

## Unit 12 - Week 10

### Course outline

How does an NPTEL online course work?

### Prerequisite Assignment

Week 1

Week 2

Week 3

Week 4

Week 5

Week 6

Week 7

Week 8

Week 9

Week 10

Computer aided drug design - II

Virtual screening - I

Virtual screening - II

QSAR - I

QSAR - II

Quiz : Assignment 10

Bio-Informatics:Algorithms and Applications : Week 10 Feedback Form

Week 11

Week 12

Download Videos

Text Transcripts

## Assignment 10

The due date for submitting this assignment has passed.  
As per our records you have not submitted this assignment.

**Due on 2020-04-08, 23:59 IST.**

1) Choose the application of docking scores

1 point

- To fix a particular position of the ligand
- To reduce the degrees of freedom
- To rank the active compounds
- All the above

No, the answer is incorrect.  
Score: 0

Accepted Answers:  
To rank the active compounds

2) Empirical scoring function depends on

1 point

- Least square fit between experimental affinity and computed parameters
- Force field of the method
- Bond length, bond angle and torsional angle
- Non-covalent interactions

No, the answer is incorrect.  
Score: 0

Accepted Answers:  
Least square fit between experimental affinity and computed parameters

3) Which of the following depends on empirical based scoring function?

1 point

- Autodock
- GOLD
- GLIDE
- PMF

No, the answer is incorrect.  
Score: 0

Accepted Answers:  
GLIDE

4) Virtual screening is used to identify

1 point

- A drug
- Probable hit compounds
- The best compound with highest binding affinity
- Types of interactions between protein and ligand

No, the answer is incorrect.  
Score: 0

Accepted Answers:  
Probable hit compounds

5) Comparison of physicochemical properties with known active compounds could reduce the initial dataset to

1 point

- 50% or less
- 95%
- 90%
- 85%

No, the answer is incorrect.  
Score: 0

Accepted Answers:  
50% or less

6) QSAR is based on the notion that

1 point

- Activity is a function of structure
- Activity is a function of molecular properties
- Activity is a function of physical properties
- All the above

No, the answer is incorrect.  
Score: 0

Accepted Answers:  
Activity is a function of molecular properties

7) IC50 is

1 point

- biased towards inhibition
- biased towards viability
- balance between inhibition and viability
- None of the above

No, the answer is incorrect.  
Score: 0

Accepted Answers:  
balance between inhibition and viability

8) 2D QSAR deals with

1 point

- Molecular properties
- Connectivity indices
- Surrounding atoms in structure
- All the above

No, the answer is incorrect.  
Score: 0

Accepted Answers:  
Connectivity indices

9) Data pre-processing involves

1 point

- Data cleaning
- Data transformation
- Feature selection
- All the above

No, the answer is incorrect.  
Score: 0

Accepted Answers:  
All the above

10) If the Pearson's correlation coefficient between the two sets of data is 0.5 then

1 point

- No correlation
- Positive correlation
- Random relationship
- Negative correlation

No, the answer is incorrect.  
Score: 0

Accepted Answers:  
No correlation