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O29: LINKING CHEMICAL STRUCTURE TO SPHEROID PHENOTYPES: AN INTERPRETABLE QSAR APPROACH FOR HEPATOTOXICITY IN THE CONTEXT OF SSBD

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In this research, we created a QSAR framework to analyse drug safety with the purpose of generating interpretable and relevant SSbD insights. We used public database containing approximately 20 000 brightfield microscopy images of human liver spheroids exposed to 108 drugs over a period of up to 7 days.^[1] CellProfiler open-source software was used to perform image segmentation and extract features related to spheroid size, shape, intensity and texture. These features were extracted from each image and exported into a CSV file, which served as input to the QSAR framework. The CSV file was further enriched with molecular fingerprints and physicochemical descriptors generated by RDKit library.^[2] We utilised scikit-learn library to train a Random Forest model, perform cross-validation and select the most relevant features. A simpler linear model was developed to compare interpretability against Random Forest model. The QSAR model investigated how the drug structure links to developed spheroid phenotype, that links to toxicity prediction. We interpreted the QSAR results using SHAP values, to identify key structural features which were further analysed in an open-source OECD QSAR Toolbox to provide mechanistic context and support grouping of compounds in line with the SSbD principles. The final output from this research is to derive conclusions of drug safety to the liver human spheroids based on correlation between chemical and structural composition of applied drugs and observed changes in spheroids upon exposure, leading to design-relevant insights, where specific aspects of drug chemical structure can be associated with toxicity level and the temporal progression of spheroid damage. These insights highlight structural motifs that should be avoided or reduced to decrease hepatotoxicity risk. Future research should include analysis of liver human spheroids toxicity response to drugs co-exposures, as combined exposures may lead to different toxicity profiles comparing to toxicity profile of single compound.

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