

Table S1. Parameters for quantitation of the compounds in the coffee fat extracts using ^1H -NMR spectroscopy and pulse length based concentration determination (PULCON).

Compound	Integration area [ppm]	Number of Protons	Molar mass [g/mol]
Kahweol	5.850 – 5.925	1	314.42
Furfuryl alcohol	7.390 – 7.411	1	98.10

Table S2. Parameters for quantitation of the compounds in the aqueous coffee extracts using ^1H -NMR spectroscopy and pulse length based concentration determination (PULCON). 5-CQA, 5-caffeoylquinic acids; NMP, N-methylpyridine; HMF, 5-hydroxymethylfurfural.

Compound	Integration area [ppm]	Number of Protons	Molar mass [g/mol]
Lactic acid	1.310 – 1.380	3	90.08
Acetic acid	1.926 – 1.955	3	60.05
5-CQA	5.286 – 5.379	1	354.31
Formic acid	8.440 – 8.490	1	46.03
NMP	8.500 – 8.572	1	94.13
Trigonelline	9.080 – 9.170	1	137.14
HMF	9.430 – 9.480	1	126.11

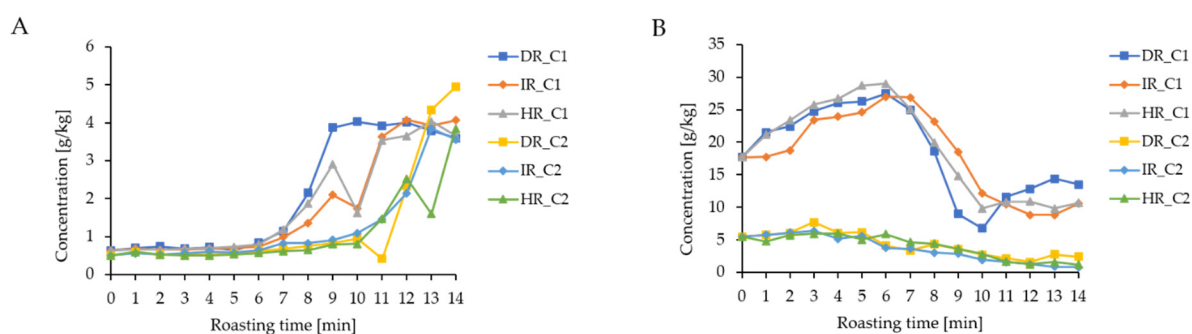


Figure S1. Evolution of (A) acetic acid and (B) 5-caffeoylquinic acid content during the roasting process of the caffeinated coffee sample (C1) and decaffeinated coffee sample (C2) in the drum roaster (DR), infrared roaster (IR) and hot air roaster (HR).

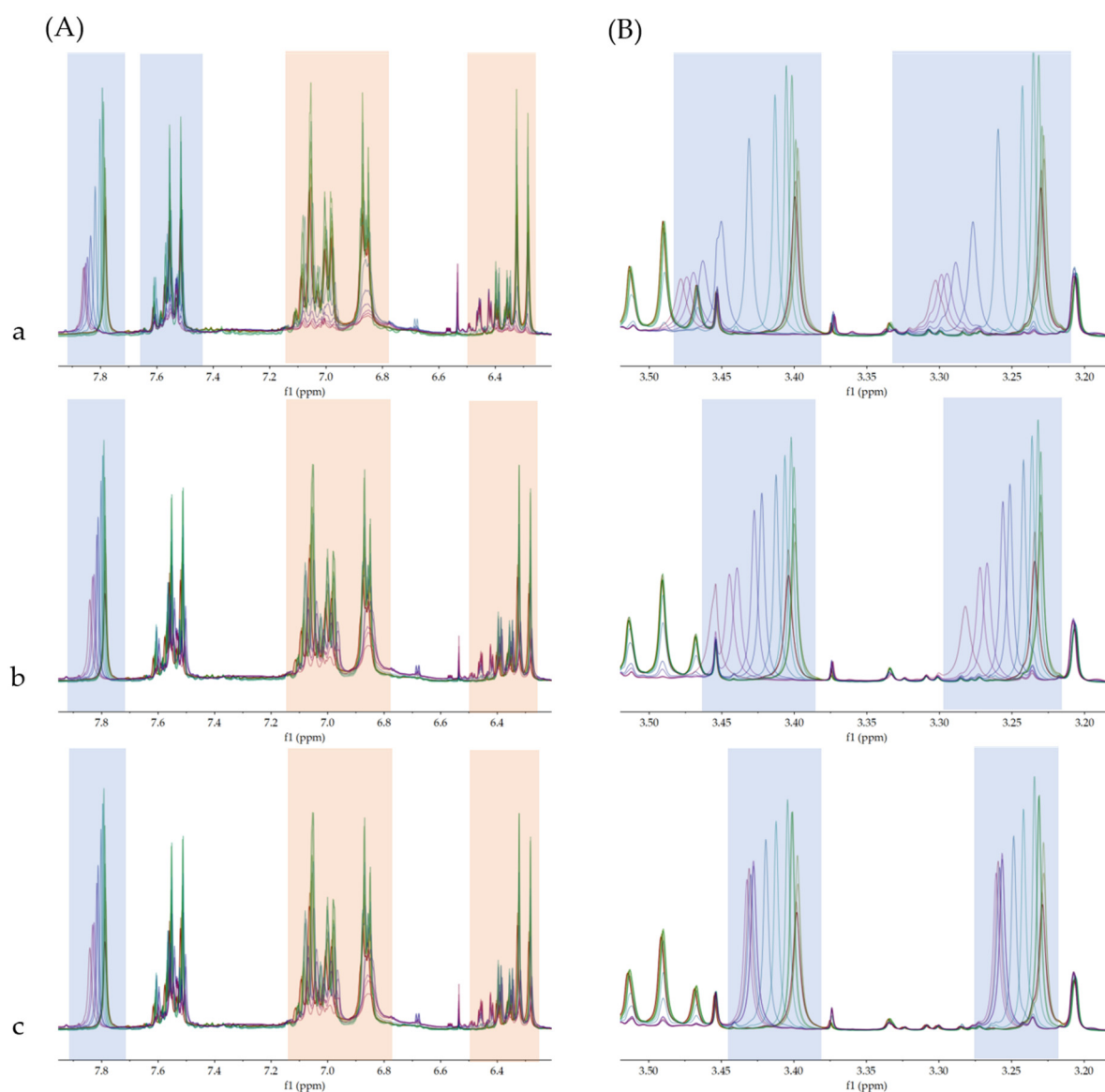


Figure S2. ^1H -NMR spectra in the region of (A) $\delta_{\text{H}} = 6.2 - 8.0$ ppm and (B) $\delta_{\text{H}} = 3.2 - 3.5$ ppm of the aqueous extracts of the caffeinated coffee samples roasted in the (a) drum roaster, (b) infrared roaster and (c) hot air roaster recorded in $\text{H}_2\text{O}/\text{D}_2\text{O}$ (9:1, v/v) using a 400 MHz NMR spectrometer. Chemical shifts were calibrated using the TSP signal at $\delta_{\text{H}} = 0.00$ ppm. For each roaster, the ^1H -NMR spectra of the aqueous extracts of the samples taken every minute are displayed in multiple layer mode. Signals of the protons of caffeine and aromatic protons of chlorogenic acid are highlighted in blue and orange.