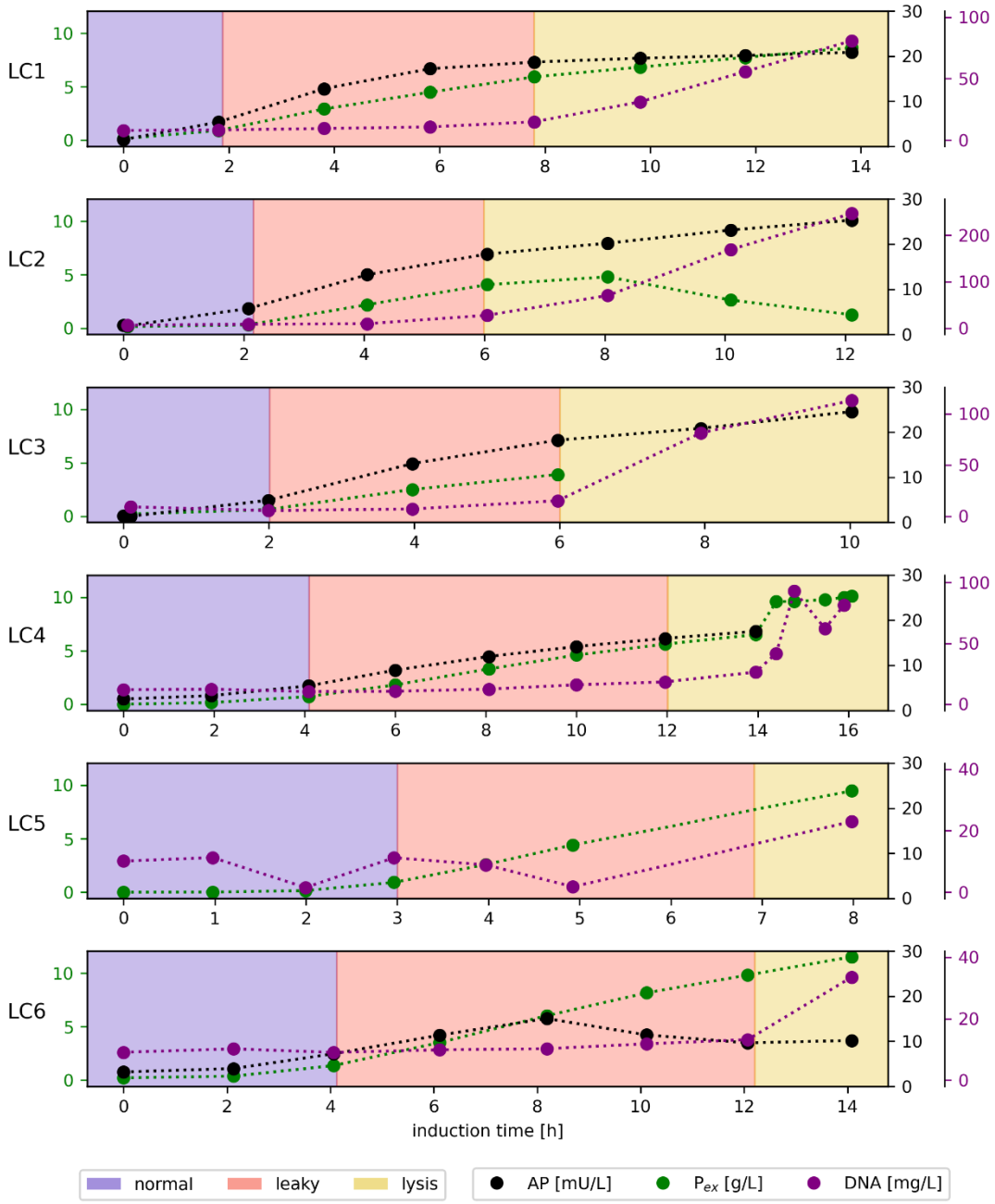

Figure S1. Reference data from the induction phase of the six bioprocesses. Cells were considered leaky when the concentration of extracellular SpA exceeded 0.5 g/L and lysis was assumed to take place when extracellular DNA exceeded 15 mg/L. Due to a gap in reference data in run LC5, the onset of lysis was estimated by linearly interpolating the DNA concentration. Due to the scale of the graphs, the standard deviation of replicate measurements is too small to be displayed.

Table S1. Number of samples and class frequency in each run. Only post-induction samples are shown since they were used for classification models.

run	total	normal	leaky	lysis
LC1	170	26	71	73
LC2	140	25	46	69
LC3	123	26	48	49
LC4	194	49	95	50
LC5	96	35	47	14
LC6	170	49	97	24

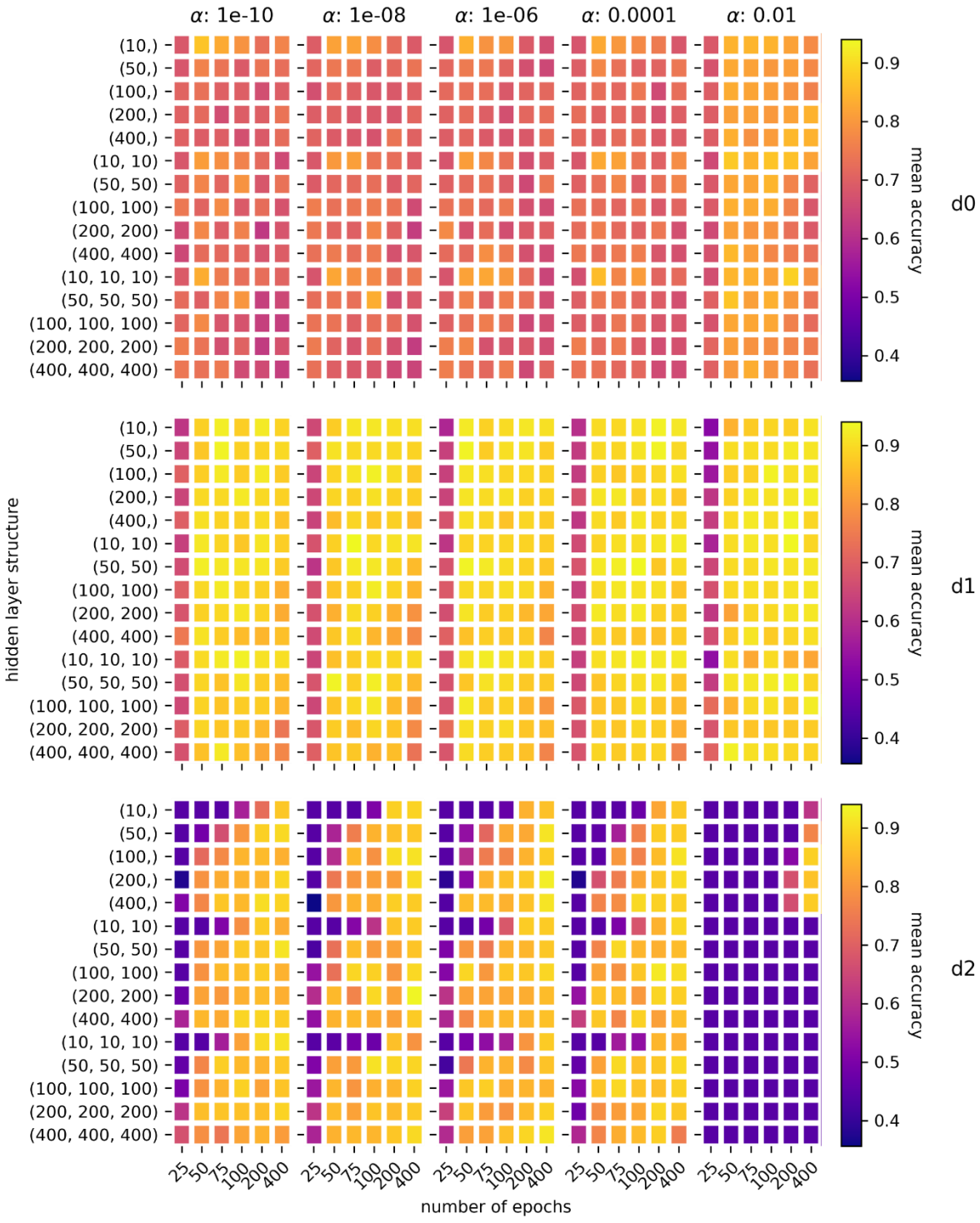

Figure S2. Hyperparameter grid search for ANN models. The searched hidden layer structures are displayed in parentheses on the left. For example, (50, 50) denotes two hidden layers with 50 nodes each. The weight penalization parameter is denoted by α. Rows show zero-oder (d0), first-order (d1) or second-order (d2) derivative.

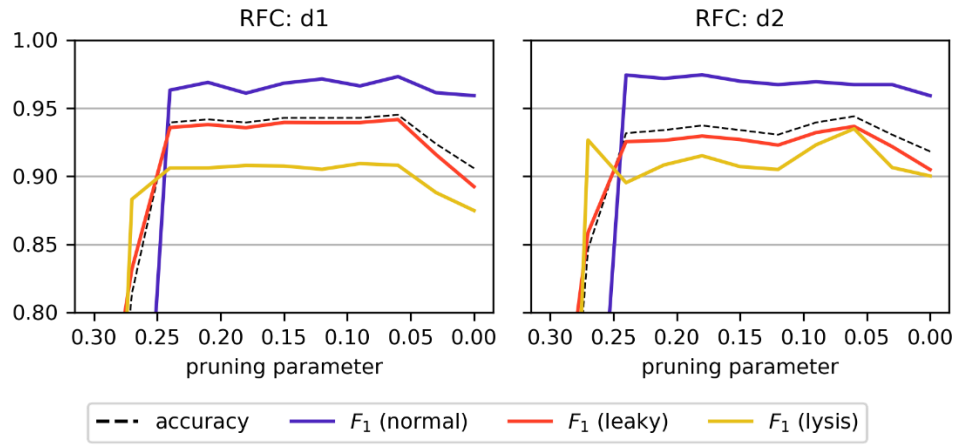

Figure S3. Magnification of Figure 6 in the main text. The figure shows the classification performance of RFC models evaluated with the first and second derivatives (d1 and d2) of baseline-corrected post-induction spectra. The x-axes are oriented such that the least complex model is on the left side and the most complex on the right side. The evaluation metrics were averaged over the six data splits (one for each run), weighted by the number of samples in each run (accuracy) or the frequency of classes in each run (F_1 score).

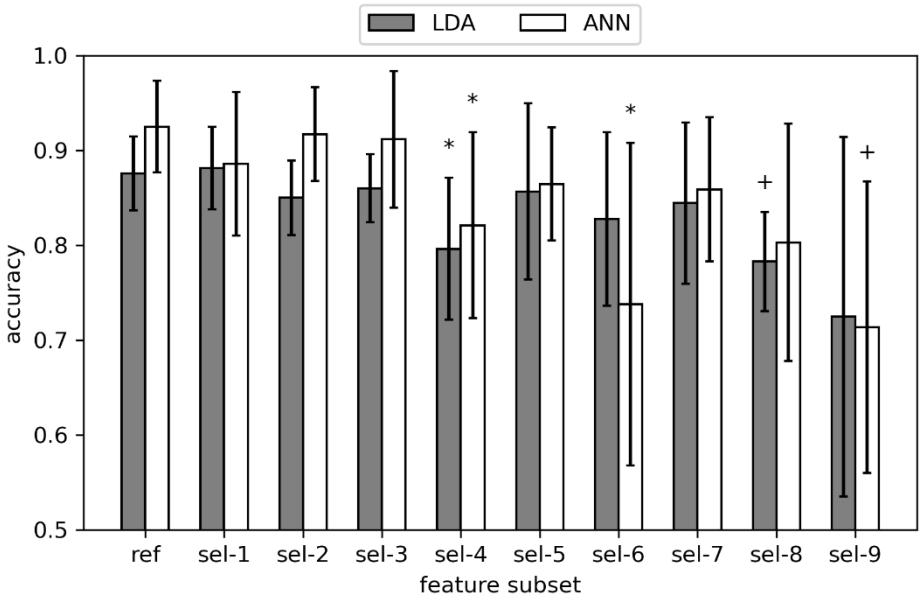

Figure S4. Classification accuracy of LDA and ANN after feature selection. Accuracy was averaged over the six different data splits (one for each run), weighted by number of samples in each run. Feature selection strategies are listed in Table 1 in the main text. Significant difference in average accuracy to the reference (ref) is denoted by * ($p < 0.05$) or + ($p < 0.01$).