Satavahana University
Department of Chemistry
Paper-II (Organic Chemistry)
Ph.D. Course Work Syllabus – 2018

Paper Title: Organic Synthesis, Spectroscopy and Heterocyclics

Unit–I: Organic reagents and reactions

Unit–II: Asymmetric and retro synthesis

Unit–III: Spectroscopic applications of organic compounds

Unit-IV: *2D-NMR spectroscopy*

Unit–V: Heterocyclics and biological evaluation

Unit –I: Organic reagents and reactions 12h

Swern oxidation, DDQ, Cr-oxidants (Jone's reagent, PCC, PDC), Corey-kim oxidation, Reductions, electrophilic metal hydride reagents-LiAlH4, NaBH4, DIBAL, Dissolving metal reductions-Birch reduction.

Reactions: Baylis-Hillmann reaction, Heck reaction, Suzuki coupling, sonogishira cross coupling, Julia-lythgoe olefination, Shapiro reaction, Mannich reaction and Witting reaction.

Unit-II: Asymmetric and retro synthesis 12h

Asymmetric synthesis: Topocity in molecules groups & faces, homotopic, heterotopic ligands and faces. Substrate selectivity, 1,2-asymmetric induction (Cram rule), chiral auxillary controlled method. Alkylation of chiral enolates, sharpless asymmetric amino hydroxylation, mukaiyama aldol reaction, Noyori-asymmetric hydrogenation.

Retro synthesis: introduction to retrosynthesis, target molecule, disconnection, synthon, selection of target molecule, chemoselectivity, regioselectivity, and stereoselcetivity, reversal of polarity, one and two group C-C, C-X disconnections, applications of retrosynthesis to synthesis of Juvabione and longifolene.

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Unit-III: Spectroscopic application of organic compounds 12h

Differentiation of possible isomers: i) $C_9H_{10}O_2$-Number of possible isomers and their detection by ^{1}H-NMR spectra. ii) Hydroxycinnamic acid- Number of possible isomers and their detection.

Differentiation pair of isomers: Differentiation of isomers using different spectra: i) IR spectra: 3-Phenylpropanaldehyde-Propiophenone;4-ethylaniline-4-methyl-N-methylaniline-N,N-dimethylaniline. ii) UV spectra: Propiophenone-phenylacetone; cis-stilbene - trans-stilbene. iii) ^{1}H-NMR spectra: vinylacetate-methylacrylate; methylpropionate-ethylacetate. iv)^{13}C-NMR spetra: 1-pentene-2-pentene; vinylacetate-methylacrylate. v) Massspectra: N,N-dimethylpropanamide-N-methylbutanamide; benzylacetate-ethylbenzoate; phenyl ethyl ketone-benzyl methyl ketone and pyrazol-imadzol; vi) All spectra: paracetamol-paramethoxybenzamide.

Unit-IV: *2D-NMR spectroscopy* 12h

Principle-Homo-2D-J-resolved and Hetero-2D-J-resolved spectroscopy, HOMO-COSY, TOCSY, Hetero-COSY, HMQC, HMBC, NOESY, and 2D-inadequate techniques by taking 1-iodo butane as example. Homo-COSY of dibutyl ketone, Hetero-COSY, HMQC, HMBC, and 2D-inadequate of Ipsenol, Homo-COSY and Hetero-COSY of menthol.

Interpretation of the structure of natural products using spectral data (IR, UV, NMR and mass): Camphor, β-Carotene, Menthol.

Unit-V: Heterocyclics and biological evaluation 12h

Heterocyclics: Synthesis and chemical reactivity of the following heterocyclic molecules like, Isoxazoles, Thiazoles, Pyrimidines, and Benzimidazoles, Pyrazines, Quinoxoline, Quinazoline, Chromones and Flavones.

Biological evaluation: Invivo and Invitro studies. Cell line assay, Enzyme inhibition, Toxicity testing, cell viability assay, High through put screening. Explanation for IC_{50}, EC_{50}, EC_{90}, LD_{50}, ED_{50}, Ki, MIC, Zone of inhibition studies. Ethical issues and regulatory affairs.

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