ACADEMIC REGULATIONS
COURSE STRUCTURE AND
DETAILED SYLLABUS

DEPARTMENT OF CHEMISTRY

For

M.Sc. Chemistry (Drugs & Pharmaceuticals)

(Two Year **Full Time** Programme)

JNTUH COLLEGE OF ENGINEERING HYDERABAD
(Autonomous)
Kukatpally, Hyderabad – 500 085
2022-23

JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY HYDERABAD
COLLEGE OF ENGINEERING HYDERABAD
(AUTONOMOUS)
Kukatpally, Hyderabad – 500 085

ACADEMIC REGULATIONS 2022

Under choice based credit system (CBCS)
M.Sc (Regular/Full Time) Program
(Effective for the students admitted into the I year from the Academic Year 2021-22 and onwards)

1.0 Post-Graduate Degree Program in M.Sc. (PGP in M.Sc.):

JNTUH offers 2 Year (4 Semesters) full-time **Master of Science** (M.Sc.) Degree Programs, under Choice Based Credit System (CBCS) at its Constituent Autonomous College - JNTUH University College of Engineering, Science & Technology Hyderabad (JNTUH UCESTH) with effect from the Academic Year 2022-23 onwards.

2.0 Eligibility for Admission:

2.1 Admissions to the PGPs shall be made subject to the eligibility, qualifications, and specializations prescribed by JNTUH College of Engineering Hyderabad, J NT University Hyderabad, for each Specialization under each M.Sc. The program, from time to time.

2.2 Admission to the PGP shall be made based on the 'common postgraduate entrance test' (CPGET), a state-level entrance test conducted by Telangana state council for higher education or Entrance Test conducted by the Jawaharlal Nehru Technological University Hyderabad or based on any other order of merit approved by the University, subject to reservations as prescribed by the Government from time to time.

2.3 The medium of instructions for all PGP s in M.Sc will be in ENGLISH only.

3.0 M.Sc. Program Structure:

3.1 The M.Sc. Program in Mathematics, Physics, and Chemistry of JNTUH-CEH are of Semester Pattern, with 4 Semesters constituting 2 Academic Years. Each Academic Year having TWO Semesters (First/Odd and Second/Even Semesters). Each Semester shall be of 22 Weeks duration (inclusive of Examinations), with a minimum of 90 Instructional Days per Semester.

3.2 UGC / AICTE specified Definitions/ Descriptions are adopted appropriately for various terms and abbreviations used in these PGPs in M.Sc - Academic Regulations.

3.2.1 **Semester Scheme:**
Each Semester having - 'Continuous Internal Evaluation (CIE)' and 'Semester End Examination (SEE)'. Choice Based Credit System (CBCS) and Credit Based Semester System (CBSS) as denoted are taken as 'references' for the present set of

Regulations. The terms 'SUBJECT' or 'COURSE' imply the same meaning here, and refer to 'Theory Subject', or 'Lab Course', or 'Design/ Drawing Subject', or 'Seminar', or 'Comprehensive Viva', or 'Project', as the case may be.

3.2.2 **Credit Courses:**
All Subjects (or Courses) are to be registered by a student in a Semester to earn Credits. Credits shall be assigned to each Subject/ Course in a Lecture Periods: Tutorial Periods: Practicals Periods: Credits(an L: T: P: C) Structure, based on the following general pattern.

3.2.3 **Course Nomenclature:**
The curriculum nomenclature or Course structure grouping for M.Sc Degree Program is as listed below

Each subject is assigned certain number of credits as specified below.

Theory Subjects	4 Periods / Week	3 Credits
Practical subjects	3 Periods / Week	2 Credits
Seminar	2 Periods / Week	2 Credits
Project		11 Credits

(Each period will be of 50 minutes duration)

4.0 Course Work:

4.1 A Student, after securing admission, shall pursue and complete the M.Sc PGP in a minimum period of 2 Academic Years (4 Semesters), and within a maximum period of 4 Academic Years (starting from the Date of Commencement of I Year).

4.2 Each student shall Register for and Secure the specified number of credits required for the completion of the PGP and Award of the M.Sc Degree in the respective Branch with the chosen Specialization.

4.3 I and II years are structured to provide typically 20 Credits (20 C) in each of the I , II III Semesters, and the IV Semester comprises, totaling 80 Credits (80 C) for the entire M.Sc Program.

5.0 Course Registration:

5.1 A 'Faculty Advisor' shall be assigned to each M.Sc Program with respective Specialization, who will advise the Students about the M.Sc Program Specialization, its Course Structure and Curriculum, Choice/ Option for Subjects/ Courses, based on his competence, progress, pre-requisites, and interest.

6.0 Attendance Requirements:

6.1 A Student shall be eligible to appear for the Semester End Examination (SEE) of any Subject if he acquires a minimum of 75% of attendance in that Subject for that Semester.

6.2 A Student's Seminar Report and Seminar Presentation shall be eligible for evaluation, only if he ensures a minimum of 75% of his attendance in Seminar Presentation Classes during that Semester.

6.3 Condoning of shortage of attendance up to 10% (65% and above, and below 75%) in each Subject or Seminar of a Semester may be granted by the College Academic Council on genuine and valid grounds, based on the Student's representation with supporting evidence.

6.4 A stipulated fee per Subject/Seminar shall be payable towards condoning of shortage of attendance.

6.5 Shortage of Attendance below 65% in any Subject/Seminar shall in NO case be condoned.

6.6 A Student, whose shortage of attendance is not condoned in any Subject(s) or Seminar in any Semester, is considered as 'Detained in that Subject(s)/ Seminar', and is not eligible to take End Examination(s) of such Subject(s) (and in case of Seminars, his/her Seminar Report or Presentation are not eligible for evaluation) in that Semester; and he has to seek Re-registration for those Subject(s)/Seminar in subsequent Semesters, and attend the same as and when offered.

7.0 Academic Requirements:

The following Academic Requirements have to be satisfied, in addition to the Attendance Requirements mentioned in Item No. 6**.**

7.1 A Student shall be deemed to have satisfied the Academic Requirements and earned the Credits allotted to each Subject/ Course, if (i) he/she secures not less than 40% Marks (28 out of 70 Marks) in the Semester end Examination, and (ii) a minimum 50% of the sum of the marks in CIE (Continuous Internal Evaluation) and SEE (Semester End Examination) both taken together; in terms of Letter Grades, this implies securing B Grade or above in that Subject.

7.2 A Student shall be deemed to have satisfied the Academic Requirements and earned the Credits allotted to - Seminar, and Comprehensive Viva-voce, if he/she secures not less than 50% of the total Marks to be awarded for each. The Student would be treated as failed, if he/she - (i) does not attend the Comprehensive Viva-voce as per the schedule given, or (ii) does not present the Seminar as required, or (ii) secures less than 50% of Marks (< 50 Marks) in -Seminar/ Comprehensive Viva-voce evaluations.
She/ he may reappear for comprehensive viva where it is scheduled again; For seminar, he has to reappear in the next subsequent Semesters, as and when scheduled.

7.3 A Student shall - register for all Subjects covering 80 Credits as specified and listed in the Course Structure for the chosen PGP Specialization, put up all the Attendance and Academic requirements for securing 80 Credits obtaining a minimum of B Grade or above in each Subject, and 'earn all 80 Credits securing SGPA $\geq$ 5.0 (in each Semester) and final CGPA (ie., CGPA at the end of PGP) $\geq$ 5.0, to successfully complete the PGP in M.Sc.

7.4 Marks and Letter Grades obtained in all those Subjects covering the above specified 90 Credits alone shall be considered for the calculation of final CGPA, which shall be indicated in the Grade Card of IV semester in II Year r.

7.5 Students who fail to earn 80 Credits as per the specified Course Structure, and as indicated above, within 4 Academic Years from the Date of Commencement of their I Year, shall forfeit their seats in M.Sc Program and their admissions shall stand cancelled.

7.6 When a Student is detained due to shortage of attendance in any Subject(s)/Seminar in any Semester, no Grade Allotment will be done for such Subject(s)/Seminar, and SGPA/ CGPA calculations of that Semester will not include the performance evaluations of such Subject(s)/Seminar in which he/she got detained. However, he becomes eligible for re-registration of such Subject(s)/Seminar (in which he got detained) in the subsequent Semester(s), as and when next offered, with the Academic Regulations of the Batch into which he gets readmitted, by paying the stipulated fees per Subject. In all these re-registration cases, the Student shall have to secure a fresh set of Internal Marks (CIE) and End Semester Examination Marks (SEE) for performance evaluation in such Subject(s), and subsequent SGPA/ CGPA calculations.

7.7 A Student eligible to appear in the End Semester Examination in any Subject, but absent at it or failed (failing to secure B Grade or above), may reappear for that Subject at the supplementary examination as and when conducted. In such cases, his/her Internal Marks (CIE) assessed earlier for that Subject/ Course will be carried over, and added to the marks to be obtained in the supplementary examination, for evaluating his performance in that Subject.

8.0 Evaluation - Distribution and Weightage of Marks:

8.1 The performance of a Student in each Semester shall be evaluated Subject-wise (irrespective of Credits assigned) with a maximum of 100 Marks for Theory, Practical and 100 marks for Seminar.

8.2 a) For Theory Subjects, Continuous Internal Evaluation (CIE) Marks shall comprise of - Mid-Term Examination Marks (for 30 Marks), and Assignment Marks (for 10 Marks) for total of 40 marks.
b) During the Semester, there shall be 2 Mid-Term examinations. Each Mid-Term examination shall be for 30 Marks (with 120 minutes duration). The better performance out of these two Mid-Term Examinations shall be considered for the award of 30 Marks. Based on the performance of the student in submitting the assignments , he/she will be awarded marks evaluated for 10 marks .This is to be done prior to the conduct of each Mid examination.

8.3 For Practical Subjects, there shall be a Continuous Internal Evaluation (CIE) during the Semester for 40 Internal Marks, and 60 Marks are assigned for Lab./Practicals End Semester Examination (SEE). Out of the 40 Marks for Internals, day-to-day work assessment in the laboratory shall be evaluated for 20 Marks; and the performance in an internal Lab./Practical Test shall be evaluated for 20 marks. The SEE for Lab./ Practicals shall be conducted at the end of the Semester by the concerned Lab. Teacher and another faculty member of the same Department as assigned by the Head of the Department.

8.4 There shall be a Seminar Presentation in I Semester II Semester and III Semester. For the Seminar, the Student shall collect the information on a specialized topic, and submit to the Department which shall be evaluated by a Departmental committee consisting of the Head of the Department and two faculty members both appointed by HOD at the time of Seminar Presentation. The Seminar Presentation shall be

evaluated for 100 Marks. There shall be no SEE or External Examination for Seminar.

8.5 a) Every PGP Student shall be required to execute his/her M.Sc Project, under the guidance of the Supervisor assigned to him/her by the Head of Department. The PGP Project shall start immediately after the completion of the II Year I Semester, and shall continue through II Year II Semester. The Student shall carry out the literature survey, select an appropriate topic and submit a Project Proposal within 2 weeks (immediately after his II Year I Semester End Examinations), for approval by the Project Review Committee (PRC). The PRC shall be constituted by the Head of Department, and shall consist of the Head of Department, Project Supervisor, and a Senior Faculty Member of the Department both appointed by HOD. The Student shall submit his/ her Project Work Proposal to the PRC, on whose approval he can 'REGISTER for the PG Project'. Every Student must compulsorily register for his/her M.Sc Project Work, within the 2 weeks of time-frame as specified above. After Registration, the Student shall carry out his work, and continually submit 'a fortnightly progress report' to his/her Supervisor throughout the Project period. The PRC will monitor the progress of the Project Work Presentation and submission of M.Sc Project Work Report/ Dissertation.

b) The PRC shall evaluate the entire performance of the Student and declare the Project Report as 'Satisfactory' or 'Unsatisfactory'.

8.6 a) In cases, where the Board declared the Project Work Performance as 'unsatisfactory', the Student is deemed to have failed in the Project Viva-voce Examination, and he/she has to reappear for the Viva-voce Examination as per the Board recommendations. If he/she fails in the second Viva-voce Examination also, he will not be considered eligible for the Award of the Degree, unless he/she is asked to revise and resubmit his/her Project Work by the Board within a specified time period.

9.0 Re-Admission / Re-Registration:

9.1 **Re-Admission for Discontinued Students:**
Students, who have discontinued the M.Sc Degree Program due to any reasons what so ever, may be considered for 'Readmission' into the same Degree Program (with same specialization) with the Academic Regulations of the Batch into which he/she gets readmitted, with prior permission from the concerned authorities, subject to Item 4.1.

9.2 Re-Registration for Detained Students:
When any Student is detained in a Subject (s)/ Seminar due to shortage of attendance in any Semester, he/she may be permitted to re-register for the same Subject in the 'same category' (Core or Elective Group) or equivalent Subject if the same Subject is not available, as suggested by the Board of Studies of that Department, as when offered in the sub-sequent Semester(s), with the Academic Regulations of the Batch into which he/she seeks re-registration , with prior permission from the concerned authorities, subject to Item 4.1.

10.0 Grading Procedure:

10.1 Marks will be awarded to indicate the performance of each student in each Theory Subject, or Lab/Practicals, or Seminar, or Project, etc., based on the % marks obtained in CIE + SEE (Continuous Internal Evaluation + Semester End Examination, both taken together) as specified in Item 6 above, and a corresponding Letter Grade shall be given.

10.2 As a measure of the student's performance, a 10-point Absolute Grading System using the following Letter Grades (UGC Guidelines) and corresponding percentage of marks shall be followed:

% of Marks Secured (Class Intervals)	*Letter Grade (UGC Guidelines)*	*Grade Points*
90% and above (≥ 90% , ≤ 100%)	O (Outstanding)	10
Below 90% but not less than 80% (≥ 80% , < 90%)	A^+ (Excellent)	9
Below 80% but not less than 70% (≥ 70% , < 80%)	A (Very Good)	8
Below 70% but not less than 60% (≥ 60% , < 70%)	B^+ (Good)	7
Below 60% but not less than 50% (≥ 50% , < 60%)	B (Average)	6
Below 50% but not less than 40% (≥ 40% , < 50%)	C (pass)	5
Below 40 (< 40%)	F (fail	0
Absent	**Ab**	**0**

10.3 A student obtaining F Grade in any Subject shall be considered 'failed' and is be required to reappear as 'Supplementary Candidate' in the Semester End Examination (SEE), as and when offered. In such cases, his/her Internal Marks (CIE Marks) in those Subjects will remain the same as those he obtained earlier.

10.4 A Letter Grade does not imply any specific % of Marks.

10.5 A student earns Grade Point (GP) in each Subject/ Course, on the basis of the Letter Grade obtained by him/her in that Subject/ Course (excluding Mandatory non-credit Courses). Then the corresponding 'Credit Points' (CP) are computed by multiplying the Grade Point with Credits for that particular Subject/ Course.

Credit Points (CP) = Grade Point (GP) x Credits …. For a Course

10.6 The Semester Grade Point Average (SGPA) is calculated by dividing the Sum of Credit Points (ΣCP) secured from ALL Subjects registered in a Semester, by the Total Number of Credits registered during that Semester. SGPA is rounded off to TWO Decimal Places. SGPA is thus computed as

SGPA = { $\sum_{i=1}^{N} C_i\, G_i$ } / { $\sum_{i=1}^{N} C_i$ } …. For each Semester,

where 'i' is the Subject indicator index (takes into account all Subjects in a Semester), 'N' is the no. of Subjects 'REGISTERED' for the Semester (as specifically required and listed under the Course Structure of the parent Department), C_i is the no. of Credits allotted to the i^{th} Subject, and G_i represents the Grade Points (GP) corresponding to the Letter Grade awarded for that i^{th} Subject.

10.7 The Cumulative Grade Point Average (CGPA) is a measure of the overall cumulative performance of a student over all Semesters considered for registration. The CGPA is the ratio of the Total Credit Points secured by a student in ALL registered Courses in ALL Semesters, and the Total Number of Credits registered in ALL the Semesters. CGPA is rounded off to TWO Decimal Places. CGPA is thus computed from the I Year first semester onwards, at the end of each Semester, as per the formula

CGPA = { $\sum_{j=1}^{M} C_j \, G_j$ } / { $\sum_{j=1}^{M} C_j$ } … for all S Semesters registered (ie., upto and inclusive of S Semesters, S ≥ 1),
where 'M' is the TOTAL no. of Subjects (as specifically required and listed under the Course Structure of the parent Department) the Student has 'REGISTERED' from the 1st Semester onwards upto and inclusive of the Semester S (obviously M > N), 'j' is the Subject indicator index (takes into account all Subjects from 1 to S Semesters), C_j is the no. of Credits allotted to the j^{th} Subject, and G_j represents the Grade Points (GP) corresponding to the Letter Grade awarded for that j^{th} Subject. After registration and completion of I Year I Semester however, the SGPA of that Semester itself may be taken as the CGPA, as there are no cumulative effects.

10.8 For Merit Ranking or Comparison Purposes or any other listing, ONLY the 'ROUNDED OFF' values of the CGPAs will be used.

10.9 For Calculations listed in Item 10.5 – 10.8, performance in failed Subjects/ Courses (securing F Grade) will also be taken into account, and the Credits of such Subjects/ Courses will also be included in the multiplications and summations. However, Mandatory Courses will not be taken into consideration.

10.10 **Passing Standards :**

10.10.1 A student shall be declared successful or 'passed' in a Semester, only when he/she gets a SGPA ≥ 5.00 (at the end of that particular Semester); and a student shall be declared successful or 'passed' in the entire PGP, only when gets a CGPA ≥ 5.00; subject to the condition that he/ she secures a GP ≥ 6 (B Grade or above) in every registered Subject/ Course in each Semester (during the entire PGP) for the Degree Award, as required.

10.10.2 After the completion of each Semester, a Grade Card or Grade Sheet (or Transcript) shall be issued to all the Registered Students of that Semester, indicating the Letter Grades and Credits earned. It will show the details of the Courses Registered (Course Code, Title, No. of Credits, Grade Earned etc.), Credits earned, SGPA, and CGPA.

11.0 Declaration of Results:

11.1 Computation of SGPA and CGPA are done using the procedure listed in 10.5 – 10.8.

11.2 For Final % of Marks equivalent to the computed CGPA, the following formula may be used ..

% of Marks = (CGPA – 0.5) x 10

12.0 Award of Degree and Class:

12.1 A Student who registers for all the specified Subjects/ Courses as listed in the Course Structure, satisfies all the Course Requirements, and passes the examinations prescribed in the entire PG Programme (PGP), and secures the required number of

90 Credits (with GP ≥ 6.0), shall be declared to have 'QUALIFIED' for the award of the M.Sc Degree in the chosen specialization as he/ she admitted.

12.2 **Award of Class**

After a student has satisfied the requirements prescribed for the completion of the program and is eligible for the award of M. Tech. Degree, he/she shall be placed in one of the following four classes based on the % CGPA:

Class Awarded	CGPA
First Class with Distinction	≥ 7.75
First Class	6.75 ≤ CGPA < 7.75
Second Class	5.75 ≤ CGPA < 6.75
Pass Class	5.0 ≤ CGPA < 5.75

12.3 A student with final CGPA (at the end of the PGP) < 5.00 will not be eligible for the Award of Degree.

13.0 Withholding of Results:

13.1 If a Student has not paid fees to University/ College at any stage, or has pending dues against his name due to any reason whatsoever, or if any case of indiscipline is pending against him/her, the result of the Student may be withheld, and he/she will not be allowed to go into the next higher Semester. The Award or issue of the Degree may also be withheld in such cases.

14.0 Transitory Regulations:

14.1 A Student - who has discontinued for any reason, or who has been detained for want of attendance as specified, or who has failed after having undergone PGP, may be considered eligible for readmission to the same PGP with same set of Subjects/ Courses (or equivalent Subjects/ Courses as the case may be), and same Professional Electives (or from same set/category of Electives or equivalents as suggested), as and when they are offered (within the time-frame of 4 years from the Date of Commencement of his/her I Year I Semester).

15.0 Student Transfers:

15.1 There shall be no Branch/ Specialization transfers after the completion of Admission Process.

15.2 There shall be no transfer among the Constituent Colleges and Units of Jawaharlal Nehru Technological University Hyderabad.

16. MALPRACTICES RULES:

	Nature of Malpractices	**Punishment**
	If the candidate:	
1 (a)	Possesses or keeps accessible in examination hall, any paper, note book, programmable calculators, Cell phones, pager, palm	Expulsion from the examination hall and cancellation of the performance in that subject only.

	computers or any other form of material concerned with or related to the subject of the examination (theory or practical) in which he/ she is appearing but has not made use of (material shall include any marks on the body of the candidate which can be used as an aid in the subject of the examination)	
1 (b)	Gives assistance or guidance or receives it from any other candidate orally or by any other body language methods or communicates through cell phones with any candidate or persons in or outside the exam hall in respect of any matter.	Expulsion from the examination hall and cancellation of the performance in that subject only of all the candidates involved. In case of an outsider, he will be handed over to the police and a case is registered against him.
2	Has copied in the examination hall from any paper, book, programmable calculators, palm computers or any other form of material relevant to the subject of the examination (theory or practical) in which the candidate is appearing.	Expulsion from the examination hall and cancellation of the performance in that subject and all other subjects the candidate has already appeared including practical examinations and project work and shall not be permitted to appear for the remaining examinations of the subjects of that Semester/year. The Hall Ticket of the candidate is to be cancelled.
3	Impersonates any other candidate in connection with the examination.	The candidate who has impersonated shall be expelled from examination hall. The candidate is also debarred and forfeits the seat. The performance of the original candidate who has been impersonated, shall be cancelled in all the subjects of the examination (including practicals and project work) already appeared and shall not be allowed to appear for examinations of the remaining subjects of that semester/year. The candidate is also debarred for two consecutive semesters from class work and all examinations. The continuation of the course by the candidate is subject to the academic regulations in connection with forfeiture of seat. If the imposter is an outsider, he/she will be handed over to the police and a case is registered against him/her.
4	Smuggles in the Answer book or additional sheet or takes out or arranges to send out the question paper during the examination or answer book or additional sheet, during or after the examination.	Expulsion from the examination hall and cancellation of performance in that subject and all the other subjects the candidate has already appeared including practical examinations and project work and shall not be permitted for the remaining examinations of the subjects of that

		semester/year. The candidate is also debarred for two consecutive semesters from class work and all examinations. The continuation of the course by the candidate is subject to the academic regulations in connection with forfeiture of seat.
5	Uses objectionable, abusive or offensive language in the answer paper or in letters to the examiners or writes to the examiner requesting him to award pass marks.	Cancellation of the performance in that subject.
6	Refuses to obey the orders of the Chief Superintendent / Assistant – Superintendent / any officer on duty or misbehaves or creates disturbance of any kind in and around the examination hall or organizes a walk out or instigates others to walk out, or threatens the officer-in charge or any person on duty in or outside the examination hall of any injury to his/her person or to any of his/her relations whether by words, either spoken or written or by signs or by visible representation, assaults the officer-in-charge, or any person on duty in or outside the examination hall or any of his/her relations, or indulges in any other act of misconduct or mischief which result in damage to or destruction of property in the examination hall or any part of the College campus or engages in any other act which in the opinion of the officer on duty amounts to use of unfair means or misconduct or has the tendency to disrupt the orderly conduct of the examination.	In case of students of the college, they shall be expelled from examination halls and cancellation of their performance in that subject and all other subjects the candidate(s) has (have) already appeared and shall not be permitted to appear for the remaining examinations of the subjects of that semester/year. The candidates also are debarred and forfeit their seats. In case of outsiders, they will be handed over to the police and a police case is registered against them.
7	Leaves the exam hall taking away answer script or intentionally tears of the script or any part thereof inside or outside the examination hall.	Expulsion from the examination hall and cancellation of performance in that subject and all the other subjects the candidate has already appeared including practical examinations and project work and shall not be permitted for the remaining examinations of the subjects of that semester/year. The candidate is also debarred for two consecutive semesters from class work and all examinations. The continuation of the course by the candidate is subject to the academic regulations in connection with forfeiture of seat.
8	Possess any lethal weapon or	Expulsion from the examination hall and

	firearm in the examination hall.	cancellation of the performance in that subject and all other subjects the candidate has already appeared including practical examinations and project work and shall not be permitted for the remaining examinations of the subjects of that semester/year. The candidate is also debarred and forfeits the seat.
9	If student of the college, who is not a candidate for the particular examination or any person not connected with the college indulges in any malpractice or improper conduct mentioned in clause 6 to 8.	Student of the colleges expulsion from the examination hall and cancellation of the performance in that subject and all other subjects the candidate has already appeared including practical examinations and project work and shall not be permitted for the remaining examinations of the subjects of that semester/year. The candidate is also debarred and forfeits the seat. Person(s) who do not belong to the College will be handed over to police and, a 8police case will be registered against them.
10	Comes in a drunken condition to the examination hall.	Expulsion from the examination hall and cancellation of the performance in that subject and all other subjects the candidate has already appeared including practical examinations and project work and shall not be permitted for the remaining examinations of the subjects of that semester/year.
11	Copying detected on the basis of internal evidence, such as, during valuation or during special scrutiny.	Cancellation of the performance in that subject and all other subjects the candidate has appeared including practical examinations and project work of that semester / year examinations.
12	If any malpractice is detected which is not covered in the above clauses 1 to 11 shall be reported to the College / University for further action to award suitable punishment.	

17. GENERAL:

- **Credit**: A unit by which the course work is measured. It determines the number of hours of instructions required per week. One credit is equivalent to one hour of teaching (lecture or tutorial) or two hours of practical work/field work per week.
- **Credit Point:** It is the product of grade point and number of credits for a course.
- The Academic Regulations should be read as a whole for the purpose of any interpretation.
- The University/College reserves the right of altering the Academic Regulations and/or Syllabus/Course Structure, as and when necessary. The modifications or amendments may be applicable to all the candidates on rolls, as specified by the University/College.

- Wherever the words ‘he’ or ‘him’ or ‘his’ occur in the above regulations, they will also include ‘she’ or ‘her’ or ‘hers’.
- Wherever the word ‘Subject’ occurs in the above regulations, it implies the ‘Theory Subject’, ‘Practical Subject’ or ‘Lab.’ and ‘Seminar’.
- In case of any ambiguity or doubt in the interpretations of the above regulations, the decision of the Vice-Chancellor will be final.

JNTUH UNIVERSITY COLLEGE OF ENGINEERING, SCIENCE AND TECHNOLOGY, HYDERABAD

M.Sc. Chemistry (Drugs & Pharmaceuticals) (Full Time) w.e.f 2022-23

First Semester

S.No.	Code	Subject	L	P	Credits
1	DPS 22 101	Physical Chemistry	3	0	3
2	DPS 22102	Inorganic Chemistry	3	0	3
3	DPS 22 103	Organic Chemistry – I	3	0	3
4	DPS 22 104(E1)	Applied Chemistry	3	0	3
	DPS 22 104(E2)	Chemistry of Energy Materials			
	DPS 22 104(E3)	Principles of Medicinal Chemistry			
5	DPS 22 L11	Physical & Inorganic Chemistry Lab	0	6	3
6	DPS 22 L12	Organic Chemistry Lab-I	0	6	3
7	DPS 22 S11	Seminar	-	-	2
		Total Credits			**20**

Second Semester

S.No.	Code	Subject	L	P	Credits
1	DPS 22 201	Reagents and Formation of C-C &C=C Bonds	3	0	3
2	DPS 22 202	Organic Chemistry – II	3	0	3
3	DPS 22 203	Organic Spectroscopy	3	0	3
4	DPS 22 204(E1)	Analytical Techniques & Instrumentation Methods	3	0	3
	DPS 22 204(E2)	Bioorganic Chemistry			
	DPS 22 204(E3)	Chemistry of Polymers			
5	DPS 22 L21	Organic Chemistry Lab -II	0	6	3
6	DPS 22 L22	Applied Chemistry Lab	0	6	3
7	DPS 22 O21	MOOCS/NPTEL Online Course/Seminar	-	-	2
		Total Credits			**20**

Third Semester

S.No.	Code	Subject	L	P	Credits
1	DPS 22 301	Asymmetric Synthesis & Synthetic Strategies	3	0	3
2	DPS 22 302	Pericyclic Reactions & Photochemistry	3	0	3
3	DPS 22 303	Regulatory Guidelines in Pharmaceutical Manufacturing	3	0	3
4	DPS 22 304 (E1)	Chemistry of Natural Products	3	0	3
	DPS 22 304 (E2)	Chemistry of Synthetic Drugs & Pharmaceutical Formulations			
	DPS 22 304 (E3)	Chemistry of Antibiotics & Antivirals			
5	DPS 22 L31	Spectroscopy Lab	0	6	3
6	DPS 22 L32	Multi-Step Syntheses Lab	0	6	3
7	DPS 22 P31	Mini Project	-	-	2
		Total Credits			**20**

Fourth Semester

S.No.	Code	Subject	L	P	Credits
1	DPS 22 401	Drug Design & Advanced Medicinal Chemistry	3	0	3
2	DPS 22 402	Molecular Modeling & Computer Aided Drug Design	3	0	3
3	DPS 22 L41	Computational Chemistry Lab	0	6	3
4	DPS 22 P41	Project	-	-	11
		Total Credits			**20**

PHYSICAL CHEMISTRY

Code: DPS 22 201	L	P	C
	3	0	3

Course objectives:

1. To understand the concepts of thermodynamics, entropy and their applications.
2. To impart knowledge and importance of laws of photochemistry and Nernst distribution law.
3. To acquire knowledge on quantum chemical description of chemical bonding.
4. To study the various factors which affect the rate of a chemical reaction such as concentration, temperature, solvent, catalyst etc. and theories of chemical kinetics.
5. To impart the knowledge on Homogeneous and Heterogeneous catalysis, Michaelis Menten mechanism and adsorption theories.

Course Outcomes: The students will acquire knowledge of

1. Laws of thermodynamics, Gibbs-Duhem and Gibbs -Helmholtz equations.
2. Laws of photochemistry and its applications, Fluorescence, Phosphorescence
3. Schrodinger equation for a particle in a box and quantum chemical description.
4. Chemical kinetics, study of fast reactions and effect of structure on reactivity- Linear free energy relationship.
5. Characteristics and theories of catalysis and adsorption.

Unit-1: Thermodynamics

Introduction, Concepts involved in first, second and third law of thermodynamic, Thermodynamic equation of state, Concept of entropy, entropy change in reversible and irreversible processes. Entropy changes in an ideal gas. Entropy change with temperature, pressure and volume. Entropy change in phase transformation. Maxwell relations, Free energy and entropy of mixing, Partial molar quantities, Gibbs-Duhem equation. Helmholtz and Gibbs free energies (A and G). Criteria for reversible and irreversible processes in terms of A &G. Physical significance of A & G. Gibbs -Helmholtz equation.

Unit-2: Photochemistry & Distribution law

Photochemistry: Laws of Photochemistry- Lambert-Beer's law, Grotthus – Draper law, Stark-Einstein's law of photochemical equivalence. Quantum Yield – Quantum yield determination, photochemical reactions-high and low quantum yield reactions, Joblonski diagram – Fluorescence, Phosphorescence, Internal conversion, inter system crossing, delayed fluorescence. Chemiluminescence.

Distribution law: Nernst distribution law - Deviation of distribution law due to molecular complexity (Hit & Trial method & logarithmic method) - Applications of distribution law.

Unit-3: Quantum Mechanics

Introduction, Black body radiation – Planck's concept of quantization – Planck's equation, average energy of an oscillator (derivation not required). Wave particle duality and Uncertainity principle. Postulates of quantum mechanics. Schrodinger wave equation for hydrogen atom. Physical significance of wave function, Eigen functions, Eigen values and quantum mechanical operators. Normalisation, Orthogonality and degeneracy. Particle in a box – one dimensional and three dimensional.

Unit-4: Chemical Kinetics

Chemical Kinetics: Introduction, Rate, order and molecularity, factors influencing rate of reaction, Kinetic equations of zero, first, second, third and nth order reactions, Theories of

reaction rates: Collision theory, steric factor. Transition state theory, Activated complex. Activation parameters and their significance. Unimolecular reactions and Lindamann's theory. Complex reactions- Opposing reactions, parallel reactions and consecutive reactions (all first order type). Chain reactions-general characteristics, steady state treatment. Example- H_2-Br_2, H_2-O_2.

Unit-5: Catalysis & Surface chemistry

Characteristics of catalysis, types of catalysis: Homogeneous and Heterogeneous catalysis, Acid-base catalysis, Catalytic coefficient, Acidity functions. Enzyme catalysis: Characteristics of enzyme catalysis, factors affecting the rate of an enzyme reaction - Michaelis Menten mechanism.

Surface Chemistry: Concept of adsorption, factors influencing adsorption. Adsorption isotherms – Freundlich, Langmuir, B.E.T theory of adsorption equation. Determination of surface area using B.E.T. method. Adsorption of gases on solids – Physisorption and chemisorption, Adsorption from solutions: Positive adsorption, negative adsorption, electrostatic adsorption, Gibbs adsorption. Applications of adsorption.

Recommended Books:

1. "*Advanced Physical Chemistry*", Gurudeep Raj; Goel Publishing House, Meerut **(**24th Edition, 1999).
2. "*Physical Chemistry*", Samuel Glasstone and D. Lewis; Mc Millan India Ltd., New Delhi **(**2nd Edition, 1984).
3. "*Physical Chemistry*", Peter Atkins and J.D.Paula; ELBS, Low Price Edition (7th Edition, 2002).
4. "*Chemical Kinetics*", K.J.Laidler; Tata Mc Graw- Hill Publishing Company Ltd, New Delhi (2nd Edition, 1984).
5. "*Principles of Physical Chemistry*", Maron and Prutton; Oxford and IBH Publishing Co Pvt Ltd., New Delhi and Calcutta (4th Edition, 1966).
6. "*Catalysis- Principles and Applications*", B.Vishwanathan, S.Sivasanker; Narosa Publications, New Delhi (2002).
7. "*Essentials of Physical Chemistry*", Bahl, Tuli and Arun bahl; S. Chand and Company Ltd. New Delhi **(**Revised Edition, 2009).
8. "*Physical Chemistry*", Gordon M Barrow, Tata Mc Graw- Hill Publishing Company Ltd, New Delhi (5th Edition, 2008).
9. "*Physical Chemistry*", Thomas Engel & Philip Reid, Pearson Education.
10. "*Physical Chemistry*", David W. Ball, Thomson Brooks/Cole, (1st Edition, 2007)

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INORGANIC CHEMISTRY

Code: DPS 22 102

L	P	C
3	0	3

Course objectives:

1. To understand the concepts of Bonding in metal complexes, crystal field splitting and Magnetic properties of transition metal complexes.
2. To impart knowledge of Formation and Stability of Metal Complexes in Solution.
3. To acquire knowledge on Reaction mechanisms of Metal complexes and types of substitution reactions.
4. To study the free ion Configurations, Terms and States including Inter –electron repulsion Parameters and Spin –Orbital coupling parameters.
5. To impart the knowledge on Symmetry of molecules, Symmetry Operations - Symmetry Elements and Molecular Point Groups.

Course Outcomes: The students will acquire knowledge of

1. Bonding in metal complexes, crystal field splitting and Magnetic properties of transition metal complexes
2. Formation and Stability of Metal Complexes in Solution
3. Reaction mechanisms of Metal complexes and types of substitution reactions
4. Free ion Configurations, Terms and States including Inter –electron repulsion Parameters and Spin –Orbital coupling parameters.
5. Symmetry of molecules, Symmetry Operations- Symmetry Elements and Molecular Point Groups.

Unit-1: Bonding in metal complexes

Crystal field theory(CFT)-Salient features – Splitting of d-orbitals in Linear, Trigonal planar, Trigonal bipyrimidal, Square planar, Tetrahedral, Octahedral and Tetragonally distorted octahedral geometries - Jahn-Tellar theorem. Factors influencing the magnitude of crystal field splitting in octahedral complexes – Nature of metal ions, nature of ligands – Spectrochemical series and geometry. Calculation of Crystal field stabilization energies (CFSE) in four and six coordinated complexes. Uses of CFSE values in stabilization of Oxidation states, geometry of complexes and heats of hydration of Transition metal ions. Magnetic properties of transition metal (octahedral) complexes - Calculation of magnetic moments using Spin-only formula.

Unit-2: Formation and Stability of Metal Complexes in Solution

Thermodynamic stability, Kinetic Stability – Binary metal complexes**:** Step-wise and overall formation or stability constants and their interrelationship. Ternary complexes: Step wise and simultaneous equilibria; Factors influencing the stability of complexes – Ligand effects: Basicity, chelate effect and steric factors. Metal ion effects: Ionic potential, Crystal field effects and natural order and effective nuclear charge. Determination of stability constants of metal complexes by P^H-metric and Spectrophotometric methods (Principle only).

Unit-3: Reaction mechanisms of Metal complexes

Energy profile of a reaction – Transition state or Activated complex – Types of substitution reactions – S_E & S_N. Ligand substitution reactions in octahedral complexes: Aquation or acid hydrolysis reactions – Factors affecting acid hydrolysis, Base hydrolysis: Conjugate base

mechanism, Evidences in favour of S_N^ICB mechanism. Substitution reactions without breaking metal-ligand bond. Ligand substitution reactions in square planar complexes: mechanism –trans effect, polarization and pi-bonding theories, Applications of trans effect in the synthesis of Pt(II) complexes.Redox or electron transfer reactions: inner sphere and outer sphere mechanisms.

Unit-4: Free ion Configurations, Terms and States

Free ion terms and Energy levels: Configurations, Terms, States and Microstates- Formula for the calculation of microstates p^n and d^n configurations; L-S (Russel-Saunders) coupling scheme, J-J coupling scheme –Determination of terms for various p^n and d^n configurations of metal ions. Hole formalism –Energy Ordering of terms (Hund's rule) Inter –electron repulsion Parameters (Racah parameters) - Spin –Orbital coupling parameters. Effect of weak cubic crystal fields on S, P, D and F terms – Orgel diagrams for d^1 &d^2 configurations.

Unit-5: Symmetry of molecules

Concept of Symmetry in Chemistry- Symmetry Operations - Symmetry Elements: Rotational Axis of Symmetry and types of Rotational Axis. Plane of Symmetry and types of planes. Improper Rotational Axis of Symmetry, Inversion center and Identity element. Molecular Point Groups**:** Definition, Properties and Notation of Point Groups, Classification of Molecules into C_1,C_s,C_i C_n, C_{nv}, C_{nh} , $C_{\alpha v}$ and other point groups – Exercises in Molecular Point Groups –Symmetry criteria for Optical activity.

References:

1. Symmetry and Group theory in Chemistry, Mark Ladd, Marwood Publishers, London (2000).
2. Molecular Symmetry and Group Theory, Robert L.Carter, John Wiley & Son (1998).
3. Symmetry and Spectroscopy of Molecules. K.Veera Reddy, New Age International (P) Limited (1999).
4. Advanced Inorganic Chemistry. F.A.Cotton, G.Wilkinson, C.A.Murillo and M.Bochmann, 6th Edition, Wiley Interscience, N.Y (1999
5. Inorganic Chemistry, J.E. Huheey, K.A.Keiter and R.L.Keiter 4 th Edition Harper Cottens College Publications (1993).
6. Inorganic Chemistry, Keith F.Purcell and John C.Kotz, Holt-Saunders International Editions, London (1977).
7. Selected topics in Inorganic chemistry", W.U.Malik, G.D.Tuli &Madan, S.Chand &Co., Delhi (2002).
8. Mechanism of Inorganic reactions", M.L.Tobe and J.Burgess, Addison Wesley Longmann,(1999).
9. Metal ions in Reaction Mechanisms", K.Veera Reddy, Galgotia Publications (P) Ltd.
10. Introduction to Ligand fields, B N Figgis, Wiley Eastern Ltd, New Delhi.

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ORGANIC CHEMISTRY-I

Code: DPS 22 103

L	P	C
3	0	3

Objectives:

1. To bring adaptability to the concepts of chemistry and to acquire the required skills.
2. To impart the knowledge of stereochemistry and synthetic aspects useful for understanding reaction pathways.
3. Acquire the knowledge about chirality, elements of symmetry and optical isomerism along with the concept of aromaticity and Huckel 's ($4n+2\pi$ rule).
4. Introduction to types of organic reactions and reactive intermediates, thermodynamic and kinetic studies of reaction mechanism.
5. Thermodynamic and kinetic studies of reaction mechanism.

Outcomes:

1. The student learns the basic principles and concepts of stereochemistry and reaction mechanism from this course.
2. Student gets comprehensive knowledge of aromaticity of benzenoid and non-benzenoid aromatic compounds
3. Reaction intermediates and addition to carbon, carbon multiple bonds.
4. The concepts of pathways to study the reaction mechanism are learnt.
5. The student learns the clear concepts of thermodynamics and kinetics of reaction mechanism.

Unit-1: Stereochemistry (Optical Isomerism, Geometrical & Conformational Isomerism):

Introduction, significance and classification of isomers into structural and stereo isomers Molecular representations: Wedge, Fischer, Newman and Saw-horse formulae, their description and interconversions. Optical Isomerism – Elements of Symmetry & Chirality: Symmetry operations (Cn & Sn). Relative and Absolute configurations- Resolution of Racemic mixtures; stereospecific, stereoselective, regiospecific and regeoselective reactions - Cram's rule - Optical Isomerism of Nitrogen compounds - Concept of dynamic enantiomerism; Cis-Trans isomerism; E-Z configuration - Interconversion of geometrical isomers and determination of their configuration; Geometrical isomerism of nitrogen compounds - Conformational Isomerism of acyclic systems like ethane and n-butane and cyclic systems like cyclohexane-mono and di substituted cyclohexanes. Introduction to stereochemistry of biphenyl, allenes, spiro compounds.

Unit-2: Aromaticity-I (Benzenoid & Non-Benzenoid Aromatic hydrocarbons):

Aromaticity - Huckel's ($4n+2\pi$ electron rule) and its limitations - Classification of cyclic conjugated hydrocarbons as alternant and non- alternant, Benzenoidal hydrocarbons-Aromatic properties and general methods of synthesis of Naphthalene, Phenanthrene and Anthracene. Homo-aromatic and Anti-aromatic systems. General methods of synthesis and properties of Non-Benzenoid aromatic compounds - Cyclopropenium salts, Cyclopentadienyl salts, Cycloheptatrienyl cation, Tropinone, Ferrocene and Azulenes.

Unit-3: Reactive Intermediates:

Introduction to Classical and Non-Classical cabocations; Generation, Structure, Stability, detection and Reactivity of Carbonium ions and Carbanions; carbenes, free radicals, nitrenes and arynes; Synthesis of Acetoacetic ester & Malonic esters.

Unit-4: Study of Organic Reaction Mechanisms:
Introduction, significance and general methods of study of mechanisms of Organic Reactions, Kinetic and non-kinetic methods; Use of isotopes; Cross-over experiments; Intermediate trapping; evidence based on stereochemistry.

Unit-5: Physical Organic Chemistry:
Thermodynamics and Kinetics - Acids and Bases; HSAB principle; Kinetic versus Thermodynamic control, Hammett equation; Linear free energy relationships, Hammond's postulates.

Recommended Books:

1. "*Stereochemistry of Carbon Compounds*" by Ernest L.Eliel, Tata-Mc Graw Hill Co., New Delhi (1975). Indian Education in 2003.
2. "*Stereochemistry - Conformation and Mechanism*", by P.S. Kalsi, Wiley Eastern Ltd., New Delhi, Hyd. (1991).
3. "*Advanced Organic Chemistry*", by Jerry March, John Wiley & Sons, New York, London. (2001).
4. "*Organic Chemistry*", by R.T.Morison and R.N.Boyd, Allyn & Bacon Inc., (printed in Singapore) (2001).
5. "*Organic Chemistry*", Vol.I, by S.M.Mukherji, S.P. Singh and H.P. Kapoor, Wiley Eastern Ltd., New Delhi, Hyderabad. (1985).
6. "*Organic Reaction Mechanisms*", by Raj K. Bansal, Tata-Mc Graw Hill Co., New Delhi (1998).
7. *Guide-book to Mechanism in Organic Chemistry*", by Peter Sykes Orient Longmans Ltd., New Delhi (1976).13)
8. "*Advanced Organic Chemistry*" by Arun Bhal & B.S. Bhal, S. Chan Company Pvt. Ltd. New Delhi.
9. "*Organic Chemistry*" by Janice G. Smith, Tata McGraw Hill Company Ltd., 2nd Edition, 2008.
10. "*Organic Chemistry*" by Stanley H Pine, Tata McGraw Hill Company Ltd., 5th Edition, 2008.
11. "*Introduction to Organic Chemistry*" by Jhon Mc Murry, Cengage Pvt. Ltd. New Delhi, 2008.

APPLIED CHEMSTRY (Elective –1)

Code: DPS 22 104 (E1)	L	P	C
	3	0	3

OBJECTIVES:

1. To bring adaptability to the concepts of water technology which is essential for desing and maintan the instruments.
2. To acquire the knowledge of electrochemistry and corrosion which are essential for the Engineers in industry.
3. To gain the knowledge on existing and future upcoming polymers used in device fabrication.
4. To acquire the skills pertaining to energy sources and batteries which are highly helpful in designing.
5. To impart basic knowledge on materials and their properties and applications for material analysis.

OUTCOMES: The basic concepts included in this course will help the student to gain:

1. Differentiate hard and soft water, solve the related problems on water purification and its significance in industry and daily life.
2. Understand the principles, concepts of electrochemistry and causes of corrosion, its consequences and methods to minimize corrosion to improve industrial designs.
3. The knowledge of theories of polymerisation, conducting and biodegradable polymers.
4. The knowledge of the properties, separation techniques of natural gas, coal and crude oil along with potential applications and role of petrochemicals in national economy.
5. The knowledge of engineering materials such as Portland Cement, white cement, concrete and lubricants etc.

Unit-1: Water and its treatment:

Introduction – hardness of water – Causes of hardness. Types of hardness: temporary and permanent. Expression and units of hardness. Estimation of hardness of water by complexometric method. Potable water and its specifications. Steps involved in treatment of water – Disinfection of water by chlorination and ozonization. Boiler troubles - Scale, Sludge, Priming, Foaming and Caustic embrittlement. Treatment of boiler feed water by Calgon conditioning, Phosphate conditioning and Colloidal conditioning. External treatment of water- Ion exchange process. Desalination of water – Reverse osmosis. Numerical problems.

Unit-2: Electrochemistry and corrosion:

Electrochemistry: Electrochemical cells – Cell, Electrode, electrode potential, standard electrode potential, Nernst equation-derivation and significance-Electrochemical series and its applications. Construction and functioning of Calomel, Quinhydrone and glass electrode. Determination of pH of a solution by using quinhydrone and glass electrode. Numerical problems. Potentiometric titrations. Batteries – Primary (Lithium cell) and secondary batteries (Lead – acid storage battery and Lithium ion battery).

Corrosion: Causes and effects of corrosion – Theories of chemical and electrochemical corrosion – mechanism of electrochemical corrosion. Galvanic corrosion, Concentration cell corrosion- water-line and pitting corrosion. Factors affecting rate of corrosion, Corrosion control methods- Cathodic protection – Sacrificial anodic protection and impressed current cathodic methods. Surface coatings – metallic coatings –Methods of coating- Hot dipping, cementation, electroplating electroless plating.

Unit – 3: Polymeric materials:

Polymers: Definition, Monomer, functionality and degree of polymerisation. Classification – Types of Polymerisation -Addition & Condensation – Mechanisms of free radical addition Polymerisation. Plastics: Definition, characristics- Compounding and fabrication- Methods of Moulding- Thermoplastics and Thermosets – Preparation, properties and applications– PVC, Teflon and Bakelite. Fibres: Definition, Characteristics. Preparation, Properties and applications of Terylene, Nylon 6:6. Elastomers: Definition and characteristics. Natural rubber-structure, processing of latex, Vulcanisation. Preparation, properties and applications of BuNa-S and Butyl rubber.Conducting Polymers- Definition, Classification. Mechanism of conduction in Polyacetylene and polyaniline.Biodegradable polymers- Concept, Applicaions and advantages of biodegradable polymers.

Unit – 4: Energy sources:

Fuels: Definition, classification with examples. Calorific value. Characteristics of good fuel. Coal: Types- Analysis of coal- proximate analysis. Petroleum- Refining-Fractional distillation- composition, properties and uses of petrol, diesel and kerosene. Cracking-types, Moving bed catalytic cracking. Knocking- Octane and Cetane rating, Composition, characteristics and uses of LPG, CNG. Biodiesel-Transesterification. Advantages. Hydrogen fuel- Production, storage, advantages and limitations. Combustion- Definition, Calculation of air required for the combustion of fuel.

Unit-5: Engineering Materials:

Portland cement: Composition and constituents. Setting and hardening of cement, special cements- properties and uses of High alumina cement, White cement and water proof cement. RCC, Decay of Concrete. Refractories: Classification, Properties-Refractoriness, RUL, Chemical inertness and porocity. Characteristics of a good refractory. Engineering Applications. Failure of a refractory. Lubricants: Classification- Mechanism of Lubrication, Properties- Viscosity, Acid value, Flash & Fire point, Cloud & Pour pint.

Text Book:

1. Engineering Chemistry – PC Jain and M Jain – Dhanpath Rai and Sons, New Delhi.

Reference Books:

1. Text book of Engineering Chemistry by Ramadevi, VenktaRamana Reddy & Prshanth Rath, Cengage learning publications.
2. A text book of Engineering Chemistry by Thirumala Chary, Laxminarayana, Shashikala. Pearson Publications.

CHEMISTRY OF ENERGY MATERIALS (Elective – 2)

Code: DPS 22 104 (E2)	L	P	C
	3	0	3

Course Objectives:

1. To understand the fundamentals and basics of material science.
2. A foundation for understanding the structure, synthesis and chemistry of materials.
3. To provide an understanding of organic semiconductors.
4. To study the basics of photovoltaics and nanomaterials and their application in energy systems and devices.
5. To introduce concepts such as nanomaterias, its types and their functions and applications in energy storage.

Course outcomes: The basic concepts included in this course will help the student to gain:

1. The knowledge of the basics and properties of materials.
2. Understand how to design and develop materials and processes that reduce the use and generation of hazardous substances in industry.
3. The knowledge of organic semiconductors and photovoltaics
4. The synthesis, structure, design and reactivity of materials.
5. The concepts of nanomaterials and their preparative approaches.

Unit-1: Elements of Materials Science

Types of crystal systems, Bravais lattices, atomic packing factor, planner atomic density, Miller indices, crystal defects, solid solutions, dispersion in solids, stress and strain diagram of brittle and ductile materials, Plastic Deformation strain hardening in single crystals and polycrystalline materials, Slip of Planes perfect lattices, force on dislocation line

Unit-2: Properties of Materials

Electronic and Electric Properties: free electron theory, fermi energy density of states, elements of band theory, dielectric, piezoelectric, pyroelectric and ferroelectric effect. Magnetic properties: origin of magnetism, para-, dia-, ferro and ferri-magnetisms. Thermal Properties: specific heat, thermal conductivity and thermal expansion, thermoelectricity. Optical and optoelectronic properties. Superconductivity.

Unit-3: Organic Semiconductors

Electronic Configuration and Concept of Atomic Orbital, Hybridization and Overlapping of orbitals, Molecular Orbital, LCAO theory, Bonding and Antibonding orbitals, Sigma Bonding and pi-bonding, Material Origin of bandgap in organic semiconductors, Charge transport in organic semiconductors, Types of organic semiconductors, Optical and Electrical Properties of Organic Semiconductors Organic Semiconductor Devices: Principal and Concepts Processing of Organic Semiconducting Materials and Devices.

Unit-4: Photovoltaics

Solar energy and energy conversion, Fundamentals of semiconductor physics and photovoltaic cells, Generation-recombination in semiconductors, p-n junction, metalsemiconductor and hetero junction, Photovoltaic device fabrication and characterization, Current status of silicon based solar cells, Advancement in photovoltaic research and design of new generation solar cells (hybrid, quantum dot, dye-sensitized and perovskite solar cells)

Unit-5: Materials for energy storage

Synthesis of nanomaterials, top-down and bottom-up approaches, mechanical milling, solgel method, chemical vapour deposition (CVD), Carbon Nano-Tubes (CNT), Carbon Nano-Fibres (CNF), graphene, preparation of graphene. Fabrication of CNTs and CNFs, CNTs and CNFs for hydrogen storage.

TEXT BOOKS:

1. Anke Krueger, "Carbon Materials and Nanotechnology", Wiley-VCH , 2010.
2. Yury Gogotsi, "Carbon Nanomaterials", Taylor and Francis, 2006.

References:

1. Introduction to Solid State Physics, 8th Ed., C. Kittel, J. Wiley & Sons

2. Physics of Functional Materials, Hasse Fredriksson and Ulla Åkerlind, J. Wiley & Sons

3. Textbook of polymer science, Fred W Billmeyer, J. Wiley & Sons

4. Materials Chemistry, Fahlman, Bradley, Sp

PRINCIPLES OF MEDICINAL CHEMISTRY (Elective – 3)

Code: DPS 22 104 (E3)	L	P	C
	3	0	3

OBJECTIVES:

1. To bring adaptability to the concepts of Medicinal chemistry and to acquire the required skills to become a perfect Medicinal Chemist.
2. To impart the basic knowledge of principles of Medicinal chemistry, drug receptors, their theories and applications which makes the student to understand the process technology based on them.
3. To acquire the knowledge of Physico-chemical Properties of Organic Medicinal Agents which are essential for the Medicinal chemists in industry.
4. To acquire the knowledge pertaining to drug metabolism and mechanism of action of drugs to apply them for medicinal and pharmaceutical field etc.
5. To impart then knowledge of prodrugs and their designing useful for understanding drug reaction pathways.

OUTCOMES: The basic concepts included in this course will help the student to gain:

1. The improve knowledge of principles related to Medicinal chemistry
2. The required principles and concepts of drug receptors and mechanisms of drugs based on their receptors.
3. The required skills to get clear concepts on physicochemical properties of drugs which are very much useful to medicinal & pharmaceutical field etc.
4. The knowledge of drug metabolism
5. The concepts of pro-drugs and their requirements, drug toxicity and adverse effects.

Unit – I: Introduction & General Principles of Medicinal Chemistry:

Introduction, Historical Evaluation, Chemotherapeutic index & Therapeutic index, Fundamental aspects of drugs, classification of drugs, Nomenclature of Drugs, Rules of Drugs nomenclature, Sources of drugs, Genesis of Drugs, Routes of Drug administration, sites of drug action, Mode of drug action, Mechanism of drug action,

Unit – II: Drug Receptor interactions:

Introduction, Drug-receptor complex nomenclature, Chemical nature of receptors, Types of receptors, Drug receptor interactions, Covalent interactions, Ionic interactions, Hydrogen bonding interactions (non-ionic/neutral), Vander Waals interactions, Hydrophobic/Lipophilic interactions, Receptor site theories - Occupation theory, Rate theory, Induced-fit theory.

Unit – III: Physico-chemical Properties of Organic Medicinal Agents:

Introduction, Physico-chemical Properties - Partition coefficient, solubility, surface activity, Degree of ionization. Importance of the following: a) Solubility, b) stabilization of biopolymers, c) Drug – receptor interaction, d) Drug protein binding- hydrogen bonding, hydrophobic interaction, charge transfer complexation, ionic bonding, covalent bonding & chelation. Stereochemical properties and drug action.

Unit – IV: Drug Metabolism:

Introduction, The stereochemistry of drug metabolism, sites of metabolism, Metabolic Reactions – Phase – I reactions: Oxidation & Oxidation of carbon-heteroatom systems, N-Hydroxylation, N-Oxidation, S-Oxidation, Dealkylations - S-Dealkylation, N-Dealkylation, O-Dealkylation, Aromatic Hydroxylation - Oxidation of benzylic carbons, Oxidation of olefins, Reductive reactions. Phase – II reactions: Glucuronidation, Sulfate Conjugation, Hydrolysis of drugs, Acetylation, Factors affecting drug metabolism.

Unit – V: Chemistry of Prodrugs:

The Prodrug concept, Applications of Prodrugs, Requirements & classifications pf prodrugs, Bioprecursor prodrugs, Carrier prodrugs, Design & Development of Prodrugs, Improve patient acceptance, to reduce gastric irritation, To improve chemical stability, Prodrugs for increased water solubility, To decrease drug's toxicity and adverse effects, To improve membrane transport, Prolonged Activity, Tissue specific prodrug design, Prodrug design based on site specific conditions, Enzyme specific prodrug design.

References:

1. Principles of Organic Medicinal Chemistry, Rama Rao Nadella, New Age International Publishers, 2005.
2. Foye's Principles of Medicinal Chemistry, Fifth Edition, David A. Williams and Thomas L. Lemke; Lippincott & Wilkins, 2002.
3. Fundamentals of Medicinal Chemistry, Gareth Thomas, University of Porthsmouth, UK, Joh Wiley &Sons Ltd, 2003.
4. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, Eleventh Edition, John H. Block, John M. Beale, Jr., 2004.
5. Essentials of Medicinal Chemistry, second edition, Andreus Korolkovas, John Wiley & Sons, 1988.
6. The Handbook of Medicinal Chemistry, Principles and Practice, Andrew Davis, Simon E Ward, Royal Society of Chemistry, 2013.
7. The Practise of Medicinal Chemistry, Camille G, Wermuth, Academic Press, Second Edition, 2003.

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PHYSICAL & INORGANIC CHEMISTRY LABORATORY

Code: DPS-22-L11	L	P	C
	0	6	3

I) Chemical Kinetics:
a) Study of first order kinetics of hydrolysis of ethyl acetate (acid catalysis).
b) Study of the hydrolysis of ester by alkali and study of the order of the reaction (ethyl acetate).
c) Determining the relative strengths of two acids by studying the hydrolysis of ester.

II) Phase rule: To study the phase diagram of simple binary system (Phenol / Water).
III) Distribution Law: To determine the Distribution Coefficient of benzoic acid between benzene and water.

IV) Adsorption: To determine the adsorption isotherm of acetic acid from aqueous solution of charcoal.

V) VOLUMETRIC ANALYSIS

i)***Dichrometry***
a) Estimation of Hypo by Dichrometry.
b) Estimation of Ferrous Iron.
c) Estimation of Ferric Iron.

ii)***Permanganometry***
a) Estimation of Oxalic acid by Permanganate.
b) Estimation of Ferrous Iron.
c) Estimation of Ferric Iron.

iii)***Acid-Base Titrations***
a) Estimation of Ammonium salt.

iv)***Iodometry***
a) Estimation of Copper.

Recommended Books:

1. "*Senior Practical Physical Chemistry*" , B.D.Khosla, 6th edition V.C.Garg and A.Khosla, R.Chand & Co., Delhi (1991).
2. "*Practical Physical Chemistry*" , J.B.Yadav, 5th edition Krishna Prakash media Pvt Ltd, Meerut (1997).
3. "*Practical Physical Chemistry*" , B.Viswanathan, P.S.Raghavan, 1st edition Viva Books Pvt. Ltd (2005).
4. Vogel's *"Text book of Quantitative Chemical Analys"*.
5. *"Modern Experiments for Introductory Chemistry*", H.A. Neidig & W.J. Stratton.
6. *"A hand book of Analytical Chemistry* "Vol-1 , Dr. S.C. Rastogi & S.K. Agarwal.

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ORGANIC CHEMISTRY LABORATORY - I

Code: DPS 22 L12	L	P	C
	0	6	3

Organic Preparations and Extractions:

i) Preparation of m-dinitrobenzene from nitrobenzene by nitration.
ii) Preparation of benzanilide from benzophenone via the oxime by Beckmann Rearrangement.
iii) Preparation of benzylideneacetophenone from benzaldehyde & acetophenone by Claisen-Schmidt Reaction.
iv) Cycloaddition of anthracene with maleic anhydride by Diels – Alder Reaction.
v) Preparation of benzoic acid and benzyl alcohol from benzaldehyde using Canizzaro's Reaction.
vi) Preparation of β-napthylbenzoate using β-napthol and benzoyl chloride using Schotten – Baumann reaction.
vii) Preparation of acetylsalicylic acid (aspirin) from salicylic acid.
viii) Preparation of hippuric acid from glycine and benzoyl chloride.
ix) Preparation of 7-hydroxy-4-methylcoumarin using resorcinol and ethyl acetoacetate.
x) Preparation of azalactone from hippuric acid.
xi) Preparation of tribromo aniline from aniline.
xii) Preparation of Tribromophenol from phenol.

Recommended Books:

1) "*Quantitative and Qualitative analysis in Organic Chemistry*" ,Vogel.

2) "*Practical Organic Chemistry*", Mann and Saunders.

3) "*Laboratory Organic Manual*", R.K.Bansal.

REAGENTS AND FORMATION OF C-C &C=C BONDS

Code: DPS 22 201	L	P	C
	3	0	3

Objectives:

1. To study about the concepts of oxidizing reagents, singlet oxidation and synthetic applications of hypervalent iodine
2. To study about different reducing agents and their applications in organic synthesis.
3. To learn about removal of functional groups by using different reducing reagents.
4. To understand the concept of C-C bond formation and its synthetic applications
5. To understand the concept of C=C bond formation and its synthetic applications.

Outcomes:

1. Able to understand organic oxidation reactions, singlet oxidations and DESS-martin oxidation.
2. Acquire knowledge on various types of reducing reagents and their significance in organic chemistry
3. Acquire knowledge about the elimination of functional groups by reduction method.
4. Obtain comprehensive understanding of formation of C-C bond formation.
5. Gain the knowledge of formation of C=C bond formation and their significance in the synthetic organic chemistry.

Unit-I: Oxidizing Reagents

Oxidations: Oxidation of C=C with transition metal oxidants – KMnO4 and OsO4, Epoxidation with peroxy acids, and hydroperoxides and subsequent transformation of epoxides. Cleavage of glycols [HIO4 and $Pb(OAc)_4$]. Oxidation of alcohols to carbonyl compounds using Cr^{VI} oxidants-(PCC, PDC, Collins reagent, and Jones reagent) and Swern oxidation. Singlet oxidation– Generation of Singlet oxygen- Reaction of alkenes with Singlet oxygen and their subsequent transformation. Synthetic applications of hypervalent Iodine: 2-Iodoxybenzoic acid (IBX), Dess-Martin oxidation, and Iodobenzenediacetate.

Unit-II: Reducing Reagents-I Group III-hydride transfer reagents: $NaBH_4$, $NaBH_3CN$, $LiAlH_4$, and DIBAL to reduce carbonyl groups and other functional groups– Reduction of α,β--unsaturated ketones(1,2 and 1,4-additions) Stereochemistry of hydride reductions (Cyclohexanones). Group IV hydride donors: Trialkylsilanes (R_3SiH and Ar_3SiH) to reduce hindered alcohols and carbonyl compounds, HCOOH -Eschweiler–Clarke reaction and Hydride ion transfer in MPV reduction and Cannizzaro reaction.

Unit-III: Reducing Reagents- II Reductive removal of functional groups-reductive removal of halogen, carbonyl group, acetate and sulfonate groups with Li or Na/EtOH, Diethyl phosphorochloridate, Zn-Hg/HCl, Zn-Al/AC_2O and Zn-Al/NH_4Cl. Birch Reduction.

Unit-IV: Formation of –C-C- bond: C-C (single) bond formation: Alkylation of relatively acidic methylene group .Aldol addition reactions of Li, B, Ti enolate anions and Mukaiyama reaction. Conjugate addition of Grignard reagents in presence of copper salts. Synthetic applications of Gilman reagent in C-C bond formation -Reaction with halides, epoxides and α,ß-unsaturated carbonyl compounds. The enamine reactions in C-C bond formation– Synthetic applications of carbenes and carbenoids.

Unit-V: C=C (double) bond formation: Wittig reaction and related reactions-Phosphonate Modification (Wadsworth-Emmon reaction), Horner-Wittig reaction, Peterson Olefination reaction, Julia-Lythgoe Olefination, McMurray Olefination, Tebbe Reagent, Bamford-Stevens Reaction, and Nickel (II) Catalyzed Cross-Coupling with Grignard Reagents (Kumada Reaction). ß-Elimination reactions, Pyrolytic Syn-eliminations in amine oxides (Cope Elimination), Sulphoxides and Selenoxides.

Books Recommended:

1. "*Reagents for Organic Synthesis*" by Fieser and Fieser.
2. "*Synthetic Reagents*" Vols. I and II by Pizey.
3. "*Organic Synthesis – Special Techniques*" by V.K. Ahluwalia & Renu Aggarwal, Narosa Publishing House, New Delhi (**2001**).
4. "*Reactions, Rearrangements and Reagents*" by S.N. Sanyal, Bharati Bhawan, Publishers, Patna (**2002**).
5. "*Organic Reaction Mechanisms*" by V.K. Ahluwalia & R. K. Parashar, Narosa Publishing House, New Delhi (**2002**).

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ORGANIC CHEMISTRY - II

Code: DPS 22 202	**L**	**P**	**C**
	3	**0**	**3**

ORGANIC CHEMISTRY - II (DPS 22 202)

Course Objectives:

1. To impart knowledge on Nucleophilic Aromatic substitution reaction mechanism and synthetic utility of various kinds of molecular rearrangement reactions.
2. To understand the synthetic design with diverse chemical reactions.
3. The sound knowledge on the structure, synthesis and reactions of various simple and fused heterocyclic compounds.
4. Acquire knowledge about biological importance of heterocyclic compounds.

Outcomes:

1. The student gets enough knowledge on mechanism and synthetic applications of molecular rearrangement reactions. He also gains concept of Nucleophilic aromatic substitution reactions.
2. They acquire the concepts of different named reactions snd their mechanisms.
3. Enough knowledge on the structure, synthesis and reactions of various simple and fused heterocyclic compounds will be gained.
4. Student gets good knowledge about biological importance of heterocyclic compounds.

Unit-1: Nucleophilic Aromatic substitutions – SN^1(Ar), SN^2 (Ar), SN^i and benzyne mechanisms; evidence for the structure of benzyne. Von Richter rearrangement. Definition and types of ambident nucleophile Neighbouring group participation of oxygen, sulphur and σ, $\prod$ bonds – (anchimeric assistance, retention of configuration.).

Unit-2: **Heterocyclic Compounds - I**

Introduction, Nomenclature Synthesis and reactivity of imidazole,pyrazole, oxazole, thiazole, isoxazole, isothiazole, pyridazine, pyrimidine, pyrazine.

Unit-3: Heterocyclic Compounds - II

Introduction, Nomenclature Synthesis and reactivity of Indole, benzofuran, benzo thiazole,quinoline, isoquinoline, benzimidazole, Coumarine, chromones.

Unit-4: Molecular Rearrangements-I:

Definition and Classification; General mechanism of Molecular rearrangements; Nucleophilic, Electrophilic, Free-radical Rearrangements - Examples; Whitmore - 1, 2– shifts, Stereochemical implications. Molecular rearrangements involving Carbocations; Wagner-Meewein, Pinacol-Pinacolone, Allylic, Wolf, Arndt-Eister. Demjanov, Dienone-Phenol Rearrangements.

Unit-5: Molecular Rearrangements-II:

Molecular rearrangements involving electron - deficient oxygen – Baeyer-Villiger oxidation, Base catalysed rearrangements, Favorskii rearrangement and Benzilic acid, Smile rearrangements. Molecular rearrangement involving electron deficient nitrogen – Beckmann, Hoffmann, Lossen, Schmidt and Curtius rearrangements.

Recommended Books:

1) "*Organic Chemistry*", R.T.Morison and R.N.Boyd, Allyn & Bacon Inc., (printed in Singapore) (2001).

2) "*Advanced Organic Chemistry*", Jerry March, John Wiley & Sons, New York, London. (2001).

3) "*Heterocyclic Chemistry"* ,T.Gilchrist.

4) "*Heterocyclic Chemistry"* , Raj K.Bansal

5) Molecular Rearrangements by Jack Lee, Wiley Publications

6) "*University Chemistry*", Vols II & III ,C.P.Murthy, S.F.Mehidi Ali and P.K. Dubey, New Age International (P) Ltd., New Delhi, Hyderabad **(**1996).

7) "Organic Chemistry", Paula Yurkanis Bruice, Pearson Education (Singapore) Pvt. Ltd., Delhi (2001).

8) "*Organic Chemistry*" , Francis A Carey, Tata Mc Graw Hill, New Delhi, 7th Edition.

9) "*Fundamentals of Organic Chemistry*" , Mc Murry and Simanek, Cenagage Learning India Pvt. Ltd., New Delhi, 6th Edition.

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ORGANIC SPECTROSCOPY

Code: DPS 22 203

L	P	C
3	0	3

Objectives:

1. To introduce the basic concepts of spectroscopy, principles of UV Visible, IR radiations, molecular changes.
2. To give enough knowledge to the student, the basic and advanced concepts of NMR techniques**.**
3. To impart the knowledge of Mass spectroscopy and its applications.
4. Imparting the analysis of spectral data to elucidate te structure of molecules.

Outcomes:

1. Study and solve problems of Ultraviolet and Visible spectroscopy of organic molecules
2. Understand Infrared spectroscopy and its applications to structural problems.
3. Important terms and theory of Nuclear Magnetic Resonance spectroscopy. Its applications to structural problems.
4. Principle, working of Mass spectrometer, formation of different ions, Mclafferty rearrangement and applications
5. Problems solved based on UV, IR, NMR & MS Spectroscopy to interpret structure.

Unit- 1: UV-Visible and IR spectroscopy:

UV: Principle -Various electronic transitions - Effect of solvent on electronic transitions - Ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes and conjugated polyenes. FieserWoodward rules for conjugated dienes and carbonyl compounds - Ultraviolet spectra of aromatic and heterocyclic compounds - Steric effect in biphenyls.

IR Principle- Charecteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines - Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance.

Unit - 2: Nuclear magnetic resonance spectroscopy (NMR)-I:

Theory of NMR-Nuclear energy levels-Instrumentation-Relaxation phenomenon, spin-spin and spin-lattice relaxations. Shielding and deshielding mechanism-chemical shift. Factors affecting the chemical shift. Isotropic and anisotropic effects-alkanes, olefins, acetylenes and aromatic systems. Low and High resolution of NMR spectrum of ethyl alcohol. Spin-spin coupling of strongly and weakly coupled systems-coupling mechanism, types of coupling constants. Factor affecting coupling constants-hybridization-dihedral angle and steric effects. NMR spectra of vinyl chloride, acetophenone, benzaldehyde, ethylbenzene, p-chlolroaniline and benzoic acid. Applications of NMR spectroscopyhydrogen bonding, keto-enol tautomers, cis-trans isomers, conformational analysis and deuterium exchange reactions.

Unit - 3: Nuclear magnetic resonance spectroscopy (NMR)-II:

Applications of spin-spin coupling in determination of structure and stereochemistry of organic molecules, NOE and its applications, and Lanthanide shift reagents. Recording of 13C NMR spectra (PFT technique), Types of 13C NMR spectra: Undecoupled, proton decoupled, selective proton decoupled spectra and off-resonance decoupled spectra - Spin decoupling method-Double resonance. 13C chemical shifts and factors affecting the chemical

shifts. Calculation of chemical shifts of alkanes, alkenes and alkynes. Applications of 13C NMR spectra. Editing techniques: INEPT and DEPT methods. 2D NMR techniques: Principles of 2D NMR, Different types of 2D-experiments with suitable examples. Correlation spectroscopy (COSY): HOMOCOSY (1 H-1 H COSY) and HETERO- COSY (1 H-13C COSY), NOESY and 2D– INADEQUATE experiments.

Unit - 4: Mass spectrometry:

Origin of mass spectrum, principles of EI, FAB, SIMS, CI, MALDI mass spectrometer-Instrumentation; Types of fragments: odd electron and even electron containing neutral and charged species (even electron rule), Nitrogen rule, isotopic peaks, metastable ion peaks, determination of molecular formula and High-resolution mass spectrometry. Salient features of fragmentation pattern of organic compounds- a-cleavage, β-cleavage, McLafferty rearrangement, Retro-Diels-Alder fragmentation and ortho effect. Fragmentation pattern of individual heterocyclic systems viz., Furan, Pyrrole, Thiophene and Pyridine. Preliminary account of chemical ionization. Introduction to GC-MS and LC-MS.

Unit - 5: Combined application of UV, IR, 1 H-NMR, 13C -NMR and Mass spectra:

Combined application of UV, IR, 1 H-NMR, 13C-NMR and Mass spectra: Introduction to the analytical approach towards the structure elucidation of simple organic molecules by combined application of UV, IR, 1 H-NMR 13C-NMR and Mass spectra

Reference Books:

1. W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994.
2. P.M. Silverstein, Spectroscopic Identification of Organic Compounds, 6th ed., Wiley 1998.
3. J.R. Dyer, Applications of Absorption Spectroscopy of Organic Compds, Prentice Hall, 1965.
4. Y.R. Sharma, Elementary Organic Spectroscopy – Principles S. Chand,1992.
5. C.N. Banwell, Fundamentals of molecular Spectroscopy, 3rd ed., TMH, New Delhi, 1983.
6. B.P. Straughan and S.Walker, Spectroscopy, Vol.3, Chapman Hall, London, 1976.
7. G.M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1964.
8. P.K.Ghosh, Introduction to Photoelectron Spectroscopy, John Wiley New York, 1989.
9. P.S.Kalsi, Spectroscopy of Organic Compounds, New age international publishers, 2007

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ANALYTICAL TECHNIQUES & INSTRUMENTATIONAL METHODS (Elective –1)

Code: DPS 22 204 (E1)

L	P	C
3	0	3

OBJECTIVES:

1. To bring adaptability to the concepts of Analytical chemistry and to acquire the required skills to become a perfect Medicinal Chemist.
2. To impart the basic knowledge of principles of analytical techniques such as UV, AAS & thermoanalytical methods which makes the student to understand the process based on them.
3. To acquire the knowledge of chromatographic techniques such as GC, HPLC which are essential for the Medicinal chemists in industry.
4. To acquire the knowledge pertaining to thermal analysis of drugs and apply them for medicinal and pharmaceutical field etc.
5. To impart then knowledge of analytical techniques useful for understanding method validation in pharmaceutical industry.

OUTCOMES: The basic concepts included in this course will help the student to gain:

1. The improve knowledge of principles related to Analytical chemistry.
2. The required principles and concepts of principles of principles of analytical techniques such as UV, AAS & thermoanalytical methods based on their processes.
3. The required skills to get clear concepts on chromatographic techniques such as GC, HPLC which are very much useful to medicinal & pharmaceutical field etc.
4. The required knowledge on thermal analysis of drugs and analytical techniques useful for understanding method validation in pharmaceutical industry

Unit – I: Importance of Analytical Chemistry:

Role of Analysis, Classification of analytical methods–classical and instrumental. Selecting an analytical method, Analytical Method validation. Statistical treatment of analytical data. Sensitivity & Detection limits, Precision & Accuracy – significant figures. Errors – types of errors, determinate, indeterminate or random errors, minimisation of errors. Mean and standard deviation. Students t-test, F-test.

Unit – II: Analytical method development:

Introduction - Parameters of method validation (selectivity, specificity, accuracy, ruggedness, robustness, linearity, LOD, LOQ, Range). Demonstration of use of statistical treatment for validation of analytical method by titrimetric method. Applications of analytical techniques in the identification of bulk pharmaceuticals, detection of impurities and quality assurance, structural elucidation and drug regulation. Role of method validation in chemical analysis.

Unit – III: Techniques of Chromatography:

Introduction, Classification of chromatographic techniques, differential migration rates, partition ratio, retention time, relation between partition ratio and retention time, capacity factor, selectivity factor. Efficiency of separation- resolution, diffusion, plate theory and rate theory. GC: Principle, instrumentation, detectors- TCD, FID, ECD. Derivatisation techniques, PTGC. HPLC: Principle, instrumentation, detectors- UV detectors, Photodiode array detector, fluorescence detector. Applications: Methods of quantitation for GC and HPLC: GC analysis of hydrocarbons in a mixture, GC assay of methyl testosterone in tablets, atropine in eye drops. HPLC assay of paracetamol and asprin in tablets.

Unit-IV: Analytical techniques:

UV-Visible spectroscopy: Introduction, Principle -Various electronic transitions - Effect of solvent on electronic transitions. Beer-Lambert's law, deviations from Beer's law. Types of transitions of inorganic and organic molecules, chromophores, effect of conjugation, solvent effects, instrumentation, applications of uv-visible spectroscopy to organic compounds.

Atomic absorption spectroscopy: Introduction, principle, detection of non-metals by AAS, advantages and disadvantages, Instrumentation, operating AAS spectrometer, applications of AAS.

X-Ray Crystallography: Introduction, what is X-Ray? what is a crystal? Bragg's Law, What's in a crystal, space group symmetry, non-crystallographic symmetry, impossible symmetry, Fourier Transforms, The phase problem, Molecular replacement, Refinement and the R factor, Key things to remember about X-ray diffraction.

Unit – V: Thermal Analysis of drugs in solid state:

Introduction to thermoanalytical methods, Thermogravimetric analysis (TGA), Principles, Derivative thermogravimetry (DTG), Comparison and interpretation of TG and DTG curves, Instrumentation of TG, TGA curves of individual compounds and mixtures, Factors affecting TGA curves, Applications of TGA. Differential thermal analysis (DTA) – Principles, Instrumentation, Interpretation of DTA curves, Influence of atmosphere on DTA curves of a sample, complementary nature of TGA and DTA, Applications of DTA in the study of clays, minerals, coals and explosives. Differential Scanning Calorimetry (DSC) – Principles, Methodology, Interpretation of DSC curves, comparison between DSC and DTA, chemical and pharmaceutical applications of DSC.

References:

1. John of Kennedy, Principle of analytical Chemistry. 2nd edition, Saunders college Publishing ,1990, New York.
2. J. W. Munson, pharmaceutical Analysis, Modern methods Part A &B, 2001, Marcel Dekker.
3. Principles of Instrumental analysis: A. Skoog, James, 5th edition, Saunders college Publishing.
4. Analytical Chemistry by Gary Christian, 6th edition, Wiley Publishing House.
5. Spectrometric identification of organic compounds: Robert M. Silverstein et al, 4th edition 1981, John & Wiley Sons.
6. Chromatographic Analysis of Pharmaceuticals, John A. Anamonics, 2nd edition.
7. Practical Pharmaceutical chemistry Part II: A.H. Beckett, J. B. Stenlake, (4th Edition), CBS Publishers Ltd.
8. Instrumental method of Chemical analysis: G. R. Chatwal, Himalaya Publishers Ltd.
9. Instrumental method of Analysis: Hubert H, Willard, 7th edition. CBS Publishers.
10. Spectroscopy of Organic Compounds: P.S. Kalsi, New Age International (P), Ltd. Publishers.
11. Organic Spectroscopy: William Kemp.ELBS, McMillan London 1991.

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BIOORGANIC CHEMISTRY (Elective-2)

Code: DPS 22 204 (E2)	L	P	C
	3	0	3

OBJECTIVES:

1. To bring adaptability to the concepts of Bio-organic chemistry and to acquire the required skills to become a perfect Medicinal Chemist.
2. To impart the basic knowledge of principles of Metabolism and Metabolic reactions which makes the student to understand the process based on them.
3. To acquire the knowledge of biomolecules such as amino acids and nucleic acids which are essential for the Medicinal chemists in industry.
4. To acquire the knowledge pertaining to biomolecules such as enzymes and apply them for medicinal and pharmaceutical field etc.
5. To impart then knowledge of coenzymes useful for understanding metabolic reaction pathways.

OUTCOMES: The basic concepts included in this course will help the student to gain:

1. The improve knowledge of principles related to Bioorganic chemistry.
2. The required principles and concepts of principles of Metabolism and Metabolic reactions based on their receptors.
3. The required skills to get clear concepts on biomolecules such as amino acids and nucleic acids which are very much useful to medicinal & pharmaceutical field etc.
4. The required knowledge on enzymes and coenzymes metabolism and their role in organic synthesis.

Unit – I: Fundamentals of Bioorganic chemistry:

Introduction of Biochemistry, Amino acids: peptides, primary, secondary, tertiary, and quaternary structure of proteins. Nucleic acids: Base pairing, double helices, DNA replication, transcription and translation, Enzymatic hydrolysis of proteins to peptides; Amino acid sequencing; amino acid metabolism (biosynthesis and degradation).

Unit – II: Metabolism and Metabolic Reactions:

Overview and important relationships between glycolysis, Bioenergetics And bioenergetic principles, oxidative phosphorylation process, ATP synthetase, photophosphorylation. Fatty acid metabolism: Biological importance of fatty acids and lipids, even chain and odd chain fatty acids, saturated and unsaturated fats, ketone bodies, fatty acid metabolism, calorific value of foods, biological membranes, properties and function of lipid bilayers and liposomes. Protein-related transformations: urea cycle, uric acid and ammonia formation.

Unit – III: Biomolecules - I:

Amino acids, peptides and proteins: Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding of secondary structures, α- helix, β-sheets, super secondary structure. Tertiary structure of protein: folding and domain structure. Quaternary structure. Nucleic acids: Structure and function of physiologically important nucleotides (c-AMP, ADP, ATP) and nucleic acids (DNA and RNA), replication, genetic code, protein biosynthesis, mutation.

Unit – IV: Biomolecules – II:

Chemistry of enzymes: Introduction, nomenclature, classes and general types of reactions catalysed by enzymes. Properties of enzymes: i) Enzyme efficiency/catalytic power ii)

Enzyme specificity; Fischer's 'lock and key' and Koshland 'induced fit' hypothesis. Concept and identification of active site. Factors affecting enzyme kinetics: Substrate concentration, enzyme concentration, temperature, pH, product concentration etc. Reversible and irreversible inhibition. Mechanism of enzyme action: transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Mechanism of chymotrypsin catalysed hydrolysis of a peptide bond.

Unit – V: Biomolecules – III:

Chemistry of coenzymes. Structure, mechanism of action and bio-modelling studies of the following coenzymes: nicotinamide adenine dinucleotide, flavin adenine dinucleotide, thiamine pyrophosphate, pyridoxal phosphate, Vitamin B12, biotin, lipoic acid, Coenzyme A. Enzymes in organic synthesis. Fermentation: Production of drugs/ drug intermediates by fermentation. Production of chiral hydroxy acids, vitamins, amino acids, β-lactam antibiotics. Synthesis of chemicals via microbial transformation, synthesis of L-ephedrine. Chemical processes with isolated enzymes in free form (hydrocyanation of m-phenoxybenzaldehyde) / immobilized form (production of 6-aminopenicillanic acid).

References:

1. Bioorganic, Bioinorganic and Supramolecular chemistry, P.S. Kalsi and J.P. Kalsi. New Age International Publishers.
2. Enzyme catalysis in organic synthesis, 3rd edition. Edited by Karlheinz Drauz, Harold Groger, and Oliver May, Wiley-VCH Verlag GmbH & Co KgaA, 2012.
3. Biochemistry, Dr U Satyanarayan and Dr U Chakrapani, Books and Allied (P) Ltd.
4. Enzymes: Practical Introduction to structure, mechanism and data analysis, By Robert A. Copeland, Wiley-VCH, Inc.
5. The Organic Chemistry of Biological Pathways By John McMurry, Tadhg Begley by Robert and company publishers
6. Biochemistry By Lehninger 20. Bioorganic Chemistry- A practical approach to Enzyme action, H. Dugas and C. Penny. Springer Verlag, 1931
7. Biochemistry: The chemical reactions in living cells,By E. Metzler. Academic Press.
8. Concepts in biotechnology by D. Balasubrarnanian & others
9. Principals of biochemistry by Horton & others. 24. Bioorganic chemistry - A chemical approach to enzyme action by Herman Dugas and Christopher Penney.

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CHEMISTRY OF POLYMERS (Elective – 3)

Code: DPS 22 304 (E3)	**L**	**P**	**C**
	3	**0**	**3**

OBJECTIVES:

1. To bring adaptability to the concepts of Medicinal chemistry and to acquire the required skills to become a perfect Medicinal Chemist.
2. To impart the basic knowledge of principles of Medicinal chemistry, drug receptors, their theories and applications which makes the student to understand the process technology based on them.
3. To acquire the knowledge of Physico-chemical Properties of Organic Medicinal Agents which are essential for the Medicinal chemists in industry.
4. To acquire the knowledge pertaining to drug metabolism and mechanism of action of drugs to apply them for medicinal and pharmaceutical field etc.
5. To impart then knowledge of prodrugs and their designing useful for understanding drug reaction pathways.

OUTCOMES: The basic concepts included in this course will help the student to gain:

1. The improve knowledge of principles related to Medicinal chemistry
2. The required principles and concepts of drug receptors and mechanisms of drugs based on their receptors.
3. The required skills to get clear concepts on physicochemical properties of drugs which are very much useful to medicinal & pharmaceutical field etc.
4. The knowledge drug metabolism and prodrugs.

Unit-1: Organic Polymers: Definition and Classification; Principles of polymerization; Chain polymerization – Free radical, Anionic and Cationic types; Co-ordination polymerization – Zeigler Natta catalysts; Miscellaneous polymerizations; Inhibitors; Step growth polymerization; Types of polymers based on structural types and Tacticity.

Unit-2: Plastics: Definition and classification: Thermoplastic materials; preparation, properties and uses of Polythylenes, Teflon, Polyvinyl acetate, Polyvinylchloride, Polystyrene and Polymethyl methacrylate. Preparation, properties and uses of Thermoset plastics such as Phenol Formaldehyde resins, Urea=Formaldehyde resins, Melamine-Formaldehyde resins. Alkyl resins. Epoxy resins, Polyurethanes etc; compounding of plastics and Fabrication techniques.

Unit-3: Elastomers & Chemical Fibers: Natural rubber; its structure and processing; Synthetic rubbers - Thiokol, Neoprene, Buna-S. Buna-N etc. – Their methods of preparation, properties and uses; Compounding and vulcanization of rubber, Classification and properties of fibers; Natural fibers like Cotton, Wool and Silk; semi-synthetic fibres – Preparation properties and uses of Cuprammonium rayon, Acetate rayon, Viscose rayon, Preparation, properties and uses of Synthetic fibers – Nylon, Kevular, Polythyleneterephthlate, Polyacrylonitrile, Vinyon.

Unit-4: Physical Chemistry of Polymers: Molecular weight and size; Number average and weight average molecular weights; Significance, experimental methods for the determination of average molecular weights of polymers by Viscometry, Osmometry, Ebulloscopy, Cryoscopy, Sedimentation and light scattering methods. Degree of Polymerization;

Polydispersity and molecular weight distribution in polymers; Practical significance of polymer molecular weight; Glass transition temperature – Its determination and significance.

Unit-5: Inorganic Polymers: General Survey of inorganic polymers; Preparation, Properties and uses of Polyphosphazenes, Ply(Siloxanes), Elemento – organic polymers – Silicones; Boom Polymers.

Recommended Books:

1. Text Books of Polymer Science – Bill Meyer (Wiley Inter Science Publishers)
2. Polymer Science – V R Gowarikar
3. Plastic Materials-Brydson
4. Rubbery materials and their compounds-Brydson.
5. Rubber Technology and manufacture-C.M. Blow
6. Polymer Chemistry- Seymour& Carreher, Marcel Dekkar, NY.
7. Principles of Polymerization-Odian G, wiley Inter Science, New Delhi
8. Polymer Science -Gowarikar, Wiley Estern Ltd. New Delhi
9. Fundamentals of Polymer Science and Engineering- anilkumar & S.K. Gupta, Tata McGraw Hill, New Delhi
10. Textbook of Polymer Science - F.W. Billmeyer

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ORGANIC CHEMISTRY LABORATORY - II

Code: DPS 22 L21	**L**	**P**	**C**
	0	**6**	**3**

1. Qualitative Analysis:

Analysis of at least six binary mixtures of monofunctional organic compounds by using systematic qualitative analyses technique. The following types of mixtures may be used.

a) Solid – Solid
b) Solid – Liquid.
c) Liquid – Liquid.

2. Quantitative Analysis:

a) Estimation of Phenols
b) Estimation of Aniline
c) Estimation of Amino Acids.
e) Estimation of Glucose by Fehling's solution.

Recommended Books:

1. "*A Textbook of Practical Organic Chemistry*: *Quantitative and Qualitative analysis*" , Vogel.
2. "*Practical Organic Chemistry*" , Mann and Saunders.
3. "*Laboratory Organic Manual*" , R.K.Bansal.
4). " *Comprehensive Practical Organic Chemistry*" , V.K.Ahilwalia & Renu Aggarwal, Universties Press (India) Pvt. Ltd., New Delhi.

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APPLIED CHEMISTRY LAB

Code: DPS 22 L22

L	P	C
0	6	3

1. Estimation of Ferrous iron by Dichrometry method.
2. Estimation of Ferrous iron by Permanganometry method.
3. Estimation of Hardness of water by EDTA Complexometry method.
4. Conductometric titrations of strong acid Vs weak base.
5. Conductometric titrations of weak acid Vs strong base.
6. Estimation of a weak acid by potentiometry
7. Estimation of a strong acid by potentiometry.
8. Estimation of an acid by *p*H metry.
9. Preparation of Phenol-formaldehyde resin (Bakelite).
10. Preparation Nylon-6,6.
11. Estimation of acid value of given lubricant oil.
12. Estimation Saponification value of a lubricant oil.
13. Estimation of Viscosity of lubricant oil using Ostwald's Viscometer.
14. Determination of rate of corrosion of mild steel in the presence and absence of inhibitor.

Recommended Books:

1. Inorganic Quantitative analysis by A.I. Vogel, ELBS Publications.
2. Laboratory Manual of Engineering Chemistry by Y. Bharathi Kumari & Jyotsna C, VGS Booklinks, Vijayawada, 2009.
3. College Practical Chemistry by V.K. Ahluwalia, Narosa Publications Ltd. New Delhi (2007).
4. Engineering Chemistry Lab Manual by B. Rama Devi & P. Aparna, Cengage Publications.
5. "*Senior Practical Physical Chemistry*" , B.D.Khosla, 6th edition V.C.Garg and A.Khosla, R.Chand & Co., Delhi (1991).
6. "*Practical Physical Chemistry*" , J.B.Yadav, 5th edition Krishna Prakash media Pvt Ltd, Meerut (1997).
7. "*Practical Physical Chemistry*" , B.Viswanathan, P.S.Raghavan, 1st edition Viva Books Pvt. Ltd (2005).
8. "*Experiments in Physical Chemistry*" ,David P. Shoemaker, Carl W. Garland and Joseph W. Nibler, 5th edition Mc Graw-Hill Book Company (1989).

ASYMMETRIC SYNTHESIS & SYNTHETIC STRATEGIES

Code: DPS 22 301

L	P	C
3	0	3

Objectives:

1. To study about the concepts of prochirality, and methods to induce enenatioselectivity
2. To study about the different types of substrate controlled and reagent controlled asymmetric synthesis.
3. To learn about the various synthetic strategies for the preparation of desired compounds.
4. To understand the different new synthetic reactions.

Outcomes:

1. Able to recognize the re-si faces, and methods for inducing enantio selectivity in the molecule.
2. Gain knowledge about types asymmetric syntheses like substrate and reagent controlled reactions.
3. Acquire knowledge about the various synthetic strategies for the synthesis of molecules of importance.
4. Able to understand various new synthetic reactions viz., Beginelli, Nazerov, Shapiro reactions.

Unit – 1: Asymmetric synthesis-I:

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 chiraility 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.

Unit-2: Asymmetric synthesis-II:

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. Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using IPC2 BH and IPCBH2. Chiral catalyst controlled asymmetric synthesis: Sharpless, Jacobson & Shi asymmetric epoxidation, Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalysts. Asymmetric aldol reaction: Diastereoselective aldol reaction (achiral enolate & achiral aldehydes) its explanation by Zimmerman-Traxel model.

Unit – 3: Synthetic Strategies- I:

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.

Unit – 4: Synthetic Strategies- II:
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.

Unit - 5: New Synthetic reactions:
Metal mediated C-C and C-X coupling reactions: Suzuki, Heck, Sonogishira cross coupling, C=C Formation Reactions: Shapiro, Bamford-Stevens, and Peterson's stereoselective olefination. Multi component Reactions: Biginelli, Bergman, Ugi - Passerini reactions. Ring Formation Reactions: Pausan-Khand reaction, Nazerov cyclisation. Click Chemistry: Click reaction, 1,3-dipolar cycloadditions. Metathesis: Grubb's 1st and 2nd generation catalyst, Olefin cross coupling metathesis (OCM), ring closing metathesis (RCM), ring opening metathesis (ROM), applications. Other important synthetic reactions: Mitsunobu reaction, Stork-enamine reaction and Michael reactions.

References:

1. Asymmetric synthesis by Nogradi
2. Asymmetric organic reactions by J D Morrison and H S Moschcr
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. Problems on organic synthesis by Stuart Warren
10. Organic chemistry Jonathan Clayden, Nick Greeves and Stuart Warren 11.The logic of chemical synthesis by Elias James Corey and Xue-Min Cheng

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PERICYCLIC REACTIONS & PHOTO CHEMISTRY

Code: DPS 22 302	L	P	C
	3	0	3

Objectives:

1. To impart the knowledge on symmetry properties, definition and classification of Pericyclic reactions methods of analyzing Pericyclic reactions.
2. The concepts of Electrocyclic Cycloaddition reactions, Woodward- Hoffmann rules for these reactions are to be known.
3. The knowledge of sigmatropic reactions and the types of them are to be learnt.
4. The basic principles, mechanism of photochemical reactions are required for the student of drug chemistry**.**

Outcomes:

1. By the end of this chapter the student will be familiar with types and principles of Pericyclic reactions.
2. He learns the basics of conservation of orbital symmetry and what conrotation and disrotation. Electrocyclic reactions and rules governing them.
3. The student learns about cycloaddition reactions and sigmatropic reactions and rules governing them.
4. The concepts of photochemistry and mechanism of photochemical reactions are learnt.

Unit-1: Introduction to Pericyclic Reactions:

Introduction -Characteristics and classification of pericyclic reactions. Representation of molecular orbitals-Bonding, Nonbonding and Anti bonding, Symmetry properties with special reference to plane of symmetry and two fold axis of symmetry - Ethylene, 1,3 Butadiene, 1,3,5- Hexatriene, allyl system.

Unit-2: Eelectrocyclic and Cycloaddition Reactions:

Woodward- Hoffman correlation diagram method, FMO approach and perturbation of molecular (PMO) approach for the explanation of pericyclic reactions under thermal and photochemical conditions. Electrocyclic Reactions: Conrotatory and disotatory motions (4n) and (4n+2), allyl systems and secondary effects. Cycloadditions: Antarafacial and suprafacial additions, notation of cycloadditions, (4n) and (4n+2) systems with a greater emphasis on (2+2) and (4+4) cycloadditions, (2+2) additions of ketones.

Unit-3: Sigmatropic Rearrangements:

PMO, FMO approach and Stereochemistry of Sigmatropic rearrangements-[1,3], [1,5], [1,7], [3.3]and [5.5]. Detailed treatment of Cope, Oxy-Cope, Aza-Cope, Claisen, and Aza-Claisen rearrangements. Sommlet-Hauser reaction, Chelotropic reactions (Additions and Eliminations), Group transfer, Group elimination and Ene reactions. Exercises based on pericyclic reactions.

Unit-4: Introduction and Photochemistry of Carbonyl compounds:

Photo excitation of molecules-Electronic transitions and types of electronic transitions, Energies and life times of excited states, Fate of excited molecules, Photophysical processes-Jablonski diagram. Photochemical sensitization and Photochemical quenching. Photochemistry of carbonyl compounds- Photoreductions (Intermolecular and Intramolecular), Paterno-Buchi reaction (Intermolecular and Intramolecular including

stereochemistry) and limitations. Photochemical cleavages-Norrish Type-I and Norrish Type-II reaction (including stereochemistry).

Unit-5: Photochemistry of Olefins:

Photochemistry of Olefines, Cis-Trans isomerisation, Dimerisation, Simple additions and Inter and Intra molecular cyclo additions. Electrocyclisation and Cycloaddition reactions in conjugated dienes. Photochemistry of Aromatic compounds -Ring isomerisation, Photocyclo additions. Photorearrangements-Barton reaction, Zimmermann rearrangement and Photo-Fries rearrangement.

Recommended Books:

1. "Organic Chemistry", R.T.Morison and R.N.Boyd, Allyn & Bacon Inc., (2001).
2. "Advanced Organic Chemistry", Jerry March, John Wiley & Sons, (2001).
3. "Organic Chemistry", S.M.Mukherji, S.P. Singh and H.P. Kapoor, Wiley Eastern Ltd., (1985).
4. "Organic Chemistry", Paula Yurkanis Bruice, Pearson Education Pvt. Ltd., Delhi (2001).
5. "Photochemistry and Pericyclic Reactions",Jagdamba Singh, New Age International (P) Ltd., (2003).
6. "Molecular Reactions and Photochemistry", Charles H. Depuy and Orville L. Chapman, Prentice Hall of India (P) Ltd.,(1988).
7. " Organic Photochemistry" , Gurdeep R.Chatwal, Himalaya Publishing House,(2008).
8. "Conservation of orbital symmetry", Ian Fleming.
9. "Pericyclic Reactions ", Sankar Raman, Wiley.

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REGULATORY GUIDELINES IN PHARMACEUTICAL MANUFACTURING

Code: DPS 22 303	**L**	**P**	**C**
	3	**0**	**3**

OBJECTIVES:

1. To bring adaptability to the concepts of Good Manufacturing Practices and to acquire the required skills to become a perfect Medicinal Chemist.
2. To impart the basic knowledge of Good Laboratory Practices and Good Clinical Practices which makes the student to understand the process based on them.
3. To acquire the knowledge of Intellectual Property Rights & Patents which are essential for the Medicinal chemists in industry.
4. To acquire the knowledge pertaining to Fundamentals in Clinical trials and of Clinical trial protocol Development

OUTCOMES: The basic concepts included in this course will help the student to gain:

1. The improve knowledge of principles related to Good Manufacturing Practices.
2. The required principles and concepts of Good Laboratory Practices and Good Clinical Practices.
3. The required skills to get clear concepts on Intellectual Property Rights & Patents which are very much useful to medicinal & pharmaceutical field etc.
5. The required knowledge on Fundamentals in Clinical trials and of Clinical trial protocol Development.

Unit – I: Good Manufacturing Practices:

History of GMP, drug laws and regulations, Essential elements of GMP regulations, GMP expectations, Characteristics of GMP products, Legal consequences of GMP noncompliance, Role of quality assurance in the pharmaceutical industry, Personnel responsibilities in GMP environment, Role of procedures: SOPs, documentation, logs in GMP environment, Function and importance of specifications, Five "Ps" of GMP; "Product", "Premise", "People", "Procedure", and "Process", GMP requirements for building, facilities, and equipment.

Unit – II: Good Laboratory Practices and Good Clinical Practices:

History and the reasoning behind the GLPs, Essential and required Good Laboratory Practices GLPs, GLP and GMP Regulations for an analytical laboratory, 21 CFR Part 11, Critical operational elements of analytical laboratories, Review GLPs and GMPs and their regulations for analytical labs, Roles and responsibilities of personnel, Appropriate design and placement of laboratory equipment, Requirements for maintenance and calibration. ICH guidelines involved. Introduction to GCP and principles governing GCP.

Unit – III: Intellectual Property Rights & Patents:

Intellectual Property in Drug Discovery; Definition, Need for patenting, Types of Patents, Conditions to be satisfied by an invention to be patentable, Introduction to patent search Introduction to Patents, copyrights, GIs; Patents in the wider context of intellectual property rights; What is a Patent, What can be Patented, requirements for patentability, patent restrictions, how are patents obtained; The Power of Patents. Introduction to Patent Medicine; Role of patents in R & D.

Unit – IV: Fundamentals in Clinical trials:

Introduction to clinical Trials, History, terminologies, types of clinical research, phases of clinical research, role of clinical trial in new drug developments.

Regulatory affairs in clinical trials: IND, NDA, ANDA- Parts and contents, Safety monitory boards, FDA in various countries including India.

Unit – V: Clinical trial protocol Development:

Required Documentation including Investigator's Brochure, Case Report Forms, Serious Adverse Event (SAE) Reports, Laboratory Certification, data collection and quality control of data, closing out of clinical trial

Good Clinical Practice Concept, importance, and GCP guidelines including ICH guidelines.

References:

1. Good Manufacturing practices for pharmaceutical- A plan for Quality control, 4th Edition revised and expanded, Sidney Willig, James Stoker, Marcel Dekker.
2. Good Laboratory Practice regulations, Sandy Weinberg (3rd edn), Marcel Dekker.
3. Quality Assurance and Quality Management in Pharma Industry, Prof. Y. Anjanayuli, Dr. R. Marayya, Pharma Book Syndicate.
4. Good pharmaceutical manufacturing practice, by Sharp John.
5. ICH guidelines
6. A textbook of clinical pharmacy practice-essential concepts and skills, Parthasarathi, Nyfort-hansen Nahata, Publisher: Orient Longman.
7. Quality Assurance of pharmaceuticals-A compendium of guidelines and related materials, Vol I, Pharma Book Syndicate.
8. Pharmaceutical Pre-approval inspections-guide to regulatory success, 2ndedn,-Martin D, III(edt) Hynes, Informa Healthcare.
9. Drugs & Cosmetics Act, 1940 and Rules, 1945.
10. Good Manufacturing Practices, Philosophy and Applications by John Sharp, Inter Pharma Press, IL 60089, USA.
11. Quality Assurance Guide (Vol I & Vol II) by Organisation of Pharmaceutical producers of India.
12. N.R. Subbaran, what everyone should know about Patent, Pharma Book Syndicate (2nd edition).
13. Current Patent Acts of various countries.
14. Patents for Chemicals Pharmaceuticals & Biotechnology 4th edition, Philip W Grubb-Oxford University Press.

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CHEMISTRY OF NATURAL PRODUCTS (Elective-1)

Code: DPS 22 304(E1)	L	P	C
	3	0	3

OBJECTIVES:

6. To bring adaptability to the concepts of Medicinal chemistry and to acquire the required skills to become a perfect Medicinal Chemist.
7. To impart the basic knowledge of principles of Medicinal chemistry, drug receptors, their theories and applications which makes the student to understand the process technology based on them.
8. To acquire the knowledge of Physico-chemical Properties of Organic Medicinal Agents which are essential for the Medicinal chemists in industry.
9. To acquire the knowledge pertaining to drug metabolism and mechanism of action of drugs to apply them for medicinal and pharmaceutical field etc.
10. To impart then knowledge of prodrugs and their designing useful for understanding drug reaction pathways.

OUTCOMES: The basic concepts included in this course will help the student to gain:

5. The improve knowledge of principles related to Medicinal chemistry
6. The required principles and concepts of drug receptors and mechanisms of drugs based on their receptors.
7. The required skills to get clear concepts on physicochemical properties of drugs which are very much useful to medicinal & pharmaceutical field etc.
8. The knowledge drug metabolism and prodrugs.

Unit-I: Chemistry of Alkaloids:

Definition, nomenclature and physiological action, occurrence isolation, general methods of structure elucidation, degradation classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following : morphine, codeine, reserpine.

Unit-II: Chemistry of Terpenoids:

Terpenes and Terpenoids: Definition, classification based on isoprene unit, isoprene rule, and special isoprene rule. Isolation, structure elucidation and synthesis of citral, aterpineol, camphor and a-pinene. Biogenesis of terpenoids.

Unit-III: Chemistry of Steroids: Introduction, occurance, structure, stereochemistry and synthesis of cholesterol, Androsterone, Testosterone, Oestrone, Progesterone and Cortisone.

Unit-IV: Chemistry of Flavanoids: Classification of Flavanoids, General methods of synthesis of Anthocyanins, Flavones, Flavonols and Flavanones. Chemistry of Pelargonidin, Cyanidin, Delphinidin chloride, Chrysin, Quercitin and Diadzein.

Unit-V: Biosynthesis of Natural products: Introduction, Major biosynthetic pathways: (a). Acetate hypothesis and its use in construction of Aromatic rings and Polyphenolic compounds (b). Mevalonic acid pathway-Ruzicka biogenetic isoprene rule, Biosynthesis of mono, sesqui and diterpenes – formation of the Presqualene alcohol and biosynthesis of triterpenes. (c) Shikimic acid pathway: Biosynthesis of essential amino acids (Phenyl alanine,

Tyrosine and Tryptophan), Flavonoids, Porphyrins and Alkaloids (Morphine and Indole group alkaloids).

Recommended Books:

1. Biosynthesis - Geismann
2. Biosynthesis - Bernfeld
3. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
4. Organic chemistry - Vol. 2, Finar
5. An introduction to the chemistry of terpenoids and steroids -William Templeton
6. Steroids - Fieser arid Fieser
7. Alkaloids - Bentley
8. The chemistry of terpenes - A Pinder
9. Terpenoids - Mayo
10. Alkaloids - Pelletier
11. Total synthesis of Natural Products - Apsimon (Vol 1-5)

CHEMISTRY OF SYNTHETIC DRUGS & PHARMACEUTICAL FORMULATIONS
(Elective – 2)

Code: DPS 22 204 (E2)	**L**	**P**	**C**
	3	**0**	**3**

OBJECTIVES:

1. To bring adaptability to the concepts of Drug Development and to acquire the required skills to become a perfect Medicinal Chemist.
2. To impart the basic knowledge on Anti-bacterial Drugs, Antifungal agents & Antihistamines.
3. To acquire the knowledge of Anti-inflammatory Agents & Anti-ulcerants which are essential for the Medicinal chemists in clinical industry.
4. To acquire the knowledge pertaining to Antiemetic Agents & Antiamoebic Agents, Sedatives & Hypnotics and Anti-Cancer Agents etc.
5. To impart then knowledge of Anti-malarials, Anti-diabetics & Pharmaceutical Formulations.

OUTCOMES: The basic concepts included in this course will help the student to gain:

1. The improve knowledge of principles related to Drug Development.
2. The required principles and concepts of Anti-bacterial Drugs, Antifungal agents & Antihistamines.
3. The required skills to get clear concepts Antiemetic Agents & Antiamoebic Agents, Sedatives & Hypnotics and Anti-Cancer Agents
4. The required knowledge on Anti-malarials, Anti-diabetics & Pharmaceutical Formulations.

Unit-1: General - Drug development:

Introduction and Historical background; Paul Ehrlisch's development of arsephenamine and his concept of Chemotherapy; Sulphas as wonder drugs; Importance of heterocyclic chemistry in drug synthesis; Natural Products as Lead molecules; Medicinal Chemistry and drug development.

Unit-2: Anti-bacterial Drugs, Antifungal agents & Antihistamines:

Sulphonamides; Sulphamethoxazole – Synthesis and mechanism of action, dosage forms; Trimethoprim, synthesis and dosage forms, its mechanism of action; Norfloxacin and Ciprofloxacin – Synthesis, dosage forms, structure-activity relationships. Mebendazole & Thiabendazole – Synthesis and applications. Antihistaminic agents; Diphenhydramine (benadryl) and Cetrazine – synthesis, therapeutic use and dosage forms; Cimetidine & Ranitidine – synthesis, dosage forms and applications.

Unit-3: Anti-inflammatory Agents & Anti-ulcerants:

Antipyretics, Analgesics and anti-inflammatory agents - General study; Non-steroidal anti-inflammatory agents: Ibuprofen, structure, synthesis, dosage forms and activity studies. Indomethacin & Piroxicam – Synthesis, dosage forms & mechanism of action. Steroidal anti-inflammatory agents like betamethasone; Anti-ulcer agents (PPI) – Omeprazole, Pantoprazole and Rabeprazole.

Unit-4: Antiemetic Agents & Antiamoebic Agents, Sedatives & Hypnotics and Anti-Cancer Agents:

Trimethobenzamide, Diphenidol, Metaclopramide – synthesis and therapeutic uses; Metronidazole – synthesis, uses & dosage forms. Definition and Classification of Sedative

and hypnotic agents; Chlorodiazepoxide, Diazepam, Nitrazepam etc.; Chemotherapy of Cancer; Synthesis and uses of Fluorouracil.

Unit-5: Anti-malarials, Anti-diabetics & Pharmaceutical Formulations:
Introduction; Malaria- its causes, control & treatment; Anti-malarials – Chlroquine, Pamaquin & Mepacrine; Mechanism of action & dosage forms. Introduction to Diabetes – its causes & types; Role of Insulin; Anti-diabetic agents – Sulphonylureas, Biguanides & Thiazolidinediones (Rosiglitazone, Pioglitazone & Ciglitazone); Mechanism of action & dosage forms; Formulations - Need for the conversion of drugs into medicines; Additives & their role; Route-wise and Form-wise dosage forms; Solid dosage forms, liquid dosage forms & semi-solid dosage forms; Ointments and Creams.

Books Recommended:

1. "*Chemistry of Synthetic Drugs*" , N. Evers and D. Caldwell, Ernest Benn Ltd. London.
2. Berger's "*Medicinal Chemistry*", Vols. I & II.
3. "*Essentials of Medicinal Chemistry*", A. Kotolkavas and J.H. Burckhalter, Wiley Interscience.
4. "*Medicinal Chemistry*", Ashutosh Kar, New Age International Ltd.
5. "*Drugs*" , G.L. David Krupadanam, D. Vijaya Prasad, K. Varaprasada Rao, K.L.N. Reddy and C. Sudhakar, Universities Press (India) Ltd., Hyderabad (2001).
6. "*Synthetic Drugs and Polymers*" , D. Dasarath, Sri Vani Publishers, Mumbai (2002).
7. "*Principles of Organic Medicinal Chemistry*" , Rama Rao Nadendla, New Age International (P), Ltd., Publisher, New Delhi, Hyderabad (2005).
8. "*Medicinal Chemistry*" , D. Sriram & P.Yogeeswari, Pearson Edication Ltd., New Delhi (2008).
9. "*Synthetic Drugs*" , G.R.Chatwal, Himalaya Publishing House Ltd., New Delhi (2009).
10. "*Medicinal Chemistry*" , G.R.Chatwal, Himalaya Publishing House Ltd., New Delhi (2008).

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CHEMISTRY OF ANTIBIOTICS & ANTIVIRALS (Elective -3)

Code: DPS 22 304(E3)	L	P	C
	3	0	3

OBJECTIVES:

1. To bring adaptability to the concepts of Bioorganic chemistry and to acquire the required skills to become a perfect Medicinal Chemist.
2. To impart the basic knowledge of principles of Metabolism and Metabolic reactions which makes the student to understand the process based on them.
3. To acquire the knowledge of biomolecules such as amino acids and nucleic acids which are essential for the Medicinal chemists in industry.
4. To acquire the knowledge pertaining to biomolecules such as enzymes and apply them for medicinal and pharmaceutical field etc.
5. To impart then knowledge of coenzymes useful for understanding metabolic reaction pathways.

OUTCOMES: The basic concepts included in this course will help the student to gain:

1. The improve knowledge of principles related to Bioorganic chemistry.
2. The required principles and concepts of principles of Metabolism and Metabolic reactions based on their receptors.
3. The required skills to get clear concepts on biomolecules such as amino acids and nucleic acids which are very much useful to medicinal & pharmaceutical field etc.
4. The required knowledge on enzymes and coenzymes metabolism and their role in organic synthesis.

Unit - I: Chemistry of Flavanoids: Classification of Flavanoids, General methods of synthesis of Anthocyanins, Flavones, Flavonols and Flavanones. Chemistry of Pelargonidin, Cyanidin, Delphinidin chloride, Chrysin, Quercitin and Diadzein.

Unit – II: Chemistry of Prostaglandins, Porphyrins and Carotenoids:
Prostaglandins- Occurrence, Nomenclature, Classification and Physiological activity. Structure determination and synthesis of PGE2 and PGF2α - Porphyrins: Structure and synthesis of HAemoglobin and Chlorophyll. Carotenoids: Structure determination and synthesis of α-Carotene, β-Carotene, γ-Carotene and Lycopene.

Unit – III: Biosynthesis of Natural Products:
Introduction, Major biosynthetic pathways: (a). Acetate hypothesis and its use in construction of Aromatic rings and Polyphenolic compounds (b). Mevalonic acid pathway-Ruzicka biogenetic isoprene rule, Biosynthesis of essential amino acids (Phenyl alanine, Tyrosine and Tryptophan), Flavonoids, Porphyrins and Alkaloids (Morphine and Indole group alkaloids).

Unit – IV: Chemistry of Antibiotics:
Classification of Antibiotics-Isolation, Structure determination, Synthesis and Stereochemistry of Tetramycin, Pencillin-G, Cephalosporin-C, Streptomycin and Chloramphenicol.

Unit – V: Chemistry of Antivirals:
Introduction to antiviral agents, structure of virus, virus life cycle, classification of antiviral agents, Synthesis, mechanism of action, properties and uses of adamantane derivatives, purine nucleotides, pyrimidine nucleotides, phosphorous derivatives, anti-retroviral agents.

References:

1. Biosynthesis - Geismann
2. Biosynthesis - Bernfeld
3. Chemistry of natural products, Vol 12, by Atta-Ur-Rahman
4. Organic chemistry - Vol. 2, Finar
5. Foye's principles of medicinal chemistry, 5th edition, David A.
6. Williams and Thomas L. Lemke, Lippincott Williams and Wilkins.
7. Medicinal Chemistry (Organic Pharmaceutical Chemistry), G.R Chatwal, Himalaya Publishing house.
8. Wilson & Gisvold; Text book of Medicinal Chemistry,
9. Philadelphia Williams & Lippinctt Wilkins.
10. Burger, Medicinal Chemistry (John Wiley & Sons N.Y).
11. Medicinal Chemistry, D. Shriram, P. Yogeshwari, Pearson Education.
12. Textbook of Pharmaceutical Chemistry by ,Jayshree Ghosh, S. Chand & company Ltd.
13. Pharmaceutical Chemistry by Dr. S. Lakshmi, Sultanchand & Sons.
14. Drug Synthesis by Gogte

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SPECTROSCOPY LABORATORY

Code: DPS 22 L31	L	P	C
	0	6	3

1) Spectroscopy:
Identification of unknown organic compounds by the interpretation of their UV – Visible, IR, NMR (Proton & Carbon) and Mass Spectra with special reference to petrochemicals, drugs and industrial intermediates.

2) Syntheses:
Formulation of detailed schemes of syntheses for different types of Petrochemicals, drugs and industrial intermediates from basic stage.

3) Mixture Analyses:
Analyses of three component mixtures of organic compounds using systematic method of separation (based on solubility data and organic identification (based on functional group analyses). Three Mixtures may be analyzed.

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MULTI-STEP SYNTHESES LABORATORY

Code: DPS 22 L32

L	P	C
0	6	3

1. Preparation of p-bromoaniline using the sequence of reactions (protecting and deprotecting)

   Aniline ⟶ Acetanilide ⟶ p-Bromoacetanilide ⟶ p-Bromoaniline

2. Preparation of 1-methyl-2-styrylbenzimidazole using the sequence of reactions. (using phase transfer catalytic method)

   OPDA ⟶ 2-Methylbenzimidazole ⟶ 2-Styrylbenzimidazole ⟶ 1-Methyl-2-Styrylbenzimidazole

3. Preparation of N- methyl-2-phenylindole using the sequence of reactions given below

   Aniline ⟶ Phenylhydrazine ⟶ Phenylhydrazone ⟶ 2-Phenylindole ⟶ N-Methyl-2-phenylindole

4. Preparation of benzilic acid using the sequence (Molecular Rearrangement)

   Benzoin ⟶ Benzil ⟶ Benzilic acid

5. Preparation of Benzopinacolone using the sequence (Photochemical Reaction)

   Benzophenone ⟶ Benzpinacol ⟶ Benzpinacolone

Books Recommended(For DPS 12 L32 & DPS 12 L33)

1. "*Spectrometric Identification of Organic Compounds",* R.M. Silverstein, G.C. Bassler and T.C. Morill, John Wiley & Sons, New York (1981).
2. "*Organic Structures from Spectra*", L.D. Field, S. Sternhell and J.R. Kalman, John Wiley & Sons, New York (2002).
3. "Chromatography", B.K. Sharma.
4. "*A Textbook of Practical Organic Chemistry*: *Quantitative and Qualitative analysis*" , Vogel.
5. "*Practical Organic Chemistry*", Mann and Saunders.
6. "*Laboratory Organic Manual*", R.K. Bansal.

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DRUG DESIGN & ADVANCED MEDICINAL CHEMISTRY

Code: DPS 22 401

L	P	C
3	0	3

OBJECTIVES:

1. To bring adaptability to the concepts of Drug designing in Medicinal chemistry and to acquire the required skills to become a perfect Medicinal Chemist.
2. To impart the basic knowledge of principles of QSAR studies, their theories and applications which make the student to understand the process technology based on them.
3. To acquire the knowledge of drug discovery processes which are essential for the Medicinal chemists in industries?
4. To acquire the knowledge pertaining to molecular drug targets and mechanism of action of drugs to apply them for medicinal and pharmaceutical field etc.
5. To impart then knowledge of clinical trials, useful for understanding drug development and testing processes.

OUTCOMES:

1. The basic concepts included in this course will help the student to gain:
2. The improve knowledge of principles related to drug design and Medicinal chemistry
3. The required principles and concepts of QSAR studies based on the structure of drug molecules and their activities.
4. The required skills to get clear concepts on drug discovery processes which are very much useful to medicinal & pharmaceutical field etc.
5. The knowledge molecular drug targets and clinical trials

Unit – I: Basic Principles of Drug Design & Advanced Medicinal Chemistry:

Introduction, History of Drug designing, Recent trends in drug designing, Structure-Based Drug Design (SBDD) - Docking ligands, Drug design based on leads, Lead Optimization, The SAR and QSAR approaches to drug design, The stereochemistry of the lead, Introduction of new substituents, The introduction of a group in an unsubstituted position, The introduction of a group by replacing an existing group.

Definitions and Objectives: Medicinal chemistry and related disciplines and terms, Drugs and drug substances, Stages of drug development, Drug Activity Phases: The pharmaceutical phase, The pharmacokinetic phase, The pharmacodynamic phase, Drug classification systems, classification by target and mechanism of action & other classification systems.

Unit – II: Quantitative structure–activity relationships (QSARS):

Introduction, Relationship between molecular structure and biological activity, Selectivity of drug action and drug receptors, Physicochemical properties of drug action: Acid-base properties, predicting degree of ionization of a molecule, Solubility of drugs, hydrogen bonding, lipophilicity parameters, electronic effects/parameter, steric parameters, chelation parameters, Hansch analysis. Free-Wilson analysis, their application, relationship between Hansch and Free-Wilson analysis (the mixed approach), non-linear relationship.

Unit – III: Process of Drug discovery:

Drug discovery by random screening of synthetic organic compounds, by targeted dedicating screening & Rational drug design, drug discovery by drug metabolism studies, drug discovery from observation of side effects, Refinement of the lead structure: determination of the pharmacophore, alterations in alkyl chains, Functional group modification: Bioisosterism, classical and non-classical bioisosters.

Unit – IV: Molecular drug targets:
Introduction, Drug binding, affinity and selectivity, Enzymes as drug targets, Membrane transporters as drug targets, ion channels as drug targets, Receptors- Structure, functions and the mechanism of drug action (Receptor Response), Design of agonist and antagonists, Receptor theories, Models and their types. GPCRs, nuclear receptors as drug targets.
Drug targets identification, validation and screening: Introduction, drug target identification, Hit-To-Lead Screening, cell based screening, intracellular receptors, intracellular enzymes, Current trends in the field of drug discovery and design.

Unit – V: Fundamentals in Clinical Trials:
Introduction to clinical Trial History, terminologies, types of clinical research, phases of clinical research, role of clinical trial in new drug developments. Regulatory affairs in clinical trials, Ethical issues in clinical trials: Principal, responsible conduct, supervision of ethics, (Informed Consent, Institutional Review Board (Role responsibility, members and auditing), Protection of participants, The Nuremberg Code, The Declaration of Helsinki, The Belmont Report.

Clinical trial design - Designs used in clinical trials, advantages and disadvantages, hypothesis, risks and benefits, subject selection, inclusion and exclusion criteria, randomization, blinding and controls. Clinical trial protocol Development Good Clinical Practice - Concept, importance, and GCP guidelines including ICH guidelines.
Management of Clinical trials - Role and responsibilities of Stakeholders of clinical trials (FDA, CRO, Sponsor, Physicians, Nurses, Health professionals, Hospitals, Patient), monitoring of clinical trials, Publications of clinical trials. Bioavailability, bioequivalence and Therapeutic Drug Monitoring, Data analysis issues in Clinical Trials.

References:

1. Foye's principles of medicinal chemistry, 5th edition, David A. Williams and Thomas L. Lemke, Lippincott Williams and Wilkins.
2. Principles of Organic Medicinal Chemistry, Rama Rao Nadella, New Age International Publishers, 2005.
3. Fundamentals of Medicinal Chemistry, Gareth Thomas, University of Porthsmouth, UK, Joh Wiley &Sons Ltd, 2003.
4. Wilson and Gisvold's Textbook of Organic Medicinal and Pharmaceutical Chemistry, Eleventh Edition, John H. Block, John M. Beale, Jr., 2004.
5. Essentials of Medicinal Chemistry, second edition, Andreus Korolkovas, John Wiley & Sons, 1988.
6. The Handbook of Medicinal Chemistry, Principles and Practice, Andrew Davis, Simon E Ward, Royal Society of Chemistry, 2013.
7. The Practise of Medicinal Chemistry, Camille G, Wermuth, Academic Press, Second Edition, 2003.
8. Medicinal Chemistry (Organic Pharmaceutical Chemistry), G.R Chatwal, Himalaya Publishing house.
9. Wilson & Gisvold; Text book of Medicinal Chemistry, Philadelphia Williams & Lippinctt Wilkins.
10. Medicinal Chemistry, D. Shriram, P. Yogeshwari, Pearson Education.
11. Textbook of Pharmaceutical Chemistry by Jayshree Ghosh, S. Chand & company Ltd

MOLECULAR MODELLING & COMPUTER AIDED DRUG DESIGN

Code: DPS 22 402

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3	0	3

OBJECTIVES:

1. To bring adaptability to the concepts of Molecular modeling aided drug design and to acquire the required skills to become a perfect Medicinal Chemist.
2. To impart the basic knowledge and principles of computer aided drug design which makes the student to understand the structure activity relationship studies.
3. To acquire the knowledge of Quantitative Structure Activity Relationships which are essential for the Medicinal chemists in industry.
4. To acquire the knowledge pertaining to Molecular Modeling and Docking and apply them for medicinal and pharmaceutical field etc.
5. To impart then knowledge of Molecular Properties and Drug Design useful for understanding metabolic reaction pathways.

OUTCOMES: The basic concepts included in this course will help the student to gain:

1. The improve knowledge of principles related to Molecular modeling aided drug design.
2. The required principles and concepts of principles of computer aided drug design.
3. The required skills to get clear concepts Quantitative Structure Activity Relationships and Molecular Modeling and Docking.
4. The required knowledge on Molecular Properties and Drug Design.

Unit – I: Introduction to Computer Aided Drug Design (CADD):

History, different technique sand applications, Quantitative Structure Activity Relationships: Basics, History and development of QSAR: Physicochemical parameters and methods to calculate physicochemical parameters: Hammett equation and electronic parameters (sigma), lipophilicity effects and parameters (log P, pi substituent constant), steric effects (Taft steric and MR parameters), Experimental and theoretical approaches for the determination of these physicochemical parameters.

Unit – II: 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 – III: Molecular Modeling and Docking:

Molecular and Quantum Mechanics in drug design, Energy Minimization Methods: comparison between global minimum conformation and bioactive conformation, 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 – IV: 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 modelling and generation of 3D-structure of protein.

Unit – V: Pharmacophore Mapping and Virtual Screening Concept of pharmacophore: pharmacophore mapping, identification of Pharmacophore features and Pharmacophore modelling; 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.

References:

1. Computational and structural approaches to drug discovery, Robert M Stroud and Janet. F Moore, RCS Publishers.
2. Introduction to Quantitative Drug Design by Y.C. Martin, CRC Press, Taylor & Francis group.
3. Drug Design by Ariens Volume 1 to 10, Academic Press, 1975, Elsevier Publishers.
4. Principles of Drug Design by Smith and Williams, CRC Press, Taylor & Francis.
5. The Organic Chemistry of the Drug Design and Drug action by Richard B. Silverman, Elsevier Publishers.
6. Medicinal Chemistry by Burger, Wiley Publishing Co.
7. An Introduction to Medicinal Chemistry –Graham L. Patrick, Oxford University Press.
8. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Ippincott Williams & Wilkins.
9. Comprehensive Medicinal Chemistry – Corwin and Hansch, Pergamon Publishers.
10. Computational and structural approaches to drug design edited byRobert M Stroud and Janet. F Moore.

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COMPUTATIONAL CHEMISTRY LAB

Code: DPS 22 L 41

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0	6	3

COMPUTATIONAL CHEMISTRY:

1. Introduction to computers – DOS and LINUX [Basics]
2. HTML
3. Creating Database – Creation of tables and Insertion of rows using MYSQL (Ligand Database), Chemical Databases ,SQL and Oracle
4. Searching Database (Online)
5. Visualizing molecules using different softwares [RASMOL, Swiss PDB Viewer]
6. Conformational analysis of small molecules [Ethane]
7. Building Molecules and Energy minimization.
8. Data Processing and Curve fitting by MS- Exel.
9. Study of molecules using chemoffice.

COLUMN CHROMATOGRAPHY:

Separation of Organic Compounds like *o*- and *p*-nitroanilines.

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