Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary Information

Novel method of nicotine quantification in electronic cigarette liquids and aerosols

Mumiye A. Ogunwale, M.S.[1,4]; Yizheng Chen, Ph.D.[2]; Whitney S. Theis, M.S.[3,4]; Michael H. Nantz, Ph.D.[1,4]; Daniel J. Conklin, Ph.D.[3,4], Xiao-An Fu, Ph.D.[2,4*]

[1]Department of Chemistry, [2]Department of Chemical Engineering, [3]Diabetes and Obesity Center, and [4]American Heart Association – Tobacco Regulation and Addiction Center, University of Louisville, Louisville, KY 40208

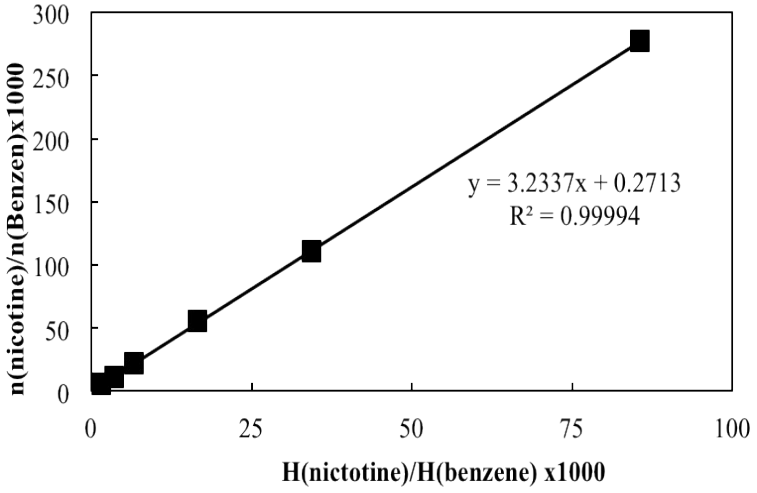

Figure S1 Plot of n(nicotine)/n(benzene) vs. H(nicotine)/H(benzene), serving as a calibration curve for ^{1}H NMR measurement of nicotine protonation.

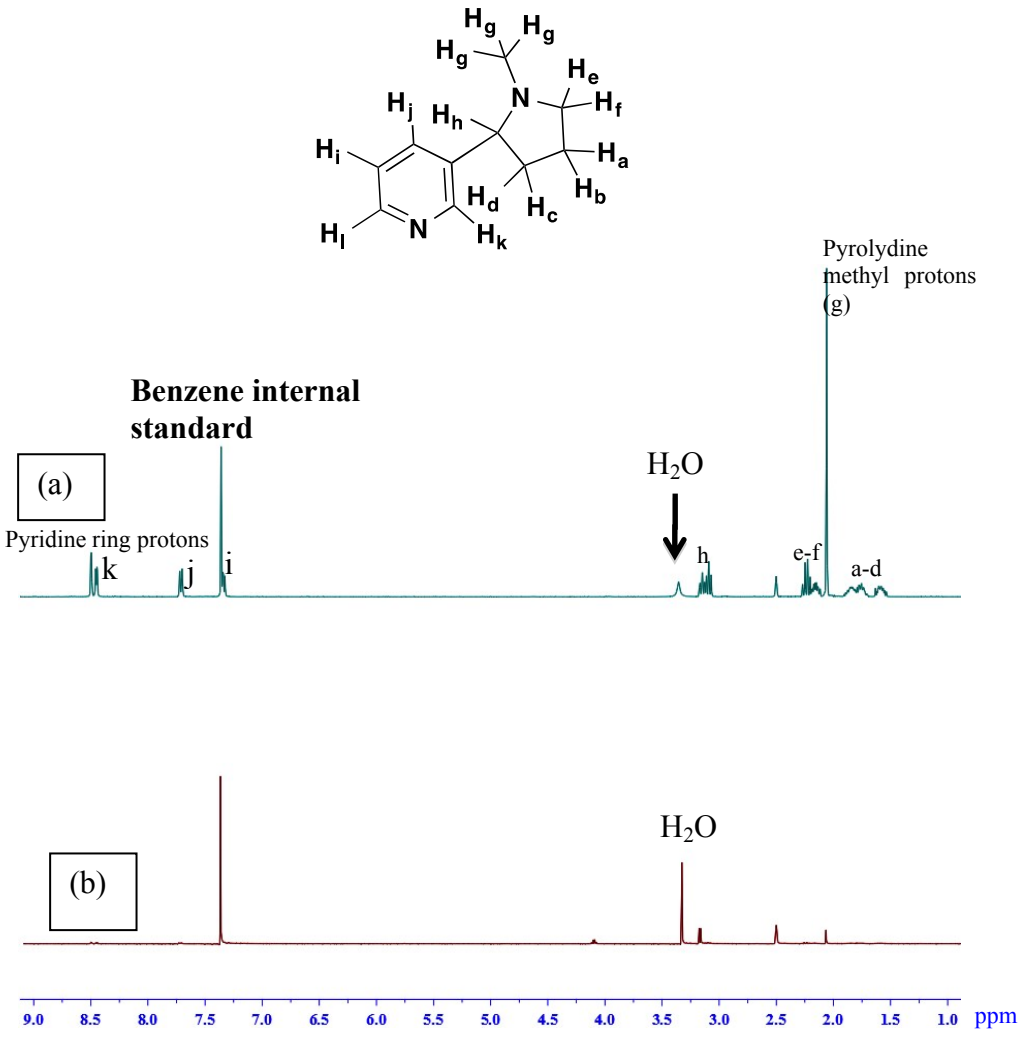

Figure S2. (a) ^{1}H NMR spectra (DMSO-d_6) of neutral nicotine and (b) ^{1}H NMR spectra (DMSO-d_6) of extracted nicotine after 30 minutes of protonation in water and HCl mixture (Less than 2% of free base left unprotonated). Quantification achieved by introduction of benzene as internal standard.

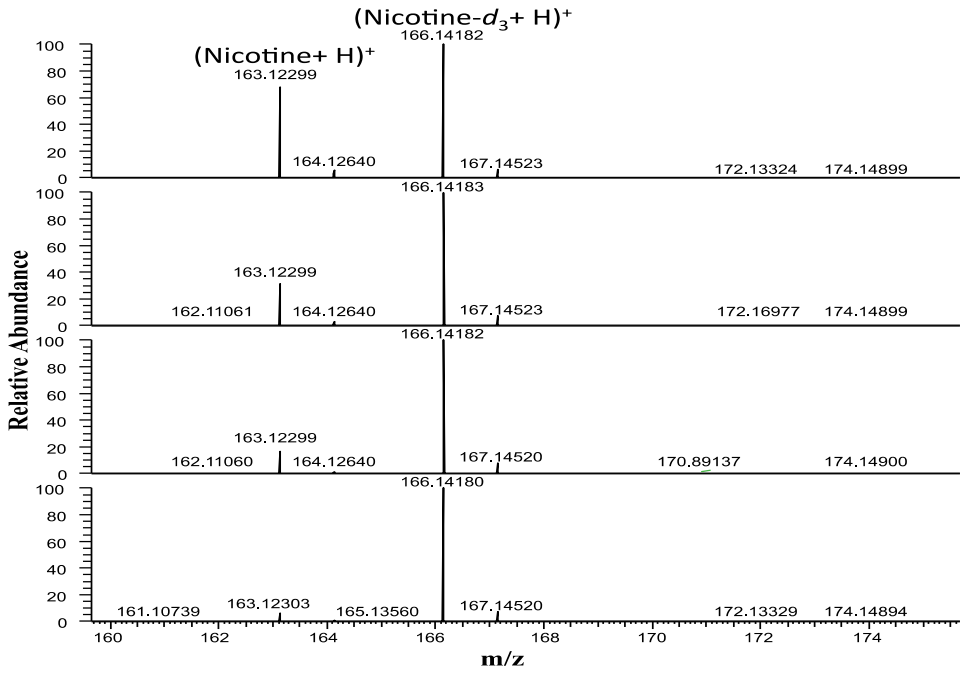

Figure S3. Comparison of FT-ICR-MS spectra of standard calibration curve working solutions, each spiked with 7.78 nmol nicotinium-d_3 as an internal standard. The nicotine peak grows relative to the internal standard peak as the nicotine concentration increases.