APPLICATIONS

TN-2094 Optimal Separation of PAH Compounds including Chrysene & Triphenylene using Zebron™ ZB-PAH-SeleCT GC column

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Introduction

Polycyclic aromatic hydrocarbons (PAHs) are carcinogenic substances that must be monitored in food and environment as per local regulations. There are numerous PAH compounds that have structural similarities including Chrysene and Triphenylene that are hard to resolve on a traditional GC column. Chromatographically, there are 3 components that contributes to improve resolution of peaks. It comprises of Efficiency term, Selectivity term, and Retention term. Among the three terms, Selectivity is most influential in drastic resolution improvement. For optimal resolution of Chrysene and Triphenylene, several combinations of stationary phases were explored. Presented in this study is an optimal stationary phase Zebron ZB-PAH-SeleCT that was utilized for separation of EU 15+1 PAHs along with Triphenylene to evaluate overall separation of PAH and separation of critical pairs Chrysene and Triphenylene.

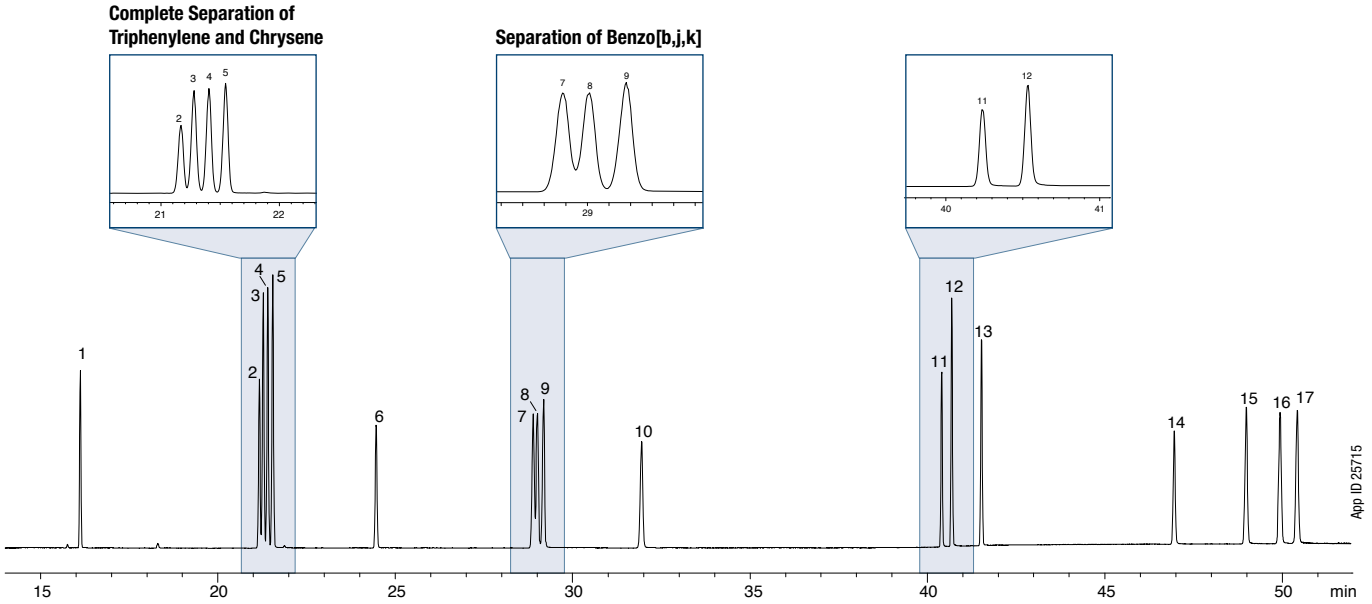
Figure 1.
Master Resolution Equation

$$R_s = \frac{\sqrt{N}}{4} \times \frac{\alpha - 1}{\alpha} \times \frac{k}{k+1}$$

Efficiency | Selectivity | Retention

N = theoretical plates **α** = k_2/k_1 **k** = $(t_R - t_0)/t_0$

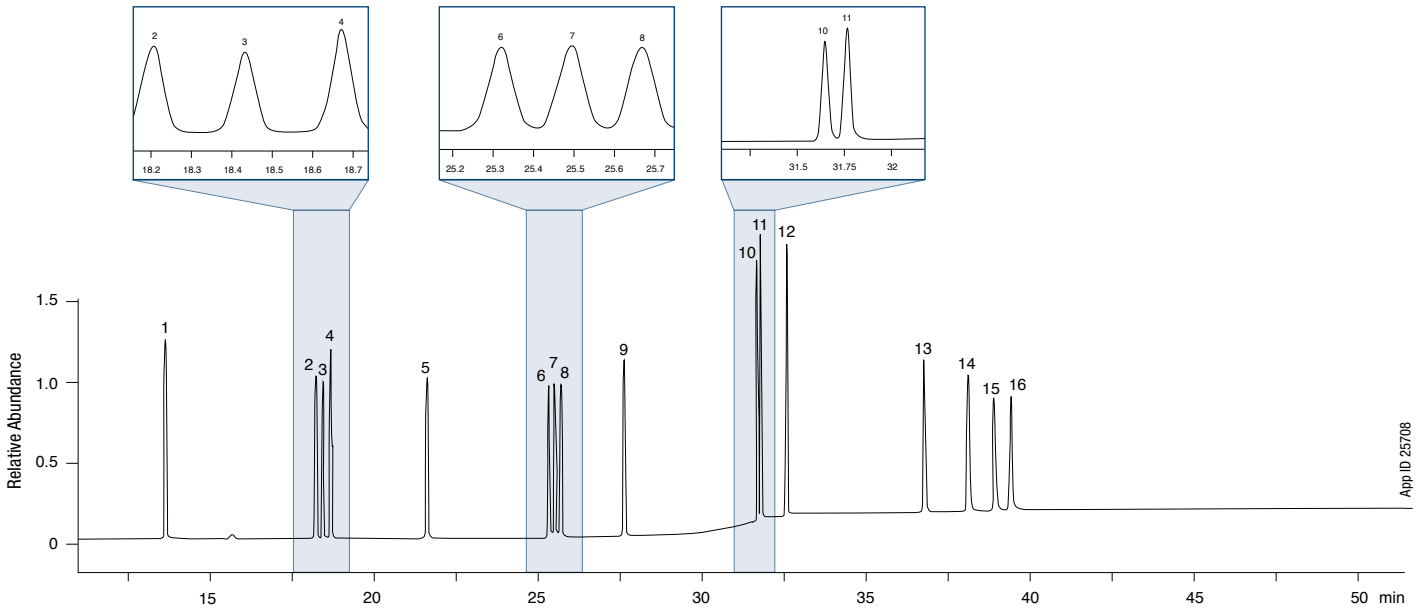
Figure 2.
EU 15+1 PAH and Triphenylene on a Zebron ZB-PAH-SeleCT GC column



Column: Zebron ZB-PAH-SeleCT
Dimensions: 40 meter x 0.18 mm x 0.14 µm
Part No.: 7PD-G044-47
Injection: Split 30:1 @ 320 °C, 1 µL
Recommended Liner: Zebron PLUS Single Taper Z-Liner™
Liner Part No.: AG2-4B13-05 (for Shimadzu® 2010 GC)
Carrier Gas: Helium @ 78 psi (constant pressure)
Oven Program: 45 °C for 0.8 min to 200 °C @ 45 °C/min to 265 °C @ 3 °C/ min for 5 min to 270 °C @ 1 °C/min to 320 °C @ 10 °C/min for 15 min
Detector: MSD (Shimadzu® GC-MS-QP2010 Ultra)
Mode: SIM
SIM Ions: 216, 226, 228, 242, 252, 276, 278, 302 m/z
Transfer line Temperature: 300 °C
Source Temperature: 300 °C

Sample:
1. Benzo[c]fluorene
2. Cyclopenta[c,d]pyrene
3. Benz[a]anthracene
4. Triphenylene
5. Chrysene
6. 5-MethylChrysene
7. Benzo[b]fluoranthene
8. Benzo[j]fluoranthene
9. Benzo[k]fluoranthene
10. Benzo[a]pyrene
11. Indeno[1,2,3-c,d]pyrene
12. Dibenz[a,h]anthracene
13. Benzo[g,h,i]perylene
14. Dibenzo[a,l]pyrene
15. Dibenzo[a,e]pyrene
16. Dibenzo[a,i]pyrene
17. Dibenzo[a,h]pyrene

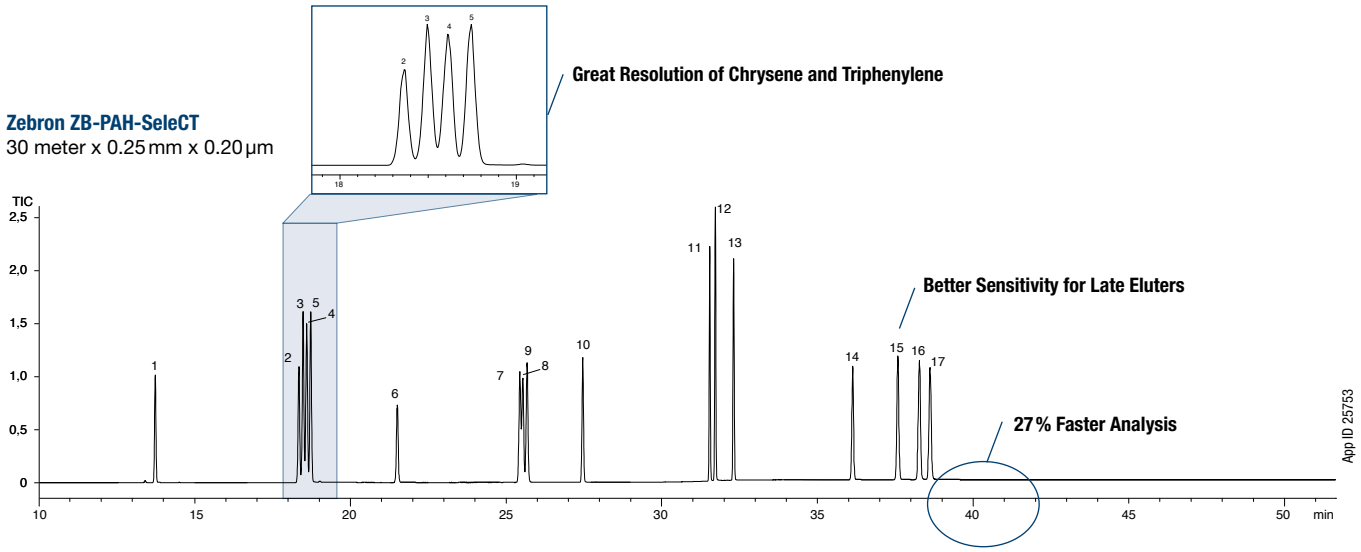
Figure 3.
EU 15+1 PAH on a Zebron ZB-PAH-EU GC column



Column: Zebron ZB-PAH-EU
Dimensions: 30 meter x 0.25 mm x 0.20 µm
Part No.: 7HG-G043-10
Injection: Split 5:1 @ 330 °C, 1 µL
Recommended Liner: Zebron PLUS Single Taper Z-Liner™
Liner Part No.: AG2-4B13-05 (for Shimadzu® 2010 GC)
Carrier Gas: Helium @ 24 psi (constant pressure)
Oven Program: 45 °C for 0.8 min to 200 °C @ 45 °C/min to 226 °C @ 3 °C/min for 0 min to 320 °C @ 10 °C/min for 20 min
Detector: MSD, 50-500 m/z
Transfer line Temperature: 300 °C
Source Temperature: 300 °C

Sample:
1. Benzo[c]fluorene
2. Benz[a]anthracene
3. Cyclopenta[c,d]pyrene
4. Chrysene
5. 5-MethylChrysene
6. Benzo[b]fluoranthene
7. Benzo[k]fluoranthene
8. Benzo[j]fluoranthene
9. Benzo[a]pyrene
10. Indeno[1,2,3-cd]pyrene
11. Dibenz[a,h]anthracene
12. Benzo[g,h,i]perylene
13. Dibenzo[a,l]pyrene
14. Dibenzo[a,e]pyrene
15. Dibenzo[a,i]pyrene
16. Dibenzo[a,h]pyrene

Figure 4.
Comparison of Analysis of EU 15+1 PAHs and Triphenylene

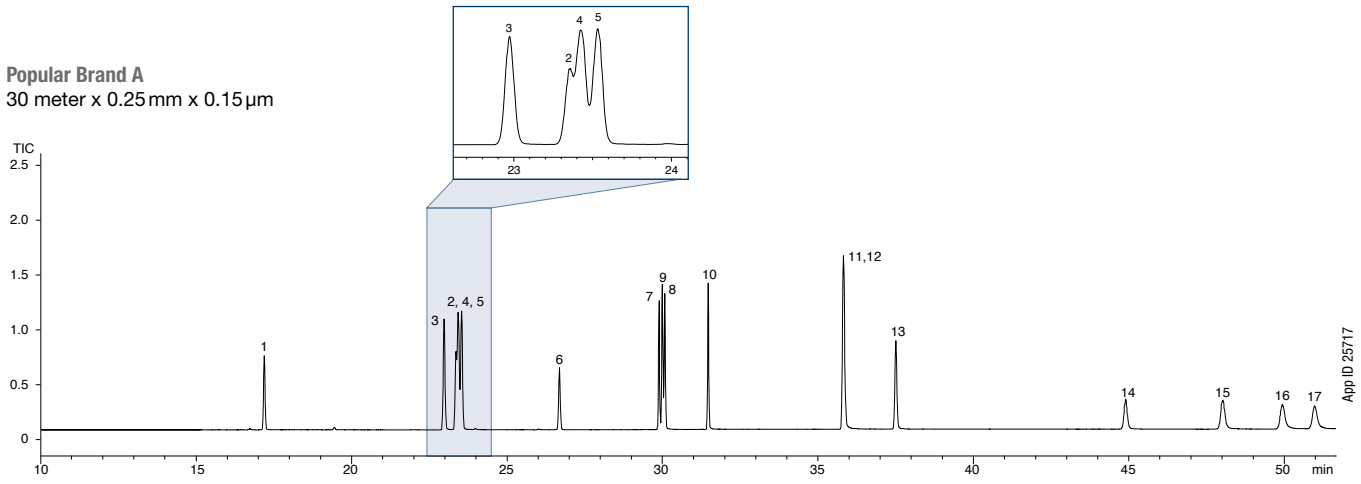


GC-MS conditions for both applications:

Column: As Indicated
Dimensions: As Indicated
Part No.: 7HG-G044-10 (Zebron ZB-PAH-SeleCT)
Injection: Split 15:1 @ 320 °C, 1 µL
Recommended Liner: Zebron PLUS Single Taper Z-Liner™
Liner Part No.: AG2-4B13-05
Carrier Gas: Helium @ 23.7 psi (constant pressure)
Oven Program: 45 °C for 0.8 min to 200 °C @ 45 °C/min to 266 °C @ 3 °C/ min for 0 min to 320 °C @ 10 °C/ min to 320 °C for 20 min
Detector: MSD (Shimadzu® GC-MS-QP2010 Ultra)
Mode: SIM
SIM Ions: 216, 226, 228, 242, 252, 276, 278, 302 m/z
Transfer line Temperature: 300 °C
Source Temperature: 300 °C

Sample:
1. Benzo[c]fluorene
2. Cyclopenta[c,d]pyrene
3. Benz[a]anthracene
4. Triphenylene
5. Chrysene
6. 5-MethylChrysene
7. Benzo[b]fluoranthene
8. Benzo[j]fluoranthene
9. Benzo[k]fluoranthene
10. Benzo[a]pyrene
11. Indeno[1,2,3-c,d]pyrene
12. Dibenz[a,h]anthracene
13. Benzo[g,h,i]perylene
14. Dibenzo[a,l]pyrene
15. Dibenzo[a,e]pyrene
16. Dibenzo[a,i]pyrene
17. Dibenzo[a,h]pyrene

VS.



Comparative separations may not be representative of all applications.

APPLICATIONS

Results and Discussion

Separation of PAH isomers are quite challenging as there are many PAH components that have structural similarities. Specifically, Chrysene and Triphenylene are one such hard to separate critical pairs. In the present study, unique selectivity of ZB-PAH-SeleCT was utilized to resolve EU 15+1 and Triphenylene. As shown in **Figure 2**, the 40 meter x 0.18 mm x 0.14 µm ZB-PAH was able to completely resolve Chrysene from Triphenylene. In addition, ZB-PAH-SeleCT also provided a peak order switch for certain PAH analytes compared to ZB-PAH-EU, including Benz[a]anthracene, Cyclopenta[c,d]pyrene (Peak 2 and 3 in **Figure 2** and 3); Benzo[b,j,k] fluoranthene (Peak 7, 8, 9 in **Figure 2** and peak 6, 7, 8 in **Figure 3**) due to the unique selectivity. The selectivity change and enhanced resolution of Chrysene and Triphenylene helps avoid false positives in the analysis. In addition to resolving Chrysene and Triphenylene completely, ZB-PAH-SeleCT in a 40 meter dimension provided the highest resolution of 2.6 for Benzo[b,k]fluoranthene

Further, EU 15+1 and Triphenylene mix was evaluated on a 30 meter ZB-PAH-SeleCT and 30 meter Popular Brand A GC column under identical chromatographic conditions. As shown in **Figure 4**, ZB-PAH-SeleCT shows better resolution of Chrysene and Triphenylene, better sensitivity for heavy PAH, and 27% faster run time because of the unique stationary phase selectivity.

Conclusion

Zebron ZB-PAH-SeleCT provides complete resolution of Chrysene and Triphenylene in addition to other EU 15+1 PAHs with a 40 meter column dimension. In addition to providing great resolution of Chrysene and Triphenylene, ZB-PAH-SeleCT provides high resolution for Benzo[b,k]fluoranthene, gives better sensitivity for heavy PAH, and provides 27% faster run time than common PAH GC columns.

Ordering Information

Zebron™ ZB-PAH-SeleCT GC Column

Length (meter)	ID (mm)	df (µm)	Temp. Limits (°C)	Part No.
20	0.18	0.14	40 to 320/340	7FD-G044-47
30	0.25	0.20	40 to 320/340	7HG-G044-10
40	0.18	0.14	40 to 320/340	7PD-G044-47

Zebron™ ZB-PAH-EU GC Column

Length (meter)	ID (mm)	df (µm)	Temp. Limits (°C)	Part No.
10	0.10	0.08	40 to 340/360	7CB-G043-59
20	0.18	0.14	40 to 340/360	7FD-G043-47
30	0.25	0.20	40 to 340/360	7HG-G043-10
60	0.25	0.20	40 to 340/360	7KG-G043-10

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