### **COURSE OUTCOMES**

- \* ACD Chem Sketch software:Introduction, download and
  installation process, Drawing
  various chemical structures
  (acyclic, cyclic, polycyclic,
  heterocyclic), name generation
  from structures, conversion of
  name of molecule into its
  structure, calculation of physical
  properties such as density,
  molecular weight, molecular
  formula, refractive index from
  structural formula, bond angles,
  bond lengths, dihedral angles
- \* downloading research papers using keywords in Scopus, Science direct, and google scholar, reaction search, product search, reactant search, structure search, markush search using Sci-finder. Introduction to End Note and its applications.

Head, Dept. of Chemistry

## **Objectives**

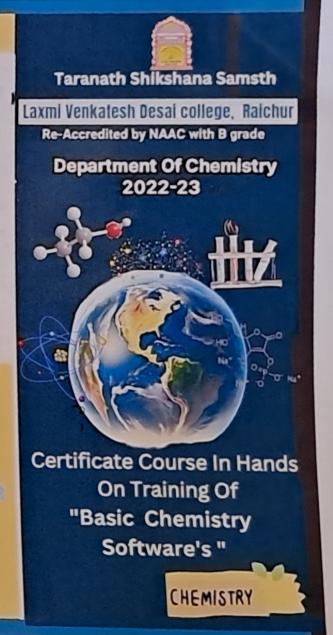
Department of chemistry LVD College, Raichur offers 30 hours Certificate course in hands on HC training of basic chemistry softwares. This course aimed at cimparting skills on use of various open source chemistry tools that are essential for any student or researcher with chemistry as a major subject. At the end of course, the participants will be able to use these softwares for drawing chemical structures. generation of their names. structure calculations, chemical reaction pathways prediction Eligibility-All B.Sc. final year students

#### TO JOIN CONTACT-

PRINCIPAL

Laxmi Venkatesh Desai College,

RAICHUR





# Taranath Shikshana Samsthe Laxmi Venkatesh Desai College, Raichur



Affiliated to Gulbarga University, Kalaburagi & Re-accredited by NAAC with B Grade

#### Index for Add-On Course

Title: Certificate Course in Hands on Training of Basic Chemistry Software's

**Academic year : 2021 - 2022** 

S.No	Particulars .	Page no
l	Declaration	1
2	Permission letter	2
3	Request letter of BOS for chairman	3-4
4	Notice	5
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6	Timetable	8
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10	Model Question Paper/Answer scripts	14-16
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# LAXMI VENKATESH DESAI COLLEGE, RAICHUR-584103. (Affiliated to Raichur University, Raichuri. Re-Accredited by NAAC with \*B\* Grade)

Dr. Venkatesh B. Devaru, M.Sc., Ph.D., MBA.

Office of the Principal Ph:( 08532)-240286, 240707 Fax:+918532 240707 e-mail: \u00favdrer@gmail.com

e-mail: Ndrcregman.com Website: www.lvdcollege.com

Date: 22-03-2022

#### TO WHOMEVER IT MAY CONCERN

This is to certify that, the college has introduced the Add\_On course on, "Certificate Course in Hands on Training of Basic Chemistry software's" with the duration of 30 hours introduced in 2022. The said programme is apart from the existing course curriculum.

Head of the Department
Head, Dept. of Chemistry
L.V.D. College, KAICHUR.

PRINCIPAL
Laxmi Venkatesh Desai College,
RAICHUR.



Date: 10-01-2022

To The Principal, LVD College, Raichur.

From HoD, Chemistry Department.

Respected Sir,

Sub: Permission to start an Add On course

With respect to the above cited subject I, the undersigned request you to grant permission to start an Add-on course titled "Certificate course in Hands on Training of Basic chemistry software's" to undergraduate students. The details of syllabus and duration are enclosed. This course helps students to build up their skills. Kindly grant the permission.

Thanking You,

Yours Faithfully, Head, Dept. of Chemistry L.V.D. College, RAICHUR.

PRINCIPAL PAICHUROS.

#### Taranatha Shikshana Samsthe

#### Laxmi Venkatesh Desai College, Raichur

(Affiliated to Raichur University Raichur, Reaccredited with "B"grade)

Dr. Venkatesh B Devaru MSc., PhD., MBA

Principal

office of the principal Ph:(08532) - 240286,240707 Fax: +918532 240707

email: lvdrcr@gmail.com website: www.lvdcollege.com

Date: 22-02-2022

ORDER Sub: Meeting of Board of Studies members

A meeting of the following BOS constituted is hereby convened on 22-02-2022 at 11:00 AM in the Department of Chemistry, LVD College, Raichur

## BOARD OF APPOINTMENT OF BOS MEMBERS FOR ADD-ON COURSE

1)	DR. Vittal Reddy Associate Professor Department of Chemistry BVB College Bodar	Chairman (S)
2)	DR. Pushpa Assistant Professor Department of Chemistry GFGC, Raichur	Member PRINCIPAL Covt. First Grade College For Womens
3)	Dr. Jayateertha N.S Department of Chemistry LVD College, Raichur	Member Head, Dept. of Chemistry L.V.D. College, RAICHUR.

The Chairman and the members are requested to make it convenient to attend THE BOS Meeting

TO COLLEGE A PAICHUR

PRINCIPAL
PRINCIPAL
L.V.D. COLLEGE RAICHUR

Date: 28-02-2022

To The Principal, LVD College, Raichur.

Respected Sir,

Sub: Acceptance to be a Member of BOS.

with reference to the above-cited subject I, Smt. Pushpa Assistant Professor, Department of Chemistry, GFGC. Raichur, received your letter of request to be a Member of BOS, for the Add-on Course to be conducted by your college

Hence, I give my consent and accept your request as a BOS Member.

Thanking You,

Yours Sincerely

Govt. First Grade College For Womens
RAICHUR-584 101



Affiliated to Gulbarga University, Kalaburagi& Re-Accredited by NAAC with B Grade

### **Department of Chemistry**

#### Notice

All the B.Sc VI Semester students are here by informed to join and get benefit of the Add-on course titled "Certificate course in Hands on Training of Basic chemistry software's" starting from

#### 22<sup>nd</sup> March, 2022 at 5 to 6 pm

This course enables you to create awareness about the importance of chemistry software's for the advance learning of subject; hence it is most useful to the students in future.

Signature of HoD Head, Dept. of Chemistry L.V.D. College, RAICHUR.

PRINCIPAL PAICHUR-03

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(Bsc XI Sem)



### Certificate course in Hands on Training of Basic Chemistry Softwares (30 Hour)

#### **Objectives**

Department of chemistry L V D College, Raichur offers 30 hours Certificate course in hands on training of basic chemistry softwares. This course aimed at imparting skills on use of various open source chemistry tools that are essential for any student or researcher with chemistry as a major subject. At the end of course, the participants will be able to use these softwares for drawing chemical structures, generation of their names, retrieve information about physical properties calculations, three-dimensional molecular structure calculations, spectroscopic signatures, chemical reaction pathways prediction, molecular functional groups, docking sites predictions, and other parameters efficiently.

<u>Eligibility</u>— All B.Sc. final year students having chemistry as major subject and all M.Sc. Chemistry students are eligible

#### Number of seats-30

<u>Evaluation Process</u>— Assessment of candidates will be done through theoretical assignments, projects & practical examinations after completion of each module. All successful candidates will be awarded with certificates.

Contents for certificate course in hands on training of basic chemistry softwares

Module 1 (4 hours): ACD ChemSketch software:— Introduction, download and installation process, Drawing various chemical structures (acyclic, cyclic, polycyclic, heterocyclic), name generation from structures, conversion of name of molecule into its structure, calculation of physical properties such as density, molecular weight, molecular formula, refractive index from structural formula, bond angles, bond lengths, dihedral angles.

Learning outcomes:- After successful completion of this module candidate will be able to use ACD ChemSketch for generation and processing of simple and complex chemical structures.

#### Module 2 (5 hours)

Cambridge ChemDraw Ultra software— Introduction, download and installation process, Drawing various chemical structures (acyclic, cyclic, polycyclic, heterocyclic), nomenclature generation, conversion of name into molecular structure, calculation of physical properties such as density, molecular weight, molecular formula, refractive index from structural formula. ¹H, ¹³C NMR prediction from molecular structure, Drawing structure of bigger molecules such as proteins, carbohydrates, and RNA/DNA, bio arts, use of templates, Comparison of ACD ChemSketch and Cambridge ChemDraw Ultra software.



Learning outcomes:- After successful completion of this module candidate will be able to use Cambridge ChemDraw Ultra for generation, processing and calculation of physical/chemical properties of simple and complex molecules.

#### Module 3 (8 hours)

Chem3D software:- Introduction, download and installation process, 3D structure of molecules, various 3D structure models, conversion of 2D structure into 3D structure, File extensions, Cartesian coordinates, Dihedral angles, Energy minimization, calculation of surface properties, calculation of molecular electrostatic potential (MEP) surface, electrostatic potential (ESP) surface, solvent accessible surface. Atomic charge calculations, Calculation of dipole moments, MM2 calculations, Huckel calculations, Calculation of UV and IR spectra using MM2 calculations.

Learning outcomes:- After successful completion of this module candidate will be able to study three dimensional properties of molecules which are highly useful in prediction of their chemical/ physical properties and can be applied in advanced research work.

#### Module 4 (5 hours)

Introduction to online chemical database search, Searching and downloading research papers using keywords in Scopus, Science direct, and google scholar, reaction search, product search, reactant search, structure search, markush search using Sci-finder. Introduction to End Note and its applications.

**Learning outcomes:-** After successful completion of this module candidate will be able to use online research tools efficiently and will be able to search research papers related to their topics more efficiently.

#### Module 5 (8 hours)

Chimera 1.12 software:- Introduction to Chimera software, Protein-ligand Docking, Protein data bank structure search, preparation of ligands and proteins for docking, Sites searching for ligand binding analysis, Docking of simple molecules over active site of protein molecules and analysis of docking results.

**Learning outcomes:-** After successful completion of this module candidate will be able to study drug-receptor interactions through docking. The knowledge of these interactions is a fundamental requirement for modern drug discovery process.

#### Salient features of certificate course

Theory and practical session as per curriculum

· Lectures include entire process of downloading and installation of these softwares.

· Hands on training on all these softwares

 At end of course candidate will be able to use these open source software's independently for their work.

A certificate will be issued to the suggessful candidates

PRINCIPAL LV.D. College, RAICHUR-03.

Hende Ranchur.



Taranath Shikshana Samsthe

## LAXMI VENKATESH DESAI COLLEGE, RAICHUR

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L.V.D. College, RAICHUR,

Name of the Staff: Miss. Jasmeen

Principal Laxm! Venkatesh Desai College RAICHIE

Affiliated to Gulbarga University, Kalaburgi & Re-Accredited by NAAC with B Grade

#### **Attendance Sheet**

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Erad, Dept. of Chemistry L.v.D. College, R-MCHUR. Signature of Principal PRINCIPAL LV.D. College, RAICHUR-03.

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Affiliated to Gulbarga University, Kalaburgi & Re-Accredited by NAAC with B Grade

#### **Attendance Sheet**

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Head, Dept. of Chemistry

L.V.D. College, RAICHUR.

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L.V.D. College, RAICHUR-03.

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Affiliated to Guibarga University, Kalaburgi & Re-Accredited by NAAC with B Grade

#### **Attendance Sheet**

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Signature of HOD

Head, Dept. of Chemistry

L.V.D. College, RAICHUR

Signature of Principal PRINCIPAL

LV.D. College, RAICHUR-03





#### Laxmi Venkatesh Desai College, Raichur Affiliated to Gulbarga University, Kalaburagi & Re-Accredited by NAAC with B Grade

## Department of Chemistry Report of Add on course

Title of the Add on course: Certificate course in Hands on Training of Basic Chemistry.

software's

Duration: 30 Hours

Started on: 22 - 3 - 2022,

Completed on: 21 - 4 - 2022,

Name of the faculty: Dr. Anganeya Oblesha, & Miss, Jasmeen Total No. of students admitted: 25

Total No. of students admitted:

Total No. of classes taken: 30

Total No. of students benefited: 35

Learning outcomes: After successful completion of this add on course students will be able to use ACD Chemsketch and Cambridge ChemDraw Ultra software for generation & processing of simple and complex chemical structures.



L.V.D. College, RAICHUR





Taranath Shikshana Samsthe

## LAXMI VENKATESH DESAI COLLEGE RAICHUR

(Re-Accredited by NAAC with 'B' Grade)



This is to Certify that Miss. 19	no Lax	mi
of B.SC VI Semest		ed the Certificate Course in
Certificate course on		
Conducted by the Department of	Chemistry	from
22-3-22 10 21-4-20	DAR V	
		The state of the s
Head of the Department		Principal

### Taranath Shikshana Samsthe's LAXMI VENKATESH DESAI COLLEGE, RAICHUR ADD ON COURSE, INTERNAL ASSESSMENT **TOPIC - TRAINING OF BASIC CHEMISTRY SOFTWARES** BSC VI SEMESTER - 2022

Time: 5:00 to 6:00 pm

Date: 08 - 04 - 2022

Max.Marks: 20M

Name: Anjali Register No: 1953406

Instructions: Choose and tick the correct answer

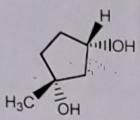
- 1. Organic compounds are broadly classified as
- a) Open chain compounds and acyclic compounds
- b) Open chain compounds and linear chain compounds
- c) Cyclic compounds and alicyclic compounds
- alicyclic compounds and acyclic compounds
- Aliphatic compound is the other name for \_\_\_
- Acyclic compounds
  - b) Alicyclic compounds
  - c) Ring compounds
  - d) Closed chain compounds
  - 3. Which among the following is not an example of alicyclic compound?
- a) Cyclohexane
- b) Cyclohexene
- c) Tetrahydrofuran
- Acetic acid
- 4. Hydrocarbons are organic compounds with element
- Both hydrogen and carbon
- b) Carbon
  - c) Hydrogen
  - d) Oxygen
  - 5. Which of the following bond is made up of a large number of organic compounds?
  - a) Metallic bond
- () b) Dipolar bond
  - Ionic bond
  - d) Covalent bond

- 6. Which of the following organic compound with molecular formula C<sub>3</sub>H C<sub>12</sub> exhibits only one signal in the <sup>1</sup>H NMR spectrum?
- a) 1, 2-dichloropropane
- b) 1. 1-dichloropropane
- 1 (2) 2, 2-dichloropropane
  - d) 1, 3-dichloropropane
  - 7. Which of the following is an organic compound having the molecular formula  $C_{10}H_{14}$  exhibited two singlets in the <sup>1</sup>H NMR spectrum and three signals in the <sup>13</sup>C NMR?

- 8. An organic compound (MF; C<sub>8</sub>H<sub>10</sub>O) exhibited the following <sup>1</sup>H NMR special data: 62.5 (3H, s), 3.8 (314, s), 6.8 (2H, d, J 8 Hz), 7.2 (2H, d, J 8 Hz) ppm. Which of the following is that compound among the choices?
- a) 4-methylbenzyl alcohol
- 4-methyl anisole
- c) 4-ethylphenol
- d) 2-ethylphenol



9. What is the complete IUPAC name of the following substance?

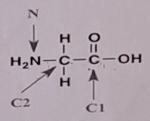


(1R,3S)-1-methylcyclopentane-1,3-diol

- b) (1S,3R)-1-methylcyclopentane-1,3-diol
- c) (1S,3S)-1-methylcyclopentane-1,3-diol
- d) (1R,3R)-1-methylcyclopentane-1,3-diol
- 10. Which set of approximate bond angles at C1, C2, and N of the following molecule indicates the correct shape?

C1 120°, C2 120°, N 120°

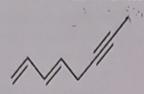
- b) C1 120°, C2 120°, N 109.5°
- c) C1 109.5°, C2 120°, N 120°
- d) C1 120°, C2 109.5°, N 109.5°
- 11. Which set of hybridization states of C1, C2, and N of the following molecule is. correct?



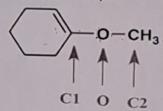
(a) C1 sp<sup>2</sup>, C2 sp<sup>3</sup>, N sp<sup>3</sup>

- b) C1 sp<sup>3</sup>, C2 sp<sup>2</sup>, N sp<sup>3</sup>
- c) C1 sp<sup>3</sup>, C2 sp<sup>2</sup>, N sp<sup>2</sup>
- d) C1 sp<sup>2</sup>, C2 sp<sup>2</sup>, N sp<sup>3</sup>

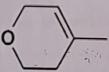
12. Which is the correct molecular formula of the following molecule?



- a) C<sub>8</sub>H<sub>8</sub>
- (b) C8H10
  - c) C7H8
  - d) C<sub>7</sub>H<sub>10</sub>
  - 13. Which set of approximate bond angles at C1, O, and C2 of the following molecule indicates the correct shape?



- 1
- a) C1 120°, O 120°, C2 120°
- b) C1 120°, O 120°, C2 109.5°
- c) C1 120°, O 109.5°, C2 120°
- d) C1 120°, O 109.5°, C2 109.5°
- 14. Which is the correct molecular formula of the following molecule?



- a) C<sub>7</sub>H<sub>10</sub>O
- b) C<sub>7</sub>H<sub>12</sub>O
- c) C<sub>6</sub>H<sub>8</sub>O
- (A) C6H10O
- 15. Expand ACD in ACD Chemsketch.
- (a) Advanced Chemistry development
- b) Automatic Chemsketch drawing
- Advanced Chemsketch development
- d) Advanced Chemistry structures drawing

- 16. How many gm moles oxygen are there in 88 gms carbon dioxide?
- b) 2
- c) 3
- - 17. What is the main application of ACD chemsketch software.
  - a) Quiet easy
- create and modify images of chemical structures.
  - c) Molecular modelling
  - d) Dimensional images
  - 18. Which of the following is a not a five membered ring?
  - a) Pyridine
- by Pyrrole
  - c) Furan
  - d) Thiophene
  - 19. The correct bond order in the following species is -
  - a)  $O_2^+ < O_2^- < O_2^{2+}$
- $\begin{array}{ccc} \text{(b)} & O_2^- < O_2^+ < O_2^{2+} \\ \text{c)} & O_2^{2+} < O_2^+ < O_2^- \end{array}$ 

  - d)  $O_2^{2+} < O_2^{-} < O_2^{+}$
  - 20. The bond angle around an atom which uses sp2 hybridization is -
  - W 120°
- 1 b) 180°
  - c) 107°
  - c) 107° d) 109°. 28'

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#### Marks list



#### **Department of Chemistry**

Class: B.Sc. VI Semester

Course title: Training of basic chemistry software's

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Sl.No	Register No	Name of the Student	Marks	Signature of Student
1	1953113	Marikeshwari	18	Me.
2	1953137	Mahesh. K.	16	- AV
3	1953155	Savita.	17	Su
4	1953172	Prayeen. K	19	B
5	1953179	Laxmi	18	James
6	1953185	Meghana	18	Maghan
7	1953 203	Tolveni	18	Theri
8	1953221	Abhechek.	16	Abbished.
9	1953212	Revati	18	Rain
10	1953233	B. Vibha	19	Brithe
11	1953.255		16	Neene
12	1953242	<u> </u>	17	2 within
13	1953270		17	Bahh
14	1953235	Bharat	17	Por
15	1953315	Rahul	18	Rahel
16	1953281	Kaveri	19	Kaveri
17	1953311	Anil	18	Anils
18	1953358	Geeta	17	Geetha
19	1953328	P. Ganesh	18	Grenet
20	1953 406	Anjali	19	Augusi
21	1953118	Lakelmana.	18	Ashma
22	1953117	Akshata.B.	16	Achata
23	1953126	Ankita.	16	ANKITA
24	1953131	Usha	18	Usha
25	1953134		19	Dell-
26	1953147	Gayatri	18	Gru
27	1953159	Pooja. K	19	989
28	1953148	Anusha	16	tolog

Signature of Faculty

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#### Marks list



### Department of Chemistry

Class: B.Sc. VI Semester

Course title: Training of basic chemistry software's

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29	1953154	Lakshmi	18	Kashmi
30	1953 143	Laxmi	19	Znù_
31	1953 150	Sangeeta	16	504
32	1953 177	G. Shouti	17	Gi, Shouti Satishs
-33	1953181	S. Satish	18	Salishs
34	1953188	Pavithra.	19	Ru_
35	1953173	Ashevini	18	Ash
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