

Supplementary Materials For:

Headspace-SIFT-MS Workflows for Rapid Screening and Quantitation of Hazardous Volatile Impurities in Personal Care Products

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Table S1. Benzene concentrations (ng g^{-1}) in nine haircare and skincare products using the method of standard additions with SIFT-MS. Values reported in the main article are calculated from the ‘good’ amounts shown in green. Values in gray are subject to significant interference for the product.

Product Number or Calibration	Standard Conc. (ppb) or Parameter	Benzene Product Ions			
		$\text{H}_3\text{O}^+ 79$	$\text{NO}^+ 78$	$\text{NO}^+ 108$	$\text{O}_2^+ 78$
1	0	11.5	1.36	28.6	2.15
	20	53.9	45.9	70.1	46.6
	40	119	108	121	109
	60	163	151	168	151
	Slope	2.598	2.555	2.346	2.545
	Intercept	8.91	-0.088	26.56	0.845
	R^2	0.9929	0.9948	0.9985	0.9942
	LOQ	1.62	1.01	1.78	1.72
	Amount (ng/g)	<LOQ	<LOQ	4.93	<LOQ
2	0	24.4	21.2	45.3	22
	20	60.4	52	72.4	55.9
	40	102	92.9	112	99.6
	60	141	135	146	134
	Slope	1.957	1.912	1.709	1.899
	Intercept	23.24	17.93	42.67	20.92
	R^2	0.9993	0.9951	0.9952	0.9975
	LOQ	2.15	1.34	2.44	2.30
	Amount (ng/g)	5.17	4.08	10.9	4.79
3	0	9.8	5.75	233	12.6
	20	29.8	22.6	249	29.7
	40	53.2	49.4	268	55.6
	60	72.5	67.5	287	71.4
	Slope	1.058	1.060	0.905	1.012
	Intercept	9.6	4.505	232.1	11.98
	R^2	0.9987	0.9922	0.9984	0.9911
	LOQ	3.98	2.42	4.61	4.33
	Amount (ng/g)	<LOQ	<LOQ	111.6	5.15
4	0	2520	2320	3040	2420
	1000	3590	3330	3880	3360
	2000	4440	4080	4700	4190
	3000	5680	5300	5840	5380
	Slope	1.033	0.969	0.922	0.971
	Intercept	2508	2304	2982	2381
	R^2	0.9952	0.9920	0.9934	0.9944
	LOQ	4.07	2.65	4.52	4.51
	Amount (ng/g)	1056	1034	1407	1067
5	0	5.36	2.84	136	7.09
	20	40.4	37.3	165	38.8
	40	89.7	83.1	204	84.4
	60	123	114	232	117

Product Number or Calibration	Standard Conc. (ppb) or Parameter	Benzene Product Ions			
		H ₃ O ⁺ 79	NO ⁺ 78	NO ⁺ 108	O ₂ ⁺ 78
6	Slope	2.011	1.896	1.635	1.877
	Intercept	4.282	2.418	135.2	5.523
	R ²	0.9943	0.9948	0.9958	0.9949
	LOQ	2.09	1.36	2.55	2.33
	Amount (ng/g)	<LOQ	<LOQ	36.0	<LOQ
	0	7.38	3.12	37.4	3.71
	20	41.7	34.9	66.6	35.6
	40	85.9	77.4	104	74.9
	60	114	102	131	109
	Slope	1.820	1.696	1.591	1.776
7	Intercept	7.636	3.484	37.02	2.527
	R ²	0.9935	0.9907	0.9964	0.9985
	LOQ	2.31	1.52	2.62	2.46
	Amount (ng/g)	<LOQ	<LOQ	10.1	<LOQ
	0	42.5	4.38	1400	7.27
	20	81.7	36.2	1450	39.5
	40	139	80.6	1490	84.4
	60	179	122	1530	121
	Slope	2.334	1.986	2.150	1.930
	Intercept	40.53	1.206	1403	5.129
8	R ²	0.9943	0.9956	0.9968	0.9964
	LOQ	1.80	1.29	1.94	2.27
	Amount (ng/g)	7.55	<LOQ	283.9	<LOQ
	0	29.5	6.44	539	75.3
	20	47.6	30.5	489	94.9
	40	74.1	49.4	527	117
	60	95.8	68.4	545	131
	Slope	1.127	1.024	0.28	0.946
	Intercept	27.94	7.968	516.6	76.17
	R ²	0.9953	0.9963	0.0827	0.9925
9	LOQ	3.73	2.51	14.89	4.62
	Amount (ng/g)	10.8	3.39	802.6	35.0
	0	35.4	2.89	380	6.56
	20	62.9	33.8	409	36.2
	40	93.6	66.8	439	69.3
	60	125	91.5	465	97.9
	Slope	1.498	1.494	1.425	1.536
	Intercept	34.3	3.923	380.5	6.422
	R ²	0.9991	0.9966	0.9991	0.9993
	LOQ	2.81	1.72	2.93	2.85
Aqueous Cal.	Amount (ng/g)	9.96	<LOQ	116.2	<LOQ
	0	3.01	0.249	33.2	1.11
	20	62.5	60.8	63.1	60.4

Product Number or Calibration	Standard Conc. (ppb) or Parameter	Benzene Product Ions			
		H ₃ O ⁺ 79	NO ⁺ 78	NO ⁺ 108	O ₂ ⁺ 78
	40	125	118	119	116
	60	182	179	174	177
	80	238	236	233	233
	100	305	290	271	285
	Slope	2.991	2.908	2.505	2.855
	Intercept	3.053	1.959	23.619	2.686
	R ²	0.9995	0.9997	0.9928	0.9995
Aqueous Cal.: High Benzene	0	19.1	0.661	13.7	0.824
	1000	3080	3020	2950	3030
	2000	6090	6000	5720	5950
	3000	9540	9300	8800	9330
	4000	12500	12200	11900	12400
	5000	15200	14700	14300	14900
	Slope	3.065	2.956	2.888	3.019
	Intercept	87	176	70	65
	R ²	0.9983	0.9978	0.9983	0.9978

Table S2. 1,4-Dioxane concentrations ($\mu\text{g g}^{-1}$) in nine haircare and skincare products using the method of standard additions with SIFT-MS. Values reported in the main article are calculated from the 'good' amounts shown in green. Values in gray are subject to significant interference for the product.

Product Number or Calibration	Standard Conc. (ppm) or Parameter	1,4- Dioxane Product Ions				
		$\text{H}_3\text{O}^+ 89$	$\text{NO}^+ 87$	$\text{NO}^+ 88$	$\text{O}_2^+ 58$	$\text{O}_2^+ 88$
1	0	46	26.2	3230	8700	61
	2	100	82.9	3050	8260	123
	4	157	144	3140	8160	180
	6	215	208	3040	8030	249
	Slope	28.2	30.325	-24	-105.5	31.05
	Intercept	44.9	24.3	3187	8604	60.1
	R ²	0.9997	0.9993	0.4861	0.8782	0.9986
	LOQ	0.31	0.37	0.49	0.42	0.37
	Amount ($\mu\text{g/g}$)	0.796	0.401	-66.4	-40.8	0.968
2	0	175	36.9	73.1	299	84.1
	2	229	102	136	344	146
	4	296	160	196	396	206
	6	342	216	244	439	265
	Slope	28.4	29.765	28.635	23.6	30.135
	Intercept	175.3	39.43	76.37	298.7	84.87
	R ²	0.9954	0.9988	0.9964	0.9988	0.9999
	LOQ	0.31	0.38	0.41	1.88	0.38
	Amount ($\mu\text{g/g}$)	3.09	0.662	1.33	6.33	1.41
3	0	169	90.2	165	349	145
	2	234	160	231	407	204
	4	279	208	280	443	266
	6	350	267	345	504	320
	Slope	29.4	28.92	29.45	25.05	29.35
	Intercept	169.8	94.54	166.9	350.6	145.7
	R ²	0.9934	0.9951	0.9969	0.9911	0.9993
	LOQ	0.30	0.39	0.40	1.77	0.39
	Amount ($\mu\text{g/g}$)	2.89	1.63	2.83	7.00	2.48
4	0	923	69.1	880	2410	1040
	2	954	123	946	2480	1050
	4	981	172	927	2280	1060
	6	1090	226	1000	2410	1190
	Slope	26.4	25.985	17.05	-10	23
	Intercept	907.8	69.57	887.1	2425	1016
	R ²	0.8806	0.9996	0.7865	0.0957	0.7101
	LOQ	0.33	0.43	0.69	4.43	0.50
	Amount ($\mu\text{g/g}$)	17.2	1.34	26.0	-121.3	22.1
5	0	114	37.1	69.2	401	92.9
	2	174	95.7	124	429	154
	4	235	164	188	499	217

Product Number or Calibration	Standard Conc. (ppm) or Parameter	1,4- Dioxane Product Ions				
		H ₃ O ⁺ 89	NO ⁺ 87	NO ⁺ 88	O ₂ ⁺ 58	O ₂ ⁺ 88
	6	312	224	253	557	278
	Slope	32.75	31.45	30.77	26.9	30.915
	Intercept	110.5	35.85	66.24	390.8	92.73
	R ²	0.9961	0.9992	0.9985	0.9750	1.0000
	LOQ	0.27	0.36	0.38	1.65	0.37
	Amount (µg/g)	1.69	0.570	1.08	7.26	1.50
6	0	145	35.3	58.5	248	81.3
	2	210	105	124	301	150
	4	258	155	172	336	202
	6	303	215	232	383	252
	Slope	26.1	29.455	28.425	22	28.205
	Intercept	150.7	39.21	61.35	251	86.71
	R ²	0.9920	0.9961	0.9968	0.9945	0.9939
	LOQ	0.34	0.38	0.41	2.01	0.41
	Amount (µg/g)	2.89	0.666	1.08	5.70	1.54
7	0	309	26.4	82.5	325	105
	2	359	85.5	138	379	164
	4	413	143	196	419	226
	6	485	213	273	484	297
	Slope	29.1	30.865	31.475	25.85	31.9
	Intercept	304.2	24.38	77.95	324.2	102.3
	R ²	0.9923	0.9979	0.9935	0.9921	0.9981
	LOQ	0.30	0.36	0.37	1.71	0.36
	Amount (µg/g)	5.23	0.395	1.24	6.27	1.60
8	0	3010	60	132	1450	864
	2	3080	149	232	1400	955
	4	3190	233	311	1490	1080
	6	3280	353	440	1670	1180
	Slope	46	48.15	50.15	37.5	53.65
	Intercept	3002	54.3	128.3	1390	858.8
	R ²	0.9934	0.9931	0.9909	0.6781	0.9966
	LOQ	0.19	0.23	0.23	1.18	0.21
	Amount (µg/g)	32.6	0.564	1.28	18.5	8.00
9	0	50.5	83.7	69.8	356	402
	2	109	138	128	403	447
	4	176	194	187	437	511
	6	230	261	245	498	573
	Slope	30.275	29.395	29.23	23	28.85
	Intercept	50.55	80.99	69.76	354.5	396.7
	R ²	0.9985	0.9974	1.0000	0.9880	0.9944
	LOQ	0.29	0.38	0.40	1.93	0.40
	Amount (µg/g)	0.835	1.38	1.19	7.71	6.88
Aqueous Cal.	0	3.75	4.73	7.06	30.3	4.94

Product Number or Calibration	Standard Conc. (ppm) or Parameter	1,4- Dioxane Product Ions				
		H ₃ O ⁺ 89	NO ⁺ 87	NO ⁺ 88	O ₂ ⁺ 58	O ₂ ⁺ 88
	2	61.7	63.1	60.7	75	69.7
	4	116	122	121	125	126
	6	182	184	190	180	192
	8	227	238	229	221	241
	10	281	288	283	270	287
	Slope	27.83	28.62	27.91	24.16	28.43
	Intercept	6.09	6.90	8.92	29.40	11.28
	R ²	0.9981	0.9989	0.9956	0.9989	0.9960

Table S3. Formaldehyde concentrations ($\mu\text{g g}^{-1}$) in nine haircare and skincare products using the method of standard additions with SIFT-MS. Values reported in the main article are calculated from the 'good' amounts shown in green. Values in gray are subject to significant interference for the product.

Product Number or Calibration	Standard Conc. (ppm) or Parameter	Formaldehyde Product Ion $\text{H}_3\text{O}^+ 31$
1	0	8.82
	10	47.3
	20	79.7
	30	130
	Slope	3.959
	Intercept	7.064
	R^2	0.9919
	LOQ	3.30
	Amount ($\mu\text{g/g}$)	<LOQ
2	0	8.87
	10	47.9
	20	88.4
	30	129
	Slope	4.009
	Intercept	8.409
	R^2	0.9999
	LOQ	3.26
	Amount ($\mu\text{g/g}$)	<LOQ
3	0	302
	10	339
	20	394
	30	440
	Slope	4.69
	Intercept	298.4
	R^2	0.9949
	LOQ	2.78
	Amount ($\mu\text{g/g}$)	31.8
4	0	549
	10	581
	20	600
	30	632
	Slope	2.680
	Intercept	550.3
	R^2	0.9907
	LOQ	4.87
	Amount ($\mu\text{g/g}$)	102.7
5	0	10.6
	10	45.5
	20	87.2

Product Number or Calibration	Standard Conc. (ppm) or Parameter	Formaldehyde Product Ion H_3O^+ 31
	30	127
	Slope	3.909
	Intercept	8.940
	R ²	0.9987
	LOQ	3.34
	Amount (µg/g)	<LOQ
	6	0
	10	48.6
	20	82.4
	30	115
	Slope	3.562
	Intercept	9.958
	R ²	0.9969
	LOQ	3.66
	Amount (µg/g)	<LOQ
	7	0
	10	45.7
	20	83.3
	30	118
	Slope	3.698
	Intercept	8.106
	R ²	0.9995
	LOQ	3.53
	Amount (µg/g)	<LOQ
	8	0
	10	75.1
	20	(outlier)
	30	179
	Slope	5.595
	Intercept	13.15
	R ²	0.9962
	LOQ	2.33
	Amount (µg/g)	<LOQ
	9	0
	10	47.6
	20	85.6
	30	122
	Slope	3.810
	Intercept	8.569
	R ²	0.9996
	LOQ	3.43
	Amount (µg/g)	<LOQ
Aqueous Cal.	0	7.41

Product Number or Calibration	Standard Conc. (ppm) or Parameter	Formaldehyde Product Ion H ₃ O ⁺ 31
	10	45.3
	20	78.9
	30	122
	40	152
	50	180
	Slope	3.503
	Intercept	10.02
	R ²	0.9960