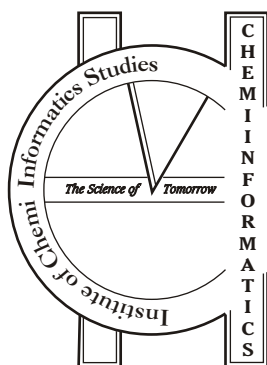


Industry Program in Cheminformatics

Examination Assignment

April 2011



ICIS

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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 April 2011.

The assignments have to be submitted to:

The Program Coordinator

Institute of Cheminformatics Studies

C-56A/28, 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.

Modern Combinatorial Chemistry

Max. Marks: 100

Attempt any five Questions:

5 × 20 Marks

1. Write short note on:
 - A. Matrix assisted Laser Desorption Ionization (MALDI)
 - B. Screening and Deconvolution
2. Explain the application of biological display libraries in Cheminformatics.
3. Give the combinatorial synthesis scheme for the chemical complexes of the following:
 - a) 2-Arylquinolines
 - b) Benzamide/urea Phenols
 - c) Benzodiazepine-2,5-diones
 - d) Bicyclooctanes
4. Mass spectrometry helps in the examination of molecular recognition and screening for lead drug candidates. Discuss.
5. Explain the following:
 - a) Halo aromatic Tags
 - b) Isotopic Tags
 - c) Autotagging
6. Write a note on the following:
 - a) Library quality control.
 - b) Cloning.
 - c) Insert design.
7. Write note on the following:
 - a) Automation for solid phase combinatorial chemistry.
 - b) Mutational SURF
 - c) Iterative deconvolution.

Chemical Database Design & Their Management

Max. Marks: 100

Attempt any five Questions:

5 × 20 Marks

1. Explain the databases relational model and relational query language.
2. Write a short notes on the following:
 - a) Wildcard characters
 - b) Comparison operators
 - c) Queries-AND/OR criteria
 - d) Queries-Multiple Table
3. What is a HITSET? How can HITSET be modified?
4. Write a short on failed reaction database. Explain its uses DBMS. How are use the failed reactions database in Accord.
5. Write down the SQL statement for the following:
 - a. Count the number of elements in the table name periodic and field EI_name.
 - b. Find the color field of EI_name = lithium in the table name periodic.
 - c. Select rows which are within the range of Neutron field between 25 to 40 in table name is periodic.
 - d. Sort out the table name periodic where crystal column is like 'cubic.
6. Explain the Data Modeling Components in detail?
7. Explain the following:
 - a) Why use DBMS to store Data?
 - b) Database Level
 - c) Database Concept
 - d) How we loose Data
 - e) Key features of Database system

Basic of Cheminformatics

Max. Marks: 100

Attempt any five Questions:

5 × 20 Marks

1. Define Cheminformatics. State the uses of Cheminformatics. Also give the list of the some companies engaged in Cheminformatics work.
2. Write short notes on the following:
 - a) CHUCKLES
 - b) PEPTIES
3. Explain the following:
 - a) Chemical information.
 - b) From chemical information to chemoinformatics.
 - c) From Cheminformatics to combichem.
4. Write short notes on the following:
 - a) Charts: Searching.
 - b) Biophore identification algorithm.
 - c) 3D-QSAR active site models.
5. Write note on the following:
 - a) Emergence of chemoinformatics.
 - b) From chemoinformatics to cheminformatics.
 - c) Current interest in 3D similarity measures
6. What is Apex - 3D expert system for drug design and its architecture? Explain general principle of basic Apex 3D algorithm and its application.
7. Give the nomenclature, symbols, and structural diagrams related to chemical information sciences and write about its abstract, reviews, compilations, and indexes.

Medicinal Chemistry

Max. Marks: 100

Attempt any five Questions:

5 × 20 Marks

1. Explain the important scientific revolutions of last few decades.
2. Write short notes on the following:
 - a) Carrier Protein Blocking
 - b) Antimetabolites
 - c) Intercalating agents
 - d) Alkylating agents
3. Describe the in vitro methods used for the testing drugs.
4. Explain the effect of pH on solubility of aqueous biological fluid with examples.
5. Write note on the following:
 - a) Glutathione conjugation.
 - b) Methylation and acylation
 - c) Oxidation of aromatic rings and carbon-nitrogen centres.
6. Explain the following:
 - a) Ligand - receptor complexes and mode of action.
 - b) Concept of hard and soft acid and base.
 - c) Scientific revolutions.
7. Write short notes on the following:
 - a) Full synthesis and semi-synthesis of drugs.
 - b) Biosynthesis of drugs.
 - c) The use of non-stereoselective reactions to produce stereospecific centers.

Data Sequencing Mining & Visualization

Max. Marks: 100

Attempt any five Questions:

5 × 20 Marks

1. Differentiate the following:
 - A. Data mining vs. Machine learning
 - B. OLALP vs. OLTP
 - C. Data mining Verification vs. Discovery
2. What is “ON-LINE ANALYTICAL PROCESSING”? Give example.
3. Write short notes on:
 - a) Computational Gene Discovery
 - b) Sequence similarity searching.
4. Explain the following softwares:
 - a) AUTOCORR
 - b) C@ROL
5. Write a note on Red Brick Systems and its software products.
6. Explain
 - a) LOGKOW
 - b) METEROR
 - c) MIDLSCREEN
 - d) SYNLIB
7. Define proteomics. Define and list Proteome database. Explain the process of proteome database mining.

Drug Design & Discovery

Max. Marks: 100

Attempt any five Questions:

5 × 20 Marks

1. Explain the following:
 - a) Drug action and response.
 - b) Adverse reactions and effectiveness & safety.
 - c) Drug interactions.

2. In silico drug discovery is playing a vital role in the drug discovery process. Explain

3. What is meant by Pharmacodynamics? Describe with the help of an example the pharmacodynamics in drug designing.

4. Explain the term pharmacodynamics. Describe the mechanism with the help of diagrams and equations.

5. Explain the five classic steps of development of a drug.

6. What is chelation? Explain the role of chelates in medicines.

7. Explain the following:
 - a) Methods for design of enzyme inhibitors.
 - b) Synthesis of lead compound.
 - c) Technology map

Chemical Information Sources

Max. Marks: 100

Attempt any five Questions:

5 × 20 Marks

1. Write short notes on the following:
 - a) Web search engines
 - b) Costs and benefits of online searching.
 - c) Current awareness, reviews, and document delivery.
 - d) Boolean search operators
2. Explain the achievement of current science on the internet. Write about electronic conference on the World Wide Web.
3. Computers searching helps to extract the information. State its advantages and limitations.
4.
 - a) What are basic necessities of chemical safety and toxicology information? Describe
 - b) Why National Library of Medicine's Toxnet system and the canadian centre for occupational health and safety database help in chemical safety.
5. Write short notes on the following:
 - a) Distributed teaching models on the World Wide Web.
 - b) Future of the scientific information communication.
 - c) Chemical application of the www System.
6. Write short notes on the following:
 - a) Electronic Publishing
 - b) Electronic Preprints
7. Write note on the following:
 - a) Patent.
 - b) Chemical abstracts in print.
 - c) Molecular formula index

Computational Chemistry

Max. Marks: 100

Attempt any five Questions:

5 × 20 Marks

1. Define Computational Chemistry. Describe its role in chemical research.
2. A. What is the important software used in computational chemistry?
Give a brief introduction of each.

B. How the following tools help in computational chemistry?
 1. COLUMBUS
 2. DB Watcher
 3. MODELLER
 4. PROCHECK
3. Define biopolymers. Explain briefly various biopolymers.
4. Write short note on Ramachandran Map/Plot.
5. Describe briefly the mathematical equation of DIIS.
6. Write a short note on Software CHARMM.
7. Explain the following:
 - a) SCRF
 - b) PCM
 - c) COSMO