

Supplementary Materials

Comparison of carrier gases for the separation and quantification of mineral oil hydrocarbon (MOH) fractions using online LC-GC-FID

M. Gorschke^{1,2}, R. Becker²

¹ Axel Semrau GmbH, Sprockhövel, Germany

² Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

7 Pages

2 Tables

8 Figures

Table S1 contains the comparison of resolutions R_s and peak width $w_{0.5}$ for the critical pairs (1-MN & 2-MN; Cycy & C13) in the internal quantification standard using different nitrogen carrier gas flows and oven ramps, with absolute injected masses of 100 ng (1-MN and 2-MN, Cycy) and 50 ng (C13).

The highlighted option using a flow of 4 mL/min and a ramp of 15 K/min was selected as the best compromise of resolution and peak width (see Table 1 of the main text).

Table S1: Optimisation of nitrogen carrier gas flow and oven ramp

N ₂ flow	R_s [1MN]	$w_{0.5}$ [1MN]	R_s [C13]	$w_{0.5}$ [C13]	Ramp
5 mL/min	1.69	0.067	2.29	0.071	10 K/min
4 mL/min	1.85	0.061	2.26	0.064	10 K/min
3 mL/min	2.09	0.054	2.20	0.054	10 K/min
5 mL/min	1.65	0.050	1.88	0.052	15 K/min
4 mL/min	1.85	0.044	1.80	0.047	15 K/min
3 mL/min	2.03	0.039	1.60	0.040	15 K/min
5 mL/min	1.63	0.040	1.60	0.042	20 K/min
4 mL/min	1.77	0.036	1.47	0.037	20 K/min
3 mL/min	2.03	0.031	1.20	0.032	20 K/min

Table S2: All gas flows applied to optimised chromatographic conditions (see Table 1 of the main text). In all cases the same total gas flow arrived at the flame ionisation detector.

Carrier gas flow (mL/min)	FID gas flows (mL/min)		
	H ₂ (fuel)	N ₂ (makeup)	air
N ₂	4	30	26
He	5	30	25
H ₂	5	25	30

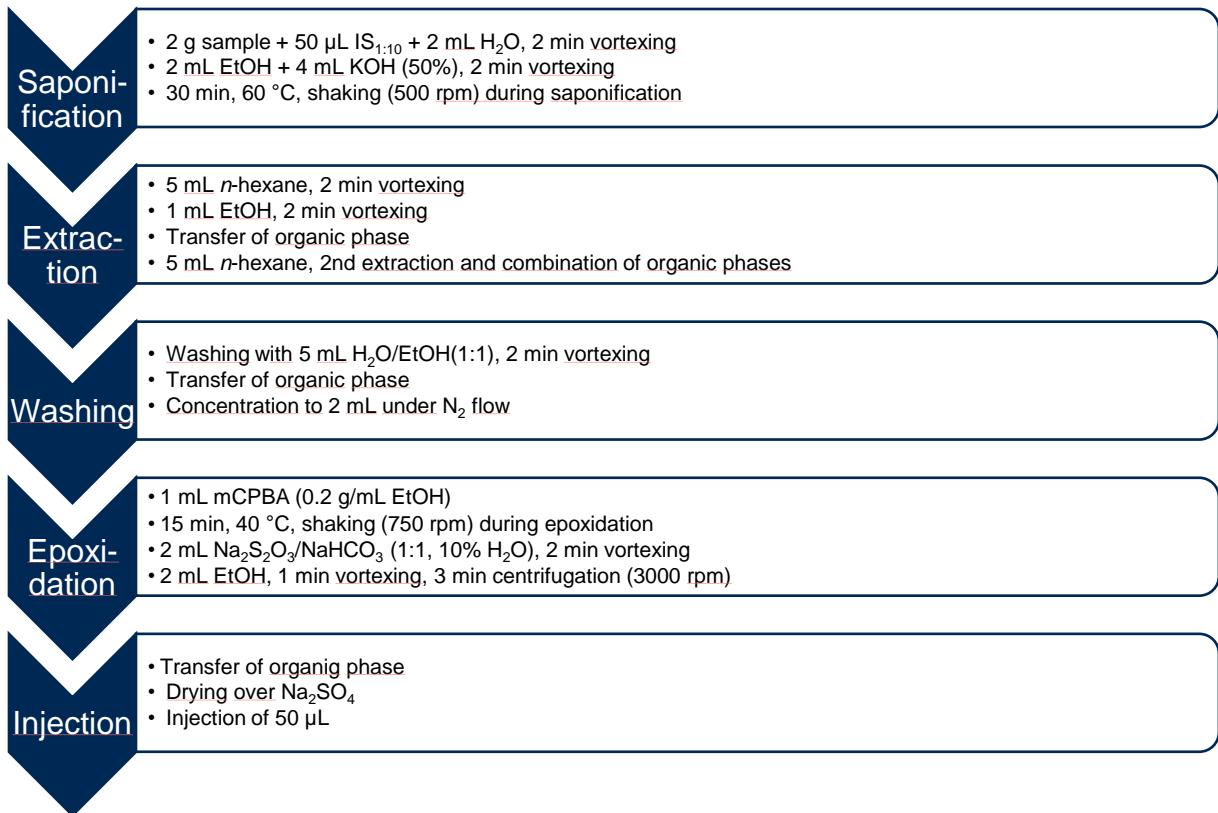


Fig. S1: Sample preparation of infant formula samples

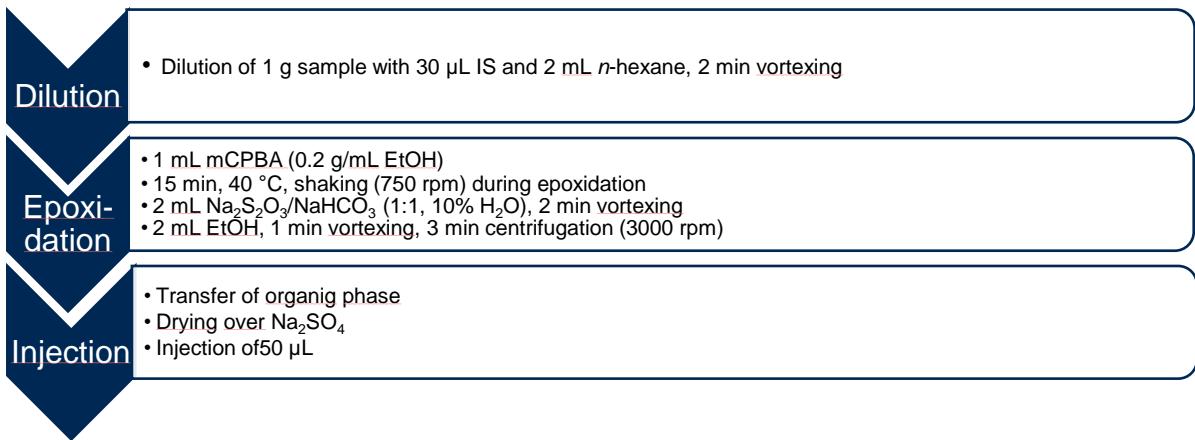


Fig. S2: Sample preparation of coconut oil samples

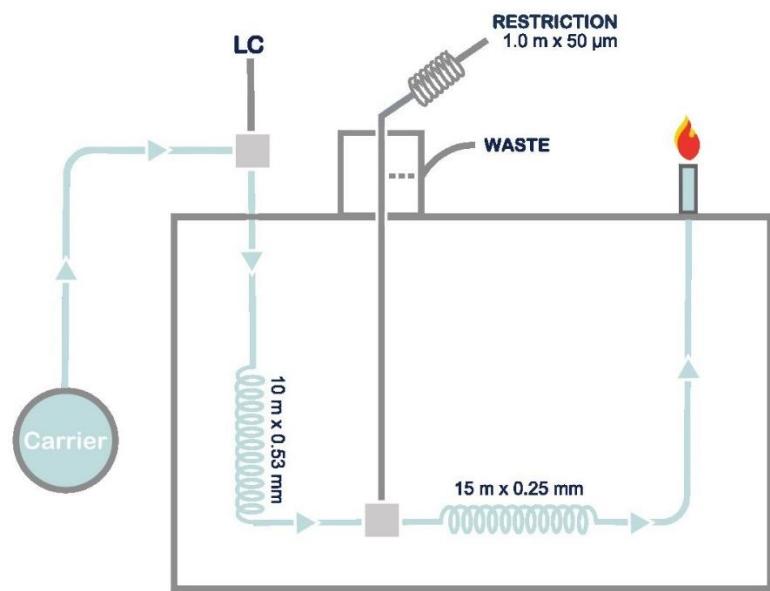
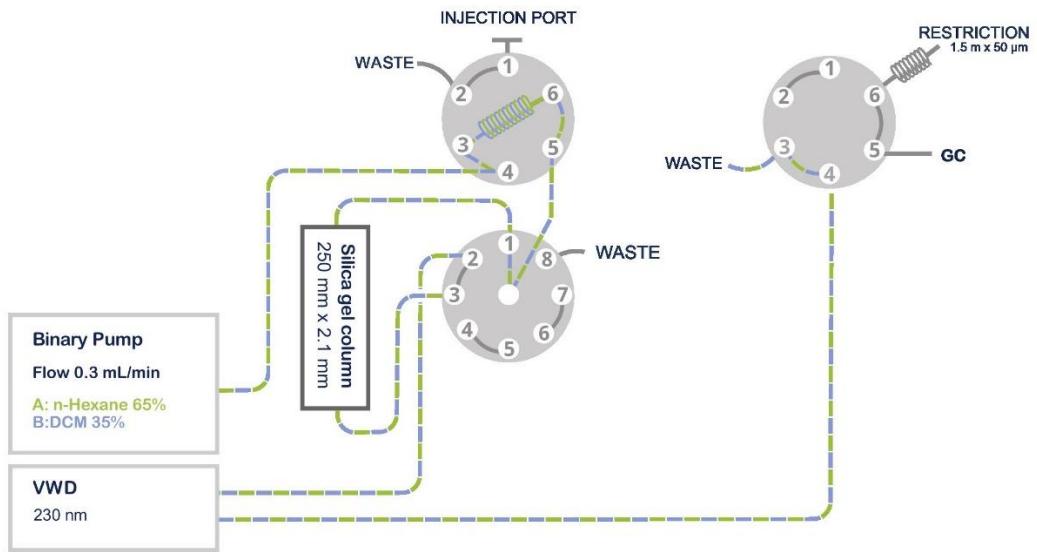


Fig. S3: LC-GC-FID configuration. Above: LC. Below : GC-FID

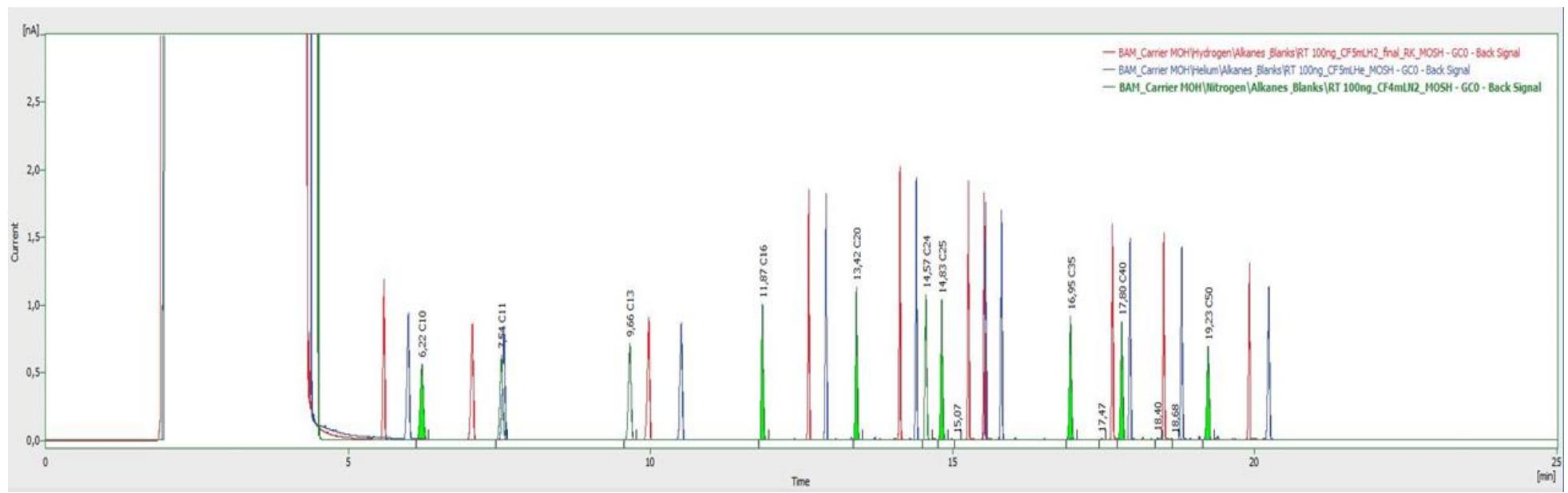


Fig. S4: Alkanes (retention time standard, each compound 100 ng absolute). Overlay of chromatograms obtained with the different carrier gases: H₂ – red; He – blue; N₂ – green

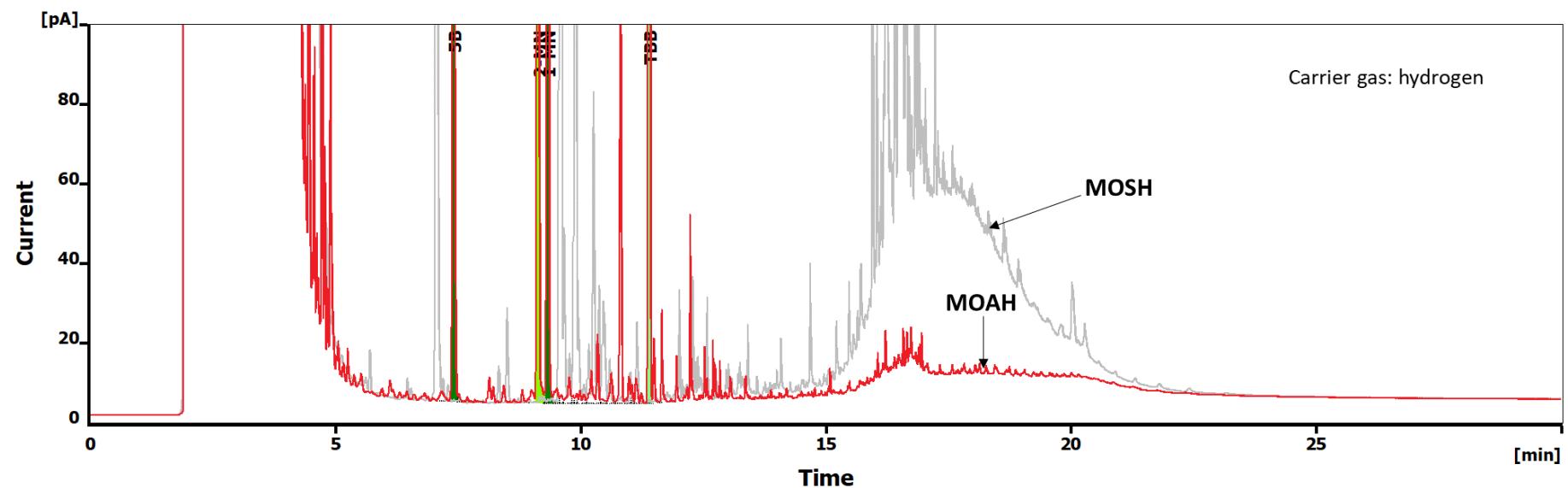
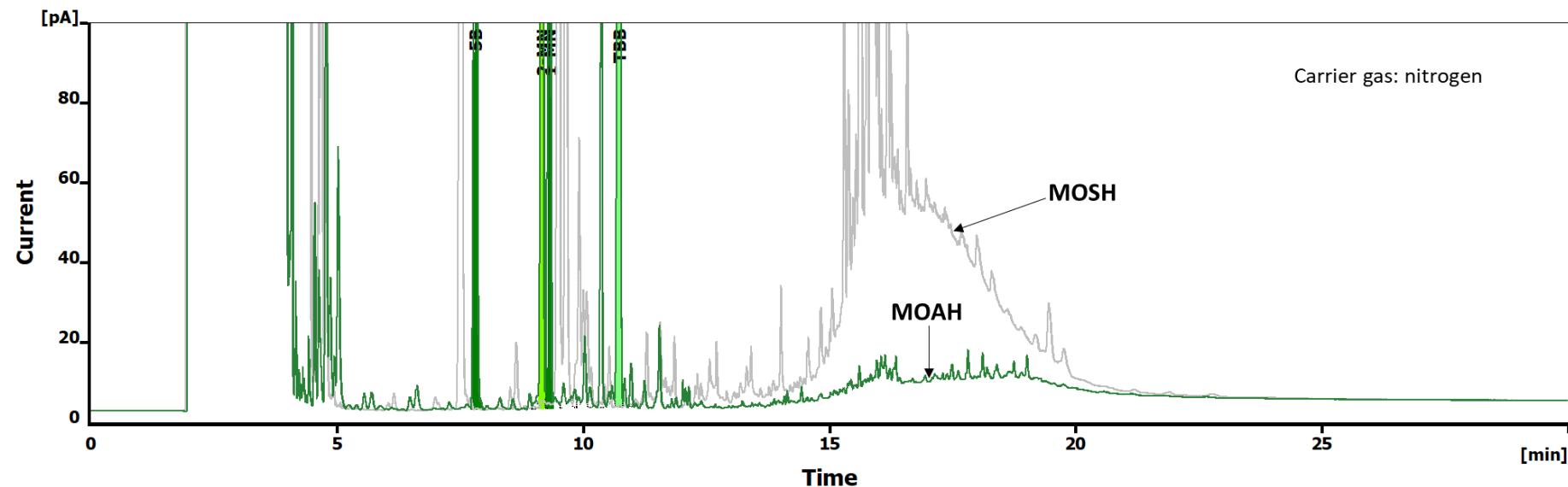


Fig. S5: Comparison of chromatograms (coconut oil 2) obtained with the three carrier gases. Overlay MOSH and MOAH fractions

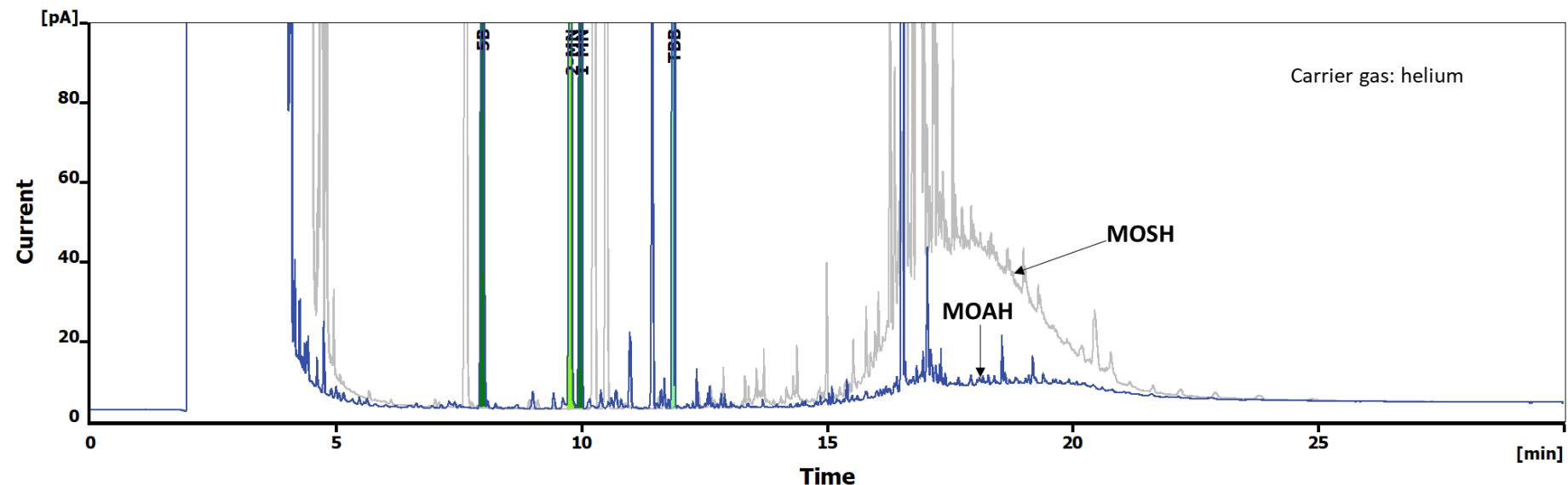


Fig. S5, continued: Comparison of chromatograms (coconut oil 2) obtained with the three carrier gases. Overlay MOSH and MOAH fractions