CH 3090- PRACTICAL COMPUTATIONAL CHEMISTRY

ASSIGNMENT 3

An Introduction to ChemDraw

Bsc Hons In Computational Chemistry

July 15, 2025

Mandini Palihawadana

16467

**Objectives**

1. To draw the complex organic compounds accuretly.
2. To showcase the mechanisms of the synthesis of compounds.
3. To enhanse the sturcural details of the compounds.

**Introduction**

ChemDraw is a chemical drawing software developed by PerkinElmer, widely used by chemists, researchers, and students for creating and visualizing chemical structures. It offers a user-friendly interface for drawing complex organic molecules, reaction mechanisms, and biological pathways with precision and clarity. It is used to drae two dimentional structures. ChemDraw supports features such as structure-to-name conversion, spectral data prediction (NMR, IR, mass spectra), and chemical property calculations, and professional chemical research. By integrating with databases and other software in the ChemOffice suite, ChemDraw streamlines documentation, reporting, and communication of chemical information in a visually intuitive format.

**Methodology**

The new ACS document type was selected from file menu. I was renamed and saved before starting the drawings.using the tools such as the different bond types, text tools, selection tools benzene, chair conformation like templates the sturctures were drawn.the structures were copied to a word document finally.

**Results**

01)



Myxovirescin A1







02) Synthesis of Salbutamol



03) Synthesis of Morphine



± Morphine

04) Synthesis of (R)-(+)-nor-Roefractine

