Overview of the Course Scheme for PhD programme

As per the university ordinance and new guidelines, the research scholars who are provisionally registered under the PhD programme will have to undergo a pre-PhD coursework. The pre-PhD coursework shall have three components. Every student admitted to the PhD programme (Chemistry) will have to pass a 'coursework' with minimum of 14 credits. The candidate can submit his/her thesis only after passing the course work.

Component one (Core Courses)

This component will comprise of three courses of 10 credits which are general to a PhD programme in Chemistry and every research scholar will have to opt for these courses mandatorily. It will have following courses:

i. Research and Publication Ethics
ii. Research Methodology
iii. Tools and Techniques in Chemistry

Component two (Research Centric)

The course is based on recent developments on the particular research topic assigned to the research student to envisage the recent developments in the available literature.

Component three (Discipline Centric Elective Courses)

This component will comprise of a basket of courses belonging to different research fields. Each course will be of 2 credits and out of the available basket of courses; students will have to opt for at least one course that will be mandatory for completion of the PhD course work.

Semester	Course Code	Course Title	Course Type	Maximum Marks			Credit Distribution			Credits
				Internal*	Final	Total	L	T	P	
Core	CHM900C	Research and Publication Ethics	Core	25	25	50	2	0	0	2
	CHM901C	Research Methodology	Core	50	50	100	3	1	0	4
	CHM902C	Tools and Techniques in Chemistry	Core	50	50	100	3	1	0	4
Research Centric	CHM903C	Seminar on Recent Developments in the Area of Research	Core	Write-up-50 Presentation-30 Viva-20		100				2
Discipline Centric Elective	CHM904E	Biopolymers and Hydrogels	Elective	25	25	50	2	0	0	2
	CHM905E	Modern methods of Electronic Structure	Elective	25	25	50	2	0	0	2
	CHM906E	Computational Quantum Chemistry	Elective	25	25	50	2	0	0	2
	CHM907E	Nanoscience and Nanotechnology	Elective	25	25	50	2	0	0	2
	CHM908E	Catalysis and its application	Elective	25	25	50	2	0	0	2
	CHM909E	Medicinal Chemistry	Elective	25	25	50	2	0	0	2
	CHM910E	Supramolecular Chemistry	Elective	25	25	50	2	0	0	2
Total Credits										14

*(Midterm 30 marks +Assignment/Attendance 20 marks

PhD (Coursework)

Core Course

Course Title: Research and Publication Ethics

Course Code: CHM 900C

Credits: 2

Marks: 50

The course comprises of six modules listed in table below. Each module has 4-5 units

Modules	Unit Title	Teaching Hours
Theory		
PRE 01	Philosophy and Ethics	4
PRE 02	Scientific Conduct	4
PRE 03	Publication Ethics	7
Practice		
PRE 04	Open Access Publishing	4
PRE 05	Publication Misconduct	4
PRE 06	Databases and Research Metrics	7
	Total	**30**

THEORY

RPE 01: Philosophy and Ethics (3 HRS)

1. Introduction to philosophy: definition, nature and scope, concept, branches 2. Ethics: definition, moral philosophy, nature of moral judgments and relations.

RPE 02: Scientific Conduct (5 HRS)

1. Ethics with respect to science and research
2. Intellectual honesty and research integrity
3. Scientific misconducts: falsification, fabrication, and plagiarism.
4. Redundant publications: duplicate and overlapping publications, salami slicing 5. Selective reporting and misrepresentation of data.

RPE 03: Publication Ethics (7 HRS)

1. Publication ethics: definition, introduction and importance
2. Best practices/standards setting initiatives and guidelines: COPE, WAME, etc.
3. Conflicts of interest
4. Publication misconduct: definition, concept, problems that lead to unethical behaviour and vice versa, types
5. Violation of publication ethics, authorship and contributor ship
6. Identification of publication misconduct, complaints and appeals
7. Predatory publishers and journals

PRACTICE

RPE 04: Open Access Publishing (4 HRS)

1. Open access publications and initiatives
2. SHERPA/RoMEO online resources to check publisher copyright and self-archiving policies.
3. Software tool to identify predatory publications developed by SPPU
4. Journal finder/ journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggested, etc.

RPE 05: Publication Misconduct (4 HRS)

A. Group Discussions (2hrs)

1. Subject specific ethical issues, FFP, authorship
2. Conflicts of interest
3. Complaints and appeals: examples and fraud from India and abroad

B. Software tools (2hrs)

Use of plagiarism software like Turnitin, Urkund and other open source software tools.

RPE 06: Databases and Research Metrics (7 HRS)

A. Databases (4 hrs)

Indexing databases, Citation databases: Web of Science, Scopus, etc.

B. Research Metrics (3 hrs)

Impact Factor of journal as per journal citation report, SNIP, SJR, IPP, Cite Score. Metrics: h-index, g index, i10 index, altmetrics

Books Recommended:

1. Indian National Science Academy (INSA) Ethics in Science and Education, research and government (2019) ISBN: 978-81939482-1-7 http://www.insaindia.res.in/pdf/Ethics_Books.pdf
2. P.Chaddah, (2018) Ethics in competitive Research , Do not get scooped; do not get plagiarized, ISBN: 978-9387480865
3. Beall, J (2012). Predatory publishers are corrupting open access, Nature ,(489 (7415), 179-179, http://doi.org/10.1038/489179a
4. Resnik, D.B(2011) What is ethics in research and why it is important , National Institute of Environmental Health Sciences , 1-10, retrieved from, http://niehs.nih.gov/research/resources/bioethics/whatis/index.cfm
5. National Academy of Sciences, National Academy of Engineering and Institute of Medicine (2009) on being a scientist : guide to Responsible conduct in research : Third Edition, National Academies Press
6. Bird,A. (2006) Philosophy of Science, Routledge
7. Maclntyre, Alasdair (1967) A short story of Ethics, London

PhD (Coursework)
Core Course
Course Title: Research Methodology

Course Code: CHM901C
Credits: 4
Marks: 100

Unit I : Research Proposal

Origin of a research proposal: Selection of research area; Review of latest literature; Overview of status of research area; Identification of the research problem; Importance of the proposed project; Aims and objectives; Hypothesis building ; Work plan, materials and methodology to be followed; Instrumentation required; Instruments available in the PI's department / University. Collaboration with other Institutions for use of advanced instrumentation. Conflict of interest statement.

Unit II: Thesis writing

Types of technical documents: Full length research paper, Short/Brief communications, Letters to editor, Book chapter, Review, Conference report. Components of thesis/full length research paper. Topic/Title; Abstract, key words; Introduction, Rationale of the paper, Materials & methods; Results and discussion; Key issues and arguments; result summary & conclusion; Acknowledgement. Bibliography

Technical resumes & components of the cover letter.

Unit III: Errors & Error Analysis

Error Analysis, Determinate and indeterminate errors, Accuracy and precision, Mean, Median, Average deviation and standard deviation, Tests of significance: Comparison of methods: F-test and T-test, Rejection of data based on Q-test, Correlation and regression ANOVA– One-way and Two-way, Multiple-range test.

Unit IV: Use of Software in Data Analysis

Concepts and difference between sensitivity, LOD and LOQ, Usage of ORIGIN, EXCEL for data analysis, Method of least squares and successive approximation, Correlation and regression– Linear and non-linear fitting (quadratic, exponential, polynomial); Multiple variable matrix and its analysis, Drawing of good fit lines, Slopes, Correlation coefficients and their significance.

Books Recommended

1. Research Methodology - R Panneerselvam, 2nd Edition, 2014
2. Research Methodology, Methods Techniques, C.R.Kothari, ViswaPrakashan, 2ndEdition, 2009.
3. Research Methods-A Process of Inquiry, Graziano, A.M., Raulin, M. L, Pearson Publications,7th Edition,2009.
4. Research Methodology: Methods & techniques, CR Kothari, 2008
5. Instrumental Methods of Analysis, 7th Ed., Willard, Merritt, Dean and Settle, CBS Publishers, New Delhi.
6. Instrumental methods of Chemical Analysis, 5thedn., G.W. Ewig, McGraw Hill Book Co., 1985.
7. KV Raman, Computers in Chemistry, Tata McGraw Hill, 1993

PhD (Coursework)
Core Course

Course Title: Tools and Techniques in Chemistry

Course Code: CHM902C

Credits:4

Marks: 100

Unit: I Spectroscopic Characterization

Infra-red spectroscopy- Interpretation of Spectra; Characteristic group frequencies of molecules.

Mass spectroscopy- Instrumentation; Mass spectrum; Determination of molecular formula; Recognition of molecular ion peak; Ionization techniques; Fragmentation and rearrangements; Quantitative applications of mass spectrometry.

Spectral interpretation and structural determination of some organic compounds using Nuclear Magnetic Resonance, Electron Spin Resonance, UV-Vis spectroscopy.

Unit: I Thermal and Separation Methods

Thermo analytical methods: Differential thermal analysis; Differential Scanning Calorimetry

An introduction to chromatographic separations; Gas chromatography; Gas chromatographic columns and stationary phases; Principles and applications of gas-liquid chromatography; High-Performance Liquid Chromatography (HPLC), Application of GC-MS and LC-MS.

Unit: III Surface Characterization by Spectroscopy and Microscopy

X-ray diffraction- Lattice; Lattice symmetry; Characterization of powder and single X-ray Crystallography, Surface Properties (XPS, BET)

Microscopic methods (Polarized optical microscope, SEM, TEM, AFM),

Unit: IV Electro Analytical Methods

Potentiometry. Potentiometric titrations, titration curves and their evaluation. pH measurements, standard buffer solutions, pH electrodes. Polarography: Determination of trace metal ions in pharmaceutical products and estimate drugs that contain metal ions as constituents. Cyclic Voltammetry: Anodic, cathodic and adsorptive stripping voltammetry. Reversible process (Randles-Sevcik equation) and irreversible (Delahay equation)

Books recommended.

1. J.M. Hollas, 2004, Modern Spectroscopy, 4th Edition. John Wiley and Sons, Chichester
2. R.M. Silverstein and F.X. Webster, 2003, Spectroscopic Identification of Organic Compounds, 6th Edition. John Wiley, New York.
3. D.A. Skoog, F.J. Holler and T.A. Nieman, 1998, Principles of Instrumental Analysis, 5th Edition, Harcourt Brace & Company, Florida
4. C.N. Banwell and E.M. Mc Cash, 1994, Fundamentals of Molecular Spectroscopy, 4th Edition. Tata McGraw Hill, New Delhi.
5. R.S. Drago, 1992, Physical Methods in Chemistry, International Edition, Affiliated East-West Press, New Delhi.
6. J.R.Dyer, 1978, Application of Absorption Spectroscopy of Organic Compounds. Prentice Hall, New Delhi.
7. R.L. Pecsok, L. D. Shields, T. Cairns and L.C. Mc William, 1976, Modern Methods of Chemical Analysis, 2nd Edition. John Wiley, New York.

PhD (Coursework)
Core Course

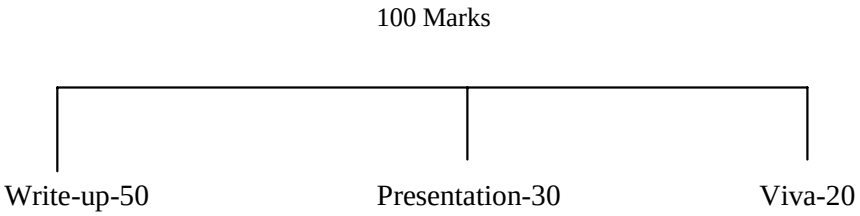
Course Title: Seminar on Recent Developments in the Area of Research

Course Code: CHM903C

Credits: 2

Marks: 100

Review of published literature: Preparation of a comprehensive and critical review of the already published literature in his/her proposed field of study in same may be submitted to a refereed/reputed journal as notified by UGC. The candidate will be evaluated on the basis of a comprehensive report to be submitted and a seminar to be delivered at the end of the semester.



PhD (Coursework)

Discipline Centric

Course Title: Biopolymers and Hydrogels

Course Code: CHM904E

Credits: 2

Marks: 50

Unit I Fundamentals of Biopolymers

Definition of biopolymers and types of biopolymers, Description of certain biopolymers like starch, cellulose, chitosan, gelatin, alginate, keratin, fatty acids, lipids, aliphatic polyesters (PLA, PHB), Cellulose derivatives and cellulose regenerating processes, Bio based composites, natural biodegradable polymer, synthetic biodegradable polymer and modified naturally biodegradable polymer, Concept of biocompatibility and responsiveness, Technically important forms of polymers (Hydrogel, bioceramics, bioelastomers and membranes), Mechanical properties (elasticity, yield stress, ductility, toughness, strength, fatigue, hardness and wear resistance) of biomaterials.

Unit II Synthesis and Characterization of Hydrogels

Introduction to hydrogel and brief historical overview, Classification of hydrogels based on origin, type of interaction, and ionic/non-ionic characteristics, Different types of gel forming techniques (Physically and chemically cross-linked hydrogels), Evaluation of swelling behaviors of hydrogels (Swelling capacity and water retention capacity) and kinetic analysis, Effect of pH, ionic strength and temperature on swelling properties of hydrogels, Relationship between morphology and swelling properties, Mechanical and rheological properties of hydrogel, smart hydrogels, characterization of hydrogels, Application of hydrogels.

Books Recommended:

1. Michael Niaounakis, Biopolymers: Applications and Trends, William Andrew Publication, 2015.
2. Odian, G., Principles of Polymerization, John Wiley & Sons (2001).
3. Gowarikar, V. R., Polymer Science, New Age International Pvt. Ltd., New Delhi (1997).
4. Campbell D. and White J.R., "Polymer Characterization: Physical Techniques", Chapman & Hall, London, 1989. 4. Schnabel W., "Polymer Degradation:
5. Principles and Practical Applications", Carl Hanser Verlag, 1981 5. Hawki
6. Cantor, C.R., and Schimmel, P.R., Biophysical Chemistry, Freeman (1980)
7. https://nptel.ac.in/courses/102/106/102106057/
8. https://iopscience.iop.org/article/10.1088/1742-6596/3/1/004/pdf
9. https://www.chemistrylearner.com/biopolymer.html

PhD (Coursework)

Discipline Centric Elective

Course Title: Modern Methods of Electronic Structure

Course Code: CHM905E

Credits: 2

Marks: 50

Unit: I Multi-electron systems and Hartree-Fock Approximation

Many electron operators and wave functions, Born-Oppenheimer approximation, Antisymmetry principle, Spin and space orbitals, Hartree product and Slater determinant wave functions.

Hartree-Fock approximation, Minimal basis H_2 model, One and two electron integrals, Coloumb and exchange operators/integrals in light of minimal basis H_2 model

Roothan equations and their matrix form, Self-consistent procedure, Basis sets, Limitations of Harttree-Fock model, Electron correlation, Brief introduction to multi-determinant wave function methods (Configuration interaction and Coupled Cluster methods).

Unit: II Introduction to Density Functional Theory

Density functional theory: Electron density as basic variable**,** Hohenberg-Kohn theorems, Kohn-Sham approach, Orbitals and the non-interacting reference system, Kohn-Sham equations and potential.

Exchange-Correlation energy in the Kohn-Sham scheme, Exchange-correlation functional, Local density and local spin-density approximations, Generalized gradient approximation, Hybrid functionals,

Books Recommended:

1. Quantum Chemistry- Ira. N. Levine, Prentice Hall, 7th Edn.; 2013.
2. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedmann, (Oxford, 2008).
3. A Chemist's Guide to Density Functional Theory. Second Edition W. Koch and M. C. Holthausen (Wiley-VCH Verlag GmbH, 2001)
4. Molecular Electronic-Structure Theory T. Helgaker, P. Jorgensen and J. Olsen, (Wiley, 2000)
5. Density Functional Theory of Atoms and Molecules, R.G. Parr and W. Yang, Oxford(1989)
6. Modern Quantum Chemistry Introduction to Advanced electronic structure theory A. Szabo & N. S. Ostlund, (Macmillan, 1982, Dover 1996).

PhD (Coursework)

Discipline Centric Elective

Course Title: Computational Quantum Chemistry

Course Code: CHM906E

Credits: 2

Marks: 50

Unit I: Linux Operating System and GUIs QM Calculations

Linux operating system: Installation and some basic commands, Making directories and files in Linux, Installation of GUIs such as Molden, Gauss View, Xcrysden, VESTA. Building simple molecules with different GUIs and saving in different formats. Visualizing bond lengths, bond angles, dihedral angles. Building units cells and slabs using VESTA.

Unit: II Basic Input and Output for QM Calculations

Sections of input file for Gaussian calculation, Geometry optimization and single point calculations on CH_4 and O_2 molecules. Frequency calculations to compute IR and Raman spectra, Visualising the output file using different GUIs, Important parameters in the output file. Calculation of some basic properties such as HOMO-LUMO gap, IP, EA of CH_4 and O_2. Plotting molecular orbitals for CH_4 and O_2

Books Recommended:

1. Linux for Beginners: An Introduction to the Linux Operating System, Jason Cannon
2. Linux Command Line and Shell Scripting Bible, Richard Blum, Wiley, Third Edition
3. (a) https://www3.cmbi.umcn.nl/molden/(b)http://www.xcrysden.org/ (c) http://www.jp-minerals.org/vesta/en/
4. GAUSSIAN Manual, Gaussian Inc
5. Exploring chemistry with electronic structure methods, Foresman J.B., Frisch A., Gaussian Inc
6. Gaussian 16 Users Reference | Gaussian.com

PhD (Coursework)

Discipline Centric Elective

Course Title: Nanoscience and Nanotechnology

Course Code: CHM907E

Credits: 2

Marks: 50

Unit: I Synthesis of Nanomaterials

Definition**,** Types of nanostructures, properties and applications**:**

One dimensional, Two dimensional and Three dimensional nanostructured materials, Quantum dots shell structures, metal oxides, semiconductors, composites, mechanical-physical-chemical properties, application as ferroelectric materials, coating, molecular electronics and nanoelectronics, biological and environmental, membrane based application, polymer based application, nanocatalysis, basic principle. Synthesis and preparation of Nanomaterials and Synthetic Techniques**:** Synthesis of bulk nanostructured materials - Sol Gel processing- bulk and nano composite materials - Grinding - high energy ball milling- injection moulding - extrusion - melt quenching and annealing, Self assembly-Self Assembled Monolayers (SAM) - Vapour Liquid Solid (VLS) approach - Chemical Vapour Deposition (CVD), Hydrothermal and microwave method.

Unit: II Carbon nanotube and Graphene

Carbon nanostructures: Synthesis, separation and characterization of Fullerene and its derivatives, applications, toxicity. Carbon nanotube (CNT), structure, synthesis and functionalization of CNT, Electronic, Vibrational, Mechanical and Optical properties of CNT, Graphene, structure, synthesis and functionalization of Graphene, Graphene composites, Electronic applications of Graphene, Graphene Oxide. The environmental effects of carbon based nanomaterials**.**

Books Recommended:

1. Instrument E L Principe, P Gnauck and P Hoffrogge, Microscopy and Microanalysis (2005), Cambridge University Press.
2. Naostructures and Nanomaterials: Synthesis, properties and applications, Imperical College Press, 2004 - G.Cao
3. Chemistry of nanomaterials : Synthesis, properties and applications –C.N.R. Rao (2004)
4. Nanoparticles: From theory to applications, Wiley Weinheim , G. Schmidt,.2004
5. Biosensors: A Practical Approach, Oxford University Press, 2004 - J. Cooper & C. Tass,
6. Advances in Nanotechnology and the Environment, CRC Press, Taylor and Francis Group - Juyoung Kim
7. Chemical Sensors and Biosensors, Wiley; New York, Chichester, 2002 - Brian R Eggins.
8. Handbook of nanoscience, Engg. and Technology, CRC Press, 2002 - W. Gaddand, D. Brenner, S. Lysherski and G. J. Infrate (Eds)

PhD (Coursework)

Discipline Centric Elective

Course Title: Catalysis and Its Application

Course Code: CHM908E

Credits: 2

Marks: 50

Unit: I Homogeneous Catalysis

Catalysis: Terminology in catalysis, TO(Turnover),TON(Turnover number), TOF(Turnover frequency), Sequences involved in a catalysed reaction, Other terms used in catalysis, enentioselectivity, stereoselectivity, chemoselectivity, regioselectivity, Asymmetric synthesis using a catalyst. Hydroformylation: Importance, Cobalt catalyst for hydroformylation, Phosphinemodified cobalt catalysis, Rhodium-Phosphine catalyst, Factors affecting n/iso ratio of hydroformylation product, Enantioselective hydroformylation. Methanol Carbonylation and Olefin Oxidation: Monsanto process of conversion of methanol to acetic acid.

Unit: II Heterogeneous Catalysis

Heterogeneous catalysis: Broad categories of catalysts metals, bimetals, semiconductors, insulators, zeolites, oxides and nano materials.

Preparation of metal catalysts: Supported metal catalysts and non- metallic catalysts. Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method. Pore size and specificity of catalysts. Surface acidity of catalyst & determination of surface acidity by indicator method, IR spectroscopic method and TPD method.

Steps in heterogeneous catalyzed reactions: Catalytic activity the determining factors. Structure sensitive and structure insensitive catalysts. Mechanism of surface-catalyzed reactions.

Books Recommended:

1. Basic Organometallic Chemistry, Concept, Synthesis and Applications, Universities PressB. D. Gupta and A. J.Elias 2013
2. Catalysis, Principles and applications, edited by B. Vishwanathan, S. Sivasanker & A. V. Rama Swamy, NarosaPublishing House, 2011
3. Applied Homogeneous Catalysis,Wiley VCH, Weinheim, 2002- B. Cornils, W. A. Hermann, Homogeneous Catalysis, John Wiley, 2002 S. Bhaduri and D. Mukesh
4. Principles of Heterogeneous Catalysis in practice, G. C. Bond, Oxford Publishing, 1987
5. Recent Achievements, Trends and Prospects in Homogeneous Catalysis, F. J. Waller, Journal of MolecularCatalysis, 31 (1985) 123 136
6. Heterogeneous Catalysis, C. Satte rfield, McGraw Hill, 1981

PhD (Coursework)

Discipline Centric Elective Course

Course Title: Supramolecular Chemistry

Course Code: CHM910E

Credits = 2

Max. Marks = 50

Course Outcome:

- **Comprehension of the fundamental concepts of supramolecular chemistry**
- **Learn the skills to design, analyse, and manipulate molecular assemblies**
- **To know the practical applications of supramolecular chemistry**
- **To know the Interdisciplinary nature of supramolecular chemistry**

Unit-1. Principles of Supramolecular Chemistry 16 hrs

Concept of Supramolecular systems, various supramolecular interactions: Host-Guest Chemistry, Molecular Host systems, Macrocycles, Binding Constant.

Unit-2. Supramolecular Cages, Macrocycles and Frameworks 16 hrs

Design strategy of Schiff-based organic cages and macrocycles. Covalent Organic Frameworks (COFs) Applications of organic cages and macrocycles in recognition of different guest molecules.

Coordination driven self-assembly, cis-block Pd (II) and Pt (II) based metal acceptors, Nitrogen containing donor ligand systems, Design strategy of coordination cages and macrocycles. Application of coordination cages in catalysis. Metal Organic Framework (MOFs)

Books Recommended:

1. Lehn, Jean-Marie. Supramolecular chemistry. Vol. 1. 1995, .New York: Vch, Weinheim,

2. H. J. Schneider and A. Yatsimirsky, Principles and Methods in Supramolecular Chemistry, 28, 2000, Wiley, New York.

3. J. W. Steed and J. L. Atwood, Supramolecular Chemistry, 73, 2009. John Wiley & Sons,

4. Beer, Paúl, Paul D. Beer, Timothy A. Barendt, and Jason YC Lim. Supramolecular Chemistry: Fundamentals and Applications 2022. Oxford University Press.

Research Articles

1. Chakrabarty, P. S. Mukherjee, P. J. Stang, Chem. Rev. 2011, 111, 6810–6918.

2. Ding, San-Yuan, and Wei Wang. & quot; Covalent organic frameworks (COFs): from design to applications." Chemical Society Reviews 42, no. 2 (2013): 548-568.

3. Schmidt, A., Casini, A., & Kühn, F. E. (2014). Self-assembled M2L4 coordination cages: Synthesis and potential applications. Coordination Chemistry Reviews, 275, 19–36.

4. Kirchon, Angelo, Liang Feng, Hannah F. Drake, Elizabeth A. Joseph, and Hong-Cai Zhou. "From fundamentals to applications: a toolbox for robust and multifunctional MOF materials." Chemical Society Reviews 47, no. 23 (2018): 8611-8638.

5. Acharyya, Koushik, and Partha Sarathi Mukherjee. "Organic imine cages: molecular marriage and applications.& quot; Angewandte Chemie 131, no. 26 (2019): 8732-8745.

PhD (Coursework)

Discipline Centric Elective Course

Course Title: Medicinal Chemistry

Course Code: CHM909E

Credits = 2

Max. Marks = 50

Course outcome:

- **Students should understand the principles and processes involved in drug discovery.**
- **Skills for isolating and characterizing of Natural Products from different sources and**
- **various analytical techniques used in the field, including chromatography, NMR and mass spectroscopy.**
- **Designing the schemes for carrying chemical derivatization to modulate biological Activities**

Unit-I: Natural products and Medicinal Chemistry 16 h

Introduction to natural products. General classification and extraction procedures for the Isolation of NPs. Isolation and purification of organic compounds (solids and liquids) with special emphasis on chromatographic techniques: TLC, column chromatography, flash and HPLC, GC and LCMS. Role of natural products as anticancer, analgesics, antipyretic, anti-inflammatory agents, antibiotics: antibacterial, antifungal and antiviral agents

Unit –II: Disconnection approach of synthesis 16 h

Disconnection approach of synthesis: Introduction, main synthetic strategies, Group disconnection, Umpolung Strategies, α functionalization of carbonyl compounds. Synthetic approach to cyclic systems. Retro synthetic and reconnection strategies of some representative drugs such as analgesics agents, antipyretic agents, antiinflammatory agents (Aspirin, paracetamol, lbuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim), etc. Concept of Chemical derivatization using common bioactive scaffolds.

Books Recommended:

1. Warren, S., & Wyatt, P. (2008). Organic synthesis: the disconnection approach. John Wiley & Sons.
2. Stephen H, Simon G, and B L. Merner (2013) Design and strategy in organic synthesis: from the Chiron approach to catalysis, Wiley-VCH Verlag GmbH & Co. KGa
3. Mandal, S. C., Mandal, V., & Konishi, T. (Eds.). (2018). Natural Products and Drug Discovery: An Integrated Approach. Elsevie In Annual Reports in Medicinal Chemistry (Vol. 55, pp. 1-44). Academic Press.
4. Silverman, R. B., & Holladay, M. W. (2014). The organic chemistry of drug design and drug action. Academic press.
5. Worwood, V. A. (2016). The complete book of essential oils and aromatherapy revised and expanded: over 800 natural, nontoxic, and fragrant recipes to create health, beauty, and safe home and work environments. New World Library.
6. Samuelsson, G. (2004). Drugs of natural origin: a textbook of pharmacognosy, 5th Swedish Pharmaceutical Press. Stockholm, Sweden.
7. Newman, D. J., Cragg, G. M., & Snader, K. M. (2000). The influence of natural