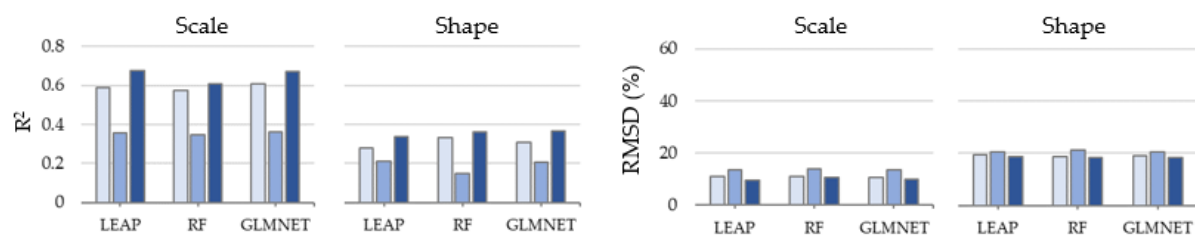
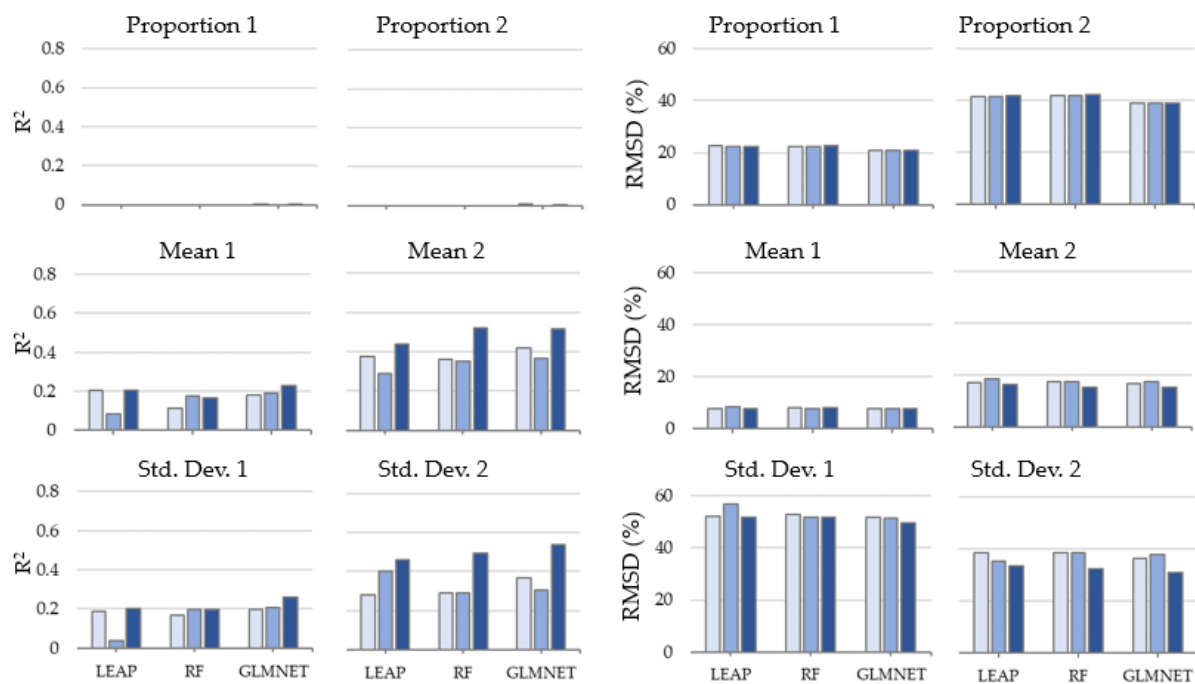


Differentiated unimodal



Differentiated bimodal



Undifferentiated

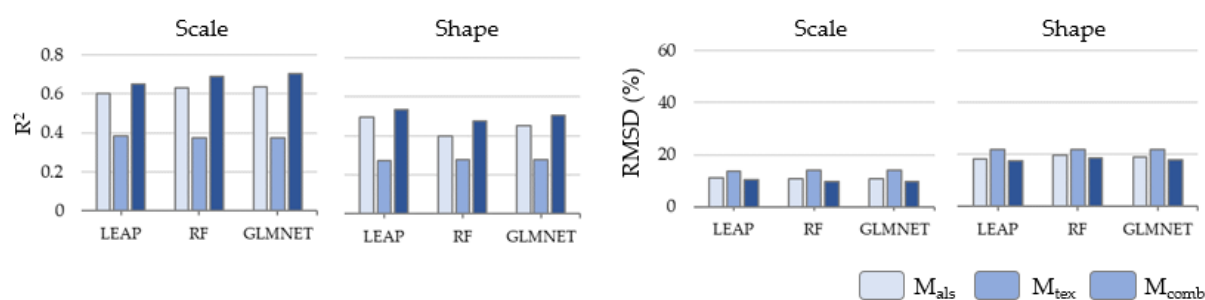


Figure S1: Average of 5 repeated cross-validation performance measures (R^2 , RMSD%) derived during model development using the various SDD modality plot groupings, ALS metric sets and modelling techniques