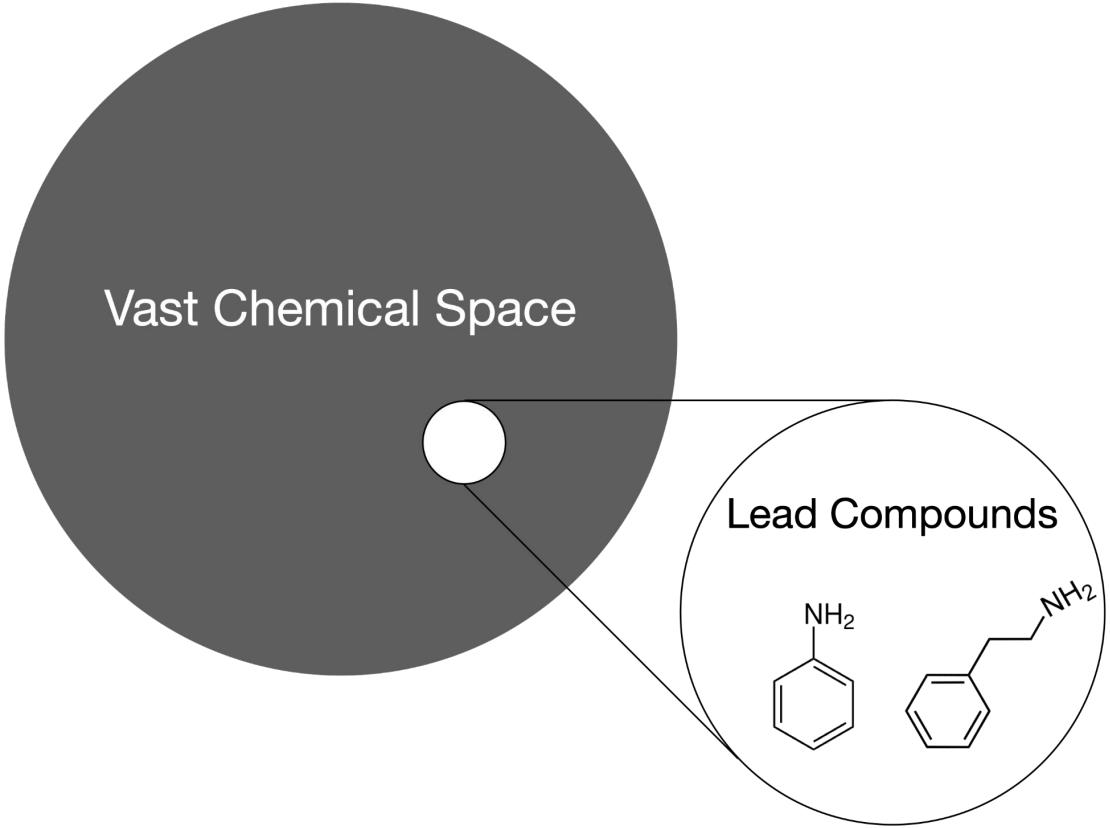
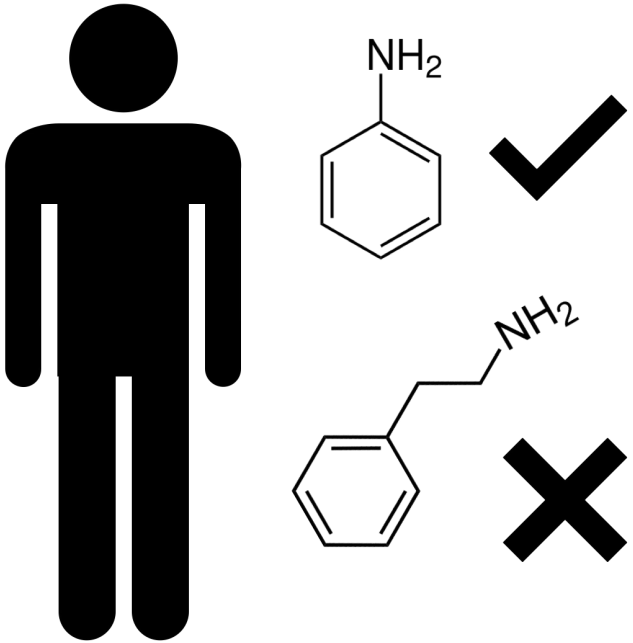
Inference of drug activity scores from transcriptomics data

Peters Couto, Badia-i-Mompel et al in progress

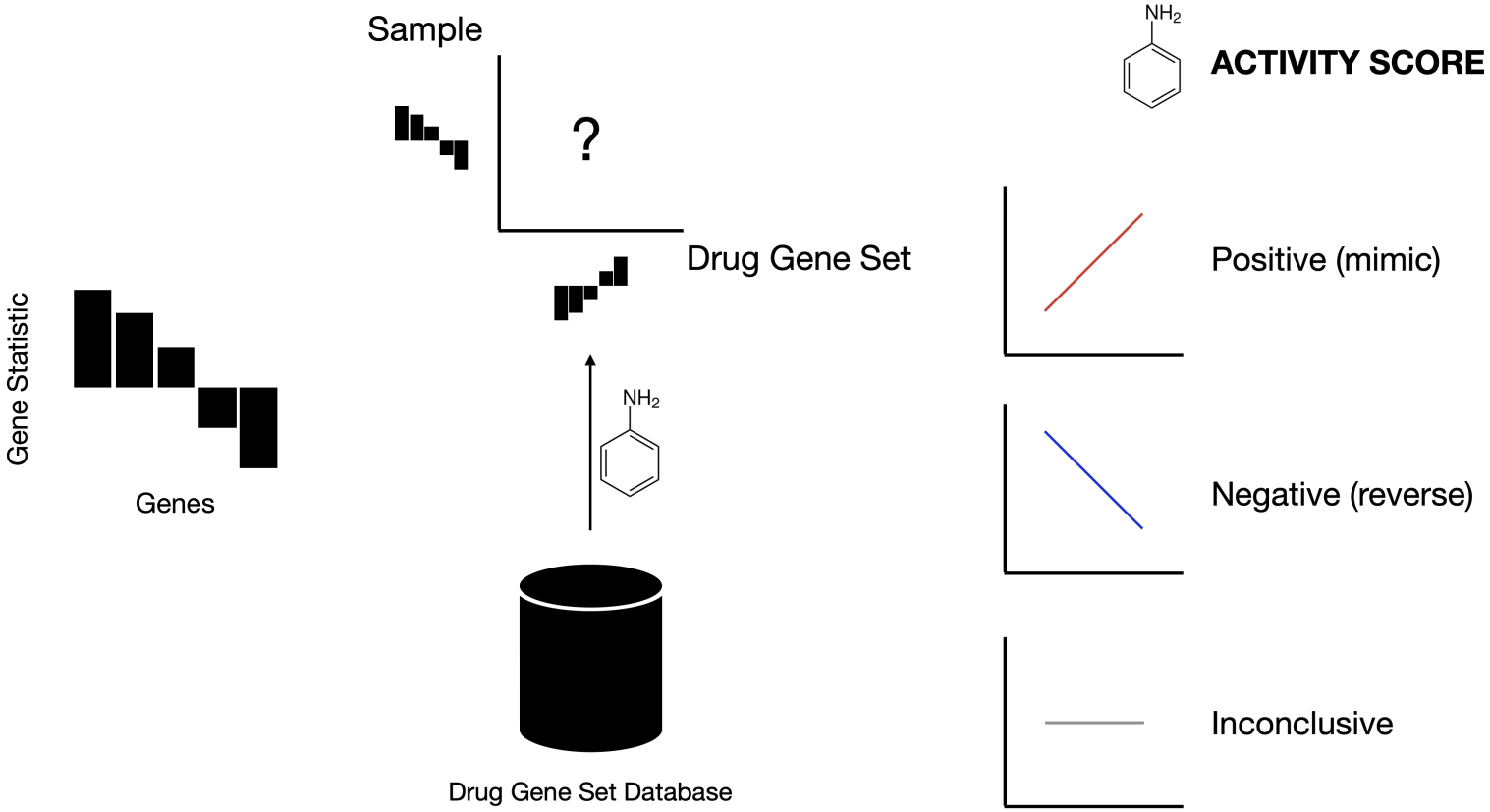
Saez-Rodriguez Group

Narrowing down the chemical space

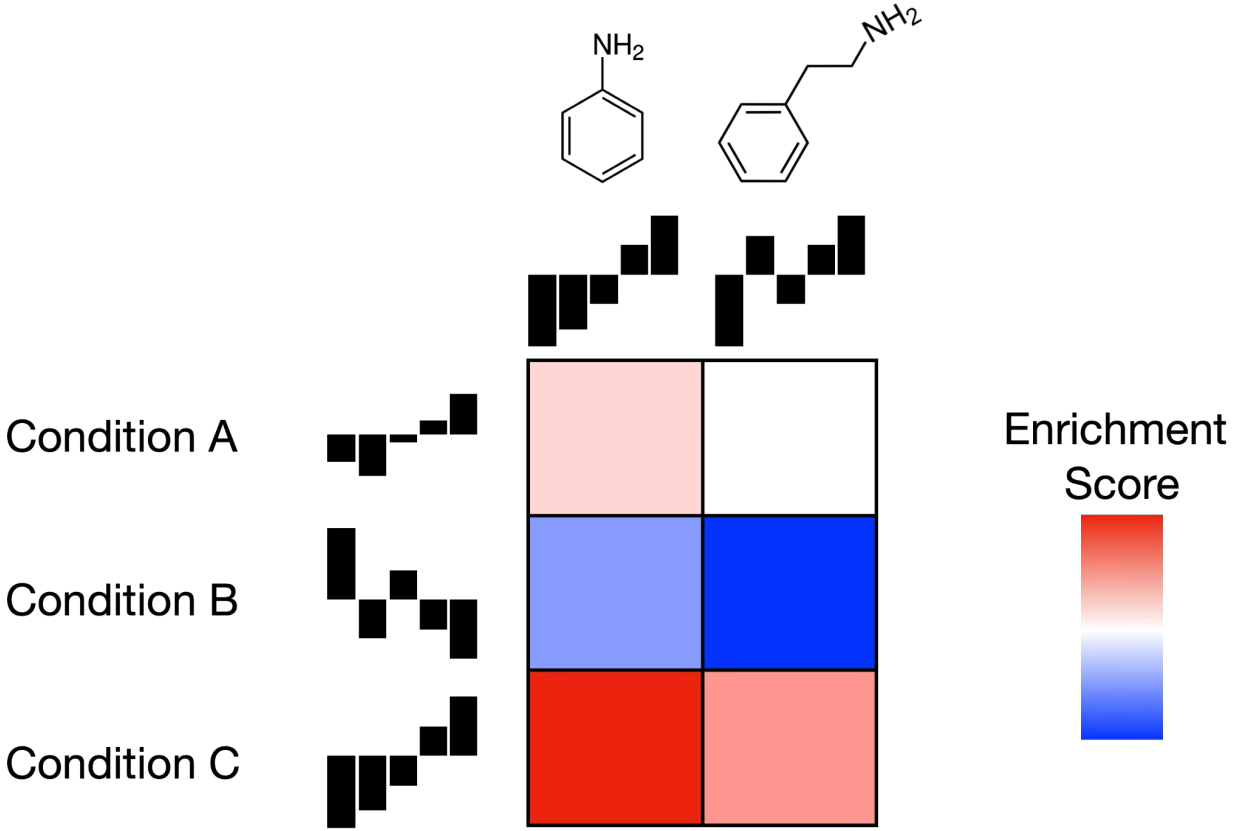




Drug activity scoring with enrichment



Drug signature matching



Current opportunities with signature matching

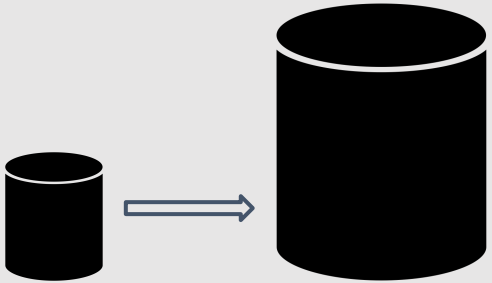
Gene Set Comparison

Protein-based

vs

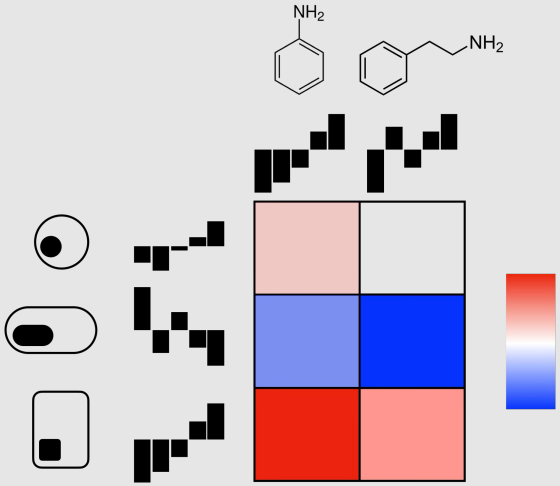
Gene-based

Large scale



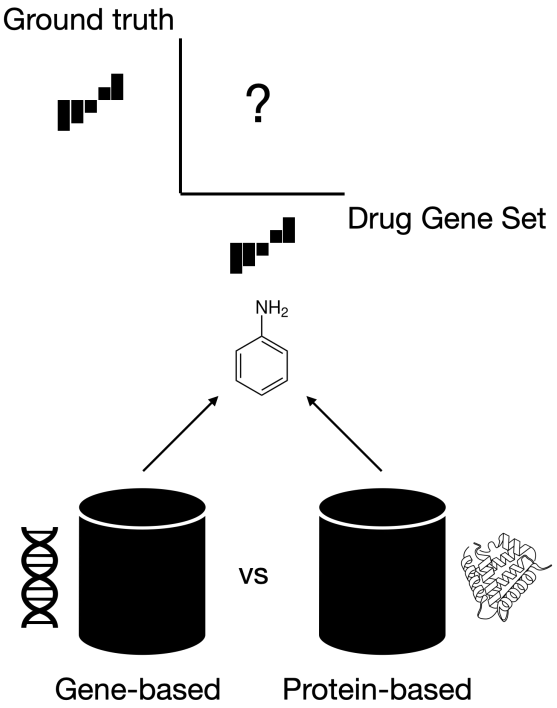
Drug gene set databases

Single cell

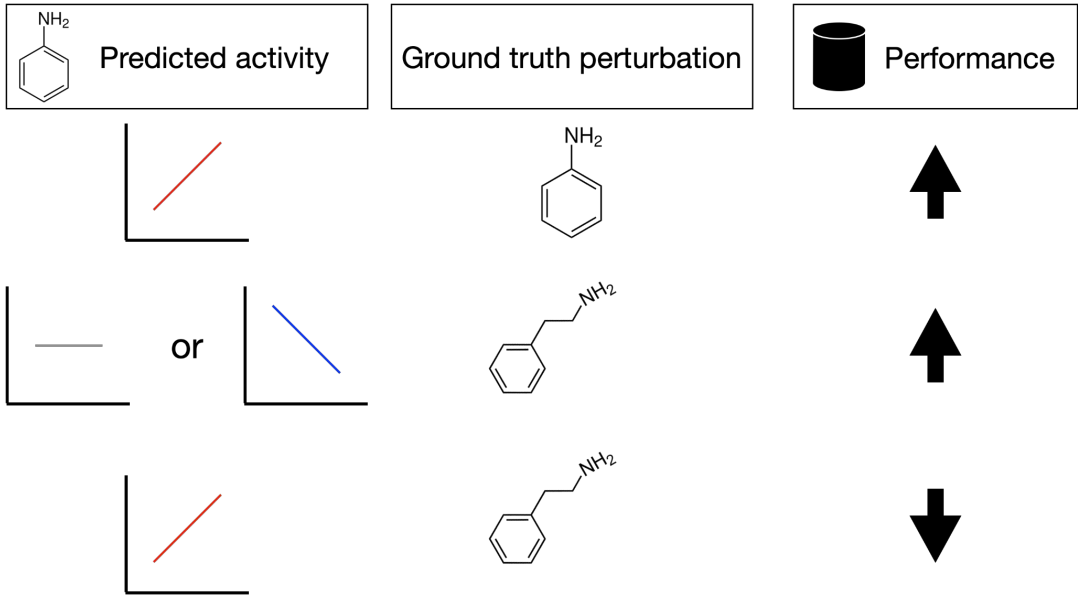


Comparing drug gene sets

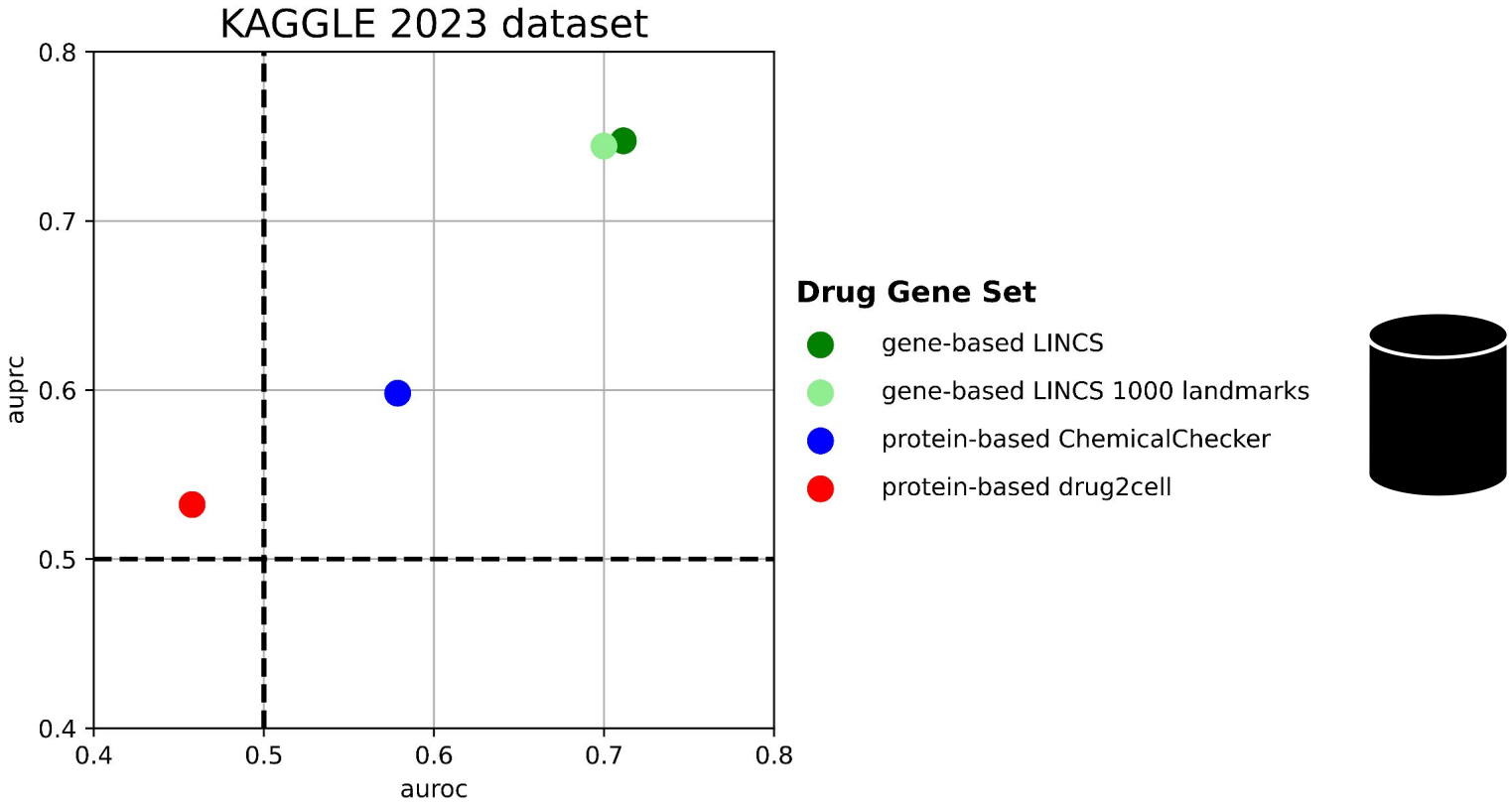
1) Drug activity scoring



2) Benchmarking



Drug gene sets perform better when gene-based than protein-based

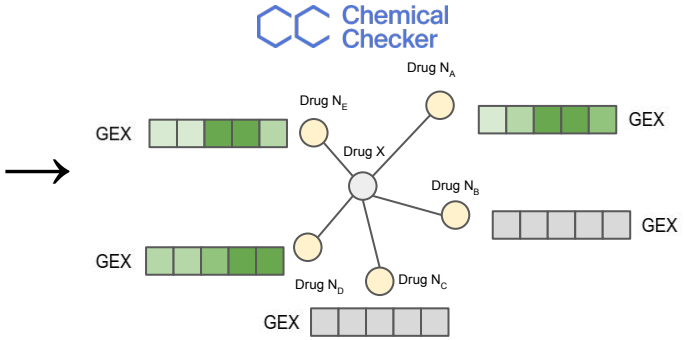


Expanding drug signatures

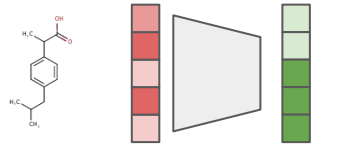
Collaboration with
Patrick Aloy lab

1)

?



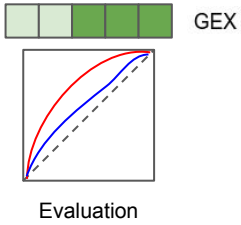
2)



Morgan Fingerprint

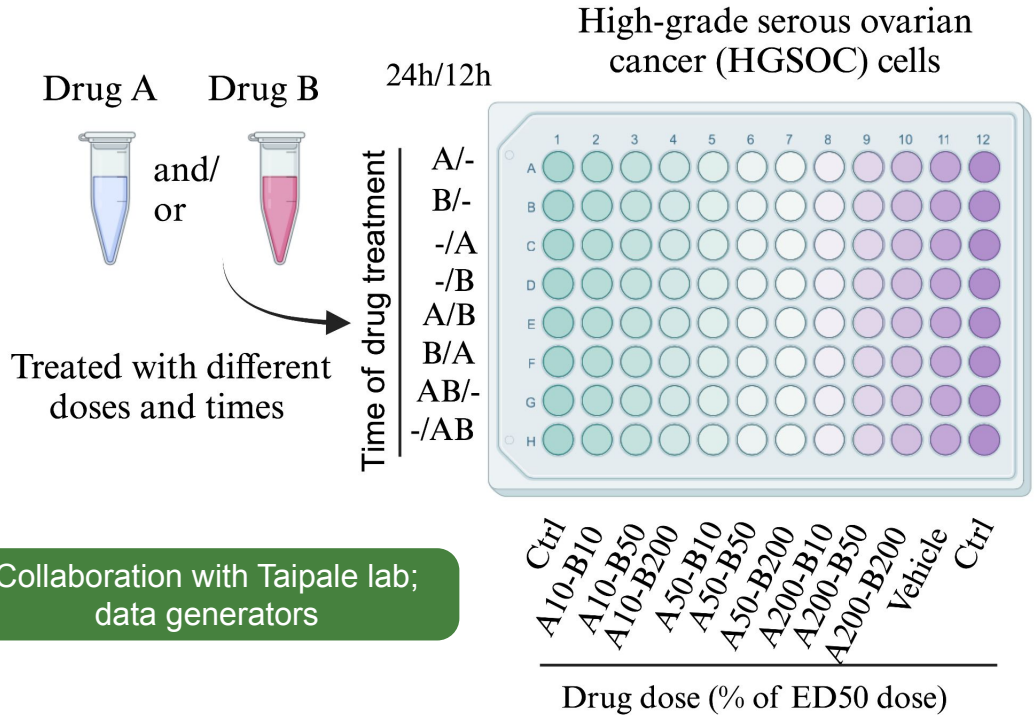
Genes

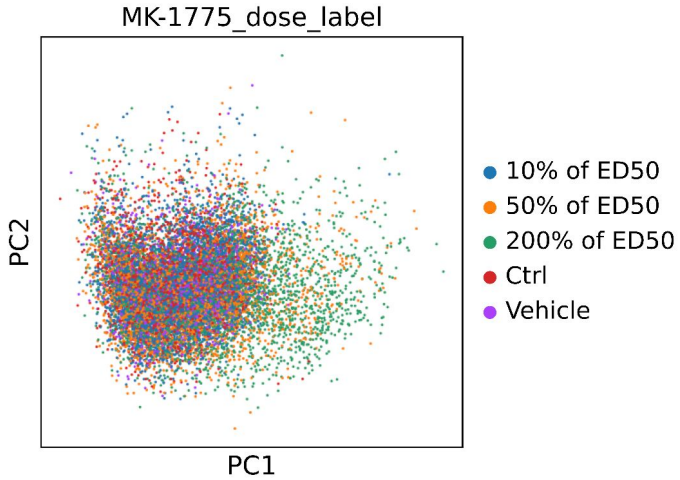
3)



Evaluation

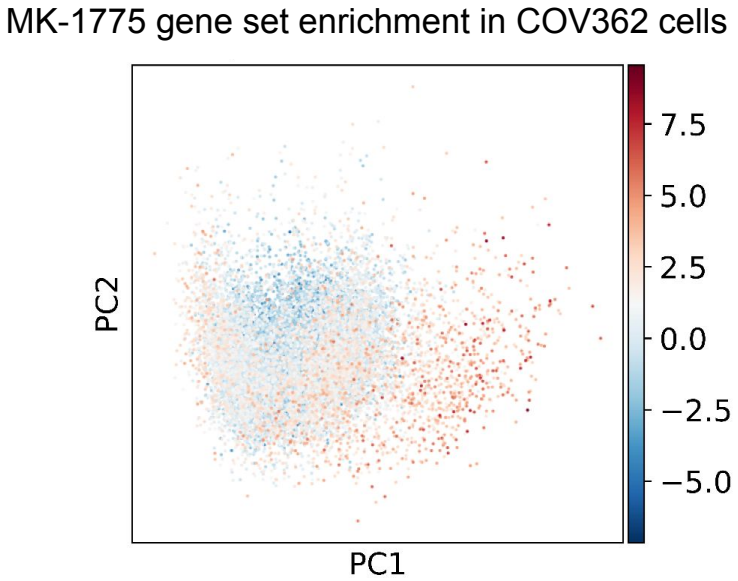
Signature matching at single cell resolution

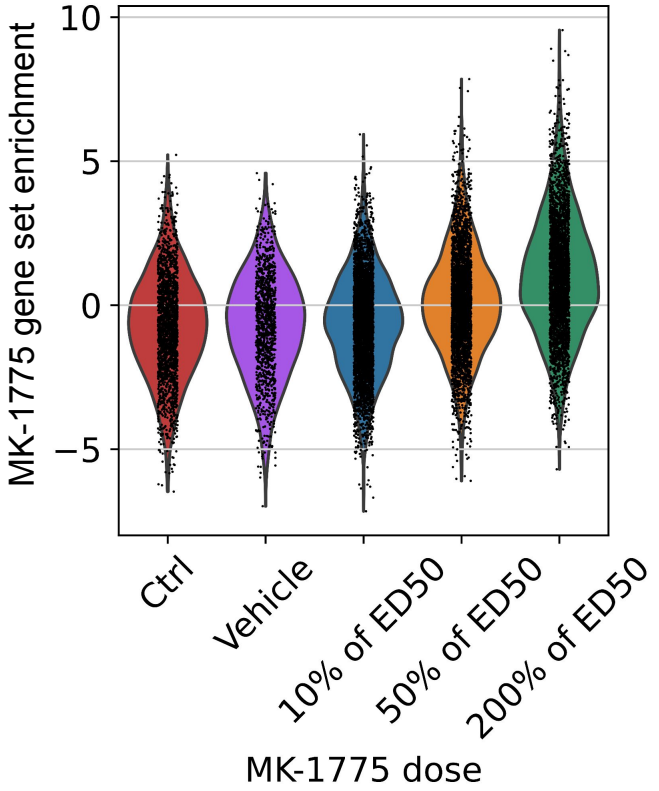




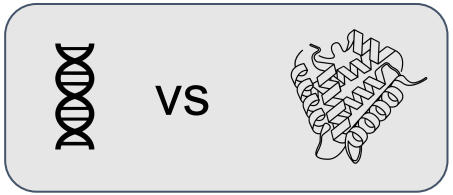
Collaboration with Taipale lab; data generators

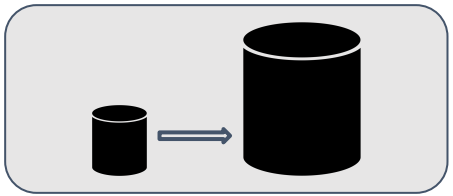
Drug gene set is associated with increasing drug dose

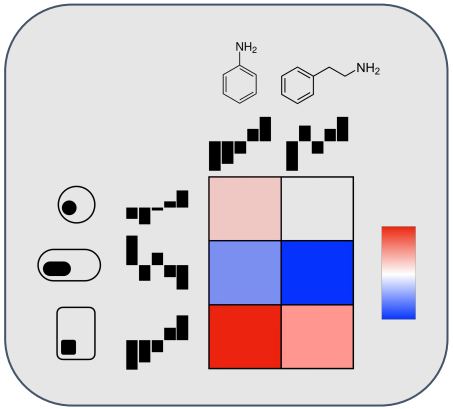




Summary

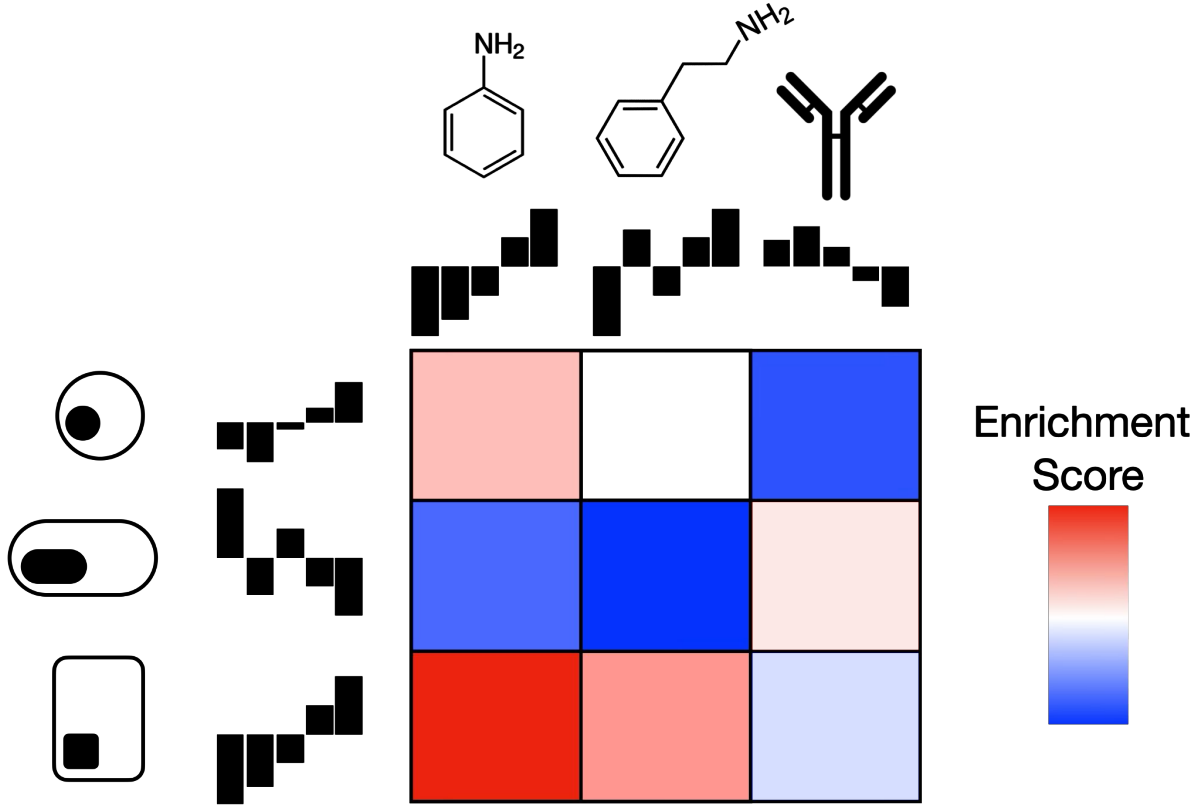






- Drug gene sets perform **better when gene-based** than when protein-based
- Currently **increasing coverage** of drug gene sets
- We are using **drug activity scoring** to study **drug response heterogeneity** at the single cell level

Using drug scoring for targeted therapy discovery



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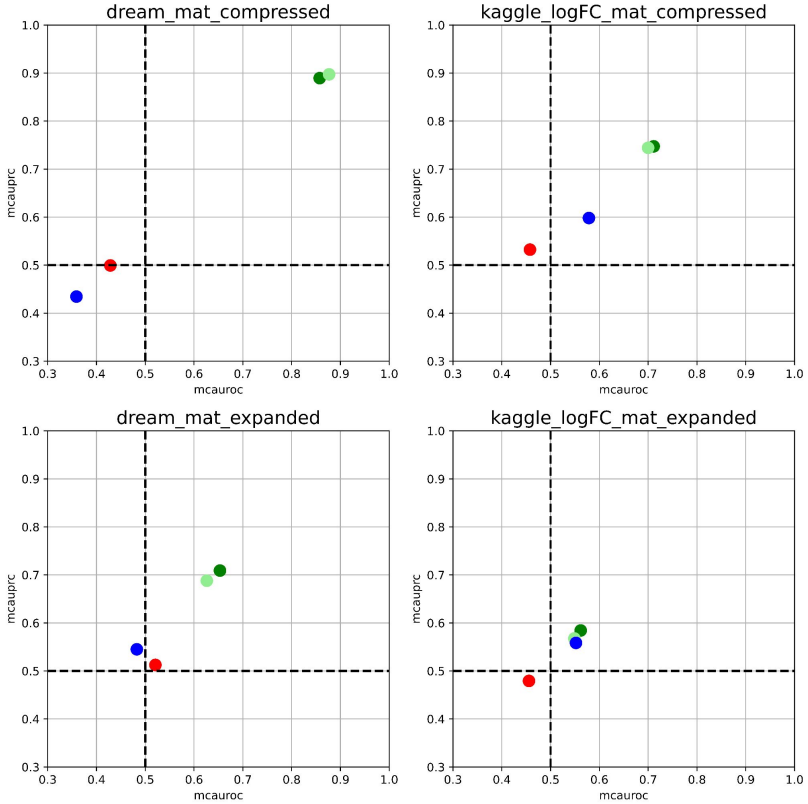
Extra slides



Drug Gene Set

- gene-based LINCS
- gene-based LINCS 1000 landmarks
- protein-based ChemicalChecker
- protein-based drug2cell