

Supplementary Information

A headspace collection chamber for whole body volatilomics

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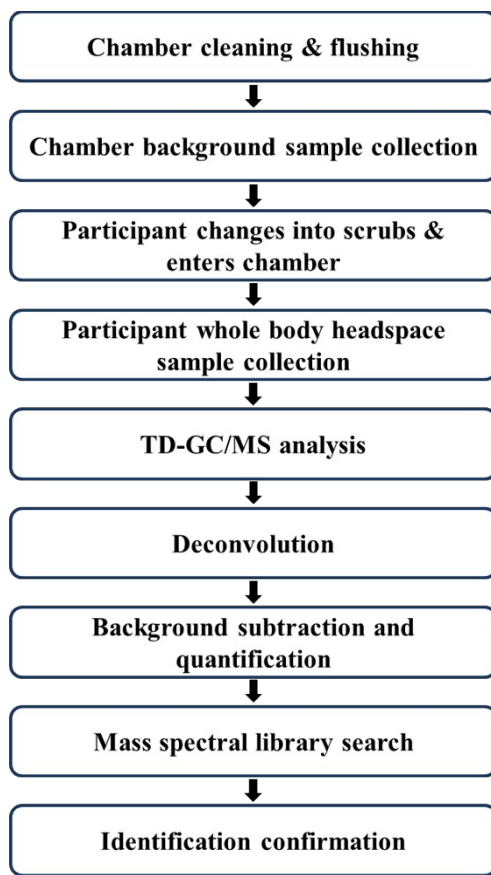


Figure S1. Schematic of the experimental workflow.

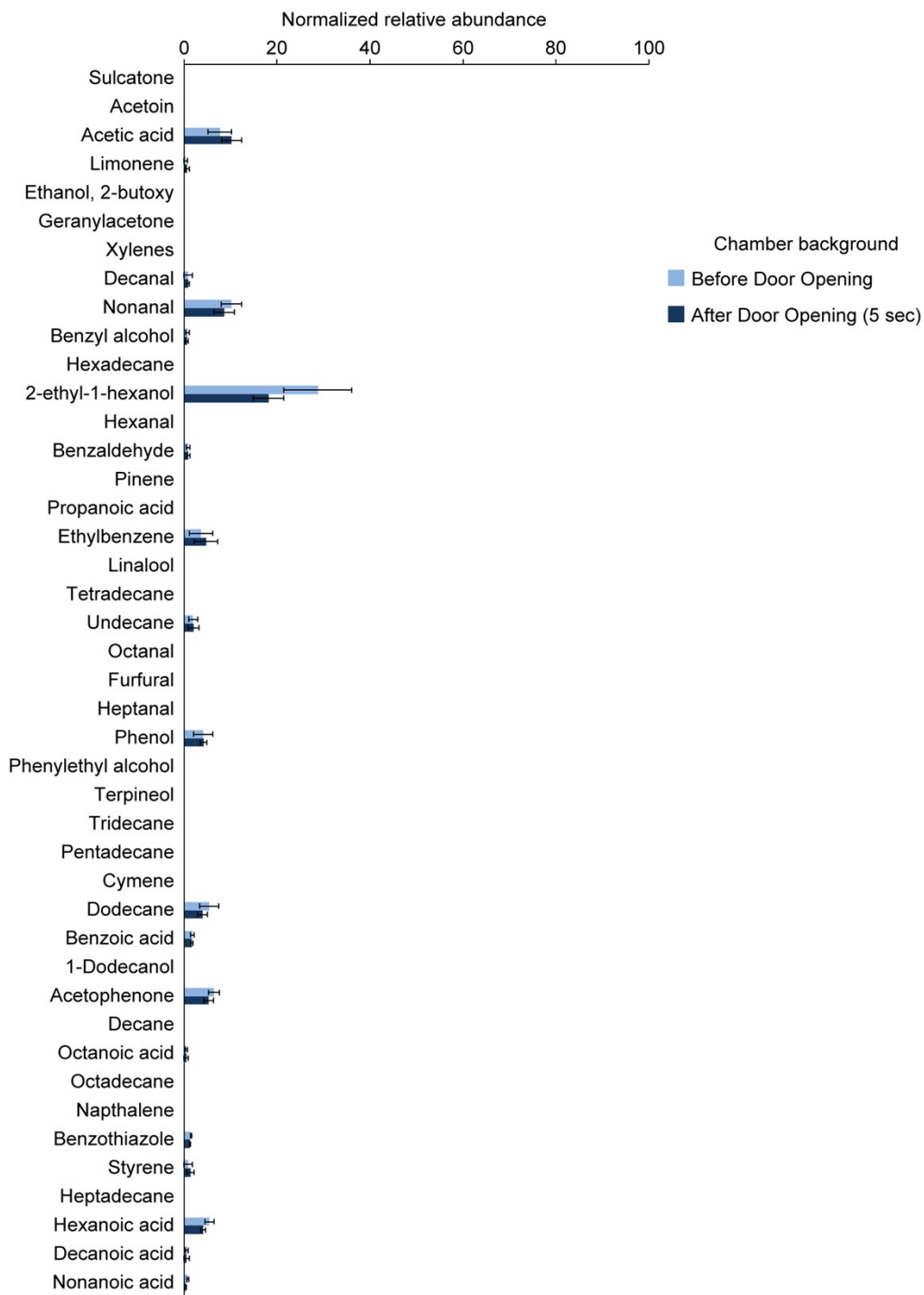


Figure S2. Normalized abundance of background traces of all human VOCs detected in the chamber background before and after opening the chamber door for 5 seconds. The majority of human VOCs were not detected in the background traces. Normalized to internal standard, standard error bars, n = 3.

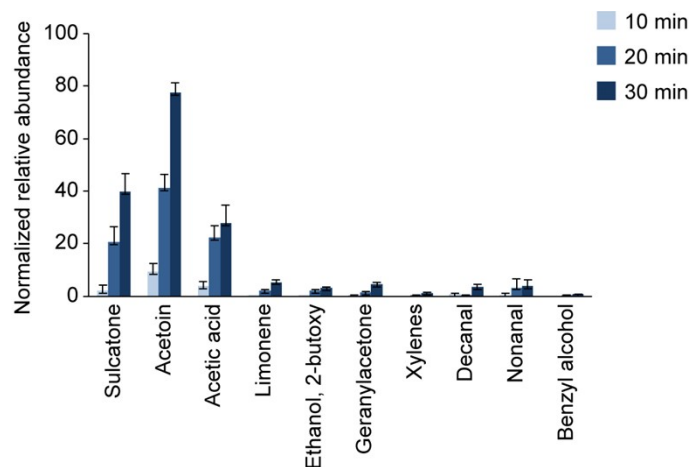


Figure S3. Normalized abundance of ten most abundant human VOCs sampled for 10, 20 and 30 minutes from a single participant. Normalized to internal standard, standard error bars, n = 3.

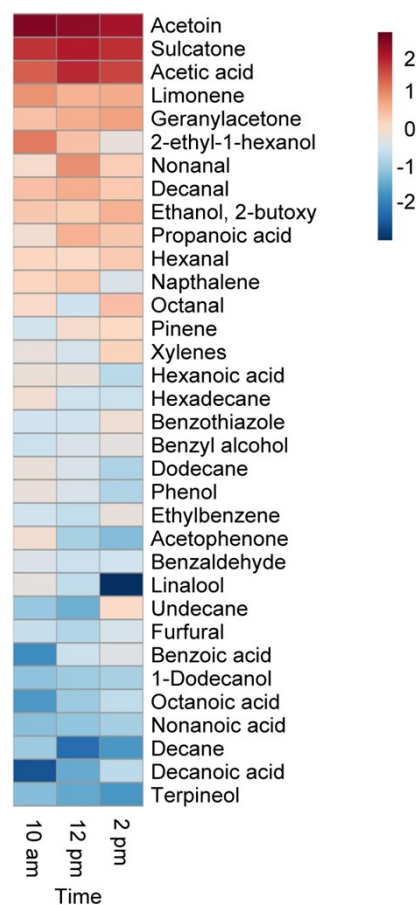


Figure S4. Human whole body odor sampled from a single participant at 10am, 12pm and 2pm. Normalized to internal standard. n = 3 for 10 and 20 minute timepoints, n = 6 for 30 minute timepoints.

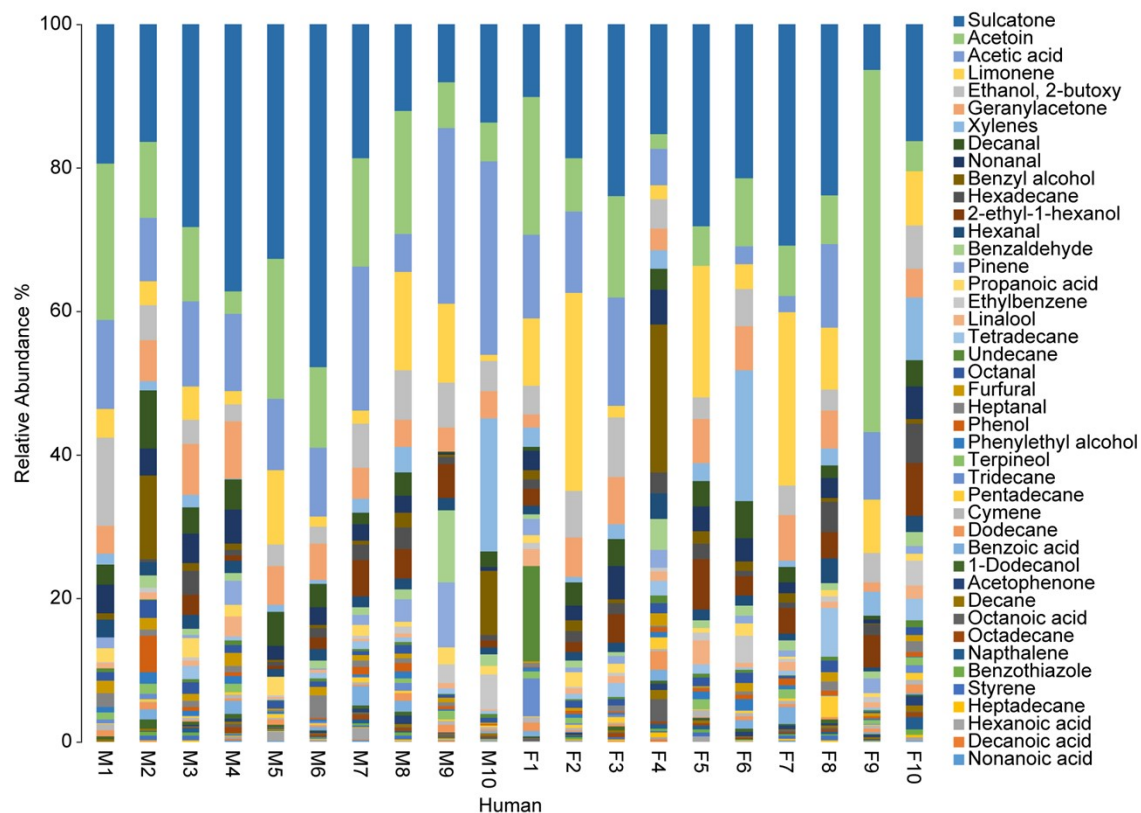


Figure S5. Relative abundances of 43 volatile organic compounds detected in whole body headspace from humans. Columns represent relative VOC signatures from individual humans, with compounds organized approximately from most to least abundant. n = 20 participants. M = male, F = female.

Table S1. Sampling chamber and blood oxygen levels across 10 participants at the start (0 mins) and end (30 mins) of whole body headspace sampling.

Participant	Sex	Weight (kg)	Starting Chamber O2 (%)	Ending Chamber O2 (%)	Chamber O2 Change (%)	Starting SpO2 (%)	Ending SpO2 (%)	SpO2 Change (%)
1	Female	48	20.9	20.9	0	99	98	-1
2	Male	111	20.9	20.3	0.6	95	97	+2
3	Male	79	20.9	20.9	0	98	97	-1
4	Female	68	20.9	20.9	0	97	97	0
5	Female	68	20.9	20.9	0	99	97	-2
6	Female	45	20.9	20.9	0	97	98	+1
7	Female	61	20.9	20.9	0	99	98	-1
8	Female	59	20.9	20.9	0	97	98	+1
9	Female	61	20.9	20.9	0	99	98	-1
10	Male	67	20.9	20.9	0	98	98	0

Table S2. Cohort metadata including sex, height, weight, smoking/vaping behavior, sampling time, CO₂ emission rate, total CO₂ concentration in the headspace collection chamber at the end of 30 min sampling period, and the mean number of MS features detected in background (BG) and whole body (WB) headspace (inclusive of background) from each participant. The mean number of MS features from WB samples with NIST library hits are denoted.

Participant	Sex	Height (cm)	Weight (kg)	Smokes/Vapes	Sampling Time	CO ₂ Emissions (ppm/min)	CO ₂ Total Concentration (ppm)	Mean BG Features	Mean WB Features	Mean WB Features with NIST Hits
M1	Male	192	113	No	10:00	197	6407	913	1140	371
M2	Male	185	82	No	10:00	147	4834	940	1110	358
M3	Male	180	73	No	10:00	139	4601	934	1079	352
M4	Male	186	76	Occasionally vapes	10:00	132	4349	869	1030	333
M5	Male	173	64	No	13:00	157	5096	711	827	274
M6	Male	183	68	No	10:00	119	3986	733	797	269
M7	Male	183	73	No	12:00	117	3913	716	882	293
M8	Male	185	104	No	9:00	196	6317	780	945	319
M9	Male	178	91	No	10:00	154	5057	863	945	322
M10	Male	173	77	No	9:00	140	4648	824	907	306
F1	Female	168	64	No	10:00	116	3934	892	1093	355
F2	Female	176	64	No	10:00	134	4409	888	1110	373
F3	Female	163	68	No	10:00	126	4186	905	1046	341
F4	Female	178	78	No	9:00	119	3984	849	1030	339
F5	Female	158	50	No	9:00	89	3130	811	965	324

F6	Female	169	68	No	10:00	137	4567	844	1017	334
F7	Female	178	68	Occasionally vapes	10:00	149	4888	754	933	315
F8	Female	157	60	No	13:00	104	3548	750	873	295
F9	Female	165	69	No	10:00	104	3581	808	965	322
F10	Female	163	88	No	10:00	126	4207	640	960	319