Supporting Information for:

Evaluation and application of a passive air sampler for atmospheric volatile organic compounds

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SI Table 1. Performance of PAS in this study for 28 VOCs. SRs are at 298 K and 1013 hPa. NR: The molecular diffusion coefficient of the analytes in air are not reported, and the corresponding theoretical SRs cannot be determined.

Compounds	MDL ($\mu g\ m^{-3}$)	MQL ($\mu g\ m^{-3}$)	Repeatability %	Recovery %	Uncertainty at 2σ %	SR ($ml\ min^{-1}$)	Theoretical SR ($ml\ min^{-1}$)
2,2-Dichloropropane	0.16	0.53	4.1 ± 3.5	95.6 ± 6.5	11.9 ± 5.1	59.68 ± 6.43	NR
cis-1,2-Dichloroethylene	0.17	0.56	4.1 ± 3.2	99.9 ± 7.0	11.9 ± 4.8	55.26 ± 3.70	NR
Bromochloromethane	0.05	0.16	3.8 ± 3.8	101.7 ± 8.8	11.3 ± 5.4	66.63 ± 7.40	76.93
Carbon tetrachloride	0.09	0.31	7.6 ± 9.2	91.2 ± 6.9	18.9 ± 10.8	60.12 ± 6.70	66.84
Benzene	0.03	0.10	3.2 ± 2.2	99.8 ± 7.5	10.1 ± 3.8	77.11 ± 6.47	75.23
Trichloroethylene	0.03	0.11	3.9 ± 4.3	98.0 ± 6.7	11.5 ± 5.9	64.04 ± 4.64	70.63
1,2-Dichloropropane	0.07	0.23	4.8 ± 4.8	98.3 ± 7.7	13.3 ± 6.4	63.79 ± 5.91	NR
Toluene	0.02	0.07	4.6 ± 2.9	97.3 ± 8.1	12.9 ± 4.5	66.01 ± 5.74	68.53
Tetrachloroethylene	0.03	0.12	2.6 ± 2.7	97.8 ± 8.9	8.9 ± 4.3	58.02 ± 7.22	64.33
Ethylbenzene	0.02	0.07	3.5 ± 3.1	96.7 ± 9.4	10.7 ± 4.7	63.07 ± 6.57	60.94
m/p-Xylene	0.04	0.13	4.0 ± 2.9	97.1 ± 9.4	11.7 ± 4.5	56.22 ± 7.54	54.81
o-Xylene	0.04	0.13	3.4 ± 2.9	95.3 ± 9.8	10.5 ± 4.5	60.29 ± 7.47	58.68
Styrene	0.03	0.12	2.3 ± 0.3	87.1 ± 9.3	4.3 ± 1.9	55.59 ± 6.38	56.58
Bromoform	0.03	0.11	7.3 ± 5.3	98.1 ± 10.1	18.3 ± 6.9	64.69 ± 8.94	61.91
1,1,2,2-Tetrachlorethane	0.04	0.12	4.3 ± 2.5	100.8 ± 9.6	12.3 ± 4.1	64.17 ± 7.35	58.28
1,2,3-Trichloropropane	0.06	0.19	1.3 ± 0.8	98.5 ± 10.0	6.3 ± 2.4	62.39 ± 8.29	NR
n-Propylbenzene	0.07	0.24	3.4 ± 2.6	93.9 ± 10.1	10.5 ± 4.2	54.90 ± 5.73	54.00
tert-Butylbenzene	0.05	0.15	2.8 ± 1.2	100.3 ± 9.8	7.3 ± 2.8	46.25 ± 6.39	NR
1,2,4-Trimethylbenzene	0.05	0.18	2.6 ± 1.8	95.5 ± 10.0	8.9 ± 3.4	47.42 ± 5.38	NR
sec-Butylbenzene	0.03	0.14	2.5 ± 2.2	101.1 ± 9.0	8.7 ± 3.8	47.09 ± 5.58	NR
p-Isopropyltoluene	0.04	0.13	2.6 ± 2.6	99.8 ± 10.2	8.9 ± 4.2	46.93 ± 5.17	NR
1,3-Dichlorobenzene	0.11	0.37	7.2 ± 8.3	95.2 ± 11.2	18.1 ± 9.9	47.07 ± 4.69	NR
1,4-Dichlorobenzene	0.09	0.31	7.8 ± 9.6	90.4 ± 11.3	19.3 ± 11.2	48.22 ± 4.22	NR

n-Butylbenzene	0.04	0.13	2.0 ± 0.9	99.2 ± 11.2	5.7 ± 2.5	46.44 ± 5.75	NR
1,2-Dichlorobenzene	0.10	0.33	7.8 ± 8.4	88.1 ± 11.2	5.3 ± 2.0	46.39 ± 4.63	NR
1,2-Dibromo-3-chloropropane	0.03	0.10	6.5 ± 9.1	91.8 ± 4.7	16.7 ± 10.7	55.53 ± 4.47	55.37
hexachloro-1,3-butadiene	0.04	0.13	7.3 ± 7.0	96.3 ± 8.7	18.3 ± 8.6	46.63 ± 4.25	NR
1,2,3-Trichlorobenzene	0.10	0.32	7.3 ± 8.6	92.3 ± 7.5	18.3 ± 10.2	42.70 ± 3.25	NR

SI Table 2. Performance of PASs for BTEX from published studies. NR: not reported.

Name	Sorbent material	Analyte	Analytical method	Deployment time	SR at 298 K (ml min^{-1})	MDL (µg m^{-3})	Recovery (%)	Repeatability (%)	Uncertainty (2σ) (%)	References
3M OVM	Activated carbon	BTEX	CS_2 desorption and GC-MS	24 h	21.5 - 45.0 (3M)	0.04 - 0.16	> 95	NR	NR	(Demirel et al., 2014)
ACFL-SPMS	Activated carbon and florisil	BTEX	Head-space GC-MS	24 h	~ 0.01 - 0.13 L/h	0.001µg	NR	< 7	NR	(Esteve-Turrillas et al., 2009)
Analyst	Graphitized charcoal	BTEX	CS_2 desorption and GC-MS	8 h	6.93 - 8.93	0.05 - 1	80 ± 5 – 110 ± 3	NR	NR	(Moussaoui et al., 2012)
GABIE	Active charcoal	Toluene	CS_2 desorption and GC-MS	4 h	36.3	NR	NR	NR	NR	(Langlois, 2008)
ORSA-5	Not reported	BTX	CS_2 desorption and GC-FID	21 d	NR	< 0.5	NR	NR	NR	(Gallego et al., 2008)
PCB	Polypyrrole	Xylene	TD GC-FID	8 h	16.2	NR	NR	< 10	NR	(Saelim et al., 2013)
Perkin Elmer tube	Tenax TA	Toluene	TD GC-MS	4 h	0.34	NR	NR	NR	NR	(Langlois, 2008)
	Carbopack X	Benzene	TD GC-FID	1 w	0.59	NR	NR	NR	NR	(Gustafson et al., 2007)
POD	Carbopack X	BTEX	TD GC-FID	24 h	1.50 ± 12.6 – 8.88 ± 5.9 at 293 K	0.045 - 0.283	NR	NR	NR	(Ballesta et al., 2016)
Radiello	Activated charcoal	BTEX	CS_2 desorption and GC-MS	1 w	65 ± 2.5 - 80 ± 1.8 (Sigma Aldrich)	0.007 - 0.014	NR	NR	NR	(Joos et al., 2003; Buczynska et al., 2009)

Shibata	Activated carbon	BTX	CS_2 desorption and GC-FID	1 - 30 d	42.2 - 54.8	0.04 - 0.05	NR	NR	NR	(Yamada et al., 2004)
SKC Ultra	Carbopack X	Benzene	TD GC-FID	24 h	16	0.03	NR	NR	NR	(Gustafson et al., 2007)
SPME	Carboxen	BTEX	TD GC-MS	1 - 95 h	0.0055 - 0.016	NR	NR	NR	NR	(Gong et al., 2008)
Tailor-made diffusive sampler	Activated carbon	BTEX	CS_2 desorption and GC-MS	24 h and 1 w	9.26 ± 4.50 – 7.79 ± 3.56	0.02 - 0.11	92.83 ± 6.51 - 101.76 ± 10.80	5.9 ± 1.4 - 13.0 ± 1.8	11.2 ± 7.90 - 13.8 ± 8.10	(Can et al., 2015; Özden Üzmez et al., 2015)
THPDS	Silica zeolites	BTX	TD GC-MS	24 h	0.76 ± 0.22 – 5.44 ± 1.46	6.1 - 11.0	NR	7.4 - 10.5	16.9 - 23.3	(Du et al., 2013; Du et al., 2014)
TOPAS	Tenax	BTEX	TD GC-MS	5 h	0.5 ± 0.1 – 2.6 ± 0.2 L/h	0.5	> 80	NR	NR	(E et al., 2001)
PAS	Activated charcoal	BTEX	CS_2 desorption and GC-FID	1w, 2w, 3w, and 1 month	56.22 ± 7.54 – 77.11 ± 6.47	0.02 – 0.04	95.3 ± 9.8 - 99.8 ± 7.5	3.2 ± 2.2 - 4.6 ± 2.9	10.1 ± 3.8 - 12.9 ± 4.5	This study

SI Table 3. Monthly mean atmospheric concentrations of 28 VOCs at NUEORS derived from the PAS in this study (μg m^{-3}).

Month	2,2-Dichloro-propane	cis-1,2-Dichloro-ethylene	Bromochloro-methane	Carbon tetrachloride	Benzene	Trichloro-ethylene	1,2-Dichloro-propane	Toluene	Tetrachloro-ethylene	Ethyl-benzene
Nov	7.62 ± 0.82	10.91 ± 0.73	6.45 ± 0.72	16.02 ± 1.78	1.97 ± 0.17	4.37 ± 0.32	2.44 ± 0.23	4.90 ± 0.43	1.56 ± 0.19	2.93 ± 0.31
Dec	11.17 ± 1.20	18.41 ± 1.23	11.31 ± 1.26	28.90 ± 3.22	3.14 ± 0.26	6.74 ± 0.49	2.78 ± 0.26	7.76 ± 0.67	2.39 ± 0.30	5.25 ± 0.55
Jan	8.17 ± 0.88	10.92 ± 0.73	6.33 ± 0.70	19.00 ± 2.12	2.82 ± 0.24	4.75 ± 0.34	2.01 ± 0.19	4.88 ± 0.42	1.73 ± 0.22	3.07 ± 0.32
Feb	8.26 ± 0.89	12.42 ± 0.83	7.03 ± 0.78	17.87 ± 1.99	2.24 ± 0.19	5.78 ± 0.42	1.95 ± 0.18	4.85 ± 0.42	1.85 ± 0.23	3.88 ± 0.40
Mar	6.34 ± 0.68	8.54 ± 0.57	4.93 ± 0.55	12.81 ± 1.43	2.15 ± 0.18	3.28 ± 0.24	1.75 ± 0.16	4.30 ± 0.37	1.48 ± 0.18	3.03 ± 0.32
Apr	5.45 ± 0.59	10.32 ± 0.69	6.32 ± 0.70	16.41 ± 1.83	1.78 ± 0.15	4.01 ± 0.29	1.91 ± 0.18	4.06 ± 0.35	1.29 ± 0.16	2.32 ± 0.24
May	2.68 ± 0.29	5.01 ± 0.34	3.04 ± 0.34	9.82 ± 1.09	1.29 ± 0.11	2.75 ± 0.20	1.17 ± 0.11	1.95 ± 0.17	1.09 ± 0.14	1.42 ± 0.15
Jun	2.91 ± 0.31	3.63 ± 0.24	2.44 ± 0.27	9.72 ± 1.08	1.01 ± 0.09	1.68 ± 0.12	1.08 ± 0.10	2.30 ± 0.20	0.94 ± 0.12	1.16 ± 0.12
Jul	2.93 ± 0.32	3.27 ± 0.22	2.30 ± 0.26	6.62 ± 0.74	0.98 ± 0.08	1.46 ± 0.11	1.01 ± 0.09	2.05 ± 0.18	0.88 ± 0.11	1.05 ± 0.11
Aug	2.46 ± 0.27	4.07 ± 0.27	2.72 ± 0.30	9.54 ± 1.06	1.14 ± 0.10	1.78 ± 0.13	0.98 ± 0.09	1.90 ± 0.17	0.97 ± 0.12	1.24 ± 0.13
Sep	3.05 ± 0.33	4.68 ± 0.31	2.95 ± 0.33	6.55 ± 0.73	1.06 ± 0.09	1.98 ± 0.14	0.95 ± 0.09	2.47 ± 0.21	1.03 ± 0.13	1.30 ± 0.14
Oct	3.37 ± 0.36	4.89 ± 0.33	3.23 ± 0.36	7.95 ± 0.89	1.04 ± 0.09	1.95 ± 0.14	1.19 ± 0.11	2.50 ± 0.22	0.97 ± 0.12	1.37 ± 0.14

Month	m/p-Xylene	o-Xylene	Styrene	Bromoform	1,1,2,2-Tetrachlor-ethane	1,2,3-Trichloro-propane	n-Propyl-benzene	tert-Butyl-benzene	1,2,4-Trimethyl-benzene	sec-Butyl-benzene
Nov	4.08 ± 0.55	3.20 ± 0.40	0.84 ± 0.10	5.96 ± 0.82	4.46 ± 0.51	0.86 ± 0.11	2.54 ± 0.27	1.34 ± 0.18	2.21 ± 0.25	1.29 ± 0.15
Dec	7.26 ± 0.97	5.29 ± 0.65	0.95 ± 0.11	7.29 ± 1.01	7.25 ± 0.83	0.94 ± 0.13	3.46 ± 0.36	1.38 ± 0.19	2.51 ± 0.29	1.03 ± 0.12
Jan	4.50 ± 0.60	3.33 ± 0.41	0.83 ± 0.10	3.87 ± 0.53	6.51 ± 0.75	0.83 ± 0.11	2.39 ± 0.25	1.22 ± 0.17	1.92 ± 0.22	1.14 ± 0.14
Feb	5.77 ± 0.77	4.08 ± 0.51	0.80 ± 0.09	3.45 ± 0.48	5.29 ± 0.61	0.82 ± 0.11	2.48 ± 0.26	1.24 ± 0.17	2.01 ± 0.23	0.96 ± 0.11
Mar	4.60 ± 0.62	3.31 ± 0.41	0.77 ± 0.09	3.48 ± 0.48	4.88 ± 0.56	0.83 ± 0.11	2.60 ± 0.27	1.28 ± 0.18	1.72 ± 0.19	0.95 ± 0.11
Apr	3.37 ± 0.45	2.53 ± 0.31	0.83 ± 0.10	3.78 ± 0.52	4.29 ± 0.49	0.96 ± 0.13	2.25 ± 0.23	1.43 ± 0.20	1.98 ± 0.22	1.28 ± 0.15
May	1.96 ± 0.26	1.68 ± 0.21	0.70 ± 0.08	2.02 ± 0.28	3.22 ± 0.37	0.71 ± 0.09	1.24 ± 0.13	0.99 ± 0.14	1.21 ± 0.14	0.89 ± 0.10
Jun	1.60 ± 0.21	1.34 ± 0.17	0.68 ± 0.08	1.59 ± 0.22	2.52 ± 0.29	0.69 ± 0.09	1.15 ± 0.12	0.92 ± 0.13	1.13 ± 0.13	0.90 ± 0.11
Jul	1.29 ± 0.17	1.18 ± 0.15	0.69 ± 0.08	3.15 ± 0.44	2.66 ± 0.31	0.68 ± 0.09	0.98 ± 0.10	0.98 ± 0.13	1.02 ± 0.12	0.99 ± 0.12
Aug	1.66 ± 0.22	1.26 ± 0.16	0.70 ± 0.08	2.73 ± 0.38	4.64 ± 0.53	0.77 ± 0.10	1.52 ± 0.16	1.25 ± 0.17	1.60 ± 0.18	1.05 ± 0.12

Sep	1.78 ± 0.24	1.53 ± 0.19	0.71 ± 0.08	2.23 ± 0.31	2.63 ± 0.30	0.71 ± 0.09	1.64 ± 0.17	1.04 ± 0.14	1.46 ± 0.17	1.00 ± 0.12
Oct	2.04 ± 0.27	1.72 ± 0.21	0.70 ± 0.08	1.86 ± 0.26	2.21 ± 0.25	0.69 ± 0.09	1.38 ± 0.14	0.94 ± 0.13	1.30 ± 0.15	0.94 ± 0.11

Month	p-Isopropyl-toluene	1,3-Dichloro-benzene	1,4-Dichloro-benzene	n-Butyl-benzene	1,2-Dichloro benzene	1,2-Dibromo-3-chloropropane	hexachloro-1,3-butadiene	1,2,3-Trichloro-benzene
Nov	1.27 ± 0.14	3.38 ± 0.34	1.74 ± 0.15	1.35 ± 0.17	1.41 ± 0.14	8.65 ± 0.70	11.56 ± 1.05	4.30 ± 0.33
Dec	0.92 ± 0.10	3.22 ± 0.32	1.67 ± 0.15	1.29 ± 0.16	1.01 ± 0.10	2.14 ± 0.17	2.25 ± 0.20	1.79 ± 0.14
Jan	0.93 ± 0.10	7.18 ± 0.72	1.11 ± 0.10	1.13 ± 0.14	0.95 ± 0.10	3.12 ± 0.25	5.45 ± 0.50	1.89 ± 0.14
Feb	0.91 ± 0.10	2.57 ± 0.26	1.50 ± 0.13	1.14 ± 0.14	0.95 ± 0.10	3.20 ± 0.26	6.22 ± 0.57	2.76 ± 0.21
Mar	0.88 ± 0.09	8.44 ± 0.84	1.33 ± 0.12	1.05 ± 0.13	0.94 ± 0.09	4.64 ± 0.37	9.66 ± 0.88	3.47 ± 0.26
Apr	1.30 ± 0.14	4.21 ± 0.42	1.82 ± 0.16	1.37 ± 0.17	1.78 ± 0.18	5.04 ± 0.41	3.85 ± 0.35	3.08 ± 0.23
May	0.85 ± 0.09	6.23 ± 0.62	0.99 ± 0.09	0.89 ± 0.11	1.01 ± 0.10	1.33 ± 0.11	1.26 ± 0.12	1.06 ± 0.08
Jun	0.93 ± 0.10	1.86 ± 0.19	0.98 ± 0.09	0.87 ± 0.11	1.01 ± 0.10	3.26 ± 0.26	0.57 ± 0.05	0.42 ± 0.03
Jul	0.91 ± 0.10	5.23 ± 0.52	1.01 ± 0.09	0.86 ± 0.11	0.98 ± 0.10	1.91 ± 0.15	2.64 ± 0.24	1.99 ± 0.15
Aug	1.26 ± 0.14	10.85 ± 1.08	1.87 ± 0.16	1.26 ± 0.16	2.58 ± 0.26	12.42 ± 1.00	5.93 ± 0.54	5.86 ± 0.45
Sep	0.86 ± 0.09	4.09 ± 0.41	1.07 ± 0.09	0.90 ± 0.11	0.97 ± 0.10	1.06 ± 0.09	1.24 ± 0.11	1.33 ± 0.10
Oct	0.79 ± 0.09	1.65 ± 0.16	1.08 ± 0.09	0.93 ± 0.11	0.96 ± 0.10	1.17 ± 0.09	0.42 ± 0.04	0.64 ± 0.05

References

Ballesta, P.P., Grandesso, E., Field, R.A. and Cabrerizo, A. (2016). Validation and modelling of a novel diffusive sampler for determining concentrations of volatile organic compounds in air. *Anal. Chim. Acta.* 908: 102-112.

Buczynska, A.J., Krata, A., Stranger, M., Locateli Godoi, A.F., Kontozova-Deutsch, V., Bencs, L., Naveau, I., Roekens, E. and Van Grieken, R. (2009). Atmospheric btex-concentrations in an area with intensive street traffic. *Atmos. Environ.* 43: 311-318.

Can, E., Özden Üzmez, Ö., Döğeroğlu, T. and Gaga, E.O. (2015). Indoor air quality assessment in painting and printmaking department of a fine arts faculty building. *Atmos Pollut Res.* 6: 1035-1045.

Demirel, G., Ozden, O., Dogeroglu, T. and Gaga, E.O. (2014). Personal exposure of primary school children to btex, no(2) and ozone in eskisehir, turkey: Relationship with indoor/outdoor concentrations and risk assessment. *Sci. Total Environ.* 473-474: 537-548.

Du, Z., Mo, J., Zhang, Y., Li, X. and Xu, Q. (2013). Evaluation of a new passive sampler using hydrophobic zeolites as adsorbents for exposure measurement of indoor btx. *Anal. Methods.* 5: 3463.

Du, Z., Mo, J., Zhang, Y. and Xu, Q. (2014). Benzene, toluene and xylenes in newly renovated homes and associated health risk in guangzhou, china. *Build. Environ.* 72: 75-81.

E, K.-B., B, R., K, C. and G, B. (2001). Topas / tds d – badge-type thermodesorption passive sampler based on tenax for air sampling -development study. *Https://www.researchgate.net/publication/269691316.*

Esteve-Turrillas, F.A., Ly-Verdu, S., Pastor, A. and de la Guardia, M. (2009). Development of a versatile, easy and rapid atmospheric monitor for benzene, toluene, ethylbenzene and xylenes determination in air. *J. Chromatogr. A.* 1216: 8549-8556.

Gallego, E., Roca, F.X., Guardino, X. and Rosell, M.G. (2008). Indoor and outdoor btx levels in barcelona city metropolitan area and catalan rural areas. *J. Environ. Sci.* 20: 1063-1069.

Gong, Y., Eom, I.Y., Lou, D.W., Hein, D. and Pawliszyn, J. (2008). Development and application of a needle trap device for time-weighted average diffusive sampling. *Anal. Chem.* 80: 7275-7282.

Gustafson, P., Barregard, L., Strandberg, B. and Sallsten, G. (2007). The impact of domestic wood burning on personal, indoor and outdoor levels of 1,3-butadiene, benzene, formaldehyde and acetaldehyde. *J. Environ. Monit.* 9: 23-32.

Joos, P.E., Godoi, A.F.L., De Jong, R., de Zeeuw, J. and Van Grieken, R. (2003). Trace analysis of benzene, toluene, ethylbenzene and xylene isomers in environmental samples by low-pressure gas chromatography–ion trap mass spectrometry. *J. Chromatogr. A.* 985: 191-196.

Langlois, E. (2008). Gabie and perkin elmer passive sampler performance under fluctuating concentration conditions. *Ann. Occup. Hyg.* 52: 239-247.

Moussaoui, Y., Cecinato, A., Assami, K. and Meklati, B.Y. (2012). Indoor and outdoor voc emissions in urban areas of northern algeria. *Fresen. Environ. Bull.*21: 1090-1098.

Özden Üzmez, Ö., Gaga, E.O. and Döğeroğlu, T. (2015). Development and field validation of a new diffusive sampler for determination of atmospheric volatile organic compounds. *Atmos. Environ.* 107: 174-186.

Saelim, J., Kanatharana, P., Thavarungkul, P. and Thammakhet, C. (2013). Novel fabricated silver particles/polypyrrole printed circuit board passive samplers for volatile organic compounds monitoring. *Microchem. J.* 108: 180-187.

Yamada, E., Hosokawa, Y., Furuya, Y., Matsushita, K. and Fuse, Y. (2004). Simple analysis of volatile organic compounds (vocs) in the atmosphere using passive samplers. *Anal. Sci.* 20: 107-112.