

# Features of JChemPaint

**Talk to a Teacher**

<http://spoken-tutorial.org>

**National Mission on Education through ICT**

<http://sakshat.ac.in>

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**23 September 2014**



# Learning Objectives



Talk to a Teacher



# Learning Objectives

We will learn to change



# Learning Objectives

We will learn to change

- Background color of the Panel



# Learning Objectives

We will learn to change

- Background color of the Panel
- Look and feel of the window



# Learning Objectives

We will learn to change

- Background color of the Panel
- Look and feel of the window
- **User interface language**



# Learning Objectives



Talk to a Teacher



# Learning Objectives

We will also learn to





# Learning Objectives

We will also learn to

- **Insert Templates**



Talk to a Teacher

# Learning Objectives

We will also learn to

- Insert Templates
- Generate SMILES and InChi keys for a given structure



Talk to a Teacher

# Learning Objectives

We will also learn to

- Insert **Templates**
- Generate **SMILES** and **InChi keys** for a given structure
- **Insert SMILES and InChi keys to generate structures**



Talk to a Teacher

# System Requirement



Talk to a Teacher



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- Ubuntu Linux OS v 12.04



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- Ubuntu Linux OS v 12.04
- JChemPaint version 3.3-1210



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- JChemPaint version 3.3-1210
- Java version 7



# Pre-requisites





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You should be familiar with



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You should be familiar with

- JChemPaint chemical structures editor



# Pre-requisites

You should be familiar with

- JChemPaint chemical structures editor
- If not, for relevant tutorials please visit

<http://spoken-tutorial.org>



# Assignment

- 1 Try various color combinations using  
Choose background color window



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# Assignment

- 1 Load other **Templates** of your choice onto the Panel



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# SMILES



# SMILES

- SMILES is simplified molecular input line entry system



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- **SMILES** is simplified molecular input line entry system
- It describes chemical structures using short **ASCII** strings





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- **Molecular Editors import SMILES strings, to convert structures into 2D drawings**



# SMILES

- **SMILES** is simplified molecular input line entry system
- It describes chemical structures using short **ASCII** strings
- Molecular Editors import **SMILES strings**, to convert structures into 2D drawings
- **CCCCCC** is canonical SMILES of Hexane



# InChi Keys



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- Inchi is International Chemical Identifier



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- **Atoms** and their bond connectivity
- **Isotopic, stereochemical and electronic charge information**



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# InChi Keys

- Inchi is International Chemical Identifier
- It describes a chemical in terms of layers of information
- **Atoms** and their bond connectivity
- **Isotopic, stereochemical** and **electronic charge** information
- **InChI=1S/C3H8/c1-3-2/h3H2,1-2H3**  
**InChi key of Propane**





# Assignment

Insert the given **SMILES** and **InChi keys** to obtain various structures

- 1 CC1=CC=CC=C1
- 2 CC(C(=O)O)N
- 3 InChI=1S/C5H10/c1-2-4-5-3-1/h1-5H2
- 4 InChI=1S/H2O4S/c1-5(2,3)4/h(H2,1,2,3,4)



# Summary

- Background color of the Panel
- Look and feel of the window
- User interface language
- Insert Templates
- Generate SMILES and InChi keys for a given structure
- Insert SMILES and InChi keys to generate structures



# About the Spoken Tutorial Project

- Watch the video available at [http://spoken-tutorial.org/What\\_is\\_a\\_Spoken\\_Tutorial](http://spoken-tutorial.org/What_is_a_Spoken_Tutorial)
- It summarises the Spoken Tutorial project



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- It summarises the Spoken Tutorial project
- If you do not have good bandwidth, you can download and watch it



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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](mailto:contact@spoken-tutorial.org)



# Acknowledgements

- Spoken Tutorial Project is a part of the Talk to a Teacher project
- 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>

