

Department of Chemistry, St. John's College Anchal

Add-on Course "Software Tools Essential for Chemical Sciences"

The Department of Chemistry, St. John's College Anchal is offering a 50 hour Add-on course in software tools essential for chemical sciences. It is an entire essential software learning package for chemistry scientific paper writing / project writing.

Eligibility requirement

B. Sc. With Chemistry as major or optional subject and must have obtained a minimum of 80% of marks in aggregate/optional subjects put together from all the years.

Course Start Date: 01st December 2022

Course Content

SCIENTIFIC GRAPHING(5hours)

Softwares for communication and publication of scientific documents

Structure Drawing Softwares

Online resources for research

Reference managing softwares/Introduction to Citation Management

Infrastructural Facilities

Worldclass research lab

Classroom with multimedia projection

24x7 wi-fi facilities

Researchlab with HPLC, GC, Electrochemical workstation, AAS, UV –Visible spectroscopy,PH meter, Turbidity meter, Conductimeter, Potentiometer etc.

Central library and INFLIBNET services

Academic Excellence

Experienced and highly qualified teachers

Well equipped laboratories

Ph.D. programmes

Other Facility

Student placement Cell

Student association

Campus placement

Department of Chemistry is interacting to provide placements after successful completion of the course in reputed industries and research organizations

Application and Admission

The application form can download from the college website and filled application is submitted to email chemistry@stjohns.ac.in.

For any queries please contact Course coordinator: 9526439368



COURSE SUMMARY REPORT

2022-2023

Name of Course	Add-on "Software Tools Essential for Chemical Sciences"(CHE-ADO-22-001)
Course Duration	50 Hours
Department offering the Course	Department of Chemistry
Faculty In Charge	Dr Thomas Mathew
Number of Students Enrolled	12
Start Date & End Date	01/12/2022 to 01/04/2023

The add-on course on Software Tools Essential for Chemical Sciences"(CHE-ADO-22-001)has been coordinated by the Department of Chemistry, St John's College, Anchal. The course was specially designed to provide essential software tools required in chemistry for scientific paper writing(data processing, presentation and interpretation). The course had a well-defined syllabus and was approved by the IQAC. The certificate course was coordinated by Dr Thomas Mathew, Assistant Professor, Department of Chemistry. The course was properly planned and organised to provide maximum support to students during their learning and hands on practice process. The course duration was 50 hours. Twelve students enrolled for the program. The course started on 01.12.2022 and ended on 01.04.2023. During the end of course, an examination was conducted. All students appeared for the examination. Final assessment was done based on the marks secured by them during the written and hands own practice session. All students passed in the examination. Certificates were also provided to them after the successful completion of the course.

Course Coordinator

Principal
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Anchal-691 306,





Module 3(15 hours)

Structure Drawing Softwares

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.

Cambridge Chem Draw 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

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.

Introduction to basic features of Chemdraw, Chemical structure to name conversion, Chemical name to structure conversion, NMR spectrum simulation(both ¹H NMR & ¹³C NMR), Mass spectrum simulation, structure clean up, export to SVG, PDF. Introduction to Chems sketch-Molecular modelling, create and modifying images of chemical structures, write and perform chemical equations and diagrams.

Course Coordinator

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Software Tools Essential for Chemical Sciences"

COURSE DESCRIPTION:

Kerala university syllabus instruct project works for UG & PG students. There is a great demand of familiarizing various research tools such as Chemdraw, Chems sketch, Origin and many computational chemistry softwares which are the widely used in their studies. Chemdraw and chemsketch are used for the purpose of molecular modeling and structure designing. The scientific graphing and data analysis are done by using origin software. The add-on course mainly focused on equipping students with chemistry drawing and computational softwares. It also focused to teach students scientific data processing/interpretation for scientific paper writing and project writing etc.

COURSE OUTCOME:

Applying chemdraw and chemsketch softwares for molecular modeling, writing structures and chemical equations. To equip students with chemical structure drawing, computational, graphing and data analysis/interpretation software's for chemical data analysis, presentation and interpretation.

Total Hours :50

COURSE SYLLABUS (CHE-ADO-22-001)

Module 1

SCIENTIFIC GRAPHING (5hours)

Introduction to Origin, basic features like Scientific graphing, drawing various 2D & 3D plots, Data analysis, statistics, signal processing, curve and Surface fitting, peak analysis and conversion of graph to various file format like JPEG, GIF, EPS.

Module 2 (14 hours)


Softwares for communication and publication of scientific documents



Latex

Introduction to latex (includes download and installation). Create your first document, Fonts and paragraphs Lists. Making tables. Tabbing Line, page and word breaks, Spacing. Labels and references, Labelling and referencing figures and tables, Picture Environment, Importing Pictures, Making Special Parts such as Cover Page, Abstract, Other Front Matter, Back Matter, Footnotes. Create posters and presentations using latex. Beamer environment, Tikzposter.

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