

## SUPPORTING INFORMATION

### Advanced data preprocessing for Comprehensive two-dimensional Gas Chromatography with Vacuum Ultraviolet Spectroscopy detection

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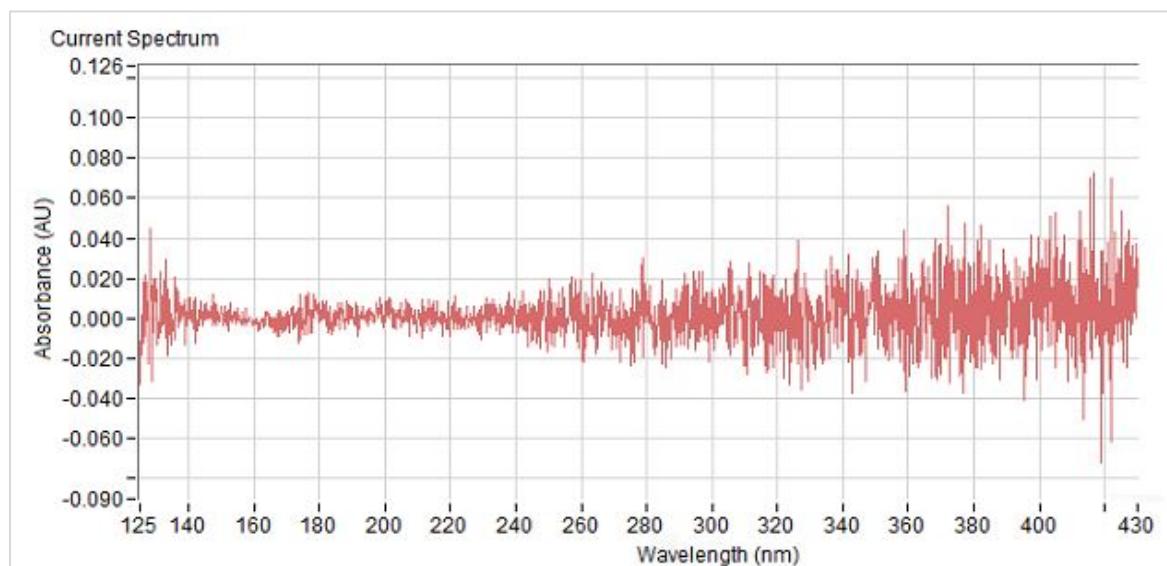


Figure S1 Measured detector blank spectrum.

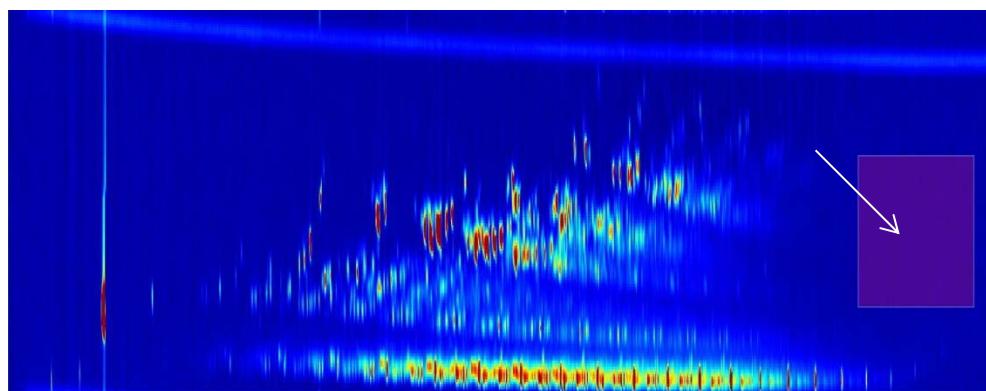
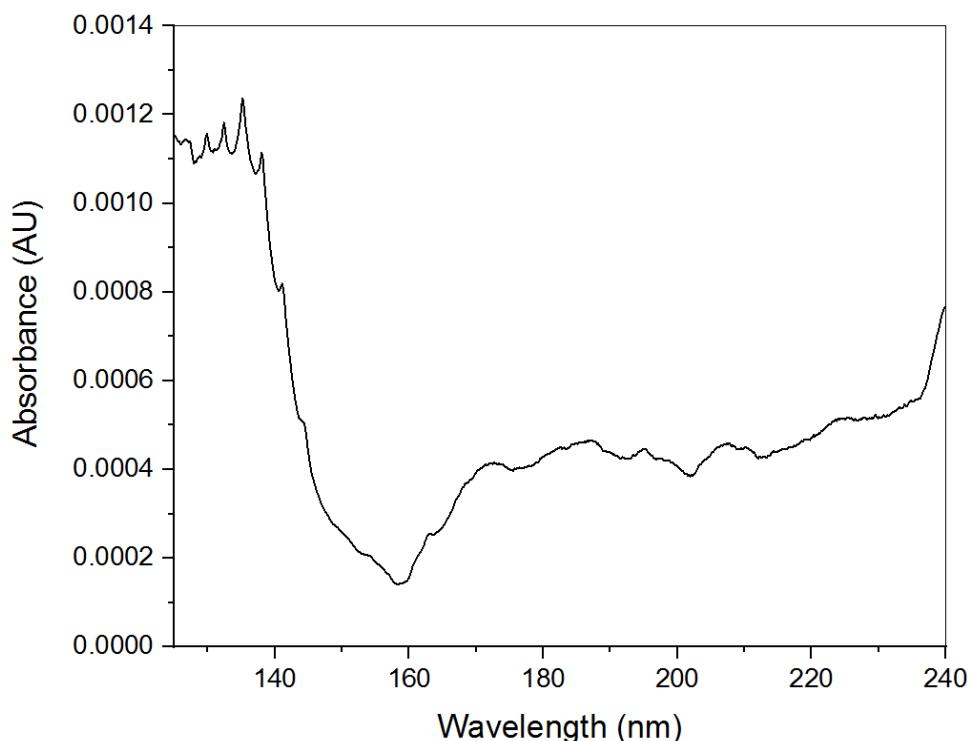


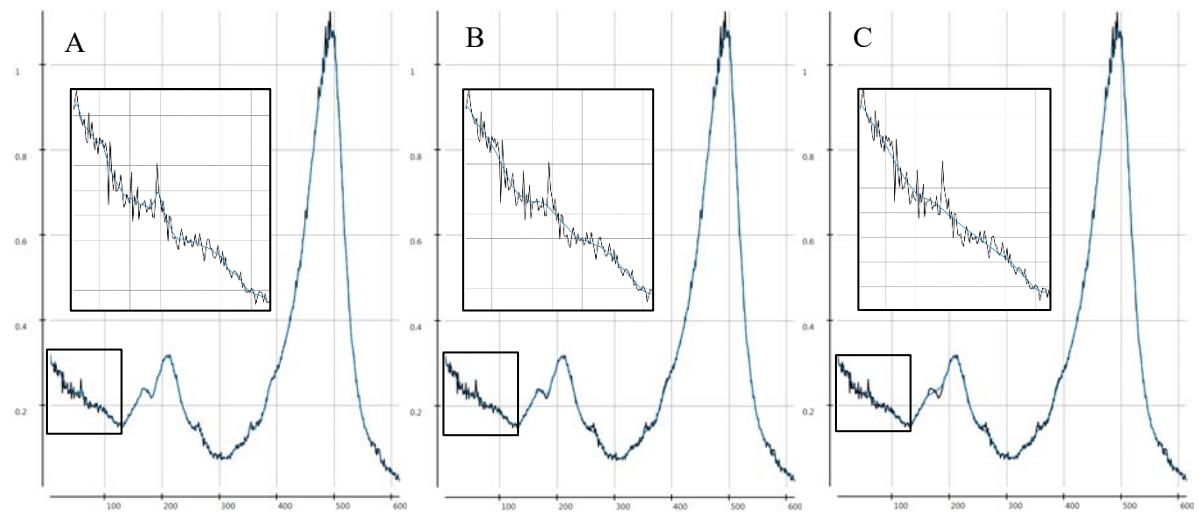
Figure S2 Selection of a zone for extracting detector blank signal.



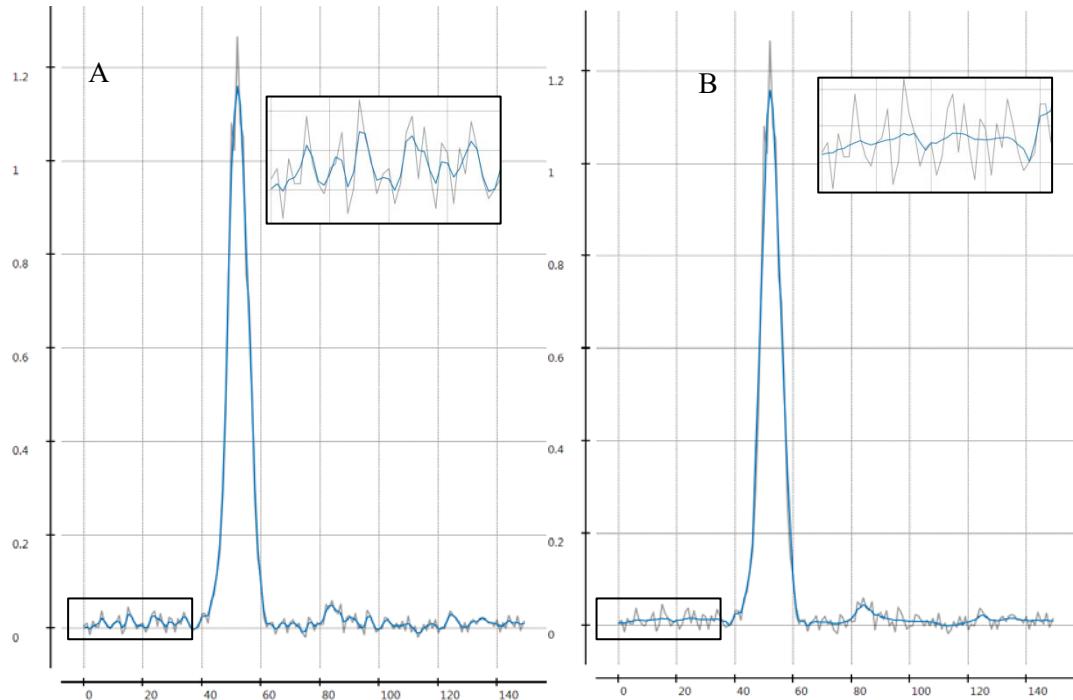
**Figure S3 Detector blank signal.**

**Table S1 Composition of standard mixture in toluene for investigation of the limits of detection of the GC $\times$ GC/VUV method.**

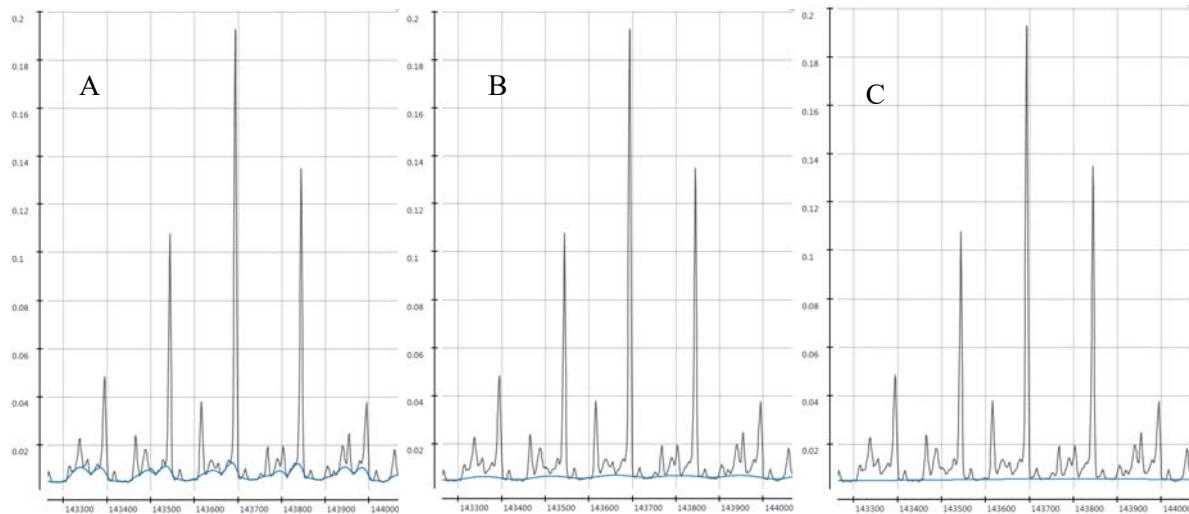
Compound	m/m% in solution
n-C8	1.07
n-C10	1.14
n-C12	0.96
n-C14	1.07
n-C16	1.07
n-C17	1.26
n-C18	1.03
1,13-tetradecadiene	1.07
1,2-cyclooctadiene	1.05
<i>trans</i> -2-octene	1.06
1,7 octadiene	1.00
<i>cis</i> -decalin	0.59
<i>trans</i> -decalin	0.70
1-decene	1.54
1-undecene	0.97
1,3,5-trimethylbenzene	1.06
1,2,3-trimethylbenzene	1.36
1-phenyldecane	0.84
1-phenyldodecane	0.89
<i>m</i> -xylene	1.19
Propylbenzene	1.09



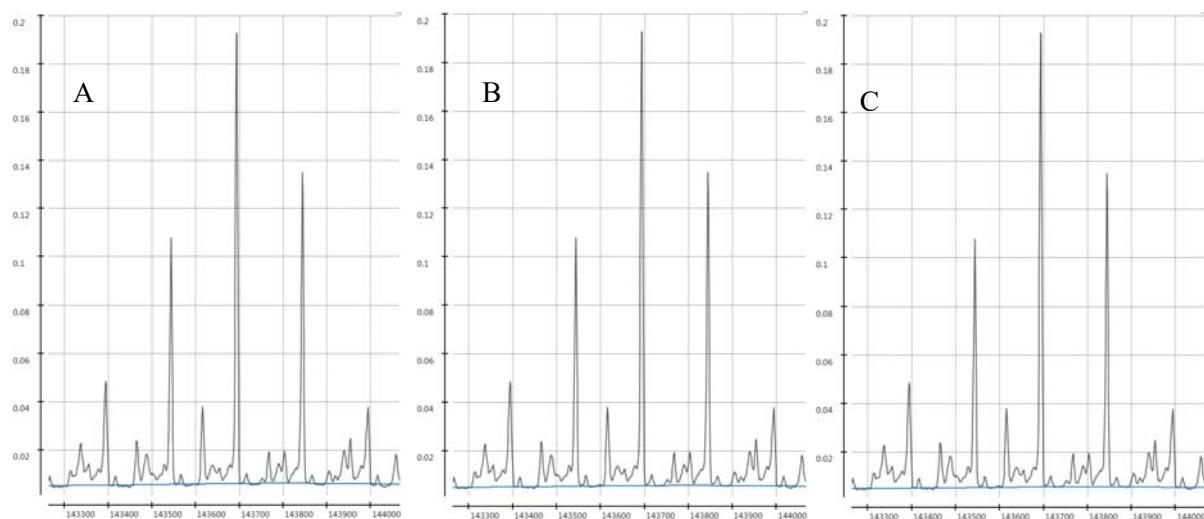
**Figure S4 Spectrum at a chosen chromatogram point (in grey) smoothed by choosing following filter M values (in blue) (A) 5, (B) 15, (C) 20.**



**Figure S5 Illustration of the noise correction: input signal in grey and resultant signal in blue. Noise filter M value (A) 2, (B) 5. One modulation period 125 nm chromatogram is shown.**



**Figure S6** Estimated baseline (in blue) for a VUV signal (in grey) depending on the chosen convolution kernel sizes; (A) 5, (B) 20, (C) 100, number of iterations is 15 (125 nm).



**Figure S7** Estimated baseline (in blue) for a VUV signal (in grey) depending on the chosen number iterations; (A) 5, (B) 10, (C) 15, convolution kernel size is 100 (125 nm).

**Table S2 Estimation of spectral similarity with corresponding VUV library spectrum - test mixture 150 x dilution.**

Compound	No preprocessing		With preprocessing	
	$\text{Chi}^2$	$R^2$	$\text{Chi}^2$	$R^2$
<b>n-decane</b>	0.008170	0.48	0.001530	0.96
<b>1-decene</b>	0.002730	0.87	0.000836	0.97
<b>m-xylene</b>	0.010200	0.61	0.000474	0.98

**Table S3 Peak volume and signal to noise ratio for selected peaks, for different dilutions of the test mixture with baseline correction in GC Image. GC Image was used for integration of Avg. 125-240 nm chromatogram.**

Compound	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N
n-C10	11400	11.54	2214.63	5770	6.20	1147.38	1238	1.41	280.33	571	0.65	135.85	251	0.33	57.46
n-C12	9600	4.59	1122.90	4859	2.46	680.08	1042	0.56	235.26	481	0.28	112.96	211	0.13	46.00
n-C14	10700	5.01	1484.44	5416	2.65	917.50	1162	0.63	280.78	536	0.29	123.66	235	0.13	50.59
n-C16	10700	4.90	1050.22	5416	2.64	847.81	1162	0.59	294.33	536	0.30	111.33	235	0.15	56.85
n-C17	12600	5.85	1658.04	6378	3.16	969.53	1368	0.69	350.43	631	0.34	162.32	277	0.17	87.47
n-C18	10300	4.85	1122.15	5213	2.65	968.00	1118	0.59	254.27	516	0.29	162.41	226	0.13	52.61
1-decene	15400	16.77	3167.40	7795	9.17	1914.10	1672	1.98	484.52	772	0.94	292.33	338	0.46	119.76
1-undecene	9700	6.07	1783.45	4910	3.33	1058.84	1053	0.72	229.03	486	0.34	137.06	213	0.17	59.26
m-xylene	11900	15.63	3478.45	6023	8.62	2395.94	1292	1.87	551.68	596	0.85	287.17	261	0.39	114.49
Propylbenzene	10900	13.18	2572.56	5517	7.20	1887.33	1183	1.59	558.55	546	0.73	282.18	240	0.33	121.60
1,3,5-trimethylbenzene	10600	13.90	3075.52	5365	7.58	2023.89	1151	1.64	607.21	531	0.78	260.15	233	0.37	110.20
1,2,3-trimethylbenzene	13600	14.92	3066.36	6884	8.25	2206.04	1477	1.77	591.59	682	0.85	259.77	299	0.38	112.28
<i>trans</i> -decalin	7000	2.89	773.79	3543	1.58	496.78	760	0.35	100.73	351	0.16	53.80	154	0.09	26.68
<i>cis</i> -decalin	5900	2.46	642.82	2986	1.35	397.74	641	0.32	78.37	296	0.14	47.94	130	0.08	21.73
1-phenyldecane	8400	6.84	2040.22	4252	3.77	1245.21	912	0.81	357.23	421	0.39	200.63	185	0.19	73.10
1-phenyldodecane	8900	6.99	1821.50	4505	3.77	1415.59	966	0.83	365.46	446	0.39	155.85	196	0.19	69.32
1,2-cyclooctadiene	10500	9.38	2171.68	5315	5.00	1304.07	1140	1.08	256.46	526	0.51	152.18	231	0.28	65.33
1,13-tetradecadiene	10700	7.56	2311.23	5416	4.10	1687.16	1162	0.89	399.65	536	0.42	176.76	235	0.22	79.22
Compound	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N
n-C10	121.4	0.17	28.78	81.98	0.13	21.17	64.64	0.11	17.16	39.37	0.07	11.16	25.25	0.06	7.27
n-C12	102.2	0.05	19.93	69.04	0.07	14.62	54.43	0.03	6.92	33.16	0.02	6.26	21.26	0.02	5.87
n-C14	113.9	0.08	24.08	76.95	0.04	14.49	60.67	0.04	9.94	36.95	0.04	8.29	23.70	0.02	5.68
n-C16	113.9	0.07	28.02	76.95	0.05	19.18	60.67	0.05	14.95	36.95	0.02	8.14	23.70	0.02	6.28
n-C17	134.2	0.10	40.27	90.61	0.06	28.39	71.44	0.06	17.77	43.52	0.04	13.66	27.91	0.03	6.59
n-C18	109.7	0.07	23.50	74.07	0.06	20.37	58.40	0.04	12.07	35.57	0.03	10.96	22.81	0.04	6.55
1-decene	164.0	0.22	44.03	110.75	0.15	36.04	87.32	0.12	27.06	53.19	0.07	12.08	34.11	0.06	8.50
1-undecene	103.3	0.06	20.10	69.76	0.05	12.08	55.00	0.03	9.23	33.50	0.03	5.66	21.49	0.00	
m-xylene	126.7	0.21	45.71	85.58	0.17	34.87	67.47	0.10	22.00	41.10	0.08	18.19	26.36	0.04	9.80
Propylbenzene	116.1	0.16	50.17	78.39	0.11	31.71	61.80	0.09	23.80	37.65	0.06	12.06	24.14	0.02	7.71
1,3,5-trimethylbenzene	112.9	0.19	43.29	76.23	0.12	30.32	60.10	0.10	24.51	36.61	0.06	15.55	23.48	0.03	7.19
1,2,3-trimethylbenzene	144.8	0.17	52.74	97.80	0.12	35.56	77.11	0.08	24.44	46.97	0.07	16.66	30.12	0.03	7.33
<i>trans</i> -decalin	74.5	0.04	10.15	50.34	0.02	8.57	39.69	0.03	7.80	24.18	0.02	4.61	15.51	0.00	6.04
<i>cis</i> -decalin	62.8	0.03	11.94	42.43	0.02	8.83	33.45	0.02	6.46	20.38	0.01	4.39	13.07	0.00	5.29
1-phenyldecane	89.4	0.09	34.62	60.41	0.07	23.32	47.63	0.04	16.89	29.01	0.03	9.85	18.61	0.02	7.73
1-phenyldodecane	94.8	0.09	33.19	64.00	0.06	19.77	50.46	0.04	12.27	30.74	0.03	7.81	19.71	0.03	6.23
1,2-cyclooctadiene	111.8	0.11	30.37	75.51	0.08	20.03	59.54	0.07	12.19	36.26	0.03	7.87	23.26	0.03	7.31
1,13-tetradecadiene	113.9	0.10	37.28	76.95	0.08	27.16	60.67	0.05	20.10	36.95	0.04	11.07	23.70	0.03	7.79

**Table S4 Peak volume and signal to noise ratio for selected peaks, for different dilutions of the test mixture with preprocessing in plug im! software (noise, baseline correction and detector blank subtraction). GC Image was used for integration of Avg. 125-240 nm chromatogram.**

Compound	Conc (ppm)*	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N
Compound	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N
n-C10	11400	12.32	10146.80	5770	6.64	6750.49	1238	1.52	2032.03	571	0.72	884.71	251	0.44	462.64
n-C12	9600	4.88	6937.21	4859	2.70	4574.22	1042	0.63	1419.38	481	0.33	702.99	211	0.17	332.55
n-C14	10700	5.48	7550.75	5416	2.82	5527.42	1162	0.68	1341.73	536	0.34	761.13	235	0.16	297.42
n-C16	10700	5.07	6177.10	5416	2.79	4789.25	1162	0.64	1899.53	536	0.35	689.09	235	0.18	370.86
n-C17	12600	6.06	7815.90	6378	3.25	4361.52	1368	0.74	1698.04	631	0.36	613.32	277	0.21	465.15
n-C18	10300	4.96	7377.31	5213	2.73	5190.62	1118	0.66	1416.61	516	0.34	624.20	226	0.16	316.81
1-decene	15400	7.25	11995.34	7795	9.44	12148.47	1672	2.11	3302.40	772	1.06	1951.60	338	0.55	867.24
1-undecene	9700	7.22	11506.68	4910	3.55	6845.71	1053	0.81	1231.01	486	0.38	879.22	213	0.22	346.71
m-xylene	11900	7.99	12667.19	6023	9.10	14171.27	1292	1.97	3041.43	596	0.94	2299.64	261	0.45	616.58
Propylbenzene	10900	6.44	11269.94	5517	7.71	12197.06	1183	1.70	3101.11	546	0.82	1741.96	240	0.39	722.42
1,3,5-trimethylbenzene	10600	17.44	15028.42	5365	8.84	12930.31	1151	1.90	4016.70	531	0.97	1661.07	233	0.44	933.01
1,2,3-trimethylbenzene	13600	3.10	6467.49	6884	7.94	12848.24	1477	1.81	3441.14	682	0.89	1655.29	299	0.43	682.90
<i>trans</i> -decalin	7000	2.62	3789.06	3543	1.70	3138.50	760	0.40	550.18	351	0.21	366.57	154	0.14	166.04
<i>cis</i> -decalin	5900	15.82	20950.58	2986	1.43	2819.71	641	0.36	418.80	296	0.19	281.52	130	0.10	131.11
1-phenyldecane	8400	14.38	15829.45	4252	4.03	6629.14	912	0.91	1935.31	421	0.44	1018.36	185	0.24	469.11
1-phenyldodecane	8900	14.10	14534.28	4505	3.94	7912.15	966	0.92	2479.57	446	0.43	801.70	196	0.23	425.39
1,2-cyclooctadiene	10500	10.05	12620.19	5315	5.25	8248.81	1140	1.14	1429.86	526	0.59	1080.24	231	0.34	405.50
1,13-tetradecadiene	10700	16.47	19964.52	5416	4.49	10182.49	1162	0.97	2176.97	536	0.48	1234.71	235	0.27	486.49
Compound	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N	Conc (ppm)	Blob volume	S/N
n-C10	121.4	0.21	200.64	81.98	0.16	167.22	64.64	0.20	110.00	39.37	0.07	73.87	25.25	0.00	
n-C12	102.2	0.07	115.54	69.04	0.08	74.94	54.43	0.06	46.51	33.16	0.03	37.47	21.26	0.05	27.19
n-C14	113.9	0.13	164.23	76.95	0.06	74.78	60.67	0.07	54.58	36.95	0.06	46.37	23.70	0.08	29.71
n-C16	113.9	0.11	174.38	76.95	0.09	113.75	60.67	0.10	80.15	36.95	0.05	49.65	23.70	0.05	25.59
n-C17	134.2	0.13	196.66	90.61	0.10	150.95	71.44	0.08	93.77	43.52	0.06	70.81	27.91	0.02	20.49
n-C18	109.7	0.09	131.06	74.07	0.08	147.08	58.40	0.06	74.34	35.57	0.07	57.09	22.81	0.02	26.58
1-decene	164.0	0.26	313.12	110.75	0.19	246.48	87.32	0.17	175.41	53.19	0.11	116.02	34.11	0.10	60.21
1-undecene	103.3	0.10	129.24	69.76	0.07	71.78	55.00	0.05	52.48	33.50	0.06	44.92	21.49	0.04	28.24
m-xylene	126.7	0.27	333.19	85.58	0.22	199.27	67.47	0.14	140.90	41.10	0.11	114.86	26.36	0.07	69.40
Propylbenzene	116.1	0.22	341.12	78.39	0.16	215.14	61.80	0.12	142.46	37.65	0.08	73.42	24.14	0.05	42.85
1,3,5-trimethylbenzene	112.9	0.23	298.26	76.23	0.14	215.10	60.10	0.12	161.49	36.61	0.13	95.32	23.48	0.02	16.39
1,2,3-trimethylbenzene	144.8	0.27	279.86	97.80	0.19	210.57	77.11	0.14	148.90	46.97	0.12	93.17	30.12	0.07	33.97
<i>trans</i> -decalin	74.5	0.08	82.85	50.34	0.05	52.65	39.69	0.05	47.40	24.18	0.03	30.74	15.51	0.02	20.77
<i>cis</i> -decalin	62.8	0.07	80.38	42.43	0.05	58.05	33.45	0.07	32.99	20.38	0.03	25.17	13.07	0.04	19.82
1-phenyldecane	89.4	0.14	207.39	60.41	0.10	133.76	47.63	0.10	84.03	29.01	0.05	51.30	18.61	0.06	24.29
1-phenyldodecane	94.8	0.13	164.04	64.00	0.08	121.18	50.46	0.09	70.28	30.74	0.06	46.84	19.71	0.06	39.40
1,2-cyclooctadiene	111.8	0.16	207.64	75.51	0.14	119.11	59.54	0.10	85.26	36.26	0.10	47.78	23.26	0.05	35.51
1,13-tetradecadiene	113.9	0.15	223.72	76.95	0.11	153.79	60.67	0.08	112.60	36.95	0.09	70.54	23.70	0.08	33.75

\* At this level detector saturation could be present.

**Table S5 Estimation of spectral similarity with corresponding VUV library spectrum - test mixture 500 x dilution.**

Compound	No preprocessing		With preprocessing	
	Chi <sup>2</sup>	R <sup>2</sup>	Chi <sup>2</sup>	R <sup>2</sup>
<b>m-xylene</b>	0.007580	0.25	0.001640	0.94