Post Graduate Diploma in Chemoinformatics
Annual Examination 2006

Paper PGDC – 101
Basics of Chemoinformatics

Time Allowed: Three Hours | Maximum Marks: 80

SECTION – I

Q1. Attempt all the objective type questions given below:- 1X20

(i) Chemoinformatics term was introduced by :
- a) Dr. Charles Brown.
- b) Dr. Frank Brown.
- c) Dr. Smith Kline
- d) Dr. Tom Brown

(ii) Chemoinformatics techniques do not include:
- a) Docking
- b) Virtual Screening
- c) Compound History
- d) Data-base mining

(iii) Spectral data information can not be obtained through:
- a) ^1H – NMR
- b) MASS spectra
- c) HPLC
- d) IR

(iv) CONCORD is a source of
- a) 2D structural data
- b) 3D structural data
- c) clogP data
- d) None of these

(v) For drugs targeted for CNS, values of log BB, for distribution of a drug to brain should be in the range of
- a) >0.3,<-1.0
- b) >1.1,<-3.0
- c) >3.0,<1.0
- d) >0.5,<1.5

(vi) American Chemical Society was founded in New York in
- a) 1846
- b) 1876
- c) 1947
- d) 1840

(vii) In 1980, the following ACS publication was made available online
   a) JMC (Journal of Medicinal Chemistry)
   b) Chemical Review
   c) Journal of Biochemistry
   d) Journal of Computational Chemistry

(viii) The first sites appeared on the World Wide Web (WWW) in
   a) 1990
   b) 1991
   c) 1992
   d) 1993

(ix)First issue of Chemical Abstract (CA) was published in
   a) 1900
   b) 1907
   c) 1908
   d) 1909

(x) NCBI (National Center for Biotechnology) was established in 1988 to oversee the
   a) Human Genome Project
   b) Genetic Information Forum
   c) Gene Therapy Project
   d) Gene Replication Project

(xi)The most important drug used to beat AIDS
   a) AZT
   b) Cyclosporin
   c) Ciprafloxcin
   d) Ciphalosporin

(xii) Major Stage in pre clinical drug discovery and informatics component does not refer to
   a) Identification of a novel drug target
   b) Characterization of biological function of target proteins
   c) Development of in vitro analysis
   d) X-ray analysis

(xiii) According to the "rule-of-five" calculated log p (clogP) must be
   a) >5.0
   b) >2.0
   c) >0.1
   d) >0.05

(xiv) Optimization of a drug means
   a) to synthesize a new drug
   b) to improve pharmacological properties of a drug
   c) to enhance the solubility of a drug
   d) none of these

(xv) An enzyme is chemically
   a) complex protein
   b) non-proteinaceous moiety
   c) inorganic compound
   d) polymer of nucleic acids

(xvi) Molar refractivity is related with
a) Size and polarization of a molecule
b) 3D structure of a molecule
c) Stereo-isomerism
d) Fragment of a compound

(xvii) High through put screening (HTS) is efficient, trial and error evaluation of a compound in a
a) Target based assay
b) Non-target-based assay
c) Genetic assay
d) Grand mass level assay

(xviii) CoMFA is a
a) 3D QSAR method
b) QSAR method
c) HTS method
d) Physio-chemical method

(xix) Liphophilicity of a molecule can not be measured by
a) RTHPLC
b) Partitian coefficient (in.1-Octanol/Water)
c) TLC
d) Column chromatography

(xx) AMBER is a molecular mechanics program for calculation on
a) Non-proteinous substance
b) Only DNA
c) Protein and nucleic acid
d) None of these

SECTION – II

Q2. Attempt any five questions. All questions carry equal marks. 6 X 5

(i) What is open access publishing (OAP)? Explain its worldwide use.
(ii) What is meant by ADME-analysis? How does it affect the properties of a drug?
(iii) What techniques can be used for lead-identification?
(iv) Differentiate between the following terms
a) Combinatorial chemistry
b) Computational chemistry
(v) Distinguish between the terms bio availability and bio assay.
(vi) What is the energy minimization process? Explain with examples.
(vii) "New soft wares for docking method are more useful to explain the actual binding sites on the substrate". Explain and support with examples.
(viii) Why do we study chemo-informatics? Describe its future perspective.

SECTION – III

Q3. Attempt any three questions. All questions carry equal marks. 10X3

1. Make a detailed comment about importance of integration, access and transformation of data, knowledge and tools etc.
2. What is the role of computers and connectivity in information services? How is CIS different from other research fields?
3. What is Rational Drug Discovery (RDD)? Describe the applications of chemoinformatics in RDD process.
4. Explain the clinical challenges for chemo informatics in the field of Drug Discovery.
5. Describe all computational methods for the prediction of 'Drug-likeness".