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Molecular Descriptors and Drug-Likeness

Practical 21 - Molecular modelling practical

Aim

To calculate and compare molecular descriptors for selected medicinal compounds.

Principle

Descriptor values depend on the encoded structure, algorithm and molecular form. Log P, molar refractivity, hydrogen-bond donor and acceptor counts describe different properties; ionisation affects their interpretation.

Materials and Requirements

- Benign reference structures with verified stereochemistry and protonation basis
- Institution-approved software with version, parameters and model documentation
- Independent reference or validation dataset
- Approved method or teaching-data pack and a dated record sheet

Procedure

1. Define the preparation or dataset, study question and method version. Record identities, units and the criteria to be used before examining the outcome.
2. Define the endpoint and retain unmodified input structures and identifiers. Standardise salts, tautomers and stereochemistry using a documented rule.
3. Verify each structure and calculate molecular mass, predicted log P, predicted molar refractivity and donor/acceptor counts with named algorithms.
4. Compare neutral and relevant ionised forms and inspect why counts or predictions change.
5. Apply any drug-likeness rule as a stated heuristic, recording exceptions rather than labelling all violations as inactive.
6. Save input/output files, failures, parameter choices and independent validation results so the analysis can be reproduced.
7. Retain the original observations and calculations. State deviations, missing information and the limits of the conclusion; do not replace measured values with expected results.

Observations and Record

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

Molecule / model	Input / settings	Output / diagnostic	Interpretation / limitation
Reference	Document	Record	Evaluate
Test molecules	Document	Record	Evaluate
Independent check	Document	Record	Evaluate

Calculations

- For a measured refractive-index model, molar refractivity = [(n^2 - 1)/(n^2 + 2)] x molar mass / density; this is distinct from a software fragment-based prediction.

Worked Example

Illustrative a neutral alcohol O-H can contribute one donor and one acceptor, whereas a protonated amine is generally not an acceptor. Use the software definition for the exact encoded structure.

A predicted log P of 2 corresponds to a neutral-species partition ratio of 100 under the definition; it is not automatically log D at physiological pH.

Result and Interpretation

- Deliver a structure-descriptor table with algorithms, units, form and interpretation.
- Predictions are not measured biological activity, clinical safety or regulatory approval.

Precautions

- Avoid training/test leakage and unsupported extrapolation.
- State software and model version and applicable domain.
- Do not select the best-looking model using the final test set.

Viva Questions and Answers

Why inspect protonation?

It changes encoded charge and can alter counts and behaviour.

Is predicted log P measured?

It is an algorithm-based estimate.

Do drug-likeness rules prove efficacy?

They are screening heuristics, not efficacy tests.

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