Ticket 1

Reference: Shityakov, S. and T. Dandekar (2010). "Lead expansion and virtual screening of Indinavir derivative HIV-1 protease inhibitors using pharmacophoric - shape similarity scoring function." Bioinformation 4(7): 295-299.

1) Could you define chemoinformatics? What are the areas of its implementation?

2) How does chemoinformatics differ from bioinformatics?

3) Can you describe the standard pipeline in chemoinformatics?

Ticket 2

Reference: Shityakov, S., et al. (2013). "Analyzing molecular polar surface descriptors to predict blood–brain barrier permeation." Int J Comput Biol Drug Des 6(1-2): 146-156.

1) What are the two main in silico methods within the chemoinformatics paradigm, and how do they differ?

2) Why is investigating and understanding the blood–brain barrier mechanism crucial for chemoinformatics?

3) How does chemoinformatics leverage experimental data for learning? Can you provide examples?

Ticket 3

Reference: Shityakov, S. and C. Forster (2014). "In silico predictive model to determine vector-mediated transport properties for the blood–brain barrier choline transporter." Adv Appl Bioinform Chem 7: 23-36.

1) What is the primary objective of chemoinformatics? How can computational methods in chemoinformatics be classified based on accuracy?

2) Which metrics (Python) are commonly used in chemoinformatics, and could you provide some examples?

3) What are the advantages and disadvantages of molecular scaffolds?

Ticket 4

Reference: Shityakov, S., et al. (2014). "Evaluation and prediction of the HIV-1 central polypurine tract influence on foamy viral vectors to transduce dividing and growth-arrested cells." ScientificWorldJournal 2014: 487969.

1) What are the advantages and disadvantages of the pharmacophore concept? Can you discuss the types of pharmacophores?

2) How is molecular docking utilized in chemoinformatics? Could you elaborate on the types of molecular docking?

3) What software is commonly used for molecular docking, and what are its advantages and disadvantages?

Ticket 5

Reference: Shityakov, S., et al. (2021). "Scaffold Searching of FDA and EMA-Approved Drugs Identifies Lead Candidates for Drug Repurposing in Alzheimer's Disease." Front Chem 9: 736509.

1) Could you discuss the algorithms commonly used for molecular docking?

2) What are the principles behind machine learning algorithms used in molecular docking?

3) What is the drawback of using genetic algorithms in molecular docking?

Ticket 6

Reference: Fareed, M. M., et al. (2022). "In-silico analysis of nonsynonymous single nucleotide polymorphisms in human beta-defensin type 1 gene reveals their impact on protein–ligand binding sites." Comput Biol Chem 98: 107669.

1) Which proteins are typically preferred for molecular docking and protein–ligand interaction studies? Can you provide some examples?

2) What is the standard error, particularly for the largest cluster, in the molecular docking technique? How can this error be minimized?

3) Could you describe the types of protein–ligand binding sites and their influence on molecular docking?

Ticket 7

Reference: Kovalenko, A. A., et al. (2023). "Using novel click chemistry algorithm to design D3R inhibitors as blood–brain barrier permeants." Future Med Chem 15(11): 923-935.

1) Can you outline the algorithms commonly used for protein–protein molecular docking? How do they differ from the algorithms used for protein–ligand molecular docking in terms of methodology?

2) What is molecular dynamics simulation, and what are its various types? Why is it considered important for chemoinformatics? Could you discuss its advantages and disadvantages?

3) How are chemical calculations utilized in cheminformatics for rational drug design and discovery?

Ticket 8

Reference: Shityakov, S., et al. (2023). "Ergodicity Breaking and Self-Destruction of Cancer Cells by Induced Genome Chaos." Entropy (Basel) 26(1).

1) Could you list some software commonly used for molecular dynamics simulations and provide examples of their applications?

2) What are the different force fields utilized in molecular dynamics simulations? Can you describe their types and discuss their respective advantages and disadvantages?

3) What are the key parameters typically employed in molecular dynamics (MD) simulations to evaluate protein flexibility, stability, and function?

Ticket 9

Reference: Isakova, A. M., et al. (2024). "NeuroClick: software for mimicking click reaction to generate drug-like molecules permeating the blood–brain barrier." Future Med Chem 16(5): 389-398.

1) Can you elaborate on computational synthetic biology and its connection to chemoinformatics? Could you provide some examples of how these fields intersect?

2) What is graph theory, and why is it important for synthetic biology and chemoinformatics?

3) Could you explain the concept of QSAR and QSPR? What are the different types of QSAR/QSPR approaches used in chemoinformatics and rational drug design and discovery?

Ticket 10

Reference: Dutta, K., et al. (2024). "Analyzing the Effects of Single Nucleotide Polymorphisms on hnRNPA2/B1 Protein Stability and Function: Insights for Anticancer Therapeutic Design." ACS Omega 9(5): 5485-5495.

1) Could you explain the differences and similarities between the Monte Carlo and simulated annealing methods? How are they utilized in chemoinformatics and synthetic biology?

2) What is drug repurposing, and why is it considered a promising tool for chemoinformatics and synthetic biology?

3) Which chemical databases are commonly used in chemoinformatics and synthetic biology research?

Ticket 11

Reference: Shityakov, S., et al. (2023). "Voronoi Entropy as a Ligand Molecular Descriptor of Protein–Ligand Interactions." ACS Omega 8(48): 46190-46196.

1) Can you define what a molecular descriptor is and provide some examples? Additionally, which descriptors are commonly used in blood–brain barrier research?

2) What are the typical chemical formats utilized in chemoinformatics and synthetic biology?

3) What are the primary molecular descriptors used in QSAR/QSPR studies? Could you provide some examples?

Ticket 12

Reference: Shityakov, S., et al. (2022). "Topological bioscaling analysis as a universal measure of protein folding." R Soc Open Sci 9(7): 220160.

1) Can you explain what protein folding is and why understanding its mechanisms is crucial for both chemoinformatics and computational synthetic biology?

2) What is PCR (polymerase chain reaction), and what are the available silico methods or software for running it? Additionally, could you describe the processes involved in experimental and computational site-directed mutagenesis of protein structures?

3) What are the different sequencing techniques available? Could you provide examples? How is gene expression analyzed in silico, particularly using Affymetrix microarray data?

Ticket 13

Reference: Shityakov, S., et al. (2023). "Folding-unfolding asymmetry and a RetroFold computational algorithm." R Soc Open Sci 10(5): 221594.

1) Could you elaborate on how chemical reactions are modeled in silico using chemoinformatics approaches? It would be helpful to provide examples such as click reactions.

2) How is chemoinformatics integrated into chemical reaction generators? Could you provide some examples to illustrate this integration?

3) What are the algorithms commonly used in chemoinformatics and computational synthetic biology to analyze molecular folding?

Ticket 14

Reference: Shityakov, S., et al. (2012). "α-Cyclodextrin dimer complexes of dopamine and levodopa derivatives to assess drug delivery to the central nervous system: ADME and molecular docking studies." Int J Nanomedicine 7: 3211-3219.

1) Could you provide insights into the implementation of ML/DL methods for chemoinformatics and computational synthetic biology? It would be beneficial to discuss the algorithms involved and offer some examples.

2) What are the advantages and disadvantages of ML/DL methods compared to classical molecular modeling algorithms (such as search-based and physics-based methods)?

3) How are conformational search and symmetry addressed in chemoinformatics? Additionally, could you elaborate on the application of Voronoi tessellation and Voronoi entropy in chemoinformatics and computational synthetic biology?

Ticket 15

Reference: Shityakov, S. and C. Forster (2013). "Multidrug resistance protein P-gp interaction with nanoparticles (fullerenes and carbon nanotube) to assess their drug delivery potential: a theoretical molecular docking study." Int J Comput Biol Drug Des 6(4): 343-357.

1) How is chemoinformatics implemented in materials science and supramolecular chemistry? Could you provide some examples to illustrate its application in these fields?

2) What is the standard protocol for molecular dynamics simulations? It would be helpful to have a description of the typical steps involved in this protocol.

3) Could you outline the standard protocol for molecular docking, using AutoDock or AutoDock Vina as an example?

Ticket 16

Reference: Tamaian, R., et al. (2023). "Exhaustive in silico design and screening of novel antipsychotic compounds with improved pharmacodynamics and blood–brain barrier permeation properties." J Biomol Struct Dyn 41(24): 14849-14870.

1) Could you explain the ADME/ADMET concept as it is used in chemoinformatics and computational synthetic biology?

2) What specific molecular descriptors are commonly utilized for calculating ADME properties?

3) What is the scaffold hopping method used in chemoinformatics, and what are its advantages and disadvantages?

Ticket 17

Reference: Shityakov, S., et al. (2020). "Modeling of shotgun sequencing of DNA plasmids using experimental and theoretical approaches." BMC Bioinformatics 21(1): 132.

1) Why do retroviral proteases and cyclodextrins favor systems for protein–ligand or host-guest interaction analysis?

2) What molecular fingerprints are typically employed in chemoinformatics and computational synthetic biology?

3) Could you clarify the distinction between molecular fingerprints and molecular descriptors used in chemoinformatics and computational synthetic biology?