

## SUPPLEMENTARY INFORMATION: The impact of indoor surfaces on indoor air chemistry following cooking and cleaning activities

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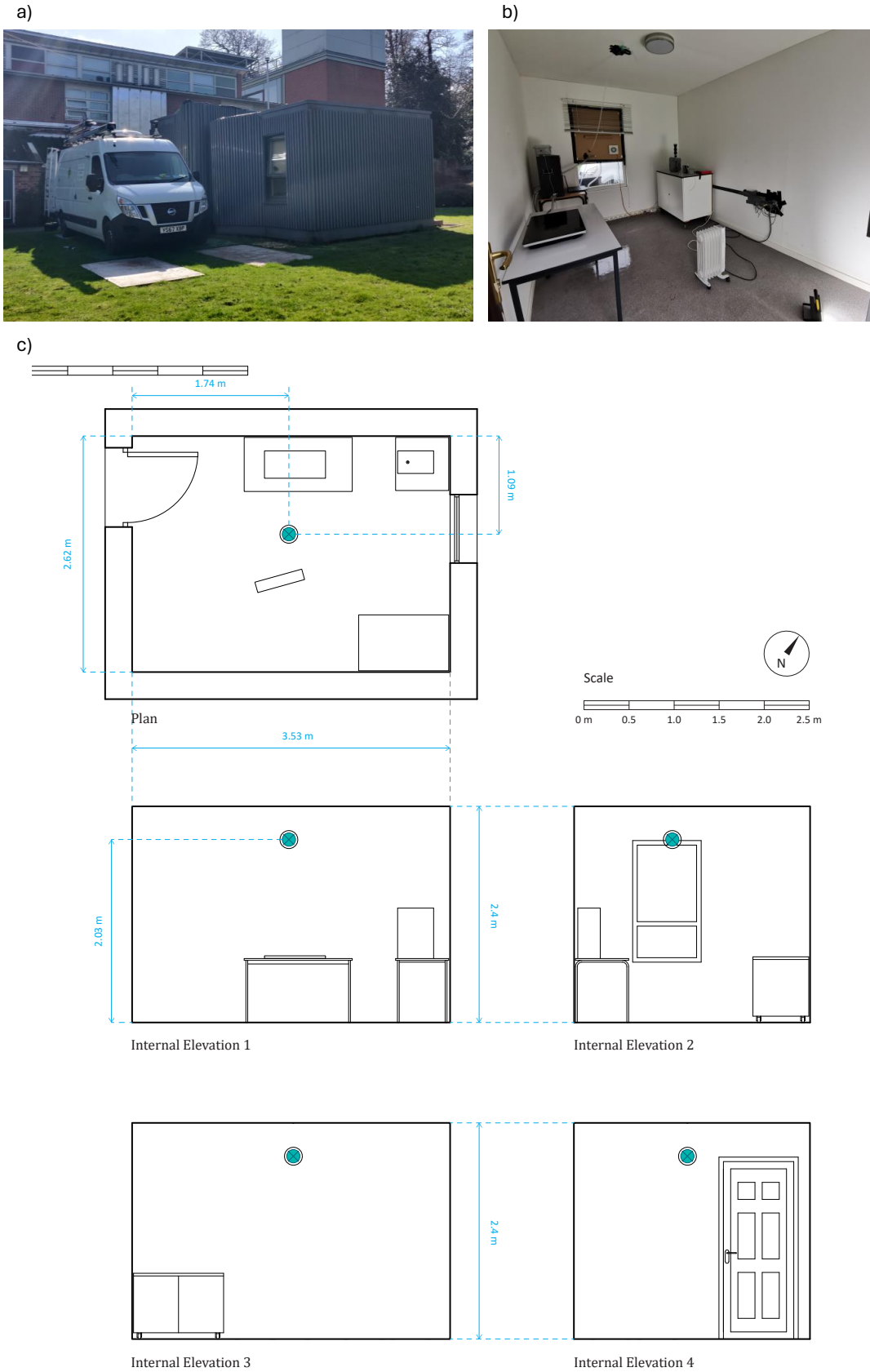
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**Figure S1:** a) External view of experimental (Part L) pod and WACL Air Sampling Platform (WASP), b) Internal view of test pod, c) Floor plan and internal elevations of test pod. Sampling location denoted by blue circle.

# 1 SIFT-MS

The VOCs measured using each reagent ion in the SIFT-MS method are shown in Table S1, along with the species molecular weights, product ions, rate coefficients and branching ratios. Whether or not a particular product ion was used for quantification is also shown in the ‘Included in Analysis’ column.

Table S2 shows the species that were measured by SIFT-MS, their limits of detection (LOD), and whether or not the species are calibrated against a gas standard. The background concentrations of dihydromyrcenol and citral were not measured during the first two instrument calibrations of the campaign due to differences in the SIFT-MS selected ion monitoring (SIM) methods used. Therefore, the average background concentrations measured during the final four instrument calibrations for these species were assumed to be an appropriate estimation of the background concentrations at the start of the campaign and were subtracted from the data. The LODs for dihydromyrcenol and citral reported in Table S2 are an average of the final four instrument calibrations only. Lactic acid was not included in any SIM method used to perform calibration and zero air measurements throughout the campaign. Consequently, the instrument background was not corrected for this species, and no LOD was available.

**Table S1:** The compounds measured by SIFT-MS during cooking, cleaning, or both experiments using each reagent ion, and their corresponding product ion molecular masses (MM), chemical formulae, rate coefficients and branching ratios. Whether or not the product ion was used for quantification is also shown in the ‘included in analysis’ column.

Reagent ion	Compound	MM (g mol <sup>-1</sup> )	Product ion	Reaction rate ( $\times 10^{-9}$ cm <sup>3</sup> molecule <sup>-1</sup> s <sup>-1</sup> )	Branching ratio (%)	Clean	Cook	Both	Included in analysis
H <sub>3</sub> O <sup>+</sup>	2,4-decadienal	153	C <sub>10</sub> H <sub>17</sub> O <sup>+</sup>	4.9	100		✓		
		171	C <sub>10</sub> H <sub>17</sub> O <sup>+</sup> · H <sub>2</sub> O				✓		
	2-phenethyl acetate	105	C <sub>8</sub> H <sub>9</sub> <sup>+</sup>	3.5	80	✓			✓
	acetaldehyde	45	C <sub>2</sub> H <sub>4</sub> O · H <sup>+</sup>	3.7	100			✓	✓
	acetonitrile	42	CH <sub>3</sub> CN · H <sup>+</sup>	5.1	100			✓	✓
		60	CH <sub>3</sub> CN · H <sup>+</sup> · H <sub>2</sub> O				✓		
	acrylamide	72	C <sub>2</sub> H <sub>3</sub> NH <sub>2</sub> CO · H <sup>+</sup>	2.1	100		✓		✓
	benzoic acid	123	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> · H <sup>+</sup>	3.0	100		✓		✓
	benzyl benzoate	151	C <sub>8</sub> H <sub>7</sub> O <sub>3</sub> <sup>+</sup>	3.7	60	✓			
		169	C <sub>8</sub> H <sub>7</sub> O <sub>3</sub> <sup>+</sup> · H <sub>2</sub> O			✓			
	cinnamaldehyde	133	C <sub>9</sub> H <sub>8</sub> OH <sup>+</sup>	2.0	100	✓			
	citral	153	C <sub>10</sub> H <sub>17</sub> O <sup>+</sup>	3.0	60	✓			✓
		171	C <sub>10</sub> H <sub>17</sub> O <sup>+</sup> · H <sub>2</sub> O			✓			
	decane	161	H <sub>3</sub> O <sup>+</sup> · C <sub>10</sub> H <sub>22</sub>	1.6	100		✓		✓
	ethanol	47	C <sub>2</sub> H <sub>7</sub> O <sup>+</sup>	2.7	100			✓	✓
	formaldehyde	31	CH <sub>3</sub> O <sup>+</sup>	3.4	100			✓	✓
	heptanal	115	C <sub>7</sub> H <sub>15</sub> O <sup>+</sup>	3.7	80			✓	✓
	hexanal	101	C <sub>6</sub> H <sub>13</sub> O <sup>+</sup>	3.7	95		✓		✓
		119	C <sub>6</sub> H <sub>13</sub> O <sup>+</sup> · H <sub>2</sub> O				✓		
		127	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub> · H <sup>+</sup>			4.0	100		✓
	maltol	145	C <sub>6</sub> H <sub>6</sub> O <sub>3</sub> · H <sub>3</sub> O <sup>+</sup>	2.7	100		✓		✓
		33	CH <sub>5</sub> O <sup>+</sup>				✓		
	methanol	163	C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> · H <sup>+</sup>	3.4	100		✓		✓
		181	C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> · H <sup>+</sup> · H <sub>2</sub> O				✓		
	n-methylpyrrole	82	C <sub>5</sub> H <sub>7</sub> N · H <sup>+</sup>	3.0	100		✓		✓
	nonanal	143	C <sub>9</sub> H <sub>19</sub> O <sup>+</sup>	2.5	86		✓		✓
	octanal	129	C <sub>8</sub> H <sub>17</sub> O <sup>+</sup>	3.8	85		✓		✓
	pinonaldehyde	107		2.0	33	✓			✓
	propanal	59	C <sub>3</sub> H <sub>7</sub> O <sup>+</sup>	3.6	100		✓		✓
	total monoterpenes	137	C <sub>10</sub> H <sub>17</sub> <sup>+</sup>	2.6	30			✓	
		155	C <sub>10</sub> H <sub>17</sub> · H <sub>2</sub> O <sup>+</sup>				✓		
	total sesquiterpenes	205	C <sub>15</sub> H <sub>25</sub> <sup>+</sup>	2.5	64			✓	✓
	NO <sup>+</sup>	1,2,4-trimethylbenzene	120	C <sub>9</sub> H <sub>12</sub> <sup>+</sup>	1.9	100		✓	

1-propanol	59	$C_3H_7O^+$	0.6	100		✓		✓
	77	$C_3H_7O \cdot H_2O^+$				✓		
2,4-decadienal	151	$C_{10}H_{15}O^+$	4.2	80		✓		✓
2-heptenal	111	$C_7H_{11}O^+$	3.9	85		✓		✓
2-phenethyl acetate	104	$C_8H_8^+$	2.9	85	✓			
2-tert-butylcyclohexyl acetate	138	$C_{10}H_{18}^+$	2.8	40	✓			✓
acetaldehyde	43	$CH_3CO^+$	0.7	80	✓			
	61	$CH_3CO^+ \cdot H_2O$			✓			
acetic acid	90	$NO^+ \cdot CH_3COOH$	0.9	100			✓	✓
acetone	88	$NO^+ \cdot C_3H_6O$	1.0	100		✓		✓
acrolein	55	$C_3H_3O^+$	1.6	60		✓		✓
	86	$C_3H_4O \cdot NO^+$		40		✓		
benzene	78	$C_6H_6^+$	1.5	55		✓		✓
benzoic acid	105	$C_7H_5O^+$	3.0	60		✓		
benzyl benzoate	180	$C_9H_{10}O_2NO^+$	2.5	45	✓			✓
cinnamaldehyde	132	$C_9H_8O^+$	2.0	100			✓	
cinnamyl acetate	176	$C_{11}H_{12}O_2^+$	3.0	100		✓		✓
citral	151	$C_{10}H_{15}O^+$	2.5	35	✓			
diallyl disulfide	146	$(C_3H_5)_2S_2^+$	2.4	100		✓		✓
dimethyl disulfide	94	$(CH_3)_2S_2^+$	2.4	100		✓		✓
ethanol	45	$C_2H_5O^+$	1.2	100	✓			
	63	$C_2H_5O^+ \cdot H_2O$			✓			
eucalyptol	154	$C_{10}H_{18}O^+$	2.4	94			✓	✓
eugenol	164	$C_{10}H_{12}O_2^+$	2.4	100			✓	✓
furan	68	$C_4H_4O^+$	1.7	100		✓		✓
hexanal	99	$C_6H_{11}O^+$	2.5	100		✓		
lactic acid	120	$NO^+ \cdot C_3H_3OCOOH$	2.5	50	✓			✓
maltol	126	$C_6H_6O_3^+$	2.5	100		✓		✓
methyl cinnamate	162	$C_{10}H_{10}O_2^+$	1.4	100		✓		
	163	$C_{10}H_{10}O_2 \cdot H^+$				✓		
toluene	92	$C_7H_8^+$	2.2	100		✓		✓
total monoterpenes	88		2.2	25	✓			
	136	$C_{10}H_{16}^+$	2.2	75			✓	✓
total sesquiterpenes	204	$C_{15}H_{24}^+$	2.0	38			✓	
undecane	155	$C_{11}H_{23}^+$	3.8	84		✓		
xylene + ethylbenzene	106	$C_8H_{10}^+$	2.0	100		✓		✓
$O_2^+$								
2-phenethyl acetate	104	$C_8H_8^+$	3.0	100	✓			
2-tert-butylcyclohexyl acetate	57	$C_4H_9^+$	4.5	45	✓			
cinnamaldehyde	132	$C_9H_8O^+$	2.0	100			✓	✓
cinnamyl acetate	134	$C_9H_{10}O_2^+$	1.5	100		✓		

dihydromyrcenol	59	$C_3H_7O^+$	2.9	50	✓		✓
	77	$C_3H_7O \cdot H_2O^+$			✓		
dimethyl sulfide	47	$CH_3S^+$	2.2	25		✓	
	62	$(CH_3)_2S^+$		60		✓	✓
dimethyl trisulfide	111	$CH_3S_3^+$	2.2	15		✓	✓
eugenol	164	$C_{10}H_{12}O_2^+$	1.9	100			✓
furan	68	$C_4H_4O^+$	1.6	100		✓	
maltol	126	$C_6H_6O_3^+$	2.5	100		✓	
nonane	99	$C_7H_{15}^+$	2.1	10		✓	✓
octane	85	$C_6H_{13}^+$	1.6	50		✓	✓
undecane	156	$C_{11}H_{24}^+$	3.2	31		✓	✓

**Table S2:** Species identified by SIFT-MS, their limits of detection (average  $\pm$  standard deviation), and whether or not their concentrations were calibrated against a gas standard

Species	Average LOD (ppb)	Calibrated
1,2,4-trimethylbenzene	0.16 $\pm$ 0.1	
1-propanol	0.76 $\pm$ 0.1	
2,4-decadienal	0.07 $\pm$ 0.0	
2-heptenal	0.14 $\pm$ 0.0	
2-phenethyl acetate	0.20 $\pm$ 0.1	
2-tert-butylcyclohexyl acetate	0.25 $\pm$ 0.1	
acetaldehyde	1.41 $\pm$ 0.4	✓
acetic acid	0.61 $\pm$ 0.1	
acetone	0.80 $\pm$ 0.1	✓
acetonitrile	0.70 $\pm$ 0.2	✓
acrolein	0.37 $\pm$ 0.1	
acrylamide	0.18 $\pm$ 0.0	
benzene	0.23 $\pm$ 0.0	
benzoic acid	0.13 $\pm$ 0.0	
benzyl benzoate	0.44 $\pm$ 0.1	
cinnamaldehyde	0.12 $\pm$ 0.0	
cinnamyl acetate	0.26 $\pm$ 0.1	
citral	0.18 $\pm$ 0.1	
decane	0.28 $\pm$ 0.1	
diallyl disulfide	0.11 $\pm$ 0.0	
dihydromyrcenol	1.70 $\pm$ 0.6	
dimethyl disulfide	0.20 $\pm$ 0.0	
dimethyl sulfide	0.46 $\pm$ 0.1	
ethanol	5.88 $\pm$ 0.7	✓
eucalyptol	0.12 $\pm$ 0.0	
eugenol	0.14 $\pm$ 0.0	
formaldehyde	1.52 $\pm$ 0.3	
furan	1.04 $\pm$ 0.2	✓
heptanal	0.22 $\pm$ 0.1	
hexanal	0.39 $\pm$ 0.0	
maltol	0.11 $\pm$ 0.0	
methanol	8.22 $\pm$ 1.4	✓
methyl cinnamate	0.20 $\pm$ 0.0	
n-methylpyrrole	0.07 $\pm$ 0.0	
nonanal	0.31 $\pm$ 0.1	
nonane	4.98 $\pm$ 0.9	
octanal	0.22 $\pm$ 0.1	
octane	1.20 $\pm$ 0.3	
pinonaldehyde	0.34 $\pm$ 0.1	
propanal	1.85 $\pm$ 0.3	
toluene	0.52 $\pm$ 0.1	✓
total monoterpenes	0.51 $\pm$ 0.2	✓
total sesquiterpenes	1.50 $\pm$ 0.7	
undecane	0.40 $\pm$ 0.2	
xylenes + ethylbenzene	0.15 $\pm$ 0.0	

## 2 SIFT calibration and uncertainty

Calibration of the SIFT-MS was performed 6 times throughout the campaign using a custom-built automated gas calibration unit (AGCU). The AGCU was used to perform stepwise dilutions of calibrant gas, which were measured by the SIFT-MS to generate a multi-point calibration curve per compound. Two gas standards were used for SIFT-MS calibration: a 14-component gas standard (1 ppm certified National Physical Laboratory, UK) and a limonene only standard (1 ppm in N<sub>2</sub>). The limonene standard was prepared in-house by injecting a controlled amount of liquid standard (Sigma Aldrich, 99.8 % purity) into an evacuated gas cylinder and subsequently pressurising the cylinder with research-grade N<sub>2</sub> (N6, BOC). The resulting limonene concentration was determined via GC-FID (calibrated using 1 ppm limonene in N<sub>2</sub> standard, NPL) after 7 days equilibration at room temperature. Each gas standard was diluted in the AGCU using zero air which was provided by a heated palladium alumina-based zero air generator. The 14-component gas standard was diluted to a concentration range of 1 to 10 ppb, while the limonene gas standard was diluted to a range of 1.8 to 18 ppb. Each concentration step was measured for 3 minutes, with the first and last 30 seconds of each step being discounted to minimise the error associated with instrument equilibration between concentration steps. The resulting data was used to generate a multi-point calibration curve, from which the calibration factor was derived by linear regression analysis. The average and standard deviation of calibration factors determined from the 6 calibration runs during the campaign are shown in Table S3.

**Table S3:** Mean  $\pm$  standard deviation of the SIFT-MS calibration factors obtained during the Nottingham Pod campaign.

Species	Average calibration factor $\pm$ standard deviation
acetaldehyde	1.84 $\pm$ 0.01
acetone	0.72 $\pm$ 0.01
acetonitrile	2.94 $\pm$ 0.03
ethanol	0.94 $\pm$ 0.01
furan	0.84 $\pm$ 0.00
total monoterpenes <sup>a</sup>	1.28 $\pm$ 0.02
methanol	0.85 $\pm$ 0.01
toluene	1.15 $\pm$ 0.01

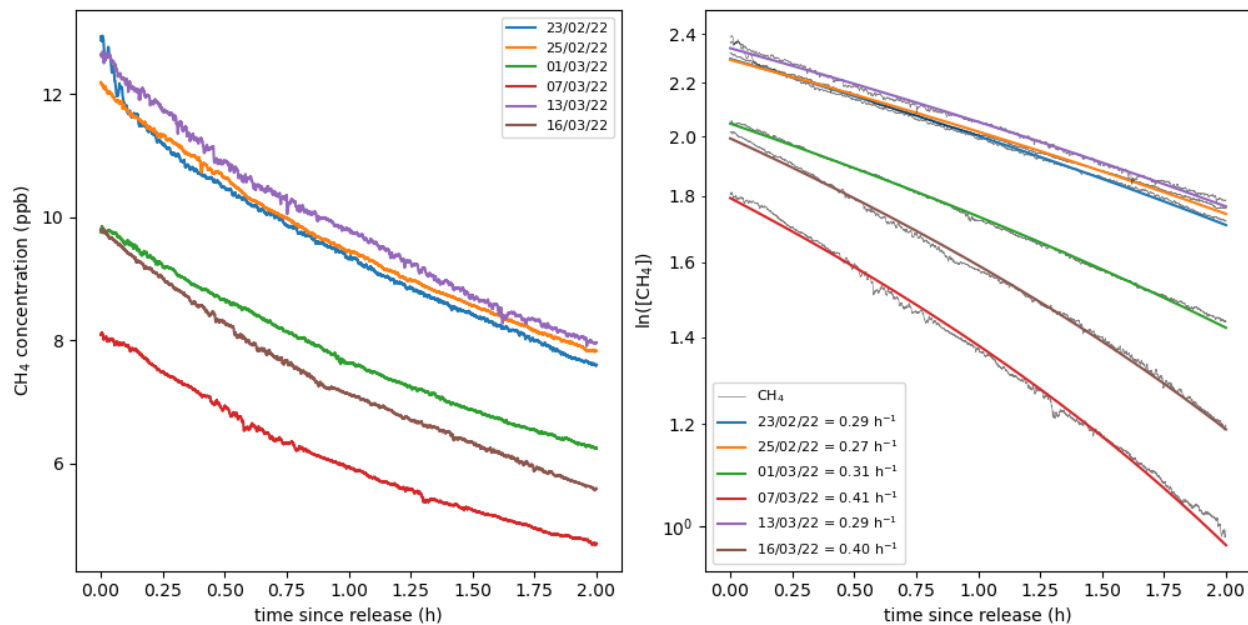
<sup>a</sup> Limonene used as calibration gas

For uncalibrated species, the SIFT-MS measurements were calculated using the ion-molecule reaction rate coefficients and branching ratios given in Table S1 (taken from Syft Technologies kinetic database). The uncertainty in these uncalibrated measurements is assumed to be  $\pm$  35 %, as recommended in Syft training resources<sup>1,2</sup>.



### 3 Air Change Rate

The air change rate in the test pod was measured 6 times during the campaign using methane tracer releases. The methane decays for each day is shown in Fig. S2a. The background methane concentration was subtracted from the calibrated methane concentration ( $C_t - C_b$ ), then the natural log was taken on the resulting concentration. After the release, the initial 10 minute mixing period was discounted, then a decay curve was fitted to the next 2 hour period, shown in Fig. S2b.



**Figure S2:** a) Concentration of methane over 2 hours following tracer release on 6 days during the campaign. b) Log-linear regression of the methane concentration decay, and the corresponding ACR for the 6 days.

## 4 VOC emission rates

The VOC emission rates input to INCHEM-Py are shown in Table S4 and S5 for the average cooking and cleaning activities occurring at 12:00 and 13:00, respectively. Emission rates were determined from SIFT-MS measurements, and calculated as the rate of increase in species concentrations during the cooking/cleaning activity. The total monoterpene emissions from the cleaning experiment were speciated using data from Harding-Smith *et al.*<sup>3</sup> for cleaner ‘SR1’, while those from the cooking experiment were speciated using data from Davies *et al.*<sup>4</sup>. Model emissions of butyl pyruvate were used as a proxy for measured emissions of 2-tert-butylcyclohexyl acetate, with mass correction. All emission rates were corrected to account for the difference between experimental and simulated room volumes.

**Table S4:** VOC emission rates determined from the averaged SIFT-MS measurements during the cooking experiment. For species where multiple gradients were observed in the emission peak, individual emission rates are reported as emission rates 1, 2 and 3. The time, in seconds from midnight, during which the emissions occurred is also shown for clarity.

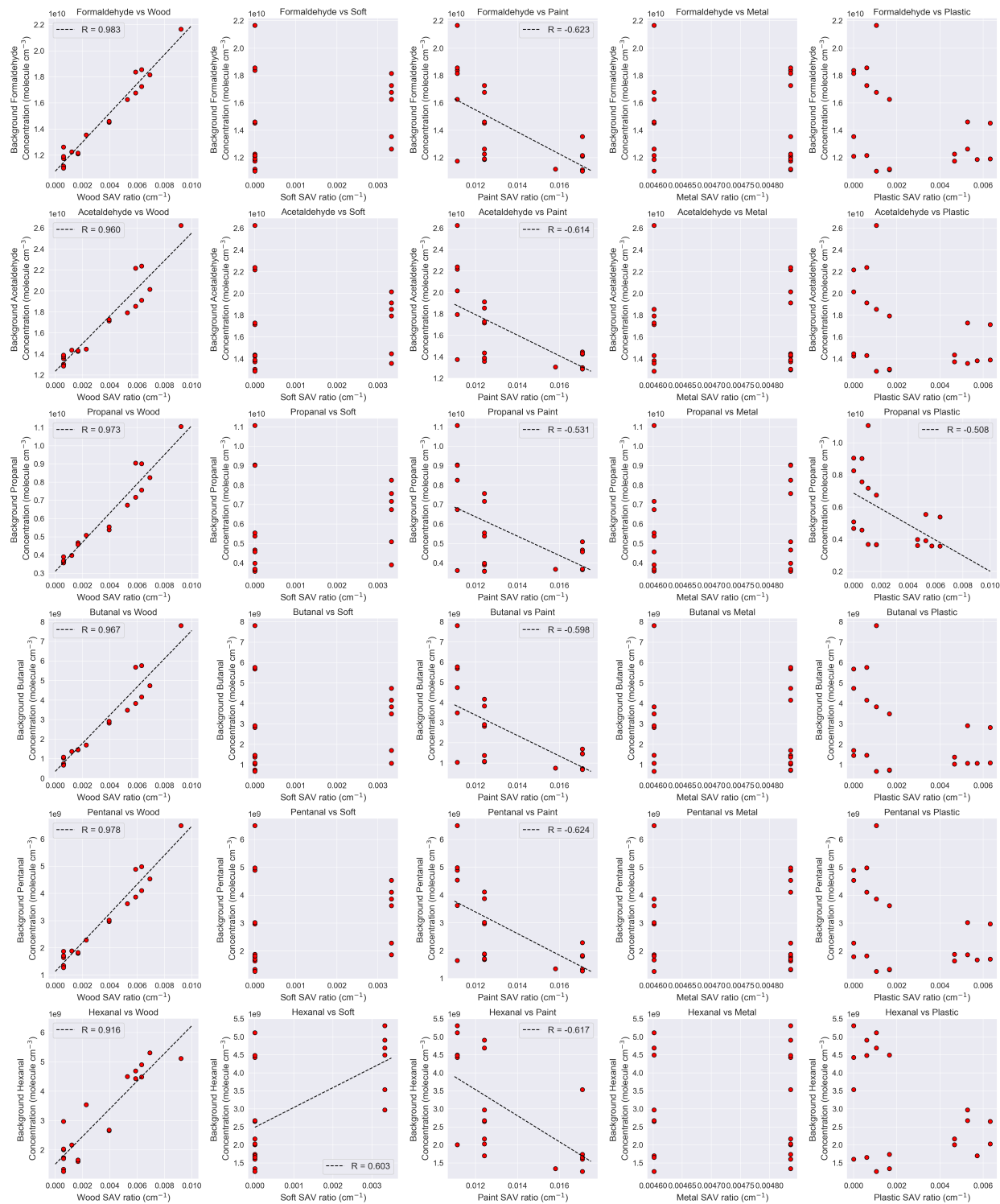
Species	$t_{start}$ (s)	$t_{end}$ (s)	Emission rate 1 (molecule $\text{cm}^{-3} \text{s}^{-1}$ )	$t_{start}$ (s)	$t_{end}$ (s)	Emission rate 2 (molecule $\text{cm}^{-3} \text{s}^{-1}$ )	$t_{start}$ (s)	$t_{end}$ (s)	Emission rate 3 (molecule $\text{cm}^{-3} \text{s}^{-1}$ )
acetaldehyde	43230	43347	$1.74 \times 10^9$	43615	43810	$1.15 \times 10^9$	43808	43977	$2.38 \times 10^8$
hexanal	43227	43351	$4.27 \times 10^8$	43602	44011	$3.70 \times 10^7$	-	-	-
methanol	43653	43846	$3.51 \times 10^{10}$	-	-	-	-	-	-
ethanol	43244	43351	$1.39 \times 10^9$	43712	43794	$6.50 \times 10^8$	43901	44015	$8.22 \times 10^9$
heptanal	43271	43361	$2.93 \times 10^8$	43729	43980	$5.16 \times 10^7$	-	-	-
octanal	43265	43419	$1.36 \times 10^8$	-	-	-	-	-	-
nonanal	43313	43516	$3.04 \times 10^8$	-	-	-	-	-	-
acrolein	43220	43323	$1.22 \times 10^9$	43595	43925	$7.71 \times 10^7$	-	-	-
limonene	42587	42776	$6.80 \times 10^7$	43609	43874	$5.26 \times 10^7$	-	-	-
camphene	42587	42776	$2.38 \times 10^8$	43609	43874	$1.84 \times 10^8$	-	-	-
$\alpha$ -pinene	42587	42776	$7.18 \times 10^7$	43609	43874	$5.55 \times 10^7$	-	-	-
1,2,4-trimethyl benzene	43612	43812	$1.45 \times 10^8$	-	-	-	-	-	-
<i>n</i> -octane	43230	43323	$1.60 \times 10^9$	43347	43984	$1.54 \times 10^8$	-	-	-
<i>n</i> -nonane	43213	43326	$2.61 \times 10^9$	43650	43849	$1.79 \times 10^9$	-	-	-
dimethyl sulphide	43216	43426	$1.42 \times 10^8$	43622	43915	$1.96 \times 10^8$	-	-	-

**Table S5:** VOC emission rates determined from the averaged SIFT-MS measurements during the cleaning experiment. For species where multiple gradients were observed in the emission peak, individual emission rates are reported as emission rates 1, 2 and 3. The time, in seconds from midnight, during which the emissions occurred is also shown for clarity.

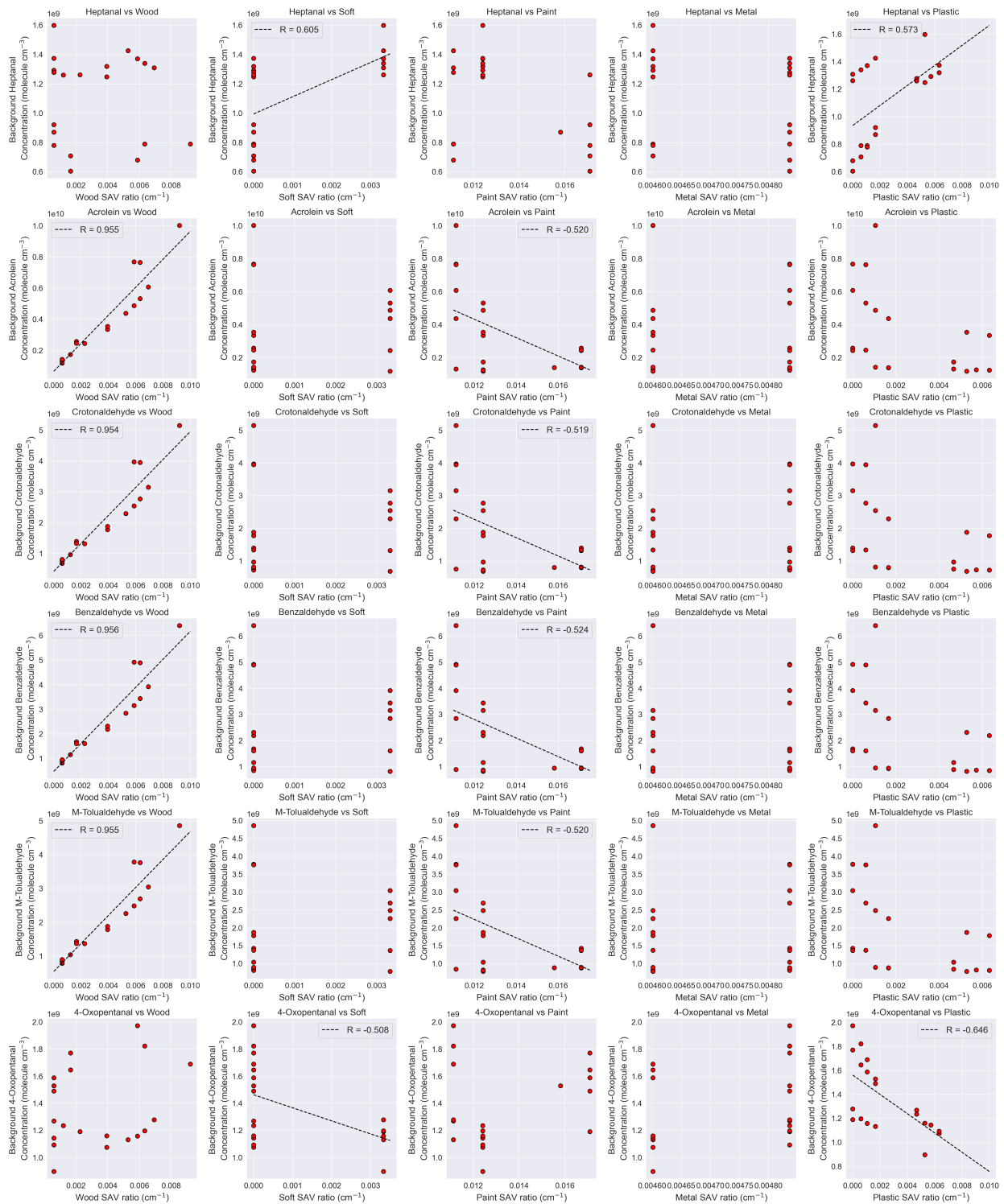
Species	$t_{start}$ (s)	$t_{end}$ (s)	Emission rate 1 (molecule $\text{cm}^{-3} \text{s}^{-1}$ )	$t_{start}$ (s)	$t_{end}$ (s)	Emission rate 2 (molecule $\text{cm}^{-3} \text{s}^{-1}$ )	$t_{start}$ (s)	$t_{end}$ (s)	Emission rate 3 (molecule $\text{cm}^{-3} \text{s}^{-1}$ )
acetaldehyde	46839	46982	$1.46 \times 10^8$						
methanol	46842	46956	$1.34 \times 10^9$						
ethanol	46840	46927	$3.88 \times 10^8$						
limonene	46806	46874	$1.34 \times 10^7$	46874	46914	$6.19 \times 10^7$	46874	46914	$1.23 \times 10^7$
carene	46806	46874	$3.41 \times 10^7$	46874	46914	$1.57 \times 10^8$	46874	46914	$3.13 \times 10^7$
camphene	46806	46874	$3.66 \times 10^7$	46874	46914	$1.69 \times 10^8$	46874	46914	$3.35 \times 10^7$
terpinolene	46806	46874	$1.22 \times 10^6$	46874	46914	$5.62 \times 10^6$	46874	46914	$1.12 \times 10^6$
$\alpha$ -pinene	46806	46874	$3.54 \times 10^7$	46874	46914	$1.63 \times 10^8$	46874	46914	$3.24 \times 10^7$
$\alpha$ -terpinene	46806	46874	$1.22 \times 10^6$	46874	46914	$5.62 \times 10^6$	46874	46914	$1.12 \times 10^6$
$\alpha$ - phellandrene	46806	46874	$1.22 \times 10^6$	46874	46914	$5.62 \times 10^6$	46874	46914	$1.12 \times 10^6$
butyl pyruvate	46835	47010	$1.57 \times 10^7$						
dihydromyrcenol	46789	47090	$1.07 \times 10^8$						

## 5 Correlations between surface materials and surface-emitted species

Figures S3 and S4 shows the correlations between the surface areas of wooden, soft, painted and plastic surfaces surfaces, and the corresponding background concentrations of surface-emitted species with a CV > 0.2 (Table 2, main text), in each of the 20 kitchen permutations.



**Figure S3:** Relationship between the surface area to volume ratios of wooded, soft, painted, metal and plastic surfaces (columns) and the background concentrations (averaged between noon and midnight) of formaldehyde, acetaldehyde, propanal, butanal, pentanal and hexanal (rows), where each point is one of the 20 kitchen permutations. Pearson correlation coefficients (R) are plotted and shown when  $R > 0.5$ , and when the correlations are statistically significant ( $p < 0.05$ ).



**Figure S4:** Relationship between the surface area to volume ratios of wooden, soft, painted, metal and plastic surfaces (columns) and the background concentrations (averaged between noon and midnight) of heptanal, acrolein, crotonaldehyde, benzaldehyde, m-tolualdehyde and 4-oxopentanal (rows), where each point is one of the 20 kitchen permutations. Pearson correlation coefficients ( $R$ ) are plotted and shown when  $R > 0.5$ , and when the correlations are statistically significant ( $p < 0.05$ ).

## 6 References

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