

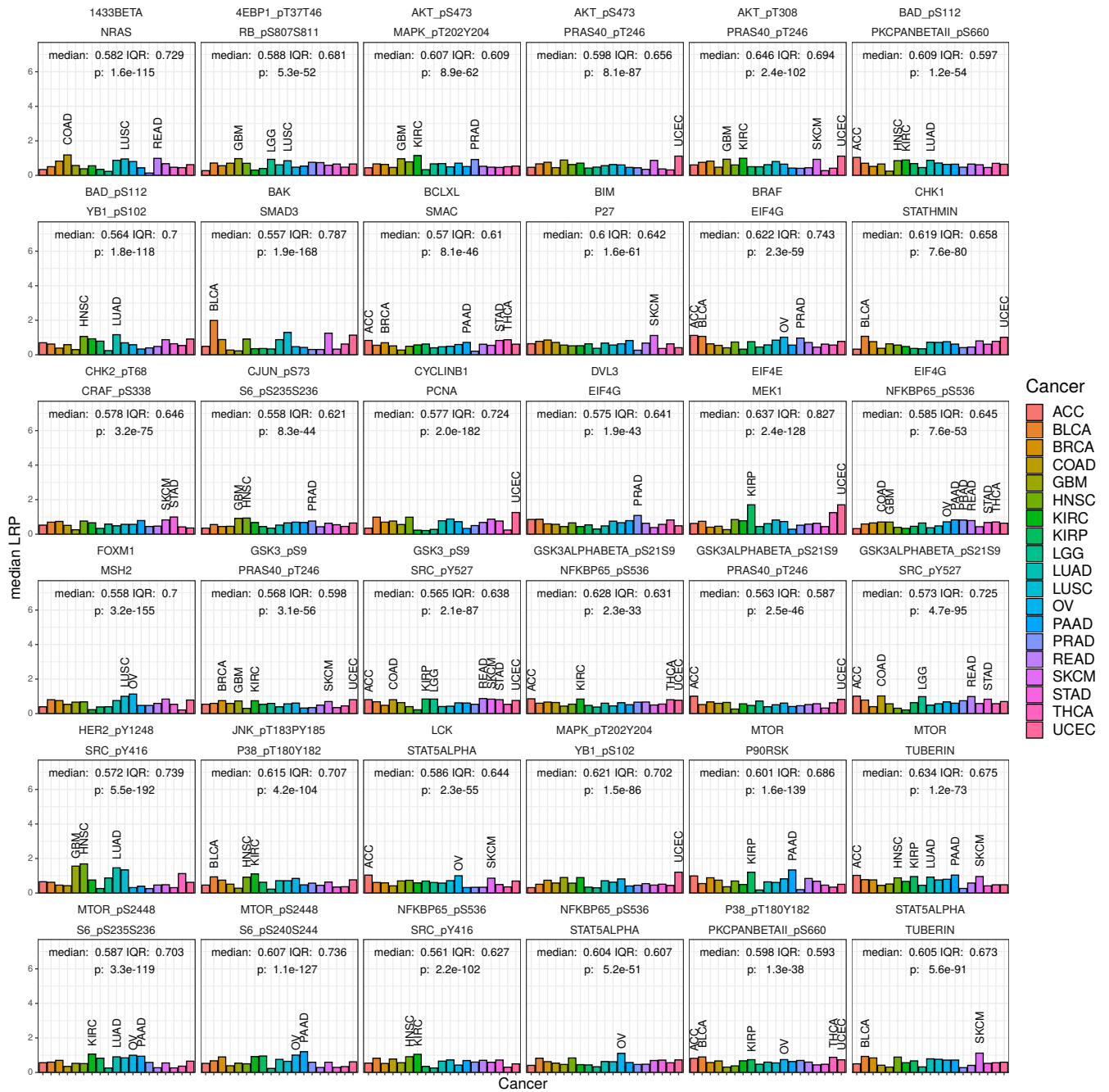
# Supplementary information for “Patient-level proteomic network prediction by explainable artificial intelligence”

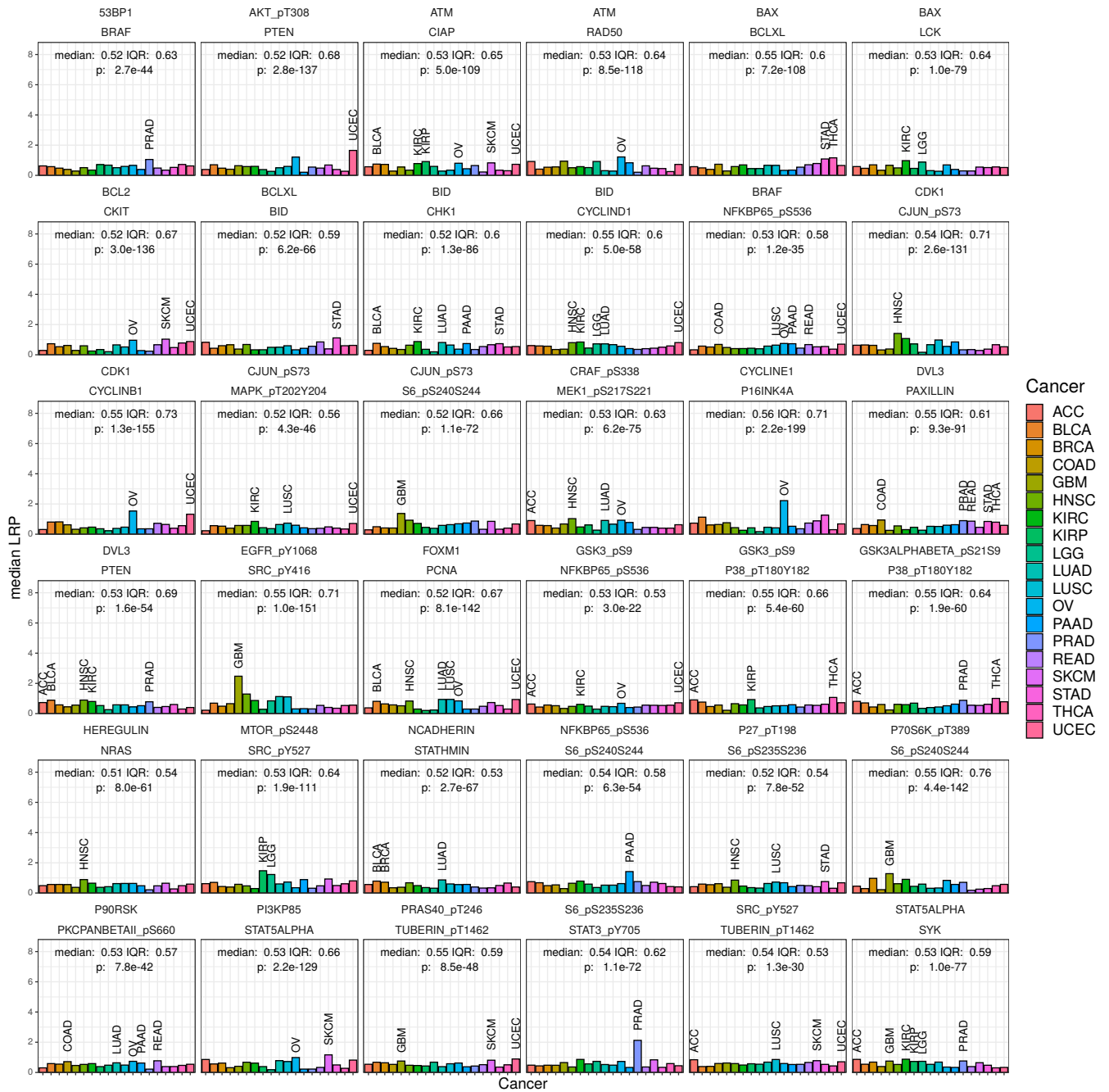
Philipp Keyl<sup>†</sup>, Michael Bockmayr<sup>†</sup>, Daniel Heim, Gabriel Dernbach,  
Grégoire Montavon\*, Klaus-Robert Müller\*, and Frederick Klauschen\*

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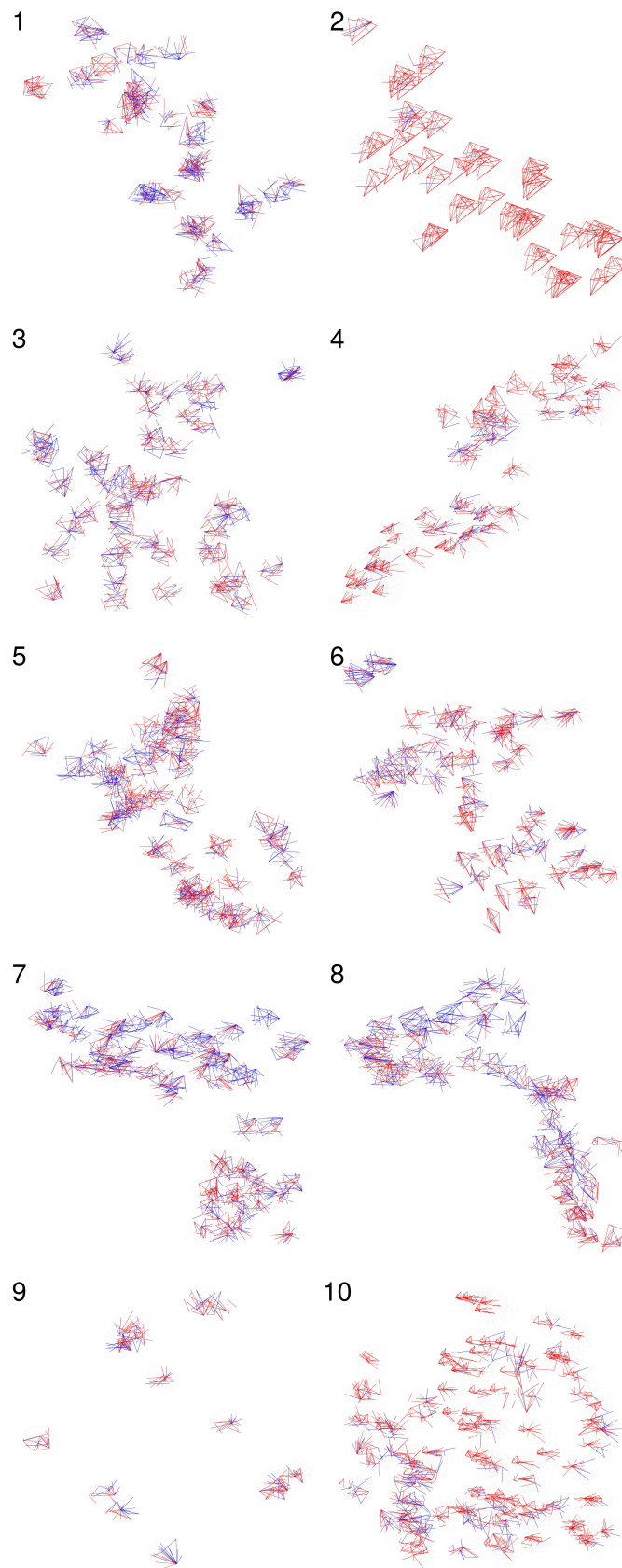
<sup>†</sup>These authors contributed equally to this work.

\*Corresponding authors. E-mail: G. M. [gregoire.montavon@tu-berlin.de](mailto:gregoire.montavon@tu-berlin.de), K-R.M. [klaus-robert.mueller@tu-berlin.de](mailto:klaus-robert.mueller@tu-berlin.de) and F. K. [f.klauschen@lmu.de](mailto:f.klauschen@lmu.de).

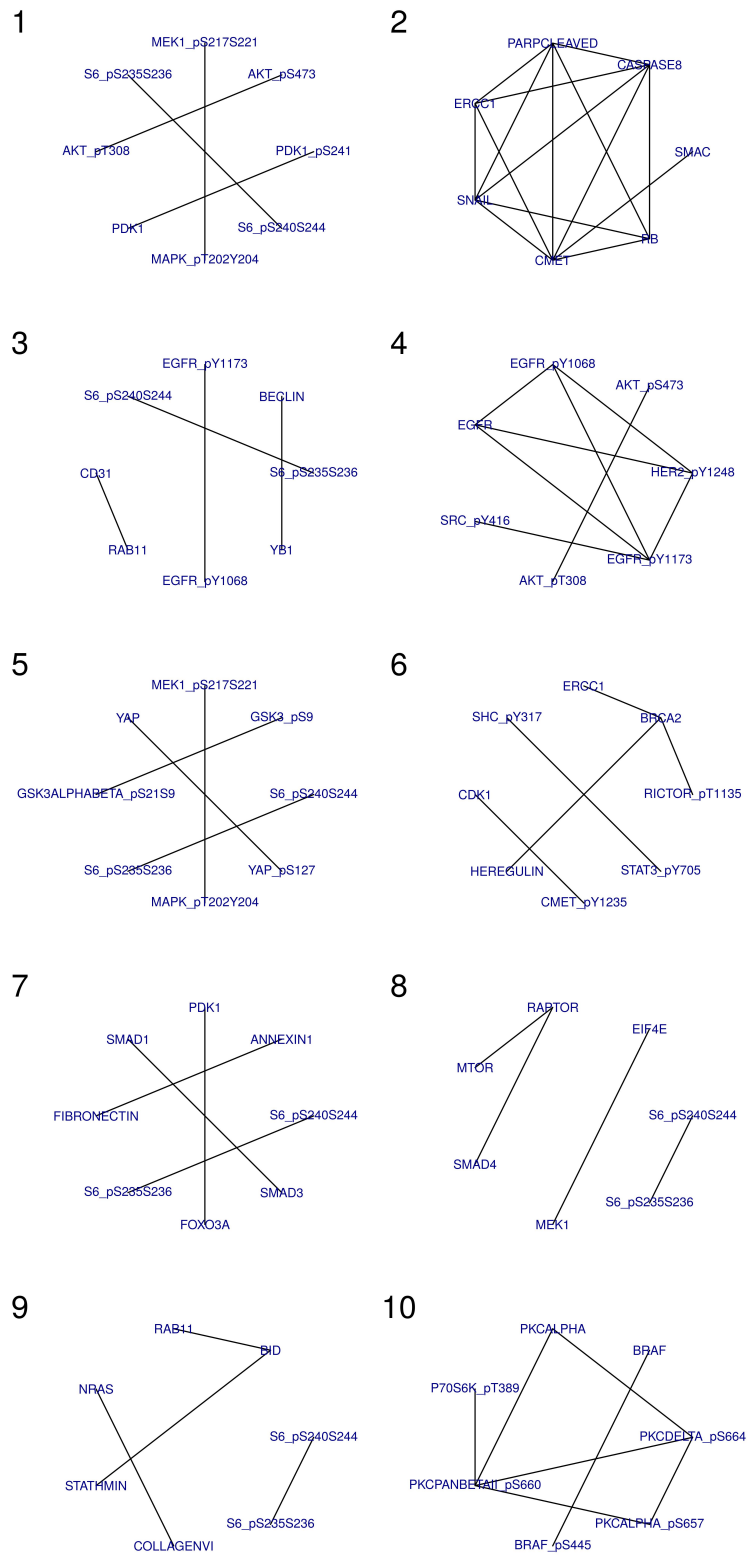




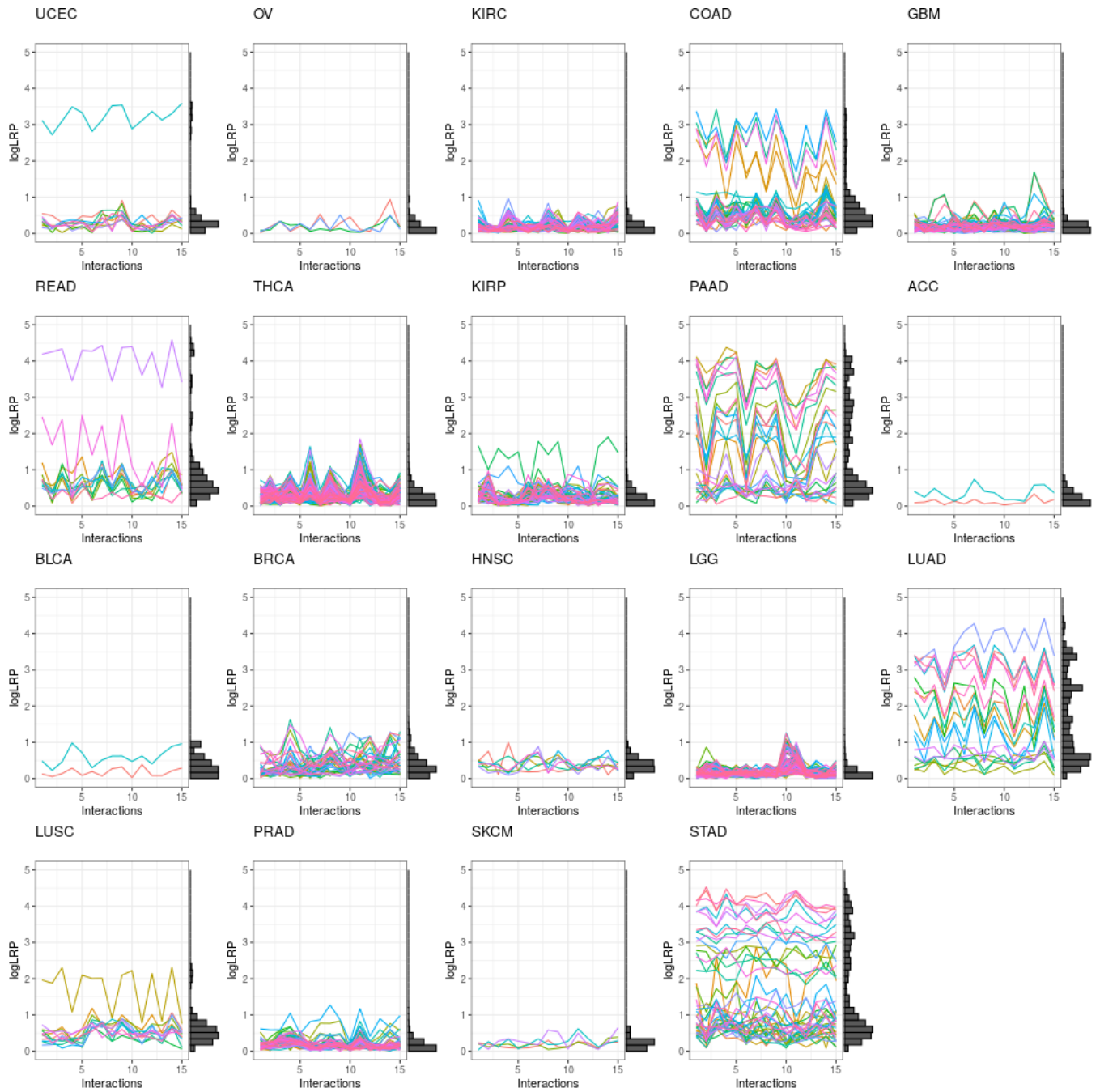
Supplementary Figure 2: Strongest inferred interactions for the TCPA data set: 73-108. Supplementary data for Figure 1 of the main manuscript.



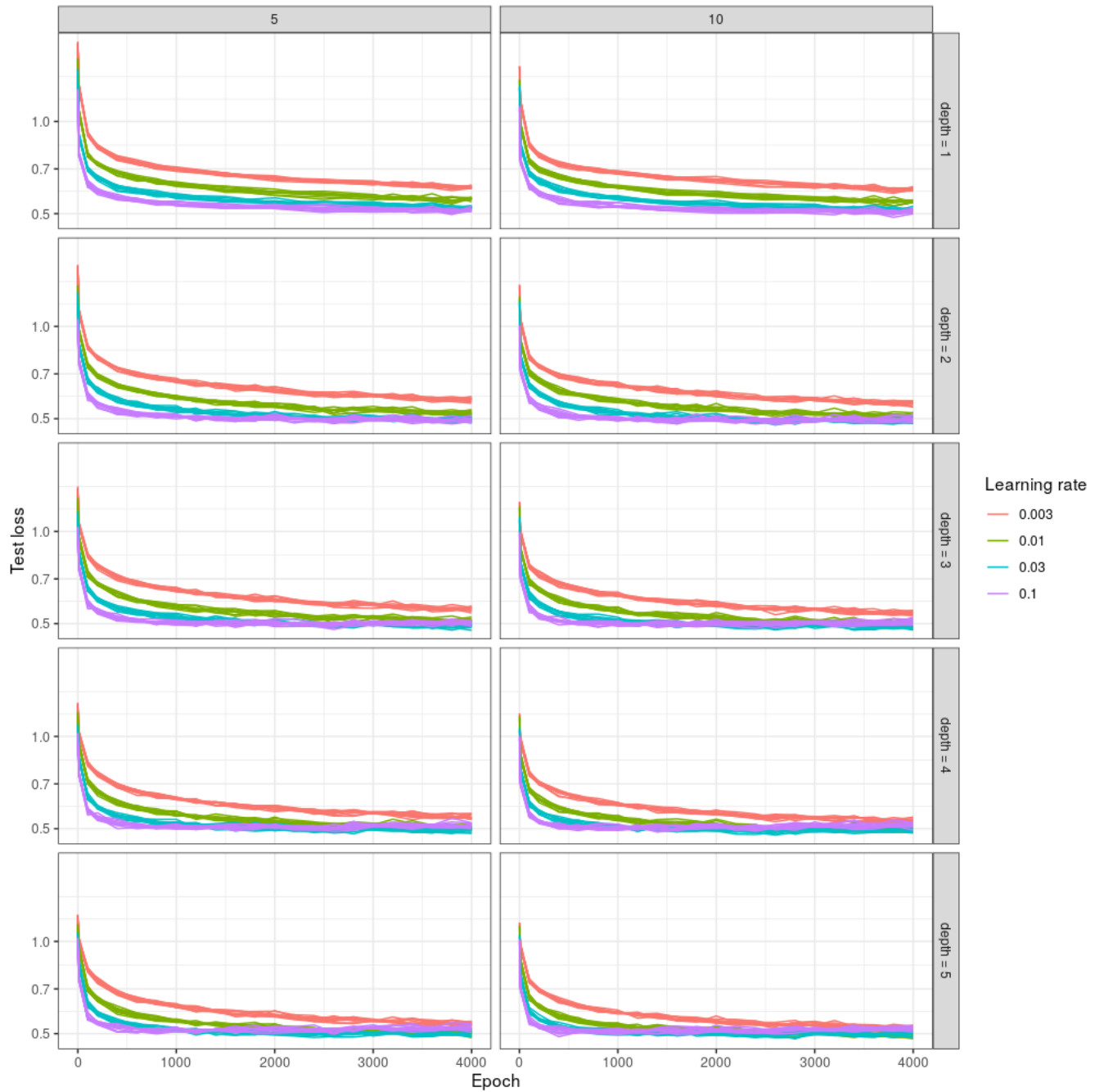
Supplementary Figure 3: Protein interaction networks for individual patients. Supplementary data for Figure 2A of the main manuscript.



Supplementary Figure 4: Averaged interaction networks for clusters of Figure S3. Supplementary data for Figure 2B of the main manuscript.



Supplementary Figure 5: Analysis of the 15 different interactions (x-axis) existing between the proteins c-MET, Snail, Caspase-8, ERCC-1, PARPcleaved and RB for the data subset used in Figure 2. The vertical axis displays the logarithm of the  $LRP_{au}$  score.  $LRP_{au}$  scores that belong to one patient are connected by a colored line. Each subplot relates to one cancer type. The distribution of  $LRP_{au}$  scores is displayed on the right side of each subplot. While in some cancers,  $LRP_{au}$  scores are overall low between these proteins, for the cancers UCEC, PAAD, LUAD, LUSC, COAD, STAD and READ interactions between these proteins show a bimodal pattern. In many cases, all  $LRP_{au}$  scores are either high or low, which could suggest that these proteins are regulated by a common mechanism.



Supplementary Figure 6: Crossvalidation for model selection. We tested different choices for ‘hidden layers’ (rows: 1-5), ‘number of neurons per layer’ (columns: [5,10] x number of proteins), ‘learning rate’ ([0.003, 0.01, 0.03, 0.1]) and ‘number of epochs’ (up to 4000). Every combination of hyperparameters was tested 10 times.