Figure 5. A PLS Model Accurately Predicts Phenotypic Responses from Time-Resolved Molecular Signals

(A) Principal components analysis of covariation between signals. Scores plot represents an aggregate measure of the signaling response for each cell type under each treatment condition at a specified time, as indicated by the colors and symbols in the legend.

(B and C) Scores and loadings for a PLS model. (B) Scores calculated and plotted as in (A), except the principal components now reflect covariation between signals and responses. (C) PLS loadings plotted for specific signals and responses projected into principal component space.

(D–I) BT-20 cell line-specific model calibration. (D) R^2, Q^2, and RMSE for BT-20 models built with increasing numbers of principal components. (E and F) Scores and loadings plots, respectively, for a two-component model of BT-20 cells. (G–I) Apoptosis as measured by flow cytometry or as predicted by our model using jack-knife cross-validation. R^2 reports model fit, and Q^2 reports model prediction accuracy. (G) Final refined model of apoptosis in BT-20. (H) BT-20 model minus targets identified as DEGs in microarray analysis. (I) Model using only the top four signals: c-caspase-8, c-caspase-6, p-DAPK1, and pH2AX.