Supplementary Information (SI) for Digital Discovery.
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Supporting Information: Schedule Optimization for Chemical Library Synthesis

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S1 Supporting figures

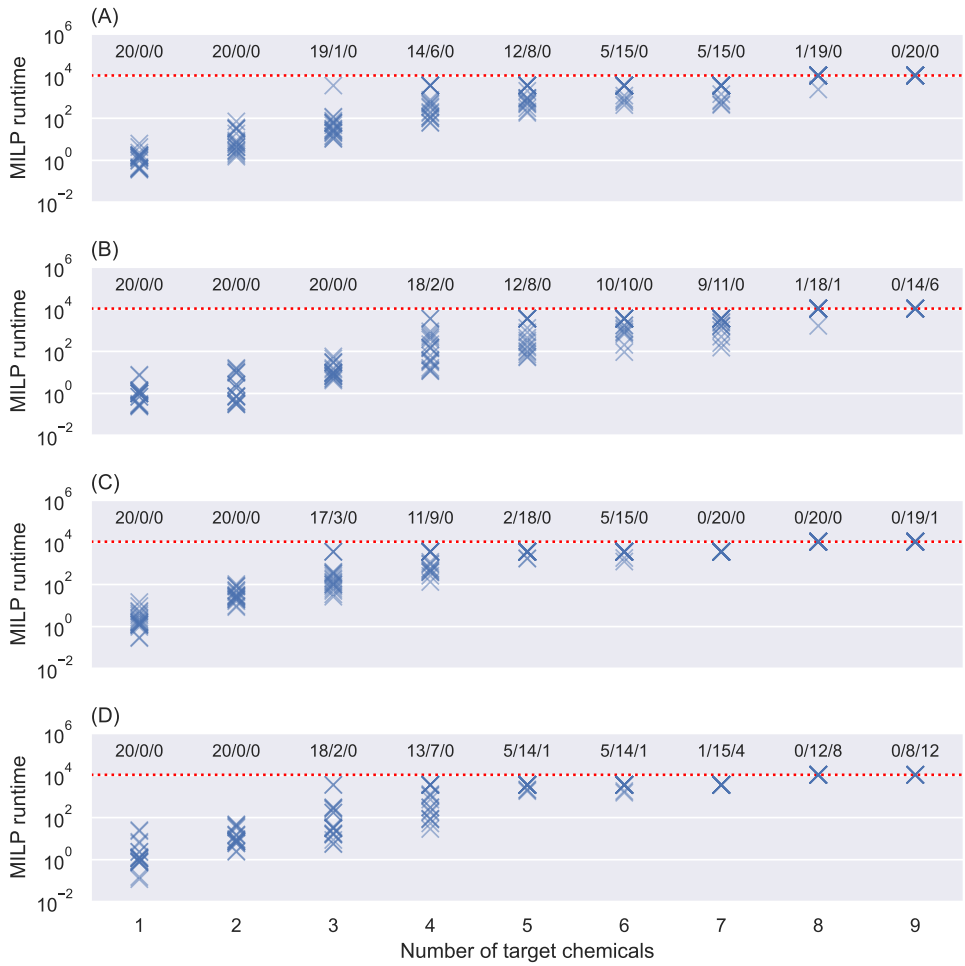

Figure S1: Runtime distributions for finding optimal schedules. Red dashed lines indicate the solver time limit of three hours. Each column (strip plot) represents the results of a library group scheduled on LAB-1 and LAB-2, totaling 20 scheduling instances. (A) FDA libraries scheduled without work shift constraints; (B) FDA libraries scheduled with work shift constraints; (C) VS libraries scheduled without work shift constraints; (D) VS libraries scheduled with work shift constraints. The columns are annotated with triples of the format "x/y/z", where "x", "y", and "z" represent the number of "Optimal", "Suboptimal", and "No solution" instances, respectively, as defined in Figure 3 caption.

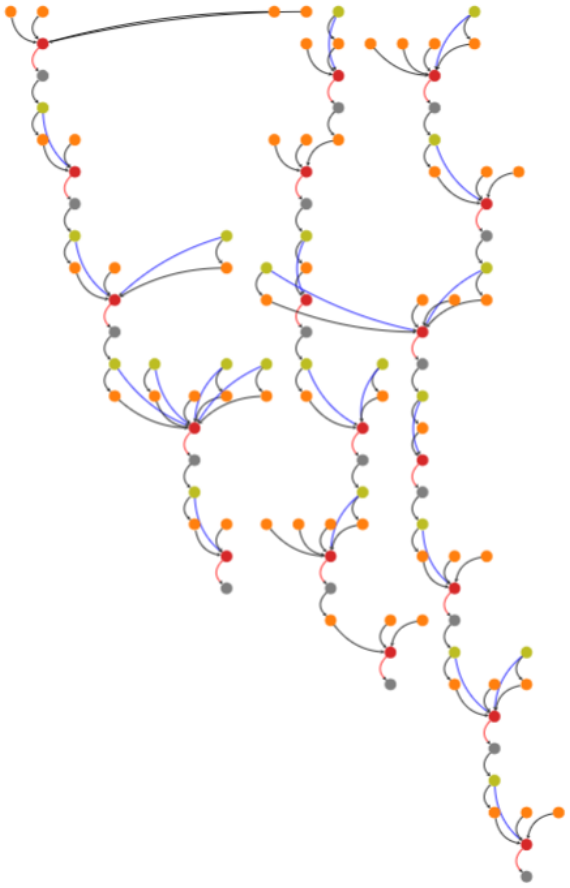

Figure S2: Operation network constructed for FDA.03.09. The orange, red, gray, and yellow markers represent `LiquidTransfer`, `Heating`, `ConcentrationAndPurification`, and `Makesolution` operations, respectively. The blue (red) edges indicate minimum (maximum) lag time constraints. This is a screenshot taken from the visualization interface.

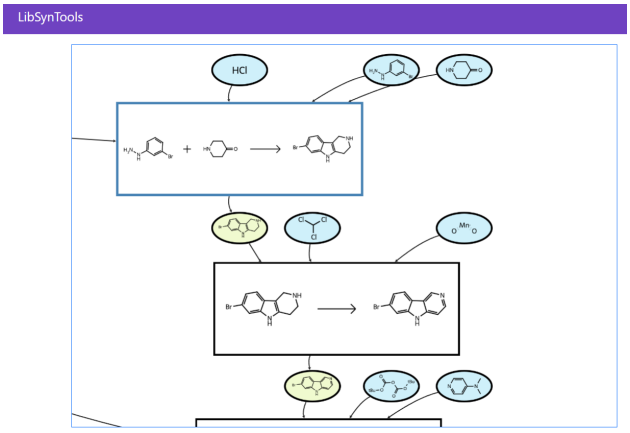

Figure S3: Part of the reaction network for FDA.03.09 from a screenshot taken from the visualization interface. Molecules with blue and green backgrounds represent starting (include solvents and reagents) and intermediate molecules, respectively.

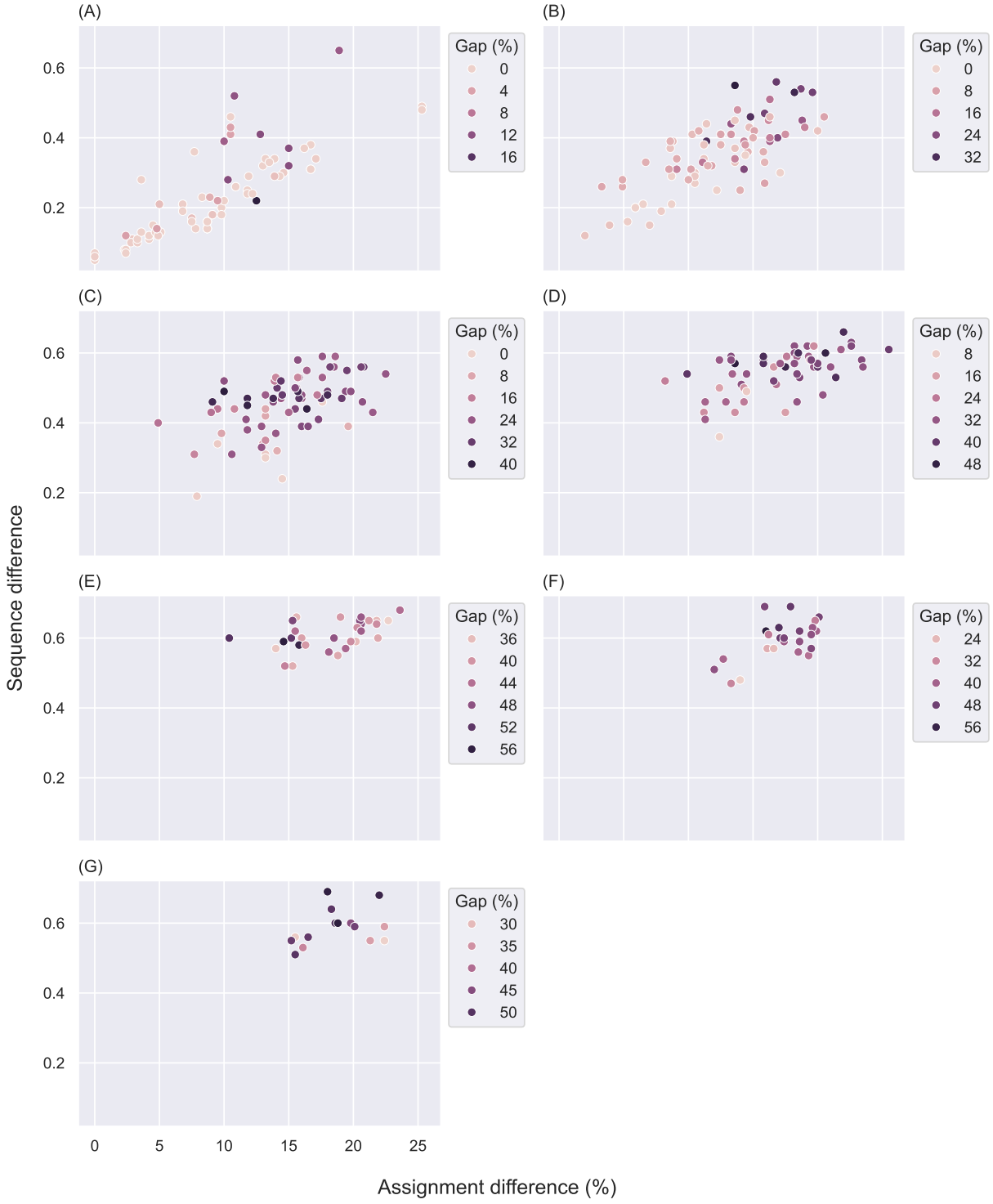

Figure S4: Schedule difference between optimal and baseline schedules. Scheduling instances are grouped by the number of target chemicals in (A) - (G) for number of target chemicals from 1 to 7.