

Pharm.D - Year 3

Medicinal Chemistry

Complete subject manual: 4 practicals and activities. Each chapter includes a student observation or work record.

Use the PDF bookmarks to navigate. The table gives each practical's content-page count; the combined manual has continuous page numbers.

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Assays of Assigned Pharmaceutical Drugs

Experiment 1 - Practical Notes

Name: _____ Roll no.: _____ Date: _____

Aim

To assay the allocated medicinal substances using the prescribed analytical methods.

Principle

An assay reports content on a specified chemical and dosage-form basis. Method selection, standard identity, stoichiometry and interference control determine the validity of the result.

Requirements

- Assigned drug substances and monographs, reference standards or standardised titrants, prescribed reagents and calibrated equipment.

Procedure

1. Plan each assay

Enter drug identity, chemical form, test portion, method version and specification.

2. Prepare the test and standard

Use the method-specific preparation, record dilution and account for anhydrous/dried or salt basis if required.

3. Measure

Obtain the prescribed endpoint or instrumental signal with blank and control results.

4. Calculate content

Use the monograph factor or validated calibration, including all dilution and chemical-form corrections.

5. Report

Compare replicates and the assigned acceptance requirement; state content, units and basis.

Medicinal Chemistry

Observations and Record

Drug / form	Method / endpoint	Content and basis
Assigned drug 1	_____	_____
Assigned drug 2	_____	_____
Assigned drug 3	_____	_____

Worked Example

The numbers below are illustrative; enter your own observations in the record.

- Content (%) = determined analyte mass / test-portion mass × 100, if both are expressed on the same basis.
- Example: 0.198 g determined in a 0.200 g portion gives 99.0% on that stated basis.

Result

Record the completed observations, calculations and conclusion with units. State any limitation of the observation.

Precautions

- Do not substitute one drug salt, hydrate or method factor for another.
- An illustrative numerical example does not set the official specification.

Viva Questions and Answers**1. Why state the chemical form?**

Salt and hydration state change formula mass and the content basis.

2. What does a blank correct?

Response not attributable to the analyte in the stated measurement system.

Drug and Intermediate Preparations - Acetylation Study

Experiment 2 - Practical Notes

Name: _____ Roll no.: _____ Date: _____

The institution assigns the drug or intermediate preparations for this subject. The acetylation options below provide a complete supervised teaching record for aspirin and acetanilide; other allocated preparations require their own approved reaction scheme and method.

Aim

To study the specified organic preparation, isolate the assigned product and calculate its yield.

Principle

Acetylation introduces an acetyl group at a suitable nitrogen or oxygen site. Acetanilide is an amide; aspirin is acetylsalicylic acid.

Requirements

- Instructor-approved reaction scheme, reagent quantities and laboratory procedure for the selected route.
- Reaction glassware, suitable ventilation, separation apparatus, balance and melting-point apparatus.

Procedure

1. Plan the selected route

Write the balanced reaction and identify the functional-group change, limiting reagent, expected product and hazards. Use the assigned supervised method for the selected option.

2. Carry out the assigned reaction

Measure the prescribed reagents and follow the authorised addition sequence and temperature controls. Record actual reaction observations and the method used.

3. Isolate the product

Complete the assigned quench, allow crystallisation and collect the solid by filtration. Wash as specified to remove soluble residual reagents.

4. Purify and dry

Apply the assigned recrystallisation or purification method. Record solvent, observations, dry mass and melting range where appropriate.

5. Assess the product

Calculate theoretical and percentage yield. Compare the measured physical properties and assigned identity test; explain that yield alone does not prove purity.

Medicinal Chemistry**Preparations and Reaction Scheme**

Route / product	Starting material and change
Acetanilide	Aniline to an acetamide derivative.
Aspirin	Salicylic acid to its phenolic O-acetyl derivative.

Observations and Record

Record	Student entry
Selected route / balanced equation	_____
Limiting reagent and molar mass	_____
Theoretical product mass	_____
Dry product mass / melting range	_____
Percentage yield / identity finding	_____

Worked Example

The numbers below are illustrative; enter your own observations in the record.

- Theoretical product mass = moles of limiting reagent $\times$ stoichiometric product ratio $\times$ product molar mass.
- Percentage yield = dry product mass / theoretical product mass $\times$ 100.
- Illustration: 0.020 mol of a limiting reagent gives 0.020 mol of a 150 g/mol product. The theoretical mass is 3.00 g; 2.40 g isolated product gives 80.0% yield.

Result

Product: _____. Route: _____. Dry mass: _____. Yield: _____. Physical property / identity evidence: _____.

Precautions

- Use the specific supervised procedure and facilities for corrosive, toxic, oxidising or flammable reagents.
- Record the selected preparation option rather than combining different reaction routes.
- Use dry product mass for yield and the stated test conditions for comparison.

Viva Questions and Answers**1. Which group is acetylated in aspirin?**

The phenolic hydroxyl group of salicylic acid.

2. What group is formed in acetanilide?

An amide group.

3. Why dry the crystals?

Residual solvent can falsely increase yield and alter melting behaviour.

Monograph Analysis of Pharmaceutical Drugs

Experiment 3 - Practical Notes

Name: _____ Roll no.: _____ Date: _____

Aim

To read and apply the identity, purity and assay requirements of an assigned medicinal substance.

Principle

A monograph defines a named material and its quality requirements; tests address distinct attributes and must be read with the relevant general instructions.

Requirements

- Institution-assigned current or syllabus-prescribed drug monographs and coded teaching analysis records.

Procedure

1. Establish scope

Enter title, edition, chemical form, formula mass and content basis.

2. Map tests

Classify description, identification, impurity/related-substance tests, water or loss on drying and assay.

3. Review methods

Record sample preparation, standards, measurement and acceptance rule for each assigned test.

4. Evaluate data

Apply the stated rules to supplied results and explain any failed or invalid test.

5. Conclude

A complete conformity conclusion needs all required results; a passing assay alone is not enough.

Observations and Record

Monograph element	Requirement / finding
Title / edition / form	_____
Identity	_____
Purity / related substances	_____
Water or drying basis	_____
Assay and overall conclusion	_____

Result

Record the completed observations, calculations and conclusion with units. State any limitation of the observation.

Precautions

- Use the correct edition and all cross-referenced general instructions.
- Do not create numerical acceptance limits absent from the assigned monograph.

Viva Questions and Answers

1. Does a high assay prove purity?

No. Different impurity and identity requirements also apply.

2. Why read general notices?

They define how the individual monograph requirements are interpreted.

Physicochemical Parameters for QSAR

Experiment 4 - Practical Notes

Name: _____ Roll no.: _____ Date: _____

Aim

To calculate partition, ionisation and molar-refractivity parameters from assigned data.

Principle

QSAR uses defined descriptors to relate chemical structure and measured activity in an explicit dataset. A descriptor or correlation alone does not prove a biological mechanism.

Requirements

- Supplied equilibrium concentration, pKa, density, refractive-index and activity datasets; calculator or spreadsheet.

Procedure

1. Partition coefficient

Use neutral-species equilibrium concentrations in the stated immiscible phases and calculate P and logP. Distinguish pH-dependent distribution D from neutral-species partition P.

2. Ionisation

Use the assigned pKa and pH model for the acid or base; record which chemical species the fraction refers to.

3. Molar refractivity

Apply the Lorentz-Lorenz equation using refractive index, formula mass and density on consistent units.

4. Compare descriptors

Prepare a compound-by-descriptor table and examine the assigned relationship with activity, noting dataset size and confounding.

5. Report

State descriptor definitions, units, conditions and the limits of an observed correlation.

Observations and Record

Descriptor	Input	Calculated result
P / logP	_____	_____
pKa / ionisation fraction	_____	_____
Molar refractivity	_____	_____
Activity relationship	_____	_____

Worked Example

The numbers below are illustrative; enter your own observations in the record.

- $P = \text{Corganic(neutral)} / \text{Caqueous(neutral)}$; $\log P = \log_{10}(P)$. Example: $20/2 = 10$, so $\log P = 1$.
- For a monoprotic weak acid, ionised fraction = $1/[1 + 10^{(pK_a - pH)}]$. At $pH = pK_a$, it is 0.5. For a base, the protonated fraction = $1/[1 + 10^{(pH - pK_a)}]$.
- Molar refractivity = $[(n^2 - 1)/(n^2 + 2)] \times M/\rho$. Example: $n = 1.5$, $M = 100 \text{ g/mol}$ and $\rho = 1 \text{ g/cm}^3$ give $29.41 \text{ cm}^3/\text{mol}$.

Result

Record the completed observations, calculations and conclusion with units. State any limitation of the observation.

Precautions

- State phase composition, pH and temperature; do not compare undefined partition measurements.
- Use an appropriate ionisation model rather than applying a monoprotic relation to every compound.

Viva Questions and Answers

1. How do logP and logD differ?

LogP describes neutral-species partitioning; logD includes the distribution of species at a stated pH.

2. Does a QSAR association prove mechanism?

No. It must be validated and interpreted within the model and dataset.

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