Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Effects of modular ion-funnel technology onto analysis of breath VOCs by means of real-time mass spectrometry

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Table S1 Details and operating conditions for the modular IF

Number of electrodes	12 (6 RF+; 6 RF-)
Length	2.2 cm
I.D. reduction	1 cm to 0.2 cm
Electrodes distance	0.1 cm
Pressure	2.3 mbar
Temperature	75 °C
RF voltage	40-200 V_{p-p}
RF frequency	4.5 MHz
DC field	4.5-27 V/cm

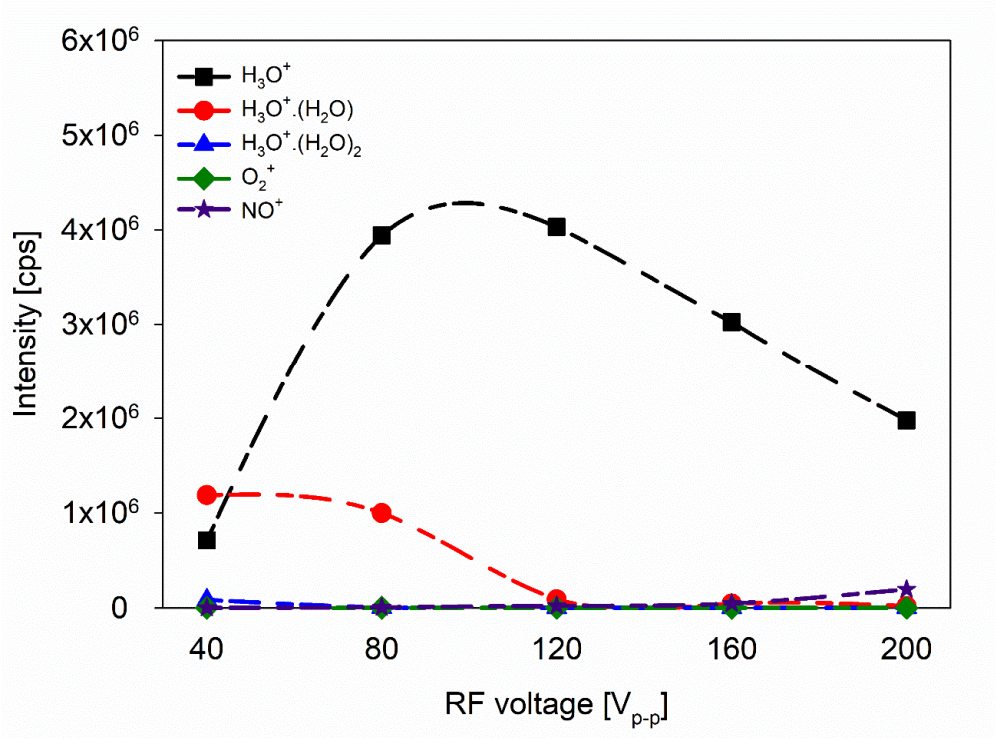
Table S2 Experimental design conducted for the ion funnel characterization

	E_{drift} [V/cm]	RF voltage [V_{p-p}]	DC field [V/cm]
Dry samples	66	40	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		80	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		120	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		160	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		200	4.5/ 9 / 13.5 / 18 / 22.5 / 27
	48	40	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		80	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		120	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		160	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		200	4.5/ 9 / 13.5 / 18 / 22.5 / 27
Humid samples	66	40	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		80	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		120	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		160	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		200	4.5/ 9 / 13.5 / 18 / 22.5 / 27
	48	40	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		80	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		120	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		160	4.5/ 9 / 13.5 / 18 / 22.5 / 27
		200	4.5/ 9 / 13.5 / 18 / 22.5 / 27

Table S3 Participant list with demographic parameters

Volunteer ID	Sex	Age	Weight (Kg)	Height (cm)	Smoker
01	M	30	78	175	YES
02	M	28	60	176	NO
03	F	38	80	165	NO
04	M	41	80	185	NO
05	M	37	85	187	YES
06	M	31	62	170	YES
07	M	39	85	192	NO
08	M	35	105	195	NO
09	M	34	105	183	NO
10	M	28	68	180	YES
11	F	20	65	171	YES
12	F	32	58	175	YES
13	M	26	65	170	YES
14	M	30	75	180	NO
15	M	44	82	177	NO
16	M	19	95	171	YES
17	M	47	92	188	NO
18	M	40	64	170	YES
19	M	29	75	180	NO
20	M	48	105	195	NO
21	M	54	85	179	YES

a)



b)

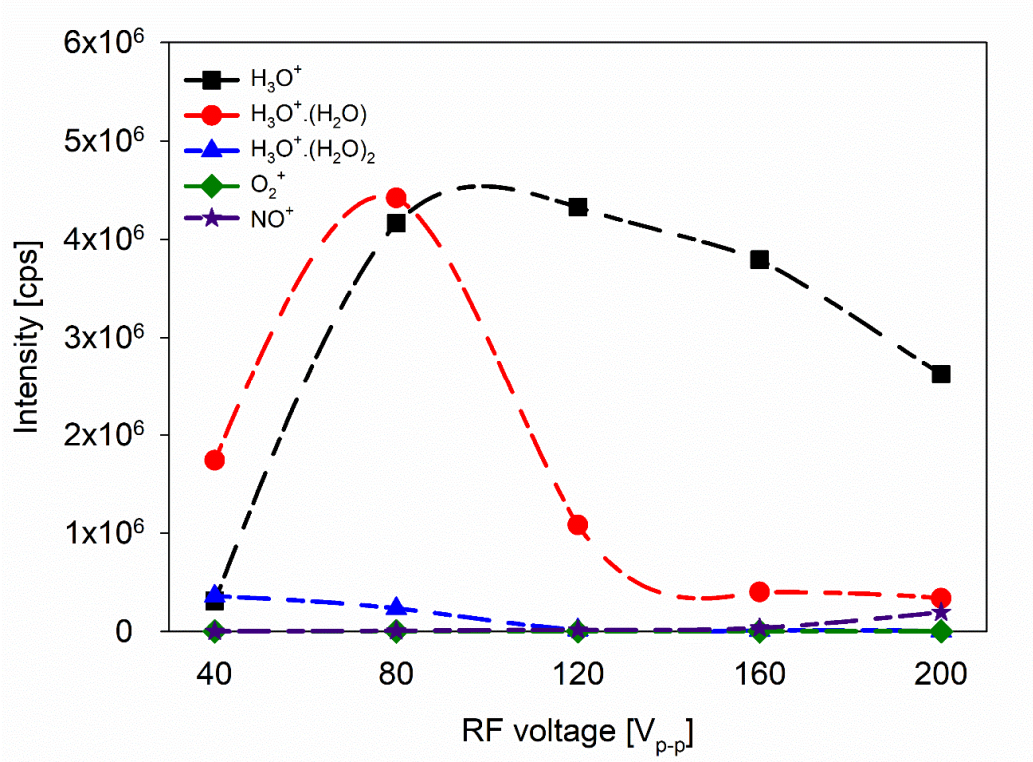
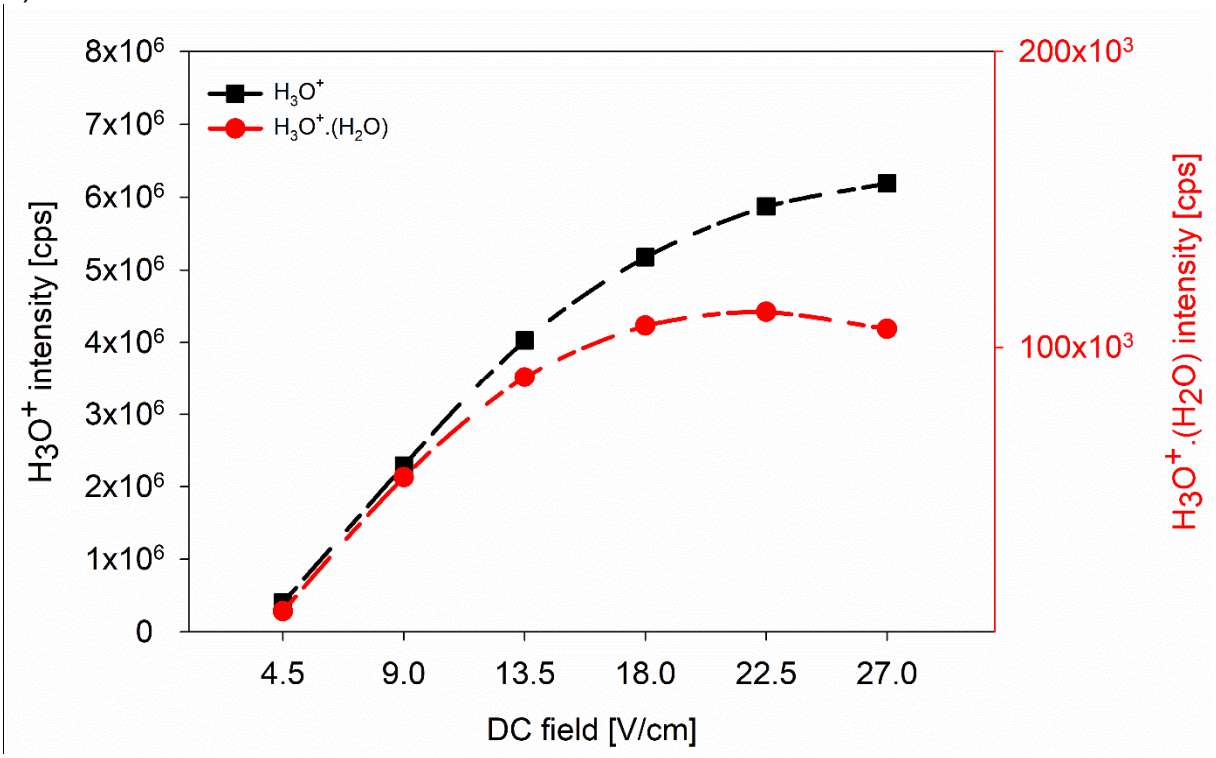


Fig. S1 Ion intensities in counts per second (cps) of the water reagent ions ($H_3O^+.(H_2O)_n$, n = 0, 1 and 2) and as well as parasitic ions O_2^+ and NO^+ present in the drift tube under dry (a) and humid (b) conditions as a function of RF voltage. DC was 13.5 V/cm and E_{drift} was 48 V/cm

a)



b)

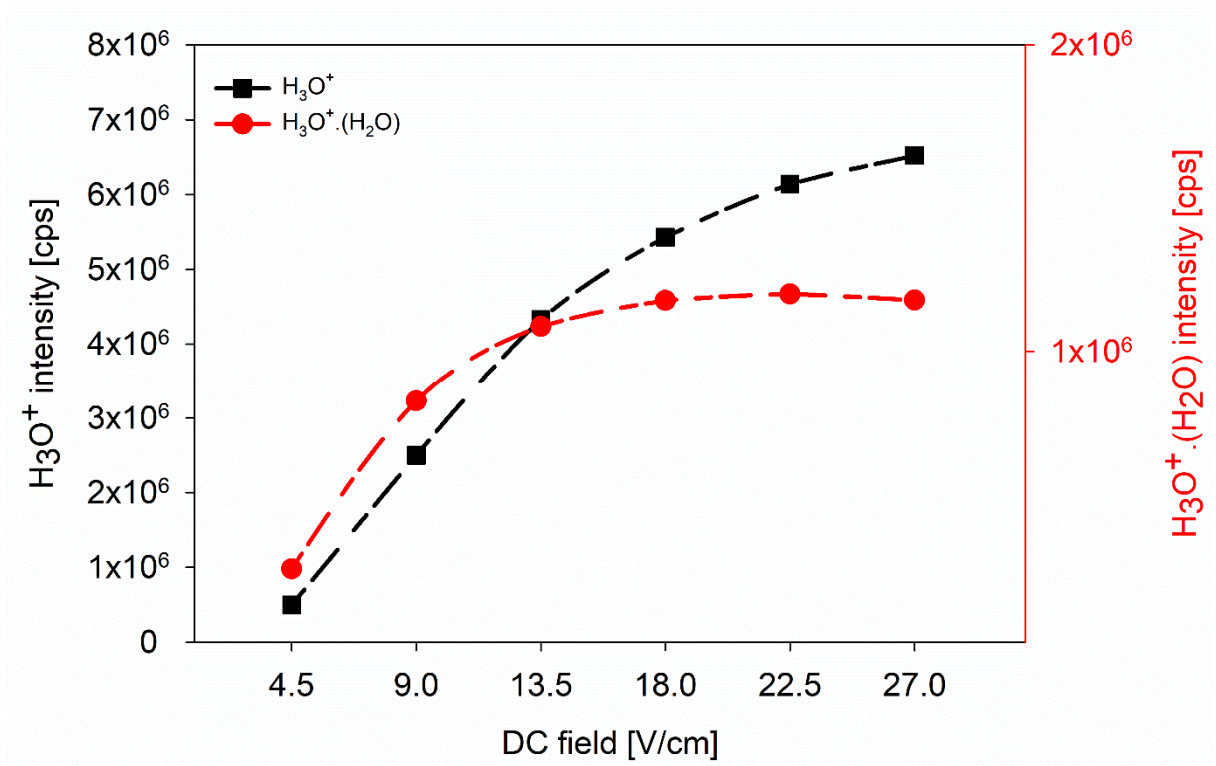


Fig. S2 Ion intensities in counts per second (cps) of H_3O^+ and $H_3O^+.(H_2O)$ present in the drift tube under dry (a) and humid (b) conditions as a function of the DC field (V/cm). RF voltage was 120 V_{p-p} and E_{drift} was 48 V/cm

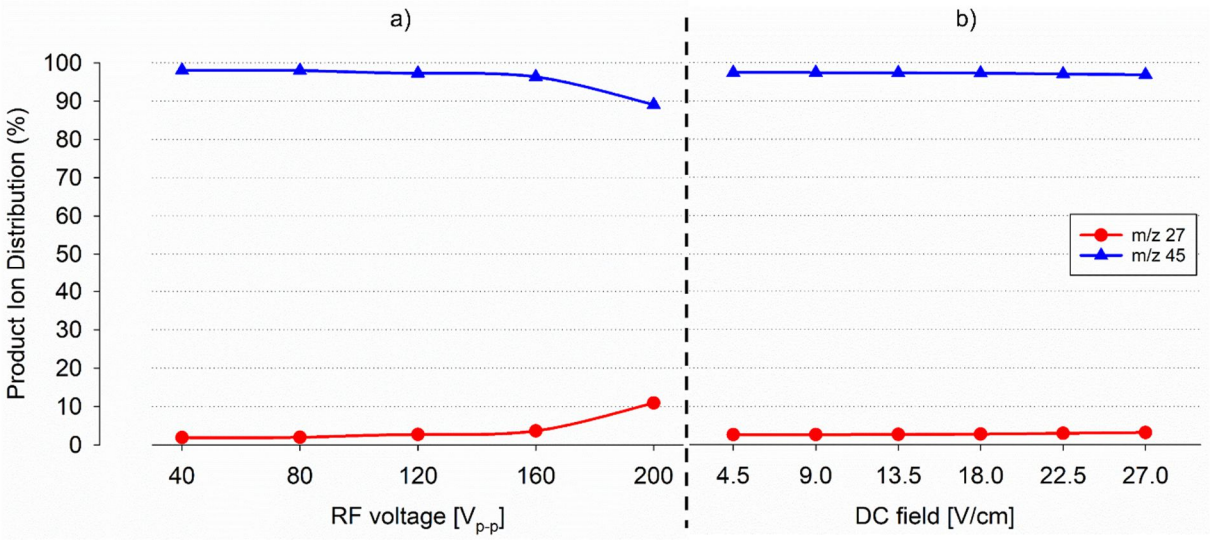


Fig. S3 Relative signal variation for protonated acetaldehyde ($C_2H_5O^+$, *m/z* 45) and its fragment ($C_2H_3^+$, *m/z* 27) as function of RF voltage (panel a; DC = 13.5 V/cm, E_{drift} = 66 V/cm) and DC voltage (panel b; RF = 120 V_{p-p}, E_{drift} = 66 V/cm)