

Supplementary Methods and Materials

Polymer isolation from sample

Using a beaker, add methanol in a proportion of 1:4 (w:v) to the sample. Afterwards mixture is blended for 5 min and let stand at room temperature for 2h. Then, it is placed at $-30\text{ }^{\circ}\text{C}$ overnight. Next, the sample is centrifuged at 1250 g for 10 min at room temperature. The Solvent is collected and eliminated in a rotatory evaporator.

Shotgun QTOF

Sample was prepared in isopropanol at 1 mg/mL with 0.1% formic acid. Then, 1 μL was directly injected in Impact II QTOF (Bruker, Karlsruhe, Germany). Ionization voltage was +4.5 kV in positive, end plate offset 0.5 kV mode; nebulizing gas pressure was 1.8 bar (8 L/min) and drying temperature $220\text{ }^{\circ}\text{C}$. Spectra were acquired within the range of m/z 150–2000.

LC-MS analyses

Analyses conditions were as reported by Sarafian et al. [1]. Thus, chromatographic analyses were performed using an ELUTE LC series system (Bruker, Karlsruhe, Germany) coupled to an Impact II QTOF (Bruker, Karlsruhe, Germany). Separation of compounds was conducted using a C18 Intensity Solo column (100 mm x 2.1 mm, 2 μm) at $55\text{ }^{\circ}\text{C}$ and 0.400 mL/min. A binary mobile system was used for the elutions of compounds i) phase A consists of ACN/ H_2O (60:40, v:v) mixed with 10 mM ammonium formate and 0.1% formic acid and ii) mobile phase B IPA/ACN (90:10, v:v) mixed with 10 mM ammonium formate and 0.1% formic acid. Gradient was as described by Sarafian et al [1]. The injection volume was 3 μL . FDR samples treated with methanol were dissolved at a concentration of 0.3 mg/mL in phase B and analyzed in positive mode: Ionization voltage was +4.5 kV, end plate offset 0.5 kV; nebulizing gas pressure was 1.8 bar (8 L/min) and drying temperature $220\text{ }^{\circ}\text{C}$; spectra were acquired within the range of m/z 150–2000.

Supplementary results

Figure S1. Chromatographic overlay of the triterpene eluting region of the assayed samples.

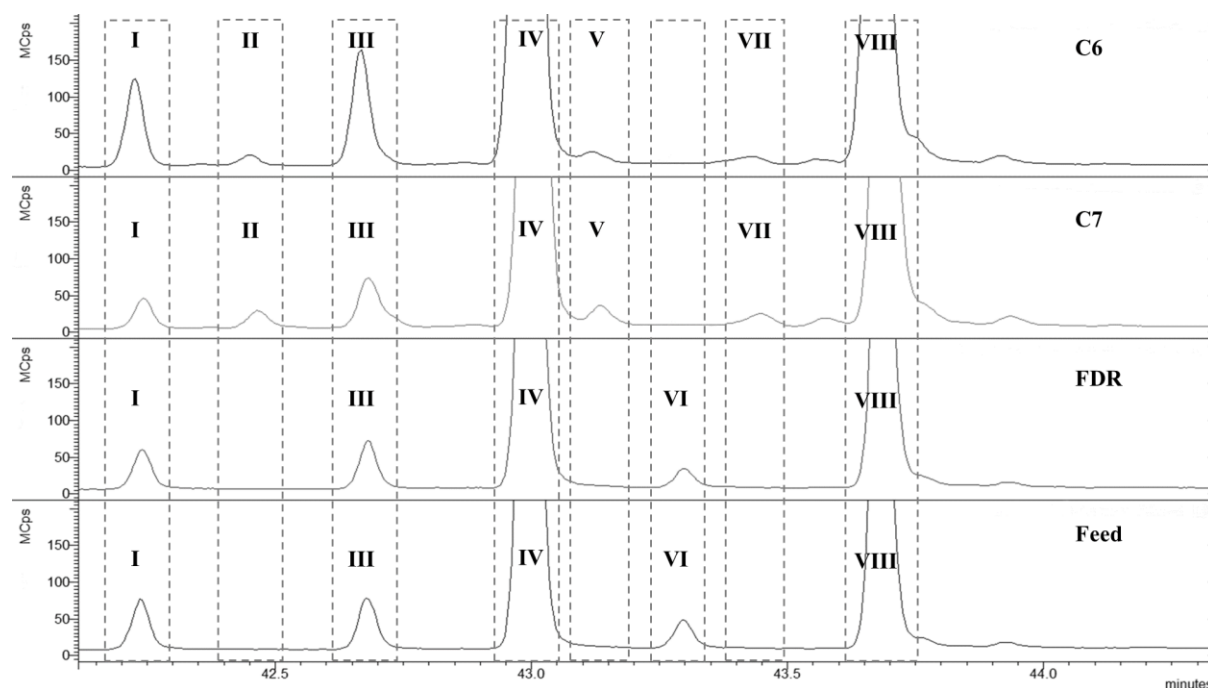


Figure S2. Mass spectra (GC-MS) of triterpene I in the assayed samples.

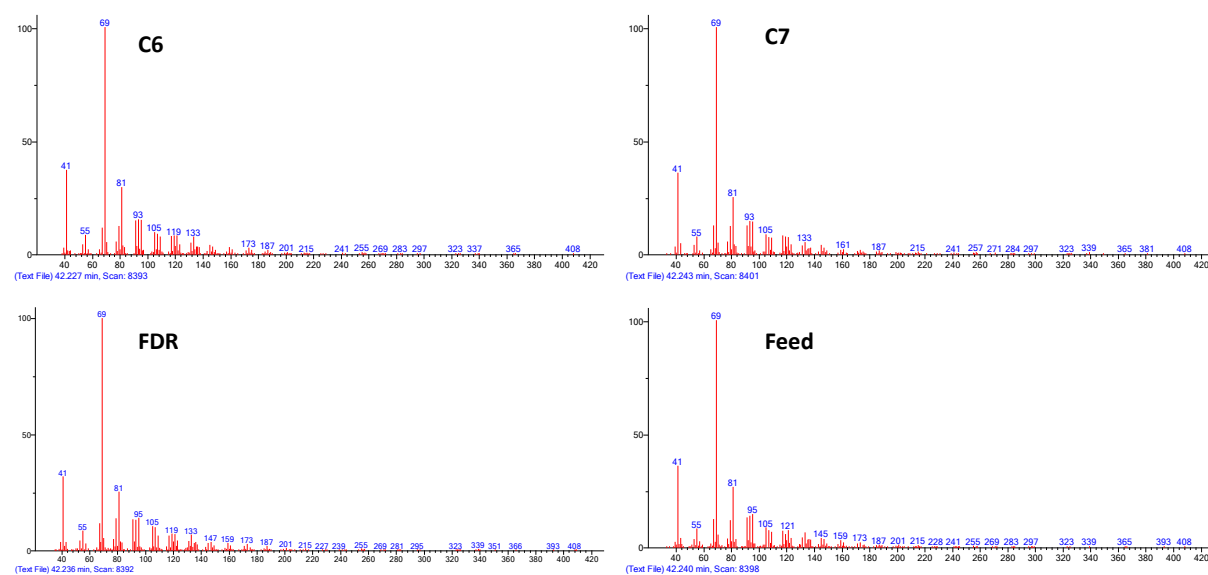


Figure S3. Mass spectra (GC-MS) of triterpene III in the assayed samples.

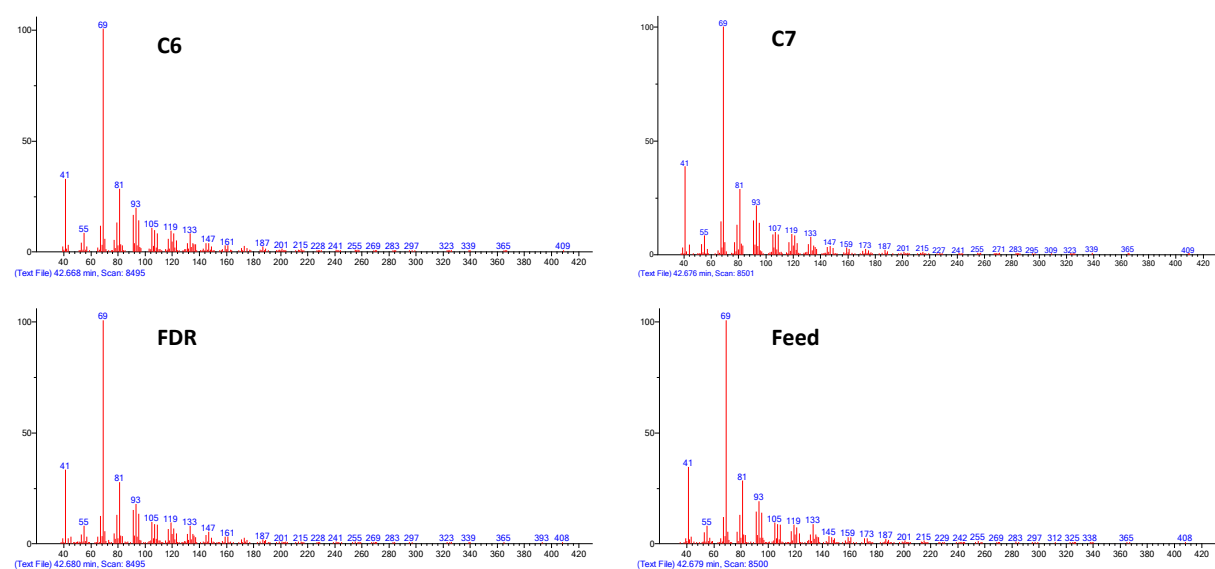


Figure S4. Mass spectra (GC-MS) of triterpene IV in the assayed samples.

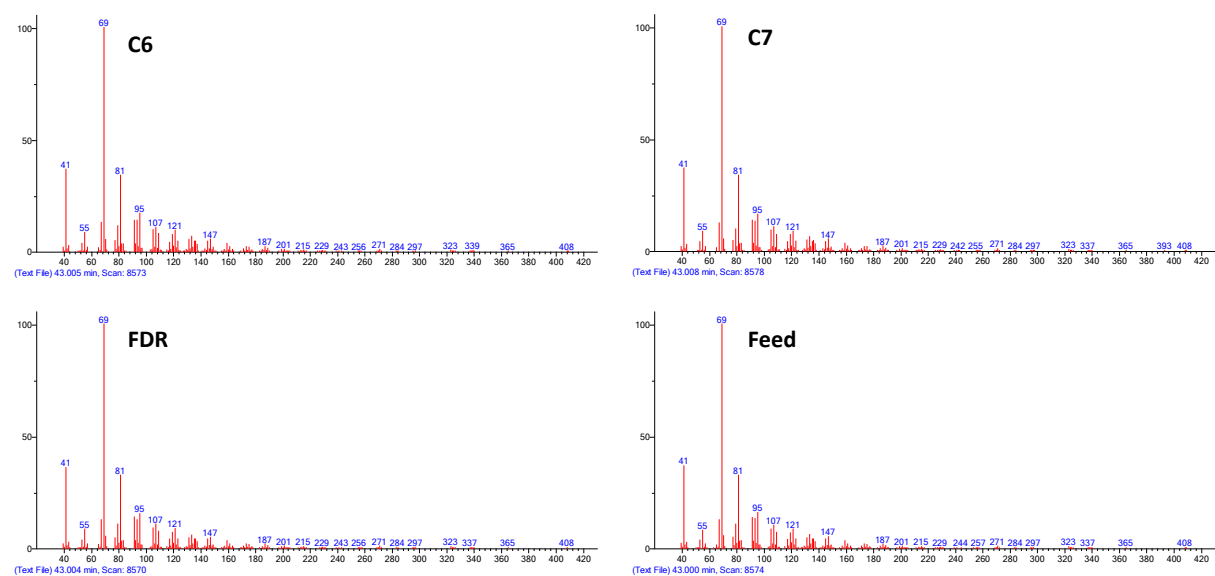


Figure S5. Mass spectra (GC-MS) of triterpene VIII in the assayed samples.

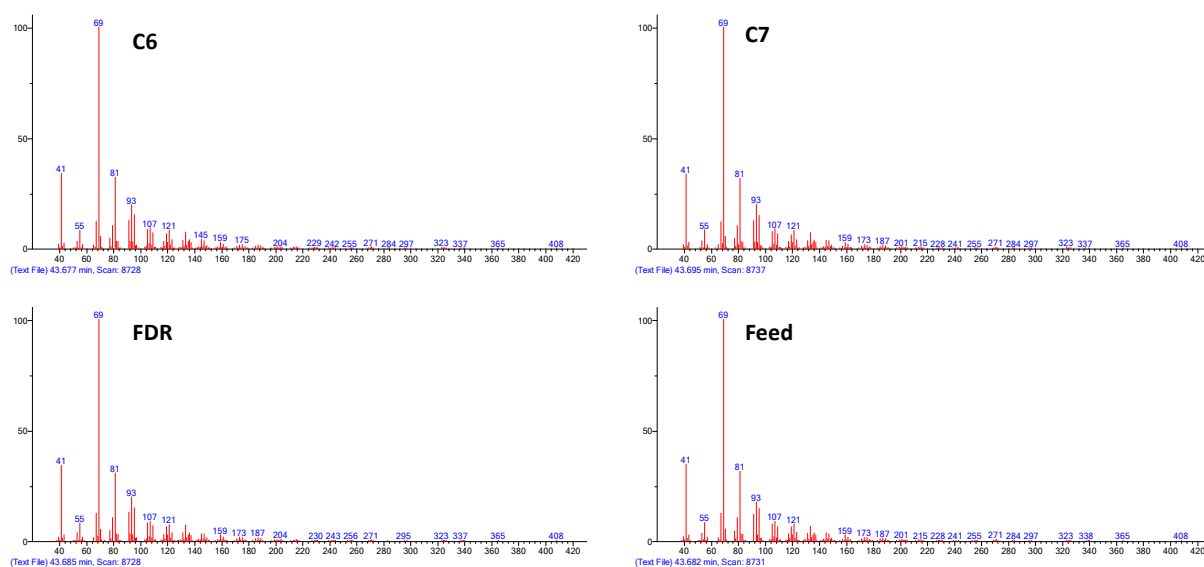


Figure S6. Mass spectra (GC-MS) of squalene (Standard from Sigma).

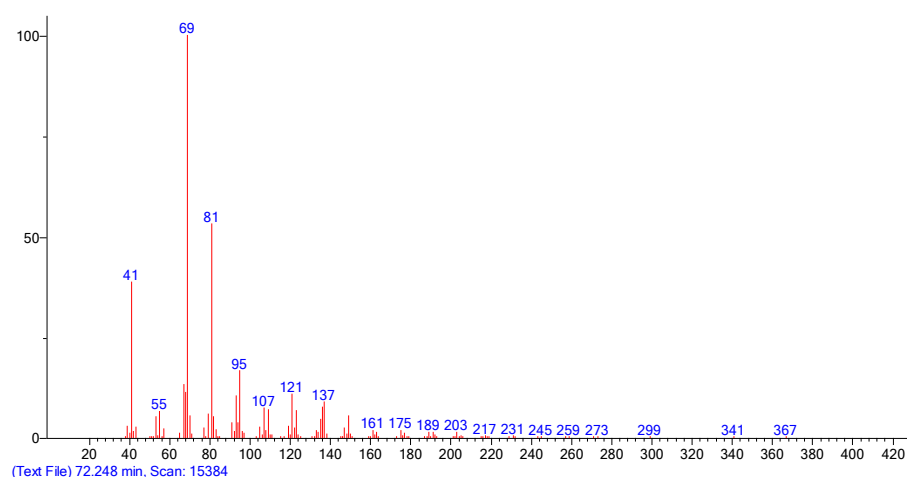


Figure S7. Direct infusion on QTOF of FDR sample treated with methanol showed a gaussian distribution of ions.

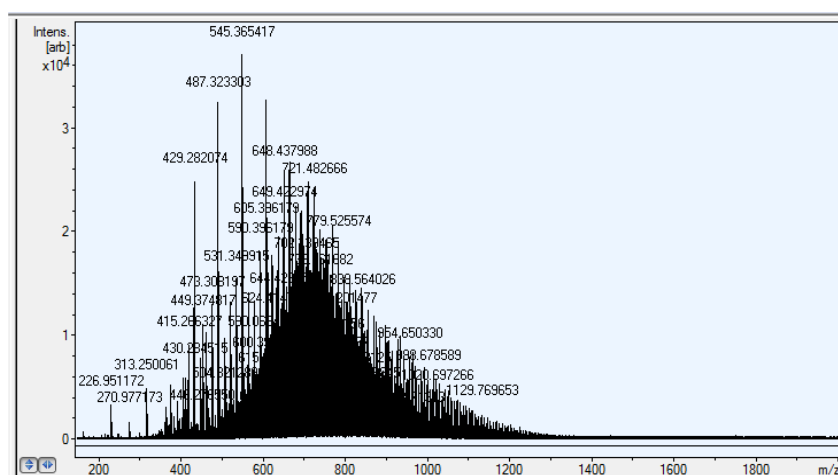


Figure S8. Mass spectra (LC-QTOF) at start (A), middle (B) and end (C) of eluting peak of methanol-treated FDR sample.

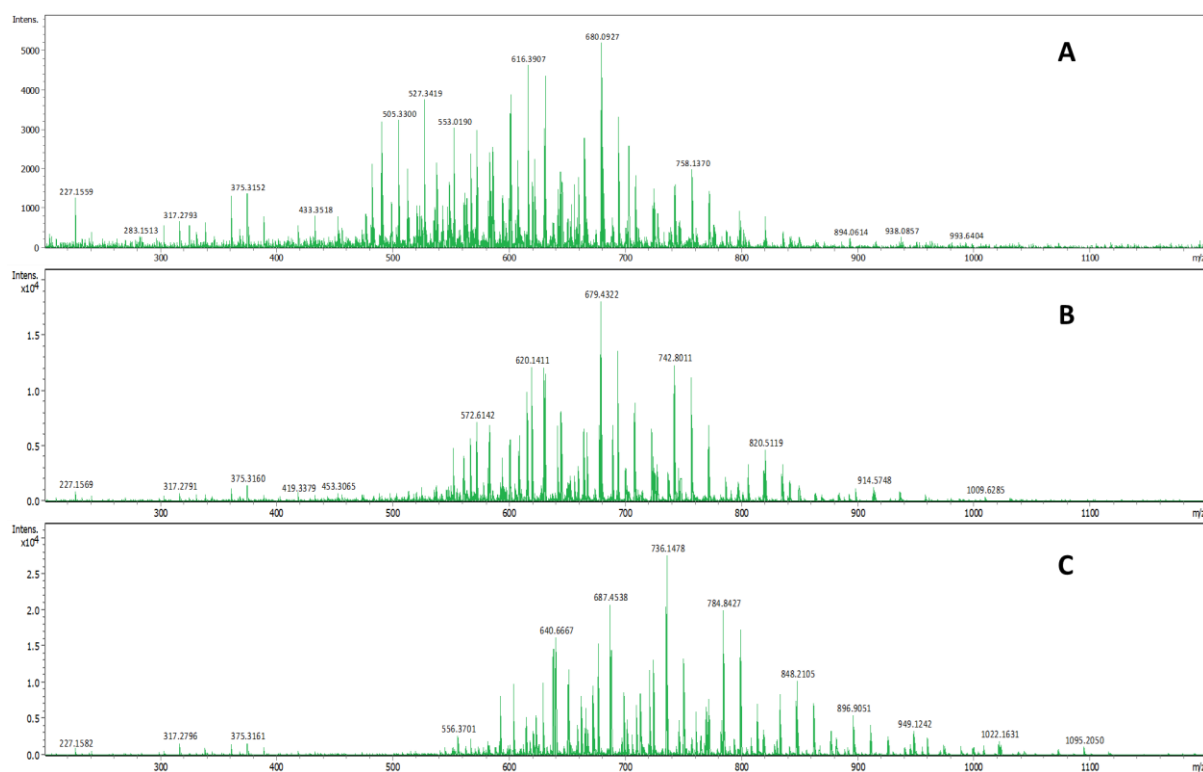


Figure S9. PCA of data obtained from GC-MS (A) and HPLC-ELSD (B).

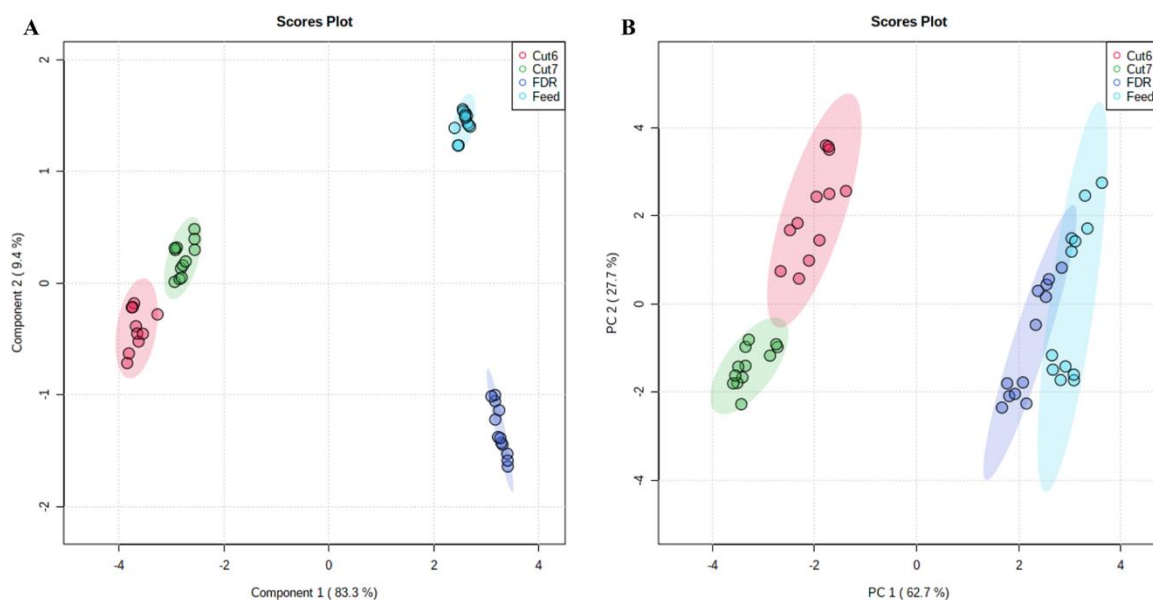


Figure S10. Heatmap of GC-MS data from the assayed samples.

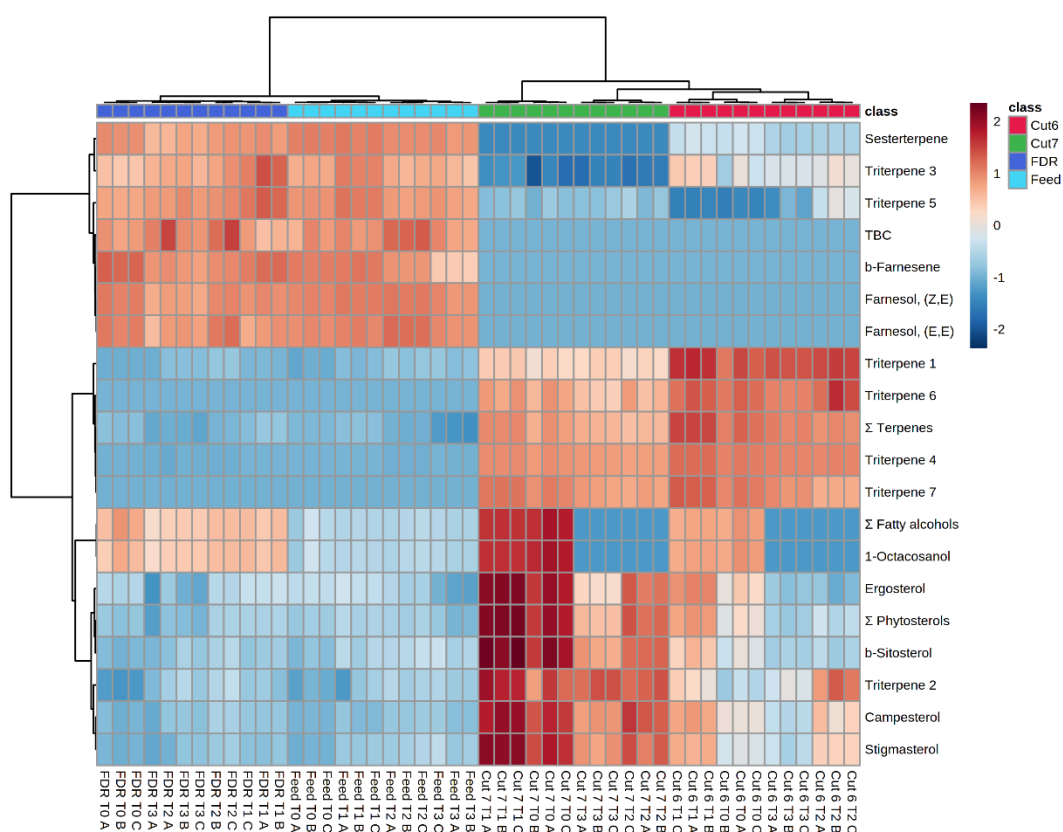


Figure S11. Heatmap of HPLC-ELSD data from the assayed samples.

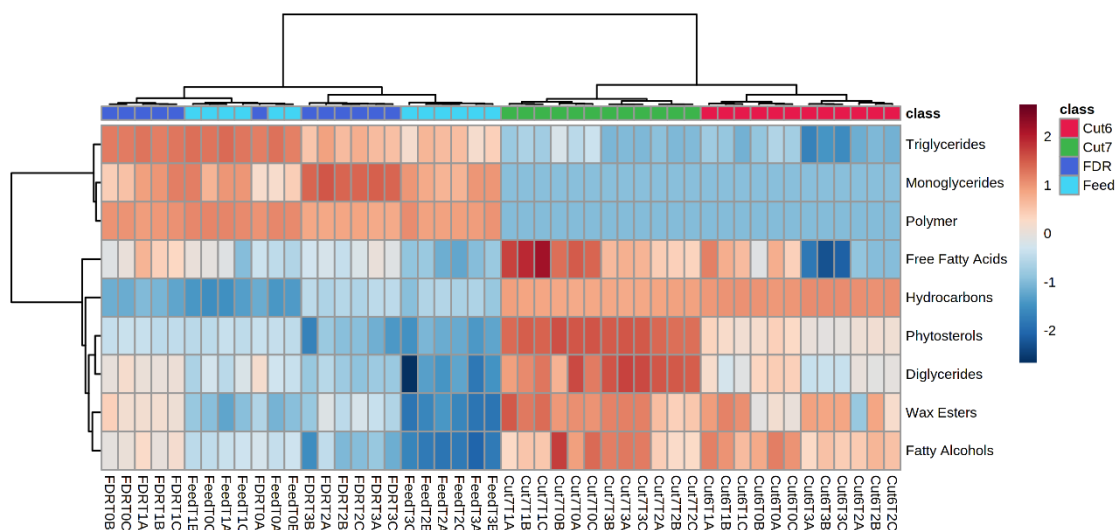


Table S1.Mobile phase gradient (%).

| Time (min.) | Mobile phase (percent) | | | | Flow-rate (mL/min.) |
|----------------|------------------------|-----|----|----|------------------------|
| | A | B | C | D | |
| 0.0 | 100 | 0 | 0 | 0 | 0.275 |
| 1.5 | 100 | 0 | 0 | 0 | 0.275 |
| 1.6 | 97 | 3 | 0 | 0 | 0.275 |
| 9.0 | 94 | 6 | 0 | 0 | 0.275 |
| 11.0 | 70 | 30 | 0 | 0 | 0.275 |
| 14.0 | 45 | 55 | 0 | 0 | 0.275 |
| 15.0 | 45 | 55 | 0 | 0 | 0.275 |
| 16.0 | 40 | 55 | 5 | 0 | 0.275 |
| 20.0 | 35 | 55 | 10 | 0 | 0.275 |
| 20.1 | 33 | 50 | 17 | 0 | 0.275 |
| 25.0 | 38 | 45 | 17 | 0 | 0.275 |
| 25.1 | 48 | 35 | 17 | 0 | 0.275 |
| 30.0 | 53 | 30 | 17 | 0 | 0.275 |
| 40.0 | 40 | 0 | 60 | 0 | 0.275 |
| 40.1 | 0 | 100 | 0 | 0 | 0.275 |
| 42.0 | 0 | 100 | 0 | 0 | 0.275 |
| 42.1 | 50 | 0 | 0 | 50 | 0.275 |
| 45.0 | 50 | 0 | 0 | 50 | 0.275 |
| 47.0 | 100 | 0 | 0 | 0 | 0.275 |
| 55.0 | 100 | 0 | 0 | 0 | 0.275 |

Table S2. FTIR frequencies interpretation table.

| Wavenumber (cm ⁻¹) | Origin | Assignment |
|--------------------------------|--|--|
| 3486-3390 | -OH stretching | Alcohols |
| 2969-2849 | C-H stretching (-CH ₃ , -CH ₂ and -CH) | Aliphatic chains |
| 1741-1738 | -C=O stretching | Esters, Carboxylic Acids, Ketones, Aldehydes |
| 1714-1712 | -OH bending | Alcohols |
| 1671 1641 | C=C stretching | Unsaturated aliphatic chains |
| 1595 | RONH ₂ | Amines |
| 1451-1374 | C-H bending | Aliphatic chains |
| 1347 | CH ₃ deformation | Aliphatic chains |
| 1297 | (unsat.) -CH deformation | Unsaturated aliphatic chains |
| ~1251 | CH ₃ symmetric deformation | Aliphatic chains |
| 1108-1102 1014 | CH ₃ CO Rocking | Ketones |
| 984 | CH deformation | Aliphatic chains |
| 904-892 | CH deformation (out of plane) | Aliphatic chains |
| ~888 | CH ₂ out of plane deformation | Unsaturated aliphatic chains |
| 836-833 | CH ₂ rocking vibration | Aliphatic chains |
| 744 | CH ₂ twisting | Unsaturated aliphatic chains |
| 719 | Rotational deformation of CH ₂ in chain | High aliphatic chains |

Table S3. Quantification of IL-1 β , IL-6, IL-8 and TNF- α levels in macrophages without and with inflammatory stimulus (LPS).

| | No stimulus | LPS stimulus |
|--------------------------------|--------------------|---------------------|
| IL-1β | | |
| Untreated cells | 0.38 \pm 0.08 | 6.32 \pm 0.19 |
| Ibuprofen | - | 8.47 \pm 0.36*** |
| C6 T0 | 0.25 \pm 0.05 | 7.15 \pm 0.23 |
| C6 T3 | 0.32 \pm 0.06 | 7.40 \pm 0.56 |
| C7 T0 | 0.18 \pm 0.08 | 6.98 \pm 0.15 |
| C7 T3 | 0.18 \pm 0.05 | 7.10 \pm 0.11 |
| IL-6 | | |
| Untreated cells | n.d. | 76.8 \pm 7.4 |
| Ibuprofen | - | 24.9 \pm 5.0**** |
| C6 T0 | n.d. | 5.00 \pm 0.26**** |
| C6 T3 | n.d. | 4.40 \pm 0.40**** |
| C7 T0 | n.d. | 5.05 \pm 0.40**** |
| C7 T3 | n.d. | 4.58 \pm 0.67**** |
| IL-8 | | |
| Untreated cells | 17.4 \pm 0.9 | 219 \pm 32 |
| Ibuprofen | - | 195 \pm 31 |
| C6 T0 | 24.5 \pm 0.1**** | 255 \pm 44 |
| C6 T3 | 28.8 \pm 0.6**** | 237 \pm 44 |
| C7 T0 | 22.3 \pm 0.7*** | 221 \pm 38 |
| C7 T3 | 18.9 \pm 0.4 | 236 \pm 48 |
| TNF-α | | |
| Untreated cells | 0.42 \pm 0.05 | 96.7 \pm 6.9 |
| Ibuprofen | - | 76.0 \pm 4.8 |
| C6 T0 | 0.40 \pm 0.01 | 60.2 \pm 8.1** |
| C6 T3 | 0.45 \pm 0.06 | 57.7 \pm 6.4** |
| C7 T0 | 0.28 \pm 0.02 | 58.9 \pm 8.7** |
| C7 T3 | 0.20 \pm 0.04** | 56.0 \pm 7.4** |

Values are expressed as pg of cytokine normalized to the total protein content. Ibuprofen at 1 mM was used as an anti-inflammatory control. One-way ANOVA was used for statistical analyses.

Supplementary References

1. Sarafian, M.H.; Gaudin, M.; Lewis, M.R.; Martin, F.P.; Holmes, E.; Nicholson, J.K.; Dumas, M.E. Objective set of criteria for optimization of sample preparation procedures for ultra-high throughput untargeted blood plasma lipid profiling by ultra performance liquid chromatography-mass spectrometry. *Anal. Chem.* **2014**, *86*, 5766–5774, doi:10.1021/ac500317c.