



CONCEPT LIFE SCIENCES

DELIVERING SCIENCE

DATA SHEET

LogD

The organic solvent-water partition coefficient (LogD or LogP) is measured using the shake flask methodology. The aqueous phase used is a 10mM solution of sodium phosphate buffer adjusted to pH 7.4. Octanol is typically used as the organic solvent, but this may be substituted with the desired choice of alternative organic solvent that best models the environment in which the test compound is intended to be applied.

The lipophilicity of n-octanol is considered to resemble lipid-bilayer membranes, and distribution of chemicals between n-Octanol and the aqueous phase simulates their ability to passively diffuse across biological membranes.

CUSTOMER PROVIDES

Compound identifier and molecular formula.

Test: 30µL of 10mM in DMSO or 0.5mg solid.

CONDITIONS

As standard, Buffer/Octanol partitioning at pH7.4 is used.

However different pH or organic solvents can be used if requested.

PROTOCOL

10mM DMSO compound is added to 490µL of Octanol saturated with pH7.4 buffer. The samples are centrifuged to remove any un-dissolved material. An aliquot of this stock is added to buffer saturated with Octanol. The samples are then shaken to achieve equilibrium between the two

phases. Post incubation, the samples are centrifuged, aliquots of the Octanol layer are taken for analysis. Excess Octanol is then removed to waste. The buffer layer is also sampled.

Quantitation of test compound in both phases is via LC-MS/MS.

POSITIVE CONTROLS

Propranolol is used in each assay run.

QUANTITATION

The analytical samples are analysed by LC-MS/MS using Concept Life Sciences generic analytical methods to measure the test compound, and quantify against a 5-point standard curve. Validated assay range is LogD -1.0 to 5.5.





DATA ANALYSIS AND RESULTS

For each test compound injection:

$$\text{Response ratio} = \frac{\text{Test peak area}}{\text{Internal standard peak area}}$$

Quantitation is via the standard curve.

The LogD of test compound bound is calculated from:

$$\text{LogD} = \text{Log} \left(\frac{\text{Octanol Response Ratio AP}}{\text{Buffer Response Ratio}} \right)$$

CONCEPT LOG D PH7.4

