

**P R O G R A M M E PROJECT REPORT (PPR)**

**POST GRADUATE DIPLOMA IN CHEMOINFORMATICS  
(OPEN AND DISTANCE LEARNING MODE)**



**School of Open And Distance Learning**

**JAMIA HAMDARD**

(Deemed University)

Hamdard Nagar, New Delhi-110062

## **Jamia Hamdard**

Late Janab Hakeem Abdul Hameed sb, the founder of Jamia Hamdard, had a vision to develop Jamia Hamdard into an institution of excellence imparting modern professional education with special emphasis on Unani medicine and Islamic studies. Today, it has evolved into an excellent centre of higher learning, fulfilling the objective of the *wakf*, which has been funding the University ever since its inception.

As a mark of tribute and thanks to the Almighty Allah for bestowing his guiding spirit to its founder and his associates, Jamia Hamdard adopted a seal inscribed with the following

*“He (The Prophet may peace be upon him)  
Instructs them in the Book and Wisdom”*

Ever since the inception of Jamia Hamdard, this holy verse (*ayat*) has been a source of inspiration and guidance for all those associated with its management and administration. As an Islamic charity, *wakf* has played the vital financial role in the making of Jamia Hamdard. He (PBUH) preached his followers that

*“Wisdom is (like) the lost animal of a believer  
wherever he finds it, catches hold of it”*

Inspired by the Holy Qur’an and exhorted by the Prophet (PBHU), Muslims became the torch-bearers of knowledge and civilization in the medieval period, but are lagging behind in present times. Late Hakeem Abdul Hameed Sahib wisely chose education and pursuit of knowledge as his prime objective when he decided to convert *Hamdard Dawakhana* into a *wakf*, a charity dedicated to fulfilling educational and health care needs of Indian Muslims. Hamdard (*wakf*) continues to provide generous grant to the university for building, equipments and salaries of staff and other development activities.

Jamia Hamdard was inaugurated by late Shri Rajiv Gandhi, the then Prime Minister of India, on August 01, 1989. In his impressive speech, the Prime Minister applauded the efforts of Hakeem Abdul Hameed Sahib in setting up institutions of higher learning, which were emerging in the form of a “Deemed to be University.” He said, “This will enable (the Muslim) minority to go forward and thus help India to march forward.”

The University offers professional courses, which equip the students to get placements in the highly competitive job market. On the basis of the record of performance of the University and quality of infrastructure including staff, the university has been accredited by NAAC in category ‘A’ of Indian Universities.

## **Mission & Objective**

The Study programme aims to provide contemporary education and training to meet the challenges of the evolving global scenario and changing environment in business administration. The objective of the project is to help the students develop ability to apply multi-disciplinary concepts, tools and technique to solve organizational problem.

### **Jamia Hamdard Mission and Goal in relevance of the programme**

Jamia Hamdard's study programmes under ODL are selective and customized to meet the learning requirements of knowledge seekers as well as to ensure that they learn at their own pace and convenience. Within the financial means of University, due care has been taken to keep the cost of education low, so that educationally backward sections can take advantage of University's programmes through ODL mode. This goal in view, the DODL of Jamia Hamdard has made concerted efforts to offer professional and job oriented courses with regular updates of curricula and study material and introduction of tools of Information Technology.

### **Targeted Group**

The distance education has potential to reach to unreached and even marginalized and excluded group of the society such as tribal populations and Muslims women. Jamia Hamdard, SODL programme provides an opportunity to students for acquiring new knowledge and skills that are needed for their development. Jamia Hamdard being in education for a long time has taken initiatives to offer an opportunity to those students who are unable to get on campus education and those who have limited access to educational resources. ODL programme of Jamia Hamdard also envisage to provide an opportunity to girls from Muslim community, who by and large have been left out by the national education endeavors.

## **DEPARTMENT OF CHEMISTRY**

The Department of Chemistry was established in 1990 as a research department. The faculty members are pursuing research in different fields of Chemistry such as Natural Product Chemistry, Surface Chemistry and Micro Emulsion, Synthetic Organic Chemistry, Polymer Chemistry etc. The department had launched M.Sc. course in Chemistry (Industrial Applications) in the year 2001 leading to M.Sc. degree in Chemistry with as objective to produce professionally trained post graduate chemist for pharmaceutical, foods, cosmetic, polymer, petroleum and allied industries and with initial intake of seven students. The first batch of the M.Sc. Chemistry (Industrial Applications) had passed out in 2003 with all seven students getting the placements in different Industries. At present the strength has been raised to 15 students including two seats for foreign nationals/NRI students. Ph.D. degrees are also being awarded in the different fields of Chemistry.

The major areas of research include the isolation and characterization of biopharmaceuticals from natural source, synthesis of new compounds of industrial interest as well as emerging technologies in drug delivery system.

Department of Chemistry has initiated academia-industry interaction and shall be organizing a series of seminar lectures on Analytical Science from October 2004 onward.

Programme offered through Open and Distance Mode

Apart from the full time regular courses, the department has decided to offer one programme through distance mode for those students who are not able to afford the expenses of education in Delhi or who have not been able to make it to the courses offered by the universities and colleges in traditional mode. However, our endeavor will be to provide the best quality education, keeping with the traditions of Jamia Hamdard, through the selected Study Centres spread over the various parts of the country. The programme to be offered is:

Post Graduate Diploma in Chemo-informatics - Programme code 652

### **BASIC INFORMATION ON CHEMOINFORMATICS**

Chemo-informatics is a generic term that encompasses the design, creation, organization, management, retrieval, analysis, dissemination, visualization and use of chemical information.

The use of information technology and management has become a critical part of the drug discovery process. Chemo-informatics is the judicious use of information resources to transform data into information and information into knowledge for the intended purpose of making better decisions faster in the area of drug lead identification and organization.

The development of future chemical informatics systems will require people with a solid grounding in chemistry and an expert knowledge of the available computer technology. Chemical, agrochemical, pharmaceutical, and biotechnology companies will increasingly depend on chemical informatics and people with extensive knowledge of chemistry and the computer skills to handle the data generated by chemical researchers. In addition, database producers, chemical software developers, and those in the primary and secondary chemical publishing areas offer attractive opportunities for students of the chemical informatics programme.

The course is designed for graduates willing to make a career in the area of pharmaceutical sciences, veterinary sciences, food sciences, agricultural sciences, biotechnology, physics, chemistry, mathematics, and statistics.

### **POST GRADUATE DIPLOMA IN CHEMOINFORMATICS (PGDC)**

#### **OBJECTIVE**

PGDC aims to create a workforce, with solid grounding in chemistry and expert knowledge in computer technology in the upcoming fields of Agrochemical/Pharmaceutical/Biotechnology industry. The curriculum is designed to combine strong, universally applicable fundamentals with some breadth in training.

**Nature** - Distance Mode

## The Course

Highlights of the course are described in the following table:

a.	Name of the course	Post Graduate Diploma in Chemo informatics (PGDC)
b.	Nature	Open and Distance Mode
c.	Duration	Minimum: 1 year (2 Semesters of Six months each) Maximum: 2 years
d.	Medium of Instruction and Examinations	English
e.	Eligibility Criteria Educational Requirements	A candidate who has passed B.Sc. in Biology, or equivalent examination with Chemistry as one of subject from a any recognized University shall be eligible for admission
f.	Commencement of the course	January / July. Twice in a year
h.	Mode of Admission	As per the norms prescribed by Jamia Hamdard from time to time.
i.	Period of Completion (Span Period)	Not more than 02 years
j.	Fees	Rs. 7,000 per semester and 14,000/- per year)

## Admission:

- a. A candidate, aspiring for admission to PGDC programme, shall have to apply in the prescribed application form that is complete in all respects, on or before the last date of submission.
- b. The Admission committee shall display/publish the list of candidates that are declared eligible for admission, after the due approval of the competent authority.
- c. Eligible candidates shall have to complete the prescribed formalities, for completion of admission, within the stipulated period of time; otherwise they will forfeit the right to admission.
- d. After having completed the formalities of admission, the candidate will be required to associate themselves with the selected Study Centres for the purpose of counseling and practicals.

e. No Migration Certificate will be required for admission.

#### THE COURSE STRUCTURE

Papers	Nomenclature	Marks	
		External	Internal
PGDC 101	Basics of Chemo-informatics	80	20
PGDC 102	Medicinal Chemistry-Receptor Ligand Interaction	80	20
PGDC 103	Modern Combinatorial Chemistry	80	20
PGDC 104	Chemo-informatics Database Design and their Management	80	20
PGDC 105	Chemical Information Sources	80	20
PGDC 106	Computational Chemistry	80	20
PGDC 107	Data Sequencing, Mining and Visualization	80	20
PGDC 108	Drug Design and Discovery	80	20

For the one-year programme, every core subject will have one paper, carrying a maximum of 100 marks.

For continuous study and assessment, there will be two tutor mark assignments for the session for each course subjects. The higher of the scores of these assignments will be taken into account for each course subject per session.

In order to pass in any session of the programme and examinee must obtain a minimum of 40% of total marks for each course subject in the session of examination. Candidates who pass in each of the courses will qualify for the award of PGDC in determining the result of the entire programme aggregate of performance of the students. Students securing 60% and more marks will be placed in first class, those securing 50% or more but less than 60% will be placed in second class and those securing 40% or more but less than 50% in third class.

There shall be supplementary examination giving only one chance to candidates who fail in only one exam paper. This supplementary exam will be held along with the next main exam.

The delivery of the programme consists of audio/video support/assignments, contact classes, library consultation etc. A minimum of 60% of attendance in contact classes, submission of assignments will be necessary conditions for the eligibility of the candidate, to appear in session end examination.

**PGDC 101**  
**(BASICS OF CHEMOINFORMATICS)**

<b>S. No.</b>	<b>Topics</b>
1.	Introduction
2.	Evolution of Chemo-informatics
3.	History of Chemical Information Science
4.	Use of Chemo-informatics
5.	Prospects of Chemo-informatics
6.	Chemo-informatics Glossary

**PGDC 102**  
**(MEDICINAL CHEMISTRY-RECEPTOR LIGAND INTERACTION)**

<b>S. No.</b>	<b>Topics</b>
1.	Introduction
2.	Drugs, Ligands and Receptors
3.	Major Classification of Drugs
4.	Medicinal Chemistry
5.	Drug Discovery
6.	Target Oriented drug-Design
7.	Drug Solubility

**PGDC 103**  
**(MODERN COMBINATORIAL CHEMISTRY)**

<b>S. No.</b>	<b>Topics</b>
1.	Introduction: concepts and Terms
2.	Solid-phase Strategies <ul style="list-style-type: none"> <li>I. General Strategies and Concepts</li> <li>II. Specific Implementation Issues</li> </ul> Chemical International resources Specific Implementation issues Anchoring Chemistry Coupling Chemistry Protection Schemes <ul style="list-style-type: none"> <li>1. Analytical methods</li> </ul>
3.	Solution Phase Strategies
4.	High Through put Screening
5.	Design of Combinatorial Libraries
6.	Glossary of Combinatorial Chemistry Terms

**PGDC 104**  
**(CHEMOINFORMATICS DATABASE DESIGN AND THEIR MANAGEMENT)**

<b>S. No.</b>	<b>Topics</b>
1.	Database Concepts
2.	Database Architecture
3.	Code Rules
4.	Normalization
5.	Access 200 database
6.	Accord 2000 Chemo-informatics Database for Access
7.	Introduction to Structured Query Language
8.	Data manipulation Language
9.	Data Definition Language
10.	SQL Reserved Words Overview
11.	SQL commands comparison for ACCESS, ORACLE and SQL Server
12.	Chemical Database Design and their tools
13.	Structure based Searches

**PGDC 105**  
**(CHEMICAL INFORMATION SOURCES)**

<b>S. No.</b>	<b>Topics</b>
1.	History and Future of the Science Internet
2.	Chemical Literature <ul style="list-style-type: none"> <li>➤ Types of Publication</li> <li>➤ Journals/Technical Report/Patents/Conference Papers/Dissertations/Electronic Publications</li> </ul>
3.	Chemical Information Searches <ul style="list-style-type: none"> <li>➤ Advantages/Limitation of Computer Searching</li> <li>➤ Strategies and Tactics for Searches</li> <li>➤ Patent Searching Techniques, Patent Search at a Patent and Trademark Depository Library</li> <li>➤ Computer Searching of Chemical Abstracts</li> <li>➤ Substructure Searching in Chemical Abstracts</li> <li>➤ Keyword-based General Bibliographic Searches</li> <li>➤ Chemical Connectivity and Structure Searches (2-D)</li> <li>➤ Chemical Structure, Property and Shape Based Searches (3-D)</li> <li>➤ Searching for the Synthesis or Reactions of Specific Compounds of Classes of Compounds</li> </ul>
4.	Communication in Chemistry <ul style="list-style-type: none"> <li>➤ Chemistry Newsgroups and Discussion Lists</li> <li>➤ Molecular Visualization Tools and Sites</li> <li>➤ The Publication Process: Primary, Secondary and Tertiary Sources</li> </ul>



	<ul style="list-style-type: none"> <li>➤ Analytical Chemistry</li> <li>➤ Physical Property Information</li> <li>➤ Chemical Safety and Toxicology Information</li> <li>➤ Chemical History, Biography, Directories and Industry sources.</li> </ul>
5.	<p>Chemical Information sources</p> <ul style="list-style-type: none"> <li>➤ Guides to Chemical Information Sources and Databases.</li> </ul>

**PGDC 106**  
**(COMPUTATIONAL CHEMISTRY)**

<b>S. No.</b>	<b>Topics</b>
1.	<p>Introduction</p> <ul style="list-style-type: none"> <li>➤ Building Molecules</li> <li>➤ Conformation Searching</li> <li>➤ Molecular Dynamics</li> </ul>
2.	<p>Introductory Quantum Chemistry</p> <ul style="list-style-type: none"> <li>➤ Basic Principles</li> <li>➤ Extended Huckel Theory and Photoelectron Spectroscopy</li> <li>➤ Symmetry and Z-matrix</li> <li>➤ Ab initio Hartree-Fock Theory, basis sets closed and open-shell molecules.</li> <li>➤ Geometry optimization, transition structure optimization, potential energy surface.</li> <li>➤ Semiempirical Methods, ZDO, CNDO, INDO, MNDO/AMI/PM3, parameterization and performance-</li> </ul>
3.	<p>Molecular Mechanics and Force Fields</p> <ul style="list-style-type: none"> <li>➤ Force fields, potential energy functions, inter and intramolecular interactions, Empirical parameters.</li> <li>➤ Molecular mechanics calculation, energy minimization, conformational</li> <li>➤ Analysis vibrational frequencies and normal mode analysis.</li> </ul>
4.	<p>Condensed Phase Modeling</p> <ul style="list-style-type: none"> <li>➤ Debye-Huckel Theory, continuum solvation models (classical and SCRF)</li> <li>➤ Explicit simulations methods, Monte Carlo, Molecular Dynamics, Brownian Dynamics.</li> <li>➤ Free energy simulation methods, and discussion of applications</li> </ul>

5.	Biopolymers <ul style="list-style-type: none"> <li>➤ Protein structure, PDB.</li> <li>➤ Energy minimization, molecular dynamics, enzyme active site, and discussion of Applications</li> <li>➤ Nucleic Acid Structure, DNA sequence, database.www.</li> </ul>
6.	Software and Hardware <ul style="list-style-type: none"> <li>➤ Insight II/Discover</li> <li>➤ MOPAC</li> <li>➤ Databases</li> <li>➤ Quanto</li> </ul>
7.	Glossary

**PGDC 107  
(DATA SEQUENCEING, MINING AND VISULIZAITON)**

<b>S. No.</b>	<b>Topics</b>
1.	An introduction to Data Mining
2.	What is Data Mining?
3.	How Data Mining Works?
4.	An architecture for Data Mining
5.	Differences between Data mining and Machine Learning
6.	Data Visualization
7.	Visualizing Data Mining Models
8.	Decision Tree
9.	Data Warehousing
10.	Data Mining and Analytic Technology
11.	Comparing Different Models using Visualization
12.	Software-past and present Developments

**PGDC 108  
(DRUG DESIGN AND DISCOVERY)**

<b>S. No.</b>	<b>Topics</b>
1.	Structure-Based Drug Design
2.	Computational Techniques in the Drug Design Process
3.	Molecular Modeling using Computers
4.	Drug Metabolism
5.	Prodrugs and Soft Drugs
6.	Chemical and Physicochemical Parameters in Drug Design
7.	Development of New Drugs
8.	Design of Enzyme Inhibitors

## **Students' Support Services**

The coordinators of the respective courses would display a copy of such important circulars/ notifications on the notice board for the benefit of all the students. Therefore, it is important for all the students to keep in regular touch with the Jamia Hamdard so as to get advance information about assignments, submission schedule, examination forms, list of students admitted to particular examination, declaration of results, etc.

## **Supply of Study Material**

One book per course will be supplied to the students as study material. However, the fast pace of computer industry necessitates that students must read some other reference materials. Studying the supplied printed material alone may not be sufficient for the knowledge of the subject. Therefore, it is strongly recommended that the students take the help of other reference materials/ websites for the preparation of their assignments and other examinations.

## **Counseling Sessions**

In distance education, face -to-face contact between the learners and their teachers/ counselors is relatively less and, therefore, is an important activity. The purpose of such a contact is to answer some of the questions and clarify the doubts, which may not be possible through any other means of communication. It also intends to provide an opportunity to meet the fellow students. There are academic counselors at the Study Centers to provide counselling and guidance to the students in the courses that they have chosen for study. These sessions will be held at the Study Centers during week ends (**Saturdays and Sundays**)

It may be noted that the counseling sessions would be very different from the classroom teaching or lectures. Counsellors will not be delivering lectures as in conventional teaching. They will try to help the students to overcome difficulties, which they face while studying for the Programme. In these sessions, they must try to resolve their subject-based difficulties and any other related problems.

**Before the students go to attend the counselling sessions, they are expected to go through the course materials supplied to them and make a plan of the points to be discussed. Unless they have gone through the Units, they may not find much to be discussed with course counsellors.**