inclusion to 7.3 after. Following the endeavour, the children gave extremely good and encouraging feedback. A majority of the students expressed that they found CHEMDRAW to be a demanding educational platform including lively illustrations and engaging visuals, and they would want to have this kind of software included in their chemistry classes from the beginning. More variables, such as their mindset toward learning chemistry and their in-depth mental awareness of chemicals, may be examined in the future.

According to Manish Kaushik, just little changes can already be made to improve the drawing capabilities of pure chemistry. ChemDraw and ChemSketch are currently the most powerful chemical drawing applications available. ChemDraw and ChemSketch are essentially identical. ChemSketch could only be somewhat better when it comes to creating detailed drawings using the available graphical elements. Specifically, take care while building with ChemDraw or templates. Along with the Chemistry 4-D Draw tool of ChemBioDraw,

these applications offer several preset template pages of different ring systems, amino acids, carbohydrates, etc., that may be quickly added to the document.

Other templates (which are not available in Accelrys Draw) are available, such as lab glassware. With the apps, the user may create own templates. In actuality, every program has a unique setup and usage procedure for templates; ChemSketch can have the most complex setup and resolution. Many other chemical, biochemical, biological, industrial, etc. templates are included with ChemDraw and may be obtained as support files from the Cambridge Soft website.

CONCLUSION:

There are still a number of difficulties in using conventional synthesis and testing techniques to investigate bioactive chemical compounds. Among these restrictions are the need for significant time, financial, and material investments as well as intensive optimization efforts. One possible way to get around these challenges may be to use chemical computation to create and build a number of software applications.

Over the past few years, computer software has advanced quickly, presenting both new opportunities and difficulties for chemistry instruction. Utilizing a computer to learn chemistry produces superior results, as demonstrated by the diverse individual and psycho-emotional capacities of students (interests, work, beliefs, skills, and emotional growth). By using computers to schedule chemistry lessons, teachers may foster students' creativity and pique their interest in the natural sciences. Moreover, it encourages creativity in research projects. This document provides basic instructions for many pieces of chemistry software and several helpful examples. We anticipate that this will support classroom instruction in chemistry.

As the program is constantly being enhanced and the improvements are easily noticeable, it should be regarded as a major release rather than a patched and upgraded version. We are thrilled with the feature options this version provided and urge everyone to choose this improved major release.

We concluded that modelling tools such as the CHEMDRAW application should be used in chemistry education. The mean score improved from 5.7 before CHEMDRAW was included to 7.3 after CHEMDRAW was incorporated, which is really amazing. After the session, the children gave incredibly helpful and positive feedback. The majority of students found that CHEMDRAW was a challenging learning environment with dynamic images and interactive visualizations, and they voiced their want for this sort of software to be immediately included into chemistry courses. Future studies should look into other aspects as well, such students' perceptions of chemistry education and their thorough conceptual understanding of the subject.

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