Structures from Database

Talk to a Teacher
http://spoken-tutorial.org
National Mission on Education through ICT
http://sakshat.ac.in

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Learning Objectives

- **Load chemical structures from** *Pubchem* **database**

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- **Convert 2D structures drawn in** *GChemPaint* **to 3D models in Jmol**

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- **Mozilla Firefox browser 22.0**

Identification of the Molecule

- **Common name or IUPAC name**
- **CAS number (Chemical Abstracts Service registry number)**
- **CID number (Compound Identification Number)**

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- **InChi identifier (IUPAC International Chemical Identifier)**
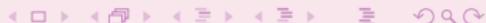- **SMILES identifier (Simplified Molecular Input Line Entry System)**

Assignment

- **Load structure of** *caffeine* **from Pubchem database https://pubchem.ncbi.nlm.nih.gov**
- **Highlight the important features in the molecule**
- **Modify the display to** *wireframe*

About GChemPaint

- **Open source software for drawing 2D chemical structures**

- **Tutorials on GChemPaint are available at http://spoken-tutorial.org**

- **To draw structures and save in .mol format, refer to** *Analysis of Compounds* **tutorial**

Summary

- **Load chemical structures from** *Pubchem* **database**
- **Modify the display of Phenol and Cholesterol**

Summary

- **Convert 2D structures drawn in** *GChemPaint* **to 3D models in Jmol**
- **Convert 2D structures of Alanine, Adenosine and Alpha-D-glucopyranose to 3D models**

Assignment

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- **Draw 2D structures of the following aminoacids in** *GChemPaint*

  Cysteine

  Histidine

  Phenylalanine

- **Save as .mol files**

- **Open the files in Jmol and modify display**

About the Spoken Tutorial Project

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Spoken Tutorial Workshops

The Spoken Tutorial Project Team

- ▶ **Conducts workshops using spoken tutorials**
- ▶ **Gives certificates to those who pass an online test**
- ▶ **For more details, please write to contact@spoken-tutorial.org**

Acknowledgements

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- **It is supported by the National Mission on Education through ICT, MHRD, Government of India**
- **More information on this Mission is available at http://spoken-tutorial.org /NMEICT-Intro**