



RAMAIAH

College of Arts, Science &
Commerce

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M S Ramaiah College of Arts, Science and Commerce

Re-accredited 'A' by NAAC, Permanently Affiliated to Bengaluru City University,

Approved by Government of Karnataka, Approved by AICTE, New Delhi,

Recognized by UGC under 2f & 12B of UGC act 1956



(National Institutional Ranking Framework, Ministry of Education, Govt of India)

Ranked 62nd in NIRF India Ranking by MHRD, New Delhi

DBT Star College Scheme

Ref. No: MSRCASC/ CHEM-BIOCHEM/21-22/23

Date: 24/04/2022

CIRCULAR

DEPARTMENT OF CHEMISTRY/BIOCHEMISTRY

Department of Chemistry/ Biochemistry is organizing Value Added Programme on Software used in Chemistry & Biochemistry Research from 02/05/2022 to 31/05/2022 for B.Sc. IV Semester and M.Sc. II Semester students. Interested students can register their names using the link provided below on or before 30/04/2022.

Registration link:

<https://forms.gle/rVh6Xd6Ug8QYCez38>

Event Coordinators:

Dr. Vibha Vinayakumar Bhat

Assistant Professor

Department of Chemistry/Biochemistry


MSRCASC, Bengaluru

Dr. Ashly P. C.

Assistant Professor

Department of Chemistry/Biochemistry

MSRCASC, Bengaluru


Head of the Department
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PATRONS

Sri. M. R. Janakiram
Hon'ble Director, GEF

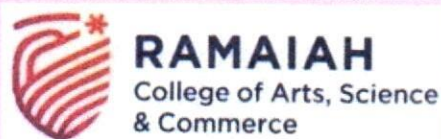
Sri. M. R. Kodandaram
Hon'ble Director, GEF

Sri. B. S. Ramaprasad
Chief Executive, E & GS, GEF

Sri. G. Ramachandra
Chief of Finance, E & GS, GEF

Dr. Nagarathna. A
Principal, MSRCASC

Mr. Prasanna Kumar S. G.
Head of the Department, MSRCASC



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**DEPARTMENT OF CHEMISTRY
& BIOCHEMISTRY**

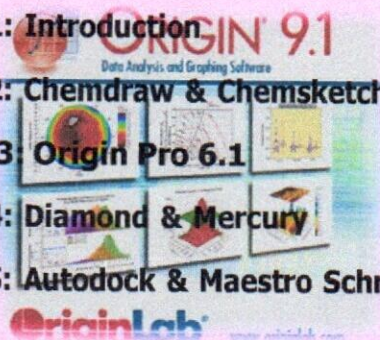
**VALUE-ADDED
PROGRAM**

ON

**SOFTWARES USED IN
CHEMISTRY &
BIOCHEMISTRY
RESEARCH**

PROGRAM DETAILS

- Module 1: Introduction**
Module 2: Chemdraw & Chems sketch
Module 3: Origin Pro 6.1
Module 4: Diamond & Mercury
Module 5: Autodock & Maestro Schrödinger



OBJECTIVES

The main objective of this program is to inculcate technical skills among students about the different types of software that are useful in carrying out research and analysis in chemical and biochemical sciences. This knowledge would be beneficial in both academic and industrial research in future for the students.

RESOURCE PERSONS

Dr. Vibha Vinayakumar Bhat
Assistant Professor
Department of Chemistry & Biochemistry,
MSRCASC

Dr. Ashly P C
Assistant Professor
Department of Chemistry & Biochemistry,
MSRCASC



Event Coordinators:

Dr. Vibha Vinayakumar Bhat
Assistant Professor
Department of Chemistry & Biochemistry
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Dr. Ashly P C
Assistant Professor
Department of Chemistry & Biochemistry
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Target Students:

- **M.Sc. Chemistry & Biochemistry**
- **B.Sc. Chemistry & Biochemistry**

From: 02/05/2022 – 31/05/2022

Duration: 30 hours

M S Ramaiah College of Arts, Science and Commerce (MSRCASC)

Dr. M.S Ramaiah, a visionary and philanthropist established "Gokula Education Foundation (GEF)", in the year 1962, to deliver education and healthcare for the betterment of mankind. Under the umbrella of GEF, M.S Ramaiah college of Arts, Science and Commerce (MSRCASC) was established in the 1994. MSRCASC is Re-accredited with "A" Grade by NAAC, affiliated to Bengaluru Central University (BCU), and approved by AICTE. The college offers seven UG courses and four PG courses in Arts, Science, and Commerce, to around 2000 students.

Department of Chemistry and Biochemistry

The Department of Chemistry and Biochemistry was established in the year 1994 and currently conducts both UG and PG courses in Chemistry and Biochemistry. The syllabus is constantly supported by current-day, real-life applications carrying utility value. The department has very good infrastructural facilities to carry out teaching and research activities. Highly qualified faculties are assigned theory and practical classes and are instructed to emphasize the 'learning' of the students.

ABOUT THE PROGRAM

The value-added program is a short-term program that can impart career-oriented skills which are important for students in upskilling themselves with the ongoing technology required for jobs as well as academic research. This would expose the students in taking challenges with confidence and learning important and relevant new skills beyond the syllabus. This will assist students to meet the industry expectations easily.

OUTCOME

Students will learn the basic Softwares that are used in chemistry and biochemistry research in designing the experiments, data analysis, and industrial approaches. This will help in building the *in-silico* skills among students and upskilling their knowledge according to the present requirements and relevance.

Registration link

<https://forms.gle/rVh6Xd6Ug8QYCEz38>

ORGANIZING COMMITTEE

Mr. Prasanna Kumar S. G.
Head of the Department,
Department of Chemistry/Biochemistry, MSRCASC

Dr. Vibha Vinayakumar Bhat
Event Coordinator
Department of Chemistry/Biochemistry, MSRCASC

Dr. Ashly P C
Event Coordinator
Department of Chemistry/Biochemistry, MSRCASC

CONTACT DETAILS

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M S RAMAIAH COLLEGE OF ARTS, SCIENCE AND COMMERCE

DEPARTMENT OF CHEMISTRY/BIOCHEMISTRY

Value-Added Program on Software used in Chemistry & Biochemistry

Research

SYLLABUS

Number of Hours: 30

Module 1: Introduction

2 hrs

Introduction to the software: ChemDraw, OriginPro, Diamond, PCD, Autodock & Maestro Schrödinger and their applications

Module 2: ChemDraw & Chems sketch

8 hrs

Basic features of ChemDraw and Chems sketch, download and installation process, drawing chemical structures: acyclic, cyclic, aromatic, heterocycles, nucleotides, Haworth and Fischer structures of sugars, conversion of structure to IUPAC name and IUPAC name to structure, identification of molecular mass, melting point, prediction of ^1H -NMR and ^{13}C -NMR spectra, prediction of the molecular ion peak in mass spectrum, drawing reaction mechanism.

Hands-on sessions

Module 3: OriginPro 8.0

5 hrs

Salient features of OriginPro, download and installation process, importing the experimental data, plotting of graphs (single and multiple), plotting of UV-Visible spectra, cyclic voltammograms, viscosity plots, analysis of spectral data, signal processing, peaks and baseline corrections, mathematical analysis, linear progression curves, non-linear fit curves. Mathematical calculations using OriginPro.

Hands-on sessions

Module 4: Diamond, Mercury and PCD

10 hrs

Salient features of Diamond & Mercury, storing and analysis of crystal structural data, atomic parameters, cell parameters and space-group, anisotropic displacement parameters, chemical and bibliographic data, input data: SHELX-93, Crystallographic Information File (CIF), XYZ format and MDL MOL formats, Auto-Builder and automatic creation of crystal picture, interconversion of crystal and molecular structures: adding and removal of cell and symmetry information, calculation of powder XRD data: Radiation type, wavelength, 2θ range,

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Diffraction diagram, Table of reflection parameters with zoom in/zoom out and tracking through 2θ range and Calculation of distances and angles.

Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds, salient features, chemical system matrix view for a 2D or 3D graphical representation, entry report for data sheet, a 3D picture of the crystal structure, the calculated powder diffraction pattern, and the table of interatomic distances.

Module 5: Autodock & Maestro Schrödinger

5 hrs

Salient features, download and installation process, downloading of protein from RCSB and ligand from PubChem, preparation of ligand and protein, Grid: macromolecule, grid box, set map types, docking: search parameters, genetic algorithm, output parameters: Lamarckian algorithm, analysis using play ranked energy and visualization of the docked molecule using python molecular view.

Hands-on sessions.

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DBT Star College Scheme

REPORT ON VALUE-ADDED PROGRAM ON SOFTWARE USED IN CHEMISTRY & BIOCHEMISTRY RESEARCH

Date: 02/05/2022 – 31/05/2022**Number of Participants: 30****Course Facilitators: Dr. Vibha Vinayakumar Bhat****Dr. Ashly P. C.**

To inculcate technical skills among science students, the Department of Chemistry and Biochemistry organized Value-Added Program on Software used in Chemistry & Biochemistry Research for B.Sc. IV Semester and M.Sc. II Semester students from 02/05/2022 to 31/05/2022. The program was taught under different modules and students were introduced to the soft skills which are used in chemical and biochemical research.

The program started with Module 1 Introduction by Dr. Vibha Vinayakumar Bhat. Herein, the students were introduced to the types of software used to draw chemical structures, plotting of graphs, analysis of the experimental data, etc. Module 2 was based on ChemDraw Ultra 8.0 and Chems sketch software. The program facilitator described the installation of ChemDraw software. Students were taught about the different options in working with the software. The first few hours of the module dealt with the basic operating skills of the software; selection of single, double and triple bonds, coordinate bonds, wedge and dashed bonds, cyclic structures, aromatic structures etc. Later sessions dealt with the drawing of reaction mechanisms using straight arrows, half-headed arrows, and so on. Students learnt to save the ChemDraw images as .cdx, .sdf, .tiff file formats and also a 3D ball and stick image format. Students had Hands-on training on this software.

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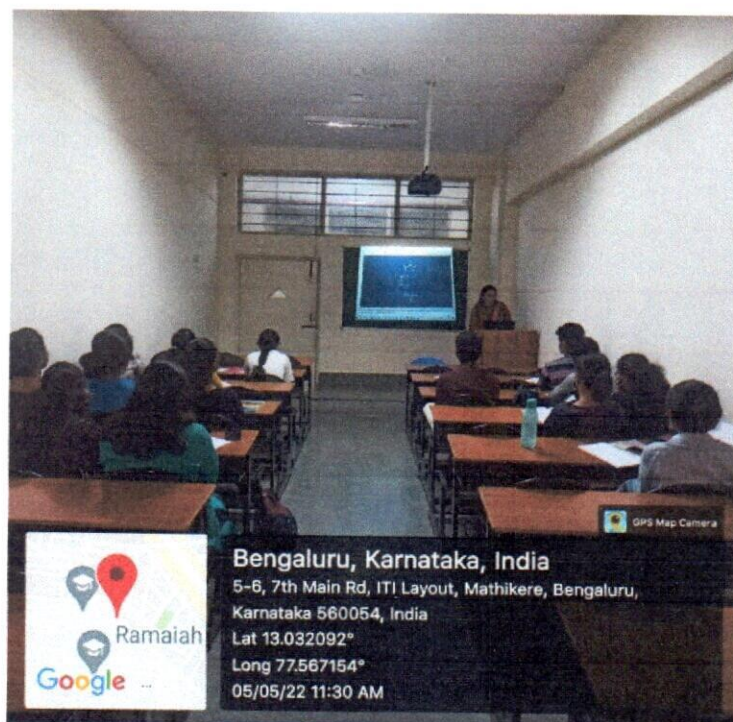
Modules 3 and 4 were taught by Dr. Ashly P. C. She introduced the students to Origin software which is used for the analysis of experimental data. The module dealt with the operating skills of Origin software in importing the experimental data, extracting values from the notepad or excel format, and plotting the graphs. Students were introduced to the data analysis using the software. Data analysis includes signal processing, peaks and baseline corrections, mathematical analysis, linear progression curves, non-linear fit curves, etc.

Module 5 dealt with Diamond, Mercury & PCD software for single crystal data analysis. It is software to visualize the molecular and crystal structure. The sessions dealt with the working of this software in detail and its understanding of the integration of a multitude of functions, which enhances the work with crystal structure data - in research and education as well as for publications and presentations. They learned the storage of data in Diamond where it can store and display structure data sets in a document with atomic parameters, cell parameters, and space-group, anisotropic displacement parameters, chemical and bibliographic data. The software supports input data in the form of SHELX-93, Crystallographic Information File (CIF), XYZ format, and MDL MOL format. Students learned how to calculate the powder pattern with a variation of diffraction parameters such as Radiation type, wavelength, 2theta range, and Diffraction diagram (styles, colors and line weights can be configured), table of reflection parameters with zoom in/zoom out and tracking through 2θ range and calculation of distances and angles using the software. PCD was introduced to students about working. With chemical system matrix view, one can get a 2D or 3D graphical representation of the available chemical systems (element combinations). Using all this information students can get a quick overview of the currently selected entry and can watch the different views change while they walk through the list of entries in the Entry report.

Module 5 dealt with Autodock & Maestro Schrödinger. In this module, students have learned about the structure-activity relationship by docking the chemical compound as a ligand and its interaction with biomolecules such as protein and DNA. Here, students learned about the protein and ligand preparation in PDB and pdbqt formats for further docking studies. Drawing of the Grid box around the docked region and their analysis using the Lamarckian algorithm. Analyzed data were visualized in Python molecular viewer software to identify the interaction site and the amino acids in protein and nucleotides in DNA during an interaction. Students had practical experience of using the software during Hands-on sessions on all the software.


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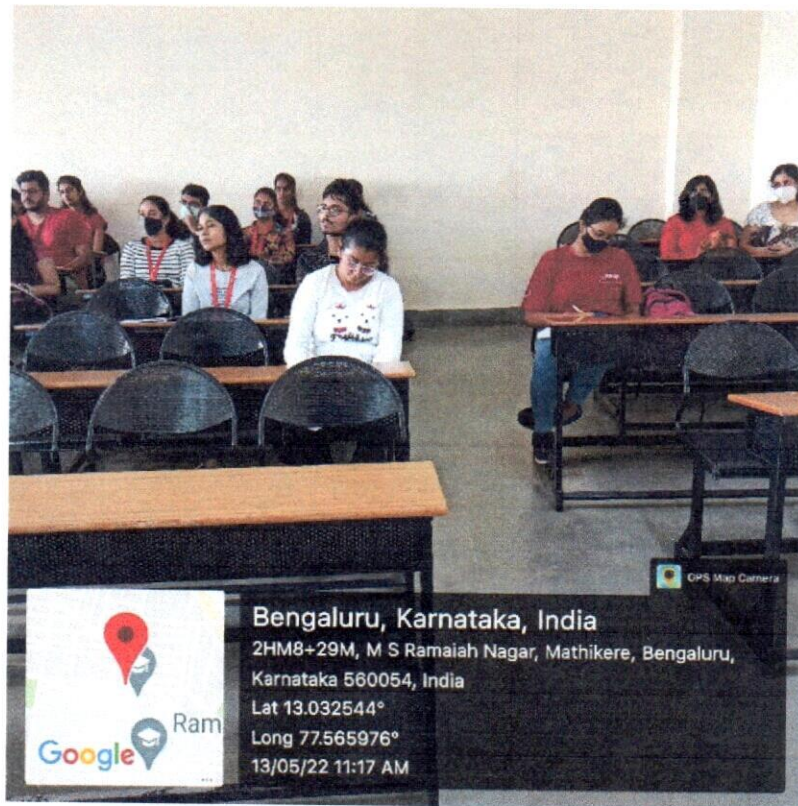
Teaching ChemDraw ultra software



Students attending the Value-added Program

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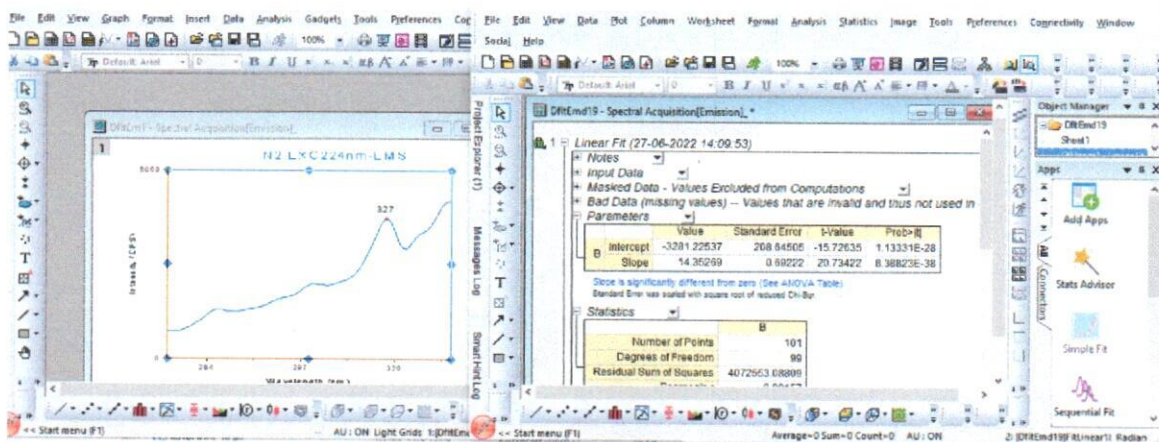
Students attending the Value-added Program



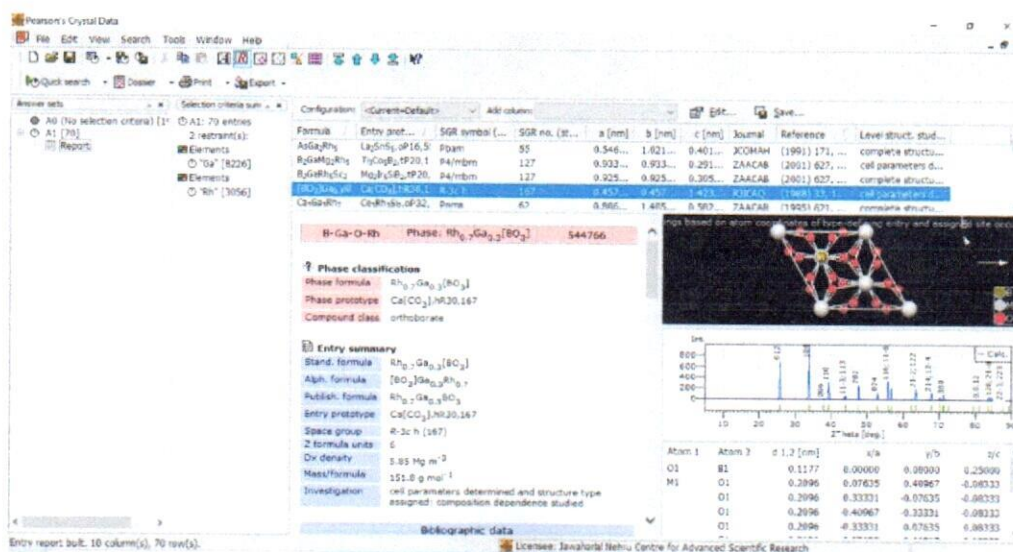
Students attending the Value-added Program

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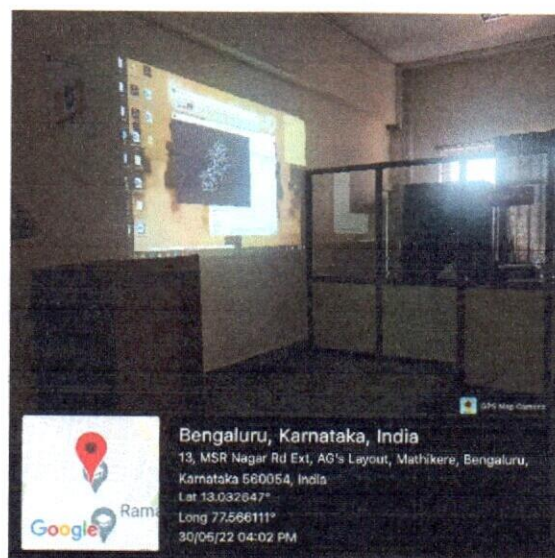
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Data analysis using OriginPro software



PCD software showing the crystal structure of inorganic compound



Demonstration of protein-ligand interaction using Autodock software

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M S Ramaiah College of Arts, Science and Commerce
Department of Chemistry/ Biochemistry
Students Attendance of Value-Added Program

on

“SOFTWARE USED IN CHEMISTRY & BIOCHEMISTRY RESEARCH”

Sl.No.	Students Name	Reg. No	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	
1	ANIRUDH BHAT M L	P18EV21 S0032	02/05	02/05	03/05	04/05	04/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	05/05	
2	ASHRITHA REDDY	P18EV21 S0036	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	
3	GIRISH KUMAR	P18EV21 S0043	1	2	3	4	5	6	7	8	9	10	A	A	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29
4	HRIINAVAI J	P18EV21 S0068	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	
5	JAMUNA MK	P18EV21 S0022	1	2	3	4	5	6	7	8	9	10	A	A	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29
6	LAVANYASHREE	P18EV21 S0005	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	
7	MANIKANTA V	P18EV21 S0017	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	
8	NIKITHA M	P18EV21 S0025	1	2	3	4	5	6	A	A	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29
9	POORNIMA R	P18EV21 S0046	1	2	3	4	A	A	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29
10	RAKSHITHA BAI	P18EV21 S0029	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	
11	SACHI K PATIL	P18EV21 S0063	1	2	3	4	5	6	A	A	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29
12	SANJANA R	P18EV21 S0030	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	

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13	SPANADANA GR	P18EV21 S0051	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
14	PRADEEP KUMAR N	P18EV21 S0016	1	2	3	4	A	A	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
15	SUCHITHRA V	P18EV21 S0027	1	2	3	4	A	A	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
16	ATULYA P	S2014471	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
17	AYUSHMA PAUL	S2014472	1	2	3	4	5	6	A	A	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
18	DEVANGI SATPATHY	S2014490	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
19	DIKSHA H	S2014493	1	2	3	4	A	A	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
20	DILIP KUMAR S	S2014495	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
21	NEHA S	S2014546	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
22	PAVITHRA S	S2014555	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
23	PRAJWAL G	S2014558	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	A	17	18	19	20	21	22	23	24	25	26	27	28	29
24	PRAJWAL PH	S2014560	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
25	PRITHVIKAR	S2014563	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	A	20	21	22	23	24	25	26	27	28	29
26	POOJA T	S2014557	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	A	25	26	27	28	29
27	SANKET SUDHEER HEGDE	S2014586	1	2	3	4	5	6	A	A	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28
28	SAMPRIITI MACHHAN	S2014581	1	2	3	4	5	6	A	A	7	8	9	10	11	12	13	14	15	16	17	A	18	19	20	21	22	23	24	25	26	27
29	RAKSHITHA A	S2014568	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	A	18	19	20	21	22	23	24	25	26	27	28	29
30	YASHAS V	S2014612	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30

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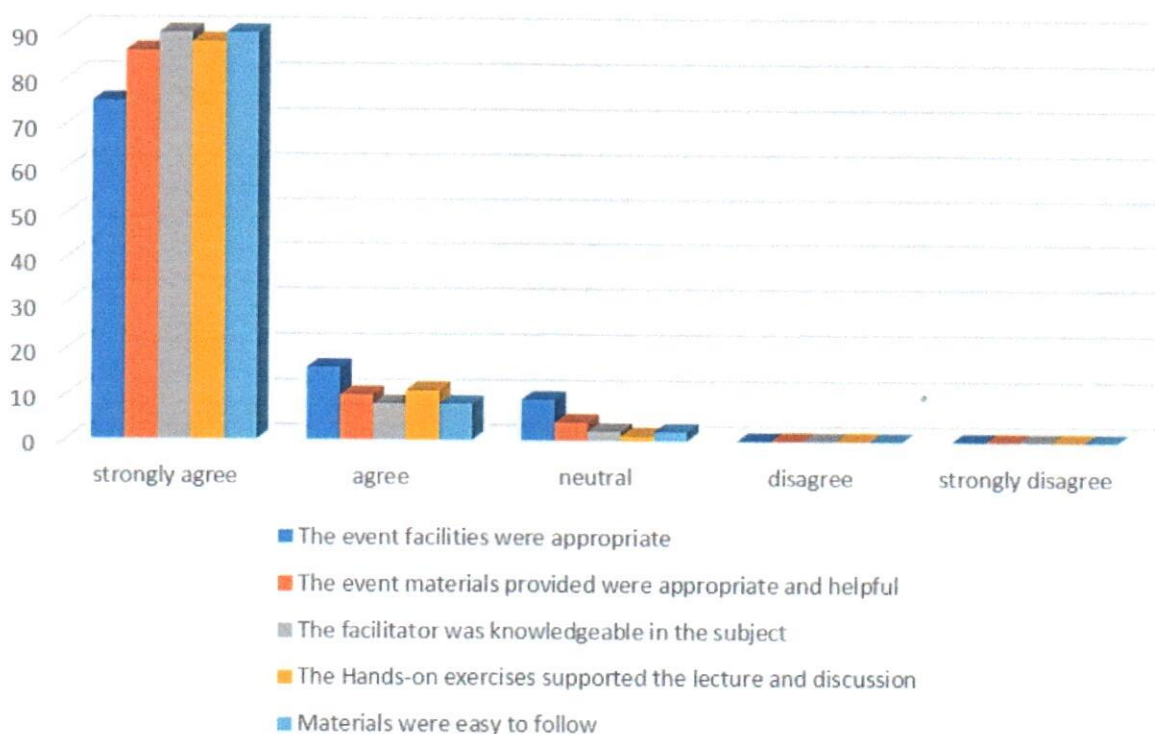
Department of Chemistry/ Biochemistry

Feedback on Value-added program

“SOFTWARE USED IN CHEMISTRY & BIOCHEMISTRY RESEARCH”

Contents	strongly agree	agree	neutral	disagree	strongly disagree
The event facilities were appropriate	75	16	9	0	0
The event materials provided were appropriate and helpful	86	10	4	0	0
The facilitator was knowledgeable in the subject	90	8	2	0	0
The Hands-on exercises supported the lecture and discussion	88	11	1	0	0
Materials were easy to follow	90	8	2	0	0

Cosolidated Feedback from the Participants



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M S Ramaiah College of Arts, Science and Commerce

Department of Chemistry/ Biochemistry

Assessment Procedure for Value-added program on Software used in chemistry & biochemistry research

Department of Chemistry/Biochemistry conducted Value-Added Program on Software used in chemistry and biochemistry research for M.Sc II Semester and B.Sc. IV Semester students from 02/05/2022 – 31/05/2022. The course facilitators were Dr. Vibha Vinayakumar Bhat and Dr. Ashly P. C. 30 students participated in the program and benefitted from the theoretical and Hands-on sessions. The assessment was done based on their performance in theoretical as well as practical sessions. Certificates were issued to the participants after the completion of the program.

Sl. No	Students Name	Reg. No	Attendance (5)	Viva (10)	Practical Skills (15)	Total (30)
1	ANIRUDH BHAT M L	P18EV21S0032	5	8	14	27
2	ASHRITHA REDDY	P18EV21S0036	5	10	15	30
3	GIRISH KUMAR	P18EV21S0043	5	7	12	24
4	HRIINAVAI J	P18EV21S0068	5	9	13	27
5	JAMUNA M K	P18EV21S0022	5	7	12	24
6	LAVANYASHREE	P18EV21S0005	5	10	15	30
7	MANIKANTA V	P18EV21S0017	5	9	14	28
8	NIKITHA M	P18EV21S0025	5	8	13	26
9	POORNIMA R	P18EV21S0046	5	7	12	24
10	RAKSHITHA BAI	P18EV21S0029	5	7	13	25
11	SACHI K PATIL	P18EV21S0063	5	7	13	25
12	SANJANA R	P18EV21S0030	5	8	14	27
13	SPANADANA G R	P18EV21S0051	5	9	15	29
14	PRADEEP KUMAR N	P18EV21S0016	5	6	13	24
15	SUCHITHRA V	P18EV21S0027	5	7	13	25
16	ATULYA P	S2014471	5	7	14	26
17	AYUSHMA PAUL	S2014472	5	8	15	28
18	DEVANGI SATPATHY	S2014490	5	10	15	30

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19	DIKSHA H	S2014493	5	9	14	28
20	DILIP KUMAR S	S2014495	5	10	15	30
21	NEHA S	S2014546	5	9	14	28
22	PAVITHRA S	S2014555	5	9	14	28
23	PRAJWAL G	S2014558	5	8	13	26
24	PRAJWAL P H	S2014560	5	7	12	24
25	PRITHVIKA R	S2014563	5	10	15	30
26	POOJA T	S2014557	5	9	14	28
27	SANKET SUDHEER HEGDE	S2014586	5	8	13	26
28	SAMPRIITI MACHHAN	S2014581	5	10	15	30
29	RAKSHITHA A	S2014568	5	10	15	30
30	YASHAS V	S2014612	5	7	12	24

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