Supplementary figures

Applicability domain of active learning in chemical probe identification: convergence in learning from non-specific compounds and decision rule clarification

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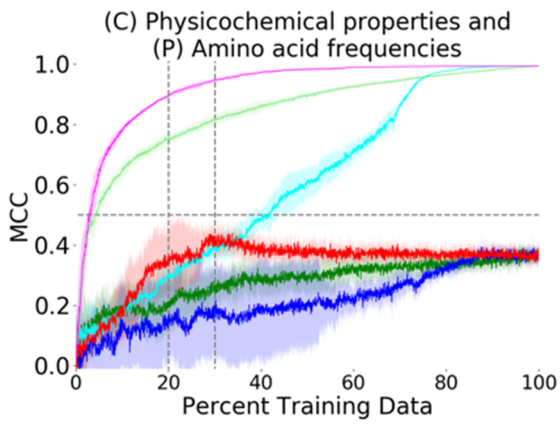
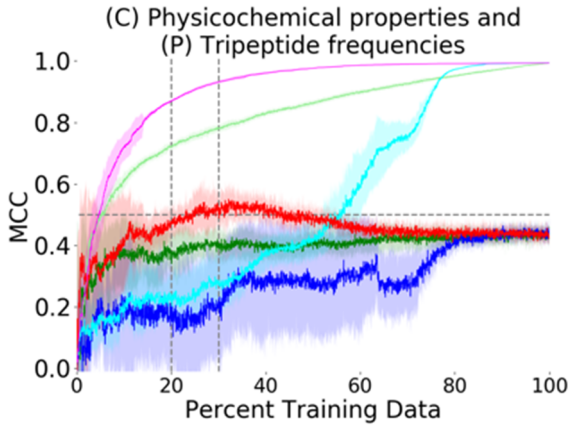
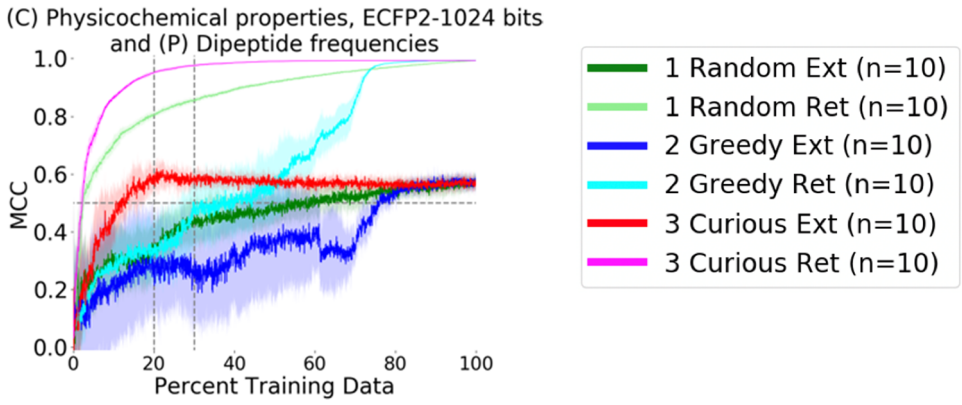
Figure S1a. (a,b) Experiments with physicochemical properties and either amino acid or tripeptide frequency protein descriptors. (c) Experiments with combination physicochemical and ECFP descriptors, using dipeptide frequency.



(a)

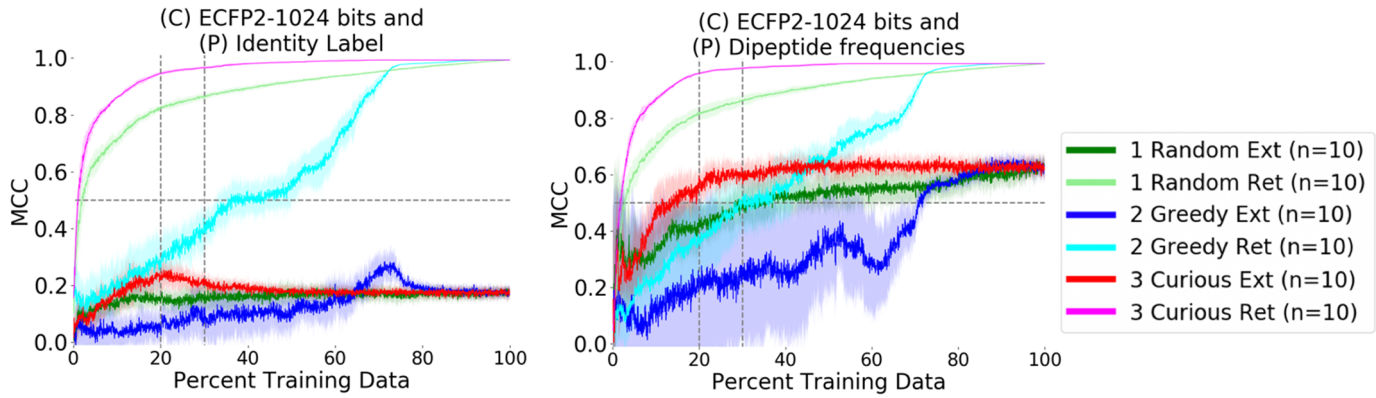


(b)



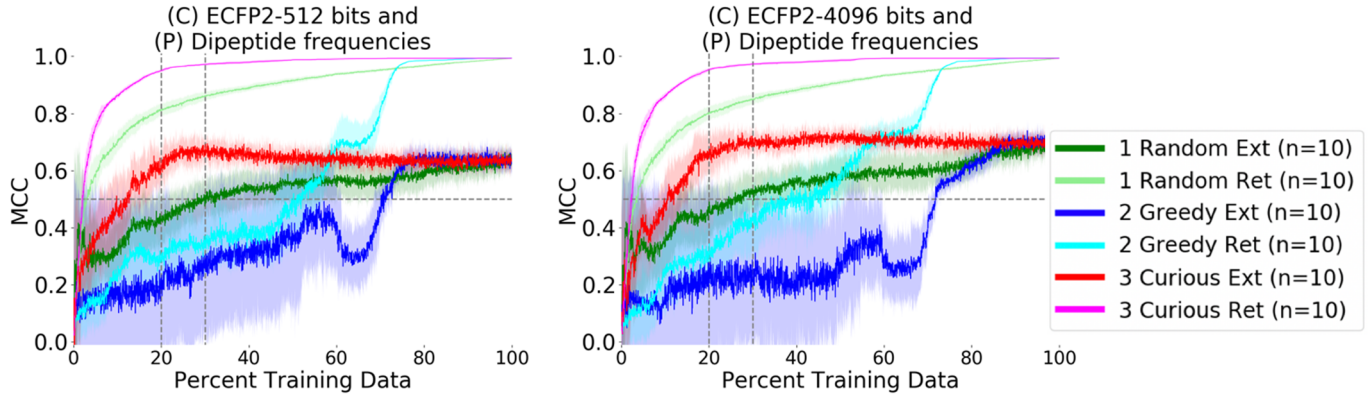
(c)

Figure S1b. Dipeptide frequency **(b)** with ECFPr2-1024 results in higher performance compared to the identity protein descriptor **(a)**.



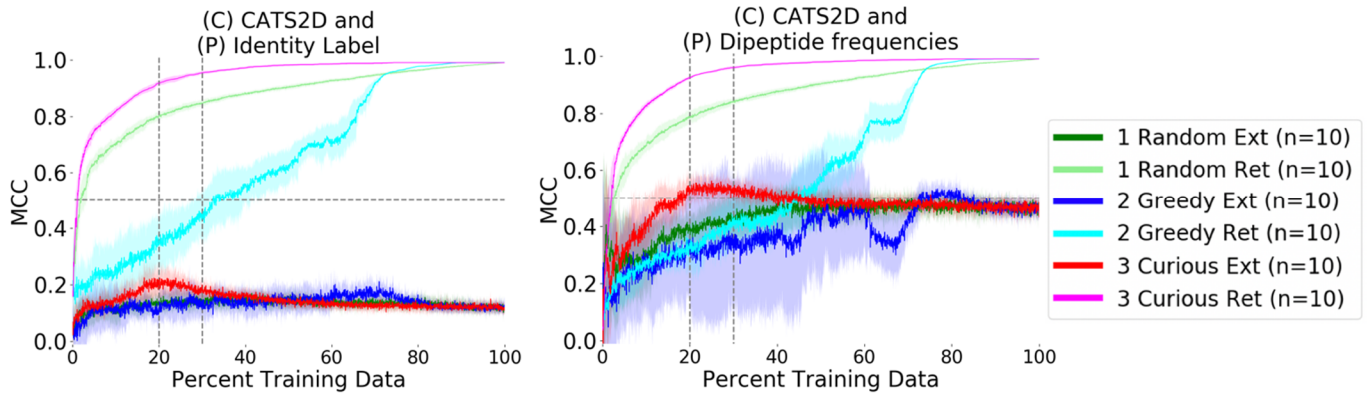
(a) **(b)**

Figure S1c. ECFPr2-4096 bits **(b)** in combination with dipeptide frequency results in equal or slightly better performance compared to the ECFPr2-512 bit fingerprints **(a)**, and a notable improvement over ECFPr2-1024 bit fingerprints.



(a) **(b)**

Figure S1d. CATS2D descriptors with dipeptide frequency **(b)** display better performance compared to identity protein descriptors **(a)** and physicochemical-based descriptors.



(a) **(b)**

Figure S1e. CATS2D descriptors with tripeptide frequency and tetrapeptide frequency display better performance on the external set compared to dipeptide frequency, amino acid frequency and identity protein descriptors.

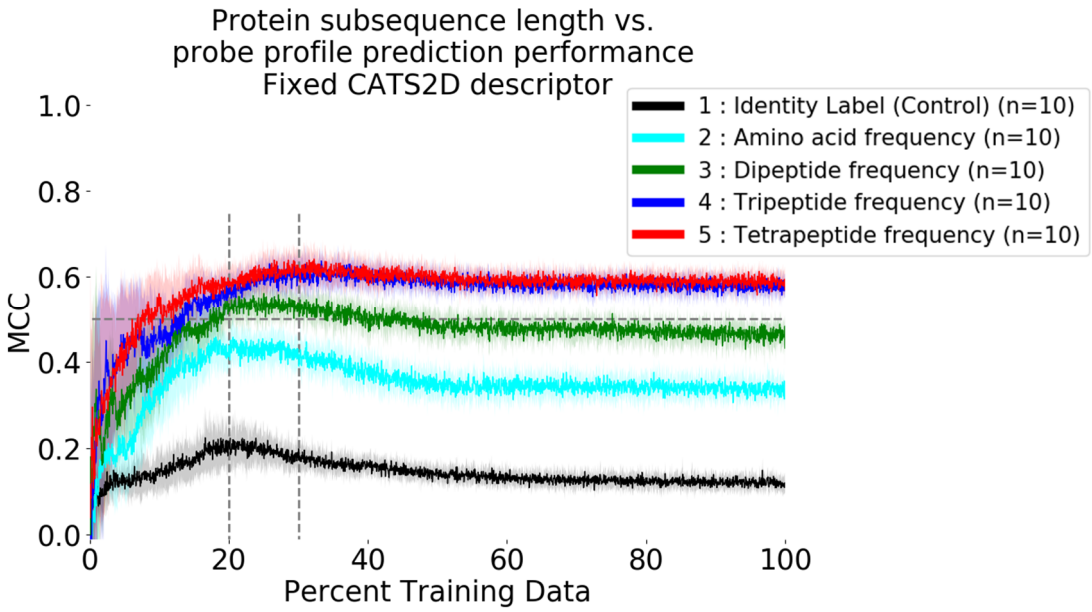


Figure S2. (a) Active projection for pChem-dipeptide description of ligand-target interactions; **(b)** pChem-tripeptide frequency descriptor-based model evolution.

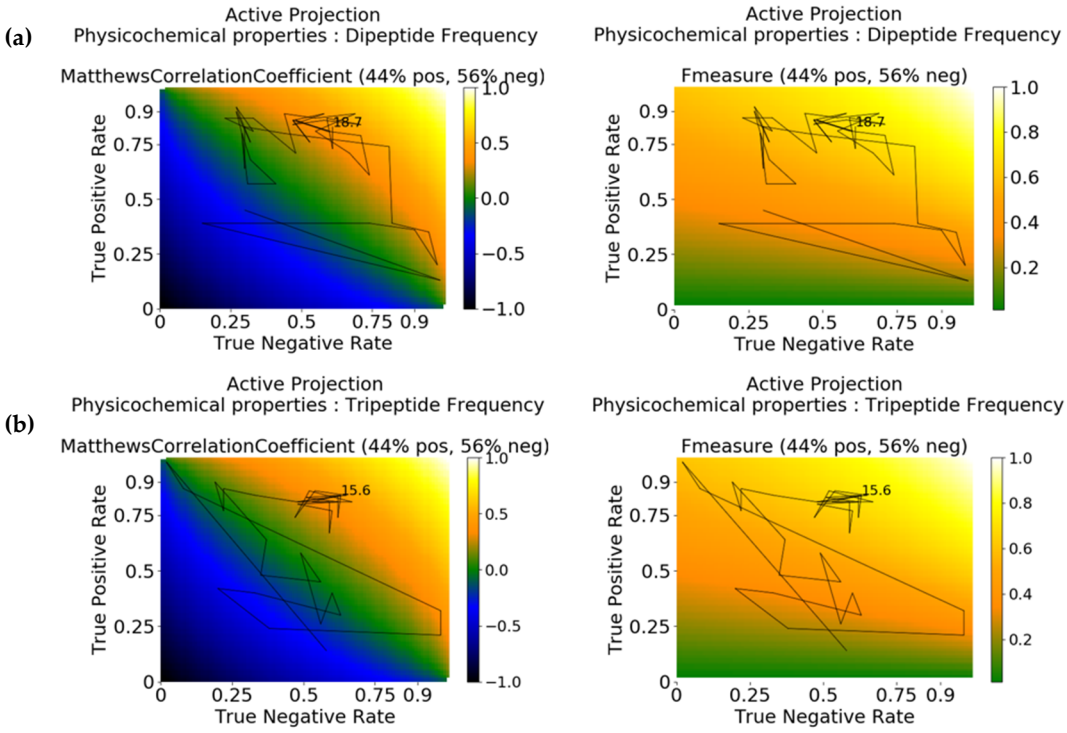


Figure S3a. Feature weight time series shows the evolving relative weights of each CATS2D-dipeptide descriptor used during model construction. Compound descriptors are the highest weighted features, whereas protein dipeptide frequencies are less weighted yet still non-trivial.

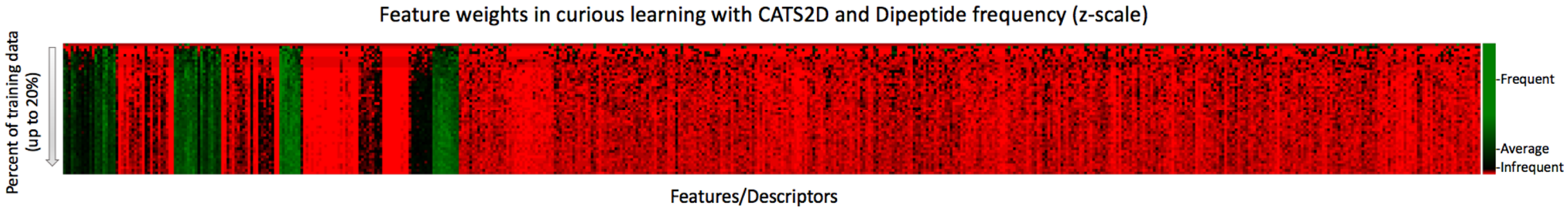
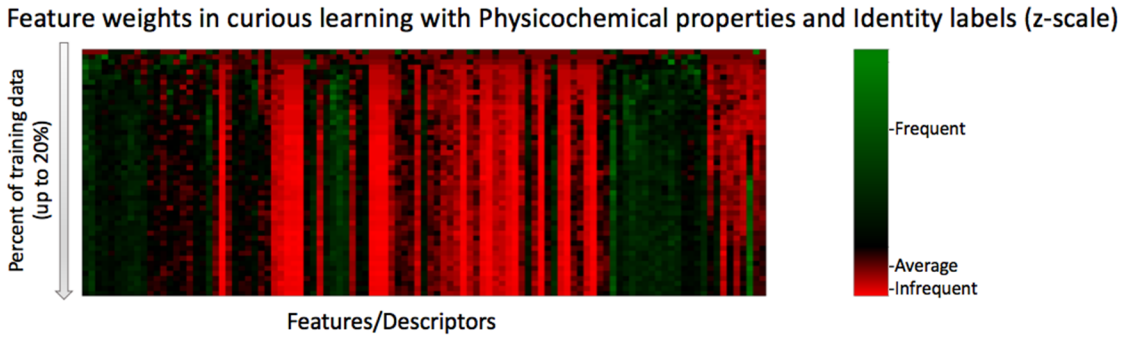


Figure S3b. Feature weight analysis of pChem-identity **(a)** and pChem-dipeptide experiments **(b)**.

(a)



(b)

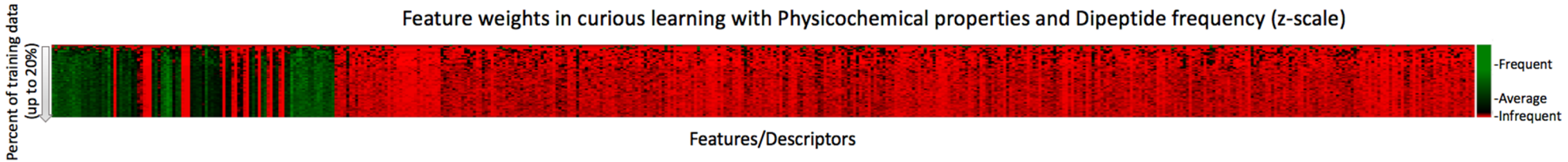


Figure S4a. A diagram showing how the protein tripeptide descriptors unique to a protein appeared in a specific decision tree. Many tripeptide rules could be found in multiple trees.

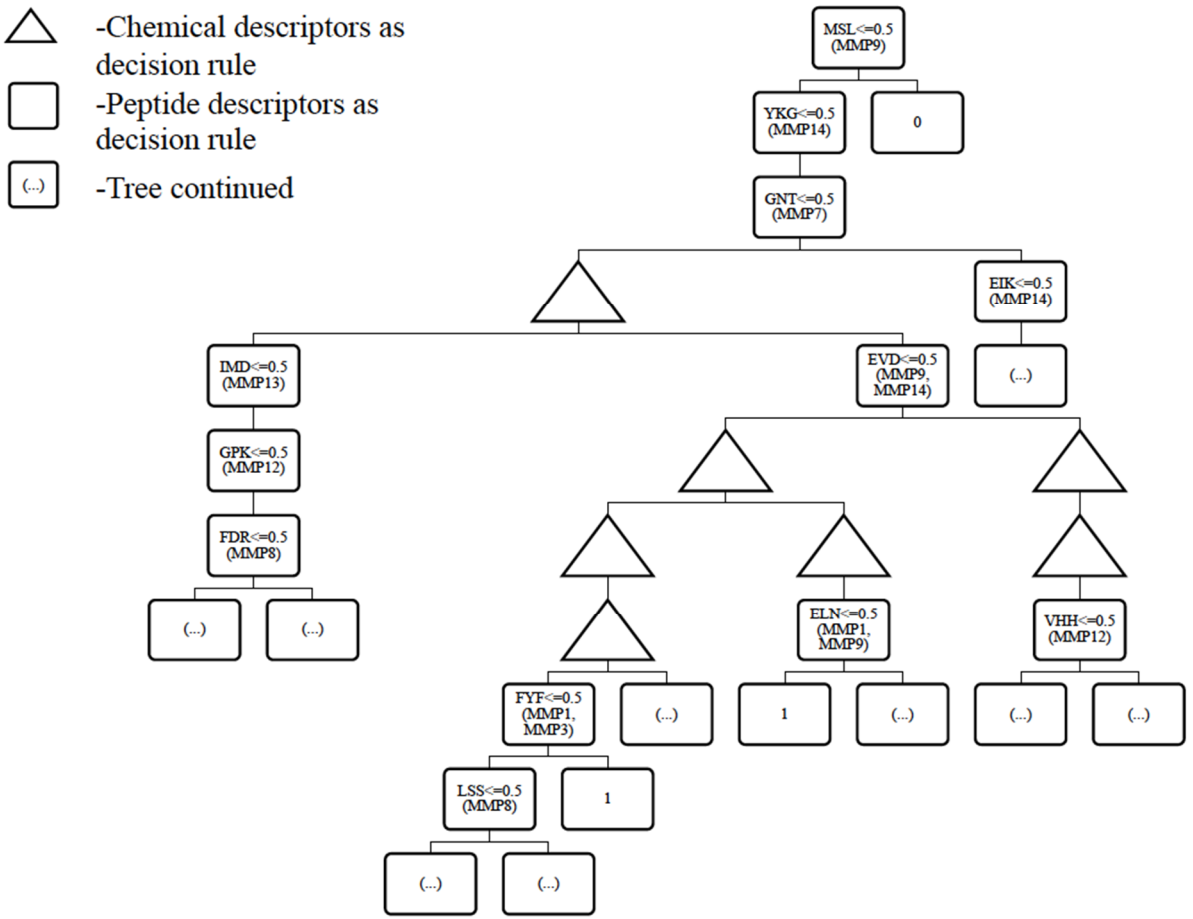


Figure S4b. A decision tree built on 20% of the training data with a predictive ability of MCC=0.50, F1=0.73 on the external probe dataset.