

## Supporting Information

### **Characterizing the distribution of aromatic amines between polyester, cotton, and wool textiles and air**

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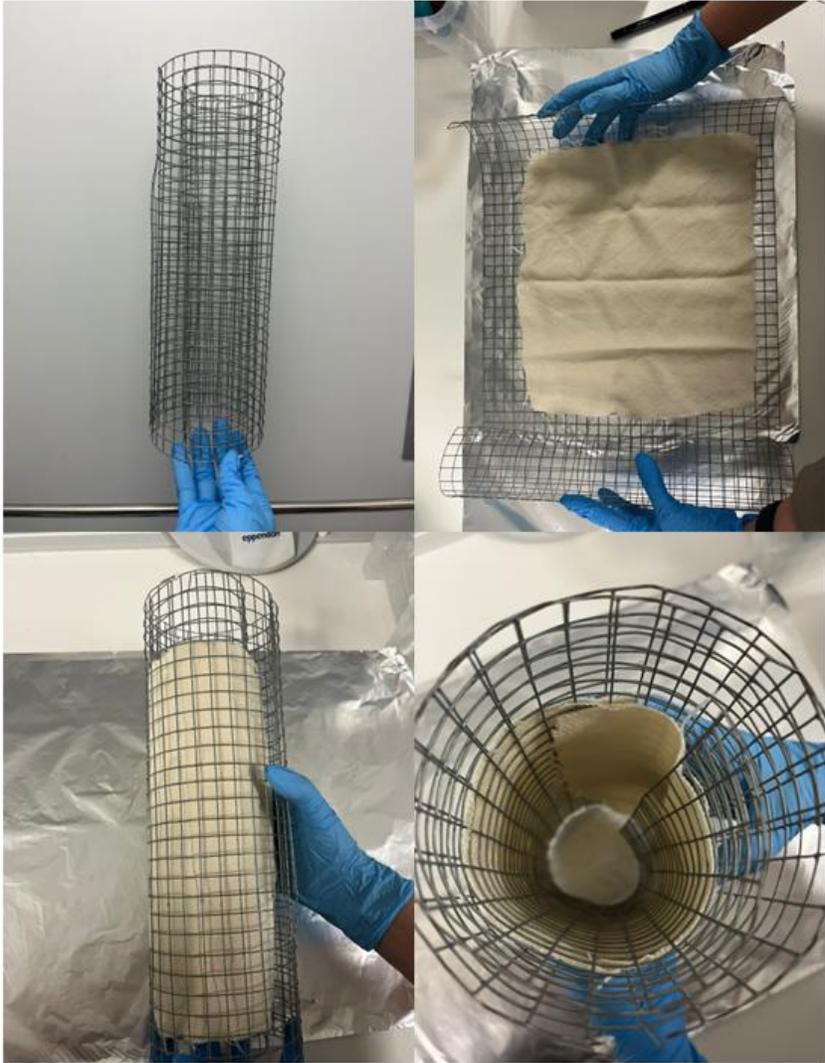


Figure S1. Details of the chamber set-up with the textile wrapped around the mesh

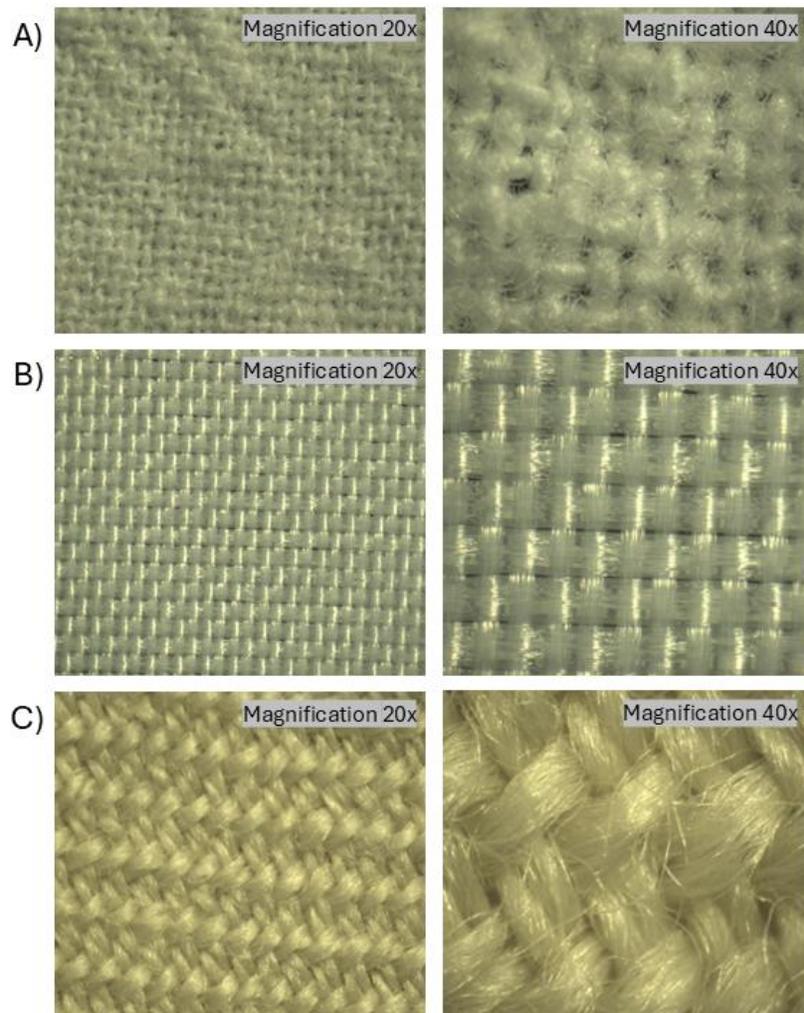


Figure S2. Microscopic structure of 3 types of textiles; A) Cotton, B) Polyester and C) Wool (Zoom Stereo Microscope; Olympus-SZ61, Tokyo, Japan).

## Text S1. Details of textile preparation

*Materials.* Three types of fabrics were procured for the study:

Plain weave Cotton: Sourced from Classic Fabrics ([classicfabrics.nl](http://classicfabrics.nl)), this fabric was white

Diagonal Twill Wool: Also from Classic Fabrics, this undyed white fabric

Polyester: Purchased from DůmLátek.cz, this fabric was white

*Preparation.* The fabrics were cut using the textile cutting board and textile cutter knife into sections measuring 27 cm by 8 cm to test different extraction procedures.

*Cleaning and Drying Procedure.* The cleaning process involved using an overhead tumbler (Fig. S2), which functioned similarly to a washing machine. The fabrics were added to a washing cycle with water only (no detergent) for two hours, simulating a standard washing procedure to remove any surface contaminants. This cleaning protocol was uniformly applied to all three types of textiles. The textiles were transferred onto aluminum foil and placed in an oven to dry. Once dried, the fabrics were wrapped in aluminum foil until further use.



*Figure S3. Overhead Tumbler for textile washing*

*Table S1. Textile properties*

<b>Textile type</b>	<b>Density (g/cm<sup>3</sup>)</b>	<b>Thickness (cm)</b>	<b>Length (cm)</b>	<b>Mass (g)</b>	<b>Width (cm)</b>
Wool	0.3	0.11	300	1221	148
Cotton	0.2	0.09	300	630	140
Polyester	0.1	0.05	300	258	148

Table S2. AA compounds and identifiers (CAS number, InChIKey, molecular formula)

Compound	Abbreviation	CAS RN	InChIKey	Molecular Formula
Aniline	ANI	62-53-3	PAYRUJLWNCNPSJ-UHFFFAOYSA-N	C6H7N
2-Aminopyridine	2APY	504-29-0	ICSNLGPSRYBMBD-UHFFFAOYSA-N	C5H6N2
o-Toluidine	OTLD	95-53-4	RNVCVTLRINQCPJ-UHFFFAOYSA-N	C7H9N
o-Anisidine	OANI	90-04-0	VMPITZXILSNTON-UHFFFAOYSA-N	C7H9NO
4-Chloraniline	4CHA	106-47-8	QSNCSYFYORTR-UHFFFAOYSA-N	C6H6ClN
p-Cresidine	PCRE	120-71-8	WXWCDTXEKCVRRO-UHFFFAOYSA-N	C8H11NO
3-Chloro-o-Toluidine	3CHOT	87-60-5	ZUVPLKVDZNDZCM-UHFFFAOYSA-N	C7H8ClN
4-Chloro-o-Toluidine	4CHOT	95-69-2	CXNVOWPRHWWCQR-UHFFFAOYSA-N	C7H8ClN
2-Amino-4-nitrotoluene	2A4NT	99-55-8	DSBIJCMXAIIKKKI-UHFFFAOYSA-N	C7H8N2O2
Benzidine	BNZD	92-87-5	HFACYLZERDEVXS-UHFFFAOYSA-N	C12H12N2
o-Aminoazotoluene	OAAT	97-56-3	PFRYFZZSECNQOL-UHFFFAOYSA-N	C14H15N3
1-Naphthylamine	1NAPA	134-32-7	RUFPHBVGCFYCNW-UHFFFAOYSA-N	C10H9N
2-Naphthylamine	2NAPA	91-59-8	JBIJLHTVPXGSAM-UHFFFAOYSA-N	C10H9N
p-Aminoazobenzene	PAAZB	60-09-3	QPQKUYVJSJWQSDY-UHFFFAOYSA-N	C12H11N3
3,3'-Dichlorobenzidine	33DCB	91-94-1	HUWXDEQWWKGHRV-UHFFFAOYSA-N	C12H10Cl2N2
o-Dianisidine	ODAN	119-90-4	JRBJSXQPQWSCCF-UHFFFAOYSA-N	C14H16N2O2
4,4'-Methylenebis(2-chloroaniline)	MBOCA	101-14-4	IBOFVQJTBBUKMU-UHFFFAOYSA-N	C13H12Cl2N2
2-Aminobiphenyl	2AMB	90-41-5	TWBPWBPGNQWFSJ-UHFFFAOYSA-N	C12H11N
4-Aminobiphenyl	4AMB	92-67-1	DMVOXQPQNTYEKQ-UHFFFAOYSA-N	C12H11N

## Text S2. Dosing procedure of aromatic amines to textiles

To ensure homogeneously spiked solutions on textiles, homogeneity tests were performed using three different dosing procedures prior to conducting chamber tests.

*Dosing with Tray.* The first method involved dosing with a tray (Figure S3). The tray was lined with aluminum foil, and textiles were placed in it. A dosing solution was prepared, with 1 ml of dosing standards added to acetone and diluted to ensure a sufficient volume for uniform application. Acetone was chosen as the solvent due to its rapid evaporation. The diluted solution was then applied to the textiles in the tray, which was subsequently placed in a fume hood to allow for complete evaporation. Following evaporation, 15 textile pieces were taken and extracted for analysis. The coefficient of variation (CV) for this method is presented in Table S1.

*Dosing with Rotary Evaporator.* The second method involved using a rotary evaporator (Figure S4). The textiles and diluted solution were prepared similarly to the tray method. However, in this procedure, the textile pieces were placed in a rotary flask and mixed thoroughly. The mixture was rotated in the rotary evaporator to ensure an even distribution of the analytes. After rotation, the solvent evaporated by rotation of the sample under mild vacuum (556 mbar, 40°C). This procedure was conducted with two different exposure times: a one-hour dosing period followed by evaporation, and a six-hour dosing period followed by evaporation. The results for these trials are detailed in Figure S2.

These preliminary tests were crucial in determining the most effective method for achieving homogeneously spiked textiles, essential for the reliability and accuracy of subsequent chamber tests. The coefficient of variation was used to assess the relative variability of data. When the CV exceeds 30 %, it often signals inconsistencies.<sup>1</sup> The lowest CV values were achieved with the 6-hour exposure design with a rotary evaporator, so this method was adopted to dose textiles for the subsequent chamber experiments.



Figure S4. Dosing with the tray

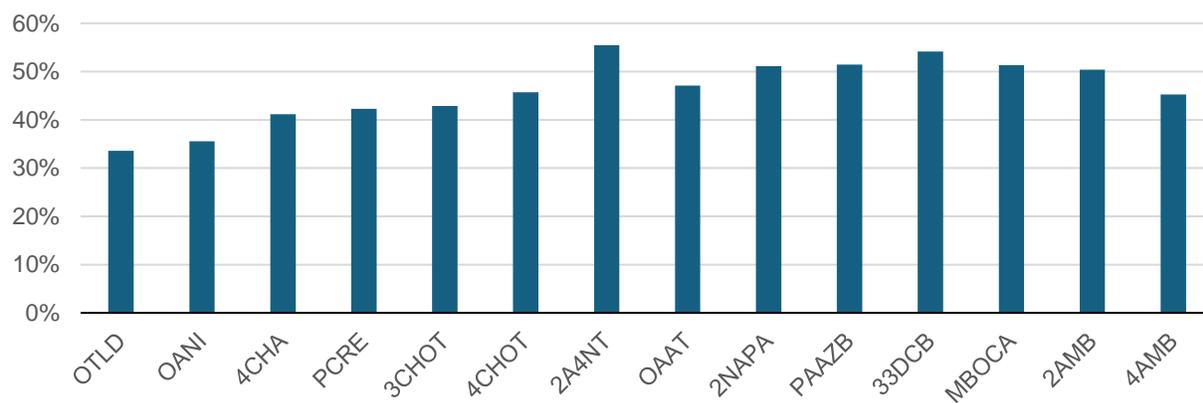


Figure S5. CV of AAs in polyester to evaluate homogeneity of fabrics based on dosing with the tray

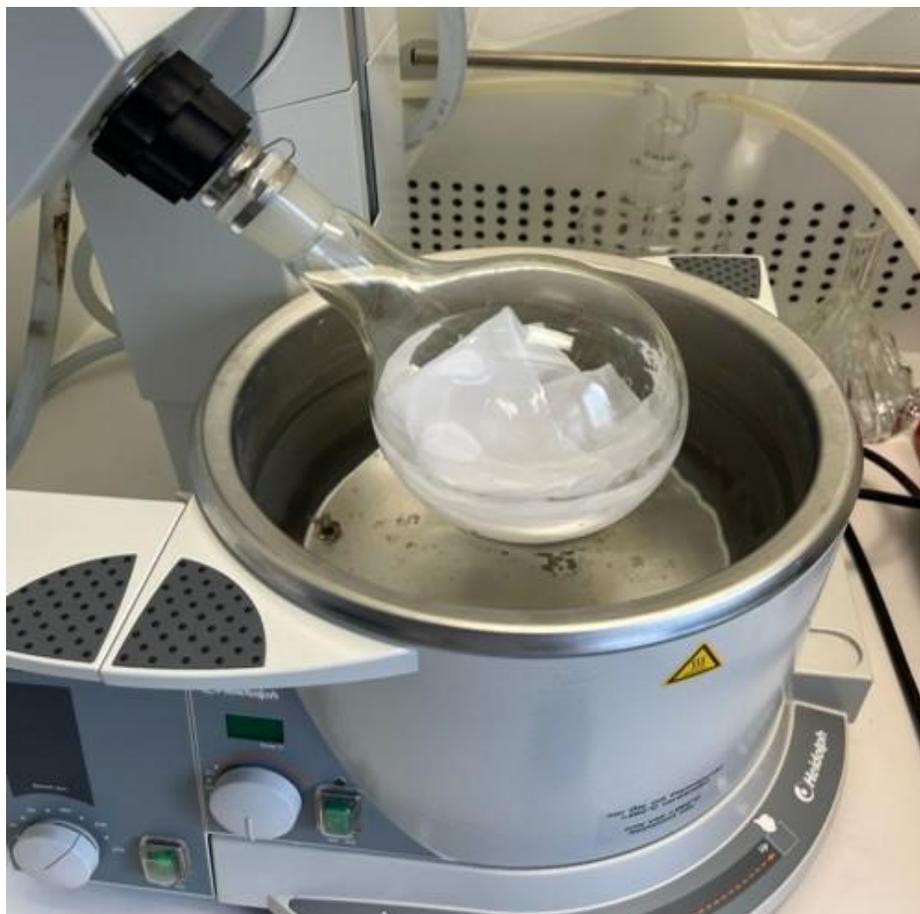


Figure S6. Dosing with Rotary Evaporator

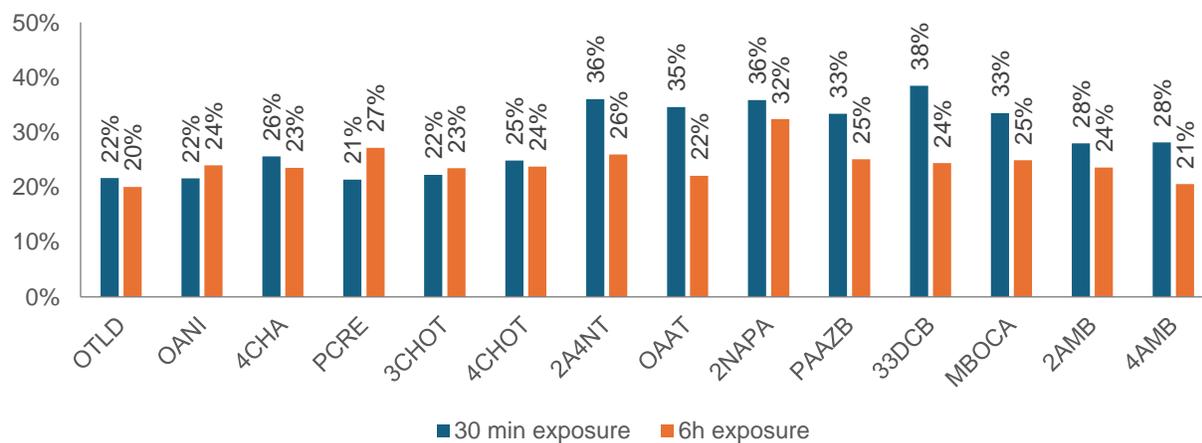


Figure S7. CV of AAs in polyester to evaluate the homogeneity of spiked AAs in fabrics based on dosing with rotary evaporator

Table S3. Nominal concentration of dosed AA on an 864 cm<sup>2</sup> area of textile surface

Compounds	Nominal Concentrations of spiked AAs (µg)	Producer
ANI	20	Chemcruz, Germany
2APY	40	Sigma-Aldrich, USA
OTLD	10	
OANI	40	
4CHA	20	
PCRE	30	
3CHOT	40	AccuStandard, USA
4CHOT	40	
2A4NT	20	
BNZD	60	Sigma-Aldrich, USA
OAAT	90	AccuStandard, USA
1NAPA	20	Tokyo Chemical Industry (TCI Co.), Japan
2NAPA	20	AccuStandard, USA
PAAZB	70	fluorochem, UK
33DCB	20	Sigma-Aldrich, USA
ODAN	50	AccuStandard, USA
MBOCA	40	
2AMB	40	
4AMB	40	Sigma-Aldrich, USA

### Text S3. Extraction tests of aromatic amines from textiles

*Acetonitrile.* Initial tests used 1% NH<sub>3</sub> in 180 mL acetonitrile (ACN) as the extraction solvent. The extraction method was adapted from Krupčíková et al.,<sup>2</sup> Textile pieces (27 x 8 cm) were placed in a 250 ml amber bottles. Primary AA standards (o-Toluidine, o-Anisidine, 4-Chloraniline, p-Cresidine, 3-Chloro-o-Toluidine, 4-Chloro-o-Toluidine, 2-Amino-4-nitrotoluene, o-Aminoazotoluene, 2-Naphthylamine, p-aminoazobenzene, 3,3'-Dichlorbenzidine, 4,4'-methylenebis(2-chloroaniline), 2-Aminobiphenyl, 4-Aminobiphenyl) spiked (500 ng/ml) on to textiles. Subsequently, the solvent was added, and the mixture was shaken on a flat orbital shaker for approximately 24 hours. This extraction process was performed three times, with only pure ACN used for the second and third extractions. The collected extracts were then concentrated to approximately 0.5 mL using a multi-position Buchi Syncore Analyst rotary evaporator. The extracts were filtered through a nylon syringe filter (Chromafil Xtra PA-20/13, pore size 0.20 µm, diameter 13 mm, Macherey-Nagel, Germany) into clean GC minivials to ensure purity and readiness for subsequent analysis.

*Acetone.* Acetone was used as the extraction solvent. Textile pieces (27 x 8 cm) were placed in 250 mL amber bottles. Textiles were dosed with the same analytes with the acetonitrile method and placed in vials. The extraction process began with the addition of 180 mL of acetone to each vial. The samples were then subjected to ultrasonication for 15 minutes. Extract transferred to the Syncore Evaporator bottles. This extraction step was repeated to maximize analyte recovery. The combined extracts were then concentrated using a Syncore Evaporator, reducing the solvent volume to approximately 0.5-1 mL. The concentrated extract underwent the same clean-up procedure with ACN to eliminate any remaining impurities. The extracts were filtered through a nylon syringe filter (Chromafil Extra PA-20/13, pore size 0.20  $\mu\text{m}$ , diameter 13 mm, Macherey-Nagel, Germany) into clean mini-vials.

*Methyl-tert-butyl Ether (MTBE).* The same procedure as for acetone was followed, using MTBE as the extraction solvent.

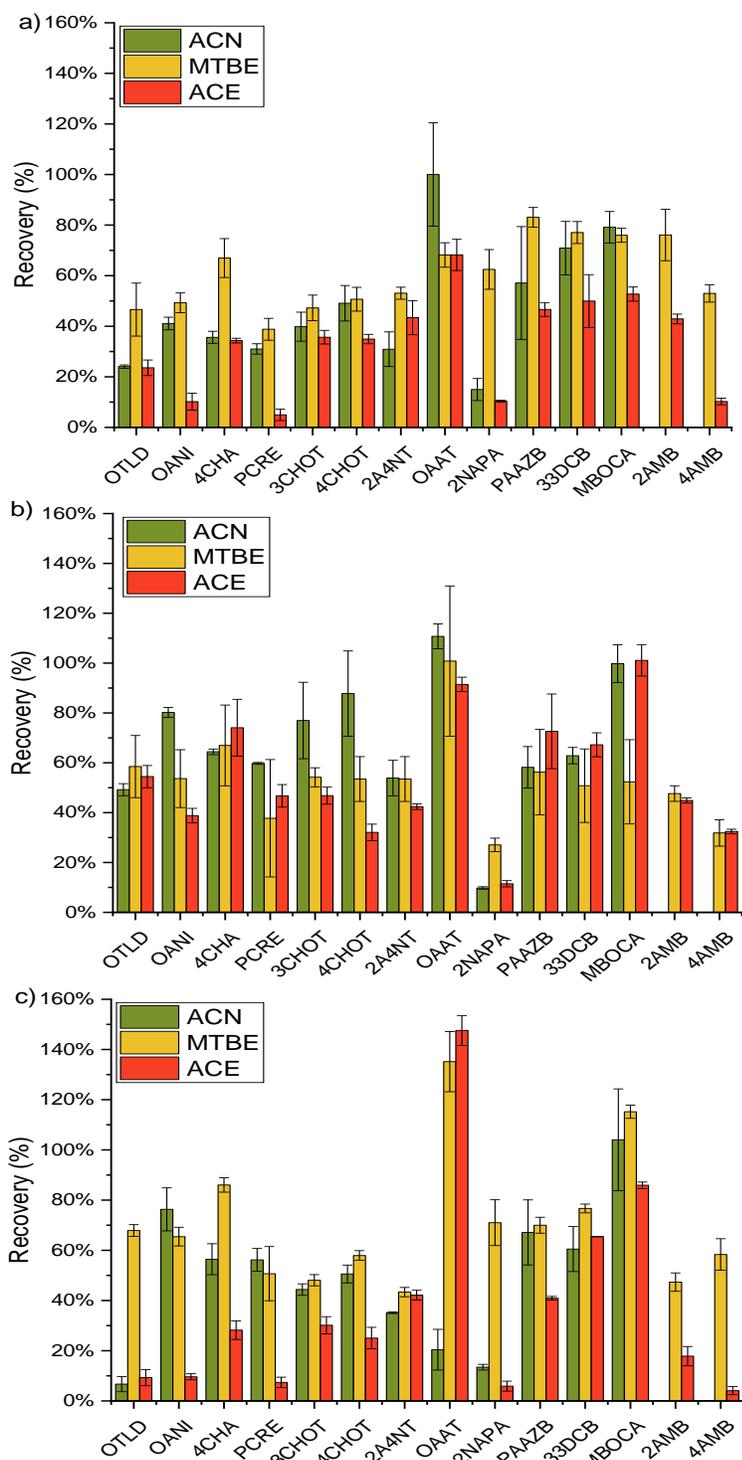


Figure S8. Extraction efficiencies for 3 different extraction solvents for a) polyester, b) cotton and c) wool. MTBE demonstrated high extraction efficiency across various textile types, particularly for compounds such as o-toluidine and 2-naphthylamine. Acetone shows effective performance for certain compounds in wool and polyester, although its efficiency is less consistent across different analytes. Acetonitrile, while exhibiting moderate efficiency comparable to acetone, generally falls short of the effectiveness observed with MTBE. MTBE is the most consistent and efficient solvent for extracting a range of analytes from diverse textile materials, highlighting its suitability for comprehensive textile analysis.

Table S4. Target analytes and internal standards (ISTDs; labelled in yellow, see section 2.5. Analysis in the main text).

Compound	Ret. Time (s)	Exact Mass [M+H] <sup>+</sup>	Precursor Ion	Product Ion		Collision Energy (V)	
2-Aminopyridine <sup>4</sup>	1.27	95.06037	95.01	78	51	20	35
Nicotine <sup>1</sup>	1.32	162.1157	163.1	132	130	15	20
Benzidine <sup>1</sup>	1.44	185.10732	185.1	168	141	20	30
Benzidine- <i>d</i> 8 <sup>1</sup>	1.45	193.1575	193.2	176	149	20	30
Aniline <sup>1</sup>	1.45	94.06513	94.1	77	67	14	14
Dianilinomethane- <i>d</i> 4 <sup>1</sup>	1.45	203.1481	203.1	186	108	15	30
<i>o</i> -Anisidine <sup>4</sup>	2.00	124.07569	124.1	109	80	14	30
<i>o</i> -Anisidine- <i>d</i> 3 <sup>4</sup>	2.00	127.0945	127.1	109	80	20	30
<i>o</i> -Toluidine- <i>d</i> 3 <sup>2</sup>	2.12	111.0996	111.1	94	67	18	30
<i>o</i> -Toluidine <sup>4</sup>	2.14	108.08078	108.1	91	65	18	26
<i>p</i> -Cresidine <sup>4</sup>	2.80	138.09134	138.1	123	106	14	22
<i>o</i> -Dianisidine <sup>5</sup>	2.89	245.12845	245.1	230	187	10	30
4-Chloraniline- <i>d</i> 4 <sup>3</sup>	3.19	132.0513	132.1	115	97	22	18
4-Chloraniline <sup>3</sup>	3.24	128.02615	128.0	111	93	22	18
2-Naphthylamine <sup>4</sup>	3.84	144.08078	144.1	127	77	20	30
1-Naphthylamine <sup>4</sup>	4.14	144.08078	144.1	127	77	20	35
4-Chloro- <i>o</i> -toluidine <sup>4</sup>	4.55	142.04180	142.0	125	107	18	14
4-Aminobiphenyl- <i>d</i> 9 <sup>4</sup>	4.62	179.1529	179.2	162	160	22	30
4-Aminobiphenyl <sup>4</sup>	4.69	170.09643	170.1	152	128	30	26
3-Chloro- <i>o</i> -toluidine <sup>4</sup>	5.01	142.04180	142.0	125	107	18	14
2-Amino-4-nitrotoluene <sup>2</sup>	5.22	153.06585	153.1	107	90	14	26
2-Aminobiphenyl <sup>4</sup>	5.42	170.09643	170.1	152	128	30	26
Aniline yellow <sup>4</sup>	6.19	198.10257	198.1	93	77	22	18
3,3'-Dichlorobenzidine- <i>d</i> 6 <sup>5</sup>	6.28	259.0670	259.1	223	188	18	30
3,3'-Dichlorobenzidine <sup>5</sup>	6.30	253.02938	253.0	217	182	18	30
MBOCA <sup>4</sup>	6.33	267.04503	267.0	231	140	18	30
<i>o</i> -Aminoazotoluene <sup>4</sup>	6.97	226.13387	226.1	107	91	22	22

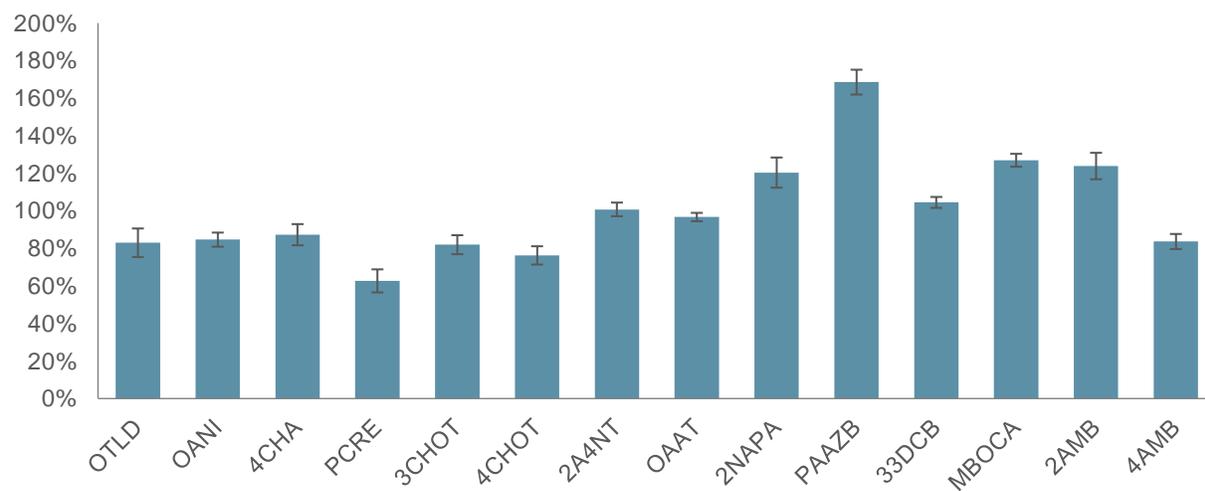


Figure S9. Tenax tubes (n=3) extraction efficiency for method development

Table S5. Breakthrough test results. Breakthrough tests were conducted using a second Tenax tube connected to the chamber system to ensure no breakthrough occurred that could affect the chamber concentration. Breakthrough percentage calculations based on the concentrations (ng/L) from the second Tenax tube (control) divided by the concentrations from the first Tenax tube, expressed as percentages.

Textile in chamber	Duration	ANI	2APY	OTLD	OANI	4CHA	PCRE	3CHOT	4CHOT	2A4NT	BNZD	OAAT	1NAPA	2NAPA	PAAZB	33DCB	ODAN	MBOCA	2AMB	4AMB
Wool	8H	34%	6%	4%	0%	0%	0%	0%	0%	0%	0%	0%	1%	0%	0%	0%	0%	0%	0%	0%
Wool	8H	12%	2%	3%	0%	1%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Wool	8H	15%	3%	6%	1%	1%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Cotton	8H	1%	1%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Cotton	8H	7%	1%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Cotton	8H	7%	2%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Poly-ester	8H	2%	2%	0%	1%	1%	6%	0%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Poly-ester	8H	3%	1%	0%	1%	2%	3%	0%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Poly-ester	8H	1%	2%	1%	2%	3%	7%	1%	2%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Wool	24H	40%	4%	3%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Wool	24H	1%	1%	2%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Wool	24H	4%	3%	2%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Cotton	24H	0%	0%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Cotton	24H	2%	1%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Cotton	24H	16%	2%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Poly-ester	24H	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Poly-ester	24H	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Poly-ester	24H	0%	1%	0%	0%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%

Table S6. Recoveries (average and standard deviation) of AAs from textiles after chamber exposure, deuterated standards d8-benzidine (BNZD-d8) and d3-o-anisidine (OANI-d3), 100 ng/sample.

Samples	8h Polyester		8h Cotton		8h Wool		24h Polyester		24h Cotton		24h Wool	
	OANI-d3	BNZD-d8	OANI-d3	BNZD-d8	OANI-d3	BNZD-d8	OANI-d3	BNZD-d8	OANI-d3	BNZD-d8	OANI-d3	BNZD-d8
<b>n</b>	27	27	26	26	27	27	27	27	27	27	27	27
<b>Range</b>	44-91%	20-54%	70-85%	53-73%	35-79%	14-76%	44-114%	7-71%	46-76%	31-66%	61-81%	43-76%
<b>Average</b>	65%	39%	78%	65%	66%	43%	87%	42%	66%	51%	72%	62%
<b>Standard deviation</b>	13	8	4	6	12	17	16	21	7	8	6	10

Table S7. Recoveries of AAs from Tenax after chamber test exposure, deuterated standards d8-benzidine and d3-o-anisidine, 100 ng/sample.

Samples	8h Polyester		8h Cotton		8h Wool		24h Polyester		24h Cotton		24h Wool	
	OANI-d3	BNZD-d8	OANI-d3	BNZD-d8	OANI-d3	BNZD-d8	OANI-d3	BNZD-d8	OANI-d3	BNZD-d8	OANI-d3	BNZD-d8
<b>Average</b>	90%	77%	83%	90%	84%	95%	118%	103%	81%	88%	85%	98%
<b>Standard deviation</b>	5	7	3	3	2	4	3	9	2	4	2	4

## Text S4 Uncertainty calculation and formula for the $K_{TA}$

The formula calculates the uncertainty in the  $K_{TA}$  by considering the calculation of uncertainties associated with several input variables. The general formula is:

$$SDK_{TA} = K_{TA} \sqrt{RSD_{NT}^2 + RSD_{VA}^2 + RSD_{MT}^2 + RSD_{NA}^2}$$

Where:

- $K_{TA}$ : The textile-air partition coefficient
- NT: Variability of textiles (textile recoveries)
- VA: Volume of air (pump and flow meter-related uncertainties)
- MT: Mass of the textiles (scale-related uncertainties)
- NA: Variability in the air (Tenax tubes recoveries)
- SD: Standard deviation
- RSD: Relative standard deviation

This approach quantifies how measurement variability in each contributing factor affects the overall uncertainty in  $K_{TA}$  calculations.

*Table S8. Volume normalized distribution coefficient data ( $\text{Log}K_{vol}$ ). Recalculated from  $K_{TA}$  values (Table 1. in the main text)*

<b>AAs</b>	<b>Log<math>K_{vol}</math> Polyester</b>	<b>Log<math>K_{vol}</math> Cotton</b>	<b>Log<math>K_{vol}</math> Wool</b>
ANI	4.4	4.8	4.9
2APY	5.1	6.1	5.9
OTLD	4.5	4.7	4.9
OANI	5.0	5.4	5.5
4CHA	5.3	5.4	5.8
PCRE	5.6	5.7	5.8
3CHOT	5.0	5.3	5.5
4CHOT	5.3	5.4	5.7
2A4NT	7.0	7.3	7.3
BNZD	7.9	8.5	8.1
OAAT	8.3	-	-
1NAPA	6.8	6.6	6.8
2NAPA	6.6	6.9	7.1
PAAZB	8.0	-	-
33DCB	7.0	7.6	7.5
ODAN	6.6	-	-
MBOCA	8.7	-	-
2AMB	5.8	6.1	6.2
4AMB	7.3	7.5	7.4

- : Indicates that air concentration data was unavailable, preventing the calculation of  $K_{vol}$  values.

Table S9. Summary of statistical tests across replicates and durations to see if the results are statistically different.

<b>Textile Type</b>	<b>Experiment Duration</b>	<b>Replicates Number</b>	<b>ANOVA Test (<math>\alpha = 0.05</math>) - Significant Difference (Yes/No)</b>
Polyester	8H	1-2	No
Polyester	8H	1-3	No
Polyester	8H	2-3	No
Polyester	24H	1-2	No
Polyester	24H	1-3	No
Polyester	24H	2-3	No
Polyester	8H-24H	1-2	No
Polyester	8H-24H	1-3	No
Polyester	8H-24H	2-3	No
Wool	8H	1-2	Yes
Wool	8H	1-3	Yes
Wool	8H	2-3	No
Wool	24H	1-2	Yes
Wool	24H	1-3	Yes
Wool	24H	2-3	No
Wool	8H-24H	1-2	Yes
Wool	8H-24H	1-3	Yes
Wool	8H-24H	2-3	No
Cotton	8H	1-2	Yes
Cotton	8H	1-3	Yes
Cotton	8H	2-3	No
Cotton	24H	1-2	Yes
Cotton	24H	1-3	Yes
Cotton	24H	2-3	No
Cotton	8H-24H	1-2	Yes
Cotton	8H-24H	1-3	Yes
Cotton	8H-24H	2-3	No

Table S10. Cotton fabric  $\text{Log}K_{\text{vol}} - \text{Log}K_{\text{OA}}$  linear fit parameters. AAs [This study], phthalates<sup>3</sup>, and PCBs<sup>4</sup> : At a significance level of 0.05, the slope of the regression model is significantly different from zero, showing a meaningful relationship between  $\text{Log}K_{\text{vol}} - \text{Log}K_{\text{OA}}$ .

Equation	$\text{Log}K_{\text{vol}} = \text{Intercept} + \text{Slope} \times \text{Log}K_{\text{OA}}$					
Plot	AAs [This study]	PCBs <sup>5</sup>	Phthalates <sup>3</sup>	Phthalates <sup>5</sup>	PCBs <sup>4</sup>	Meth-amphetamine <sup>7</sup>
Intercept	1.70 ± 1.33	16.76 ± 2.69	-3.65 ± 0.24	-1.89 ± 3.66	4.87 ± 0.48	--
Slope	0.77 ± 0.17	-1.33 ± 0.33	1.20 ± 0.03	0.97 ± 0.45	0.32 ± 0.10	--
Pearson's r	0.75	-0.94	1.00	0.83	0.61	--
R-Square (COD)	0.56	0.89	1.00	0.70	0.37	--
Standard Error	0.17	0.33	0.03	0.45	0.1	-
Adj. R-Square	0.54	0.83	1.00	0.55	0.33	--
Prob> t	0.0038	0.06	2.2E-6	0.2	0.006	-

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