National Workshop on

Synergetic Research Approach through RSM, Molecular Docking and SPSS for Scientific Computation

Sponsored by

M.P. Council of Science and Technology
4th to 6th January 2024

Organized by:
Department of Chemistry

St. Aloysius College(Autonomous), Jabalpur, M.P.

Re-Accredited 'A+' Grade By NAAC(3.68/4.00)
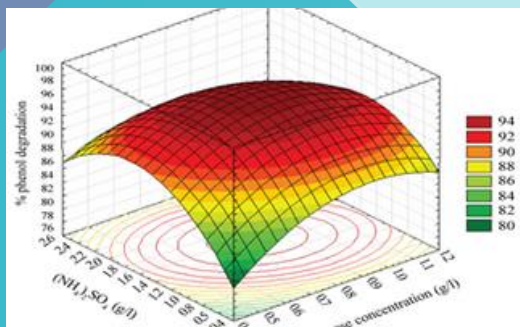College with Potential for Excellence by UGC
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ABOUT THE COLLEGE

St. Aloysius' College is a premier autonomous educational Institute in Madhya Pradesh. The college has been Re-accredited 'A+' by NAAC, Bangalore. It has carved a niche for itself by being the only college in the state, to have been awarded the highest CGPA (3.68/4.00) in all three cycles of NAAC accreditation and is also awarded with College with Potential for Excellence, DST-FIST Supported and Star College Scheme by DBT. St. Aloysius' College is synonymous with quality and has a legacy of efficiency. With its best infrastructure and rich academic ambience, the college holds glories of success in providing excellence in education and character building of the students proving its motto "*Virtus in Arduo*".

ABOUT THE NATIONAL WORKSHOP

Redman and Moore defined research as a systematized effort to gain new knowledge, a movement from known to unknow. It utilizes acceptable scientific methodology to solve problems and create new knowledge which is applicable. It aims at developing new technologies and solving practical problems, using procedures which are relevant, appropriate and justified.

TOOLS FOR RESEARCH DEVELOPMENT

RSM (Response Surface Methodology)

RSM, available in MINITAB and other proprietary softwares, combines statistical and mathematical techniques for process development, improvement, and optimization. It plays a crucial role in new product design and enhances existing ones. RSM identifies optimum factors for optimal results, making it a robust tool for manipulating and analyzing research data. Its applications extend to designing, developing, and formulating new products.

Molecular Docking

Molecular docking models the interaction between small molecules and proteins at the atomic level, revealing behavior within binding sites and elucidating biochemical processes. The process involves predicting ligand conformation, position, and orientation (pose) and assessing binding affinity. Molecular docking is pivotal for understanding chemical compound interactions with molecular targets, aiding drug discovery. The increasing number of studies on molecular docking demonstrates its importance in identifying structural determinants for efficient ligand-receptor binding and advancing accurate docking methods.

SPSS (Statistical Package for the Social Sciences)

SPSS Statistics, developed by IBM, is a widely-used software suite for data management, advanced analytics, and multivariate analysis. Acquired by IBM in 2009, it is particularly popular in human behavior research. SPSS offers a user-friendly graphical interface for compiling non-parametric and parametric analyses, descriptive statistics, and graphical depictions. It also supports advanced statistical processing and script automation.

OBJECTIVES OF THE WORKSHOP

- To cover fundamental principles and functionality of software tools, including RSM, SPSS, and Molecular Docking, and develop diverse data analysis methods for qualitative and quantitative data.
- To provide participants with timely updates and offer comprehensive training in powerful software tools like RSM, SPSS, and Molecular Docking, relieving researchers from computational complexities.
- To emphasize the importance of defining, organizing, and analyzing data, drawing meaningful conclusions, and evaluating their robustness and uncertainties.
- To focus on deep research and complex data analysis using SPSS, explore process optimization with RSM, and showcase molecular docking's predictive role in biochemical reactions.
- To foster high-quality contributions to scientific research, particularly in Life Sciences instrumentation.
- To assess and stay abreast of advancements in scientific analysis.

GUEST SPEAKERS

Dr. Gaurav Dwivedi
Topic: "Response Surface Methodology"
MANIT, Bhopal, M.P.

Dr. Nilanjana Jain
Topic: "Molecular docking and drug designing"
Govt College, Udaynagar, Dewas, M.P.

Dr. Jai Anand Shukul
Topic: "SPSS"
Mangalaytan University, Jabalpur, M.P.