



**Figure S4: Selection frequency of signature genes**

The figure depicts a histogram showing the number of genes selected twice or more times as informative genes for compound class prediction. For the generation of this figure, we considered 8 predicted signatures for solving 4 binary classification tasks (C vs. NC, GC vs. NGC, GC vs. NC, NGC vs. NC) after 3 days and 14 days of repeated dosing, respectively. The genes selected 4 and 5 times, respectively, are listed next to the histogram.