

Drawing Drug Structures and Reactions in ChemDraw

Practical 14 | Medicinal Chemistry III

Aim

To study Drawing Drug Structures and Reactions in ChemDraw, and interpret the recorded observations.

Principle

- Chemical drawing software must preserve connectivity, bond order, stereochemistry and formal charge. A tidy drawing can still be chemically wrong.
- Choose the calculation or statistical model appropriate to the data structure and assumptions.
- Units, paired or independent observations, and the direction of the measured effect must be explicit.

Materials and Apparatus

- ChemDraw or equivalent drawing software, assigned drug list and verified structural information.
- Instructor-provided dataset and the stated study/model assumptions.
- Calculator or spreadsheet/statistical software and a record sheet.

Method

1. Enter the assigned structure with the correct ring and bond connectivity.
2. Check valence, aromaticity, formal charge and the exact salt or hydrate convention.
3. Add required wedge/dash bonds and verify the stereochemical meaning.
4. Arrange reaction arrows, reagents and products without overlapping labels.
5. Use the software check tools, then inspect the structure independently.
6. Export a clear figure and retain the editable file with an informative name.

Observation Record

Complete this record using actual laboratory findings or the provided teaching data.

Observation / parameter	Record / finding
Drug name	_____
Connectivity	_____
Charge and salt form	_____
Stereochemistry	_____
Reaction annotations	_____
Export quality	_____

Calculations and Interpretation

- For a neutral compound, verify the molecular formula and molar mass generated by the software.
- For salts, document whether the displayed mass refers to the base, salt or entire drawn composition.

Result

Record the actual finding, calculated value with units where relevant, and a conclusion supported by the observations.

Finding: _____

Conclusion: _____

Precautions

- Do not interchange paired and independent analyses.
- Keep unit conversions explicit and round at the final reporting stage.
- A model estimate or p-value does not by itself establish a causal or clinical conclusion.

Viva Questions

1. Does a software structure check establish the intended drug identity?

No. A valence-valid structure can still have the wrong connectivity, isomer or salt form.

2. Why state assumptions?

An equation or test can give a misleading answer when its underlying assumptions do not hold.

3. Why keep intermediate calculations?

They make the result reproducible and expose unit or transcription errors.

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