GOVERNMENT COLLEGE
KASARAGOD

VIDYANAGAR, KASARAGOD, KERALA, 671123

www.gck.ac.in

NAAC 3RD CYCLE ACCREDITATION

ADD ON COURSE
APPLICATIONS OF COMPUTER AIDED
DESIGNS IN SCIENCE
(ACADS)
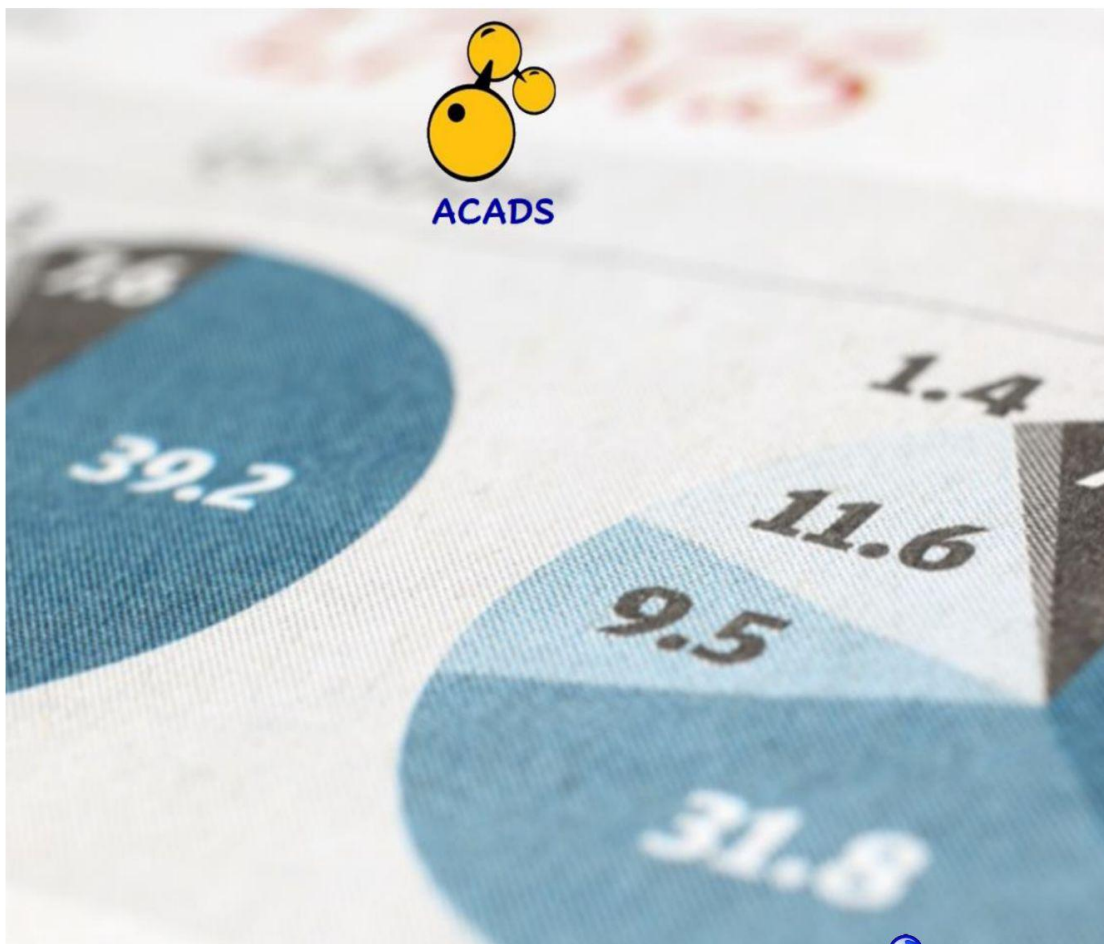
Brochure:

ACADS

Applications of Computer Aided Designs in Science

Course Brochure

DEPARTMENT OF CHEMISTRY, GCK

Date................

Name and Signature of the Principal
Dr.Ananthapadmanabha.A.L

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ACADS

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Dr.Ananthapadmanabha.A.L

Government College Kasaragod
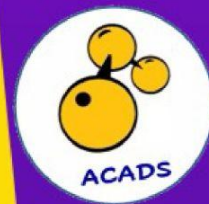
Add-on Course
Applications of Computer Aided Designs in Science
ACADS

REGISTER NOW!
bit.ly/acads2022

MOLECULAR GRAPHICS TOOLS
Introdicing molecular visualization soft wares: Gaussview, Avogadro, Chemdraw, ChemSketch, JMol & Chemcraft. Learn how to design computational chemistry inputs from theses softwares

GaussView 5 GAUSSIAN, INC.
ChemDraw
ChemCraft
ChemSketch
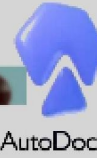
BASIC COMPUTATIONAL SCIENCE
Introducing Quantum Chemistry softwares: Gaussian, GAMESS, Molpro, NWChem, ORCA, Quantum espresso etc..

ORCA NWCHEM
HIGH-PERFORMANCE COMPUTATIONAL CHEMISTRY SOFTWARE
Molpro Quantum Chemistry Software
GAMESS
Gaussian
QUANTUMESPRESSO

IN SILICO DURG DESIGNING
Design your first ever drug using Autodock PyMol and Discovery Studio Visualizer. Crystal structure in CRYSTAL program

PyMOL
CRYSTAL 17
DISCOVERY STUDIO
AutoDock

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Certificate Course on

APPLICATIONS OF COMPUTER AIDED DESIGNS IN SCIENCE (ACADS)

Offering department: CHEMISTRY

Course Objectives:

- To understand the drug biomolecular interactions for the rational drug design and drug discovery
- To enable the learner to use the graphical softwares for designing 2D and 3D molecules.
- To enable the learner to understand the quantum chemistry softwares leading them to carry out small computational chemistry projects.
- To understand the concepts and calculations in quantum chemistry and analytical chemistry using spreadsheets
- To enable the learner to understand numerical computing softwares for visualizing important mathematical functions and their properties through 2D and 3D plots

Learning Outcomes:

At the end of the course, the learners should be able to:

➢ Perform molecular docking using Autodock / Autodock Vina and analyse the binding affinity and determine the effectiveness of the drug on a target.

➢ Draw molecules in 2D and 3D space and convert them to digital identifiers

➢ Create GAMESS/NWChem/ORCA/Gaussian/Molpro input files, run, analyse and visualize the output files

Course Syllabus

(Total contact hours: 30 hours)

✸ **MODULE I: In Silico Drug Designing**:

Introducing protein data bank – retrieving target file from protein database - preparation of target, ligand and docking files using Autodock – performing automated docking calculations using bash script in Cygwin software – analysing the output and preparing quality images with autodock, pymol, discovery studio, UCSF Chimera and LigPlot softwares. Introducing other docking softwares such as Vina, Smina, iDock etc.

[10 Hours including laboratory sessions]

✸ **MODULE II: Molecular Graphics Visualization**:

Preparation of 2D molecules using ChemSketch and Chemdraw - Molecular editor and visualization in 3D using Avogadro, GaussView, McMolPlt and Chemcraft

[6 Hours including laboratory sessions]

✸ **MODULE III: Basic Computational Science**:

Theoretical background of computational chemistry – Installing GAMESS in Linux and Windows PC – using python code to run GAMESS files - introduction to basic theory of computational chemistry – designing input files manually using text editor – designing input files using Avgadro and GaussView - Calculation of Molecular parameters using MOLPRO/GAUSSIAN/GAMESS Softwares – Analysing the output file manually and using molecular visualization softwares – Calculation of single point energy – minimization of molecular structures by geometry optimization – examining optimization results

[14 Hours including laboratory sessions]

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ENROLMENT LIST FOR THE ADD-ON COURSE (ACADS 2022)

Sl. No.	Name	M/F	Department	Sem	Faculty?	Course
1	Dr.ANJANA GEORGE	F	Chemistry	N/A	Yes	N/A
2	Dr.KEERTHI MOHAN A	F	Chemistry	N/A	Yes	N/A
3	Mrs.VIJI K	F	Chemistry	N/A	Yes	N/A
4	Mrs.DHANUSHA KK	F	Chemistry	N/A	Yes	N/A
5	Ms.AKHILA M V	F	Chemistry	4	No	PG
6	Ms.AMINATH SUMAYYA K B	F	Chemistry	1	No	PG
7	Ms.DEEPTHI N	F	Chemistry	2	No	PG
8	Ms.FATHIMATH SAFA.M	F	Chemistry	2	No	PG
9	Ms.FATHIMATH SHAHEERA R P	F	Chemistry	4	No	PG
10	Ms.GOPIKA M	F	Chemistry	2	No	PG
11	Ms.GOPIKA R KRISHNAN	F	Chemistry	4	No	PG
12	Ms.JYOTHILAKSHMI M	F	Chemistry	4	No	PG
13	Ms.MAYOOKHA. M	F	Chemistry	4	No	PG
14	Ms.NISARGA K	F	Chemistry	4	No	PG
15	Ms.PRAVEENA K V	F	Chemistry	2	No	PG
16	Ms.SARIGA DAS	F	Chemistry	4	No	PG
17	Ms.SETLANA A V S	F	Chemistry	2	No	PG
18	Ms.SHABNA	F	Chemistry	2	No	PG
19	Ms.SHRIDEVI E	F	Chemistry	2	No	PG
20	Ms.SREELAKSHMI C	F	Chemistry	4	No	PG
21	Ms.VISMAYA BHASKARAN	F	Chemistry	2	No	PG
22	Ms.ANAGHA A K.	F	Chemistry	2	No	UG
23	Ms.ANAGHA K	F	Chemistry	2	No	UG
24	Ms.BINITHA K	F	Chemistry	4	No	UG
25	Ms.KEERTHI M	F	Chemistry	2	No	UG
26	Ms.NAVYA M C	F	Chemistry	2	No	UG
27	Ms.SANGEETHA G K	F	Chemistry	4	No	UG
28	Ms.YASHWITHA U B	F	Chemistry	2	No	UG

Name and Signature of the Principal
Dr.Ananthapadmanabha.A.L

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Attendance Sheet:

No	Name	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	Dr.ANJANA GEORGE															
2	Dr.KEERTHI MOHAN A															
3	Mrs.VIJI K															
4	Mrs.DHANUSHA KK															
5	Ms.AKHILA M V															
6	Ms.AMINATH SUMAYYA K B															
7	Ms.DEEPTHI N															
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No	Name	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
		15/11/22	16/11/22	2/12/22	13/12/22	05/01/23	06/01/23	11/01/23	2/01/23	2/01/23	20/01/23	3/01/23	2/01/23	03/01/23	15/03/23	16/03/23
1	Dr.ANJANA GEORGE															
2	Dr.KEERTHI MOHAN A															
3	Mrs.VIJI K															
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Model Certificate:

CERTIFICATE
OF COMPLETION

PROUDLY PRESENTED THIS

GOPIKA R KRISHNAN

For successfully completed the add-on course entitled "Applications of Computer Aided Designs in Sciences (ACADS)" conducted by the department of chemistry , Government College Kasaragod during the academic year 2022 -23

HONOURED MENTION

SIGNATURE
(COORDINATOR, ACADS 2022)

SIGNATURE
(HEAD, DEPARTMENT OF CHEMISTRY)

Name and Signature of the Principal
Dr.Ananthapadmanabha.A.L

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ACADS REPORT

ADD-ON COURSE 2022 -23

GOVERNMENT COLLEGE KASARAGOD

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Report on add-on course
APPLICATIONS OF COMPUTER AIDED DESIGNS IN SCIENCE (ACADS)
YEAR 2022 – 23

Offering Department: **Chemistry**
Government College Kasaragod

Executive Summary:
This report provides an overview of the successful implementation of the add-on course titled "Applications of Computer-Aided Designs in Sciences," offered by the Department of Chemistry at our college. This specialized course was designed to bridge the gap between traditional chemistry education and modern computational tools, equipping students with valuable skills in computer-aided design (CAD) as applied to scientific research. The report outlines implementation process, outcomes, challenges, and future recommendations. Curriculum and learning outcomes were already mentioned in the syllabus. 30 hours course included theory and hands on training.

Introduction:
In an era characterized by the integration of technology into scientific research and experimentation, the Department of Chemistry recognized the need to offer a course that equips students with essential skills in skills in computer-aided design (CAD). The "Applications of Computer-Aided Designs in Sciences" course aimed to empower chemistry students with the ability to use CAD software effectively for data visualization, molecular modeling, and scientific simulations.

Implementation Process:
The implementation process included the following steps:
1. Faculty Selection: An experienced faculty member with expertise in CAD and chemistry was chosen to teach the course. Dr. VC Saheer, Assistant professor in the department of chemistry has been selected for this course.
2. Computer Lab Facilities: Dedicated computer labs with skills in CAD software were made available to students.
3. Curriculum Development: The curriculum was meticulously designed to ensure alignment with the course objectives.
4. Teaching Methodology: A blend of lectures, hands-on lab sessions, and project work encouraged active learning and practical application of CAD tools.

Key Outcomes:
The course yielded significant outcomes:
1. CAD Proficiency: Students developed proficiency in using skills in CAD software, allowing them to create accurate molecular models and visualizations.

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2. Interdisciplinary Perspective: Exposure to skills in CAD applications in various scientific fields broadened students' perspectives.
3. Research Competence: Students applied skills in CAD techniques to research projects, enhancing their research skills and scientific communication abilities.
4. Career Readiness: Graduates of the course are well-equipped with skills in demand in scientific research and industry.

Challenges Faced:

While the course was successful, it faced some challenges:
1. Technical Requirements: Ensuring access to skills in CAD software and hardware for all students required careful planning and resource allocation.
2. Diverse Skill Levels: Students entered the course with varying levels of skills in CAD and chemistry knowledge, necessitating adaptable teaching methods.

Future Recommendations:

To build upon the success of the course, the following recommendations are made:
1. Resource Expansion: Increase the availability of skills in CAD software and training resources to accommodate a larger number of students.
2. Advanced Levels: Consider offering advanced skills in CAD courses tailored to specific scientific disciplines.
3. Collaboration: Explore opportunities for interdisciplinary collaboration with other departments to expand skills in CAD applications.

In conclusion, the "Applications of Computer-Aided Designs in Sciences" course offered by the Department of Chemistry has enriched our curriculum, fostering interdisciplinary education and equipping students with valuable CAD skills. The course's success exemplifies our commitment to providing cutting-edge scientific education and preparing students for future research and industry challenges in chemistry and related fields.

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