Supporting Information:

Multivariate Analysis to Quantify Species in the Presence of Direct Interferents: Micro-Raman Analysis of HNO_3 in Microfluidic Devices

Amanda M Lines[1]*; Gilbert L Nelson[2]; Amanda J Casella[1]; Job M Bello[3]; Sue B. Clark[1,4], and Samuel A Bryan[1]*

[1]Energy and Environment Directorate, Pacific Northwest National Laboratory, Richland, WA 99352
[2]College of Idaho, Department of Chemistry, 2112 Cleveland Blvd, Caldwell, ID 83605
[3]Spectra Solutions Inc. , 1502 Providence Highway, Norwood, MA, 02062-4643.
[4]Washington State University, Department of Chemistry, Pullman, WA 99164

*corresponding author

CORRESPONDING AUTHORS

Dr. Samuel Bryan: sam.bryan@pnnl.gov
Phone:509-375-5648
Dr. Amanda Lines: amanda.lines@pnnl.gov
Phone:509-375-5689

ABSTRACT

Microfluidic devices are a growing field with significant potential for applications to small scale processing of solutions; however, fast, reliable, and cost effective means of monitoring streams during processing are needed. Here we apply a novel micro-Raman probe to the on-line monitoring of streams within microfluidic and micro-flow devices. Details regarding the calibration sets used to build chemometric models are described here.

Table S1: Solution set 1

Sample name	HNO_3 M	$NaNO_3$ M	Total NO_3^- M
S2_1	0	0	0
S2_2	0	0.502	0.502
S2_3	0	0.998	0.998
S2_4	0	1.983	1.983
S2_5	0	2.496	2.496
S2_6	0	2.908	2.908
S2_7	0	3.982	3.982
S2_8	0.52	0	0.52
S2_9	0.52	0.529	1.049
S2_10	0.52	1.026	1.546
S2_11	0.52	1.994	2.514
S2_12	0.52	2.524	3.044
S2_13	0.52	2.902	3.422
S2_14	0.52	3.893	4.413
S2_15	0.99	0	0.99
S2_16	0.99	0.52	1.51
S2_17	0.99	1.014	2.004
S2_18	0.99	1.989	2.979
S2_19	0.99	2.6	3.59
S2_20	0.99	3.056	4.046
S2_21	0.99	4.01	5
S2_22	1.96	0	1.96
S2_23	1.96	0.504	2.464
S2_24	1.96	1.009	2.969
S2_25	1.96	2.002	3.962
S2_26	1.96	2.514	4.474
S2_27	1.96	3.031	4.991
S2_28	1.96	3.997	5.957
S2_29	2.96	0	2.96
S2_30	2.96	0.525	3.485
S2_31	2.96	1.003	3.963
S2_32	2.96	2.002	4.962
S2_33	2.96	2.516	5.476
S2_34	2.96	2.989	5.949
S2_35	2.96	4.013	6.973
S2_36	3.95	0	3.95
S2_37	3.95	0.509	4.459
S2_38	3.95	1.021	4.971

S2_39	3.95	2.014	5.964
S2_40	3.95	2.497	6.447
S2_41	3.95	3.042	6.992
S2_42	3.95	3.996	7.946
S2_43	5.86	0	5.86
S2_44	5.86	0.493	6.353
S2_45	5.86	1.006	6.866
S2_46	5.86	2.02	7.88
S2_47	5.86	2.564	8.424
S2_48	5.86	3.041	8.901
S2_49	5.86	3.996	9.856
S2_50	7.94	0	7.94
S2_51	7.94	0.522	8.462
S2_52	7.94	1.04	8.98