In-tube extraction dynamic headspace coupled to gas chromatography-mass spectrometry for the sensitive analysis of volatile compounds in aqueous samples

Eleni Zymvrakaki, Nikos Anagnostou, Urania Menkissoglu-Spiroudi

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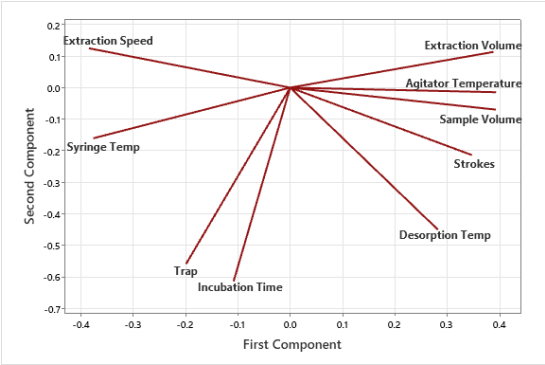
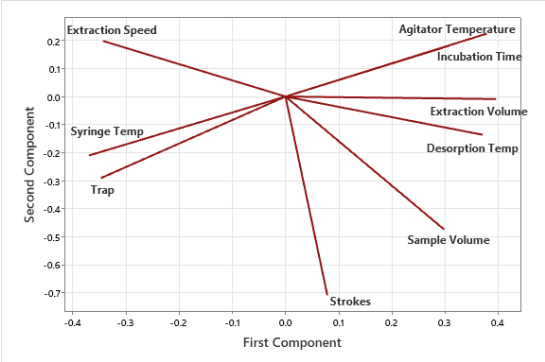
Supplementary materials 1	
Figure S1–10	Figure S1–10



Eigenvectors

Variable	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9
Agitator Temperature	0.393	-0.015	-0.208	0.299	-0.177	0.172	-0.577	-0.276	0.492
Extraction Speed	-0.385	0.125	-0.263	-0.232	-0.795	0.182	-0.131	0.165	-0.069
Extraction Volume	0.388	0.113	-0.131	-0.491	-0.030	-0.159	-0.228	-0.455	-0.542
Incubation Time	-0.108	-0.615	-0.373	0.065	-0.163	-0.219	0.411	-0.460	0.112
Desorption Temp	0.282	-0.450	-0.225	-0.457	0.187	0.519	0.028	0.384	0.079
Sample Volume	0.393	-0.070	-0.061	-0.102	-0.224	-0.705	0.005	0.499	0.172
Strokes	0.347	-0.214	0.717	0.031	-0.459	0.206	0.227	-0.113	-0.033
Syringe Temp	-0.376	-0.161	0.380	-0.552	0.116	-0.210	-0.304	-0.188	0.445
Trap	-0.199	-0.560	0.135	0.296	0.019	-0.103	-0.533	0.182	-0.460

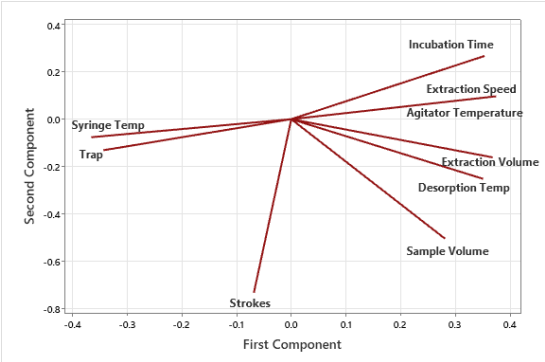
Figure S1. PCA-biplot of all variables applied for benzene



Eigenvectors

Variable	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9
Agitator Temperature	0.378	0.225	-0.027	0.496	-0.238	0.055	0.592	-0.093	-0.376
Extraction Speed	-0.343	0.199	-0.459	0.042	0.495	0.323	0.085	0.378	-0.362
Extraction Volume	0.396	-0.009	0.063	0.054	-0.324	0.615	-0.441	0.396	-0.038
Incubation Time	0.307	0.181	-0.631	-0.124	-0.212	-0.514	-0.337	0.047	-0.185
Desorption Temp	0.370	-0.137	0.329	0.380	0.590	-0.334	-0.259	0.225	-0.116
Sample Volume	0.298	-0.474	-0.206	-0.267	0.039	-0.073	0.492	0.484	0.298
Strokes	0.079	-0.710	-0.279	0.076	0.094	0.223	-0.114	-0.488	-0.310
Syringe Temp	-0.370	-0.211	-0.246	0.707	-0.243	-0.108	-0.109	0.190	0.373
Trap	-0.347	-0.291	0.312	-0.108	-0.361	-0.266	-0.005	0.360	-0.596

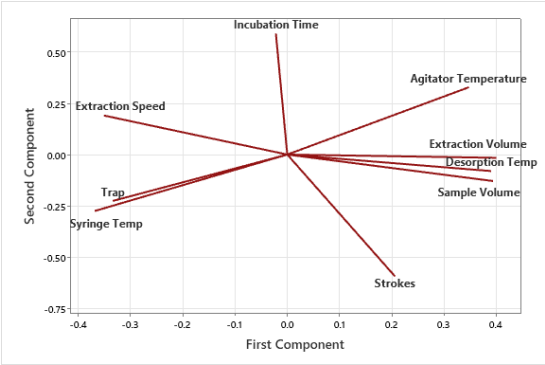
Figure S2. PCA-biplot of all variables applied for toluene



Eigenvectors

Variable	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9
Agitator Temperature	0.375	0.097	-0.104	-0.188	-0.210	0.707	-0.425	0.143	-0.243
Extraction Speed	0.375	0.097	-0.104	-0.188	-0.210	-0.707	-0.425	0.143	-0.243
Extraction Volume	0.368	-0.162	0.150	-0.395	0.225	0.000	0.622	0.303	-0.360
Incubation Time	0.353	0.268	-0.087	0.089	0.711	0.000	-0.120	-0.510	-0.085
Desorption Temp	0.351	-0.253	0.325	-0.366	-0.301	0.000	0.044	-0.516	0.464
Sample Volume	0.281	-0.506	0.022	0.227	0.366	0.000	-0.255	0.461	0.449
Strokes	-0.068	-0.735	-0.304	0.149	-0.064	0.000	-0.048	-0.358	-0.454
Syringe Temp	-0.366	-0.077	-0.454	-0.722	0.265	0.000	-0.146	0.029	0.202
Trap	-0.344	-0.132	0.737	-0.191	0.237	0.000	-0.382	0.002	-0.286

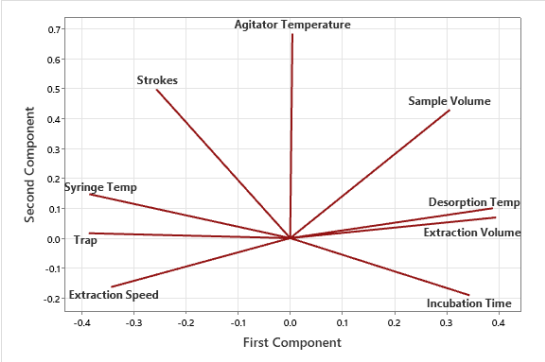
Figure S3. PCA-biplot of all variables applied for ethylbenzene



Eigenvectors

Variable	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9
Agitator Temperature	0.347	0.329	-0.201	-0.019	-0.623	0.104	-0.508	-0.033	0.268
Extraction Speed	-0.351	0.191	-0.464	-0.195	-0.090	0.405	0.352	-0.532	0.092
Extraction Volume	0.400	-0.016	-0.056	0.142	-0.197	-0.454	0.640	-0.094	0.390
Incubation Time	-0.022	0.591	0.627	0.173	0.244	0.130	0.004	-0.276	0.274
Desorption Temp	0.390	-0.081	0.228	0.267	-0.285	0.541	0.313	-0.003	-0.496
Sample Volume	0.393	-0.129	-0.028	-0.451	0.356	0.468	0.076	0.304	0.425
Strokes	0.206	-0.596	0.150	0.066	0.093	0.017	-0.294	-0.677	0.148
Syringe Temp	-0.368	-0.276	-0.021	0.612	-0.127	0.301	0.009	0.277	0.480
Trap	-0.334	-0.227	0.522	-0.508	-0.522	-0.008	0.133	0.059	0.115

Figure S4. PCA-biplot of all variables applied for *p,m*-xylene



Eigenvectors

Variable	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8	PC9
Agitator Temperature	0.347	0.329	-0.201	-0.019	-0.623	0.104	-0.508	-0.033	0.268
Extraction Speed	-0.351	0.191	-0.464	-0.195	-0.090	0.405	0.352	-0.532	0.092
Extraction Volume	0.400	-0.016	-0.056	0.142	-0.197	-0.454	0.640	-0.094	0.390
Incubation Time	-0.022	0.591	0.627	0.173	0.244	0.130	0.004	-0.276	0.274
Desorption Temp	0.390	-0.081	0.228	0.267	-0.285	0.541	0.313	-0.003	-0.496
Sample Volume	0.393	-0.129	-0.028	-0.451	0.356	0.468	0.076	0.304	0.425
Strokes	0.206	-0.596	0.150	0.066	0.093	0.017	-0.294	-0.677	0.148
Syringe Temp	-0.368	-0.276	-0.021	0.612	-0.127	0.301	0.009	0.277	0.480
Trap	-0.334	-0.227	0.522	-0.508	-0.522	-0.008	0.133	0.059	0.115

Figure S5. PCA-biplot of all variables applied for *o*-xylene

Concetration	Mean Peak Area	Deviation	RSD Drift (%)
50.00	4810931.67	24377.33	0.51
100.00	12840368.33	96013.29	0.75
250.00	38409984.00	732224.25	1.91
500.00	76196283.56	1231577.40	1.62
1000.00	157444776.00	732224.25	0.47
2000.00	314889551.33	15716298.18	4.99

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.99997214
R Square	0.999944281
Adjusted R Square	0.999930351
Standard Error	990926.0199
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	7.04877E+16	7.04877E+16	71784.51861	1.16426E-09
Residual	4	3.92774E+12	9.81934E+11		
Total	5	7.04916E+16			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-2550755.401	558886.104	-4.563998609	0.010307545	-4102471.989	-999038.8132	-4102471.989	-999038.8132
X Variable 1	158947.8021	593.2518903	267.9263306	1.16426E-09	157300.6708	160594.9334	157300.6708	160594.9334

Concetration	Mean Peak Area
50	4840801
50	4781089
50	4810905
100	12904918
100	12704639
100	12911548
250	37438259
250	39205752
250	38585941
500	77884548
500	74981345
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1000	152338234
1000	155212345
1000	164783749
2000	297691176
2000	311295915
2000	335681563

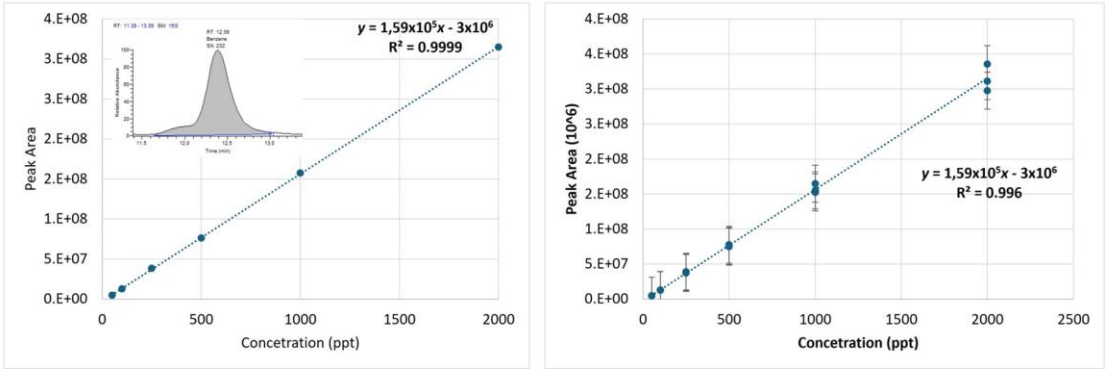


Figure S6. Calibration curve for benzene and statistical analysis data

Concetration	Mean Peak Area	Deviation	RSD Drift (%)
50.00	15565600	595518.31	3.83
100.00	31809281	1272677.55	4.00
250.00	85190436	1948203.39	2.29
500.00	170500886	2759490.90	1.62
1000.00	332501144	14861377.76	4.47
2000.00	665002288	12651288.24	1.90

SUMMARY OUTPUT

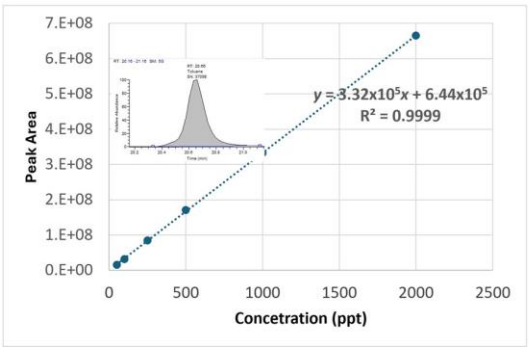
Regression Statistics	
Multiple R	0.99997908
R Square	0.999958161
Adjusted R Square	0.999947701
Standard Error	1914293.131
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	3.50328E+17	3.50328E+17	95599.94806	6.56456E-10
Residual	4	1.46581E+13	3.66452E+12		
Total	5	3.50342E+17			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-3567342.36	1079668.723	3.304108274	0.029818434	-6564983.3	569701.4198	-6564983.3	569701.4198
X Variable 1	354352.2279	1146.05732	309.1924127	6.56456E-10	351170.2626	357534.1931	351170.2626	357534.1931

Concetration	Mean Peak Area
50	14799835
50	15644895
50	16252071
100	30678897
100	31161527
100	33587418
250	83096155
250	84687179
250	87787975
500	170027701
500	174092215
500	167382742
1000	334129986
1000	313540071
1000	349833375
2000	679383847
2000	648594095
2000	667028922



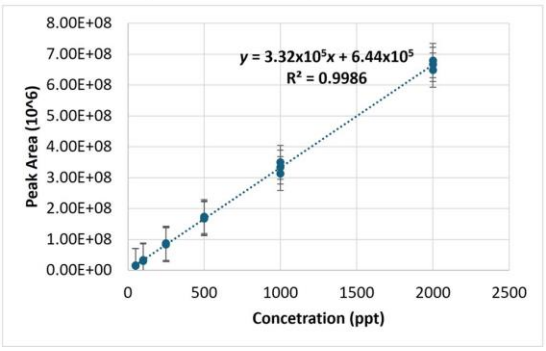


Figure S7. Calibration curve for toluene and statistical analysis data

Concetration	Mean Peak Area	Deviation	RSD Drift (%)
50	2158304	90160.64	4.18
100	5250703	212789.47	4.05
250	17912995	378888.62	2.12
500	38534618	1346922.95	3.50
1000	73332184	1929056.26	2.63
2000	146664370	7656757.23	5.22

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.999732976
R Square	0.999466022
Adjusted R Square	0.999332528
Standard Error	1429021.87
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.52891E+16	1.52891E+16	7486.950455	1.06944E-07
Residual	4	8.16841E+12	2.0421E+12		
Total	5	1.52973E+16			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-808588.3087	805973.8564	-1.003243843	0.372510561	-3046330.477	1429153.86	-3046330.477	1429153.86
X Variable 1	94026.84724	855.5330155	86.52716599	1.06944E-07	71651.50679	76402.1877	71651.50679	76402.1877

Concetration	Mean Peak Area
50	2035396
50	2190372
50	2249145
100	5452149
100	5343587
100	4956373
250	18407676
250	17487321
250	17843987
500	37190468
500	38037827
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1000	71159562
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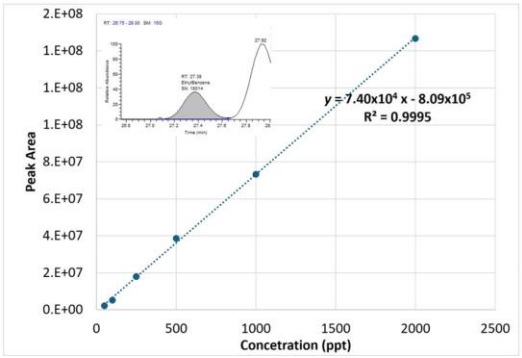
1000	75847366
2000	154512974
2000	149200598
2000	136279537



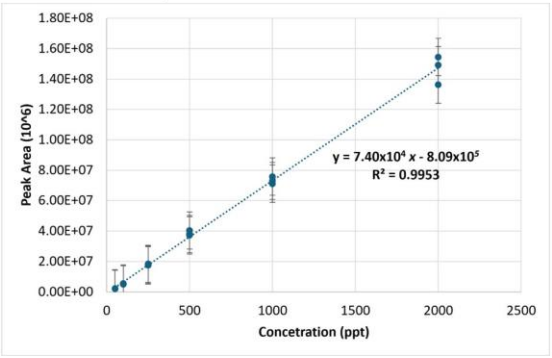


Figure S8. Calibration curve for ethylbenzene and statistical analysis data

Concetration	Mean Peak Area	Deviation	RSD Drift (%)
50.00	6607506	59072.46	0.89
100.00	15200997	613130.60	4.03
250.00	48651474	627477.18	1.29
500.00	93610726	961768.94	1.03
1000.00	194076490	10575365.72	5.45
2000.00	388152979	12435680.05	3.20

SUMMARY OUTPUT

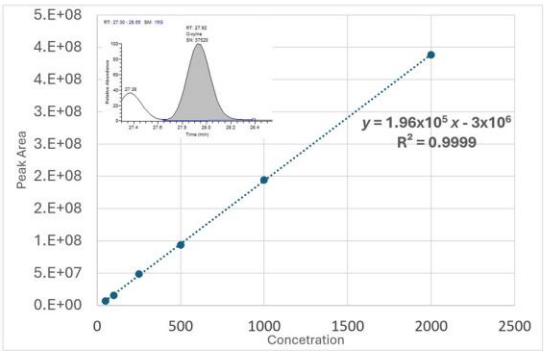
Regression Statistics	
Multiple R	0.999940899
R Square	0.999881801
Adjusted R Square	0.999852251
Standard Error	1777371.054
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.06893E+17	1.06893E+17	33837.13278	5.23936E-09
Residual	4	1.26362E+13	3.15905E+12		
Total	5	1.06906E+17			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-2845644.528	910444.1418	-2.838706327	0.04692908	-5628875.659	-62413.39723	-5628875.659	-62413.39723
X Variable 1	195736.933	1064.084216	183.9487232	5.23936E-09	192782.5616	198691.3044	192782.5616	198691.3044

Concetration	Mean Peak Area
50	6525489
50	6662271
50	6634758
100	14438349
100	15939630
100	15225012
250	49472136
250	48533506
250	47948779
500	94723196
500	93732213
500	92376769
1000	196190249
1000	180197498
1000	205841722
2000	400241095
2000	393171349
2000	371046494



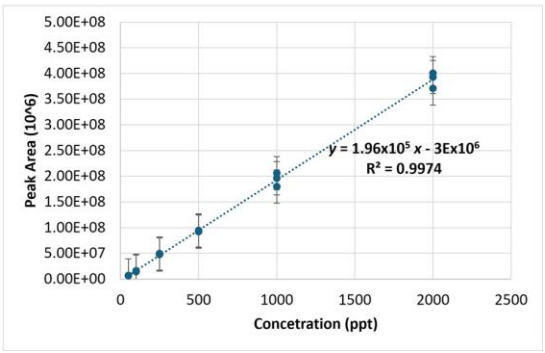


Figure S9. Calibration curve for *p,m*-xylene and statistical analysis data

Concetration	Mean Peak Area	Deviation	RSD Drift (%)
50.00	2599672	152828.33	5.88
100.00	5855122	158032.73	2.70
250.00	21130254	997868.53	4.72
500.00	46969282	1796569.44	3.82
1000.00	92030164	793048.53	0.86
2000.00	184060328	7394828.94	4.02

SUMMARY OUTPUT

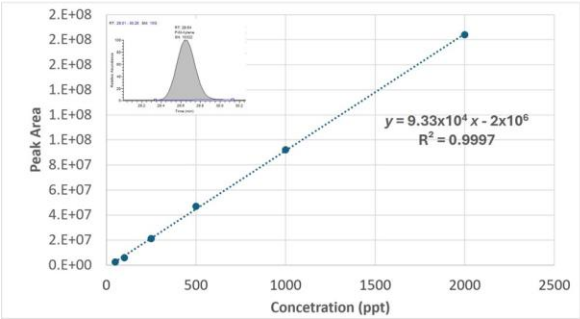
Regression Statistics	
Multiple R	0.999828965
R Square	0.999657959
Adjusted R Square	0.999572449
Standard Error	1441936.301
Observations	6

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	2.43067E+16	2.43067E+16	11690.51	4.39E-08
Residual	4	8.31672E+12	2.07918E+12		
Total	5	2.4315E+16			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*Lower 95.0%*	*Upper 95.0%*
Intercept	-1895881.096	813257.6454	-2.331218289	0.080145	-4153846	362084.1126	-4153846.305	362084.1
X Variable 1	93338.48938	863.264683	108.122678	4.39E-08	90941.68	95735.29638	90941.68238	95735.3

Concetration	Mean Peak Area
50	2739731
50	2387086
50	2672199
100	5799161
100	6070487
100	5695719
250	22249297
250	19826139
250	21315326
500	45318995
500	49467419
500	46121432
1000	91099775
1000	91952983
1000	93037734
2000	187034489
2000	191256047
2000	173890447



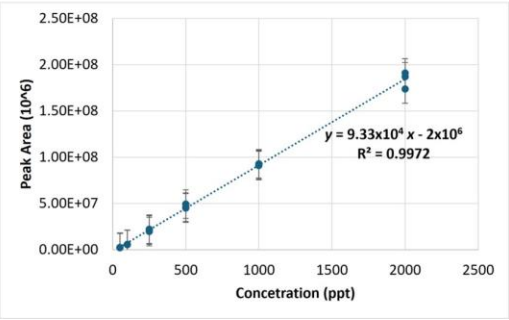


Figure S10. Calibration curve for *o*-xylene and statistical analysis data