Electronic Supplementary Material (ESI) for Analytical Methods.

Supporting Information

Experimental and Numerical Investigation of Microdialysis Probes for Ethanol Metabolism Studies

Tse-Ang Lee,[1] Jessie Peng,[1] Divjot Walia,[1] Rueben Gonzales,[2] Tanya Hutter[1,3]*

[1] Department of Mechanical Engineering, The University of Texas at Austin, Austin, TX 78712, USA
[2]College of Pharmacy, Division of Pharmacology and Toxicology, The University of Texas at Austin, Austin, TX 78712, USA
[3]Materials Science and Engineering Program and Texas Materials Institute, The University of Texas at Austin, Austin, TX 78712, USA
*Corresponding author: tanya.hutter@utexas.edu

Calibration of the GC-FID for in vitro studies

Standard solutions of ethanol and acetaldehyde were prepared at concentrations of 0.5, 2.5, 5, 10, and 20 mM, and were measured using GC-FID for quantification. Fig. S1 shows the measured peak heights of ethanol and acetaldehyde at different concentrations. The equation of the linear regression lines in the figure has high linearity and can be used to calculate the concentration of ethanol and its metabolites in the dialysate samples.

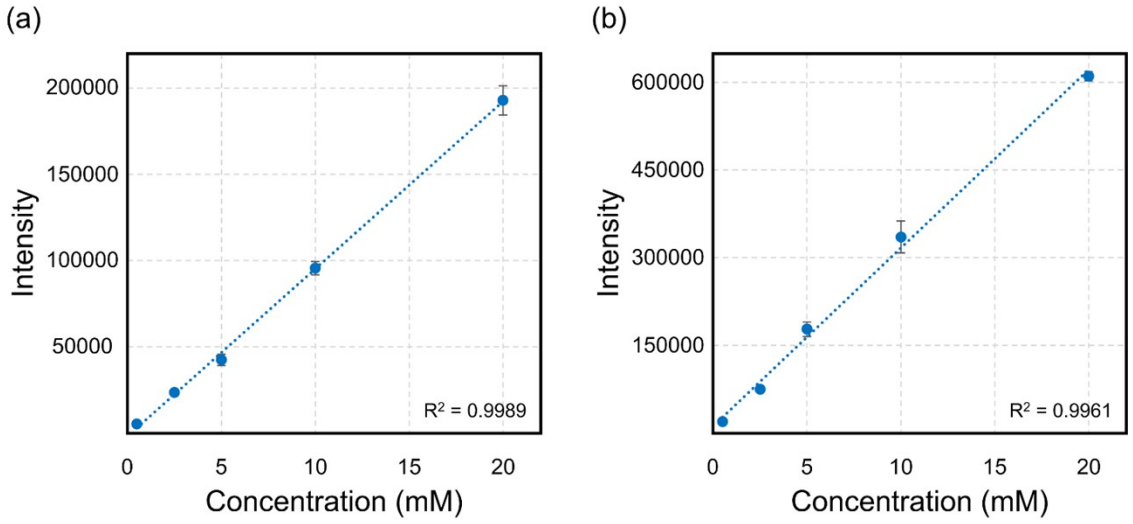

Fig. S1 *GC-FID calibration for in vitro experiments. Error bars represent the standard deviation (N=3) for (a) ethanol and (b) acetaldehyde.*

Calibration of UV-VIS spectrometer

Acetate solutions were prepared as standards at concentrations of 0.5, 2.5, 5, 10, and 20 mM, and were measured using UV-VIS spectrometer for quantification. Fig. S2 illustrates the measured peak heights of acetate at different concentrations. The linear regression line in the figure has high linearity, as expected by Beer-Lambert law, and can be used to calculate the acetate concentration in the dialysate samples.

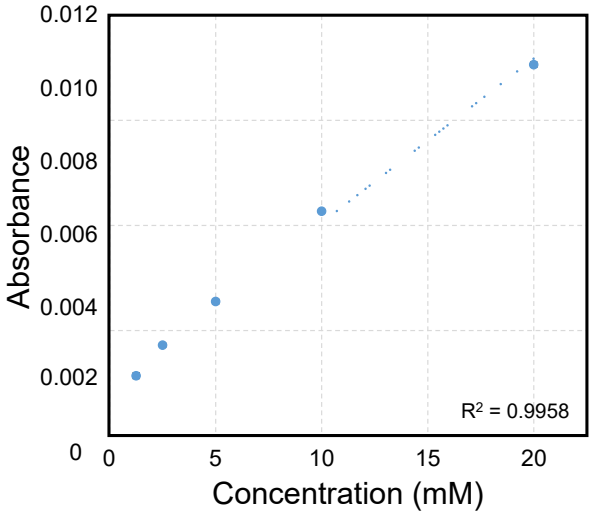

Fig. S2 *Calibration of UV-VIS spectrometer (N=3). The error bars are too small to visibly see.*

Physical Model for COMSOL simulation

Fig. S3 illustrates the physical model created in COMSOL. The probe was generated with dimensions identical to the actual probe. A surrounding cylinder was employed to simulate the striatum region in the rat's brain.

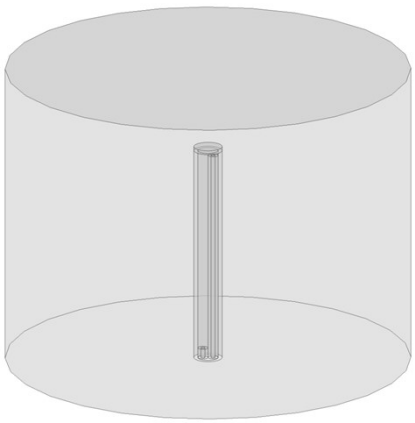

Fig. S3 *Physical model of the microdialysis probe and brain.*

Calibration of the GC-FID for in vivo studies

Standard solutions of ethanol were prepared at 0.5, 2.5, 5, 10, and 20 mM. Acetaldehyde standard solutions were prepared at 1, 0.5, 0.25, 0.125, 0.063, 0.03135 and 0.0156 mM. Methyl acetate was prepared at concentrations of 2, 1, 0.5, 0.25, 0.125, and 0.0625 mM. All the standards were measured using GC-FID for quantification. Fig. S2 shows the measured peak heights of ethanol and acetaldehyde at different concentrations.

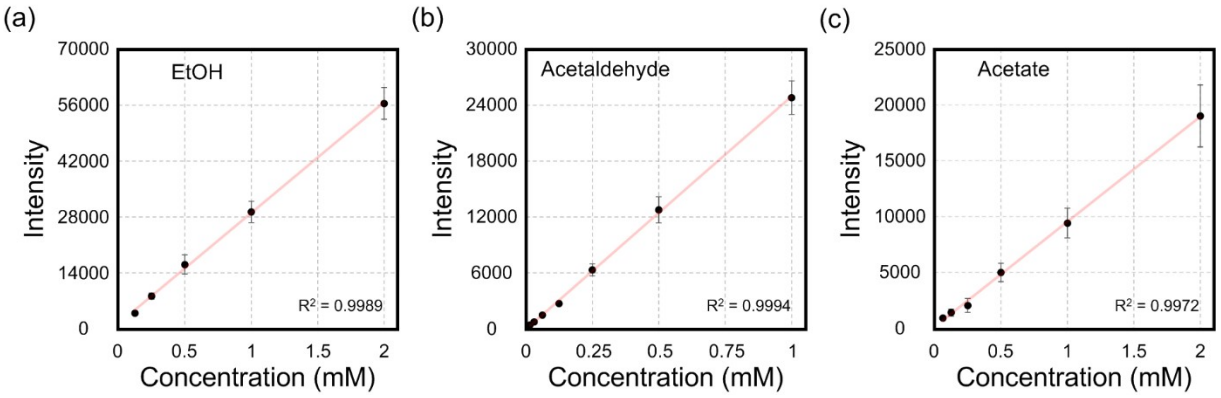

Fig. S4 *GC-FID calibration for in vivo experiments. Error bars represent the standard deviation (N=3) for (a)ethanol, (b)acetaldehyde, and (c) acetaldehyde.*

Calibration of infrared spectrometer

Spectra of the mixture at 5, 10, 15, and 20 mM for each analyte were taken to calibrate the concentration of the dialysate sample, as shown in Fig. S4(a). Distinctive peaks at 1046 cm^{-1}, 1175 cm^{-1}, and 1280 cm^{-1}, corresponding to C-O stretch, C=O stretch, and C-O stretch, were used for the quantification of ethanol, acetaldehyde, and acetate, respectively. Local absorbance at 1062 cm^{-1}, 1196 cm^{-1}, and 1203 cm^{-1} were subtracted to calculate their peak heights. Fig. S4(b) shows the measured peak heights of the three analytes at different concentrations. The linear regression line equation in the figure has high linearity (R^2>0.99) and can be used to calculate the concentration of ethanol in the dialysate samples.

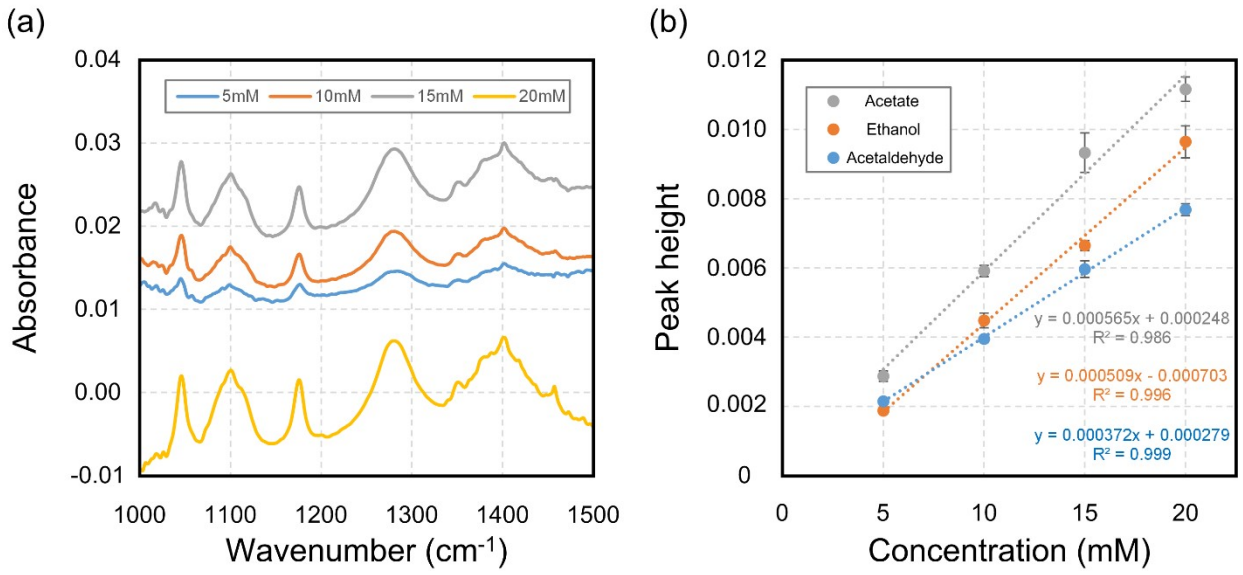

Fig. S5 *Calibration of infrared spectrometer. (a) Infrared absorbance spectra of three mixtures of ethanol, acetate and acetate at different concentrations. (b) Peak height as a function of concentration for each analyte.*

Backpressure measurements at 25 °C and 37°C

Backpressure measurements were performed using lab-made microdialysis probes with a 2 mm membrane. Various flow rates of 0.5, 1, 2, 4, and 6 µL/min were applied to the probes to induce backpressure at 25°C and 37°C. Each pressure level was held for 15 minutes to ensure that the system reached a steady state. Results from three different probes were reported as average ± standard deviation (N=10), as shown in Fig S6. The back pressure difference between 25°C and 37°C was within 5% for all measurements.

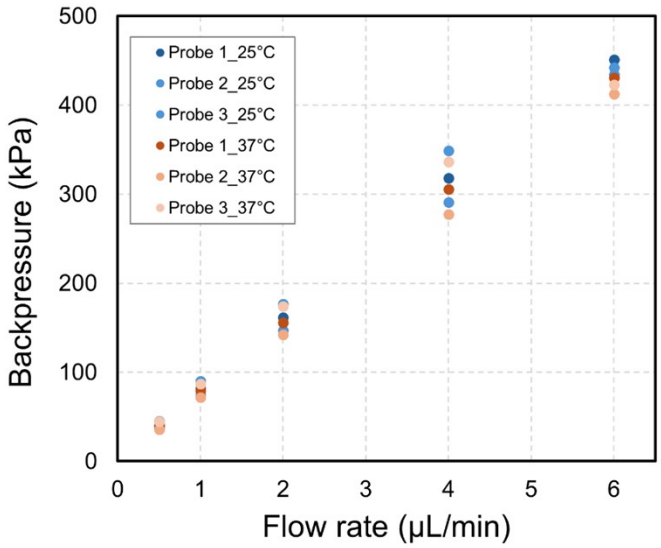

Fig. S6 *Backpressure measurements at different flow rates and temperatures. The error bars are too small to be visible.*