

M. SC. BIOINFORMATICS SEM.-III (2013 COURSE)
(CHOICE BASED CREDIT SYSTEMS) : WINTER - 2017

SUBJECT : CHEMINFORMATICS & DRUG DESIGN

Day : Saturday
Date : 28/10/2017

W-2017-1016

Time : 02.00 PM TO 05.00 PM
Max. Marks : 60

N.B :

- 1) **Q. 1 and Q. 5 are Compulsory.** Out of the remaining questions, attempt **any 2** from each sections.
- 2) Figures to the right indicate **Full** marks.
- 3) Answers to both the sections should be written in **Separate** answer books.

Section - I

- Q. 1** Define : (10)
- | | |
|---|---|
| a) Hosoya index
c) E-state
e) Molecular Shape | b) Adjacency Matrix
d) Pharmacophore |
|---|---|
- Q. 2**
- | | |
|--|----------------------|
| a) Explain SMARTS.
b) Describe electro-topological and refracto-topological descriptors.
c) Write short note on cheminformatics. | (02)
(04)
(04) |
|--|----------------------|
- OR**
- c) Define descriptors. Explain shape indices descriptors.
- Q. 3**
- | | |
|---|---|
| a) What is Vertex partition algorithm?
b) Explain followings:
1) Tanimoto coefficient
c) Explain Multiple Linear Regression (MLR). | 2) Euclidean distance
(02)
(04)
(04) |
|---|---|
- OR**
- c) How molecular databases are important in drug discovery research?
- Q. 4**
- | | |
|---|----------------------|
| a) Define principal moment of inertia.
b) Write short note on ADMET.
c) How combinatorial library play important role in drug discovery research? | (02)
(04)
(04) |
|---|----------------------|
- OR**
- c) Discuss Lipinski's rule of five and define lead molecule.

Section - II

- Q. 5** Answer in brief: (10)
- | | |
|---|--|
| a) Name any four 3D descriptors.
b) Define SMIRKS
c) Write full form of SMILES.
d) What is Tversky Index?
e) Write a brief account on Autodock. | |
|---|--|
- Q. 6**
- | | |
|--|--------------|
| a) What is lead optimization?
b) Differentiate between ligand-based and structure-based drug design approaches with examples. | (02)
(04) |
|--|--------------|
- OR**
- | | |
|---|------|
| b) How can you identify and validate target site?
c) Discuss ab-initio drug design approach. | (04) |
|---|------|
- Q. 7**
- | | |
|---|----------------------|
| a) Define structure-activity relationship (SAR).
b) Differentiate between 2D and 3D QSAR techniques with examples.
c) Explain stepwise derivation of 2D QSAR model. | (02)
(04)
(04) |
|---|----------------------|
- OR**
- c) Why validation of in-silico models are important?
- Q. 8**
- | | |
|--|--------------|
| a) Define virtual screening.
b) Differentiate between flexible and rigid docking. | (02)
(04) |
|--|--------------|
- OR**
- | | |
|---|--------------|
| b) Write short note on Scoring function.
c) Define pharmacophore. Explain steps of derivation of pharmacophore models. | (04)
(04) |
|---|--------------|

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