

M.Pharm Syllabus

Semester 02

Pharmaceutical Chemistry

Subjects

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MPC201T - Advanced Spectral Analysis

Theory

Unit 1

- UV and IR spectroscopy: Woodward - Fieser rule for 1,3-butadienes, cyclic dienes and α , β -carbonyl compounds and interpretation compounds of enones.
- ATR-IR, IR Interpretation of organic compounds.

Unit 2

- NMR spectroscopy: 1-D and 2-D NMR, NOESY and COSY, HECTOR, INADEQUATE techniques, Interpretation of organic compounds.

Unit 3

- Mass Spectroscopy Mass fragmentation and its rules, Fragmentation of important functional groups like alcohols, amines, carbonyl groups and alkanes, Meta stable ions, McLafferty rearrangement, Ring rule, Isotopic peaks, Interpretation of organic compounds.

Unit 4

- Chromatography:
- Principle, Instrumentation and Applications of the following :
- GC-MS b) GC-AAS c) LC-MS d) LC-FTIR e) LC-NMR f) CE-MS g) High Performance Thin Layer chromatography h) Super critical fluid chromatography i) Ion Chromatography j) I-EC (Ion-Exclusion Chromatography) k) Flash chromatography

Unit 5

- . Thermal methods of analysis Introduction, principle, instrumentation and application of DSC, DTA and TGA.
- . Raman Spectroscopy Introduction, Principle, Instrumentation and Applications.
- . Radio immuno assay Biological standardization , bioassay, ELISA, Radioimmuno assay of digitalis and insulin.

MPC202T - Advanced Organic Chemistry II

Theory

Unit 1

- Green Chemistry:
- Introduction, principles of green chemistry
- Microwave assisted reactions: Merit and demerits of its use, increased reaction rates, mechanism, superheating effects of microwave, effects of solvents in microwave assisted synthesis, microwave technology in process optimization, its applications in various organic reactions and heterocycles synthesis
- Ultrasound assisted reactions: Types of sonochemical reactions, homogenous, heterogeneous liquid-liquid and liquid-solid reactions, synthetic applications
- Continuous flow reactors: Working principle, advantages and synthetic applications.

Unit 2

- Chemistry of peptides
- Coupling reactions in peptide synthesis
- Principles of solid phase peptide synthesis, t-BOC and Fmoc protocols, various solid supports and linkers: Activation procedures, peptide bond formation, deprotection and cleavage from resin, low and high HF cleavage protocols, formation of free peptides and peptide amides, purification and case studies, site-specific chemical modifications of peptides
- Segment and sequential strategies for solution phase peptide synthesis with any two case studies
- Side reactions in peptide synthesis: Deletion peptides, side reactions initiated by proton abstraction, protonation, over-activation and side reactions of individual amino acids.

Unit 3

- Photochemical Reactions Basic principles of photochemical reactions. Photo-oxidation, photo-addition and photo-fragmentation.
- Pericyclic reactions Mechanism, Types of pericyclic reactions such as cyclo addition, electrocyclic reaction and sigmatropic rearrangement reactions with examples

Unit 4

- Catalysis:
- Types of catalysis, heterogeneous and homogeneous catalysis, advantages and disadvantages
- Heterogeneous catalysis - preparation, characterization, kinetics, supported catalysts, catalyst deactivation and regeneration, some examples of heterogeneous catalysis used in synthesis of drugs.
- Homogeneous catalysis, hydrogenation, hydroformylation, hydrocyanation, Wilkinson catalysts, chiral ligands and chiral induction, Ziegler-Natta catalysts, some examples of homogeneous catalysis used in synthesis of drugs
- Transition-metal and Organo-catalysis in organic synthesis: Metal-catalyzed reactions

- Biocatalysis: Use of enzymes in organic synthesis, immobilized enzymes/cells in organic reaction.
- Phase transfer catalysis - theory and applications

Unit 5

- Stereochemistry & Asymmetric Synthesis
- Basic concepts in stereochemistry - optical activity, specific rotation, racemates and resolution of racemates, the Cahn, Ingold, Prelog (CIP) sequence rule, meso compounds, pseudo asymmetric centres, axes of symmetry, Fischers D and L notation, cis-trans isomerism, E and Z notation.
- Methods of asymmetric synthesis using chiral pool, chiral auxiliaries and catalytic asymmetric synthesis, enantiopure separation and Stereo selective synthesis with examples.

MPC203T - Computer Aided Drug Design

Theory

Unit 1

- Introduction to Computer Aided Drug Design (CADD) History, different techniques and applications.
- Quantitative Structure Activity Relationships: Basics History and development of QSAR: Physicochemical parameters and methods to calculate physicochemical parameters: Hammett equation and electronic parameters (σ), lipophilicity effects and parameters ($\log P$, π -substituent constant), steric effects (Taft steric and MR parameters) Experimental and theoretical approaches for the determination of these physicochemical parameters.

Unit 2

- Quantitative Structure Activity Relationships: Applications Hansch analysis, Free Wilson analysis and relationship between them, Advantages and disadvantages; Deriving 2D-QSAR equations.
- 3D-QSAR approaches and contour map analysis.
- Statistical methods used in QSAR analysis and importance of statistical parameters.

Unit 3

- Molecular Modeling and Docking
- Molecular and Quantum Mechanics in drug design.
- Energy Minimization Methods: comparison between global
- Molecular docking and drug receptor interactions: Rigid docking, flexible docking and extra-precision docking.
- Agents acting on enzymes such as DHFR, HMG-CoA reductase and HIV protease, choline esterase (AChE & BchE)

Unit 4

- Molecular Properties and Drug Design
- Prediction and analysis of ADMET properties of new molecules and its importance in drug design.
- De novo drug design: Receptor/enzyme-interaction and its analysis, Receptor/enzyme cavity size prediction, predicting the functional components of cavities, Fragment based drug design.
- Homology modeling and generation of 3D-structure of protein.

Unit 5

- Pharmacophore Mapping and Virtual Screening Concept of pharmacophore, pharmacophore mapping, identification of Pharmacophore features and Pharmacophore modeling; Conformational search used in pharmacophore mapping.
- In Silico Drug Design and Virtual Screening Techniques Similarity based methods and Pharmacophore based screening, structure based In-silico virtual screening protocols.

MPC204T - Pharmaceutical Process Chemistry

Theory

Unit 1

- Process chemistry Introduction, Synthetic strategy Stages of scale up process: Bench, pilot and large scale process.
- In-process control and validation of large scale process.
- Case studies of some scale up process of APIs.
- Impurities in API, types and their sources including genotoxic impurities

Unit 2

- Unit operations
- Extraction: Liquid equilibria, extraction with reflux, extraction with agitation, counter current extraction.
- Filtration: Theory of filtration, pressure and vacuum filtration, centrifugal filtration,
- Distillation: azeotropic and steam distillation
- Evaporation: Types of evaporators, factors affecting evaporation.
- Crystallization: Crystallization from aqueous, non-aqueous solutions factors affecting crystallization, nucleation. Principle and general methods of Preparation of polymorphs, hydrates, solvates and amorphous APIs.

Unit 3

- Unit Processes - I
- Nitration: Nitrating agents, Aromatic nitration, kinetics and mechanism of aromatic nitration, process equipment for technical nitration, mixed acid for nitration,
- Halogenation: Kinetics of halogenations, types of halogenations, catalytic halogenations. Case study on industrial halogenation process.
- Oxidation: Introduction, types of oxidative reactions, Liquid phase oxidation with oxidizing agents. Nonmetallic Oxidizing agents such as H₂O₂, sodium hypochlorite, Oxygen gas, ozonolysis.

Unit 4

- Unit Processes - II
- Reduction: Catalytic hydrogenation, Heterogeneous and homogeneous catalyst; Hydrogen transfer reactions, Metal hydrides. Case study on industrial reduction process.
- Fermentation: Aerobic and anaerobic fermentation.
- Production of
- Antibiotics; Penicillin and Streptomycin, ii. Vitamins: B₂ and B₁₂ iii. Statins: Lovastatin, Simvastatin
- Reaction progress kinetic analysis
- Streamlining reaction steps, route selection, ii. Characteristics of expedient routes, characteristics of cost-effective routes, reagent selection, families of reagents useful for scale-up.

Unit 5

- Industrial Safety
- MSDS (Material Safety Data Sheet), hazard labels of chemicals and Personal Protection Equipment (PPE)
- Fire hazards, types of fire & fire extinguishers
- Occupational Health & Safety Assessment Series 1800 (OHSAS-1800) and ISO-14001 (Environmental Management System), Effluents and its management

MPC205P - Pharmaceutical Chemistry II

Practical

- Synthesis of organic compounds by adapting different approaches involving
- Oxidation
- Reduction/hydrogenation
- Nitration
- Comparative study of synthesis of APIs/intermediates by different synthetic routes
- Assignments on regulatory requirements in API
- Comparison of absorption spectra by UV and Woodward - Fieser rule
- Interpretation of organic compounds by FT-IR
- Interpretation of organic compounds by NMR
- Interpretation of organic compounds by MS
- Determination of purity by DSC in pharmaceuticals
- Identification of organic compounds using FT-IR, NMR, CNMR and Mass spectra
- To carry out the preparation of following organic compounds
- Preparation of 4-chlorobenzhydrylpiperazine. (an intermediate for cetirizine HCl).
- Preparation of 4-iodotoluene from p-toluidine.
- NaBH₄ reduction of vanillin to vanillyl alcohol
- Preparation of umbelliferone by Pechmann reaction
- Preparation of triphenyl imidazole
- To perform the Microwave irradiated reactions of synthetic importance (Any two)
- Determination of log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares
- Calculation of ADMET properties of drug molecules and its analysis using softwares Pharmacophore modeling
- 2D-QSAR based experiments
- 3D-QSAR based experiments
- Docking study based experiment
- Virtual screening based experiment

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