GURU GOBIND SINGH INDRAPRASTHA UNIVERSITY

Guru Gobind Singh Indraprastha University
Sector – 16C Dwarka, New Delhi – 110078

(Coordination Branch)
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F.No.: GGSIPU/Co-ord./46th AC/2019/17 Dated: 13 August 2019

CIRCULAR

The 46th meeting of the Academic Council of the University was held on 22.07.2019. Please find enclose herewith the minutes of the 46th meeting of the Academic Council for kind information.

(Brig. P.K. Upmanyu)
Registrar

F.No.: GGSIPU/Co-ord./46th AC/2019/17 Dated: 13 August 2019

To

1. Dean- USBAS/ USBT/ USCT/ USEM/ USICT/ USHSS/ USMC/ USLLS/ USM&PMHS/ USMS/ USAP/ USE, GGSIP University
2. Director- Academic Affairs/ Coordination/ Students' Welfare/ CDMS/ Development/ International Affairs/ CEPS/ Research and Consultancy/ Legal Aid / IUIIC, GGSIP University
3. Librarian, GGSIP University
4. Prof. P.K. Jhulka, (Retired), Max Institute of Cancer Care, 26-A Ring Road, Nirmal Puri, Nirmal Colony, Block-2, Lajpat Nagar-IV, New Delhi-110024
5. Prof. M.C. Sharma, 109, Nav Shakti Sadan, Sector 13, Rohini, New Delhi-110085
6. Prof. Karmeshu, (Retired), 150, Deepali, Road No. 42, Pitampura, Delhi-110034
7. Sh Arvind Misra, 5/101, Mathura Road, Agra-282002
8. Shri. Sandeep Gupta, 100 UB Jawahar Nagar, Delhi-110007
9. Prof. Rajiv Bhat, School of Biotechnology, Jawaharlal Nehru University, New Delhi
10. Prof. (Dr.) Pradeep Kulshrestha, Dean, School of Law, Sharda University, Plot No. 32 & 34, Knowledge Part-III, Greater Noida-201306 (UP)
11. Dr. Rupal S. Randhawa, 204-A, Pocket B, Mayur Vihar, Phase-2, New Delhi-110091
12. Prof. P.N. Varshney, E-30, Greater Kailash-III, New Delhi-110048
13. Dr. Jagdish Lal Gupta, CP-18, Maurya Enclave, Pitam Pura, Delhi-110034
14. Prof. M.N. Hooda, Director, Bharti Vidyapeeth's Institute of Computer Application & Management, A-4, Paschim Vihar, Rohtak Road, New Delhi-110063
15. Dr. Surendra Kumar, Principal, Delhi Institute of Rural Development, Holambi Khurd, Delhi-110082
16. Dr. Maharaj Krishen Bhat, Director, Maharaja Agrasen Institute of Management Studies, Maharaja Agrasen Camp, Plot No.1, Sec-22, Rohini, Delhi-110086

Contd.....2/-

17. Dr. Dhirendra Srivastava, Principal, ESIC Dental College & Hospital, Sector-15, Rohini, New Delhi -110085
18. Prof. Sanjiv Mittal, University School of Management Studies, GGSIP University
19. Prof. U.K. Mandal, University School of Chemical Technology, GGSIP University
20. Prof. Udyan Ghosh, University School of Information Communication & Technology, GGSIP University
21. Dr. Nimisha Sharma, Associate Professor University School of Biotechnology, GGSIP University
22. Dr. Gulshan Dhamija, Asst. Professor, University School of Basic and Applied Science, GGSIP University

Copy for information of the Competent Authority:
(i) AR to the Vice Chancellor, GGSIP University
(ii) AR to the Registrar, GGSIP University

Shikha

(Shikha Agarwal)
Dy.Registrar (Co-ordination)

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GURU GOBIND SINGH
INDRAPRASTHA
UNIVERSITY

FORTY SIXTH MEETING OF THE ACADEMIC COUNCIL

DATE : 22ND JULY, 2019 (Monday)

TIME : 03:00 P.M.

VENUE : VC SECTT., (Conference Hall)

MINUTES FOR 46TH ACADEMIC COUNCIL MEETING

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Agenda Item No. AC 46.16: **To consider and approve the Scheme of Examinations (up to 4 semesters) and syllabus of the 1st semester for M.Voc. (Interior Design) programme proposed to be introduced from Academic Session 2019-20.**

The Academic Council considered and approved the Scheme of Examinations (up to 4 semesters) and syllabus of the 1st semester for M.Voc. (Interior Design) programme proposed to be introduced from Academic Session 2019-20.

Agenda Item No. AC 46.17: **To consider and approve the syllabus of Ph.D. Program offered by CEPS**

The Academic Council considered and approved the syllabus/course content of Ph.D. Course Work for Ph.D. programme offered by CEPS.

Agenda Item No. AC 46.18: **To consider and approve the syllabus of M. Pharm. (Pharmaceutical Chemistry) offered by CEPS.**

The Academic Council considered and approved the syllabus/course content of M. Pharm. (Pharmaceutical Chemistry) programme offered by CEPS.

Agenda Item No. AC 46.19: **To consider and approve the syllabus of M.Sc (Medicinal Chemistry & Drug Design) offered by CEPS.**

The Academic Council considered and approved the syllabus/course content of M.Sc. (Medicinal Chemistry & Drug Design) programme offered by CEPS.

Agenda Item No. AC 46.20: **Finalization of Admission Brochure from the Academic Session 2020-2021 and onwards.**

The Academic Council appreciated the efforts of the University for timely planning of the activities of the next academic session. All the members approved the proposal for constitution of the committee as posed in agenda regarding finalization of Admission Brochure for the Academic Session 2020-2021 by 30th November, 2019 and also approved that thereafter the Admission Brochure should be finalized by 30th November of every year for the next academic session.

Guru Gobind Singh Indraprastha University
Sector-16C, Dwarka, New Delhi-110078

STRUCTURE and SYLLABUS

For

Ph.D. Course Work

Under

Centre of Excellence in Pharmaceutical Sciences

EntrepreneurshipEmployabilitySkill Development

CONTENTS

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Objectives of the Ph.D. Course Work: CEPS

The Ph.D. course work is designed to impart knowledge and to validate the concepts. Further courses/seminars would help develop the scholar's intellectual skills for free and objective inquiry courage and integrity, truthfulness awareness, and sensitivity to the needs and demands of society.

Programme Outcomes

1. The scholastic educational module and research programs have been structured with new information and a bird eye to developing fields of Pharmaceutical sciences.
2. Research pathway centre around different pharmaceutical medication conveyance frameworks, , natural product , Pharmacology, synthesis and other push regions such as bioinformatics, microbiology, sensors of Pharmaceutical Research.
3. The programme consistently distributes their exploration research in reputed international journals.
4. The course concentrates on research and coursework identifying with the improvement, and activity of medications in the body.
5. The centre works towards promoting multidisciplinary, team-based approach to drug delivery, embracing a variety of activities in the broad area of drug formulation and delivery.
6. Major areas of emphasis include quality education with professionalism by considering the recent requirements in different aspect of pharmaceutical fields.

Programme Specific Outcomes

- To provide quality education, practical based training and research in pharmaceutical sciences and allied areas for the well-being of people.
- Impart knowledge of medicinal chemistry as basic objective of education. A Scientific attitude to make students create open minded and curiosity who can take up responsibilities as pharmaceutical sciences professionals, suitable for community, industries and institutions.
- Provide infrastructure and research facilities to disseminate the advanced knowledge to the students in various branches pharmaceutical sciences through innovative teachinglearning processes with inter-disciplinary approach such that they grow their wisdom to acquire all kinds of knowledge and generate new ideas.
- Educate and train manpower for the development of the medicinal chemistry and establish linkages with industries for the promotion of science and technology.
- Develop the spirit of internationalism and competitiveness in students such that they develop new original ideas and make new discoveries and inventions to make a strong society.
- Encourage students for, acquiring self-confidence, self- respect and self-dependence and instill moral values in students making them well disciplined and pay special attention to the improvement of the social and economic conditions
- Develop skills in practical work experiments, equipments and laboratory use along with collection and interpretation of data.

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Rules and Regulations: CEPS

1. These regulations shall be called Guru Gobind Singh Indraprastha University regulations for programs leading to the degree of Doctor of Philosophy (Ph.D.).

2. These regulations are meant to clarify and supplement the provisions of Ordinance 12 (hereafter referred to as the Ph.D. ordinance) to facilitate its uniform interpretation and implementation.

3. These regulations will come into force immediately from the date of notification on the University website. The regulations will also be displayed on the University website.

4. Eligibility Criteria for admission to Ph.D. program would be M.Sc. in Pharmaceutical Chemistry/Organic Chemistry or M.Pharm. in PharmaceuticalChemistry/Pharmacology or M.Sc. (Bioinformatics) or M.Sc. (Microbiology) or M. Tech. (Bioinformatics) or MD/MS, B.Tech.(Physical Sciences/Life Science) (Gate qualified).

5. The Ph.D. program in each available discipline shall be run by the concerned USS, with its Centre Research & Consultancy (CRC) Committee and Steering Committee in compliance with clause 1 of the Ph.D. Ordinance 12

6. Meetings of the CRC may be held as frequently as needed, but at least once in a semester, or at the written request of one-fourth of the total number of CRC members of the school/discipline. The quorum shall be more than half of the total number of CRC members of the school/discipline. The meeting notice shall be released at least three days in advance, clearly mentioning the agenda items. The minutes of all meetings of the CRC and Steering Committee must be circulated to all the faculty members of the school within one week of the meeting.

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Ph.D. Course Work Structure: CEPS

1. The Ph.D. Course Work shall be offered as a Credit System.

2. The Course Work will be for a minimum of One Semester and shall be treated as pre Ph.D. Preparation.

3. The course work will have14 credits maximum and six credits minimum to be of sixmonths semester duration.

4. **4** credits for Research Methodology, which includes Research Methodology, quantitative methods, computer application, tools, and techniques include instrumentation, communicationskills, seminar presentation and review of research paper and is mandatory and two credits for Research and Publications Ethics (RPE). The course is meant for awareness about thepublication ethics and publication misconduct.

5. **8** credits for subject (3 subjects of specialization) course work.

S. No.	Particulars of the Course	Learning Hours per week	Examination Type	Examination Scheme			Credits
				Mid Term (01)	End Term (02)	Sum Total (01+02)	
1.	Research Methodology (R.M.)	04	Theory	25	75	100	04
2.	Research and Publication Ethics(RPE)	02	Theory	12.5	37.5	50	02
3.	Subject Specialization (01)	02	Theory	12.5	37.5	50	02
4.	Subject Specialization (02)	04	Theory	25	75	100	04
5.	Subject Specialization (03)	04	Theory	25	75	100	04
6.	Subject Specialization (04)	02	Theory	12.5	37.5	50	02
7.	Subject Specialization (05)	02	Theory	12.5	37.5	50	02
8	Subject Specialization (06)	04	Theory	25	75	100	04
9	Subject Specialization (07)	04	Theory	25	75	100	04
10	Subject Specialization (08)	04	Theory	25	75	100	04
11	Subject Specialization (09)	04	Theory	25	75	100	04
12.	*Subjection Specialization along with Practical	08	Theory + Practical	25	75	100	06
Total				250	750	1000	**42**

* 1 &2 are compulsory, and ten credits may opt from 3-12

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Research Methodology (RM)

Course Code: PPC-601 **Maximum Marks: 25 + 75 (CE)**
Credits: 04

Instruction to Paper Setters:	**Time: 3 hours**
Attempt five questions	
• Student has to attempt any **five questions** from eight questions.	
• All questions are of 15 marks each.	

Course Objectives:

1. To provide students with knowledge, general competence, and analytical skills in Research Methodology.
2. To build their foundation for research in interdisciplinary areas like Mathematics, Bio Sciences, Physics, Chemistry and Pharmaceutical sciences.
3. To familiarize participants with basic of research and the research process.
4. To enable the participants in conducting research work and formulating research synopsis and report.
5. To identify and discuss the concepts and procedures of sampling, data collection, analysis and reporting.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- Develop understanding on various kinds of research, objectives of doing research, research process, research designs and sampling.
- Have basic knowledge on qualitative research techniques.
- Have adequate knowledge on measurement & scaling techniques as well as the quantitative data analysis.
- Have basic awareness of data analysis-and hypothesis testing procedures.

1. **Foundations of Research:** Meaning, Objectives, Motivation, Utility. Concept of theory, empiricism, deductive and inductive theory. Characteristics of scientific method-Understanding the language of research-Concept, Construct, Definition, Variable. Research Process. **(6 hrs.)**
   Problem Identification & Formulation-Research Question-Investigation Question-Measurement Issues-Hypothesis-Qualities of a good Hypothesis-Null Hypothesis & Alternative Hypothesis. Hypothesis Testing-Logic & Importance. **(6 hrs.)**
2. **Research Design:** Concept and Importance in Research-Features of a good research design-Exploratory Research Design-concept, types and uses, Descriptive Research Designs-concept, types, and uses. **(5hrs.)**
   Experimental Design: Concept of Independent & Dependent variable **(1hr)**
3. **Qualitative and Quantitative Research:** Qualitative research-Quantitative research-Concept of measurement, causality, generalization, replication. Merging the two approaches. **(6hrs.)**

4. **Measurement:** Concept of measurement-what is measured? Problems in measurement in research-Validity and Reliability. Levels of measurement-Nominal, Ordinal, Interval, Ratio. **(4hrs.)**
5. **Sampling:** Concepts of Statistical Population, Sample, Sampling Frame, Sampling Error, Sample Size, Non-Response. Characteristics of a good sample. Probability Sample-Simple Random Sample, Systematic Sample, Stratified Random Sample & Multi-stage sampling. Determining the size of the sample-Practical considerations in sampling and size. **(8 hrs)**
6. **Data Analysis:** Data Preparation-Univariate analysis (frequency tables, bar charts, pie charts, percentages), Bivariate analysis-Cross tabulations, and Chi-square test, including the testing hypothesis of association. **(4 hrs.)**
   Interpretation of Data and Paper Writing-Layout of a Research Paper, Journals in Sciences, Impact factor of Journals, When and Where to publish? Ethical issues related to publishing, Plagiarism, and Self-Plagiarism. **(5hrs.)**
7. Use of Encyclopedias, Research Guides, Handbook, etc., Academic Databases for Computer Science Discipline. **(3 hrs.)**
8. **Use of Tools/Techniques for Research:** Methods to search required information effectively, Reference Management Software like Zotero/Mendeley, Software for paper formatting like LaTeX/M.S. Office, Software for detection of Plagiarism. **(8 hrs.)**

Suggested Reading:

1. Kothari C.R., *Research Methodology,* New Age International Publishers, 2nd Edition, (2006).
2. Cooper Donald and Schindler Pamela, *Business Research Methods,* TMGH, 9th Edition, (2006).
3. Black, Ken, *Business Statistics, Wile Black, Ken, Business Statistics: For Contemporary Decision Making*, Wiley, 5th Edition, (2007).
4. Zikmund, William G., *Business Research Methods,* Thomson, 7th Edition, (2006).
5. Kumar Ranjit, *Research Methodology,* Delhi: Pearson Education, (2006).
6. Gibaldi Joseph, *MLA Handbook for Writers of Research Papers,* New Delhi: Affiliated East-West Press, 5th Edition, (1999).
7. Kothari C.K., *Research Methodology: Methods and Techniques,* Wilsey Eastern Limited, New Delhi, (1980).
8. Bryman Alan & Bell Emma, *Business Research Methods,* Oxford University Press.

Reference:

1. Web Sources
2. Relevant Research Articles from the original research work and review articles published in peer-reviewed journals of international repute.

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Research and Publication Ethics (RPE)

Paper Code: PPC-603 **Maximum Marks: 25+75 (CE)**
Credits: 02

Instruction to Paper Setters: **Time: 3 hours**

Attempt five questions

- Student has to attempt any **five questions** from eight questions.
- All questions are of 15 marks each.

Course Objectives:

1. To build an ethical research and publishing culture through awareness.
2. To promote academic integrity and publication ethics among doctoral students, researchers and faculty members.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- By the end of the Course, students will be able to understand the importance of being ethics in carrying out research and publication activities.
- They will be able to differentiate the quality publication practices
- The learners will also get acquainted with the software/databases which are necessary for carrying out research work.
- The learner would have sound knowledge of Indexing and citation databases, open access publications, research metrics (citations, h-index, Impact Factor etc).
- The student would be able present plagiarism tools for a valid and ethical research report.

1. Philosophy and Ethics **(3 hrs.)**

Introduction to Philosophy:definition, nature and scope, concept, branches
Ethics: definition, moral philosophy, nature of moral judgments and reactions

2. Scientific conduct **(5 hrs.)**

Ethics with respect to Science and Research
Intellectual honesty and research integrity
Scientific misconducts: Falsification, Fabrication, and Plagiarism(FFP)
Redundant publications: Duplicate and overlapping publications, salami slicing
Selective reporting and misrepresentation of data

3. Scientific conduct **(7 hrs.)**

Publication ethics: definition, introduction, and importance
Best practices/standard-setting initiatives and guidelines: COPE, WAME, etc
Conflict of interest
Publication misconduct: definition, concept problems that lead to unethical behavior and vice versa types
Violation of publication ethics, authorship, and contributorship
Identification of publication misconduct, complaints, and appeal
Predatory publishers and Journals
Practice

4. Open access Publishing **(4hrs.)**

Open access publications and initiatives
SHERPA/RoMEO online resource to check publisher copyright & self-archiving policies
A software tool to identify predatory publications developed by SPPU
Journal finder / Journal suggestion tools viz. JANE, Elsevier Journal Finder, Springer Journal Suggester, etc.

5. Publication Misconduct **(4hrs.)**

A. Group Discussions

Subject-specific ethical issues, FFP, authorship
Conflicts of interest
Complaints and appeals: examples and fraud from India and abroad

B. Software tools

Use of plagiarism software like Turnitin, Urkund, and other open-source software tools

6.Databases and Research Metrics ((7hrs.)

A. Databases

Indexing databases
Citation databases: Web of Science, Scopus, etc.

B. Research Metrics (3 hrs.)

Impact Factor of a journal as per Journal Citation Report, SNIP, SJR, IPP, Cite Score.
Metrics: h-index, g index, i10 index, altmetrics

References

1. Bird A., *Philosophy of Science*, Routledge (2006).
2. MacIntyre Alasdair,*A Short History of Ethics,*London(1967).
3. Chaddah P.,*Ethics in Competitive Research: Do not get scooped; do notget plagiarized*, ISBN:9789387480865 (2018).
4. National Academy of Sciences, National Academy of Engineering and Instituteof Medicine, *On Being a Scientist: A Guide to Responsible Conduct inResearch*, Third Edition, National Academies Press(2009).
5. Resnik D. B.,*What is ethics in research & why is it important*. National Institute of Environmental Health Sciences, 1—10. Retrievedfrom https://www.niehs.nih.gov/researcwresources&bioethics/whatis/index.cfm(2011).
6. Beal J., *Predatory publishers are corrupting open access.* Nature, 489(7415), 179 -179. (https://doi.org/l O. 1038/489179a) (2012)
7. Indian National Science Academy (INSA), *Ethics in Science Education, Research and Governance*, ISBN:978-81-939482-l-7(2019).https://www.insaindia.res.in/pdf/ Ethics_book.pdf

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Pharmaceutical Chemistry (PC)

Paper Code: PPC-605 **Maximum Marks: 25 + 75 (CE)**
Credits: 02

Instruction to Paper Setters: **Time: 3 hours**

Attempt five questions

- Student has to attempt any **five questions** from eight questions.
- All questions are of 15 marks each.

Course Objectives:

1. To give the knowledge of organic chemistry at an advanced level and mainly aimed at the stereochemistry and different organic named reactions including preparations of reactive intermediates.
2. To design a stereo selective synthesis of new chemical entities (NCE) for the treatment of different diseases in new Drug Discovery Program.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- Understand the chemistry of drugs with respect to their pharmacological activity.
- Understand the drug metabolic pathways, adverse effect and therapeutic value of drugs.
- Know the Structural Activity Relationship (SAR) of different class of drugs.
- Account for reactivity/stability of compounds.

1. **Pharmaceutical Organic Chemistry:** Methods of determining reaction mechanisms (kinetic and non-kinetic methods); Energy profile diagrams, reaction intermediates, crossover experiments, and isotopic labeling; Order of reactions, reversible, consecutive and parallel reactions, solvent, ionic strength, and salt effects; Multi-component reactions of pharmaceutical importance such as Biginelli reaction, Hantzsch reaction, Ugi reaction, Passerini reaction, and Strecker synthesis. **(10 hrs.)**

2. **Pharmaceutical Medicinal Chemistry:** General principles, Identification, and study of targets for development of various therapeutic agents, Rational approach for drug design, Computer-aided drug design, a study of recently developed drugs and molecules in the development pipeline. **(9 hrs.)**

3. **Organic Chemistry of Drug Design & Drug Action:** Structure-based drug designing and target-based drug designing, case studies with successful examples. **(9 hrs.)**

Suggested Reading:

1. Wolff Manfred E., *Burgers Medicinal Chemistry,* 8th Edition, 8 Volume Set, John Wiley & Sons, (2010).
2. Roberts S.M. and Price B.J., *Medicinal Chemistry-The Role of Organic Chemistry in Drug Research,* Academic Press, (1985).
3. Wilson and Gisvold, *Textbook of Medicinal and Pharmaceutical Chemistry,* 12th Edition, Lippincott Williams & Wilkins, New York.
4. Foye William, *Principles of Medicinal Chemistry,* Lippincott Williams & Wilkins, New York, (2014).

5. Smith Michael B., *Organic Synthesis,* 3rd Edition, Mac Graw Hill, (2001).

Reference:

1. Web Sources
2. Relevant Research Articles from the original research work and review articles published in peer-reviewed journals of international repute.

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Natural Product (NP)

Paper Code: PPC-607 **Maximum Marks: 25 + 75 (CE)**
Credits: 04

Instruction to Paper Setters: **Time: 3 hours**

Attempt five questions

- Student has to attempt any **five questions** from eight questions.
- All questions are of 15 marks each.

Course Objectives:

1. To learn about nomenclature, Structure and physiological action of Alkaloids, Steroids, Terpenes, Carbohydrates etc..
2. Classification, structural elucidation by chemical degradation.
3. To learn source, extraction, processing, chemistry & applications of natural products used in pharmaceutical industry.
4. Synthesis of Natural products and drugs by using proper mechanisms.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- Understand & explain tools & techniques used in study of biosynthetic pathways in plants.
- Explain source, chemistry & applications of drugs.
- Understand & explain underlying reasons as why natural products are appropriate material in discovering new drugs.
- Explain source, extraction, processing, chemistry & applications of natural products used in pharmaceutical industry.

1. Introduction use of natural products in traditional medicines, the potential of natural products, Natural products in drug discovery and development, Drugs from nature. **(4 hrs.)**

2. **Recent Development in the Research on Natural Medicinal Products**: Introduction, Biological and Pharmacological activities, Isolation, and characterization studies of the different classes of Phytoconstituents (Alkaloids, Glycosides, Steroids, Saponins, etc.). **(10 hrs.)**
3. **Natural Product Drug Discovery from Different Sources (Marine, Microbial, Mineral, etc.)**: Introduction, recent development, methods of extraction and Isolation, applications, etc. **(10 hrs.)**
4. **Extraction and Isolation Techniques:** Introduction, Principle, and Applications of different extraction & isolation methods viz. Soxhlet extraction, microwave extraction, supercritical fluid extraction, solid-phase extraction, Column chromatography, Flash chromatography, etc. **(16 hrs.)**
5. **Biosynthesis &Biomemetic Synthesis:** Biosynthesis of mono-, sesqui-, di & triterpenoids, squalene, chalcones&stilbene biosynthesis, biomimetic synthesis with the latest examples. **(14 hrs.)**

Suggested Reading:

1. Mabry & Markham, *Systematic Identification of Flavonoid Compounds,* Springer (1970).
2. Apsimon John, T*otal Synthesis of Natural Products,* Vol 18, (1992).
3. Thomson R.H., *The Chemistry of Natural Products,* 2nd Ed., Springer (2007).
4. Rahman Atta-Ur, *Chemistry of Natural Products,* Vol 1-46, Elsevier (Science Direct), (2015).
5. Ross Ivan A., *Medicinal Plants of the World,* Vol. 1-3, Springer, (2005).
6. Kirtikar K.R. &BasuBishen D., *Indian Medicinal Plants,* 2nd Edition, Vol. 1-4, (1991).
7. Runeckles V.C. (Ed.), *Recent Advances in Phytochemistry,* Vol. 1-9, Elenum Press, (1975).
8. Nakanishi Koji (Ed.), *Natural Products Chemistry,* Vol. 1-3, (1983).
9. Trease and Evans, *Pharmacognosy,* 16th Edition, Baillier-Tindall, (2009).

Reference:

1. Web Sources
2. Relevant Research Articles from the original research work and review articles published in peer-reviewed journals of international repute.

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Asymmetric Synthesis (AS)

Paper Code: PPC-609 **Maximum Marks: 25 + 75 (CE)**
Credits: 04

Instruction to Paper Setters: **Time: 3 hours**

Attempt five questions

- Student has to attempt any **five questions** from eight questions.
- All questions are of 15 marks each.

Course Objectives:

1. Develop a fundamental understanding of the concepts of stereoisomerism, optical activity and chirality.
2. Learn the principle methods that are used to prepare enantiomerically pure products from achiral starting materials.
3. Learn various commercial processes from individual case-studies involving chiral synthesis currently practiced in the pharmaceutical sectors including (a) classical resolutions, (b) asymmetric synthesis, (c) biological methods (d) immobilization and membrane technologies.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- Discover reactions that will reliably provide optically pure compounds in a wide variety of systems.
- Determine which strategic bond constructions can be used most effectively to obtain synthetic targets with high stereoselectivity.
- Develop effective strategies for using chiral auxiliaries, catalysts, and the substrate to control stereochemical relationships.
- Become adept at identifying strengths and weaknesses of particular methods, and determine which one will be optimal for a particular synthetic operations.

1. **General Concept:** Differentiation of molecules, group selectivity, topicity and prochirality, substrate and product selectivities, necessary conditions for stereoselectivity, the concept of enantio/diastereo differentiation, methods of inducing stereo-selectivity, strategies for stereoselective synthesis, kinetics and thermodynamics of stereoselective reactions, modifications of CIP classification of chirality- constitutional properties of a CIP system, continuous symmetry measure of chirality-degree of shape chirality, topological chirality and significance of drug stereochemistry. Use of Chiral auxiliaries in the synthesis of chiral drugs. **(14 hrs.)**

2. **Determination of EnantiomericPurity:** Various tools, chiral derivatizing agents, chiral shift reagents, chiral solvating agents. Racemization, Separation of enantiomers by Kinetic resolution, enzymatic resolution, and chromatography.

(9hrs.)

3. **EnantioselectiveSynthesis:** Stereoselective catalytic reduction- homogeneous hydrogenation (chiral ligands, the effect of solvent/ pressure/ temperature/ addendum, substrate dependence of enantioselectivity, mechanistic aspects), stereoselective heterogeneous hydrogenation, hydrogenation, hydrosilylation, hydrocyanation; stereoselective oxidation – enantio /diastereoselective epoxidation and dihydroxylation, ligand accelerated catalysis; Asymmetricalkylation; Self-replication of chirality- catalytic self-replicating molecules, control of Chirality memory, Pi -stacking effect, selectivity and mechanism of asymmetric catalytic synthesis.

(18 hrs.)

4. **Stereoselective C-C Bond Formation:** Nucleophilic addition to C=X (X=C, O, S, N), Stereoselectivehydroformylation, Pericyclic reaction – asymmetric induction in [3+2] and [2+2] cycloaddition,stereoselectivecarbene addition, chirality transfer in sigmatropic rearrangements.Ring annulations with reference to Baldwin's rule. **(14hrs.)**

Suggested Reading:

1. Nasipuri D., *Stereochemistry of Organic Compounds – Principles & Applications,* 2nd Ed., New Age Publication, (2005).
2. Eliel Ernest L. &Wilen Samuel H., *Stereochemistry of Organic Compounds,* 1st Ed., Wiley, (1994).
3. Bassendale Alan, *The Third Dimension in Organic Chemistry,* 3rd Ed., John Wiley & Sons, (1984).
4. Stephenson G.R., Nogradi, *Asymmetric Synthesis,* 3rd Ed., John Wiley, and Sons, (1984).
5. Izumi Y. & Akira Tai, *Stereo Dif ferentiating Reactions,* 3rd Ed., Academic Press, (1977).
6. Morrison J.D. and Moscher H.S., *Asymmetric Organic Reactions,* Vol. 3, Academic Press, (1984).
7. Hawley Robert E. & Aube Jeffrey, *Principles in Asymmetric Synthesis,* 2nd Ed., Elsevier, (2012).
8. Smith Michael B. and March Jerry, *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure,* (2007).
9. Warren Stuart, *Designing Organic Synthesis,* 1st Edition, (1978).
10. Carey Francis A., Sundberg Richard J., *Advanced Organic Chemistry: Reactions and Synthesis,* Part-B, *Reaction & Mechanism,* (2007).
11. Carruthers William, Coldha Lain, *Modern Methods of Organic Synthesis,* (2004).
12. Gould, *Mechanism, and Structure in Organic Chemistry,* (2010) Digitized.

Reference:

1. Web Sources
2. Relevant Research Articles from the original research work and review articles published in peer-reviewed journals of international repute.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL CHEMISTRY
GURU GOBIND SINGH INDRAPRASTHA UNIVERSITY
SECTOR-16C, DWARKA, NEW DELHI-110078

Principles of Peptide Chemistry (PPC)

Paper Code: PPC-611 **Maximum Marks: 25 +75 (CE)**
Credits: 02

Instruction to Paper Setters: **Time: 3 hours**

Attempt five questions

- Student has to attempt any **five questions** from eight questions.
- All questions are of 15 marks each.

Course Objectives:

1. Ability to define common research objectives of those involved in research of biological, biochemical and physicochemical properties of peptides and proteins.
2. Introduce the structure and biological activity of peptides and proteins.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- Understand the basic concept of peptide synthesis.
- Understand the strategy and mode of peptide synthesis.
- Understand the synthesis of peptidomimetrics and structure activity relationship of biologically active peptides.

1. Importance of peptides in drug discovery, peptidomimetics in drug discovery. **(1hrs.)**

2. **Protection and Deprotection of Amino Acids:** General aspects, need for protection, minimal versus global protection, protection of amino group by acid and labile base groups, protection of carboxyl group, the concept of orthogonal protection in peptide synthesis, importance of side-chain functional groups protection and details of protective groups used for masking individual amino acids, methods used for deprotection. **(7 hrs.)**

3. **Coupling reactions in peptide synthesis.** **(4hrs.)**

4. **Side Reactions in Peptide Synthesis:** Deletion peptides, side reactions initiated by proton abstraction, protonation, over-activation, and side reactions of individual amino acids. **(4 hrs.)**
5. **Segment and sequential strategies for solution-phase peptide synthesis with case studies**. **(5hrs.)**

6. **Principle of Solid Phase Peptide Synthesis, t-BOC and FMOC Protocols, Various Solid Supports and Linkers:** Activation procedures, peptide bond formation, deprotection and cleavage from the resin, low and high H.F. cleavage protocols, the formation of free peptides and peptide amides, purification and case studies, site-specific chemical modifications of peptides. **(7hrs.)**

Suggested Reading:

1. Varki A., Cummings Richard, Esko Jeffrey, Hart Hudson Freeze Gerald, Marth Jerrey (Ed.), *Essentials of Glycobiology,* Gold Spring Harbar Lab Press, (1999).
2. Wong Chi Huey and Whitesides G.M., *Enzymes in Synthetic Organic Chemistry,* Vol. 12, Pergamon, (2013).
3. Glasel J.A. and Dentscher Murray P. (Ed.), *Introduction to Biophysical Methods in Protein and Nucleic Acid Research,* Academic Press, (1995).
4. Wang Y. John and Pearlmer Rodney, *Stability and Characterization of Protein & Peptide of Drugs,* Springer, (1993).
5. Reid Ronard E. (Ed.), *Peptide and Protein Drug Analysis,* Marcell Deckker, (2000).
6. Nolting B., *Methods in Modern Biophysics,* Springer, (2010).

Reference:

1. Web Sources
2. Relevant Research Articles from the original research work and review articles published in peer-reviewed journals of international repute.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL CHEMISTRY
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SECTOR-16C, DWARKA, NEW DELHI-110078

Carbohydrate Chemistry (CC)

Paper Code: PPC-613 **Maximum Marks: 25 + 75 (CE)**
Credits: 02

Instruction to Paper Setters: **Time: 3 hours**

Attempt five questions

- Student has to attempt any **five questions** from eight questions.
- All questions are of 15 marks each.

Course Objectives:

1. Aims to provide a sound understanding of the fundamentals of the chemistry of carbohydrates.
2. Discuss the chemistry and functions of Carbohydrates.
3. Describe methods for identification of carbohydrates.
4. Illustrate the chemical structure and stereochemistry of carbohydrates.
5. Know and recognize aldose/ketose, hexose/pentose, pyranose/furanose,α / β.
6. Know the factors that influence the properties of polysaccharides.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- Learn the importance of carbohydrates with examples.
- Classify carbohydrates with examples.
- Discuss isomerism of carbohydrates with examples.
- Explain the chemical reactions of monosaccharides.
- Enumerate the biologically important sugar derivatives of monosaccharides with examples.
- Understand the reducing sugar assay and the total sugar assay.

Definition and Classification of Sugars, Nomenclature, Aldoses, and Ketoses, Configuration of (+)- Glucose: The Fischer proof, ring structures, and conformation, mutarotation, anomericity, naturally occurring monosaccharides, oligosaccharides and polysaccharides, the three-dimensional structure of macromolecular carbohydrates. **(4 hrs.)**

Methods for Isolation, purification, structural analysis, complete and partial hydrolysis, methylation analysis, Smith degradation, chromatographic and electrophoretic techniques, and advanced spectroscopic techniques including fast atom bombardment mass spectrometry and two-dimensional NMR. **(6 hrs.)**

Chemical reactions of carbohydrates, oxidation, reduction, formation of derivatives, glycosides, ethers esters and cyclic acetals, modern chemical transformations, methods for the formation and cleavage of O-glycosidic bond, use of protecting groups, chemical and enzymatic synthesis of oligosaccharides, carbohydrates as chiral synthons for natural products synthesis. **(10 hrs.)**

Carbohydrate biopolymers, animal glycoproteins, blood-group substances, plant and algal glycoproteins, proteoglycans and glycosaminoglycans, glycolipids, the structural basis for the biological functions of glycan chains in glycoconjugates, carbohydrates and biological molecular recognition, carbohydrate components of nucleic acids, and antibiotics. **(8 hrs.)**

Suggested Reading:

1. Osborn H.M.I., *Carbohydrates,* Academic Press, (2003).
2. Khan Shaheer H. and O'Neill Roger 'A', *Modern Methods in Carbohydrate Synthesis,* Harward Publishing Publishers, (1996).
3. Hale K.J. and Boons G.J., *Organic Synthesis with Carbohydrates,* Academic Press, (2008).
4. Collins J.M. and Ferrier Rober J.,*Monosaccharides.Their Chemistry and Their Roles in Natural Products,* Wiley and Son, (1995).
5. Varki A., Cummings Richard, Esko Jeffrey, Hart Hudson Freeze Gerald, Marth Jerrey (Ed.), *Essentials of Glycobiology,* Gold Spring Harbar Lab Press, (1999).
6. Kennedy J.F. and White *C.A., Bioactive Carbohydrates*, Ellis Horwood, New York, (1983).
7. Binkley, R.W., *Modern Carbohydrate Chemistry,* Marcell and Dekker, New York, (1988).
8. Kennedy J.F., *Carbohydrate Chemistry,* Oxford University Press, Oxford, (1988).
9. Hanessian S., *Total Synthesis of Natural Products: The Chiron Approach,* Pergamon, Oxford, (1983).

Reference:

1. Web Sources
2. Relevant Research Articles from the original research work and review articles published in peer-reviewed journals of international repute.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL CHEMISTRY
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SECTOR-16C, DWARKA, NEW DELHI-110078

Advanced Topics in Drug Action and Drug Design (ATDD)

Paper Code: PPC-615 **Maximum Marks: 25 + 75 (CE)**
Credits: 04

Instruction to Paper Setters: **Time: 3 hours**

Attempt five questions

- Student has to attempt any **five questions** from eight questions.
- All questions are of 15 marks each.

Course Objectives:

1. Develop your knowledge and understanding of how drugs and medicines are made and used safely.
2. Learn about research methods which are key to understanding modern drug discovery and development.
3. Focus on small molecule drug discovery.
4. The basis of the drug discovery process will be described and the phases of drug development discussed.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- The latest screening protocols for lead identification from large compound libraries.
- The inherent toxicity problems of synthetic, small molecule drugs.
- Learn a range of targets for drug discovery.
- Learn how small molecule drug affects.

1. Molecular recognition and supramolecular chemistry; Molecular associations involving weakinteractions; Solvation effects on molecular associations, hydrogen bonding especially weak, cation-π interaction, π-π interaction, and arenes interactions. **(18hrs.)**

2. Metalloenzymes in medicinal chemistry; Metals in medicine- reversible and irreversible enzyme inhibition; Mechanisms of drug activation; Enzyme activation of drugs; Bioprocess prodrugs, the chemistry of metabolic reactions; Organic chemistry of drug metabolism-conjugation reactions, reductive reactions, oxidative reactions. **(18 hrs.)**

3. Molecular interaction fields- Molecular electrostatic potentials in understanding drug action; Drug action on biomembranes- organic chemistry of drug permeability through membranes; Molecular similarity and molecular diversity in drug design. **(18 hrs.)**

Suggested Reading:

1. Patrick Graham, *Introduction to Medicinal Chemistry,* 5th Ed., Oxford (1995).
2. Silverman R.B., *The Organic Chemistry of Drug Design and Drug Action,* 3rd Ed., Academic Press, (2011).
3. Nogrady T., Weaver D.F., *Medicinal Chemistry: A Molecular and Bio-Chemical Approach,* 3rd Ed., Oxford, (2005).

4. Roth Herman J., Kelemon Axel, Wenger T. Beiss, Horwood Ellis, *Pharmaceutical Chemistry and Drug Synthesis,* (1988), Digitized (2008).
5. Ledneiser Daniel, *Strategies for Organic Drug Synthesis and Design,* 2nd Ed., Wiley, (2008).
6. Sheldon Roger A., *Chirotechnology Industrial Synthesis of Optically Active Compound,* Marcel Decker (1993).
7. Wolf Manfred B., *Burger's Medicinal Chemistry and Drug Discovery,* Wiley, (2014) Digitized.
8. Hantzsch J.B., *Comprehensive Medicinal Chemistry,* Vol 1-5.
9. Ledneiser D., *Organic Drug Synthesis,* Vol 1-7, Wiley, (2007).
10. NassarAla F., *Drug Metabolism Handbook Concepts and Applications Edited,* Wiley, (2000).
11. Gringauz A., *Introduction toMedicinal Chemistry How Drugs Act and Why,* Wiley, (2006).
12. Buckingham A.D., *Principles of Molecular Recognition,* Academic Press, (1993).

Reference:

1. Web Sources
2. Relevant Research Articles from the original research work and review articles published in peer-reviewed journals of international repute.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL CHEMISTRY
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SECTOR-16C, DWARKA, NEW DELHI-110078

Synthetic Strategies in the Total Synthesis of Complex Organic Molecules (SSOM)
Paper Code: PPC-617 **Maximum Marks: 25 + 75 (CE)**
Credits: 04

Instruction to Paper Setters: **Time: 3 hours**

Attempt five questions

- Student has to attempt any **five questions** from eight questions.
- All questions are of 15 marks each.

Course Objectives:

1. The complete chemical synthesis of a complex molecule, often a natural product, from simple, commercially-available precursors.
2. To gain a better understanding of their structures. Synthesis also enables chemists to produce compounds that do not form naturally for research purposes.
3. To provide opportunities to test the applicability and scope of newly developed methods, to discover and develop new synthetic reactions, and to render natural and designed. molecules readily available for biological investigations.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- The application of retrosythetic analysis in organic synhtesis.
- Understand the special emphasis on bio-active natural products synthesis which gives an idea of planning, design, understanding the mechanistic implications.
- Execute of synthetic organic chemistry which is pivotal in organic chemistry.
- Theoretically devise strategies for the synthesis of simple to complex organic molecules synthesis.

1. **Retrosynthetic Analysis, Disconnections, and Reliability of ReactionsSynthons:**Donor and acceptor, functional group interconversions, one group carbon-heteroatom, and carbon-carbon disconnections, two group carbon-heteroatom and carbon-carbon disconnections, chemo-,regio-and stereoselectivity considerations, natural reactivity and umpolung. **(14hrs.)**

2. **General Synthetic Reaction Patterns and Strategies:**Aliphatic nucleophilic and electrophilicsubstitutions, aromatic nucleophilic and electrophilic substitutions, addition to carbon-carbon and carbon-heteroatom multiple bonds, eliminations, rearrangements, oxidations, and reductions. **(14hrs.)**

3. **Chemistry of Protecting Groups and Deprotection:**Protection and Deprotectionfor alcohols, carbonyl groups, carboxylic groups, and amino groups. **(14 hrs.)**

4. **Applications of Synthetic Strategies in the Total Synthesis of Selected Organic Molecules:**(a) Progesterone (b) Reserpine (c) Penicillin (d) Prostaglandin (e) Taxol with case studies. **(14 hrs.)**

Suggested Reading:

1. Carruthers W., *Some Modern Methods of Organic Synthesis,* 1st Ed., Reprint, Cambridge University Press, (1986).
2. Smith B. Micheal, *Organic Synthesis,* 3rd Ed., Elsevier, (2011).
3. Meckie R.K., Smith D.M. &Atken R.A., *Guidebook to Organic Synthesis,* 3rd Ed., Longman Publishing Co., (1990).
4. Fieser&Fieser, *Reagents for Organic Synthesis,* Vol. 1-26, Wiley, (2011).
5. Reich and Rigby, *Handbooks of Reagents for Organic Synthesis,* Set of Volume, (2007).
6. Warren S., *Designing Organic Synthesis,* Wiley, (1978)
7. Carruthers W., *Some Modern Methods of Organic Synthesis,* 4th Ed., Cambridge University Press, (2004).
8. House H.O. &Benjamin W.A., *Modern Synthetic Reactions*2nd Ed., (1965).

Reference:

1. Web Sources
2. Relevant Research Articles from the original research work and review articles published in peer-reviewed journals of international repute.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL CHEMISTRY
GURU GOBIND SINGH INDRAPRASTHA UNIVERSITY
SECTOR-16C, DWARKA, NEW DELHI-110078

Organometallic and Sustainable Chemistry in Synthesis of Pharmaceuticals (OSCP)

Paper Code: PPC-619 **Maximum Marks: 25 + 75 (CE)**
Credits: 04

Instruction to Paper Setters: **Time: 3 hours**

Attempt five questions

- Student has to attempt any **five questions** from eight questions.
- All questions are of 15 marks each.

Course Objectives:

1. The course is intended that the students acquire the right skills to know and relate the structure, properties, reactivity, and applications of main-group and transition-metal derived organometallic compounds in organic synthesis.
2. This course is intended to acquire skills in the synthesis and manipulation of organometallic compounds as well as in the use of appropriate technique for the study and characterization of these compounds.
3. To make students understand the principles and goals of green chemistry.
4. To acquaint with the concept of green solvents and to understand the need for alternative solvents.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- Recognize and classify the different types of main-group and transition-metal derived organometallic compounds.
- Know about the stability and reactivity (stoichiometric and catalytic) of the various types of organometallic compounds.
- Apply the appropriate characterization technique to the analysis of organometallic compounds.
- Know and demonstrate the utility of the organometallic compounds to the synthesis of drugs, especially by catalytic methods.
- Distinguish between a green-process and non-green process.
- Design alternative routes of synthesis which is greener, cleaner and cost-effective.

1. **Carbon-Carbon and Carbon-Heteroatom Coupling Reactions:** Suzuki, Hiyama, Stille, Negishi, Kumada, Heck, Sonogashira, Ullmann, Chan-Lam, Buchwald-Hartwig reactions; Cross-coupling of unactivated arenes; Use in the synthesis of pharmaceutically important molecules. **(10 hrs.)**

2. **Metathesis:**Grubbs (first and second generation) and Schrock catalysts, Olefin, alkyne, ring-closing,ring-opening, and multiple metatheses; Application in the synthesis of heterocycles, natural products, andpharmaceuticals. **(10 hrs.)**

3. **Green Chemistry:** Principles, metrics, pharmaceutical industries; Green discoveries, greener reactions, catalysis, alternative reaction media, greener technologies; Sustainable synthesis of pharmaceuticals. **(10 hrs.)**

4. **Click Chemistry:** Click reactions, criteria, water as a solvent; Huisgencycloaddition, nucleophilic ring-opening of epoxide and aziridine; Use in creating new drug candidates, combinatorial, structure-based, and in situ click chemistry. **(12 hrs.)**

5. **Multi-component Reactions:** Ugi, Passerini, Biginelli, Hantzsch, Mannich, Petasis, Strecker, Kabachnik-fields reactions; Diversity oriented synthesis; Convergent synthesis of pharmaceutically relevant molecules. **(14 hrs.)**

Suggested Reading:

1. Meckie R.K., Smith D.M. &Atken R.A., *Guidebook to Organic Synthesis,* 3rd Ed., Longman Publishing Co., (1990).
2. Fieser&Fieser, *Reagents for Organic Synthesis,* Vol. 1-26, Wiley, (2011).
3. Reich and Rigby, *Handbooks of Reagents for Organic Synthesis,* Set of Volume, (2007).
4. Warren S., *Designing Organic Synthesis,* Wiley, (1978)
5. Carruthers W., *Some Modern Methods of Organic Synthesis,* 4th Ed., Cambridge University Press, (2004).
6. House H.O. &Benjamin W.A., *Modern Synthetic Reactions*2nd Ed., (1965).
7. Warren Stuart, *Designing Organic Synthesis,* 1st Edition, (1978).
8. Gould, *Mechanism, and Structure in Organic Chemistry,* (2010) Digitized
9. Warner John and Anastas Paul,*Green Chemistry: Theory and Practice*, 1st Ed., Oxford University Press (2000) Reprint.
10. Lancaster Mike, Scott Janet, Wilson Karen, *Green Chemistry: Introductory Text*, 1st Ed., Royal Society of Chemistry (London) (2010).
11. Ryan M.A. and Tinnesand M., *Introduction to Green Chemistry*, 1st Ed., American Chemical Society (Washington) (2003).
12. Matlack*, Introduction to Green Chemistry*, 2nd Ed., CRC Press, (2010).
13. TundoPietro, PerosaAlvise, Zecchin F., *Methods, and Reagents for Green Synthesis: An Introduction,* 1st Ed., Wiley, (2007).
14. Cann Michael C. and Connelly M.E., *Real-world cases in Green Chemistry*, American Chemical Society (Washington), (2000).
15. Cann M.C. and Umile T.P., *Real world cases in Green Chemistry* (Vol 2), American Chemical Society (Washington) (2000).
16. Anastas Paul T., PeroraAlvize, Selva Maurizio, *Handbook of Green Chemistry-Green Catalysis,* 1st Ed., Wiley-VCH, (2013).

Reference:

1. Web Sources
2. Relevant Research Articles from the original research work and review articles published in peer-reviewed journals of international repute.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL CHEMISTRY
GURU GOBIND SINGH INDRAPRASTHA UNIVERSITY

Principles of Biological Sciences

Paper Code: PPC-621 **Maximum Marks: 25 + 75 (CE)**
Credits: 04

Instruction to Paper Setters: **Time: 3 hours**

Attempt five questions

- Student has to attempt any **five questions** from eight questions.
- All questions are of 15 marks each.

Course Objectives:

1. To demonstrate the basic knowledge of immunological processes at a cellular and molecular level.
2. To understand the basic of genetic analysis at the gene, genome and population levels.
3. To understand the basic organization of prokaryotic and eukaryotic genomes.
4. To understand the process of neurotransmission, especially chemicals used in the brain and elsewhere to carry signals from nerve terminals to the structures they innervate.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- Identify the cellular and molecular basis of immune responsiveness.
- Understand gene expression and regulation mechanisms.
- Solve genetic problems.
- Examine neurotransmitter release, activation of ligand-gated ion channels, receptor-mediated modulation of neuronal excitability, and neurotransmitter clearance.
- Describe neurotransmitter and receptor mechanisms and an insight into how membrane excitability elicits functional effects in individual neurons and neuronal networks.

1. **Immunology**: Evolution of immune system, Adaptive and Innate Immunity, Types of Adaptive immunity, Cardinal features of Adaptive immune responses, Features of Innate immune recognition, Mammalian Toll-like receptors, Components of Innate Immunity, Pathways of complement activation, Components of Immune cells, Hematopoiesis/ Maturation, Lymphocyte Classes, Antigen-Recognition Molecules of theImmune System, Antigen binding molecules, Antibody Structure, Fragments of Igmolecule, Hypervariable regions in Ig, Antibody Isotypes, MHC Molecules ClassI andClassII, Germline organization of TCR loci, V(D)J recombination, Junctional Diversity,Positive or Negative selection, Immunity to extracellular bacteria, Mechanisms of immune evasion by bacteria, Immune responses against viruses, Vaccine. **(14 hrs.)**

2. **Genome organization and Gene expression**: Organization of genes in a genome, Gene families and superfamilies: Organization of *sigH*paralogs in the genome. Prokaryotic Gene expression: Synthesis of fatty and mycolic acids, Scheme of FAS II elongation pathways, Promoter's utility in the development of novel screen system, Comparative studies on the organization of kas operon genes in two mycobacterial species, Reporter gene expression for promoter assessment, Differential gene expression

Eukaryotic Genome: Human genome, Genetic and Physical map of Genome, Human Chromosome X, and Mapping position of pF1 on Y-Chromosome Genomic Organization and in silico expression profiling of WDR13 gene; the genesis of ESTs (Expressed Sequence Tag): Exon-Intron Boundaries of Human WDR13 Gene,

Expression analysis of WDR13 in human tissues samples, expression extends across the phylogeny with significant variations in defined tissue-types. **(14 hrs.)**

3. Basic Principal of Pharmacology: Definitions: Pharmacology Drug, Branches of Pharmacology, Sources, and routes of administration of drugs, Absorption, distribution andexcretion of drugs, Bio-transformation of drugs, Mechanisms of action of drugs, Drug toxicity, development of new drugs, The official Publications: Pharmacoepias and Formularies.**(14 hrs.)**

4. Neurotransmitters and Receptor: Neuroeffectorjunctional sites, Transmission at Junctional Regions, Neurotransmitter (N.T.), Criteria for a Neurotransmitter, Synthesis, and Storage of N.T., Release of N.T., Termination of action of N.T., Regulation of Turnover, Receptor, Types and Function Of Receptor, Signal Transduction Pathway, G-Protein Coupled Receptor (GPCR), Effect of agonist, P-agonist, antagonist and reverse antagonist, Dose-response curve, in vivo and in vitro study of receptors, Cloning of Receptors, Non-NT Neurochemicals Influencing Neuronal Activity. **(14 hrs.)**

Suggested Reading:

1. CoicoRichard, Sunshine Geoffrey, *Immunology*, A Short Course, 7th Edition, Wiley-Blackwell (2015).
2. Paul William E., *Fundamental Immunology*, 7th Edition, Lippincot Williams and Wilkinsons, (2013).
3. Primrose Sandy B., TwymanRichard, *Principles of Genome Analysis and Genomics*, John Wiley & Sons, (2009).
4. Golan David E., *Principles of Pharmacology*, Lippincott Williams & Wilkins, (2008).
5. Clark Michelle A., Harvey Richard A., FinkelRichard, Rey Jose A., Whalen Karen, *Pharmacology*,6th Edition, Lippincott Williams & Wilkins, (2011).
6. HalbachOliver Von Bohlen Und, DermietzelRolf, *Neurotransmitters and Neuromodulators*, John Wiley & Sons, (2006).

Reference:

1. Cantor Charles R., Smith Cassandra L., Genomics, *The Science and Technology Behind the Human Genome Project*, John Wiley & Sons, (2004).
2. Pevsner Jonathan, *Bioinformatics, and Functional Genomics*, John Wiley & Sons, (2015).
3. SchermanDaniel, *Advanced Textbook on Gene Transfer, Gene Therapy, and Genetic Pharmacology*, Imperial College Press, (2013).
4. Yoshida HagiharaH., Y., EbashiS., *Neurotransmitters, Receptors*, *Proceedings of the 8th International Congress of Pharmacology*, Elsevier, (2013).
5. Webster Roy, Neurotransmitters, *Drugs and Brain Function*, John Wiley & Sons, (2001).
6. Web Sources
7. Relevant Research Articles from the original research work and review articles published in peer-reviewed journals of international repute.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL CHEMISTRY
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SECTOR-16C, DWARKA, NEW DELHI-110078

Concepts in Drug Design (CDD)

Paper Code: PPC-623 **Maximum Marks: 25 + 75 (CE)**
Credits: 04

Instruction to Paper Setters: **Time: 3 hours**

Attempt five questions

- Student has to attempt any **five questions** from eight questions.
- All questions are of 15 marks each.

Course Objectives:

1. This course will explore the process of drug development, from target identification to final drug registration.
2. It will present drug development as a process involving target selection, lead discovery using computer-based methods and combinatorial chemistry/high-throughput screening.
3. Learn about molecular recognition, computeraided drug design, and toxicology as applied to the development of new medicines.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- Describe the process of drug discovery and development.
- Discuss the challenges faced in each step of the drug discovery process.
- Have gained a basic knowledge of computational methods used in drug discovery.
- Organize information into a clear report.

1. **Computational Molecular Modeling:** Molecular Mechanics (MM), Force Field, Energy minimization, Geometry optimization methods: Linear and non-linear methodsof minimization, Confirmation search different methods: (Systematic Search, RandomSearch, Monte Carlo Methods, Tabu Search, Simulated Annealing, Matrix MethodGenetic Algorithmsetc) Advantages and limitations of a different method. **(4 hrs.)**

2. **Structure-Based Drug Design:** Introduction, Molecular interactions; Protein structure selection-preparation; Binding Site Analysis; Docking; Search algorithms; Scoring methods: Molecular Mechanics, Empirical functions, Knowledge-based, consensus scoring; Grid-based docking, validation of the results; Comparison of different docking software; Rigid docking Vs. Flexible docking methods; Induced fit docking; Covalent docking; Binding affinity calculations; Hydration thermodynamics in lead optimization; Structure-based Virtual screening workflow; De-novo Drug Design methods: Fragment-based drug design, Combinatorial library generation, Scaffold hopping. **(8 hrs.)**

3. **Protein Structure Prediction and Biologics:** Introduction: Homology modeling, Threading method; Template identification; Sequence alignment methods: Sequence-based alignment, Fold based alignment; Model building; Protein-loop refinement; Protein model validation; Protein-protein Docking; Antibody modeling, Protein Engineering tools: Cysteine Scanning, Residue Scanning, protein aggregation analysis. **(6 hrs.)**

4. **Ligand Based Drug Design:** Introduction; 3D-Pharmacophore; Hypothesis development; Validation of the pharmacophore; energy-based pharmacophore; Shape-based search methods for virtual screening.

(8 hrs.)

5. **Quantitative Structure-Activity Relationship (QSAR):** Introduction; Physicochemical properties; Electronic effects: Hammett equation; lipophilicity effects: Hansch equation; steric effects: Taft equation; Descriptors for QSAR: Physicochemical descriptors, Steric descriptors: 1D, 2D, 3D-QSAR; atom-based QSAR, Field-based QSAR; ADME Screening. **(10 hrs.)**

6. **Quantum Mechanics (QM):** Introduction; Difference between Q.M. and MM; Introduction of Hartee-Fock and DFT calculation with the selection of basic set, single point energy calculation, geometry optimization, prediction of pKa, interpretation, and prediction of U.V./Vis, IR and Raman Spectra, identifying HOMO and LUMO-visualization of molecular orbitals and normal modes of vibrations. **(12 hrs.)**

7. **Molecular Dynamics:** Introduction and theory; Ensembles: Canonical and micro-canonical ensemble, Free Energy perturbation method; Total free energy calculation. **(8 hrs.)**

8. **Chemo-informatics Methods in Drug Design:** Introduction to chemo-informatics, Structure fingerprint methods; Structure similarity search/Clustering methods; R-group analysis. **(4 hrs.)**

***To be taken along with practical.**

Suggested Reading:

1. Young David C., *Computational Drug Design: A Guide for Computational and Medicinal Chemist,* Wiley (2009).
2. Silverman R.B., *Organic Chemistry of Drug Design and Drug Action,* 3rd Edition, Academic Press, (2014).
3. Charifson P.S., *Practical Applications of Computer-Aided Drug Design,* Marcel Deckker, (1997).
4. Cohen N.C., *Molecular Modeling in Drug Design,* Online.
5. Goodman J., *Chemical Applications of Molecular Modeling,* RSC, (2004).
6. Guner O.F., *Pharmacophore Perception, Development, and Use in Drug Design,* International University, (2000).
7. Lemke Thomas L. and William David A., *Berger'sMedicinal Chemistry and Drug Design,* 6th Edition, Lippincott, (2008).
8. Purcell William P., *Strategies of Drug Design,* RSC, (2011).
9. Abraham Donald J. and Rotella D.P., *Foye's Medicinal Chemistry,* Vol. 1-8, 7th Edition, Wiley, (2010).
10. Korolkovas A. and Burckhalter J.H., *Essentials of Medicinal Chemistry,* John Wiley, (1976).
11. Veerapandion Pandi, *Structure-Based Drug Design,* Monograph, Vol. II and III, Academic Press.

Reference:

1. Leach A.R., *Molecular Modeling.*

1.

CENTRE OF EXCELLENCE IN PHARMACEUTICAL CHEMISTRY
GURU GOBIND SINGH INDRAPRASTHA UNIVERSITY
SECTOR-16C, DWARKA, NEW DELHI-110078

Computational Drug Design Practical (CDDP)

Paper Code: PPC-651 **Maximum Marks: 25 + 75 (CE)**
Credits: 04

Course Objectives:

1. Providing students with the basic concepts and tools to manage the 3D structure of proteins in the perspective of drug design using Web-based and stand-alone tools.
2. Covering the key areas of computational chemistry methods as applied to the modelling of biological processes.
3. Rationalizing drug design, building interactions, medicinal chemistry, molecular simulations and case studies.
4. Learn how applying some web-based and stand-alone tools to resolve simple drug design problems, e.g. the docking of a drug, the definition of a pharmacophore, etc.

Expected Course Outcome:

Upon completion of this course, the students will be able to:

- Handle experimental and predicted protein structures.
- Describe protein-ligand docking and the empirical/knowledge-based scoring functions employed.
- Discuss empirical scoring, de-novo design and virtual screening.
- Describe simulations of ligand binding thermodynamics.
- Describe the relation between IC50 and Kd, and discuss biophysical methods used.
- Analyse the 3D structure of proteins paying particular attention to the interaction between drugs and their targets.
- Know how to use software such as KNIME, CDK, AutoDock and Sire.

Topics:

1. Visualization of small / Macro-molecule structure, drawing of small molecules, and optimization of a small molecule (ligand Preparation).
2. Sequence Database: Swiss-Prot/Uniprot; Protein Database (PDB); Selection and optimization of the protein structure (Protein Preparation).
3. Docking: Protein grid generation, small molecule docking, and analysis of docking results.
4. Flexible protein docking: Induced fit docking.
5. Covalent docking.
6. Homology modeling generation; Model refinement and validation of the generated model.
7. De-novo structure-based drug design: Combinatorial library design and Identification of potential molecule by virtual screening workflow.
8. Pharmacophore generation and virtual screening of databases.
9. 2D-QSAR, 3D-QSAR development for series of molecules by atom-based QSAR and Field-based QSAR techniques and ADME Toxicity predictions.
10. Energy-based Pharmacophore (E-Pharmacophore) generation and Shape based virtual screening.

11. Antibody modeling, model validation, Antigen-Antibody docking, or Protein-Protein Docking.
12. Residue-scanning and associated property predictions, Cysteine scanning, Reactive hot spots prediction, and Affinity Maturation.
13. Q.M.: Small molecule Geometry optimization, Single-point energy calculation, spectral (U.V./Visible, VCD, I.R., NMR, Raman), and molecular property calculation(HOMO and LUMO, molecular orbitals, density, potential).
14. Molecular Dynamics Simulations and trajectory analysis.
15. Chemoinformatics analysis of chemical database (Binary fingerprint analysis, Similarity search, Clustering, Scaffold decomposition)

Note: Any experiment may be introduced/deleted in the practical class based on the availability/non-availability of the instruments/chemicals.

Reference:

1. Web Sources
2. Relevant Research Articles from the original research work and review articles published in peer-reviewed journals of international repute.