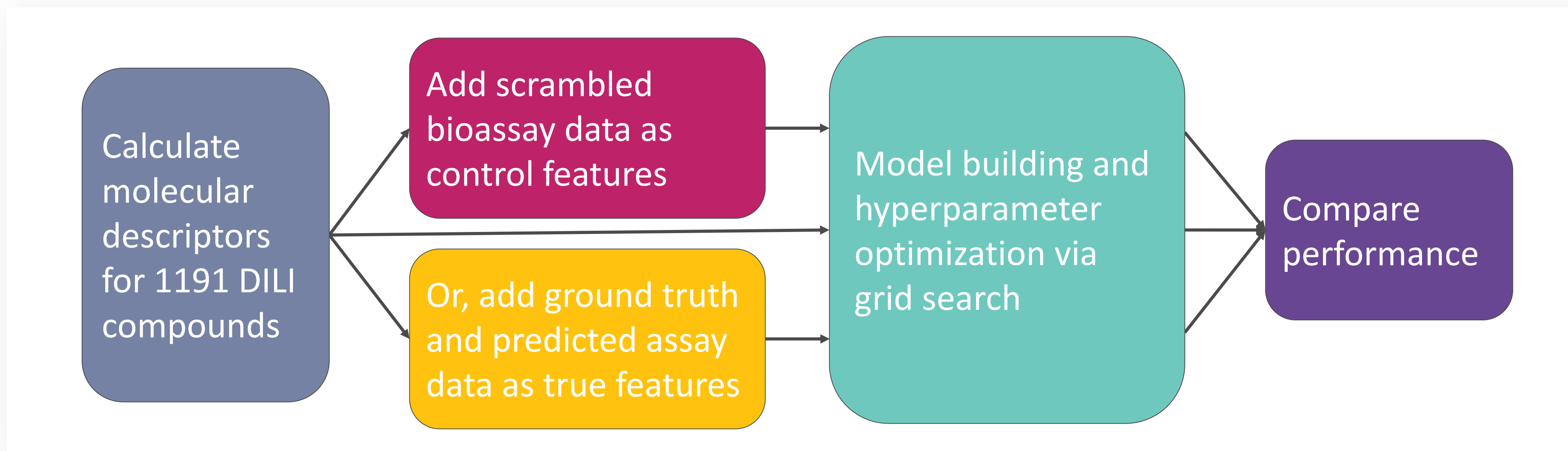


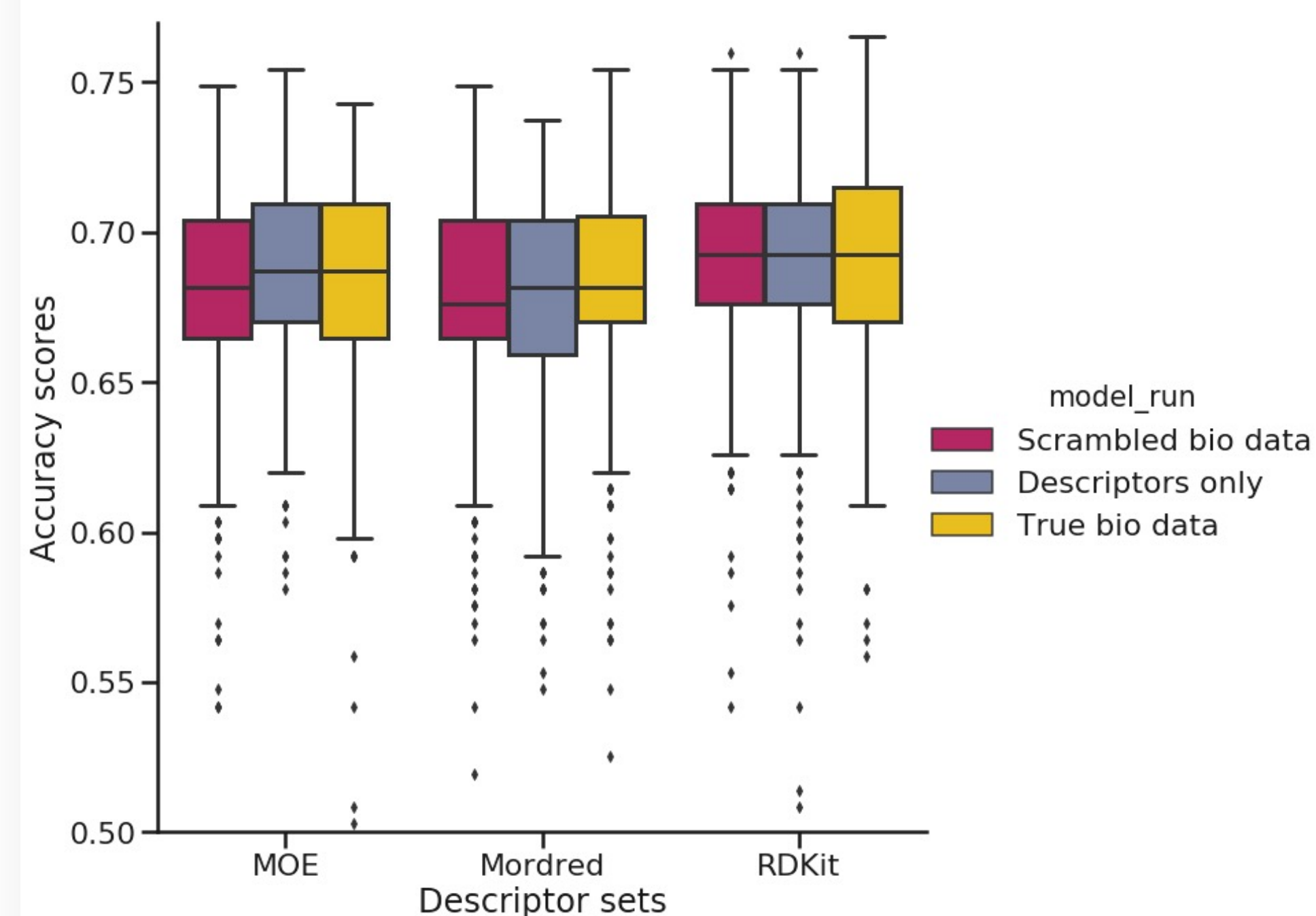
Cell biology assay data can improve prediction of drug-induced liver injury compared to chemical descriptors alone.

Method

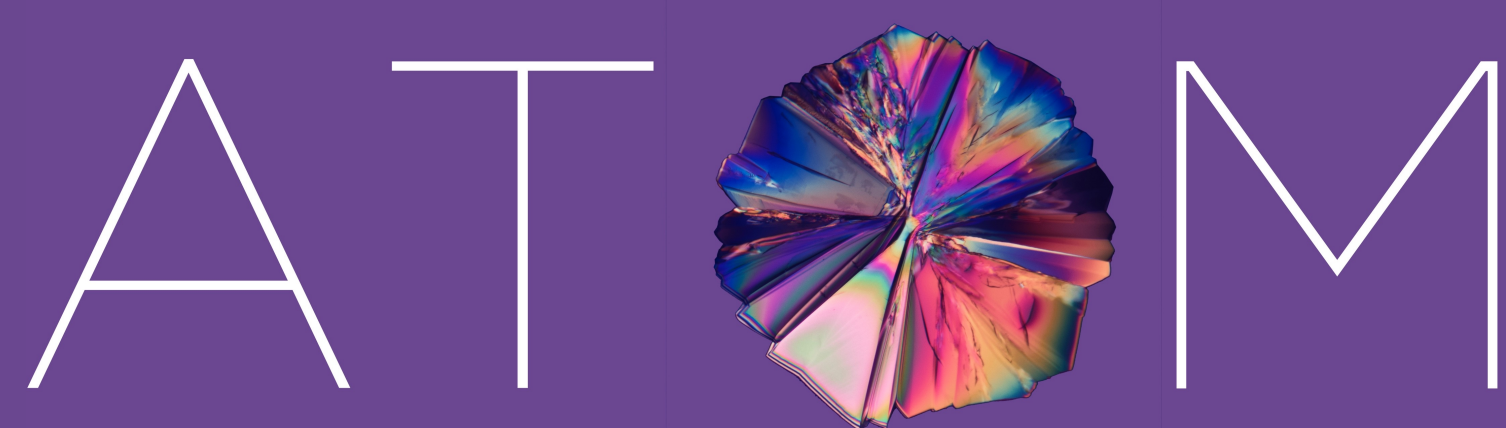
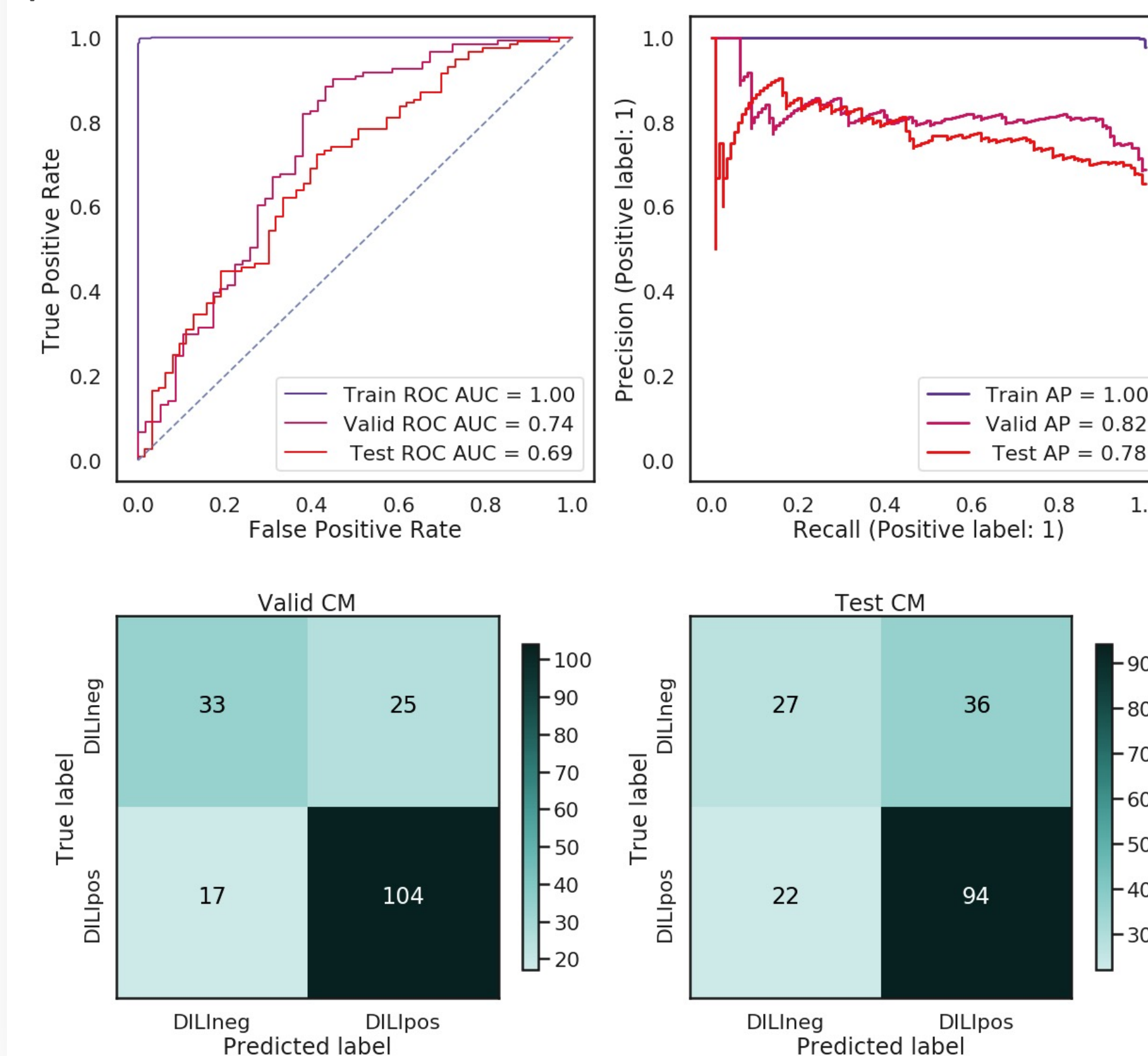


Results

For each set of molecular descriptors, **including biological data yields models that perform as well or better** than either descriptors alone or scrambled bioassay data, suggesting that biological information improves the accuracy of DILI prediction.



The **best performing model** is a random forest using RDKit descriptors and transporter inhibition predictions for MRP3, MRP4 and BSEP.



Towards a data-driven DILI prediction platform

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