*Comptes Rendus*
*Chimie*
Supplementary material to the article available at:
https://doi.org/10.5802/crchim.286

# Supplementary material: Development of an analytical method for the simultaneous determination of 22 Polycyclic Aromatic Hydrocarbons (PAHs) in maternal and umbilical cord blood

**Stéphanie Swiha** [a, b], **Valérie Pichon** [*, a, c], **Thierry Fournier** [b, d, e], **Sophie Gil** [b, d, e] **and Nathalie Delaunay** [a]

[a] Laboratory of Analytical and Bioanalytical Sciences and Miniaturization, UMR CBI 8231 CNRS – ESPCI Paris, PSL University, Paris, France

[b] INSERM U1139, Faculté de Pharmacie, Paris, France

[c] Sorbonne Université, Paris, France

[d] Université Paris Descartes, UMR-S 1139, Sorbonne Paris Cité, Paris, France

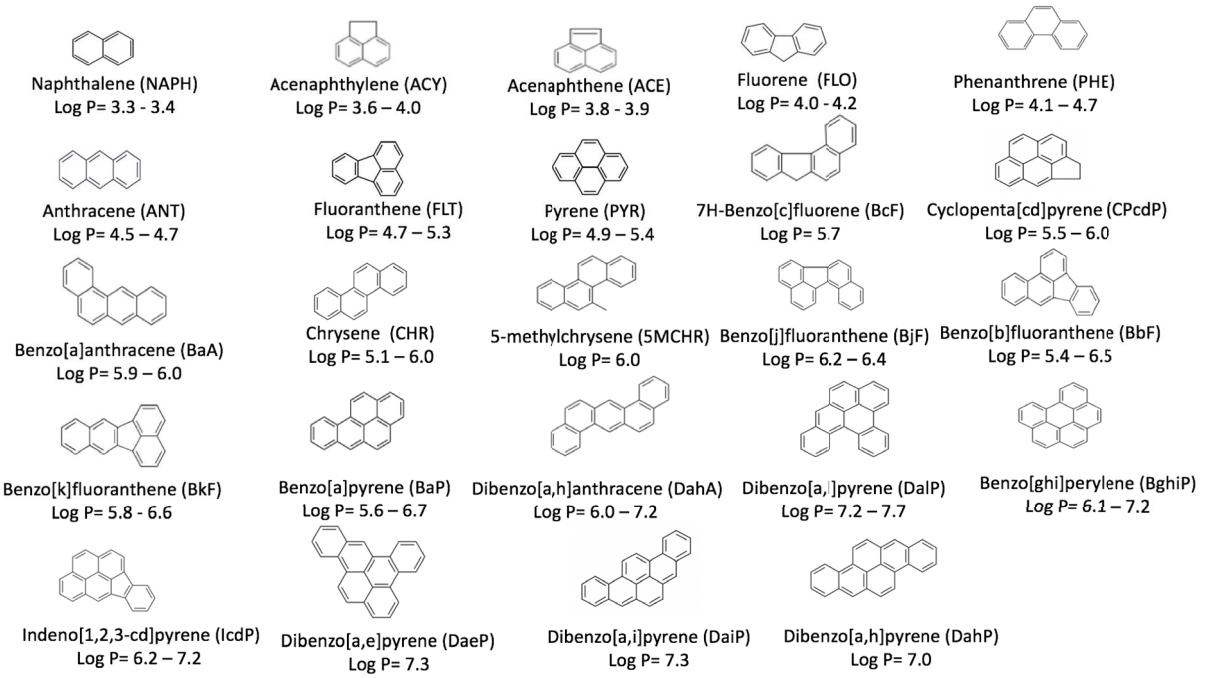
[e] Fondation PremUP, Paris, France

*Current address:* LSABM, UMR CBI 8231 CNRS – ESPCI Paris, PSL University, 10 rue Vauquelin, 75231 Paris cedex 05, France (V. Pichon)

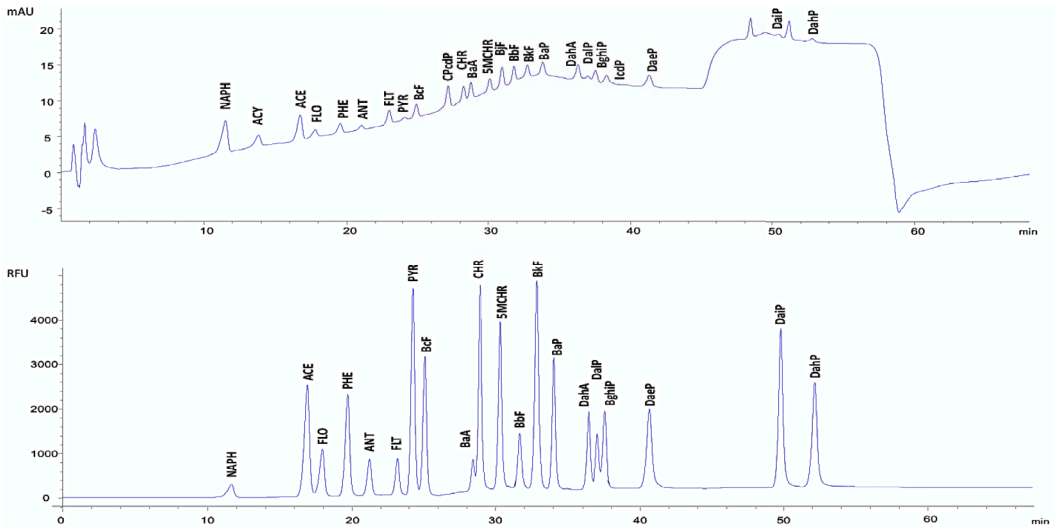
*E-mail:* valerie.pichon@espci.fr (V. Pichon)

*Not yet published*

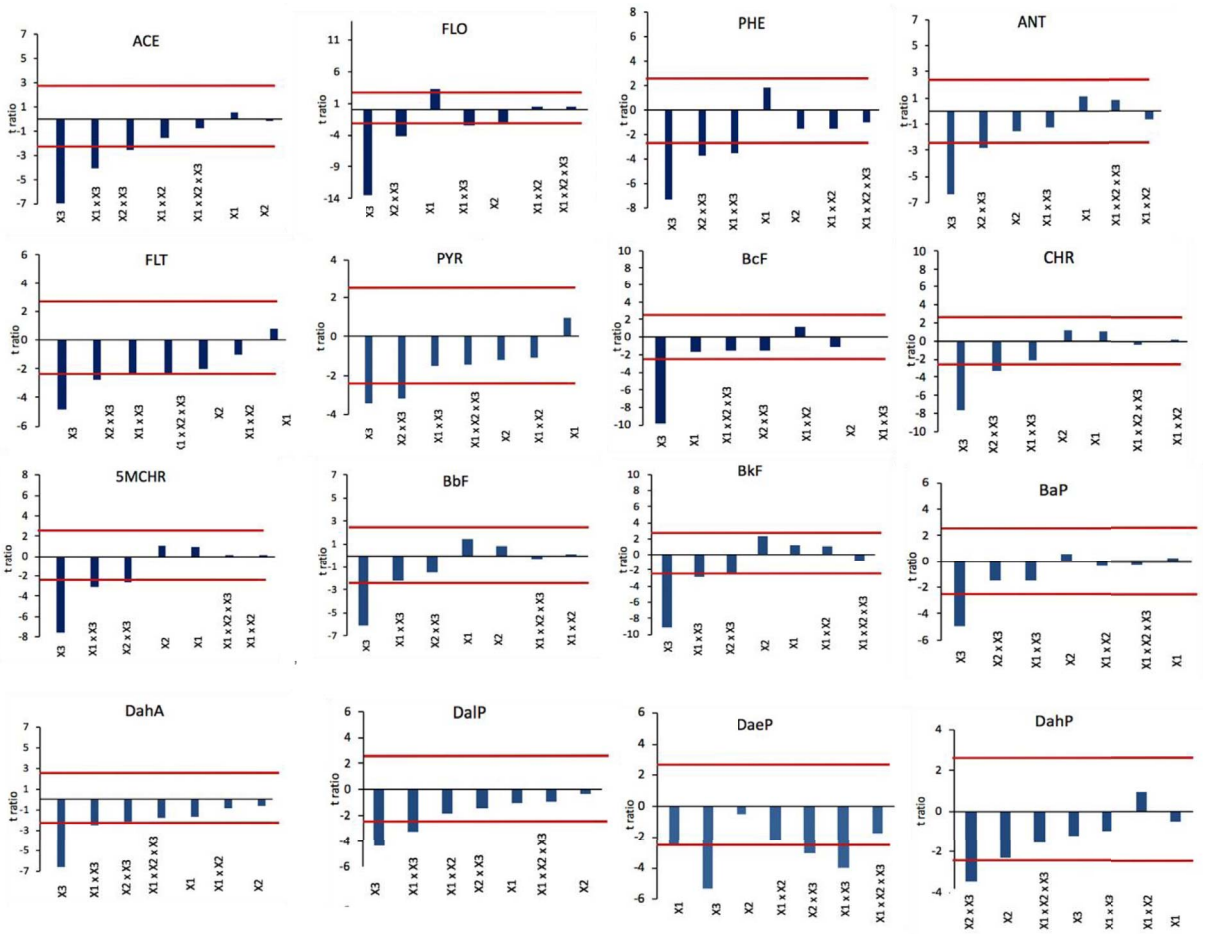
* Corresponding author.



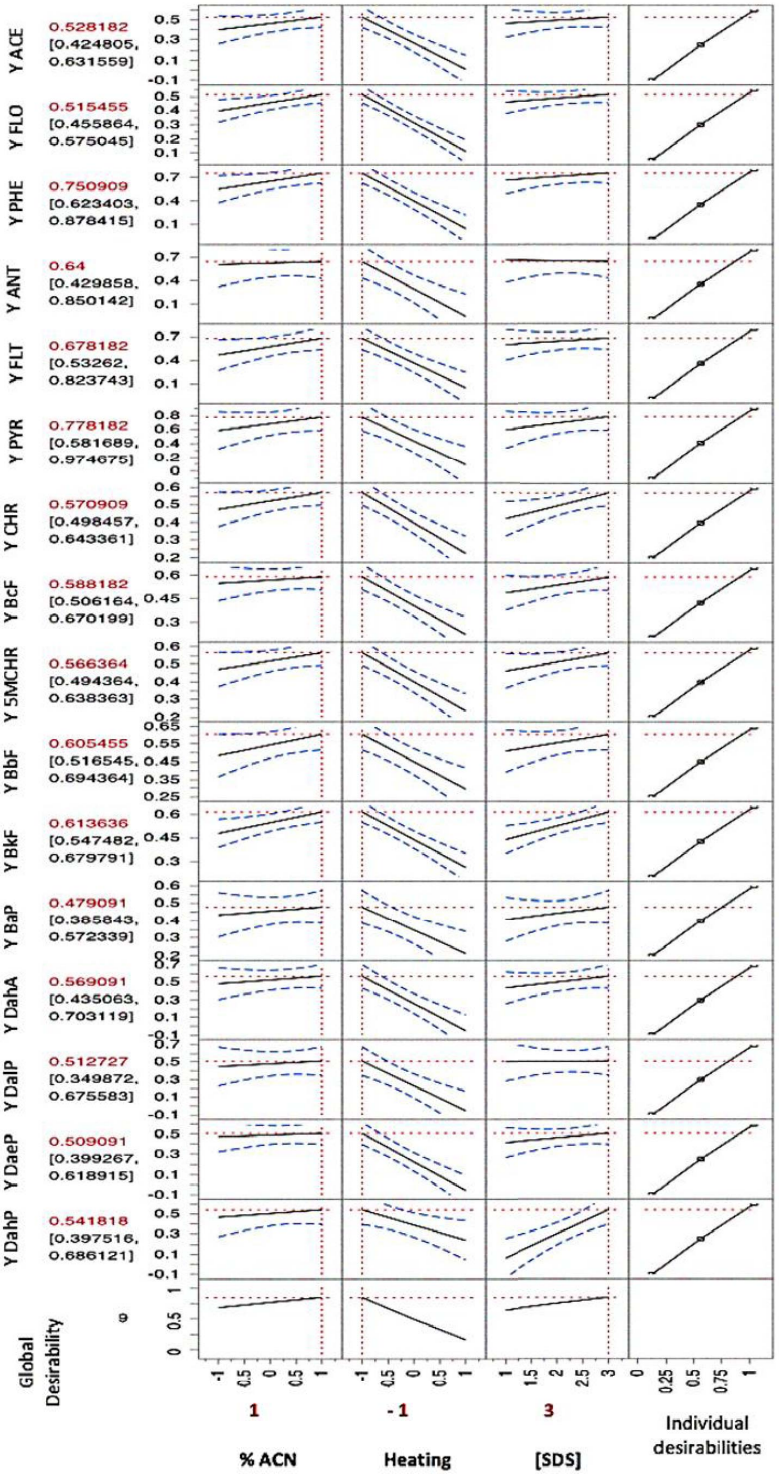

**Supplementary Figure S1.** Chemical structure and log P values of the 24 regulated PAHs [9–12].



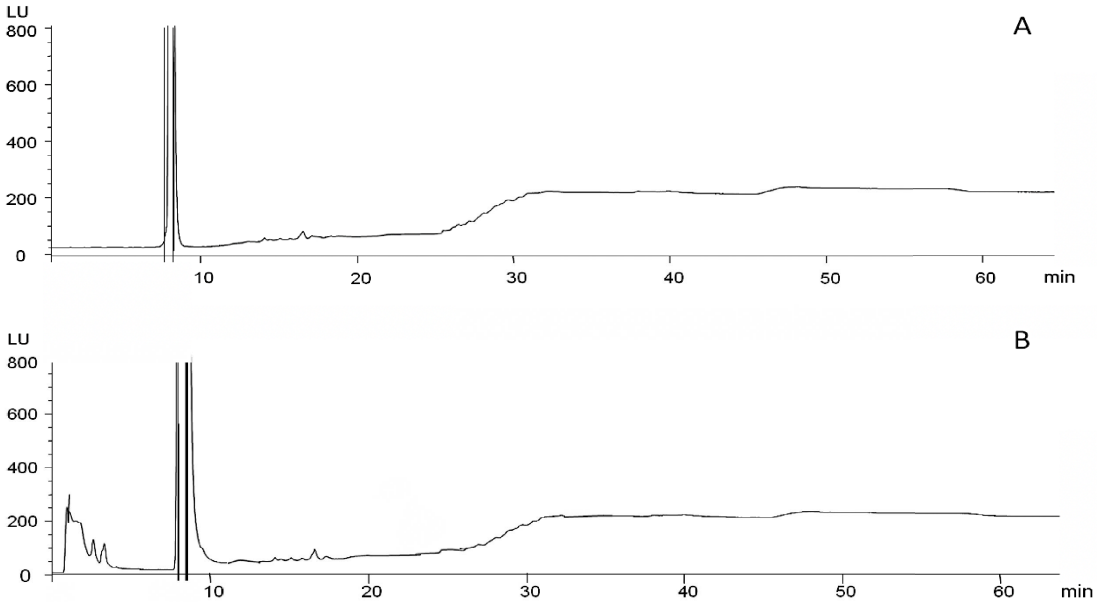

**Supplementary Figure S2.** LC-UV/FD chromatograms of a standard solution of 24 PAHs at 100 μg/L in $CH_3CN/H_2O$ (1/1, v/v) with (A) UV detection at 220 nm and (B) Fluorescence detection. Other conditions: see Section 2.2.




**Supplementary Figure S3.** Effect of the 3 studied factors ($CH_3CN$ percentage, SDS concentration and heating) and their interactions on each PAH recovery. X1: % ACN, X2: [SDS], X3: heating.




**Supplementary Figure S4.** Optimization carried out by means of the prediction profiler of JMP software. The sixteen responses of interest correspond to the first sixteen rows with their individual desirability function represented in the last column. The last row gives the global desirability as a function of the 3 studied factors ($CH_3CN$ percentage, SDS content, and temperature), represented at optimum coded values in the first 3 columns. Values appearing under the global desirability and each response are the values at the predicted optimized conditions (±95% confidence interval).




**Supplementary Figure S5.** LC-FD chromatograms of extracted (A) maternal and (B) umbilical cord pooled sera without spiking. Other conditions: see Section 2.2.

**Supplementary Table S1.** Optimization of the precipitation step: experimental design matrix with experimental responses (extraction recoveries for each PAH)

| Factor 1 Proportion of ACN | Factor 2 Heating | Factor 3 Proportion of SDS | ACE | FLO | PHE | ANT | FLT | PYR | BcF | CHR | 5MCHR | BbF | BkF | BaP | DahA | DalP | DaeP | DahP |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 3 | <8% | 13% | <8% | <20% | <13% | <5% | 24% | 23% | 26% | 32% | 28% | 23% | <20% | <25% | <15% | 26% |
| 1 | 1 | 1 | 21% | 25% | 40% | 35% | 47% | 54% | 31% | 33% | 30% | 35% | 28% | 29% | 29% | 30% | 33% | 36% |
| 1 | 1 | 1 | - | - | - | - | - | - | 28% | 39% | 32% | 49% | 31% | 28% | 24% | 30% | 28% | 34% |
| −1 | −1 | 2 | 30% | 35% | 43% | 39% | 47% | 52% | 39% | 62% | 40% | 44% | 43% | 40% | 48% | 37% | 38% | 37% |
| 1 | −1 | 2 | 59% | 51% | 79% | 73% | 73% | 82% | 54% | 61% | 56% | 62% | 54% | 48% | 62% | 66% | 52% | 43% |
| 1 | −1 | 3 | 54% | 48% | 73% | 52% | 59% | 71% | 58% | 57% | 56% | 58% | 60% | 39% | 52% | 41% | 47% | 43% |
| 1 | −1 | 3 | 47% | 54% | 73% | 72% | 72% | 78% | 54% | 57% | 55% | 60% | 62% | 55% | 56% | 54% | 52% | 59% |
| −1 | −1 | 3 | 42% | 41% | 57% | 65% | 47% | 59% | 49% | 53% | 48% | 49% | 48% | 43% | 48% | 46% | 49% | 47% |
| −1 | 1 | 1 | 19% | 22% | 36% | 27% | 39% | 43% | 35% | 33% | 34% | 38% | 30% | 29% | 29% | 30% | 36% | 34% |
| −1 | 1 | 1 | 28% | 27% | 45% | 43% | 49% | 53% | 31% | 40% | 36% | 34% | 34% | 31% | 32% | 33% | 33% | 25% |
| 1 | −1 | 1 | 42% | 45% | 62% | 62% | 55% | 53% | 40% | 45% | 44% | 48% | 43% | 39% | 38% | 43% | 39% | <13% |
| 1 | 1 | 2 | 14% | 14% | 33% | <20% | 38% | 55% | 23% | 25% | 21% | 26% | 22% | 21% | <20% | <25% | <15% | 25% |
| −1 | 1 | 2 | 28% | 12% | 24% | <20% | 29% | 37% | 23% | 27% | 25% | 26% | 23% | 24% | 22% | 29% | 32% | 21% |
| −1 | 1 | 3 | 21% | 9% | 28% | <20% | 34% | 34% | 29% | 30% | 31% | 36% | 32% | 30% | 31% | 39% | 37% | 28% |
| −1 | −1 | 1 | 29% | 36% | 43% | 41% | 50% | 46% | 38% | 61% | 37% | 42% | 40% | 35% | 45% | 33% | 36% | 28% |