

## SUPPLEMENTARY MATERIALS

### 1. Rad-Score

To simplify the logistic regression model for interpretability, we defined the Rad-score as a substitute for the 13 principal components. The Rad-score is computed based on a weighted sum of selected principal components derived from the logistic regression model. First, the features are standardized to ensure consistency across scales. Then, a logistic regression model is trained on the standardized features using grid search to identify the optimal regularization parameter. The model assigns each feature a coefficient, reflecting its contribution to the prediction. The Rad-score is calculated as the sum of each feature multiplied by its respective coefficient, representing an aggregated predictive score for the model. In our model, its calculation formula is:

$$\text{Rad-score} = 1.491*PC1 + -0.300*PC2 + -0.466*PC3 + -0.329*PC4 + 0.203*PC5 + -0.077*PC6 + 0.065*PC7 + 0.123*PC8 + 0.178*PC9 + -0.044*PC10 + -0.208*PC11 + 0.157*PC12 + -0.198*PC13$$

### 2. Feature Selection

#### 1) Least Absolute Shrinkage and Selection Operator

Least absolute shrinkage and selection operator (LASSO) was

first applied to select the most relevant features from the dataset. Using cross-validation ( $cv=5$ ), the optimal hyperparameter ( $\alpha$ ) for LASSO was determined, minimizing the mean squared error. Supplementary Fig. 1 demonstrates that the model's mean squared error is minimized at  $\alpha=0.0473$ , with the selected features listed in Supplementary Table 3.

#### 2) Principal Component Analysis

Principal component analysis (PCA) was used for further feature dimensionality reduction. PCA is a method that converts a set of possibly correlated features into a smaller set of linearly uncorrelated components, known as principal components. By setting ' $n\_components=0.95$ ', the number of principal components was chosen such that they capture 95% of the cumulative variance. A total of 13 principal components (PC1–PC13) were retained for calculating the Rad-score (Supplementary Fig. 2). Supplementary Fig. 3 visualizes how the first 3 principal components capture key variance in the data to differentiate between classes. Supplementary Fig. 4 is a heatmap of the correlation coefficient matrix for PC1–PC13, demonstrating the very low correlations between the principal components.