

SUPPLEMENTARY INFORMATION

Analysis of oxylipins in human plasma: comparison of ultrahigh-performance liquid chromatography and ultrahigh-performance supercritical fluid chromatography coupled to mass spectrometry

Róbert Berkecz^{a,b}, Miroslav Lísa^a, Michal Holčapek^{a*}

^a*Department of Analytical Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentská 573, 53210 Pardubice, Czech Republic*

^b*Department of Medical Chemistry, Faculty of Medicine, University of Szeged, Dóm tér 8, H-6720, Szeged, Hungary*

* **Corresponding author:** Michal Holčapek, Tel.: +420-466037087; E-mail: Michal.Holcapek@upce.cz

Table: 1

Figure: 1

Table S1 Structural information of oxylipin and fatty acid standards.

Abbreviation	Subclass	Isomeric group	Theoretical m/z of [M-H] ⁻	Structure
tetranor-PGDM	Prostaglandins	-	327.1449	
6-keto-PGF1 α	Prostaglandins	1	369.2283	
TXB2	Thromboxanes			
8-iso-PGF2 α	Prostaglandins	2	353.2334	
PGF2 α				
13,14-dihydro-15-keto-PGF2 α				
2,3-dinor-6-keto-PGF1 α	Prostaglandins	-	341.1970	
PGD3	Prostaglandins	-	349.2021	

Table S1 Structural information of oxylipin and fatty acid standards (continuing).

Abbreviation	Subclass	Isomeric group	Theoretical m/z of [M-H] ⁻	Structure
PGH2	Prostaglandins	3	351.2177	
PGE2				
15-keto-PGF2α				
PGD2				
13,14-dihydro-15-keto-PGE2				
Resolvin D1	Docosanoids	-	375.2177	
PGA2	Prostaglandins	4	333.2071	
PGJ2				
PGB2				
15-deoxy-δ-12,14-PGD2				

Table S1 Structural information of oxylipin and fatty acid standards (continuing).

Abbreviation	Subclass	Isomeric group	Theoretical m/z of [M-H] ⁻	Structure
8,15-DiHETE	Hydroxy/hydroperoxyeicosatetraenoic acids	5	335.2228	
5,15-DiHETE				
6-trans LTB4	Leukotrienes			
LTB4				
5,6-DiHETE	Hydroxy/hydroperoxyeicosatetraenoic acids			
12,13-DiHOME	Other octadecanoids	-	313.2384	
19,20-DiHDPE	Docosanoids	-	361.2384	
tetranor-12-HETE	Hydroxy fatty acids	-	265.1809	
14,15-DiHETrE	Hydroxy/hydroperoxyeicosatrienoic acids	6	337.2384	
5,6-DiHETrE				

Table S1 Structural information of oxylipin and fatty acid standards (continuing).

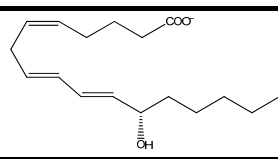
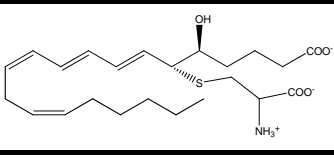
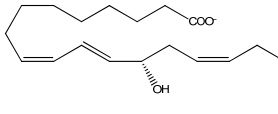
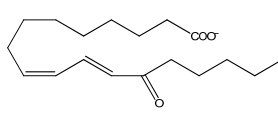
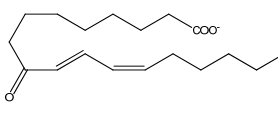
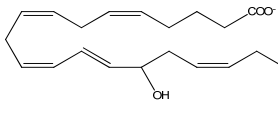
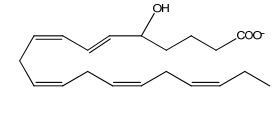
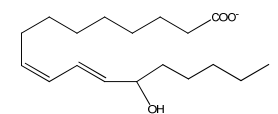
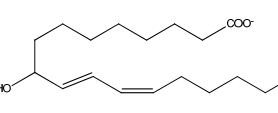
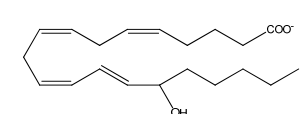
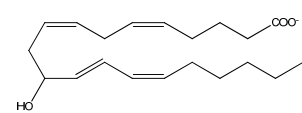
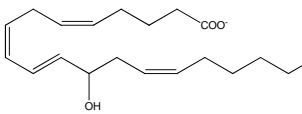
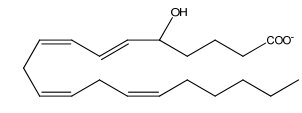
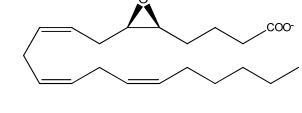
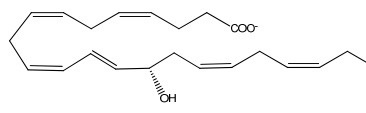
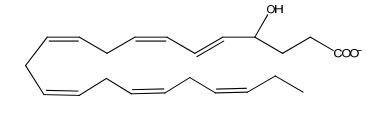
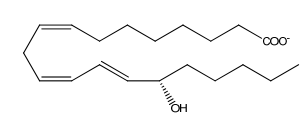
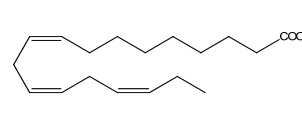
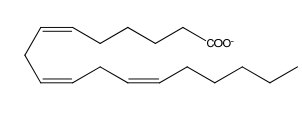
Abbreviation	Subclass	Isomeric group	Theoretical m/z of [M-H] ⁻	Structure
12-HHTrE	Hydroxy/hydroperoxyeicosatrienoic acids	-	279.1966	
LTE4	Leukotrienes	-	438.2320	
13-HOTrE	Other octadecanoids	7	293.2122	
13-OxoODE				
9-OxoODE				
15-HEPE	Hydroxy/hydroperoxyeicosapentaenoic acids	8	317.2122	
5-HEPE	acids			
13-HODE	Other octadecanoids	9	295.2279	
9-HODE				

Table S1 Structural information of oxylipin and fatty acid standards (continuing).

Abbreviation	Subclass	Isomeric group	Theoretical m/z of [M-H] ⁻	Structure
15-HETE	Hydroxy/hydroperoxyeicosatetraenoic acids	10	319.2279	
11-HETE				
12-HETE				
5-HETE				
11,12-EET				Epoxyeicosatrienoic acids
5,6-EET				
14-HDoHE	Docosanoids	11	343.2279	
4-HDoHE				
15-HETrE	Hydroxy/hydroperoxyeicosatrienoic acids	-	321.2435	
α-Linolenic acids	Unsaturated fatty acids	12	277.2173	
γ-Linolenic acids				

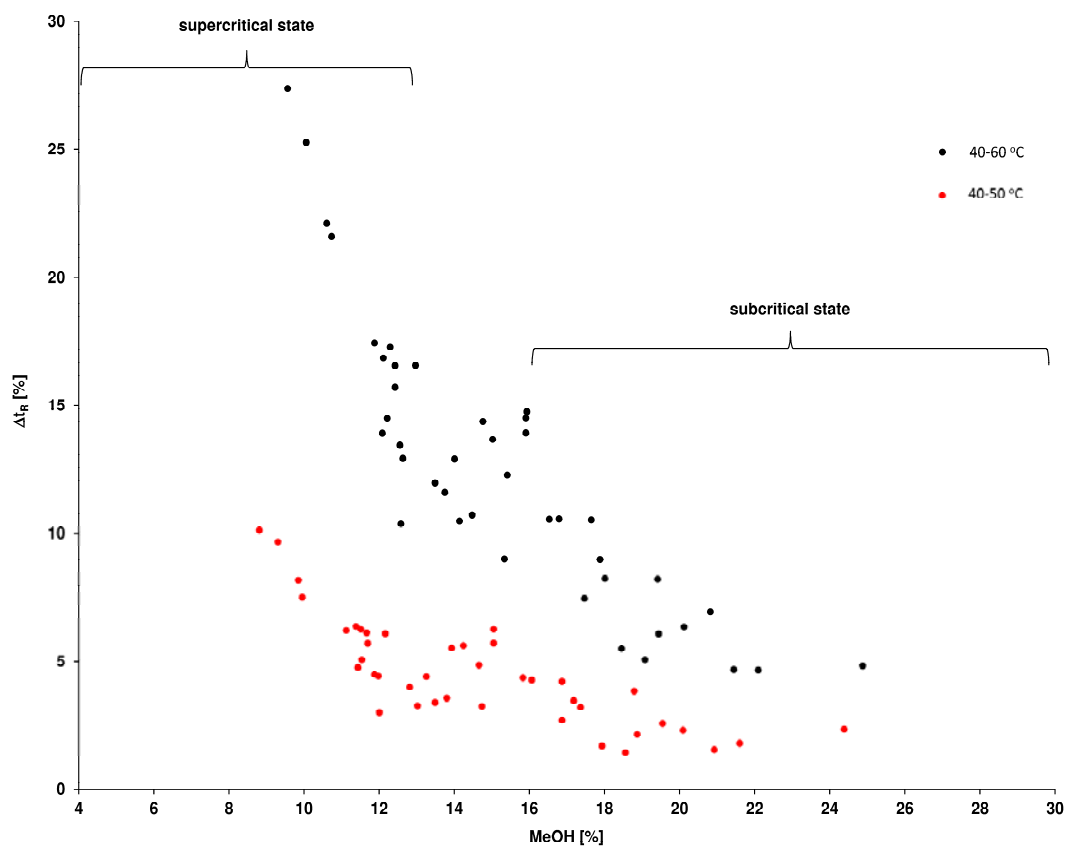


Fig. S1. Dependence of retention times on the concentration of methanol in modifier in UHPSFC/ESI-MS. The methanol content was calculated from retention times and the gradient program.