

Chapter 15: Computers in medicinal chemistry

Type: multiple choice question

Title: Chapter 15 - Question 01

01) Which of the following operations or calculations would generally be carried out using quantum mechanics?

Feedback: Quantum mechanics is used for the calculation of partial atomic charges. The other calculations or procedures are generally done using molecular mechanics.

Page reference: 326-327

- a. Energy minimisation
- b. Identifying stable conformations
- *c. Partial atomic charges
- d. Energy calculations for specific conformations

Type: multiple choice question

Title: Chapter 15 - Question 02

02) Which of the following software programs is not used for drawing 2D chemical structures?

Feedback: Chem3D is a general molecular modelling software program.

Page reference: 327

- a. ChemDraw
- b. Chem/Window
- *c. Chem3D
- d. Isis/Draw

Type: multiple choice question

Title: Chapter 15 - Question 03

03) Which of the following software programs is not dedicated to the creation of 3D chemical models?

Feedback: DOCK was one of the early software programs for docking a ligand to a binding site.

Page reference: 327-328, 345

- *a. DOCK
- b. Alchemy
- c. Hyperchem
- d. Discovery Studio Pro

Type: multiple choice question

Title: Chapter 15 - Question 04

04) Which of the following is associated with conformational searching?

Feedback: The Monte Carlo method is used in searching for different conformations of a molecule. LUDI is a software program used in de novo drug design. DOCK is used in docking molecules into binding site. CoMFA is used in 3D QSAR.

Page reference: 337-338

- a. LUDI
- b. DOCK
- *c. Monte Carlo method
- d. CoMFA

Type: multiple choice question

Title: Chapter 15 - Question 05

05) Molecular dynamics can be used to search for different conformations of a molecule. Which of the following statements is false?

Feedback: Measurements are calculated after each femtosecond of movement.

Page reference: 335-337

- a. A variety of different conformations are generated by 'heating' the molecule to 900K.
- *b. The position and velocity of each atom is measured after each nanosecond of movement
- c. The programme treats each atom as a moving sphere
- d. Each atom is only allowed to move a fraction of a bond length between each cycle of calculations

Type: multiple choice question

Title: Chapter 15- Question 06

06) Which of the following statements regarding molecular mechanics is untrue?

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Harry J. Witchel, Michael W. Lee



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conduct their search for and design of new drug entities In contrast to competing books it focuses on the chemistry rather than pharmacological concepts or descriptions of the various therapeutic classes of drugs Most medicinal chemists working in the pharmaceutical industry are organic synthetic chemists who must acquire a strong knowledge of medicinal chemistry as they enter the industry This book aims to be their practical handbook a complete guide to the drug discovery process The only book available dealing with the practical aspects of medicinal chemistry Serves as a complete guide to the drug discovery process from conception of the molecules to drug production Updated chapters devoted to the discovery of new lead compounds including combinatorial chemistry Secrets of Success: Getting into Medical School Viyaasan

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education In this regard the authors highlight how educational technology is both a bridge and barrier to student access and inclusivity Further they address the ongoing discussion as to whether students need to be present for lectures and on how having agency in their own learning can improve both retention and conceptual understanding To link the content to current events the authors also shed light on the impact that the COVID 19 pandemic is having on the continuity of educational programs and on the growing importance of educational technologies Consequently the book offers life science educators valuable guidance on the technologies already available and an outlook on what is yet to come *Educart CBSE Class 12 Chemistry One Shot Question Bank 2026 (Includes PYQs for 2025-26) ,*

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