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Review

Chemical structure and reaction schemes using chemdraw

Garamsandh Gandhi Velusamy[1], Kamalakannan Dhanabalan[2], R. Manivannan[3], Blessalya Mathiyalagan[4], Boopathi Selvaraj[4], Deepak kumar Anguraj[4], Harish Kanagaraj[4], Yaswanth Sengottuvel[4], Yasotha selvan*[4]

Associate professor[1], Professor & Head[2], Professor & Principal[3], Scholar[4]
Excel College of Pharmacy, Namakkal, Tamil Nadu, India

*Author for Correspondence: Yasotha selvan
Email: yasothaselvan@gmail.com

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Abstract

CHEMDRAW is a software program used for creating chemical structures and reactions. It provides a user-friendly interface for drawing and editing chemical structures, including 2D and 3D depictions, and allows for the creation of reaction schemes and predictions of chemical properties. It is widely used in the field of chemistry for research, teaching, and scientific communication. CHEMDRAW supports various file formats for exporting and importing chemical structures and is compatible with many chemical databases, making it a valuable tool for chemical information management.

Keywords: Chemdraw, Chemical Structures, Molecular Drawing, Reaction Schemes, Structural Formulas.

INTRODUCTION

CHEMDRAW offers several advanced tools for chemical modeling, including prediction of reaction pathways and energies, and calculation of molecular properties such as molecular weight and rotational constants. It also includes a set of spectral analysis tools for interpretingNMR and mass spectrometry data, and tools for creating publication-quality figures and reports. Another important aspect of CHEMDRAW is its compatibility with a range of other software programs, such as chemical databases, molecular modeling programs, and scientific word processors. This integration allows for seamless transfer of chemical information between different tools, reducing errors and increasing efficiency in research and publication. Overall, CHEMDRAW is an essential tool for chemists, chemical engineers, and researchers in relatedfields, providing a comprehensive suite of tools for chemical structure drawing, reaction design, and data analysis. CHEMDRAW is a software program that allows for the creation of chemical structures and reaction schemes. With its user-friendly interface, users can easily draw

and edit chemical structures in 2D and 3D depictions. It supports various chemical file formats,making it easy to import and export structures to and from different sources. In CHEMDRAW, users can create complex chemical structures by adding atoms, bonds, and functional groups, and modifying their properties such as charge, stereo-chemistry, and hybridization. The program also includes tools for designing reaction schemes, where users can add reactants, catalysts, and products, and specify the conditions and reaction pathways. Additionally, CHEMDRAW provides a set of tools for predicting chemical properties and modeling chemicalreactions, such as the calculation of molecular weight and rotational constants, prediction of reaction pathways and energies, and interpretation of NMR and mass spectrometry data. The chemical structure represent a range of target from very simple molecules (E.g. such as proteins). Therefore, a computer program was sought since the beginning for creating and modifying representation of chemical structure and reaction currently, several computerprograms included,

i. Standalone programs (E.g. ACD/CHEMSKETCH, ARGUSLAH, BK chem. Elemental (software) MARVINSKETCH/view etc...
ii. Java applets (E g ACCLYR JDRAW, JCHEMPAINT, JME molecule editor, Marvinspace, Marvin sketch, Flame etc...
iii. JAVASCRIPT embeddable editors (Eg. ANGULAR DRAWCHEM, KETCHER, Marvin JS, MOLINSPIRATION WEBME, molecule editor and VIWER, PUBCHEM online etc.
iv. Mobile editor apps (CHEMDOODLE Mobile Structure and reaction)

The computer program Cambridge softs CHEMDRAW is a user-friendly and industry leads inchemical and reaction drawing. In addition it analyzes properties of provides sophisticated search and information function. CHEMDRAW is operated by a combination of tools compounds that can be selected from tools PALLOOTTE usually for a no of frequently used structure components (E g Benzene, Imidazole, etc.,) and menu, respectively. The cost of entrylevel commercial CHEMDRAW prime 16.0 is about X9.65 lacs with a perpetual license and its academic price is about X0.10 lacs with one year LICENCES.

Basic steps to use ChemDraw

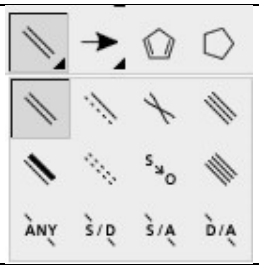
1. Opening ChemDraw:
   - Once installed, launch the software. You'll be greeted with a blank workspace.
2. Drawing Atoms and Bonds:
   - To draw atoms, simply select the text tool (usually represented by an "A" icon) and click on the workspace. Type the elemental symbol (e.g., "C" for carbon).
   - To draw bonds, select the bond tool (usually represented by a line icon). Click and drag to draw single, double, or triple bonds. ChemDraw will automatically adjust bond angles based on the type of atom and hybridization.
3. Drawing Rings and Complex Structures:
   - ChemDraw has templates for common structures like benzene rings. You can drag and drop these into the workspace and modify as needed.
4. Drawing Reaction Schemes:
   - Use the arrow tool to draw reaction arrows.
   - You can place reactants on the left, the arrow in the middle, and the products on the right.
   - For side products, conditions, or catalysts, you can use the text tool to type above or below the arrow.
5. Cleaning Up Structures:
   - If your structure looks a bit off or you want to optimize the layout, there's usually a "clean up structure" or "clean up reaction" option in the toolbar or under one of the menus. This automatically adjusts the drawn structure to look neater and more professional.
6. Adding Text and Annotations:
   - Use the text tool to add labels, reaction conditions, or any other textual information to your drawing.
7. Saving and Exporting:
   - Once you've completed your drawing, save your work. ChemDraw files typically have a ".cdx" extension.
   - You can also export your drawing to various formats like PDF, image files (JPEG, PNG), etc., depending on your needs.
8. Advanced Features:
   - ChemDraw often comes with advanced features like predicting NMR spectra, calculating molecular properties, and more, depending on the version you have.

General procedure

Tools	Description
	Lasso Make freehand selection of irregular areas
	Marquee Selection Select all or part of a molecule, reaction, or any other object or text string within arectangle
	Undo

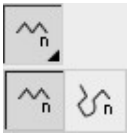
Tools	Description
	Cancel your last action and go back to the previous state (can be applied multipletimes)
	Redo Redo an action (can be applied multiple times)
	Magnify View an enlarged view of objects
	Reduce Reduce the size of objects
	Copy Copy the current drawing area drawing/content.
	Paste Paste drawing/content into the drawing area.
	Eraser Remove all or sections of objects
	Solid Bond Draw single bonds
	Dashed Bond Draw dashed bonds
	Bold Bond Draw bold bonds
	Hashed Bond Draw hashed bonds
	Wedged Bond

Tools	Description
	Draw wedged bonds
	Hashed Wedged Bond Draw hashed wedged bonds
	Hollow Wedged Bond Draw hollow wedged bonds
	Wavy Bond Draw wavy bonds
	Multiple Bonds Let's you access the Multiple Bonds toolbar to draw various bonds such as double bond, triple bond, and dative bonds. Long-click on this icon to access the secondarytools as shown.



Acyclic Chain

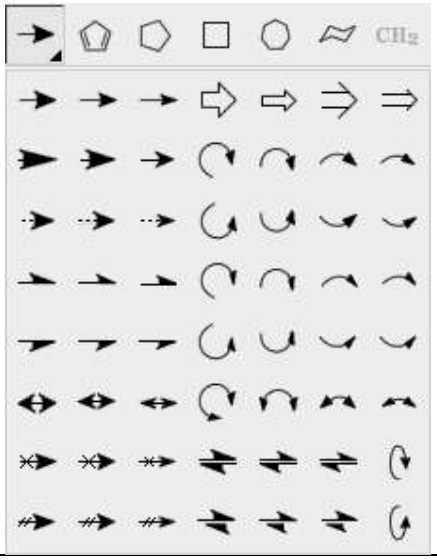
Lets you access the Acyclic Chain palette to draw acyclic chains and snaking chainsof different lengths. Long-click on this icon to access the secondary tools as shown.



Arrows

Let's you access the Arrow palette to draw various arrows such as solid arrow, boldarrow, and hollow arrows. Long-click on this icon to access the secondary tools as shown.

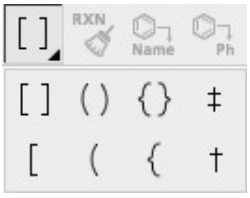
Tools	Description



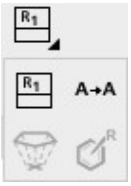
	Benzene Insert benzene rings
	Cyclopentadiene Insert Cyclopentadiene rings
	Cyclohexane Ring Insert Cyclohexane rings
	Cyclopentane Ring Insert Cyclopentane rings
	Cyclopropane Ring Insert Cyclopropane rings
	Cyclobutane Ring Insert Cyclobutane rings

	Cyclooctane Ring Insert Cyclooctane rings

Tools	Description
	Cycloheptane Ring Insert Cycloheptane rings
	Chair Cyclohexane Insert one of the two chair Cyclohexane conformations
	Chair Cyclohexane Insert one of the two chair Cyclohexane conformations
A	**Text** Insert and edit text. The text can be a linear formula or a chemical structure, or canbe text used as a caption or annotation.
CH_2	**Formula** Let's you change the atom label into a proper chemical formula using Subscript and Superscript where necessary
X^2	**Superscript** Enter text as superscript
X_2	**Subscript** Enter text as subscript
	Group Group multiple objects into one object.
	Ungroup Ungroup a grouped object
	Integral Create groups so that individual objects in the group cannot be selected (integralgroup).

Tools	Description
[ ]	**Brackets** Let's you access the Brackets palette to draw various brackets such as braces, brackets, and parentheses. Long-click on this icon to access the secondary tools asshown. 
	Clean Up Structure Clean up a structure drawn in the drawing window. You must first select the drawingyou want to clean up (using the Marquee Selection tool or the Lasso tool) to enable the Structure Cleanup tool.
RXN	**Clean Up Reaction** Clean up a reaction drawn in the drawing window. You must first select the drawingyou want to clean up (using the Marquee Selection tool or the Lasso tool) to enablethe Reaction Cleanup tool.
Name	**Name To Structure** Let's you convert chemical names into their corresponding chemical structures
Name	**Structure To Name** Let's you generate the name of structures you have drawn

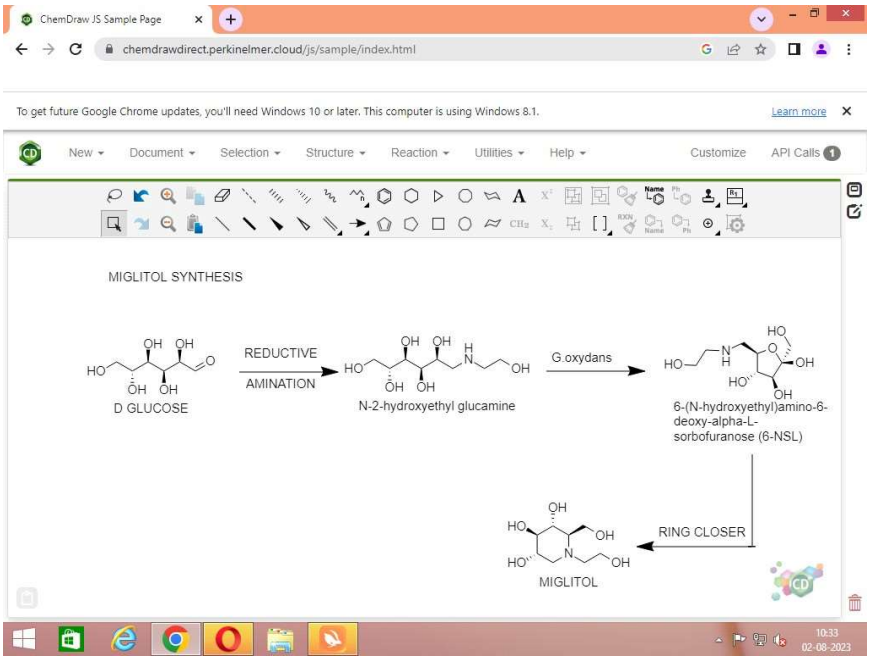
	Expand Label Let's you expand the labels into full structure
	Contract Label Let's you collapse the full structure back to its label
	Templates

Tools	Description
	Let's you access the templates library which contains pre-drawn molecularstructures to help you draw structures.
	Chemical Symbols Tool Let's you access the Chemical Symbol tool palette to use Electron Pushing and Radical Pushing tools to illustrate electron transfer. Long-click on this icon to accessthe secondary tools as shown. 
	Query Tools Let's you access the Query Tools palette to use different Query tools suchas *Alternative Group* tool, *Reaction Atom Map* tool, *Add Multi-Centre Attachment* tool, and *Add Variable Attachment* tool. Long-click on this icon toaccess the secondary tools as shown. 
	Show Properties Let's you specify or assign properties to atoms in a structure.

Procedure for anti-diabetic drugs

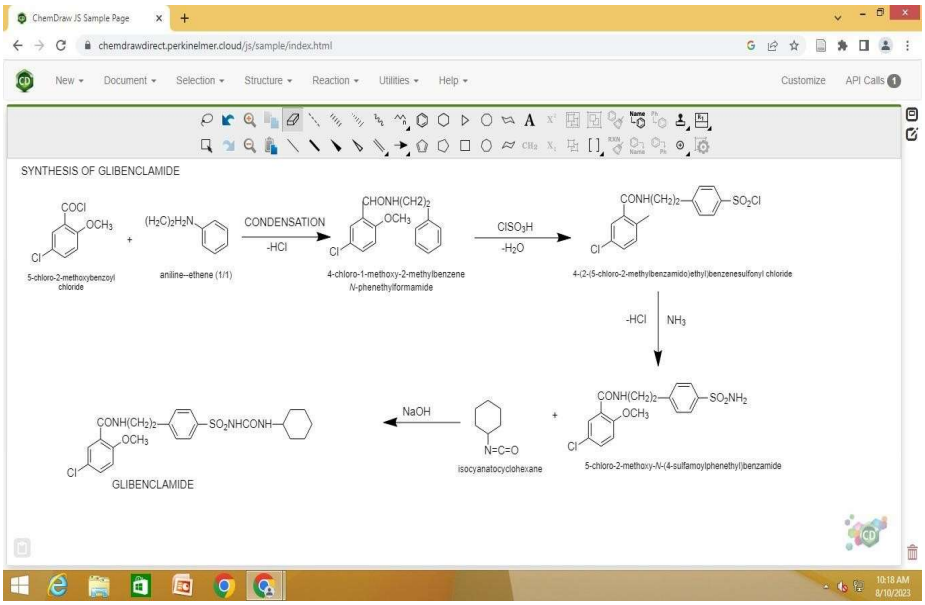
1. MIGLITOL

1. Choose the cyclohexane from the "MAIN TOOL BAR" on the right.
2. Place the "N" atom at a 1st position with a use of TEXT BOX "A".
3. Place the Acyclic chain at the 1st position from the main tool bar.
4. Place the OH group with the help of functional group tool bar and make stick to 1stposition.
5. To draw a "HASHED BOND" select the "HASHED BOND" tool and attached to3rd position.
6. Place the OH functional group with the help of functional group tool bar and to makestick to 3rd position.
7. To draw a "WEDGE BOND" select the "WEDGE BOND" tool and attached 4thposition.
8. Place the OH functional group with the help of functional tool bar and make stick to4th position.
9. To draw a "HASH BOND " select the "HASH BOND" tool and attach to 5th position.
10. Place the OH functional group with help of functional group tool bar and to makestick to 5th position
11. To draw "WEDGE BOND" select the "WEDGE BOND" tool and attached to 6thposition.
12. To draw a "single bond" select the "solid bond" tool and attached to "WEDGEBOND".
13. Place the OH group with the help of functional tool bar and to make stick to 6thposition.
14. Complete the structure of "**MIGLITOL".**



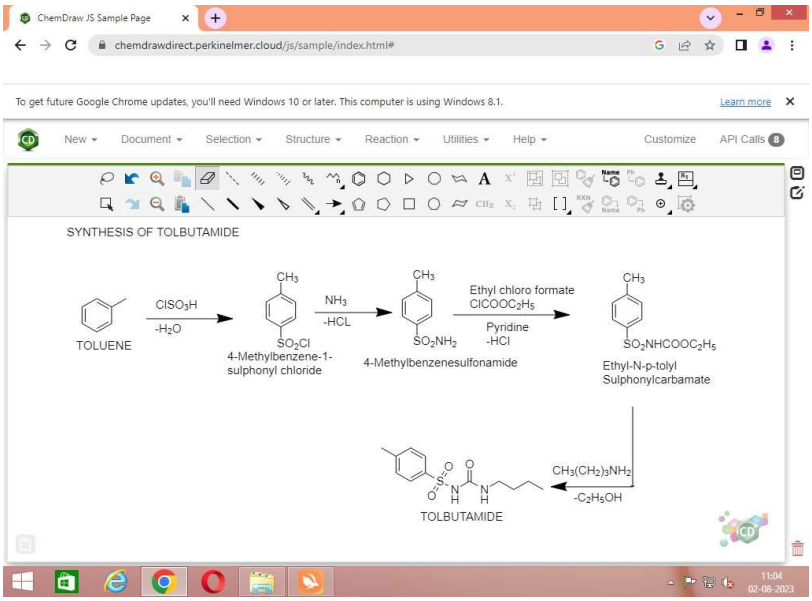
Glibenclamide

15. Choose the benzene from the "MAIN TOOL BAR" the left.
16. Choose the "SOLID BOND" tool and add to the benzene at 1st position.
17. By the use of FUNCTIONAL GROUP tool bar, select the "KETONE" group and attached to ethyl amine from the help of TEXT BOX "A".
18. Again attached to benzene from the TOOL BAR paste it at 1st position of by use of "FUNCTIONAL GROUP" tool bar, select the SULPHONAMIDE group attached with amide from the help of TEXT BOX "A".
19. Again attached to cyclohexane ring from the "TOOL BAR" at 1stpostion.
20. Select the single bond from the "TOOL BAR" at 2nd position.
21. Place the O atom and methyl group at 2nd position with the use of TEXT BOX "A".
22. Place the chlorine atom by using the TEXT BAR at 5th position.
23. Complete the structure of "**GLIBENCLAMIDE"**.



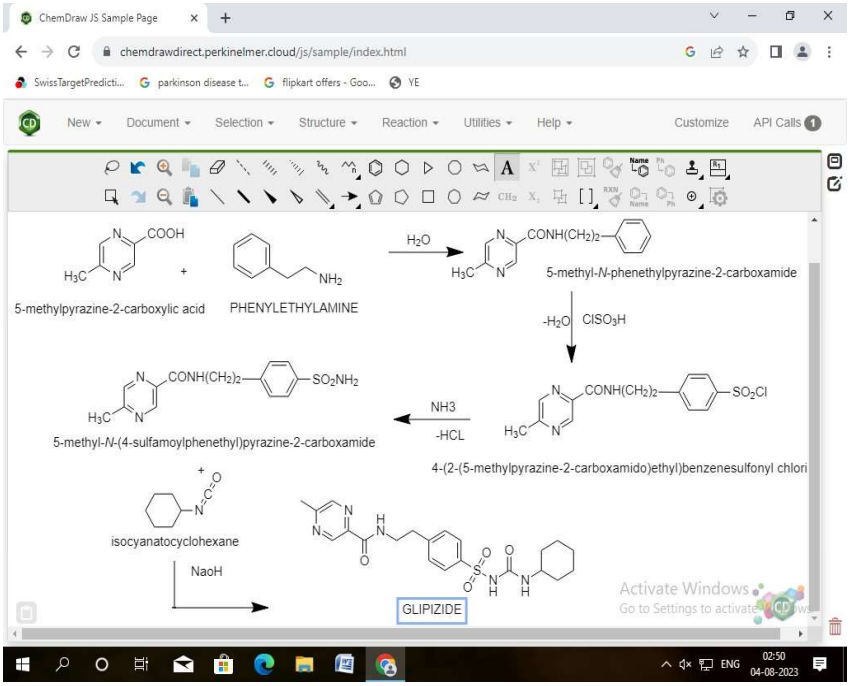
Tolbutamide

24. Choose the benzene from "MAIN TOOL BAR" on the left.
25. Similarly choose the "SOLID BOND" tool and add on the benzene at 1st position tocomplete the structure of tolbutamide.
26. To introduce sulphonyl group into a given structure using "TEMPLATES" from themain tool bar.
27. To draw a single bond, select the "SOLID BOND" tool and attach to sulphonyl group.
28. Place a NH group using text box "**A**".
29. To introduce ketone group into a given structure using "TEMPLATES" from the maintool bar.
30. Place a NH group using text box "**A**".
31. Place the acyclic ring to the NH group.
32. To draw a single bond at 4thposition select a solid bond tool.
33. Complete the structure of "**TOLBUTAMIDE"**.



Glipizide

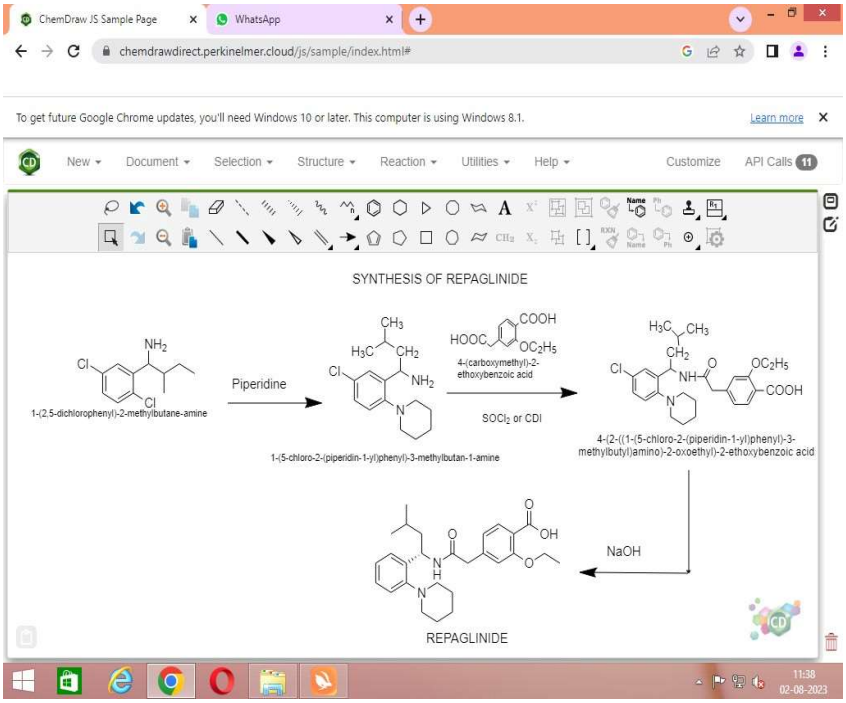
34. Choose the benzene ring MAIN TOOL BAR on the left.
35. Choose the "SOLID BOND" from the main tool bar.
36. Place the single bond on the 1st position of the benzene.
37. Place the SULPHONYL functional group using the functional tool bar.
38. Place the single bond using "SOLID BOND" tool.
39. Place the NH group using text box "A".
40. Place the acyclic chain using the acyclic chain.
41. Place the ketone group on a cyclic ring.
42. Place the single bond using "SOLID BOND" tool.
43. Place the acyclic chain on the 4th position of the benzene.
44. Place the NH group using text box "A".
45. Place the acyclic ring using functional group tool bar.
46. Benzene is added to the acyclic ring from MAIN TOOL BAR.
47. The "N" atom is added on 1st position of benzene using text box "A".
48. Select the solid bond to place single bond on 5th position.
49. To Complete the Structure of "**GLIPIZIDE**".



Repaglinide

50. Choose the benzene from the "MAN TOOL BAR" on left.
51. Similarly choose the "HASH BOND" tool and added onto the benzene ring at 1STposition.
52. Select the "SOLID BOND" tool and attach to the hash bond.
53. Place the acyclic chain on the bond using the cyclic side chain "MAIN TOOL BAR".
54. Place NH group using TEXT BOX "A".
55. To place the acyclic chain choose the acyclic side chain from "MAIN TOOL BAR"and attached onto the NH group.
56. Place the KETONE functional group with the help of "FUNCTIONAL GROUP"
57. tool bar and make attach to the acyclic ring.
58. Select the benzene ring the "MAIN TOOL BAR" and place it on the acyclic ring.
59. Place the acyclic chain in the 1st position of the benzene ring.
60. Place the KETONE functional group with the help of "FUNCTIONAL GROUP" toolbar and make attach to the acyclic ring.
61. Place the KETONE functional group with the help of "FUNCTIONAL GROUP" toolbar and make attach to the acyclic ring.

62. Using the TEXT BOX "A" attach oh group.
63. Place the single bond on 2nd position using "SOLID BOND" tool.
64. Using the TEXT BOX "A" attach oh group.
65. To place the acyclic chain choose the acyclic side chain from "MAIN TOOL BAR"and attached it to the 'O' atom.
66. Place the CYCLOHEXANE ring at the 2 nd position benzene using the
67. CYCLOHEXANE tool on "MAIN TOOL BAR".
68. Place the 'N' atom using TEXT BOX "A".
69. Complete the structure of "**REPAGLINIDE**"



Report

The chemical synthesis of **"ANTIDIABETIC DRUGS"** was drawn and finalized byusing **"CHEMDRAW"** Software.

CONCLUSION

It is widely used in the field of chemistry for research, teaching, and scientific communication. CHEMDRAW supports various file formats for exporting and importing chemical structures and is compatible with many chemical databases, making it a valuable toolfor chemical information management.

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