

Input of an off-line comprehensive three-dimensional method (CPCxSFC/HRMS) to quantify polycyclic aromatic hydrocarbons in vacuum gas oils

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Supplementary material

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Table S1: Model mix for separation and detection method optimizations

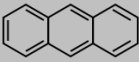

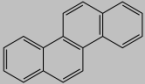
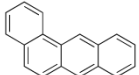
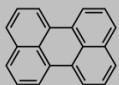
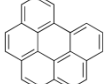

Standard name	Structure	Boiling point (°C)	Chemical formula	DBE	Molar mass (g/mol)
Anthracene		341	C ₁₄ H ₁₀	10	178.234
Pyrene		404	C ₁₆ H ₁₀	12	202.256
Chrysene		448	C ₁₈ H ₁₂	13	228.294
Benz[a]anthracene		438	C ₁₈ H ₁₂	13	228.294
Perylene		400	C ₂₀ H ₁₂	15	252.316
Benzo[ghi]perylene		500	C ₂₂ H ₁₂	17	276.331
Coronene		525	C ₂₄ H ₁₂	19	300.352

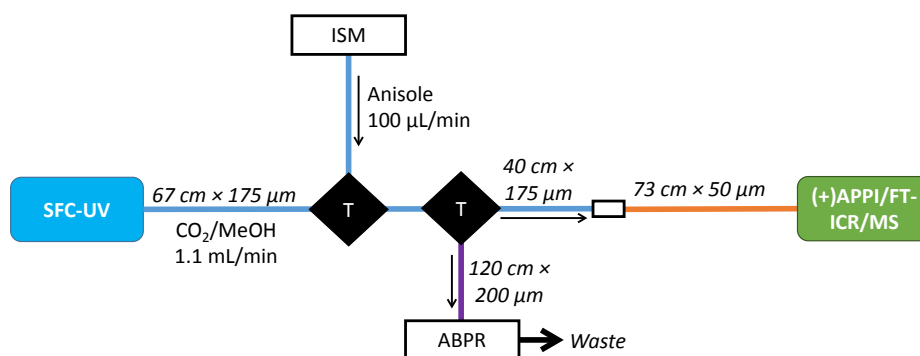
Figure S1: Scheme of the SFC-UV/MS interface

Figure S2: Retention times of pyrene and coronene for the different screening conditions in SFC.

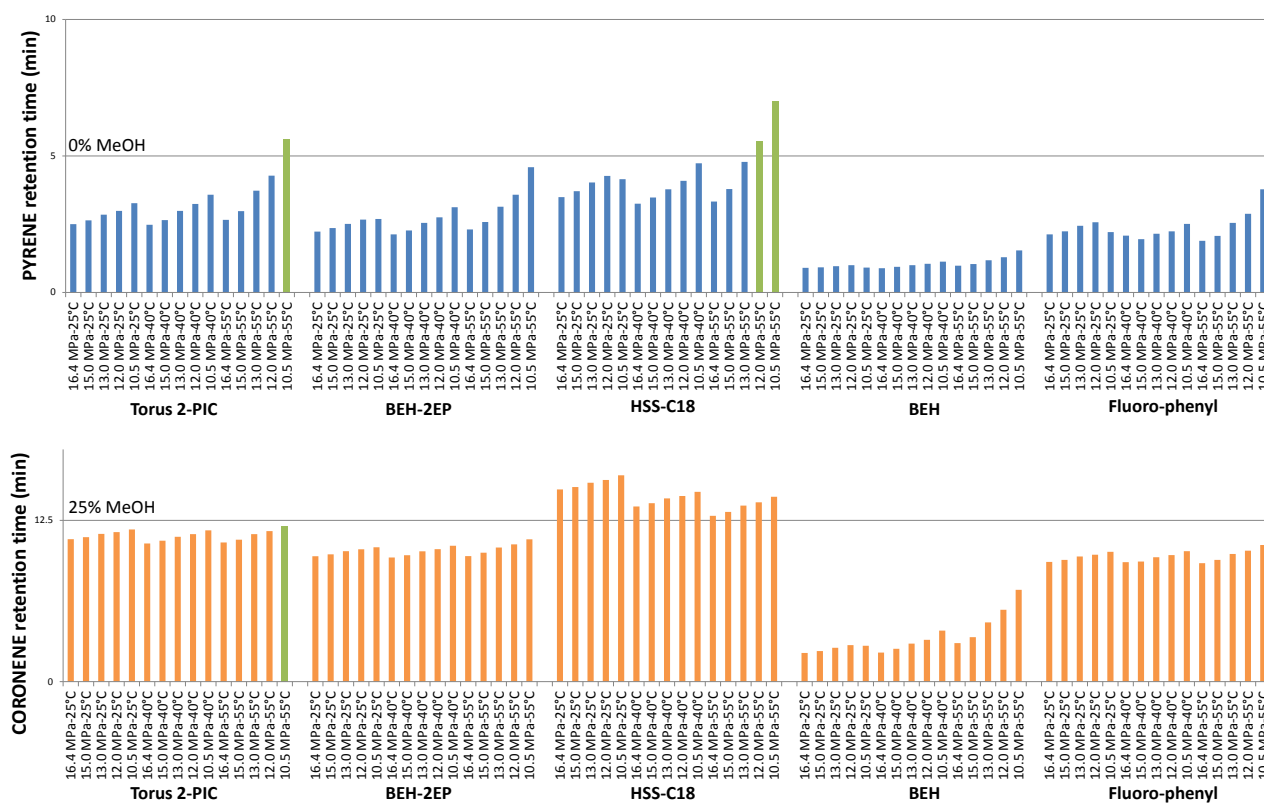


Figure S3: Extracted Ion Chromatograms of (A) pyrene (m/z 202.07-202.08) and (B) coronene (m/z 300.09-300.10) using toluene (red) or anisole (black) as dopant

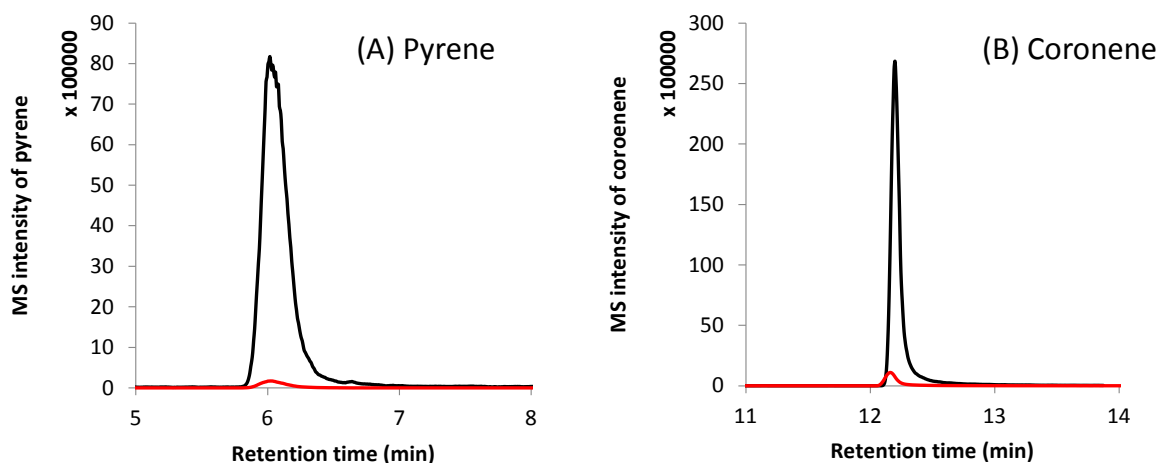


Figure S4: Mass spectra of spiked UCO (A) and spiked VGO 1 (B) using SFC/MS method

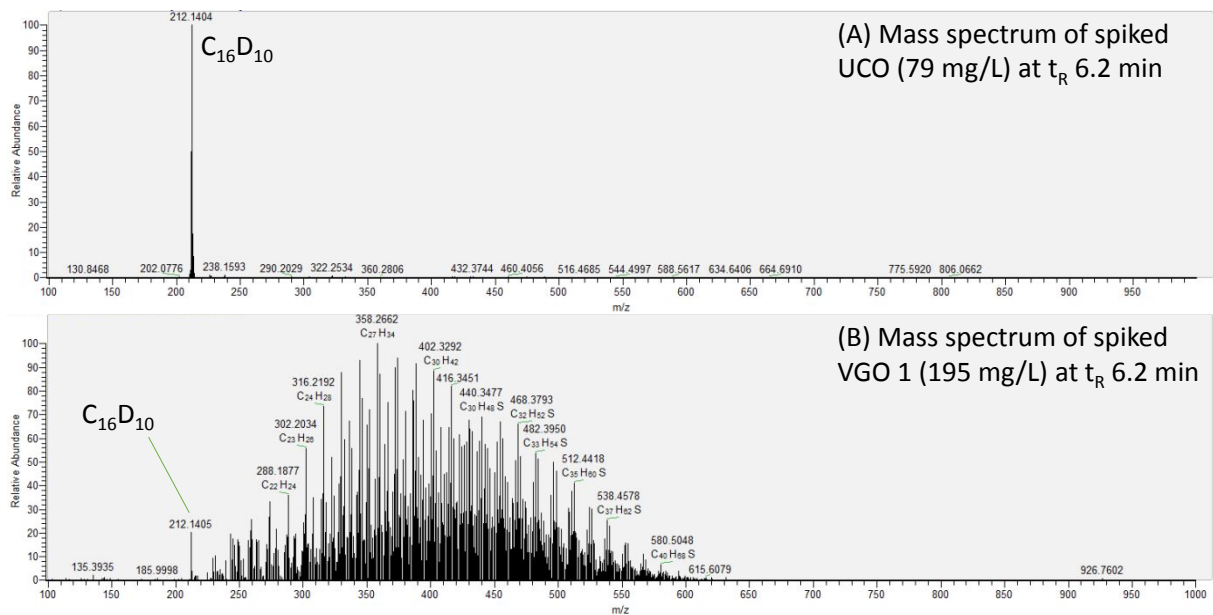


Figure S5: CPC chromatograms at several UV wavelengths for HPAH model mixture, UCO and the three VGO

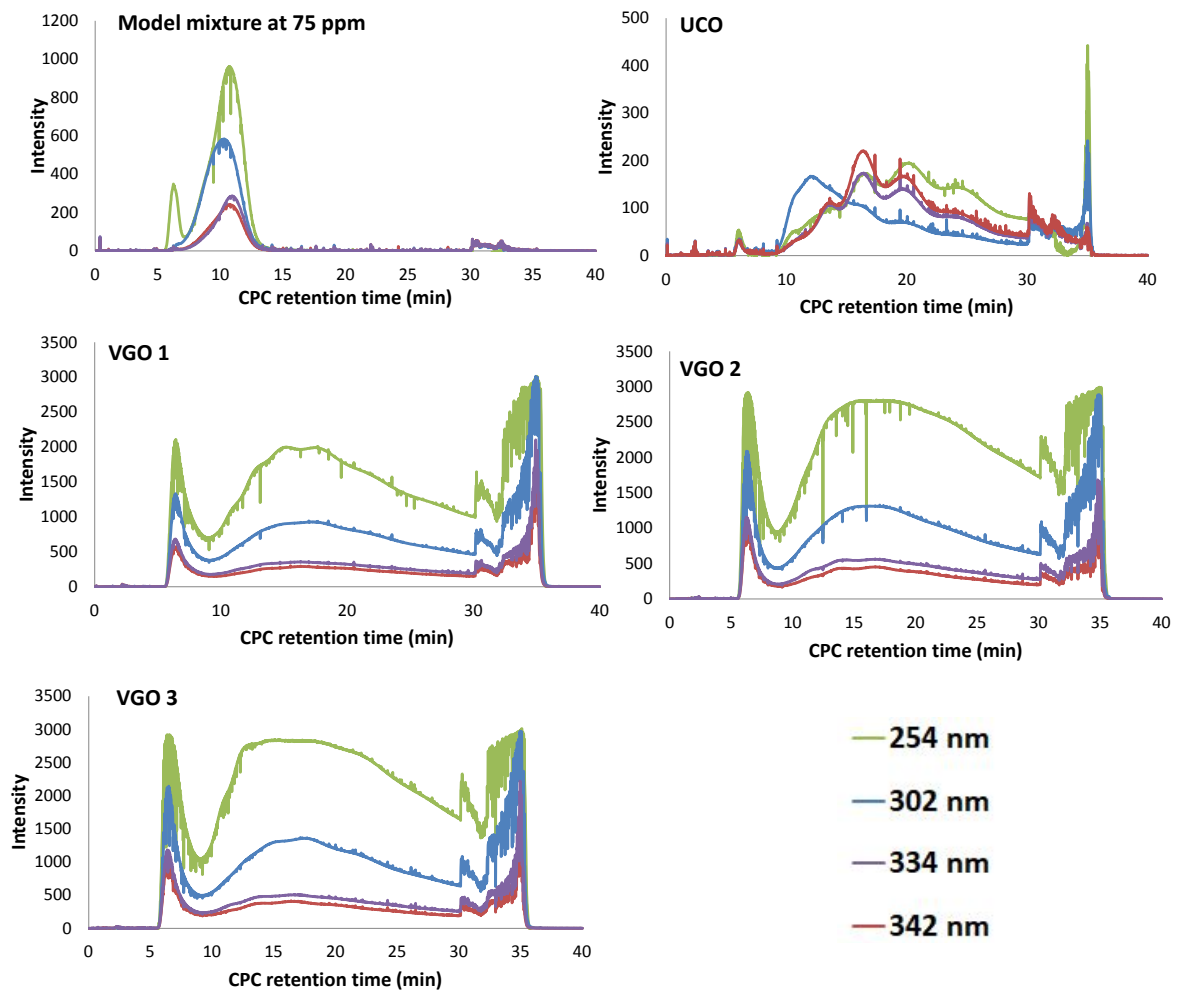


Figure S6: CPC×SFC-UV max plots (between 250 and 400 nm) of UCO (A) and VGO 1 (B).

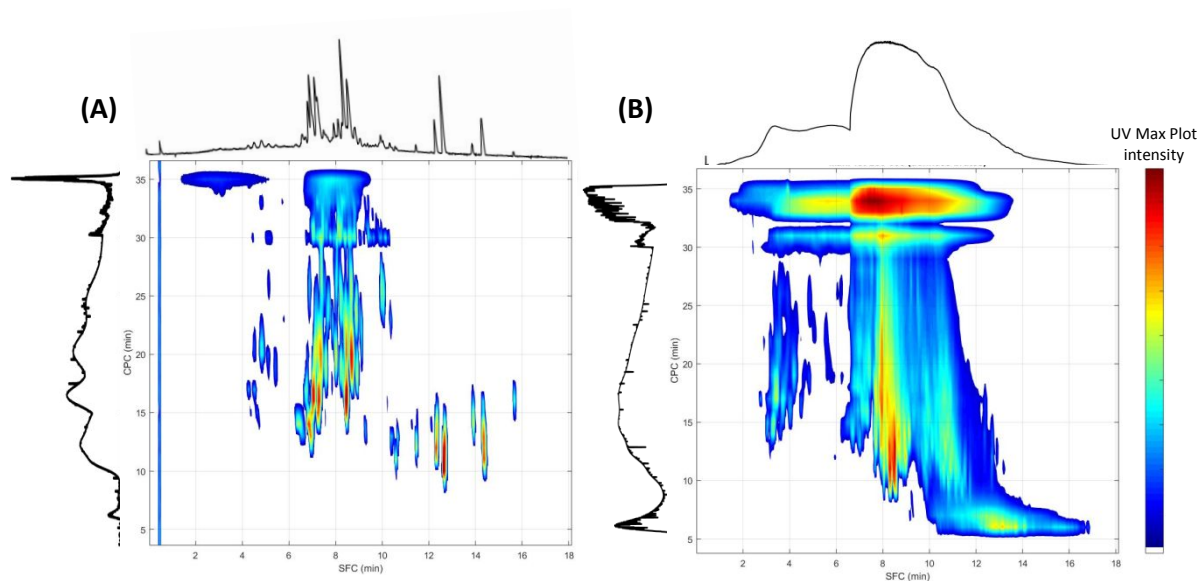


Figure S7: DBE = f(nC) for the different chemical families detected in VGO 1

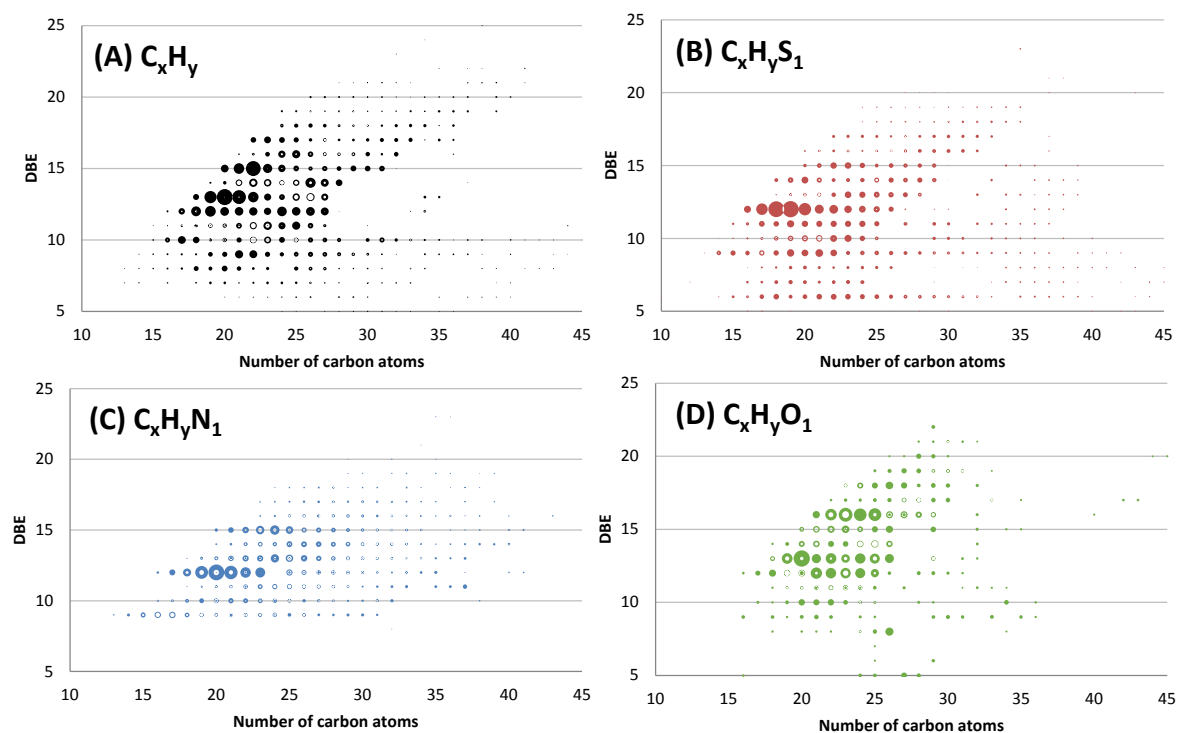


Figure S8: UV spectra of compounds with a DBE of 13 detected in (A) VGO and (B) UCO, compared to (C) standard of pyrene and (D) standard of chrysene.

