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PG Program in Cheminformatics

Examination Assignments

November 2012

INSTRUCTIONS FOR EXAMINATION ASSIGNMENTS

- Electronic (email, fax) submission of the assignments is not acceptable.
- The assignments have to be submitted by the student on standard A4 size paper in legible hand written, typed or printed format only.
- Do not copy from the answers of other participants. If it is noticed the assignment of such participants will not be accepted.
- The assignment for each paper should be written separately. Do not write the assignment for all the papers in continuity. However, all the assignments are to be submitted together.
- No two or more participants should submit their assignments in one envelope.
- The participants should mention their name and enrollment number on each page of submitted assignment copy.
- The last date of submission of Assignments is 30th November, 2012.

  The assignments have to be submitted to:
  The Program Coordinator
  ICIS
  C-56A/28, 1st Floor, Sector-62, Noida-201301
  U.P. INDIA
- Participants are advised to keep a photocopy of submitted assignments.
- The participants should mention their name and enrollment number at the top of the envelope.
- The participant should also mention **Examination Assignment** at the top of the envelope.

Basic of cheminformatics

Max. Marks: 100

SECTION A

Very Short Answer Type Questions (30-40 Words)

Attempt any four Questions : 4 × 5 = 20 Marks

1. What do you mean by data storage and management .
2. What do you understand by virtual screening?
3. Define & Explain the term internet.
4. Define the terms:
   a) Portability b) Comprehensiveness
   c) Conciseness d) Parsability
5. Differentiate between biophore sites and secondary sites.
6. What do you mean by pharmacophore.
7. Define the terms:
   a) Active transport b) Address- message concept
   c) Affinity .

SECTION B

Short Answer Type Questions (150-200 words)

Attempt any four Questions: 4 × 10 = 40 Marks

1. Explain briefly computational chemistry and retrieving chemical data
2. Explain briefly 2D substructure searching and 3D substructure searching.
3. Explain CHORTLES and the limitations of CHORTLES.
4. Explain biophore identification algorithm
5. Explain briefly linking sugars and modifying sugars
6. Explain intrinsic activity, ligand – based design and phage display .

SECTION C

Long Answer Type Questions (800-1000 words)

Attempt any two Questions: 2×20=40 Marks

1. What do you understand by cheminformatics, uses of cheminformatics its scope along with information use and information acquirement.
2. Briefly explain the following:
   a) Chemical information system b) Chemical Similarity
   c) Looking at small molecules d) From cheminformatics to combichem
3. Explain the size of the chemical information and computing capacity? Briefly explain peptides along with the example of diazepines.
4. Explain briefly library design, determining the overlap of libraries, library registration and chemically generated screening libraries.

Medicinal Chemistry

Max. Marks: 100

SECTION A

Very Short Answer Type Questions (30-40 Words)

Attempt any four Questions : 4 × 5 = 20 Marks

1. Define active principle of drugs.
2. Explain with the help of labelled diagrams
   (i) Metabolism of protonsil to sulfanilmide.
   (ii) Hydrolysis of penicillin by B- Lactamase
3. Define the following terms:
   (i) Topoisomerases (ii) Antimetabolites
4. List out the lead compound obtained from the following sources
   (i) Marine Sources (ii) Micro organisms
5. Define 'Drug potency'. Explain Dose response curve with example.
6. Explain the need of patent protection in case of drugs.
7. List the number of methods for structural optimization. Explain the characteristics of x-ray crystallographic data.

SECTION B

Short Answer Type Questions (150-200 words)

Attempt any four Questions: 4 × 10 = 40 Marks

1. Explain herbal remedies What are the benefits and possible limitations of herbal medicines.
2. What are Prodrugs? Explain the concept of prodrug technology.
3. Differentiate between intercalating agents and alkylating agents
4. Explain the process of catalysis by enzymes with the help of well labelled diagrams.
5. What are the various ways of improving water solubility.
6. Differentiate between
   (i) Diastereomers and Epimers.
   (ii) Competitive and Non Competitive inhibitors.

SECTION C

Long Answer Type Questions (800-1000 words)

Attempt any two Questions: 2×20=40 Marks

1. What do you understand by drugs. Explain the classification criteria of drugs. Also explain the scientific revolutions of drugs.
2. Describe soft drugs and also explain the various uses of soft drug principle.
3. Explain drug metabolism and how drug metabolic reactions are classified? Explain the irreversible removal of drugs by different routes in body.
4. Explain how to assess crystallographic data. What are the main types of co-ordinate system used in molecular modelling. Explain with suitable examples of each type.

Modern combinatorial chemistry

Max. Marks: 100

SECTION A

Very Short Answer Type Questions (30-40 Words)

Attempt any four Questions : 4 × 5 = 20 Marks

1. What do you understand by solid support mediated solution synthesis? Give few example of solid supported reagents.
2. Define linkers write down some examples of linkers
3. Write down the basic difference between phage and phagemid. Explain lytic cycle with the help of labelled diagram.
4. Write down the basic differences between synthetic and natural V - regions. Give a list of natural sources of V - regions.
5. Write down the uses of solid supported catalysts.
6. Define the following
   i) Assay ii) Target
7. Explain the factors governing selection of primary phage libraries

SECTION B

Short Answer Type Questions (150-200 words)

Attempt any four Questions: 4 × 10 = 40 Marks

1. Write down the main characteristics of chemically encoded libraries & mechanically encoded libraries, also discuss the main differences between them
2. Explain resin capture approach with its applications
3. Explain the key components of HTS.
4. Explain noncovalently bound tags with example.
5. How to design diverse libraries by analyzing product space and also explain database comparisons.
6. Define biological library display and explain its construction with the help of suitable diagrams

SECTION C

Long Answer Type Questions (800-1000 words)

Attempt any two Questions: 2 × 20 = 40 Marks

1. Explain the drug discovery process.
2. Name and explain the analytical techniques used in combinational library development.

3. Explain
   i) Designing screening assays for binding
   ii) Designing screening assays for functions
   iii) Need for improving antibody affinities. What are its advantages.
   iv) Downstream use of antibodies
4. Explain
   i) Vectors ii) Biopanning in vivo
   iii) Cloning iv) Bacterial display libraries

Chemical Database Design & Their Management

Max. Marks: 100

SECTION A

Very Short Answer Type Questions (30-40 Words)

Attempt any four Questions : 4 × 5 = 20 Marks

1. Explain key features of database system.
2. What is database concept. Explain
3. Give overview of MOS Database.
4. List the issues arising from file based systems.
5. Give an overview of the relational model.
6. How to remove duplicate rows of SQL Data.
7. Explain failed reactions chemical database.

SECTION B

Short Answer Type Questions (150-200 words)

Attempt any four Questions: 4 × 10 = 40 Marks

1. Explain chemical databases in terms of biocatalysis.
2. Explain chemical databases in terms of Metabolism.
3. Explain CODD's Rules.
4. Explain Data Modeling Components.
5. Write down the steps for creating tables using table wizard after database creation.
6. Explain antibody catalysis and cross linking.

SECTION C

Long Answer Type Questions (800-1000 words)

Attempt any two Questions: 2 × 20 = 40 Marks

1. What is DBMS. Explain the uses and the components of Database Management System.
2. Explain HITSET? How can HITSET be modified.
3. Explain protecting groups database.
4. Explain solid phase synthesis database with its database content and the selection criteria of reactions for inclusion in the database.

Chemical Information Sources

Max. Marks: 100

SECTION A

Very Short Answer Type Questions (30-40 Words)

Attempt any four Questions : 4 × 5 = 20 Marks

1. Give overview of chemical literature with its main types.
2. Write about primary literature the major forms of primary scientific publication.
3. Explain spectral complications.
4. Explain biomolecule sequence and structure databases.
5. Define and give overview of Beilstein and Gmelin.
6. Explain patents.
7. What is Molecular formula index.

SECTION B

Short Answer Type Questions (150-200 words)

Attempt any four Questions: 4 × 10 = 40 Marks

1. What do you mean by CAS. Explain the basic rules of CAS Nomenclature.
2. Write a short note on chemistry on www.
3. Differentiate between basic search skills and electronic search skills.
4. Describe the procedure of structure searching by using scifinder scholar.
5. Write short note on chemical connectivity and structure searches (2-D).
6. Write short note on chemical structure, property and shape based searches (3-D).

SECTION C

Long Answer Type Questions (800-1000 words)

Attempt any two Questions: 2 × 20 = 40 Marks

1. Explain structure searching and its uses.
2. Explain chemical safety and toxicology information.
3. (A) What are basic necessities of chemical safety and toxicology information? Describe.
   (B) Why National library of medicines TOXNET system and the canadian centre for occupational health and safety database help in chemical safety.
4. Write down notes on “current science on internet”. Give list of chemical applications of World Wide Web.

Computational Chemistry

Max. Marks: 100

SECTION A

Very Short Answer Type Questions (30-40 Words)

Attempt any four Questions : 4 × 5 = 20 Marks

1. What do you understand by photoelectric effect
2. Define the term inactive orbitals
3. What is carcinogenicity
4. What do you mean by photo-induced toxicity
5. What do you understand by torsion energy
6. Differenciate between stretching energy and binding energy
7. Define the following term:
   a) Monte carlo methods b) Intermolecular potentials
   c) Car – parrinello methods d) Gibbs duhem method
   e) Molecular dynamics methods

SECTION B

Short Answer Type Questions (150-200 words)

Attempt any four Questions: 4 × 10 = 40 Marks

1. Explain molecular mechanics and its method
2. Explain Hartree – fock energy expression and its equations
3. Describe Dirac Notation and properties predicted by electronic structure theory
4. Drive the expression "The mathematics of DIIS and explain programming DIIS
5. Describe all four continuum solvation methods
6. Explain, understanding the relative free energy Hamiltonian along with the advantage and disadvantage of slow growth method

SECTION C

Long Answer Type Questions (800-1000 words)

Attempt any two Questions: 2 × 20 = 40 Marks

1. Briefly explain computational chemistry, roles, its application and components of computational chemistry. Describe performance targets for the mesoscale
2. Briefly describe the symmetry & sample Z – matrix
3. Explain briefly the software used in computational chemistry
4. Describe biopolymers and briefly explain beta glucan technologies .

Data Sequencing mining and visualization

Max. Marks: 100

SECTION A

Very Short Answer Type Questions (30-40 Words)

Attempt any four Questions : 4 × 5 = 20 Marks

1. Define and given overview of two types of data mining models with suitable examples.
2. What are the basic differences between data warehouses and conventional databases?
3. Define and give overview of proteomics
4. Differentiate between uniform and rectilinear mapping methods
5. Write a short note on genomics
6. Define and explain any one data mining technique.
7. What are modules? List out its main characteristics.

SECTION B

Short Answer Type Questions (150-200 words)

Attempt any four Questions: 4 × 10 = 40 Marks

1. Write a note on application of data mining
2. Differentiate between data mining and machine learning
3. Compare OLAP and OLTP
4. Discuss the problems associated with data ware housing and explain the criteria for data warehouse
5. What are the problems associated with data mining
6. Write down short notes on
   i) Biotool
   ii) Oracle

SECTION C

Long Answer Type Questions (800-1000 words)

Attempt any two Questions: 2×20=40 Marks

1. What do you understand by data mining? Explain the scope of data mining. Describe how data mining works
2. Explain the various software applications of data mining
3. List out the different softwares used for chemical data mining. Explain any 15 softwares with their features.
4. What do you understand by gen expression and gen expression databases? What are datafieleds that should include in gene expression databases? What are the benefits of gene expression database mining?

Drug Design & Discovery

Max. Marks: 100

SECTION A

Very Short Answer Type Questions (30-40 Words)

Attempt any four Questions : 4 × 5 = 20 Marks

1. What do you mean by inhalation
2. Differenciate between disjunction and conjunction
3. What do you understand by molecular modeling kits and X-ray crystallography
4. What is ferguson principle
5. What do you mean by quinones
6. Define the following term:-
   a) Production b) Marketing
   c) Formulation d) Generic production
7. Define the term hybrids

SECTION B

Short Answer Type Questions (150-200 words)

Attempt any four Questions: 4 × 10 = 40 Marks

1. Explain injection route, sublingual route and rectal route
2. Explain the comparison of traditional and modern drug discovery
3. Explain four stereochemistry of enzymes
4. Briefly explain parameter space
5. Explain strategies for drug discovery, participants in drug discovery and describe any one management issues in discovery
6. Explain the types of need of drug discovery

SECTION C

Long Answer Type Questions (800-1000 words)

Attempt any two Questions: 2 × 20 = 40 Marks

1. Explain briefly the history and economies of drug discovery along with exploitation of side effects of drugs? How to testing of intermediates in drug synthesis
2. Explain ionization constants, briefly describe prediction of bioactivities based on certain physicochemical constants and prediction of bioactivities by manual methods of topliss, prediction of bioactivities by side chains
3. How drug design is necessary for T-cell functioning. Briefly explain design of inhibitors along with synthesis of lead compound and technology map.
4. Explain drug discovery process, current roles of the computer in drug design, challenge face by drug design and draw a graphical structure of drug discovery pipeline? Give some overview about template driven structure generation.