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Computational Modelling of Drug Disposition

Practical 16 - Software and data-analysis practical

Aim

To compare compartmental or physiologically motivated models of drug disposition.

Principle

Disposition models describe distribution and elimination using defined structures and parameter relationships. Additional compartments can improve description but also increase the evidence needed to estimate parameters reliably.

Keep the supplied data, transformations, software version, analysis settings and complete output together. Record units explicitly and distinguish assumptions from observations.

Materials and Requirements

- Supplied concentration-time data and model candidates
- Dose, route, physiological assumptions and parameter bounds
- Spreadsheet or institution-approved analysis software
- Raw-data dictionary and analysis worksheet

Procedure

1. Define the analysis question and the variables, units, identifiers and missing-data conventions in the dataset.
2. Import a working copy and check values against the original file. Inspect ranges, duplicates, timing and unit consistency.
3. Draw the proposed structure and state which data inform absorption, distribution and elimination.
4. Fit or simulate the selected structures with consistent units and meaningful parameter bounds.
5. Inspect residual patterns, uncertainty and parameter correlations rather than selecting only the smallest residual sum.
6. Compare candidates using the prespecified model-selection approach and interpret the model parameters within that structure.
7. Retain diagnostics, intermediate calculations and the selected analysis settings. Explain exclusions and sensitivity checks.
8. Write a conclusion that addresses the stated question and the limitations of the design rather than relying on one fitted statistic.

Observations and Record

Enter actual measurements or the supplied teaching data. Record the method, material identity, conditions and units.

Candidate model	Assumptions	Fit / prediction evidence	Reason for selection
One-compartment	Record	Record	Assess
Two-compartment or other candidate	Record	Record	Assess
Sensitivity or validation scenario	Record	Record	Assess

Calculations

• For a one-compartment linear model, elimination rate constant = CL/V
• Changing model structure changes the interpretation of fitted rate constants and volumes.

Worked Example

Illustrative CL = 4 L/h and V = 20 L give elimination rate constant 0.20 h^-1 and half-life ln(2)/0.20 = 3.466 h. A second model may fit better because it represents a distribution phase. Compare the supporting diagnostics and parameter uncertainty before interpreting that improvement.

Result and Interpretation

• Explain the selected structure and the observations supporting it. Treat simulations outside the data range as extrapolations.

Precautions

• Avoid mixing rate constants with clearance units.
• Use independent validation where available.
• Do not interpret a compartment as a literal organ without the model supporting that meaning.
• Preserve the original dataset and a reproducible record of the analysis.

Viva Questions and Answers

Is every compartment an organ?

No; many compartmental models are mathematical descriptions.

Why can too many parameters be a problem?

The data may not identify them reliably.

Why inspect residuals?

They can reveal systematic model inadequacy.

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