KARPAGAM ACADEMY OF HIGHER EDUCATION
(Deemed to be University)
(Established Under Section 3 of UGC Act 1956)
Coimbatore – 641 021.
(For the candidates admitted from 2017 onwards)

DEPARTMENT OF CHEMISTRY

SUBJECT NAME: CHEMINFORMATICS-PRACTICAL SUBJECT CODE: 17CHU511A
SEMESTER: V CLASS: III B.Sc CHEMISTRY

Programme objectives
The course helps the student to
1. Understand and apply the applications of chemiinformatics in drug design.

Programme objectives
The course enable the student to
1. Apply the applications of chemiinformatics in drug design.

Hands-on Exercises
Application of Chemoinformatics in Drug Design

Suggested Readings

Text Books:

1. Andrew R. Leach & Valerie, J. Gillet. (2007). *An introduction to Chemoinformatics.* Springer: The Netherlands.
1. Gasteiger, J. & Engel, T. (2003).*Chemoinformatics: A text-book.* Wiley-VCH.

Reference Book

1. Gupta, S. P. (2011). *QSAR & Molecular Modeling.* New Delhi: Anamaya Pub.

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LECTURE PLAN

Total no. of hours: 48

S.NO	LECTURE DURATION	TOPICS TO BE COVERED	SUPPORT MATERIALS
1.	3	Procedure writing	W
2.	3	Drawing Chemical structure using chemdraw	W
3.	3	Elemental Analysis, Molecular weight & m/z values	W
4.	3	Predict the ^{1}H-NMR using chemdraw	W
5.	3	Predict the C^{13}-NMR using chemdraw	W
6.	3	Determination of chemical properties, melting point and boiling point etc	W
7.	3	Convert name into structure and vice versa	W
8.	3	Find the structure using protein bank	
9.	3	Molecular docking	
10.	3	Viva-voce	
11.	3	Model examination	
12.	3	Model examination	

W: www.kj-gibbs.uio.no/kjemi/manuals/chemBioDraw10-E.pdf

Experiment.1

Draw the chemical structure using Chemdraw

Aim

To learn how to draw the chemical structure of the organic compounds using Chemdraw Ultra 8.0 software

Tutorial on the Use of ChemDraw.

On the laptop, double click on the Macintosh HD icon. Double click on the Applications folder and look for the CS ChemOffice 2004 folder. Double click on the CS ChemDraw Pro icon. (Alternatively, if the ChemDraw icon is present in the dock, you may simply select that.)

To insert structures or reactions into another document such as Word, select the structuresor reactions as described below, then copy and paste into the document.

On the left is a tool palette. This is where you choose various tools for drawing structures.

Select the single bond tool (straight line) and click in the main window. A bond will be drawn. This is actually a line representation of Ethane, CH3-CH3. Click on one end of the bond. A second bond forms. This would be propane, CH3-CH2-CH3. Next click on the end of a bond and instead of letting the mouse button go, drag the mouse around. This will add another carbon but it allows you to place it at a different angle. Letting it add the carbon by itself produces a "normal-looking" structure.

Select the six-membered ring (cyclohexane) and click in the main window. A cyclohexane line drawing is produced. You can select the single bond tool and connect a CH3 to one of the carbons of cyclohexane to make methylcyclohexane.

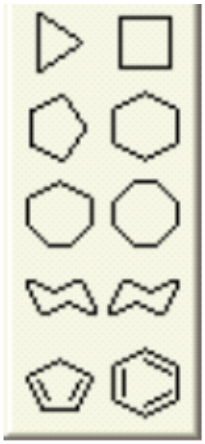
Selecting and moving objects. Select the lasso or marquee tool and click on a molecule. One click selects an atom or bond and double clicking selects the entire molecule. Several molecules and objects may be selected by surrounding the objects with one of the selection tools. The selection may be moved around by dragging it with the mouse.

To make a double bond, you can select the bond you would like to convert to a double bond, and by clicking on it with the single bond tool, it will change it into a double bond. If you would like to hange it back to a single bond, you may use the eraser tool to do so. Just select the eraser tool and click on the atom or bond that you wish to erase.

To add a functional group, for example, OH, select the text tool and click on the atom that you want to change to that group. Type in OH and an alcohol will be drawn.

Result:

We learned the draw the chemical structure of the Ethane, Propane, Cyclohexane, Methyl cyclohexane Butane, Benzene, Naphthalene, Anthracene and methane structures.

Cyclopropane		*Cyclobutane*
Cyclopentane		*Cyclohexane*
Cycloheptane		*Cyclooctane*
Cyclohexane Chair (1)		*Cyclohexane Chair (2)*
Cyclopentadiene		*Benzene*

Experiment: 2

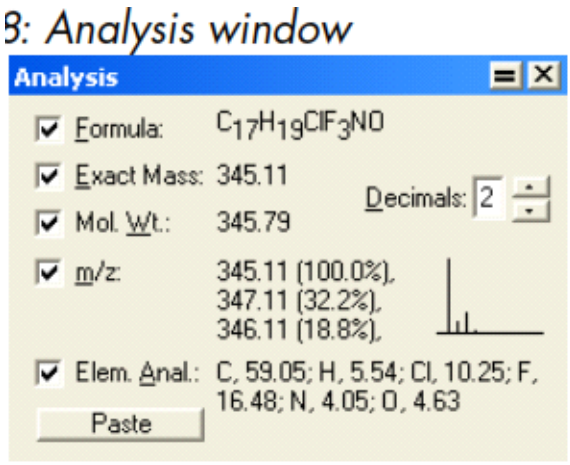
ELEMENTAL ANALYSIS, MOLECULAR WEIGHT, AND m/z VALUES

Aim

To learn how to analysis the chemical structure of the organic compounds using Chemdraw Ultra 8.0 software

The Analysis window displays the chemical formula, exact mass, molecular weight, m/z, and elemental analysis for the entire document, a structure, part of a structure, or a caption in Formula style. To view analysis information, click the ShowAnalysis Window command on the View menu. The Analysis window appears.

Figure : Analysis window



Values for selected objects in the document window are shown. If no structure is selected in your document, values for the entire document are shown. You can have this window open as you draw in the document. It shows the current values as you draw. The Decimals setting applies to Exact Mass,
Molecular Weight, and m/z only.

Property Description
Formula: The molecular formula showing the exact number of atoms of each element in the molecule and charges, radicals, and isotopes.
Exact Mass: The exact molecular mass of the structure, where atomic masses of each atom are based on the most common isotope for the element.
Molecular Weight: The average molecular mass of the structure, where atomic masses are based on the natural abundance of all isotopes of the element.
Property Description
m/z Mass/charge, where charge =1. The weights of the most common isotopes and a graphical representation of the isotopic abundance is shown. The molecular weight shown takes the isotopes for each atom and their natural abundance into account. Where there is more than one abundant isotope,
ChemDraw computes multiple molecular weights.Low abundance combinations (whether because the isotope is in low abundance or because it includes
Many moderate-abundance contributions) are not taken into account. You cannot paste the graph in adocument.

Elemental Analysis: The percent by weight of each element in the structure.

To paste information about a structure as a caption:
1. Click the check boxes for the information that you want to paste.
2. Click Paste.
The information appears as a multiline caption below the structure. You can edit this information with the text tool.

Result:

We learned the elemental analysis, molecular weight, and m/z values of the organic compounds using Chemdraw Ultra 8.0 software

Experiment: 3

PREDICT THE ^{1}H - NMR STRUCTURE OF CHEMICAL COMPOUND USING CHEMDRAW

Aim

To learn how to predict the 1H - NMR structure of the organic compounds using Chemdraw Ultra 8.0 software

ChemNMR (Ultra Feature)

Using ChemNMR, you can estimate and display proton and Carbon-13 chemical shifts for a selected molecule.As with ChemBioDraw, you can also use ChemBio3D to predict NMR. ChemBio3D includes several interfaces tocomputational chemistry packages which predict NMR. Some packages predict IR spectra and other spectra as well.For more information on ChemBio3D packages, which have NMR predictions, and their available parameters, see the Chem& Bio 3D User Guide.

Setting Parameters Values in ChemNMR

Use the ChemNMR option in Preferences dialog to set the parameter values in ChemNMR. See the example below:

Solvent

The solvent is not user-definable in ChemNMR, except by adding new custom shift correction data. Most spectra in

the default ChemNMR database are run in deuterated chloroform, but the database is intended to be solvent-free. In

ChemBioDraw, you can set either deuterated chloroform, or deuterated dimethyl sulfoxide as solvent from the Preferences

dialog. Spectral shifts which depend on the solvent are generally indicated as "rough" predictions.

Spectrometer Frequency

ChemNMR' s default for estimating proton NMR is a spectrometer frequency of 300 MHz. To change the default frequency,

either set the new frequency using the Preferences dialog, or hold the <Alt> key while selecting Predict 1HNMR

Shifts, and enter a frequency in MHz and run the spectrum. The new frequency will apply until you reset it,

including after closing ChemBioDraw. The spectrometer frequency parameter only applies to proton NMR.

Result:

We learned the predict the 1H - NMR structure of the organic compounds using Chemdraw Ultra 8.0 software

Experiment: 4

PREDICT THE C^{13} – NMR STRUCTRUE USING CHEMDRAW

Aim

To learn how to predict the C^{13} – NMRstructure of the organic compounds using Chemdraw Ultra 8.0 software

NMR Shifts

ChemNMR estimates chemical shifts for all hydrogen or carbon atoms for which additivity rules are available. Followinga hierarchical list, it first identifies key substructures of a molecule. A substructure provides the base value forthe estimated shift. For example, benzene would be the key substructure of trinitrotoluene.When a substructure is a ring system not available in the data, ChemNMR approximates its base shift using embeddedrings and, if necessary, will disassemble the ring into acyclic substructures.

ChemNMR views remaining parts of the molecule as substituents of a substructure. Each substituent adds to, or subtractsfrom, the base shift of the substructure to which it is attached. Additivity rules determine the increment of eachcontribution. If an increment for a substituent cannot be determined, ChemNMR uses embedded substituents—smallerstructural units with the same neighboring atoms. Or, it will use increments of identical, or embedded substituents,of a corresponding substructure by assuming that the effects of the substituents are of the same magnitude.

ChemNMR provides a detailed protocol of the estimation process applied. It gives substructures as names, compoundclasses in most cases, substituents in the form of a linear code, respectively.

It also implements models for ethylenes (cis/trans) and cyclohexanes (equatorial/axial)

To view ^{1}H or ^{13}C NMR information:

1. Select a structure.
2. Navigate to **Structure**>**Predict 1H-NMR Shifts** or **Predict 13C-NMR Shifts**.

ChemNMR redraws the molecule with the estimated shifts and displays the information and line spectrum in a newwindow.

Modifying NMR Frequency

You can change the default NMR frequency of 300 Mhz in ChemDraw Proton NMR predictions.

To change the frequency:

Result:

We learned the predict the C^{13} – NMRstructure of the organic compounds using Chemdraw Ultra 8.0 software

Experiment: 5

DETERMIANATION OF CHEMICAL PROPERTIES OF THE ORGANIC COMPOUNDS

Aim

To learn how to analysis the chemical properties of the organic compounds using Chemdraw Ultra 8.0 software

Viewing the Chemical PropertiesWindow

To view predicted properties for a selected structure:

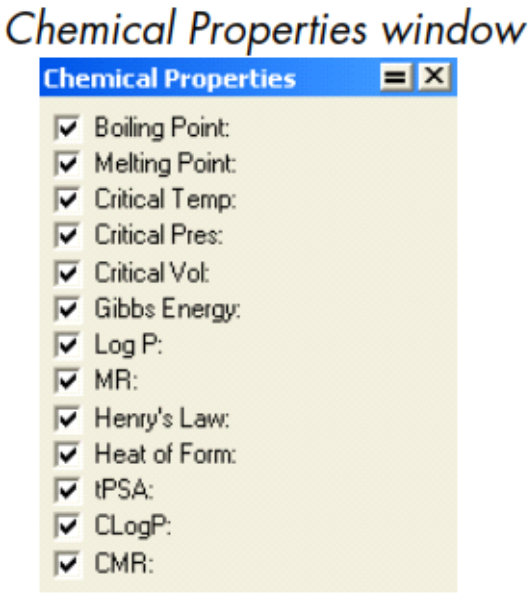
1. Select the structure to analyze.
2. Click

the Show Chemical Properties Window

command on the View menu.

The Chemical Properties window appears.

Figure Chemical properties window



The following basic values are displayed.

Property Description

Boiling Point: The boiling point for thestructure. Reported in Kelvin at 1 atm.

Melting Point: The melting point for thestructure. Reported in Kelvinat 1 atm.

Critical Temperature: The temperature above whichthe gas form of the structurecannot be liquefied, no matterthe applied pressure (T).Reported in Kelvin.

Critical Pressure: The minimum pressure thatmust be applied to liquefy thestructure at the criticaltemperature (Pc). Reported inbars.

Critical Volume: The volume occupied at thecompound's critical temperatureandpressure (Vc). Reportedin cm^3/mol.

Gibbs Energy: The Gibbs free energy, ΔG,for the structure. Reported inkJ/mol at 1 atm and 298.15K.

Henry's Law: The inverse of the logarithmof Henry's law constant[-log (H)] (no units).

Result:

We learned the chemical properties ofthe organic compounds using Chemdraw Ultra 8.0 software

Experiment: 6

DETERMINATION OF MELTING POINT AND BOILING POINT OF COMPOUNDS

AIM:

To determine the melting point and boiling point of chemical compounds using chemdraw.

Chemical Properties:

ChemDraw Pro and Ultra, using an add-on, ChemProp, calculate predicted values for the physical and thermodynamic properties of a selected structure of up to 100 atoms. You can view the values in the Chemical Properties window. The properties are calculated using the most reliable methods for calculation for the given structure. Log P and MR values based on literature values rather than a calculation are included in the report file. Viewing the Chemical Prop- erties Window

To view predicted properties for a selected struc- ture: 1. Select the structure to analyze. 2. Click the Show Chemical Properties Window command on the View menu. The Chemical Properties window appears. Figure 6 - 9: Chemical properties window

To paste the basic properties into your document: • Click Paste. To create a report and view results for other fragmentation methods including the Broto, Crippen, Viswanadhan, Joback, and Joback/Stein methods: • Click Report.

Property Description

Boiling Point The boiling point for the structure. Reported in Kelvin at 1 atm.

Melting Point The melting point for the structure. Reported in Kelvin at 1 atm.

Critical Temperature

The temperature above which the gas form of the structure cannot be liquefied, no matter the applied pressure (Tc). Reported in Kelvin.

Critical Pressure The minimum pressure that must be applied to liquefy the structure at the critical temperature (Pc). Reported in bars.

Critical Volume The volume occupied at the compound's critical tempera- ture and pressure (Vc). Reported in cm3/mol.

Gibbs Energy The Gibbs free energy, ΔG, for the structure. Reported in kJ/mol at 1 atm and 298.15K.

Henry's Law The inverse of the logarithm of Henry's law constant [-log (H)] (no units).

Heat of Forma- tionThe heat of formation, ΔHf, for the structure. Reported in kJ/mol at 1 atm and 298.15K.tPSA Calculation of polar surface area based on fragment contributions.CLogP The calculated n-octanol/water partition coefficient (log Pow).CMR The calculated Molar Refrac- tivity

RESULT:

We learned about the melting point and boiling point of the organic compound using chem draw.

Experiment: 7

CONVERT STRUCTUREINTO NAMEOF THE ORGANIC COMPOUND USING CHEMDRAW

AIM:

To learn to draw the structure into name of the organic compound using chemdraw

Struct=Name (Ultra Feature)

ChemBioDraw includes two features for generating structures and chemical names—*Name>Struct*and *Struct>Name*. Collectively, these features are called *Struct=Name*.

Struct>Name generates the names of chemical structures using the Cahn-Ingold-Prelog rules for stereochemistry.

Using this option, you can generate the name of structures you have drawn.

Name>Struct lets you convert chemical names into their corresponding chemical structures. It is designed to interpret

chemical names as they are used by chemists. In other words, it recognizes the shorthand and slang of everyday usage, in addition to recognizing most of the official IUPAC, IUBMB, and CAS rules and recommendations.

Struct>Name

Struct>Name can interpret a variety of chemical structures. This means that you can draw a structure and Struct>Name will provide its name. It also updates the name when you modify the structure.

Using Struct>Name

To generate the name of your structure:

1. Select the structure.
2. Navigate to **Structure**>**Convert Structure to Name**. The name appears under the structure.

Supported Structures

However, Struct>Name will interpret:

RESULT:

We learned how to convert the structure into name of the chemical compounds using chem draw.

Experiment: 8

CONVERT THE NAME OF THE COMPOUND TO CHEMICAL STRUCTURE USING CHEMDRAW

AIM

To learn to draw the name into strucure of the organic compound using chemdraw.

Name=Struct

You can draw a structure automatically from a chemical name using Name=Struct. Name=Struct recognizes most organic nomenclature. Inorganic chemistry is also usually recognized, especially when the rules closely match those for organic chemistry.

The following are not supported:

- Coordination complexes
- Polyborane
- Polymers

- Some highly-bridged ring systems, including fullerenes and porphyrins/porphines
- Some stereochemistry designators: +, -, +/-, +-, D, L, DL, endo, exo, syn, anti, r, t, c

Although some trade names are supported, Name=Struct is not intended to interpret trade or common names. A chemical database, such as chemfinder.com, is more appropriate for obtaining structures for trade or common names. See “Finding Information on ChemFinder.com” on page 258 for more information.

NOTE: Because the syntax of German is very similar to that of English, Name=Struct can also interpret many German names. Chemical names in other languages, however, will generally not be recognized.

Converting Names to Struc- tures

There are two ways to insert a name into the document window as a structure:

- Insert Structure dialog box
- Paste Special command

Insert Structure

Insert Structure is designed for typed-in entries. For example, to insert 2-bromobenzoic acid:

1. Choose Convert Name to Structure from the Structure menu.

The Insert Structure dialog box appears.

2. Type 2-bromobenzoic acid.

NOTE: You can also copy a name to the clipboard and type Crtl+V or Command+V to paste the name into the dialog box.

3. Click OK. The molecular structure and name (if “Paste name below structure” is selected) appear in the drawing area. If you should happen to type the name incorrectly, Insert Structure will try to correct the error.

Click OK to accept the suggested spelling, or click Cancel and start again to make a manual correction.

Paste Special The Paste Special command allows you to paste a name, copied to the clipboard from another application, as a structure in ChemDraw. To paste a name from the clipboard: 1. Click in the document window.

2-bromobenzoic acid

130•Struct<=>Name CambridgeSoft Name=Struct

Administrator

2. Point to Paste Special on the Edit menu, and choose Name as Structure. The structure appears in your document. Converting Captions to Structures

If a caption is already present in the drawing area you can convert it to a structure as follows: 1. Select the caption.

Figure 7 - 6: Selecting a caption

2. Choose Convert Name to Structure from the Structure menu. The molecular structure and name appear in the drawing area. Types of Structures Supported by Struct=Name Struct=Name can name compounds in the following classes of structures:

RESULT:

We learned how to convert the name into structure of the chemical compounds using chem draw.

Experiment: 9

MOLECULAR DOCKING STUDIES

Aim.

To learn how to perform molecular docking of the organic compounds using Chemdraw.

Docking and Floating

You can dock or float any standard toolbar. When you dock a toolbar, it becomes attached to the drawing window. Thefloating toolbars appear in front of the document window and you can move them around in the drawing window.Double-clicking the toolbar restores it to the last, or default, or docked position.

To dock a toolbar, do one of the following:

Click and drag the toolbar to any edge outside the drawing window.

Right-click the toolbar and select **Dock Toolbar**.To float a toolbar, do one of the following:

Double-click the docked toolbar.Click and drag the docked toolbar into the drawing window.

Right-click the toolbar and select **Float Toolbar**.

Docking and UndockingToolbars

The standard toolbars, can be docked or undocked.Docked toolbars can attach to any edge of the

ChemDraw window. Undocked toolbars can floatanywhere on your monitor screen.

To dock a toolbar:

• Drag the toolbar to the edge of the ChemDraw screen where you want it to dock.

• Double-click the toolbar background. This will dock the toolbar in the default position. (Alltoolbars default to the top of the ChemDrawwindow, except for the Tools toolbar whichdefaults to the left side.)

To undock a toolbar do one of the following:

• Drag the toolbar into the position you want.

• Double-click the toolbar.

Result:

We learnedabout the molecular docking of the organic compounds using Chemdraw.