

**NIZAM COLLEGE
DEPARTMENT OF CHEMISTRY**

LESSON PLAN

FOR THE ACADEMIC YEAR
2017-18 onwards

M. Sc. Chemistry (Second Year)
Spl: Pharmacoinformatics

Semester-III
Course/Paper - I

CH(CPI)301 T : Database Management, Sources and Scripting Languages

Unit: CPI - 09: Chemical Information Sources and Searches

Topics to be covered	No. of Hours required
Introduction to information sources	1
searching strategies, tactics for searches	2
Advantages and Limitations of computer searching	1
Keyword based general bibliographic searches, Chemical connectivity and structure searches (2D)	2
Chemical structure, property and shape based searches (3D), Searching for the synthesis (or) reactions of specific compounds or classes of compounds, Searching of chemical abstracts	2
Types of Publications: Journals, Technical reports, Patents, Conference Papers, Dissertations, Electronic Publications	2
Types of databases: Public databases - NCBI, RCSB, CSD, Expasy, Swiss-Prot and Paid databases - CAT'STN and SciFinder	2
Web-based cross platform solutions for Cheminformatics: BLAST, ClustalW, SAVES, ProSA	3
	15hrs

Unit: CPI - 10: Database Design and Management

Topics to be covered	No. of Hours required
Computers & it's components, Operating System (Windows & Linux)	1
Introduction to DBMS, Database concepts	2
Database models and ER diagrams	2
Normalization	1
Introduction to SQL, DDL, DML, DCL, and TCL;	2
Creation of databases, Searching database using SQL	1
Built-in-functions, String manipulation, improving query performance (where, 'Group By', having Clause)	1
cursors, stored procedures	1
Introduction to MySQL, configuring and running MySQL on Linux	2
Data Processing, Information systems and computing	1
Data presentation for computing, Distributed processing	1
	15hrs

Unit: CPI - 11: Data Sequencing and Mining

Topics to be covered	No. of Hours required
Introduction to Data Mining	2
working principles of Data Mining	2
Architecture form of data Mining	1
Difference between Data Mining and Machine learning techniques	2
Supervised and unsupervised learning methods and its application to QSAR	3
Data Visualization: Visualizing Data mining models, Decision Tree	2
Data warehousing: Data mining and analytic technology	2
Comparing different Models using visualization	1
	15hrs

Unit: CPI – 12 : Scripting Languages

Topics to be covered	No. of Hours required
Introduction to Shell scripting	1
Common Linux commands (Bash)	1
Basic shell Programming: addition, subtraction, loops, conditional-loops, un-conditional loops, Linux text editors (Vi)	1
Perl: Introduction, basics, sequences	2
Perl: uses, implementation issues, changes from other languages	2
advantages, and disadvantages	1
Strings: operations, support with Perl, advantages	2
accessing MySQL database using Perl, getting id, Sequence from a Database Object	2
matching a sequence in a Database Object, Subroutines	1
Introduction to Bio-Perl, Perl for Cheminformatics / Bioinformatics	2
	15hrs

Course/Paper - II

CH(CPI)302 T : Computational Chemistry, Molecular Modeling &Its Applications.

Unit: CPI – 13 : Computational Chemistry -I

Topics to be covered	No. of Hours required
Introduction to Molecular Modeling	1
Single molecule calculations, assemblies of molecules and reactions of molecules	2
Co-ordinate systems: Cartesian and Internal Co-ordinates, Z-matrix	1
Potential energy surface - Conformational search; Global minimum, Local minimum	2
Conformational analysis of ethane	1
Force field - Features of Molecular Mechanics	1
Bonded and Non-bonded interactions, Bond Stretching, Angle Bending	2
Torsional Terms (Improper Torsions, out of Plane Bending Motions, Cross Terms)	2
Non Bonded Interactions (Electrostatic Interactions, Van-der Waals interactions)	2
Hydrogen Bonding Interactions	1
	15hrs

Unit: CPI – 14 : Computational Chemistry -II

Topics to be covered	No. of Hours required
Force Field Equation in Energy minimization (Energy as function of r, θ, ω)	2
Introduction to Derivative Minimization Methods (First Order Minimization)	2
Types of energy minimization Methods; Steepest Descent, Conjugate Gradient	3
Conformational Search procedures - Geometry optimization procedures	2
Molecular Dynamics: Introduction, description of Molecular Dynamics	2
basic elements of Monte-Carlo method, differences between Molecular Dynamics and Monte-Carlo method	2
Qualitative exposure to Molecular Dynamics Simulations	2
	15hrs

Unit: CPI – 15 : Drug Design Methods I - Ligand Based

Topics to be covered	No. of Hours required
Lead Molecule, Structure Activity Relationship (SAR)	1
Quantitative Structure Activity Relationship (QSAR), Distinguish between SAR and QSAR	1
Physicochemical parameters: Electronic effects, Hydrophobicity,	1
Physicochemical parameters: Steric Factors Taft's Steric function, Molar Refractivity, Verloop Steric factor	1
Molecular Descriptor analysis: Craig plot, Topliss scheme	2
Bioisosteres - Hansch model, Free-Wilson model for QSAR equations	2
Regression analysis: Multi Linear Regression and Partial Least Square (terms: n, SD, r, r ² , r ² %, F)	2
Examples for linear and non-linear equations	2
3D QSAR: CoMFA and CoMSIA	2
Differences between 2D and 3D QSAR	1
	15hrs

Unit: CPI – 16 : Drug Design Methods II - Structure Based

Topics to be covered	No. of Hours required
Database similarity searches, Pair-wise alignment: Global sequence analysis (Needleman-Wunsch),	1
Local Sequence Alignment (Smith Waterman), Multiple Sequence Alignment	1
Homology Modeling: Query sequence, Template selection,	1
Alignment, Backbone Modeling, Loop Modeling, Side chain Modeling,	2
Model optimization, Energy minimization	2
Model Evaluation: Ramachandran Plot, Verify 3D, Errata and ProSA	2
Active site Identification - Docking	1
Docking Algorithms: Genetic Algorithm, Incremental construction	2
Molecular Interactions, Scoring functions	1
Virtual Screening: Ligand Based and Structure Based	1
De novo ligand design and its limitations	1
	15hrs

Course/Paper - III

CH(CPI)303 T: Elective-3A: Synthetic Reagents, Advanced NMR, Conformational Analysis and ORD

Unit: CPI – 17 : Synthetic Reagents-I

Topics to be covered	No. of Hours required
i) Protecting groups:	
a) Protection of alcohols by ether, silyl ether and ester formation	2
b) Protection of 1,2-diols by acetal, ketal and carbonate formation	1
c) Protection of amines by benzyloxycarbonyl, t-butyloxycarbonyl, fmoc and triphenyl methyl groups.	1
d) Protection of carbonyls by acetal, ketal and thiolacetal (Umpolung) groups	1
e) Protection of carboxylic acids by ester and ortho ester (OBO) formation.	1
ii) Organometallic Reagents:	
Preparation and application of the following in organic synthesis:	1
1) Organo lithium 2) Organo copper reagents	
3) Organo boranes in C-C bond formation	1
4) Organo silicon reagents: reactions involving β -carbocations and α carbanions, utility of trimethyl silyl halides, cyanides and triflates	2
iii) Carbonyl methylenation:	
a) Phosphorous ylide mediated olefination	2
1) Wittig reaction, 2) Horner-Wordsworth-Emmons reaction.	
b) Titanium- Carbene mediated olefination 1) Tebbe reagent	1
2) Petasis reagent 3) Nysted reagent	1
iv) Carbene insertions: Rh based carbene complexes, cyclopropanations.	
v) C-H Activation: Introduction, Rh catalysed C-H activation.	1
	15hrs

Unit: CPI – 18 : Synthetic Reagents-II

Topics to be covered	No. of Hours required
i) Oxidations: a) Oxidation of active C-H functions: DDQ and SeO ₂ .	2
b) Alkenes to diols: Prevost and Woodward oxidation	1
c) Alcohol to carbonyls: Cr(VI) oxidants (Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation	2
d) Oxidative cleavage of 1,2-diols: Periodic acid and Lead tetra acetate.	1
ii) Reductions	1
a) Catalytic hydrogenation: Homogenous (Wilkinson's catalytic hydrogenation) and heterogeneous catalytic reduction.	2
b) Non-metallic reductions: Diimide reduction	1
c) Dissolving metal reductions: Birch reduction.	2
d) Nucleophilic metal hydrides: LiAlH ₄ , NaBH ₄ , Modifications LAH, SBH.	1
e) Electrophilic metal hydrides: BH ₃ , AlH ₃ and DIBAL.	1
f) Use of tri-n-butyl tin hydride: Radical reductions	1
	15hrs

Unit: CPI – 19: ^{13}C NMR and 2D NMR spectroscopy

Topics to be covered	No. of Hours required
i) Introduction, Types of ^{13}C NMR spectra (uncoupled, proton- decoupled and off-resonance decoupled (ORD) spectra).	2
^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds	2
Calculation of chemical shifts of alkanes, alkenes and alkynes.	1
Homonuclear (^{13}C , ^{13}C J) and heteronuclear (^{13}C , ^1H J and ^{13}C , ^2H J) coupling.	1
Applications of ^{13}C -NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules.	2
^{13}C NMR spectral editing techniques:	1
principle and applications of APT, INEPT and DEPT methods.	1
ii) Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMO COSY (^1H - ^1H COSY) , TOCSY	2
Hetero COSY (^1H , ^{13}C COSY, HMQC), long range ^1H , ^{13}C COSY (HMBC),	1
Homonuclear and Heteronuclear 2D-J-resolved spectroscopy,	1
NOESY and 2D-INADEQUATE experiments and their applications.	1
	15hrs

Unit: CPI – 20: Conformational analysis (Cyclic systems) & ORD

Topics to be covered	No. of Hours required
Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes	2
cyclohexanone (2-alkyl and 3-alkyl ketone effect), 2-halo-cyclohexanones, cycloheptane	2
Stereo chemistry of bicyclo[3,3,0]octanes, hydrindanes, decalins and perhydro-anthracenes.	2
Conformational structures of piperidine, N-Methyl-piperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolizidine.	3
Factors governing the reactivity of axial and equatorial substituents in cyclohexanes.	1
Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring	1
Optical rotation, circular birefringence, circular dichroism Cotton effect.	1
Plain curves and anomalous curves.	1
Empirical and semi-empirical rules-The axial halo-ketone rule, the octant rule, Helicity rule, Exciton chirality method.	1
Application of the rules to the study of absolute configuration and organic molecules	1
	15hrs

Course\Paper-III:

CH(CPI)303 T:Elective 3B: Advanced Natural Products

Unit: CPI-21: Biosynthesis of natural products

Topics to be covered	No. of Hours required
Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis	2
Methods for determination of biosynthetic mechanism. Isolation and identification of Biosynthetic precursors, Feeding experiments	2
use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation	2
Identification of the position of labels in labeled natural products by chemical degradation and spectral methods	2
Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds	2
2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids	3
3) Mevalonic acid pathway : Biosynthesis of terpenes – mono, sesqui, di, tri (β -amyrin) and carotenoids, steroids – cholesterol	2
	15hrs

Unit: CPI-22: Structure determination of natural products by chemical methods.

Topics to be covered	No. of Hours required
Determination of structure and stereochemistry of morphine	3
Determination of structure and stereochemistry of reserpine	3
Determination of structure and stereochemistry of abietic acid	3
Determination of structure and stereochemistry of cholesterol	3
Determination of structure and stereochemistry of rotenone	3
	15hrs

Unit: CPI-23: Structure determination and stereochemistry of natural products by spectral methods.

Topics to be covered	No. of Hours required
Spectroscopic techniques IR, UV	2
^1H nmr, ^{13}C nmr	2
COSY, HETEROCOSY, NOESY, 2D-INADEQUATE	2
MS in the structure elucidations of natural products, Examples, flavones, biflavones, flavanones, isoflavones, coumarins, quinolines, isoquinolines.	2
Study of the following solved problems: Mass, IR, ^1H , ^{13}C NMR, HOMOCOSY, HECTOR, DEPT, 2D-INADEQUATE and NOE of Geraniol, INEPT of menthol, APT of apparicine	3
Heteronuclear 2D-J resolved spectrum of stricticine	1

NOESY of buxaquamarine	1
HETEROCOSY of strictanol	1
2D-INADEQUATE of α -picoline and β -methyl tetrahydran furan	1
	15hrs

Unit: CPI-24: Total stereo selective synthesis of natural products.

Topics to be covered	No. of Hours required
Nicalou's synthesis of Dynemicin A	2
Corey's synthesis of prostaglandins (E2, F2 α) and paeoriflorin	3
Sharpless synthesis of L-hexoses	2
Nicolaous synthesis of taxol	2
Danishefsky synthesis of indolizomycin	2
Takasago synthesis of menthol	2
Hoffmann-LaRoche synthesis of Biotin	2
	15hrs

Course\Paper-IV

CH(CPI)304 T:ELECTIVE 4A: Modern Organic Synthesis

Unit: CPI - 25 : Asymmetric Synthesis

Topics to be covered	No. of Hours required
Introduction: Brief revision of classification of stereo selective reactions	1
Prostereoisomerism: Topicity in molecules Homotopic, stereo-heterotopic (enantiotopic and diastereotopic) groups and faces-symmetry criteria.	1
Prochiral nomenclature: Pro chirality and Pro-R, Pro-S, Re and Si. Conditions for stereo selectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivity.	2
Analytical methods: %Enantiomeric excess and diastereomeric ratio. Determination of enantiomeric excess: specific rotation, Chiral NMR; Chiral derivatizing agents, Chiral solvent, Chiral shift reagents and Chiral HPLC.	2
Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.	2
Chiral auxiliary controlled asymmetric synthesis: α -Alkylation of chiral enolates, Evan's oxazolidinone, 1, 4-Asymmetric induction and Prelog's rule.	2
Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC2 BH and IPCBH2.	2
Chiral catalyst controlled asymmetric synthesis: Sharpless epoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphin catalyst.	2
Asymmetric aldol reaction: Diastereoselective aldol reaction (achiral enolate & achiral aldehydes) its explanation by Zimmerman-Traxel model.	1
	15hrs

Unit: CPI - 26 : Synthetic strategies

Topics to be covered	No. of Hours required
Introduction: Terminology, Target, synthon, synthetic equivalent, functional group inter-conversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis.	2
Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations.	2
Order of events: S-Salbutamol, Propoxycaine.	1
One group C-C and C-X disconnections: Introduction .One group C-C disconnections in alcohols and carbonyl compounds. One group C-X disconnections in Carbonyl compounds, alcohols, ethers and sulphides.	2
Two group C-C and C-X disconnections : Introduction, Two group C-X disconnections in 1,1-difunctionalised, 1,2-difunctionalised and 1,3-difunctionalised compounds.	2
Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.	2
Control in carbonyl condensations: oxanamide and mevalonic acid.	1

Strategic bond: definition, guidelines for disconnection; disconnection of C-X bonds, disconnect to greatest simplification, using symmetry in disconnection, disconnection corresponding to known reliable reaction, high yielding steps and recognizable starting materials. Retrosynthesis of Retronecene, longifoline.	3
	15hrs

Unit: CPI - 27 : New Synthetic reactions

Topics to be covered	No. of Hours required
Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.	3
C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions, Julia-Lythgoe olefination and Peterson's stereoselective olefination.	3
Multicomponent Reactions: Ugi, Passerini, Biginelli, Bergman and Mannich reactions.	2
Ring Formation Reactions: Pausan-Khand reaction, Nazarov cyclisation.	1
Click Chemistry: Click reaction, 1,3-dipolar cycloadditions.	1
Metathesis: Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), Ring Closing Metathesis (RCM), Ring Opening Metathesis (ROM), applications.	2
Other important synthetic reactions: Baylis-Hilman reaction, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction, Stork-enamine reaction and Michael reactions.	3
	15hrs

Unit: CPI - 28 : Chiral Drug

Topics to be covered	No. of Hours required
Introduction to chiral drugs. Three-point contact model	1
Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule.	1
Synthesis and pharmacological activity of Menthol, S-Naproxen, S-Ibuprofen (anti inflammatory)	1
Synthesis and pharmacological activity of S-Timolol, oxazolidone, Captopril, Enalapril, Diltiazam (Calcium antagonist)	2
Synthesis and pharmacological activity of Indinavir sulphate (HIV-1-protease inhibitor)	2
Synthesis and pharmacological activity of Ethambutal (anti-tubercular). Cloxacillin, Cephalexin (Antibiotic)	2
Synthesis and pharmacological activity of Oxybutynine hydrochloride (Antispasmodic Agent), Dexormaplatin (Antitumour Agent)	2
Synthesis and pharmacological activity of indacrinone (Diuretic), Griseofulvin, (Antifungal)	2
Synthesis and pharmacological activity of Levocitrizine (Antihistamine) and Metoprolol (β_1 - blocker)	2
	15hrs

Course\Paper-IV

CH(CPI)304 T:ELECTIVE 4B: Intellectual Property Rights

Unit: CPI - 29 : Introduction

Topics to be covered	No. of Hours required
Introduction to Legal Rights and obligations	2
Concept of Property	1
Kinds of Property	1
General concept and Significance of Intellectual Property (IP)	2
Intellectual Property Rights (IPR),	1
Intellectual property, Introduction to IPR	2
contents of IPR and their protection	1
Recent Developments, IP Organisations	2
Introduction to Patents	1
Trademarks, Copyrights, Trade secrets,	1
Industrial designs and Geographical indications	1
	15hrs

Unit: CPI - 30 : International Organizations & Treaties

Topics to be covered	No. of Hours required
Paris Convention for the Protection of Industrial Property	1
Berne Convention for the Protection of Literary and Artistic Works	2
Patent Cooperation Treaty (PCT) which facilitates obtaining of patents in several countries by filing a single application	2
World Trade Organization (WTO), Trade Related Aspects of Intellectual Property (TRIPS)	2
Madrid system for the international registration of marks	2
The Hague system for the international deposit of industrial designs	2
Budapest treaty on the international recognition of the deposit of microorganisms for the purpose of patent procedure	2
International convention for the protection of new varieties of plants	2
	15hrs

Unit: CPI - 31 : Patent Search

Topics to be covered	No. of Hours required
What is a patent search.	1
Who needs a patent search	1
Patent Search Types and Methodologies,	2
Novelty Searches, Validity Searches	2
Infringement Searches, State-of the-art searches	2
Searching in Patent Databases: Free search databases: USPTO, EPSPACE, WIPO, Free Patents Online, Fresh Patents and JSPTO	2
Paid search databases: Micropat, Delphion, DialogPro, Patent Optimiser, Aureka and PatentCafe,	2
Structure based search: STN search, SciFinder	1
	15hrs

Unit: CPI - 32 : IP Reports Generation

Topics to be covered	No. of Hours required
Novelty search reports	1
Infringement search reports	1
Prior-art search reports	1
Patent invalidation reports	1
Competitive search reports	1
Business analysis reports	1
Patent Filing and Drafting	2
Patent filing procedures	2
Indian patent act	1
patent drafting	2
PCT applications, provisional and complete specifications	2
	15hrs

LABORATORY COURSES

Course\Paper-V:

CH(CPI)351 P : Molecular Modeling Lab

No. of Hours Allotted: 15 weeks x 9 hrs

Topics to be covered	No. of Weeks required
Dos and Linux commands; Shell Scripting : if, if else, for, do while	1
Perl Scripting : if, if else, for, while; Perl scripting for accessing MySQL database objects using DDL, DML, DCL	1
Creating Database : Creation of tables and Insertion of rows using MySQL	1
Perl scripting for Sequence analysis : a. Translate DNA sequence into RNA sequence b. Finding common Ktup (k = 1, 2, 3) between two sequences c. Local and global alignment of two sequences (DNA/RNA/Protein) d. Multiple sequence alignment	2
Drawing and minimizing molecules in modeling software, calculating physicochemical parameters.	2
2D QSAR Studies (COX 1 and 2, DHFR inhibitors).	1
3D QSAR: Pharmacophore model generation and pharmacophore match searching in database.	2
Homology Modeling: Retrieving Query Sequence, Finding Template, Pair-wise alignment, 3D model generation, energy minimization and structure validation.	2
Molecular Docking of COX 1 and 2, DHFR inhibitors into respective receptors.	3
	15 Weeks

Course\Paper-VI:

CH(CPI)352 P : Synthesis, Isolation and Mixture separation of Organic Compounds

No. of Hours Allotted: 15 weeks x 9 hrs

Topics to be covered	No. of Weeks required
Synthesis of Drugs: Benzocaine (Anaesthetic)	1
Antipyrine (Antipyretic)	1
Clofibrate(Anti-lipidemic)	1
Sulphonamide (antibacterial)	1
2-phenyl-Indole, Quinoxalinone, Isoniazid (Anti-Tubercular)	1
Benzillic acid rearrangement, Beckmann rearrangement and stereo selective reduction of ethyl acetoacetate by bakers yeast.	2
2. Isolation of Herbal Drugs: 1.Piperine from black Pepper 2. Caffeine from tea leaves 3. Cineole from Eucalyptus leaves	2
3. Mixture Separation	
a) Solid - Solid - 3 mixtures	2
b) Solid - Liquid – 3 mixtures	2
c) Liquid - Liquid – 3 mixtures	2
	15 Weeks

(Semester-IV)
Course/Paper - I

CH(CPI) 401 T: Pharmacokinetics

Unit: CPI - 33: Biopharmaceutics

Topics to be covered	No. of Hours required
Introduction to Biopharmaceutics, definition of pharmacokinetics	2
pharmacodynamics, ADME processes	1
Rate, Rate Constants and order of reactions- zero order kinetics, first order kinetics, mixed order kinetics	2
Routes of administration: Enteral (oral, sublingual, buccal, rectal) perenteral (intravenous, intramuscular and subcutaneous), topical (dermal, trans dermal, ophthalmic, intranasal), advantages and disadvantages.	2
Plasma drug concentration vs time profile: pharmacokinetic parameters (Peak plasma concentration, time of peak concentration, AUC), pharmacodynamic parameters (MEC, MSC, Therapeutic range, onset of action, onset of time, duration of action, intensity of action)	2
Dissolution: Definition and theories of drug dissolution, Diffusion layer model, Danckwert's model & interfacial barrier model.	3
Factors influencing dissolution, dissolution tests for tablets and capsules (basket apparatus, paddle apparatus, flow through cell apparatus).	1
In vitro - in vivo correlation of dissolution.	2
	15hrs

Unit: CPI-34: Drug Absorption and Distribution

Topics to be covered	No. of Hours required
Absorption: Structure of cell membrane	1
Mechanism of drug absorption- Passive diffusion, Pore-transport, facilitated diffusion	1
active transport, ionic or electrochemical diffusion,	1
ion-pair transport, endocytosis	1
Factors influencing drug absorption: Dosage form, pH (pH partition hypothesis) Lipophilicity, Gastric emptying	2
Bioavailability: Objectives of bioavailability studies,	1
absolute versus relative bioavailability	1
Plasma level- time studies (single dose and multiple dose)	1
Concept of steady state concentration.	1
Distribution: Volume of distribution	1
Apparent volume of drug distribution and its determination	1
Factors affecting drug distribution	1
Plasma protein binding	2
	15hrs

Unit: CPI-35: Drug Metabolism and Excretion

Topics to be covered	No. of Hours required
Definition of biotransformation, drug metabolizing organs, drug metabolizing enzyme. Chemical pathways of drug biotransformation- Phase-I reactions and Phase-II reactions.	2
Phase-I reactions: A) Oxidative reactions, Cytochrome-P450 Oxidation-reduction cycle i) Aromatic hydroxylation (Acetanilide),	1
ii) Aliphatic hydroxylation (Ibuprofen), iii) N-Dealkylation (Diazepam),	1
iv) Oxidative deamination (Amphetamine), v) N-Hydroxylation (Paracetamol), vi) S- oxidation (Phenothiazine).	1
B) Reductive reactions- i) Reduction of carbonyls (Chioral hydrate) ii) N-Compounds (Nitrazepam). c) Hydrolytic reactions (Asprin).	1
Phase-II reactions: (Real detoxication pathways). i) Conjugation with D-Glucuronic acid (Benzoic acid), ii) Conjugation with Sulfate moieties (Paracetamol), iii) Conjugation with α -Amino acids (Salicylic acid). iv) Acetylation (p-Amino Salicylic acid), v) Methylation (Histamine).	3
Factors affecting biotransformation of drugs i) physiochemical properties of drugs, ii) chemical factors, iii) biological factors, Bioactivation and tissue toxicity.	2
Excretion of drugs. Definition of excretion, Types of excretion- (Renal and non-renal excretion).	1
The process of Renal excretion of drugs-Glomerular filtration, Active tubular secretion and active or passive tubular reabsorption, concept of clearance, factors effecting renal excretion, nonrenal routes of excretion, biliary excretion, salivary excretion and pulmonary excretion.	3
	15hrs

Unit: CPI-36: Pharmacokinetic Models

Topics to be covered	No. of Hours required
Definition, classification of models(mammillary and catenary)	1
One Compartment open model (I.V bolous, IV infusion, Extravascular administration)	2
Two Compartment open model (I.V bolous, IV infusion, Extravascular administration)	2
Application of these models to determine the various pharmacokinetic parameters	3
Calculations and non- compartmental approaches to pharmaco kinetics	2
Non-linear pharmaco kinetics: causes of nonlinearity	2
Michaels-Menten kinetics- characteristics	2
basic kinetic parameters	1
	15hrs

Course/Paper-II

CH(CPI)402 T : Principles of Drug Discovery, Drug Targets and chemistry of Pharmacology

Unit: CPI - 37: Principles of Drug Discovery and SAR Studies

Topics to be covered	No. of Hours required
Introduction to drug discovery. Folklore drugs, stages involved in drug discovery- disease, drug targets, bioassay	2
Discovery of a lead - screening of natural products and synthetic compound libraries.	1
Natural products as lead structures in drug discovery – Pharmacophore - structure pruning technique e.g. morphine	2
Discovery of lead structure from natural hormones and neurotransmitters	1
Principles of design of agonists (Salbutamol), antagonists (cimitidine) and enzyme inhibitors (captopril).	1
Drug discovery without lead – serendipity - Penicillin and Librium as examples. Principles of Prodrug design; Existing drugs as leads (me too drugs). Introduction to drug patents and Clinical trials.	2
SAR Introduction; 1. Binding role of hydroxy group, Amino group, aromatic ring, double bond, ketones and amides.	2
2. Variation of substituents- alkyl substituents, aromatic substituents, extension of structure, chain extension, ring expansion/contraction, ring variation, ring fusion.	2
3. Simplification of the structure, rigidification, conformational blockers, X-ray crystallographic studies. Ex: A case study of Oxaminquine (schistosomiasis), Sulpha drugs (antibacterial), and Benzodiazepines (Hypnotics).	2
	15hrs

Unit: CPI-38: General Principles of Pharmacology and drug Targets, drugs acting on ANS and CNS

Topics to be covered	No. of Hours required
Nature and sources of drugs - Routes of administration of drugs – Classification. Drug absorption – bioavailability - Drug distribution.	1
Biotransformation and excretion drugs - Biological half-life and its significance/toxicity - Mechanism of action including drug receptor - Interactions and factors influencing them - Dose response relationship.	1
Introduction to macromolecular targets- Enzymes, cell wall, Cell membrane, Genetic material (DNA/RNA) Ion Channels, and drug classification. Structural architecture of Human Cell structure and Bacterial Cell wall,	1
Pharmacology of Drugs Acting on ANS and CNS, Introduction, classification of ANS and CNS. Structure of neuron. definitions of Somatic and autonomic nervous systems	1
Importance of acetyl choline – Biosynthesis. pathway of Cholinergic signalling systems .Uptake process – choline esterase. Cholinergic agonist-Acetyl choline. Degeneration- alzheMER. carbachol- synthesis & activity. Choline Esterase inhibitors. phsostigmine.	1
Cholinergic agonist – Atropine. Local Anaesthetics. Architecture of Na ⁺ ion channel on nerve membrane. H and M gates. Synthesis and mode of	1

action of procaine	
Adrenergic Receptors- α / β 1 & 2 receptors - Occurrence- Effect of activation and its Physiological effect.	1
Biosynthesis of Adrenalin and Nor adrenalin – α 1 and α 2 receptors importance of α 2 and NE. Synthesis of NE and E. Adrenergic Stimulants - Methyl DOPA – synthesis and mode of action.	1
Adrenergic antagonist- Mode of action and synthesis of Doxazocin. Anti Ulcer agent Synthesis and Mode of action. CNS neurotransmitters. Classification of CNS stimulants, Analeptic – Nikethamide; Psycho motor stimulants – amphetamine.	1
Anti Depressants; imipramine – synthesis and mode of action.	1
Hypnotics and Anxiolytics- Classification . Chlorpromazine – synthesis and mode of action as anti psychotic agent	1
Anti-epileptic Agents-Brief description about epilepsy – types of epilepsy- Phenytoin – synthesis and mode of action.	1
General Anesthetics: Classification - Inhalation anaesthetic- Haloethanes synthesis and mode of action.	1
(I.V. anesthetic) – Thiopentone; Synthesis and mode of action.	1
Neurodegenerative disorders – classification – Importance of Acetyl Choline and Dopamine. Parkinsons Disease- Symptoms. Synthesis of Levo Dopa, Mode of action. Alzheimer Disease-loss of Neurons- Donepezil.	1
	15hrs

Unit – CPI-39: Drugs Acting on Cardio Vascular and Respiratory System

Topics to be covered	No. of Hours required
General considerations-Pharmacology of drugs used in the treatment of congestive heart failure	1
Anti-arrythmics - Classification with examples, Anti-hypertensives, ACE inhibitors (captopril), beta1-blockers (Propranolol)	2
Drugs acting on Ion channels - Ca^{2+} , Na^+ and Cl^- channels and their mode of action	1
Structural formulae of Tetracaine and synthesis and of Amlodipine, Nifedipine, Diltiazem, Tetracine and 4-Aminopyridine	2
α -Adrenoreceptor stimulant (Clonidine), α - Adrenoreceptor blocking agent (Prazocin), Anti-hyperlipedemic (Clofibrate).	2
Pharmacology of Drugs affecting Respiratory System: Drugs used in the treatment of disorders of Respiratory Function and Bronchial Asthma	2
Broncho dilators - i) β -adrenergic agents (Albuterol) ii) Phosphodiesterase inhibitors (Aminophylline)	1
Anticholinergic agents (Atropine), Corticosteroids (Beclomethasone)	1
Inhibitors of mediator release (Cromolyn Sodium), Anti-tussives (Codeine) and Expectorants (Guaifenesin)	1
Pharmacology of Drugs affecting Gastro intestinal System - H^+/K^+ -ATPase inhibitors (omeprazole)	1
Pharmacology of purgatives/laxatives (Dulcolax), Anti-diarrhoeals (Lopramide)	1
	15hrs

Unit: CPI-40: Drugs acting on metabolic process, cell wall, genetic material and immune system

Topics to be covered	No. of Hours required
a)Drugs acting on metabolic process: Antifolates - Discovery and mechanism of action of sulphonamides, Structure of sulfomethoxazole, and dapsons. Diaminopyrimidines - trimethoprim, and drug synergism.	3
b)Drugs acting on cell wall: β -Lactam antibiotics - mechanism of action of penicillins and cephalosporins. Resistance to penicillins, broad spectrum penicillins - ampicillin and amoxicillin. β -Lactamase inhibitors - Structural formulae and mode of action of clavulanic acid and sulbactam.	3
Drugs acting on genetic material: Introduction, classification and mechanism of action.	1
a)DNA-intercalating agents -Anti-cancer and Anti-malarial agents. Structural formulae of Daunomycin, Amsacrine and Chloroquine.	1
b)DNA- Binding and nicking agents: Antiprotozoal drugs, Metronidazole, and Tinidazole.	2
c)DNA-Polymerase inhibitors: Antiviral agents - AZT.	
d)DNA-Topoisomerase inhibitors: Anti bacterial agents. Structural formulae of Ciprofloxacin and Norfloxacin	1
e)Inhibitors of transcribing enzymes: Anti-TB and anti-leprosy agents, structural formulae of Rifamycins.	1
f)Drugs interfering with translation process: Antibacterial drugs, Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin.	1
Drugs acting on immune system: Introduction to immune system. Immuno-suppressing agent - structural formula of Cyclosporin. Immunoenhancers-use of vaccines and structural formula of levamisol.	2
	15hrs

Course/Paper - III

Course\CH(CPI)403 T: ELECTIVE 3A: Pharmaceutical Analysis

Unit: CPI - 41: Spectral Methods in Pharmaceutical Analysis

Topics to be covered	No. of Hours required
Ultraviolet and Visible Spectroscopy: Introduction, principle, instrumentation, calibration	1
UV spectra of some representative drug molecules : Steroid enones, Ephedrine [the benzoid chromophore], ketoprofen [extended benzene chromophore], Procaine [amino group auxochrome], Phenylephrine [hydroxyl group auxochrome].	1
Application of UV-Vis Spectrophotometry to Pharmaceutical quantitative Analysis: Assay of Frusemide in tablet, Assay of Penicillin by derivatization.	1
Assay of Drugs by i) Direct UV method ii) Suitable Chromogens and iii) Charge transfer Complexes and Difference spectrophotometry, Derivative Spectra	1
Applications of UV-Visible Spectrophotometry in Pre-formulation and formulation	1
Infrared Spectroscopy - Introduction, principle, instrumentation, Sample preparation methods	1
Application of IR Spectrophotometry in Structure Elucidation, interpretation of IR spectra of Paracetamol, aspirin, dexamethasone and phenoxymethyl penicillin potassium.	1
Examples of IR Spectra of Drug molecules, IR Spectrophotometry as a fingerprint technique	1
Near IR analysis (NIRA) : Introduction, Examples of NIRA application	1
Examples of NIRA application – determination of particle size in United states Pharmacopia grade Aspirin, determination of blend uniformity, determination of active ingredients in multi- component dosage forms, moisture determination	1
Nuclear Magnetic Resonance Spectroscopy – Introduction, principle, instrumentation, general application.	1
¹ H NMR : Application of NMR to Structure Confirmation in some drug molecules, ¹ H NMR spectral analysis of Benzocaine, Phenacetin, Clofibrate and phenylephrine	2
¹³ C NMR : ¹³ C NMR spectrum of Salbutamol sulphate, Two Dimensional NMR Spectra – Proton- proton correlation spectrum of Tranexamic acid, Application of NMR to quantitative analysis	2
	15hrs

Unit: CPI - 42: Chromatography in Pharmaceutical Analysis-I

Topics to be covered	No. of Hours required
Chromatography – Introduction to chromatography, principle – physical basis of chromatography – adsorption and partition coefficients, stationary and mobile phases, classification of chromatographic methods	1
Thin Layer Chromatography (TLC): principle, adsorbents, preparation of TLC plates, drying of plates, sample application – spotting, solvents for	1

development, choice of solvents	
Visualization and detection of spots – UV light, Iodine chamber etc., preparative TLC, applications of TLC – qualitative identification tests, Limit tests; HPTLC - Introduction to HPTLC, principle, advantages over TLC	1
High performance TLC (HPTLC): , instrumentation, steps involved in HPTLC – sample preparation, selection of chromatographic layer, plates, prewashing, condition of plates, sample application, preconditioning, mobile phases	1
HPTLC – chromatographic development, detection of spots, scanning and documentation, Applications of HPTLC – assay of rifampicin, isoniazide and pyrazinamide	1
High Performance Capillary Electrophoresis: Introduction to electrophoresis, electrokinetic phenomenon, Electro-Osmotic Flow (EOF), migration of ionic and neutral species in CE	1
CE – Instrumentation , types of electrophoresis – Zone and Capillary electrophoresis, stationary and mobile phases, electrodes, control of separation – migration time, electrodispersion	1
Applications of CE – Separation of Atenolol and related impurities based on charge, assay of NSAIDs by CE and separation of anions based on ionic radius	1
Micellar Electrokinetic Chromatography (MECC): introduction, principle, separation mechanism - combination of electrophoresis, electro-osmosis and chromatography	1
MECC – Partition – micellar phase and pseudo stationary phase, surfactants – micelle-separation of anionic, cationic and neutral micelles, detection – electropherogram, application of MECC- determination of flavonoids	1
Gas Chromatography (GC): Introduction, principle, theoretical considerations-retention time, retention volume, plate theory – equilibrium plates, calculation of no. of theoretical plates, resolution, Rate theory – Van De Meter's equation – Eddy Diffusion, Longitudinal Diffusion, Mass transfer; Instrumentation, stationary and mobile phases – carrier gas, detectors	1
GC: selectivity of liquid stationary phases – Kovat's indices, Mc Reynolds Constants; Derivatization in GC; Applications of GC – External and Internal standard methods	1
Quantitative applicants of GC: determination of manufacturing residues – detection of pivalic acid in dipivefrin eye drops, determination of residual solvents – purge trap GC, applications of GC in bio-analysis. HPLC – introduction and principle	1
High Performance Liquid Chromatography (HPLC) - instrumentation, stationary and mobile phases, elution methods, detectors, structural factors governing elution of drugs, qualitative analysis of drugs by HPLC	1
Assay of hydrocortisone in cream, assays involving specialized techniques – assay of adrenaline by anionic ion-pairing agent	1
	15hrs

Unit: CPI - 43: Chromatography in Pharmaceutical Analysis-II

Topics to be covered	No. of Hours required
Potentiometric Titrations: - Introduction, principle, instrumentation.	1
Assay of Aspirin, Assay of Iron(II) succinate in ferromynS tablets, Introduction to ISE	1
Determination of fluoride in tablets and solutions by Fluoride Ion Selective Electrode. Fundamentals of radioactivity	1
Measurement of radioactivity, Radiopharmaceuticals - requirements, radiochemical methods	1
Isotope dilution analysis IDA, Radioimmuno , assay RIA-Thyroxin, and thyroid stimulating Hormone	1
Introduction to thermal methods, classification,application of drug phenacetin	1
Detection of polymorphisim and pseudopolymorphisim in pharmaceutical by DSC/DTA.	1
Introduction to electro-analytical techniques, classification	2
Polarography, theory, polarogram	2
applications of polarography in analysis of Antibiotics, Alkaloids	1
applications of polarography in analysis Trace metals and metal containing drugs	1
applications of polarography in analysis Blood serum and cancer diagnosis, insecticides,	1
applications of polarography in analysis Vitamins, Hormones.	1
	15hrs

Unit: CPI-44: Titrimetry, Chemical and Extraction methods in Pharmaceutical Analysis

Topics to be covered	No. of Hours required
Introduction - Qualitative analysis, quantitative analysis, classical methods of analysis, Types of chemical reactions and primary and secondary solutions.	1
Acid-base titrations ,Terminology, indicator principle, direct acid-base titrations in the aqueous phase, Indirect titrations in aqueous phase, estimation of alcohols and hydroxyl values by reaction with acetic anhydride.	1
Non-aqueous titrations -Theory, types of non-aqueous solvents, titrations of weak acids, Analysis of phenylephrine using perchloric acid.	1
Argentimetric Titrations – Principle, procedure for assays of Sodium chloride, potassium chloride, thiamine hydrochloride and carbromal.	1
Complexometric Titrations – Principle, types of complexometric titrations, metallochromes used, criteria of complexation and detection, effect of pH on complexation, estimation of metal ions, stability of metal complexes.	1
Redox Titrations - principle, types of redox titrations, assays of ferrous salts, hydrogen peroxide, sodium perborate and benzoyl peroxide by titration with $KMnO_4$.	1
Iodometric Titrations – principle, Assay of phenolglycerol injection.	1
Ion-pair Titrations - titrations using indicator dyes, titrations using iodide as a lipophilic anion	1
Diazotization Titrations – principle, assay of sulphanilamide.	2
Karl-Fischer Titrations - principle and procedure.	1
Introduction to extraction methods.	1

Commonly used excipients in formulations – (i) tablets and capsules (ii) suspensions and solutions (iii) creams and ointments. Solvent Extraction methods - extraction of organic bases and acids utilizing their ionized and un-ionized forms.	1
Partition between organic solvents and ion pair extraction.	1
Solid phase extraction – Introduction, methodology, types of adsorbents used in Solid phase extraction – (i) Lipophilic silica gels (ii) Polar surfaced modified silica gels.	1
	15hrs

Course/Paper - III

Course\CH(CPI)403 T: ELECTIVE 3B: Bioorganic Chemistry

Unit: CPI-45: Carbohydrates

Topics to be covered	No. of Hours required
Introduction to the importance of Carbohydrates.	2
Types of naturally occurring sugars.	1
Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions	1
C=C Formation Reactions: Importance of double bonded compounds; Introduction to C=C Formation Reactions	1
Shapiro, Bamford-Stevens and McMurrey reactions	1
Julia-Lythgoe olefination and Peterson's stereoselective olefination	1
Multicomponent Reactions: Importance of Multi-component reactions; Ugi and Passerini reactions	1
Biginelli, Hantzsch and Mannich reactions	1
Ring Formation Reactions: Pausan-Khand reaction, Bergman cyclisation, Nazarov cyclisation	1
Click Chemistry: Overview of Click Reactions; Criteria for Click reaction	1
Sharpless azides cycloadditions	1
Metathesis: Grubb's 1st and 2nd generation catalyst; Olefin cross coupling metathesis(OCM), ring closing metathesis(RCM), ring opening metathesis(ROM), applications	1
Other important synthetic reactions: Baylis-Hilman reaction and Eschenmoser-Tanabe fragmentation	1
Mitsunobu reaction, Stork-enamine reaction and Michael reactions	1
	15hrs

Unit: CPI-46: Nucleic acids and Lipids

Topics to be covered	No. of Hours required
Nucleic acids: Retro synthetic analysis of nucleic acids	1
Nucleotides, Nucleosides, Nucleotide bases and Sugars	2
Structure and synthesis of nucleosides and nucleotides	2
Primary, secondary and tertiary structure of DNA. Types of mRNA, tRNA and rRNA	2
Replication, transcription and translation. Genetic code. Protein biosynthesis. DNA finger printing	2
Lipids: Introduction and classification of lipids. Stereochemical notation in lipids	2
Chemical synthesis and biosynthesis of phospholipids and glycolipids	2
Properties of lipid aggregates, micelles, bilayers, liposomes and biological membranes	2
	15hrs

Unit: CPI-47: Proteins and Enzymes

Topics to be covered	No. of Hours required
Proteins: Introduction. Peptide bond, classification and nomenclature of peptides	1
Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis	1
Peptide synthesis by solution phase and solid phase synthesis methods	1
Proteins - Biological importance and classification - Primary, secondary and tertiary structure of proteins	2
Enzymes: Definition. Classification based on mode of action	2
Mechanism of enzyme catalysis - Lock and Key, Induced- Fit and three point contact models	3
Enzyme selectivity –chemo, regio, diastereo and enantio selectivity– illustration with suitable examples	2
Factors affecting enzyme catalysis	1
Enzyme inhibition - reversible and irreversible inhibition	1
Enzymes in organic synthesis. Immobilised enzymes	1
	15hrs

Unit: CPI-48: Coenzymes and Vitamins

Topics to be covered	No. of Hours
Coenzymes: Introduction, Co-factors - cosubstrates - prosthetic groups	1
Classification-Vitamin derived coenzymes and metabolite coenzymes	1
Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP)	1
oxidized and reduced forms of i) nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP+ NADPH)	1
ii) Flavin adenine nucleotide FAD, FADH ₂ and iii) Flavin mononucleotide (FMN, FMNH ₂) lipoic acid, biotin, tetrahydrofolate and ubiquinone.	2
Adenosine triphosphate (ATP) and adenosine diphosphate (ADP), S-adenosyl methionine (SAM) and uridine diphospho sugars (UDP-sugars) Mechanism of reactions catalyzed by the above coenzymes	2
Vitamins: Introduction, classification and biological importance of vitamins	1
Structure determination and synthesis of vitamins A, B ₁ , and B ₂	3
Synthesis of vitamins - B ₆ , C, E and K. Structure of vitamin B ₁₂	3
	15hrs

Course/Paper - IV

Course\CH(CPI)404 T: ELECTIVE 4A: Advanced Heterocyclic Chemistry

Unit: CPI - 49: Non aromatic heterocyclics & Aromaticity

Topics to be covered	No. of Hours required
Different types of strains, interactions and conformational aspects of non-aromatic heterocycles	1
Synthesis, reactivity and importance of Azirines, Aziridines	2
Synthesis, reactivity and importance of Oxiranes, Oxaziridines	2
Synthesis, reactivity and importance of Diazirenes, Diaziridines	2
Synthesis, reactivity and importance of Thiiranes, Azetidines	2
Synthesis, reactivity and importance of Oxetanes, thietanes	2
Aromaticity introduction, Aromatic and anti aromatic compounds, Criteria for aromaticity	1
Huckel's $4n+2$ electron rule for benzene and non benzenoid aromatic compounds	1
Cyclopropenium ion, cyclopentadienyl ion, cycloheptatrienium ion, azulene and annulenes	2
	15hrs

Unit: CPI - 50: Five and six membered heterocyclics with two hetero atoms

Topics to be covered	No. of Hours required
Synthesis, reactivity, aromatic character & importance: Pyrazole, Imidazole	3
Synthesis, reactivity, aromatic character & importance: Oxazole, Isoxazole	3
Synthesis, reactivity, aromatic character & importance:Thiazole, Isothiazole	3
Synthesis, reactivity, aromatic character & importance: Pyridazine	1
Synthesis, reactivity, aromatic character & importance: Pyrimidine	1
Synthesis, reactivity, aromatic character & importance: Pyrazine	1
Synthesis, reactivity, aromatic character & importance: Oxazine, thiazine	1
Synthesis, reactivity, aromatic character & importance: benzimidazole, benzoxazole and benzthiazole	2
	15hrs

Unit: CPI - 51: Heterocyclics with more than two hetero atoms

Topics to be covered	No. of Hours required
Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3- triazoles, 1,2,4-triazoles	2
Synthesis, reactivity, aromatic character and importance of Tetrazoles	1
Synthesis, reactivity, aromatic character and importance of 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5- oxadiazole	2
Synthesis, reactivity, aromatic character and importance of 1,2,3-thiadiazoles, 1,3,4- thiadiazoles, 1,2,5- thiadiazoles	2
Synthesis, reactivity, aromatic character and importance of 1,2,3-triazine, 1,2,4- triazine, 1,3,5- triazine	2

Synthesis, reactivity, aromatic character and importance of tetrazines	2
Synthesis and importance of purines and pteridines	2
Synthesis of Caffeine, theobromine and theophylline	2
	15hrs

Unit: CPI - 52: Larger ring and other hetero cyclics

Topics to be covered	No. of Hours required
Introduction and nomenclature to heterocyclic compounds	1
AZEPINES: Synthesis, structure, stability and reactivity of Azepines	1
OXEPINES: Synthesis, structure, stability and reactivity of Oxepines	1
THIEPINES: Synthesis, structure, stability and reactivity of Thiepin.	1
DIAZEPINES: Synthesis of Diazepines, Rearrangement of 1,2-Diazepines	1
Synthesis and Reactivity of Benzoazepines.	1
Synthesis and Reactivity of Benzodiazepines	1
Synthesis and Reactivity of Benzooxepines	1
Synthesis and Reactivity of Benzothiepin	1
Synthesis and Reactivity of Azocines	1
Synthesis and Reactivity of Azonines	1
Synthesis and Reactivity of Selenophenes	1
Synthesis and Reactivity of Tellerophenes	1
Synthesis and Reactivity of Phospholes	1
Synthesis and Reactivity of Boroles	1
	15hrs

Course/Paper - IV

Course\CH(CPI)404 T: ELECTIVE 4B: Green chemistry and Organic materials

Unit: CPI - 53: Principles of Green chemistry

Topics to be covered	No. of Hours required
Green chemistry: Introduction, Designing a Green Synthesis using these principles	1
Prevention of Waste/by-products; maximum incorporation of the starting materials used in the synthesis into the final products (Atom Economy)	2
prevention/minimization of hazardous/toxic products; designing safer chemicals	2
selection of appropriate auxiliary substances - green solvents, ionic liquids and solvent-free synthesis	2
energy requirements for reactions - use of microwaves, ultrasonic energy in organic synthesis	2
prevention of unnecessary derivatization – careful use of protecting groups	1
use of catalytic reagents in preference to stoichiometric reagents	1
designing of biodegradable products; prevention of chemical accidents	2
strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes	2
	15hrs

Unit: CPI - 54: Green Synthesis

Topics to be covered	No. of Hours required
i) Microwave Assisted Organic Synthesis (MAOS): introduction, benefits and limitations	1
a) Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Claisen rearrangement and Diels- Alder reaction	2
b) Microwave assisted Solvent-free reactions: Deacetylation, saponification of esters, alkylation of reactive methylene compounds and synthesis of nitriles from aldehydes	2
ii) Ultrasound Assisted Organic Synthesis: introduction, applications of ultrasound-Cannizzaro reaction, Reformatsky reaction and Strecker synthesis	2
iii) Organic Synthesis in Green Solvents: introduction	1
a) Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, Hoffmann elimination, Claisen-Schmidt condensation hydrolysis and dihydroxylation reactions	2
b) Organic Synthesis using Ionic liquids: Introduction, applications-Beckmann rearrangement Suzuki Cross-Coupling Reaction and Diels- Alder reaction	2
iv) Green Catalysts in organic synthesis: introduction	
a) Phase Transfer Catalysts in Organic Synthesis: Introduction, Williamson ether synthesis and Wittig reaction	2
b) Biocatalysts in Organic Synthesis: Biochemical (microbial) oxidations and reductions	1
	15hrs

Unit: CPI - 55: Organic nanomaterials

Topics to be covered	No. of Hours required
Introduction: The ‘top-down’ approach, the ‘bottom-up’ approach and Nanomanipulation	1
Molecular Devices: Photochemical devices, Liquid crystals, Molecular wires, Rectifiers, Molecular switches and Molecular Muscles	2
New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes	2
Growth, Chemical Synthesis and optoelectronic properties of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs)and Graphenes	3
Structures of aromatics belts, nano car and molecular machines	2
Optoelectronic molecules: OLEDs, Organic Solar Cells (Basic OLED mechanism and structures)	3
Natural Benz heterazoles and their synthetic modifications as optoelectronic molecules	2
	15hrs

Unit: CPI - 56: Supramolecular chemistry

Topics to be covered	No. of Hours required
Introduction: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation- π , anion- π , π - π and Van der Walls interactions), Ionophore and molecular receptors	3
Host-Guest Chemistry: Lock and key analogy, Structures and applications of Cryptands, Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicaricrands	4
Self-assembly: Ladder, polygons, helices, rotaxanes, catanenes, Molecular necklace, dendrimers, self-assembly capsules their synthesis, properties and applications	4
Enantioselective molecular recognition: Cyclodextrins, Crown ethers with chiral frame work, Chiral receptor from Kemp’s triacid. Chiral receptors for tartaric acid	4
	15hrs

**SEMESTER -IV
PRACTICALS**

Course\Paper-V: CPI – 451P: Quantitative Analysis of Pharmaceuticals

No. of Hours Allotted: 15 weeks x 9 hrs

Topics to be covered	No. of Hours required
Assay of pharmaceuticals - Redox titrations Assay of analgin in tablets by iodometry Assay of ascorbic acid in raw material by iodometry Assay of ascorbic acid in tablets by cerimetry Determination of hydrogen peroxide in medicament by Permanganometry	2
Assay of pharmaceuticals - Complexometric titrations Assay of Calcium in Calcium gluconate Assay Zinc in Bacitracin zinc Assay of pharmaceuticals - Non-aqueous titrations: Assay of diphenylhydramine hydrochloride in tablets Assay of ephedrine hydrochloride in capsules Assay of Ibuprofen in tablets	2
Assay of pharmaceuticals – Potentiometry/Conductometric Potentiometric estimation of Sulphanilamide Potentiometric estimation of Atropine Conductometric estimation of analysis Amidazophen (aminophenazone) Conductometric estimation of analysis Aspirin	2
Assay of pharmaceuticals - UV-Visible Spectrophotometry Assay of Riboflavin in tablets Assay of Diazepam in tablets Assay of Nimuselide in nimuselide tablets	1
Assay of pharmaceuticals – by other methods Dissolution profile of paracetamol & ampicillin Determination of Sodium and potassium ions in pharmaceuticals by flame photometry Determination of Quinine sulphate & Riboflavin by fluorimetry.	2
1) Identification of unknown organic compounds by interpretation of IR, UV, ¹ H-NMR, ¹³ C-NMR and mass spectral data Aspirin, p-Chloroacetophenone, clofibrate, Ibuprofen, Phenylacetic acid, p-MethylBenzoylchloride, L-Dopa, Benzocaine	3
2) Thin layer chromatography: Determination of purity of a given sample, monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the R _f values of known standards.	1
3. Separation by column chromatography: Separation of a mixture of <i>ortho</i> and <i>para</i> nitroanilines using silicagel as adsorbant and chloroform as the eluent. The column chromatography should be monitored by TLC.	2
	15 weeks

Course\Paper-VI: CPI - 452P: PROJECTWORK No. of Hours Allotted: 15 weeks x 9 hrs