

SEMESTER –IV
ADVANCED HETEROCYCLICS AND NATURAL PRODUCTS-II
THEORY

Programme: M.Sc.
Course Code: P20/CHE/DSE/403
Type of course: DSE – 7
No. of credits : 4

Max.Hours : 60
Hours /week: 4
Max.Marks: 100

COURSE OBJECTIVES

- Advanced Natural products deals with the Biosynthesis of secondary metabolites like terpenoids, alkaloids and steroids.
- Within the field of organic chemistry, natural products are produced by the pathways of primary or secondary metabolism . Some of studied natural products include , Morphine, rotenone, cholesterol, Reserpine and Abietic acid .
- Step wise total stereoselective synthesis of natural products

COURSE OUTCOME

CO1: Discuss the synthesis, reactivity, aromatic character and importance of heterocyclics with more than two hetero atoms

CO2: Discuss the synthesis and importance of purines and pteridines.

CO3: Outline the synthesis of Caffeine, theobromine and theophylline.

CO4: Discuss the synthesis, structure, stability, rearrangements and reactivity of Azepines, Oxepines and Thiopines, Diazepines, benzo fused heterocycles. Outline the synthesis of selenophenes, Tellerophenes, Phospholes and Boroles.

CO5: Outline the synthesis of selenophenes, Tellerophenes, Phospholes and Boroles.

CO6: Determine structure and stereochemistry of Morphine, Reserpine, Abietic acid, Cholesterol and Rotenone

CO7: Determine Structure of natural products through Spectroscopic techniques.

CO8: Study of solved problems of Geraniol, Menthol, Apparicine, Stricticine, Buxaquamarine, α -Picoline and β -Methyl furan.

MODULE1: HETEROCYCLICS WITH MORE THAN TWO HETERO ATOMS**(15 Hrs)**

Synthesis, reactivity, aromatic character and importance of the following Heterocycles: 1,2,3-triazoles, 1,2,4-triazoles, Tetrazoles, 1,2,4-oxadiazole, 1,3,4-oxadiazole, 1,2,5-oxadiazole, 1,2,3-thiadiazoles, 1,3,4-thiadiazoles, 1,2,5-thiadiazoles, 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.

MODULE 2: LARGER RING AND OTHER HETEROCYCLES**(15 Hrs)**

Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiopines. Synthesis of Diazepines rearrangements of 1,2-diazepines. Synthesis of Benzoazepines, Benzodiazepines, Benzooxepines, Benzothiopines, Azocines and Azonines. Synthesis of selenophenes, Tellerophenes, Phospholes and Boroles.

MODULE-3: STRUCTURE DETERMINATION OF NATURAL PRODUCTS-I (15Hrs)

Determination of structure and stereochemistry of morphine, reserpine, abietic acid, cholesterol and rotenone.

MODULE4: STRUCTURE DETERMINATION OF NATURAL PRODUCTS-II**(15 Hrs)**

Spectroscopic techniques IR, UV, ¹Hnmr, ¹³Cnmr, COSY, HETEROCOSY, NOESY, 2D-INADEQUATE and MS in the structure elucidations of natural products, Examples, flavones, biflavones, flavanones, isoflavones, coumarins, quinolines, isoquinolines.

Study of the following solved problems: Mass, IR, ¹H, ¹³C NMR, HOMOCOSY, HECTOR, DEPT, 2D-INADEQUATE and NOE of Geraniol, INEPT of menthol, APT of apicarine, Heteronuclear 2D-J resolved spectrum of stricticine, NOESY of buxaquamarine, HETEROCOSY of strictanol, 2D-INADEQUATE of α -picoline and β -methyl tetrahyranfuran.

Reference books:

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
5. Handbook of Heterocyclic Chemistry, A.R.Katritzky
6. Non-benzenoid aromatic compounds by D.Ginsberg
7. Nonbenzenoid compounds by Lloy
8. Textbook of organic chemistry, Vol II by I L Finar.
9. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
10. An introduction to the chemistry of terpenoids and steroids, by William templeton
11. Systematic identification of flavonoid compounds by Mabry &Markham
12. Steroids by Fieser and Fieser
13. Alkaloids by Manske
14. Alkaloids by Bentley
15. The chemistry of terpenes by A Pinder
16. The terpenes by Simenson
17. Terpenoids by Mayo
18. Alkaloids by Pelletier
19. Principles of organic synthesis 3rdEd.R O C Norman and J M Coxen
20. One and two dimensional nmr spectroscopy by Atta Ur Rahman
21. Spectrometric identification of organic compounds by Silverstein and Webster

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Time: 2½ Hrs

SECTION –A (Essay Questions)

I. Answer the following

4 x 10 = 40 M

1. (a) Discuss the chemical reactivity of Tetrazole.(CO1)
(b) Outline the synthesis of Caffeine and Theophylline.(CO3)

OR

2. (a) Discuss the reactivity of 1,3,5- Triazine. (CO1)
(b) Outline the synthesis of 1,2,5 – thiadiazoles. (CO1)
3. (a) Explain the rearrangement reactions of diazepines.(CO4)
(b) Give the synthesis of Benzoxepines and Azonines. (CO4)

OR

4. (a) Give one method of synthesis of oxepine and discuss its reactivity. (CO4)
(b) Describe the synthesis of Selenophenes and Phospholes.(CO5)
5. (a)Discuss how the structure of Reserpine was established? (CO6)

OR

6. (a) Discuss the structure determination of Rotenone.(CO6)
(b)Write stereochemistry of Abietic Acid.(CO6)
7. (a)Explain the structural elucidation of Quinolines by IR, UV, ¹HNMR, ¹³CNMR spectral analysis.(CO7)
(b)Discuss NOESY of Buxaquamarine. (CO8)

OR

8. (a) Explain the spectral analysis of monoterpenes.(CO7)
(b) Briefly explain 2D-INADEQUATE spectrum of α-picoline and β-methyl tetrahydranfuran. (CO8)

SECTION –B**II Answer any five****5 x 4 = 20 M**

8. Outline the synthesis of 1,2,4-oxadiazole.(CO1)
9. Give the importance of Purins and Pteridines.(CO2)
10. Outline the synthesis of Phospholeand Borole.(CO4)
11. Discuss the chemical reactivity of azepine (CO4)
12. How do you determine the position of double bond in Cholesterol?(CO6)
13. Discuss the stereochemistry of Reserpine. (CO6)
14. Explain the UV spectral analysis of Flavanoid taking suitable example. (CO7)
15. Briefly give the Mass spectral and ¹H NMR analysis of Umbelliferone.(CO7)