Supporting Information

Submillisecond mixing in a continuous-flow, microfluidic mixer utilizing mid-infrared hyperspectral imaging detection

Drew P. Kise,[a] Donny Magana,[a] Michael J. Reddish,[a] and R. Brian Dyer*[a]

Table S1: Settings for the FPA detector used in all IR flow experiment data acquisitions

Setting	Value
Integration Time	40 µs
Detector Bias	12
Gain	1
Offset	216
Frame Rate	1610 Hz

COMSOL simulations.

Numerical simulations were carried out to assess the the mixing performance of the mixer and to compare the results to experiment. A 2D finite element model was computed on COMSOL Multiphysics Version 4.3a software (Comsol Inc., Stockholm, Sweden) using the parameters listed below (Table S2) and an extra-fine mesh. The model was built in COMSOL using the dimensions and angles of the mixer, which were measured on a visible microscope. The simulations were performed by solving the incompressible Navier-Stokes equations to calculate the velocity vector at each element, which was then used in the convective-diffusion equation to calculate the concentration profile of the mixer. The calculations used the physics package "Transport of Dilute Species & Laminar Flow" to model the mixing process.

Table S2: Parameters for theoretical modeling in COMSOL for H_2O/D_2O mixing experiment

Parameter	Value/Setting
Diffusion Coefficient	2.2×10^{-9} m^2/s, isotropic
Sample flow velocity	0.0013 m s^{-1} (for 0.60 µL min^{-1})
Sheath flow velocity	0.0270 m s^{-1} (for 17 µL min^{-1}
Material	Water, liquid
Inflow sample concentration	100 mM
Inflow sheath concentration	0 mM

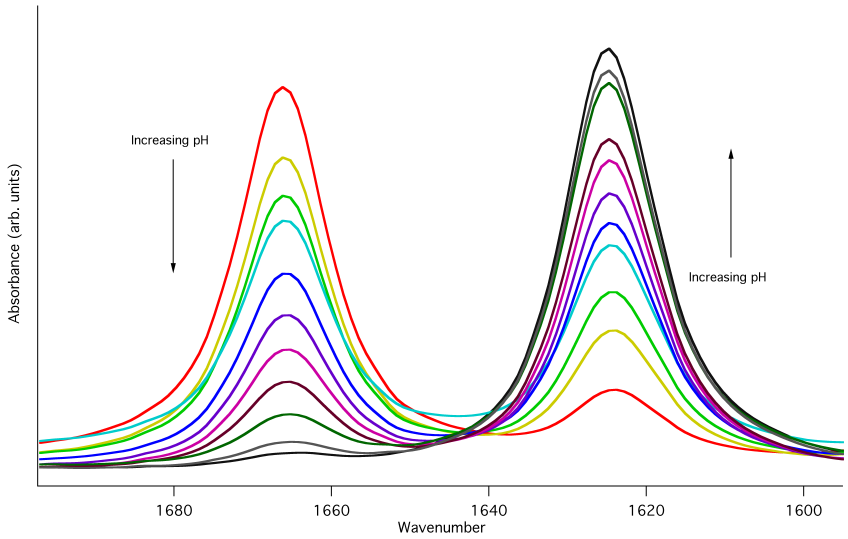

Figure S1: Equilibrium FTIR data of the pD titration of AMP in D2O (from red to black, pD = 3.2, 3.65, 3.85, 4.0, 4.2, 4.4, 4.6, 4.8, 5.1, 5.5, 5.8). These data were used to create the pD titration curve based on the ratio of the 1666 and 1624 cm^{-1} peaks

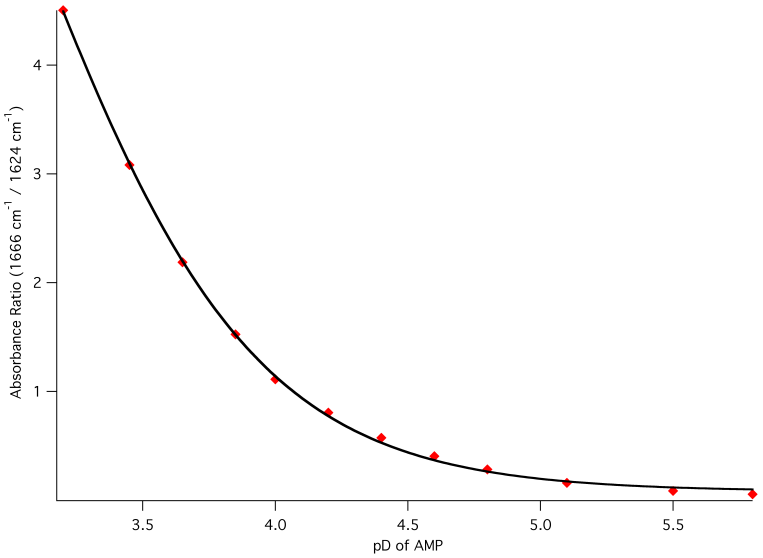

Figure S2: The titration curve established from the pD dependent equilibrium FTIR data for AMP in D_2O, shown in Fig. S1. The ratio of absorbance peak maxima at 1666 and 1624 cm^{-1} is plotted as a function of the pD. The data were fit to a sigmoid curve with the center fixed at the pK_a value of AMP, 3.4 (in pD units). The fit was used to obtain the pD values of the AMP sample in the flow experiments.

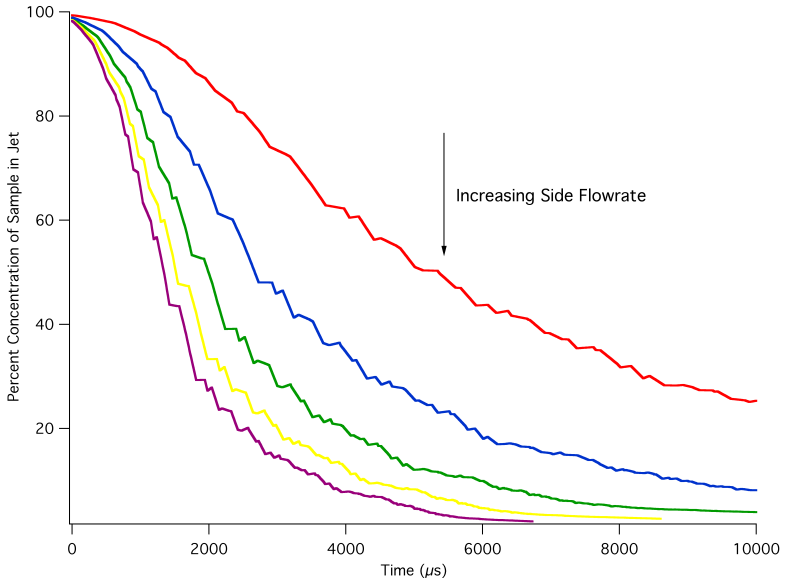

Figure S3: Simulated concentration decays versus time computed with COMSOL. The different traces correspond to different side flow rates where the red, blue, green, yellow, and purple traces correspond to 5, 10, 15, 20, and 25 µL min^{-1} side flows, respectively. The slower the flow rate, the longer the sample stays in the jet but the fatter the jet and subsequently the longer the mixing time. In contrast, the faster the flow rate, the faster the sample and sheath solutions mix, but also the concentration decreases more rapidly ($D=2.2x10^{-9}$ m^2 s^{-1} for all simulations).