Supplementary Information

APCI(+)FT-ICR MS Analysis of Hydrocarbons Using Isooctane as Ionizing Reagent - A Comparison with HTGC-FID, GC×GC-MS and NMR

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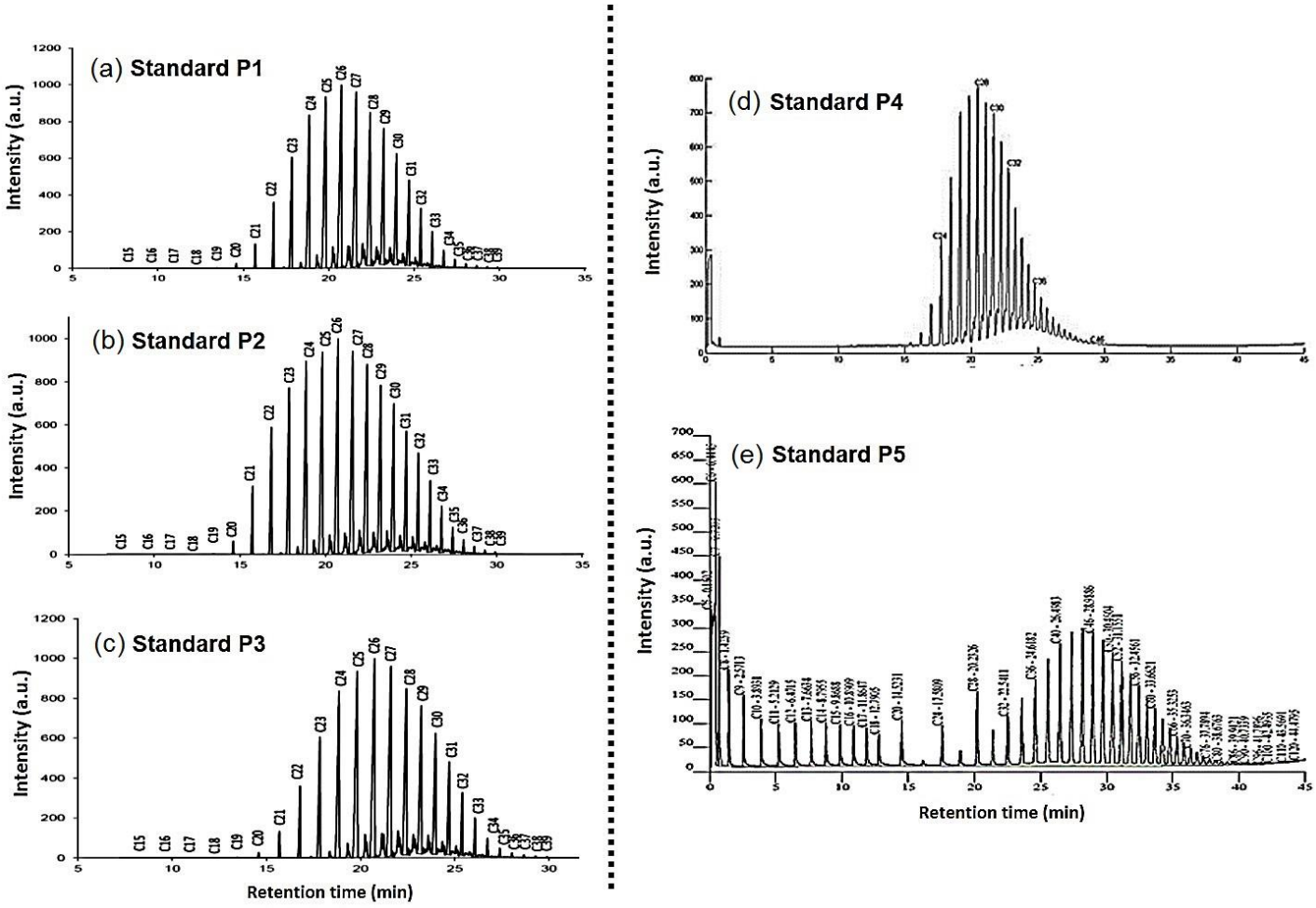

Figure S1. HTGC analysis of five paraffin standards (P1-P5). The CNs of the *n*-paraffins were marked above the chromatogram based on the retention times of the *n*-paraffins model.

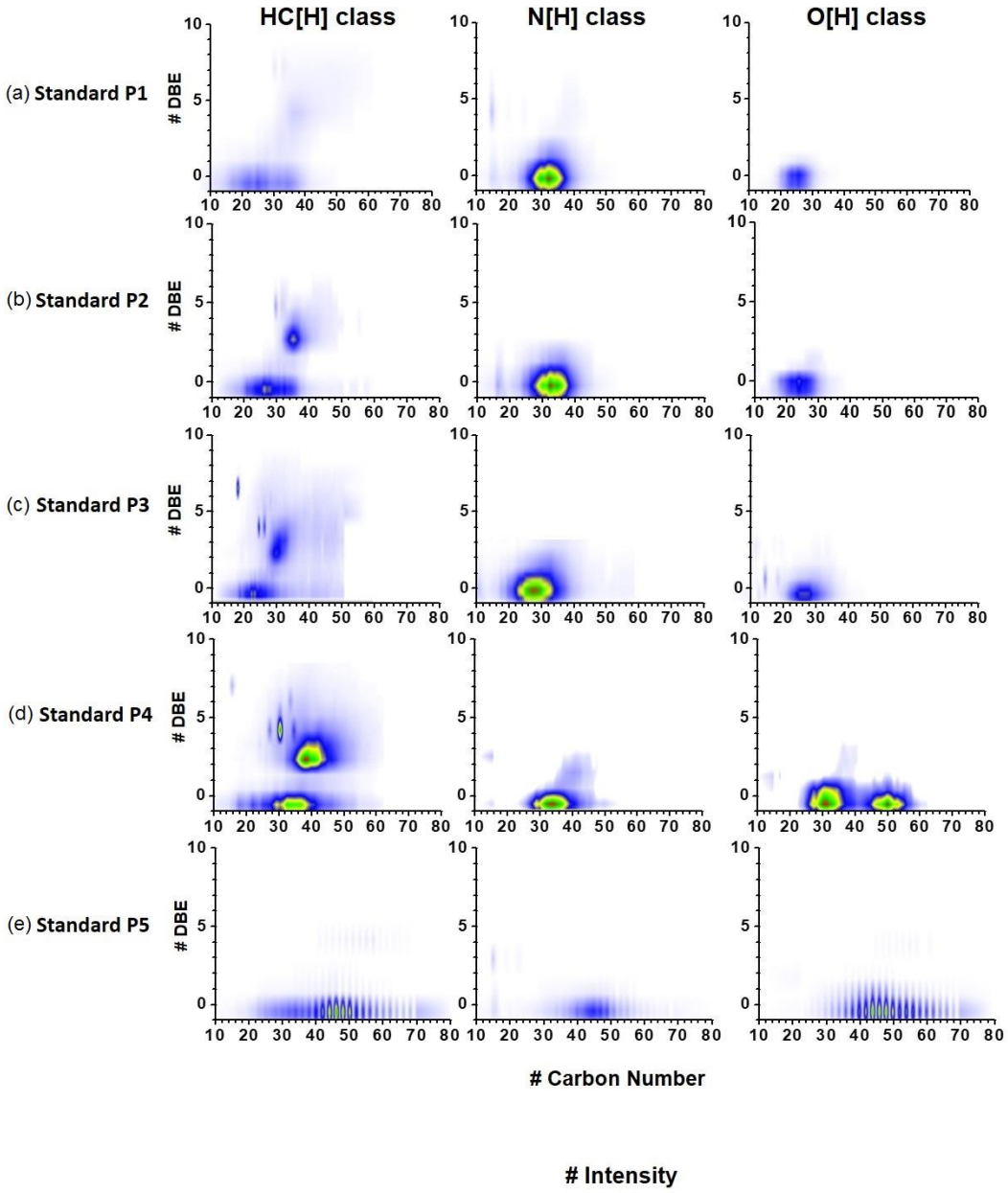

Figure S2. DBE *versus* CN plots for the HC[H], N[H] and O[H] classes for five paraffin standards (P1-P5).

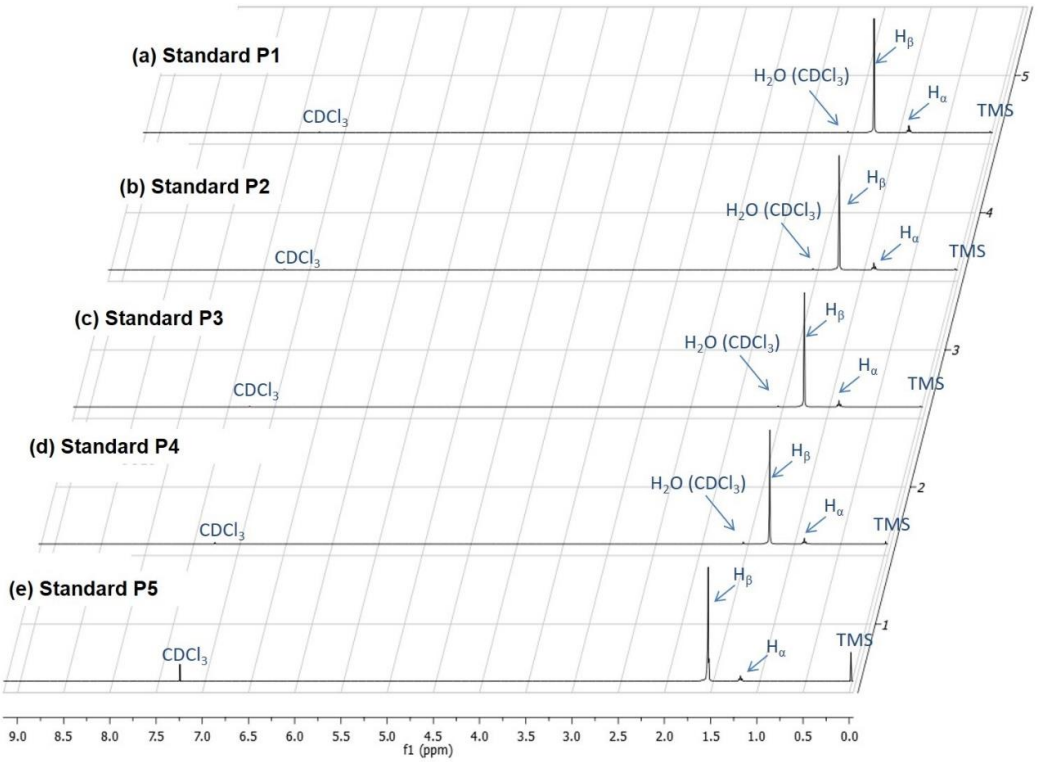

Figure S3. ^{1}H NMR spectra (6410.3 Hz, deuterated chloroform) recorded for the five paraffin standards (P1-P5).

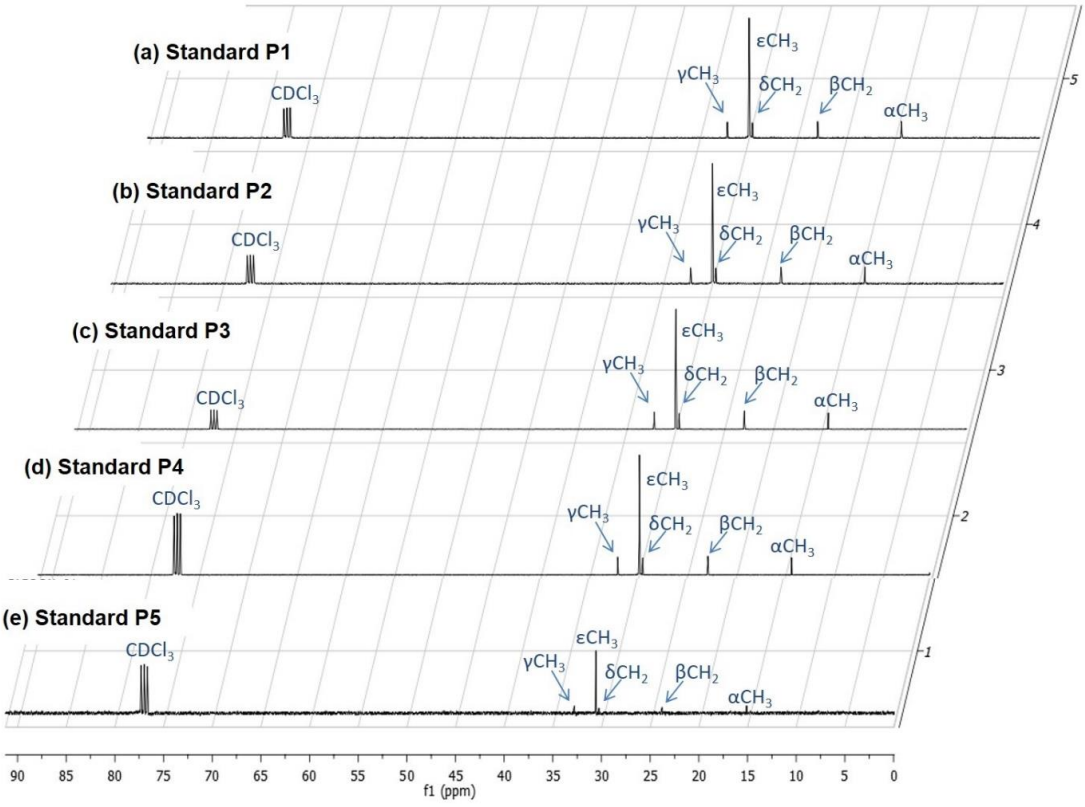

Figure S4. ^{13}C NMR spectra (25510.2 Hz, deuterated chloroform) recorded for the five paraffin standards (P1-P5).

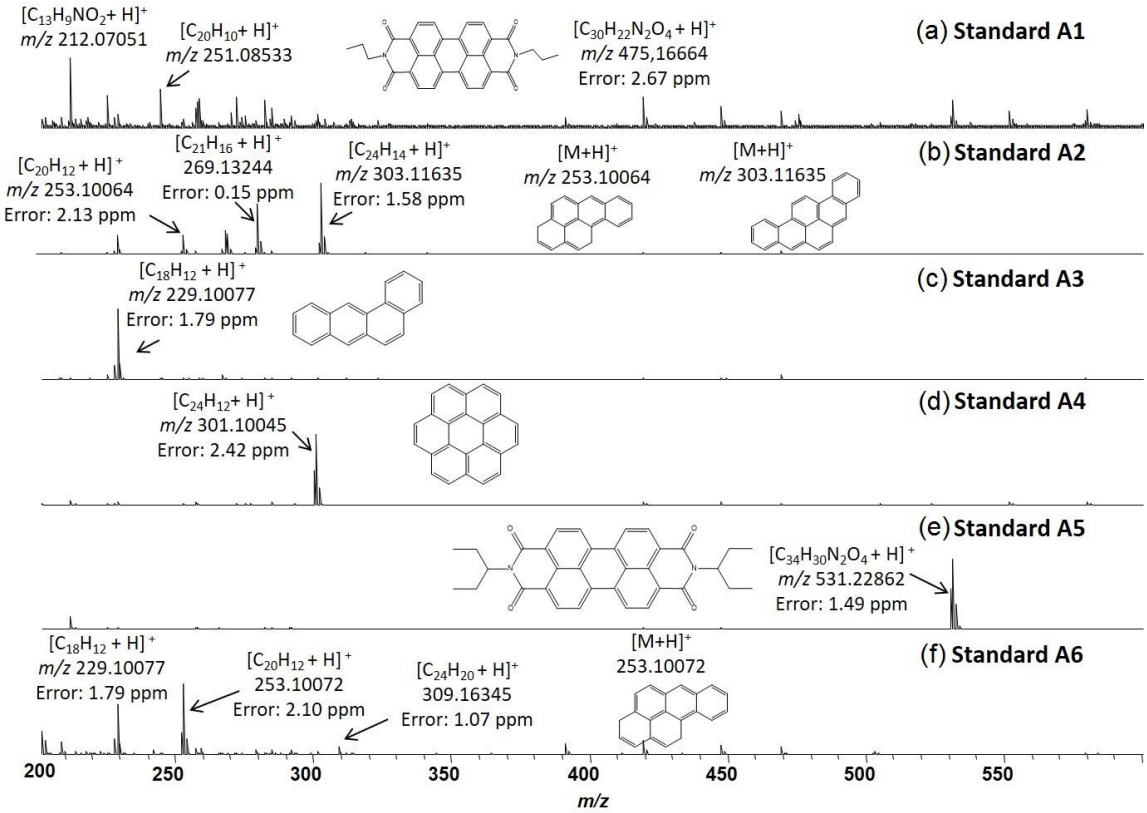

Figure S5. APCI(+)FT-ICR mass spectra for PAH standards A1-A6.

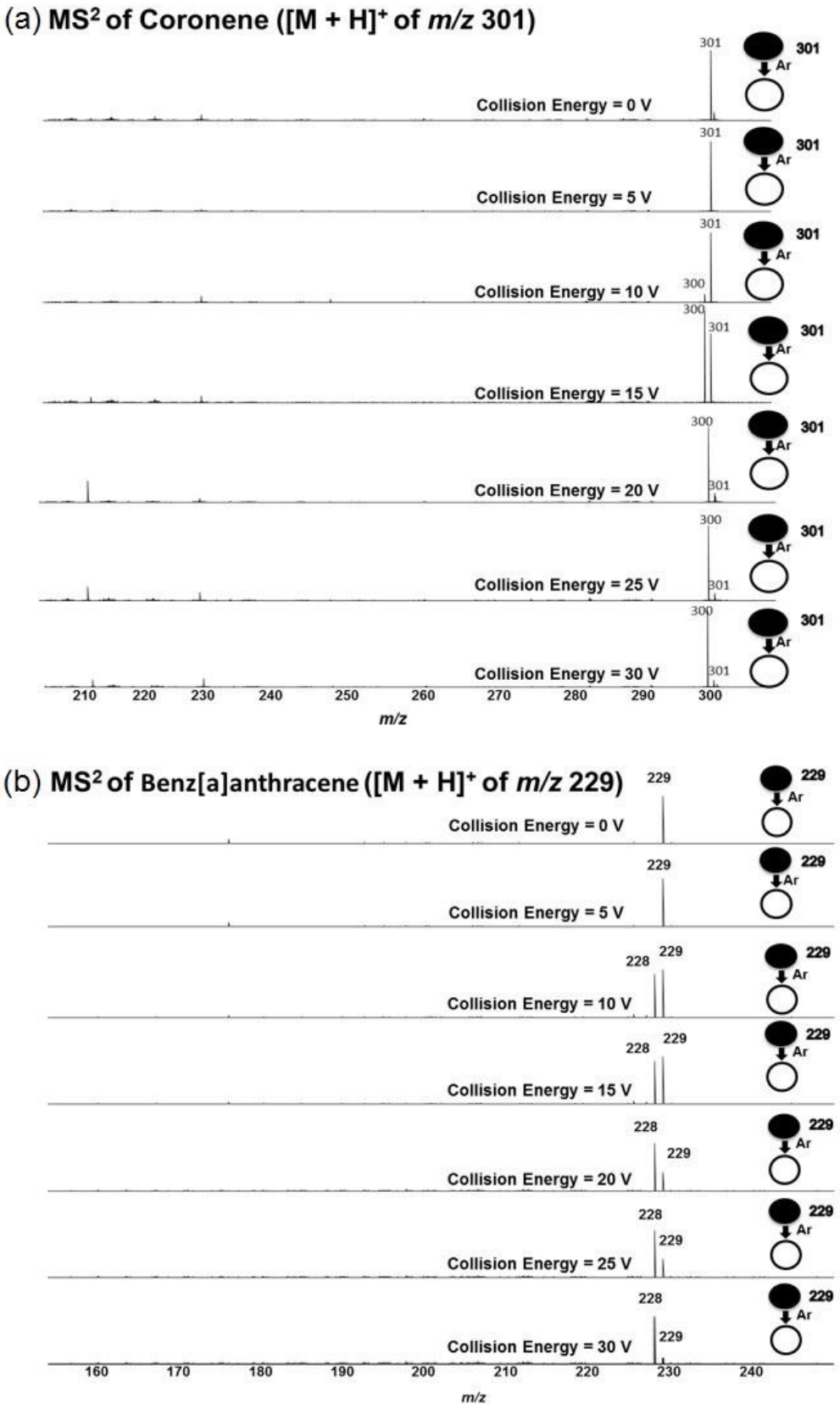

Figure S6. APCI(+)-MS/MS of PAH standards: (a) coronene; (b) benzoantracene, with the collision energy varying from 0 to 30 V.

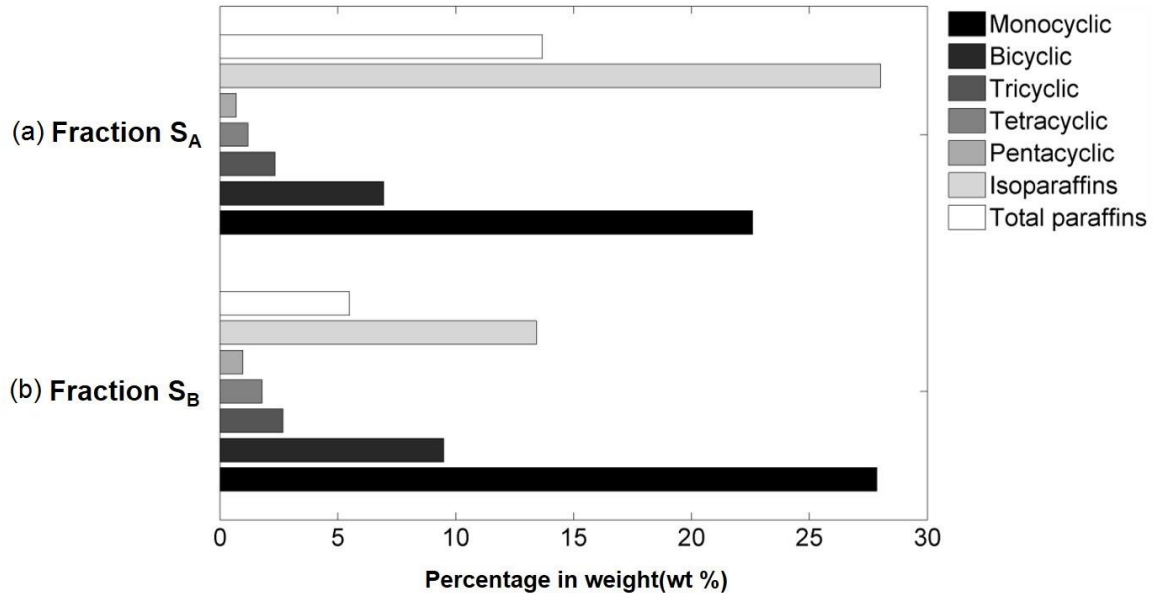

Figure S7. Percentage in weight (wt.%) of linear HCs, branched HCs, mono-, bi-, tri-, tetra- and penta-cyclic HCs identified in the two saturated fractions by GC×GC-MS