

M.Sc. CHEMISTRY (ORGANIC CHEMISTRY SPECIALISATION)

Syllabus for III and IV Semesters

[Under Restructured CBCS Scheme]

(for the batches admitted in academic year 2023-24 onwards under CBCS pattern)

Grand total marks and credits (all 4 semesters) 2400 marks – 80 credits

(Approved in the P.G. BOS meeting held on 27-01-24)

Semester - III (Organic Chemistry)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(OC)301T (Core)	3	50 marks	50 marks	100 marks	3
CH(OC)302T (Core)	3	50 marks	50 marks	100 marks	3
CH(OC)303T (Elective)	3	50 marks	50 marks	100 marks	3
CH(OC)304T (Elective)	3	50 marks	50 marks	100 marks	3
CH351P (OC LAB1)	4		50 marks	50 marks	2
CH352P (OC LAB2)	4		50 marks	50 marks	2
CH353P (OC LAB3)	2		25 marks	25 marks	1
CH354P (OC LAB4)	2		25 marks	25 marks	1
Seminar	2		50 Marks	50 Marks	2
Total				600 marks	20

Semester - IV (Physical Chemistry)

	Hrs/week	Internal assessment	Semester exam	Total	Credits
CH(OC)401T (Core)	3	50 marks	50 marks	100 marks	3
CH(OC)402T (Core)	3	50 marks	50 marks	100 marks	3
CH(OC)403T (Elective)	3	50 marks	50 marks	100 marks	3
CH451P (OC LAB1)	4		50 marks	50 marks	2
CH452P (OC LAB2)	4		50 marks	50 marks	2
CH453P (OC LAB3)	2		25 marks	25 marks	1
CH454P (Project)	12	50 marks	125 marks	175 marks	6
Total				600 marks	20

Grand total marks and credits (all 4 semesters) 2400 marks - 80 credits

M.Sc. SEMESTER - III
ORGANIC CHEMISTRY SPECIALIZATION
 (for the batches admitted in academic year 2023-24 & later under CBCS pattern)

PAPER I CH (OC) 301T(CORE): SYNTHETIC REAGENTS, ^{13}C AND 2D NMR
 OC-07: Synthetic Reagents-I
 OC-08: Synthetic Reagents-II
 OC-09: ^{13}C NMR and 2D NMR spectroscopy

PAPER II CH (OC) 302T(CORE): MODERN ORGANIC SYNTHESIS
 OC-10: Asymmetric synthesis
 OC-11: Synthetic strategies
 OC-12: New Synthetic reactions

PAPER III CH (OC) 303T (ELECTIVE IIIA): BIOORGANIC CHEMISTRY AND CONFORMATIONAL ANALYSIS (CYCLIC SYSTEMS) & ORD
 OC(CB1)-13: Carbohydrates, Nucleic acids & Coenzymes
 OC(CB1)-14: Proteins, Enzymes and Lipids
 OC(CB1)-15: Conformational analysis-II (Cyclic Systems) & ORD

PAPER III CH (OC) 303T (ELECTIVE IIIB): PROCESS CHEMISTRY AND DEVELOPMENT
 OC(CB1)-13: Process chemistry and Principles
 OC(CB1)-14: Process Development /Optimization
 OC(CB1)-15: Process Development /Optimization

PAPER IV CH (OC) 304T (ELECTIVE IVA: GREEN CHEMISTRY AND NEW TECHNIQUES
 OC (CB2) -16: Principles of Green chemistry and Green Synthesis
 OC (CB2) -17: Organic nanomaterials and Supramolecular chemistry
 OC (CB2) -18: New techniques and concepts in organic synthesis

PAPER IV CH (OC) 304T (ELECTIVE IVB): PESTICIDES
 OC (CB2) - 16: Introduction to pesticides
 OC (CB2) - 17: Synthetic insecticides
 OC (CB2) - 18: Natural insecticides & herbicides

LABORATORY COURSES

Paper-V CH (OC) 351P: Synthesis of organic molecules
 Paper-VI CH (OC) 352P: Separation and identification of organic compounds
 Paper-VII CH (OC) 353P: Isolation of natural products and Thin layer chromatography
 Paper-VIII CH (OC) 354P: Separation of three component mixtures by chemical methods and Column chromatography

SEMINAR

Handwritten signatures and initials:
 of Lauke Vijayulu KR Reddy
MM 22/11/24 V Phani

M.Sc. SEMESTER - IV
ORGANIC CHEMISTRY SPECIALIZATION
 (for the batches admitted in the academic year 2023-24 and later under CBCS pattern)

PAPER-1 CH (OC) 401T(CORE): DRUG DESIGN AND DRUG DISCOVERY

OC-19: Principles of Drug design and drug discovery

OC-20: Lead modification and SAR Studies

OC 21: QSAR studies and computer aided drug design

PAPER-II CH (OC) 402T(CORE): ADVANCED HETEROCYCLIC CHEMISTRY

OC-22: Heterocyclic compounds, Nonaromatic heterocyclics and Five membered heterocyclics with two heteroatoms

OC-23: Six membered heterocyclics with two heteroatoms and Five membered heterocyclics with more than two heteroatoms

OC-24: Six membered heterocyclics with more than two heteroatoms and Larger ring heterocyclics

PAPER-III CH (OC) 403 T(ELECTIVE IIIA): DRUG SYNTHESIS AND MECHANISM OF ACTION

OC(CB1)-25: Drugs acting on metabolic process, cell wall and specific enzymes

OC(CB1)-26: Drugs acting on genetic material and immune system

OC(CB1)-27: Drugs acting on receptors and ion channels

PAPER III CH (OC) 403 T(ELECTIVE IIIB): ADVANCED NATURAL PRODUCTS

OC(CB1)-25: Biosynthesis of natural products

OC(CB1)-26: Structure determination of natural products

OC(CB1)-27: Total stereo selective synthesis of natural products.

LABORATORY COURSES

Paper-IV CH (OC) 451P: Spectroscopic identification of organic compounds

Paper-V CH (OC) 452P: Synthesis of following drugs

Paper-VI CH (OC) 453P: Practice of chemistry software programmes

PROJECT CH(OC)454P

V. Jayashree *MAR 27/2024*

M.Sc. SEMESTER - III
ORGANIC CHEMISTRY Specialization
 (for the batches admitted in academic year 2023-24 and later under CBCS pattern)

PAPER I

CH (OC) 301T(CORE): SYNTHETIC REAGENTS, ¹³C AND 2D NMR

OC-07: Synthetic Reagents-I
 OC-08: Synthetic Reagents-II
 OC-09: ¹³C NMR and 2D NMR spectroscopy

OC-07: Synthetic Reagents-I

15 Hrs

- i) Protecting groups:
 a) Protection of alcohols by silyl ether (TBDMS, TBPS) and ester formation
 b) Protection of 1,2-diols by acetal, ketal and carbonate formation
 c) Protection of amines by t-butyloxycarbonyl, fmoc groups.
 d) Protection of carbonyls by thiol acetal (Umpolung) groups.
 e) Protection of carboxylic acids ortho ester (OBO) formation.
 ii) Organometallic Reagents: Preparation and application of the following in organic synthesis: 1) Organo lithium 2) Organo copper reagents 3) Organo boranes in C-C bond formation 4) Organo silicon reagents: reactions involving β -carbocations and α -carbanions, utility of trimethyl silyl halides, cyanides and triflates.
 iii) Carbonyl methylenation: a) Phosphorous ylide mediated olefination 1) Wittig reaction, 2) Horner-Wordsworth-Emmons reaction.
 iv) Carbene insertions: Rh based carbene complexes, cyclopropanations.
 v) C-H Activation: Introduction, Rh catalysed C-H activation.

OC-08: Synthetic Reagents-II

15 Hrs

- i) Oxidations:
 a) Oxidation of active C-H functions: DDQ and SeO₂.
 b) Alkenes to diols: Prevost and Woodward oxidation
 c) Alcohol to carbonyls: Crv oxidants Jones reagent, PCC, PDC) IBX, DMP, CAN, TEMPO, TPAP, Swern oxidation.
 ii) Reductions:
 a) Catalytic hydrogenation: Homogenous (Wilkinson's catalytic hydrogenation) and heterogeneous catalytic reduction.
 b) Non-metallic reductions: Diimide reduction
 c) Dissolving metal reductions: Birch reduction.
 d) Nucleophilic metal hydrides: LiAlH₄, NaBH₄, and their modifications.
 e) Electrophilic metal hydrides: BH₃, AlH₃ and DIBAL.
 f) Use of tri-n-butyl tin hydride: Radical reductions.

Sube m/w .d.124 K.P. Reddy

OC-09: ^{13}C NMR and 2D NMR spectroscopy**15 Hrs**

i) ^{13}C NMR spectroscopy: Introduction, Types of ^{13}C nmr spectra: uncoupled, proton-decoupled and off-resonance decoupled (ORD) spectra. ^{13}C chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and alkynes. Homonuclear (^{13}C , ^{13}C J) and heteronuclear (^{13}C , ^1H J and ^{13}C , ^2H J) coupling. Applications of ^{13}C -NMR spectroscopy: Structure determination, stereochemistry, reaction mechanisms and dynamic processes in organic molecules. ^{13}C -NMR spectral editing techniques: principle and applications of APT, INEPT and DEPT methods.

ii) 2D-NMR spectroscopy: Principles of 2D NMR, Classification of 2D-experiments. Correlation spectroscopy (COSY) HOMO COSY (^1H - ^1H COSY), TOCSY (Total Correlation Spectroscopy), Hetero COSY (^1H , ^{13}C COSY, HMQC), long range ^1H , ^{13}C COSY (HMBC), Homonuclear and Heteronuclear 2D-J-resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

BOOKS SUGGESTED:

1. Modern methods of organic synthesis by W. Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic Synthesis by O House
4. Organic synthesis by Micheal B Smith
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11 (1984)
6. Organic synthesis by Robert E Ireland
7. Handbooks of reagents for organic synthesis by Reich and Rigby, Vol-I-IV
8. Organic chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
9. Organic Reactions and their mechanisms by P.S.Kalsi
10. Organic reaction mechanisms by V.K.Ahulwalia and Rakesh Kumar Parashar
11. Spectroscopic identification of organic compounds, RM Silverstein, G C Bassler and T B Morrill
12. Organic Spectroscopy by William Kemp
13. Spectroscopic methods in Organic chemistry by DH Williams and I Fleming
14. Modern NMR techniques for chemistry research by Andrew B Derome
15. NMR in chemistry - A multinuclear introduction by William Kemp
16. Spectroscopic identification of organic compounds by P S Kalsi
17. Introduction to organic spectroscopy by Pavia
18. Carbon-13 NMR for organic chemists by GC Levy and O L Nelson
19. Nuclear Magnetic Resonance Basic principles by Atta-ur-Rahman
20. Basic one and two-dimensional NMR spectroscopy by Horst Friebolin
21. NMR spectroscopy by H.Gunther
22. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri
23. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. Wilen
24. Stereochemistry: Conformation & Mechanism by P S Kalsi
25. The third dimension in organic chemistry, by Alan Bassendale
26. Stereo selectivity in organic synthesis by R S Ward.
27. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
28. Optical rotatory dispersion by C Djerassi
29. Optical rotatory dispersion and circular dichroism by P Crabbe
30. Mechanism and Structure in Organic chemistry by S Mukherjee

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PAPER II CH (OC) 302T(CORE): MODERN ORGANIC SYNTHESIS

OC-10: Asymmetric synthesis
 OC-11: Synthetic strategies
 OC-12: New Synthetic reactions

OC-10: Asymmetric synthesis

15 Hrs

Introduction: Brief revision of classification of stereo selective reactions

Prostereoisomerism: Topicity in molecules Homotopic, stereoheterotopic (enantiotopic and diastereotopic) groups and faces- symmetry criteria.

Prochiral nomenclature: Pro chirality and Pro-R, Pro-S, Re and Si.

Conditions for stereoselectivity: Symmetry and transition state criteria, kinetic and thermodynamic control. Methods of inducing enantioselectivity.

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.

Chiral Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.

Chiral auxiliary controlled asymmetric synthesis: α -Alkylation of chiral enolates, Evan's oxazolidinone, 1, 4-Asymmetric induction and Prelog's rule. Asymmetric Diels-Alder reaction.

Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC2 BH and IPCBH2.

Chiral catalyst controlled asymmetric synthesis: Sharpless epoxidation. Asymmetric hydrogenations using chiral Wilkinson biphosphine catalyst. **Asymmetric aldol reaction:** Diastereoselective aldol reaction (achiral enolate & achiral aldehydes) its explanation by Zimmerman-Traxel model.

OC-11: Synthetic Strategies

15 Hrs

Introduction: Terminology, Target, synthon, synthetic equivalent, functional group interconversion (FGI), functional group addition. Criteria for selection of target. Linear and convergent synthesis. Retrosynthetic analysis and synthesis involving chemoselectivity, regioselectivity, reversal of polarity and cyclizations. .

Order of events : S-Salbutamol, Propoxycaine..

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.

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.

Two group C-C disconnections: Diels-Alder reaction, 1,3-difunctionalised compounds, 1,5-difunctionalised compounds, Michael addition and Robinson annulation.

Control in carbonyl condensations: oxanamide and mevalonic acid.

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.

OC-12: New Synthetic reactions**15 Hrs**

1. Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions.
2. C=C Formation Reactions: Shapiro, Bamford-Stevens, McMurrey reactions, Julia- Lythgoe olefination and Peterson's stereoselective olefination.
3. Multicomponent Reactions: Ugi, Passerini, Biginelli and Bergman reactions.
4. Ring Formation Reactions: Pausan-Khand reaction, Nazarov cyclisation.
5. Click Chemistry: Click reaction, 1,3-dipolar cycloadditions.
6. Metathesis: Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications.

BOOKS SUGGESTED:

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moscher
3. Principles in Asymmetric synthesis by Robert E. Gawley & Jeffrey aube
4. Stereo differentiating reactions by Izumi
5. Some modern methods of organic synthesis by W Carruthers
6. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
7. Organic synthesis by Michael B Smith
8. Organic Synthesis-The disconnection approach by S Warren
9. Organic Synthesis by C Willis and M Willis
10. Problems on organic synthesis by Stuart Warren
11. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
12. The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng
13. Name reactions by Jie Jacj Ji

PAPER III CH (OC) 303T (ELECTIVE IIIA): BIOORGANIC CHEMISTRY AND CONFORMATIONAL ANALYSIS (CYCLIC SYSTEMS) & ORD
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OC(CB1)-13: Carbohydrates, Nucleic acids & Coenzymes

OC(CB1)-14: Proteins, Enzymes and Lipids

OC(CB1)-15: Conformational analysis-II (Cyclic systems) & ORD

OC(CB1)-13: Carbohydrates, Nucleic acids & Coenzymes

15Hrs

Carbohydrates: Introduction to the importance of Carbohydrates. Types of naturally occurring sugars. Deoxy sugars, aminosugars, branched chain sugars. Determination of configuration and determination of ring size of D-glucose and D-Fructose. Conformational analysis of monosaccharides. Synthesis of amino, halo and thio sugars. Conformational structures of sucrose. Structure and biological functions of starch, cellulose, glycogen and chitin.

Nucleic acids: Retro synthetic analysis of nucleic acids - Nucleotides, Nucleosides, Nucleotide bases and Sugars. Structure and synthesis of nucleosides and nucleotides. Primary, secondary and tertiary structure of DNA.

Coenzymes: Introduction. Co-factors, cosubstrates, prosthetic groups.

Classification — Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of nicotinamide adenosine dinucleotide / their phosphates (NAD), NADH, NADP+ NADPH)

OC(CB1)-14: Proteins, Enzymes and Lipids

15 Hrs

Proteins: Introduction. Peptide bond, classification and nomenclature of peptides. Amino acid sequence of polypeptides and proteins: terminal residue analysis and partial hydrolysis. Peptide synthesis by solution phase and solid phase synthesis methods.

Enzymes: Definition. Classification based on mode of action. Mechanism of enzyme catalysis - Lock and Key, Induced- Fit and three point contact models. Enzyme selectivity -chemo, regio, diastereo and enantio selectivity - illustration with suitable examples. Factors affecting enzyme catalysis.

Lipids: Introduction and classification of lipids. Stereochemical notation in lipids. Chemical synthesis and biosynthesis of phospholipids and glycolipids.

OC(CB1)-15: Conformational analysis-II (Cyclic systems) & ORD

15 Hrs

Conformational analysis-II (Cyclic systems): Study of conformations of cyclohexane, mono, di and tri substituted cyclohexanes, (1,3,5-trimethyl cyclohexanes and Menthols), cyclohexanone (2-alkyl and 3'-alkyl ketone effect), 2-halocyclohexanones, cycloheptane. Stereo chemistry of bicyclo [3,3,0] octanes, hydrindanes, decalins and perhydroanthracenes. Conformational structures of piperidine, N-Methylpiperidine, tropane, tropine, pseudotropine, decahydroquinoline and quinolidine. Factors governing the reactivity of axial and equatorial substituents in cyclohexanes.

(oxidation, SN2 reaction, rearrangements, Ester hydrolysis) Stereochemistry of addition to the carbonyl group of a rigid cyclohexanone ring.

Optical Rotatory Dispersion (ORD) and CD Spectroscopy: Optical rotation, circular birefringence, circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical

Handwritten note: 1. 2. 3. 4. 5. 6. 7. 8. 9. 10. 11. 12. 13. 14. 15. 16. 17. 18. 19. 20. 21. 22. 23. 24. 25. 26. 27. 28. 29. 30. 31. 32. 33. 34. 35. 36. 37. 38. 39. 40. 41. 42. 43. 44. 45. 46. 47. 48. 49. 50. 51. 52. 53. 54. 55. 56. 57. 58. 59. 60. 61. 62. 63. 64. 65. 66. 67. 68. 69. 70. 71. 72. 73. 74. 75. 76. 77. 78. 79. 80. 81. 82. 83. 84. 85. 86. 87. 88. 89. 90. 91. 92. 93. 94. 95. 96. 97. 98. 99. 100. 101. 102. 103. 104. 105. 106. 107. 108. 109. 110. 111. 112. 113. 114. 115. 116. 117. 118. 119. 120. 121. 122. 123. 124. 125. 126. 127. 128. 129. 130. 131. 132. 133. 134. 135. 136. 137. 138. 139. 140. 141. 142. 143. 144. 145. 146. 147. 148. 149. 150. 151. 152. 153. 154. 155. 156. 157. 158. 159. 160. 161. 162. 163. 164. 165. 166. 167. 168. 169. 170. 171. 172. 173. 174. 175. 176. 177. 178. 179. 180. 181. 182. 183. 184. 185. 186. 187. 188. 189. 190. 191. 192. 193. 194. 195. 196. 197. 198. 199. 200. 201. 202. 203. 204. 205. 206. 207. 208. 209. 210. 211. 212. 213. 214. 215. 216. 217. 218. 219. 220. 221. 222. 223. 224. 225. 226. 227. 228. 229. 230. 231. 232. 233. 234. 235. 236. 237. 238. 239. 240. 241. 242. 243. 244. 245. 246. 247. 248. 249. 250. 251. 252. 253. 254. 255. 256. 257. 258. 259. 260. 261. 262. 263. 264. 265. 266. 267. 268. 269. 270. 271. 272. 273. 274. 275. 276. 277. 278. 279. 280. 281. 282. 283. 284. 285. 286. 287. 288. 289. 290. 291. 292. 293. 294. 295. 296. 297. 298. 299. 300. 301. 302. 303. 304. 305. 306. 307. 308. 309. 310. 311. 312. 313. 314. 315. 316. 317. 318. 319. 320. 321. 322. 323. 324. 325. 326. 327. 328. 329. 330. 331. 332. 333. 334. 335. 336. 337. 338. 339. 340. 341. 342. 343. 344. 345. 346. 347. 348. 349. 350. 351. 352. 353. 354. 355. 356. 357. 358. 359. 360. 361. 362. 363. 364. 365. 366. 367. 368. 369. 370. 371. 372. 373. 374. 375. 376. 377. 378. 379. 380. 381. 382. 383. 384. 385. 386. 387. 388. 389. 390. 391. 392. 393. 394. 395. 396. 397. 398. 399. 400. 401. 402. 403. 404. 405. 406. 407. 408. 409. 410. 411. 412. 413. 414. 415. 416. 417. 418. 419. 420. 421. 422. 423. 424. 425. 426. 427. 428. 429. 430. 431. 432. 433. 434. 435. 436. 437. 438. 439. 440. 441. 442. 443. 444. 445. 446. 447. 448. 449. 450. 451. 452. 453. 454. 455. 456. 457. 458. 459. 460. 461. 462. 463. 464. 465. 466. 467. 468. 469. 470. 471. 472. 473. 474. 475. 476. 477. 478. 479. 480. 481. 482. 483. 484. 485. 486. 487. 488. 489. 490. 491. 492. 493. 494. 495. 496. 497. 498. 499. 500. 501. 502. 503. 504. 505. 506. 507. 508. 509. 510. 511. 512. 513. 514. 515. 516. 517. 518. 519. 520. 521. 522. 523. 524. 525. 526. 527. 528. 529. 530. 531. 532. 533. 534. 535. 536. 537. 538. 539. 540. 541. 542. 543. 544. 545. 546. 547. 548. 549. 550. 551. 552. 553. 554. 555. 556. 557. 558. 559. 560. 561. 562. 563. 564. 565. 566. 567. 568. 569. 570. 571. 572. 573. 574. 575. 576. 577. 578. 579. 580. 581. 582. 583. 584. 585. 586. 587. 588. 589. 590. 591. 592. 593. 594. 595. 596. 597. 598. 599. 600. 601. 602. 603. 604. 605. 606. 607. 608. 609. 610. 611. 612. 613. 614. 615. 616. 617. 618. 619. 620. 621. 622. 623. 624. 625. 626. 627. 628. 629. 630. 631. 632. 633. 634. 635. 636. 637. 638. 639. 640. 641. 642. 643. 644. 645. 646. 647. 648. 649. 650. 651. 652. 653. 654. 655. 656. 657. 658. 659. 660. 661. 662. 663. 664. 665. 666. 667. 668. 669. 670. 671. 672. 673. 674. 675. 676. 677. 678. 679. 680. 681. 682. 683. 684. 685. 686. 687. 688. 689. 690. 691. 692. 693. 694. 695. 696. 697. 698. 699. 700. 701. 702. 703. 704. 705. 706. 707. 708. 709. 710. 711. 712. 713. 714. 715. 716. 717. 718. 719. 720. 721. 722. 723. 724. 725. 726. 727. 728. 729. 730. 731. 732. 733. 734. 735. 736. 737. 738. 739. 740. 741. 742. 743. 744. 745. 746. 747. 748. 749. 750. 751. 752. 753. 754. 755. 756. 757. 758. 759. 760. 761. 762. 763. 764. 765. 766. 767. 768. 769. 770. 771. 772. 773. 774. 775. 776. 777. 778. 779. 780. 781. 782. 783. 784. 785. 786. 787. 788. 789. 790. 791. 792. 793. 794. 795. 796. 797. 798. 799. 800. 801. 802. 803. 804. 805. 806. 807. 808. 809. 810. 811. 812. 813. 814. 815. 816. 817. 818. 819. 820. 821. 822. 823. 824. 825. 826. 827. 828. 829. 830. 831. 832. 833. 834. 835. 836. 837. 838. 839. 840. 841. 842. 843. 844. 845. 846. 847. 848. 849. 850. 851. 852. 853. 854. 855. 856. 857. 858. 859. 860. 861. 862. 863. 864. 865. 866. 867. 868. 869. 870. 871. 872. 873. 874. 875. 876. 877. 878. 879. 880. 881. 882. 883. 884. 885. 886. 887. 888. 889. 890. 891. 892. 893. 894. 895. 896. 897. 898. 899. 900. 901. 902. 903. 904. 905. 906. 907. 908. 909. 910. 911. 912. 913. 914. 915. 916. 917. 918. 919. 920. 921. 922. 923. 924. 925. 926. 927. 928. 929. 930. 931. 932. 933. 934. 935. 936. 937. 938. 939. 940. 941. 942. 943. 944. 945. 946. 947. 948. 949. 950. 951. 952. 953. 954. 955. 956. 957. 958. 959. 960. 961. 962. 963. 964. 965. 966. 967. 968. 969. 970. 971. 972. 973. 974. 975. 976. 977. 978. 979. 980. 981. 982. 983. 984. 985. 986. 987. 988. 989. 990. 991. 992. 993. 994. 995. 996. 997. 998. 999. 1000.

method. Application of the rules to the study of absolute configuration and conformations of organic molecules.

BOOKS SUGGESTED:

1. Organic Chemistry Vol.I and Vol.II by I.L.Finar
2. Carbohydrate Chemistry by Barton Volumes
3. Carbohydrate chemistry by G.J.Boons
4. The chemistry of natural products:vol.V - carbohydrates by S.F.Dyke
5. Organic Chemistry by McMurry
6. Nucleic acids in Chemistry and Biology by G M Blackburn MI Gait
7. Lehninger Principles of Biochemistry by D L Nelson and M M Coxon
8. Outlines of Biochemistry by Conn and Stumpf
9. Enzyme structure and mechanism by Fersht and Freeman
10. Enzymes for green organic synthesis by V.K.Ahluwalia
11. Biotransformations in Organic Chemistry by K Faber.
12. Principles of biochemistry by Horton & others.
13. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.
14. Concepts in Biotechnology by D.Balasubramanian & others
15. Chemistry and physiology of the vitamins by H.R.Rosenberg. 22. Stereochemistry of organic compounds — Principles & Applications by D Nasipuri 23. Stereochemistry of Carbon compounds by Ernest L Eliel & Samuel H. Wilen
16. Stereochemistry: Conformation & Mechanism by P S Kalsi
17. The third dimension in organic chemistry, by Alan Bassendale
18. Stereo selectivity in organic synthesis by R S Ward.
19. Advanced organic chemistry. Part A Structure & Mechanism by Francis A. Corey and Richard J. Sundberg
20. Optical rotatory dispersion by C Djerassi
21. Optical rotatory dispersion and circular dichroism by P Crabbe
22. Mechanism and Structure in Organic chemistry by S Mukherjee

PAPER III CH (OC) 303T (ELECTIVE IIIB): PROCESS CHEMISTRY AND DEVELOPMENT.

- OC(CB1)-13: Process chemistry and Principles
 OC(CB1)-14: Process Development /Optimization - I
 OC(CB1)-15: Process Development /Optimization - II

OC(CB1)-13: Process Chemistry and Principles

15 Hrs

Introduction to Pharmaceutical Industry, Product life cycle and its different functions in product life cycle management, Research & Development, Production/Manufacturing, Quality Control, Quality Assurance, Intellectual Property, Regulatory Affairs.

Route selection: SELECT (Safety, Environmental, Legal, Economics, Control, Throughput)

Safe route, Environment friendly route, Legal (more insights into Intellectual Property on patent infringement related topic), Economic and commercially viable route, Control & Scalable route, Feasibility of selected route/s for optimum throughput (Depends on number of routes proposed for development), Structure confirmation of product at each stage by IR, NMR, Mass, Conclusion of feasibility study

OC(CB1)-14: Process Development / Optimization - I

15 Hrs

Process Chemistry: Introduction & importance of process optimization in product development, Starting material/s : Definition, Reagent/s: Definition, different types of reagents; Catalysts, stoichiometry calculations, Solvent/s: Definition, different types of solvents and their compatibility. **Process Safety Engineering:** Reaction condition/s: Definition, different reaction conditions, exothermic & endothermic conditions (DSC / TSU, Reaction calorimetry and gas evolution study) endothermic conditions. **Analytical:** Reaction monitoring technique/s or In-process controls: Definition, different types of monitoring techniques: TLC, HPLC and GC, Impurity identification and their structure elucidation: UV, IR, Mass, NMR. Fixing Specifications in each stage: Definition, significance of fixing specifications, Different detectors (UV, RI, ELSD, CAD).

OC(CB1)-15: Process Development / Optimization - II

15 Hrs

Reaction Parameters: Reaction Kinetics (Homogeneous, Heterogeneous reactions, Mixing, Temperature, Time and Critical Process parameter identification). **Work up & product isolation:** Definition, different types of work ups: Quenching, extraction and distillation/concentration & isolation. **Purification:** Definition, different types of purifications: Washing, precipitation, crystallization. **Filtration study. Drying:** Different types of drying methods, ATD (Air tray dryer), VTD (Vacuum tray dryer), RCVD (Rotatory cone vacuum dryer), FBD (Fluid Bed Dryer), Lyophilization, Spray Drying. **What-if and Stability study:** Definitions & its requirement in scale up, Finalizing the Critical Process parameters based on the Optimization and what if study. Risk mitigations by considering Critical Material Attributes and critical process parameter. **Report writing**

SUGGESTED BOOKS

1. Practical Process Research & Development-Neal Anderson (Chapter-2)
2. Process Chemistry in Pharmaceutical Industry by Kumar Gadamasetti, Vol I & II, CRC Press,

Handwritten signatures and initials: - V. S. ... M. ... K. P. Reddy

3. The chemistry of process development in fine chemical & pharmaceutical chemistry. C. Someswara Rao. Asian Books Private Limited New Delhi.
4. Analytical Chemistry by D. Kealey & P. J. Haines
5. Chemical Analysis, Modern Instrumentation Methods and Techniques by Francis Rouessac and Annick Rouessac, University of Le Mans, France
6. Pharmaceutical Drug Analysis by Ashutosh Kar published by New Age International (P) Limited, Publishers.
7. HPLC and UHPLC for Practicing Scientists by Michael W. Dong,
8. Process Chemistry in Pharmaceutical Industry by Kumar Gadasetti, Vol I & II, CRC press
9. The chemistry of process development in fine chemical & pharmaceutical chemistry. C. Someswara Rao. Asian Books Private Limited New Delhi.
10. Analytical Chemistry by D. Kealey & P. J. Haines
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12. Pharmaceutical Drug Analysis by Ashutosh Kar published by New age international (P) Limited, Publishers.
13. HPLC and UHPLC for Practicing Scientists by Michael W. Dong
14. Fundamentals of Medicinal Chemistry by Thomas
15. Practical Process Research & Development by Neal G Anderson
16. P. J. Dunn, The importance of Green Chemistry in Process Research and Development, Chem. Soc. Rev., 2012, 41, 1452-1461.
17. Pharmaceutical Quality by Design: A Practical Approach by Walkiria S. Schlindwein, Mark Gibson
18. Strategies for Organic Drug Synthesis and Design by Daniel Lednicer, Wiley
19. Pharmaceutical Process Chemistry, Editor(s): Prof. Dr. Takayuki Shioiri, Dr. Kunisuke Izawa, Dr. Toshiro Konoike, Wiley
20. The Art of Process Chemistry, Editor(s): Dr. Nobuyoshi Yasuda, Wiley
22. New Horizons of Process Chemistry: Scalable Reactions and Technologies, Editors: Tomioka, Kiyoshi, Shioiri, Takayuki, Sajiki, Hironao, Springer
23. Pharmaceutical Process Development: Current Chemical and Engineering Challenges edited by John Blacker & Michael T Williams-RSC publishing
- 24) Chemical Analysis, Modern Instrumentation Methods and Techniques by Francis Rouessac and Annick Rouessac, University of Le Mans, France
- 25) Pharmaceutical Drug Analysis by Ashutosh Kar published by New age international (P) Limited, Publishers.
- 26) HPLC and UHPLC for Practicing Scientists by Michael W. Dong
- 27) Analytical Chemistry by D. Kealey & P. J. Haines
- 28) Pharmaceutical Quality by Design: A Practical Approach by Walkiria S. Schlindwein, Mark Gibson

PAPER IV CH (OC) 304T (ELECTIVE IVA): GREEN CHEMISTRY, NANOMATERIALS AND NEW TECHNIQUES IN ORGANIC SYNTHESIS

OC (CB2) -16: Principles of Green chemistry and Green Synthesis
 OC (CB2) -17: Organic nanomaterials and Supramolecular chemistry
 OC (CB2) -18: New techniques and concepts in organic synthesis

OC (CB2) -16: Principles of Green Chemistry and Green Synthesis

15 Hrs

Introduction of Green Chemistry. Principles of Green Chemistry. Introduction to alternative approaches. Microwave Assisted Organic Synthesis (MAOS): introduction, benefits and limitations
 i) Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Claisen rearrangement and Diels- Alder reaction. ii) Microwave assisted Solvent-free reactions: Deacetylation, saponification of esters, alkylation of reactive methylene compounds and synthesis of nitriles from aldehydes. iii) Ultrasound Assisted Organic Synthesis: introduction, applications of ultrasound Cannizzaro reaction, Reformatsky reaction and Strecker synthesis. iv) Organic Synthesis in Green Solvents: introduction Aqueous Phase Reactions: Diels-Alder Reaction, Heck reaction, Hoffmann elimination, Claisen-Schmidt condensation hydrolysis and dihydroxylation reactions. v) Organic Synthesis using Ionic liquids: Introduction, applications-Beckmann rearrangement Suzuki Cross-Coupling Reaction and Diels- Alder reaction. vi) Green Catalysts in organic synthesis: introduction a) Phase Transfer Catalysts in Organic Synthesis: Introduction, Williamson ether synthesis and Wittig reaction b) Biocatalysts in Organic Synthesis: Biochemical (microbial) oxidations and reductions.

OC (CB2) -17: Organic Nanomaterials and Supramolecular Chemistry

15 Hrs

Organic Nanomaterials:

Introduction: The 'top-down' approach, the 'bottom-up' approach and Nanomanipulation.

Molecular Devices: Photochemical devices, Liquid crystals.

New Carbon family: Types of Fullerenes, Types of Carbon nanotubes (Zig-Zag, Armchair and Chiral), Graphenes. Types of Fullerenes, CNTs (Zig Zag, Armchair and Chiral), singlewalled CNTs (SWCNTs) and multi walled MWCNTs) and Graphenes.

Supramolecular Chemistry :

Introduction: Supramolecular interactions (ion-ion, ion-dipole, H-bonding, cation- π , anion- π , π - π and Van der Waals interactions), Ionophore and molecular receptors.

Host-Guest Chemistry: Lock and key analogy, Structures and applications of Cryptands, Spherands, Calixerenes, Cyclodextrins, Cyclophanes, Carcerands and hemicarcerands.

Self-assembly: Ladder, polygons, helices, rotaxanes, catanenes, Molecular necklace, dendrimers, properties and applications.

OC (CB2) -18: New techniques and concepts in organic synthesis

15 Hrs

Techniques in peptide synthesis:

Solid phase peptide synthesis, commonly used resins (Rink resin, Wang resin and Ellman resin, synthesis of cross linked Merrifield resin and drawbacks of solid phase synthesis.

Solid phase oligodeoxynucleotide synthesis: Phospho triester, phosphite triester and phosphoramidite pathway

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Oligosaccharide synthesis: Glycosidation: cyclic oxocarbenium ion, glycosyl donors and glycosyl acceptors, Kahne glycosidation, convergent and linear oligosaccharide synthesis.

Phase Transfer catalysis: Onium and crown ethers as PTC.

Tandem synthesis: Tandem reactions; conjugate addition-aldol reaction, polymerization-cyclisation, electrocyclic-Diels Alder reaction.

Baldwin Rules: Exo and Endo cyclisation, tetrahedral, trigonal and diagonal systems, favoured and disfavoured cyclisations.

Chiron approach in organic synthesis: Nature's chiral pool, carbohydrates, amino acids, hydroxy acids, terpenes as chiral precursors. Synthesis of shikimic acid from D-arabinose, furanonycin from D-glucose, S-(-)-iphenol from S-leucine.

Determination of absolute configuration: Mosher's method.

BOOKS SUGGESTED:

1. P.T. Anastes & J.K. Warner: Oxford Green Chemistry- Theory and Practical, University Press (1998).
2. A.S. Matlack: Introduction to Green Chemistry, Marcel Deckkar, (2001).
3. M.C. Cann & M.E. Connely: Real-World cases in Green Chemistry, American Chemical Society, Washington (2000).
4. M.A. Ryan & M. Tinnesand, Introduction to Green Chemistry, American Chemical Society, Washington (2002).
5. V.K. Ahluwalia & M.R. Kidwai: New Trends in Green Chemistry, Anamalaya Publishers
6. Enantioselective organocatalysis, Peter I Dallco, Willey-VCH
7. Core Concepts in Supramolecular Chemistry and Nanochemistry by Jonathan W. Steed, David R. Turner and Karl J. Wallace; John-Wiley and Sons Publications
9. Supramolecular Chemistry by Jonathan W. Steed and Jerry L. Atwood, John-Wiley and Sons Publications
10. Supramolecular Chemistry-Concepts and Perspectives by J M. Lehn; Wiley-VCH (1995) Publications
11. Supramolecular Chemistry by P. D. Beer, P. A. Gale and D. K. Smith; Oxford University Press (1999)
12. Stereochemistry of organic compounds - Principles & Applications by D Nasipuri
13. Nanochemistry by G.B. Sergeev; Elsevier
14. Nanochemistry: A chemical approach to nano materials , G.A. Ozin & A.C. Arsenault; RSC publishers.
15. Stereo differentiating reactions by Izumi
16. Some modern methods of organic synthesis by W Carruthers
17. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
18. Organic synthesis by Michael B Smith
19. Organic Synthesis by C Willis and M Wil lis
20. Problems on organic synthesis by Stuart Warren
21. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren
22. The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng
33. Name reactions by Jie Jacj Li

K. P. Reddy

PAPER IV CH (OC) 304T (ELECTIVE IVB): PESTICIDES

- OC (CB2) - 16: Introduction to pesticides
 OC (CB2) - 17: Synthetic insecticides
 OC (CB2) - 18: Natural insecticides & herbicides

OC(CB2) - 16: Introduction to pesticides

15 Hrs

- i) Definition, Classification and importance of pesticides
 ii) Pest control: Different methods -chemical insecticides, fungicides, herbicides, rodenticides, fumigants, chitin synthesis inhibitors and insect repellents..
 a) Biological pheromones: Definition and classification, synthesis of Disparlure, Exobrevicomin. Endobrevicomin, frontalinal and grandiso pheromones, synthetic sex attractants.
 b) Insect juvenile hormones: JH-A, JH-B, Synthesis of juvabione. Structural formula and importance of methopren.
 c) Moulting hormones-structural formulae and mode of action of ecdysones
 d) Antibiotics and secondary metabolites of microbial origin as insecticides and fungicides in agriculture. Structural formula and importance of Blasticidin-S, Kasugamycin, Avermectin-B, Invermectin, piercidins and phytoalexins.
 iii) Environmental pollution from pesticides. iv) Integrated pest management.
 v) Pesticide formulations: Dusts, Granules, Wettable powders, Emulsions and Aerosols.
 vi) Formulation and residue analysis of organochlorine, organophosphorous and carbamate insecticides.

OC(CB2) -17: Synthetic Insecticides

15 Hrs

A. Synthetic origin:

- i) Organochlorine insecticides- synthesis and mode of action of methoxychlor, perthane and Endosulfan.
 ii) Organophosphorous insecticides synthesis and mode action of Phosphoric acid derivatives. Dichlorophos, parathion and TEPP
 iii) Carbamate insecticides- synthesis and mode of action of carbaryl and Baygon

B. Natural origin:

- i) Insecticides of plant origin-synthesis and importance of pyrethrins (I and II), Rotenone. Main constituents Neem-structural formula of Azadirachtin. Synthesis of polygodial and warbunganol Antifeedants).
 ii) Synthesis of pyrethroids: synthesis of Allethrin, Bioallethrin and Fenvalerate.
 iii) Concept of Bioinsecticides - Bacillus thuringiensis.
 iv) Concept of pro-insecticides-structure and mode of action of pro-pheromones and pre-pro-insecticides.

OC(CB2) -18: Natural insecticides & herbicides

15 Hrs

- i) Fungicides: Synthesis application and mode of action of the following classes: (a) Quinones-chloranil and Benquinox b) perchloromethylmercaptan derivative-captan, folpet Mesulfan c) Benzimidazoles-carbendazim and Thiabendazole
 ii) Rodenticides: a) Anticoagulants-synthesis and application of warfarin. Dicoumarol and

v. K. K. Reddy

Bromodiolen. b) Acute poisons- application of pindone, Ratindan, Sodium Fluoroacetate Barium fluoroacetate, Antu, Tetramine, pindone and castrix. No. of Congress reduce.
 ii) Herbicides : Synthesis, applications and mode of action of the following a) Aryloxyalkyl carboxylic acid derivative: 2,4-D. MCPA, 2,4,5-1 and 2,4,5-TP b) Carbamates- propham and chloropham, c) Urea derivatives Monouron and diuron, d) Aliphatic acids- Dalapon. ICA. e) Aromatic acids -2,3,6-TBA Dicamba and Amiben.

BOOKS SUGGESTED:

- 1) Naturally occurring insecticides: M.Jacobson and D.G.Crosby.
- 2) Insecticides for future:Jacobson
- 3) Insect juvenile hormone chemistry and action: J.J Mann and M.Beroza
- 4) Polygodial and warburganal. Terpenoid antifeedants part-II rec, Tran,chin 106
- 5) Insect antifeedants :S.V.ley & P.L Toogood,chemistry in Britain, Jan 1990 P.31
- 6) Synthesis of Insecticides Metcalf
- 7) Fungicides-Frear
- 8) Fungicides-Nene
- 9) Residue reviews vol.36: Melnikov
- 10) Safer insecticides : E. Hodgson
- 11) Crop protection agents from Nature: Leonard G Copping
- 12) Biofertilizers and Bioinsecticides: A.M.Deshmukh
- 13) Insecticides and Fungicides U Sriramulu.
- 14) Organo chlorine insecticides: persistent organic pollutants :F.Moriary
- 15) Herbicides :P.C.Kearney & D.D.Kaufnan
- 16) Analytical Method for pesticides:Z. Weig (Vol III)
- 17) Pesticide formulations: Van Valkenburg
- 18) Insecticides:A.S.Tahori
- 19) Herbicides, fungicides, formulation chemistry-A.S.Tahori
- 20) Environmental pollution by pesticides :C.A.Edwards
- 21) Pesticides managements and insecticide resistance: Watson and brown
- 22) Organo phosphorous pesticides M.eto

LABORATORY COURSES

Paper- V CH (OC) 351P: Synthesis of Organic Molecules

4 Hrs/Week

Synthesis of the following compounds:

2-Phenyl indole (Fischer indole synthesis), 7-hydroxy-3-methyl flavone (Baker - Venkatraman reaction), 2,5-Dihydroxy acetophenone (Fries reaction), 4- Chlorotoluene from p-toluidine (Sandmeyer reaction), Benzilic acid from benzoin (Benzilic acid rearrangement), Benzpinacol (photochemical reaction), 7-hydroxy coumarin (Pechman synthesis), Photo-dimerization of maleic anhydride, benzophenone (Friedel-Crafts reaction), Benzanilide (Beckmann rearrangement), Vanillyl alcohol from vanillin (NaBH_4 reduction), 2- and 4-nitrophenols (nitration and separation by steam distillation), Acridone from Phthalic anhydride.

Paper-VI CH (OC) 352P: Separation and Identification of Organic Compounds

4 Hrs/Week

Separation of two component mixtures by chemical methods and their identification by chemical reactions — separation by using solvent ether, 5 % aqueous sodium bicarbonate, 5% sodium hydroxide and dil hydrochloric acid, checking the purity of the two components by TLC; identification of the compounds by a systematic study of the physical characteristics (mp/bp), extra elements (nitrogen, halogens and sulfur), solubility, functional groups, preparation of crystalline derivatives and identification by referring to literature. A minimum of 09 mixtures should be separated and analyzed by these procedures.

Paper-VII CH (OC) 353P: Isolation of Natural Products and Thin Layer Chromatography

2 Hrs/Week

A. Isolation of the following Natural Products

Caffeine from tea leaves (solvent extraction), Piperine from pepper (Soxhlet extraction), Eucalyptus oil from leaves (steam distillation), Lycopene from tomatoes.

B. Identification of Components in the extracts by TLC

Paper-VIII CH (OC) 354P: Separation of Three Component Mixtures by Chemical Methods and Column Chromatography:

2 Hrs/Week

Separation of three component mixtures by chemical methods. A minimum of four mixtures should be separated and analyzed.

Column Chromatography: Separation of four mixtures of two components each using silica gel as adsorbent and a suitably polar eluent. The column chromatography should be monitored by TLC.

BOOKS SUGGESTED:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Ralph L. Shriner, Christine K. F. Hermann, Terence C. Morrill and David Y. Curtin

SEMINAR

2 Hrs/ week

M.Sc. SEMESTER - IV
ORGANIC CHEMISTRY SPECIALIZATION
 (For the batches admitted in academic year 2023-24 onwards under CBCS pattern)

PAPER I CH (OC) 401T (CORE): DRUG DESIGN AND DRUG DISCOVERY

OC-19: Principles of Drug Design and Drug Discovery
 OC-20: Lead Modification and SAR Studies
 OC-21: QSAR Studies and Computer Aided Drug Design

OC -19: Principles of Drug Design and Drug Discovery

15 Hrs

Introduction to drug discovery. Folklore drugs, stages involved in drug discovery disease, drug targets, bioassay, Discovery of a lead screening of natural products and synthetic compound libraries. Existing drugs as leads (me too drugs). Pharmacokinetics (ADME), pharmacodynamics. Nature of drug receptor interactions and their theories Occupancy theory, Induced fit theory, Macromolecular perturbation theory and Two-state model of receptor activation, Natural products as lead structures in drug discovery Pharmacophore - structure pruning technique e.g. morphine. Discovery of lead structure from natural hormones and neurotransmitters. Drug discovery without lead serendipity Penicillin and Librium as examples. Principles of prodrug design. Introduction to drug patents and Clinical trials.

OC-20: Lead Modification and SAR Studies

15 Hrs

SAR: Lead modification strategies. Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion and ring contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxamiquine, salbutamol, cimitidine and captopril Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, and taxol analogs.

OC-21: QSAR Studies and Computer Aided Drug Design

15 Hrs

QSAR: Introduction, physicochemical properties pKa, electronic effects and Hammett constants(6), lipophilicity constant(x), steric effects and Taft's constant, linear and nonlinear relationship between biological activity Lipophilicity Substituent constants. Lipinski rule of five. Hansch analysis, Craig's plot, Topliss scheme, Free Wilson approach, cluster significant analysis. Two case studies (QSAR study on pyranenamine and design of Crizotinib).

Computer Aided Drug Design:

Introduction, active site, allosteric binding site, use of grids in docking rigid docking flexible docking and induced fit docking of ligands, Basic principles and difference between structure and ligand based drug design, denovo drug design and utility to optimize the lead structure.

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BOOKS SUGGESTED :

1. Burger's medicinal chemistry and drug discovery by Manfred E. Wolf.
2. Introduction to Medicinal chemistry by Patrick.
3. Introduction to drug design by R Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. by William Foye
6. Biochemical approach to medicinal chemistry. by Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis by Roth and Kleeman
8. Drug design by E.J. Arienes
9. Principles of Medicinal Chemistry Vol I & II by Kadam et al
10. Medicinal chemistry An introduction by Garreth Thomas
11. Organic and Pharmaceutical chemistry By Delgrado
12. Organic Pharmaceutical chemistry By Harikishan singh
13. Medicinal Chemistry By Ashtoshkar
14. Medicinal Chemistry By Chatwal
15. Organic Drug synthesis By Ledneicer Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneicer.
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirotechnology By Roger A. Sheldon
19. Burger's Medicinal Chemistry and Drug Discovery: Principles and Practices. Vol.1.
20. Medicinal Chemistry by G. Patricks.
21. Text book of Drug Design and Discovery. Edited by Povl Krogsgaard - Larsen Tommy Liljefors.
22. Structure Based Drug Design of Crizotinib (PF-02341066), a Potent and Selective Dual Inhibitor of Mesenchymal-Epithelial Transition Factor (c-MET) Kinase and Anaplastic Lymphoma Kinase (ALK) Martin P. Edwards, J. Med. Chem., 2011, 54 (18), pp 6342-6363.
http://www.pfizer.com/news/featured_stories/featured_stories_martin_edwards.jsp

Organic Chemistry

AP

N. Jayash

Sauri

P. S. Chary

M. S. S. S. S.

K. R. Reddy

PAPER II CH (OC) 402T(CORE): ADVANCED HETEROCYCLIC CHEMISTRY

OC-22: Heterocyclic compounds, Nonaromatic heterocyclics and Five membered heterocyclics with two heteroatoms

OC-23: Six membered heterocyclics with two heteroatoms and Five membered heterocyclics with more than two heteroatoms

OC-24: Six membered heterocyclics with more than two heteroatoms and Larger ring heterocyclics

OC-22: Heterocyclic compounds, Nonaromatic heterocyclics and Five membered heterocyclics with two heteroatoms 15 Hrs

Heterocyclic compounds: Introduction, Nomenclature Synthesis and reactivity of indole, quinone, isoquinoline and acridine.

Nonaromatic heterocyclics: Synthesis, reactivity and importance of the following ring systems. Azirines, Aziridines, Oxiranes, Thiiranes, Diazirenes, Diaziridines, Oxaziridines, Azetidines, Oxetanes and Thietanes.

Five membered heterocyclics with two heteroatoms: Synthesis, reactivity, aromatic character and importance of the following Heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole.

OC-23: Six membered heterocyclics with two heteroatoms and Five membered heterocyclics with more than two heteroatoms 15 Hrs

Six membered heterocyclics with two heteroatoms: Synthesis, reactivity, aromatic character and importance of the following Heterocycles: Pyridazine, Pyrimidine, Pyrazine, Oxazine, Thiazine.

Five membered heterocyclics with more than two heteroatoms: Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole, 1,2,3-thiadiazoles, 1,2,5-thiadiazoles.

81/175

OC-24: Six membered heterocyclics with more than two heteroatoms and larger ring heterocyclics 15 Hrs

Six membered heterocyclics with more than two heteroatoms: 1,2,3-triazine, 1,2,4-triazine, 1,3,5-triazine, tetrazines. Synthesis and importance of purines and pteridines. Synthesis of Caffeine, theobromine and theophylline.

Larger ring heterocyclics: Synthesis, structure, stability and reactivity of Azepines, Oxepines, Thiepinines. Synthesis of diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiepinines, Azocines and Azonine.

BOOKS SUGGESTED:

1. Heterocyclic Chemistry, T.Gilchrist
2. An introduction to the Chemistry of heterocyclic compounds, R.M.Acheson
3. Heterocyclic Chemistry, J.A.Joule & K.Mills
4. Principles of Modern Heterocyclic Chemistry, A.Paquette

PAPER-III CH (OC) 403 T(ELECTIVE IIIA):
DRUG SYNTHESIS AND MECHANISM OF ACTION

OC(CB1)-25: Drugs acting on metabolic process, cell wall and specific enzymes

OC(CB1)-26: Drugs acting on genetic material and immune system

OC(CB1)-27: Drugs acting on receptors and ion channels

OC(CB1)-25: Drugs acting on metabolic process, cell wall and specific enzymes 15Hrs

Basic concepts of mechanism of drug action: Introduction to macromolecular targets, carbohydrates, proteins, lipids and nucleic acids as possible drug targets. Classification of drugs. Enzyme inhibition and its types.

a) Drugs acting on metabolic process:

Antifolates –Discovery and mechanism of action of sulphonamides, Synthesis of sulfomethoxazole, sulfadoxine, sulfaguanidine and dapsone.

Diaminopyrimidines -trimethoprim, bacterial resistance to sulfonamides and drug synergism

b)Drugs acting on cell wall: Structure of bacterial cell wall, β -Lactam antibiotics – mechanism of action of penicillins and cephalosporins. Synthesis of penicillin-G and cephalosporin-C, cefalexin and cycloserine. Resistance to penicillins, broad spectrum penicillins – cloxacillin, methicillin, ampicillin, amoxicillin and carbenicillin. β -Lactamase inhibitors - Structural formulae and mode of action of clavulanic acid and sulbactam

c)Drugs acting on specific enzymes: H⁺/K⁺ -ATPase inhibitors- synthesis of Omeprazole and Carbonic anhydrase inhibitors-synthesis of Acetazolamide.

OC(CB1)-26: Drugs acting on genetic material and Chiral drugs 15Hrs

Drugs acting on genetic material: Introduction, classification and mechanism of action.

a) DNA-intercalating agents-Anticancer and antimalarial agents. Structural formulae of Daunomycin, Adriamycin and Amsacrine. Synthesis of Amsacrine, Nitracrine, Quinacrine and Chloroquine.

b) DNA- Binding and nicking agents: Antiprotozoal drugs. Synthesis of Metronidazole, Dimetridazole and Tinidazole.

c) DNA-Alkylators: Synthesis of Cyclophosphamide and Bisulphan.

d) DNA-Polymerase inhibitors: Antiviral agents- Synthesis of Acyclovir and AZT.

e) DNA-Topoisomerase inhibitors: Anti bacterial agents. Synthesis of Ciprofloxacin and Norfloxacin. Structural formulae ofloxacin and Lomefloxacin.

f) Inhibitors of transcribing enzymes: Anti-TB and antileprosy agents-structural formulae of Rifamycins and partial synthesis of Rifampicin.

g) Drugs interfering with translation process: Antibacterial drugs- Structural formulae of Erythromycin, 5-Oxytetracycline and Streptomycin. Synthesis of Chloromycetin

Introduction to chiral drugs. Three-point contact model, Eutomer, Distomer and eudesmic ratio. Pfeiffer's rule. Role of chirality on biological activity: Distomers – a) with no side effects b)with undesirable side effects c) both isomers having independent therapeutic value d)combination products having therapeutic advantages e) metabolic chirality inversion.

OC(CB1)-27: Drugs acting on receptors and ion channels 15Hrs

Introduction to nervous system: structure of neuron, nerve transmission. Definition and examples of agonist, antagonist, neurotransmitters and receptors.

Drugs acting on receptors:

A - N/A K.R. Reddy

- a) Adrenergic receptors - Introduction and classification. α -Adrenergic-receptor agonists and antagonists- Synthesis and biological activity of Nor-adrenaline, Methyl L dopa and Tetrazosin. β -Adrenergic-receptor - agonists and antagonists – Synthesis and pharmacological activity of Salbutamol, Tetrabotalin, Propranolol and Atenolol.
- b) Cholinergic-receptors: Introduction and classification. Cholinergic-receptor agonists and antagonists- Structural formulae of Nicotine, Atropine and Tubocurarine. Synthesis of Acetyl choline and Succinyl choline
- c) Dopamine receptors: Introduction and classification. Dopamine- receptor agonists and antagonists- Biosynthesis of Dopamine. Synthesis of L-Dopa and Chlorpromazine.
- d) Serotonin receptors: Introduction and classification. Serotonin receptor agonists and antagonists- synthesis and pharmacological activity of Serotonin and Metoclopramide.
- e) Histamine receptors: Introduction and classification. Histamine receptor agonists and antagonists- synthesis and biological action of Histamine, Chloropheneramine, and Ranitidine.
- f) Hormones and their receptors: Introduction to estrogen receptors, Structural formulae of Tamoxifen
- Drugs acting on ion channels: Introduction to ion channels, drugs acting on Ca^{2+} , Na^{+} and Cl^{-} channels and their mode of action. Structural formulae of Tetracaine and synthesis and of Nifedipine, Diltiazem, Tetracaine and 4-Aminopyridine.

BOOKS SUGGESTED:

1. Burger's medicinal chemistry and drug discovery. By Manfred B. Wolf.
2. Introduction to Medicinal chemistry. By Graham Patrick.
3. Introduction to drug design. By R.B. Silverman
4. Comprehensive medicinal chemistry. Vol 1-5 by Hanzsch.
5. Principles of medicinal chemistry. By William O. Foye et al.
6. Biochemical approach to medicinal chemistry. By Thomas Nogrady.
7. Pharmaceutical Chemistry and Drug synthesis By Roth and Kleeman
8. Drug design By E.J. Arienes
9. Principles of Medicinal Chemistry. Vols.1 & 2 By Kadam et al
10. Medicinal chemistry An introduction By Gareth Thomas
11. Wilson and Gisvold,s text book of Organic, Medicinal and Pharmaceutical chemistry By J.N.Delgado and W.A.Remers.
12. Organic Pharmaceutical chemistry By Harikishan singh.
13. Medicinal Chemistry By Ashutoshkar
14. Medicinal Chemistry By G.Chatwal
15. Organic Drug synthesis By Ledneiser Vol 1-6
16. Strategies for organic drug synthesis and design By Daniel Ledneiser
17. Top Drugs: Top synthetic routes By John Saunders
18. Chirecchnology By Roger A. Sheldon

PAPER III CH (OC) 403 T(ELECTIVE IIIB): ADVANCED NATURAL PRODUCTS

- OC(CB1)-25: Biosynthesis of natural products
 OC(CB1)-26: Structure determination of natural products
 OC(CB1)-27: Total stereo selective synthesis of natural products.

OC(CB1)-25: Biosynthesis of Natural Products

15 Hrs

Biosynthesis of secondary metabolites: Introduction, Difference between Laboratory synthesis and biosynthesis. Methods for determination of biosynthetic mechanism. Isolation and identification of Biosynthetic precursors, Feeding experiments – use of radioisotopes Measurement of incorporation – absolute incorporation, specific incorporation. Identification of the position of labels in labeled natural products by chemical degradation and spectral methods. Major biosynthetic pathways: 1) Acetate-Malonate pathway: Biosynthesis of aromatic compounds, 2) Shikimic acid pathway ; Biosynthesis of essential amino acids – phenylalanine, tyrosine and tryptophan, carboxylic acid derivatives, flavonoids and morphine alkaloids. 3) Mevalonic acid pathway : Biosynthesis of terpenes – mono, sesqui, di, tri (β -amyrin) and carotenoids, steroids – cholesterol.

OC(CB1)-26: Structure Determination of Natural Products

15Hrs

- a) **By Chemical Methods:** Determination of structure and stereochemistry of reserpine, abietic acid and rotenone.
- b) **By Spectral Methods:**
- i) IR, UV, ^1H NMR, ^{13}C NMR, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE and MS in the structure elucidations of natural products, Examples: flavones, flavanones, coumarins, quinolines.
 - ii) DEPT and NOE of Geraniol; INEPT of menthol.
 - iii) Heteronuclear 2D-J resolved spectrum of stricticine, HETEROCOSY of strictanol.

OC(CB1)-27: Total Stereo Selective Synthesis of Natural Products

15Hrs

Takasago synthesis of Menthol, Hoffmann-LaRoche synthesis of Biotin, Corey's synthesis of Prostaglandins (E2, F2 α) and Paeoniflorin, Sharpless synthesis of L-hexoses, Danishefsky synthesis of Indolizomycin, Nicolaou's synthesis of Taxol, Meyer's synthesis of Dynemicin A.

BOOKS SUGGESTED:

1. Textbook of organic chemistry, Vol II by I L Finar
2. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
3. An introduction to the chemistry of terpenoids and steroids, by William templeton
4. Systematic identification of flavonoid compounds by Mabry & Markham
5. Steroids by Fieser and Fieser
6. Alkaloids by Manske
7. Alkaloids by Bentley
8. The chemistry of terpenes by A Pinder
9. The terpenes by Simenson
10. Terpenoids by Mayo

13. Biosynthesis by Geismann
14. Principles of organic synthesis 3rd Ed. R O C Norman and J M Coxen
15. One and two dimensional nmr spectroscopy by Atta Ur Rahman
16. Classics in total synthesis K C Nicolaou and E J Sorenson
17. Spectrometric identification of organic compounds by Silverstein and Webster

Laboratory courses

Paper-IV CH (OC) 451P: Spectroscopic Identification of Organic Compounds 4 Hrs/Week
 Identification of unknown organic compounds by interpretation of IR, UV, ^1H -NMR, ^{13}C NMR, and mass spectral data (five examples with 2D-NMR). A minimum of 25 representative examples should be studied.

Paper-V CH (OC) 452P: Synthesis of following Drugs 4 Hrs/Week
 Paracetamol, Phenytoin, Benzocaine, 6-Methyluracil, Chloritone, Fluorescein, 4-Aminobenzene sulfonamide, antipyrine and phenothiazine, 2,4,5-tri phenyl imidazole, 4-chloro benzhydryl piperazine

Paper-VII CH (OC) 453P: Practice of Chemistry Software Programmes 2 Hrs/Week
 Chem Draw, analysis of IR and NMR using ACD/Id NMR processor. EXCEL: Drawing graphs, Molecular docking.

SUGGESTED BOOKS:

1. Practical organic chemistry by Mann & Saunders
2. Text book of practical organic chemistry by Vogel
3. The systematic identification of organic compounds by Shriner et.al
4. Analytical chemistry by G N David Krupadanam et.al
5. Advanced practical medicinal chemistry by Ashutoshkar
6. Pharmaceutical drug analysis by Ashutoshkar
7. Quantitative analysis of drugs in pharmaceutical formulations by P D Sethi
8. Practical pharmaceutical chemistry part-1 and part-2 by A H Beckett and J B Stenlake
9. Spectroscopic identification of organic compounds by R M Silverstein and F X Webster

PROJECT CH (OC) 454P**12 Hrs/ week****IV Semester Project Assessment for 175 Marks****Marks Distribution for Project Assessment****INTERNAL ASSESSMENT**

Research Design Seminar	1 credit	25 marks
Progress Seminar	1 credit	25 marks

SEMESTER END ASSESSMENT

Dissertation	1 credit	50 marks
Final presentation	2 credits	50 marks
Viva Voce during final presentation	1 credit	25 marks