Supplementary Material 5



**Fig. S5.1** Identification of fatty acyl composition in the lipid hydroperoxide PCOOH 16:0/18:2. (**A**) The HRMS1 spectrum showed an identical signal at *m/z* 790.5594 as [M + H]+; (**B**) in MS2 spectrum, the signals of *m/z* 772 and *m/z* 756 indicated the existence of the hydroperoxyl group, while *m/z* 605 was assigned as the [M – H2O – headgroup + H]+; (**C**) the MS3 spectrum not only gave the signal of hydroperoxyl group cleavage as [M – H2O – O – 2H + H]+) at *m/z* 754, but also showed two pairs of signals, *m/z* 534, 516, and *m/z* 496, 478, which were assigned as [M – FA16:0 + H]+ and [M – FA18:2OOH + H]+, respectively.

**Table S5.1** LC/MS data of the identified lipid hydroperoxides

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Lipid species | Formula | Diagnostic ion | RT | Calc. *m/z* | Exp. *m/z* | Δppm |
| TGOOH52:2 | C55H102O8 | [M + NH4]+ | 12.58 | 908.7913 | 908.7939 | 2.86 |
| TGOOH52:3 | C55H100O8 | [M + NH4]+ | 12.32 | 906.7756 | 906.7769 | 1.43 |
| TGOOH52:4 | C55H98O8 | [M + NH4]+ | 12.12 | 904.7600 | 904.7610 | 1.11 |
| TGOOH54:3 | C57H104O8 | [M + NH4]+ | 12.69 | 934.8069 | 934.8064 | −0.53 |
| TGOOH54:4 | C57H102O8 | [M + NH4]+ | 12.42 | 932.7913 | 932.7908 | −0.54 |
| TGOOH54:5 | C57H100O8 | [M + NH4]+ | 12.16 | 930.7756 | 930.7763 | 0.75 |
| TGOOH56:6 | C59H102O8 | [M + NH4]+ | 12.78 | 956.7913 | 956.7936 | 2.40 |
| TGOOH56:7 | C59H100O8 | [M + NH4]+ | 12.48 | 954.7756 | 954.7762 | 0.63 |
| PCOOH34:2 | C42H80O10NP | [M + H]+ | 6.25 | 790.5593 | 790.5597 | 0.51 |
| PCOOH34:3 | C42H78O10NP | [M + H]+ | 5.66 | 788.5436 | 788.5432 | −0.51 |
| PCOOH34:4 | C42H76O10NP | [M + H]+ | 3.94 | 786.5280 | 786.5281 | 0.13 |
| PCOOH34:5 | C42H74O10NP | [M + H]+ | 3.20 | 784.5123 | 784.5119 | −0.51 |
| PCOOH36:2 | C44H84O10NP | [M + H]+ | 6.86 | 818.5906 | 818.5898 | −0.98 |
| PCOOH36:3 | C44H82O10NP | [M + H]+ | 6.49 | 816.5749 | 816.5745 | −0.49 |
| PCOOH36:4 | C44H80O10NP | [M + H]+ | 6.01 | 814.5593 | 814.5582 | −1.35 |
| PCOOH36:5 | C44H78O10NP | [M + H]+ | 5.66 | 812.5436 | 812.5432 | −0.49 |
| PCOOH36:6 | C44H76O10NP | [M + H]+ | 4.25 | 810.5280 | 810.5275 | −0.62 |
| PCOOH38:4 | C46H84O10NP | [M + H]+ | 6.68 | 842.5906 | 842.5911 | 0.59 |
| PCOOH38:5 | C46H82O10NP | [M + H]+ | 6.27 | 840.5749 | 840.5743 | −0.71 |
| PCOOH38:6 | C46H80O10NP | [M + H]+ | 5.88 | 838.5593 | 838.5584 | −1.07 |
| PCOOH38:7 | C46H78O10NP | [M + H]+ | 5.06 | 836.5436 | 836.5425 | −1.31 |
| PCOOH38:8 | C46H76O10NP | [M + H]+ | 4.52 | 834.5280 | 834.5273 | −0.84 |
| PCOOH40:6 | C48H84O10NP | [M + H]+ | 6.57 | 866.5906 | 866.5900 | −0.69 |
| PEOOH36:2 | C41H78O10NP | [M − H]− | 13.64 | 774.5291 | 774.5256 | −4.52 |
| PEOOH36:3 | C41H76O10NP | [M − H]− | 13.17 | 772.5134 | 772.5112 | −2.85 |
| PEOOH36:4 | C41H74O10NP | [M − H]− | 12.84 | 770.4978 | 770.4949 | −3.76 |
| PEOOH38:4 | C43H78O10NP | [M − H]− | 13.67 | 798.5291 | 798.5259 | −4.01 |
| PEOOH38:5 | C43H76O10NP | [M − H]− | 13.10 | 796.5134 | 796.5142 | 1.00 |
| PEOOH38:6 | C43H74O10NP | [M − H]− | 12.84 | 794.4978 | 794.4955 | −2.89 |
| PEOOH40:6 | C45H78O10NP | [M − H]− | 13.57 | 822.5291 | 822.5255 | −4.38 |
| PEOOH40:7 | C45H76O10NP | [M − H]− | 13.22 | 820.5134 | 820.5107 | −3.29 |
| PEOOH40:8 | C45H74O10NP | [M − H]− | 12.86 | 818.4978 | 818.4938 | −4.89 |
| PIOOH34:1 | C43H81O15P | [M − H]− | 14.44 | 867.5240 | 867.5263 | 2.65 |
| PIOOH34:2 | C43H79O15P | [M − H]− | 13.92 | 865.5084 | 865.5052 | −3.70 |
| PIOOH34:3 | C43H77O15P | [M − H]− | 13.79 | 863.4927 | 863.4957 | 3.47 |
| PIOOH34:4 | C43H75O15P | [M − H]− | 13.62 | 861.4771 | 861.4801 | 3.48 |
| PIOOH38:4 | C47H83O15P | [M − H]− | 12.70 | 917.5397 | 917.5370 | −2.94 |