

Kierunek: Biosciences

Specjalność: Bioinformatics

### **Zagadnienia na egzamin dyplomowy**

1. Postulates of quantum mechanics
2. Wave-particle nature of matter and light
3. Exact solutions of the Schrödinger equation
4. Electron spin and the form of the wave function of a multi-electron system
5. Methods of determining approximate wave functions of atoms and multi-electron molecules
6. Hartree-Fock method, orbitals of many-electron atoms and molecules
7. Partition functions in statistical thermodynamics.
8. Ergodic hypothesis.
9. Thermodynamic functions based on partition functions.
10. Molecular mechanics and molecular dynamics
11. Computational methods used in protein global minimum search.
12. Computational methods in bionanotechnology.
13. Intermolecular interactions: components of different nature, predictions of geometries of complexes
14. Types of chemical bonds
15. Phase-boundary interactions - adsorption phenomenon
16. Methods of numerical integration
17. Kinetic and thermodynamic description of catalyzed reactions
18. Mechanisms of catalytic reactions - homogeneous, heterogeneous, enzymatic
19. Photodegradation of organic compounds
20. Applications of nanomaterials
21. Applications of Monte Carlo methods in chemistry
22. Similarity and homology of biological sequences: measures of similarity, sequence alignments, inferring homology
23. Molecular phylogenesis
24. Automation of data processing in bioinformatics

25. Design of biologically active compounds
26. Docking and virtual screening
27. Classifications of chemical reactions
28. Reaction kinetics (rate laws) for different types of chemical reactions
29. The role of water in biochemical reactions
30. Water–protein interactions
31. Enzymes as catalysts
32. Kinetics of enzymatic reactions
33. Inhibition in enzymatic reactions
34. Methods of pharmaceuticals' analysis
35. Analytical procedures in drugs identification (spectrophotometric, colorimetric, potentiometric, etc.)