

Supporting Information

Controlled reduction of aromaticity of alkylated polyaromatic compounds by selective oxidation using H₂WO₄, H₃PO₄ and H₂O₂: A route for upgrading heavy oil fractions

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Figure S1: ^1H NMR (500MHz, CDCl_3) of *a*) 2-octadecylpyrene (**9**) and *b*) the oxidation products obtained from 2-octadecylpyrene, with marked groups of protons A and D used for calculation of % of preserved aliphatic protons.

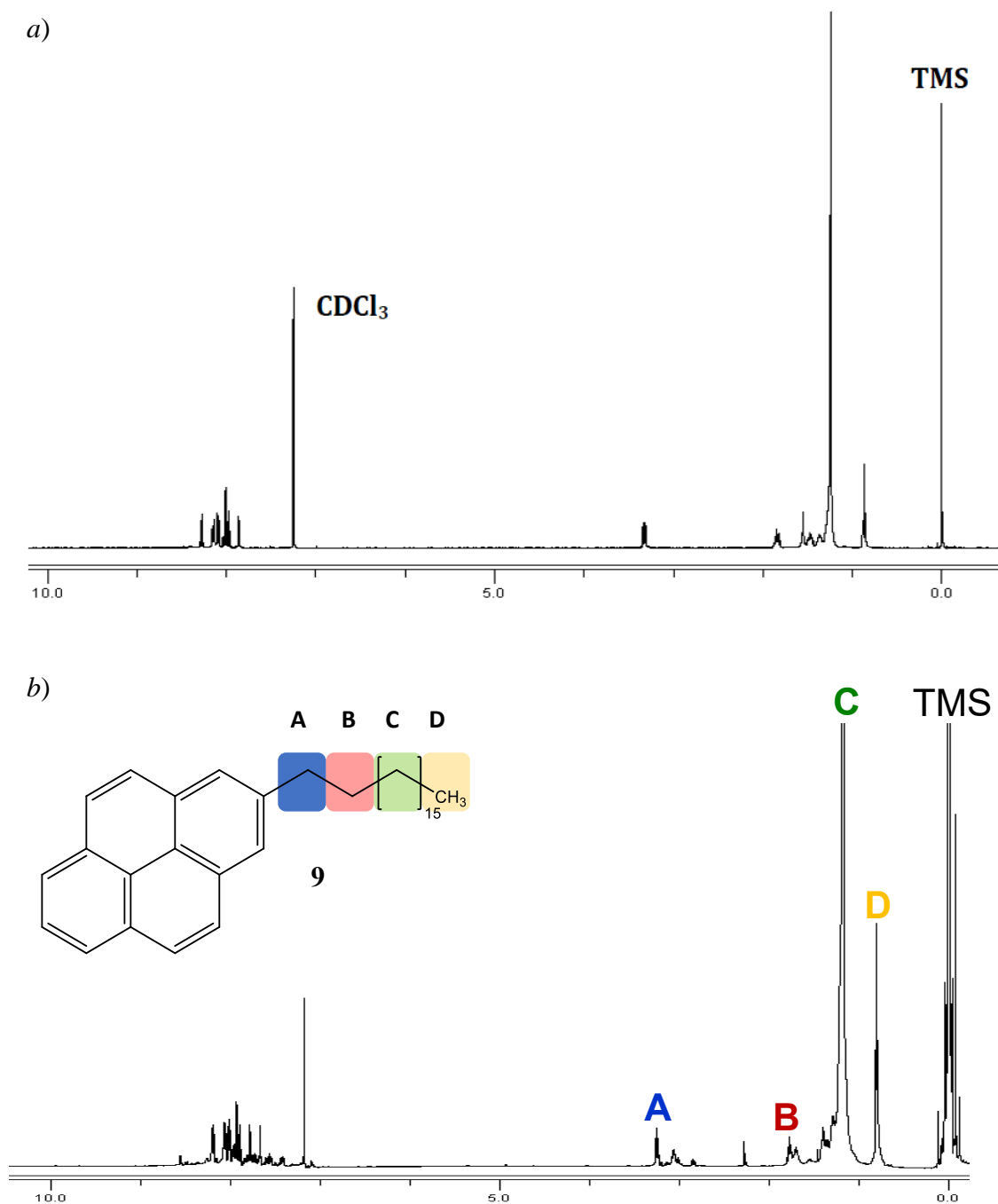


Figure S2. GC-MS analysis of 2-ethylnaphthalene oxidation products in toluene (2-ethylnaphthalene, R_t = 19.35 mins; acetophenone, R_t =22.63 mins).

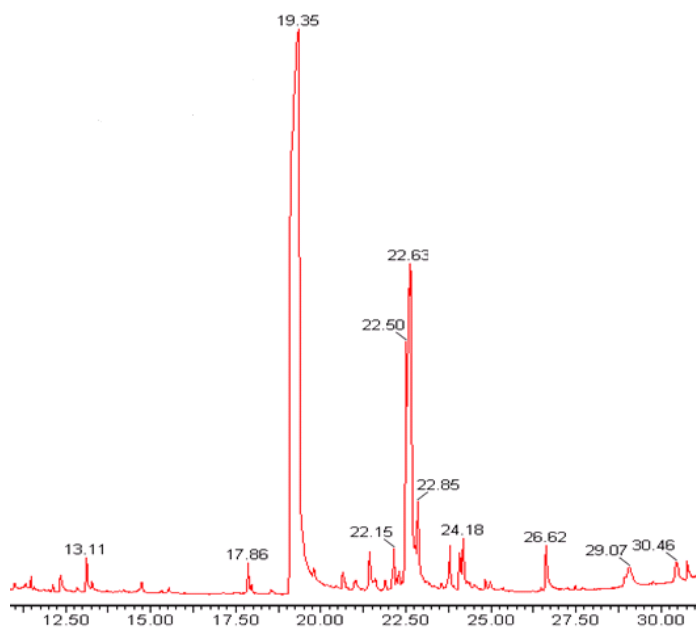


Figure S3. GC-MS analysis of 2-ethylnaphthalene oxidation products in chlorobenzene (2-ethylnaphthalene, Rt= 19.30 mins; 5-ethyl phthalic acid, Rt=21.48 mins; acetophenone, Rt=22.65 mins; Rt=23.80 mins unidentified product).

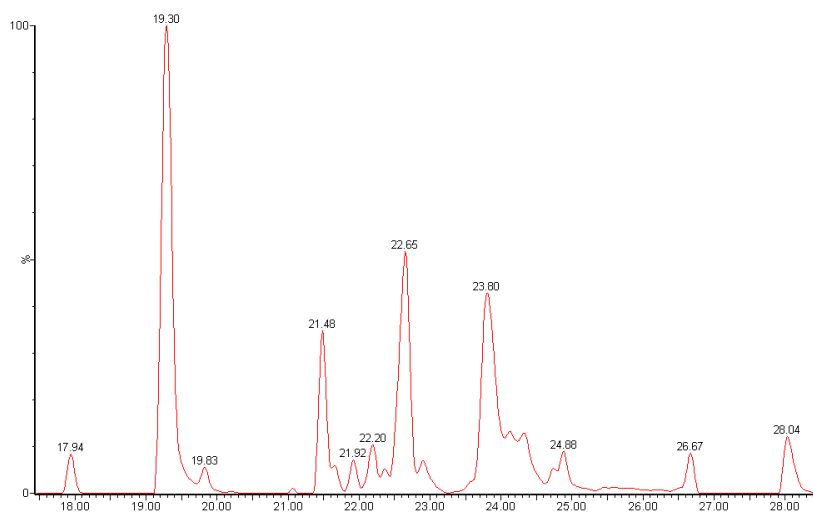


Figure S4. GC-MS analysis of 2-ethylnaphthalene oxidation products in propionitrile (2-ethylnaphthalene, $R_t=19.64$ mins; naphthalene-2-yl-ethanol, $R_t=22.51$ mins; several column bleeding and unidentified products).

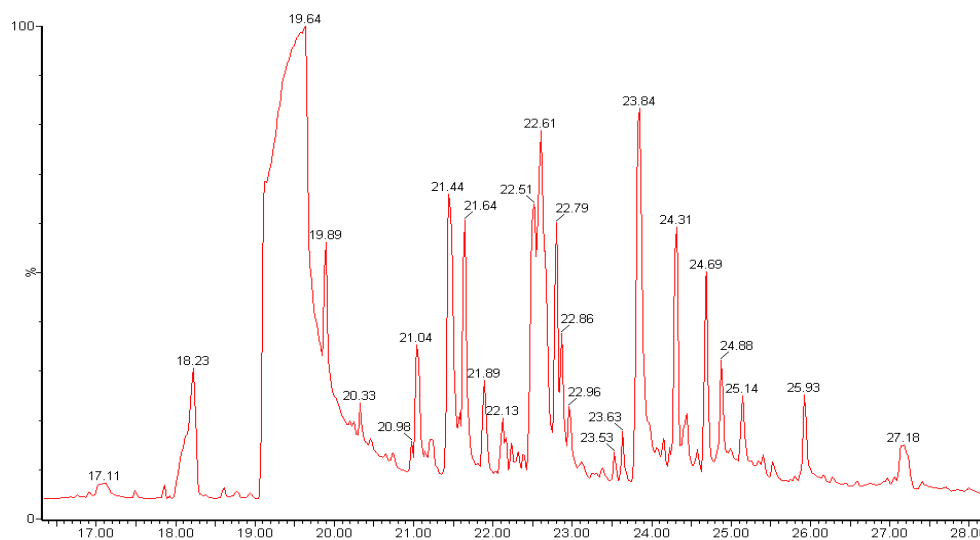


Figure S5. GC-MS analysis of 2-ethylnaphthalene oxidation products in acetonitrile.

(2-ethylnaphthalene $R_t=19.27$ mins, 5-ethyl phthalic acid, $R_t=21.51$ mins; 6-ethylnaphthalene-1,4-dione, $R_t=22.67$ mins; 6-ethyl-2-hydroxynaphthalene-1,4-dione, $R_t=23.89$ mins)

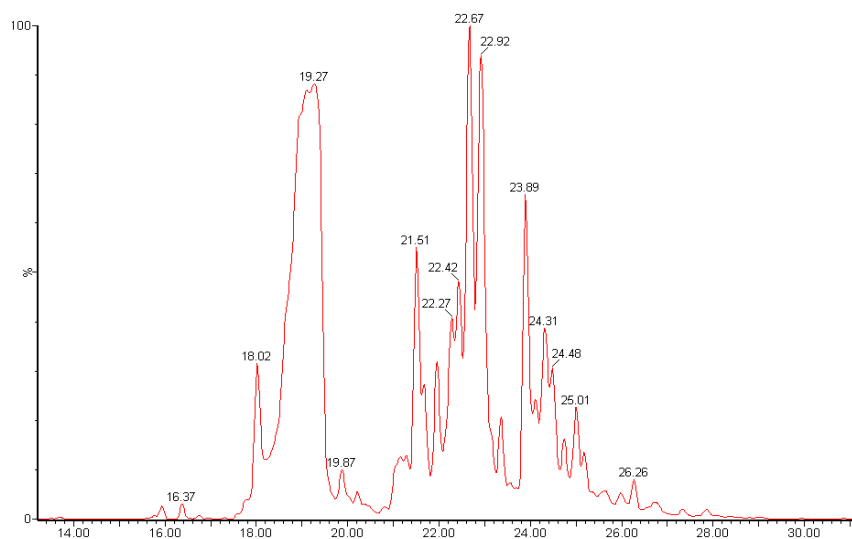


Figure S6: Comparison of ^{13}C NMR spectra of 2-acetonaphthone standard (top) and reaction mixture from 2-ethylnaphthalene oxidation (bottom)

Reaction Conditions: Substrate 18.8 mmol, H_2WO_4 0.153g (0.614mmol), H_2O_2 35% 12 ml, Aliquat 336 0.24 ml, H_3PO_4 10% 0.14 ml, CH_3CN 8 ml, $T=65^\circ\text{C}$, $t=20$ h

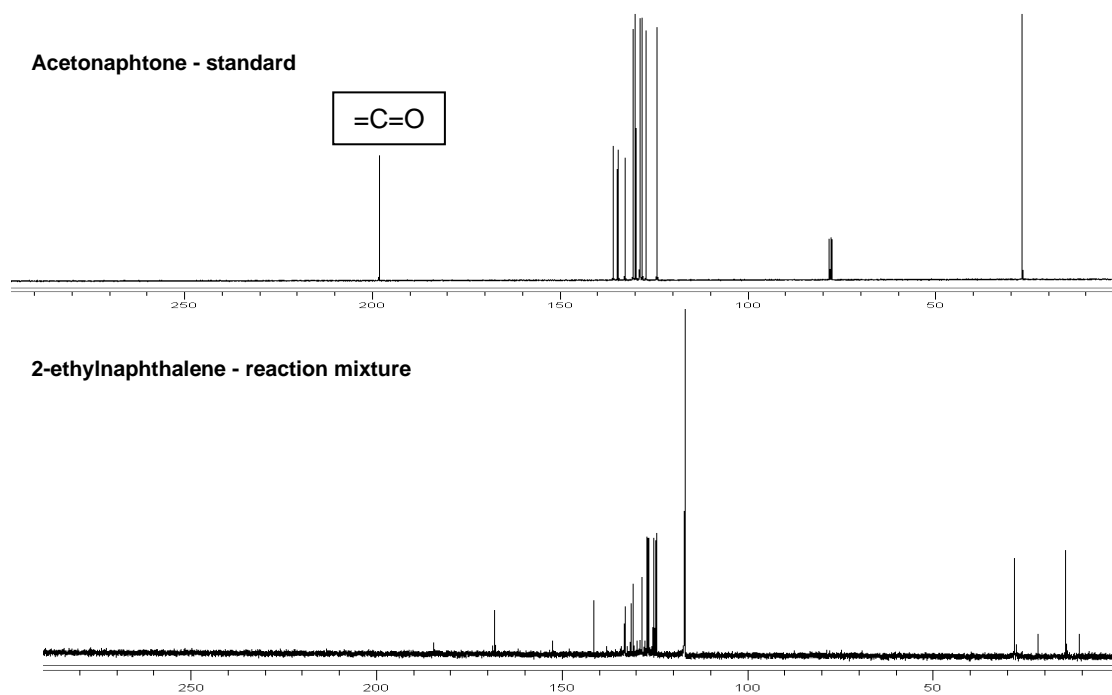


Figure S7: Structures of a) phenanthrene and b) pyrene showing standard atom numberings used in this manuscript.

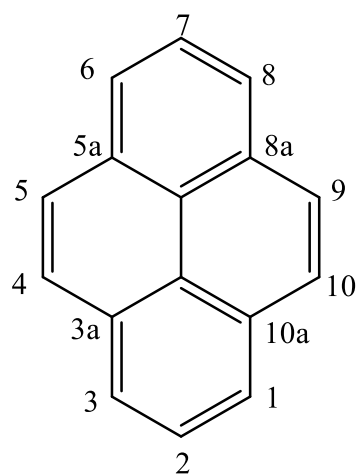
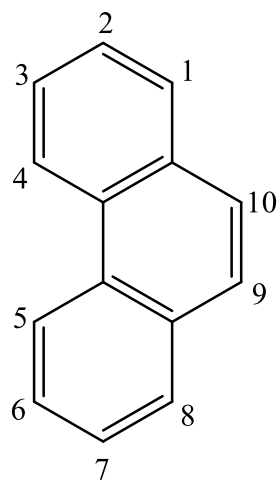


Figure S8: IR analysis of 2-octadecylpyrene oxidation products (organic layer)

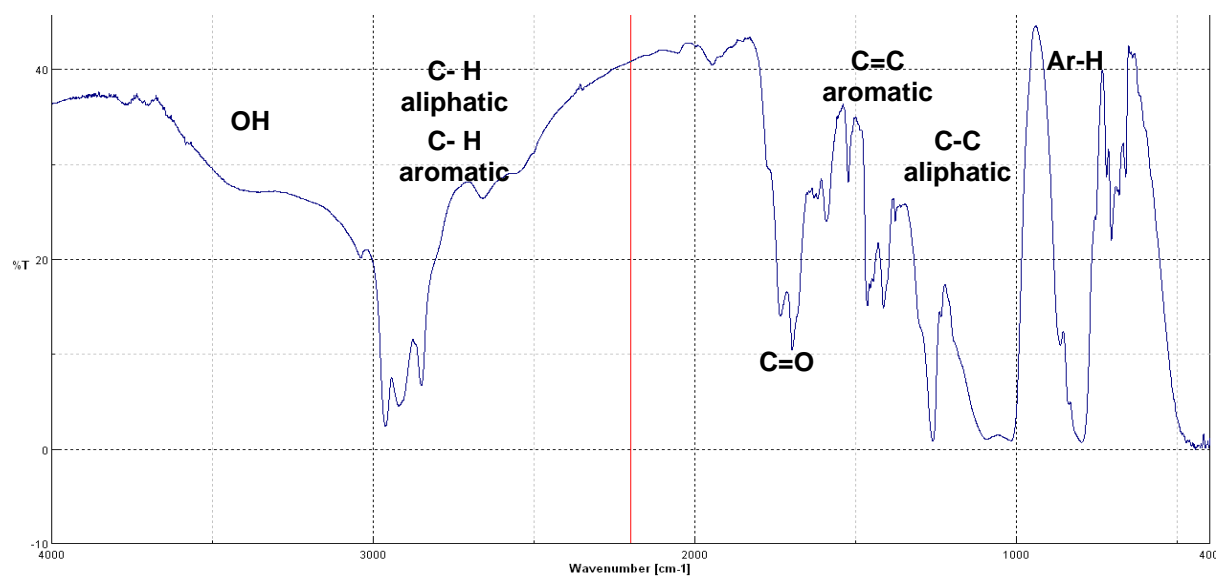


Figure S9: MS analysis of 2-octadecylpyrene oxidation products with strong signal m/z 581.31.

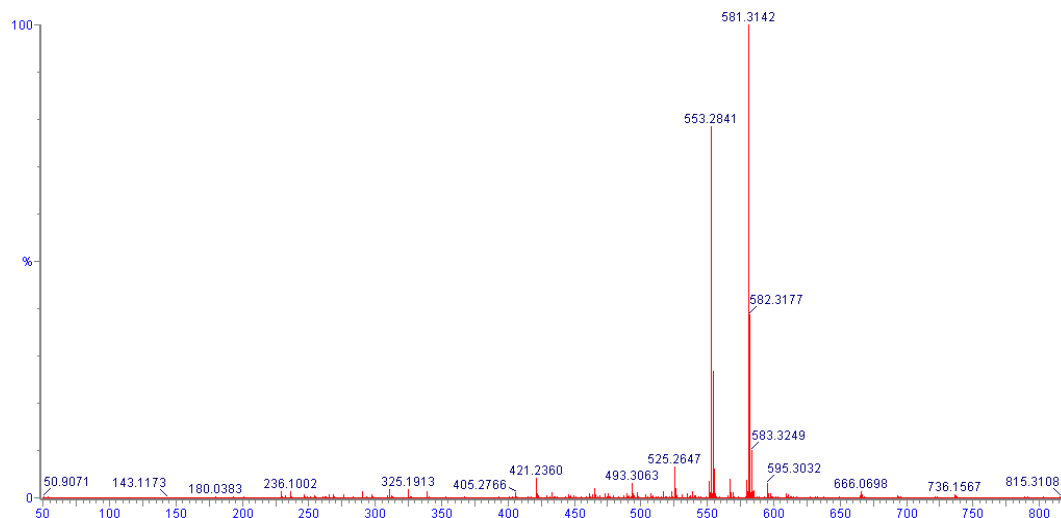


Figure S10: MS analysis of 9-octadecylphenanthrene oxidation with strong signal m/z 462.34

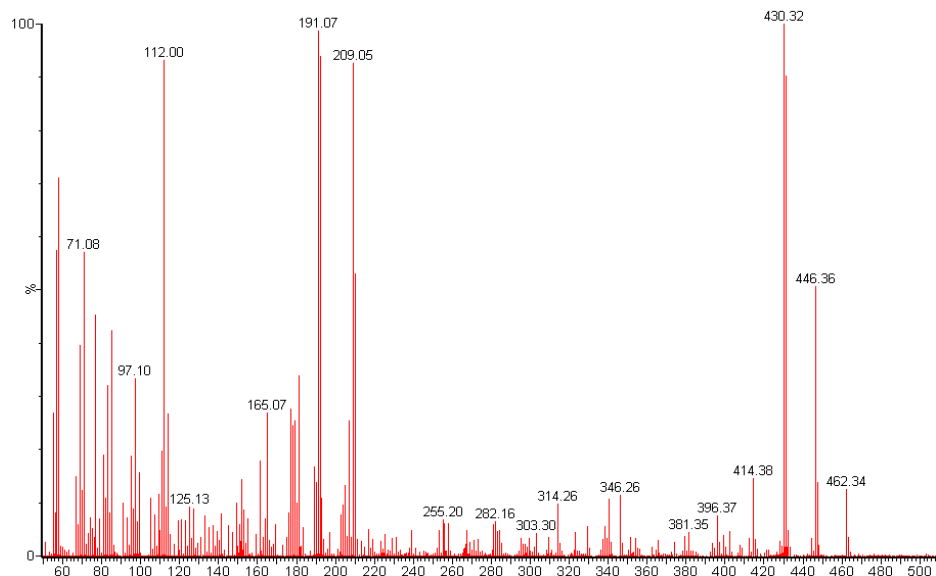


Figure S11: ^1H NMR analysis of 9-octadecylphenanthrene oxidation products (500MHz, 1% TMS in CDCl_3).

