Electronic Supplementary Information

Tube-type passive sampling of cyclic volatile methyl siloxanes (cVMSs) and benzene series simultaneously in indoor air: Uptake rate determination and field application

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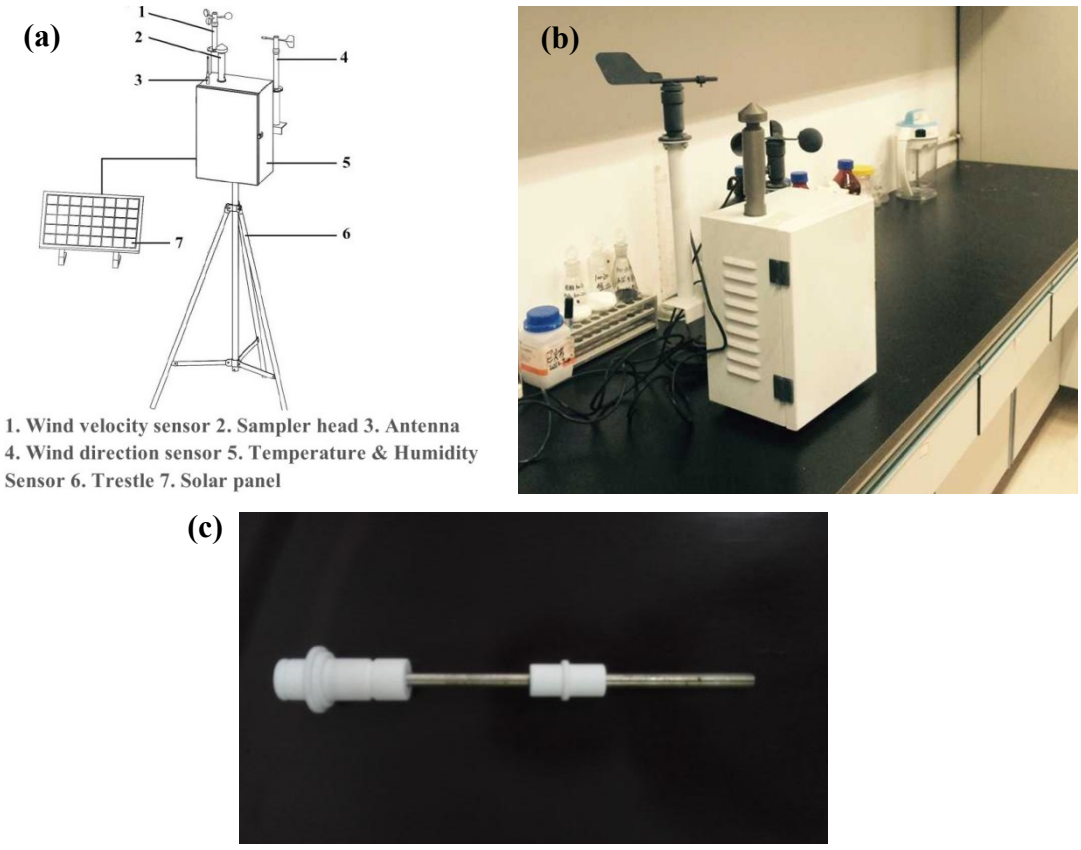

Figure S1. (a) The structure of the active low air flow sampler, and the photos of **(b)** low air flow sampler and **(c)** TD tubes with Tenax-TA.

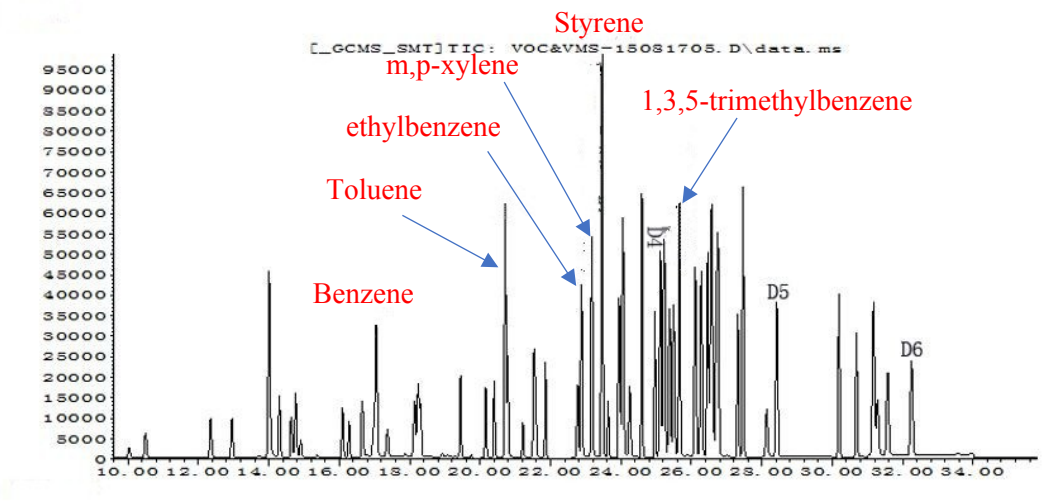

Figure S2. The total ion chromatograms.

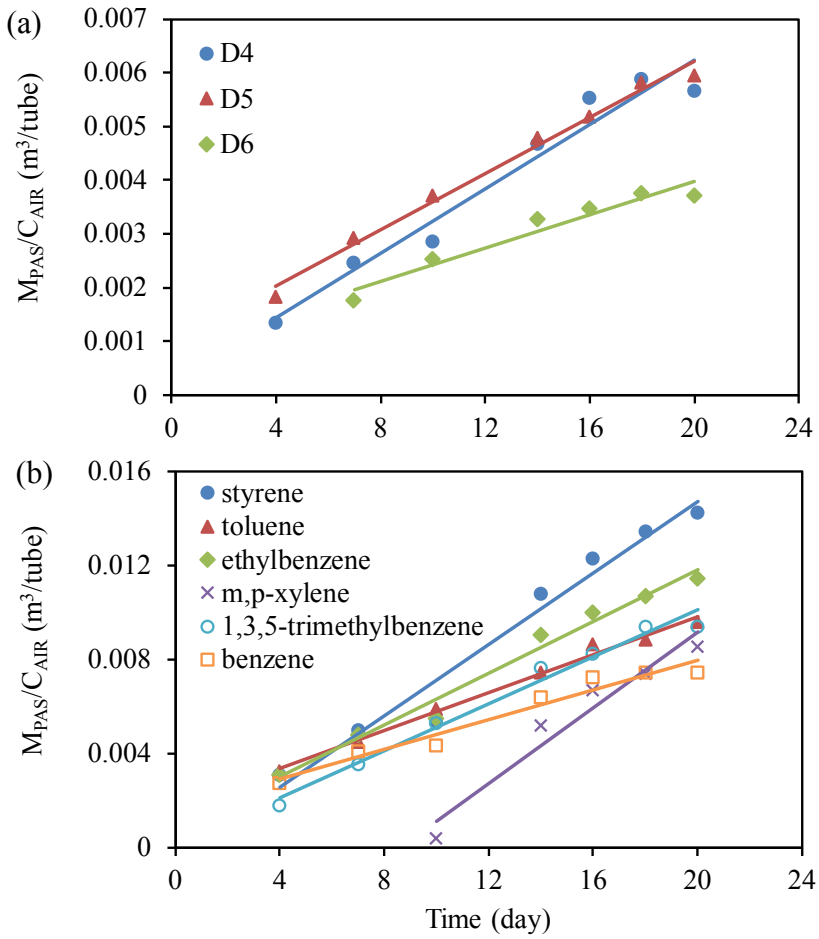

Figure S3. Calibration curves for (a) cVMSs and (b) benzene series compounds.

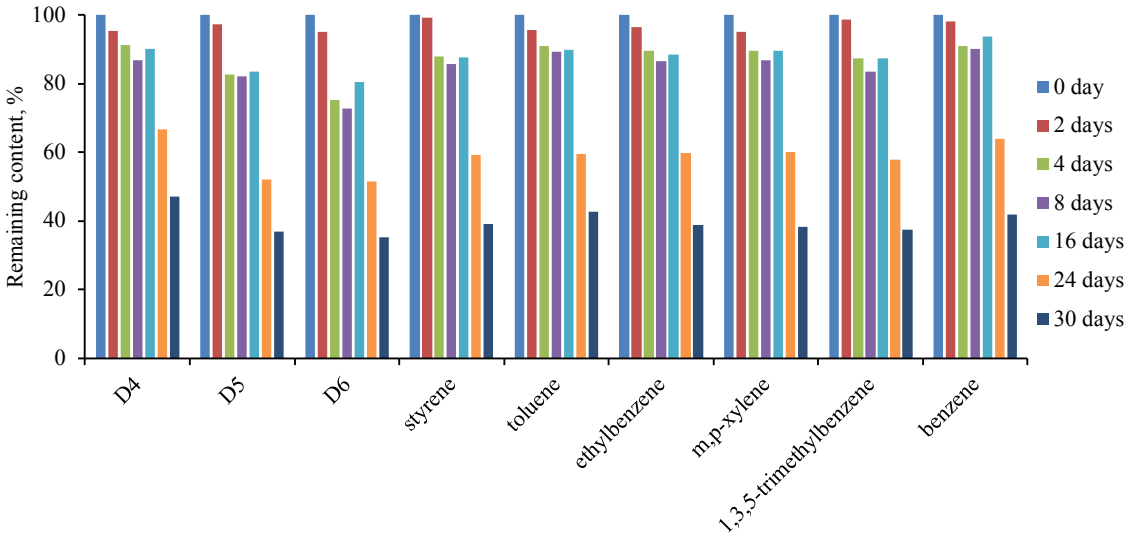

Figure S4. Temporal (30-day) changes in levels of cVMSs and benzene series compounds in the Tenax-TA-PAS samples.

Table S1. Passive air sampling time (min) for calibration.

Start time		End time		Sampling duration
(dd/mm/yyyy)	(hh:mm)	(dd/mm/yyyy)	(hh:mm)	(hr)
21/11/2015	15:30	21/11/2015	15:30	96
21/11/2015	15:30	28/11/2015	15:30	168
21/11/2015	15:30	01/12/2015	15:30	240
21/11/2015	15:30	05/12/2015	15:30	336
21/11/2015	15:30	07/12/2015	15:30	384
21/11/2015	15:30	09/12/2015	15:30	432
21/11/2015	15:30	11/12/2015	15:30	480

Table S2. Active air sampling time (min), sampling volume (mL) and sampling flow rate ($mL \cdot min^{-1}$) for calibration.

Start time		End time	Sampling duration	Sampling volume	Sampling flow rate
(dd/mm/yyyy)	(hh:mm)	(hh:mm)	(hr)	(mL)	($mL \cdot min^{-1}$)
18/11/2015	11:00	14:00	3	10800	60
20/11/2015	9:00	11:00	3	7020	39
22/11/2015	15:30	18:30	3	9360	52
25/11/2015	15:30	18:30	3	9720	54
28/11/2015	15:00	18:30	3	10440	58
1/12/2015	8:30	11:30	3	9360	52
4/12/2015	15:00	18:00	3	8820	49
7/12/2015	15:30	18:30	3	10260	57

Table S3. The indoor temperature and humidity during sampling in the indoor setting.

Time (day)	Temperature (°C)	humidity (%)
0	23	29
4	25	33
7	25	34
10	23	35
14	25	37
16	23	35
18	21	32
20	19	29

Table S4. Signal to noise ratio (S/N), limit of detection (LOD) and quantification (LOQ) for individual cVMSs and benzene series compounds.

Compound	S/N	LOD (ng/tube) [a]	LOQ (ng/tube) [b]
D4	530	0.00113	0.00377
D5	915	0.000656	0.00219
D6	570	0.00105	0.00351
styrene	315	0.00191	0.00636
toluene	180	0.00334	0.0111
ethylbenzene	760	0.000789	0.00263
m,p-xylene	1335	0.000449	0.00150
1,3,5-trimethylbenzene	194	0.00310	0.0103
benzene	175	0.00343	0.0114

[a] LOD = average of blanks + 3 × standard deviation. [b] LOQ = average of blanks + 10 × standard deviation. All samples were corrected for field blanks.

Table S5. Physicochemical properties of cVMSs and benzene series compounds.

	MW (g/mol)	BP (°C)	VP (Pa)	lg K_{OA} [a]
D4	297	175	124.5	4.42
D5	371	210	20.4	3.94
D6	445	245	4.6	5.50
styrene	104	145	666.6	3.87
toluene	92	111	2800	3.31
ethylbenzene	106	136	1333	3.64
m,p-xylene	106	138	1200	3.69
1,3,5-trimethylbenzene	120	165	266.6	3.90
benzene	78	80	12700	2.77

[a] lg K_{OA} is obtained from http://www.chemspider.com/

Table S6. The mass of passive air sampling (μg) and average concentration of active air sampling (μg·m^{-3}) in the calibration experiment.

Compounds	M_{PAS} (μg)							C_{air}
	4 d	7 d	10 d	14 d (n=4) ±STD*	16 d	18 d	20 d	(μg·m^{-3})
D4	0.0085	0.0156	0.0181	0.0296±0.0015	0.035	0.0372	0.0359	6.34±0.29
D5	0.0099	0.0159	0.0202	0.026±0.0016	0.0282	0.0316	0.0324	5.45±0.25
D6	ND	0.0037	0.0053	0.0069±0.0006	0.0073	0.0079	0.0078	2.11±0.28
styrene	0.0008	0.0013	0.0014	0.0028±0.0003	0.0032	0.0035	0.0037	0.26±0.44
toluene	0.0099	0.0137	0.0179	0.0227±0.0013	0.0263	0.0269	0.0293	3.05±0.28
ethylbenzene	0.0013	0.002	0.0023	0.0038±0.0003	0.0042	0.0045	0.0048	0.42±0.44
m,p-xylene	ND	ND	0.0001	0.0014±0.0002	0.0018	0.002	0.0023	0.27±0.58
1,3,5-trimethylbenzene	0.0003	0.0006	0.0009	0.0013±0.0001	0.0014	0.0016	0.0016	0.17±0.34
benzene	0.0031	0.0046	0.0049	0.0072±0.0003	0.0082	0.0084	0.0084	1.13±0.59

*Accuracy was calculated through the analysis of 4 replicates, d=day

Table S7. Calibration curves for cVMSs and benzene series compounds from Figure S3.

	This study		
	Linear	R^2	R (mL/min)
D4	y=0.00030x+0.0002	0.957	0.21
D5	y=0.00026x+0.0010	0.988	0.18
D6	y=0.00015x+0.0009	0.937	0.10
styrene	y=0.00076x-0.0005	0.965	0.53
toluene	y=0.00040x+0.0017	0.992	0.28
ethylbenzene	y=0.00055x+0.0008	0.980	0.38
m,p-xylene	y=0.00080x-0.0069	0.945	0.56
1,3,5-trimethylbenzene	y=0.00050x+0.00008	0.981	0.35
benzene	y=0.00032x+0.0016	0.956	0.22

Table S8. Passive uptake rate (R, mL/min) of benzene series compounds for tube-type passive samplers in this study and other papers.

Compounds	This study	Walgraeve et al. [1]	Jia and Fu [2]
styrene	0.53	0.36	0.36
toluene	0.28	0.32	0.32
ethylbenzene	0.38	0.35	0.46
m,p-xylene	0.56	0.36	0.36
1,3,5-trimethylbenzene	0.35	-	0.34
benzene	0.22	0.27	0.27

Table S9. Storage results for blank TD tubes (ng).

	0 day (n=2)	1 day (n=2)	2 days (n=2)	4 days (n=2)	6 days (n=2)	10 days (n=2)	14 days
D4	ND	ND	ND	ND	ND	ND	ND
D5	ND	ND	ND	ND	ND	ND	ND
D6	2.07±0.08	1.99±0.01	2.10±0.07	1.98±0	2.01±0	2.03±0.06	2.07
styrene	ND	ND	ND	ND	ND	ND	ND
toluene	ND	ND	ND	ND	ND	ND	ND
ethylbenzene	ND	ND	ND	ND	ND	ND	ND
m,p-xylene	ND	ND	ND	ND	ND	ND	ND
1,3,5-trimethylbenzene	ND	ND	ND	ND	ND	ND	ND
benzene	ND	ND	ND	ND	ND	ND	0.09

Table S10. The concentration of cVMSs ($\mu g \cdot m^{-3}$) in active and passive air samples in living room and office environments.

Compounds	Living room				Office environment			
	active (n=14)	STD	RSD (%)	passive (n=1)	active (n=7)	STD	RSD (%)	passive (n=1)
D4	0.36	0.21	57	0.57	0.49	0.17	35	0.52
D5	0.28	0.12	44	0.57	0.22	0.07	34	0.76
D6	0.54	0.27	50	0.90	0.35	0.11	31	0.50
styrene	0.57	0.70	123	0.14	0.50	0.03	6	0.19
toluene	10.8	9.65	90	7.64	4.52	2.53	56	5.17
ethylbenzene	3.84	2.94	76	3.96	1.05	0.12	12	0.90
m,p-xylene	3.72	3.13	84	2.40	0.98	0.22	22	0.46
1,3,5-trimethylbenzene	0.22	0.19	85	0.46	0.18	0.03	16	0.06
benzene	4.85	3.62	75	6.08	1.09	1.06	97	1.29

References

[1] C. Walgraeve, K. Demeestere, J. Dewulf, K. Van Huffel, and H. Van Langenhove, Diffusive sampling of 25 volatile organic compounds in indoor air: Uptake rate determination and application in Flemish homes for the elderly. *Atmospheric Environment*, 2011. **45**(32): p. 5828-5836.

[2] Chunrong Jia and Xianqiang Fu, Diffusive Uptake Rates of Volatile Organic Compounds on Standard ATD Tubes for Environmental and Workplace Applications. *Environments*, 2017. **4**(4): p. Article Number 87.