Electronic Supplementary Information

Rxn Rover: Automation of Chemical Reactions with User-Friendly, Modular Software

Zachery Crandall,[ab] Kevin Basemann,[ab] Long Qi,*[a] and Theresa L. Windus*[ab]

[1] U.S. DOE Ames Laboratory, Iowa State University, Ames, Iowa 50011, United States
[2] Department of Chemistry, Iowa State University, Ames, Iowa 50011, United States

*Correspondence to: twindus@iastate.edu, lqi@iastate.edu

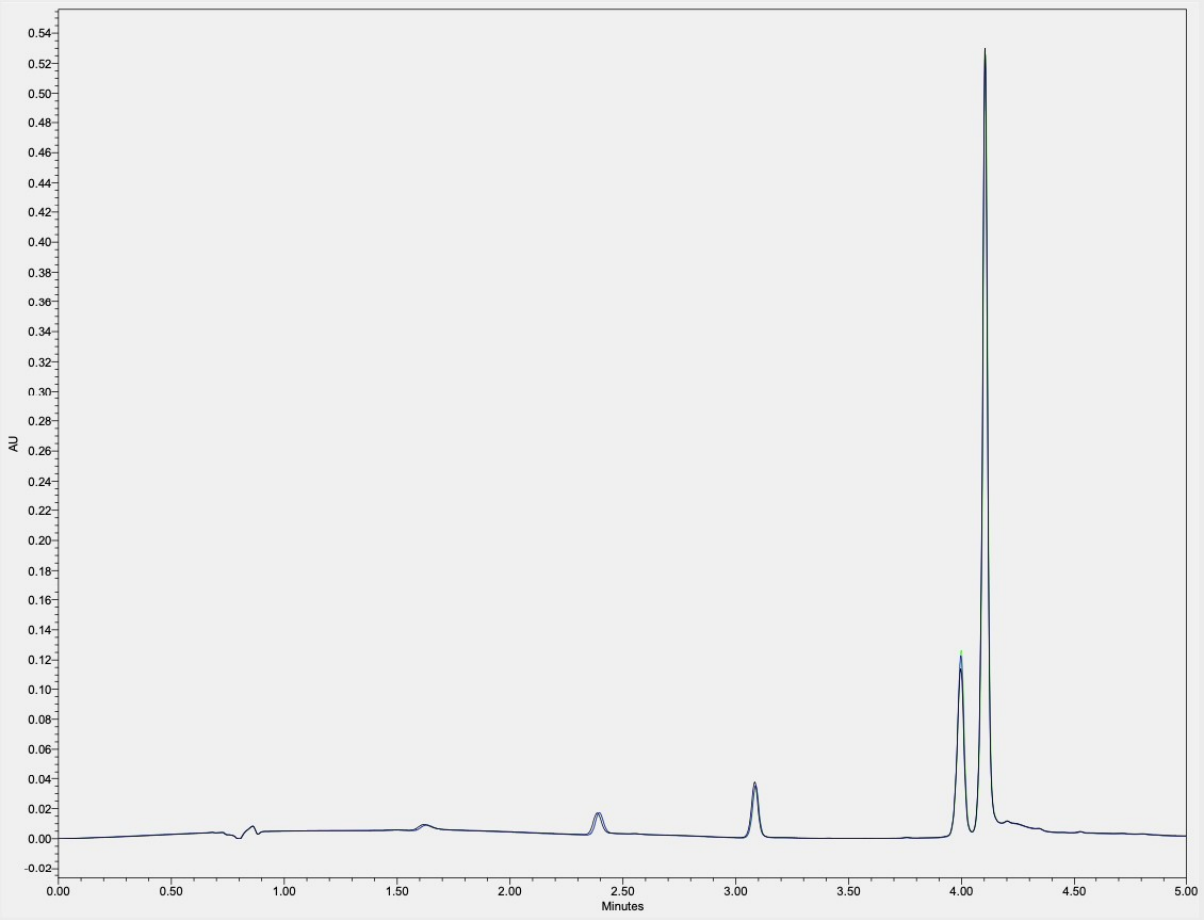

Figure S1. The representative chromatograms acquired during the automated optimization. The corresponding reaction conditions are 50% imine, 50% PMHS, 40.9 °C. All three chromatograms (blue, navy, and green) used for averaging are nearly identical, suggesting the 30 min waiting time is adequately allowing the reactor to equilibrate. Peak assignment: 4.105 min (amine), 3.998 min (imine), 3.089 min (hydrogenolysis product of imine), 2.396 min (acetophenone), and 1.633 min (aniline).

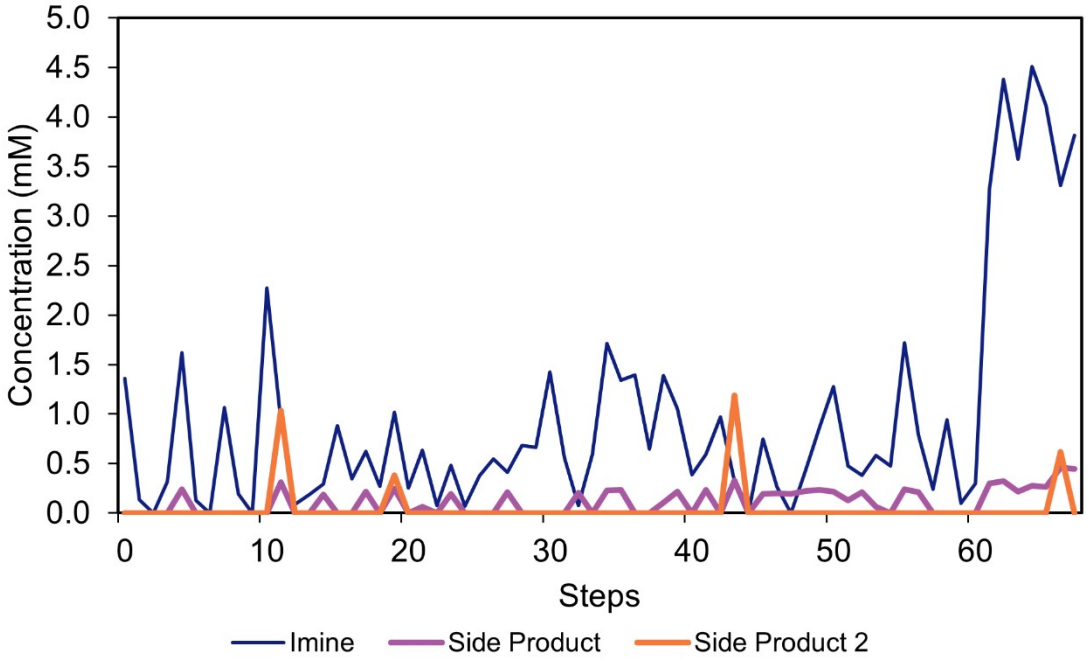

Figure S2. Concentrations of residual imine, acetophenone (side product 1) and aniline (side product 2) at different steps.

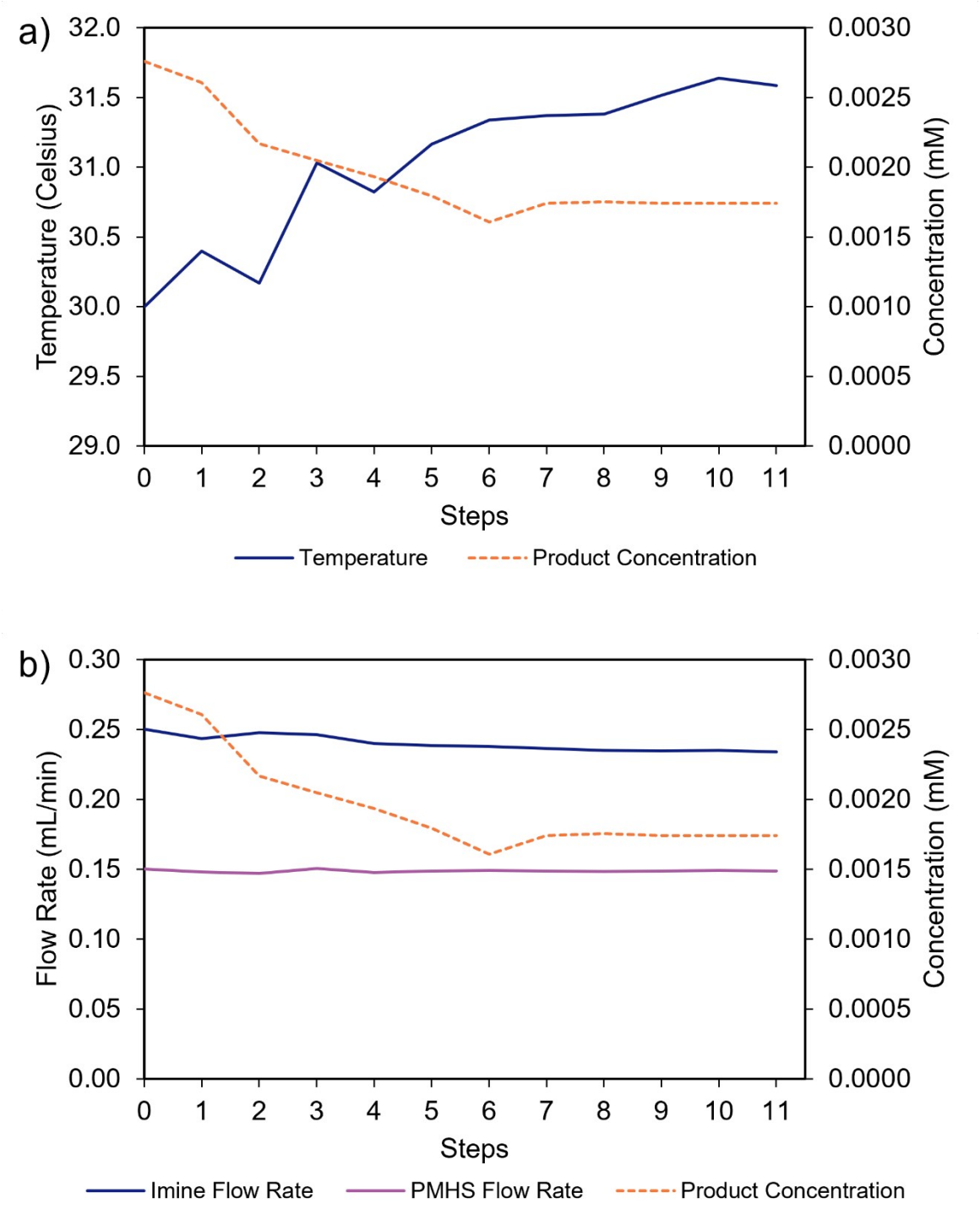

Figure S3. Reaction optimization parameters in the order of reactions performed. Deep Reaction Optimizer was used to guide the optimization. (a) Temperature (blue, solid) and concentration (orange, dashed) are plotted. (b) Imine (blue, solid) and PMHS (pink, solid) flow rates, along with product concentration (orange, dashed) are also shown.

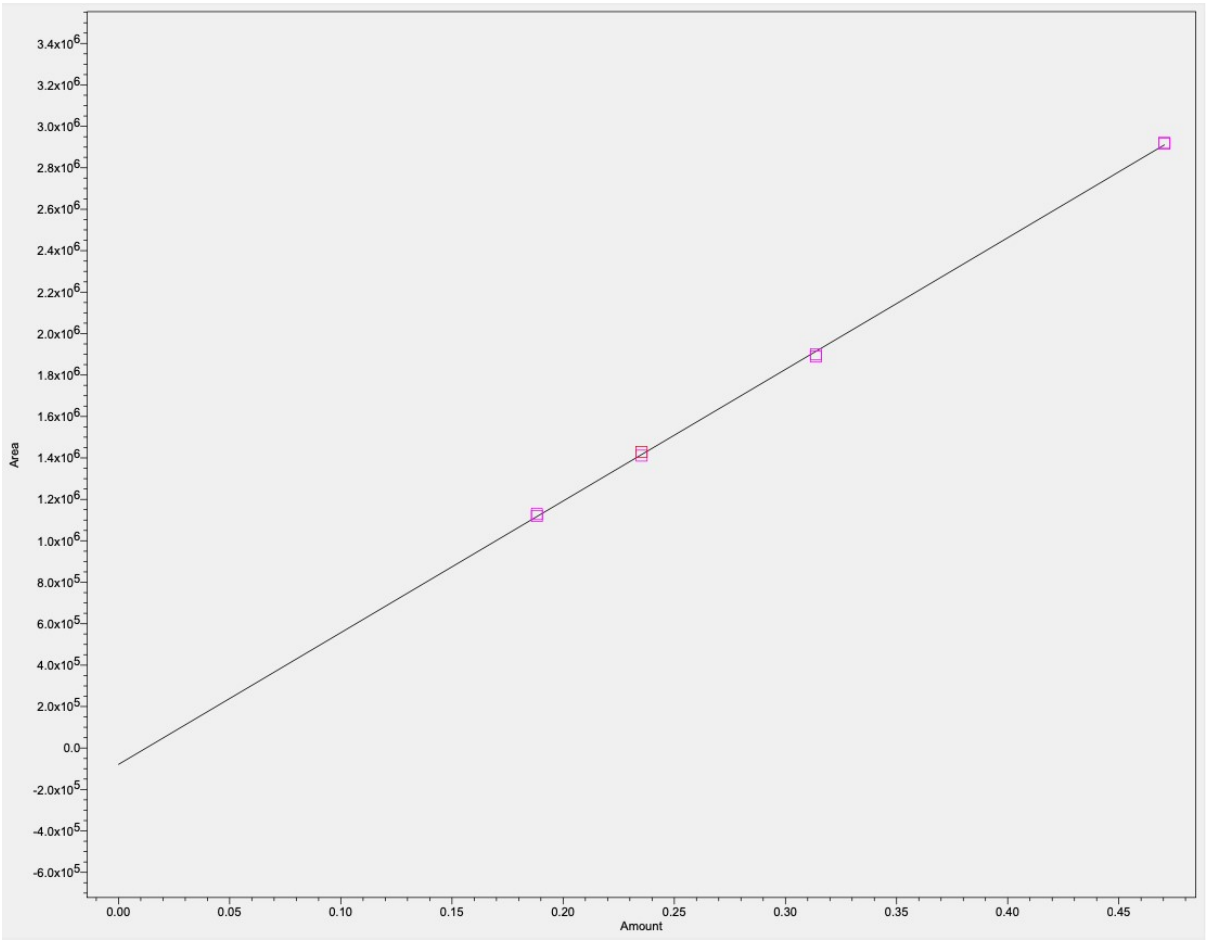

Figure S4. External at-line calibration with imine as a representative example. The default online dilution function was used as well as dilution factors of 20, 30, 40, and 50. Three repeated injections were carried out at each dilution level. The R^2 value is 0.999653.