Separation of 54 PAHs on an Agilent J&W Select PAH GC Column

Application Note

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Introduction

Polycyclic aromatic hydrocarbons (PAHs) are compounds that contain two or more aromatic rings. They are formed during incomplete combustion or pyrolysis of organic matter, industrial processes and cooking and food processing. PAHs are therefore analyzed in environmental and food samples.

The difficulty in analyzing PAHs lies in separating PAH isomers. These isomers have the same chemical structure and same ion fragment and therefore cannot be separated by mass spectrometers. The Select PAH capillary column has enhanced selectivity towards PAHs, separating the isomers and enabling accurate PAH analysis. This application note describes an optimized oven program for the Select PAH column. In PAH analysis, there is a difference between the European (EU) and American (EPA) legislation. The legislations both describe a different set of PAHs and address different matrix origins. Table 1 lists the PAH regulated by EU and EPA legislation, including the potential interferences. For this application note, we chose a sample containing 54 PAHs to demonstrate the unique selectivity of the Select PAH.

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Conditions

Technique:	GC/MS, Triple Quad
Column:	Select PAH, 30 m x 0.25 mm, df=0.15 µm (part number CP7462)
Sample Conc:	approx 0.1-0.3 µg/mL
Injection Volume:	1 µL
Temperature:	70 °C (0.7 min), 85 °C/min, 180 °C, 3 °C/min, 230 °C (7 min), 28 °C/min, 280 °C (10 min), 14 °C/min, 350 °C (3 min)
Carrier Gas:	Helium, constant flow 2 mL/min
Injector:	300 °C, Splitless mode, 1 min @ 50 mL/min
Detector:	Triple Quad, EI in SIM mode, ion source 275°C, transfer line 300°C

Results and Discussion

Figure 1 shows the separation of all 54 PAH isomers and Figures 2-6 reveal the finer details.

When performing this analysis, there are three sets of peaks that are difficult to resolve. The first set, comprising benzo[a]anthracene, cyclopenta[c,d]pyrene, chrysene and triphenylene, has different masses, m/z 226 and 228. The compounds with m/z 228 also contain some m/z 226, making it difficult to resolve this set by MS alone. The same problem occurs when separating indeno[1,2,3-c,d]pyrene, benzo[b]triphenylene and dibenzo[a,h]anthracene with m/z 276 and 278. The third set of PAH isomers difficult to resolve are the benzofluoranthenes. These three isomers, benzo[b] fluoranthene, benzo[j]fluoranthene and benzo[k]fluoranthene, have the same mass and cannot be resolved by MS.

However, the unique selectivity of Select PAH resolves all the PAH isomers and enables accurate quantification of all PAHs.

Peaks 1 and 2 show some tailing, which can be resolved by further optimization of the splitless injection conditions.

Conclusion

The Select PAH column resolves 54 PAHs in a single GC/MS run, including the hard to separate PAH isomers. The optimized GC oven program performs the run time in less than 45 minutes.

Table 1. Peak Identification for Figure 1

Peak	MW	Compound	EPA 610	SFC & EFSA PAHs (15+1)	CAS
1	136	Naphthalene-d8			1146-65-2
2	128	Naphthalene	X		91-20-3
3	142	2-Methylnaphthalene			91-57-6
4	142	1-Methylnaphthalene			90-12-0
5	152	Acenaphthylene	X		208-96-8
6	164	Acenaphthene-d10			15067-26-2
7	154	Acenaphthene	X		83-32-9
8	166	Fluorene	X		86-73-7
9	188	Phenanthrene-d10			1517-22-2
10	178	Phenanthrene	X		85-01-8
11	178	Anthracene	X		120-12-7
12	202	Fluoranthene	X		206-44-0
13	202	Pyrene	X		129-00-0
14	216	Benzo[a]fluorene			238-84-6
15	216	Benzo[b]fluorene			243-17-4
16	216	7H-Benzo[c]fluorene		X	205-12-9
17	234	Benzo[b]naphto[2,1-d]-thiophene			239-35-0
18	226	Benzo[g,h,i]-fluoranthene			203-12-3
19	228	Benzo[c]phenanthrene			195-19-7
20	228	Benz[a]anthracene	X	X	56-55-3
21	226	Cyclopenta[c,d]pyrene		X	27208-37-3
22	240	Chrysene-d10			1719-03-5
23	228	Triphenylene			217-59-4
24	228	Chrysene	X	X	218-01-9
25	242	6-Methylchrysene			175-85-7
26	242	5-Methylchrysene		X	3697-24-3
27	252	Benzo[b]fluoranthene	X	X	205-99-2
28	252	Benzo[k]fluoranthene	X	X	207-08-9
29	252	Benzo[j]fluoranthene		X	205-82-3
30	252	Benzo[a]fluoranthene			203-33-8
31	252	Benzo[e]pyrene			192-97-2
32	252	Benzo[a]pyrene	X	X	50-32-8
33	264	Perylene-d12			1520-96-3
34	252	Perylene			198-55-0
35	268	3-Methylcholanthrene			56-49-5
36	330	9,10-Diphenylanthracene			216-105-1
37	279	Dibenzo[a,h]acridine			226-36-8
38	279	Dibenzo[a,j]acridine			224-42-0
39	278	Dibenzo[a,j]anthracene			224-41-9
40	292	Dibenzo[a,h] anthracene-d14			13250-98-1
41	278	Benzo[b]triphenylene			215-58-7
42	276	Indeno[1,2,3-c,d]pyrene	X	X	193-39-5
43	278	Dibenzo[a,h]anthracene	X	X	53-70-3
44	278	Benzo[b]chrysene			214-17-5
45	278	Picene			213-46-7
46	276	Benzo[g,h,i]perylene	X	X	191-24-2
47	276	Dibenzo[def,mno]-chrysene			191-26-4
48	267	7H-Dibenzo[c,g]-carbazole			194-59-2
49	302	Dibenzo[a,l]pyrene		X	191-30-0
50	302	Dibenzo[a,e]pyrene		X	192-65-4
51	300	Coronene			191-07-1
52	302	Benzo[b]perylene			197-70-6
53	302	Dibenzo[a,i]pyrene		X	189-55-9
54	302	Dibenzo[a,h]pyrene		X	189-64-0

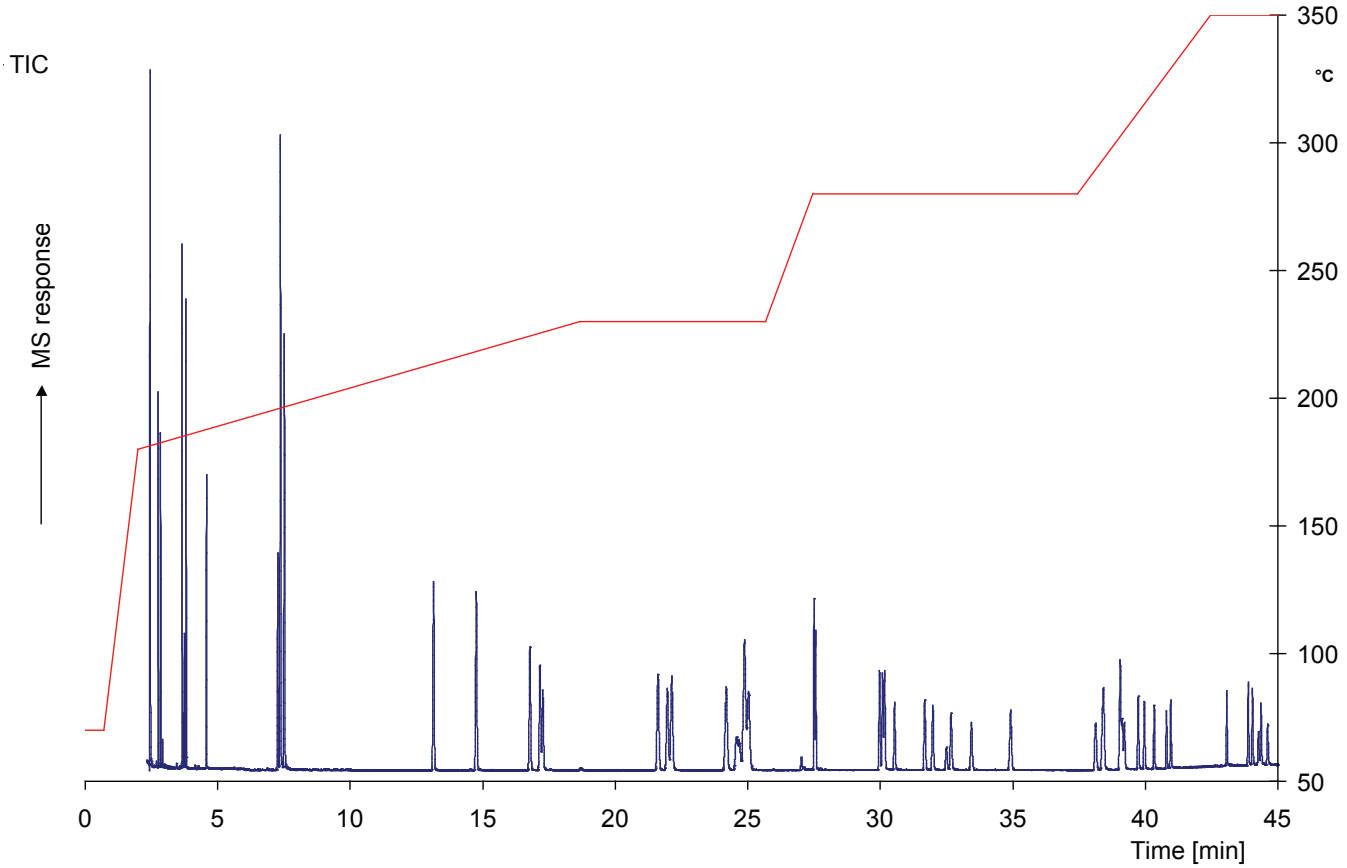

Figure 1. GC/MS analysis of EU and EPA PAHs on Select PAH column, 30 m x 0.25 mm x 0.15 µm

Table 2. Peak Identification for Figure 2

Peak	MW	Compound	EPA 610	CAS
1	136	Naphthalene-d8		1146-65-2
2	128	Naphthalene	X	91-20-3
3	142	2-Methylnaphthalene		91-57-6
4	142	1-Methylnaphthalene		90-12-0

Peak	MW	Compound	EPA 610	CAS
5	152	Acenaphthylene	X	208-96-8
6	164	Acenaphthene-d10		15067-26-2
7	154	Acenaphthene	X	83-32-9
8	166	Fluorene	X	86-73-7

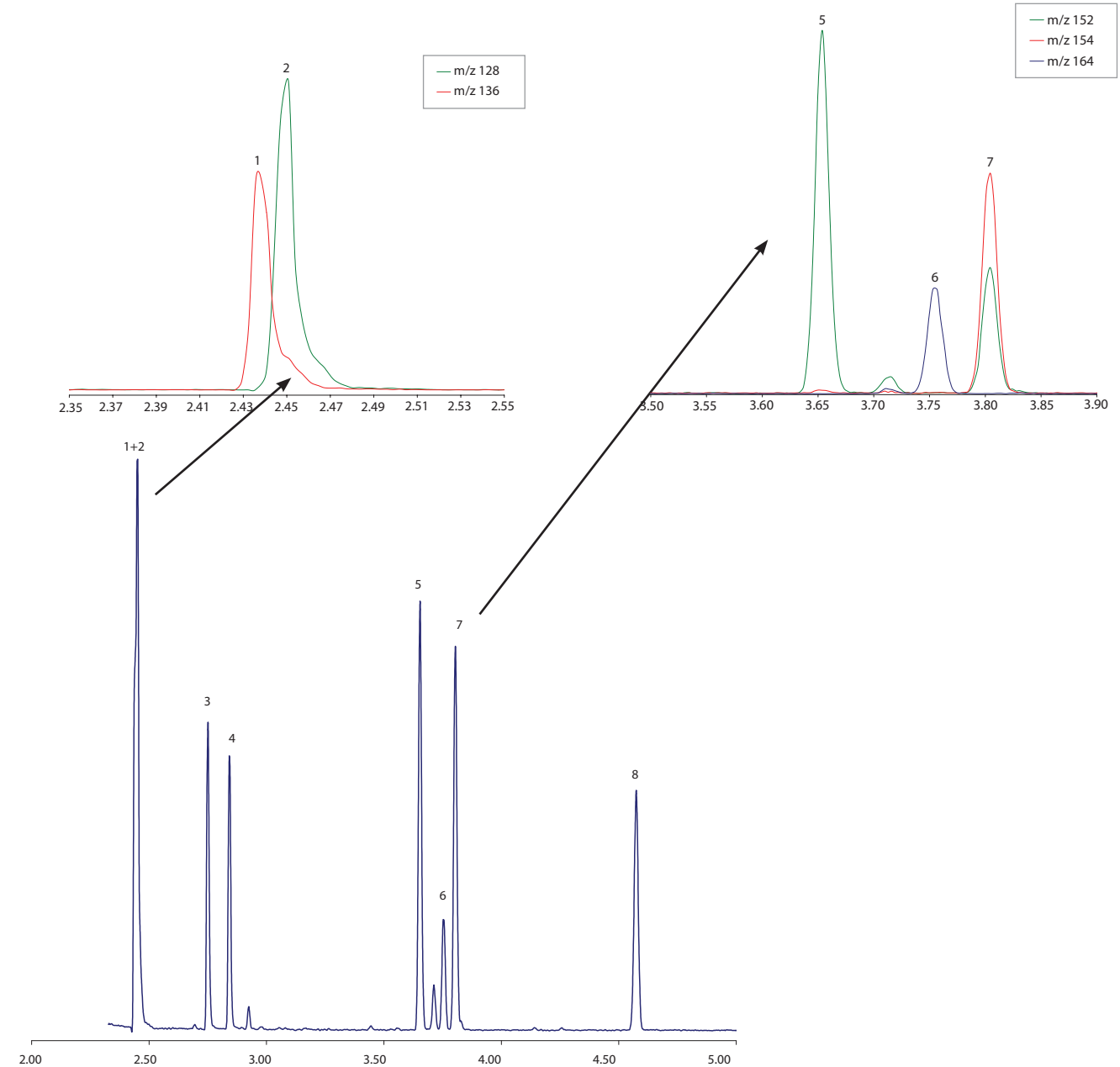

Figure 2. Details and identification of peaks 1 to 8

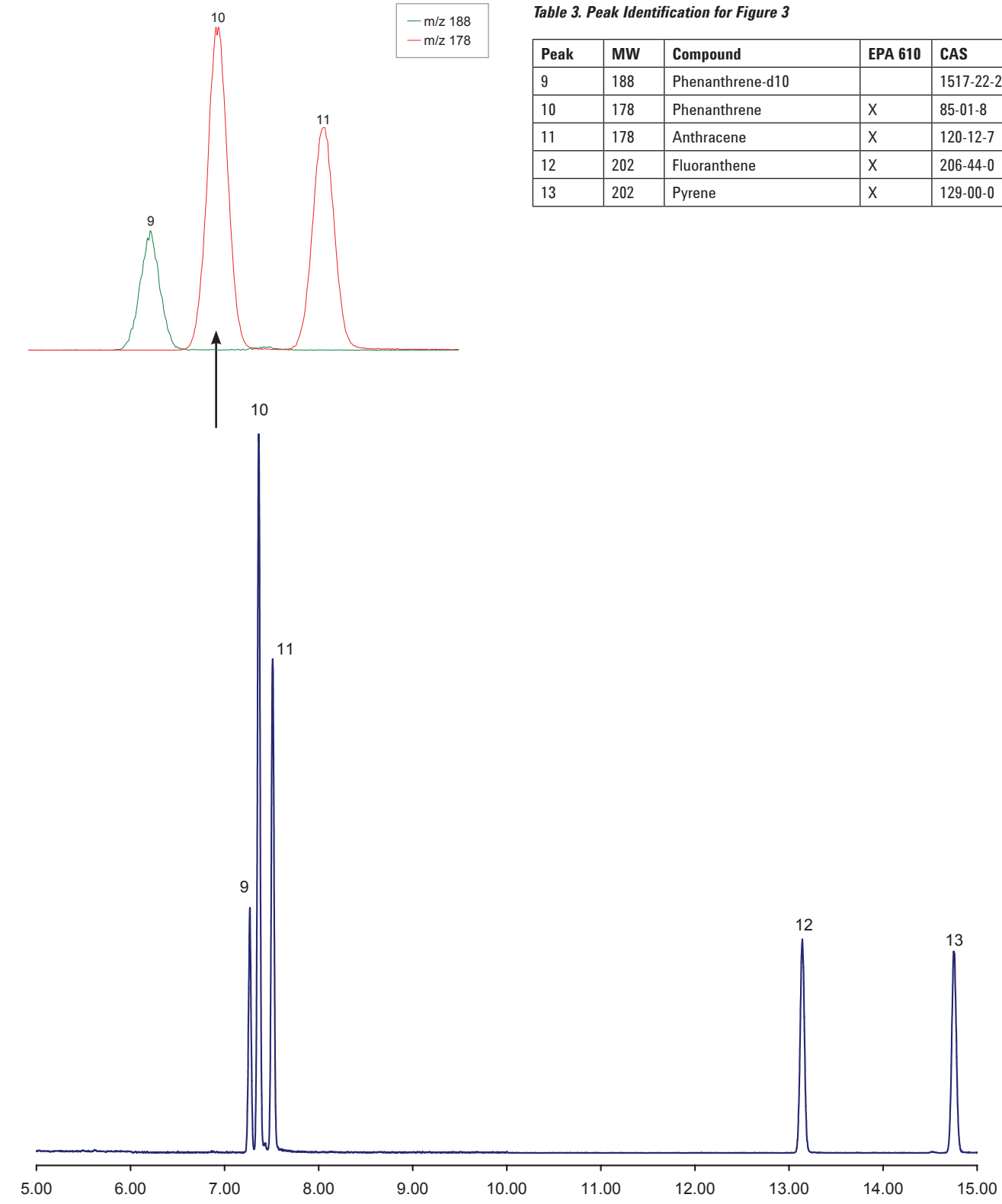

Figure 3. Details and identification of peaks 9 to 13

Table 3. Peak Identification for Figure 3

Peak	MW	Compound	EPA 610	CAS
9	188	Phenanthrene-d10		1517-22-2
10	178	Phenanthrene	X	85-01-8
11	178	Anthracene	X	120-12-7
12	202	Fluoranthene	X	206-44-0
13	202	Pyrene	X	129-00-0

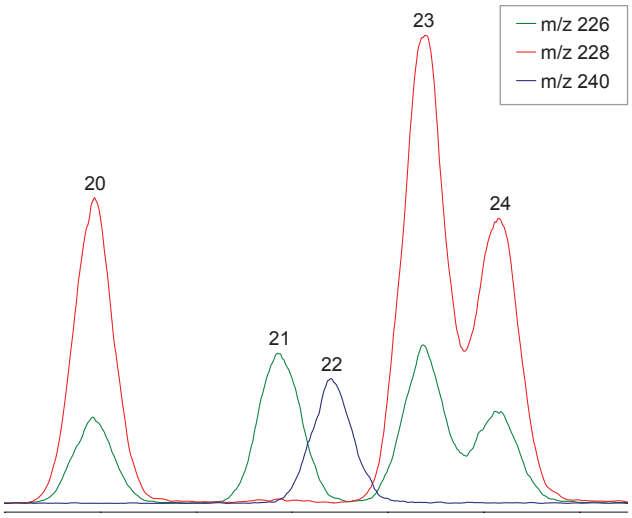

Table 4. Peak Identification for Figure 4

Peak	MW	Compound	EPA 610	SFC & EFSA PAHs (15+1)	CAS
14	216	Benzo[a]fluorene			238-84-6
15	216	Benzo[b]fluorene			243-17-4
16	216	7H-Benzo[c]fluorene		X	205-12-9
17	234	Benzo[b]naphto[2,1-d] thiophene			239.35-0
18	226	Benzo[g,h,i]fluoranthene			203-12-3
19	228	Benzo[c]phenanthrene			195-19-7
20	228	Benzo[a]anthracene	X	X	56-55-3
21	226	Cyclopenta[c,d]pyrene		X	27208-37-3
22	240	Chrysene-d10			179-03-5
23	228	Triphenylene			217-59-4
24	228	Chrysene	X	X	218-01-9

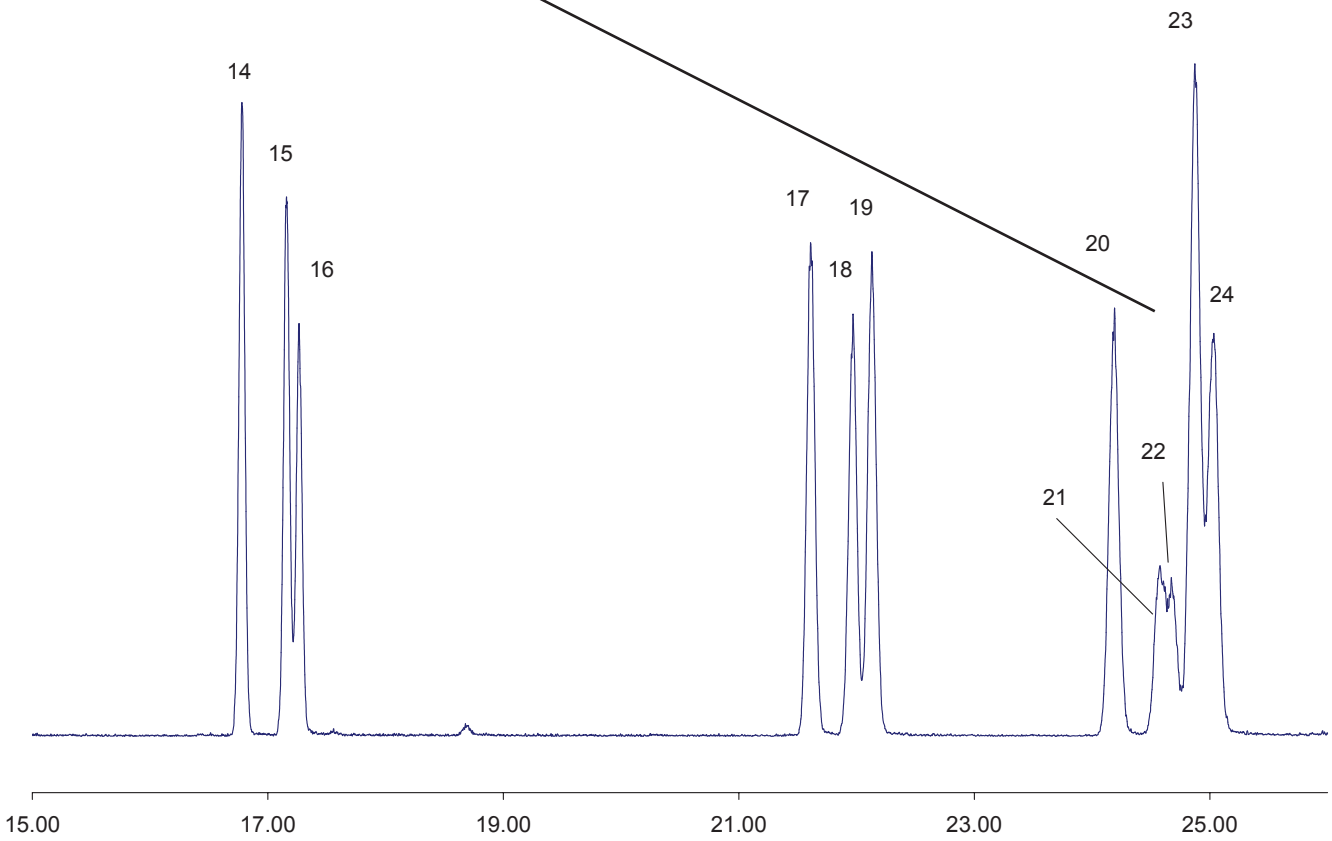

Figure 4. Details and identification of peaks 14 to 24

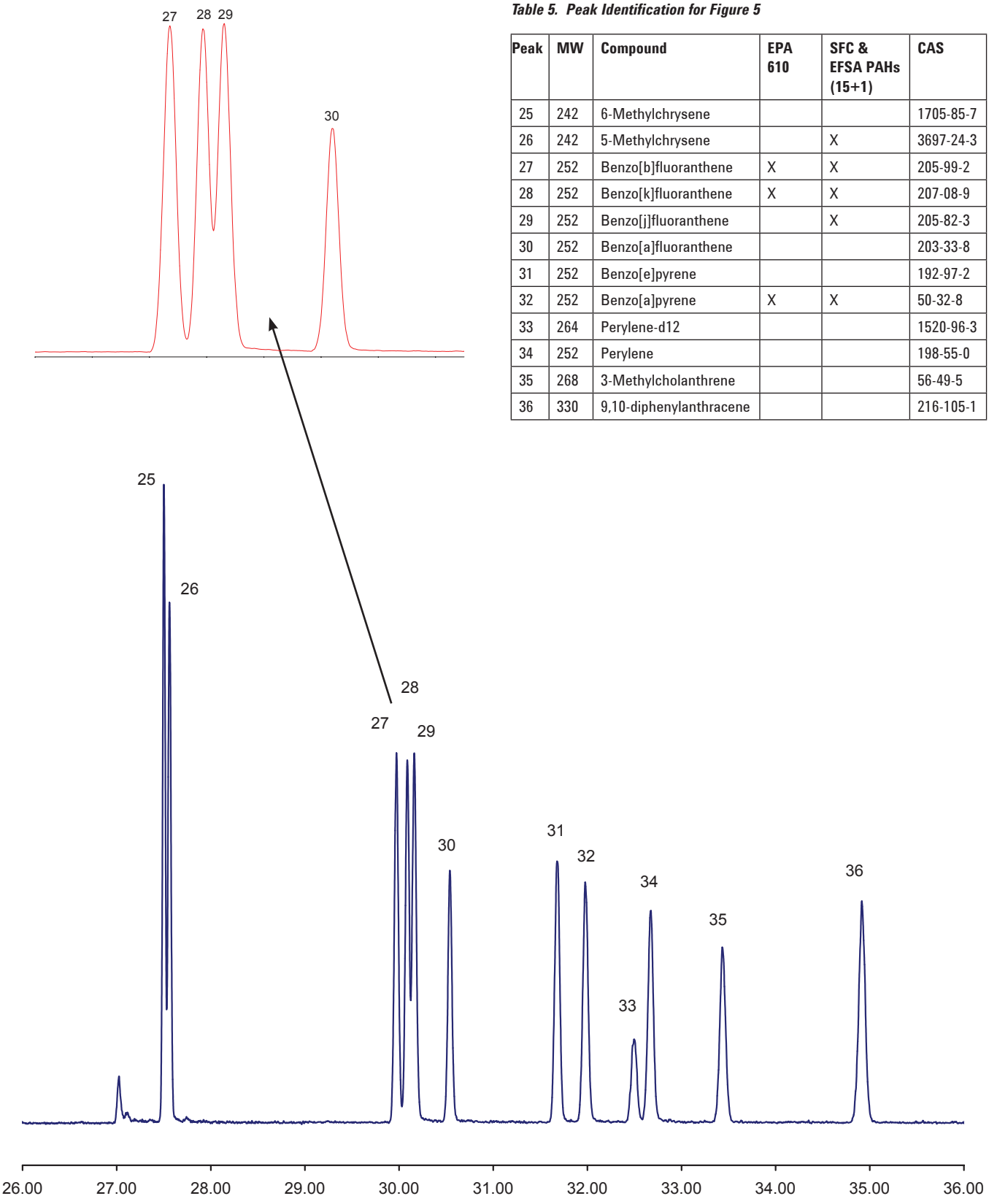

Figure 5. Details and identification of peaks 25 to 36

Table 5. Peak Identification for Figure 5

Peak	MW	Compound	EPA 610	SFC & EFSA PAHs (15+1)	CAS
25	242	6-Methylchrysene			1705-85-7
26	242	5-Methylchrysene		X	3697-24-3
27	252	Benzo[b]fluoranthene	X	X	205-99-2
28	252	Benzo[k]fluoranthene	X	X	207-08-9
29	252	Benzo[j]fluoranthene		X	205-82-3
30	252	Benzo[a]fluoranthene			203-33-8
31	252	Benzo[e]pyrene			192-97-2
32	252	Benzo[a]pyrene	X	X	50-32-8
33	264	Perylene-d12			1520-96-3
34	252	Perylene			198-55-0
35	268	3-Methylcholanthrene			56-49-5
36	330	9,10-diphenylanthracene			216-105-1

Table 6. Peak Identification for Figure 6

Peak	MW	Compound	EPA 610	SFC & EFSA PAHs (15+1)	CAS
37	279	Dibenzo[a,h]acridine			226-36-8
38	279	Dibenzo[a,j]acridine			224-42-0
39	278	Dibenzo[a,j]anthracene			224-41-9
40	292	Dibenzo[a,h] anthracene-d14			13250-98-1
41	278	Benzo[b]triphenylene			215-58-7
42	276	Ideno[1,2,3-c,d]pyrene	X	X	193-39-5
43	278	Dibenzo[a,h]anthracene	X	X	53-70-3
44	278	Benzo[b]chrysene			214-17-5
45	278	Picene			213-46-7

Peak	MW	Compound	EPA 610	SFC & EFSA PAHs (15+1)	CAS
46	276	Benzo[g,h,i]perylene	X	X	191-24-2
47	276	Dibenzo[def,mno]chrysene			191-26-4
48	267	7H-Dibenzo[c,g]carbazole			194-59-2
49	302	Dibenzo[a,l]pyrene			191-30-0
50	302	Dibenzo[a,e]pyrene		X	192-65-4
51	300	Coronene			191-07-1
52	302	Benzo[b]perylene			197-70-6
53	302	Dibenzo[a,i]pyrene		X	189-55-9
54	302	Dibenzo[a,h]pyrene		X	189-64-0

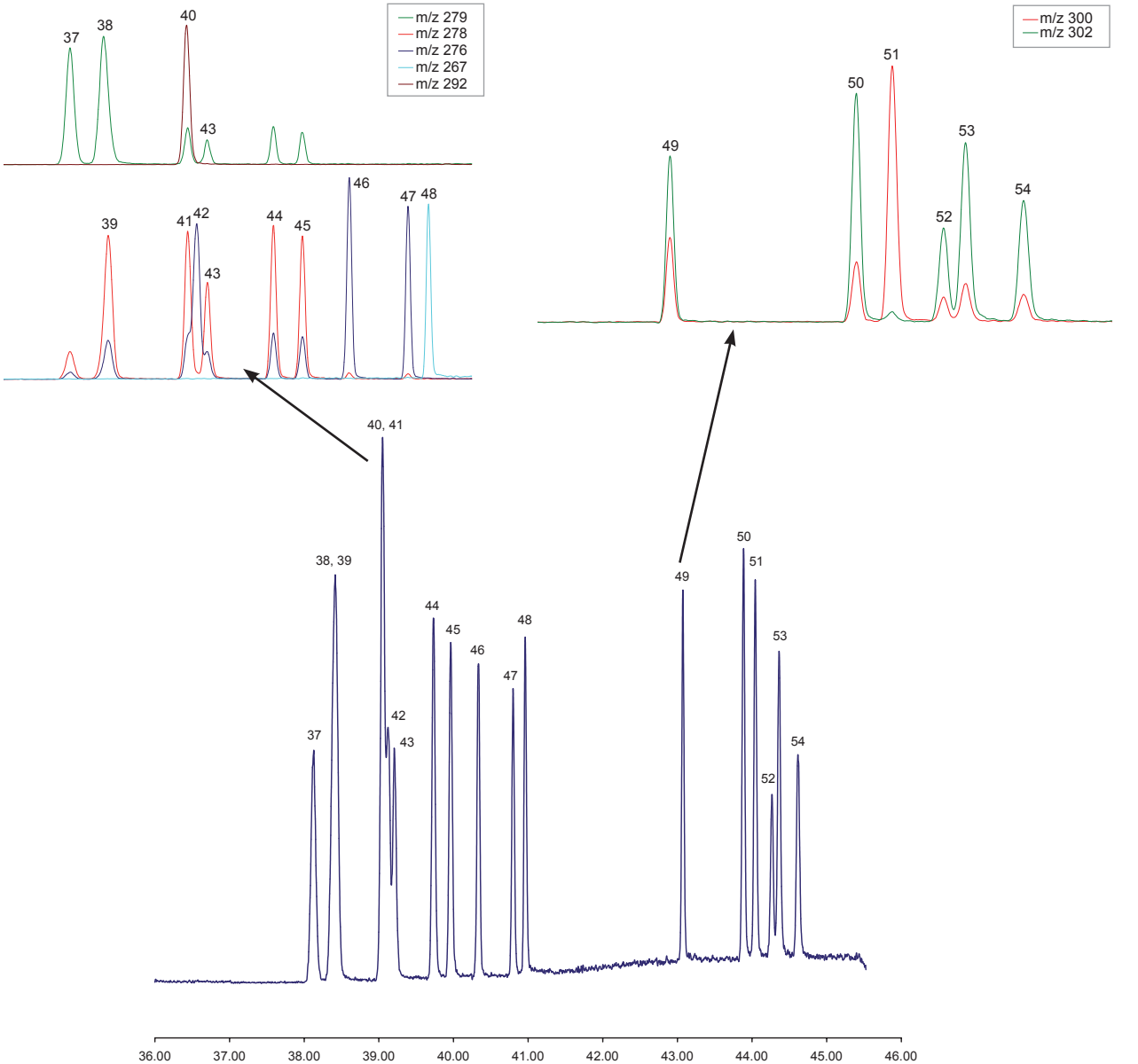

Figure 6. Details and identification of peaks 37 to 54

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