

molecular informatics

models – molecules – systems

Supporting Information

Supplementary Panel/Figure images for
manuscript
“Classifiers and their metrics quantified”

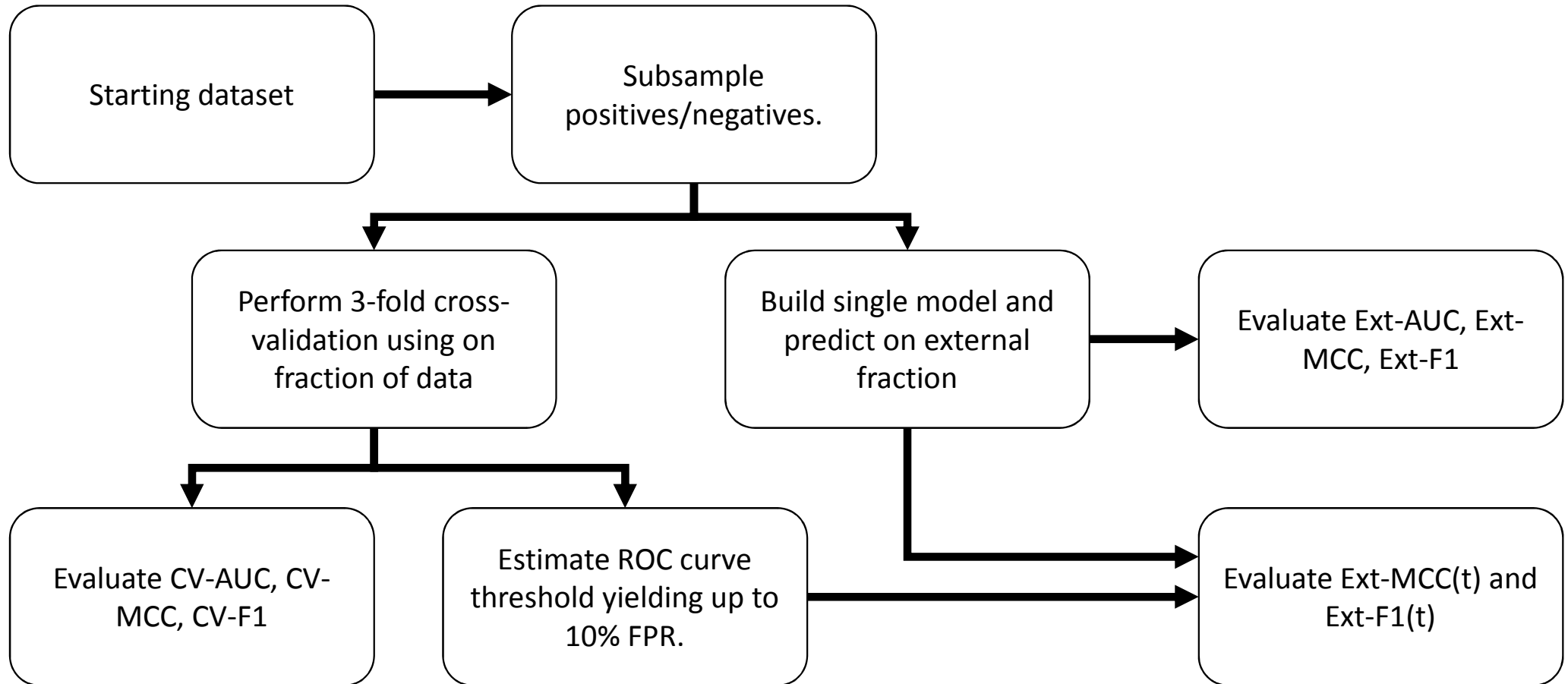
For re-submission to Molecular Informatics by

J.B. Brown , Kyoto University

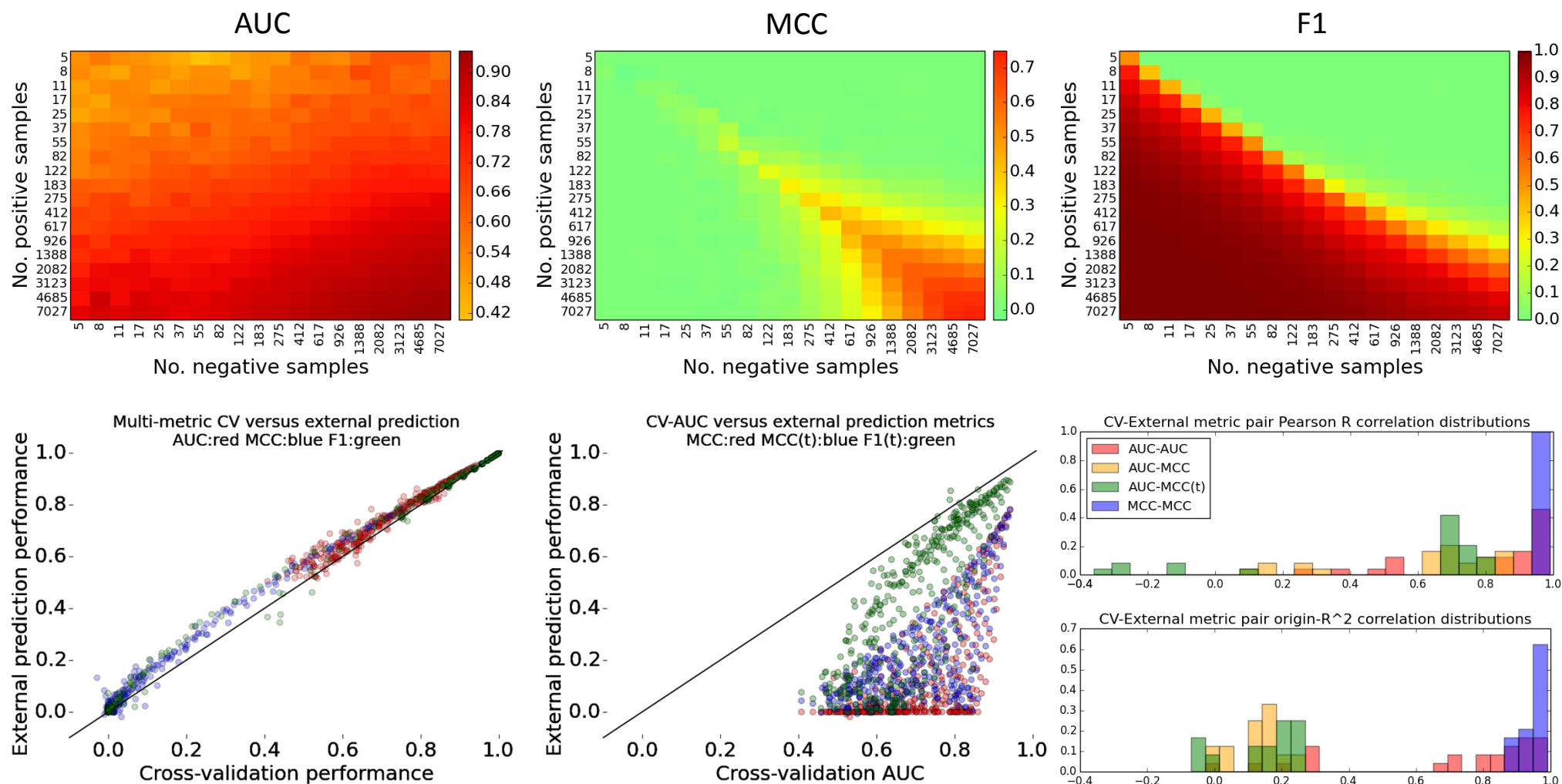
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Supplementary Figure: chemogenomic CV-external metric evaluation workflow



Supplementary Figure: Cross-validation, external prediction, metrics, and their cross-correlations (Kinase SARfari 5)



Supplementary Figure: CV-AUC versus external prediction for other parameter sets

