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Research article

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Chemical structure and reaction schemes using chemdraw

S. Yasotha^{*1}, Dr. R. Manivannan², S.R. Sathya³, K. Sankar⁴, P. Sathish Kumar⁴

¹Assistant Professor, ²Professor and Principal, ³Lecturer, ⁴Scholar
Excel College of Pharmacy, Komarapalayam, Namakkal Dist- 638183. Tamil Nadu, India.

Corresponding Author: S. Yasotha

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

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 interpreting NMR 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 related fields, 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.¹

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 chemical reactions, 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 computer programs included

- i. Standalone programs (e.g.ACD/chemsketch, Arguslah, BK chem. Elemental (software) MarvinSketch/view etc...
- ii. Java applets (e.g Accelry Jdraw, Jchempaint, JME molecule editor, Marvin space, Marvin sketch, Flame etc...
- iii. Javascript embeddable editors (e.g. Angular DrawChem, Ketcher, Marvin JS, Molinspiration WebME, molecule editor and viewer, 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 in chemical 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 palette usually for a no of frequently used structure components (eg, Benzene, Imidazole, etc..) and menu, respectively. The cost of entry level 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.

GENERAL PROCEDURE

- i. Start the program CHEMDRAW
- ii. Choose the “solid bond Tool” from the “Main Toolbar” on the left.

Draw a first bond²

- i. Click-hold-drag-release at different places in the drawing area to draw some first lines (bonds) showing into different directions.
- ii. To suppress fixed bond length and fixed bond angles, press the “Alt” key while drawing.
- iii. Just click into the drawing area to place a bond in default style directly on to the canvas.

Extend the structures

- i. Just click on an atom to automatically extend the structure.
- ii. Click several times on the same atom to add more bonds to the same center. Observe the effect on atoms of differently oriented bonds.
- iii. Choose the “Benzene” tool from the Main Toolbar on the left.
- iv. Click-hold-drag at different places in the drawing area to draw differently oriented benzene.³
- v. Just click into the drawing area to place a benzene in default style directly onto the canvas.
- vi. Erase structures, atoms, or bonds

With the “Eraser tool”

- i. Choose the “Eraser tool” from the “Main toolbar”
- ii. Click on a bond or an atom to erase it.

By “select and delete”

- i. Choose the “Lasso” tool from the “Main toolbar”
- ii. Select an atom or bond by clicking it with the “Lasso” or select an object, several objects, or a part of an object by encircling with the “Lasso”.
- iii. Select additional objects by pressing the “Shift” key and proceeding as above.
- iv. Delete selected object by using the “Delete” or “Back delete” key of your keyboard.

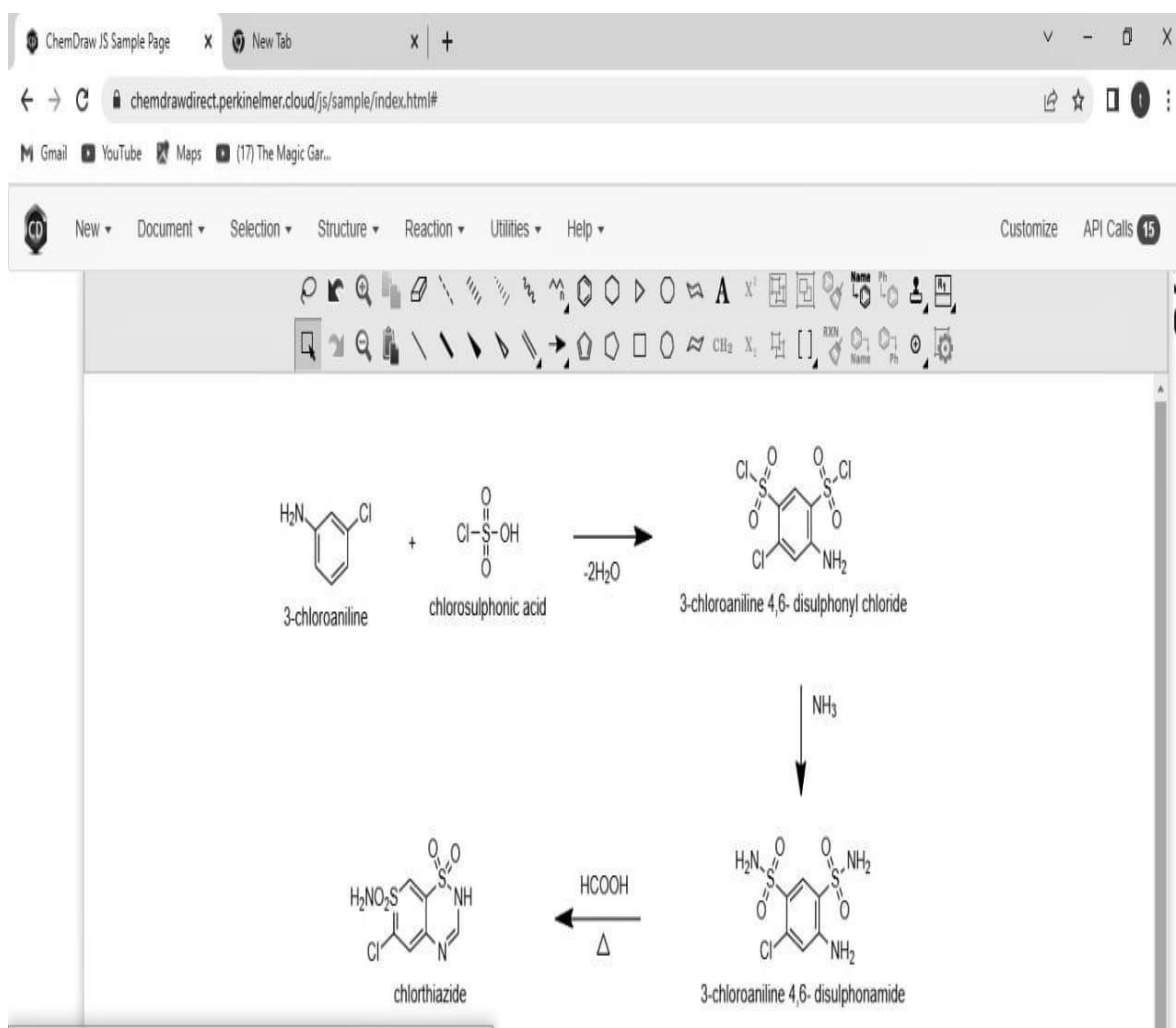
CONVERTING NAMES TO STRUCTURES⁴

- i. Once IUPAC Name of the compound is known, then structure is drawn using convert name to structure, Command Shift + Ctrl + N
- ii. A reaction scheme is drawn to keep major structural frameworks within a row or a column or they are centered horizontally or vertically.⁵
- iii. The structure is copied using Ctrl C command and pasted in word file using Ctrl + V command.

PROCEDURE FOR THIAZIDE DRUGS⁶

1. CHLORTHIAZIDE⁷

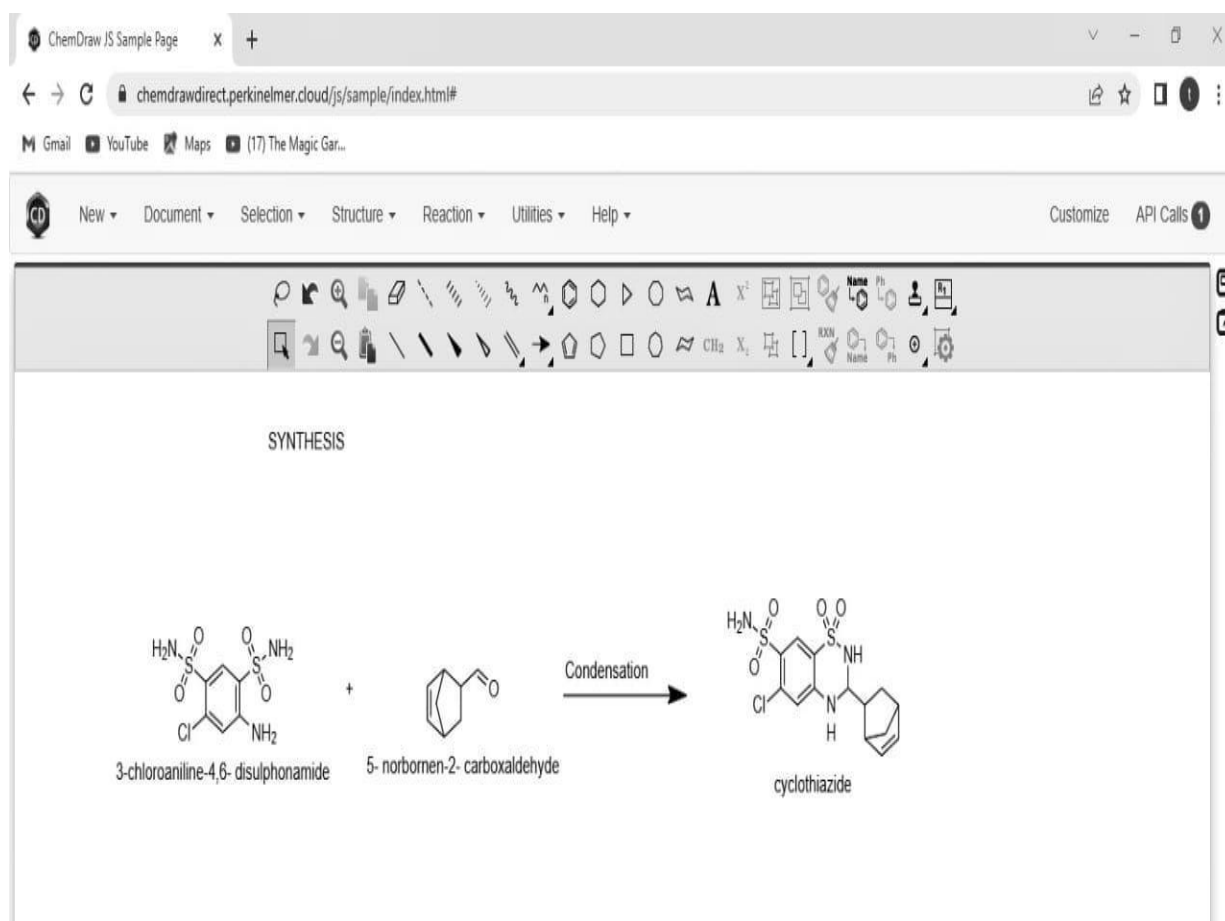
- i. Choose the benzene from the “MAIN TOOLBAR” on the left.
- ii. Similarly choose the “SOLID BOND” tool and add on to the benzene at 1st position to complete the structure of CHLORTHIAZIDE.
- iii. To introduce sulphonyl group into a given structure, using “TEMPLATES” from the main toolbar.
- iv. To draw a single bond, select the “SOLID BOND” tool and attached to the sulfonyl group.
- v. Place the NH group at 2nd position with the use of text box “A”
- vi. Choose the “FUNCTIONAL GROUP” tool bar and select the propene bond and attached to the 2nd position.
- vii. Select the N atom and attached to the 4th position and enclose the ring with the use of “SINGLE SOLID BOND”.
- viii. Place the Cl atom by using the TEXT BAR at 6th position of Chlorthiazide.
- ix. By the use of FUNCTIONAL GROUP tool bar, select the SULFONAMIDE group and attached at 7th position of Chlorthiazide.
- x. Complete the structure of Chlorthiazide.



CYCLOTHIAZIDE⁸

- Choose the benzene from the “MAIN TOOLBAR” on the left.
- Similarly choose the “SOLID BOND” tool and add on to the benzene at 1st position to complete the structure CYCLOTHIAZIDE.
- To introduce sulphonyl group into a given structure, using “TEMPLATES” from the main toolbar.
- To draw a single bond, select the “SOLID BOND” tool and attached to the sulfonyl group.
- Place the NH group at 2nd position with the use of text box “A”

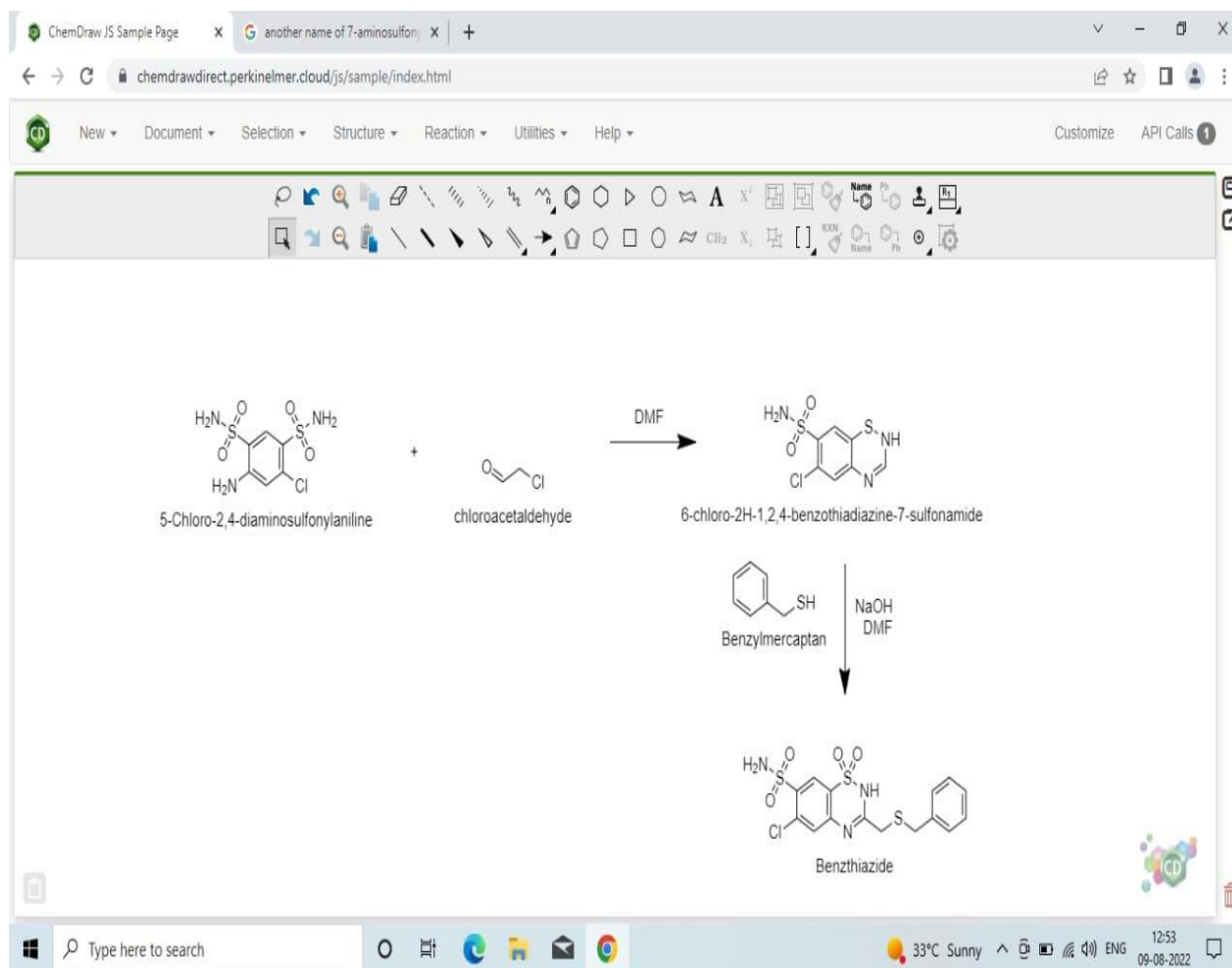
- Choose the “FUNCTIONAL GROUP” tool bar and select the propene bond and attached to the 2nd position.
- Choose the Bicyclic ring from the TOOL BAR and attached to the 3rd position of Chlorthiazide forms Cyclothiazide.
- Select the N atom and attached to the 4th position and enclose the ring with the use of “SINGLE SOILD BOND”
- Place the Cl atom by using the TEXT BAR at 6th position of Cyclothiazide.
- By the use of FUNCTIONAL GROUP tool bar, select the SULFONAMIDE group and attached at 7th position of Cyclothiazide.
- Complete the structure of Cyclothiazide.



BENZOTHAZIDE

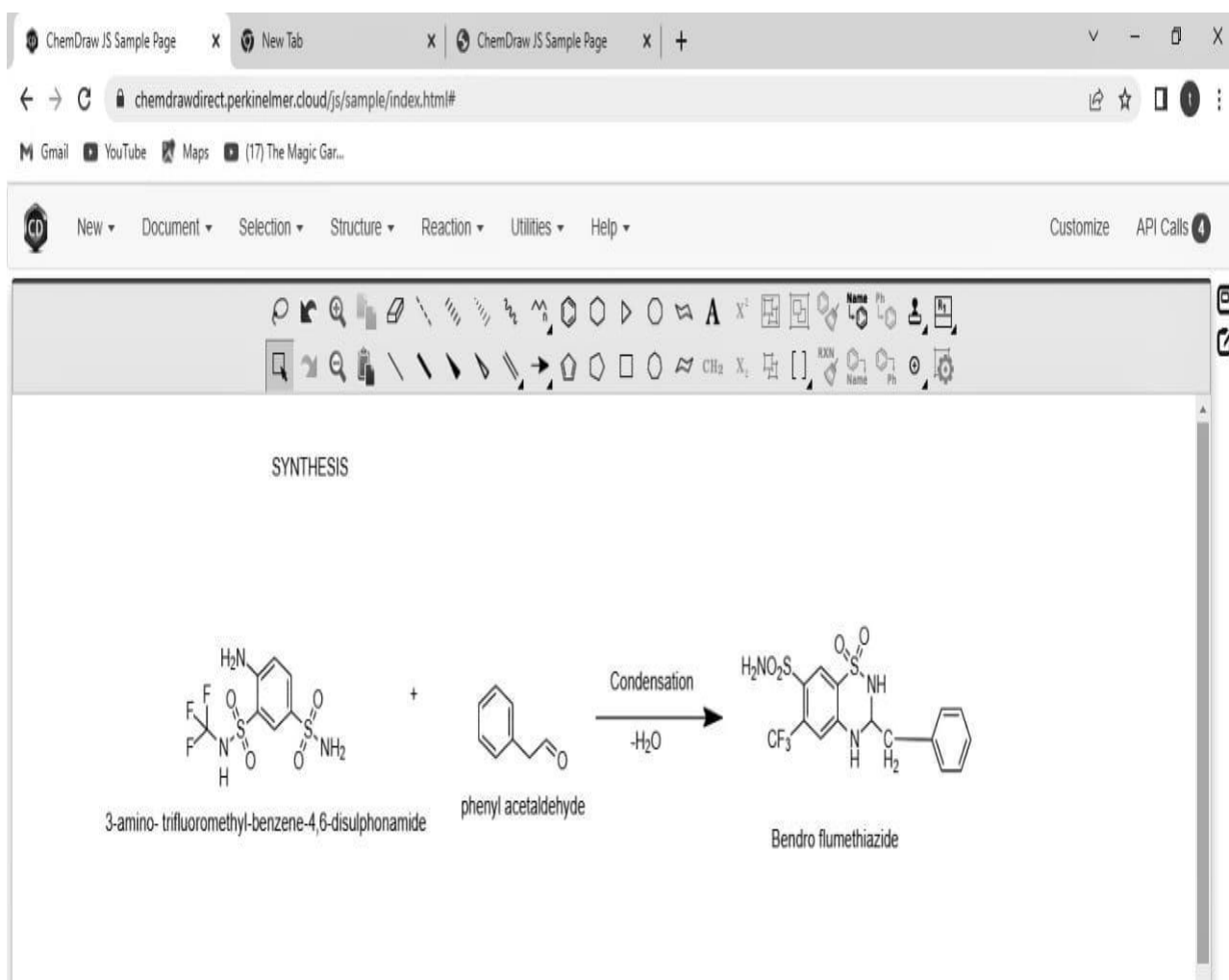
- i. Choose the benzene from the “MAIN TOOLBAR” on the left.
- ii. Similarly choose the “SOLID BOND” tool and add on to the benzene at 1st position to complete the structure BENZOTHAZIDE.
- iii. To introduce sulphonyl group into a given structure, using “TEMPLATES” from the main toolbar.
- iv. To draw a single bond, select the “SOLID BOND” tool and attached to the sulfonyl group.
- v. Place the NH group at 2nd position with the use of text box “A”
- vi. Choose the “FUNCTIONAL GROUP” tool bar and select the propene bond and attached to the 2nd position.
- vii. Select the single bond from the TOOL BAR, paste it at 3rd position of Benzthiazide and add one more bond on
- xiv.

- it.
- viii. Place the S atom to that of the bond from the help of TEXT BOX “A.”
- ix. Again create the double bond with S atom, in addition to that Benzene ring is attached.
- x. Finally it produces phenyl methyl sulfonyl methyl group at 3rd position.
- xi. Select the N atom and attached to the 4th position and enclose the ring with the use of “SINGLE SOILD BOND”.
- xii. Place the Cl atom by using the TEXT BAR at 6th position of Benzothiazide.
- i. By the use of FUNCTIONAL GROUP tool bar, select the SULFONAMIDE group and attached at 7th position of Benzothiazide.
- xiii. Complete the structure of Benzothiazide.



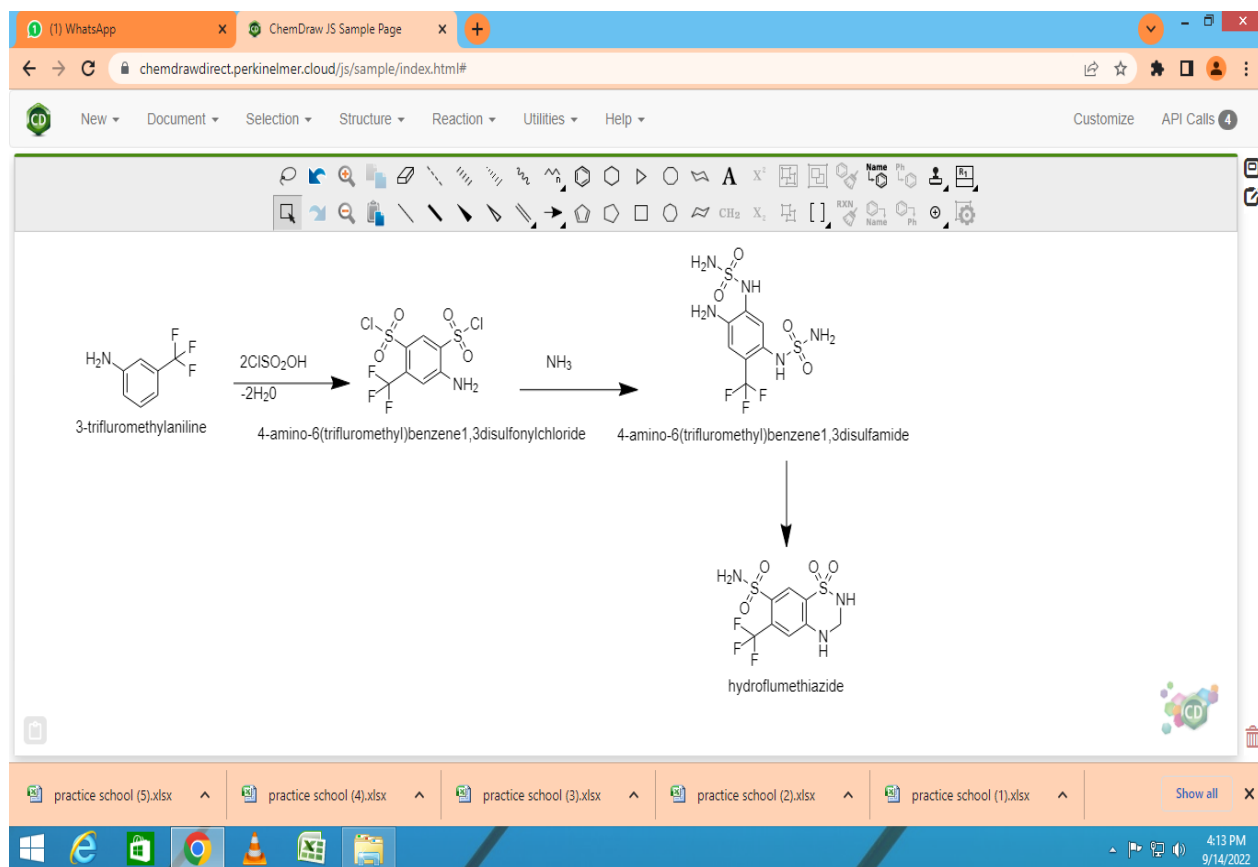
BENDROFLUMETHIAZIDE

- i. Choose the benzene from the “MAIN TOOLBAR” on the left.
- ii. Similarly choose the “SOLID BOND” tool and add on to the benzene at 1st position to complete the structure BENDROFLUMETHIAZIDE.
- iii. To introduce sulphonyl group into a given structure, using “TEMPLATES” from the main toolbar.
- iv. To draw a single bond, select the “SOLID BOND” tool and attached to the sulfonyl group.
- v. Place the NH group at 2nd position with the use of text box “A”
- vi. Choose the “FUNCTIONAL GROUP” tool bar and select the Propene bond and attached to the 2nd position.
- vii. Select the single bond from the TOOL BAR, paste it at 3rd position of Bendroflumethiazide and add one more bond on it.
- viii. Benzene is attached to that bond.
- ix. Trifluoromethyl group is selected from the tool bar and attached to 6th position of Bendroflumethiazide.
- x. By the use of FUNCTIONAL GROUP tool bar, select the SULFONAMIDE group and attached at 7th position of Bendroflumethiazide.
- xi. Complete the structure of Bendroflumethiazide.



HYDROFLUMETHIAZIDE

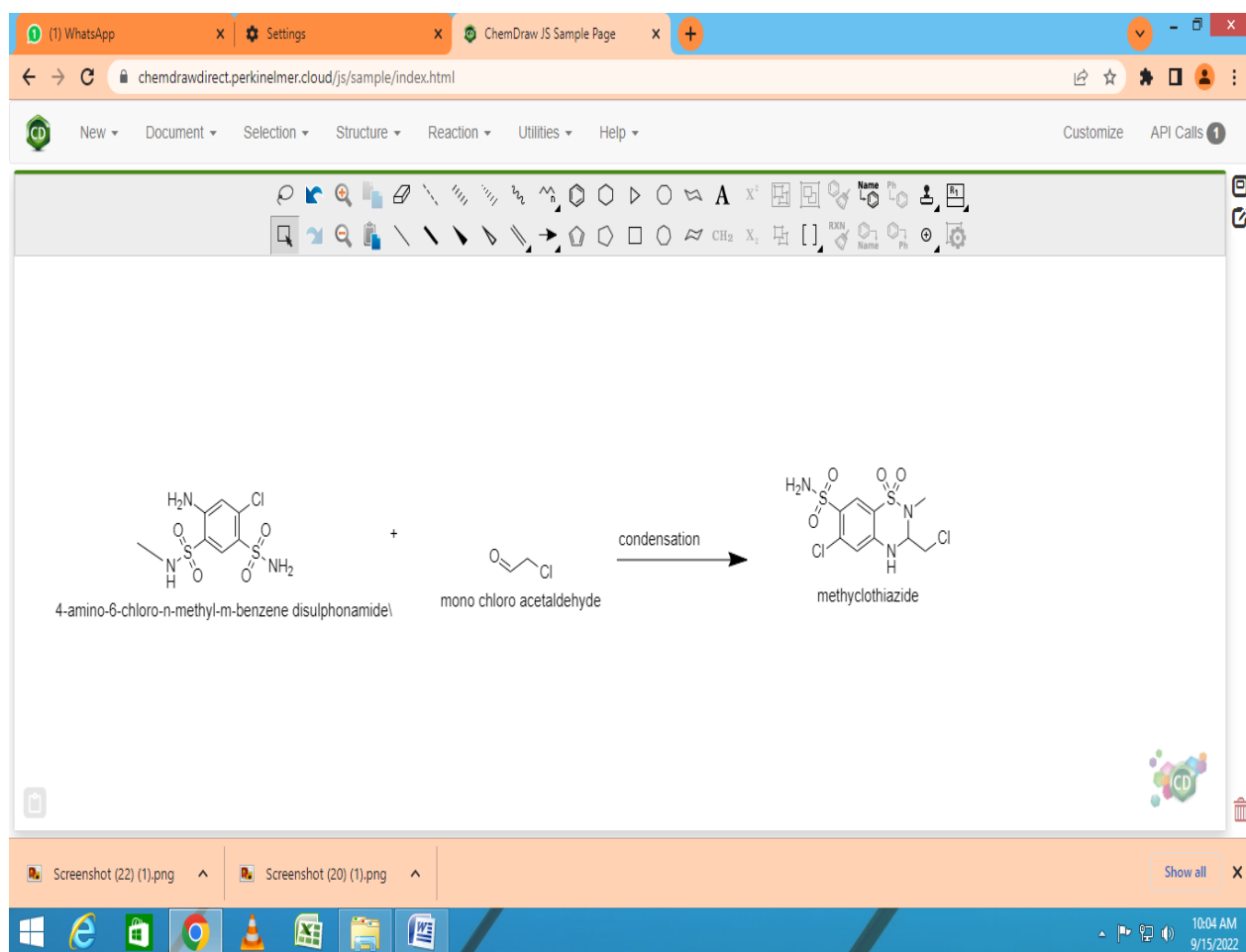
- Choose the benzene from the “MAIN TOOLBAR” on the left.
- Similarly choose the “SOLID BOND” tool and add on to the benzene at 1st position to complete the structure of HYDROFLUMETHIAZIDE.
- To introduce sulphonyl group into a given structure, using “TEMPLATES” from the main toolbar.
- To draw a single bond, select the “SOLID BOND” tool and attached to the sulfonyl group.
- Place the NH group at 2nd position with the use of text box “A”
- Choose the “FUNCTIONAL GROUP” tool bar and select the propene bond and attached to the 2nd position.
- Select the N atom and attached to the 4th position and enclose the ring with the use of “SINGLE SOILD BOND”
- Place the Trifluoromethyl group at the 6th position of Hydroflumethiazide.
- By the use of FUNCTIONAL GROUP tool bar, select the SULFONAMIDE group and attached at 7th position of Hydroflumethiazide.
- Complete the structure of Hydroflumethiazide



METHYCLOTHIAZIDE

- Choose the benzene from the “MAIN TOOLBAR” on the left.
- Similarly choose the “SOLID BOND” tool and add on to the benzene at 1st position to complete the structure of METHYCLOTHIAZIDE.
- To introduce sulphonyl group into a given structure, using “TEMPLATES” from the main toolbar.
- To draw a single bond, select the “SOLID BOND” tool and attached to the sulfonyl group.
- Choose the methyl group from the tool bar and connect to
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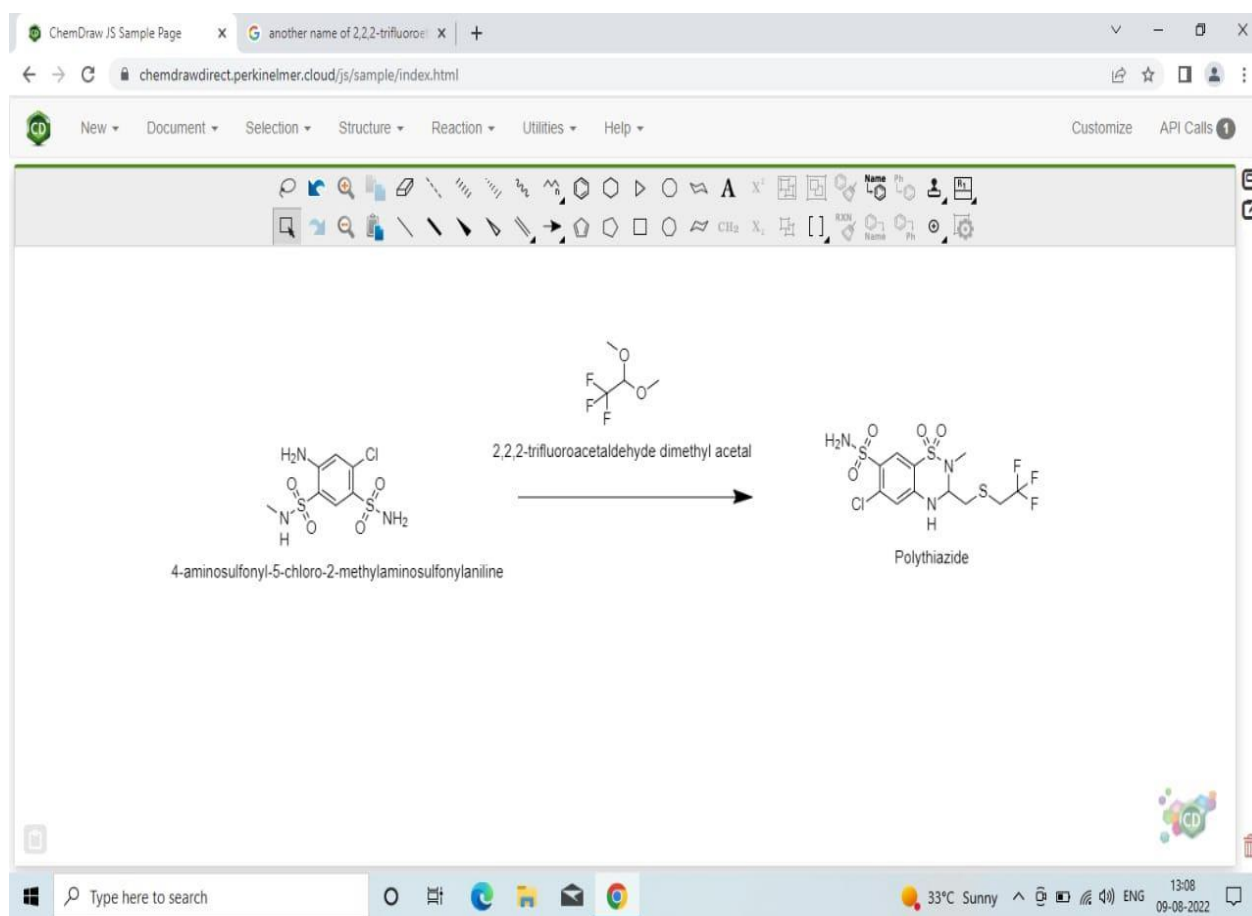
- at 2nd position.
- Place the chloromethyl group with the help of FUNCTIONAL GROUP tool bar and to make stick to the 3rd position.
- Select the N atom and attached to the 4th position and enclose the ring with the use of “SINGLE SOILD BOND”
- Place the Cl atom by using the TEXT BAR at 6th position.
- By the use of FUNCTIONAL GROUP tool bar, select the SULFONAMIDE group and attached at 7th position of Methyclothiazide.
- Complete the structure of Methyclothiazide



POLYTHIAZIDE

- i. Choose the benzene from the "MAIN TOOLBAR" on the left.
- ii. Similarly choose the "SOLID BOND" tool and add on to the benzene at 1st position to complete the structure of POLYTHIAZIDE.
- iii. To introduce sulphonyl group into a given structure, using "TEMPLATES" from the main toolbar.
- iv. To draw a single bond, select the "SOLID BOND" tool and attached to the sulfonyl group.
- v. Choose the methyl group from the tool bar and connect to at 2nd position.
- xiii.

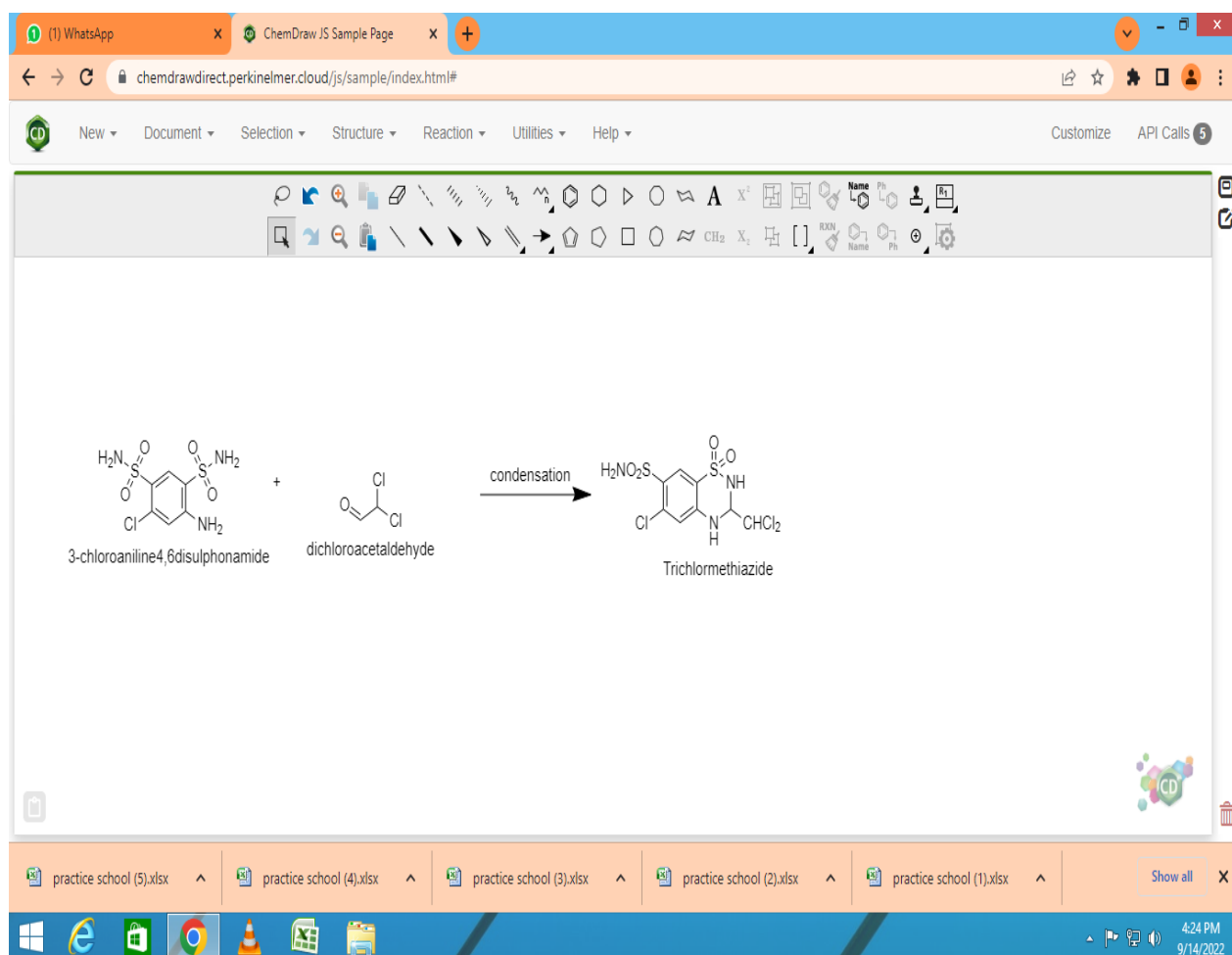
- vi. Select the single bond from the TOOL BAR, paste it at 3rd position of Polythiazide and add one more bond on it.
- vii. Place the S atom to that of the bond from the help of TEXT BOX "A".
- viii. Again create the double bond with S atom. To that Trifluoromethyl group is attached to that of the bond.
- ix. Select the N atom and attached to the 4th position and enclose the ring with the use of "SINGLE SOILD BOND"
- x. Place the Cl atom by using the TEXT BAR at 6th position.
- xi. By the use of FUNCTIONAL GROUP tool bar, select the SULFONAMIDE group and attached at 7th position of Polythiazide.
- xii. Complete the structure of Polythiazide.



TRICHLORMETHIAZIDE

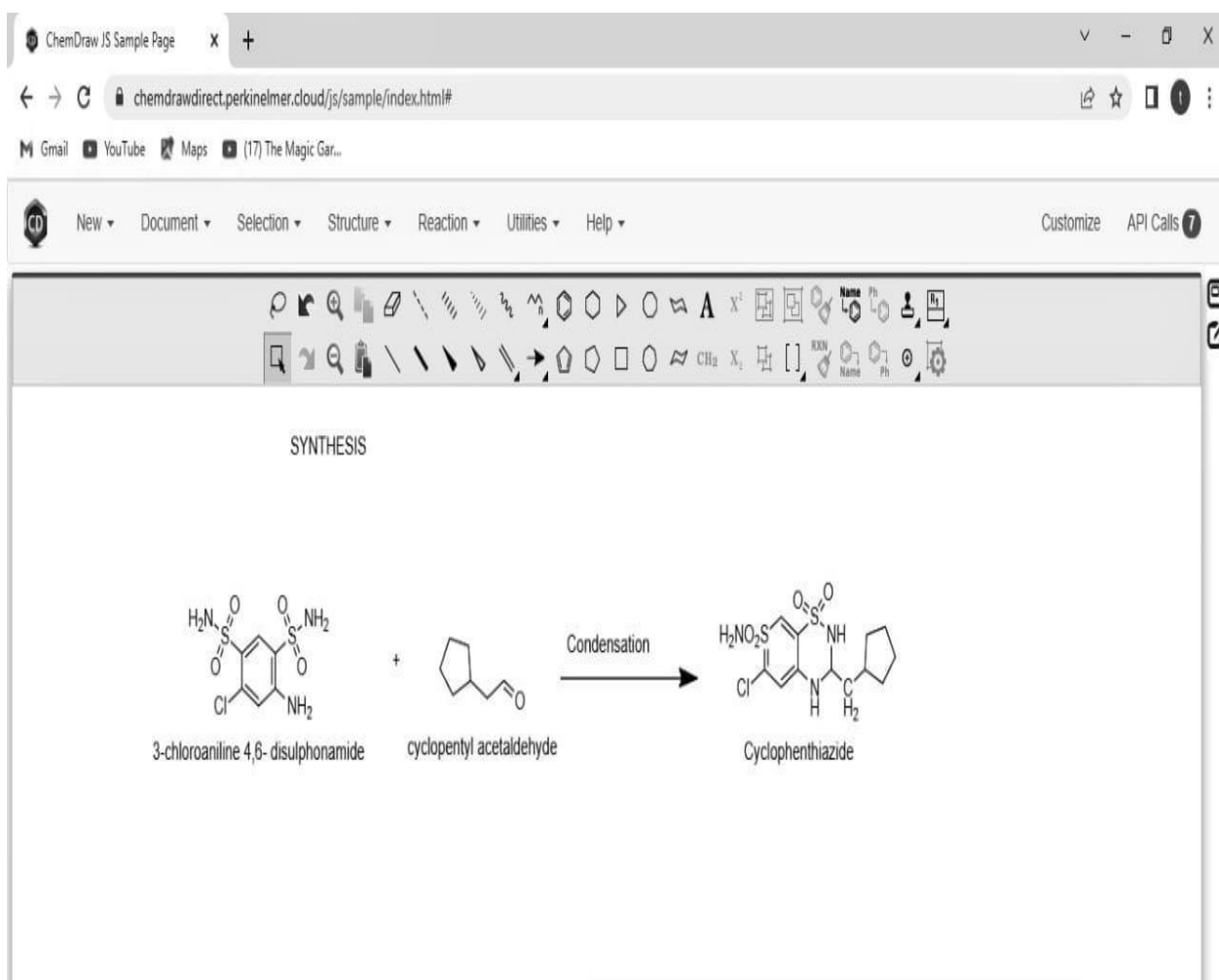
- Choose the benzene from the “MAIN TOOLBAR” on the left.
- Similarly choose the “SOLID BOND” tool and add on to the benzene at 1st position to complete the structure of TRICHLORMETHIAZIDE.
- To introduce sulphonyl group into a given structure, using “TEMPLATES” from the main toolbar.
- To draw a single bond, select the “SOLID BOND” tool and attached to the sulfonyl group.
-

- Place the NH group at 2nd position with the use of text box “A”
- Select Dichloromethyl group from the Functional group toolbar and add on to at 3rd position.
- Select the N atom and attached to the 4th position and enclose the ring with the use of “SINGLE SOILD BOND”
- Place the Cl atom by using the TEXT BAR at 6th position.
- By the use of FUNCTIONAL GROUP tool bar, select the SULFONAMIDE group and attached at 7th position of Trichlormethiazide.
- Complete the structure of Trichlormethiazide.



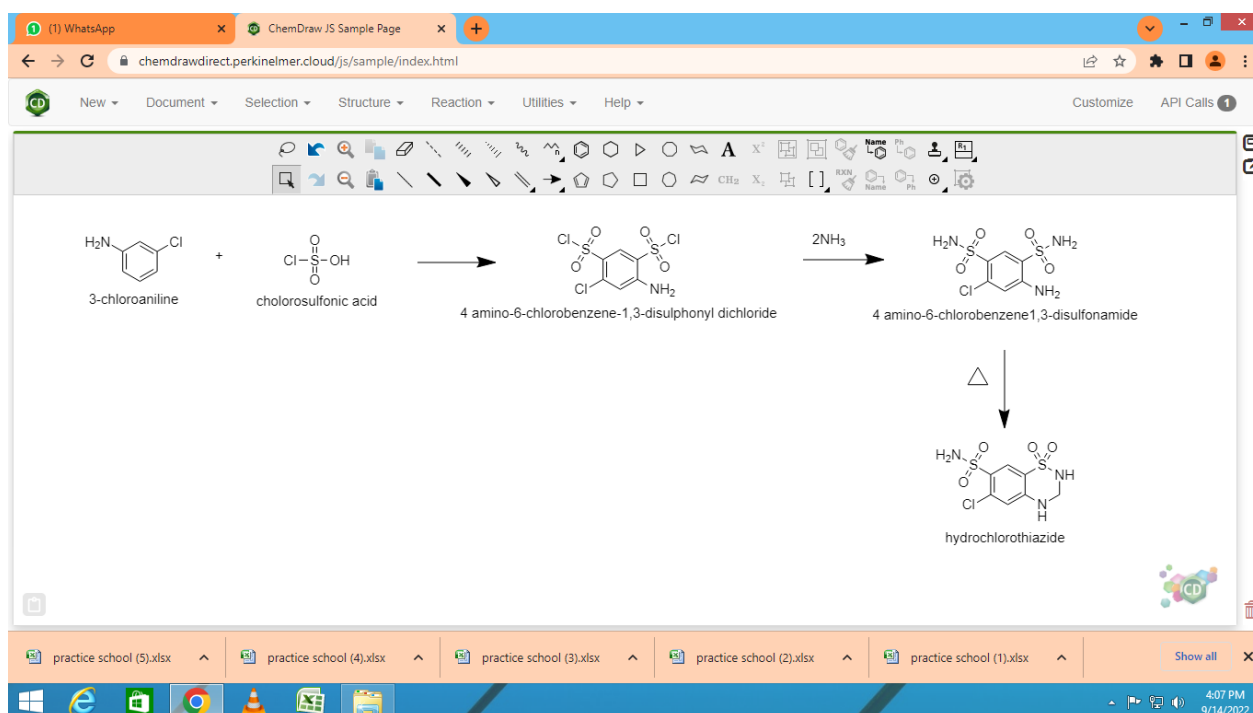
CYCLOPENTHAZIDE

- i. Choose the benzene from the "MAIN TOOLBAR" on the left.
- ii. Similarly choose the "SOLID BOND" tool and add on to the benzene at 1st position to complete the structure of CYCLOPENTHAZIDE.
- iii. To introduce sulphonyl group into a given structure, using "TEMPLATES" from the main toolbar.
- iv. To draw a single bond, select the "SOLID BOND" tool and attached to the sulfonyl group.
- xi. .
- v. Place the NH group at 2nd position with the use of text box "A"
- vi. Choose the Cyclopentyl methyl ring from the MAIN TOOL BAR and attached to the 3rd position.
- vii. Select the N atom and attached to the 4th position and enclose the ring with the use of "SINGLE SOILD BOND"
- viii. Place the Cl atom by using the TEXT BAR at 6th position.
- ix. By the use of FUNCTIONAL GROUP tool bar, select the SULFONAMIDE group and attached at 7th position of Cyclopenthiiazide.
- x. Complete the structure of Cyclopenthiiazide



HYDROCHLORTHIAZIDE

- Choose the benzene from the “MAIN TOOLBAR” on the left.
- Similarly choose the “SOLID BOND” tool and add on to the benzene at 1st position to complete the structure of HYDROCHLORTHIAZIDE.
- To introduce sulphonyl group into a given structure, using “TEMPLATES” from the main toolbar.
- To draw a single bond, select the “SOLID BOND” tool and attached to the sulfonyl group.
- Place the NH group at 2nd position with the use of text box “A”
- Choose the “FUNCTIONAL GROUP” tool bar and select the propene bond and attached to the 2nd position.
- Select the N atom and attached to the 4th position and enclose the ring with the use of “SINGLE SOILD BOND”. Hydrogen atom is bonded to that of Nitrogen atom.
- Place the Cl atom by using the TEXT BAR at 6th position of HydroChlorthiazide.
- By the use of FUNCTIONAL GROUP tool bar, select the SULFONAMIDE group and attached at 7th position of HydroChlorthiazide.
- Complete the structure of HydroChlorthiazide.



REPORT

Drawing of chemical synthesis of “DIURETICS” was finalized by using “CHEMDRAW” software.

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