BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI
First Semester 2023-2024
Mid-Semester Examination (Closed Book)

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.

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1) a) Define lead. Explain the strategies for lead discovery with suitable examples.   **(2x3=6)**
b) Write a note on failures in drug discovery. Explain risk mitigation strategies in academic pre-clinical drug discovery.

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 and distribution constant in the drug likeness prediction of NMEs.

3) a) Write the steps involved in sequencing of dimeric tripeptide? How will you determine *N*-terminus portion of the same protein using 1-fluoro-2,4-di-nitrobenzene.   **(2x3=6)**
b) List out the various methods available for protein structure prediction. Explain in detail about any one method used for proteins which do not have homologous proteins.

4) a) Enumerate the types of sequence alignment in knowledge-based protein modeling. **(2x3=6)**
b) Write a brief account on typical errors in knowledge based modeling and it's mitigation strategies.

5) a) Explain how a library that are used during earlier phase of drug discovery are designed? Write it's significance and quantifying criteria.   **(2x3=6)**
b) Write a brief account on final compound selection methodology in virtual chemical library design.