

BP807ET: COMPUTER AIDED DRUG DESIGN (THEORY)

UNIT 5: MOLECULAR MODELING

QUESTION TYPE	QUESTIONS	MAPPING (TNMGRMU / GPAT / NIPER / Pharma Exams with Year)*	BLOOM'S TAXONOMY
2 Mark	Define molecular modeling.	TNMGRMU (2021, 2023)	Remember
2 Mark	What is molecular mechanics?	TNMGRMU (2020), GPAT (2019)	Remember
2 Mark	Define quantum mechanics in drug design.	TNMGRMU (2022), GPAT (2020)	Understand
2 Mark	What is force field?	GPAT (2018, 2021)	Remember
2 Mark	List any two components of a molecular mechanics force field.	TNMGRMU (2021)	Remember
2 Mark	What is energy minimization?	TNMGRMU (2020), Pharma Interview	Understand
2 Mark	Mention any two energy minimization methods.	GPAT (2022)	Remember
2 Mark	Define conformational analysis.	TNMGRMU (2023)	Understand
2 Mark	What is global minimum energy conformation?	NIPER (2019)	Understand
2 Mark	State the importance of conformational analysis in drug design.	Pharma Exams (2022)	Apply

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5 Mark	Explain the basic principles of molecular mechanics.	TNMGRMU (2021, 2022)	Understand
5 Mark	Describe the components of a molecular mechanics force field.	GPAT (2020)	Understand
5 Mark	Compare molecular mechanics and quantum mechanics.	TNMGRMU (2020), GPAT (2019)	Analyze
5 Mark	Explain energy minimization and its significance in molecular modeling.	TNMGRMU (2023)	Apply
5 Mark	Describe steepest descent method of energy minimization.	GPAT (2021)	Understand
5 Mark	Explain conjugate gradient method for energy minimization.	NIPER (2020)	Understand
5 Mark	Discuss conformational analysis and its role in CADD.	TNMGRMU (2022)	Apply
5 Mark	Write a short note on local and global minima.	GPAT (2018)	Analyze
5 Mark	Explain the importance of global conformational minima determination.	Pharma Exams (2023)	Apply

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QUESTION BANK



10Mark	Explainmolecular mechanics in detailwith forcefieldcomponentsandappl ications.	TNMGRMU (2021,2023)	Understand
10Mark	Discuss quantummechanics approaches used indrug design.	GPAT (2020),NIPER (2019)	Understand
10Mark	Describe variousenergy minimizationmethodsused in molecular modeling.	TNMGRMU(2022)	Analyze
10Mark	Explainconformational analysis with suitable examples.	TNMGRMU(2020), GPAT (2021)	Apply
10 Mark	Discuss methods for global conformational minima determination in detail.	NIPER (2021)	Analyze
10 Mark	Compare energy minimization techniques and their applications in CADD.	GPAT (2022)	Evaluate
10 Mark	Explain the role of molecular modeling in rational drug design.	Pharma Exams (2023)	Evaluate