POST GRADUATE DIPLOMA IN CHEMOINFORMATICS
ANNUAL EXAMINATIONS-2017
BASICS OF CHEMOINFORMATICS
PGDC-101

Time Allowed: 3 Hours **Max Marks: 100**

Note: This paper is divided into three sections. Attempt all questions from Section A, any five questions from Section B and any four questions from Section C.

Section – A

Answer *all* questions briefly. **2x10=20**

1. What is CHUCKLES
2. Define Force field?
3. What are bioisosteres?
4. Which journal is considered as the first chemistry journal?
5. What are biophores?
6. How is pharmacophore mapping performed?
7. Enlist the limitations of CHORTLES
8. What is library registration?
9. What are the advantages of solid phase over solution phase synthesis?
10. What do you mean by Chemometrics?

Section – B

Attempt *any five* questions. All questions carry equal marks **6x5=30**

1. Discuss the Ontogen Approach
2. Highlight the major changes in strategies for Drug Design
3. What is extensible markup language?
4. What are the general considerations for generation of a particular library against the biological target of interest?
5. Give an account of 2D similarity searching?
6. Enumerate the steps involved in 3D-QSAR Model Building Procedure.
7. Give an overview of biologically focused library design.
8. What is molecular diversity analysis?

Section – C

Attempt *any four* questions. All questions carry equal marks **12½x4=50**

1. Give an overview of prospects of Chemoinformatics in Drug Design
2. Give a description of general principals of basic Apex-3D Algorithm?
3. What are the chemical strategies for introducing carbohydrate molecular diversity into drug discovery process?
4. Describe the advantages of structure based designing of combinatorial library
5. Discuss the High throughput Screening Strategies used in drug design?
6. Computer–aided chemistry laboratory speeds research, justify?

Your Roll no.....

P.G. Diploma in Chemo- Informatics Examination 2017

Paper-PGDC-102

Medicinal Chemistry-Receptor Ligand Interaction

Time Allowed: 3hours *Maximum marks: 100*

(Write your Roll No. at the top immediately on receipt of this question paper)

Section A is Compulsory. Answer any **six** questions from **section B** and any **four** questions from **section C**

SECTION A

Attempt all questions (2x10 =20 marks)

1. What is virtual screening?
2. Define the terms-Affinity, Efficacy and Potency
3. Give Fick's law of diffusion.
4. Give some examples of drugs developed from natural products.
5. What is 2- Fold Strategy for Innovation .
6. Define agonist and antagonist.
7. What are abused drugs?
8. What do you understand by the term drug solubility?
9. Name two analytical techniques used in drug development process.
10. What is nanotechnology?

SECTION B

Attempt any six questions (5x6 =30 marks)

1. What are the essential properties of molecule to be drug?
2. Describes the terms drugs, ligands and receptors.
3. Mention the possible steps in a drug discovery process.
4. Draw a flow chart to show experimental approach for bioassay directed isolation of cancer chemopreventive agents.
5. Explain combinatorial synthesis by giving example.
6. Discuss ADME/PK strategy..
7. What prospects medicinal chemistry has in pharmaceuticals?
8. Write note on ligand binding and lead optimization.
9. What are the applications of substructure analysis?

SECTION C

Attempt any four questions (12.5x4 =50 marks)

1. Describe in detail the structure based ligand design technologies.
2. Explain about the 'rule of 5' and its implementation in drug design. What is the rationale for measuring drug solubility in a discovery setting?
3. Write a note on molecular docking. How scoring of compounds at the binding site has been done?
4. What are the different ways by which one can generate a library? What are the different kinds of libraries generated from natural products?
5. Discuss the major classification of drugs in detail. Give examples of each class.
6. What are the challenges in medicinal chemistry? Discuss the role of medicinal chemist in drug discovery.
7. What is the role of small molecule ligands in target validation and lead discovery?

.....x.....

POST GRADUATE DIPLOMA IN CHEMOINFORMATICS
ANNUAL EXAMINATIONS-2017
MODERN COMBINATORIAL CHEMISTRY
PGDC-103

Time Allowed: 3 Hours **MM: 100**

Note: This paper is divided into three sections. Attempt all questions from Section A, any five questions from Section B and any four questions from Section C

SECTION –A

Answer *all* questions briefly. **2x10=20**

1. What is ADMET virtual screening
2. What are isotopic tags?
3. What are the advantages of synthesizing by DCR method?
4. Distinguish between discrete and pool libraries.
5. Which are the different types of optical barcoding methods?
6. Which are the parameters that can be used to generate optodiversity in the encoding colloidal particles?
7. What is magic angle spinning NMR?
8. Why are multiple component condensations (MCC) useful for the generation of combinatorial libraries
9. Which are the three major steps in designing any combinatorial library?
10. Name some non-destructive techniques used for monitoring of the solid phase organic synthesis?

Section –B

Attempt *any five* questions. All questions carry equal marks **6x5=30**

1. Discuss the use of biocatalysts as combinatorial agents for synthesis.
2. What do you understand by parallel synthesis?
3. Discuss the application of active site derived pharmacophores with informative library design
4. Write a note on 'resin capture'.
5. How can novel encoding techniques escalate throughput in screening?
6. Give different applications of biopanning.
7. How can chemical coding be used for identification of library compounds?
8. Give an overview of biologically focused library design.

Section C

Attempt *any four* questions. All questions carry equal marks **12½x4=30**

1. Discuss how biopanning can be used to identify new potential ligands against a variety of targets of interest.
2. What are the advantages of solution phase chemistry?
3. Which are the analytical methods of choice for monitoring of solid phase organic synthesis?
4. Describe the advantages of structure based designing of combinatorial library
5. What is a linker? Discuss the role of a linker in solid phase synthesis. Which are the different types of linkers used in solid phase synthesis?
6. Discuss direct methods of deconvolution?

Jamia Hamdard (Jamia University)
Hamdard Nagar, New Delhi
PGDC- 104
CHEMO-INFORMATICS DATABASE DESIGN AND THEIR MANAGEMENT
Annual Examination-2017

MM 100

Time 3HRS

Section A(20*1=20)

1) A database is ----------
2) A Databases record is uniquely identified with----------
3) A DBMS is advantageous because----------
4) Data Integrity means data consistency (T/F)
5) A file is a complete , named collection of a) data b) information
6) Individual element of a record is called a)field b) table c) key
7) A key is used to identify a) database b) record c) table
8) Accord Database Explorer is designed and developed by: a)IBM b)Acceirys
9) What is simplest method of querying database a) SQL b)Query c) Query by form
10) Database browser can be opened by clicking on a) hitset b) browser c) both
11) Complex queries can be constructor using query builder logic a) true b) false
12) We can't view past queries from hitset manager a) true b) false
13) The BioCat form searches biocatalyst data a) true b) false
14) SQL Update commands edits a table. a) true b) false
15) We can join two tables using where clause. a) true b) false
16) We can't add rows to a table after its creation. a) true b) false
17) We can have ----------primay key for a table .
18) ---------- establishes referential integrity
19) Alcohols comes under N-protection N-protection category a) true b) false

Section B(6*5=30)

Answer any six

1. Disscuss issues in file based data storage system.
2. What is relational query Language and explain its components.
3. State and explain special comparison operator
4. Discuss steps to start Accord database explorer.
5. Explain the concept of crosslinking in biocatalyst.
6. Explain the technique of solid-phase synthesis.
7. Explain the concept of entities, attributes, primary key and foreign keys with help of sutaible example.
8. Explain noramalization process and its advantages.

Section C(10* 5=50)

Attempt Any five

1. Explain CODD rules in detail.

2.Explain the concept of entities, attributes, primary key and foreign keys with help of sutaible example

3.Explain noramalization process in detail.

4.Explain different DML commands with example.

5.Discuss SQL aggregate functions in detail.

6.Explain how biocatalyst database can be used in Accord Database Explorer.

7. Explain how solid phase synthesis database can be used in Accord Database Explorer.

P.G. Diploma in Chemoinformatics-Examination 2017

Paper-PCID-105
Chemical information sources

Time: Three Hours *Maximum Marks: 100*

(Write your Roll No. On the top immediately on receipt of this question paper)

SECTION- A

Answer all questions (2x10=20 marks)

1. The best way to find chemistry related websites is to use _____
2. www stands for_____
3. A copyright does not require _____
4. What is a markush structure?
5. CAS stands for _____
6. What is the major drawback associated in computer searching?
7. What is MSDS?
8. What is database guide?
9. NNTP stands for_____
10. What is TRN?

SECTION- B

Answer <u>any five</u> questions (8x5=40 marks)

1. Describe the future of scientific internet
2. What are the essential criteria of patenting
3. Describe the advantages and disadvantages of Electronic Journals
4. What is substructure and how can it be searched in Chemical abstracts?
5. Describe the Patent searching techniques
6. Explain the goals of analytical Chemistry
7. Write a short note on physical property information.
8. Describe database selection

P.T.O.

SECTION- C

Answer any four questions (10x4=40 marks)

1. Write a detail note on Chemical Abstracts as chemical information sources?
2. Explain the different types of structure searches?
3. Describe the various databases used to search for the synthesis or reactions of specific compounds/ classes of compounds?
4. Explain in detail about Sci-Finder Scholar and Bielstein Cross fire
5. Write a detailed note on Chemical Index Search?
6. Write a detailed note of IPR and patenting
7. Write a detailed note on Chemical safety and toxicology information sources?
8. Explain the importance of Chemical dictionaries, guides, handbooks and indexes

----------OO----------

PG Diploma in Chemo-Informatics
PCDC-106
Computational Chemistry

Time: 3 Hrs

Maximum Marks 100

Section A

Answer Appropriately

10x2=20

1. Bending energy equation is based on .....
2. Total energy of a molecule is given by
   E= stretching energy + ... energy + ... energy + non-bonded interaction energy.
3. What does RSCB stands for.....
4. In molecular quantum mechanics the Potential Energy Surface is related to .....
5. Photoelectron spectroscopy utilizes ..... and ..... analysis of the emitted photoelectron to study the composition and electronic state of the surface region of a sample.
6. The weakness of standard EHM is that it does not takes into account .....
7. Proteins are macromolecules, made up of .....
8. α- helix of protein is composed of.....
9. The dielectric constant also describes.....
10. Brownian dynamic simulation are used to simulate ..... molecules in solution.

Section B

Answer any six questions:

5X8=40

1. Discuss Extended Huckel Method approximation and its strength.
2. Discuss the physical basis of photoelectron spectroscopy.
3. How is Z- matrix constructed in Gaussian format? Explain with an example
4. Write short note on SHAKE.
5. Explain the term force field parameters. Discuss Lenard Jones potential in detail.
6. What is α helix and discuss its properties in detail.
7. What does PDB stands for? Explain in detail the structure of PDB file.

Section C

Answer any five questions: 4x10=40

1. What do you understand by Continuum Solvation Model? What are its components and discuss in detail the Born and Onsager Model.
2. What are inter and intramolecular interactions, give their importance in energy minimizations.
3. Describe the basic algorithm of molecular dynamics. Discuss its structure in detail.
4. What is the need for simulation studies and what do they explain? Explain in detail the Monte Carlo Simulations.
5. How will you evaluate the quality of a Homology Model developed? What are the sources of errors and in accuracies?
6. Explain Nucleic acid structure and nucleic acid databases and its uses.

P.G. Diploma in Chemoinformatics - Examinations 2017

Paper Code –PGDC-107

Time: Three Hours

Data Sequencing, Mining and Visualization

Maximum Marks: 100

(Write your roll no. on the top immediately on receipt of the question paper)

SECTION – A

(Answer all questions)

2 x 10 = 20 Marks

1. OLAP is part of the spectrum of _____
2. The goal of data mining is to _____
3. Data mining does not replace _____ techniques
4. Midwest grocery chain used the _____ capacity of Oracle Software
5. Data are any _____ that can be processed.
6. Modelling is simply the act _____
7. Data mining allows the analyst to _____
8. Data visualization provides a _____
9. Common forms of interaction are _____
10. CART stands for _____

SECTION B

(Answer any FIVE questions)

6 x 5 = 30 Marks

1. Differentiate between data mining and machine learning.
2. Which software's we are using for chemical data mining
3. What is the warehousing? State its characteristics and advantages over conventional data bases.
4. What is Biological Data Analysis? How it helps in data mining.
5. What is Modelling?
6. Explain Data Visualisation?
7. What is the Dimension of Data?

SECTION C

(Answer any FOUR question)

12.5 x 4 = 50 Marks

1. Describe the various mapping methods in data mining
2. What is meant by model? Describe model and algorithm, model as process and model as input output mapping.
3. Differentiate algorithm and model.
4. What do you understand by information harvestor?
5. Describe the application of Data mining software.
6. What do you understand by Molecular Data Mining?
7. Describe the various mapping methods in data mining.

Your Roll No. .....

P.G. Diploma in Chemo informatics-Examination 2017
Paper Code: PGDC-108
Paper Title: Drug Design and Discovery

Time: Three hours *Maximum Marks: 100*

(Write your roll number on the top immediately on receipt of this question paper)

Section A

Answer the following questions briefly **(2x10= 20 Marks)**

1. Define prodrugs. Give examples.
2. Explain the Lipiinski "Rule of 5".
3. Give the primary methods for structure determination that are useful for drug design.
4. Explain the role of computers in molecular modeling.
5. How prediction of permeability is carried out?
6. Give the clinical significance of enzyme inhibitors.
7. Give the differences between Genetics and pharmacogenetics.
8. Name the sites where drug is metabolized in the body ?
9. How to identify ligand binding and macromolecular binding sites ?
10. Explain first pass effect.

Section B

Answer briefly *any five* questions **(6x 5= 30 Marks)**

1. Explain docking. Write the various steps involved in it.
2. Give application of energy calculations to drug design.
3. Describe enzyme inhibition and enzyme induction.
4. Discuss the six array systems used to identify the lead compounds.
5. Explain the Michaelis-Menton equation.
6. Give the significance of solvent in ligand binding. Also give the required steps during scouring in modeling.
7. Describe the salt bridges analysis of protein-ligand interaction patterns.
8. Explain the various rapid, reversible inhibitors.

Section C

Answer *any four* questions in about 500 words **(12 ½ x 4= 50 Marks)**

1. Name and explain the various forces involved in forming the enzyme-inhibitor complex.
2. Explain the mechanism of drug metabolism including phase I and II.
3. Enumerate various De Novo drug design methods.
4. What is SBDD? Explain AmpC-β-lactamase case study.
5. Name and explain various Tactile Model.
6. How will you design a
   a. Covalently binding enzyme inhibitor
   b. Non-covalently binding enzyme inhibitor
7. What are hard and soft drugs? Discuss their function.