Figure S1. LC/QTOF-MS (ESI⁻) fragmentation pattern of pinellic acid from (**a**) bread and (**b**) pure standard.
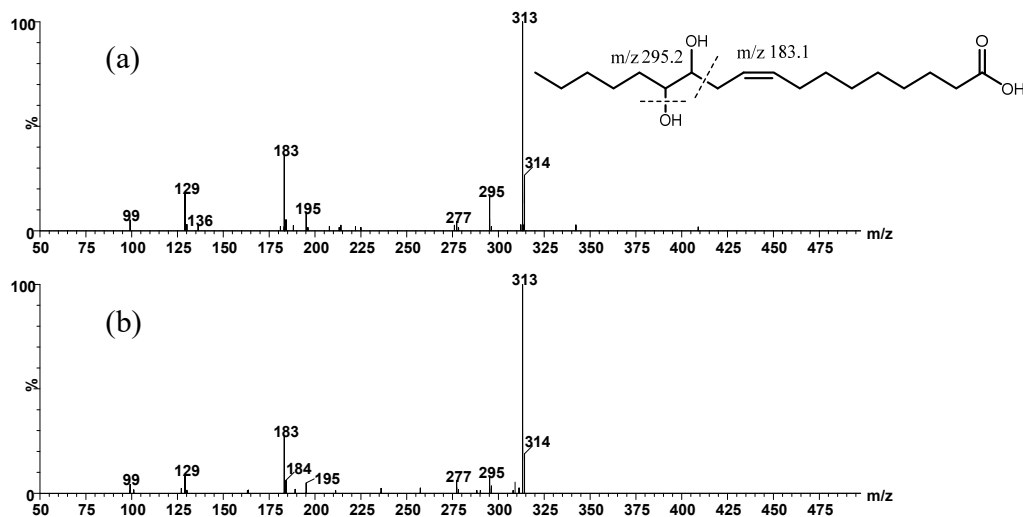

Figure S2. LC/QTOF-MS (ESI⁻) fragmentation pattern of 12,13-dihydroxy-9(Z)-octadecenoic acid from (**a**) bread and (**b**) pure standard.
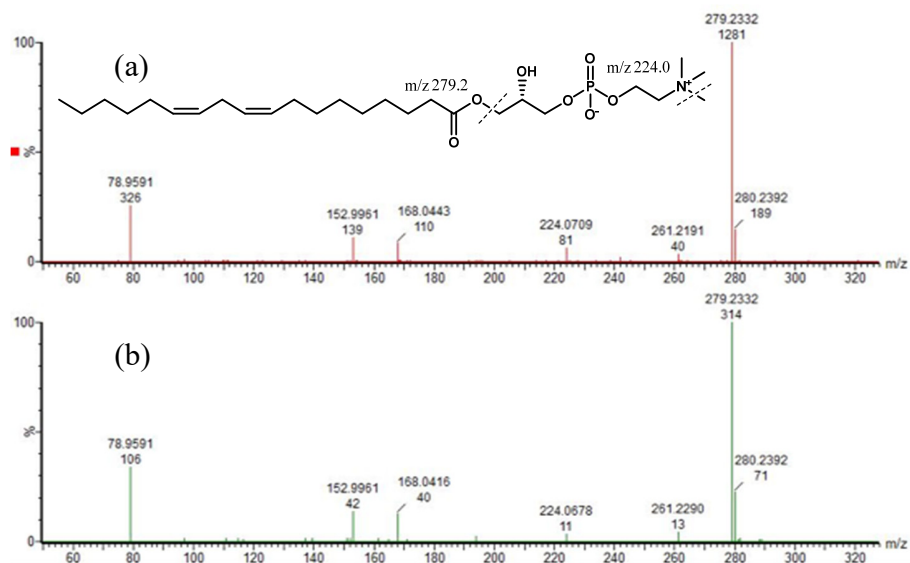
Figure S3. LC/QTOF-MS (ESI⁻) fragmentation pattern of 1-(9Z,12Z-octadecadienoyl)-*sn*-glycero-3-phosphocholine from (**a**) bread and (**b**) pure standard.
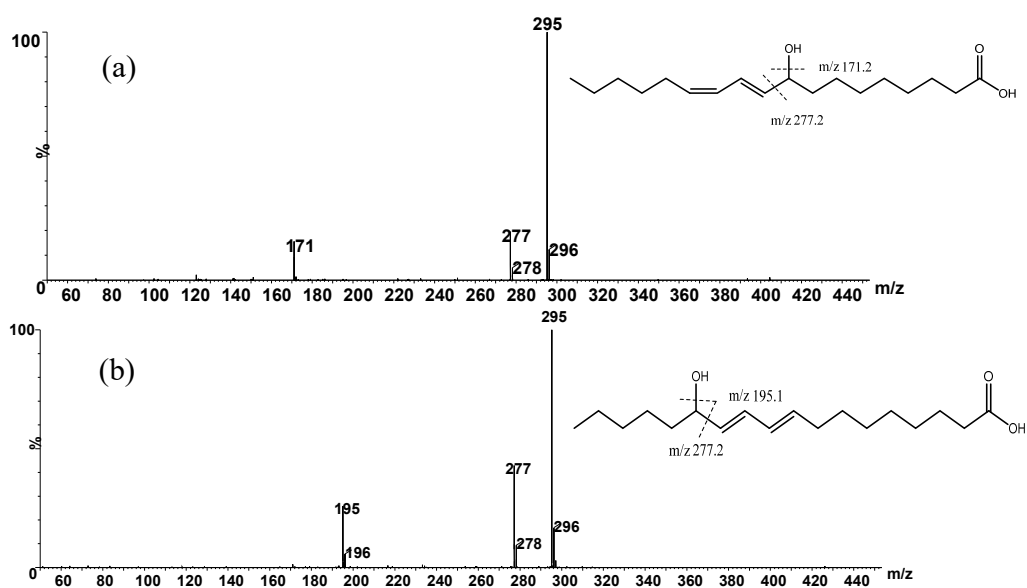

Figure S4. LC/QTOF-MS (ESI⁻) fragmentation pattern of 10(*E*),12(*Z*)-9-hydroxyoctadecadienoic acid (**a**) and 9(*E*),11(*E*)-13-hydroxyoctadecadienoic acid (**b**).
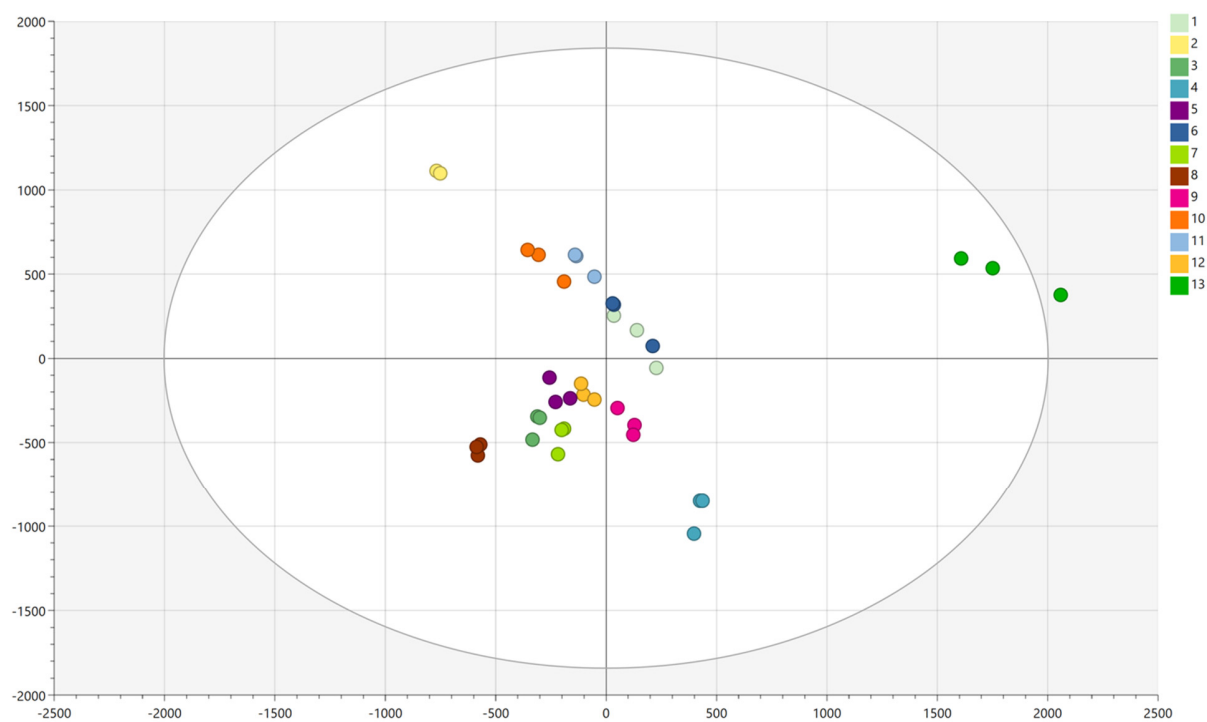
Figure S5. Scores scatter plot of PCA model (Pareto scaling) for LC/MS chemical profiling data (n = 791) from thirteen whole wheat bread samples in triplicate. Colored by sample.