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A 1H NMR-Linked PCR Modelling Strategy for Tracking the Fatty Acid Sources of Aldehydic Lipid Oxidation Products in Culinary Oils Exposed to Simulated Shallow-Frying Episodes

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Abstract : Objectives/Hypotheses: The adverse health effect potential of dietary lipid oxidation products (LOPs) has evoked much clinical interest. Therefore, we employed a ¹H NMR-linked Principal Component Regression (PCR) chemometrics modelling strategy to explore relationships between data matrices comprising (1) aldehydic LOP concentrations generated in culinary oils/fats when exposed to laboratory-simulated shallow frying practices, and (2) the prior saturated (SFA), monounsaturated (MUFA) and polyunsaturated fatty acid (PUFA) contents of such frying media (FM), together with their heating time-points at a standard frying temperature (180 ^oC). Methods: Corn, sunflower, extra virgin olive, rapeseed, linseed, canola, coconut and MUFA-rich algae frying oils, together with butter and lard, were heated according to laboratory-simulated shallow-frying episodes at 180 ^oC, and FM samples were collected at time-points of 0, 5, 10, 20, 30, 60, and 90 min. (n = 6 replicates per sample). Aldehydes were determined by ¹H NMR analysis (Bruker AV 400 MHz spectrometer). The first (dependent output variable) PCR data matrix comprised aldehyde concentration scores vectors (PC1* and PC2*), whilst the second (predictor) one incorporated those from the fatty acid content/heating time variables (PC1-PC4) and their first-order interactions. Results: Structurally complex trans,trans- and cis,trans-alka-2,4-dienals, 4,5-epxy-trans-2-alkenals and 4-hydroxy-/4-hydroperoxy-trans-2-alkenals (group I aldehydes predominantly arising from PUFA peroxidation) strongly and positively loaded on PC1*, whereas n-alkanals and trans-2-alkenals (group II aldehydes derived from both MUFA and PUFA hydroperoxides) strongly and positively loaded on PC2*. PCR analysis of these scores vectors (SVs) demonstrated that PCs 1 (positively-loaded linoleoylglycerols and [linoleoylglycerol]:[SFA] content ratio), 2 (positively-loaded oleoylglycerols and negatively-loaded SFAs), 3 (positively-loaded linolenoylglycerols and [PUFA]:[SFA] content ratios), and 4 (exclusively orthogonal sampling time-points) all powerfully contributed to aldehydic PC1* SVs (p 10⁻³to < 10⁻⁹), as did all PC1-3 x PC4 interaction ones (p 10⁻⁵ to < 10⁻⁹). PC2* was also markedly dependent on all the above PC SVs (PC2 > PC1 and PC3), and the interactions of PC1 and PC2 with PC4 (p < 10⁻⁹ in each case), but not the PC3 x PC4 contribution. Conclusions: NMR-linked PCR analysis is a valuable strategy for (1) modelling the generation of aldehydic LOPs in heated cooking oils and other FM, and (2) tracking their unsaturated fatty acid (UFA) triacylglycerol sources therein.

Keywords : frying oils, lipid oxidation products, frying episodes, chemometrics, principal component regression, NMR Analysis, cytotoxic/genotoxic aldehydes
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