

Visualizing and Analyzing the 3D Structures of Medicinal Alkaloids Using Jmol

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Abstract

This project uses Jmol to visualize and analyze the 3D molecular structures of four important medicinal alkaloids—**morphine, quinine, caffeine, and nicotine**. Structural features like **bond lengths, angles, ring systems, functional groups, and stereochemistry** were explored to understand how their structure relates to biological activity.

Aim/Objective of the Experiment

To visualize and analyze the **3D molecular structures** of selected medicinal alkaloids—**morphine, quinine, caffeine, and nicotine**—using **Jmol**, and to study their **bond lengths, angles, functional groups, ring systems, and stereochemistry**, thereby understanding the structure-activity relationship.

Introduction

Alkaloids are naturally occurring organic compounds with nitrogen atoms, often showing strong pharmacological effects. Notable examples include morphine (analgesic), quinine (anti-malarial), caffeine (stimulant), and nicotine (psychoactive). Understanding their 3D structures aids in studying receptor binding and biological activity. Jmol, an open-source molecular viewer, was used for visualization and analysis.

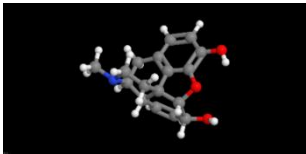
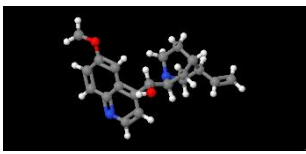
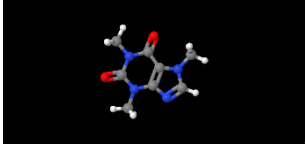

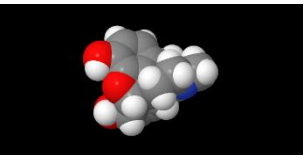
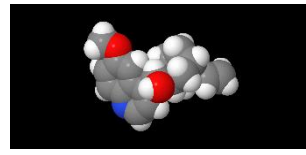
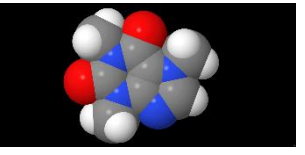
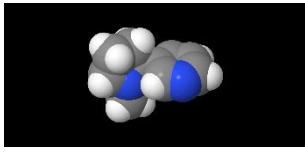

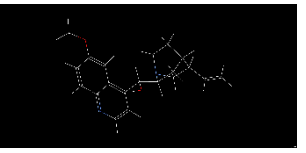
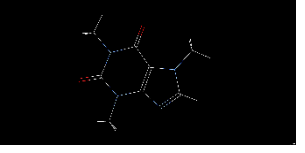
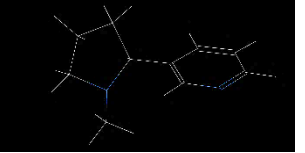
Methodology & Jmol Visuals

Steps Followed:

1. Downloaded .sdf files from PubChem.
2. Opened them in Jmol (File → Open).
3. Explored display styles: Ball-and-Stick, Wireframe, and Spacefill.
4. Measured bond lengths, bond angles, and torsions (right-click → Measure).
5. Identified rings, chiral centers, and functional groups.

Results

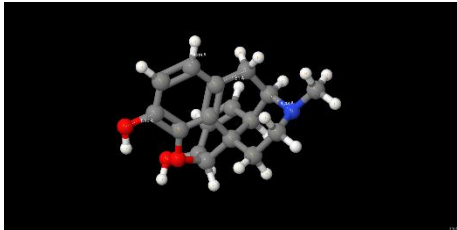
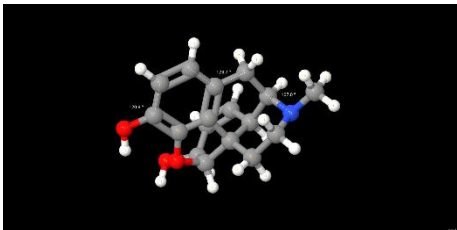
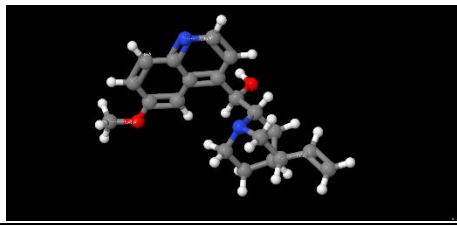
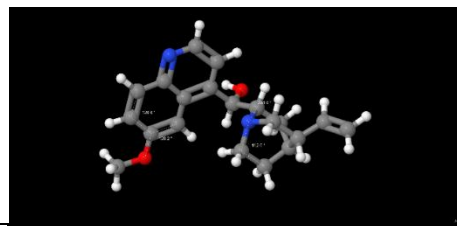
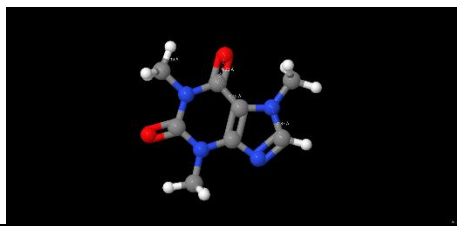
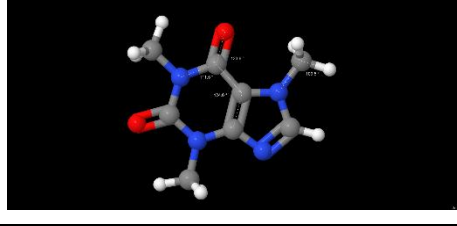
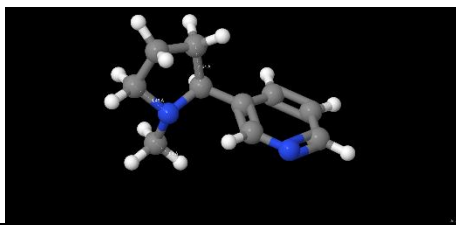
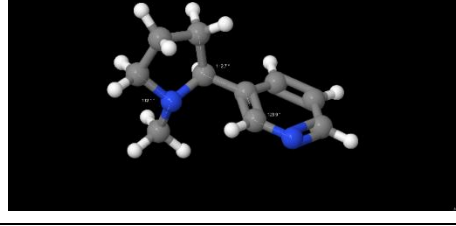
1. 3D Molecular Visualization

Morphine	Quinine	Caffeine	Nicotine
Ball-Stick Model 	Ball-Stick Model 	Ball-Stick Model 	Ball-Stick Model 
Space Filling Model 	Space Filling Model 	Space Filling Model 	Space Filling Model 
Bond Length View 	Bond Length View 	Bond Length View 	Bond Length View 

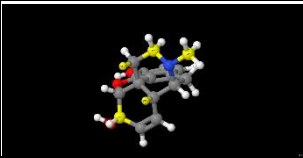
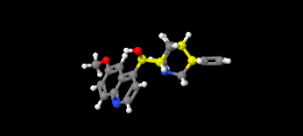
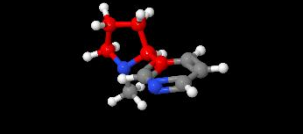
2. Bond Length & Angle Analysis

Molecule	C–O (Pheno l) (Å)	C–C (Aliphat ic) (Å)	C–N (Ami ne) (Å)	C–H (Å)	C=O (Carbo nyl) (Å)	O–H (Hydro xyl) (Å)	C–C–C (Ring) (°)	O–C–C (Ether) (°)	C–N–H (Tetra hedral) (°)	C–C–N (Arom atic) (°)
Morphine	1.36	1.51	1.48	1.09	–	0.96	123.7	120.8	109	120
Quinine	1.43	1.50	1.35	1.09	–	–	120	120.2	108	112
Caffeine	-	1.43	1.37	1.09	1.23	–	124.6	123.6	109.5	111.5
Nicotine	–	1.54	1.46	1.10	–	–	112.7	–	112.1	123.9

2.1. Bond Length and Angle Images

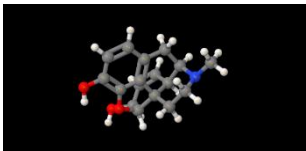
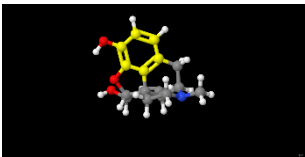
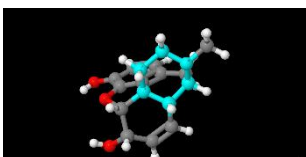
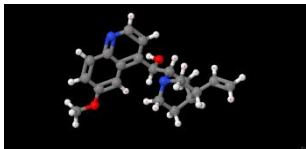
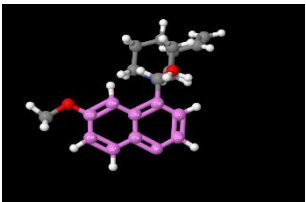
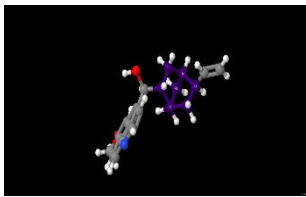
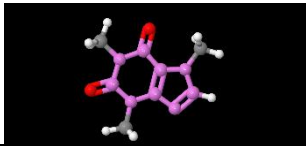
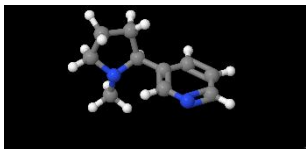
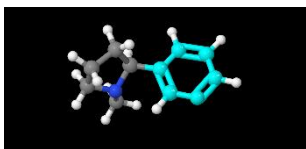
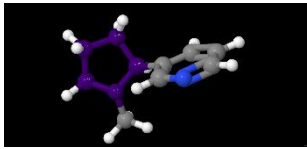
Molecule	Bond Length Image	Bond Angle Image
Morphine		
Quinine		
Caffeine		
Nicotine		

3. Stereochemistry

Molecule	Structure (Yellow color)	Number of Chiral Centers
Morphine		5
Quinine		4
Nicotine		2

*Caffeine not have chiral center

4.Functional Group & Ring System

Alkaloid	Functional Groups	Ring System
Morphine	Hydroxyl (-OH), Ether (-O-), Amine (-N-) 	Benzene ring, Piperidine ring  
Quinine	Hydroxyl (-OH), Ether (-O-), Amine (-N-), Ester (-COO-) 	Quinoline ring, Quinuclidine ring  
Caffeine	Methyl (-CH ₃), Carbonyl (C=O), Amide (-CONH) 	Purine ring (pyrimidine + imidazole)
Nicotine	Pyridine, Pyrrolidine 	Pyridine ring, Pyrrolidine ring  

References

1. PubChem Database (<https://pubchem.ncbi.nlm.nih.gov/>)
2. Jmol: An Open-Source Molecular Visualization Software (<http://jmol.sourceforge.net/>)