

SUPPLEMENTARY INFORMATION

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

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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).

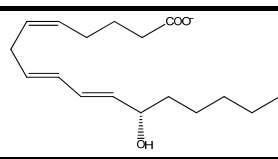
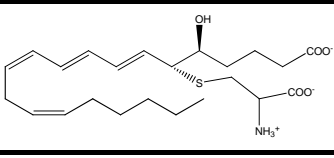
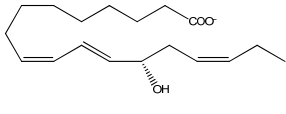
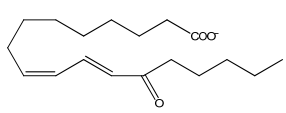
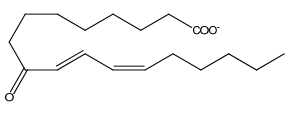
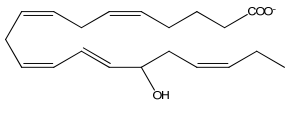
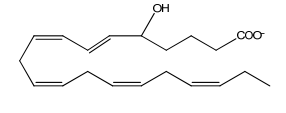
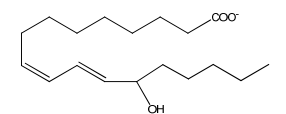
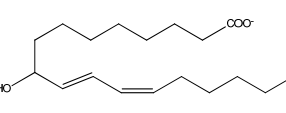
| Abbreviation | Subclass | Isomeric group | Theoretical m/z of [M-H] ⁻ | Structure |
|--------------|---|----------------|---------------------------------------|---|
| 12-HHTrE | Hydroxy/hydroperoxyeicosatrienoic acids | - | 279.1966 |  |
| LTE4 | Leukotrienes | - | 438.2320 |  |
| 13-HOTrE | Other 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 | | | | |

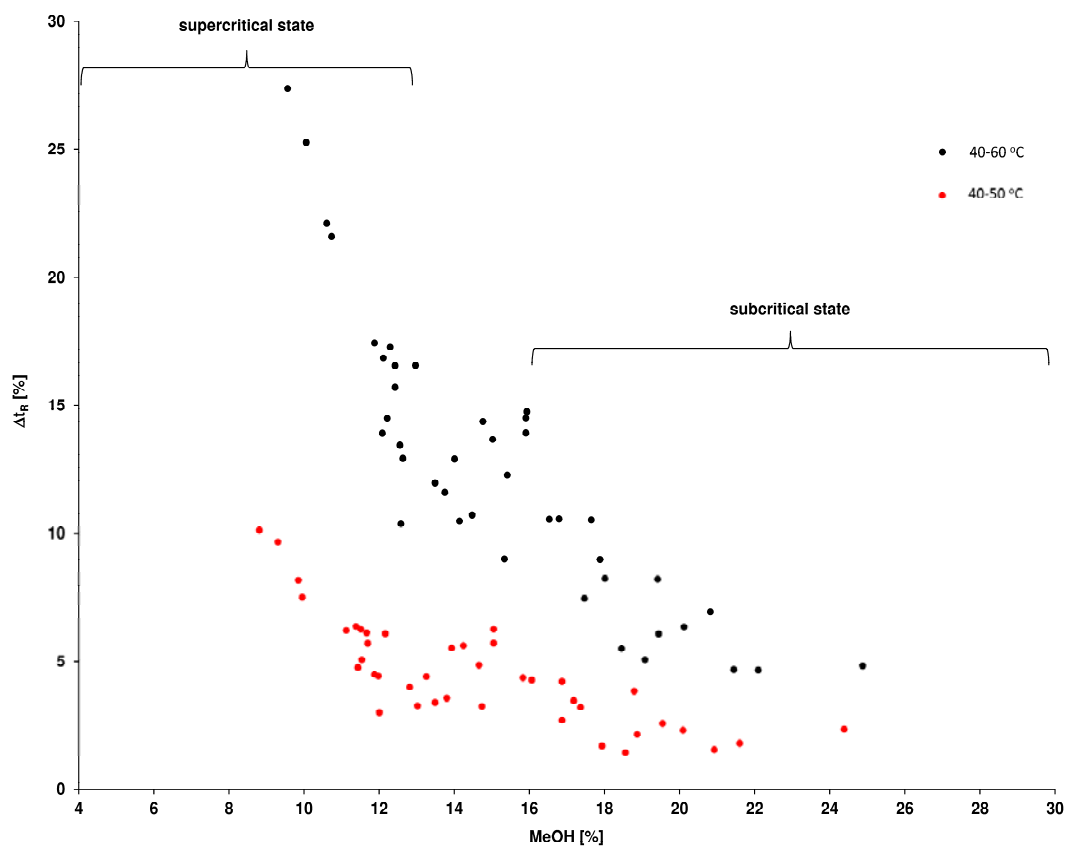


Fig. S1. Dependence of retention times on the concentration of methanol in modifier in UHPSFC/ESI-MS. The methanol content was calculated from retention times and the gradient program.