Course Name: Computer Aided Drug Design   Course No: PHA G541

Max. Marks: 30   Duration: 90 Min

Note: Answer for all questions precisely with appropriate illustrations if required.
Give the answer for all sub-parts together in one place.

1) a) Define drug target. What are the things you will consider while selection of target during

NDD?   **(2x3=6)**

b) Write about CADD techniques used in pre-clinical studies? Limitations of CADD in NDD.

2) a) Write about predictive ADR models and the approaches for their assessment.   **(2x3=6)**

b) Write the significance of synthetic accessibility prediction in Drug Discovery.

3) a) Write the steps involved in sequencing of dimeric protein? How will you determine *N*-

terminus portion of the same protein using phenyl isothiocyanate.   **(2x3=6)**

b) List out available methods for the determination of protein structure. Explain in detail about

the method that uses microscope for the same.

4) a) Enumerate the significances of sequence alignment in knowledge-based modeling. **(2x3=6)**

b) How will you validate the modeled protein built by comparative modeling.

5) a) Enumerate various types of available compound libraries. Write the workflow involved in

an efficient library design.   **(2x3=6)**

b) Write a brief account on pharmacophore based library design.