CERTIFICATE IN PHARMACOINFORMATICS

1. Program Title:	**CERTIFICATE IN PHARMACOINFORMATICS**
2. Nodal Department	CENTRE FOR BIOINFORMATICS
3a. Program Coordinator:	DR. AJIT KUMAR, Centre for Bioinformatics, MDU
3b. Program Co-Coordinator:	DR. MEHAK DANGI, Centre for Bioinformatics, MDU
4. Collaborating Departments within the University:	NIL
5. In partnership: Industry/Institutional/ other Department /s, None	NONE (At present); Planned for industrial partnership in future.
6. Program Description	Target specific drug discovery is the need of the hour. Techniques evolved in the post genomic era have given us an opportunity to accelerate discovery process by looking at many cellular processes simultaneously. Advances in combinatorial chemistry, molecular modelling, computational algorithms, and modern database mining techniques are accelerating the discovery science even more. New strategies and disciplines are emerging to identify the role of specific molecules in causing and counteracting diseases. Pharmacoinformatics, a new emerging field integrates Bioinformatics and Chemoinformatics along with pharmaceutics, pharmacology (ADME/toxicity) Pharmacy-informatics, Medical-informatics and IPR issues relevant to drug discovery.
7a. Program Objectives	1. To provide basic training of bioinformatics tools application in drug discovery and development process. 2. To abreast the student with emerging strategies and tools of computer aided drug design. 3. To learn the amalgamation of Bioinformatics and Chemo-informatics in the field of drug discovery. 4. To give an added value to the professionals of biological sciences research both academic level and at industry level. 5. To provide additional skills in Pharmaco-informatics for manpower required in pharma industries, vaccine development, clinical research projects, research, etc.
7b. Program Specific Outcomes	1. Knowledge of bioinformatics tools application in drug discovery and development process. 2. Scientific professionals with added values of pharmco-informatics in biological/pharmaceutical sciences research, at both academic level and industry level. 3. Acquisition of additional skills in Pharmaco-informatics for manpower required in pharma industries, vaccine development, clinical research projects, research, etc. 4. Added skills to students pursuing post-graduate studies in life sciences/pharmaceutical sciences/clinical sciences, etc.

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8. Duration	6 Months
9. Target Group	The course is designed for graduates pursuing postgraduates or Ph.D. and those working in industry / academics and is scheduled on weekends only.
10. Eligibility	Any of the following (minimum 50% marks required in qualifying examination): MBBS / B.D.S. / BAMS / B.H.M.S / B.Pharmacy / B.Tech-Biotech / BVSC / B.Sc. (Nursing) / M.Sc./ M.Pharm/ B.Sc. (with minimum one year relevant industry/ academic research work experience). Note: Any candidate pursuing a regular course in M.D. University, Rohtak or any other University of India, may also co-opt for this course along with their regular course.
11. Timing: Weekend/Evening/ Daytime	Weekend
12. Online/Offline/Blend of the two/Content sharing and online/Any other (please specify)	Blend of Online Content sharing and weekend Online/Offline classes.
13. Assessment and Evaluation mode	Students will be evaluated through periodic internal examination, evaluation of assignment and project work. At the end of the course, students will appear for final examination conducted by Centre for Bioinformatics, M.D. University, Rohtak. The students will be awarded as per absolute grading system, detailed in detail at Annexure I.
14. Fee structure	Rs.6,000/-
15. Any other	➢ **Intake: 20 Seats**

SEAT METRICS

	STATE QUOTA					
AIO	**HOGC**	**EWS**	**BC-A**	**BC-B**	**SC**	**PH**
03	07	01	03	02	03	01

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Annexure I

Program objectives:

The course aims to give an added value to the professionals of biological sciences research both at academic level and industry level in the areas like pharma industries, vaccine development, clinical research projects, academic research, etc.

Course syllabus outline & Scheme of examination

S.No.	Course code	Course title	Internal evaluation	End term evaluation	Credits	Total marks
1.	20CPPI11C1	Introduction to bioinformatics	20	80	4	100
2	20CPPI11C2	Chemo-informatics & Drug Design	20	80	4	100
3	20CPPI11C3	Predictive Pharmacology	20	80	4	100
4	20CPPI11C4	Project work	--	200	8	200
Total			**60**	**440**	**20**	**500**

- **Projects:** Each student will select the topic for his/her project within eight weeks of joining the course. Thus the projects can be taken by a group of students (not more than 5). Students will send their proposal to the Course Coordinator/Co-coordinator, who will help to nominate the guides. The project should involve about 10 days of research/field work.

- **Note:** This being a post graduate certificate course, students are expected to gain knowledge through interaction with the faculty, use of library /internet and shared E- course material.

- **Evaluation and Examination**

Students will be evaluated through periodic internal examination, evaluation of assignment and project work. At the end of the course students will appear for final examination conducted by Centre for Bioinformatics, M.D. University, Rohtak.

The students will be awarded as per absolute grading system, detailed below:

Interval of Marks	Grade	Grade Points
> or = 80 but <or =100	O (Outstanding)	10
> or = 70 but <80	A+(Excellent)	9
> or = 65 but <70	A (Very Good)	8
> or = 55 but <60	B+ (Good)	7
> or = 50 but <55	B (Above Average)	6
> or = 45 but <50	C (Average)	5
> or = 40 but <45	P (Pass)	4
Less than 40	F (Fail)	0
	Ab (Absent)	0

Note: A student obtaining Grade F shall be considered failed and will be required to reappear in the examination.

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Program Name	**Certificate in Phramaco-informatics**	**Program Code**	**CPPI**
Course Name	**Introduction to bioinformatics**	**Course Code**	**20CPPI11C1**
Credits	**4 [2 : 1 : 1 : : L : P : T]**	**No. of hours/Week**	**4**
Duration of End term examination	**3 Hours**	**Max. marks**	**100**

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question no. I is compulsory covering the whole syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

Course Objectives:

1. To learn the world of Bioinformatics and its evolution.
2. Assess the, different types of biological data and bioinformatics resources.
3. Assess and explain the tools and techniques of analyzing DNA and protein sequences.
4. Discuss the basic principles and applications of pharmacogenomics.
5. Utilize the different analysis packages available for different computational jobs.

Course Outcomes:

1. Understanding of bioinformatics and data mining concepts.
2. Learning of major bioinformatics resources available.
3. Learning of basic algorithms of sequence alignments of bioinformatics.
4. Learning of bioinformatics tools for sequence alignments.
5. Acquire understanding of principles and applications of pharmacogenomics.

UNIT I

Overview of Bioinformatics and Information Technology

History, Scope and application, Internet and World Wide Web; Generation of computers; Concept of Networking; Introduction to Data Mining; Application of data mining in Bioinformatics.

UNIT II

Bioinformatics Resources

Biological databases, Basic classification – Sequence & Structure; Generalized & Specialized; Primary & Secondary, with example databases (Genbank, EMBL, DDBJ, INSDC, Swiss Prot, PIR, PDB, NDB, BLOCKS, Pfam, ProSITE, etc.); Literature databases.

UNIT III

Bioinformatics techniques

Sequence comparison and alignment; Local and Global Alignment – (Smith Waterman Algorithm; Needleman Wunsch Algorithm); Concept of Gap, Gap Penalty & Scoring Matrices (PAM, BLOSSUM); Dot Plot Analysis.

UNIT IV

Bioinformatics tools

Information retrieval system (Entrez, SRS); Sequence alignment tools (BLAST, FASTA, CLUSTAL-W/X, MUSCLE, TCOFFEE), Variants of BLAST (BLASTn, BLASTp, PSI- BLAST, PHI-BLAST, etc)

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Suggested readings:

- Mount, D. W. (2004). Sequence and genome analysis. Bioinformatics: Cold Spring Harbour Laboratory Press: Cold Spring Harbour, 2.
- Selzer, P. M., Marhöfer, R. J., & Rohwer, A. (2008). Applied bioinformatics. An introduction–Springer, Verlag, Berlin, Heidelberg, Germany, 260.
- Rastogi S. C. (2014) Bioinformatics: Methods and Applications - Genomics, Proteomics and Drug Discovery: PHI Learning.
- Jones, N. C., Pevzner, P. A., & Pevzner, P. (2004). An introduction to bioinformatics algorithms. MIT press.
- Miller, W. (2006). An Introduction to Bioinformatics Algorithms.

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Program Name	**Certificate in Phramaco-informatics**	**Program Code**	**CPPI**
Course Name	**Chemo-informatics and Drug Design**	**Course Code**	**20CPPI11C2**
Credits	**4 [2 : 1 : 1 : : L : P : T]**	**No. of hours/Week**	**4**
Duration of End term examination	**3 Hours**	**Max. marks**	**100**

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question no. I is compulsory covering the whole syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

Course Objectives:

1. To learn the different structure representation systems.
2. To learn different chemical databases and its use in drug design.
3. To understand and explain the tools and methods of modeling small moleculaes.
4. Discuss the basic principles and applications of Chemo informatics.

Course Outcomes:

1. Understanding the representation systems of molecules.
2. Learning of major chemical database.
3. Learning of protein science and proteomics.
4. Learning of bioinformatics tools for functional analysis of genome and proteomes.

UNIT I

Structure representation systems

Representation of 2D and 3D structures; General introduction to chemical structure-hybridization, tetrahedron geometry etc.; The degeneracy of isomeric SMILES and introduction to unique SMILES; Reaction transformations notation like SMIRKS, Introduction to graph theory, vertex partitioning algorithms- CANGEN algorithm, Internal co-ordinates and introduction to calculation of Z matrix of simple small organic molecules.

UNIT II

Chemical Databases

Design, Storage and Retrieval methods; Introduction to database filters, property based & (drug-like)-Lipinski Rule of Five, *In silico* ADMET; QSAR approach, Knowledge-based approach**.**

UNIT III

Modeling of small molecules

Methods for interaction mapping; Chemical properties 2D and 3D; Introduction to adjacency, distance matrix and use of these matrices for calculating Weiner Index, Hosoya Index, Balban Index, Shultz Index, Randic Index. Introduction to shape indices- Kappa Shape index and calculation of molecular shape.

UNIT IV

Principles of Chemo-informatics

Role of Chemo-informatics in pharmaceutical/chemical research; Integrated databases; HTS analysis; Ligand based design of compounds; Structure based design of compounds, Chemoinformatics tools for drug discovery; Integration of active drugs; Optimization techniques; Filtering chemicals.

Suggested readings:

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- Leach, A. R., & Gillet, V. J. (2007). An introduction to chemoinformatics. Springer.
- Mannhold, R., Kubinyi, H., & Folkers, G. (2005). Chemoinformatics in drug discovery (Vol. 23). T. I. Oprea (Ed.). Weinheim:: Wiley-VCH.
- Varnek, A., & Tropsha, A. (Eds.). (2008). Chemoinformatics approaches to virtual screening. Royal Society of Chemistry.
- Mannhold, R., Kubinyi, H., & Folkers, G. (2006). Chemoinformatics in drug discovery (Vol. 23). John Wiley & Sons.

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Program Name	**Certificate in Phramaco-informatics**	**Program Code**	**CPPI**
Course Name	**Predictive Pharmacology**	**Course Code**	**20CPPI11C3**
Credits	**4 [2 : 1 : 1 : : L : P : T]**	**No. of hours/Week**	**4**
Duration of End term examination	**3 Hours**	**Max. marks**	**100**

Note: Nine questions are to be set in all and the candidates are required to attempt five questions including compulsory question. Question no. I is compulsory covering the whole syllabus. Out of remaining eight questions, two questions are to be set from each unit. Candidate is required to attempt four questions, selecting one question from each unit.

Course Objectives:

1. To learn the general principles of pharmacology.
2. To learn drug discovery and development process.
3. To learn the concept of pharmacophore and its application in drug design.
4. To understand the role of bioinformatics in pharmacological studies.

Course Outcomes:

1. Understanding of bioinformatics and data mining concepts.
2. Learning of major bioinformatics resources available.
3. Learning of basic algorithms of sequence alignments of bioinformatics.
4. Learning of bioinformatics tools in pharmacology.

UNIT I

General Pharmacology

Drug receptor interaction theories, Structure activity relationships, pharmacodynamic and pharmacokinetic aspects of chiral drugs, allosteric binding, thermodynamics of drug interactions with the receptors.

UNIT II

Drug Discovery and Development

The Lead compound, Drug Discovery Cycle, Bioinformatics in drug discovery and development, chemical databases, ADME and Toxicity , Virtual Screening, Molecular Docking, Structure and Ligand Based Drug Designing, Case studies.

UNIT III

Pharmacophore Kinetics

Characterization of chemicals by Class & by Pharmacophore. Introduction to pharmocophore Identification of pharmacophore features. Building pharmacophore hypothesis; Searching databases using pharmocophores. Design & Analysis of combinatorial libraries; Reagent and product base combinatorial library generation; Focus library and HTS library.

UNIT IV

Bioinformatics in Pharmacology

Chemical Databases – Design, Storage and Retrieval methods. Introduction to database filters, property based & (drug-like)-Lipinski Rule of Five. Chemical file formats. Drug databases and Resources (Pubchem, Drug Bank, Super Drug, Chemfinder).Chemical sketching (ISIS Draw, Chemsketch).

Suggested readings:

- Benfenati, E. (Ed.). (2016). In silico methods for predicting drug toxicity. Humana Press.
- Kenakin, T. (2016). Pharmacology in Drug Discovery and Development: Understanding Drug Response. Academic Press.
- Kenakin, T. P. (2017). Pharmacology in drug discovery and development.
- Mannhold, R., Kubinyi, H., & Folkers, G. (2006). Chemoinformatics in drug discovery (Vol. 23). John Wiley & Sons.

Program Name	**Certificate in Phramaco-informatics**	**Program Code**	**CPPI**
Course Name	**Project work**	**Course Code**	**20CPPI11C4**
Credits	**8 [0 : 8 : 0 : : L : P : T]**	**No. of hours/Week**	**4**
Duration of End term examination	**3 Hours**	**Max. marks**	**200**

Course Objectives:

1. To conceptualize a small project on a relevant topic.
2. To plan and execute the project in a time bound manner.
3. To learn scientific report writing skills.

Course Outcomes:

1. The course will help to understand the relevance of bioinformatics in biological research.
2. The course will help to learn and apply different bioinformatics tools in solving biological problems.

Each student will select the topic for his/her project within eight weeks of joining the course. Thus the projects can be taken by a group of students (not more than 5). Students will send their proposal to the Course Coordinator/Co-coordinator, who will help to nominate/select the project guides. The project should involve about 10 days of research/field work and will be evaluated by external examiner(s).