



Introduction To Chemdraw And It's Various Features

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Abstract: This manuscript offers an extensive analysis of ChemDraw, an innovative software for chemical structure depiction that was developed in 1985. Originally designed to overcome the challenges associated with manual chemical illustrations, ChemDraw has transformed into a vital resource for chemists, researchers, educators, and professionals in various industries. It enables the creation of high-quality two-dimensional and three-dimensional molecular representations, reaction mechanisms, and predictive modeling of properties. The paper delineates the historical progression of ChemDraw, significant version enhancements, and essential features such as NMR prediction, stereochemical analysis, SMILES generation, and chemical property estimation. The review underscores its wide-ranging applications within academic settings, pharmaceutical development, industrial chemistry, and chemical engineering. Notwithstanding its myriad advantages—including an intuitive user interface, cloud functionality, and educational applications—the software exhibits certain limitations, particularly in the management of intricate biomolecules, inorganic chemistry, and three-dimensional modeling. The manuscript concludes by emphasizing ChemDraw's ongoing advancement and its critical role in contemporary chemical communication and documentation.

Index Terms- Structural Formula, Reaction Mechanism, Spectral Analysis, IUPAC Naming, NMR Prediction, Mass Spectrometry (MS), SMILES String, 3D Modeling, Templates and Tools, Chemical Databases, Cheminformatics, Structure Clean-up

INTRODUCTION

ChemDraw is a specialized software application created by PerkinElmer, acclaimed for its efficacy in illustrating and disseminating chemical structures and reactions. The functionality of ChemDraw transcends professional realms, penetrating educational contexts where it operates as an interactive pedagogical tool, particularly beneficial for intricate topics such as hydrocarbons. This software has demonstrated its capacity to enrich the educational experience by rendering abstract chemical principles more comprehensible and stimulating for learners [1].

ChemDraw constitutes a fundamental application within the domain of chemistry, gaining widespread recognition for its critical role in the production of high-fidelity chemical structure illustrations intended for scholarly publications and pedagogical applications. It is regarded as the benchmark within the industry for the synthesis of publication-grade chemical illustrations, with its proprietary file format, CDX, serving as a vital element in the field of chemoinformatics. The applicability of ChemDraw transcends mere professional utilization, as it has been successfully incorporated into academic environments to augment student comprehension and involvement [2,3].

ChemDraw serves as an indispensable resource for chemists, enabling the generation of diagrams representing chemical structures of publication caliber. It facilitates the transition from two-dimensional to three-dimensional structures, a crucial aspect for formal presentations and scholarly articles [4].

This software is incorporated within a collection of independent chemical drawing applications, which are vital in the domain of cheminformatics for the processing, storage, and modification of chemical structural data [4].

ChemDraw has established itself as one of the most prevalent molecular illustration software utilized across diverse fields of chemistry. Each iteration of ChemDraw aspires to provide improved tools and functionalities that facilitate the drawing, visualization, and analysis of chemical structures. The release of version 12.0.2 reinforces this esteemed position, presenting both two-dimensional and three-dimensional drawing capabilities, molecular refinement functionalities, and an array of spectroscopic prediction instruments that serve the research community in both academic and industrial settings [29].

ChemDraw's ability to accurately create 2D representations of molecular structures makes it a highly appreciated tool. In organic and inorganic chemistry, these characteristics are particularly helpful because they enable chemists to precisely illustrate structures, describe reaction mechanisms, and communicate discoveries in publications and presentations [5].

HISTORICAL BACKGROUND

In 1985, Stewart Rubenstein, Selena "Sally" Evans, and her husband David A. Evans created the molecule editor ChemDraw (later by the cheminformatics business CambridgeSoft). PerkinElmer purchased the business in 2011. Included in the ChemOffice family of applications, ChemDraw is accessible on both Macintosh and Microsoft Windows, along with Chem3D and ChemFinder.

A personal necessity gave rise to the concept: Sally, a PhD candidate, needed an effective method for drawing chemical structures. The software was developed in part to reduce her burden and help her study under her husband, Harvard chemist David A. Evans. The first version was coded by Stewart Rubenstein, a Harvard graduate student in E. J. Corey's group. ChemDraw was shown at the Gordon Research Conference on Reactions & Processes in New Hampshire in July of that year, 1985. Stuart L. Schreiber, who was at Yale at the time, made the first purchase for \$295 (academic pricing), which was meant to circumvent institutional approval obstacles, attracting attention to this debut.

1. Pre ChemDraw Period

Chemists used laborious and frequently inaccurate manual methods to sketch chemical structures before to ChemDraw. The chemist's triangle, created by Harvard chemist Louis Fieser, was a noteworthy tool for hand-drafting structures. In his 1980 thesis, Scott E. Denmark, for example, recalls employing this approach, emphasizing how time-consuming it was. The development of ChemDraw was facilitated by this background, which emphasizes the necessity of a digital solution.

2. Commercialization and Evolution

ChemDraw was first commercialized in 1986 by Cambridge Scientific Computing, which later changed its name to CambridgeSoft. The company was sold to PerkinElmer in 2011 and it was a reflection of its financial success and incorporation into more comprehensive scientific equipment. Versions for Macintosh and Windows were added to ChemDraw over time, with the Windows version being released in 1994. The usefulness of SciFinder was increased by 2014 when ChemBioDraw 14 included direct searching. As part of the ChemOffice suite, it is now accessible on both platforms and is utilized by more than a million people globally, not only on Macs. It was extensively adopted in two years, including by all of Eli Lilly & Co.'s chemical labs, indicating its quick adoption in both academia and business.

3. Technical Growth

As ChemDraw's technology evolved, it facilitated importing and exporting formats such as MOL, SDF, and SKC along with native file formats such as CDX and CDXML. By supporting third-party plugins, e.g., Quick HotKey for HotKey configuration, its SDK enhances user interaction. With templates for important chemical journals and functionality to interact with research databases, the software is commonly applied in academic as well as industrial environments, proving its impact. It is a necessary utility for drawing, examining, and documenting complex chemical structures and reactions.

4. Modern Era of ChemDraw

The 2011 PerkinElmer purchase of CambridgeSoft placed ChemDraw in the spotlight of business success and integration into bigger scientific groups. It remains an educational, research, and industrial standard in chemistry today with more than one million users worldwide. One of CambridgeSoft's original co-founders, Stewart Rubenstein, retired in 2006, closing the book on an era.

ChemDraw, which changed how scientists share and display structures, is considered to be one of the first widely used applications of its sort. It was developed to replace laborious hand sketching in order to meet a practical requirement, and its continued evolution demonstrates how applicable it is even in the digital era of chemistry [6,7,8].

KEY EVENTS OF CHEMDRAW

Table.1: Various Key Events Of ChemDraw Software

S.No	Year	Events
1	1985	ChemDraw developed by Sally, David.A, Evans and Stewart Rubenstein. First demo at Gordon Research Conference
2	1985	First purchase by Stuart L. Schreiber at Yale University.
3	1986	Commercialization of ChemDraw in 1986 by Cambridge Scientific Computing, which later changed its name to CambridgeSoft.
4	1994	Windows Version Release
5	2011	PerkinElmer purchased the CambridgeSoft.
6	2014	ChemDraw 14 launched and introduced direct searching.

VARIOUS VERSIONS OF CHEMDRAW SOFTWARE

ChemDraw is a well-known molecular structure sketching program that comes in a variety of editions to meet the needs of various users. Designed for chemistry researchers, students, and professionals, the primary versions are ChemDraw Prime, ChemDraw Professional, and Signals ChemDraw. There are various versions of ChemDraw released till now [9][10].

S.No.	Versions	Release Year	Features
1	ChemDraw 1.0	1985	Initial release by Selena "Sally" Evans, David A. Evans, and Stewart Rubenstein. Introduced basic chemical structure drawing for Macintosh Computers.
2	ChemDraw 2.0	1986	Added additional features, such as atom numbering and bond formatting. The first ChemDraw-based PhD thesis was published in 1986–87.
3	ChemDraw 3.0	1990	Provided a new user interface and added Windows support.
4	ChemDraw 4.0	1993	New features like a structure cleaning function and reaction arrow tools were included.
5	ChemDraw 5.0	1996	Enhanced user interface and support for more file formats (such MOL and SDF). Enhanced performance and unveiled a new drawing engine.
6	ChemDraw 6.0	1999	Added a new file and more capabilities for web-based collaboration.
7	ChemDraw 7.0	2001	Improved chemical property computations, journal templates, and drawing accuracy. Brought in new features including a molecular database and 3D visualization.
8	ChemDraw 8.0	2003	A new user interface was added, and performance was enhanced. Added TLC Plate Tool and chemical query properties.
9	ChemDraw 9.0	2005	Better structural cleanup and more options for file export (CDX, CDXML). Updated the bioinformation toolkit and included support for biosequences.
10	ChemDraw 10.0	2007	Improved connection with the ChemOffice suite and improved polymer drawing. Brought in new features including a reaction planner and structure-based naming.
11	ChemDraw 11.0	2009	Enhanced usability and included capabilities for Name-to-Structure and Structure-to-Name.
12	ChemDraw Ultra 12.0	2011	Advanced reaction drawing tools, Polymer Draw, and Fragmentation Tools were added.
13	ChemDraw 13.0	2013	Enhanced functionality, cloud preview capabilities, and structure-based search.
14	ChemDraw 14.0	2014	Improved retrosynthesis tools and better ChemOffice integration.
15	ChemDraw 15.0	2015	NMR prediction and journal-specific templates were added as part of ChemOffice 15.
16	ChemDraw 16.0	2016	Clipboard enhancements, SciFinder integration, and an improved Retrosynthesis Tool.
17	ChemDraw 17.0	2017	HELM support for biopolymers, new hotkeys, and a rewrite for the macOS Cocoa framework.

18	ChemDraw 18.0	2018	Improved stability, improved cloud connectivity, and biopolymer sketching tools.
19	ChemDraw 19.0	2019	Minor feature changes, improved Office integration, and improved usability.
20	ChemDraw 19.1	2020	Bug fixes, enhanced cloud storage options, and compatibility with latest operating systems.
21	ChemDraw 20.0	2020	Performance improvements, new interface changes, and increased access to chemical databases.
22	ChemDraw 21.0	2021	Enhanced collaboration tools, cloud-native features, and the HELM editor.
23	ChemDraw 22.0	2022	Usability enhancements, Signals Notebook integration, and new hotkeys and shortcuts
24	ChemDraw 22.2	2023	Stability enhancements, minor changes, and improved biopolymer tools.
25	ChemDraw 23.0	2024	Cloud-native ecosystem, ChemDraw, Dark Mode, and Smart Paste were introduced.
26	ChemDraw 23.1	2024	Latest version of ChemDraw with enhanced user interface, better monomer choices, and refined biopolymer drawing.

Table.2: Various Versions Of ChemDraw Software

Types of ChemDraw Software.

1. **ChemDraw Professional:** ChemDraw Professional adds sophisticated capabilities appropriate for more intricate scientific work, building on the Prime version. Features like the ChemDraw Cloud program, which lets users develop and maintain chemical structures online and sync them with their desktop version, are among its features [10] [11]. A wide variety of tools are also supported by this edition, such as the Name to Structure function and an NMR forecast feature [10] [12]. Through cloud connectivity, improved collaboration features enable teams to work together smoothly, sharing and reusing drawings across many programs [14].
2. **ChemDraw Prime:** As a basic version, ChemDraw Prime offers the features required for simple molecular drawing jobs. For users who need a dependable tool for making chemical drawings without the extra capabilities available in more advanced versions, it is perfect [13].
3. **Signals ChemDraw:** Signals ChemDraw is a comprehensive platform made especially for biologists and chemists. It combines an electronic laboratory notebook (ELN) that may be accessed online with molecular sketching capabilities. Thus, data on chemicals, reactions, and properties may be efficiently collected, stored, analyzed, and shared by researchers [11] [12]. Modern scientific research requires the use of cloud features since they improve collaboration and guarantee data security [12] [13]. ChemDraw is the industry standard for chemical drawing software since each edition is customized to satisfy the various needs of its user base, which includes both industry professionals and academic researchers [9] [10].

KEY FEATURES AND FUNCTIONS OF CHEMDRAW

ChemDraw provides an extensive array of functionalities aimed at enhancing the representation and examination of chemical structures. Its fundamental features encompass both two-dimensional and three-dimensional drawing tools that address the requirements of chemists and biologists equally [23] [24].

1. Chemical Structure Drawing

ChemDraw's user-friendly drawing interface, which allows users to swiftly and effectively design complex chemical structures, is one of its best features [25] [26]. Among the many drawing tools offered by the software are specific arrow tools for representing reaction systems and bond manipulation features [27]. Additionally, ChemDraw makes drawing easier with its wide template libraries and structural cleanup tools [28]. The basic feature of ChemDraw is 2D and 3D structure drawing tool which provides highly detailed structure representation.

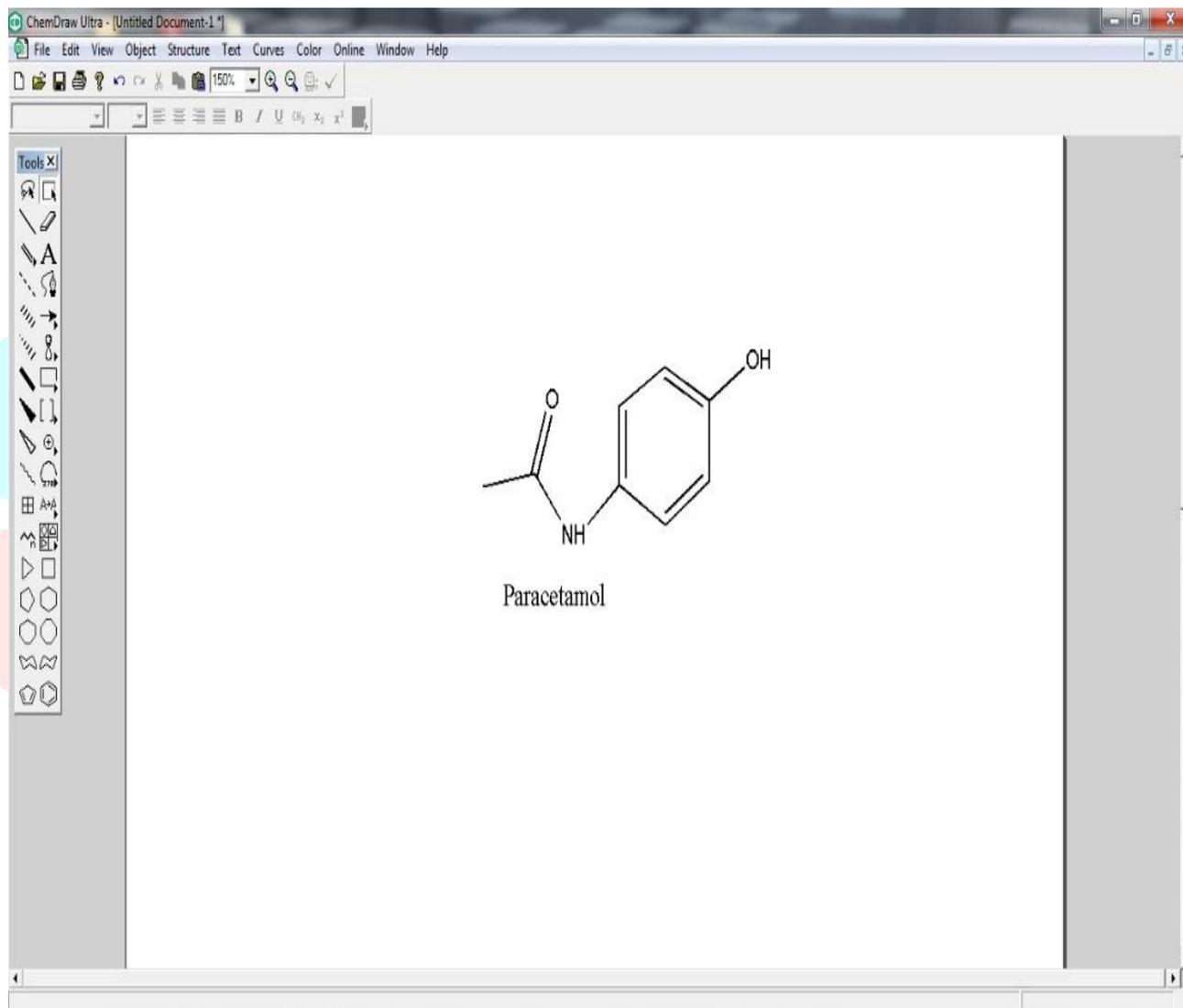


Fig.1.1. 2D Structure Drawing

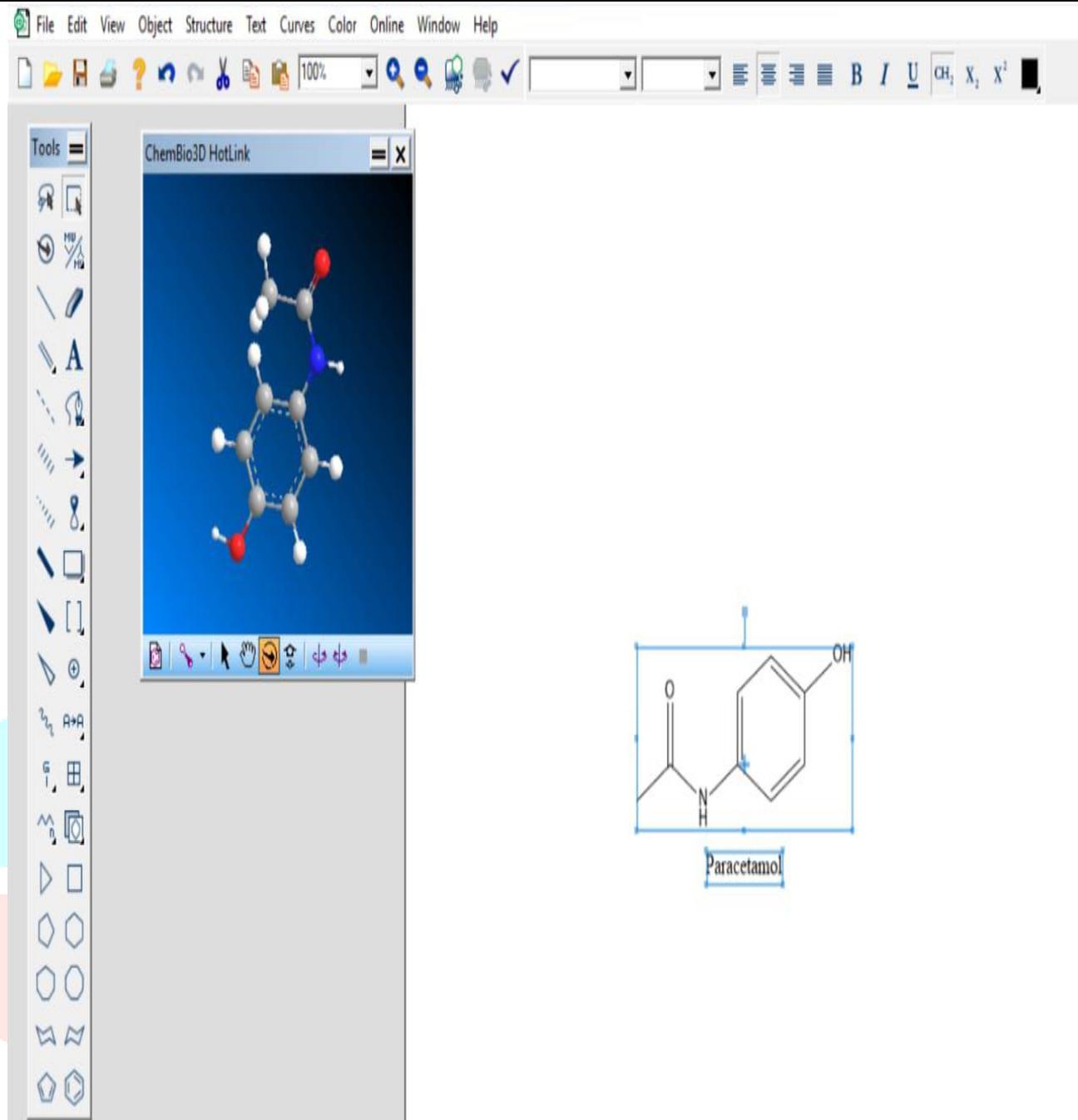


Fig.1.2. 3D Structure Drawing

2. Reaction Drawing

ChemDraw offers a wide range of features designed specifically for representing chemical reactions, making it an essential tool for chemists working in both academic and industrial settings. The software allows users to readily visualize and annotate chemical structures and reaction mechanisms, which is particularly helpful in the fields of organic and inorganic chemistry [26] [29]. Reactants, products, and intermediate species in a chemical reaction can be defined by users using ChemDraw's Reaction Drawing tool. The ability to change bond widths, arrow styles, and colors allows users to customize each graphic to meet their unique requirements [30].

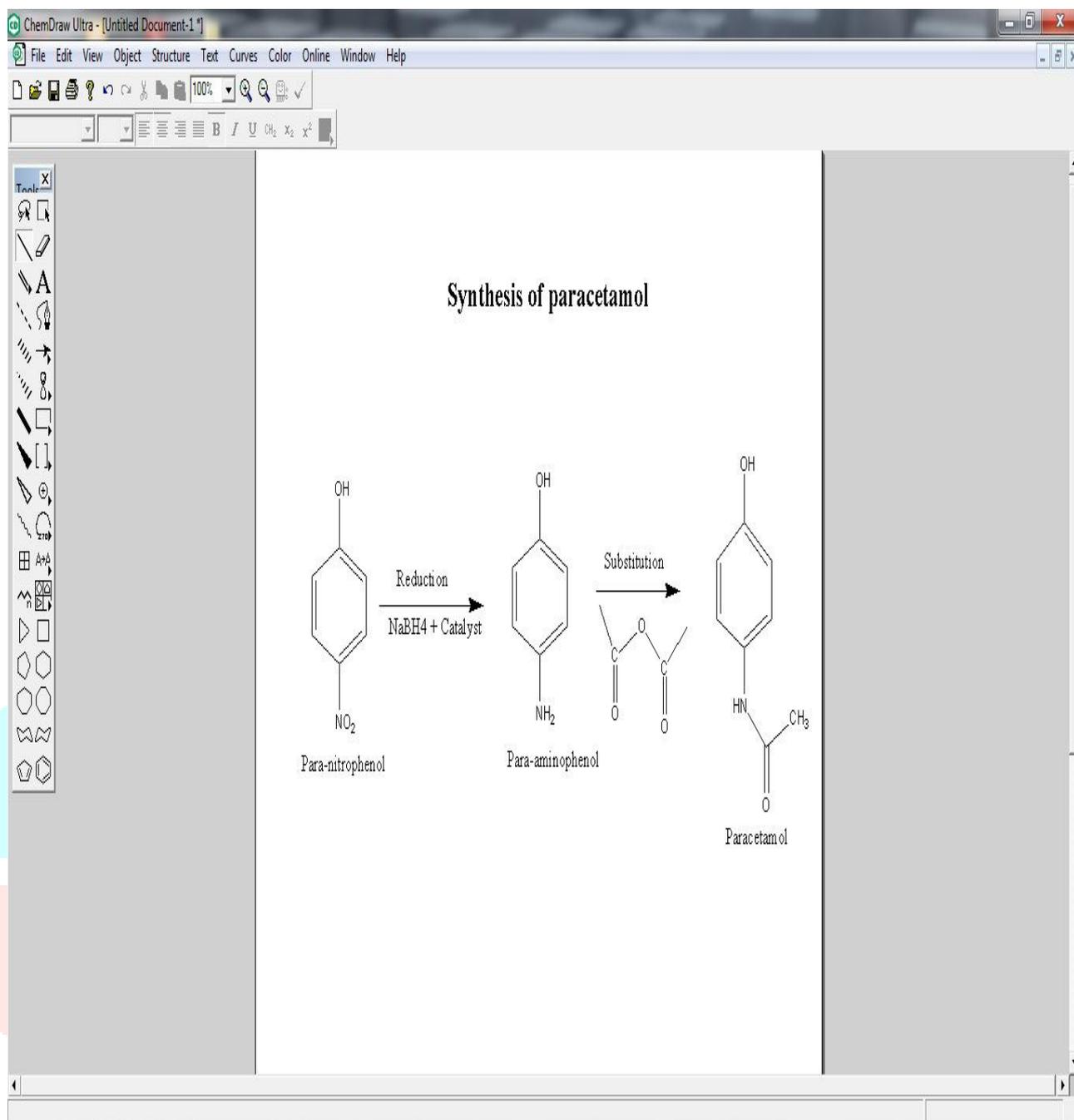


Fig.(2.1). Reaction Drawing

3. Structure Clean-up tool

The Structure Cleanup tool in ChemDraw is used to standardize bond lengths and angles in order to make chemical structures more visually clear. Users who have manually designed structures or imported them from other programs will find this tool extremely useful as it standardizes their appearance for better presentation and legibility [32] [33]. The Structure Cleanup tool's main purpose is to make molecules look better. It modifies bond lengths and angles to create uniformity and aesthetic appeal [34] [35].

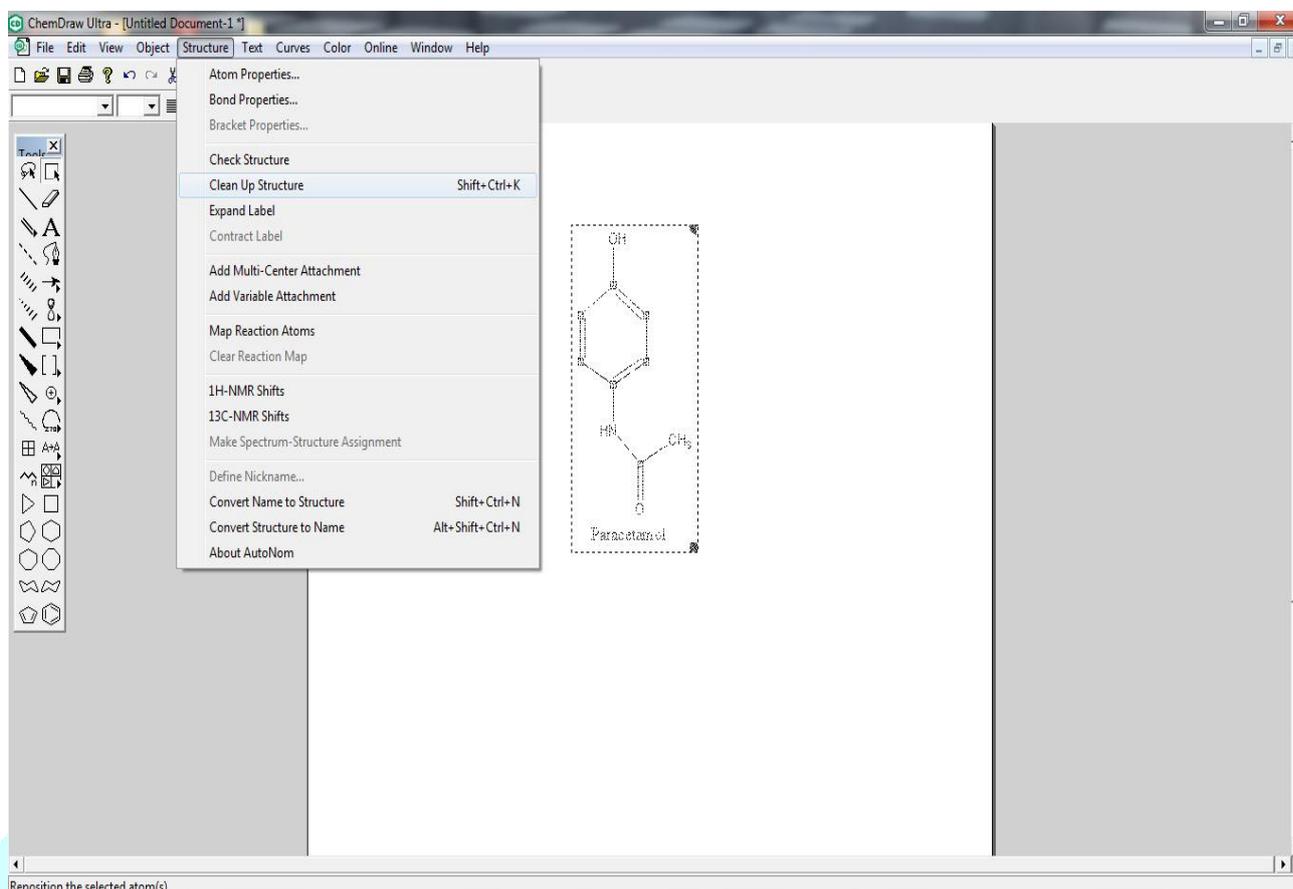


Fig.3.1. Structure Before Clean-up

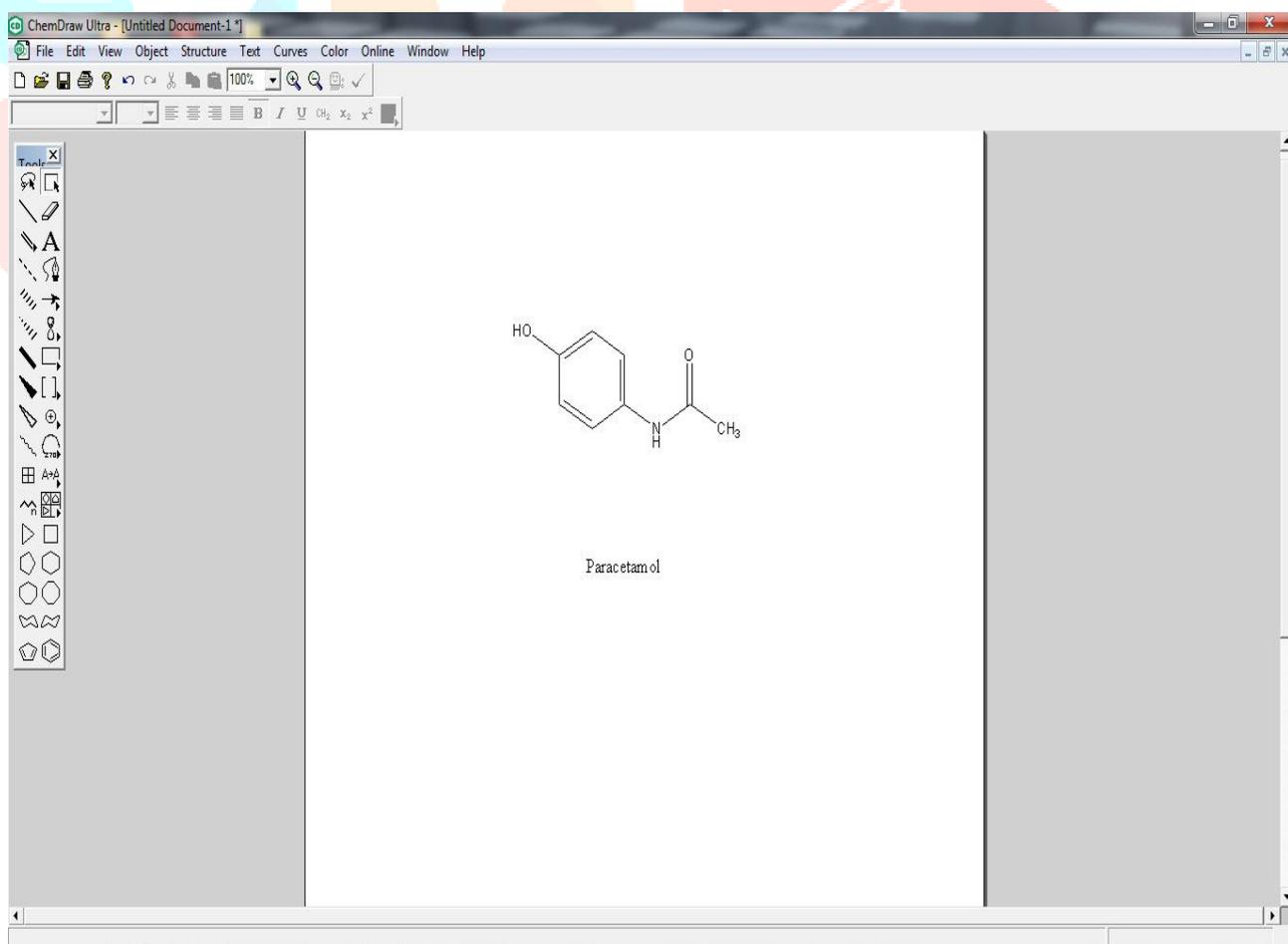


Fig.3.2. Structure After Clean-up

4. Prediction of Chemical Property

ChemDraw's capability for Chemical Property Prediction, which enables users to compute different chemical characteristics of molecular structures, is one of its primary features. A library of functions to return chemical properties directly within a worksheet is accessible in ChemDraw/Excel, where this

function is integrated [36] [37]. It greatly simplifies the process of data analysis in chemistry by allowing users to investigate a variety of approaches for forecasting values associated with chemical substances [37].

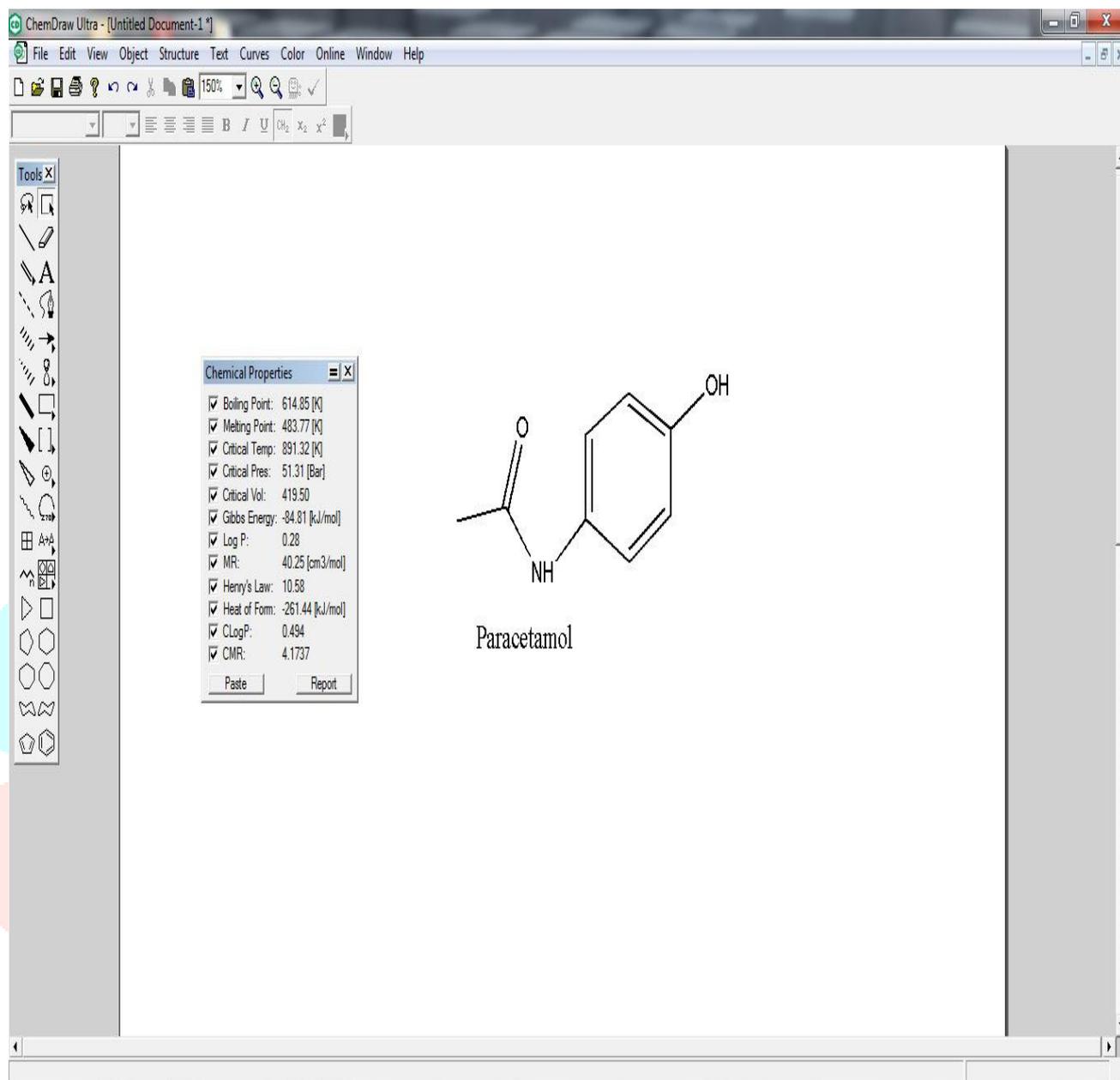


Fig.4.1. Prediction of Chemical Properties

5. Bond Angle and Length Adjustment

One essential tool for effectively representing molecular structures in chemical representations is ChemDraw's bond angle and length adjustment capability [42] [43]. Users can design molecular structures with certain bond angles in ChemDraw, which can be changed to suit their preferences. ChemDraw ensures consistency and clarity in chemical diagrams by using predefined bond lengths and angle [37] [43]. Using either an exact value specified by the user or a percentage of the bond length (ranging from 1 to 100), users can modify bond lengths and the distance between double bonds in aromatic ligands as necessary [45] [46].

6. Structure to Name and Name to Structure

Chemical structures and their matching IUPAC names can be easily converted with ChemDraw's "structure to name" and "name to structure" functionalities. While "name to structure" creates a molecular structure from a chemical name, "structure to name" transforms a drawn structure into an

IUPAC name. These features are especially helpful in domains where precise compound identification is essential, such as medicinal chemistry [29] [47].

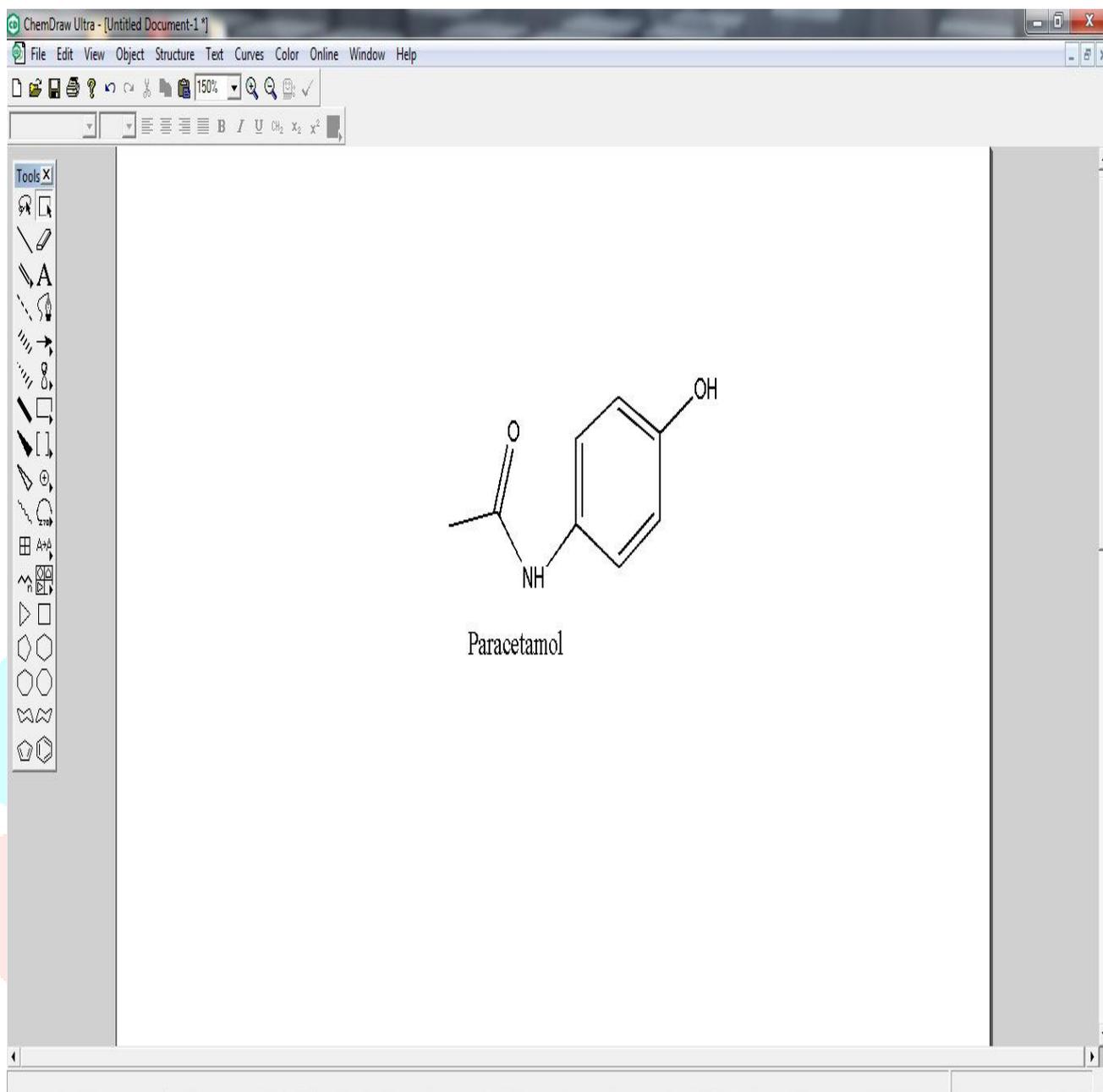


Fig.6.1. Structure to Name

7. **¹H NMR and ¹³C NMR Prediction**

Although ChemDraw can anticipate both ¹H and ¹³C NMR chemical shifts, the precision of pre¹H NMR spectroscopy reveals details about molecule structure by detecting proton chemical changes. Dictionaries can change based on the molecule and the technique [48] [49]. For instance, ChemDraw's CS ChemNMR Pro function can calculate chemical shifts for typical organic compounds, but it might not be as precise for unconventional systems [50]. A molecule's carbon skeleton can be directly observed via ¹³C NMR spectroscopy, which displays the chemical shifts of each carbon atom [51].

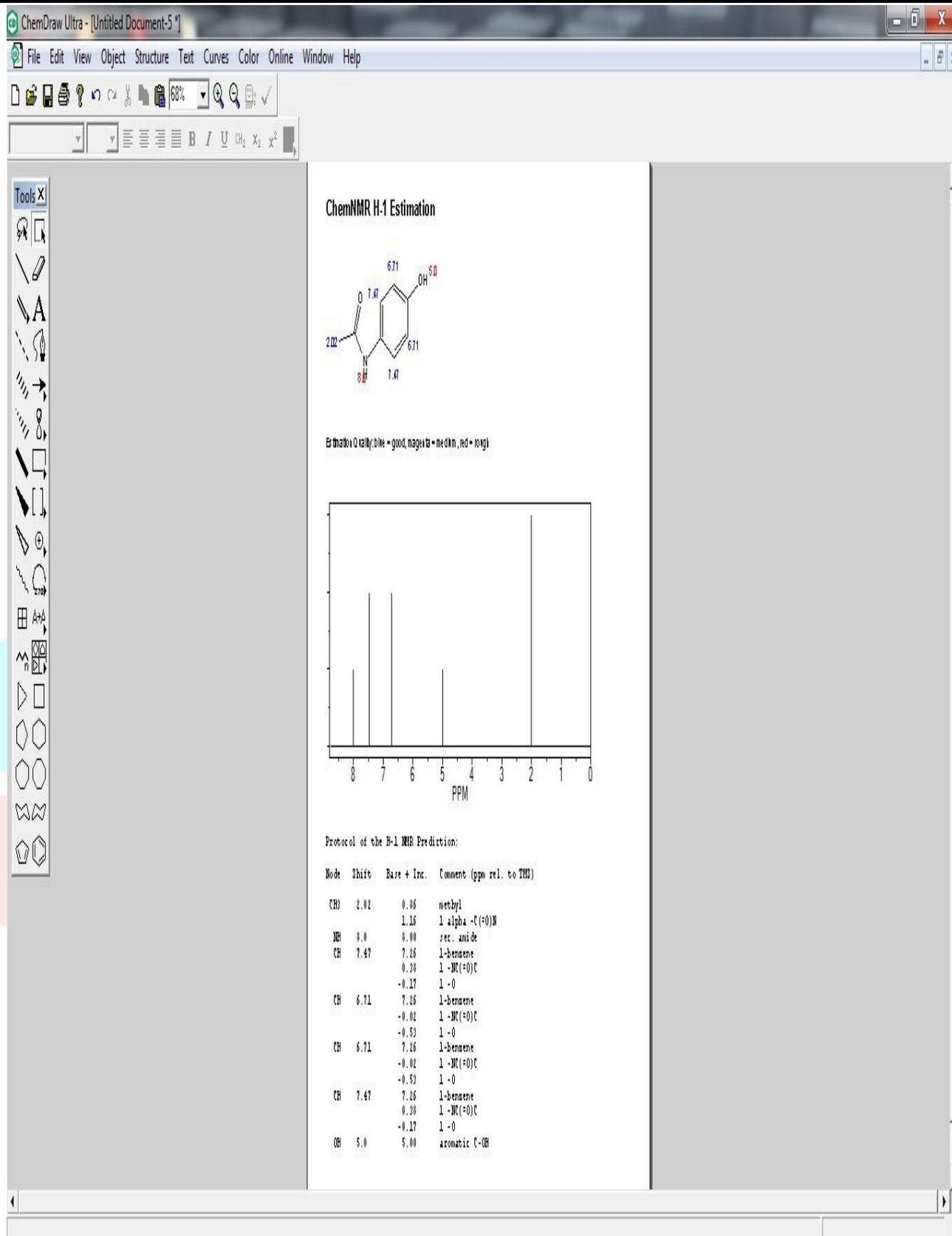


Fig.7.1. ¹H NMR Prediction

9. SMILES String Generation

SMILES (Simplified Molecular Input Line Entry System) strings can be created from drawn structures using ChemDraw. The “Copy As SMILES” tool allows you to create a SMILES representation of a drawn molecule, which you can subsequently copy and paste into other programs [55] [56].

10. Chemical Analysis

ChemDraw gives users chemical analysis tools that let them sketch, examine, and compute structures. It can produce fundamental data such as molecular weight, determine precise fragment weights, and forecast NMR spectra. Additionally, ChemDraw facilitates structure alignment and comparison, which is helpful for lead optimization and drug discovery [29] [54] [57].

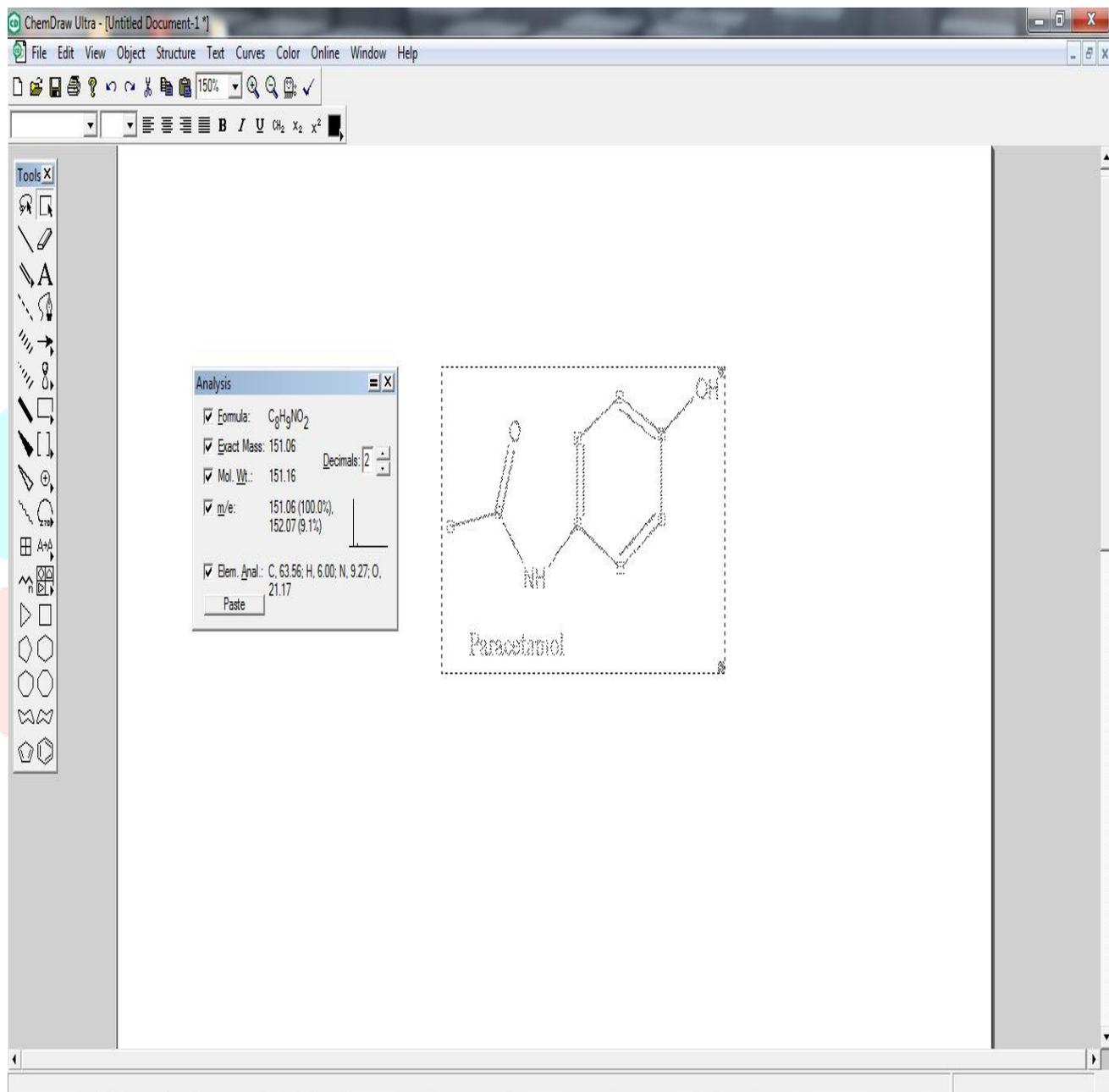


Fig.10.1. Chemical Analysis

11. Specialized Toolbar

ChemDraw offers tools for sketching chemical structures, annotations, and other features using a set of toolbars that includes the Main toolbar and other specialty toolbars. With tools for sketching bonds, atoms, and fundamental elements, the Main toolbar serves as the main toolbar. Tools for more specialized uses, such drawing annotations, brackets, arcs, and chemical symbols, are available under specialized toolbars like the Drawing Elements and Chemical Symbols toolbars [49] [54] [58].

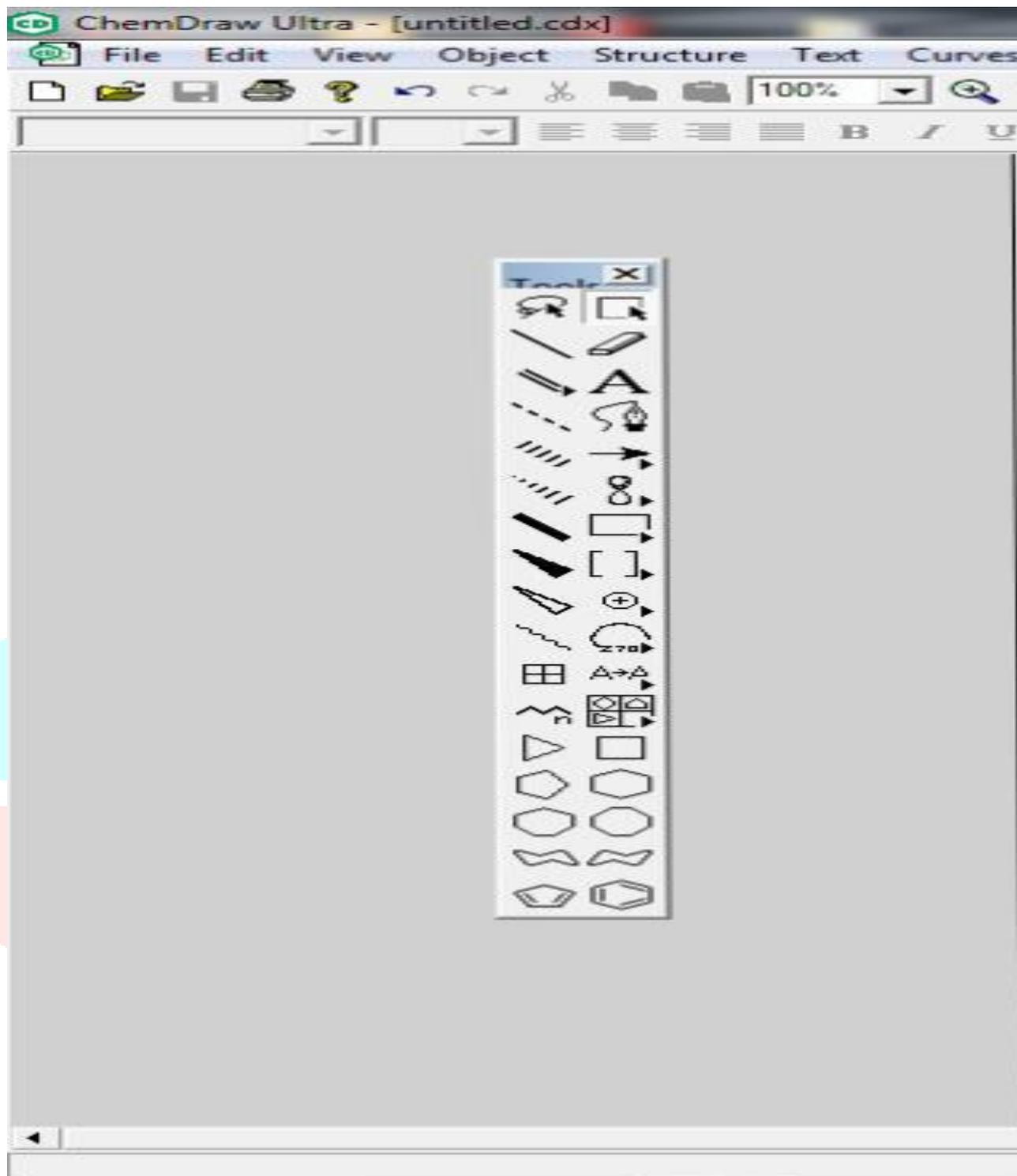


Fig.11.1. Specialized Toolbar

SOME ADDITIONAL FEATURES OF NEW CHEMDRAW 23

The latest version of ChemDraw 23 have some additional features.

1. **Cloud integration with Signals ChemDraw:** Signals ChemDraw incorporates all of the cutting-edge tools from the ChemDraw suite and takes the role of ChemOffice [65].
2. **ChemOffice+ :** Formerly called ChemDraw Collections, ChemOffice+ is a new program that allows you to better manage, find, organize, and share your computer's chemical material (molecules and reactions) by classifying them [52].
3. **HELM monomer curation features:** A tool for organizing and managing unique monomer libraries used in the creation of complex macromolecules and biopolymers is the HELM Monomer Curation application, which is a component of the Revvity Signals platform. Users can inspect libraries, manage individual monomers by restoring or deprecating them, and upload monomers in bulk. Additionally, it lets users create rules for adding monomers to libraries and offers comprehensive information on bulk imports to help find problems with uploaded monomers [17] [52].
4. **ChemDraw+ Application:** With its user-friendly interface, the "ChemDraw+ application" is a cloud-native version of ChemDraw that enables users to manage and sketch chemical structures right in the cloud [52].

ADVANTAGES OF CHEMDRAW SOFTWARE

ChemDraw has many benefits that help chemists and chemical engineers in many different fields be more productive and efficient.

1. **User Friendly Interface**
Both experts and students can use the software because of its clear layout. New users have a lower learning curve because to features like structural cleanup and large template libraries that make navigation and use simple [39] [16].
2. **Reporting and Documentation**
The software facilitates the creation of precise documentation required for publications, safety reports, and patents. Maintaining adherence to industry standards and making sure that all pertinent data is efficiently documented depend on this function [41].
3. **Time Consuming Features**
Chemical intelligence is incorporated into ChemDraw to expedite the drawing process and enable users to produce structures and visuals that are suitable for publication. In educational contexts, where time efficiency is essential for both teaching and learning, this talent is especially prized [27] [38].
4. **Advanced Searching Features**
ChemDraw offers powerful search features, such as precise structural and substructure searches. This makes it possible for users to find particular compounds in chemical databases with ease, improving research capabilities and the effectiveness of locating pertinent information [39] [41].
5. **3-D Modeling**
The capacity of ChemDraw to create 3D models from 2D structures is one of its best qualities. This feature is very helpful for understanding molecular interactions and properties by allowing you to see molecules in three dimensions [40].
6. **Integration with Other Software**
ChemDraw allows users to efficiently manage data across several platforms by integrating with Electronic Lab Notebooks (ELNs) and other tools. For contemporary research settings where teamwork is essential, this interoperability is essential [37] [41].
7. **Continuous Improvement**
ChemDraw is updated frequently, taking user input into account to improve functionality and meet new demands in the chemistry industry. Users will always have access to the newest features and tools in chemical drawing software because to this dedication to improvement [16].
8. **Educational Benefits**
Institutions give students access to the same expert tools used by working chemists by including ChemDraw into their educational programs. In addition to improving learning, this exposure gets children ready for future employment in science and technology [16].

APPLICATION OF CHEMDRAW SOFTWARE

ChemDraw is a popular software program for drawing chemical structures that provides a complete platform that makes it easy for researchers, teachers, and business professionals to make and work with molecular representations. It's also offers application in various research field, industrial field, chemical engineering etc.

1. Industrial Applications

ChemDraw is extensively used in many different industries due to its strong skills in data administration, chemical drawing, and research facilitation. Professionals working in industries like food science, petrochemicals, and pharmaceuticals can benefit greatly from its applications, which go beyond straightforward molecular representations.

2. Pharmaceutical Industry

ChemDraw is essential to drug research and discovery in the pharmaceutical industry. It enables researchers to maintain chemical datasets, produce intricate chemical structures, and illustrate intricate molecular interactions. ChemDraw speeds up experiment design and makes it easier to complete the paperwork needed for safety reports and patents by offering features like 3D visualization tools and editable templates [59] [60]. Additionally, the program offers integrated drug development methodologies, like Translational Pharmaceuticals®, which blends real-time cGMP manufacturing with clinical activities [61] [62].

3. Manufacturing and Drug Synthesis

ChemDraw is also essential to the manufacture and synthesis of medicinal substances. Route scouting, process research and development (PR&D), and small-scale Good Manufacturing Practice (GMP) manufacturing are just a few of the extensive capabilities it makes possible [16] [61]. For regulatory compliance and a successful medicine approval, the program helps researchers create correct paperwork and optimize production operations [63] [64].

4. Clinical Pharmacology

ChemDraw helps in the design of integrated pharmacology programs and first-in-human studies in clinical pharmacology. Its technologies increase the effectiveness of clinical trials and the likelihood of positive results by assisting researchers in making important decisions earlier in the drug development process [16] [62]. Pharmacological studies required for new drug approvals are further supported by the software's capacity to evaluate spectra and optimize process flows [60] [65].

5. Chemical Engineering

Beyond the pharmaceutical industry, ChemDraw is widely used in chemical engineering for activities including reactor design, process flow visualization, and chemical safety data analysis [60] [66]. Because of the software's adaptability, chemical engineers can produce intricate structures and diagrams that are necessary for effective plant design and operation [59] [64].

6. Educational and Academic Use

ChemDraw is especially well-liked in educational settings because it gives teachers and students the resources they need to effectively sketch chemicals and see molecules. ChemDraw's numerous versions meet the needs of diverse users; for academic users who need quick and neat chemical sketches, ChemDraw Prime is the best option [37] [60].

LIMITATIONS OF CHEMDRAW SOFTWARE

Despite various features and uses, ChemDraw has several limitations.

1. Inorganic Chemistry

In order to visualize inorganic structures, users must construct custom templates because the standard ChemDraw templates, such as ACS96, are made for organic chemistry and might not be the best option [67].

2. Larger Biomolecules

Some larger biomolecules can be difficult for ChemDraw to handle because to their size and complexity, which could affect the accuracy of modeling and visualization [29].

3. 3-D Modeling

Although ChemDraw has 3D modeling features, they are not as sophisticated as those of dedicated 3D modeling software, which might make it more difficult to thoroughly examine intricate 3D structures [29].

4. Customization

According to Revvity Signals, ChemDraw (vNext) does not support stylesheet customization through the Renderer Setting dialog, which means users are unable to adjust atom size or location as they did in earlier versions [68].

5. Coordinative Bonds

Coordinative bond information can be extracted using ChemScanner, but it needs to be represented in a Molfile in order to be immediately transferred to SMILES [67].

6. Log P Calculation

According to a study on the hydrophobicity of ADC payloads, LogP values determined by various software programs, such as ChemDraw, might differ greatly and could not always correctly represent true hydrophobicity [69].

7. Errors in Translation

According to a study on ChemScanner, there may be some translation issues when exporting ChemDraw documents to other formats [71].

CONCLUSION

ChemDraw is an essential tool for contemporary chemistry that makes property analysis, reaction modeling, and molecular drawing easier. As it developed from a simple illustration program to a feature-rich, cloud-integrated platform, its usefulness in research, industry, and academia has increased. It enhances efficiency and comprehension in chemical investigations with its user-friendly design and sophisticated features, such as NMR prediction and stereochemistry analysis. ChemDraw is still widely used because to its accuracy, usability, and ongoing innovation, even with its slight drawbacks when it comes to complicated biomolecules and 3D modeling. It is regarded as a vital tool for chemists everywhere.

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