Supporting information of *Technical note: Identification and quantification of gaseous and particulate organic compounds from cooking fumes by comprehensive two-dimensional gas chromatography-mass spectrometry*

Yuanzheng Gong[1,#], Kai Song[1,#], Song Guo[1,2,*], Daqi Lv[1], Yuan Zhang[1], Zichao Wan[1], Wenfei Zhu[1], Hui Wang[1], Ying Yu[1], Rui Tan[1], Ruizhe Shen[1], Sihua Lu[1], Shuangde Li[3], Yunfa Chen[3]

[1] State Key Joint Laboratory of Environmental Simulation and Pollution Control, International Joint Laboratory for Regional Pollution Control, Ministry of Education (IJRC), College of Environmental Sciences and Engineering, *Beijing* 100871, China

[2] Collaborative Innovation Center of Atmospheric Environment and Equipment Technology, Nanjing University of Information Science & Technology, *Nanjing* 210044, China

[3] State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, *Beijing* 100190, China

[#] These authors contribute equally

* **Correspondence:** Song Guo: songguo@pku.edu.cn

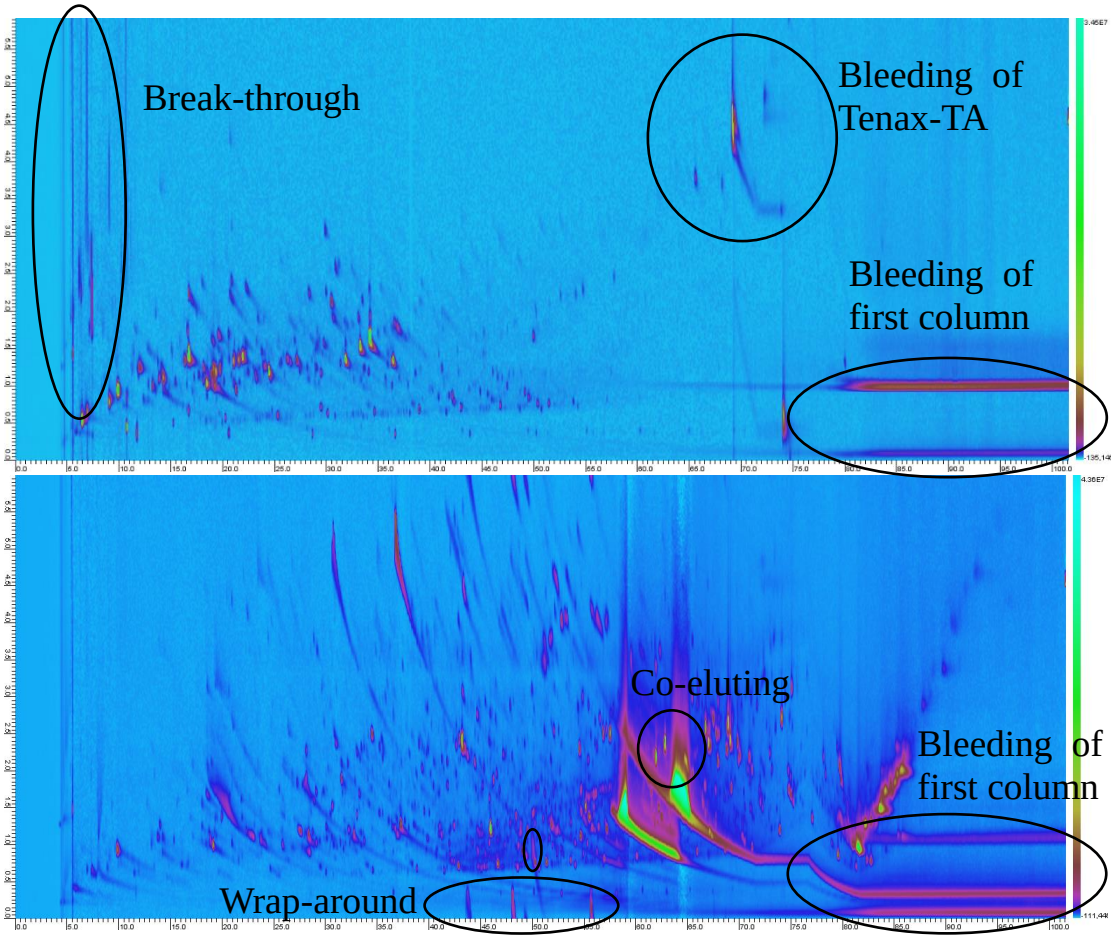

Figure S1. GCxGC chromatogram of gaseous and particulate sample emitting from fried chicken fumes.

The GCxGC chromatogram of gaseous and particulate organics emitting from fried chicken fumes are shown in Figure **S1**. Strong break-through represents in the gaseous sample for hexane and heptane as the thermo-modulator used was an electronic refrigerator with a cooling limit of -74 ℃, which cannot freeze and concentrate hexane and heptane well. In addition, some lactams in particulate samples wrapped around (i.e. the 2-D retention time of the compounds are larger than the modulation time 6s and the blobs locate at a weak-polar area). These blobs are very broad in the second dimension but most compounds besides hexahydropyrrolo[1,2-a]pyrazine-1,4-dione don't overlap with weak-polar compounds. Hence the wrap-around effects do not influence the quantification of most compounds. And the TIC response of hexahydropyrrolo[1,2-a]pyrazine-1,4-dione was carefully calculated by deducing the contribution made by the co-elute heptadecane. Fatty acids are predominant in particulate samples, of which the blobs are so large that cover several other compounds such as hexadecanamide and 9(*Z*)-octadecenenitrile. Compounds with authentic standards like hexadecanamide can be quantified with quantifier ions which are seldom influenced by the overlapped fatty acids, while compounds without authentic standards are quantified using TIC response deduced from the response of its quantifier ion and the ratio of quantifier to TIC in the NIST library. Bleedings of Tenax-TA and first column are not quantified as they are not targets from cooking fumes.

Tables

Table S1. The retention time, calibration curve, R^2, linear range and RSD of different concentration levels of authentic standards.

Table S2. The amounts of selected standards calculated by standard curves and surrogate standard curves and the difference of the semi-quantitative method.

Table S3. The retention time and concentrations of identified organics in both gaseous and particulate samples.

Table S1. The retention time, calibration curve, R^2, linear range and RSD of different concentration levels of authentic standards.

compound	1-D R.T.	2-D R.T.	slope	intercept	R^2	Linear range	RSD(n=5) 4ng	20ng	40ng	60ng	200ng
acids											
Benzoic acid	28.8	1.17	250343	-6847795	0.971	4-200ng	n.d.	n.d.	28.9%	n.d.	4.3%
Heptanoic acid	33.0	1.05	2131	-3755	0.805	4-200ng	n.d.	n.d.	n.d.	n.d.	n.d.
Phthalic anhydride	33.2	2.58	231389	22202135	0.981	4-200ng	n.d.	n.d.	6.3%	n.d.	36.0%
Undecanoic acid	59.8	1.14	812	5935	0.970	4-200ng	n.d.	n.d.	n.d.	n.d.	n.d.
aldehydes											
Hexanal	9.9	0.84	428427	9717187	0.972	4-200ng	n.d.	n.d.	2.5%	n.d.	3.3%
Heptanal	14.3	0.84	465836	8589705	0.961	4-200ng	13.7%	n.d.	1.0%	n.d.	3.3%
Benzaldehyde	16.8	1.68	440370	13599045	0.968	4-200ng	24.4%	n.d.	1.9%	n.d.	4.4%
Octanal	19.3	0.84	559030	6559260	0.992	4-200ng	2.6%	n.d.	5.2%	n.d.	3.3%
Nonanal	24.5	0.81	281558	13319080	0.977	4-200ng	5.1%	n.d.	1.5%	n.d.	2.4%
Decanal	29.5	0.78	338030	15966783	0.975	4-200ng	0.8%	n.d.	1.8%	n.d.	2.5%
Citral	32.2	1.05	338504	4634663	0.988	4-200ng	n.d.	n.d.	4.0%	n.d.	1.8%
Dodecanal	38.4	0.48	829420	7367850	0.980	4-200ng	4.9%	n.d.	1.4%	n.d.	5.8%
alkanols											
1-Butanol	6.3	0.54	173641	18107050	0.973	4-200ng	n.d.	n.d.	2.1%	n.d.	6.2%
1-Butanol, 3-methyl-	7.9	0.66	539780	8579677	0.996	4-200ng	18.1%	n.d.	1.5%	n.d.	5.1%
1-Hexanol	13.1	0.81	448439	3807097	0.991	4-200ng	n.d.	n.d.	6.7%	n.d.	3.9%
Benzyl alcohol	20.8	1.62	464912	8209089	0.979	4-200ng	n.d.	n.d.	4.3%	n.d.	1.9%
1-Hexanol, 2-ethyl-	21.1	0.72	34496	27524926	0.963	4-200ng	7.2%	n.d.	24.9%	n.d.	3.8%
Phenylethyl Alcohol	24.7	1.62	502037	20235693	0.973	4-200ng	n.d.	n.d.	5.1%	n.d.	1.6%
1-Dodecanol	41.2	0.72	1030789	2210803	0.996	4-200ng	67.7%	n.d.	1.9%	n.d.	2.5%
alkenols											

compound	1-D R.T.	2-D R.T.	slope	intercept	R^2	Linear range	RSD(n=5) 4ng	20ng	40ng	60ng	200ng
Linalool	24.5	0.75	46187	5109924	0.979	4-200ng	n.d.	n.d.	15.2%	n.d.	6.8%
Citronellol	30.7	0.81	552899	4042779	0.989	4-200ng	16.5%	n.d.	3.5%	n.d.	3.8%
amides											
Caprolactam	30.9	2.79	495849	14426984	0.958	4-200ng	n.d.	n.d.	22.7%	n.d.	4.8%
Hexadecanamide	96.8	2.16	83503	-646915	0.961	4-200ng	n.d.	n.d.	n.d.	n.d.	n.d.
aromatics											
Toluene	9.2	0.75	443121	4846746	0.998	4-100ng	5.7%	5.2%	n.d.	4.1%	n.d.
Ethylbenzene	13.0	0.87	415866	9506163	0.996	4-100ng	6.6%	3.2%	n.d.	6.1%	n.d.
Benzene, 1,3-dimethyl-	13.3	0.84	702273	21421131	0.973	4-100ng	4.7%	2.5%	n.d.	5.7%	n.d.
Styrene	14.1	1.02	472665	8554263	0.999	4-100ng	n.d.	5.9%	n.d.	7.5%	n.d.
o-Xylene	14.3	0.93	395014	12307653	0.975	4-100ng	4.6%	2.5%	n.d.	3.9%	n.d.
Benzene, (1-methylethyl)-	15.8	0.84	635195	8419191	0.986	4-100ng	4.2%	1.7%	n.d.	2.1%	n.d.
Benzene, propyl-	17.4	0.84	478544	9944618	0.972	4-100ng	3.2%	1.9%	n.d.	4.0%	n.d.
esters											
n-Propyl acetate	7.4	0.6	358155	11228820	0.977	4-200ng	3.3%	n.d.	2.7%	n.d.	16.3%
sec-Butyl acetate	8.8	0.63	556400	5542265	0.991	4-200ng	5.3%	n.d.	4.9%	n.d.	5.1%
Butanoic acid, ethyl ester	10.2	0.72	462753	7566755	0.980	4-200ng	5.7%	n.d.	2.5%	n.d.	3.7%
1-Butanol, 3-methyl-, acetate	13.5	0.75	614255	8680932	0.978	4-200ng	3.4%	n.d.	5.3%	n.d.	2.4%
Acetic acid, hexyl ester	19.3	0.72	477741	3406899	0.989	4-200ng	15.0%	n.d.	5.8%	n.d.	2.6%
Acetic acid, phenylmethyl ester	27.1	1.47	610322	6465680	0.995	4-200ng	10.5%	n.d.	4.2%	n.d.	2.9%
Benzeneacetic acid, ethyl ester	30.9	1.41	265875	15735816	0.986	4-200ng	2.3%	n.d.	5.7%	n.d.	3.5%
Acetic acid, 2-phenylethyl ester	31.4	1.38	647480	8130532	0.980	4-200ng	5.3%	n.d.	2.9%	n.d.	2.0%
Linalyl acetate	32.0	0.72	198923	6751661	0.980	4-200ng	12.8%	n.d.	7.7%	n.d.	5.9%
Dimethyl phthalate	39.6	1.95	350836	3614714	0.989	4-100ng	2.9%	2.8%	n.d.	4.2%	n.d.

compound	1-D R.T.	2-D R.T.	slope	intercept	R^2	Linear range	RSD(n=5) 4ng	20ng	40ng	60ng	200ng
Diethyl Phthalate	45.1	1.68	371204	1488632	0.980	4-100ng	7.8%	3.2%	n.d.	2.4%	n.d.
Benzyl Benzoate	51.5	2.01	830246	6059710	0.990	4-200ng	3.8%	n.d.	1.8%	n.d.	2.5%
Dibutyl phthalate	57.7	1.5	328509	15297024	0.975	4-100ng	6.6%	1.3%	n.d.	1.7%	n.d.
Benzyl butyl phthalate	68.9	2.4	459157	8652860	0.975	4-100ng	7.8%	3.0%	n.d.	5.9%	n.d.
Hexanedioic acid, bis(2-ethylhexyl) ester	70.6	1.14	649694	4949450	0.986	4-200ng	6.3%	n.d.	3.9%	n.d.	3.7%
Bis(2-ethylhexyl) phthalate	74.6	2.28	731246	6634275	0.991	4-100ng	16.7%	3.0%	n.d.	5.3%	n.d.
Di-N-octyl phthalate	80.0	1.44	919796	3612301	0.986	4-100ng	18.1%	3.0%	n.d.	5.0%	n.d.
ketones											
Cyclohexanone	13.5	1.59	707182	5939017	0.997	4-200ng	1.9%	n.d.	5.6%	n.d.	3.2%
3-Heptanone	13.7	0.81	286135	9024371	0.978	4-200ng	32.1%	n.d.	1.9%	n.d.	3.1%
2-Heptanone	13.9	0.87	292003	35369085	0.965	4-200ng	22.3%	n.d.	5.0%	n.d.	6.4%
5-Hepten-2-one, 6-methyl-	18.4	0.96	458266	11114987	0.972	4-200ng	6.5%	n.d.	2.6%	n.d.	2.2%
Acetophenone	22.2	1.68	591155	15979443	0.987	4-200ng	12.9%	n.d.	2.1%	n.d.	4.8%
Isophorone	25.0	1.32	487756	6832225	0.975	4-100ng	2.2%	0.9%	n.d.	8.6%	n.d.
Camphor	26.4	1.23	195385	22259055	0.955	4-200ng	n.d.	n.d.	4.6%	n.d.	4.8%
Quinoline	30.6	2.01	637795	8612696	0.988	4-200ng	5.1%	n.d.	5.4%	n.d.	2.4%
alkanes and alkenes											
C7	7.4	0.33	146035	3133309	0.986	4-100ng	20.3%	30.7%	n.d.	96.3%	n.d.
C8	10.7	0.39	784938	4737945	0.990	4-100ng	7.7%	2.8%	n.d.	5.5%	n.d.
C9	15.2	0.39	292422	18633044	0.978	4-100ng	7.6%	2.5%	n.d.	1.8%	n.d.
C10	20.2	0.42	598582	9039032	0.976	4-100ng	6.1%	2.9%	n.d.	2.1%	n.d.
C11	25.3	0.42	257733	17282643	0.967	4-100ng	2.3%	2.1%	n.d.	4.1%	n.d.
C12	30.1	0.42	511216	9518454	0.975	4-100ng	2.8%	1.4%	n.d.	2.2%	n.d.
C13	34.6	0.42	609010	10636341	0.980	4-100ng	0.8%	1.2%	n.d.	1.7%	n.d.

compound	1-D R.T.	2-D R.T.	slope	intercept	R^2	Linear range	RSD(n=5) 4ng	20ng	40ng	60ng	200ng
C14	38.9	0.42	483085	11803587	0.986	4-100ng	0.8%	1.2%	n.d.	2.1%	n.d.
C15	42.9	0.45	577509	24698431	0.987	4-100ng	3.8%	0.4%	n.d.	3.6%	n.d.
C16	46.7	0.45	539434	27472675	0.991	4-100ng	1.6%	0.9%	n.d.	4.1%	n.d.
C17	50.3	0.45	863756	17858175	0.978	4-100ng	2.4%	1.7%	n.d.	4.9%	n.d.
C18	53.8	0.48	409603	25656993	0.974	4-100ng	3.0%	1.7%	n.d.	3.7%	n.d.
C19	57.0	0.48	424592	19678887	0.974	4-100ng	1.3%	1.5%	n.d.	2.9%	n.d.
C20	60.1	0.51	587255	8079682	0.989	4-100ng	2.2%	1.6%	n.d.	9.5%	n.d.
C21	63.1	0.51	738093	10204776	0.979	4-100ng	3.0%	0.9%	n.d.	4.8%	n.d.
C22	66.0	0.54	703648	11095092	0.976	4-100ng	2.6%	0.8%	n.d.	5.6%	n.d.
C23	68.9	0.57	530361	19584994	0.971	4-100ng	3.8%	1.1%	n.d.	2.7%	n.d.
C24	71.3	0.72	852644	15234240	0.992	4-100ng	4.5%	1.5%	n.d.	5.4%	n.d.
C25	74.2	0.93	907839	15516191	0.983	4-100ng	9.1%	1.2%	n.d.	4.8%	n.d.
C26	77.1	0.78	1090682	9247177	0.992	4-100ng	15.1%	2.8%	n.d.	4.1%	n.d.
C27	80.2	0.63	909060	11372911	0.995	4-100ng	10.3%	1.3%	n.d.	3.4%	n.d.
C28	83.3	0.78	1030031	5203146	0.990	4-100ng	9.4%	0.9%	n.d.	5.4%	n.d.
C29	86.4	0.93	1253914	-1134576	0.973	4-100ng	10.3%	1.8%	n.d.	3.5%	n.d.
C30	89.5	1.17	1420611	-8453663	0.994	4-100ng	11.1%	4.1%	n.d.	4.9%	n.d.
C31	92.6	1.41	1304834	-2319492	0.994	4-100ng	7.2%	3.4%	n.d.	5.7%	n.d.
C32	95.7	1.74	1379389	-12026336	0.993	4-100ng	3.9%	5.3%	n.d.	5.8%	n.d.
Cyclohexane, octyl-	40.9	0.54	357541	16843976	0.991	4-200ng	3.7%	n.d.	0.6%	n.d.	2.5%
3-Carene	21.4	0.66	218769	10384090	0.987	4-200ng	1.3%	n.d.	3.7%	n.d.	3.0%
N-compounds											
1-Propanamine, N-nitroso-N-propyl-	22.5	1.26	326597	10974780	0.996	4-100ng	4.9%	1.1%	n.d.	11.4%	n.d.
Benzene, nitro-	23.1	1.8	362708	6222925	0.984	4-100ng	n.d.	1.0%	n.d.	5.5%	n.d.

compound	1-D R.T.	2-D R.T.	slope	intercept	R^2	Linear range	RSD(n=5) 4ng	20ng	40ng	60ng	200ng
Indole	32.8	2.28	627410	6842884	0.998	4-200ng	10.0%	n.d.	3.7%	n.d.	2.4%
Carbazole	54.0	2.7	1063918	7272520	0.991	4-100ng	8.0%	1.1%	n.d.	3.5%	n.d.
Benzonitrile	17.7	1.89	437203	8219380	0.978	4-200ng	8.2%	n.d.	2.1%	n.d.	3.6%
PAHs											
Naphthalene	28.5	1.56	343479	19347461	0.987	4-100ng	2.2%	3.1%	n.d.	1.3%	n.d.
Naphthalene, 2-methyl-	33.6	1.44	862618	16797341	0.975	4-100ng	3.7%	3.0%	n.d.	4.6%	n.d.
Acenaphthylene	40.1	1.89	452774	7766843	0.991	4-100ng	3.7%	1.6%	n.d.	3.4%	n.d.
Acenaphthene	41.4	1.8	523720	11138693	0.986	4-100ng	0.5%	1.1%	n.d.	2.5%	n.d.
Fluorene	45.3	1.8	835221	7374597	0.992	4-100ng	0.9%	0.9%	n.d.	2.4%	n.d.
Azobenzene	46.7	1.71	376963	6555488	0.988	4-100ng	4.7%	2.3%	n.d.	3.5%	n.d.
Phenanthrene	52.5	2.19	533657	8641899	0.984	4-100ng	2.3%	2.0%	n.d.	5.6%	n.d.
Anthracene	52.8	2.16	677343	12322203	0.992	4-100ng	2.8%	2.7%	n.d.	1.8%	n.d.
Fluoranthene	61.3	2.46	702143	14392382	0.985	4-100ng	3.2%	1.3%	n.d.	3.8%	n.d.
Pyrene	62.8	2.7	759231	18389814	0.978	4-100ng	4.0%	1.4%	n.d.	3.2%	n.d.
Benz[a]anthracene	72.0	4.17	545969	13969649	0.987	4-100ng	17.2%	2.5%	n.d.	5.1%	n.d.
Chrysene	72.3	4.38	779638	20110086	0.979	4-100ng	4.9%	1.0%	n.d.	1.9%	n.d.
Benzo[b]fluoranthene	81.4	3.78	1508220	19731914	0.975	4-100ng	4.5%	3.2%	n.d.	7.3%	n.d.
Benzo[k]fluoranthene	85.5	4.89	829561	15533128	0.986	4-100ng	n.d.	0.4%	n.d.	5.6%	n.d.
Indeno[1,2,3-cd]pyrene	93.6	3.45	1928464	-20525563	0.977	4-100ng	n.d.	9.0%	n.d.	24.4%	n.d.
Benzo[ghi]perylene	95.5	5.43	1197192	4235210	0.996	4-100ng	n.d.	8.0%	n.d.	16.9%	n.d.
phenols											
Phenol	18.6	1.29	181376	2256806	0.965	4-100ng	n.d.	6.7%	n.d.	6.8%	n.d.
Phenol, 2-methyl-	22.2	1.29	426215	-8029785	0.987	4-200ng	6.4%	n.d.	2.3%	n.d.	2.1%
Phenol, 3-methyl-	23.4	1.38	792593	-13245628	0.993	4-200ng	10.5%	n.d.	2.2%	n.d.	1.4%

compound	1-D R.T.	2-D R.T.	slope	intercept	R^2	Linear range	RSD(n=5) 4ng	20ng	40ng	60ng	200ng
Phenol, 2,6-dimethyl-	24.5	1.38	370168	23598090	0.984	4-200ng	5.1%	n.d.	2.4%	n.d.	6.1%
Resorcinol	32.8	1.92	480783	-4239934	0.972	4-200ng	n.d.	n.d.	1.7%	n.d.	1.9%
1-Naphthalenol	42.2	2.13	331227	9477848	0.973	4-200ng	12.3%	n.d.	1.2%	n.d.	2.5%
2-Naphthalenol	42.6	2.19	757947	11450570	0.986	4-200ng	n.d.	n.d.	1.8%	n.d.	0.8%
VCPs											
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	36.4	0.84	243154	2038616	0.979	4-200ng	3.6%	n.d.	4.6%	n.d.	5.9%

Semi-quantitative method and its uncertainty.

As shown in table S2, for each selected standard, a surrogate standard of the same class and a surrogate n-alkane were chose for the semi-quantification of the standard. While the true calibrated amounts were calculated by the standard curve and response of their own quantitative ions, the semi-quantifications utilize the response of their total ion current (TIC) and the surrogate standard curve of their TIC. The difference of the semi-quantification was calculated as the following forum:

$$D\% = \frac{A_s - A_d}{A_d} \times 100\%$$

where, A_s and A_d are the amounts calculated by quantification and semi-quantification. The total uncertainty of the method was calculated by the forum:

$$D_{total}\% = \sqrt{{D_1}^2 + {D_2}^2 + \cdots + {D_n}^2}$$

where, D_1, D_2…D_n are the uncertainty of each standard.

Table S2. The amounts of selected standards calculated by standard curves and surrogate standard curves and the difference of the semi-quantitative method.

Compound	True calibrated amounts (ng)	Amounts using TIC and surrogates of the same class calibration (ng)	Amounts using TIC and n-alkanes calibration (ng)	% Difference using surrogates of the same class	% Difference using n-alkanes
		Alkanols			
1-Heptanol	19.99	15.72	10.86	-21%	-46%
1-Octanol	14	17.31	1.29	24%	-91%
1-Nonanol	19.42	17.44	10.91	10%	-44%
1-Decanol	19.84	22.16	5.96	12%	-70%
1-Undecanol	9.46	9.96	d	5%	
Square average				16%	66%
		Phenols			
p-Cresol	21.08	15.31	3.8	-27%	-82%
Phenol, 2,4-dimethyl-	19.22	25.22	8.44	31%	-56%
Square average				29%	70%
		Aldehydes			
Hexanal	17.06	18.11	15.65	6%	-8%
Heptanal	32.01	30.31	16.65	-5%	-48%
Octanal	22.27	20.21	16.66	-9%	-25%
Square average				7%	32%
		Ketones			
Isophorone	19.04	18.08	6.4	-5%	-66%
2-Decanone	21.06	22.53	13.3	7%	-37%

Square average				6%	54%
		Esters			
Hexanoic acid, methyl ester	20.84	19.03	21.94	-9%	5%
Octanoic acid, methyl ester	21.56	22.52	18.64	4%	-14%
Decanoic acid, methyl ester	23.36	21.99	10.57	-6%	-55%
Undecanoic acid, methyl ester	20.99	17.65	3	-16%	-86%
Methyl (Z)-10-pentadecenoate	20.9	20.1	4.18	-4%	-80%
9-Hexadecenoic acid, methyl ester, (Z)-	18.92	22.72	1.65	20%	-91%
Square average				12%	65%
		Amides			
Hexadecanamide	19.77	50.43	7.12	155%	-64%
Octadecanamide	17.66	13.76	2.81	-22%	-84%
Square average				111%	75%
		Nitriles			
Benzonitrile	22.09	21.35	25.81	-3%	17%
Decanenitrile	17.5	19.03	7.12	9%	-59%
Square average				7%	43%
		Aromatics			
Toluene	20.83	15.22	15.99	-27%	-23%
o-Xylene	18.86	20.87	32.11	11%	70%
Benzene, propyl-	20.19	24.74	34.61	23%	71%
Benzene, dodecyl-	20.48	12.54	4.36	-39%	-79%
Square average				27%	65%
Total uncertainty				27%	69%

Table S3. The retention time and concentrations of identified organics in both gaseous and particulate samples.

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
Gaseous Sample				
Acids/Alkanoic acids				
Butanoic acid, 3-methyl-	12.3	0.81	2.42	VOCs
Butanoic acid, 2-methyl-	12.8	0.78	0.89	VOCs
Hexanoic acid	19.1	1.23	687.11	VOCs
Phenylmaleic anhydride	44	2.85	6.44	IVOCs
Aldehydes/Olefinic aldehydes				
2-Hexenal, (E)-	12	1.23	13.59	VOCs
4-Heptenal, (Z)-	14.1	1.23	2.17	VOCs
2-Heptenal, (Z)-	16.3	1.32	8.46	VOCs
2-Heptenal, (E)-	16.7	1.44	76.17	VOCs
2,4-Heptadienal, (E,E)-	19.6	1.65	14.94	VOCs
2-Octenal, (E)-	21.9	1.38	48.32	VOCs
4-Nonenal, (E)-	24.1	1.26	10.31	VOCs
2-Nonenal, (Z)-	26.5	1.32	5.09	VOCs
2-Nonenal, (E)-	27.1	1.32	16.63	VOCs
2,4-Nonadienal	28.1	1.23	6.26	IVOCs
4-Decenal, (E)-	29	1.23	5.68	IVOCs
2,4-Nonadienal, (E,E)-	29.7	1.56	8.58	IVOCs
2-Decenal, (Z)-	31.3	1.29	4.31	IVOCs
2-Decenal, (E)-	31.8	1.35	39.85	IVOCs
(Z)-3-Phenylacrylaldehyde	32.4	2.58	5.62	IVOCs
2,4-Decadienal, (E,Z)-	33.2	1.53	50.68	IVOCs
aldehyde-enes-trans-2-Dodecenal-surrogate	33.20	1.53	2.74	VOCs
cis-Undec-4-enal	33.6	1.23	2.89	IVOCs
2,4-Decadienal, (E,E)-	34.2	1.68	119.02	IVOCs
2-Undecenal, E-	35.9	1.29	4.30	IVOCs
2-Undecenal	36.4	1.32	38.26	IVOCs
2-Dodecenal	40.8	1.41	2.87	IVOCs
Aldehydes/Saturated aldehydes				
Pentanal	6.9	0.63	22.83	VOCs
2-Furanol, tetrahydro-	9.7	1.26	4.23	VOCs
Hexanal	9.9	0.93	59.61	VOCs
Heptanal	14.7	0.93	1.79	VOCs
Benzaldehyde	16.7	2.22	12.72	VOCs
Octanal	19.3	1.17	48.86	VOCs
3-Cyclohexene-1-carboxaldehyde, 1-methyl-	20.5	1.68	5.24	VOCs
Benzeneacetaldehyde	20.8	2.4	6.16	VOCs
Nonanal	24.4	1.2	52.45	VOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
Decanal	29.4	1.17	6.78	IVOCs
4-Oxononanal	30.4	2.13	23.87	IVOCs
Cyclohexanone, 2-butyl-	31.7	1.86	1.67	IVOCs
Undecanal	34	1.17	3.43	IVOCs
Dodecanal	38.5	1.17	4.34	IVOCs
Tridecanal	42.7	1.17	2.98	IVOCs
Aliphatic hydrocarbons/Alkanes				
C6	5.50	1.41	3643.08	VOCs
C7	7.4	0.33	4422.82	VOCs
C8	10.7	0.42	272.61	VOCs
C9	15.2	0.48	2.39	VOCs
Cyclopentane, butyl-	16.7	0.66	6.20	VOCs
b-alkanes-C10	19.9	0.51	6.41	VOCs
C10	20.2	0.57	3.22	VOCs
b-alkanes-C11	24.2	0.57	13.74	VOCs
C11	25.3	0.6	4.33	VOCs
b-alkanes-C12	28	0.6	3.85	IVOCs
C12	30.1	0.63	2.17	IVOCs
b-alkanes-C13	30.8	0.6	3.74	IVOCs
C13	34.6	0.66	0.75	IVOCs
b-alkanes-C14	38	0.63	3.16	IVOCs
C14	38.9	0.66	0.93	IVOCs
b-alkanes-C15	41.5	0.63	6.00	IVOCs
C15	42.9	0.69	1.50	IVOCs
b-alkanes-C16	44.8	0.69	1.07	IVOCs
C16	46.7	0.72	1.19	IVOCs
b-alkanes-C17	48.6	0.69	1.70	IVOCs
C17	50.3	0.75	0.81	IVOCs
b-alkanes-C18	50.7	0.69	0.52	IVOCs
C18	53.8	0.78	1.31	IVOCs
b-alkanes-C19	54.2	0.72	0.26	IVOCs
C19	57	0.81	0.35	IVOCs
C20	60.1	0.81	0.12	IVOCs
Aliphatic hydrocarbons/Alkenes				
1-Heptene	7.1	1.77	30.31	VOCs
1-Nonene	14.1	0.66	0.44	VOCs
1-Decene	19.6	0.63	0.52	VOCs
D-Limonene	21.3	0.93	11.65	VOCs
1,10-Undecadiene	24.4	0.6	0.41	VOCs
4-Undecene, (E)-	24.7	0.66	0.61	VOCs
2-Undecene, (E)-	26.1	0.57	0.27	VOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
alkenes-C12	28.4	0.6	0.24	IVOCs
3-Dodecene, (E)-	29.4	0.69	3.88	IVOCs
alk-di-enes-C12	31.1	0.99	1.74	IVOCs
alkenes-C13	34	0.72	0.73	IVOCs
alkenes-C14	38.3	0.75	0.43	IVOCs
alkenes-C15	42.3	0.78	2.06	IVOCs
alkenes-C16	45.9	0.81	0.37	IVOCs
alkenes-C17	49.5	0.84	1.44	IVOCs
alkenes-C17	49.50	0.84	5.06	IVOCs
alkenes-C18	52.9	0.84	1.74	IVOCs
Neophytadiene	55.2	0.78	0.28	IVOCs
Aliphatic hydrocarbons/Alkynes				
3-Nonen-1-yne, (E)-	17.1	0.9	3.20	VOCs
alkynes-C12	32.4	0.9	0.74	IVOCs
alkynes-C14	40.2	0.93	0.93	IVOCs
alkynes-C15	42.1	0.87	6.42	IVOCs
alkynes-C16	47.4	0.99	4.13	IVOCs
alkynes-C17	49.1	0.9	3.31	IVOCs
alkynes-C18	52.6	0.9	1.13	IVOCs
Aromatic hydrocarbons/Aromatics				
Toluene	8.3	0.54	0.68	VOCs
Ethylbenzene	12.8	1.02	3.37	VOCs
p-Xylene	13.2	0.99	3.64	VOCs
Benzene, (1-methylethyl)-	15.9	0.96	5.38	VOCs
Benzene, propyl-	17.2	1.11	1.36	VOCs
aromatics-C3	17.6	1.14	3.72	VOCs
aromatics-C4	22.4	1.17	6.14	VOCs
Silane, diethoxydiphenyl-	50.2	1.95	3.17	IVOCs
Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis-	52.5	2.22	2.42	IVOCs
Benzene, 1,1'-(3,3-dimethyl-1-butenylidene)bis-	54	2.19	3.33	IVOCs
Aromatic hydrocarbons/PAHs				
Naphthalene	28.3	2.22	1.76	IVOCs
Naphthalene, 1-methyl-	33.4	2.13	2.58	IVOCs
Naphthalene, 2-methyl-	34.1	2.31	2.38	IVOCs
Esters and Amides/Esters				
Acetic acid, butyl ester	10.7	0.78	0.27	VOCs
Formic acid, pentyl ester	11.3	0.84	0.01	VOCs
Butyrolactone	13.9	3.69	0.23	VOCs
2H-Pyran-2-one, tetrahydro-	20.7	4.26	0.18	VOCs
2(3H)-Furanone, 5-ethyldihydro-	20.8	3.09	0.06	VOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
n-Amyl ether	23.8	0.6	0.31	VOCs
2(5H)-Furanone, 5-(1-methylethyl)-	25.5	2.67	0.05	VOCs
2(3H)-Furanone, 5-butyldihydro-	30.8	2.58	0.34	IVOCs
Hexanoic acid, pentyl ester	33.3	1.08	3.82	IVOCs
Benzoic acid, pentyl ester	41.2	1.74	0.05	IVOCs
Benzoic acid, 2-ethylhexyl ester	49.9	1.65	0.30	IVOCs
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	54.7	2.28	4.30	IVOCs
Hexadecanoic acid, methyl ester	57.4	1.17	0.06	IVOCs
Dibutyl phthalate	57.7	2.43	1.72	IVOCs
1,3-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	80	1.29	4.87	SVOCs
Ketones/Olefinic ketones				
3-Furanmethanol	12.7	1.5	9.37	VOCs
1-Octen-3-one	18.1	1.23	6.96	VOCs
Furan, 2-pentyl-	19.2	0.99	19.74	VOCs
Acetophenone	22.2	2.31	12.04	VOCs
trans-3-Nonen-2-one	26.2	1.35	11.14	VOCs
2-N-Octylfuran	34.5	1.11	1.62	IVOCs
Ketoned/Saturated ketones				
Cyclopentanone, 2-methyl-	11.4	1.44	8.55	VOCs
2-Heptanone	13.8	1.08	5.40	VOCs
3-Ethylcyclopentanone	16.6	1.71	6.47	VOCs
2-Octanone	19	1.05	2.91	VOCs
Cyclopentanone, 3-butyl-	26.9	1.59	3.65	VOCs
1-Propanone, 1-phenyl-	27.5	1.86	1.40	VOCs
6-Dodecanone	37	1.08	2.57	IVOCs
Others/N-compounds				
Pentane, 1-nitro-	14.2	1.11	19.20	VOCs
Nitric acid, pentyl ester	15.4	1.05	0.11	VOCs
Benzonitrile	18	2.37	4.25	VOCs
Pyridine, 2-pentyl-	29.1	1.56	6.74	IVOCs
Benzothiazole	29.9	3.06	5.83	IVOCs
Others/Others				
UCM3	20.7	2.19	9.30	VOCs
1-Hexanol, 2-ethyl-	21	1.02	2.22	VOCs
Copaene	37.8	0.99	0.39	IVOCs
Oxygenated compounds/Alkanols				
1-Butanol	6.4	0.54	101.92	VOCs
1-Pentanol	9.1	0.81	47.12	VOCs
3,3-Dimethylbutane-2-ol	11.2	1.26	5.30	VOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
2-Heptanol	14.2	0.96	4.52	VOCs
2-Octanol	19.6	0.96	5.66	VOCs
Cyclohexanol, 2,4-dimethyl-	19.7	1.2	29.89	VOCs
3,4-Dimethylcyclohexanol	21	1.32	23.81	VOCs
1-Octanol	23.2	1.08	3.79	VOCs
6-Undecanol	33.6	0.96	0.89	IVOCs
1-Undecanol	36.3	0.99	1.05	IVOCs
Oxygenated compounds/Alkenols				
1-Octen-3-ol	18.4	1.02	58.86	VOCs
2-Octen-1-ol, (E)-	23.1	1.14	2.73	VOCs
alkenols-1-Tridecanol-surrogate	35.70	1.08	4.01	IVOCs
Oxygenated compounds/Oxygenated compounds				
8-Oxabicyclo[5.1.0]octane	13.7	1.32	5.22	VOCs
Cyclohexanecarboxaldehyde	15.1	1.44	7.32	VOCs
3-Hydroxy-3-phenylbutan-2-one	23.4	1.89	5.80	VOCs
oxygenated-di-isoprenes	23.7	1.44	3.16	VOCs
oxiranes-surrogate-Oxirane, decyl-	25.90	1.14	2.10	VOCs
2,4-Pentadien-1-ol, 3-pentyl-, (2Z)-	31.8	1.56	4.05	IVOCs
Benzene, 1-methoxy-4-(1-propenyl)-, (Z)-	33	1.92	0.12	IVOCs
2H-1b,4-Ethanopentaleno[1,2-b]oxirene, hexahydro-, (1a-alpha-,1b-bta-,4-bta-,4a-alpha-,5a-alpha-)-	34.20	1.92	4.51	IVOCs
cis-4,5-Epoxy-(E)-2-decenal	36.5	1.83	6.22	IVOCs
oxo-aldehyde-enes	36.8	1.77	14.82	IVOCs
2,6-Di-tert-butyl-4-hydroxy-4-methylcyclohexa-2, 5-dien-1-one	41.1	1.23	4.20	IVOCs
o-Hydroxybiphenyl	43	2.52	3.62	IVOCs
Xanthoxylin	48.7	2.64	1.48	IVOCs
Ethanone, 1,2-diphenyl-	50.7	3.15	3.85	IVOCs
Particulate Sample				
Acids/Alkanoic acids				
Acetic acid	5.7	0.39	350.94	VOCs
Propanoic acid, 2-methyl-	8.9	0.69	2.82	VOCs
Hexanoic acid	19.1	1.23	137.21	VOCs
Heptanoic acid	23.7	1.05	394.47	VOCs
Hexanoic acid, 2-ethyl-	25.8	0.99	0.25	VOCs
Octanoic acid	28.3	1.14	485.41	IVOCs
Neodecanoic acid	31.7	0.93	47.28	IVOCs
Nonanoic acid	32.7	1.14	342.90	IVOCs
1,2-Benzenedicarboxylic acid	34.6	2.97	7.84	IVOCs
n-Decanoic acid	36.9	1.14	26.71	IVOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
Dodecanoic acid, 3-hydroxy-	51.6	3.78	61.55	IVOCs
acids	51.8	1.26	207.66	IVOCs
n-Hexadecanoic acid	57.8	1.44	8484.44	IVOCs
Acids/Alkenoic acids				
2-Propenoic acid	7.4	0.66	6.17	VOCs
2-Octenoic acid, (E)-	30	1.23	91.93	IVOCs
trans-2-Decenoic acid	38.5	1.26	22.56	IVOCs
cis-5-Dodecenoic acid	52.8	4.05	53.54	IVOCs
Hematoporphyrin	53.1	0.33	7.89	IVOCs
Oleic Acid	59	2.52	857.84	IVOCs
cis-13-Octadecenoic acid	62.2	1.47	231.10	IVOCs
trans-13-Octadecenoic acid	63.3	1.23	217.06	IVOCs
9,12-Octadecadienoic acid (Z,Z)-	64.1	1.89	11053.39	IVOCs
Arachidonic acid	65.9	2.88	24.97	IVOCs
Gorlic acid-1	66.7	2.58	219.99	IVOCs
Gorlic acid-2	67	2.37	225.31	IVOCs
Linoelaidic acid	67.1	1.17	151.54	IVOCs
Gamolenic acid	67.5	2.7	107.47	SVOCs
cis-Vaccenic acid	69.6	0.93	270.43	SVOCs
Aldehydes/Olefinic aldehydes				
2-Heptenal, (Z)-	16.3	1.32	1.60	VOCs
2-Octenal, (E)-	21.9	1.38	1.47	VOCs
2,4-Decadienal, (E,Z)-	33.2	1.53	2.29	IVOCs
aldehyde-enes-trans-2-Dodecenal-surrogate	34.2	1.53	6.70	VOCs
Aldehydes/Saturated aldehydes				
Pentanal	6.9	0.63	1.23	VOCs
Hexanal	9.9	0.93	12.62	VOCs
Heptanal	14.7	0.93	0.23	VOCs
Octanal	19.3	1.17	0.24	VOCs
d-Mannose	55.2	0.3	10.48	IVOCs
Aliphatic hydrocarbons/Alkanes				
C10	20.2	0.57	0.50	VOCs
C11	25.3	0.6	0.31	VOCs
b-alkanes-C12	28	0.6	0.59	IVOCs
C12	30.1	0.63	0.55	IVOCs
b-alkanes-C13	30.8	0.6	3.40	IVOCs
C13	34.6	0.66	0.17	IVOCs
b-alkanes-C14	38	0.63	3.15	IVOCs
C14	38.9	0.66	2.45	IVOCs
3-Ethyl-2,6,10-trimethylundecane	41.4	0.63	2.28	IVOCs
b-alkanes-C15	41.5	0.63	3.15	IVOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
9-Octadecene, (E)-	42.4	0.75	1.09	IVOCs
C15	42.9	0.69	2.63	IVOCs
Pentadecane, 7-methyl-	44.7	0.69	0.75	IVOCs
Cyclohexane, hexadecyl-	44.7	0.9	2.07	IVOCs
b-alkanes-C16	44.8	0.69	6.07	IVOCs
Heptadecane, 2,6-dimethyl-	45.1	0.69	1.09	IVOCs
Eicosane, 2-methyl-	45.3	0.69	0.84	IVOCs
Pentadecane, 3-methyl-	45.6	0.72	0.58	IVOCs
Cyclohexane, 1,3,5-trimethyl-2-octadecyl-	46	0.81	0.06	IVOCs
C16	46.7	0.72	4.61	IVOCs
Tetradecane, 2,6,10-trimethyl-	47	0.69	0.76	IVOCs
Eicosane, 7-hexyl-	47.7	0.72	0.11	IVOCs
Hexadecane, 7-methyl-	48.5	0.45	0.36	IVOCs
Pentadecane, 2,6,10-trimethyl-	48.5	0.69	2.08	IVOCs
b-alkanes-C17	48.6	0.69	4.77	IVOCs
C17	50.3	0.75	3.12	IVOCs
Hexadecane, 2,6,10,14-tetramethyl-1	50.6	0.66	1.23	IVOCs
b-alkanes-C18	50.7	0.69	0.55	IVOCs
2-Hexadecene, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-	51.3	0.75	3.96	IVOCs
C18	53.8	0.78	0.87	IVOCs
Hexadecane, 2,6,10,14-tetramethyl-2	54.1	0.72	0.74	IVOCs
b-alkanes-C19	54.2	0.72	1.62	IVOCs
C19	57	0.81	1.71	IVOCs
b-alkanes-C21	57.3	0.78	2.80	IVOCs
C20	60.1	0.81	1.63	IVOCs
C21	63	0.9	12.23	IVOCs
C22	65.9	0.9	3.29	IVOCs
b-alkanes-C23	67	0.87	3.44	IVOCs
C23	68.6	0.93	5.69	SVOCs
C24	71.2	0.96	7.54	SVOCs
C25	73.9	1.2	4.72	SVOCs
b-alkanes-C25	74	0.78	6.83	SVOCs
b-alkanes-C26	76.1	1.56	3.35	SVOCs
C26	77	1.35	2.95	SVOCs
b-alkanes-C27	78.1	1.02	3.91	SVOCs
C27	80	0.33	6.59	SVOCs
C28	81.3	0.69	2.13	SVOCs
b-alkanes-C29	82.3	0.78	65.32	SVOCs
C29	82.7	0.78	8.23	SVOCs

Aliphatic hydrocarbons/Alkenes

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
1,3-Octadiene	11.5	0.6	3.28	VOCs
5,5-Dimethyl-1,3-hexadiene	13.4	0.69	2.20	VOCs
Cyclohexene,3-propyl-	14.2	0.9	2.36	VOCs
trans-3-Decene	14.6	0.54	0.11	VOCs
Cycloheptene, 1,2-dimethyl-	15.3	1.05	1.43	VOCs
1,3-Nonadiene, (E)-	16.1	0.72	3.35	VOCs
C10-alkenes	19.6	0.6	0.91	VOCs
C11-alkenes	24.6	0.66	1.85	VOCs
C12-alkenes	29.5	0.69	2.69	IVOCs
C13-alkenes	34	0.72	0.51	IVOCs
C14-alkenes	38.4	0.72	0.51	IVOCs
1,8,11-Heptadecatriene, (Z,Z)-	48.6	0.99	1.74	IVOCs
Nonacos-1-ene	49.3	0.84	2.66	IVOCs
alkenes-C17-UCM	53	0.84	0.35	IVOCs
Squalene	81.5	0.96	130.26	SVOCs
Stigmastan-3,5,22-trien	82.7	1.32	28.00	SVOCs
Aliphatic hydrocarbons/ Alkynes				
9-Octadecyne	42	0.87	0.60	IVOCs
7-Pentadecyne	47.3	0.99	2.93	IVOCs
alkyenes	52.7	0.93	0.67	IVOCs
Aromatic hydrocarbons/Aromatics				
Ethylbenzene	12.8	1.02	0.44	VOCs
Styrene	14	1.26	1.39	VOCs
Benzene, propyl-	17.2	1.11	0.25	VOCs
Benzene, N-butyl-	23	1.08	13.26	VOCs
1-Phenyl-1-butene	26	1.38	0.74	VOCs
Benzene, pentyl-	27.5	1.17	6.71	VOCs
Benzene, hexyl-	32.2	1.2	2.94	IVOCs
Benzene, 1,2,4-trimethyl-5-(1-methylethyl)-	34.5	1.98	0.13	IVOCs
Hex-1-enylbenzene	35.2	1.41	0.65	IVOCs
Benzene, heptyl-	36.7	1.2	2.84	IVOCs
Benzene, 1-heptenyl-	39.5	1.44	0.72	IVOCs
Benzene, octyl-	41	1.23	3.04	IVOCs
Benzene, 1-octenyl-	43.7	1.44	0.75	IVOCs
Benzene, nonyl-	45	1.23	0.62	IVOCs
Methyl 6,8-octadecadiynoate	45.2	1.8	2.86	IVOCs
Levodopa	45.3	2.01	1.57	IVOCs
2-Oxaspiro[5.5]undecane-1,5-dione, 3-(4-chlorophenyl)-4-methyl-	46.8	1.74	2.08	IVOCs
Benzene, (1-butylheptyl)-	47.6	1.05	0.21	IVOCs
Aromatics-C10	51.00	1.08	2.35	IVOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
Aromatics-C11	58.4	0.24	7.76	IVOCs
Aromatic hydrocarbons/PAHs				
Naphthalene	28.3	2.22	1.76	IVOCs
Naphthalene, 1-methyl-	33.4	2.13	2.21	IVOCs
Acenaphthylene	39.5	2.55	2.54	IVOCs
Benzene, (cyclopentylidenephenylmethyl)-	64.5	4.5	2.28	IVOCs
Esters and Amides/Esters				
2(5H)-Furanone, 3-methyl-	17.5	3.33	0.00	VOCs
2(3H)-Furanone-C6	20.6	3.06	0.07	VOCs
2H-Pyran-2-one, tetrahydro-	20.7	4.26	0.03	VOCs
2H-Pyran-2-one, tetrahydro-6-methyl-	22.6	3.6	4.53	VOCs
But-3-enyl (E)-2-methylbut-2-enoate	23.5	4.71	0.26	VOCs
2-Oxepanone	24.7	4.02	5.39	VOCs
2(3H)-Furanone-C7	25.6	2.82	3.38	VOCs
2(3H)-Furanone-C8	30.1	2.25	0.01	IVOCs
Tetrahydrogeranyl formate-2	30.1	1.08	0.07	IVOCs
Propanoic acid, 2-methyl-, 2-ethyl-1-propyl-1,3-propanediyl ester	31.4	1.02	0.02	IVOCs
1-Oxaspiro(4,5)decan-2-one	33.4	2.31	0.14	IVOCs
Triacetin	34.8	2.22	4.89	IVOCs
2(3H)-Furanone-C9	35.4	2.4	0.04	IVOCs
Propanoic acid, 2-methyl-, 3-hydroxy-2,2,4-trimethylpentyl ester	36.1	1.32	0.02	IVOCs
2H-Pyran-2-one, 5,6-dihydro-6-pentyl-	40.2	2.61	0.03	IVOCs
10-Methylundec-3-en-4-olide	40.4	1.77	0.04	IVOCs
Pyrrolo[1,2-c]oxazol-1(3H)-one, tetrahydro 7a-acetyl-3-(1,1-dimethylethyl)-	41.7	2.1	0.06	IVOCs
2H-Pyran-2-one, 6-hexyltetrahydro-	43.3	4.53	0.40	IVOCs
2(3H)-Furanone-C11	43.9	1.92	0.01	IVOCs
Tetrahydrofuran-2-one, 5-[1-hydroxyhexyl]-	45.4	2.94	0.07	IVOCs
10-Methyl-E-11-tridecen-1-ol propionate	45.8	1.62	0.09	IVOCs
2(3H)-Furanone-C12	48	2.19	0.06	IVOCs
2-Pentadecanone	49.5	1.2	6.85	IVOCs
Octahydrobenzo[b]pyran, 4a-acetoxy-5,5,8a-trimethyl-	50.5	1.77	0.15	IVOCs
2(3H)-Furanone-C13	51.7	2.16	0.17	IVOCs
Dotriacontyl trifluoroacetate	51.7	0.36	0.26	IVOCs
2-Pentadecanone, 6,10,14-trimethyl-	54.6	1.11	12.48	IVOCs
2-((2-Methoxyethoxy)carbonyl)benzoic acid	54.7	4.5	0.07	IVOCs
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	54.7	2.28	10.89	IVOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
Benzoic acid, decyl ester-2	55.4	1.62	0.73	IVOCs
9-Octadecene, 1,1-dimethoxy-, (Z)-	55.5	1.35	14.54	IVOCs
Benzoic acid, dec-2-yl ester	55.9	1.65	2.26	IVOCs
Benzoic acid, decyl ester-4	56.1	1.68	1.84	IVOCs
2H-Pyran-2-one, tetrahydro-6-nonyl-	56.2	2.31	0.11	IVOCs
Benzoic acid, decyl ester-5	56.8	1.77	1.84	IVOCs
benzoic esters	57.1	1.74	5.36	IVOCs
Hexadecanoic acid, methyl ester	57.4	1.17	0.11	IVOCs
Benzoic acid, decyl ester-6	57.4	1.77	1.28	IVOCs
Dibutyl phthalate	57.7	2.43	21.12	IVOCs
2(3H)-Furanone-C16	61.9	2.19	1.81	IVOCs
2H-Pyran-2-one, tetrahydro-6-undecyl-	62.8	2.4	1.37	IVOCs
Trilinolein	66.5	1.53	0.23	IVOCs
(Z)-9-Octadecen-4-olide	67.8	2.46	0.06	SVOCs
2(3H)-Furanone-C18	67.9	2.13	0.09	SVOCs
2H-Pyran-2-one, tetrahydro-6-tridecyl-	68.8	2.28	0.06	SVOCs
9,12-Octadecadienoic acid (Z,Z)-, methyl ester	68.9	2.67	0.00	SVOCs
4,8,12,16-Tetramethylheptadecan-4-olide	69.2	1.77	0.06	SVOCs
esters	69.8	2.4	0.26	SVOCs
Hexanedioic acid, bis(2-ethylhexyl) ester	70.5	1.5	0.02	SVOCs
Butyl 9,12-octadecadienoate	72	1.56	0.09	SVOCs
Hexanoic acid, 2-ethyl-, hexadecyl ester	72.8	1.35	0.03	SVOCs
Octan-2-yl palmitate	73.6	1.47	0.01	SVOCs
Phthalic acid, di(2-propylpentyl) ester	74.1	2.7	16.24	SVOCs
trans-9-Octadecenoic acid, pentyl ester	74.8	1.74	0.04	SVOCs
Di-isononyl phthlate-1	79.4	1.74	1.27	SVOCs
Phthalic acid, nonyl oct-3-yl ester	80.1	1.65	1.47	SVOCs
Esters and Amides/Olefinic amides				
Benzamide, N,N-dimethyl-	35.9	3.21	1.78	IVOCs
Niacinamide	37.4	4.5	18.08	IVOCs
Oct-3-enoylamide, N-methyl-	44.4	2.1	4.76	IVOCs
dl-Alanyl-L-leucine	51.1	3.51	16.51	IVOCs
Oct-3-enoylamide, N-isobutyl-	51.2	1.68	3.35	IVOCs
Cyclo-(glycyl-L-leucyl)	52.1	4.17	2.18	IVOCs
Cyclo(L-prolyl-L-valine)	52.3	4.59	15.00	IVOCs
Arachidonoyl-N-methyl amide	65.5	1.95	11.39	IVOCs
9-Octadecenamide, (Z)-	69.1	2.4	21.16	SVOCs
Arachidonoyl-N,N-dimethyl amide	71	2.16	57.16	SVOCs
9-Octadecenamide, N,N-dimethyl-	71.2	2.01	29.71	SVOCs
Oleic diethanolamide	78.3	1.95	10.98	SVOCs
10,13-Octadecadienooic acid, pyrrolidide	79.7	2.04	107.12	SVOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
1-Octadec-cis-9-enoylpyrrolidine	79.8	1.89	38.55	SVOCs
Esters and Amides/Saturated amides				
2-Pyrrolidinone, 1-methyl-	20.5	3.81	0.89	VOCs
Hexanamide	26.4	2.49	3.90	VOCs
Glutarimide	26.7	4.77	2.06	VOCs
2-Pyrrolidinone, 1-ethenyl-	29.8	1.71	3.13	IVOCs
Enanthamide	30.5	2.43	3.27	IVOCs
Caprolactam	30.8	4.02	0.91	IVOCs
2,4-Imidazolidinedione, 5-methyl-	34.9	4.08	2.79	IVOCs
2,5-Pyrrolidinedione, 1-butyl-	35.8	2.97	1.88	IVOCs
2,4-Dihydroxy-5,6-dimethylpyrimidine	37.4	3.42	1.63	IVOCs
Phthalimide	39.8	3.87	2.08	IVOCs
Octanoic acid, pyrrolidide	42.3	2.43	1.45	IVOCs
Hexahydropyrrolizin-3-one	42.4	5.43	1.79	IVOCs
3,6-Dimethylpiperazine-2,5-dione	42.6	4.95	12.55	IVOCs
Pentanoic acid, 3,3-dimethyl-4-semicarbazono-	43.2	3.54	3.62	IVOCs
amides	43.2	2.43	127.87	IVOCs
Dodecanamide	43.7	2.19	5.55	IVOCs
[1,3]Diazepan-2,4-dione	44.1	5.76	6.30	IVOCs
2,5-Piperazinedione, 3-methyl-6-(1-methylethyl)-	47.1	4.14	7.62	IVOCs
1,4-Diazabicyclo[4.3.0]nonan-2,5-dione, 3-methyl	48	0.27	27.24	IVOCs
3-Isopropyl-2,5-piperazine-dione	49.5	4.23	7.29	IVOCs
C12-amide	51.2	2.1	2.36	IVOCs
5,10-Diethoxy-2,3,7,8-tetrahydro-1H,6H-dipyrrolo [1,2-a:1',2'-d]pyrazine	55.6	0.12	17.98	IVOCs
Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-	56.2	4.08	26.30	IVOCs
6H-Purin-6-one, 1,7-dihydro-1-methyl-	59.5	3.48	13.40	IVOCs
Hexadecanamide	64.7	2.16	23.85	IVOCs
Hexadecanoic acid, pyrrolidide	75	3.12	47.23	SVOCs
Ketones/Olefinic ketones				
1-Octen-3-one	18.1	1.23	1.74	VOCs
Furan, 2-pentyl-	19.2	0.99	22.26	VOCs
Acetophenone	22.2	2.31	6.10	VOCs
2-Cyclopenten-1-one, 2-pentyl-	32.8	1.86	2.77	IVOCs
2-n-Octylfuran	33.7	1.05	4.31	IVOCs
5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-	40	1.41	1.57	IVOCs
Linoleyl methyl ketone	55.1	1.5	22.02	IVOCs
Ketones/Saturated ketones				
2-Propanone, 1-hydroxy-	4.6	0.21	101.93	VOCs
Cyclopentanone	9.3	1.5	1.15	VOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
4-Cyclopentene-1,3-dione	13.4	2.25	1.60	VOCs
2-Heptanone	13.8	1.08	2.68	VOCs
3-Ethylcyclopentanone	16.6	1.71	1.72	VOCs
2-Octanone	19	1.05	2.01	VOCs
2-Butyl-2-cyclopentenone	28.1	1.89	16.50	IVOCs
1H-Inden-1-one, 2,3-dihydro-	32	3.18	0.88	IVOCs
1H-Indole-1-carboxaldehyde, 2,3-dihydro-	32.1	2.1	1.86	IVOCs
Cycloheptanone, 3-butyl-	36.1	1.8	3.79	IVOCs
2-Propanone, 1-(4-methoxyphenyl)-	36.5	2.76	2.82	IVOCs
1-Hexanone, 1-phenyl-	40.1	1.95	1.34	IVOCs
ketones	40.9	1.68	13.47	IVOCs
1,4-Cyclododecanedione	44.5	1.74	2.65	IVOCs
7-Ethyl-4,6-pentadecandione	54.4	2.85	5.41	IVOCs
2-Heptadecanone	56.4	1.23	7.16	IVOCs
Others/N-compounds				
N,N-Dimethylaminoethanol	8	1.11	71.68	VOCs
Ethanamine, N-pentylidene-	10.8	0.81	3.17	VOCs
1-Propanamine, 2-methyl-N-(2-methylpropylidene)-	11.9	0.63	3.85	VOCs
Hexanenitrile	12.7	1.53	4.13	VOCs
Pentane, 1-nitro-	14.2	1.11	1.74	VOCs
Heptane, 3-ethyl-2-methyl-	16.6	0.72	2.15	VOCs
Pyridine, 3-ethyl-	17.1	2.1	1.65	VOCs
3-Pyridinecarbonitrile	18.5	3.12	4.93	VOCs
1-Azabicyclo[2.2.2]octane, 2-methyl-	18.6	2.04	2.60	VOCs
1H-Pyrazol-3-amine	19.3	3.15	6.79	VOCs
N,N-Dimethylglycine	20.6	1.47	59.21	VOCs
1H-Imidazo[1,2-b]pyrazole, 2,3-dihydro-	21	2.58	5.76	VOCs
1-Butanamine, 2-methyl-N-(2-methylbutylidene)-	21.6	0.78	1.68	VOCs
2,5-Pyrrolidinedione, 1-methyl-	22	4.62	0.39	VOCs
Pyridine, 2-butyl-	24	1.62	0.43	VOCs
Succinimide	24.4	4.74	0.87	VOCs
2,5-Pyrrolidinedione, 1-ethyl-	24.4	3.78	0.98	VOCs
Cyclohexylamine	25.8	3.96	1.00	VOCs
3-Pyridinol	26	2.01	3.69	VOCs
Pyridine, 3-butyl-	26.7	1.59	0.86	VOCs
3'H-Cycloprop(1,2)-5-cholest-1-en-3-one, 1'-carboethoxy-1'-cyano-1,2-dihydro-	26.8	0.96	2.45	VOCs
Pyrrolidine, 1-acetyl-	26.9	3.51	0.26	VOCs
1-Butanamine, 3-methyl-N-(3-methylbutylidene)-	28.4	0.9	3.77	IVOCs
Pyridine, 2-pentyl-	29.1	1.56	3.70	IVOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
1,2-Benzisothiazole	29.6	3.09	1.85	IVOCs
Amantadine	30.6	1.5	3.34	IVOCs
2,4-Imidazolidinedione, 1-methyl-	30.7	5.28	15.40	IVOCs
Pyridine, 4-pentyl-	31.6	1.68	1.05	IVOCs
Pyridine, 2-hexyl-	33.6	1.56	1.21	IVOCs
2-Methyl-5-(3-methylbutyl)pyridine	34.6	1.47	0.82	IVOCs
Adamantane, 1-isocyanato-	35.5	1.41	0.25	IVOCs
Pyridine, 2-(1-methyl-2-pyrrolidinyl)-	35.5	2.16	1.87	IVOCs
Pyridine,4-C6	35.6	1.68	0.58	IVOCs
Pyridine,2-C7	38	1.56	1.02	IVOCs
(+-)-2-Phenylbutyronitrile	38.7	1.98	0.38	IVOCs
Pyridine,4-C7	39.8	1.65	0.81	IVOCs
1-[3-Aminopropyl]-2[1H]-pyridone	39.8	2.85	3.29	IVOCs
Piperidine, 1-cyclohexyl-	41.2	2.16	1.17	IVOCs
Pyridine,2-C8	41.7	1.47	0.79	IVOCs
N-Ethyl-1-azaspiro[5,5]undecane	42.6	1.95	1.85	IVOCs
2-Methyl-6-propylpiperidine	42.6	2.34	2.74	IVOCs
1H-Indazol-5-amine, 3-methyl-	44.4	4.44	2.36	IVOCs
Pyridine,4-C8	44.7	1.65	1.33	IVOCs
4,6-Quinolinediamine	47.9	4.86	1.89	IVOCs
Hexadecanenitrile	55.9	1.5	0.49	IVOCs
11-Octadecynenitrile	61.2	1.89	25.26	IVOCs
9-Octadecenenitrile, (Z)-	61.5	1.86	13.11	IVOCs
Imidazo(1,2-a)pyrimidine, 6-methyl-5-oxo-1,2,3,5-tetrahydro-	61.8	3.69	2.11	IVOCs
1-Acetyl-6-methyl-5-oxo-1,2,3,5-tetrahydroimidazo[1,2-a]pyrimidine	61.9	3.39	3.14	IVOCs
[1,2,4]Triazolo[1,5-a]pyrimidin-7-ol, 5-methyl-	62.3	3.6	3.00	IVOCs
N-compounds	65.4	3	18.11	IVOCs
Others/Others				
Sulfur dioxide	4.4	0.21	43.56	VOCs
UCM1	15.1	0.78	1.75	VOCs
S-Methyl methanethiosulphonate	20.9	4.32	3.05	VOCs
1-Hexanol, 2-ethyl-	21	1.02	4.98	VOCs
4-Oxopentanethioic acid	21.8	1.59	2.77	VOCs
UCMs	37.2	1.29	56.47	IVOCs
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	45.9	1.23	22.88	IVOCs
Tri(2-chloroethyl) phosphate	50.4	3.54	0.21	IVOCs
2-Propanol, 1-chloro-, phosphate (3:1)	52.1	2.52	1.72	IVOCs
Bis(1-chloro-2-propyl)(3-chloro-1-propyl)phosphate	52.5	2.55	0.31	IVOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
Oxygenated compounds/Alkanols				
1-Pentanol	9.1	0.81	3.08	VOCs
1-Hexanol	13.1	0.99	0.82	VOCs
3-Methoxy-3-methylbutanol	14.7	1.44	1.98	VOCs
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	19.3	1.35	2.40	VOCs
2-Propanol, 1-(2-methoxypropoxy)-	19.9	1.35	1.99	VOCs
endo-Borneol	27	1.32	0.68	VOCs
1-Octanol, 3,7-dimethyl-	29.1	1.02	7.89	IVOCs
Cyclohexanol, 3,5-dimethyl-	30.7	0.99	10.92	IVOCs
4a(2H)-Naphthalenol, octahydro-, trans-	35.2	2.31	10.03	IVOCs
1-Undecanol	36.3	0.99	7.04	IVOCs
Cyclopentaneethanol, 2-(hydroxymethyl)- ¿ó,3-dimethyl-	38.6	1.53	1.52	IVOCs
4-Methyl-5-decanol	43.2	3.06	6.76	IVOCs
1-Tetradecanol	48.8	1.17	9.61	IVOCs
Ethanol, 2-(dodecyloxy)-	50.4	1.08	2.36	IVOCs
Phytol	52.4	0.93	6.00	IVOCs
alkanols	54.7	1.44	86.29	IVOCs
1-Hexadecanol	55.8	1.2	6.25	IVOCs
Oxygenated compounds/Alkenols				
4,4,6-Trimethyl-cyclohex-2-en-1-ol	34.5	2.49	9.81	IVOCs
2,4,7,9-Tetramethyl-5-decyn-4,7-diol	38.8	1.02	2.10	IVOCs
1-Dodecyn-4-ol	41.9	1.02	2.96	IVOCs
(Z)6-Pentadecen-1-ol	49	0.9	8.27	IVOCs
Eicosen-1-ol, cis-9-	67.3	1.11	56.54	SVOCs
E,E,Z-1,3,12-Nonadecatriene-5,14-diol	71	1.5	10.07	SVOCs
Oxygenated compounds/Cholesterols				
1H-Indene, 1-ethylideneoctahydro-, trans-	38.3	1.5	0.70	IVOCs
Ergost-5-en-3-ol, acetate, (3ß,24R)-1	82.1	1.26	299.05	SVOCs
Stigmastan-3-ol, 5-chloro-, acetate, (3ß,5α)-	83.6	1.47	801.02	SVOCs
Ergost-5-en-3-ol, acetate, (3ß,24R)-2	84.1	1.71	336.12	SVOCs
ß-Sitosterol	85	1.83	127.88	SVOCs
Cholesta-4,6-dien-3-ol, (3ß)-	85.2	1.95	171.37	SVOCs
cholesterols	85.7	2.01	998.61	SVOCs
Oxygenated compounds/Oxygenated compounds				
3-Hydroxy-3-phenylbutan-2-one	23.4	1.89	2.72	VOCs
¿ó-Asarone	46.4	2.7	2.58	IVOCs
Xanthoxylin	48.7	2.64	3.81	IVOCs
oxygenated compounds	79.8	1.35	62.38	SVOCs
Campesterol	87.8	2.88	23.88	SVOCs
¿ó-Sitosterol	89.7	3.39	15.63	SVOCs

compound	1-D R.T. /min	2-D R.T. /sec	Concentration /μg·m^{-3}	Volatility
Oxygenated compounds/ Phenols				
Phenol	18.5	1.68	4.48	VOCs
Phenol, 4-butyl-	34.4	1.74	1.51	IVOCs
Benzene, 1,1'-[1,2-ethanediylbis(oxy)]bis-	52.4	3	1.09	IVOCs
[1,1':3',1"-Terphenyl]-2'-ol	65.4	3.75	4.70	IVOCs
Oxygenated compounds/Sugars				
2,3-Anhydro-D-galactosan	28.8	3.78	1.13	IVOCs
2,3-Anhydro-D-mannosan	29.1	3.63	1.58	IVOCs
D-Allose	40.6	4.26	0.64	IVOCs