# **III SEMESTER**

ADVANCED ORGANIC CHEMISTRY									
Course Code	22MSC31	CIE Marks	50						
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50						
Total Hours of Pedagogy	50	Total Marks	100						
Credits	4	Exam Hours	3						

- To understand the reactions of organic compounds involving various reagents.
- To learn the synthesis and retro-synthesis of different organic compounds.

#### Module-1

Oxidation: (a)Metal based and non-metal based oxidations of alcohols (chromium, manganese, silver, ruthenium, DMSO, and hypervalent iodine). (b) Peracids oxidation of alkenes and carbonyls. (c) Alkenes to diols (manganese, osmium based), alkenes to carbonyls with bond cleavage (manganese, ruthenium, and lead based, ozonolysis), and alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, and selenium based allylic oxidation).

(d) Asymmetric epoxidations (Sharpless, Jacobsen, and Shi epoxidations) and Sharpless asymmetric dihydroxylation.

#### Module-2

Reduction: (a) Catalytic homogeneous and heterogeneous hydrogenation, Wilkinson catalyst. (b) Metal based reductions using Li/Na in liquid ammonia, sodium, magnesium, zinc, titanium, and samarium. (c) Hydride transfer reagents: NaBH4, L- selectride, K-selectride, Luche reduction, LiAlH4, DIBAL-H, Red-Al, Trialkylsilanes, and Trialkylstannane. (d) Enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata) and Noyori asymmetric hydrogenation.

#### Module-3

Modern Synthetic Methods: (a) Baylis-Hillman reaction, Henry reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Brook rearrangement, Tebbe olefination.

(b) Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reactions, directed ortho metalation. (c) Stereoselective synthesis of tri- and tetra-substituted olefins, Synthetic applications of Claisen rearrangement, ene reaction (metallo-ene, Conia ene).

# Module-4

Construction of Ring Systems: (a) Different approaches towards the synthesis of three, four, five, and sixmembered rings. (b) Pauson-Khand reaction, Bergman cyclization; Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization, inter-conversion of ring systems (contraction and expansion). (c) Construction of macrocyclic rings and ring closing metathesis.

#### Module-5

Retrosynthetic Analysis: Basic principles and terminology of retrosynthesis, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions Protecting groups: Protection and deprotection of hydroxy, carboxyl, carboxyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

# References

1. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996.

2. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier

Academic Press, 2005.

3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.

4. F. A. Cary and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009.

5. M. B. Smith, Organic Synthesis, 2nd Edition, 2005

6. S. Warren, Organic Synthesis, The disconnection Approach, John Wiley & Sons, 2004.

7. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21st Century, John Wiley & Sons, 2003.

8. I. Ojima, Catalytic Asymmetric Synthesis, 2nd edition, Wiley–VCH, New York, 2000.

9. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.

CO1	<b>utcomes:</b> After completion of the course, students will have Students are familiar about chemistry of oxidants and various types of oxidants used for									
	oxidation	reactions								
CO2	Better und	lerstandir	ng of reduc	ing agents	and reduct	tion reaction	on mechan	isms		
CO3	Familiar a	bout vari	ous moder	ns syntheti	c methods	and reacti	ons			
CO4	Able to co	nstruct va	rious ring	systems						
CO5	Analyse th	ne reactio	ns by Retr	o-synthetic	approach					
Iapping o	f Cos and Pos			•						
		PO1	PO2	PO3	PO4	PO5	PO6	PO7		
	CO1	X		X			X	X		
	CO2	X								
	CO3	X	X							
							<b>X</b> 7	<b>N</b> 7		
	<b>CO4</b>	X	X	X			X	X		

ADVANCED ANALYTICAL TECHNIQUES									
Course Code	22MSC32	CIE Marks	50						
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50						
Total Hours of Pedagogy	50	Total Marks	100						
Credits	4	Exam Hours	3						

- To learn sampling techniques and conventional volumetric methods and chromatographic techniques.
- To understand the concepts and applications of microscopic techniques

#### Module-1

Titrimetric Analysis: Acid-Base, Complexometric, redox, precipitartion and gravimnetric analysis Thermal Analysis: TGA, DTG, DTA, DSC - combustion calorimetry- Thermal diffusivity by the laser flash technique- simultaneous techniques including analysis for gaseous products.

Electro-analytical technique Principle and applications of : Coulometry, Polarography, Hydrodynamic voltametry , Pulse Polarography , Cyclic Voltammetry and Amperometry.

#### Module-2

Principles of chromatography- Chromatographic separations and classification of principal chromatographic separations. Chromatographic mechanisms-sorption isotherms; adsorption systems-stationary and mobile phases, partition systems-stationary and mobile phases.

Characterization of solutes-distribution ratio, retention factor, retention time and retardation factor.

Thin layer chromatography (TLC) - Principles and procedures, stationary and mobile phases, solute-detection, alternative TLC procedures and applications of TLC.

Gas chromatography (GC) - Principles and types. Mobile phases, Sample injections, columns and stationary phases. Temperature control and solute detection; thermal conductivity detector (TCD), flame ionization detector (FID), nitrogen-phosphorus detector (NPD) and electron capture detector (ECD).

High performance liquid chromatography(HPLC): Principles, mobile phases, solvent delivery systems, sample injection system, column and stationary phases.

#### Module-3

Ion-exchange chromatography (IEC): Principles, apparatus and instrumentation, and applications. Sizeexclusion chromatography (SEC): Principles, apparatus and instrumentation, and applications. Affinity chromatography (AFC): Principles, methodology and applications. Supercritical fluid chromatography (SFC): Properties of supercritical fluids, instrumentation and operating variables, comparison of SFC with other chromatographic techniques, applications. Supercritical fluid extraction (SFE): Advantages, instrumentation, choice of supercritical fluids, off-line and on-line extraction, applications. Electrophoresis (EP) and electrochromatography(EC): Principles- high performance capillary electrophoresis and capillary electrochromatography, running buffers, supporting medium, sample injection, solutes- detection, instrument control and data processing.

### Module-4

Solvent and solid phase extraction: Extraction techniques, extraction efficiency and selectivity. Solvent extraction (SE) - Extraction of organic acids and bases, extraction of metals. Methods of extraction and applications. Solvent phase sorbents, solid phase extraction (SPE) formats. Automated solid phase extraction. Solid phase micro extraction (SPME). Applications of SPE and SPME.

#### Module-5

**Microscopic Techniques**: Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM). Scanning Probe Microscopy: Atomic Force Microscopy, Scanning Tunnelling Microscopy (STM), Near field scanning optical microscopy (NSOM). Principles of Fluorescence microscopy. Confocal Laser

Scanning Microscopy.

References

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch, 8 th edition, 2005, Saunders College Publishing, New York.

- 2. Analytical Chemistry, G.D. Christian, 5th edition, 2001, John Wiley & Sons, Inc, India.
- 3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, Prentice Hall, Inc. New Delhi.
- 4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and

M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Education Pvt. Ltd., New Delhi.

5. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993 prenticeHall, Inc. New Delhi.

6. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders CollegePublishing, California, 1990.

7. Principles and Practice of Analytical Chemistry, F.W. Fifield and Kealey, 3rd edition, 2000, Blackwell Sci., Ltd. Malden, USA.

8. Modern Analytical Chemistry, David Harvey, McGraw Hill, New Delhi, 2000.

9. Principles of instrumental analysis, Douglas A Skoog, Donald M West, Saunders College, Philadelphia. **Publisher:** Cengage; 6 edition (1 November 2014) **ISBN- 13:** 978-81-315-25579.

10. X-Ray Diffraction Procedures: For Polycrystalline and Amorphous Materials, 2<sup>nd</sup> Edition - Harold P. Klug, Leroy E. Alexander,**Publisher:** Wiley-Blackwell; 2<sup>nd</sup> Revised edition edition (1 January 1974) **ISBN-13**: 978-0471493693

11. Transmission Electron Microscopy: A Textbook for Materials Science (4-Vol Set)- David B. Williams and C. Barry Carter, **Publisher:** Springer; 1st ed. 1996. Corr.6thprinting edition (15 April 2005) **ISBN-13**: 978-0306453243

12. Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AEM - Ray F. Egerton ,**Publisher:** Springer; Softcover reprint of hardcover 1st ed. 2005 edition (12 October 2010) **ISBN-13**: 978-1441938374

**Course Outcomes:** After completion of the course, students will have

CO1 Skills on sampling, purification, characterizations and data analysis using instrumental techniques.

**CO2** Knowledge of chromatographic techniques

CO3 Principle of Instrumentation and analytical applications of chromatographic techniques

**CO4** The idea of Solvent and solid phase extraction methods

**CO5** Better understanding about Microscopic techniques

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X						
CO2	X						
CO3	X	X					
<b>CO4</b>	X	Χ					
CO5	X	Χ	Χ				X

	<b>NCED INORGANIC CHEN</b>	MISTRY	
Course Code	22MSC33	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	4	Exam Hours	3
Course Learning Objectives:		· · ·	
<ul> <li>To understand the fundamental homogeneous and hetrogeneous</li> <li>To learn the concepts of metal of the second second</li></ul>	se catalysis.	emistry and general prin	ciples of
	Module-1		
Fundamental concepts: Introducti	on, Classification of organ	ometallic compounds	by bond type
nomenclature, the effective atomic nu	umber rule, complexes that dis	sobey the EAN rule, co	mmon reaction
used in complex formation.			
Organometallics of transition meta			cobalt, iron and
manganese carbonyls. Preparation and			
Ferrocene: Preparation, structure and			
Complexes containing alkene, alkyr		reparation, structure and	a bonding
	Module-2		
General principles of Catalysis: Lar			
Homogeneous catalysis - Industria			
Wacker's process, Monsanto acetic a		nthesis, alkene oligome	rizations, water
gas shift reactions. The Reppe reactio			
Heterogeneous catalysis – The natur			
catalysis, Fischer-Tropsch carbon cha		neterogeneous catalysis.	
	Module-3	~	
Zeolites as catalysts for organic tran			
Alkene metathesis, hydroboration, an		SI Heck reaction i	
			. 1
<b>Biological and Medicinal Applicati</b>			nd organoarseni
			nd organoarseni
<b>Biological and Medicinal Applicati</b> compounds.	ions: Organomercury, organol Module-4	boron, organosilicon ar	
Biological and Medicinal Applicati compounds. Chemistry of main group eleme	Module-4 ents: Diborane and its reac	boron, organosilicon ar tions, polyhedral bora	nnes(preparation
Biological and Medicinal Application compounds. Chemistry of main group element properties, structure and bonding	Module-4 ents: Diborane and its reac	boron, organosilicon ar tions, polyhedral bora	nnes(preparation
Biological and Medicinal Applicati compounds. Chemistry of main group eleme properties, structure and bonding Phosphazenes, S-N compounds.	Module-4 Module-4 ents: Diborane and its reac b). Wade's rules, carboran	boron, organosilicon ar tions, polyhedral bora les andmetallocarbora	nnes(preparation nes. Borazines
Biological and Medicinal Applicati compounds. Chemistry of main group eleme properties, structure and bonding Phosphazenes, S-N compounds. Metal clusters: Evidences and factor	<b>Module-4</b> <b>Module-4</b> <b>ents</b> : Diborane and its reac (). Wade's rules, carboran ors favoring of M-M bonding	boron, organosilicon ar tions, polyhedral bora es andmetallocarbora , Wade's-Mingo's-Laul	nnes(preparation nes. Borazines her rules, bi, tr
Biological and Medicinal Applicati compounds. Chemistry of main group eleme properties, structure and bonding Phosphazenes, S-N compounds. Metal clusters: Evidences and facto tetra, penta and hexa nuclear metal ca	Module-4 Module-4 ents: Diborane and its reac g). Wade's rules, carboran ors favoring of M-M bonding arbonyl clusters. Low and hig	boron, organosilicon ar tions, polyhedral bora es andmetallocarbora , Wade's-Mingo's-Laul	nnes(preparation nes. Borazines her rules, bi, tr
Biological and Medicinal Applicati compounds. Chemistry of main group eleme properties, structure and bonding Phosphazenes, S-N compounds. Metal clusters: Evidences and facto tetra, penta and hexa nuclear metal ca	Module-4 Module-4 ents: Diborane and its reac g). Wade's rules, carboran ors favoring of M-M bonding arbonyl clusters. Low and hig s. The isolobal analogy.	boron, organosilicon ar tions, polyhedral bora es andmetallocarbora , Wade's-Mingo's-Laul	nnes(preparation nes. Borazines her rules, bi, tr
Biological and Medicinal Applicati compounds. Chemistry of main group eleme properties, structure and bonding Phosphazenes, S-N compounds. Metal clusters: Evidences and facto tetra, penta and hexa nuclear metal co counting schemes in carbonyl clusters	Module-4 Module-4 ents: Diborane and its reac g). Wade's rules, carboran ors favoring of M-M bonding arbonyl clusters. Low and hig s. The isolobal analogy. Module-5	boron, organosilicon ar tions, polyhedral bora les andmetallocarbora , Wade's-Mingo's-Lau h nuclearity carbonyl c	nnes(preparation nes. Borazines her rules, bi, tr lusters. Electro
Biological and Medicinal Applicati compounds. Chemistry of main group eleme properties, structure and bonding Phosphazenes, S-N compounds. Metal clusters: Evidences and facto tetra, penta and hexa nuclear metal ca counting schemes in carbonyl clusters Silicates: Structure, classification - s	Module-4 Module-4 ents: Diborane and its reac by. Wade's rules, carboran ors favoring of M-M bonding arbonyl clusters. Low and hig s. The isolobal analogy. Module-5 ilicates with discrete anions, s	boron, organosilicon ar tions, polyhedral bora les andmetallocarbora , Wade's-Mingo's-Lau h nuclearity carbonyl c	nnes(preparation nes. Borazines her rules, bi, tr lusters. Electro
Biological and Medicinal Applicati compounds. Chemistry of main group eleme properties, structure and bonding Phosphazenes, S-N compounds. Metal clusters: Evidences and facto tetra, penta and hexa nuclear metal co counting schemes in carbonyl clusters Silicates: Structure, classification - s with layer structure, silicones with thr	Module-4 Module-4 ents: Diborane and its reac g). Wade's rules, carboran ors favoring of M-M bonding arbonyl clusters. Low and hig s. The isolobal analogy. Module-5 ilicates with discrete anions, so ree dimensional net-work and a	boron, organosilicon ar tions, polyhedral bora es andmetallocarbora , Wade's-Mingo's-Lau h nuclearity carbonyl c silicates containing char applications.	nnes(preparation nes. Borazines her rules, bi, tr lusters. Electro
Biological and Medicinal Applicati compounds. Chemistry of main group eleme properties, structure and bonding Phosphazenes, S-N compounds. Metal clusters: Evidences and facto tetra, penta and hexa nuclear metal ca counting schemes in carbonyl clusters Silicates: Structure, classification - s with layer structure, silicones with the Silicones: General methods of prepar	Module-4 Module-4 ents: Diborane and its reac g). Wade's rules, carboran ors favoring of M-M bonding arbonyl clusters. Low and hig s. The isolobal analogy. Module-5 ilicates with discrete anions, s ree dimensional net-work and a ation, properties. Silicone poly	boron, organosilicon ar tions, polyhedral bora es andmetallocarbora , Wade's-Mingo's-Lau h nuclearity carbonyl c silicates containing char applications.	nnes(preparation nes. Borazines her rules, bi, tr lusters. Electro
Biological and Medicinal Applicati compounds. Chemistry of main group eleme properties, structure and bonding Phosphazenes, S-N compounds. Metal clusters: Evidences and facto tetra, penta and hexa nuclear metal ca counting schemes in carbonyl clusters Silicates: Structure, classification - s with layer structure, silicones with the Silicones: General methods of prepar silicone resins, silicone rubbers and the	Module-4 Module-4 ents: Diborane and its reac g). Wade's rules, carboran ors favoring of M-M bonding arbonyl clusters. Low and hig s. The isolobal analogy. Module-5 ilicates with discrete anions, s ree dimensional net-work and a ation, properties. Silicone poly	boron, organosilicon ar tions, polyhedral bora es andmetallocarbora , Wade's-Mingo's-Lau h nuclearity carbonyl c silicates containing char applications.	nnes(preparation nes. Borazines her rules, bi, tr lusters. Electro inanion, silicate
Biological and Medicinal Applicati compounds. Chemistry of main group eleme properties, structure and bonding Phosphazenes, S-N compounds. Metal clusters: Evidences and facto tetra, penta and hexa nuclear metal ca counting schemes in carbonyl clusters Silicates: Structure, classification - s with layer structure, silicones with the Silicones: General methods of prepar	Module-4 Module-4 ents: Diborane and its reac g). Wade's rules, carboran ors favoring of M-M bonding arbonyl clusters. Low and hig s. The isolobal analogy. Module-5 ilicates with discrete anions, s ree dimensional net-work and a ation, properties. Silicone poly heir applications.	boron, organosilicon ar tions, polyhedral bora es andmetallocarbora , Wade's-Mingo's-Lau h nuclearity carbonyl c silicates containing chai applications. ymers – silicone fluids,	ines(preparation nes. Borazines her rules, bi, tr lusters. Electro inanion, silicate silicone greases

Publishing Company (1985).

3. The Organometallic Chemistry of the Transition Metals, 4th edition, Robert H. Crabtree, Wiley Interscience, (2005).

4. Organometallics - A Concise Introdution, 2nd edition, ChistophElschenbroich and Albert Salzer VCH, (1992).

5. Inorganic Chemistry, 2nd edition, C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd., (2005).

- 6. Inorganic Chemistry- 3rd edition, G.L. Miessler and D.A. Tarr, Pearson Education,(2004).
- 7. Basic Organometallic Chemistry B.D. Gupta and A.J. Elias, Universities Press (2010).
- 8. Inorganic Chemistry Principles of Structure and Reactivity: James E. Huheey, Ellen A.
- 9. Keiter, Richard L. Keiter, Okhil K. Medhi, Delhi University, New Delhi (2006)
- 10. Chemistry of the Elements N.N. Greenwood and A. Earnshaw, Pergamon Press (1985).

11. Inorganic Chemistry, 6th edition. D.F. Shriver, M. Weller. T. Overton, J. Rourke and F. Armastrong, Oxford University Press (2014).

12. Organometallic Chemistry and Catalysis, Didier Astruc, Springer (2007).

13. Transition Metal Organometallic Chemistry, Francois Mathey, Springer (2013).

#### **Course Outcomes:**

CO1	Fundamental concepts of organometallic chemistry and synthesis, structure and bonding in different organometallics and their applications.									
CO2	Homogene	Homogeneous and heterogeneous catalyst and their in applications in the synthesis of organic compounds in industries.								
CO3	Knowledg	Knowledge about zeolites, Biological and Medicinal Applications								
CO4	-			ents, metal		••				
CO5	Better und	lerstandir	ng of silica	tes and silic	ones and th	neir applica	tions in da	y to day life	e.	
apping o	of COs and PO	S	0							
		PO1	PO2	PO3	PO4	PO5	PO6	PO7		
	CO1	Χ								
	CO2	Χ								
	CO3	X								
	CO4	X								
	CO5	X	X				X	X		

POLYMERS AND COMPOSITES									
Course Code	22MSC34	CIE Marks	50						
Teaching Hours/Week (L:P:SDA)	2:0:2	SEE Marks	50						
Total Hours of Pedagogy	40	Total Marks	100						
Credits	3	Exam Hours	3						

- To understand the basics of polymers and kinetics of polymerization ٠
- To understand the basics of composites
- To familiarize about different types of composites

#### Module-1

Polymers: Fundamentals of polymers - monomers, repeat units, degree of polymerization. Linear, branched and network polymers. Classification of polymers, Polymerization - condensation, addition, free radical, ionic, co-ordination polymerization and ring opening polymerization. Molecular weight and size, polydispersion. Average molecular weight concepts - number, weight and viscosity average molecular weight. Determination of molecular weights - viscosity method, osmotic pressure method, sedimentation and light scattering methods.

#### Module-2

Kinetics of Polymerization - Condensation, addition, free radical, ionic, co-ordination polymerization. Phase transitions in polymers and thermal characterization: Glass transition, crystallinity and meltingcorrelation with the polymer structure. Polymers in solution:

Criteria of polymer solubility, thermodynamics of polymer solutions.

# Module-3

General introduction to composite materials: Concept and definition, classification of composites (CMC, MMC, PMC).Functional roles of reinforcement and matrix and importance of interface. Polymer matrix composites (PMCs): Fiber reinforced and particulate filled polymer composites. Reinforcements (glass, carbon/graphite, Kevlar), Matrices - Thermoset matrices - polyesters, epoxides, phenolics, vinyl esters, polyimides, cyanate esters - Thermoplastic matrices. Choice of reinforcements and matrices for different application needs.

#### Module-4

#### **Polymer nanocomposites**

Introduction to polymer composites, Processing of nanoparticles, binding mechanisms in nanoparticles, dispersion of nanoparticles, and stabilization of nanoparticles. Processing and fabrication of polymer nanocomposites, Melt blending, solvent casting, In-situ polymerization, solution polymerization, template synthesis, high shear mixing. Homogeneous/heterogeneous nucleation, plasma promoted nucleation.

#### **Ceramic metal nanocomposites**

Ceramic based nanoporous composites, metal matrix nanocomposites, natural nano-bioccomposites, biomimetic nanocompostes and biologically inspired nanocomposites, nanocompsites for hard coatings, DLC coatings, thin film naocomposites, modelling of nanocomposites, synthesis of various nanocomposites materials, sputtering, mechanical alloying.

# References

1. Text Book of Polymer Science, F.W. Billmeyer, Jr., John Wiley, London (1994).

2. Polymer Science. V. R. Gowrikar, N.V. Vishwanathan and J. Sreedhar, Wiley Eastern, New Delhi (1990).

3. Fundamentals of Polymer Science and Engineering. A. Kumar and S.K. Gupta, Tata – McGraw Hill

#### Module-5

New Delhi (1978).

- 4. Polymer Characterization, D. Campbell and J.R. White, Chapman and Hall, New York.
- 5. Fundamental Principles of Polymer Materials, R.L. Rosen, John Wiley and Sons, New York.

6. Nanocomposite science and technology by P.M.Ajayan, L.S. Schadler and P.V. Braun, Wiley-VCH GmbH Co. 2003.

7. Encyclopedia of Nanotechnology by H.S.Nalwa, American Scientific Publishers, 2003.

- 8. Metalopolymer nanocomposites, Ed A.D. Pomogailo and V.N.Kestelman, Springer-Verlag, 2005.
- 9. Composite materials, K.K. Chawala, 2nd ed., (1987) Springer-Verlag, New York.

CO1	Fundamen	Fundamentals of polymers and their applications in controlling the quality and waste									
	manageme	management of polymer product.									
CO2	Fundamen	Fundamentals of composites, their types, preparations and applications									
Mapping o	of CO <u>s and PO</u>	S									
		PO1	PO2	PO3	PO4	PO5	PO6	PO7			
	<b>CO1</b>	X	X	X			X	X			
	001										

NMR AND MASS SPECTROSCOPY										
Course Code	22MSC35	CIE Marks	50							
Teaching Hours/Week (L:P:SDA)	2:0:0	SEE Marks	50							
Total Hours of Pedagogy	30	Total Marks	100							
Credits	2	Exam Hours	3							

- To understand the basic concepts NMR spectroscopy.
- To familiarize with the mass spectroscopy

# Module-1

NMR Spectroscopy: Magnetic properties of nuclei (magnetic moment, g factor, nuclear spin), effect of external magnetic field on spinning nuclei, Larmor precession frequency, resonance conditions, population of nuclear magnetic energy levels, relaxation processes, relaxation time, line width and other factors affecting line width. Chemical Shift: Standards employed in NMR, factors influencing chemical shift: electronegativity, shielding and deshielding, van der Walls deshielding magnetic anisotropy, H-bonding, diamagnetic and paramagnetic anisotropies, spin-spin coupling, chemical shift values and correlation for protons bonded to carbon and other nuclei, Instrumentation. Chemical shift equivalence and magnetic equivalence, effects of chiral centre, Karplus curve-variation of coupling constants with dihedral angle.

#### Module-2

Complex NMR Spectra: Simplification of complex spectra-isotopic substitution, increased magnetic field strength, double resonance and lanthanide shift reagents, Nuclear Overhauser Effect (NOE), FT-NMR, Spectroscopy and advantages. 13CNMR Spectroscopy, multiplicity-Proton decoupling-Noise decoupling-Off resonance decoupling-Selective proton decoupling - Chemical shift, application of 13C, 19F, 31P, 11B and 15N. Applications of NMR: Structural diagnosis, conformational analysis, keto-enol tautomerism, H bonding. Solid state NMR and its applications. Multiple resonance spectroscopy: Introduction to 2D-techniques: DEPT, COSY and NOESY

#### Module-3

Mass Spectrometry: Basic principles, Instrumentation -Mass spectrometer, interpretation of mass spectra, resolution, exact masses of nuclides, molecular ions, meta-stable ions and isotope ions. Different methods of ionization (chemical ionization, electron impact, field ionization, MALDI etc.). Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement.

# Module-4

Fragmentations (fragmentation of organic compounds with respect to their structure determination) associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitro compounds, amines & nitrogen heterocycles. Fragmentation patterns of glucose, myrcene, nicotine, retro Diels-Alder fragmentation. Application in structure elucidiation and evaluation of heats of sublimation & ionization potential. Nitrogen rule. LC-MS and GC-MS, High resolution mass spectroscopy.

#### Module-5

Composite problems involving the applications of UV, IR, 1H and 13C-NMR and mass spectroscopic techniques. Structural elucidation of organic and inorganic compounds. Industrial Case studies.

# References

1. Organic Spectroscopy-3rd Ed.-W. Kemp (Pagrave Publishers, New York), 1991.

2. Spectrometric Identification of Organic Compounds - Silverstein, Bassler & Monnill (Wiley) 1981.

3. Spectroscopy of Organic Compounds-3rd Ed.-P.S. Kalsi (New Age, New Delhi) 2000.

4. E.A.V. Ebsworth, D.W.H. Ranklin and S. Cradock: Structural Methods in Inorganic Chemistry, Blackwell Scientific, 1991.

5. J. A. Iggo: NMR Spectroscopy in Inorganic Chemistry, Oxford University Press, 1999

6. C. N. R. Rao and J. R. Ferraro: Spectroscopy in Inorganic Chemistry, Vol I & II (Academic) 1970.

7. Spectroscopy, B. P. Straughan and S. Salker, John Wiley and Sons Inc., New Yourk, Vol.2, 1976.

8. Application of Absorption Spectroscopy of Organic Compounds, John R. Dyer, Prentice/Hall of India Private Limited, New Delhi, 1974.

9. Organic Spectroscopy, V. R. Dani, Tata McGraw-Hall Publishing Company Limited, New Delhi. 1995.

10. Interpretation of Carbon-13 NMR Spectra, F.W. Wehrli and T. Wirthin, Heyden, London, 1976.

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11. NMR spectroscopy-Powai

**CO3** 

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ourse C	<b>Dutcomes:</b>									
CO1	Describe the spectra.	he NMR s	spectroscoj	pic techniqu	es includin	g the basic	principles	for record	ing of NMI	
CO2	Predict the	Predict the structure of organic compounds on Mass spectral data								
CO3	The course chemistry	e related t	o understa	nd the spect	roscopic te	chniques fo	or the char	terization in	n organic	
apping o	f COs and PO	S								
		PO1	PO2	PO3	PO4	PO5	PO6	<b>PO7</b>		
	CO1	X								
	CO2	X	X	X			X	X		

X

X

ORGANIC CHEMISTRY PRACTICALS										
Course Code	22MSC36	CIE Marks	50							
Teaching Hours/Week (L:P:SDA)	0:6:0	SEE Marks	50							
Total Hours of Pedagogy	72	Total Marks	100							
Credits	3	Exam Hours	3							

- To understand synthetic methods by carrying out different experiments.
- To develop the skill for the separation and qualitative analysis of binary mixtures of organic compounds.

### PART-A

# Multistep synthesis

- 1. Preparation p-bromoaniline from acetanilide.
- 2. Preparation of n-butyl bromide from n-butyl alcohol.
- 3. Oxidation of cyclohexanol to adipic acid.
- 4. Esterification: Preparation of benzoccaine from p-nitrotoluene.
- 5. Diazotization (Sandmeyer's reaction): Preparation of p-chlorobenzoic acid from ptoluidine.
- 6. Preparation benzilic acid from benzoin.
- 7. Preparation of o-hydroxy benzophenone from phenyl benzoate via Fries rearrangement.
- 8. Preparation of benzanilide from benzophenone oxime via Beckmann rearrangement.
- 9. Preparation of benzoic acid from benzaldehyde (Cannizzaro Reaction).
- 10. Preparation of 2,4-dinitrophenylhydrazine from 2,4-dinitrochlorobenzene.
- 11. Preparation of m-nitrobenzoic acid from methylbenzoate.
- 12. Preparation of chalcone.

# PART-B

# Qualitative analysis:

Separation of binary mixtures, identification of functional groups and preparation of suitable solid derivatives.

Interpretation of Spectra: Structural elucidation of some simple organic compounds by UV, IR, NMR and mass. Spectra have to be provided by the Examiners.

# References

1. Vogel' text book of practical organic chemistry, V edition, B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatehell.

2. Elementary practical organic chemistry, Part-I: Small scale preparations, Part-II: Qualitative organic analysis, By Arthur I, Vogel.

- 3. Hand book of organic analysis, H. T. Clarke and Norman Collie.
- 4. Experiments in Organic Chemistry, Louis F. Fieser.
- 5. Laboratory manual of Organic Chemistry by B. B. Dey and M. V. Sitaraman.
- 6. Practical Organic Chemistry by Mann F. G. and Saunders.

# **Course Outcomes:**

~	04150 0	
	CO1	Students are involved in the multi-step synthesis of different organic compounds
	CO2	Understand the qualitative analysis of binary mixture of organic compounds through separation,
		identification of functional groups and preparation of some solid derivatives.

# Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X						
CO2	X	Χ	X	Χ	X	Х	Х

ANALYTICAL CHEMISTRY PRACTICALS							
Course Code	22MSC37	CIE Marks	50				
Teaching Hours/Week (L:P:SDA)	0:6:0	SEE Marks	50				
Total Hours of Pedagogy	72	Total Marks	100				
Credits	3	Exam Hours	3				

- To understand basic concepts by carrying out analytical experiments.
- The experimental results are subjected to validation of analytical parameters.

# PART-A

1. Determination of total acidity of vinegar and wines by acid-base titration.

2. Determination of purity of a commercial boric acid sample, and Na<sub>2</sub>CO<sub>3</sub> content of washing soda.

3. Analysis of chromate-dichromate mixture by acid-base titration.

4. Determination of replaceable hydrogen and relative molecular mass of a weak organic acid by titration with NaOH.

5. Determination of ephedrine and aspirin in their tablet preparations by residual acid-base titrimetry.

6. Determination of purity of aniline and assay of chlorpromazine tablets by nonaqueous acid-base titration.

7. Periodate determination of ethylene glycol and glycerol (Malprade reaction).

8. Determination of carbonate and bicarbonate in a mixture by *p*H-metric titration and comparison with visual acid-base titration.

9. Determination of purity of a commercial sample of mercuric oxide by acid-base titration.

10. Determination of benzoic acid in food products by titration with methanolic KOH in chloroform medium using thymol blue as indicator.

11. Determination of the *p*H of hair shampoos and *p*H determination of an unknown soda ash.

12. Analysis of water/waste water for acidity/alkalinity by visual, *p*H metric and conductometric titrations.

13. Determination of carbonate and hydroxide-analysis of a commercial washing soda by visual and *p*H-titrimetry.

14. Determination of ammonia in house-hold cleaners by visual and conductometric titration.

15. Potentiometric determination of the equivalent weight and Ka for a pure unknown weak acid.

17. Spectrophotometric determination of creatinine and phosphorus in urine.

18. Flame emission spectrometric determination of sodium and potassium in river/lake water.

19. Spectrophotometric determination of *p*Ka of an acid-base indicator.

# PART-B

1. Determination of percentage of chloride in a sample by precipitation titration- Mohr, Volhard and Fajan's methods.

2. Determination of silver in an alloy and Na<sub>2</sub>CO<sub>3</sub> in soda ash by Volhard method.

3. Mercurimetric determination of blood or urinary chloride.

4. Determination of total hardness, calcium and magnesium hardness and carbonate and bicarbonate hardness of water by complexation titration using EDTA.

5. Determination of calcium in calcium gluconate/calcium carbonate tablets/injections and of

calcium in milk powder by EDTA titration.

6. Analysis of commercial hypochlorite and peroxide solution by iodometric titration.

7. Determination of copper in an ore/an alloy by iodometry and tin in stibnite by iodimetry.

8. Determination of ascorbic acid in vitamin C tablets by titrations with KBrO3 and of vitamin C in citrus fruit juice by iodimetric titration.

9. Determination of iron in razor blade by visual and potentiometric titration using sodium metavanadate.

10. Determination of iron in pharmaceuticals by visual and potentiometric titration using cerium(IV) sulphate.

11. Determination of nickel in steel by synergic extraction and boron in river water/sewage using ferroin.

12. Determination of total cation concentration of tap water by ion-exchange chromatography.

13. Determination of magnesium in milk of magnesium tablets by ion-exchange chromatography.

14. Cation exchange chromatographic separation of cadmium and zinc and their estimation by EDTA titration.

15. Gas chromatographic determination of ethanol in beverages.

16. Determination of aspirin, phenacetin and caffeine in a mixture by HPLC.

17. Solvent extraction of zinc and its spectrophotometric determination.

18. Anion exchange chromatographic separation of zinc and magnesium followed by EDTA titration of the metals.

19. Separation and determination of chloride and bromide on an anion exchanger.

20. Thin layer chromatographic separation of amino acids.

# References

1. Fundamental of Analytical Chemistry, D.A. Skoog, D.M. West, Holler and Crouch 8th edition, 2005, Saunders College Publishing, New York.

2. Analytical Chemistry, G.D. Christian, 5th edition, 2001 John Wiley & Sons, Inc, India.

3. Quantitative Analysis, R.A. Day and A.L. Underwood, 6th edition, 1993, Prentice Hall, Inc. New Delhi.

4. Vogel's Textbook of Quantitative Chemical Analysis, J. Mendham, R.C. Denney, J.D. Barnes and

M.J.K. Thomas, 6th edition, Third Indian Reprint, 2003, Pearson Education Pvt. Ltd., New Delhi.

5. Analytical Chemistry Principles, John H. Kennedy, 2nd edition, Saunders College Publishing, California, 1990.

6. Practical Clinical biochemistry methods and interpretations, R. Chawla, J.P. Bothers Medical Publishers (P) Ltd., 1995.

7. Laboratory manual in biochemistry, J. Jayaraman, New Age International Publishers, New Delhi, 1981.

8. Practical Clinical Biochemistry by Harold Varley and Arnold.Heinmann, 4th edition.

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# **Course Outcomes:**

**CO2** 

X

X

Course	Juccomes.										
CO1	Develop th	Develop the skill to carry out acid-base titrimetric analysis, potentiometric and conductometric									
	methods.	methods.									
CO2	Understan	Understand the chemistry of different chemical reactions involved in the determination of									
	pharmaceu	itical, ind	ustrial and	vegetable s	amples.						
Mapping of	of COs and PO	S									
	PO1 PO2 PO3 PO4 PO5 PO6 PO7										

Х

X

X

Х

# **IV SEMESTER**

**FORENSICS CHEMISTRY** 

ELEMENTS OF FORENSIC CHEMISTRY AND TOXICOLOGY								
Course Code	22MSCF1	CIE Marks	50					
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50					
Total Hours of Pedagogy	40	Total Marks	100					
Credits	3	Exam Hours	3					

- To understand the basic concepts of chemistry and toxicology as they relate to forensic science.
- To gain proficiency in analytical techniques used in forensic chemistry, such as chromatography and spectroscopy.
- Learn to identify and quantify various toxic substances.

### Module-1

**General Forensic Chemistry:** Definition, Important cases associated with Forensic chemistry, Types of cases which require chemical analysis, Presumptive and confirmatory testing of chemical evidences.

#### Module-2

#### **Scientific Instrumentation and Equipments involving analysis of chemical evidences**: Early Analytical Techniques: Wet Chemistry, Chemistry of Color, Thin-Layer Chromatography Development of Instrumental Techniques Microscopy, Hyphenated Instruments: Separation and Detection, Spectrophotometry.

#### Module-3

**Drugs of Abuse:** Introduction and classification of Drugs of Abuse (Narcotics, Stimulants, Depressant and hallucinogens), Status of Drug abused in India, Introduction to Club drugs and Drug abuse in Sports, Drugs as Evidence.

Introduction and brief analysis of Phenolphthalein in Trap case, Petroleum adulteration. Illicit liquors and Arson and Explosives.

#### Module-4

**Forensic Toxicology**: Definition, Areas of Forensic Toxicology, Elements of Forensic Toxicology Nature of cases, Role of the Forensic Toxicologists, Laws related to Forensic Toxicology. **Poisons:** Definition of Poison, Toxin and Toxicant, Ideal Poison, Classification of poisons based on their origin and Chemical nature, mode of action.

## Module-5

**Types and Trends of Poisoning:** Animals and Human poisoning in India with special reference to Suicidal, Homicidal and accidental poisons, Major vesicants used as chemical-warfare agents. Factors affecting the poisoning, methods of administration.

Extraction methods of some important poisons and their forensic identification

# References

- 1. Modi's (1988) Medical Jurisprudence & Toxicology, M. M. Trirathi Press Ltd. Allahabd,.
- 2. Saferstein, R (1982) Forensic Science Hand Book, Vol I, II and III, Pretince Hall, NI.
- 3. Saferstein, R (2000) Criminalistics.
- 4. Curry (1986) Analytical Methods in Human Toxicology, Part II.
- 5. Curry, A.S. (1976) Poison Detection in Human Organs.
- 6. Mathew E. Johll (2009) Investigating Chemistry: A Forensic Science Perspective
- 7. Suzanne Bell (2009) Drugs, Poisons, and Chemistry
- 8. DFS Manuals of Forensic Chemistry and Narcotics.

#### **Course Outcomes:**

**CO1** Demonstrate proficiency in using analytical techniques such as chromatography and mass

	spectrome	spectrometry for substance identification and quantification.										
CO2	Apply fun evidence.	Apply fundamental concepts of chemistry and toxicology to analyze and interpret forensic evidence.										
CO3	Assess the effects of various toxic substances on human health and recognize symptoms of exposure.											
CO4	Exhibit best practices in the collection, preservation, and documentation of chemical evidence, ensuring integrity and reliability.											
apping o	of CO <u>s and PO</u>					1	r	1	•			
		PO1	PO2	PO3	PO4	PO5	PO6	PO7				
					101	105	100	10/				
	CO1	X		100	101	105	100	107				
	CO1 CO2	X X	X	X		105	100	107				
			X X				100	107				

CHEMISTRY OF NATURAL PRODUCTS								
Course Code	22MSCF2	CIE Marks	50					
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50					
Total Hours of Pedagogy	40	Total Marks	100					
Credits	3	Exam Hours	3					

- Define natural products and categorize them, with a specific focus on lipids, flavonoids, and isoflavonoids.
- Explore the biosynthetic pathways involved in the production of lipids, flavonoids, and isoflavonoids, including key enzymes and regulatory mechanisms.
- Examine the chemical structures of lipids, flavonoids, and isoflavonoids, emphasizing their functional groups and structural variations.

# Module-1

Lipids: Nomenclature, classification, purification, structure and synthesis of fatty acids, phospholipids, sphingolipids. Biological importance of lipids (Lecithin, sphingolipids, oils and fats). Prostaglandins: Introduction, classification and biological importance of PG's. Constitution of PGE1. Synthesis of PGE & F series.

#### Module-2

Terpenoids: Introduction, classification and general methods of structural elucidation. Chemistry of pinene, camphor, caryophyllene, santonin. Biosynthesis of terpenoids.

Porphyrins: Introduction, structure and biological functions of haemin. Vitamin B12: structure and as coenzyme in molecular rearrangement reactions; Chlorophyll: structure and biological importance

# Module-3

Flavonoids and Isoflavonoids: Occurrence, nomenclature and general methods of structure determination. Isolation and synthesis of Apigenin, Luteolin, Kaempferol, Quercetin, wedelolactone, Butein, Daidzein. Biosynthesis of flavonoids and isoflavonoids: Acetate Pathway and Shikimic acid Pathway. Biological importance of flavonoids and isoflavonoids

#### Module-4

Alkaloids: Introduction, classification, isolation and general methods of structural elucidation of alkaloids. Classification of alkaloids. Biological importance of alkaloids. Structural elucidation of nicotin, papavarine, quinine, reserpine and morphine. Biosynthesis of alkaloids (nicotin, conine and cocaine).

#### Module-5

Steroids: Introduction, Structural elucidation of cholesterol, bile acids, Ergosterol and its irradiation products. Sex hormones and corticosteroids: Synthesis of estrone, progesterone, androsterone, testosterone. Barton reaction for the synthesis of aldosterone. Brief discussion of homosteroids, norsteroids and oral contraceptives. Biological significance of anabolic steroids.

#### References

1. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.

2. Organic Chemistry, Vol-II by I. L. Finar.

3. Schaum's outline of theory and problems of Organic Chemistry, Harbert Meislich, Howard Nechamkin and Jocob Sharefkin.

4. Natural products: Their chemistry and biological significance, J. Mann, R. S. Davidson, J. B. Banthorpe and J. B. Harborne.

5. Synthetic drugs, Gurdeep R. Chatwal.

6. Heterocyclic chemistry by Achison.

7. Heterocyclic chemistry by Smith and Joule. 8. Heterocyclic chemistry by Pacquete.

Course Outcomes:											
CO1	Demonstr	Demonstrate a thorough understanding of the structure, classification, and properties of									
	lipids, flav	lipids, flavonoids, and isoflavonoids.									
CO2	Design and conduct research projects focused on natural products, demonstrating the ability to formulate hypotheses, collect data, and analyze results.										
		<i>.</i>		,	2						
CO3	Demonstr	ate an un	derstandin	g of the eth	ical implic	ations of u	ising natu	ral produc	ts in		
	research a	nd indust	try, includ	ing sustaina	bility and	biodiversi	ty conside	rations.			
apping o	of COs and PO	s									
		PO1	PO2	PO3	PO4	PO5	PO6	PO7	]		
	CO1	X	X								
	CO2	X	X	X							
	CO3	X	X	X			X	X	]		

]	FORENSIC DRUG ANALYSIS						
Course Code	22MSCF3	CIE Marks	50				
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50				
Total Hours of Pedagogy	40	Total Marks	100				
Credits	3	Exam Hours	3				
Course Learning Objectives:							
• To understand the basic principles of forensic science and the role of drug analysis within the forensic field.							
<ul> <li>To classify various types of controlled substances, including their chemical structures, categories, and legal implications.</li> <li>To learn forensic analytical techniques specifically applicable to the detection and analysis of drugs of</li> </ul>							
• To learn forensic analytical tech abuse in biological samples.		ne detection and anal	lysis of drugs of				
	Module-1						
Drug: Definition of Drug, Drug Use		Dependence and ch	nemistry of				
Addiction, Drug Receptors and Brain <b>Drugs of Abuse:</b> Definition, Classifie		Use Effects and Sc	hadulas				
Structure of NDPS Act and the defini							
Examples of Illegal Drugs, United Na		-	i ionnig				
Examples of megal Drugs, Onited Ne	Module-2	riogramme					
Chemistry and Analysis of Drugs o		Methods of preparat	ion Storage				
Diluents and Adulterants, Sample Ha			ion, Storage,				
Presumptive/Screening and Confirma			ion.				
Microcrystalline tests, Thin-Layer Ch	•	1					
Evaluation of TLC for Drug Screenin							
Spectrophotometry, NMR, GC-MS &							
and Opioids analgesics, Stimulants (C	· • • •	1	1				
Depressants (Barbiturates and Benzoo	· 1	1	<i>//</i>				
Mescaline), OTC, Inhalant and Volat	1 /* 0 (						
	Module-3						
Clandestine laboratory: Meaning an	nd Definition of Clandestine, Clan	destine Laboratory,	Related				
Problems, Factors Contributing to Cla		•					
Equipment Needs: Reflux, Distillati							
Cooking Methods Commonly Used in							
Synthesis Process, Tableting.	C ·						
Designer drugs: Definition, Analogs	of Fentanyl and Meperidine (both	n synthetic opioids),	Phencyclidine				
(PCP), Amphetamines and methamph	• • •	• • •	-				
	Module-4	-	• /				
Laboratory Analysis: The Chemist,	Extractions: Physical Extraction.	Drv Wash/Extractio	on.				
Liquid/Liquid Extractions, Analysis:	•	•					
Spectroscopy, Thin-Layer Chromatog	·	<b>.</b> .					
NDPS Report Writing & Court Room		0 1	2				
¥¥	Module-5						
<b>Module-5</b> <b>Drug Abuse in Sports</b> : Introduction, International Olympic Committee (IOC), World Anti-Doping Agency (WADA), classification of commonly prohibited substances and Performance enhancing Drugs, Steroids, Stack and Pyramid methods, Dope test and Blood Doping, Sampling techniques, analytical approaches.							

# References

1. Clarke's Analysis of Drugs and Poisons, (Formerly Isolation & Identification of Drugs) 3rd Ed. 2 Vol. Set.

2. Clark, E.G.C. : Isolation and identification of Drugs, VI and Vol. II, 1966, 1975-1986.

3. Modi, Text Book of Medical Jurisprudence Forensic Medicines and Toxicology (1999) CBS Pub. New Delhi

4. Saferstien (1982) Forensic Science, Handbook, Vol. I, II & III, Prentice Hall Inc. USA.

5. DFS -Working Procedure Manual- Narcotics

6. E. Stahl (1969) Thin Layer Chromatography: ALaboratory Handbook.

7. Saferstein (1976) Criminalistics.

# **Course Outcomes:**

Ľ		accomes.										
	CO1	Demonstr	Demonstrate a comprehensive understanding of the definitions, classifications, and effects of									
	commonly abused drugs.											
	CO2	2 Apply forensic analytical techniques to accurately identify and quantify drugs in various samples.										
	CO3	Conduct in	ndepende	nt researcl	n on emerg	ing trends	in drug ab	use and fo	rensic ana	lysis,		
		demonstra	ating criti	cal thinkin	g and analy	tical skills	S.					
Μ	Mapping of COs and POs											
			PO1	PO2	PO3	PO4	PO5	PO6	PO7			
										1		

X X

apping of CO	<u>s and PO</u>	S						
		PO1	PO2	PO3	PO4	PO5	PO6	I
	CO1	X	X					
	CO2	X	X	X	X		Χ	
	CO3	Χ	X	Χ	Χ	Χ	Χ	

ADVANCED FORENSIC CHEMISTRY								
Course Code	22MSCF5	CIE Marks	50					
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50					
Total Hours of Pedagogy	40	Total Marks	100					
Credits	3	Exam Hours	3					

- To develop skills to identify and analyze complex chemical evidence from crime scenes, including illicit drugs, explosives, and trace evidence.
- To conduct quantitative analyses of chemical substances, applying statistical methods to interpret data and ensure the reliability of results.
- To conduct laboratory experiments utilizing advanced analytical techniques, demonstrating proficiency in instrumentation and data analysis.

# Module-1

Introduction to Forensic Chemistry, branches of and cases involved in Forensic chemistry, preliminary and confirmatory methods used in Forensic chemistry.

**Analytical Chemistry**: Nature and scope of analytical chemistry in Forensic chemical analysis, Concepts of Structure and function of drug molecules, Concept of Mole, Molecular Mass and Molecular Weight, Atomic Number and Atomic Mass, Classification of acids, bases and salts, pH value and pH scale, Buffer solutions, Oxidizing and reducing agents in organic chemistry, Functional group analysis, Schemes of identification of unknown solids, Volumetric/Titrimetric methods of analysis, Theory of indicators, Gravimetric methods of analysis, Process of precipitation, Saturated and supersaturated solution, Methods of sample preparation in organic analytical chemistry.

**Chemical separation Techniques:** Solvent extraction (Liquid-liquid extraction), Solid phase extraction, Solid phase microextraction (SPME).

#### Module-2

**Phenolphthalein in trap case**: Chemistry and Forensic examination of Phenolphthalein used in Bribe trap cases, and related legal issues.

**Forensic significance of Cosmetics**: Introduction to cosmetics of forensic interest and their role in crime investigation, General Chemistry of Colorants, Dyes, Pigments & Polymers.

**Industrial Products:** Physical and chemical examination of adulterated and non-adulterated oils and fats, Analysis of chemical fertilizers, consumer items such as gold, silver, tobacco, tea, sugar, salts.

**Corrosive chemicals:** Hydrochloric acid, sulphuric acid, and nitric acid and alkalis' in crime exhibits of acid/alkali throwing cases.

#### Module-3

**Fire & Arson**: Light and Flame, Chemistry of Fire, Combustion reaction, Fire Triangle, Fire Tetrahedron; Backdraft, Thermo-chemistry of Fire, Heat Capacity and Phase changes, Accelerants & types of accelerants, Combustible and Flammable liquids, Flash point, Fire point, Ignition point, Auto Ignition point, vapour density, vapour pressure, Fire extinguisher.

**Arson:** Legal Definition, Arson motives, Degrees of Arson, Forensic and legal Concepts, Determining origin and cause; Fire patterns, Collection/Preservation of Arson Evidences, Flashover, Backdraught, Live or dead at time of arson; Documenting the fire or crime scene;

**Scheme of analysis**: Extraction of samples from debris (Direct and solvent extraction methods, Head Space method, SPME, Distillation), Clean-up (Filtration & Acid stripping), Analysis (GC, GC-MS, FTIR & SEM etc.), Interpretation of GC-MS spectra.

**Petroleum Products:** Introduction to Petroleum Products, Properties and Testing of Petroleum and Petroleum Products, Adulteration of petroleum products as per Prevention of Malpractices in Supply and

Distribution, Analysis of common petroleum products including, Petrol, Kerosene, Diesel, Lubricating Oil, Furnace Oil and Grease as per BIS specifications. Analysis of Dyes used in petroleum products, Chemical fingerprinting of petroleum products

# Module-4

**Explosives:** Definition of Explosives, Definition as per Indian Explosive Acts. History of Explosives, Chemistry of explosives, Deflagration and Detonation phenomenon (Redox Chemistry, Kinetics-Molecular Theory of gases & Gas Laws), Characteristics of high and low explosives, Dust explosion, Gas/vapour explosion, BLEVE, Effect of blast wave on structures & human and Pyrotechnics.

**Improvised Explosive Device**: Definition of IED, Components of IED, Explosives Initiation (Explosive Trains); Types (Molotov cocktail, Letter bomb, Pipe bomb, VBIED and CBRN), Detection of Hidden Explosives.

**Bomb Scene**: Specific approach to scene of explosion, Reconstruction of sequence of events, Evaluation and assessment of scene of explosion,

**Analysis of Explosive:** Pre-blast and Post blast residue collection, Systematic examination of explosives and explosion residues in the laboratory using chemical and instrumental techniques and interpretation of results.

### Module-5

**Liquors (Alcoholic beverages):** Definition, classification of liquors based on origin (Indian Made Foreign Liquors, Country Made Liquors and Illicit Liquors), Fermented and Distilled methods (Pot Still and Continuous Still), Characteristics of Beer, wines and Whisky, Congeners in alcoholic beverages, Laws and penalties as per Excise/ Act.

Laboratory methods of determination alcoholic strength, Forensic analysis of distilled and fermented liquors including illicit liquors.

**Report Writing & Court Room Testimony**: Evidence and testimony in court, Information required by the Forensic expert, Components of Forensic Reports, Preparation of Report, Presenting findings in a Report format.

# References

1. Modi's (1988) Medical Jurisprudence & Toxicology, M. M. Trirathi Press Ltd. Allahabd,.

- 2. Saferstein, R (1982) Forensic Science Hand Book, Vol I, II and III, Pretince Hall, NI.
- 3. Saferstein, R (2000) Criminalistics.
- 4. Curry (1986) Analytical Methods in Human Toxicology, Part II.
- 5. Curry, A.S. (1976) Poison Detection in Human Organs.
- 6. Mathew E. Johll (2009) Investigating Chemistry: A Forensic Science Perspective
- 7. Suzanne Bell (2009) Drugs, Poisons, and Chemistry
- 8. DFS Manuals of Forensic Chemistry and Narcotics.

9. ANaquest (1984) legal chemistry. a guide to the detection of poisons, examination of tea, stains, etc.

- 10. DFS -Working Procedure Manual- Chemistry, Explosives
- 11. E. Stahl (1969) Thin Layer Chromatography: ALaboratory Handbook.
- 12. Jehuda Yinon; Forensic and Environmental Detection of Explosives
- 13. Saferstein (1976) Criminalistics.

14. Saferstien: Forensic Science, Handbook, Vol. I, II & III, Prentice Hall Inc. USA

15. Yinon Jitrin (1993)Modern Methods & Application in Analysis of Explosives, John Wiley & Sons ,England

# 16. J ASiegel, P.J Saukko (2000) Encyclopedia of Forensic Sciences Vol. I, II and III, Acad. Press.

# Course Outcomes:

CO1 Collaborate effectively with professionals from other forensic disciplines, integrating

	chemical a	analysis v	vith biolog	gical, digita	l, and inve	stigative a	spects of f	orensic sci	ence.
CO2	Conduct in	ndepende	nt researcl	n, critically	evaluating	g forensic l	literature a	nd proposi	ng
	innovative	e solution	s to conter	nporary for	rensic chal	lenges.			
CO3	Effectivel	y interpre	et and repo	rt quantitat	ive data, a	oplying sta	atistical me	ethods to en	nsure the
	reliability	and valid	lity of fore	nsic analys	ses.				
apping o	of COs and PO	S							
		PO1	PO2	PO3	PO4	PO5	PO6	PO7	
	CO1	X	X						
	CO2	X	X						
	CO3	X	X	X			X	X	

ANALY	TICAL FORENSIC TOXI	COLOGY	
Course Code	22MSCF4	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3
Course Learning Objectives:		· · ·	
<ul> <li>To understand the fundamental relationships, and the classificat</li> <li>To learn proper procedures for tenvironmental samples to ensure</li> <li>To conduct laboratory experime</li> </ul>	tion of toxic substances. the collection, preservation, and e the integrity of evidence rela	d transportation of biologi ted to poisoning cases.	cal and
poisons.	M - J-1 - 1		
Samples required in Toxicological a	Module-1	1 1 0	
particular class of poison, Classes of s collection (Living and Dead person), ( and storage conditions. Alternative specimens: Hair analysis, Analysis of Exhumed and decompose	Classification of matrices, cho Drugs in oral fluid, Detection	pice of preservatives, con	1
<b>`</b>	Module-2		
Toxic properties and effects of alcoho Chemical tests for alcohol in blood an analysis of some alcoholic beverages and instrumental methods (GC), Lega Format of Report Writing & Court Ro Presenting findings in a Report format	d urine including Breath Alco in biological materials by che <u>l context to drinking and driv</u> <u>Module-3</u> oom Testimony: Information r	mical methods (Kozelka- ing.	· Hine)
••••••••••••••••••••••••••••••••••••••	Module-4		
Animal Poisons: Insects and animal t and mode of action, Effect on the bod Plant poisons: Classification and char matrices and analysis by chemical and	oxins and their examination, y as a whole, and tests for ide acteristics, method of extracti	ntifications.	
Casague Paisoning: Carbon Monovid		osphine asse significant	a signs
Gaseous Poisoning: Carbon Monoxid and symptoms, methods of diagnosis, Food Poisoning: What is food poison symptoms of food poisoning, collection from food material, Biological materia techniques.	tests for identification. ing, Food poisoning due to cl on and preservation of eviden	nemical and bacterial, Sig ce material, extraction an	gn and d isolation,
References			
<ol> <li>DFS Manual of Forensic Toxicolog</li> <li>A C Moffat Clarke's Analysis of D Ed. 2 Vol. Set.</li> <li>Constant &amp; Dell Terrischer (2002)</li> </ol>	rugs and Poisons, (Formerly l		of Drugs) 3rd
3. Casarett & Doll Toxicology (2003)	fication of Drugs, VI and Vol		

5. Curry A.S (1986) Analytical Methods in Human Toxicology, Part II, CRC Press Ohio

6. Curry, A.S. (1976) Poison Detection in Human Organs.

7. Michael J. Deverlanko et al (1995) Hand Book of Toxicology CRC Press.

8. Morgan B.J.T (1996) Statistics in Toxicology, Clarendon Press, Oxford.

9. Modi, Text Book of Medical Jurisprudence Forensic Medicines and Toxicology (1999) CBS Pub. New Delhi

10. Saferstien (1982) Forensic Science, Handbook, Vol. I, II & III, Prentice Hall Inc. USA.

# **Course Outcomes:**

CO1	Accurately conduct the analysis of biological and environmental samples for the presence of
	toxins, ensuring adherence to established protocols for evidence handling.
<b>CO2</b>	Apply knowledge of the legal framework surrounding forensic toxicology and poisoning,
	understanding the implications of toxicological evidence in judicial proceedings.
CO3	Effectively utilize advanced analytical techniques, such as GC to identify and quantify
	poisons and other toxic substances in biological samples.
Mapping of	f COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	Χ	X	X				
CO2	Χ	X	X				X
CO3	Χ	Χ	X			X	X

# NANO CHEMISTRY

SYNTHESIS A	AND PROPERTIES OF NANON	IATERIALS	
Course Code	22MSCN1	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3

- To learn various synthesis methods for nanomaterials, with a focus on physical and chemical methods.
- To investigate the applications of nanomaterials in various fields, such as medicine, electronics, energy storage, and environmental remediation.
- To examine the applications of nanomaterials in fields such as medicine, electronics, energy, and environmental science.

#### Module-1

#### **Physical Methods:**

Bottom-Up versus Top-Down; Top-down approach with examples. Ball milling synthesis, Arc discharge, RF-plasma, Plasma arch technique, Inert gas condensation, electric explosion of wires, Ion sputtering method, Laser pyrolysis, Molecular beam epitaxy and electrodeposition. Electro spinning, Physical Vapor Deposition (PVD) – Chemcial Vapour Deposition (CVD) - Atomic layer Deposition (ALD) – Self Assembly- LB (Langmuir-Blodgett) technique.

#### Module-2

# Chemical methods:

Chemical precipitation methods- Coprecipitation, Arrested precipitation, Sol-gel method, Chemical reduction, Photochemical synthesis, Electrochemical synthesis, Microemulsions or Reverse Micelles, Sonochemical synthesis, Hydrothermal, Solvothermal, Supercritical fluid process.

Module-3

#### **Combustion and Solution Methods:**

Solution combustion process, spray pyrolysis method, flame spray pyrolysis, gas phase synthesis, gas condensation process, chemical vapour condensation. Fundamental aspects of VLS (Vapour-Liquid-Solid) and SLS (Solution-Liquid-Solid) processes – VLS growth of Nanowires – Control of the size of the nanowires – Precursors and catalysts – SLS growth – Stress induced recrystallization.

Module-4

### **Biological methods:**

Use of bacteria, fungi, Actinomycetes for nanoparticle synthesis, Magnetotactic bacteria for natural synthesis of magnetic nanoparticles; Mechanism of formation; Viruses as components for the formation of nanostructured materials; Natural and artificial synthesis of nanoparticles in microorganisms; Use of microorganisms for nanostructure formation, Role of plants in nanoparticle synthesis, synthesis of nanoparticles using proteins and DNA templates.

#### Module-5

#### **Electronic Properties**

Classification of materials based on band structures - Brillouin zone – Effect of temperature on conductors – Intrinsic and extrinsic semiconductors - Electrical and electronic conductivity- Hall effect and its determination.

Dielectric Properties, Optical Properties: Photoconductivity, Optical absorption and transmission -

Photoluminescence, fluorescence and phosphorescence

#### **Mechanical behavior**

Stress-strain, tensile strength, toughness,. **Thermal properties:** Heat capacity, thermal conductivity and thermal expansion of nanomaterials. **Magnetic properties:** Magnetic hysteresis – Superparamagnetism .

# References

1.Guozhong Cao, "Nanostructures and Nanomaterials, synthesis, properties and applications", Imperial College Press, 2004

2.M.S. Ramachandra Rao, Shubra Singh, Nanoscience and Nanotechnology: fundamentals to Frontiers, Wiley 2013. Introduction to Nanotechnology - Charles P. Poole Jr. and Franks. J. Qwens

3. Hari Singh Nalwa - Encyclopedia of Nanotechnology.

4. Processing & properties of structural Naonmaterials by Leon L. Shaw (editor)

5. Chemistry of Nanomaterials : Synthesis, properties and applications by CNR Rao et.al.

6. Nanochemistry: A chemical approach to Nanomaterials Roayal Society of Chemistry, Ozin and Arsenault, Cambridge UK 2005,

7. Nanoparticles: From Theory to Applications, G.Schmidt, Wiley Weinheim 2004.

8. M.S.Vijaya, G.Rangarajan, Materials Science, Tata McGraw-Hill publishing company Ltd., New Dehli.

9. Fundamental Properties of Nanostructured Materials, Ed. D. Fiorani (World Scientific, Singapore, 1994.

10. Properties of Materials, Robert E.Newnham, Oxford University Press, 2005.

11. Nanostructured Materials, Edited by Carl C. Koch, Noyes Publications, New York, 2002.

#### **Course Outcomes:**

CO1 Understand principles and mechanisms of various synthesis and processing techniques.
 CO2 Demonstrate the knowledge to synthesize different nanomaterial choosing suitable method
 CO3 Design desired nanostructure with size and morphology controlled to get desired property.

Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X						
CO2	X						
CO3	X	Χ	X			X	X

CHARAC	<b>CTERISATION OF NANOM</b>	IATERIALS	
Course Code	22MSCN2	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3
<b>Course Learning Objectives:</b>	-		-
<ul> <li>To identify and describe vario microscopy (e.g., TEM, SEM)</li> <li>To analyze and interpret data significance of the results in the significance of the results in the second second</li></ul>	, FTIR). obtained from characterization he context of nanomaterial app	n techniques, understand	-
X-Ray based characterization	Module-1		
Principles and applications of X-ra techniques; Debye-Scherrer equatio ultra-thin films. Basics of structure r diffraction for probing structure.X-ra ray absorption techniques: XANES,	n to treat line broadening ar refinement (Reitveld). Rotati ay photoelectron spectroscopy	nd strain induced in na ng anode and synchrotr	noparticles and on based X-ray
<b>Electron microscopy techniques</b> Introduction, Principles and applic Scanning electron microscopy (SI Electron-diffraction, SAED. Scanni Microscope, Scanning Tunnelling M	EM/FESEM), transmission of ing Probe Microscopy: Princ	electron microscopy (	ΓΕΜ/HRTEM),
Microscope, Scanning Tunnening M	Module-3		
Spectroscopic techniques UV-VIS Spectrophotometers, IR/FTI gap measurements. Raman spectrosco measurement by Dynamic light scatte	opy principles and application		
	Module-4		
<b>Magnetic characterization</b> Types of magnetic materials, Magnet temperature, Curie temperature VSM	etic susceptibility, Curie-Wei		
<b>Electrical measurements</b> Cyclic Voltameter, Impedance Meas information.		ctric measurements, im	pedance spectral
References			
Books         1. Characterization of Nanostruct         2. Instrumental Methods of Anal         3. Scanning Probe Microscop         Wiesendanger         References:	lysis, 7 <sup>th</sup> edition- Willard, Mer	rritt, Dean, Settle	hnology)-Roland

- 1. X-Ray Diffraction Procedures: For Polycrystalline and Amorphous Materials, 2nd Edition Harold P. Klug, Leroy E. Alexander
- 2. Transmission Electron Microscopy: A Textbook for Materials Science (4-Vol Set)- David B. Williams and C. Barry Carter
- 3. Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AEM Ray F. Egerton.

CO1	Demonstra	ate a com	prehensiv	e understan	ding of the	e fundamer	ntal prope	rties and b	ehaviors of
	nanomater						p. op o		
CO2	Proficient analyze na	•	-	characteriz	zation tech	niques (e.g	g., TEM, S	EM, FTIR	, XRD) to
CO3	Conduct in	ndepende	nt researc	h projects i	nvolving tl	ne characte	erization o	f nanomat	erials,
	demonstra	ting the a	ability to d	lesign expe	riments and	d draw me	aningful c	onclusions	5.
apping o	of COs and PO	S							_
		PO1	PO2	PO3	PO4	PO5	PO6	PO7	
	CO1	X	Χ						
	CO2	X	X				X	X	
	CO3	V	V	V			V	V	

CARBON AN	D ADVANCED NANOSTI	RUCTURES	
Course Code	22MSCN3	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3

- To describe the various allotropes of carbon (e.g., graphene, carbon nanotubes, fullerenes) and their unique structural, electrical, and mechanical properties.
- To identify and utilize appropriate characterization techniques (e.g., Raman spectroscopy) to analyze the structural and functional properties of carbon nanostructures.

#### Module-1

**Carbon Nanotubes (CNT):** History, types of CNTs, synthesis methods, CVD method, Laser ablation and electric arc processes, growth mechanisms, purification and characterization methods, mechanical reinforcements, solid disordered carbon nanostructures.

#### Module-2

**Graphene**: Background, structure, exfoliation or synthesis methods- physical methods-micromechanical (scotch tape method), CVD, electric arc process. Chemical approaches-Hammers method, oxidation and reduction of graphite, solvothermal, supercritical fluid, solvent sonication method, chemically modified graphene, electrochemical synthesis and other methods

#### Module-3

**Fullerenes and derivatives**: Fullerenes and types, diamond like carbon, nanodiamond, clusters, metal carbide derived carbon nanostructures, synthesis and applications.

**Nanostructures**: Graphite, Whiskers, Cones, and Polyhedral crystals, structure, properties and applications. **Properties of Carbon nanostructure:** Electronic, Vibrational, Mechanical Properties of CNTs, optical properties & Raman spectroscopy of CNTs.

#### Module-4

**Functionalization of carbon nanostructures:** (CNT, Graphene and fullerenes)- reactivity, covalent functionalization-oxidative purification, defect functionalization, transformation and modification of carboxylic functionalization like amidation, thiolation, halogenations, hydrogenation, addition of radicals, sidewall functionalization through electorphilic addition, nano covalent exohedralfunctionalization, endohedro functionalization.

#### Module-5

Advanced 2D nanostructures: Introduction to 2D nanostructures, Structure and properties of metal nitrides, carbides, selenides, sulphides, metal dichalcogenides, MXenes. Synthesis methods and surface chemistry, functionalization of MXenes. Applications of 2D nanostructures

# References

# **TEXT BOOKS:**

- 1. Carbon Nanotubes: properties and applications-Mchael J. O'Connell, Taylor & Francis, 2006
- 2. Nanotubes and Nanowires-CNR Rao and A Govindaraj RSC publishing
- 3. Handbook of Carbon, YuryGagotsi, Taylor & Francis, 2006
- 4. Mxenes and their Composites Synthesis, Properties and Potential Applications. Edited by Kishor

Kumar Sadasivuni. Elsevier, 2022. https://doi.org/10.1016/C2019-0-05458-1

# Reference

- 1. Physical properties of carbon nanotube- R. Satio
- 2. Applied physics of Carbon nanotubes: fundamentals of theory, optics and transport devices-S.Subramoney and S.V.Rotkins
- 3. Carbon nanotechnology-Liming Dai

# **Course Outcomes:**

CO1				nding of the					f various
CO2	Successfu	lly perfor	m synthes	is techniqu d properties	es for carb				their
apping o	f COs and PO	S		-					
		PO1	PO2	PO3	PO4	PO5	PO6	<b>PO7</b>	
	CO1	X	X						
	CO2	X	V	Y			V	Y	

	NANOCOMPOSITES		
Course Code	22MSCN4	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3

- To explain the fundamental concepts of nanocomposites, including definitions, types, and the significance of nanoscale materials in composite formation.
- To identify and describe various synthesis methods for nanocomposites, such as sol-gel processes, melt mixing, and in situ polymerization.
- To develop skills in designing and conducting experiments related to the synthesis and characterization of nanocomposites, including data analysis and interpretation.

#### Module-1

#### Introduction to nanocomposites

Definition of composite material, Classification based on matrix and topology, Constituents of composites, Interfaces and Interphases, Distribution of constituents, Nano-composites. Advantage of composite materials, mechanical properties, Thermal, electrical and electronic and optical properties. Super hard nanocomposites-designing and mechanical properties - stress-strain relationship, toughness, strength, and plasticity.

#### Module-2

#### **Ceramic metal nanocompsites**

Ceramic based nanoporous composites, metal matrix nanocomposites, natural nano-bioccomposites, bio-mimetic nanocompostes and biologically inspired nanocomposites, nanocomposites for hard coatings, DLC coatings, thin film naocomposites, modelling of nanocomposites, synthesis of various nanocomposites materials, sputtering, mechanical alloying.

#### Module-3

#### **Polymer nanocomposites**

Introduction to polymer composites, Processing of nanoparticles, binding mechanisms in nanoparticles, dispersion of nanoparticles, and stabilization of nanoparticles. Processing and fabrication of polymer nanocomposites, Melt blending, solvent casting, In-situ polymerization, solution polymerization, template synthesis, high shear mixing. Homogeneous/heterogeneous nucleation, plasma promoted nucleation. Polymer nanocomposites with structural, gas barrier and flame retardant properties, carbon fibre reinforced polymer composites, elastomer and thermoplastic elastomer nanocomposites for propulsion systems, water borne fire-retardant nanocomposites, hybrid composites for cosmetics, protective and decorative coatings.

#### Natural nanocomposite systems

Spider silk, bones, shells; organic-inorganic nanocomposite formation through self-assembly. Biomimetic synthesis of nanocomposite material; use of synthetic nanocomposites for bone teeth replacement. Bioactive nanocomposites in bone grafting and tissue engineering, inorganic/polymer nanocomposites for dental restoration and bone replacement applications.

Module-4

#### Module-5

#### **Bio ceramics for implant coating**

Calcium phosphates-hydroxyapatites Ti<sub>6</sub>Al<sub>4</sub>V and other biomedical alloys, implant tissue interfacing-metal organic CVD-use of tricalcium phosphate-biomimetic and solution based processing- osteoporosis- osteo plastic, regeneration of bones by using bio compatible ceramics, bio interactive hydro gels- PEG coating and surface modifications, PEG hydrogels patterned on surfaces- PEG based hydrogels.

#### **References TEXT BOOKS:**

- 1. Nanocomposite science and technology by P.M.Ajayan, L.S. Schadler and P.V. Braun, Wiley-VCH GmbH Co. 2003.
- 2. Encyclopedia of Nanotechnology by H.S.Nalwa, American Scientific Publishers, 2003.
- 3. Metalopolymer nanocomposites, Ed A.D. Pomogailo and V.N.Kestelman, Springer-Verlag, 2005.
- 4. Composite materials, K.K. Chawala, 2nd ed., (1987) Springer-Verlag, New York.

#### **References:**

- 1. Biomedical nanostructures by Kenneth E.Gonsalves, Craig R. Halberstadt, Cato T. Laurencin, Lakshmi S. Nair. John-Wiley & Sons, 2008.
- 2. Nanobiotechnology II: Edited by Chad A. Mirkin and Christof M. Niemeyer, Wiley-VCH, 2006.
- 3. Handbook of Biomineralization: Biomimetic and Bioinspired, Chemistry edited by Peter Behrens, Edmund Bäuerlein John-Wiley Sons, 2006.3. Steven S Saliterman, Fundamentals of BioMEMS and Medical Microdevices, 2006

# **Course Outcomes:**

CO1	Demonstr	ate a thor	ough unde	erstanding c	of the princ	iples, type	s, and sig	nificance of	f	
	nanocomp	osites in	materials	science.	-		_			
CO2	Successfu	essfully synthesize v	Successfully synthesize various types of nanocomposites using a						hed method	ds and
	evaluate th	heir effec	tiveness b	ased on des	ired prope	rties.	-			
CO3	Analyze th	he effects	of nanosc	ale fillers c	on the over	all propert	ies of com	posites,		
	demonstra	iting an a	bility to re	late structu	re to funct	ion.				
apping o	demonstra f COs and PO	<u> </u>	bility to re	late structu	re to funct	ion.				
apping o		<u> </u>	bility to re PO2	late structu PO3	re to funct	ion. PO5	PO6	PO7		
apping o		s	•		1	1	PO6	PO7		
apping o	f COs and PO	s PO1	•		1	1	PO6 X	PO7 X		

Course Code	22MSCN5	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3

- To explain the basic principles and characteristics of organic and inorganic nanomaterials, including their unique properties at the nanoscale.
- To investigate the diverse applications of organic and inorganic nanomaterials in agriculture.
- To explore current trends and future directions in the field of nanomaterials, particularly in agricultural applications and plant protection, identifying potential innovations and challenges.

Module-1

# Agricultural Nanotechnology:

Conventional Farming: Issues and Limitations, Intensive Conventional Farming Affects Environment, Current Agricultural Production Systems, Nanotools -Nano processes, and Nanomaterials Production of Bionanomaterials from Agricultural Wastes: Cellulose and Nanocellulose from Citrus and Orange Wastes, Synthesis of Graphene Oxide from Agro wastes, Production of Amorphous Silica Nanoparticles from Agrowastes, Carbon Nanomaterials from Agrowastes,

# Module-2

# Nanoengineering Superabsorbent Materials in Agriculture:

Introduction, Formation and Structure of Cross-Linked Polyacrylates, Formation and Structure of Cross-Linked Polyacrylates; Statistical Models, Mechanisms of Swelling in Superabsorbent Polymers, Mechanisms of Swelling in Superabsorbent Polymers; Hydration, Hydrogen Bonds, Properties of Superabsorbent Polymers, Absorption of Aqueous Solution, Moisture Absorption Superabsorbent Polymers Application in Agriculture Superabsorbent/Clay Nanocomposites

#### Module-3

# Nanotechnology in plant protection:

Nanotechnology and Their Applications in Insect's Pest Control; Formulations of Nanoinsecticides-Nanoemulsions, Components, Preparation, Types and Methods, Nanoparticle-Based Plant Disease Management; Interactions between NPs, Pathogens, and Plants, Plant Disease Diagnosis Using different NPs, Nanotechnology in Microbial Plant Pathogen and insect Management, Targeted Delivery of Agrochemicals Using Nanotechnology, Nanobased Pesticides in Agriculture, Nano-based Fertilizer Efficiency, Improving Plant Traits against Environmental Stresses Using Nanotechnology, Nanotechnology and Its Applications in Water Conservation

# Module-4

# Nanoparticles in food production and diagnostics:

Food and New Ways of Food Production - Efficient Fractionation of Crops Efficient Product Structuring -Optimizing Nutritional Values - Applications of Nanotechnology in Foods: Sensing, Packaging, Encapsulation, Engineering Food Ingredients to Improve Bioavailability - Nanocrystalline Food Ingredients - Nanoemulsions - Nano-Engineered Protein Fibrils as Ingredient Building Blocks Preparation of Food Matrices - Concerns about Using Nanotechnology in food production. Diagnostics Enzyme Biosensors and Diagnostics - DNA- Based Biosensors and Diagnostics Radiofrequency Identification- Integrated Nanosensor Networks: Detection and Response- Lateral Flow (Immuno) assay -Nucleic Acid Lateral Flow (Immuno)assay - Flow-Through (Immuno)assays - Antibody Microarrays Surface Plasmon Resonance Spectroscopy.

Module-5

#### Nanotechnology in food packaging:

Crop improvement - Reasons to Package Food Products - Physical Properties of Packaging Materials -Strength - Barrier Properties Light Absorption – Structuring of Interior Surfaces - Antimicrobial Functionality - Visual Indicators – Quality Assessment - Food Safety Indication - Product Properties -Information and Communication Technology - Sensors -Radiofrequency Identification Technology-Risks - Consumer and Societal Acceptance

#### References

## Books

- 1) Nanobiotechnology Applications in Plant Protection by Kamel A. Abd-Elsalam and Ram Prasad, Volume 2, Springer, 2018.
- 2) Nanotechnology an Agricultural Paradigm by Ram Prasad, Manoj Kumar, Vivek Kumar Springer, 2017.
- 3) Nanoscience in Food and Agriculture by Shivendu Ranjan, Volume 1, Springer, 2016.
- 4) Nanotechnology and Plant Sciences by Manzer H. Siddiqui, Springer, 2015.
- 5) Nanoparticle Assemblies and Superstructures by Nicholas A. Kotov, CRC, 2006.
- 6) Nanotechnology in agriculture and food production by Jennifer Kuzma and Peter VerHage, Woodrow Wilson International, 2006.
- 7) Bionanotechnology by David S Goodsell, John Wiley & Sons, 2004.
- 8) Nanobiomaterials Handbook by Balaji Sitharaman, Taylor & Francis Group, 2011.

# **Course Outcomes:**

CO1	Demonstrate a comprehensive understanding of the properties, characteristics, and											
	classifications of both organic and inorganic nanomaterials.											
CO2	Successfu	lly synth	esize a var	iety of orga	nic and in	organic na	nomateria	ls using es	tablished			
	methodol	ogies and	evaluate t	heir effectiv	veness bas	ed on spec	ific criteri	a.				
CO3	Conduct i	ndepende	ent researc	h related to	organic ar	nd inorgan	ic nanoma	terials, inc	luding			
	designing	experim	ents, data c	collection, a	inalysis, ar	nd interpre	tation.		-			
apping o	of COs and PO	)s							_			
		PO1	PO2	PO3	PO4	PO5	PO6	PO7				
	CO1	X										
	CO2 X X											
	CO2	CO2 X X										

# PHARMACEUTICAL CHEMISTRY

BA	SIC MEDICINAL CHEMIS	STRY						
Course Code	22MSCP1	CIE Marks	50					
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50					
Total Hours of Pedagogy	40	Total Marks	100					
Credits								
Course Learning Objectives:	5	Lixuiii 110uis	5					
	iples of medicinal chemistry, i	ncluding drug design de	evelopment and					
the chemical properties of bio	1	neruding drug design, de	velopment, and					
<ul> <li>To understand how changes in</li> </ul>	<b>č</b> <i>i</i> 1	a activity and effectiven	000					
•								
To explore basic methods for	synthesizing organic compour	ids relevant to medicinal	chemistry.					
T 1 A /** C /* / T / 1 /	Module-1							
Local Anti-infective agents: Introduct	tion, classification, mechanism	of action, Synthesis and S	AR of					
nitrofurazone and furazolidos	tion mochanism of action form	havin and CAD of sulfing						
<b>Sulfonamides:</b> Introduction, classification sulfamethoxazoles	tion, mechanism of action, Synt	nesis and SAR of suffiso	oxazoles and					
Antibiotics: Introduction, classificat	tion machanism of action	Sunthagia and SAD a	f Donisillin C					
cephalosporins, and tetracyclins.	tion, mechanism of action,	Synulesis and SAR O	or Peniciliin G,					
cephalospornis, and tetracyclins.	Module-2							
Antituboroular and antilopratio again		machanism of action for	uthania of					
Antitubercular and antileprotic agen		mechanism of action, Sy	nthesis of					
isoniazid, ethambutal, clofazimine, dap		machanism of action S	wath agin of					
Analgesic and anti-inflammatory age Ibuprofen, phenylbutazone, acetaminop		i, mechanism of action, S	ynthesis of					
Anticancer/antiviral, hypoglycemic		nation mode of estion	Synthesis of 5					
flurouracil, azidothymadine, Tolbutam		auon, mode of action,	Synthesis of 5-					
nurouracii, azidotnymatine, roioutam	Module-3							
Antihistamine: Introduction, classifica		of Phenarimine maleate	nyrilamine					
ranitidine, cimetidine	tion, mode of action, Synthesis	of Thenarmine maleate,	pymannie,					
Cardiovascular Agents: Introduction,	classification mechanism of a	ction Synthesis of Antia	rythmicggents					
verapamil,			i y tilline agents					
Antihypertensive agent clonidine and	hydralazine derivatives							
Then per consider ugene elemente una	Module-4							
Antimalarials Introduction, classificat		hesis of Chloroquine met	Joquine					
primaquine. SAR of antimalarial agent		liesis of emologume, me	noquine,					
Antiamoebic agents Introduction, class		Synthesis of Metronidaz	ole and					
iodoquinol	sincution, incentinisin of action	, Synthesis onvietionadz	ore and					
1	ntroduction, classification, r	nechanism of action,	Synthesis of					
Benzodiazepines: diazepam, Phenothia			Synanesis of					
	Module-5	, so y mile.						
Anticonvulsant Introduction, classifica		thesis of Phenytoin sodiu	m					
carbamazepine.		linesis on nenytoin soura	,					
Sedatives and hypnotics Introduction.	classification mechanism of a	ction Synthesis of Phenol	parbital					
Chlordiazepoxide								
General anesthetics Introduction, clas	sification, mechanism of action	. Synthesis of Halothane	Methahexital					
sodium		, ~ j indicolo of finite indication,						
References								
1. Principles of Medicinal chemistry-Fe	ove.Vargheese and Co.							
2. Drug discovery and development-M								
2. Drug discovery and development-lift	. 5. Chorgade, 101-2.							

- 3. Wilson and Gisvold's: Text Book of Medicinal Chemistry
- 4. Comprehensive Medicinal Chemistry-C. Hansch, Series 1-VI, Academic press.
- 5. Burgers Medicinal Chemistry Volume-1 to Volume 6

# Course Outcomes:

- **CO1** Understand key concepts in medicinal chemistry, including how drugs work.
- CO2 Demonstrate basic methods for synthesizing medicinal compounds.
- **CO3** Clearly present key concepts and findings in medicinal chemistry.

### Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X	X					
CO2	X	X					X
CO3	Χ	X	X			Χ	X

DRU	G DESIGN AND DEVELOP	MENT	
Course Code	22MSCP2	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50
Total Hours of Pedagogy	40	Total Marks	100
Credits	3	Exam Hours	3
Course Learning Objectives:	5		5
<ul><li>To understand the basic princicon compound optimization.</li><li>To explain the roles of pharma</li></ul>	ples of drug design, including t acokinetics and pharmacodynam of drug formulation, including d	nics in drug design an	nd development.
Drug discovery from natural produ	Module-1	ition. Introduction	mig discovery and
design a historical outline, Sources administration, the pharmaceutical pha the pharmacodynamic phase. Introduc biological screening, methods for comp brief explanation on the development of	of drugs and lead compound se, Introduction to drug action: tion to medicinal plants: prepara bound structure elucidation and i f natural product drugs.	ds, Classification of ADME process. Bioavation of initial extract	drugs, Route of vailability of drug, s and preliminary
	Module-2		
<b>Drug design:</b> General approach to disco principles of drug action – drug stere design – docking - molecular modeling	to chemistry -drug action - 3D	database search - cor	nputer aided drug
<i>discovery</i> : Introduction, stereochemistr Solubility and drug design: The import incorporation of water solubilizing g attached groups, the position of water s	ance of water solubility, solubilit roups in structure: The type of	y and drug structure, s group. Reversibility	alt formation. The and irreversibility
Introduction, relationship between mo		activity selectivity o	f drug action and
drug receptors. Discovery and structu screening of synthetic compounds. Ref	ral modification of lead compo- inement of lead structure. Function	ounds. Drug discovery	y through random
	Module-5		
Vitamins: Introduction, classification, importance (Occurrence, Chemical pro Thiamine (B1), Ascorbic acid, Pantath Lipids: nomenclature, classification, p sphingolipids. Biological importance o	perties, Deficiency and Excess de onic acid, Vitamin K. urification, structure and synthes	efect), of following Vi is of lipids, phospholip	tamins: Retinal,
References	wa Warahaaga ay 1 Ca		
1. Principles of medicinal Chemistry-F			
2. Text Book of Medicinal Chemistry-			
3. Comprehensive Medicinal Chemistr	· · · · · · · · · · · · · · · · · · ·		
4. Fundamentals of medicinal chemistr			
5. Organic Synthesis, The disconnectio		aui wyatt,2nd edition,	
6. Natural Products-Gurdeep and Chaty	vai, Himaiya Publishers.		
7. Terpenoids-V. K. Ahluwalia			
8. Biochemistry-Jain			

Course O	utcomes:										
C01	Demonstrate a thorough understanding of the drug design process, including target identification and lead optimization.										
CO2		Demonstrate basic methods for synthesizing new drugs.									
				2	<u> </u>	<u> </u>	<u>a</u> 1				
CO3		1	armacokii	netics and p	harmacod	ynamics ir	ifluence dr	rug action.			
Mapping of	f CO <u>s and PO</u>	S									
		PO1	PO2	PO3	PO4	PO5	PO6	PO7			
	CO1	X		X							
	CO2	X	Χ								
	CO3	Χ	Χ	X				X			

CI	<b>IEMISTRY OF DRUG ACTI</b>	ON						
Course Code	22MSCP3	CIE Marks	50					
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50					
Total Hours of Pedagogy								
Credits								
Course Learning Objectives:								
<ul> <li>systems at the molecular level</li> <li>To describe the mechanisms b other biomolecules.</li> </ul>	ples of drug action, including ho by which drugs exert their effects and advancements in the chemist	s on target receptors,	enzymes, and					
therapies and biotechnology.	Module-1							
confirmation, configuration. Solubility structure, salt formation. The incorp	<b>Module-1</b> Introduction to drug discovery: Introduction, stereochemistry and drug design: structurally rigid groups confirmation, configuration. Solubility and drug design: The importance of water solubility, solubility and drug structure, salt formation. The incorporation of water solubilizing groups in structure: The type of group Reversibility and irreversibility attached groups, the position of water solubilizing group, methods o							
	Module-2							
Introduction, relationship between modular drug receptors. Discovery and structure screening of synthetic compounds. Reference of the selective examples of drug action at a disrupt cell membranes and walls-Antiti Ionophoric antibiotic action, Cell wall a Irreversible inhibition, Transition state	ral modification of lead compo- inement of lead structure. Function Module-3 some common target areas: Intra- fungal agents, Azoles, Allylamine synthesis inhibition, Drugs that tar	unds. Drug discovery nal group modificatio oduction, Examples o es, Phenols, Antibacter	/ through random n. f drugs that rial agents-					
Drugs that target receptors- Agonis Antimetabolites, Enzyme inhibitors, In agents, Antiviral drugs-Nucleic acid s protein synthesis.	ntercalation agents, Alkylating ag	gents, Antisense drug	s, Chain cleaving					
	Module-5							
<b>Drug receptor Interaction and Adverse Drug receptor:</b> Introduction, history, affinity - the role of chemical bonding, conformation, stereochemistry of labetalol.Drug receptors, Drug action, sites of drug action, Mechanism of drug action, drug receptors, types of receptors-ligand gated ion channels, voltage gated ion channels, G-protein coupled receptors, intracellular receptors, dose response relationship, adverse drug relationship. Drug allergy.								
References 1. Principles of medicinal Chemistry-F 2. Text Book of Medicinal Chemistry-V 3. Comprehensive Medicinal Chemistry 4. Fundamentals of medicinal chemistry 5. Organic Synthesis, The disconnection 6. Natural Products-Gurdeep and Chatw 7. Terpenoids-V. K. Ahluwalia	Wilson and Gisvold's. y-Series 1-VI , (Academic press) y-Gareth Thomas John Wiley & S n approach, Stuart Warren and Pa							

8. Biochemistry-Jain

- 9. Pharmacology and Pharmacotherapeutics-Satoshkar et al.
- 10. Drug Discovery and Evaluation: Pharmacological assays, 3rd edition, Vol 2. H. G. Vogel.

## **Course Outcomes:**

CO1	Explain the mechanisms by	y which drugs exert their effec	ts on specific targets.
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CO2 Analyze specific drugs to illustrate their mechanisms of action and therapeutic uses.

**CO3** Analyze how changes in chemical structure affect drug efficacy and safety.

## Mapping of COs and POs

	PO1	PO2	PO3	PO4	PO5	PO6	PO7
CO1	X						
CO2	X	Χ	X				
CO3	X	Χ	X		X	X	X

MEDICINAL CHEMISTRY OF NATURAL PRODUCTS									
Course Code	22MSCP4	CIE Marks	50						
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50						
Total Hours of Pedagogy	40	Total Marks	100						
Credits	3	Exam Hours	3						

#### **Course Learning Objectives:**

- To learn the significance of natural products in medicinal chemistry and their historical role in drug discovery.
- To understand techniques for the isolation and characterization of natural products, including chromatography and spectroscopy.
- To explore the structures, properties, and biological activities of alkaloids, flavonoids, and terpenoids, highlighting their medicinal applications.

#### Module-1

Study of Natural products as leads for new pharmaceuticals for the following class of drugs a) Drugs Affecting the Central Nervous System: Morphine Alkaloids b) Anticancer Drugs: Paclitaxel and Docetaxel, Etoposide, and Teniposide c) Cardiovascular Drugs: Lovastatin, Teprotide and Dicoumarol d) Neuromuscular Blocking Drugs: Curare alkaloids e) Anti-malarial drugs and Analogues f) Chemistry of Macrolide antibiotics: (Erythromycin, Azithromycin, Roxithromycin, and Clarithromycin) and  $\beta$  - Lactam antibiotics (Cephalosporins and Carbapenem)

#### Module-2

**a)** Alkaloids: General introduction, Classification, Isolation, Purification, Molecular modification and Biological activity of Alkaloids, General methods of Structural determination of alkaloids, structural elucidation and stereochemistry of ephedrine, morphine, ergot, emetine and reserpine.

**b)** Flavonoids Introduction, isolation and purification of flavonoids, General methods of structural determination of flavonoids; Structural elucidation of quercetin.

c) Steroids General introduction, chemistry of sterols, sapogenin and cardiac glycosides. Stereochemistry and nomenclature of steroids, Chemistry of contraceptive agents, male & female sex hormones (Testosterone, Estradiol, Progesterone), adrenocorticoids (Cortisone), contraceptive agents and steroids (Vit – D).

#### Module-3

a) Terpenoids Classification, isolation, Isoprene rule and General methods of structural elucidation of Terpenoids; Structural elucidation of drugs belonging to mono terpenoids (citral, menthol, camphor), di terpenoids (retinol, Phytol, taxol) and tri terpenoids (Squalene, Ginsenoside) carotinoids (β carotene).
b) Vitamins Chemistry and Physiological significance of Vitamin A, B1, B2, B12, C, E, Folic acid and Niacin.

#### Module-4

a). Recombinant DNA technology and drug discovery rDNA technology, hybridoma technology, New pharmaceuticals derived from biotechnology; Oligonucleotide therapy. Gene therapy: Introduction, Clinical application and recent advances in gene therapy, principles of RNA & DNA estimation
b). Active constituent of certain crude drugs used in Indigenous system Diabetic therapy – Gymnema sylvestre, Salacia reticulate, Pterocarpus marsupiam, Swertia chirata, Trigonella foenum graccum; Liver

dysfunction – Phyllanthus niruri; Antitumor – Curcuma longa Linn

#### Module-5

Structural Characterization of natural compounds Structural characterization of natural compounds using IR, 1HNMR, 13CNMR and MS Spectroscopy and of specific drugs e.g., Penicillin, Morphine, Camphor,

Vit-D, Quercetin and Digitalis glycosides.

# References

1. Modern Methods of Plant Analysis, Peech and M.V.Tracey, Springer - Verlag, Berlin, Heidelberg.

2. Phytochemistry Vol. I and II by Miller, Jan Nostrant Rein Hld.

3. Recent advances in Phytochemistry Vol. I to IV – Scikel Runeckles, Springer Science & Business Media.

- 4. Chemistry of natural products Vol I onwards IWPAC.
- 5. Natural Product Chemistry Nakanishi Gggolo, University Science Books, California.
- 6. Natural Product Chemistry "A laboratory guide" Rapheal Khan.
- 7. The Alkaloid Chemistry and Physiology by RHF Manske, Academic Press.
- 8. Introduction to molecular Phytochemistry CHJ Wells, Chapmannstall.

9. Organic Chemistry of Natural Products Vol I and II by Gurdeep and Chatwall, Himalaya Publishing House.

- 10. Organic Chemistry of Natural Products Vol I and II by O.P. Agarwal, Krishan Prakashan.
- 11. Organic Chemistry Vol I and II by I.L. Finar, Pearson education.
- 12. Elements of Biotechnology by P.K. Gupta, Rastogi Publishers.
- 13. Pharmaceutical Biotechnology by S.P.Vyas and V.K.Dixit, CBS Publishers.
- 14. Biotechnology by Purohit and Mathur, Agro-Bios, 13th edition.
- 15. Phytochemical methods of Harborne, Springer, Netherlands.
- 16. Burger's Medicinal Chemistry.

	Dutcomes:			<u> </u>	1 1 0			1 01	• • •	
CO1	Demonstrate understanding of synthetic methods for producing alkaloids, flavonoids, and terpenoids.									
CO2	Demonstra medicinal		U	e significa	nce of natu	ral produc	ts in drug	discovery	and their	
CO3	Describe t	he proces	sses involv	ed in devel	loning drug	os from na	tural produ	ucts inclu	ding testing	
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		tion.			ioping uru	55 110111 114				
	and regula	tion.	PO2	PO3	PO4	PO5	PO6	PO7	]	
	and regula	ition. s				-	-	-	]	
	and regula of COs and PO	s PO1				-	-	-	]	

ADVANCED MEDICINAL CHEMISTRY									
Course Code	22MSCP5	CIE Marks	50						
Teaching Hours/Week (L:P:SDA)	3:0:0	SEE Marks	50						
Total Hours of Pedagogy	40	Total Marks	100						
Credits	3	Exam Hours	3						

#### **Course Learning Objectives:**

- To gain a comprehensive understanding of advanced concepts in medicinal chemistry, including contemporary drug design methodologies.
- To investigate detailed mechanisms of action of various drug classes at the molecular and cellular levels.
- To analyze complex structure-activity relationships to predict drug efficacy and optimize lead compounds.
- To explore advanced synthetic methodologies for the development of novel therapeutic agents, including asymmetric synthesis and combinatorial chemistry.

#### Module-1

Fundamental aspects of drugs: Forms, application, biological action, placebo effect, metabolism, drug interactions, adverse effects, classification of drugs, nomenclature of drugs, drug combinations, selection of essential drugs.

Physicochemical properties of drug molecules in relation to biological activity; solubility, partition coefficient, hydrogen bonding, protein binding, chelation, pka values, isomerism, Geometrical and optical isomers, steric effect, ionization.

#### Module-2

**SAR and QSAR:** SARs, Changing size and shape, introduction of new substituents-the introduction of a group in an unsubstituted position, the introduction of a group by replacing the existing group. QSAR- Lipophilicity, partition coefficient (log P), lipophilic substitution constants( $\pi$ ). Electronic effect (Hammet constant  $\sigma$ ), steric effect, Taft's steric parameter (Es), Hansch analysis and application, craigs plot, Free-Wilson analysis and application.

#### Module-3

**Prodrugs:** Enzyme activation of drugs, Utility of prodrugs, types of prodrugs, mechanism of drug activation-Carrier linked prodrugs, carrier linkages for various functional groups, carrier linked bipartite prodrugs. Bioprecurssor prodrugs(Proton activation, hydrolytic activation, elimination activation, oxidative activation, reductive activation, nucleotide activation, phosphorylation activation, sulfation activation, decorboxylation activation

#### Module-4

**Combinatorial Chemistry:** Introduction, the design of combinatorial synthesis, the general techniques used in combinatorial synthesis, the solid support method, parallel synthesis, Furka's mix and split techniques, Encoding methods-Sequential chemical tagging method, stills binary core tag system, computerized tagging, combinatorial synthesis in solution, screening and deconvolution.

#### Module-5

**Drug metabolism:** Introduction, sites of drug biotransformation, phase-I and phase-II reactions, role of Cytochrome P-450, Factors affecting drug metabolism.

## References

- 1. Introduction to quantitative Drug Design-Y.C.Martin.
- 2. Comprehensive Medicinal chemistry-Crowin and Hansch.
- 3. Medicinal Chemistry-Burger.
- 4. Principles of Drug Design-Smith.

- 5. Principles of Medicinal Chemistry- William Foye.
- 6. Drug design volumes-Ariens.
- 7. Strategy of drug design-Brucell.
- 8. The Organic Chemistry of drug design and drug action-Richard. B. Silverman.
- 9. Fundamentals of medicinal chemistry-Gareth Thomas. John Wiley and sons England.

CO1	Demonstrate an in-depth understanding of advanced concepts in medicinal chemistry and								
	their application in drug discovery.								
CO2	Understand and articulate the regulatory processes involved in drug approval, including the significance of clinical trials.								
CO3	Demonstrate proficiency in advanced synthetic methodologies, including combinatorial chemistry, for the development of novel therapeutic agents.								
apping of	of COs and PO	s							
		PO1	PO2	PO3	PO4	PO5	PO6	PO7	
	<b>CO1</b>	X	X						
	CO2	X	Χ	X					