Real-time quantification of amino acids in the exhalome by secondary electrospray ionization-mass spectrometry: A proof-of-principle study

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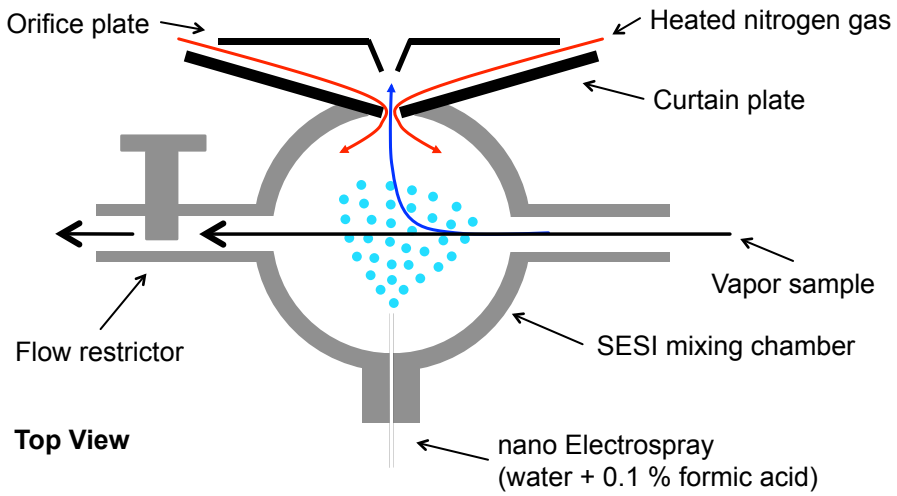
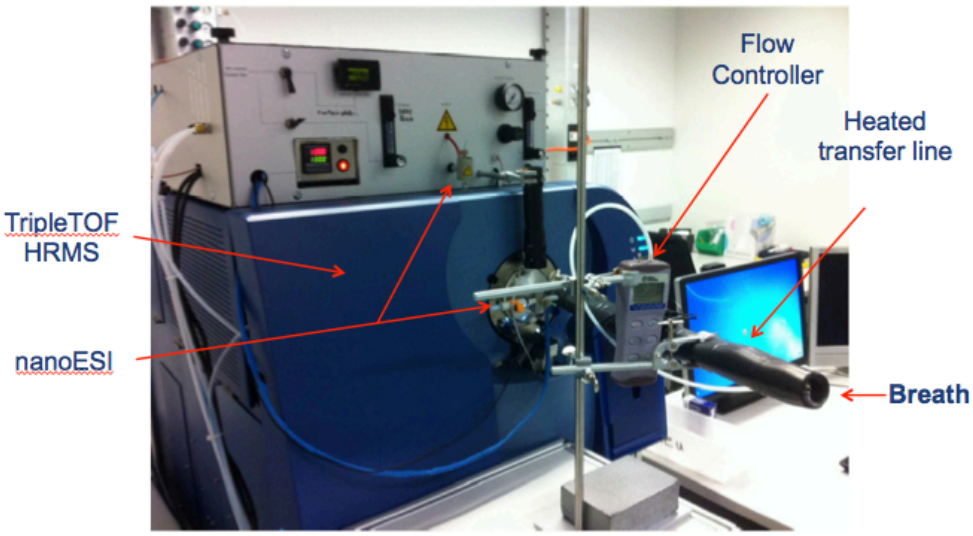
Supplemental Figure 1. Scheme and picture of the secondary ESI instrumentation





Supplemental Table 1. Baseline characteristics for training and test sets

	Training set N=25	**Test set N=12**	**p-value**
Gender, M/F (% male)	22/3 (88)	7/5 (58)	0.19
Age, years	27±11	30±6	0.39
BMI, kg/m^2	22±2.3	23±1.9	0.20

Supplemental Table 2. Passing-Bablok regression equations (y=a+bx where y= D4-Ala normalized signal and x= plasma free concentration in mmol/L).

Amino acid	Slope (b) (L/mmol)	Intercept (a)	Pearson's *r*	Spearman's ρ	Range (μmol/L)
A	1.6±0.3	-0.3±0.2	0.9113	0.9468	230-675
J	2.8±0.7	0.0±0.2	0.8811	0.8739	89-317
G	0.4±0.1	0.00±0.03	0.8936	0.8513	137-479
P	4±1	-0.2±0.4	0.8635	0.8539	168-432
V	9±2	-1.2±0.6	0.9105	0.9342	120-361
K	29±7	-3±2	0.9262	0.9377	108-256
Orn	6±1	-0.1±0.2	0.8529	0.8569	31-137
F	16±3	-0.3±0.2	0.9282	0.9138	40-97

Supplemental Table 3. Coefficients of variation (CV) for blood (HPLC method with two identical setups 1 & 2) and breath (SESI-HRMS) determination of amino acids.

Amino acid	HPLC 1 CV (%) n=119	HPLC 2 CV (%) n=134	SESI-HRMS CV (%) n=25
A	2.2	1.8	4.4
V	2.3	1.7	3.6
J	2.6	1.8	9.6
G	2.4	1.8	5.7
P	2.6	2.3	7.7
K	2.8	1.9	9.9
F	2.7	1.9	9.0
Orn	2.5	1.9	8.4