Supplemental Information

A Real-Time Fast-Flow Tube Study of VOC and Particulate Emissions from Electronic, Potentially Reduced-Harm, Conventional, and Reference Cigarettes

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Equations

The following equations were used for the calculations of cigarette emissions in the fast flow tube (Fig. 1) experiments. Note that these equations served as a guideline to the data analysis; the actual measurements relied on explicit calibration measurements described in the text. The parameters used in these equations include: R_m = mass delivery rate of injection of a specific chemical standard (by a cigarette or a calibration syringe pump); C_{XA} = concentration of chemical at stage "A"; F_A and F_B = flow of chemical at stage "A" or "B"; f_A, f_B, and f_C = fraction of flow of chemical in stage "A", "B", or "C"; and DF = dilution factor between stage "B" and stage "C".

S1
$$R_m\left(\frac{\mu g}{s}\right) = R_v\left(\frac{\mu L}{hr}\right)\cdot\frac{10^{-3}cm^3}{\mu L}\cdot\frac{1hr}{3600s}\cdot\rho\left(\frac{g}{cm^3}\right)\cdot\frac{10^6\mu g}{g}$$

S2
$$R_N\left(\frac{molec}{s}\right) = R_m\left(\frac{g}{s}\right)\cdot\frac{N_A}{MW\left(\frac{g}{mol}\right)}$$

S3
$$C_{XA}\left(\frac{molec}{cm^3}\right) = \frac{R_N\left(\frac{molec}{s}\right)}{F_A\left(\frac{cm^3}{s}\right)}\text{, assuming STP inside flowtube}$$

S4
$$f_A = \frac{C_{XA}\left(\frac{molec}{cm^3}\right)}{C_0\left(\frac{molec}{cm^3}\right)}\text{, assuming STP inside flowtube}$$

S5
$$f_B = f_A\cdot\frac{F_A\left(\frac{cm^3}{s}\right)}{F_A\left(\frac{cm^3}{s}\right)+F_1\left(\frac{cm^3}{s}\right)}\text{, assuming STP inside flowtube}$$

S6
$$f_C = f_B\cdot\frac{F_B\left(\frac{cm^3}{s}\right)}{F_B\left(\frac{cm^3}{s}\right)+F_2\left(\frac{cm^3}{s}\right)}\Rightarrow f_B\cdot DF$$

Figure S1. PTMRS mass spectra of well resolved $[M+H]^+$ peaks for the fifth puff of a 3R4F cigarette: a) CO_2 (*m/z* 44.998) was not detected, but acetaldehyde (*m/z* 45.034) was clearly observed; b) both the acrolein (*m/z* 57.034) and butenes (*m/z* 57.070) are well resolved.

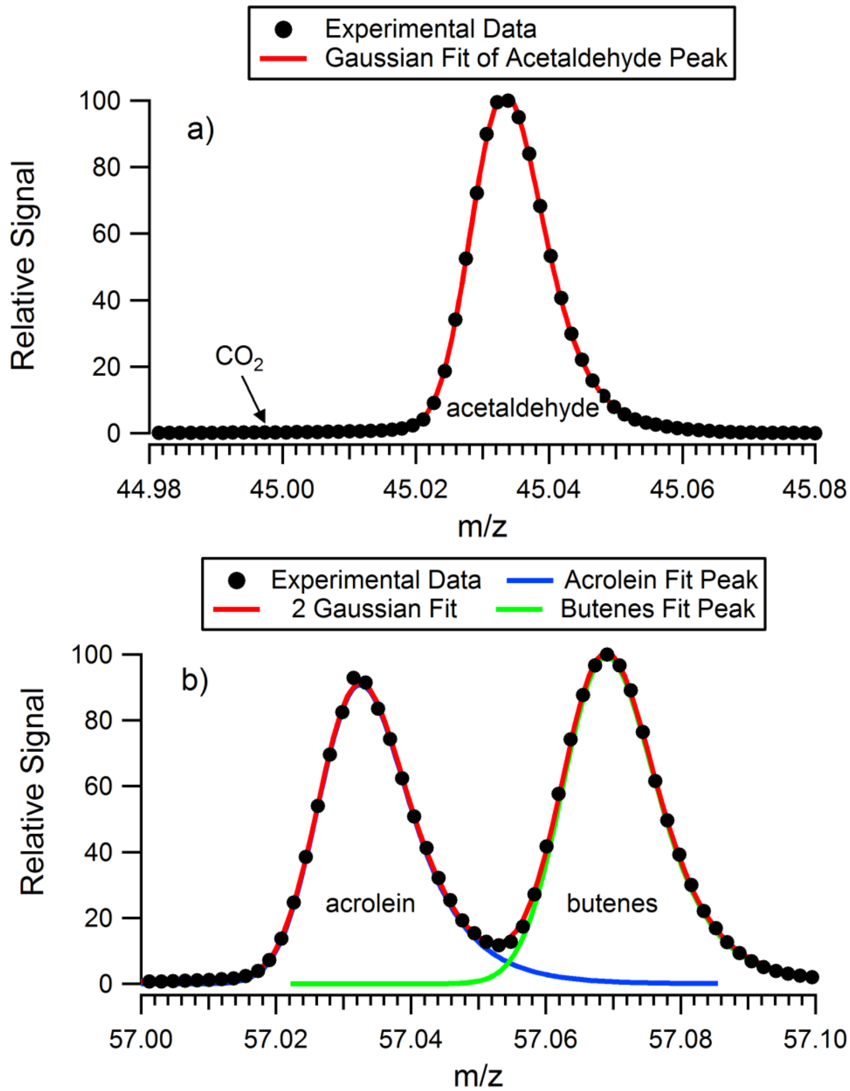

Figure S2. PTMRS time profile of 1R5F at a frequency of 1 puff/min for fast flow tube experiments. The contributions from the individual puffs are clearly resolved with the present time resolution. The first spike near t=0 corresponds to the 1st puff and there are 9 puffs total.

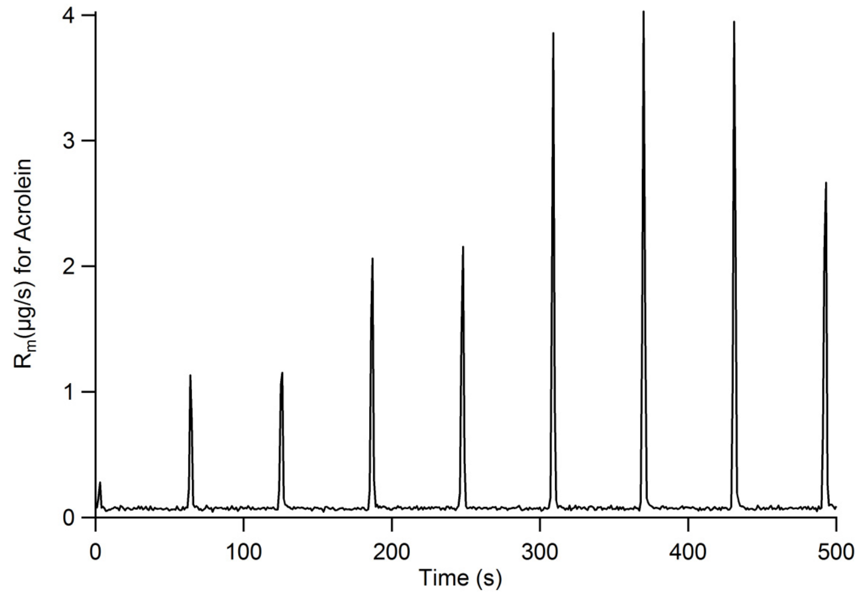

Figure S3. CPC time profile of 1R5F at a frequency of 1 puff/min for fast flow tube experiments. The first spike near t=0 corresponds to the 1st puff and there are 9 puffs total.

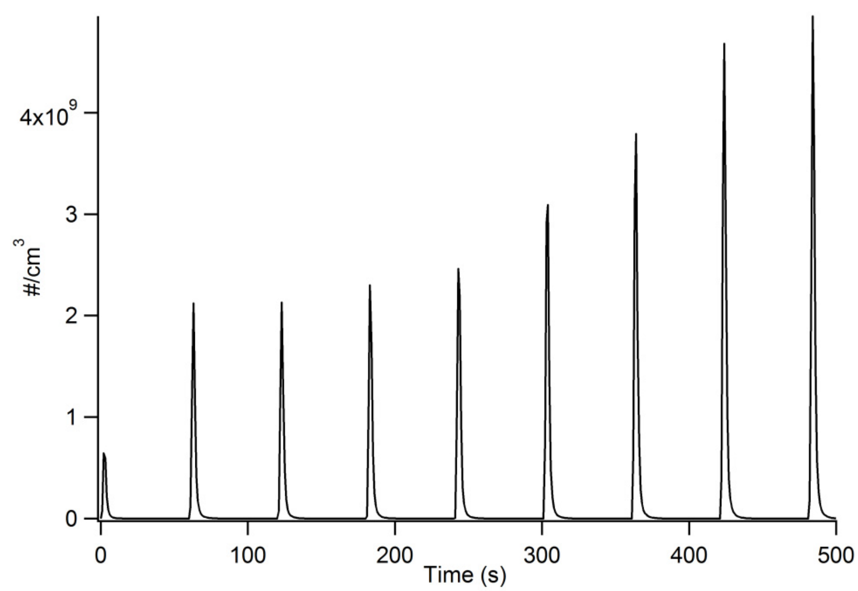

Figure S4. PTMRS time profile of e-cigarette-2 at a frequency of 4 puff/min for fast flow tube experiments. As this figure shows, the contributions from different puffs would overlap at higher puff frequencies complicating the quantitative analysis of the PTRMS data. Therefore, most PTRMS measurements reported in the paper were done at 1 puff/min puffing rate.

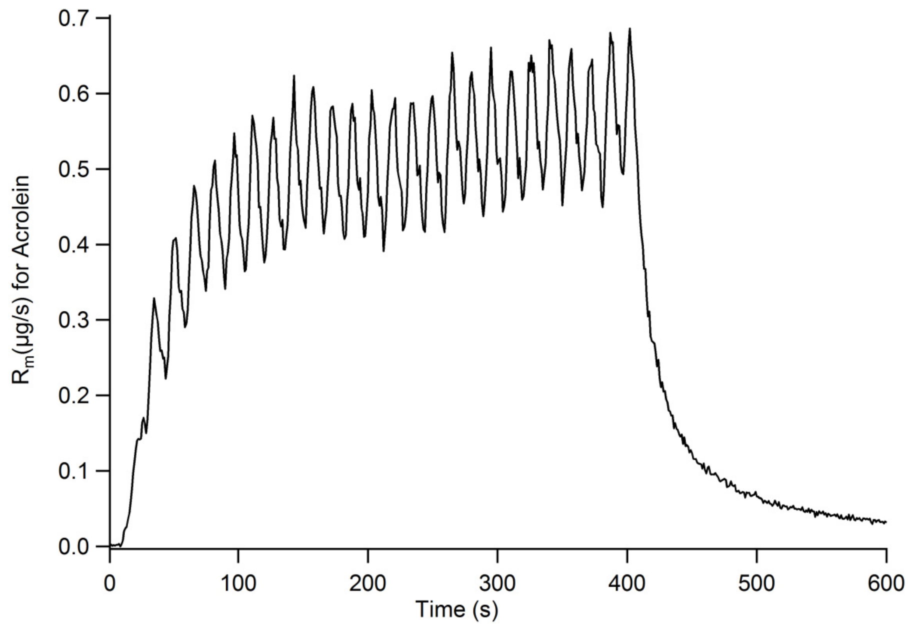

Figure S5. CPC time profile of e-cigarette-2 at a frequency of 4 puff/min for fast flow tube experiments. The first spike near t=0 corresponds to the 1st puff and there are 9 puffs total. Unlike the convoluted PTRMS signal shown in Figure S3, the CPC signal for each puff was clearly resolved even at the highest puff frequency probed here (4 puff/min).

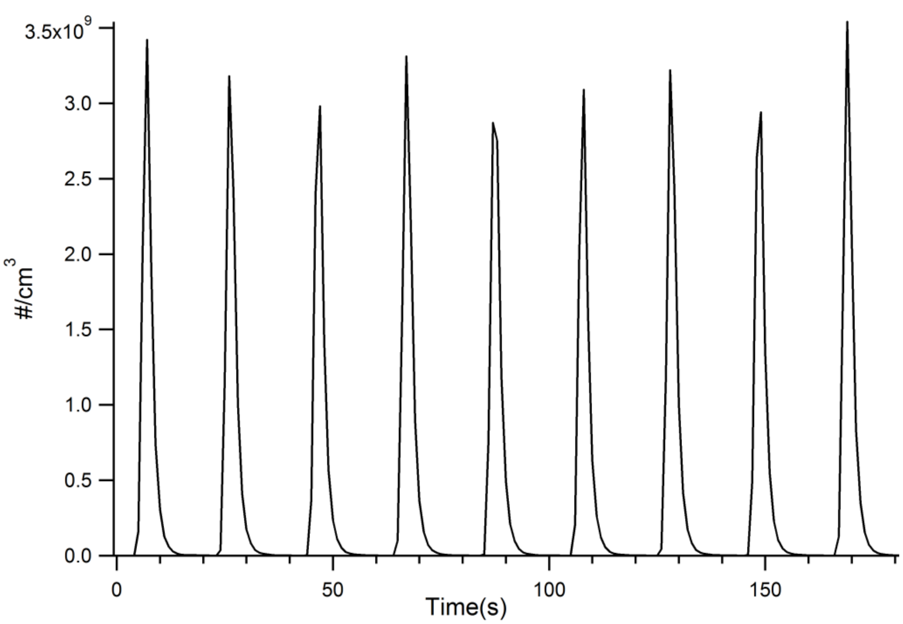

Figure S6. Puff frequency dependence of selected VOCs emitted by 1R5F in fast flow tube experiments. There is no quantifiable difference in the VOCs in the cigarettes for different puff frequencies.

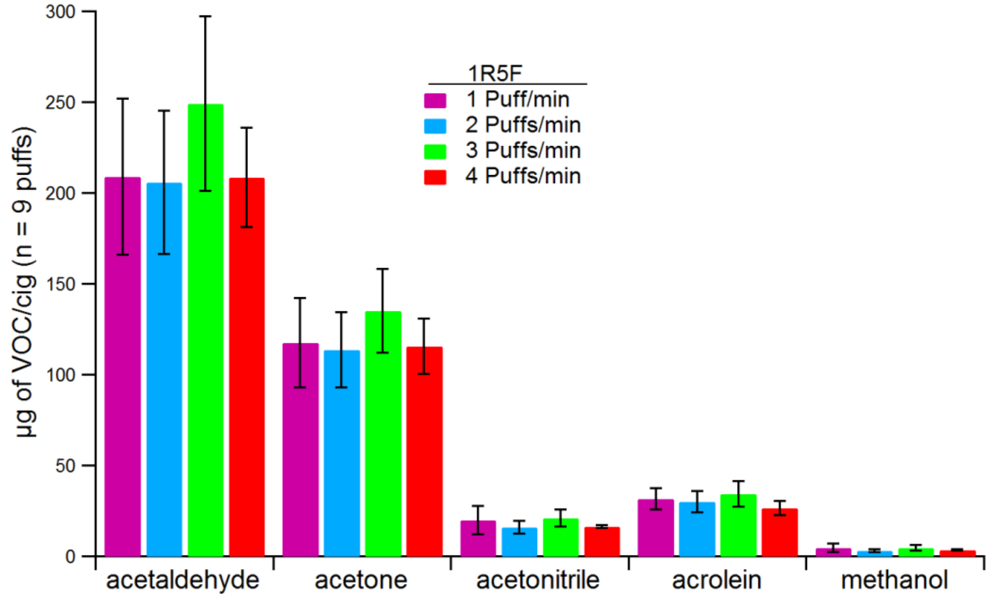

Figure S7. Puff frequency dependence of the number of particles emitted in fast flow tube experiments. The particle concentration similarly has no puff frequency dependence except for menthol light-5 and original-5 where the 1 puff/min frequency had somewhat larger particle emissions than the other frequencies.

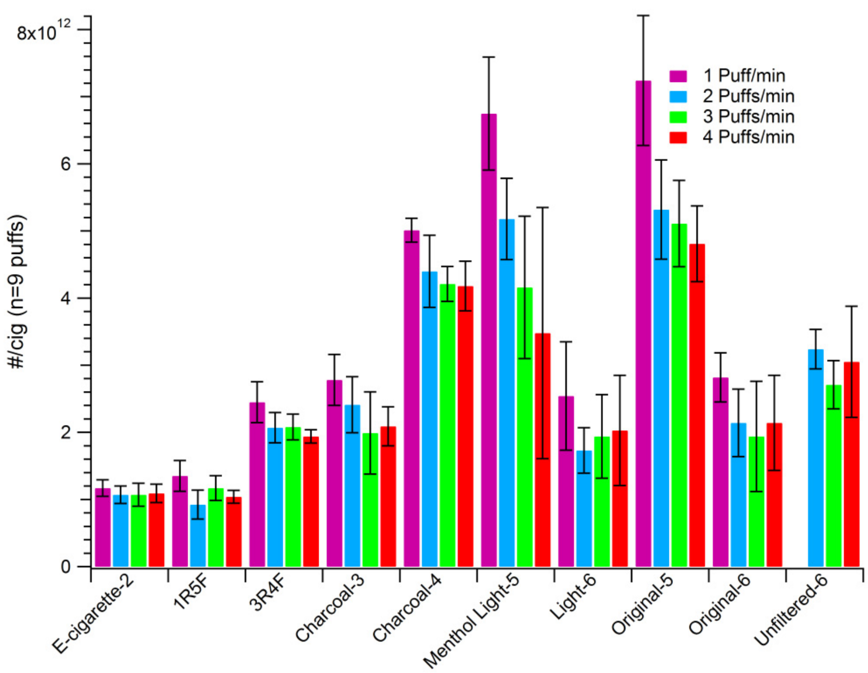

Figure S8. Amount of selected VOCs in conventional cigarettes for a puff frequency of 2 puffs/min in fast flow tube experiments.

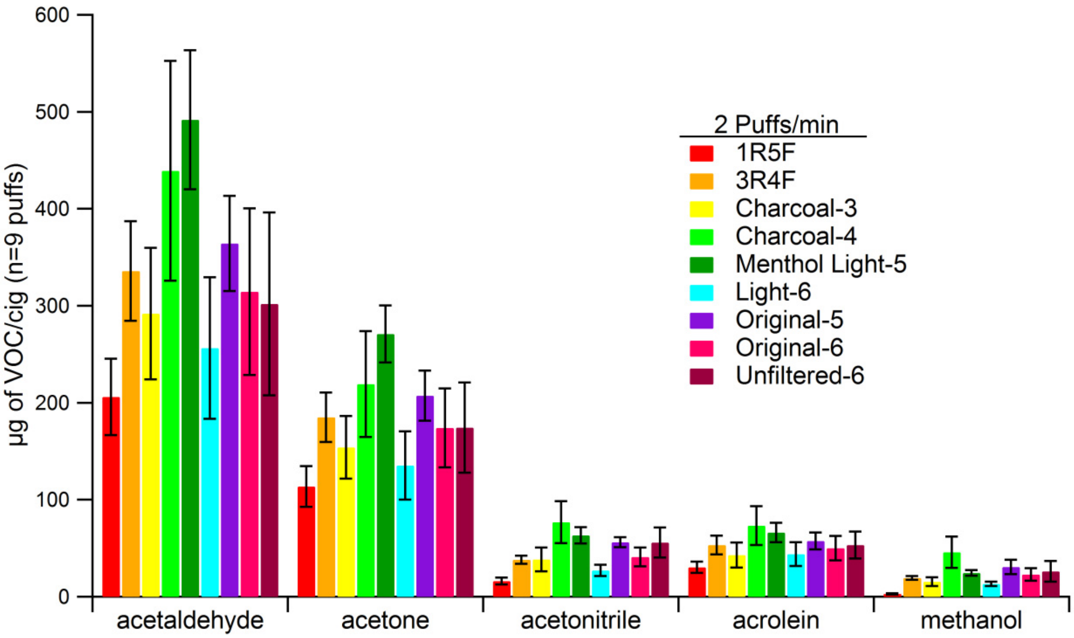

Table S1. Amount (µg in 9 puffs) of selected VOCs emitted by conventional cigarettes for n=3 samples and (standard deviation) for a puff frequency of 2 puffs/min in fast flow tube experiments.

VOC (2 puffs/min)	Acetaldehyde	Acetone	Acetonitrile	Acrolein	Methanol
1R5F	206 (40)	114 (21)	16.1 (3.7)	30.2 (5.8)	2.96 (0.69)
3R4F	336 (52)	185 (25)	38.3 (4.2)	53.2 (9.7)	19.5 (2.0)
charcoal-3	292 (68)	154 (32)	38.4 (12.3)	43.1 (12.9)	15.4 (4.5)
charcoal-4	439 (113)	219 (55)	76.8 (21.8)	73.4 (20.0)	45.9 (16.3)
menthol light-5	492 (72)	271 (29)	63.3 (8.3)	66.4 (10.2)	24.6 (3.0)
light-6	256 (73)	135 (35)	27.2 (5.8)	43.9 (12.3)	13.4 (2.2)
original-5	364 (49)	207 (26)	56.1 (5.1)	57.4 (8.6)	30.8 (7.3)
original-6	315 (86)	174 (41)	40.9 (9.8)	50.1 (12.6)	22.8 (6.6)
unfiltered-6	302 (94)	175 (46)	56.0 (15.6)	53.4 (13.9)	26.2 (10.8)

Figure S9. Amount of selected VOCs in conventional cigarettes for a puff frequency of 3 puffs/min in fast flow tube experiments.

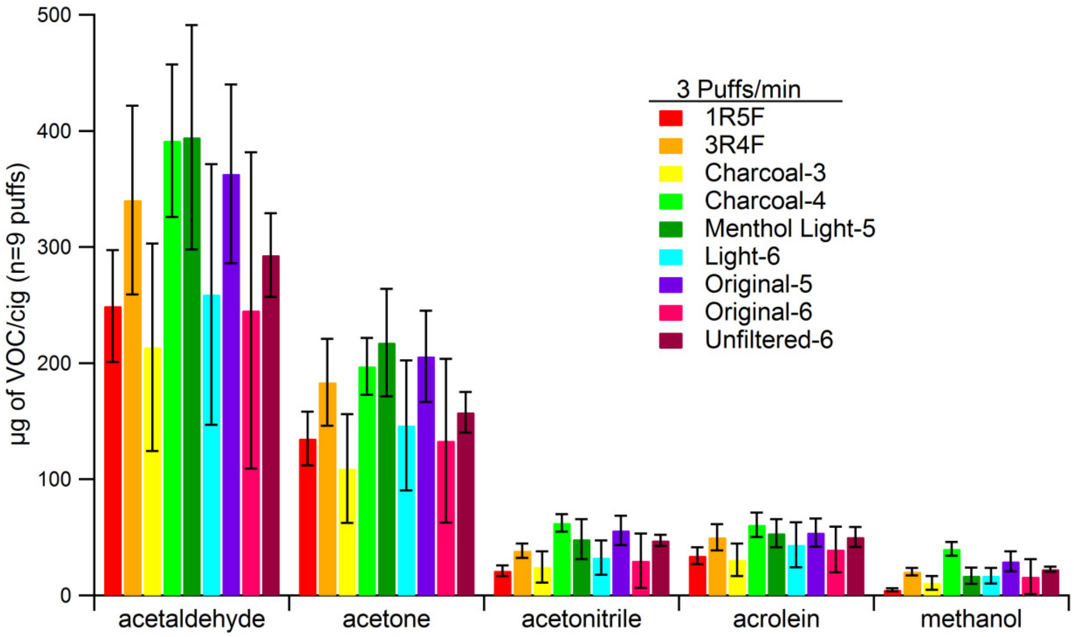

Table S2. Amount (µg in 9 puffs) of selected VOCs emitted by conventional cigarettes for n=3 samples and (standard deviation) for a puff frequency of 3 puffs/min in fast flow tube experiments.

VOC (3 puffs/min)	Acetaldehyde	Acetone	Acetonitrile	Acrolein	Methanol
1R5F	249 (48)	135 (23)	21.2 (4.7)	34.3 (7.2)	4.76 (1.37)
3R4F	341 (81)	184 (38)	38.6 (6.2)	50.0 (11.3)	20.6 (3.3)
charcoal-3	214 (89)	109 (47)	24.5 (13.5)	30.6 (14.0)	10.7 (5.9)
charcoal-4	392 (66)	197 (24)	62.4 (7.7)	60.9 (5.9)	40.0 (5.9)
menthol light-5	395 (97)	218 (46)	48.3 (17.2)	53.7 (12.2)	17.0 (6.9)
light-6	259 (112)	147 (56)	32.5 (14.8)	43.6 (19.3)	16.8 (6.8)
original-5	363 (77)	206 (39)	55.8 (12.6)	54.0 (12.0)	29.4 (8.5)
original-6	245 (136)	133 (70)	29.8 (23.4)	39.6 (19.8)	16.1 (15.2)
unfiltered-6	293 (36)	158 (18)	47.3 (4.8)	50.4 (8.7)	22.5 (2.2)

Figure S10. Amount of selected VOCs in conventional cigarettes for a puff frequency of 4 puffs/min in fast flow tube experiments.

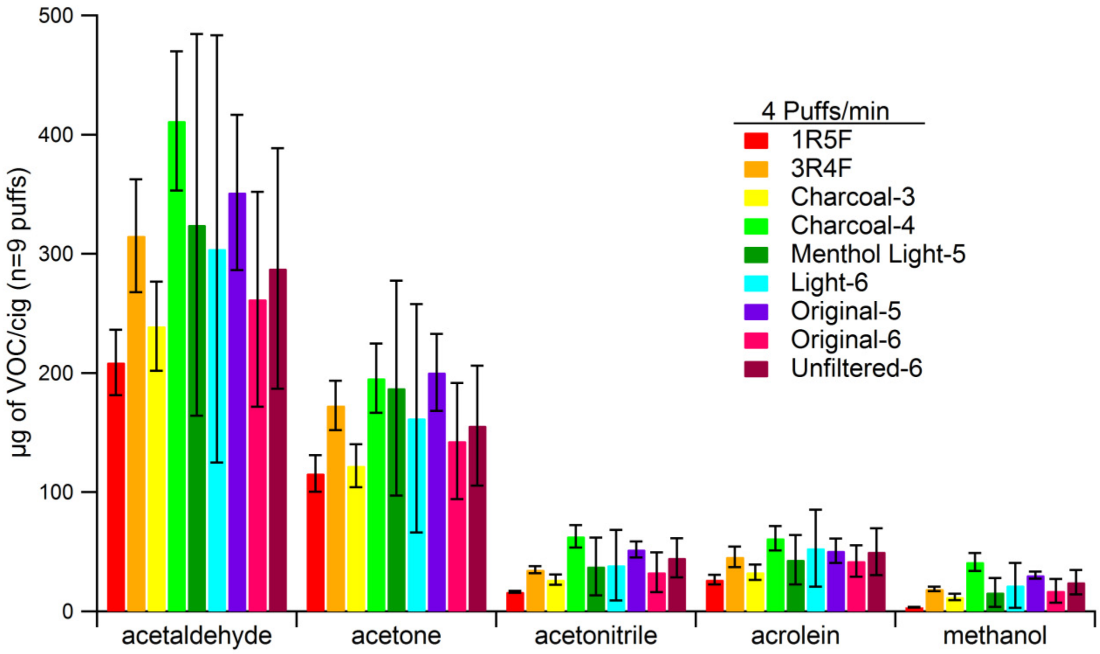

Table S3. Amount (µg in 9 puffs) of selected VOCs emitted by conventional cigarettes for n=3 samples and (standard deviation) for a puff frequency of 4 puffs/min in fast flow tube experiments.

VOC (4 puffs/min)	Acetaldehyde	Acetone	Acetonitrile	Acrolein	Methanol
1R5F	208.7 (27.4)	115 (15)	16.3 (0.8)	26.7 (4.1)	3.40 (0.27)
3R4F	315 (47)	173 (21)	35.1 (2.9)	45.6 (8.6)	19.0 (2.0)
charcoal-3	239 (37)	122 (18)	26.7 (4.2)	32.8 (6.5)	12.2 (2.7)
charcoal-4	411 (58)	196 (29)	62.9 (9.3)	61.4 (10.2)	41.3 (7.5)
menthol light-5	324 (160)	187 (90)	37.6 (24.2)	43.3 (20.7)	15.9 (12.0)
light-6	304 (179)	162 (96)	38.8 (29.6)	52.9 (32.4)	21.8 (18.8)
original-5	351 (65)	200 (32)	51.9 (6.7)	50.8 (10.4)	30.4 (3.0)
original-6	262 (90)	142.9 (48.7)	33.0 (16.6)	42.2 (13.3)	17.2 (10.0)
unfiltered-6	288 (101)	156 (50)	44.8 (16.5)	50.1 (19.6)	24.4 (10.2)