

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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Arun Syamal



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Mahalingasivam, Marc Gladman, Manoj Ramachandran, 2020-10-07 Applying to medical school has become increasingly competitive with greater numbers of students applying every year Applicants must take every available opportunity to make themselves stand out amongst the competition if they want to have a chance of getting into the school of their choice *Secrets of Success: Getting into Medical School* is written for all potential medical students and is intended to guide applicants on making the right choices in choosing schools and optimizing their performance in the application process The Pearson General Studies Manual 2009, 1/e Showick Thorpe Edgar Thorpe, 2009 This latest edition of The Pearson General Studies Manual continues to provide exhaustive study material for the General Studies paper of the UPSC Civil Services Preliminary Examination This student friendly book has been completely revised thoroughly updated and carefully streamlined and is strictly exam centric In this new edition a large number of new boxes and marginalia with additional and relevant information have been added to provide cutting edge information to the aspirant Readers will find that important facts and information have been presented in the form of well structured tables and lists *Gcse Biology Study Guide* Daniel W Foster Professor of Medical Ethics John Sadler, 2007-10 Written by examiners and practising teachers each book in this series contains activities and useful features intended to aid understanding Knowledge is tested throughout with progress checks at the end of every chapter and practice questions at the end of each section *Hepatology* Jawad Ahmad, Scott L. Friedman, Henryk Dancygier, 2014-04-14 Mount Sinai Expert Guides Hepatology will provide gastroenterology and hepatology trainees with an extremely clinical and accessible handbook covering the major liver diseases and symptoms their diagnosis and clinical management Perfect as a point of care resource on the hospital wards and also as a refresher for board exam preparation the focus throughout is on providing rapid reference essential information on each disease to allow for quick easy browsing and assimilation of the must know information All chapters follow a consistent template including the following features An opening bottom line key points section Classification pathogenesis and prevention of disease Evidence based diagnosis including relevant algorithms laboratory and imaging tests and potential pitfalls when diagnosing a patient Disease management including commonly used medications with dosages when to perform surgery management algorithms and how to prevent complications How to manage special populations ie in pregnancy children and the elderly The very

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Drug Design and Development Chris Rostron, 2020 Drug Design and Development outlines the processes involved in the design and development of new drugs and emphasises the significance of these processes to the practice of pharmacy The book highlights why it is important that all practicing pharmacists including those working in hospitals or high street stores have a solid understanding of the process of the design and development of the drugs they interact with It adopts an integrated approach formulated to complement courses which are designed in line with the General Pharmaceutical Council s new curriculum requirements Furthermore this is the only integrated textbook to consider both drug design and development within one volume Throughout the book the journey of the drug from discovery to market is presented in an integrated fashion emphasising the interconnection of all the processes involved *Competition Science Vision*, 2000-10 Competition Science Vision monthly magazine is published by Pratiyogita Darpan Group in India and is one of the best Science monthly magazines available for medical entrance examination students in India Well qualified professionals of Physics Chemistry Zoology and Botany make contributions to this magazine and craft it with focus on providing complete and to the point study material for aspiring candidates The magazine covers General Knowledge Science and Technology news Interviews of toppers of examinations study material of Physics Chemistry Zoology and Botany with model papers reasoning test questions facts quiz contest general awareness and mental ability test in every monthly issue *Pratiyogita Darpan*, 2008-02 Pratiyogita Darpan monthly magazine is India s largest read General Knowledge and Current Affairs Magazine Pratiyogita Darpan English monthly magazine is known for quality content on General Knowledge and Current Affairs Topics ranging from national and international news issues personality development interviews of examination toppers articles write up on topics like career economy history public administration geography polity social environment scientific legal etc solved papers of various examinations Essay and debate contest Quiz and knowledge testing features are covered every month in this magazine **Technologies in Biomedical and Life Sciences Education** Harry J. Witchel, Michael W. Lee, 2022-06-24 This contributed volume focuses on understanding the educational strengths and weaknesses of mediated content including media as a learning supplement in comparison to traditional face to face learning Each chapter includes research on and a broad brush summary of approaches to combining life sciences education with educational technologies The chapters are organized into four main sections each of which focuses on a key question regarding the consequences of incorporating

media into 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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