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Application of lipophilicity, protein and phospholipid binding measured by HPLC for prediction of ADME properties and toxicity of compounds

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The chromatographic separation principle is suitable for measuring the physicochemical properties of compounds using generic HPLC methods with standardised retention times. When phospholipids (IAM, immobilised artificial membrane) and proteins (albumin and glycoprotein) are used as stationary phases, the measured data can be used for predicting the toxicity and in vivo distribution of compounds. Thus, compounds' volume of distribution, brain tissue binding, lung retention, skin penetration, phospholipidotic and cardiotoxicity potential can be predicted.
These measurements will be part of an AI/machine learning (ML) platform developed by AsedaSciences®, integrating other high-content cellular and zebrafish embryo toxicity screens. The chromatographic, cellular and zebrafish screening results and associated ML-based predictions and visualisation will be available on an AWS cloud-based platform called 3RnD®. Scientists from any academic Institution or drug discovery company will be able to compare the results for their own compounds to a library of thousands of compounds, helping to predict toxicity risk earlier. This approach helps scientists select safer scaffolds, understand SAR's impact, and prioritise safer compounds, improving R&D productivity by preventing later-stage attrition.