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# Computer Simulation of Pharmacokinetics and Pharmacodynamics

Practical 15 - Software and data-analysis practical

## Aim

To simulate a concentration-time profile and connect exposure to an explicit pharmacodynamic model.

## Principle

A pharmacokinetic model describes drug disposition, while a pharmacodynamic model relates concentration or exposure to a measured response. The model assumptions determine which quantities can be interpreted. Hysteresis or delayed responses may require more than a direct concentration-effect relationship.

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

## Materials and Requirements

- Declared model parameters and initial conditions
- Supplied or simulated concentration and response data
- 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. Specify the route, model structure, parameter units and whether the task is simulation or fitting.
4. Construct a time grid suitable for the processes being represented and simulate the concentration profile.
5. Apply the selected response relationship and inspect how changes in clearance, volume, Emax or EC50 alter the output.
6. Compare predictions with any provided observations and review residuals and parameter identifiability.
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.

| Model component | Parameter / units | Input value | Prediction / sensitivity |
|---|---|---|---|
| PK model | Clearance and volume | Record | Concentration profile |
| PD model | Emax and EC50 | Record | Response profile |
| Scenario | One changed parameter | Record | Compare outputs |

## Calculations

- For a simple one-compartment IV-bolus model, $C(t) = \text{Dose}/V \times \exp(-CL \times t/V)$

• Direct Emax model: E = E0 + Emax x C/(EC50 + C)

### Worked Example

Illustrative direct-response model: E0 = 0, Emax = 100 response units and EC50 = 5 concentration units.
At C = 5, E = 50 units. At C = 15, E = 75 units.
These are model outputs. They do not define a patient dosing regimen or prove that a real biological system follows the selected equation.

## Result and Interpretation

• Present the model, parameters and outputs together. Explain what the simulation can and cannot answer.

## Precautions

• State model and unit assumptions.
• Inspect predictions over plausible parameter ranges.
• Separate fitting quality from biological plausibility.
• Preserve the original dataset and a reproducible record of the analysis.

## Viva Questions and Answers

### What does EC50 represent?

The concentration giving half the modelled maximal increment in response.

### Why perform sensitivity analysis?

It shows how parameter changes influence model predictions.

### Can a model be fitted well but interpreted poorly?

Yes; structure and parameter identifiability still require assessment.

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