**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**

|  |  |  |  |
| --- | --- | --- | --- |
| **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 |

**1. 3D Molecular Visualization**

**2. Bond Length & Angle Analysis**

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Molecule** | **C–O (Phenol) (Å)** | **C–C (Aliphatic) (Å)** | **C–N (Amine) (Å)** | **C–H (Å)** | **C=O (Carbonyl) (Å)** | **O–H (Hydroxyl) (Å)** | **C–C–C (Ring) (°)** | **O–C–C (Ether) (°)** | **C–N–H (Tetrahedral) (°)** | **C–C–N (Aromatic) (°)** |
| **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 |

|  |  |  |
| --- | --- | --- |
| **Molecule** | **Bond Length Image** | **Bond Angle Image** |
| **Morphine** |  |  |
| **Quinine** |  |  |
| **Caffeine** |  |  |
| **Nicotine** |  |  |

**2.1.**Bong Length and Angle Images

**3.Sterochemistry**

|  |  |  |
| --- | --- | --- |
| **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 (-CH3), 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/**](https://pubchem.ncbi.nlm.nih.gov/)**)**
2. **Jmol: An Open-Source Molecular Visualization Software (http://jmol.sourceforge.net/)**