

# Continue Learning with FirstHope

## Complete Notes on the FirstHope App

**Complete subject and semesters are available on FirstHope app only.**

- Get complete subject and semester notes in the FirstHope app.
- Available for B.Pharm, D.Pharm, M.Pharm and Pharm.D students.

**[Click here to get the FirstHope app](#)**

## Join the FirstHope Telegram Channel

Join FirstHope Notes and keep up with channel updates.

**[Click here to join Telegram](#)**

## Instagram

@firsthope.official

**[Click here to follow Instagram](#)**

## YouTube Channel

FirstHope-Pharmacy / Live streams

**[Click here to watch the YouTube channel](#)**

## WhatsApp Channel

Follow FirstHope on WhatsApp.

**[Click here to join the WhatsApp channel](#)**

## FirstHope Website

firsthopenotes.com

**[Click here to visit the website](#)**

# Semester 6 - Practical Notes

## Medicinal Chemistry III

### Complete Subject Manual

15 practicals and activities. Use the PDF bookmarks to move between practicals. Page numbers restart within each practical; the page counts below exclude the promotion pages.

### Contents

| No. | Practical / Activity                                     | Pages |
|-----|----------------------------------------------------------|-------|
| 1   | Preparation of Sulphanilamide                            | 2     |
| 2   | Preparation of 7-Hydroxy-4-Methylcoumarin                | 2     |
| 3   | Preparation of Chlorobutanol                             | 2     |
| 4   | Preparation of Triphenylimidazole                        | 2     |
| 5   | Preparation of Tolbutamide                               | 2     |
| 6   | Preparation of Hexamine                                  | 2     |
| 7   | Assay of Isonicotinic Acid Hydrazide                     | 2     |
| 8   | Assay of Chloroquine                                     | 2     |
| 9   | Assay of Metronidazole                                   | 2     |
| 10  | Assay of Dapsone                                         | 2     |
| 11  | Assay of Chlorpheniramine Maleate                        | 2     |
| 12  | Assay of Benzylpenicillin                                | 2     |
| 13  | Microwave-Assisted Synthesis of an Assigned Intermediate | 2     |
| 14  | Drawing Drug Structures and Reactions in ChemDraw        | 2     |
| 15  | Physicochemical Descriptors and Lipinski Rule of Five    | 2     |

# Preparation of Sulphanilamide

Practical 01 | Medicinal Chemistry III

## Aim

To prepare Sulphanilamide, and interpret the recorded observations.

## Principle

- The sulphonamide group and para amino group define the sulphanilamide scaffold. A protected aniline route illustrates why functional-group protection can be needed before introducing the sulphonamide functionality.
- A chemical transformation changes selected functional groups while retaining or constructing the required molecular skeleton.
- Product identity and purity require analytical evidence; appearance alone cannot establish either.
- Identify the protection, functional-group conversion and deprotection stages in the assigned reaction scheme.
- Reaction record: draw starting material and product structures, mark the functional-group change, and retain the assigned stoichiometry.
- Characterization record: compare the assigned melting range, TLC or spectral evidence. A narrow melting interval can support purity but cannot alone establish complete identity.

## Materials and Apparatus

- Assigned protected aromatic intermediate and instructor-demonstrated sulphonamide route.
- Assigned starting materials and instructor-selected reagents.
- Balance, reaction glassware, stirring/heating arrangement, condenser where required, filtration equipment and identity/purity test apparatus.

## Method

1. Write the assigned reaction scheme and balance the transformation before calculating reagent requirements.
2. Identify the limiting reactant and document the approved reaction scale, solvent and conditions.
3. Observe the instructor-directed reaction sequence and record changes without substituting reagents or conditions.
4. Complete the prescribed work-up to separate the product from reaction liquids and by-products.
5. Purify the product by the assigned method, dry it appropriately and determine the recovered mass.
6. Record the assigned identity and purity observations and compare them with the expected product.

## Observation Record

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

| Observation / parameter       | Record / finding |
|-------------------------------|------------------|
| Assigned route                | _____            |
| Limiting-reactant calculation | _____            |
| Process observations          | _____            |
| Dry recovery                  | _____            |
| Identity/purity evidence      | _____            |

## Calculations and Interpretation

- Theoretical product mass = limiting-reactant amount (mol)  $\times$  product stoichiometric ratio  $\times$  product molar mass.
- Percentage yield = dry product mass / theoretical product mass  $\times$  100.

### Worked Illustration

Illustration: a theoretical product mass of 2.00 g and dry recovery of 1.50 g give 75.0% yield.

The values in this illustration are for calculation practice.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Use the approved reaction conditions and suitable ventilation.
- Keep product, starting material and waste streams separately labelled.
- Calculate yield from dry product and the limiting reactant; never use wet mass as pure-product mass.

## Viva Questions

### 1. Why inspect the final molecular structure?

The intended connectivity and substituent positions distinguish the product from related intermediates or isomers.

### 2. What is the limiting reactant?

The reactant whose available amount permits the smallest theoretical amount of product.

### 3. Does a high yield establish purity?

No. Residual solvent, impurities and unreacted material can increase recovered mass.

# Preparation of 7-Hydroxy-4-Methylcoumarin

Practical 02 | Medicinal Chemistry III

## Aim

To prepare 7-Hydroxy-4-Methylcoumarin, and interpret the recorded observations.

## Principle

- A Pechmann-type condensation of a suitable phenol with a beta-ketoester can construct the coumarin ring. Substituent positions must be checked on the final structure.
- A chemical transformation changes selected functional groups while retaining or constructing the required molecular skeleton.
- Product identity and purity require analytical evidence; appearance alone cannot establish either.
- Trace ring construction and identify the lactone carbonyl, 7-hydroxy group and 4-methyl group.
- Reaction record: draw starting material and product structures, mark the functional-group change, and retain the assigned stoichiometry.
- Characterization record: compare the assigned melting range, TLC or spectral evidence. A narrow melting interval can support purity but cannot alone establish complete identity.

## Materials and Apparatus

- Assigned phenolic precursor, beta-ketoester and approved condensation system.
- Assigned starting materials and instructor-selected reagents.
- Balance, reaction glassware, stirring/heating arrangement, condenser where required, filtration equipment and identity/purity test apparatus.

## Method

1. Write the assigned reaction scheme and balance the transformation before calculating reagent requirements.
2. Identify the limiting reactant and document the approved reaction scale, solvent and conditions.
3. Observe the instructor-directed reaction sequence and record changes without substituting reagents or conditions.
4. Complete the prescribed work-up to separate the product from reaction liquids and by-products.
5. Purify the product by the assigned method, dry it appropriately and determine the recovered mass.
6. Record the assigned identity and purity observations and compare them with the expected product.

## Observation Record

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

| Observation / parameter       | Record / finding |
|-------------------------------|------------------|
| Assigned route                | _____            |
| Limiting-reactant calculation | _____            |
| Process observations          | _____            |
| Dry recovery                  | _____            |
| Identity/purity evidence      | _____            |

## Calculations and Interpretation

- Theoretical product mass = limiting-reactant amount (mol)  $\times$  product stoichiometric ratio  $\times$  product molar mass.
- Percentage yield = dry product mass / theoretical product mass  $\times$  100.

### Worked Illustration

Illustration: a theoretical product mass of 2.00 g and dry recovery of 1.50 g give 75.0% yield.

The values in this illustration are for calculation practice.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Use the approved reaction conditions and suitable ventilation.
- Keep product, starting material and waste streams separately labelled.
- Calculate yield from dry product and the limiting reactant; never use wet mass as pure-product mass.

## Viva Questions

### 1. Why inspect the final molecular structure?

The intended connectivity and substituent positions distinguish the product from related intermediates or isomers.

### 2. What is the limiting reactant?

The reactant whose available amount permits the smallest theoretical amount of product.

### 3. Does a high yield establish purity?

No. Residual solvent, impurities and unreacted material can increase recovered mass.

# Preparation of Chlorobutanol

Practical 03 | Medicinal Chemistry III

## Aim

To prepare Chlorobutanol, and interpret the recorded observations.

## Principle

- The assigned acetone/chloroform transformation forms a tertiary alcohol bearing a trichloromethyl group. Product form and residual reagents matter when interpreting recovery.
- A chemical transformation changes selected functional groups while retaining or constructing the required molecular skeleton.
- Product identity and purity require analytical evidence; appearance alone cannot establish either.
- Compare the ketone starting functionality with the tertiary alcohol in the product; record the exact product form.
- Reaction record: draw starting material and product structures, mark the functional-group change, and retain the assigned stoichiometry.
- Characterization record: compare the assigned melting range, TLC or spectral evidence. A narrow melting interval can support purity but cannot alone establish complete identity.

## Materials and Apparatus

- Instructor-demonstrated chlorobutanol reaction materials.
- Assigned starting materials and instructor-selected reagents.
- Balance, reaction glassware, stirring/heating arrangement, condenser where required, filtration equipment and identity/purity test apparatus.

## Method

1. Write the assigned reaction scheme and balance the transformation before calculating reagent requirements.
2. Identify the limiting reactant and document the approved reaction scale, solvent and conditions.
3. Observe the instructor-directed reaction sequence and record changes without substituting reagents or conditions.
4. Complete the prescribed work-up to separate the product from reaction liquids and by-products.
5. Purify the product by the assigned method, dry it appropriately and determine the recovered mass.
6. Record the assigned identity and purity observations and compare them with the expected product.

## Observation Record

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

| Observation / parameter       | Record / finding |
|-------------------------------|------------------|
| Assigned route                | _____            |
| Limiting-reactant calculation | _____            |
| Process observations          | _____            |
| Dry recovery                  | _____            |
| Identity/purity evidence      | _____            |

## Calculations and Interpretation

- Theoretical product mass = limiting-reactant amount (mol)  $\times$  product stoichiometric ratio  $\times$  product molar mass.
- Percentage yield = dry product mass / theoretical product mass  $\times$  100.

### Worked Illustration

Illustration: a theoretical product mass of 2.00 g and dry recovery of 1.50 g give 75.0% yield.

The values in this illustration are for calculation practice.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Use the approved reaction conditions and suitable ventilation.
- Keep product, starting material and waste streams separately labelled.
- Calculate yield from dry product and the limiting reactant; never use wet mass as pure-product mass.

## Viva Questions

### 1. Why inspect the final molecular structure?

The intended connectivity and substituent positions distinguish the product from related intermediates or isomers.

### 2. What is the limiting reactant?

The reactant whose available amount permits the smallest theoretical amount of product.

### 3. Does a high yield establish purity?

No. Residual solvent, impurities and unreacted material can increase recovered mass.

# Preparation of Triphenylimidazole

Practical 04 | Medicinal Chemistry III

## Aim

To prepare Triphenylimidazole, and interpret the recorded observations.

## Principle

- A multicomponent condensation using an assigned diketone, aldehyde and nitrogen source constructs an imidazole ring carrying phenyl substituents.
- A chemical transformation changes selected functional groups while retaining or constructing the required molecular skeleton.
- Product identity and purity require analytical evidence; appearance alone cannot establish either.
- Identify the two ring nitrogens and distinguish the imidazole product from imidazoline or imidazolidine.
- Reaction record: draw starting material and product structures, mark the functional-group change, and retain the assigned stoichiometry.
- Characterization record: compare the assigned melting range, TLC or spectral evidence. A narrow melting interval can support purity but cannot alone establish complete identity.

## Materials and Apparatus

- Assigned diketone/aldehyde precursors and approved nitrogen-source system.
- Assigned starting materials and instructor-selected reagents.
- Balance, reaction glassware, stirring/heating arrangement, condenser where required, filtration equipment and identity/purity test apparatus.

## Method

1. Write the assigned reaction scheme and balance the transformation before calculating reagent requirements.
2. Identify the limiting reactant and document the approved reaction scale, solvent and conditions.
3. Observe the instructor-directed reaction sequence and record changes without substituting reagents or conditions.
4. Complete the prescribed work-up to separate the product from reaction liquids and by-products.
5. Purify the product by the assigned method, dry it appropriately and determine the recovered mass.
6. Record the assigned identity and purity observations and compare them with the expected product.

## Observation Record

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

| Observation / parameter       | Record / finding |
|-------------------------------|------------------|
| Assigned route                | _____            |
| Limiting-reactant calculation | _____            |
| Process observations          | _____            |
| Dry recovery                  | _____            |
| Identity/purity evidence      | _____            |

## Calculations and Interpretation

- Theoretical product mass = limiting-reactant amount (mol)  $\times$  product stoichiometric ratio  $\times$  product molar mass.
- Percentage yield = dry product mass / theoretical product mass  $\times$  100.

### Worked Illustration

Illustration: a theoretical product mass of 2.00 g and dry recovery of 1.50 g give 75.0% yield.

The values in this illustration are for calculation practice.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Use the approved reaction conditions and suitable ventilation.
- Keep product, starting material and waste streams separately labelled.
- Calculate yield from dry product and the limiting reactant; never use wet mass as pure-product mass.

## Viva Questions

### 1. Why inspect the final molecular structure?

The intended connectivity and substituent positions distinguish the product from related intermediates or isomers.

### 2. What is the limiting reactant?

The reactant whose available amount permits the smallest theoretical amount of product.

### 3. Does a high yield establish purity?

No. Residual solvent, impurities and unreacted material can increase recovered mass.

# Preparation of Tolbutamide

Practical 05 | Medicinal Chemistry III

## Aim

To prepare Tolbutamide, and interpret the recorded observations.

## Principle

- Tolbutamide contains a sulphonylurea linkage. Structural study distinguishes the sulphonylurea nitrogen substitution from an ordinary sulphonamide.
- A chemical transformation changes selected functional groups while retaining or constructing the required molecular skeleton.
- Product identity and purity require analytical evidence; appearance alone cannot establish either.
- Trace the sulphonylurea linkage and the aromatic and alkyl substituents on the assigned scheme.
- Reaction record: draw starting material and product structures, mark the functional-group change, and retain the assigned stoichiometry.
- Characterization record: compare the assigned melting range, TLC or spectral evidence. A narrow melting interval can support purity but cannot alone establish complete identity.

## Materials and Apparatus

- Instructor-demonstrated tolbutamide teaching intermediates and assigned product-identity data.
- Assigned starting materials and instructor-selected reagents.
- Balance, reaction glassware, stirring/heating arrangement, condenser where required, filtration equipment and identity/purity test apparatus.

## Method

1. Write the assigned reaction scheme and balance the transformation before calculating reagent requirements.
2. Identify the limiting reactant and document the approved reaction scale, solvent and conditions.
3. Observe the instructor-directed reaction sequence and record changes without substituting reagents or conditions.
4. Complete the prescribed work-up to separate the product from reaction liquids and by-products.
5. Purify the product by the assigned method, dry it appropriately and determine the recovered mass.
6. Record the assigned identity and purity observations and compare them with the expected product.

## Observation Record

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

| Observation / parameter       | Record / finding |
|-------------------------------|------------------|
| Assigned route                | _____            |
| Limiting-reactant calculation | _____            |
| Process observations          | _____            |
| Dry recovery                  | _____            |
| Identity/purity evidence      | _____            |

## Calculations and Interpretation

- Theoretical product mass = limiting-reactant amount (mol)  $\times$  product stoichiometric ratio  $\times$  product molar mass.
- Percentage yield = dry product mass / theoretical product mass  $\times$  100.

### Worked Illustration

Illustration: a theoretical product mass of 2.00 g and dry recovery of 1.50 g give 75.0% yield.

The values in this illustration are for calculation practice.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Use the approved reaction conditions and suitable ventilation.
- Keep product, starting material and waste streams separately labelled.
- Calculate yield from dry product and the limiting reactant; never use wet mass as pure-product mass.

## Viva Questions

### 1. Why inspect the final molecular structure?

The intended connectivity and substituent positions distinguish the product from related intermediates or isomers.

### 2. What is the limiting reactant?

The reactant whose available amount permits the smallest theoretical amount of product.

### 3. Does a high yield establish purity?

No. Residual solvent, impurities and unreacted material can increase recovered mass.

# Preparation of Hexamine

Practical 06 | Medicinal Chemistry III

## Aim

To prepare Hexamine, and interpret the recorded observations.

## Principle

- Hexamine is a cage-like nitrogen-containing compound formed in the assigned formaldehyde/ammonia condensation. Its identity is different from the individual starting substances.
- A chemical transformation changes selected functional groups while retaining or constructing the required molecular skeleton.
- Product identity and purity require analytical evidence; appearance alone cannot establish either.
- Balance the assigned overall equation and inspect the cage connectivity in the product structure.
- Reaction record: draw starting material and product structures, mark the functional-group change, and retain the assigned stoichiometry.
- Characterization record: compare the assigned melting range, TLC or spectral evidence. A narrow melting interval can support purity but cannot alone establish complete identity.

## Materials and Apparatus

- Instructor-demonstrated formaldehyde/ammonia teaching system and identity records.
- Assigned starting materials and instructor-selected reagents.
- Balance, reaction glassware, stirring/heating arrangement, condenser where required, filtration equipment and identity/purity test apparatus.

## Method

1. Write the assigned reaction scheme and balance the transformation before calculating reagent requirements.
2. Identify the limiting reactant and document the approved reaction scale, solvent and conditions.
3. Observe the instructor-directed reaction sequence and record changes without substituting reagents or conditions.
4. Complete the prescribed work-up to separate the product from reaction liquids and by-products.
5. Purify the product by the assigned method, dry it appropriately and determine the recovered mass.
6. Record the assigned identity and purity observations and compare them with the expected product.

## Observation Record

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

| Observation / parameter       | Record / finding |
|-------------------------------|------------------|
| Assigned route                | _____            |
| Limiting-reactant calculation | _____            |
| Process observations          | _____            |
| Dry recovery                  | _____            |
| Identity/purity evidence      | _____            |

## Calculations and Interpretation

- Theoretical product mass = limiting-reactant amount (mol)  $\times$  product stoichiometric ratio  $\times$  product molar mass.
- Percentage yield = dry product mass / theoretical product mass  $\times$  100.

### Worked Illustration

Illustration: a theoretical product mass of 2.00 g and dry recovery of 1.50 g give 75.0% yield.

The values in this illustration are for calculation practice.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Use the approved reaction conditions and suitable ventilation.
- Keep product, starting material and waste streams separately labelled.
- Calculate yield from dry product and the limiting reactant; never use wet mass as pure-product mass.

## Viva Questions

### 1. Why inspect the final molecular structure?

The intended connectivity and substituent positions distinguish the product from related intermediates or isomers.

### 2. What is the limiting reactant?

The reactant whose available amount permits the smallest theoretical amount of product.

### 3. Does a high yield establish purity?

No. Residual solvent, impurities and unreacted material can increase recovered mass.

# Assay of Isonicotinic Acid Hydrazide

Practical 07 | Medicinal Chemistry III

## Aim

To assay Isonicotinic Acid Hydrazide, and interpret the recorded observations.

## Principle

- Isoniazid is an isonicotinic-acid hydrazide. The assigned assay may use its defined redox or other analytical response; calculate with the exact reaction and validated method factor.
- The property is obtained from a defined observable under controlled conditions.
- Replicate measurements, instrument checks and consistent units are needed before comparison.

## Materials and Apparatus

- Assigned isoniazid, reference or standardized analytical reagents and completed/observed assay readings.
- Assigned test material and calibration or comparison material.
- The apparatus specified for this property, a balance or volumetric equipment where relevant, and a record sheet.

## Method

1. Identify the exact analyte form, assay method and reporting basis assigned to the exercise.
2. Record the standardized reagent factor or the reference-standard potency used.
3. Prepare the measured test portion and comparison/blank according to that method.
4. Obtain replicate endpoint or instrumental responses and retain the raw readings.
5. Apply reaction stoichiometry, reference potency and dilution corrections as applicable.
6. Report content on the specified mass or potency basis and compare only with the assigned criterion.

## Observation Record

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

| Observation / parameter     | Record / finding |
|-----------------------------|------------------|
| Analyte form                | _____            |
| Test portion                | _____            |
| Method and reference/factor | _____            |
| Raw assay response          | _____            |
| Dilution                    | _____            |
| Assay result                | _____            |

## Calculations and Interpretation

- Titrimetric method:  $\text{analyte mass} = \text{corrected volume} \times \text{verified method factor} \times \text{dilution correction}$ .
- Instrumental method: obtain concentration from the valid reference calibration and correct for preparation/dilution.
- Assay (%) =  $\text{measured analyte amount} / \text{nominal analyte amount} \times 100$  on equivalent units and form.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Keep temperature and test conditions consistent across comparative readings.
- Record raw readings before rounding calculated values.
- Do not compare results obtained with different methods as if they were interchangeable.

## Viva Questions

### 1. Why is the analyte form part of the calculation?

Salt, hydrate and declared potency conventions can change the factor and reporting basis.

### 2. Why control the test conditions?

A change in conditions may alter the measured property independently of the intended variable.

### 3. Why retain replicate readings?

They show repeatability and help identify an anomalous measurement.

# Assay of Chloroquine

Practical 08 | Medicinal Chemistry III

## Aim

To assay Chloroquine, and interpret the recorded observations.

## Principle

- Basic sites and the declared chloroquine salt determine the analytical preparation and reporting basis. A factor for the free base cannot be silently transferred to a salt.
- The property is obtained from a defined observable under controlled conditions.
- Replicate measurements, instrument checks and consistent units are needed before comparison.

## Materials and Apparatus

- Assigned chloroquine form, method reagents/reference and assay apparatus.
- Assigned test material and calibration or comparison material.
- The apparatus specified for this property, a balance or volumetric equipment where relevant, and a record sheet.

## Method

1. Identify the exact analyte form, assay method and reporting basis assigned to the exercise.
2. Record the standardized reagent factor or the reference-standard potency used.
3. Prepare the measured test portion and comparison/blank according to that method.
4. Obtain replicate endpoint or instrumental responses and retain the raw readings.
5. Apply reaction stoichiometry, reference potency and dilution corrections as applicable.
6. Report content on the specified mass or potency basis and compare only with the assigned criterion.

## Observation Record

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

| Observation / parameter     | Record / finding |
|-----------------------------|------------------|
| Analyte form                | _____            |
| Test portion                | _____            |
| Method and reference/factor | _____            |
| Raw assay response          | _____            |
| Dilution                    | _____            |
| Assay result                | _____            |

## Calculations and Interpretation

- Titrimetric method:  $\text{analyte mass} = \text{corrected volume} \times \text{verified method factor} \times \text{dilution correction}$ .
- Instrumental method: obtain concentration from the valid reference calibration and correct for preparation/dilution.
- Assay (%) =  $\text{measured analyte amount} / \text{nominal analyte amount} \times 100$  on equivalent units and form.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Keep temperature and test conditions consistent across comparative readings.
- Record raw readings before rounding calculated values.
- Do not compare results obtained with different methods as if they were interchangeable.

## Viva Questions

### 1. Why is the analyte form part of the calculation?

Salt, hydrate and declared potency conventions can change the factor and reporting basis.

### 2. Why control the test conditions?

A change in conditions may alter the measured property independently of the intended variable.

### 3. Why retain replicate readings?

They show repeatability and help identify an anomalous measurement.

# Assay of Metronidazole

Practical 09 | Medicinal Chemistry III

## Aim

To assay Metronidazole, and interpret the recorded observations.

## Principle

- Metronidazole assay measures the defined analyte under the assigned validated method. Metronidazole and metronidazole benzoate are different reporting bases.
- The property is obtained from a defined observable under controlled conditions.
- Replicate measurements, instrument checks and consistent units are needed before comparison.

## Materials and Apparatus

- Assigned metronidazole form, analytical reference/reagents and assay readings.
- Assigned test material and calibration or comparison material.
- The apparatus specified for this property, a balance or volumetric equipment where relevant, and a record sheet.

## Method

1. Identify the exact analyte form, assay method and reporting basis assigned to the exercise.
2. Record the standardized reagent factor or the reference-standard potency used.
3. Prepare the measured test portion and comparison/blank according to that method.
4. Obtain replicate endpoint or instrumental responses and retain the raw readings.
5. Apply reaction stoichiometry, reference potency and dilution corrections as applicable.
6. Report content on the specified mass or potency basis and compare only with the assigned criterion.

## Observation Record

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

| Observation / parameter     | Record / finding |
|-----------------------------|------------------|
| Analyte form                | _____            |
| Test portion                | _____            |
| Method and reference/factor | _____            |
| Raw assay response          | _____            |
| Dilution                    | _____            |
| Assay result                | _____            |

## Calculations and Interpretation

- Titrimetric method:  $\text{analyte mass} = \text{corrected volume} \times \text{verified method factor} \times \text{dilution correction}$ .
- Instrumental method: obtain concentration from the valid reference calibration and correct for preparation/dilution.
- Assay (%) =  $\text{measured analyte amount} / \text{nominal analyte amount} \times 100$  on equivalent units and form.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Keep temperature and test conditions consistent across comparative readings.
- Record raw readings before rounding calculated values.
- Do not compare results obtained with different methods as if they were interchangeable.

## Viva Questions

### 1. Why is the analyte form part of the calculation?

Salt, hydrate and declared potency conventions can change the factor and reporting basis.

### 2. Why control the test conditions?

A change in conditions may alter the measured property independently of the intended variable.

### 3. Why retain replicate readings?

They show repeatability and help identify an anomalous measurement.

# Assay of Dapsone

Practical 10 | Medicinal Chemistry III

## Aim

To assay Dapsone, and interpret the recorded observations.

## Principle

- Dapsone contains two primary aromatic amino groups and a sulphone linkage. The stoichiometry of the assigned assay must reflect the actual analytical reaction.
- The property is obtained from a defined observable under controlled conditions.
- Replicate measurements, instrument checks and consistent units are needed before comparison.

## Materials and Apparatus

- Assigned dapsone, standardized analytical system or reference and assay apparatus.
- Assigned test material and calibration or comparison material.
- The apparatus specified for this property, a balance or volumetric equipment where relevant, and a record sheet.

## Method

1. Identify the exact analyte form, assay method and reporting basis assigned to the exercise.
2. Record the standardized reagent factor or the reference-standard potency used.
3. Prepare the measured test portion and comparison/blank according to that method.
4. Obtain replicate endpoint or instrumental responses and retain the raw readings.
5. Apply reaction stoichiometry, reference potency and dilution corrections as applicable.
6. Report content on the specified mass or potency basis and compare only with the assigned criterion.

## Observation Record

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

| Observation / parameter     | Record / finding |
|-----------------------------|------------------|
| Analyte form                | _____            |
| Test portion                | _____            |
| Method and reference/factor | _____            |
| Raw assay response          | _____            |
| Dilution                    | _____            |
| Assay result                | _____            |

## Calculations and Interpretation

- Titrimetric method:  $\text{analyte mass} = \text{corrected volume} \times \text{verified method factor} \times \text{dilution correction}$ .
- Instrumental method: obtain concentration from the valid reference calibration and correct for preparation/dilution.
- Assay (%) =  $\text{measured analyte amount} / \text{nominal analyte amount} \times 100$  on equivalent units and form.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Keep temperature and test conditions consistent across comparative readings.
- Record raw readings before rounding calculated values.
- Do not compare results obtained with different methods as if they were interchangeable.

## Viva Questions

### 1. Why is the analyte form part of the calculation?

Salt, hydrate and declared potency conventions can change the factor and reporting basis.

### 2. Why control the test conditions?

A change in conditions may alter the measured property independently of the intended variable.

### 3. Why retain replicate readings?

They show repeatability and help identify an anomalous measurement.

# Assay of Chlorpheniramine Maleate

Practical 11 | Medicinal Chemistry III

## Aim

To assay Chlorpheniramine Maleate, and interpret the recorded observations.

## Principle

- The assay distinguishes the active base from its maleate salt and follows the method-specified endpoint or instrumental response. Salt stoichiometry changes the mass factor.
- The property is obtained from a defined observable under controlled conditions.
- Replicate measurements, instrument checks and consistent units are needed before comparison.

## Materials and Apparatus

- Assigned chlorpheniramine maleate, method reagents/reference and assay apparatus.
- Assigned test material and calibration or comparison material.
- The apparatus specified for this property, a balance or volumetric equipment where relevant, and a record sheet.

## Method

1. Identify the exact analyte form, assay method and reporting basis assigned to the exercise.
2. Record the standardized reagent factor or the reference-standard potency used.
3. Prepare the measured test portion and comparison/blank according to that method.
4. Obtain replicate endpoint or instrumental responses and retain the raw readings.
5. Apply reaction stoichiometry, reference potency and dilution corrections as applicable.
6. Report content on the specified mass or potency basis and compare only with the assigned criterion.

## Observation Record

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

| Observation / parameter     | Record / finding |
|-----------------------------|------------------|
| Analyte form                | _____            |
| Test portion                | _____            |
| Method and reference/factor | _____            |
| Raw assay response          | _____            |
| Dilution                    | _____            |
| Assay result                | _____            |

## Calculations and Interpretation

- Titrimetric method:  $\text{analyte mass} = \text{corrected volume} \times \text{verified method factor} \times \text{dilution correction}$ .
- Instrumental method: obtain concentration from the valid reference calibration and correct for preparation/dilution.
- Assay (%) =  $\text{measured analyte amount} / \text{nominal analyte amount} \times 100$  on equivalent units and form.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Keep temperature and test conditions consistent across comparative readings.
- Record raw readings before rounding calculated values.
- Do not compare results obtained with different methods as if they were interchangeable.

## Viva Questions

### 1. Why is the analyte form part of the calculation?

Salt, hydrate and declared potency conventions can change the factor and reporting basis.

### 2. Why control the test conditions?

A change in conditions may alter the measured property independently of the intended variable.

### 3. Why retain replicate readings?

They show repeatability and help identify an anomalous measurement.

# Assay of Benzylpenicillin

Practical 12 | Medicinal Chemistry III

## Aim

To assay Benzylpenicillin, and interpret the recorded observations.

## Principle

- The beta-lactam structure is susceptible to degradation. The declared salt/form and the method-specific potency or mass basis must be retained throughout the assay.
- The property is obtained from a defined observable under controlled conditions.
- Replicate measurements, instrument checks and consistent units are needed before comparison.

## Materials and Apparatus

- Assigned benzylpenicillin form, reference/reagents and the selected validated analytical records.
- Assigned test material and calibration or comparison material.
- The apparatus specified for this property, a balance or volumetric equipment where relevant, and a record sheet.

## Method

1. Identify the exact analyte form, assay method and reporting basis assigned to the exercise.
2. Record the standardized reagent factor or the reference-standard potency used.
3. Prepare the measured test portion and comparison/blank according to that method.
4. Obtain replicate endpoint or instrumental responses and retain the raw readings.
5. Apply reaction stoichiometry, reference potency and dilution corrections as applicable.
6. Report content on the specified mass or potency basis and compare only with the assigned criterion.

## Observation Record

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

| Observation / parameter     | Record / finding |
|-----------------------------|------------------|
| Analyte form                | _____            |
| Test portion                | _____            |
| Method and reference/factor | _____            |
| Raw assay response          | _____            |
| Dilution                    | _____            |
| Assay result                | _____            |

## Calculations and Interpretation

- Titrimetric method:  $\text{analyte mass} = \text{corrected volume} \times \text{verified method factor} \times \text{dilution correction}$ .
- Instrumental method: obtain concentration from the valid reference calibration and correct for preparation/dilution.
- Assay (%) =  $\text{measured analyte amount} / \text{nominal analyte amount} \times 100$  on equivalent units and form.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Keep temperature and test conditions consistent across comparative readings.
- Record raw readings before rounding calculated values.
- Do not compare results obtained with different methods as if they were interchangeable.

## Viva Questions

### 1. Why is the analyte form part of the calculation?

Salt, hydrate and declared potency conventions can change the factor and reporting basis.

### 2. Why control the test conditions?

A change in conditions may alter the measured property independently of the intended variable.

### 3. Why retain replicate readings?

They show repeatability and help identify an anomalous measurement.

# Microwave-Assisted Synthesis of an Assigned Intermediate

Practical 13 | Medicinal Chemistry III

## Aim

To study Microwave-Assisted Synthesis of an Assigned Intermediate, and interpret the recorded observations.

## Principle

- Microwave-assisted synthesis couples electromagnetic energy to the reaction system. Heating behaviour depends on the material and apparatus; a shorter heating time does not alone prove higher purity or yield.
- A chemical transformation changes selected functional groups while retaining or constructing the required molecular skeleton.
- Product identity and purity require analytical evidence; appearance alone cannot establish either.
- Use a purpose-built laboratory system and its rated operating arrangement.
- The reaction temperature and pressure record are more informative than a nominal power setting alone.
- Reaction record: draw starting material and product structures, mark the functional-group change, and retain the assigned stoichiometry.
- Characterization record: compare the assigned melting range, TLC or spectral evidence. A narrow melting interval can support purity but cannot alone establish complete identity.

## Materials and Apparatus

- Instructor-selected reaction, rated laboratory microwave system and completed comparison records.
- Assigned starting materials and instructor-selected reagents.
- Balance, reaction glassware, stirring/heating arrangement, condenser where required, filtration equipment and identity/purity test apparatus.

## Method

1. Write the assigned reaction scheme and identify the limiting reactant.
2. Review the instrument-rated vessel, reaction scale and operating limits with the instructor.
3. Observe the trained microwave demonstration and record its monitored conditions.
4. Review the assigned work-up and purification stages.
5. Calculate dry yield and compare identity/purity with the conventional teaching record.
6. Discuss differences in energy coupling, process time and analytical outcome.

## Observation Record

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

| Observation / parameter     | Record / finding |
|-----------------------------|------------------|
| Assigned reaction           | _____            |
| Instrument settings         | _____            |
| Reaction time               | _____            |
| Temperature/pressure record | _____            |
| Yield and purity comparison | _____            |

## Calculations and Interpretation

- Theoretical product mass = limiting-reactant amount (mol)  $\times$  product stoichiometric ratio  $\times$  product molar mass.
- Percentage yield = dry product mass / theoretical product mass  $\times$  100.

### Worked Illustration

Illustration: a theoretical product mass of 2.00 g and dry recovery of 1.50 g give 75.0% yield.

The values in this illustration are for calculation practice.

## Result

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

Finding: \_\_\_\_\_

Conclusion: \_\_\_\_\_

## Precautions

- Use the approved reaction conditions and suitable ventilation.
- Keep product, starting material and waste streams separately labelled.
- Calculate yield from dry product and the limiting reactant; never use wet mass as pure-product mass.

## Viva Questions

### 1. What is the limiting reactant?

The reactant whose available amount permits the smallest theoretical amount of product.

### 2. Does a high yield establish purity?

No. Residual solvent, impurities and unreacted material can increase recovered mass.

# 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.

# Physicochemical Descriptors and Lipinski Rule of Five

Practical 15 | Medicinal Chemistry III

## Aim

To study Physicochemical Descriptors and Lipinski Rule of Five, and interpret the recorded observations.

## Principle

- Drug-design software estimates descriptors for a specific drawn structure. The rule of five is a screening heuristic for oral absorption/permeability tendencies, not proof of efficacy or bioavailability.
- 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.
- LogP describes neutral-species partitioning; logD is pH-dependent total-species distribution.
- cLogP is a calculated prediction. State the model rather than reporting it as a measured value.
- Molar refractivity is an additional descriptor and is not one of the four rule-of-five thresholds.

## Materials and Apparatus

- Assigned drug structures, descriptor software and a spreadsheet for consistent comparisons.
- Instructor-provided dataset and the stated study/model assumptions.
- Calculator or spreadsheet/statistical software and a record sheet.

## Method

1. Choose a consistent structural convention for each assigned drug.
2. Check connectivity, charges, stereochemistry and whether counterions are included.
3. Record software/version and the descriptor model used.
4. Calculate molar mass, logP/cLogP, molar refractivity and donor/acceptor counts.
5. Compare the results with the stated rule-of-five thresholds.
6. Explain exceptions and distinguish a screening flag from an experimental conclusion.

## Observation Record

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

| Observation / parameter | Record / finding |
|-------------------------|------------------|
| Drug/form               | _____            |
| Molar mass              | _____            |
| LogP or cLogP           | _____            |
| Molar refractivity      | _____            |
| H-bond donors           | _____            |
| H-bond acceptors        | _____            |
| Rule violations         | _____            |

## Calculations and Interpretation

- Common screening thresholds: molar mass not above 500 g/mol; H-bond donors not above 5; acceptors not above 10; cLogP not above 5.
- Count violated thresholds consistently; values are screening descriptors rather than acceptance specifications.

## 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. Can a compound outside the rule of five be a useful drug?

Yes. The rules are empirical screening guidance and have exceptions, including mechanisms or delivery routes outside their intended context.

### 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.

# Continue Learning with FirstHope

## Complete Notes on the FirstHope App

**Complete subject and semesters are available on FirstHope app only.**

- Get complete subject and semester notes in the FirstHope app.
- Available for B.Pharm, D.Pharm, M.Pharm and Pharm.D students.

**[Click here to get the FirstHope app](#)**

## Join the FirstHope Telegram Channel

Join FirstHope Notes and keep up with channel updates.

**[Click here to join Telegram](#)**

## Instagram

@firsthope.official

**[Click here to follow Instagram](#)**

## YouTube Channel

FirstHope-Pharmacy / Live streams

**[Click here to watch the YouTube channel](#)**

## WhatsApp Channel

Follow FirstHope on WhatsApp.

**[Click here to join the WhatsApp channel](#)**

## FirstHope Website

firsthopenotes.com

**[Click here to visit the website](#)**