Unit 9 - Week 7

Course outline

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Week 7

- 3D QSAR
- Pharmacophore modelling
- Target based drug design
- Target based drug design
- Target based drug design
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Text Transcription

Assignment 7

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

Due on 2019-09-18, 23:59 IST.

1) Molecule A has 14 finger prints and Molecule B has 9 finger prints. They have 3 finger prints in common. Calculate the Tanimoto Coefficient?

Hint

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Range) 0.148,0.152

1 point

2) Which is not a pharmacophore in this list ***1 point***

- aromatic
- rotatable bond
- hydrogen bond donor
- hydrophobic

No, the answer is incorrect.
Score: 0
Accepted Answers:
rotatable bond

3) If the binding constant for a ligand protein interaction is 2.1, calculate the molar Gibbs free energy $-\Delta Go$ at 30ºC in kJ/mol

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Range) 1.75,2.0

1 point

4) A relationship is developed between the binding energy of drugs with their activities as pIC50 =- 1.73 - 0.84 * binding energy. If the binding energy for a new molecule is -9.0 kcals/mol, calculate its activity, IC50, in micro mol

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Range) 1.46,1.5

1 point

5) Sequence A has 400 AA, while Sequence B has 600 AA. Using BLAST a pair wise alignment was done. 90 amino acids are identical. What is the % Identity

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Range) 22.0,23.0

1 point

6) In problem 5, if 25 amino acids that are different by conservation substitution, what is the % Similarity

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Range) 28.7,28.8

1 point

7) Disulfide bonds contribute to protein stability mainly by reducing the conformational entropy of the denatured state as ΔS = −2.1 − (3/2) R ln(n). n is the number of residues in the loop formed by the crosslink. If the number of residues in the loop increases from 5 to 10 , what is the increase in % stability

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Range) 38.5,39.5

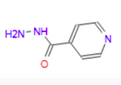
1 point

8) A protein and ligand interact through van der waals force. If the ligand moves away by 10%, what is the decrease in the van der waals force in %

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Range) 56,57

1 point

9) What is the Uniprot number of the most probable target of



No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: String) P21397

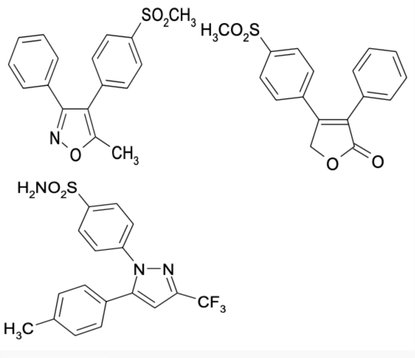
1 point

10)When you run a BLAST search with the above target what is the Uniprot number of the protein which has 100% identity

No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: String) Q53YE7

1 point

11)Perform a pharmacophore model of the following three molecules using Pharmagist. What is the highest alignment score reported?



No, the answer is incorrect.
Score: 0
Accepted Answers:
(Type: Range) 15.3,15.5

1 point