Government Degree College Shadnagar

Rangareddy district-509216
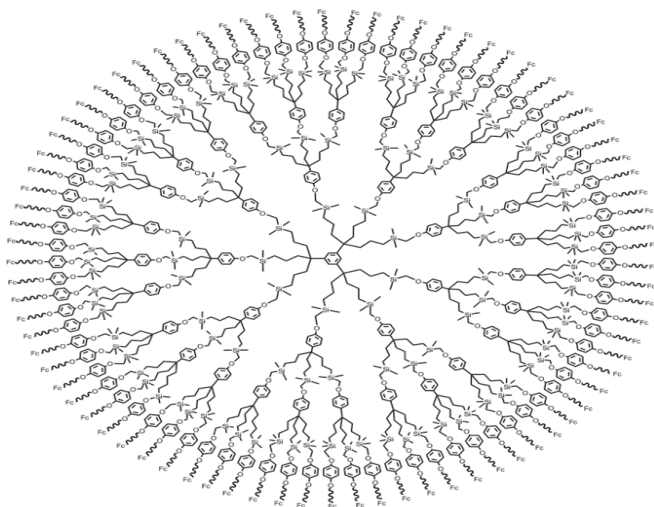
(Affiliated to Palamuru University)

CERTIFICATE COURSE

On

CHEMDRAW

ACADEMIC YEAR 2021-22(FROM 3-11-2022 TO 30-11-2022)

DEPARTMENT OF CHEMISTRY

Number of participants: 22

Number of hours: 30   **Time :4:00 p.m**.

Government Degree College Shadnagar
Rangareddy district, Telangana
Department of chemistry

<u>Circular</u>

Date: 28-10-2022

All the students, teaching staff are hereby informed that the chemistry department would like toconduct **"A CERTIFICATE COURSE IN CHEMDRAW" for a period of 30 hours for the academic year 2021-22**. classes will conduct on zero hours that is from 4.00 pm-5.00 pm. Interested Students are asked to give their names to M.Srilatha Asst.prof of chemistry on or before 03-11-2022.

PRINCIPAL
Govt. Degree College
Shadnagar.
Ranga Reddy Dist.

Principal

Department of Chemistry

Description:

Chemical structure drawing program i.e., ChemDraw is used to draw and manipulate different organic chemistry structures. Programs like these are used to draw chemical structures included in your text books. How to draw chemical structures, as well as doing various manipulations on them, is a technique that all the students must learn.

Therefore, this course is designed to illustrate fundamental drawing techniques. Each tutorial introduces new techniques. So, we request sincerely all the students must participate fully in these tutorials and do exercises because you will be working independently later on doing similar exercises.

Objectives:

As a result of successful completion of the workshop, participants will be able to:

1. Draw bonds, bond order and bond types
2. Assigning atomic/group labels to molecules
3. Drawing rings, modifying, rotating them and duplicating
4. Assigning chemical properties to the structures
5. Drawing Fischer and Newman projections of molecules
6. Assigning stereochemical indicators.
7. Assigning colours to the structures.

Curriculum Design:

- The total workload of this certificate course will be 6 hours (1 hour/day).
- It contains a total of 6 modules (one module each day), followed by doubts clarifying session.

Assessment and Evaluation:

- Participants are evaluated through the practical examination at the end of the course.
- Certificates are issued based on the performance.

Teaching Pedagogy:

- ☑ The entire course, as it is said in the title of the course, will be taught entirely through online mode.

☑ Doubts sessions and hands on experience sessions will also be conducted through online mode.

☑ Reading materials will be provided to practice at home.

Course Index

- -

Module 1:

☑ How to create a bond?

☑ How to change bond order (double/triple bond/fraction of bonds)?

☑ How to add atom labels?

☑ How to draw a ring?

☑ How to increase the size of the rings?

☑ How to duplicate the structure?

Module 2:

☑ How to add a bond between the duplicated structures?

☑ How to rotate a ring/structure?

☑ How to add captions to the structure?

☑ How to view the basic properties of the structure and paste the information into the document?

☑ How to draw Newman Projection Formula?

☑ How to assign stereochemical indicators?

Module 3:

➔ Tutorial 1: How to draw acetone structure?

➔ Tutorial 2: How to draw fused rings?

Module 4:

➔ Tutorial 3: How to create Fischer Projection formula of glucose?

➔ Tutorial 4: How to create a perspective drawing of α – D – Glucose?

Module 5:

Appendix:

 List of Hot Keys

Module 1

Topic 1:   How to create a bond?

- Navigate to View>Show Main Toolbar.
- On the Main toolbar, select the Solid Bond tool.
- Click in the document window. A bond appears.
- To add a second bond, click the right-end of the bond you just created. The two bonds form a 120-degree angle.
- To create a tertiary carbon, click the same place, as shown in step 4 above.

Topic 2:   How to change bond order (double/triple bond/fraction of bonds)?

To create the double bond, either hover over the centre of the bond and type "2" or click on the bond.

Topic 3:   How to add atom labels?

1. Using the Text tool, click the end of the double-bond. A text box appears at the end of the bond.
2. Type an uppercase O in the text box.
3. Press the <Esc> key on your keyboard to close the text box, or choosing another tool.
4. An alternative is hover over the atom at the end of the double bond and hit the "o" key. This is utilizing the Hotkey functionality of ChemDraw.

Topic 4:   How to draw a ring?

1. Click the **Ring tools**.

2. Click in an empty area of a document window. A cyclohexane ring appears.

Topic 5:   How to increase the size of the rings?

1. Go to **Edit>Select All** (or type CTRL+A).

2. Click-drag the ring corner adjustment handle to increase the size of the ring to 150%.

Topic 6:   How to duplicate the structure?

1. Click a selection tool. The last structure you drew is selected.

2. To create a duplicate, hold down the **CTRL key** while dragging the selection rectangle upward to the right of the original. The selection box disappears while you are dragging.

Module 2

1. Click the Solid Bond tool.

2. Click and drag from the tertiary carbon atom of the lower fragment to the other tertiary carbon.

Topic 8:   How to rotate a ring/structure?

1. Go to Edit>Select All (or type CTRL+A).

2. Go to Object>Rotate (or type CTRL+R)

3. In the Rotate Objects dialog box, enter 30 degrees for an angle and click Rotate. The cyclohexane ring rotates.

Topic 9:   How to add captions to the structure?

1. Using the Text tool, click below and to the left of the structure. A text box appears.

2. In the text box, type "2-propanone".

3. Press the <Esc> key on your keyboard to close the text box, or choose another tool.

Topic 10: How to view the basic properties of the structure and paste the information into the document?

1. Click a selection tool to select the last structure drawn. If the structure is not selected, double-click the structure.

2. Go to View>Show Analysis Window.

3. In the Analysis window, click Paste. The analysis information appears as a caption below the structure.

Topic 11: How to draw Newman Projection Formula?

1. Click the Orbital tool, and select the s (Open) orbital.
2. Point to the left centre carbon and click-drag outward.
3. Click the Marquee tool. The orbital is selected. Click an empty space to deselect it.
4. Point above the structure and drag around the upper fragment to select the three bonds. Do not select the bond connecting the two fragments.

Topic 12: How to assign stereochemical indicators?

1. Select the entire structure with the Lasso or Marquee tool.
2. Go to Object>Show Stereochemistry. The S marker appears.
3. Select the structure and go to Object>Flip Horizontal. The R marker appears.
4. With the structure selected, go to Object>Rotate 180° Vertical. You can also use the object toolbar to rotate the structure.
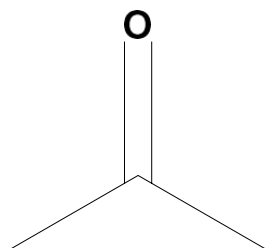
The Wedged bond becomes hashed and the (R) stereochemistry is preserved.

Module 3

Tutorial 1:

Drawing a Structure

In this tutorial, we explain how to draw this structure:

O

Note: If you want the bond angles and lengths to be fixed, navigate to Object>Fixed Lengths and Fixed Angles. This ensures that bond lengths and bond angles are consistent throughout the structure.

To Create Bonds:

1. Navigate to View>Show Main Toolbar.

2. On the Main toolbar, select the Solid Bond tool.

3. Click in the document window. A bond appears.

4. To add a second bond, click the right-end of the bond you just created. The two bonds form a 120-degree angle.

5. To create a tertiary carbon, click the same place, as shown in step 4 above.

Changing Bond Order

To create the double bond, either hover over the centre of the bond and type "2" or click on the bond.

Adding Atom Labels

1. Using the Text tool, click the end of the double-bond. A text box appears at the end of the bond.

2. Type an uppercase O in the text box.

3. **Press the <Esc> key** on your keyboard to close the text box, or choosing another tool.

4. An alternative is hover **over the atom at the end of the double bond** and hit the **"o" key**. This is utilizing the Hotkey functionality of ChemDraw.

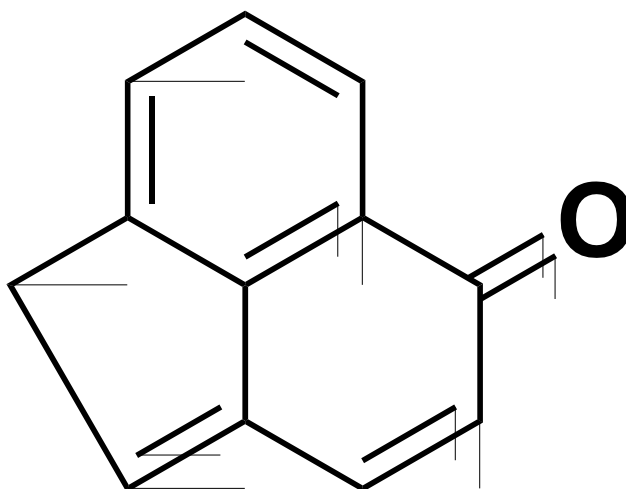## *Adding Captions:*

To name the molecule:

1. **Using the Text tool**, click below and to the left of the structure. A text box appears.

2. In the text box, **type "2-propanone".**

3. **Press the <Esc> key** on your keyboard to close the text box, or choose another tool.

The structure is complete

Tutorial 2:

Drawing rings

In this tutorial we use rings to create this structure:

To create the ring system:

1. Using the Benzene tool, click in an empty area of the document.

2. Point to the centre of the lower right bond in the benzene ring.

3. Click to fuse another ring.

4. In the final structure, there are two double bonds in the second ring. To correct the current structure, hover the mouse over one of the double bonds in the second ring and type '1'.

5. To create the double bond in the second ring, either hover the mouse over the bond and type '2' or click it.

6. Using the bond tool, click the carbon atoms. Three new bonds will appear.

7. Hover your mouse over one of the bonds and type '2'. Do the same for the other bond.

8. Hover the mouse over the right-most terminal carbon and type the letter 'o' to create the ketone functional group.

9. To connect the left terminal carbons, select the solid bond tool and click-drag a bond from one carbon to the other.

The structure is complete.

Module 4

Tutorial 3:

Fischer projections

This tutorial demonstrates how to create a Fischer projection of glucose:
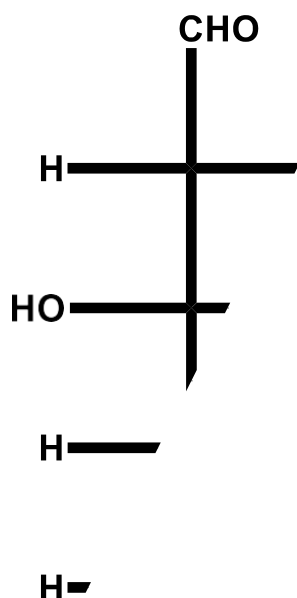
Chemical Formula: $C_6H_{12}O_6$
Exact Mass: 180.06
Molecular Weight: 180.16
m/z: 180.06 (100.0%), 181.07 (6.5%), 182.07 (1.2%)
Elemental Analysis: C, 40.00; H, 6.71; O, 53.28

To draw the first bond:

1. Click the Solid Bond tool.

2. Point in the document window. Drag downward to draw the first bond.

3. Point to the lower atom, and drag downward again to draw the second bond. The red wavy box appears because Show Chemical Warnings is selected. We will keep it selected for now.
4. Repeat step 3 there are five bonds.

Add horizontal bonds to the second atom in the string of bonds you created:

1. To add a horizontal bond, point to the uppermost Chemical Warning box and click it. Note that the red wavy box disappears when you add a bond.
2. Click again to add a horizontal bond in the opposite direction.
3. Repeat steps 1 and 2 with each Chemical Warning box until all horizontal bonds are added.

Add labels to the first and last carbon atoms:

1. Select the Text tool.
2. Click the uppermost carbon atom to create a text box, and type CHO.
3. Click the lower-most carbon atom, and type CH2OH.

Add the repeating labels for the hydrogens and hydroxyl groups:

1. Click the atom shown in *A* below and type the letter H.
2. Double-click each of the other atoms labelled as hydrogen.
3. Click one of the remaining atoms and type O.
4. Double-click the remaining atoms to repeat the label.

View the basic properties of the structure and paste the information into your document:

1. Click a selection tool to select the last structure drawn. If the structure is not selected, double-click the structure.

2. Go to View>Show Analysis Window.

3. In the Analysis window, click Paste. The analysis information appears as a caption below the structure.

The structure is complete.

Tutorial 4:

Perspective Drawings

In this tutorial, we explain how to create a perspective drawing by creating a model of a–D–glucose as a Haworth projection.

Create a new document using the default style:
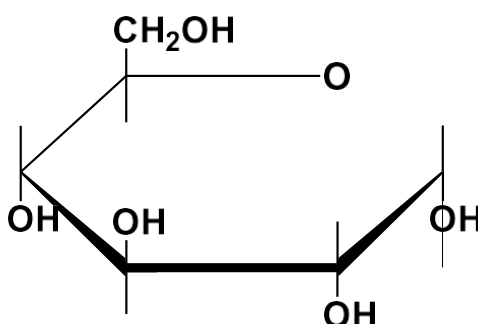
Go to File>Open Style Sheets>New Document.

Draw a ring:

1. Click the Cyclohexane Ring tool.

2. Click in an empty area of a document window. A cyclohexane ring appears.

Rotate the ring:

1. Go to Edit>Select All (or type CTRL+A).

2. Go to Object>Rotate (or type CTRL+R)

3. In the Rotate Objects dialog box, enter 30 degrees for an angle and click Rotate. The cyclohexane ring rotates.

Change cyclohexane to tetrahydropyran:

1. Click outside the structure to deselect it.

2. Point to the atom, and type the letter 'o'.

Resize horizontally:

1. Go to Edit>Select All (or type CTRL+A).

2. Using a selection tool, click-drag the right-side handle to horizontally resize the ring. Release the mouse button when the ring is stretched about 200%.

Enlarge the ring:

1. Go to Edit>Select All (or type CTRL+A).

2. Click-drag the ring corner adjustment handle to increase the size of the ring to 150%.

Add vertical bonds:

1. Click the Solid Bond tool.

2. Point to the atom shown in the figure below and drag upward to create a bond.

3. Point to the same atom, and drag downward to create another bond.

4. Repeat this procedure four more times, adding the pairs of vertical bonds shown below:

Create OH labels:

1. Select the Solid Bond tool, point to the atom shown in the figure below, and double-click to open a text box. Type OH.

2. Move the pointer to the other atoms as shown, and triple-click to repeat the atom label.

Add the CH2OH label:

1. Triple-click the upper atom of C5.

2. Press ENTER to open the atom label text box. Type CH2 before the OH.

Change the type of the front bonds:

1. Click the Bold Bond tool.

2. Click the bond to which we want to apply.

3. The cursor changes to a bold arrow as you point to the bond.

4. Click the Wedge bond tool.

5. Click each ring bond adjacent to the bold bond.

The structure is complete.

Module 5

Tutorial 5:

Newman projections

This tutorial demonstrates how to draw a Newman projection of ethane:
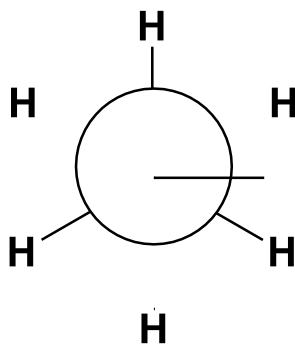
Draw ethane:

1. Click the Solid Bond tool.

2. In the document window, click-drag downward to create the first bond.

3. Click the atom at the bottom of the bond to add a second bond.

4. Click the bottom atom again to add a third bond.

5. Hover the mouse over the end of each bond (without clicking) and type **H** to add the hydrogen atoms.

Duplicate the structure:

1. Click a selection tool. The last structure you drew is selected.

2. To create a duplicate, hold down the CTRL key while dragging the selection rectangle upward to the right of the original. The selection box disappears while you are dragging.

Add a bond between the duplicated structures:

1. Click the Solid Bond tool.

2. Click and drag from the tertiary carbon atom of the lower fragment to the other tertiary carbon.

When you release the mouse button, the ethane structure is complete. Now, create its Newman projection.

Drawing the Newman projection

In this step, you draw the hollow circle that is particular to Newman projections.

1. Click the Orbital tool, and select the s (Open) orbital.

2. Point to the left centre carbon and click-drag outward.

3. Click the Marquee tool. The orbital is selected. Click an empty space to deselect it.

4. Point above the structure and drag around the upper fragment to select the three bonds. Do not select the bond connecting the two fragments.

Rotate the selection:

1. Double-click the rotation handle to open the Rotate Objects dialog box.

2. Type 180 in the Angle text box and click Rotate.

3. Go to Object>Bring to Front (there is no visible change when you do this).

Move the front part of the structure to create a Newman projection:

1. Point within the Selection Rectangle so the pointer changes to a hand.

2. Drag the selection until the tertiary carbon is centered within the orbital

3. Release the mouse button and click outside the Selection Rectangle to deselect the structure.

The structure is complete.

Tutorial 6:

Stereochemistry

This tutorial demonstrates stereochemistry markers and the Flip command.

2-amino-3-methylbutanoic acid
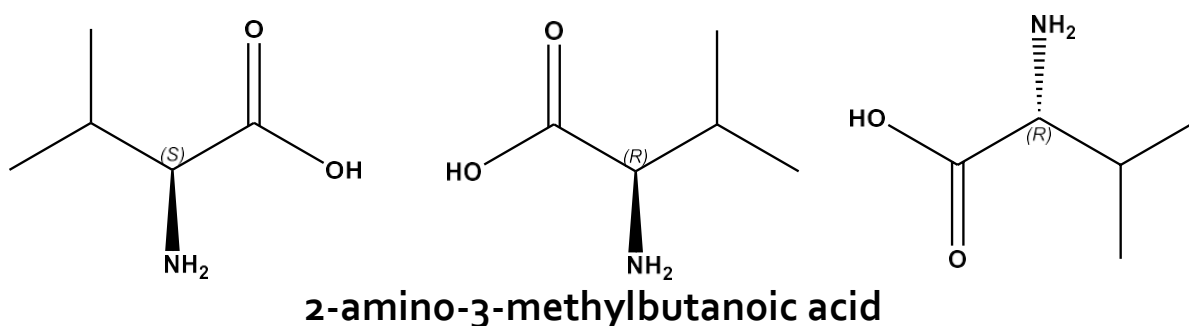
To draw the structure:

1. Click the Solid Bond tool.

2. In the document window, click and drag downward to create the first bond.

3. Point at the lower atom and click to add a second bond.

4. Continue pointing at the same atom and click again to add a third bond.

5. Point to the atom and click twice to create two bonds.

6. Pointing to the bond, right-click, and select Double>Plain from the context menu.

7. Click the Wedged Bond tool, point to the atom below, and then click.

Adding atom labels

1. With the Text tool selected, click the atom shown below, and then type 'NH2' in the text box that appears.

2. With the Text tool selected, click the atom shown below, and then type 'O' in the text box that appears.

3. With the Text tool selected, click the atom shown below, and then type 'OH' in the text box that appears.

Displaying stereochemical markers

We now display the stereochemical markers, (R) and (S) for the two isomers. To add the markers:

1. Select the entire structure with the Lasso or Marquee tool.

2. Go to Object>Show Stereochemistry. The S marker appears.

3. Select the structure and go to Object>Flip Horizontal. The R marker appears.

4. With the structure selected, go to Object>Rotate 180° Vertical. You can also use the object toolbar to rotate the structure.

The Wedged bond becomes hashed and the (R) stereochemistry is preserved.

The structure is complete.

APPENDIX

- -

Hot Keys

Atom Hotkey	o ; q	n ; w	s	Enter	Shift + s	l or Shift + c	c	b	Shift + b	Shift + a	p	Shift + p	m	e	x	d	h	f	r	i
		OH	NH₂	SH		SiH₃	Cl	CH₃	Br	BH₂	Ac	PH₂	Ph	Me	Et	X	D	H	F	R	

Atom Hotkey	0	1	2	3 ; a	4	5	6	7	8	9	z

Bond Hotkey	a	z	1	2	3	v	4	5	6	7	8	9	0

Bond Hotkey	w	h or Shift+w	b	Shift+b	y	Shift+h	d

Moving the hotspot:

Hover over an atom or a bond with your mouse to activate a hotspot. While the mouse cursor is not over an atom or bond, you can move it by pressing keyboard arrows. Pressing arrows will make move from atom to bond to atom to bond. By holding shift while you press the arrows you can move from atom to atom, or bond to bond.

Example   "2 n 1 3 1 o"
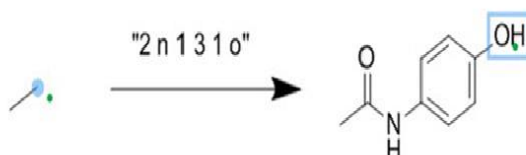
B.Sc.(B.Z.C.-II Yr) (E.M)-
2021-22 STUDENT LIST ATTENDED FOR CERTIFICATE COURSE

Sl.No	Name of the Student	Student Enrolment Number
1	A.Anusha	21033067 445 1001
2	B. Vinod Kumar	21033067 445 1002
3	B. Yamini	21033067 445 1004
4	B. Manisha	21033067 445 1005
5	B. Sreevani	21033067 445 1006
6	B. Girija	21033067 445 1007
7	B. Anitha	21033067 445 1008
8	D. Swapna	21033067 445 1010
9	G. Sruthi	21033067 445 1011
10	J. Naveen Prakash	21033067 445 1012
11	K.Anusha	21033067 445 1014
12	K. Sandhya Rani	21033067 445 1017
13	K. Jahnavi	21033067 445 1018
14	L. Rama Devi	21033067 445 1019
15	M. Sony	21033067 445 1020
16	M. Babu	21033067 445 1021
17	R. Shireesha	21033067 445 1025
18	S.Swathi	21033067 445 1027
19	T. Rajeshwari	21033067 445 1028
20	T. Kamakshi	21033067 445 1029
21	V. Ankitha	21033067 445 1031
22	V. Lokeshwari	21033067 445 1033

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Shadnagar,
Ranga Reddy Dist.

FEEDBACK ON CERTIFICATE PROGRAM

("chemdraw")

Tick (√) the appropriate option(s)

➢ **Why did you enroll in the programme**

◯ *General educational requirement*

◯ *General elective*

◯ *General necessity*

➢ **How did you find this programme**

◯ *Excellent*

◯ *Good*

◯ *Average*

➢ **Why did you find the lectures/training of the resource persons for this programme**

◯ *Excellent*

◯ *Good*

◯ *Average*

➢ **How did you find the lab/infrastructure facility provided**

◯ *Excellent*

◯ *Good*

◯ *Average*

➢ **How did the Department organize the programme**

◯ *Excellent*

◯

Good

◯ *Average*

➢ **How did you find the pace of the programme**

◯ *It was too fast*

◯ *It was manageable*

◯ *It was too slow*

My personal remarks :

_____

_____

_____

_____

_____

Date :

Station :

THANK YOU

Certificate course Inauguration by Principal G .Bhanuprakash Garu

Shadnagar, Telangana, India
36F5+VVX, Raghavendra Colony, Shadnagar, Telangana
509216, India
Lat 17.074418°
Long 78.209742°
03/11/22 02:56 PM GMT +05:30
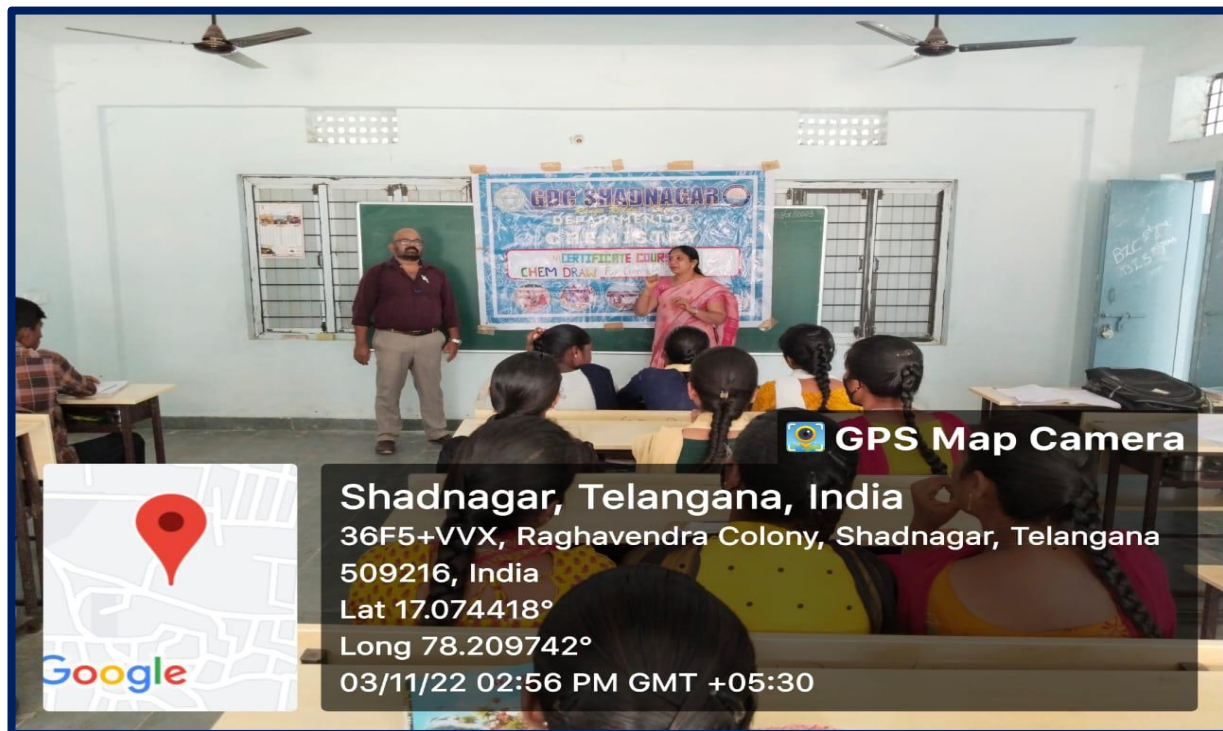
GDC SHADNAGAR
Ranga Reddy - Dist

Department of Chemistry

A Certificate Course in

CHEMDRAW

Certificate of Participation

This is to Certify that -------------------------- has participated in

"ChemDraw"

which is conducted by Department of Chemistry in this Academic Year 2021 - 22.
In this course his/her performance is Excellent.

Department of Chemistry   Principal

Certificate distribution by Principal G.Bhanuprakash garu

Certificate course Chemdraw student attendance

2021-22

30hrs

Sl.No	Name of the Student	3/11 2hr	4/11 2hr	7/11 2hr	8/11 2hr	9/11 2hr	10/11 2hr	11/11 2hr	14/11 2hr	15/11 2hr	16/11 2hr	21/11 2hr	26/11 2hr	28/11 2hr	29/11 2hr	30/11
1	A.Anusha	P	P	P	P	P	P	P	P	P	P	P	P	P	P	P
2	B. Vinod Kumar	P	P	P	A	P	P	P	P	P	P	P	P	P	P	P
3	B. Yamini	P	P	P	P	P	A	P	P	P	A	P	P	P	P	P
4	B. Manisha	P	P	P	A	P	P	P	P	P	P	P	P	P	P	P
5	B. Sreevani	P	P	A	P	P	P	P	P	P	P	A	P	P	P	P
6	B. Girija	P	P	P	P	P	P	P	P	P	P	P	P	A	P	P
7	B. Anitha	P	P	P	A	P	P	P	P	P	P	P	P	P	P	P
8	D. Swapna	P	P	P	P	P	A	P	P	P	A	P	P	P	P	P
9	G. Sruthi	P	P	P	P	P	P	P	P	P	A	P	P	A	P	P
10	J. Naveen Prakash	P	P	P	A	P	P	P	P	P	P	A	P	P	P	P
11	K.Anusha	P	P	P	P	P	A	P	P	P	P	A	P	P	P	P
12	K. Sandhya Rani	P	P	A	P	P	P	P	P	P	A	P	P	P	P	P
13	K. Jahnavi	P	P	P	P	P	A	P	P	P	A	P	P	P	P	P
14	L. Rama Devi	P	P	P	P	P	P	P	P	A	A	P	P	P	P	P
15	M. Sony	P	P	P	P	P	P	P	P	P	A	P	P	A	P	P
16	M. Babu	P	P	P	P	A	P	P	P	P	P	P	P	P	P	P
17	R. Shireesha	P	P	P	P	P	P	P	P	P	P	P	P	P	P	P
18	S.Swathi	P	P	P	P	P	P	P	P	P	A	P	P	P	P	P
19	T. Rajeshwari	P	P	A	P	P	P	P	A	P	P	P	A	P	P	P
20	T. Kamakshi	P	P	P	A	P	P	P	P	P	A	P	P	P	P	P
21	V. Ankitha	P	P	P	P	P	A	P	P	P	P	P	P	P	P	P
22	V. Lokeshwari	P	P	P	P	P	P	P	A	P	P	A	P	P	P	P

Principal
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