

Supplementary Information for

Fully automated portable comprehensive 2-dimensional gas chromatography device

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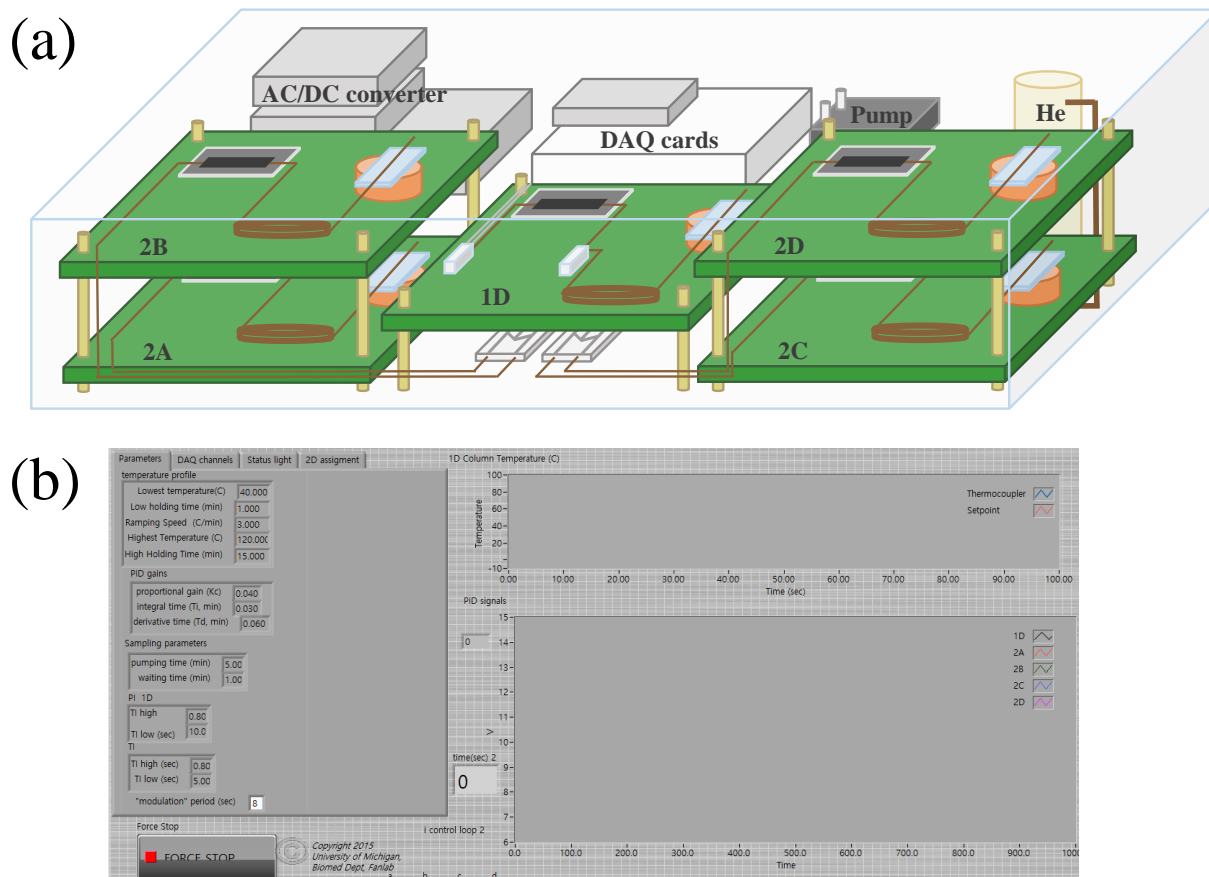


Figure S1. (a) Layout of the portable 1x4-channel GC x GC device. (b) The screen shot of Labview™ user interface.

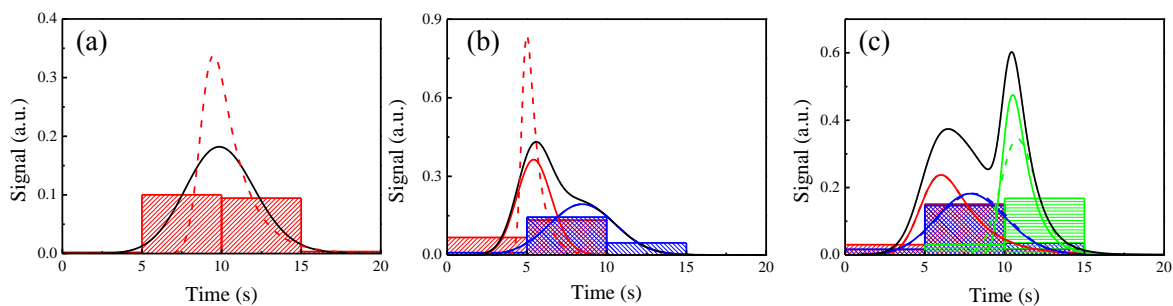


Figure S2. Reconstruction of (a) single peak, (b) coeluted two peaks, (c) coeluted three peaks using the same EMG model as in Fig. 2, but without the assist of the 1D chromatogram.

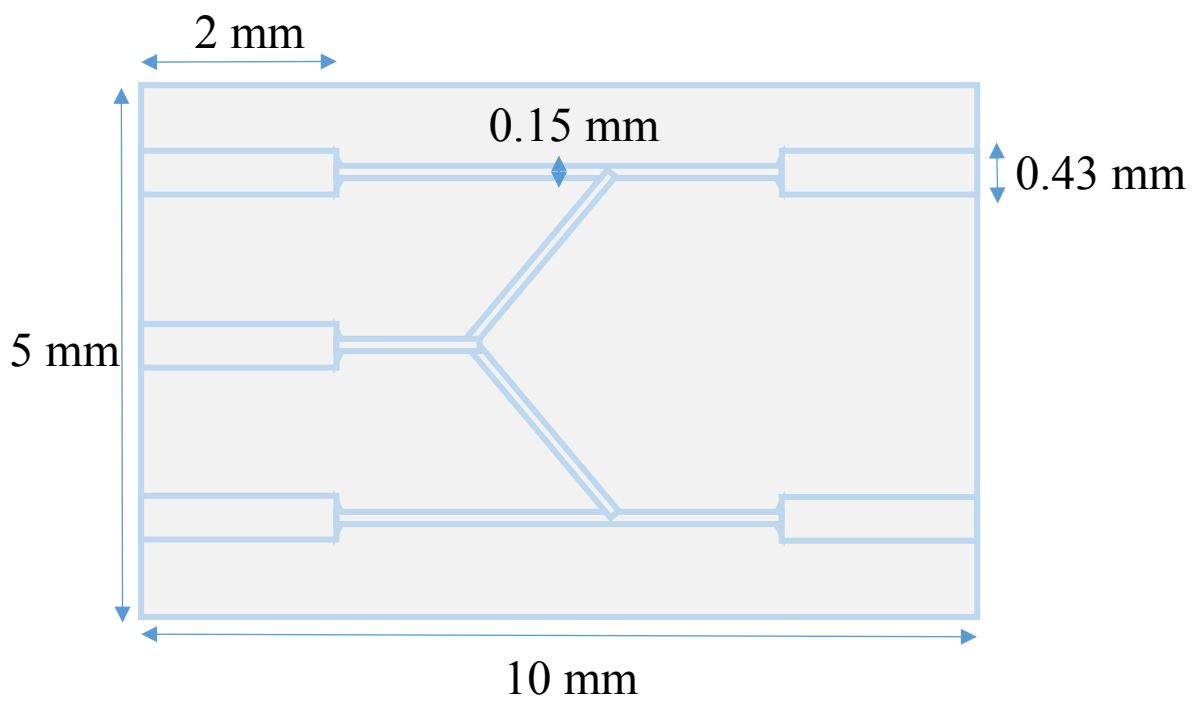


Figure S3. The dimensions of the μ DS.

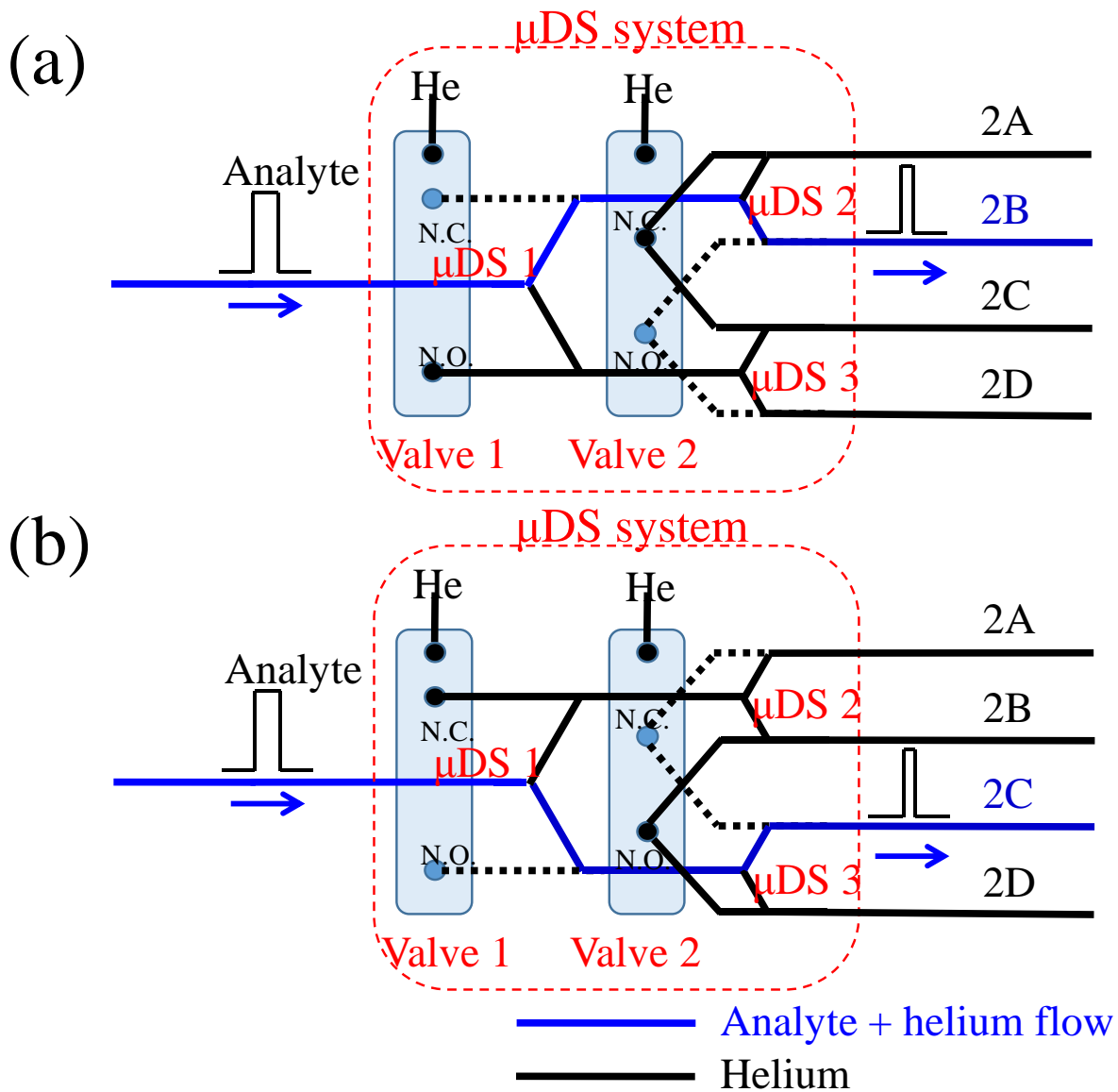


Figure S4. Schematic showing how the switching module sends analytes to (a) 2B and (b) 2C.

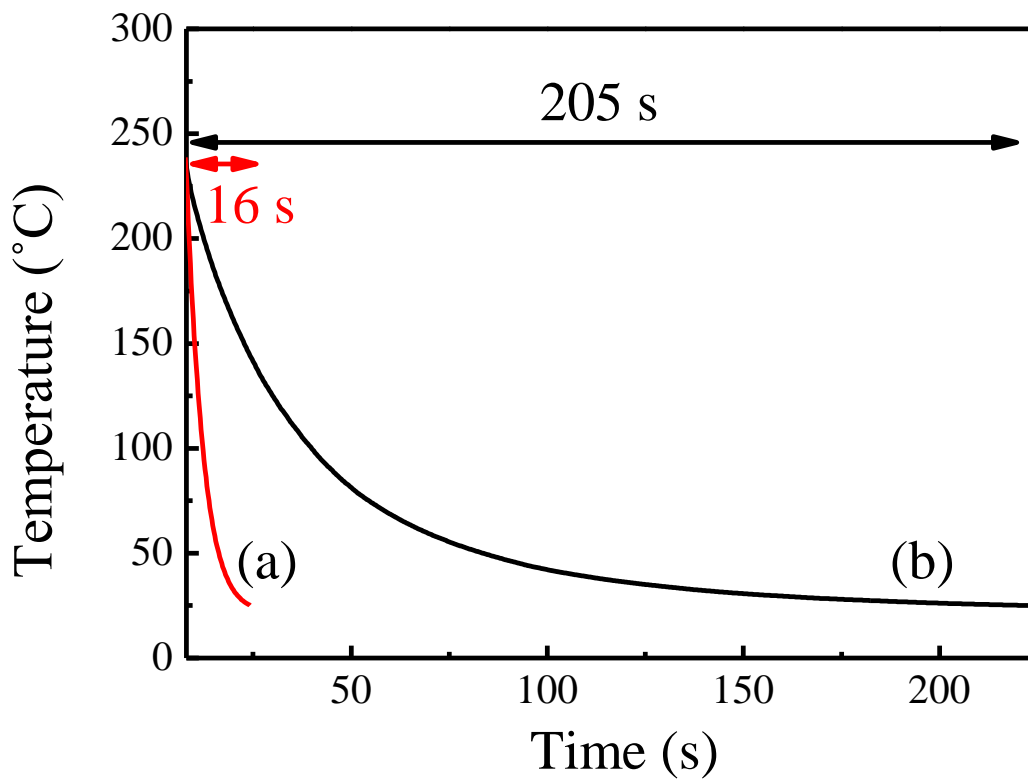


Figure S5. The cooling process of the μ TI with (a) and without (b) a coaxial fan. With the fan, it takes 16 seconds for the μ TI to cool from 240 °C to 25 °C.

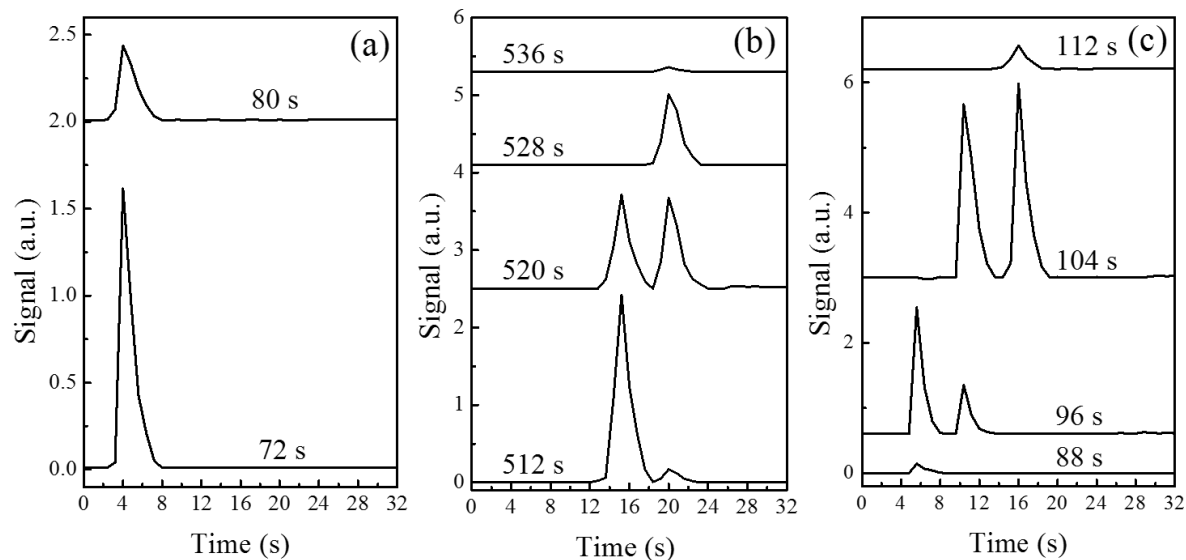


Figure S6. ^2D separation of (a) cyclohexane for the modulation at 72 s (detected by PID 2B) and 80 s (detected by PID 2C), (b) 3-chlorotoluene and 1,3-dichlorobenzene for the modulation at 512 s (detected by PID 2A), 520 s (detected by PID 2B), 528 s (detected by PID 2C), and 536 s (detected by PID 2D), and (c) heptane, 1,4-dioxane, and methylisobutylketone for the modulation at 88 s (detected by PID 2D), 96 s (detected by PID 2A), 104 s (detected by PID 2B), and 112 s (detected by PID 2C).

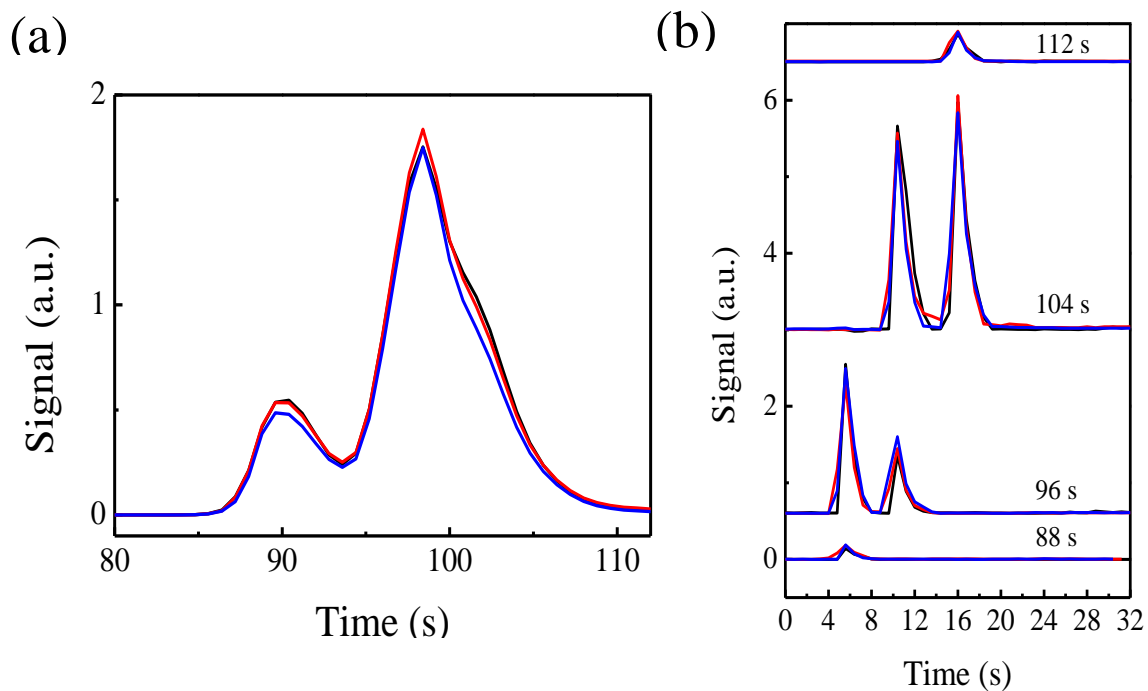


Figure S7. (a) ^1D chromatogram obtained with PID 1 for a mixture of heptane, 1,4-dioxane, and methylisobutylketone. The black, red, and blue curves were obtained in a few days. The standard deviation for two peaks at 90 s and 98 s is 0.11 s and 0.06 s, respectively. (b) ^2D separation of heptane, 1,4-dioxane, and methylisobutylketone for the modulation at 88 s (detected by PID 2D), 96 s (detected by PID 2A), 104 s (detected by PID 2B), and 112 s (detected by PID 2C). The black, red, and blue curves were obtained in a few days. The standard deviation for heptane, 1,4-dioxane, and methylisobutylketone is 0.02 s, 0.03 s, and 0.6 s, respectively.

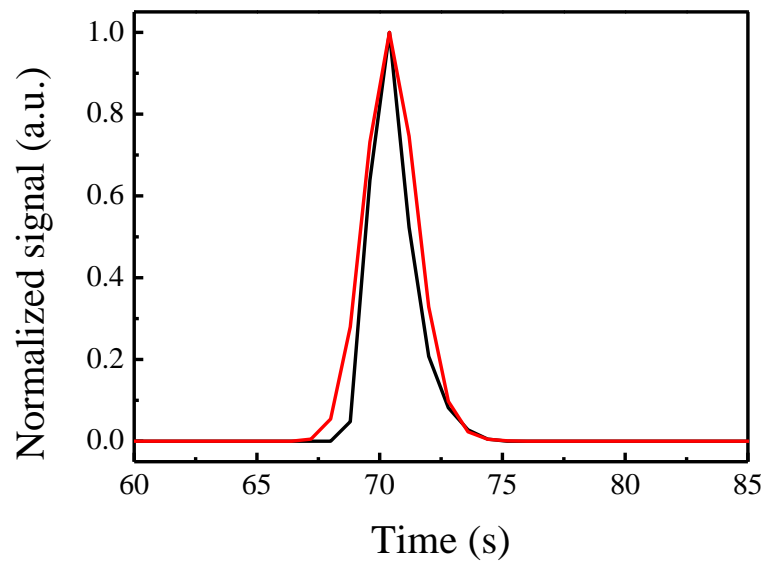


Figure S8. Comparison of the normalized peak (black) of cyclohexane obtained with PID 1 and the corresponding reconstructed peak (red).

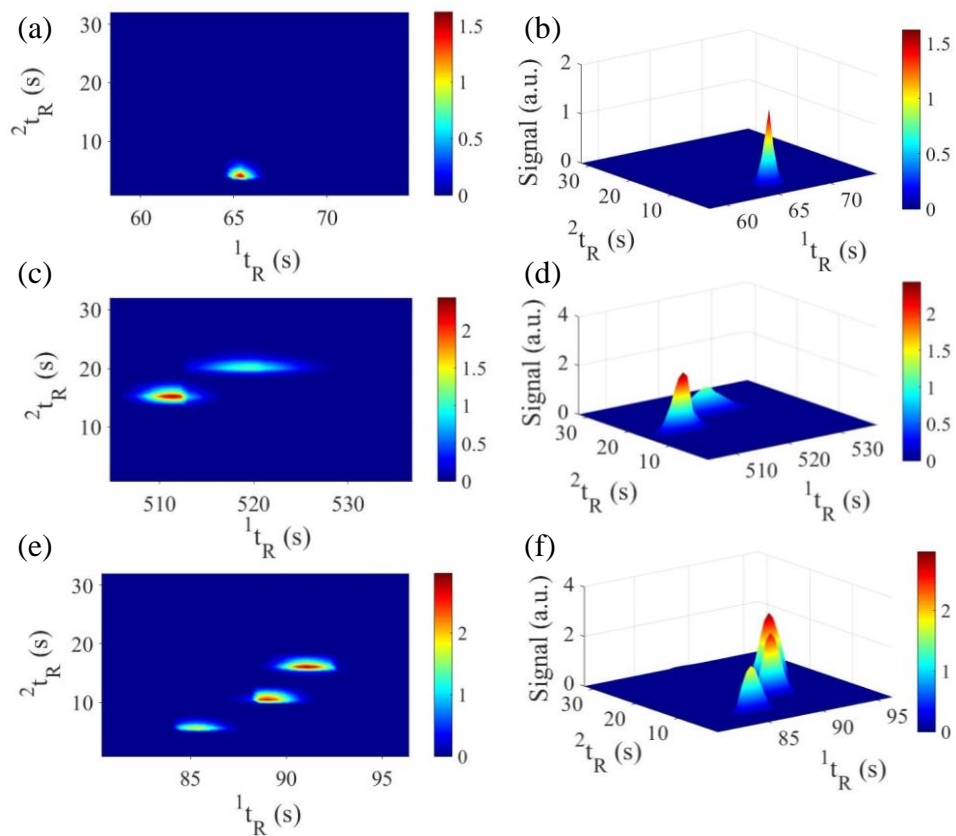


Figure S9. 2-D and 3-D contour plots of Figs. S8 and 6 using Eqs. (9) and (10). For comparison, the corresponding contour plots using the traditional method are shown in Fig. S10.

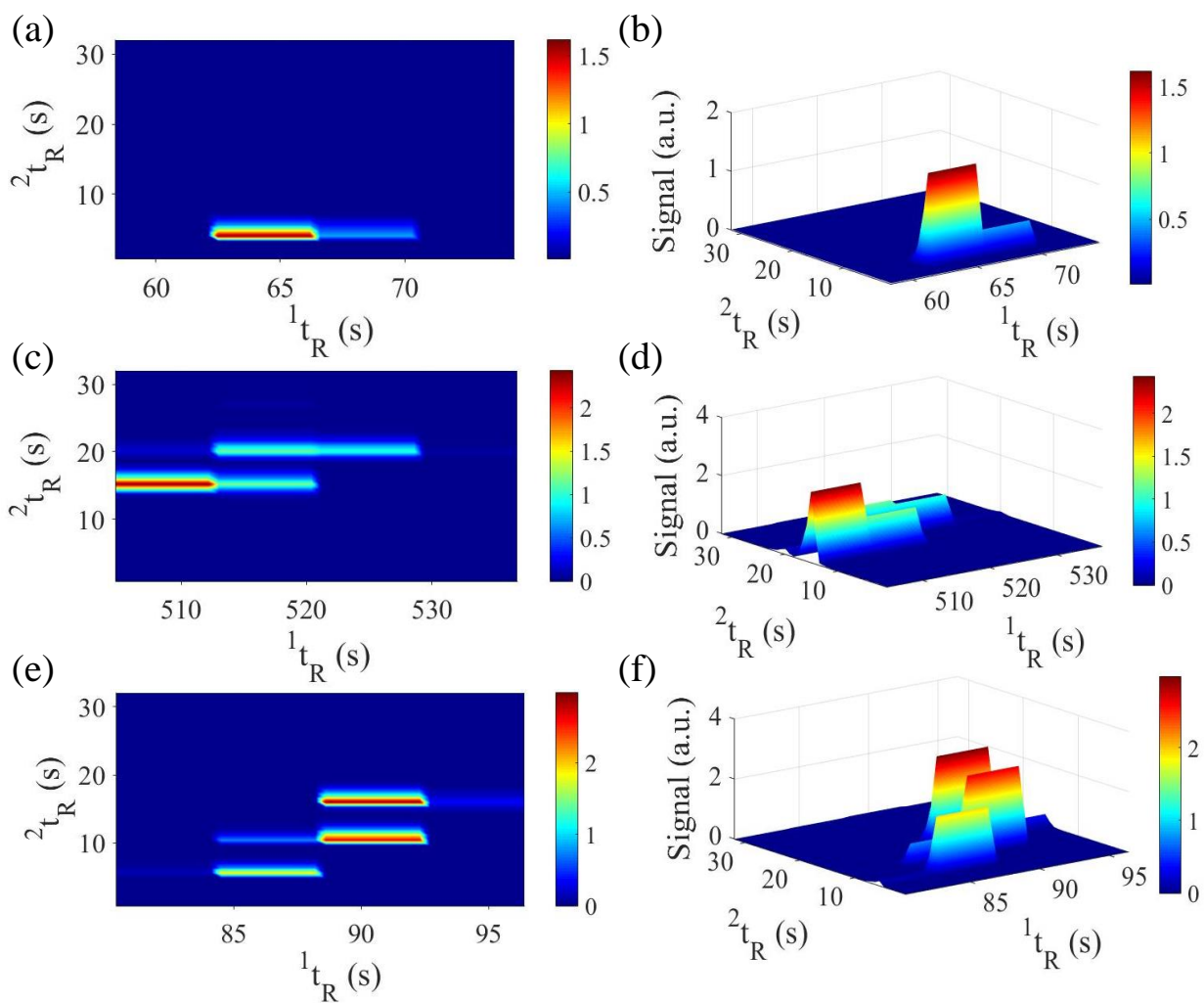


Figure S10. 2-D and 3-D contour plots corresponding to Fig. S9 using the traditional method.

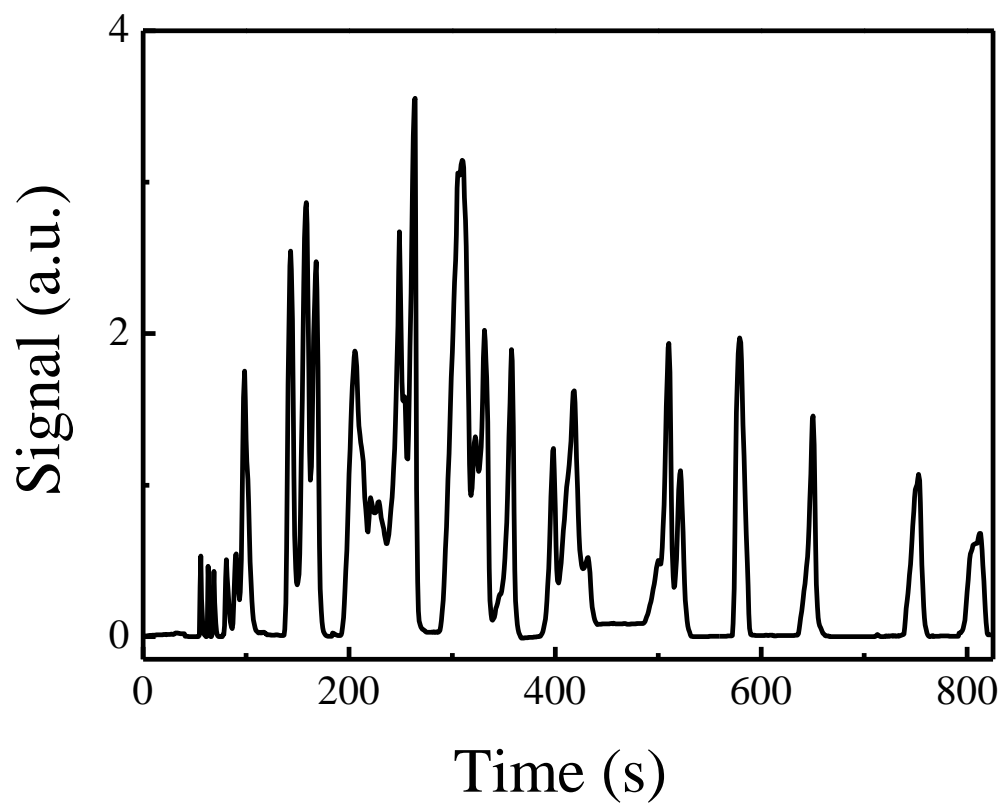


Figure S11. ^1D chromatogram of the 50 VOCs detected by PID 1.

Analyte	¹ t _R	¹ FWHM	² t _R	² FWHM	Analyte	¹ t _R	¹ FWHM	² t _R	² FWHM		
1	Hexane	56	1.5	5.7	1	26	Nonane	310	10.9	10.4	1.4
2	2-methylfuran	63	1	10.3	1	27	1,2-dichlorobenzene	323	10.2	19.2	1.6
3	Cyclohexane	70	1.7	4	1.3	28	Cumene	331	9.2	18.4	1.22
4	Benzene	80	3.2	8	1.25	29	2-ethoxyethyl acetate	333	7.2	24.7	1.2
5	Heptane	90	4	5.6	1	30	Propylbenzene	355	9.03	16	1.56
6	1,4-dioxane	97	4.2	10	0.95	31	(+)- α -pinene	357	6.18	12	1.12
7	Methylisobutylketone	102	4.5	16	1.34	32	4-ethyltoluene	396	5.8	11.9	1.4
8	Methylcyclohexane	142	4.6	5.57	1.23	33	Benzaldehyde	401	9	16	1.1
9	Toluene	144	6.91	8.8	1.12	34	2-chlorotoluene	411	7.92	22.4	1.5
10	Cyclopentanone	156	5.99	11.1	1.34	35	Mesitylene	418	11.8	20	1.2
11	2-hexanone	160	8.1	14	1.45	36	4-chlorotoluene	419	6	16	1.4
12	Hexanal	168	8.8	12.8	1.12	37	Phenol	427	5.5	12	1.34
13	Octane	168	7.1	7.9	1.1	38	2-ethyltoluene	500	10.3	19	1.31
14	Trans-2-hexen-1-al	202	10.7	12	1.23	39	1,2,4-trimethylbenzene	508	7.2	22.4	1.6
15	Chlorobenzene	206	8.37	19.1	1.33	40	3-chlorotoluene	511	5.5	15.2	1.5
16	Ethylbenzene	213	7.53	8.8	1.24	41	1,3-dichlorobenzene	519	8.5	19.8	1.6
17	Xylene	221	5.36	12	1.34	42	1-heptanol	522	8	21.6	1.29
18	1-hexanol	228	4.1	15.3	1.09	43	2-octanone	577	6	22.4	1.3
19	Cyclohexanol	236	8.7	17.5	1.2	44	Decane	581	8.3	12	1.8
20	Styrene	248	10.8	13.5	1.17	45	(R)-(+)-limonene	646	9.45	15.2	1
21	Cyclohexanone	250	11	12	1.3	46	3-octanol	650	7	21.6	1.26
22	2-heptanone	260	6.7	20	1.14	47	Nonanal	749	12.3	21.5	1.36
23	Anisol	264	11	22.3	1.2	48	Undecane	752	11	16	1.6
24	Heptanal	300	10	12.7	1.34	49	1-octen-3-ol	805	10.5	20	1.81
25	2,5-hexadione	305	11.4	16.8	1.8	50	Dodecane	812	11	16	1.57

Table S1. 50 VOCs used in experiments, and their ¹D and ²D retention time and peak width.

	Analyte	1t_R	1FWHM	2FWHM	n_{GCxGC}	$n_{GCxGC}/^1t_R$
#29	2-ethoxyethyl acetate	333 s	7.2 s	1.2 s	430	77/min
#33	Benzaldehyde	401 s	9 s	1.1 s	455	68/min
#50	Dodecane	812 s	11 s	1.57 s	526	40/min

Table S2. Calculation of the peak capacity and peak capacity production of the portable 1x4-channel GC x GC device based on Eqs. (12) and (13).