SUPPORTING INFORMATION

Improved Separation of Complex Polycyclic Aromatic Hydrocarbon Mixtures Using Novel Column Combinations in GC×GC/ToF-MS

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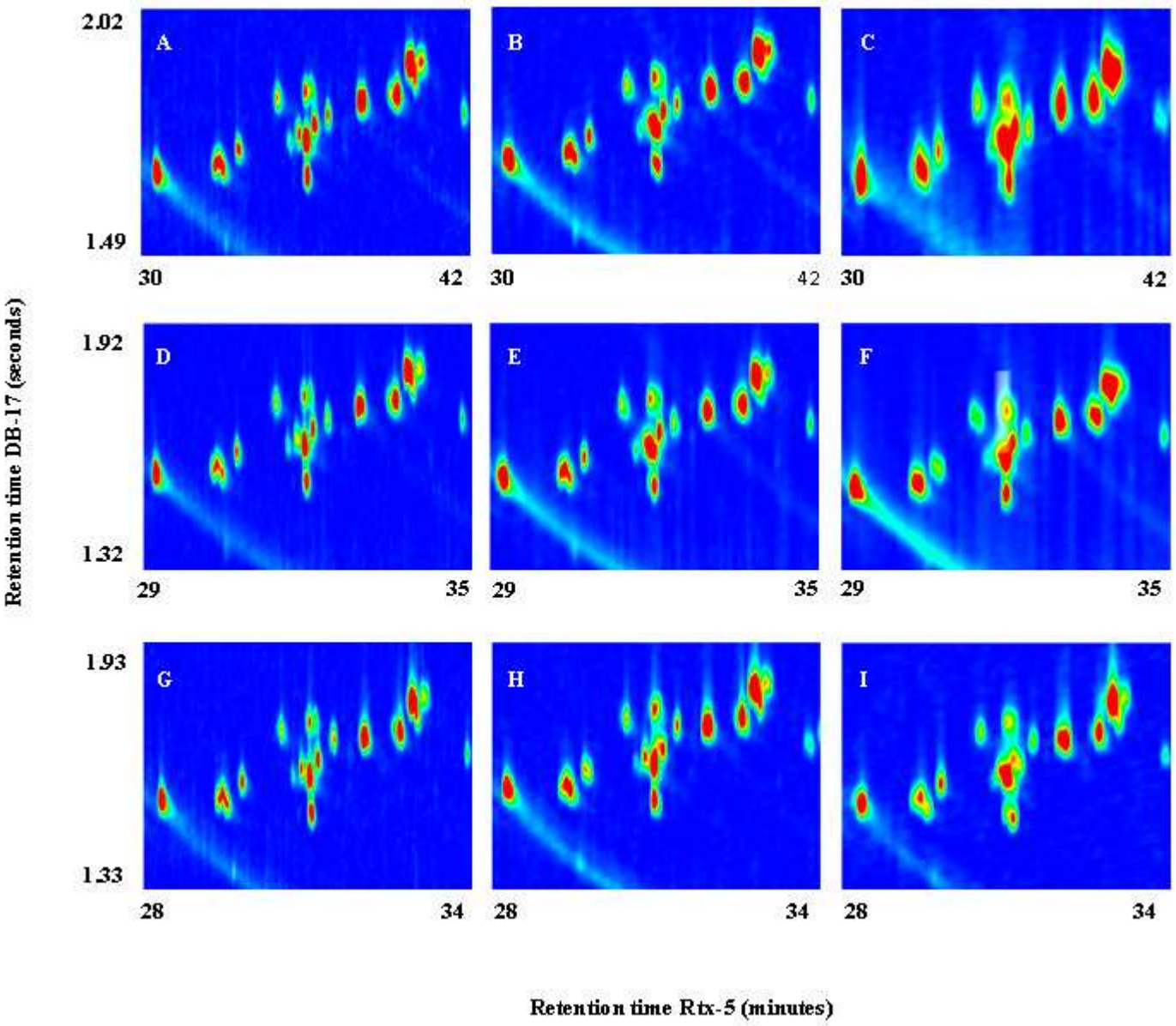

Figure S1: Chromatographic separation of PAHs using an Rtx-5ms in the first dimension and an Rxi-17 in the second dimension. A critical section of the chromatogram where more than three PAHs co-elute close together is shown. The boxes represent different conditions of separation, with modulation period (M, in seconds) and gas flow rate (F, in mL/min): A) M=3, F=0.8; B) M=5, F=0.8; C) M=7, F=0.8; D) M=3, F=1; E) M=5, F=1; F) M=7, F=1; G) M=3, F=1.2; H) M=5, F=1.2; I) M=7, F=1.2.

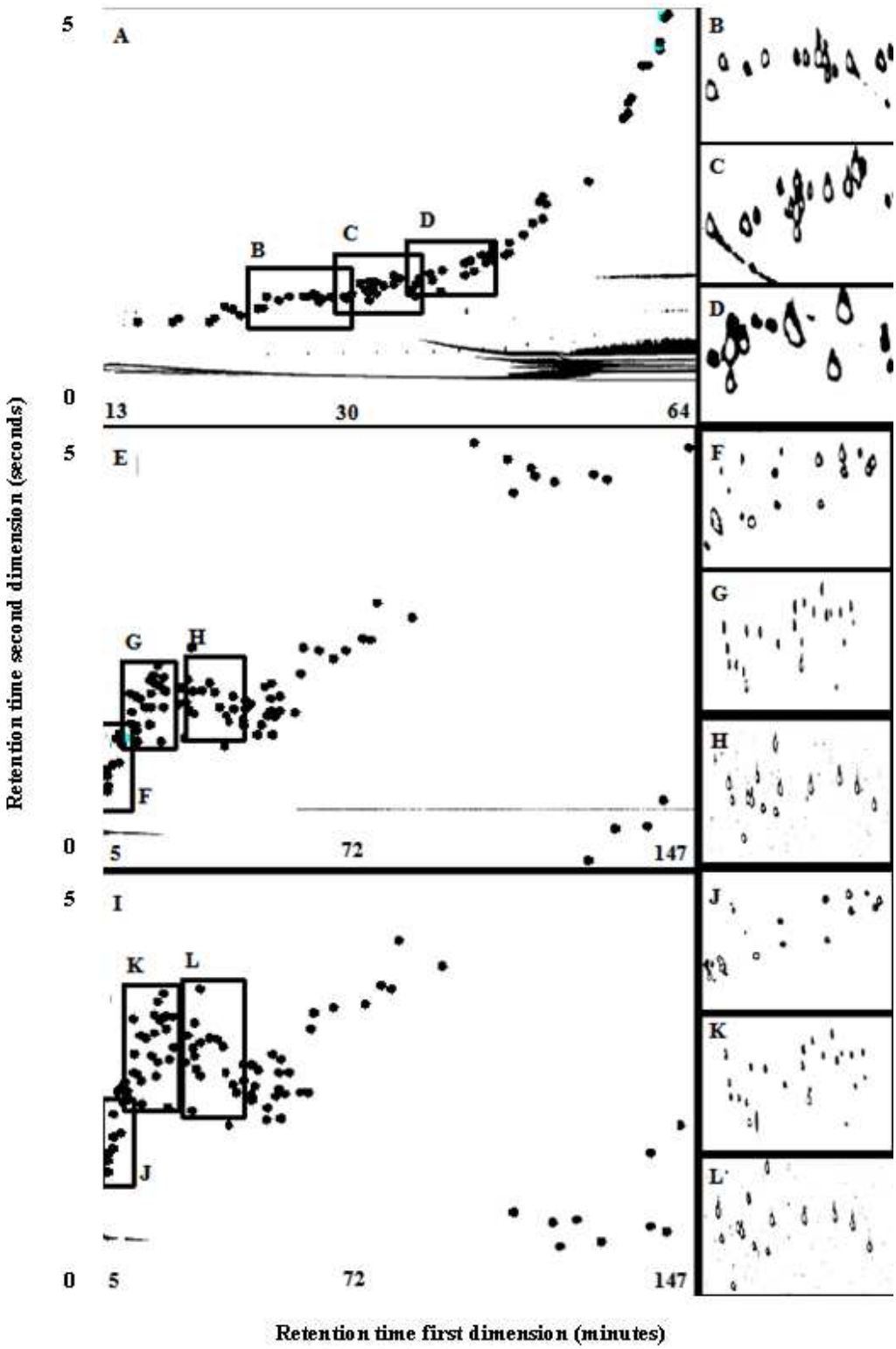

Figure S2: Black and white version of TICs showing the separation of 97 PAHs by GC×GC/ToF-MS with 3 column combinations: (A) Combination "A1" showing co-elution of PAHs at (1D 'minutes', 2D 'seconds'): (B) 23.57, 1.19 to 30.24, 1.79; (C) 28.41, 1.30 to 34.24, 1.80; (D) 33.90, 1.37 to 37.23, 1.97. (E) TIC for Combination "B", improved separation at (F) 5, 0.75 to 10.83, 1.65; (G) 10.58, 1.19 to 23.91, 2.69; (H) 22.99, 1.17 to 36.32, 2.67. (I) TIC for combination "C" further improvement in separation at: (J) 5, 1.00 to 11.67, 2.50; (K) 11.40, 1.68 to 24.75, 3.68; (L) 25.40, 1.89 to 38.73, 3.39.

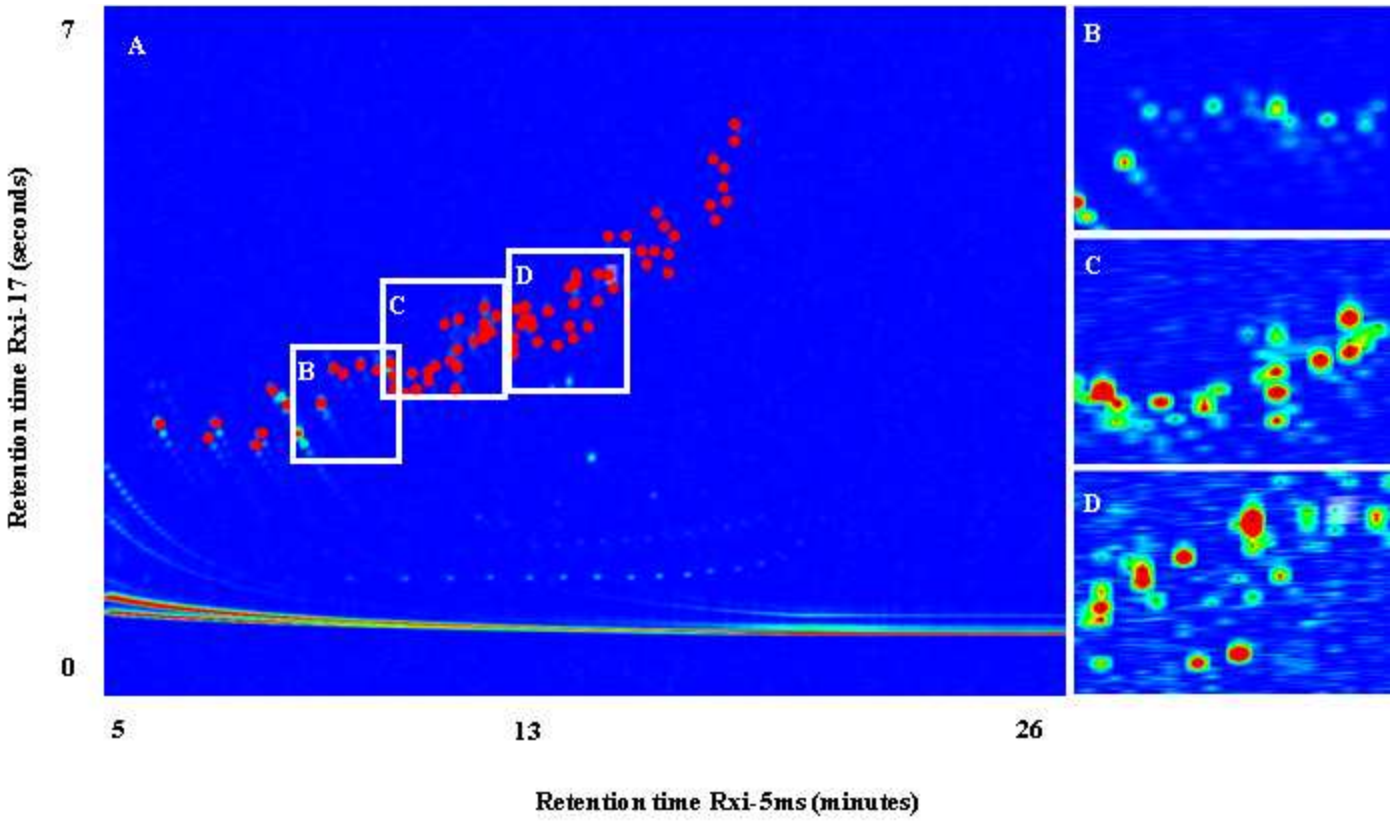

Figure S3: (A) Chromatogram showing the separation of 97 PAHs using column combination "A2". The boxes show a closer view to the separation of PAHs at different sections in the chromatogram (1D 'minutes', 2D 'seconds'): (B) 9.08, 1.47 to 12, 3.97; (C) 10.71, 2.79 to 13.21, 4.54; (D) 13.28, 2.89 to 15.78, 4.51.

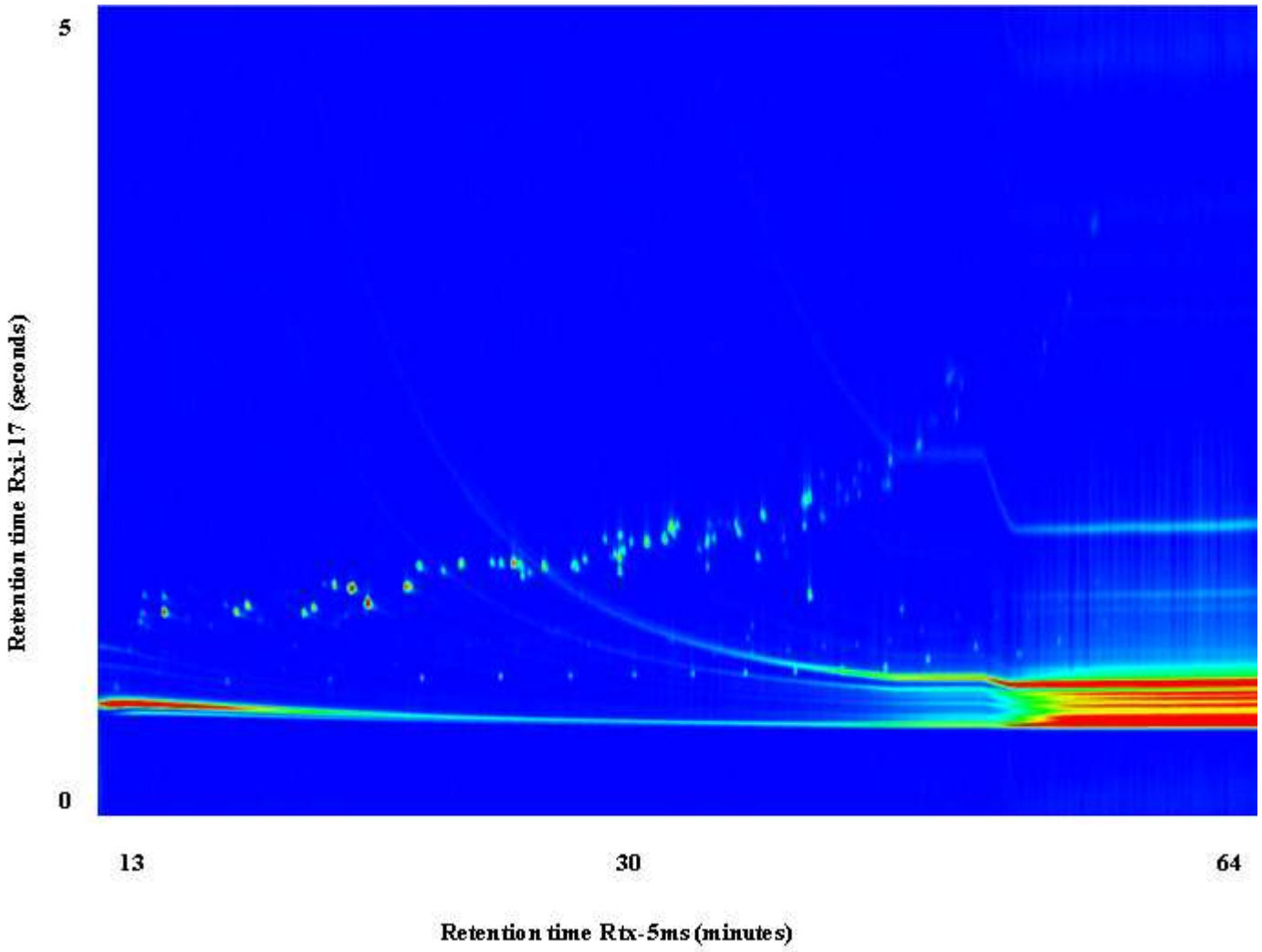

Figure S4: TIC showing the separation of 97 PAHs by GC×GC/ToF-MS using column combination "A1" (Rtx-5ms × Rxi-17)

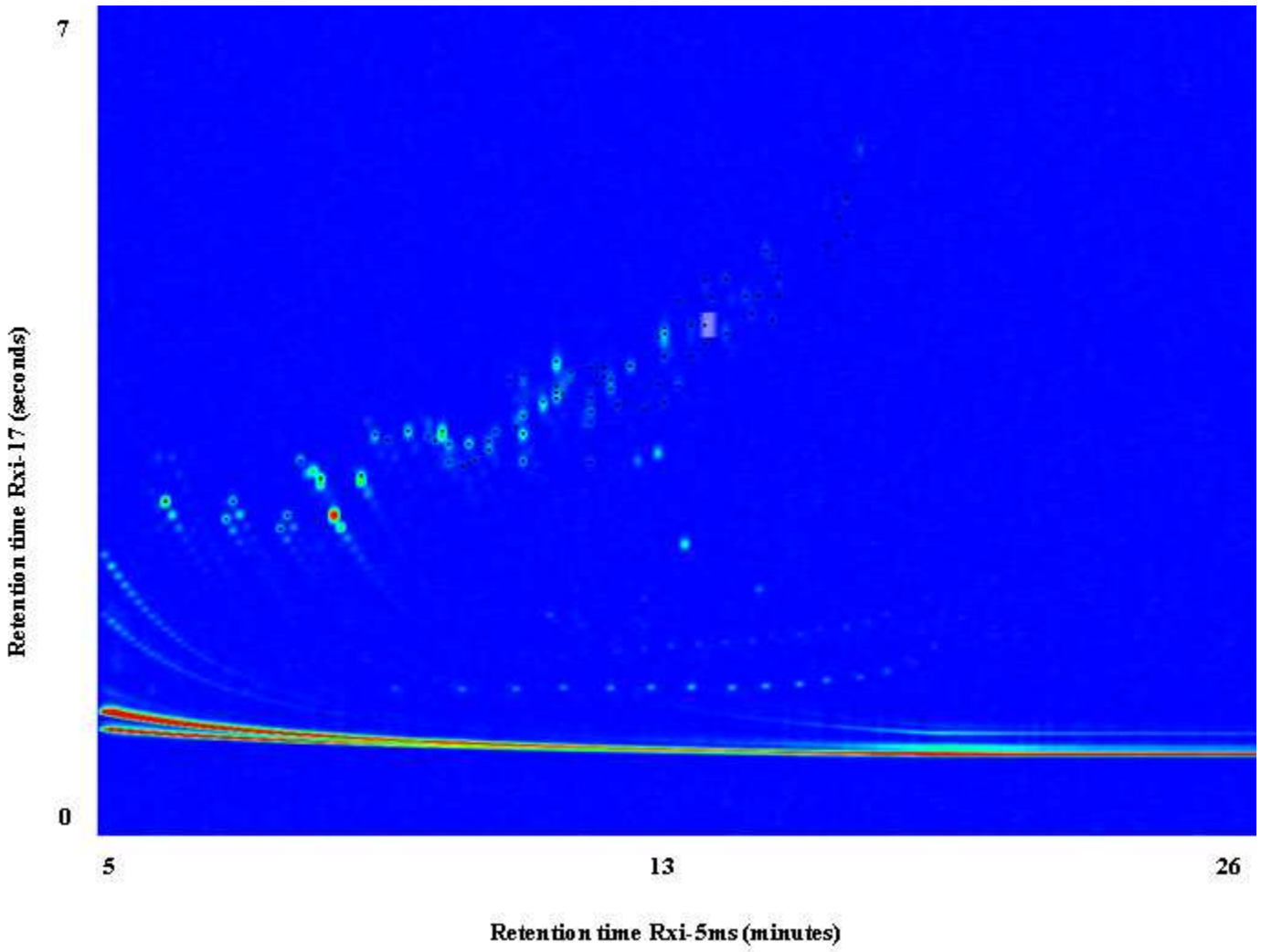

Figure S5: TIC showing the separation of 97 PAHs by GC×GC/ToF-MS using column combination "A2" (Rxi-5ms × Rxi-17)

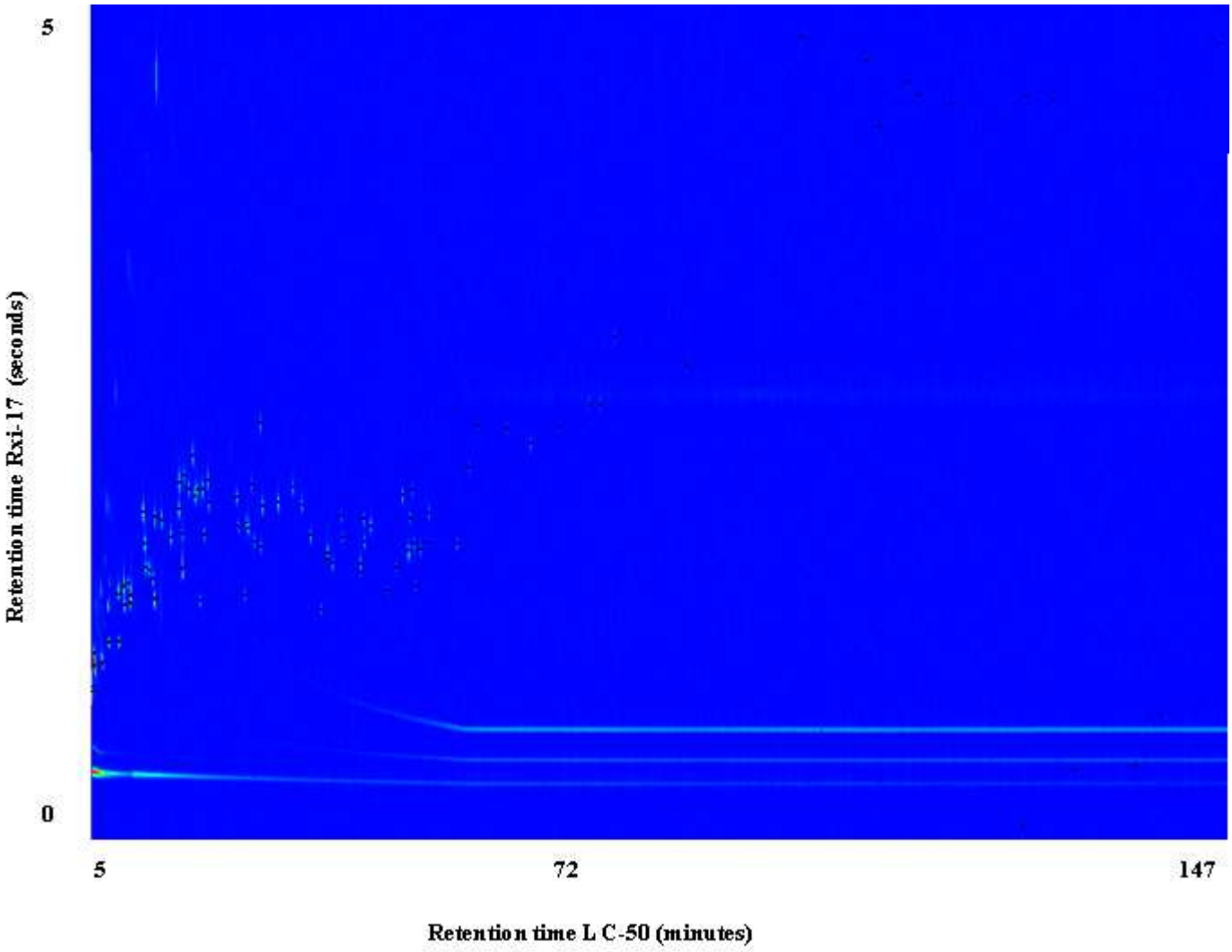

Figure S6: TIC showing the separation of 97 PAHs by GC×GC/ToF-MS using column combination "B" (LC-50 × Rxi-17)

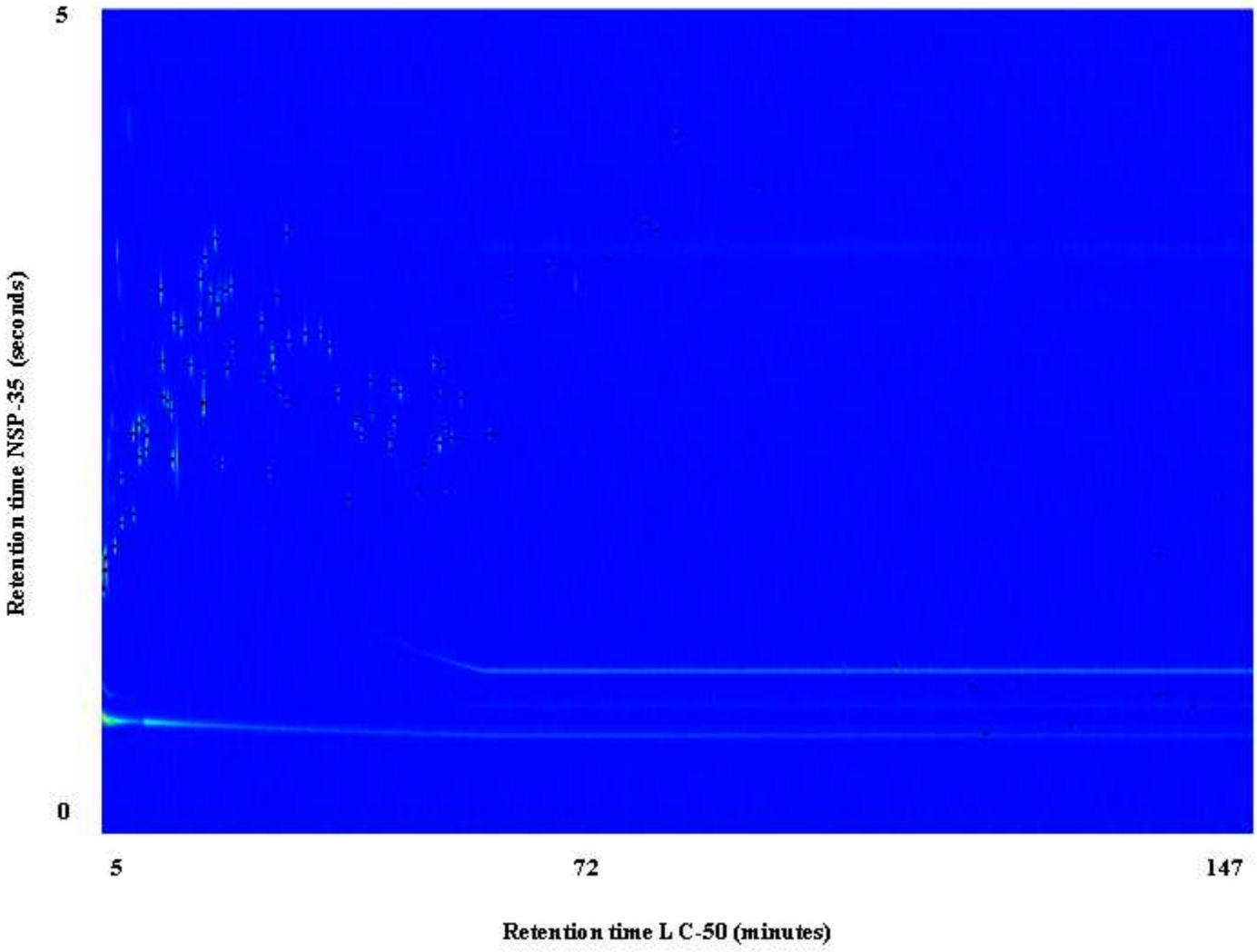

Figure S7: TIC showing the separation of 97 PAHs by GC×GC/ToF-MS using column combination "C" (LC-50 × NSP-35)

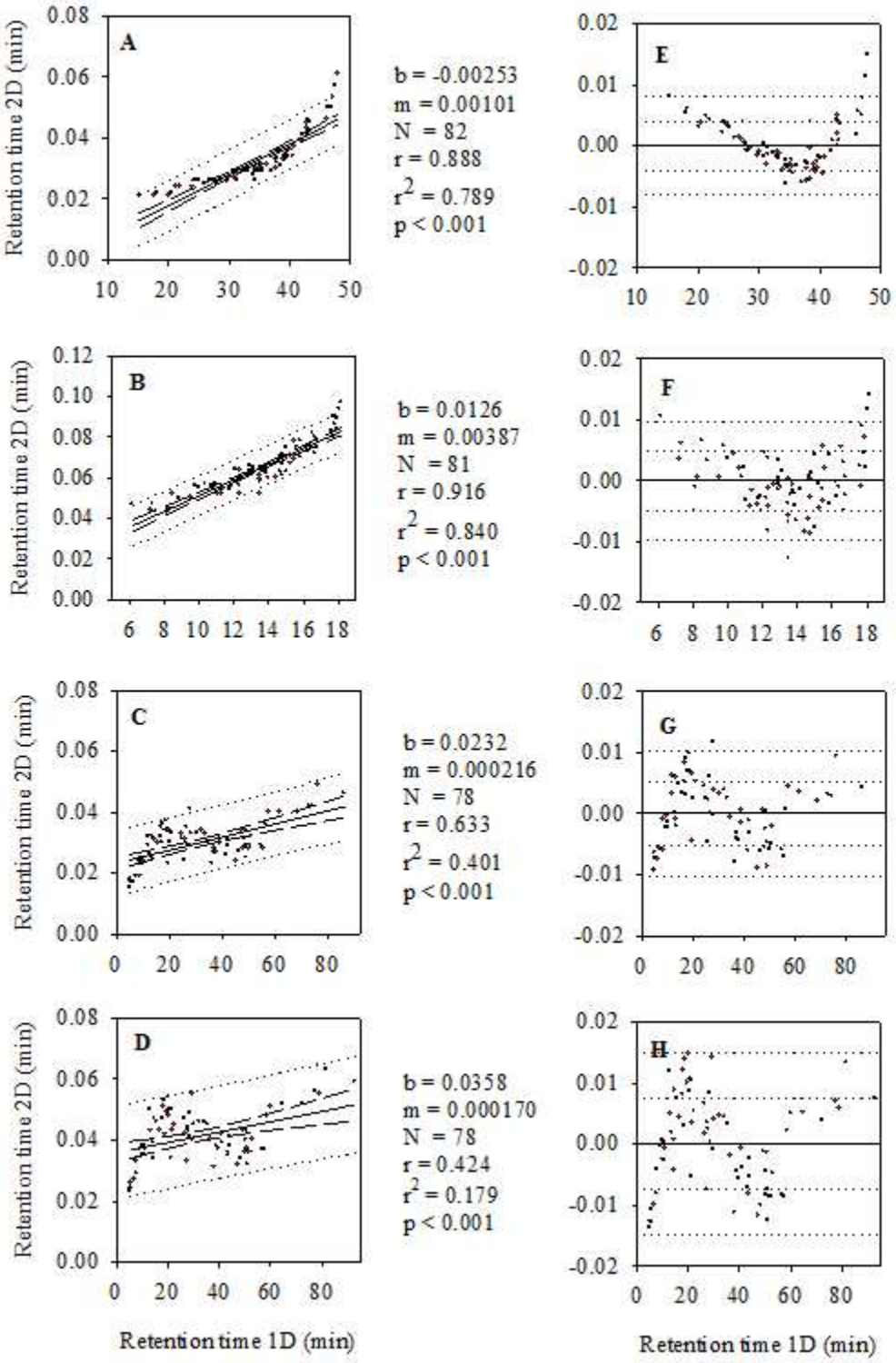

Figure S8: Correlation of 1D retention time with 2D retention time for PAHs analyzed with four different column combinations: (A) Combination "A1", (B) Combination "A2", (C) Combination "B", and (D) Combination "C". Values for the slope, y-intercept, and correlation coefficients are shown; the larger dashed lines represent the 95% CI for the regression and the smaller dashed lines the 95% CI for the population. Scatter plot residuals for the linear regression for the four different column combinations used: (E) Combination "A1", (F) Combination "A2", (G) Combination "B", and (H) Combination "C". The dashed lines represent the upper and lower control limit and upper and lower specification being 2 and 3 standard deviations, respectively.

A

0	0	0	0	0	0	0	2
0	0	0	0	0	0	0	2
0	0	0	0	0	0	1	4
0	0	0	0	0	0	7	0
0	0	0	0	0	2	4	0
0	0	0	0	1	12	1	0
0	0	5	12	16	2	0	0
3	4	2	2	0	0	0	0

Hx	2.81
Hy	2.43
Hy|x	0.85
Φ	34.68%

B

0	0	0	0	0	0	0	2
0	0	0	0	0	0	0	5
0	0	0	0	0	0	4	3
0	0	0	0	0	5	8	1
0	0	0	1	4	5	2	0
0	0	1	2	11	6	0	0
0	2	3	8	3	0	0	0
3	2	0	0	0	0	0	0

Hx	2.77
Hy	2.74
Hy|x	1.33
Φ	48.59%

C

0	0	0	0	0	0	0	2
0	0	1	0	0	0	2	0
0	1	0	0	1	1	1	0
2	9	5	1	3	1	0	0
2	4	5	4	7	0	0	0
8	0	1	4	2	0	0	0
2	1	0	1	0	0	0	0
7	0	0	0	0	0	0	0

Hx	2.65
Hy	2.55
Hy|x	1.64
Φ	64.42%

D

0	0	0	0	0	0	1	1
0	2	1	0	0	0	2	0
1	5	1	0	1	2	1	0
3	5	6	0	2	0	0	0
5	2	3	5	2	0	0	0
4	1	1	4	6	0	0	0
3	0	0	2	1	0	0	0
5	0	0	0	0	0	0	0

Hx	2.63
Hy	2.74
Hy|x	1.94
Φ	70.85%

Figure S9: Orthogonality calculation based on conditional entropy for the four different column combinations used: (A) Combination "A1", (B) Combination "A2", (C) Combination "B", (D) Combination "C". The numbers represent the number of PAHs eluting in each box of the normalized separation space and its distribution represent the distribution of PAHs in the two-dimensional space. Conditional entropy ($H(Y|X)$) and orthogonality (Φ) calculated for four column combinations are also shown.

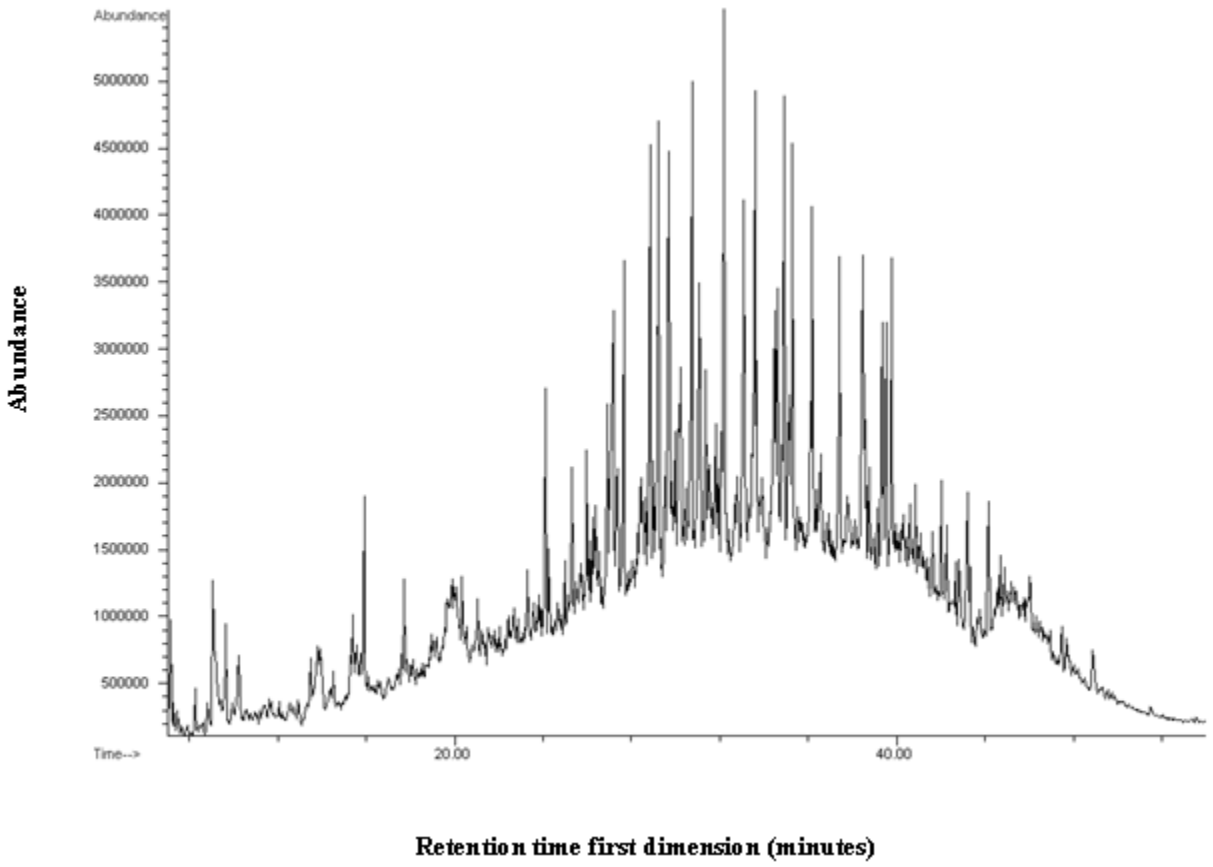

Figure S10: TIC for Beijing atmospheric $PM_{2.5}$ sample extract analyzed using a one-dimensional GC/MS with a 30m × 0.25mm × 0.25μm DB-5ms.

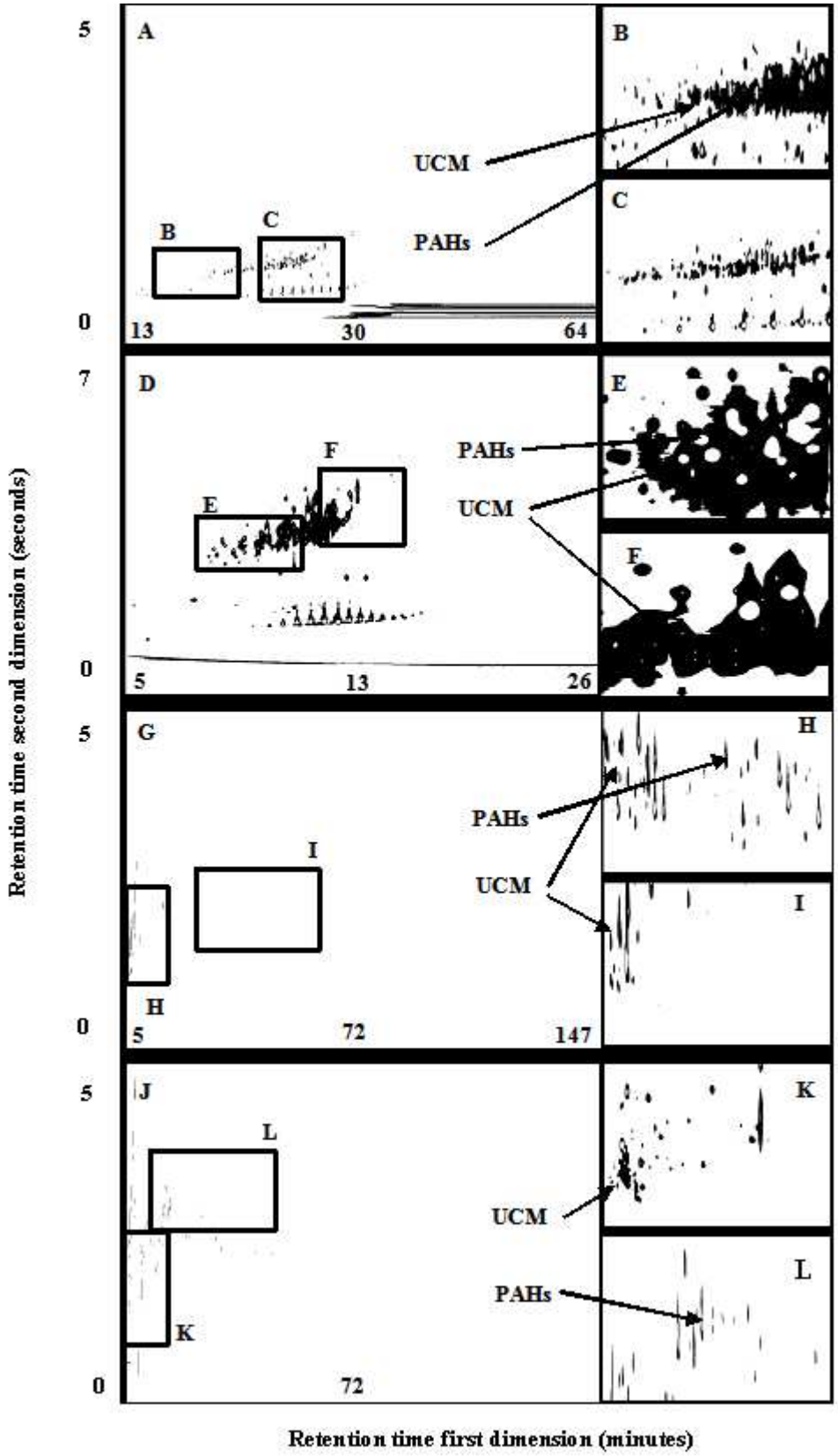

Figure S11: TIC for Beijing atmospheric $PM_{2.5}$ sample extract analyzed using the four different column combinations: (A) Combination "A1" (D) Combination "A2", (G) Combination "B", (J) Combination "C". The inner boxes show the UCM distributed in different places in the four chromatograms.

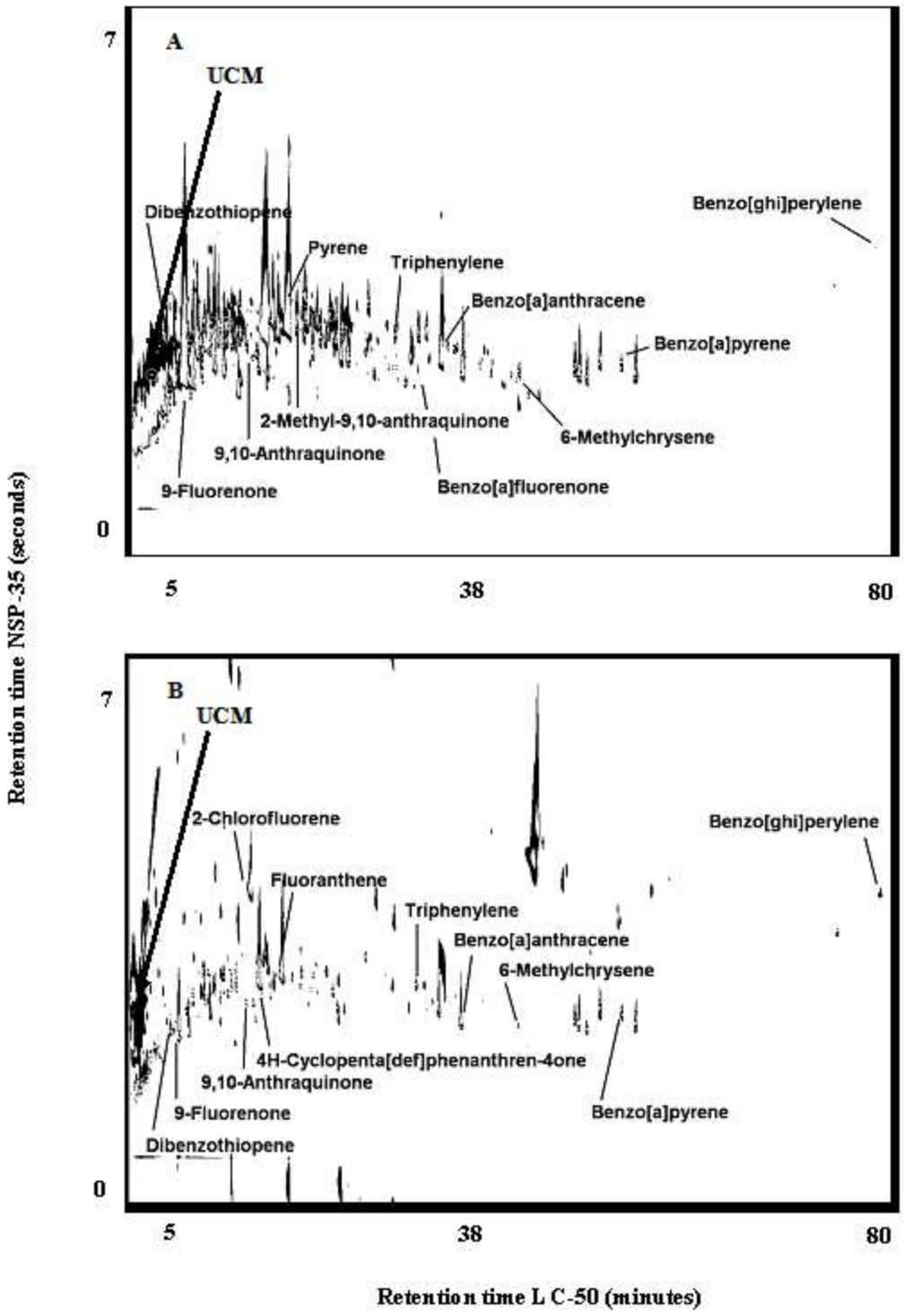

Figure S12: TIC of environmental samples analyzed using column combination "C". (A) Soil sample extract from St. Maries Creosote Superfund Site and (B) Sediment sample extarct from Portland Harbor Superfund Site. Some of the PAHs identified have been labeled.

Table S1: PAHs analyzed using a GC×GC/ToF-MS system. Parent PAHs (PPAHs), alkylated PAHs (MPAHs), chloro-PAHs (ClPAHs), bromo-PAHs (BrPAHs), nitro-PAHs (NPAHs), thio-PAHs (SPAHs), oxy-PAHs (OPAHs) and PAHs with molecular weight ≥ 300 Da (HMW PAHs) are shown

N°	Name	Abbreviation	Ions (m/z)	"A1" (min)		"A2" (min)		"B" (min)		"C" (min)	
				1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt
	PPAHs										
1	Naphthalene	NAP	128	15.33	0.021	6.17	0.047	n.d.[a]	n.d.[a]	n.d.[a]	n.d.[a]
2	Acenaphthylene	ACY	152	21.33	0.024	8.5	0.052	5.416	0.017	5.666	0.024
3	Acenaphthene	ACE	153	21.99	0.024	8.85	0.05	5.333	0.018	5.666	0.026
4	Fluorene	FLO	166	23.99	0.024	9.55	0.05	6.582	0.017	6.832	0.027
5	Phenanthrene	PHE	178	27.66	0.026	10.95	0.057	9.413	0.025	10.08	0.038
6	Anthracene	ANT	178	27.82	0.026	10.95	0.057	10.41	0.024	11.16	0.037
7	Fluoranthene	FLA	202	32.32	0.029	12.7	0.061	19.16	0.034	20.57	0.048
8	Pyrene	PYR	202	33.15	0.03	12.93	0.066	16.91	0.032	18.24	0.047
9	Benzo(a)anthracene	BaA	228	37.81	0.032	14.79	0.067	34.81	0.03	36.73	0.04
10	Chrysene	CHR	228	37.98	0.033	14.79	0.07	37.23	0.028	39.06	0.038
11	Triphenylene	TRI	228	37.98	0.033	14.79	0.07	32.4	0.034	34.31	0.046
12	Benzo(b)fluoranthene	BbF	252	41.81	0.039	16.19	0.075	48.97	0.029	50.97	0.037
13	Benzo(k)fluoranthene	BkF	252	41.89	0.039	16.31	0.073	49.88	0.028	51.88	0.036
14	Benzo(e)pyrene	BeP	252	42.81	0.045	16.54	0.082	50.97	0.032	53.13	0.04
15	Benzo(a)pyrene	BaP	252	42.98	0.046	16.66	0.08	54.8	0.029	56.88	0.037
16	Indeno(1,2,3-c,d)pyrene	IcdP	276	47.06	0.053	17.94	0.089	72.87	0.042	77.61	0.056
17	Dibenzo[a.h]anthracene	DahA	278	47.06	0.053	17.94	0.089	74.28	0.042	79.28	0.055
18	Benzo[g,h,i]perylene	BghiP	276	47.97	0.061	18.18	0.097	76.2	0.049	81.77	0.063
19	Picene	PIC	278	47.56	0.057	18.06	0.094	86.19	0.046	92.85	0.059

N°	Name	Abbreviation	Ions (m/z)	"A1" (min)		"A2" (min)		"B" (min)		"C" (min)	
				1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt
	MAPHs										
20	1-Methylnaphthalene	1 met NAP	142	17.91	0.021	7.22	0.044	n.d.[a]	n.d.[a]	n.d.[a]	n.d.[a]
21	2-Methylnaphthalene	2 met NAP	142	18.25	0.022	7.33	0.047	n.d.[a]	n.d.[a]	n.d.[a]	n.d.[a]
22	Retene	RET	219	34.4	0.026	13.51	0.052	17.57	0.036	18.91	0.053
23	1,3-Dimethylnaphthalene	1,3 met NAP	156	20.24	0.021	8.15	0.043	5.08[b]	0.015[b]	5.167[b]	0.024[b]
24	2,6-Dimethylnaphthalene	2,6 met NAP	156	20.58	0.022	8.26	0.045	5.17[b]	0.015[b]	5.250[b]	0.023[b]
25	2-Methylanthracene	2 met ANT	192	29.82	0.026	11.76	0.054	13.41	0.025	14.41	0.039
26	1-Methylphenanthrene	1 met PHE	192	30.07	0.027	11.88	0.056	12.24	0.029	13.24	0.043
27	2,3-Dimethylphenanthrene	2,3 met PHE	206	31.32	0.026	12.35	0.052	11.99	0.032	12.99	0.05
28	6-Methylchrysene	6 met CHR	242	39.73	0.034	15.49	0.069	39.06	0.032	40.97	0.042
29	1-Methylpyrene	1 met PYR	216	35.4	0.031	13.86	0.064	24.73	0.033	26.48	0.047
	Cl PAHs										
30	2-Chloroanthracene	2 Cl ANT	212	31.49	0.028	12.35	0.056	13.58	0.024	14.74	0.047
31	9-Chloroanthracene	9 Cl ANT	212	31.56	0.028	12.35	0.059	14.49	0.031	15.74	0.046
32	9,10-Dichloroanthracene	9,10 Cl ANT	246	34.4	0.029	13.51	0.058	19.41	0.034	20.91	0.05
33	1,9-Dichlorophenanthrene	1,9 Cl PHE	246	34.65	0.029	13.51	0.059	20.07	0.034	21.57	0.05
34	3,9-Dichlorophenanthrene	3,9 Cl PHE	246	34.07	0.028	13.51	0.061	18.82	0.037	20.24	0.054
35	9-Chlorofluorene	9 Cl FLO	200	27.91	0.025	11.06	0.052	10.25	0.023	11	0.035
36	1-Chloropyrene	1 Cl PYR	236	36.32	0.031	14.21	0.066	28.32	0.033	30.15	0.045
37	3-Chlorofluoranthene	3 Cl FLA	236	35.48	0.03	13.86	0.062	26.07	0.031	27.82	0.044

N°	Name	Abbreviation	Ions (m/z)	"A1" (min)		"A2" (min)		"B" (min)		"C" (min)	
				1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt
38	8-Chlorofluoranthene	8 Cl FLA	236	35.57	0.029	13.98	0.06	26.32	0.031	28.07	0.043
39	3,9,10-Trichloropenanthrene	3,9,10ClPHE	280	37.07	0.029	14.44	0.06	26.73	0.035	28.57	0.049
40	1,3-Dichlorofluorathene	1,3 Cl FLA	270	37.81	0.03	14.68	0.063	30.40[c]	0.033[c]	32.31[c]	0.046[c]
41	3,8-Dichlorofluoranthene	3,8 Cl FLA	270	38.51	0.031	14.79	0.061	37.14[c]	0.027[c]	39.81[c]	0.037[c]
42	3,4-Dichlorofluoranthene	3,4 Cl FLA	270	39.31	0.033	15.03	0.063	37.81[c]	0.027[c]	43.55[c]	0.036[c]
43	7-Chlorobenzo(a)anthracene	7 Cl BaA	262	40.56	0.034	15.84	0.07	42.14	0.031	44.14	0.041
44	3-Chlorobenzanthrone	3 Cl Benzan	264	40.81	0.037	15.84	0.078	48.22	0.028	50.3	0.036
45	6,12-Dichlorochrysene	6,12 Cl CHR	296	43.14	0.042	16.66	0.072	47.39	0.034	49.47	0.043
46	7,12-Dichlorobenzo(a)anthracene	7,12 Cl BaA	296	43.31	0.045	16.78	0.075	48.72	0.034	50.8	0.043
	BrPAHs										
47	2-Bromofluorene	2 Br FLO	244	29.74	0.026	11.76	0.055	12.91	0.026	13.91	0.04
48	9-Bromophenanthrene	9 Br PHE	256	32.9	0.029	12.93	0.061	16.99	0.035	18.32	0.051
49	9-Bromoanthracene	9 Br ANT	256	33.23	0.029	13.05	0.062	18.24	0.034	19.66	0.049
50	9,10-Dibromoanthracene	9,10 Br ANT	176	37.73	0.033	14.68	0.07	27.98	0.029	29.82	0.055
51	1-Bromopyrene	1 Br PYR	280	37.98	0.033	14.79	0.071	33.65	0.033	35.56	0.045
52	7-Bromobenzo(a)anthracene	7 Br BaA	226	42.94	0.041	17.59	0.083	48.38	0.031	50.47	0.04
53	7,11-Dibromobenzo(a)anthracene	7,11 Br BaA	226	46.14	0.046	17.71	0.08	56.46[d]	0.036[d]	58.88[d]	0.048[d]
54	7,12-Dibromobenzo(a)anthracene	7,12 Br BaA	226	46.31	0.05	17.71	0.09	57.54[d]	0.04[d]	60.13[d]	0.051[d]
55	4,7-Dibromobenzo(a)anthracene	4,7 Br BaA	226	46.31	0.05	17.83	0.086	61.62[d]	0.04d	64.79[d]	0.052[d]
56	5,7-Dibromobenzo(a)anthracene	5,7 Br BaA	226	46.89	0.05	17.94	0.084	68.62[d]	0.04d	72.70[d]	0.052[d]

N°	Name	Abbreviation	Ions (m/z)	"A1" (min)		"A2" (min)		"B" (min)		"C" (min)	
				1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt
	NPAHs										
57	1-Nitropyrene	1 N PYR	201	39.81	0.036	15.49	0.078	46.47	0.027	48.47	0.034
58	2-Nitropyrene	2 N PYR	201	40.06	0.036	15.61	0.075	49.13	0.025	51.13	0.032
59	2-Nitrofluoranthene	2 N FLA	247	38.98	0.033	15.26	0.067	41.72	0.026	43.72	0.035
60	3-Nitrobenzanthrone	3 N Benzan	200	43.28	0.045	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
61	2-Nitrofluorene	2 N FLO	165	24.69	0.026	12.93	0.063	25.82	0.024	27.48	0.033
62	3-Nitrofluoranthene	3 N FLA	247	39.06	0.034	15.26	0.071	45.39	0.024	47.39	0.032
63	2-Nitroanthracene	2 N ANT	223	35.15	0.03	13.75	0.065	36.31	0.023	38.14	0.031
64	3-Nitrophenanthrene	3 N PHE	223	34.48	0.03	13.63	0.063	27.98	0.041	29.82	0.04
65	9-Nitroanthracene	9 N ANT	176	33.4	0.03	13.16	0.065	20.99	0.033	22.49	0.045
66	5-Nitroacenaphthalene	5 N ACE	152	31.4	0.029	12.35	0.064	17.41	0.03	18.74	0.042
67	1-Nitronaphthalene	1 N NAP	127	24.32	0.026	9.78	0.056	8.75	0.019	7.748	0.029
68	2-Nitronaphthalene	2 N NAP	127	25.16	0.026	10.01	0.055	7.33	0.019	7.748	0.033
69	6-Nitrochrysene	6 N CHR	273	42.91	0.043	16.43	0.075	55.55	0.028	57.71	0.037
70	9-Nitrophenanthrene	9 N PHE	165	34.4	0.03	13.51	0.065	24.99	0.031	26.73	0.042
71	2-Nitrobiphenyl	2 N BiPhe	152	25.96	0.025	10.36	0.057	13.58	0.032	14.58	0.034
72	3-Nitrobiphenyl	3 N BiPhe	152	28.16	0.025	11.3	0.052	10	0.025	10.75	0.038
73	4-Nitrobiphenyl	4 N BiPhe	152	28.65	0.026	11.41	0.055	10	0.025	10.75	0.038
74	7-Nitrobenz(a)anthracene	7 N BaA	215	42.14	0.041	16.78	0.078	50.72	0.029	52.71	0.036
75	3-Nitrodibenzofuran	3 N Diben	213	30.85	0.027	12.23	0.057	19.82	0.023	21.24	0.034

N°	Name	Abbreviation	Ions (m/z)	"A1" (min)		"A2" (min)		"B" (min)		"C" (min)	
				1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt
	SPAHs										
76	Dibenzothiophene	Dibenzoth	184	27.16	0.026	10.83	0.055	8.66	0.024	9.247	0.037
77	2-Nitrodibenzothiophene	2 N Dib	229	35.31	0.029	13.75	0.064	27.15	0.029	28.9	0.041
	OPAHs										
78	9,10-Anthraquinone	9,10 ANTq	208	30.82	0.029	12.11	0.064	15.83	0.03	16.99	0.043
79	9-Fluorenone	9 Fluo	180	26.82	0.026	10.71	0.056	9.5	0.023	10.16	0.035
80	2-Methyl-9,10-anthraquinone	2 met ANTq	222	32.9	0.029	12.93	0.062	20.32	0.03	21.82	0.043
81	Benzanthrone	Benzan	230	38.4	0.036	15.03	0.075	39.22	0.03	41.22	0.039
82	Benz(a)anthracene-7,12-dione	BaAq	258	39.56	0.035	15.49	0.071	42.22	0.029	44.22	0.038
	HMW PAHs										
83	Coronene	COR	300	53.22	0.078	n.d.[g]	n.d.[g]	147.23	0.007	n.d.	n.d.
84	Naphtho[1,2-b]fluoranthene	DahPYR	302	51.22	0.063	n.d.[g]	n.d.[g]	101.43[e]	0.08[e]	111.3[e]	0.016[e]
85	Naphtho[2,3-j]fluoranthene	DaePYR	302	51.47	0.064	n.d.[g]	n.d.[g]	110.25[e]	0.078[e]	121.6[e]	0.014[e]
86	Dibenzo[a,e]fluoranthene	DalPYR	302	51.55	0.065	n.d.[g]	n.d.[g]	111.92[e]	0.071[e]	123.3[e]	0.01[e]
87	Dibenzo[b,k]fluoranthene	DaiPYR	302	n.d.[f]	n.d.[f]	n.d.[g]	n.d.[g]	115.83[e]	0.076	127.9[e]	0.014[e]
88	Dibenzo[a,k]fluoranthene	N23aPYR	302	n.d.[f]	n.d.[f]	n.d.[g]	n.d.[g]	117.33[e]	0.074[e]	134.6[e]	0.01[e]
89	Dibenzo[j,l]fluoranthene	N23ePYR	302	51.64	0.067	n.d.[g]	n.d.[g]	121.75[e]	0.074[e]	146.3[e]	0.013[e]
90	Dibenzo[a,l]pyrene	DbkFLA	302	51.8	0.069	n.d.[g]	n.d.[g]	131.82[e]	0.074[e]	146.3e	0.026[e]
91	Naphtho[2,3-k]fluoranthene	N12bFLA	302	n.d.[f]	n.d.[f]	n.d.[g]	n.d.[g]	131.90[e]	0.002[e]	150.97[e]	0.012[e]

N°	Name	Abbreviation	Ions (m/z)	"A1" (min)		"A2" (min)		"B" (min)		"C" (min)	
				1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt	1D Rt	2D Rt
92	Naphtho[2,3-e]pyrene	DelPYR	302	53.8	0.069	n.d.[g]	n.d.[g]	135.73[e]	0.074e	154.97[e]	0.031[e]
93	Dibenzo[a,e]pyrene	DakFLA	302	53.64	0.073	n.d.[g]	n.d.[g]	138.90[e]	0.007[e]	164.38[e]	0.034[e]
94	Dibenzo[e,l]pyrene	DjlFLA	302	52.7	0.073	n.d.[g]	n.d.[g]	150.72[e]	0.012[e]	n.d.[f]	n.d.[f]
95	Naphtho[2,3-a]pyrene	DaeFLA	302	54.08	0.077	n.d.[g]	n.d.[g]	157.97[e]	0.079[e]	n.d.[f]	n.d.[f]
96	Benzo[b]perylene	N23jFLA	302	55.38	0.082	n.d.[g]	n.d.[g]	n.d.[f]	n.d.[f]	n.d.[f]	n.d.[f]
97	Dibenzo[a,h]pyrene	BbPER	302	54.75	0.082	n.d.[g]	n.d.[g]	n.d.[f]	n.d.[f]	n.d.[f]	n.d.[f]

n.d.: PAHs non detected, [a] PAHs eluted with the solvent line in less than 5 min, [b] Compounds share the same ions (146, 251 m/z), order may be reverted, [c] Compounds share the same ion (270 m/z), order may be reverted, [d] Compounds share the same ions (226, 386 m/z), order may be reverted, [e] Compounds share the same ions (302 m/z), order may be reverted, [f] not detected due to possible co-elution, [g] few broad signals detected, no compound was assigned.

Table S2: Retention times of co-eluting slices for some critical pairs of PAHs analyzed in a GC×GC/ToF-MS with three different column combinations.

	PAHs pairs	1D Rt	2D Rt	1D Rt	2D Rt	Δ1D	Δ2D
Combination "A1"	CHR - TRI	2278.8	1.98	2278.8	1.98	0	0
	BbF - BkF	2508.69	2.32	2508.69	2.32	0	0
	IcdP - DahA	2823.45	3.192	2823.45	3.165	0	0.027
	2 Cl ANT - 9 Cl ANT	1889.16	1.654	1889.16	1.654	0	0
	3 Cl FLA - 8 Cl FLA	2128.97	1.787	2128.97	1.787	0	0
	7,12 Br BaA - 4,7 Br BaA	2778.48	3.027	2778.48	3.027	0	0
Combination "A2"	CHR - TRI	887.4	4.2	887.4	4.2	0	0
	BbF - BkF	971.4	4.5	971.4	4.38	0	0.12
	IcdP - DahA	1076.4	5.34	1076.4	5.34	0	0
	2 Cl ANT - 9 Cl ANT	741	3.36	741	3.54	0	0.18
	3 Cl FLA - 8 Cl FLA	831.6	3.72	831.6	3.6	0	0.12
	7,12 Br BaA - 4,7 Br BaA	1062.6	5.4	1062.6	5.16	0	0.24
Combination "B"	CHR - TRI	2233.8	1.68	1944	2.04	289.8	0.36
	BbF - BkF	2938.2	1.74	2992.8	1.68	54.6	0.06
	IcdP - DahA	4372.2	2.52	4456.8	2.52	84.6	0
	2 Cl ANT - 9 Cl ANT	814.8	1.44	869.4	1.44	54.6	0
	3 Cl FLA - 8 Cl FLA	1564.2	1.86	1579.2	1.86	15	0
	7,12 Br BaA - 4,7 Br BaA	3452.4	2.4	3697.2	2.4	244.8	0
Combination "C"	CHR - TRI	2343.6	2.28	2058.6	2.76	285	0.48
	BbF - BkF	3058.2	2.22	3112.8	2.16	54.6	0.06
	IcdP - DahA	4656.6	3.36	4756.8	3.3	100.2	0.06
	2 Cl ANT - 9 Cl ANT	884.4	2.82	944.4	2.76	60	0.06
	3 Cl FLA - 8 Cl FLA	1669.2	2.64	1684.2	2.58	15	0.06
	7,12 Br BaA - 4,7 Br BaA	3607.8	3.06	3887.4	3.12	279.6	0.06