Supplementary Data 2. MS^2 fragmentation patterns for oxidatively truncated and full-length oxygenated lipids.

Table of Contents

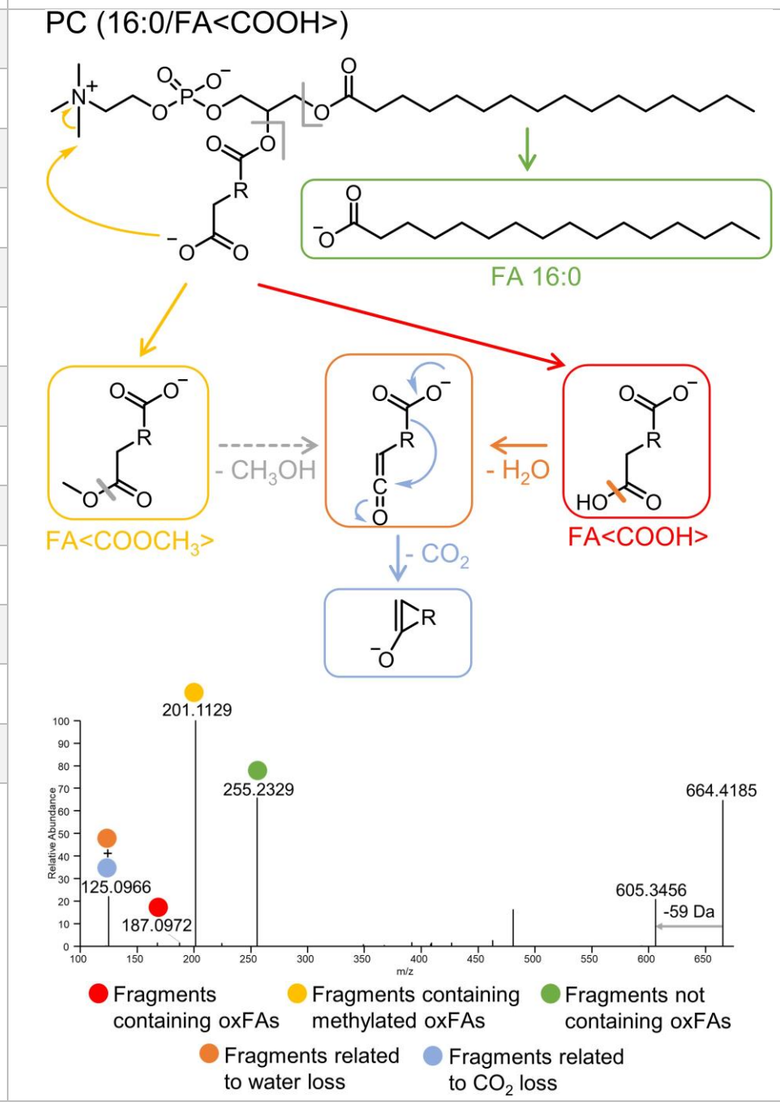
General notes:

1. All *m/z* values given in the table were calculated considering the charge.
2. Representative MS^2 spectra do not always contain signals corresponding to the position-specific fragments (the latter were acquired in MS^3 experiments).
3. For simplicity, only *E*-conformers of PUFAs are depicted. Fragmentation patterns do not allow to elucidate the configuration of a double bond, but keep in mind the natural *Z*-configuration for some double bonds in (ox)PUFAs.
4. Modification- and position-specific fragments: the most intense ones are highlighted in **bold**, the intermediate intensity ones are regular, and the weak ones are grayed out.

PHOSPHATIDYLCHOLINES

Oxidatively truncated: <COOH>

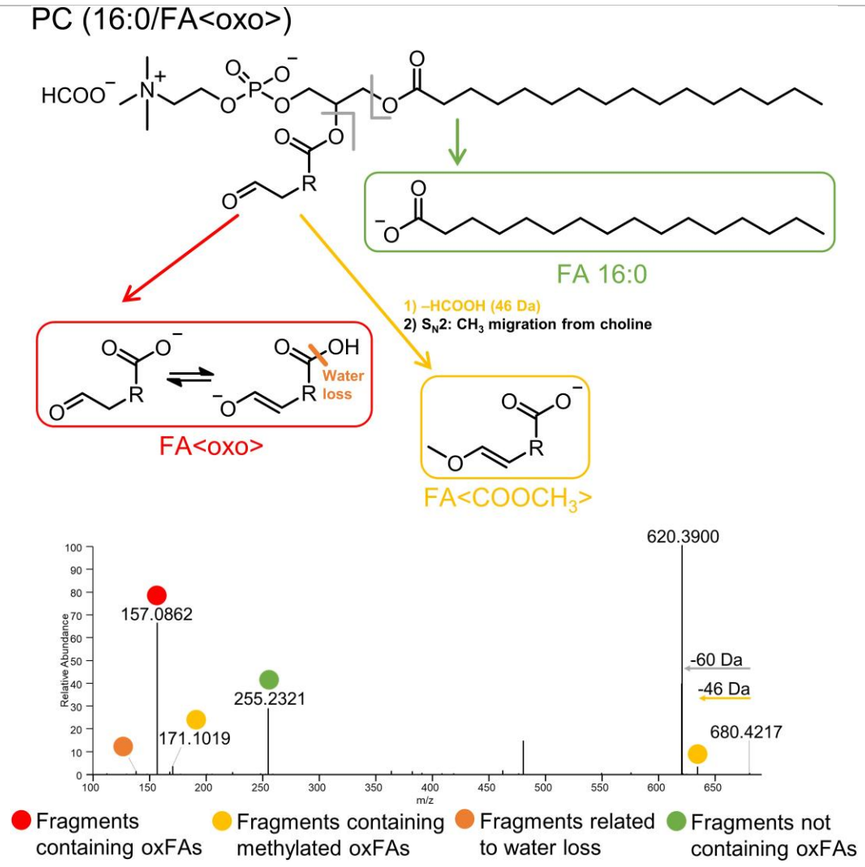
$[M-H]^-$ adducts (precursors)

Mod. position	Precursor	Chemical Formula	*m/z*	MS² Fragmentation	Mod./pos.-specific fragment[1]	Chemical Formula	*m/z*
4	PC(16:0/4:0<COOH>)	$C_{28}H_{53}O_{10}NP$	594.3413		FA(4:0<$COOCH_3$>)	$C_5H_7O_4$	131.0350
5	PC(16:0/5:0<COOH>)	$C_{29}H_{55}O_{10}NP$	608.3569		FA(5:0<$COOCH_3$>)	$C_6H_9O_4$	145.0506
7	PC(16:0/7:0<COOH>)	$C_{31}H_{59}O_{10}NP$	636.3882		FA(7:0<$COOCH_3$>)	$C_8H_{13}O_4$	173.0819
8	PC(16:0/8:0<COOH>)	$C_{32}H_{61}O_{10}NP$	650.4039		FA(8:0<$COOCH_3$>)	$C_9H_{15}O_4$	187.0976
9	PC(16:0/9:0<COOH>)	$C_{33}H_{63}O_{10}NP$	664.4195		FA(9:0<COOCH3>)	$C_{10}H_{17}O_4$	201.1132
10	PC(16:0/10:0<COOH>)	$C_{34}H_{65}O_{10}NP$	678.4352		FA(10:0<$COOCH_3$>)	$C_{11}H_{19}O_4$	215.1289
	PC(16:0/10:1<COOH>)	$C_{34}H_{63}O_{10}NP$	676.4195		FA(10:1<$COOCH_3$>)	$C_{11}H_{17}O_4$	213.1132
11	PC(16:0/11:1<COOH>)	$C_{35}H_{65}O_{10}NP$	690.4352		FA(11:1<$COOCH_3$>)	$C_{12}H_{19}O_4$	227.1289
	PC(16:0/11:2<COOH>)	$C_{35}H_{63}O_{10}NP$	688.4195		FA(11:2<$COOCH_3$>)	$C_{12}H_{17}O_4$	225.1132
12	PC(16:0/12:1<COOH>)	$C_{36}H_{67}O_{10}NP$	704.4508		FA(12:1<$COOCH_3$>)	$C_{13}H_{21}O_4$	241.1445
	PC(16:0/12:2<COOH>)	$C_{36}H_{65}O_{10}NP$	702.4352		FA(12:2<$COOCH_3$>)	$C_{13}H_{19}O_4$	239.1289
13	PC(16:0/13:2<COOH>)	$C_{37}H_{67}O_{10}NP$	716.4508		FA(13:2<$COOCH_3$>)	$C_{14}H_{21}O_4$	253.1445
	PC(16:0/13:3<COOH>)	$C_{37}H_{65}O_{10}NP$	714.4352		FA(13:3<$COOCH_3$>)	$C_{14}H_{19}O_4$	251.1289
14	PC(16:0/14:3<COOH>)	$C_{38}H_{67}O_{10}NP$	728.4508		FA(14:3<$COOCH_3$>)	$C_{15}H_{21}O_4$	265.1445

[1] Although other characteristic fragments can be formed occasionally, "Mod./pos.-specific fragment" column contains the most reproducible fragment ion *m/z*. Such fragments as FA<COOH>, FA<COOH>-CO_2, FA<COOH>-H_2O (or FA<$COOCH_3$>-CH_3OH) were occasionally observed, and might be also used as supporting the annotation.

Oxidatively truncated: <oxo>

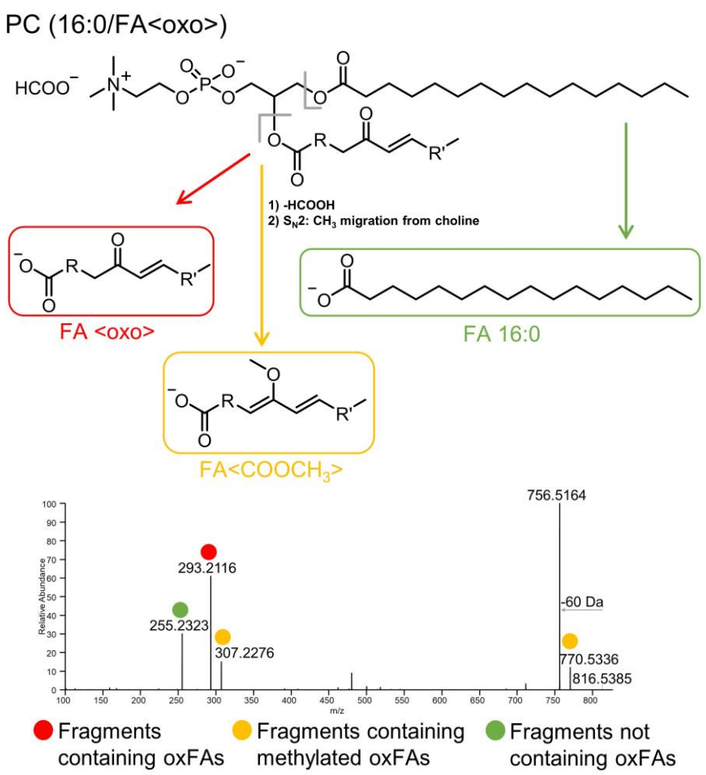
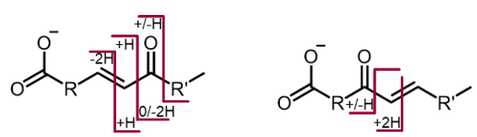
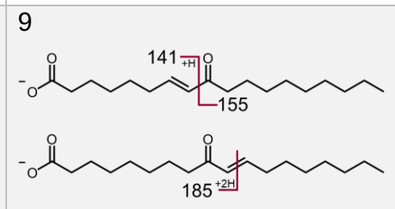
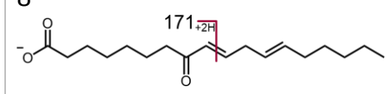
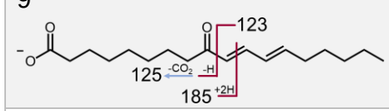
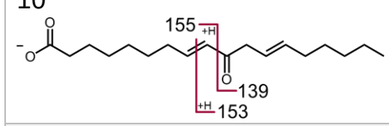
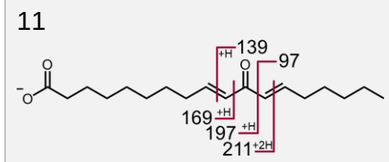
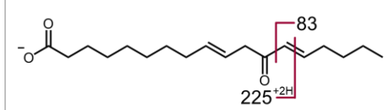
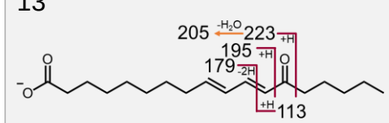
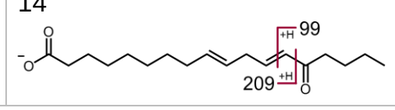
[M+HCOO]$^-$ adducts (precursors)

Mod. position	Precursor	Chemical Formula	*m/z*	MS^2 Fragmentation	Mod./pos.-specific fragment[2]	Chemical Formula	*m/z*
4	PC(16:0/4:0<oxo>)	$C_{29}H_{55}O_{11}NP$	624.3518		FA(4:0<oxo>)	$C_4H_5O_3$	101.0244
5	PC(16:0/5:0<oxo>)	$C_{30}H_{57}O_{11}NP$	638.3675		FA(5:0<oxo>)	$C_5H_7O_3$	115.0401
7	PC(16:0/7:0<oxo>)	$C_{32}H_{61}O_{11}NP$	666.3988		FA(7:0<oxo>)	$C_7H_{11}O_3$	143.0714
8	PC(16:0/8:0<oxo>)	$C_{33}H_{63}O_{11}NP$	680.4144		FA(8:0<oxo>)	$C_8H_{13}O_3$	157.0870
9	PC(16:0/9:0<oxo>)	$C_{34}H_{65}O_{11}NP$	694.4301		FA(9:0<oxo>)	$C_9H_{15}O_3$	171.1027
10	PC(16:0/10:0<oxo>)	$C_{35}H_{67}O_{11}NP$	708.4457		FA(10:0<oxo>)	$C_{10}H_{17}O_3$	185.1183
	PC(16:0/10:1<oxo>)	$C_{35}H_{65}O_{11}NP$	706.4301		FA(10:1<oxo>)	$C_{10}H_{15}O_3$	183.1027
11	PC(16:0/11:1<oxo>)	$C_{36}H_{67}O_{11}NP$	720.4457		FA(11:1<oxo>)	$C_{11}H_{17}O_3$	197.1183
	PC(16:0/11:2<oxo>)	$C_{36}H_{65}O_{11}NP$	718.4301		FA(11:2<oxo>)	$C_{11}H_{15}O_3$	195.1027
12	PC(16:0/12:1<oxo>)	$C_{37}H_{69}O_{11}NP$	734.4614		FA(12:1<oxo>)	$C_{12}H_{19}O_3$	211.1340
	PC(16:0/12:2<oxo>)	$C_{37}H_{67}O_{11}NP$	732.4457		FA(12:2<oxo>)	$C_{12}H_{17}O_3$	209.1183
13	PC(16:0/13:2<oxo>)	$C_{38}H_{69}O_{11}NP$	746.4614		FA(13:2<oxo>)	$C_{13}H_{19}O_3$	223.1340
	PC(16:0/13:3<oxo>)	$C_{38}H_{67}O_{11}NP$	744.4457		FA(13:3<oxo>)	$C_{13}H_{17}O_3$	221.1183
14	PC(16:0/14:3<oxo>)	$C_{39}H_{69}O_{11}NP$	758.4614		FA(14:3<oxo>)	$C_{14}H_{19}O_3$	235.1340

[2] + additional weak signals in MS^2 spectra: FA<COOH> -H_2O (or FA<$COOCH_3$>-CH_3OH), FA<COOH>-CO_2.

Full-length oxygenated: <oxo>

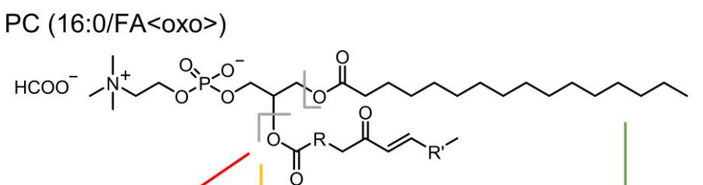
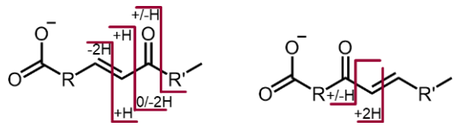
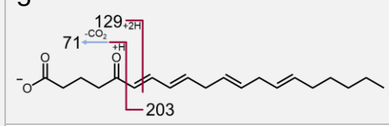
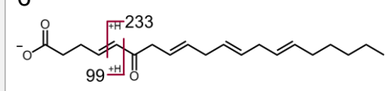
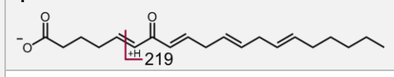
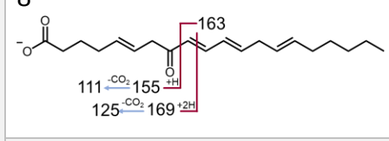
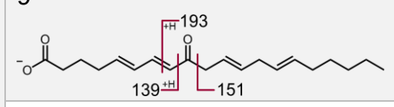
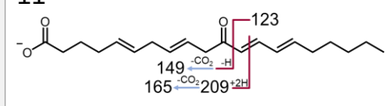
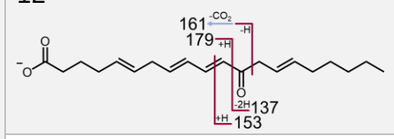
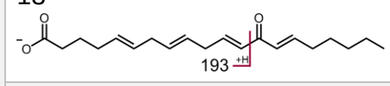
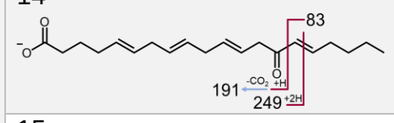
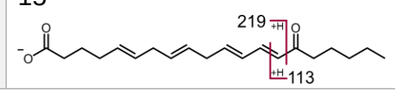
[M+HCOO]$^-$ adducts (precursors)

Precursor	Chemical Formula & *m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula & *m/z*	Pos.-specific fragmentation	Chemical Formula	*m/z*
PC(16:0/18:1<oxo>)	$C_{43}H_{81}O_{11}NP$ 818.5553	 * Signal of precursor ion might not always be present in MS^2 spectra due to the intensive fragmentation **FA fragmentation pattern:** 	**FA(18:1<oxo>)** Methylation CO_2 loss	**$C_{18}H_{31}O_3$** **295.2279** $C_{19}H_{33}O_3$ 309.2435 $C_{17}H_{31}O$ 251.2380	9 	$C_8H_{13}O_2$ $C_{10}H_{19}O$ $C_{10}H_{17}O_3$	141.0921 155.1441 185.1183
					8 	**$C_9H_{15}O_3$**	**171.1027**
					9 	C_9H_{15} $C_8H_{13}O$ **$C_{10}H_{17}O_3$**	123.1179 125.0972 **185.1183**
					10 	**$C_9H_{15}O$** $C_{10}H_{17}O$ $C_9H_{15}O_2$	**139.1128** 153.1285 155.1078
PC(16:0/18:2<oxo>)	$C_{43}H_{79}O_{11}NP$ 816.5396		**FA(18:2<oxo>)** Methylation CO_2 loss	**$C_{18}H_{29}O_3$** **293.2122** $C_{19}H_{31}O_3$ 307.2279 $C_{17}H_{29}O$ 249.2224	11 	C_7H_{13} $C_9H_{15}O$ $C_{10}H_{17}O_2$ $C_{11}H_{17}O_3$ $C_{12}H_{19}O_3$	97.1023 139.1128 169.1234 197.1183 211.1340
					12 	C_6H_{11} $C_{13}H_{21}O_3$	83.0866 225.1496
					13 	**$C_7H_{13}O$** $C_{11}H_{15}O_2$ $C_{12}H_{19}O_2$ $C_{13}H_{17}O_2$ $C_{13}H_{19}O_3$	**113.0972** 179.1078 195.1391 205.1234[3] 223.1340[4]
					14 	$C_6H_{11}O$ $C_{13}H_{21}O_2$	99.0815 209.1547

[3] The signal is seen in the case of FA(18:2<OOH{13}>).
[4] The signal is seen in the case of FA(18:2<OOH{13}>).

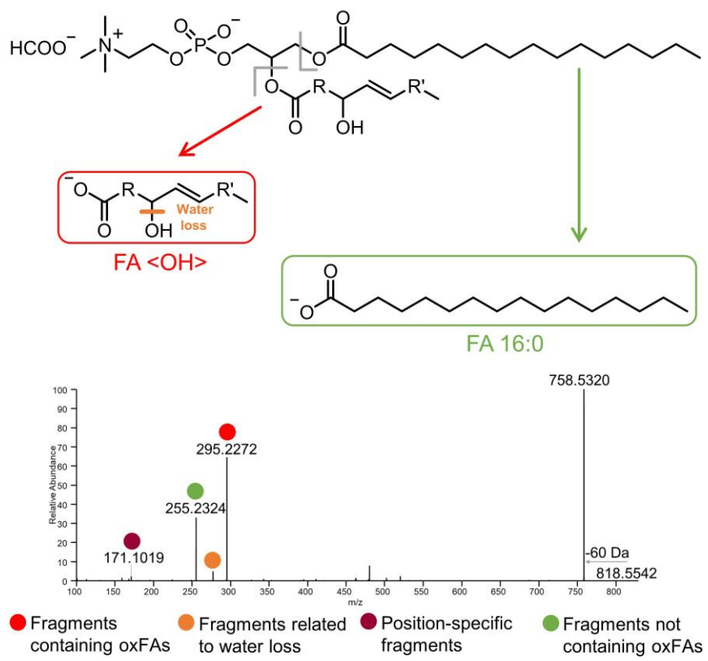
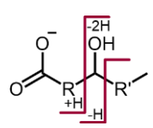
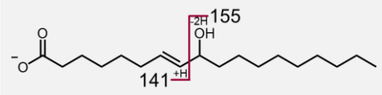
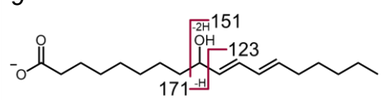
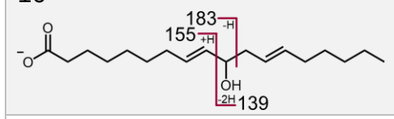
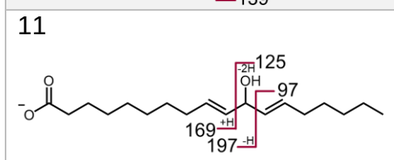
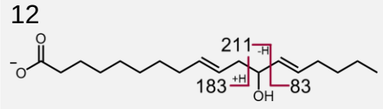
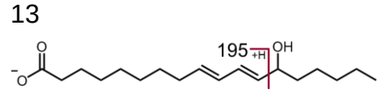
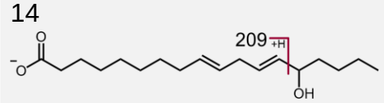
Full-length oxygenated: <oxo> (continued)

[M+HCOO]$^-$ adducts (precursors)

Precursor	Chemical Formula & *m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula & *m/z*	Pos.-specific fragmentation	Chemical Formula	*m/z*
PC(16:0/20:4<oxo>)	$C_{45}H_{79}O_{11}NP$ 840.5396	PC (16:0/FA<oxo>)  ● Fragments containing oxFAs ● Fragments containing methylated oxFAs ● Fragments not containing oxFAs * The precursor ion m/z may not always present in MS^2 spectra due to the intensive fragmentation **FA fragmentation pattern:** 	**FA(20:4<oxo>)** Methylation CO_2 loss	**$C_{20}H_{29}O_3$** **317.2122** $C_{21}H_{31}O_3$ 331.2279 $C_{19}H_{29}O$ 273.2224	5 	C_4H_7O $C_6H_9O_3$ **$C_{15}H_{23}$**	71.0502 129.0557 **203.1805**
					6 	$C_5H_7O_2$ $C_{16}H_{25}O$	99.0452 233.1911
					7 	$C_{15}H_{23}O$	219.1754
					8 	$C_7H_{11}O$ $C_8H_{13}O$ $C_8H_{11}O_3$ $C_{12}H_{19}$ $C_9H_{13}O_3$	111.0815 125.0972 155.0714 163.1492 169.0870
					9 	$C_8H_{11}O_2$ $C_{11}H_{19}$ $C_{13}H_{21}O$	139.0765 151.1492 193.1598
					11 	C_9H_{15} $C_{10}H_{13}O$ $C_{11}H_{17}O$ $C_{12}H_{17}O_3$	123.1128 149.0972 165.1285 209.1183
					12 	$C_9H_{13}O$ **$C_{10}H_{17}O$** $C_{11}H_{13}O$ $C_{11}H_{15}O_2$	137.0972 **153.1285** 161.0971 179.1078
					13 	$C_{12}H_{17}O_2$	193.1234
					14 	C_6H_{11} **$C_{13}H_{19}O$** $C_{15}H_{21}O_3$	83.0866 **191.1441** 249.1496
					15 	$C_7H_{13}O$ $C_9H_{15}O$ $C_{14}H_{19}O_2$	**113.0972** 139.1128 219.1391

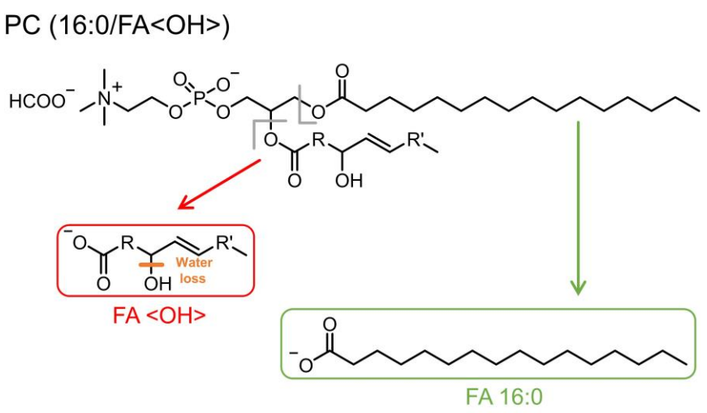
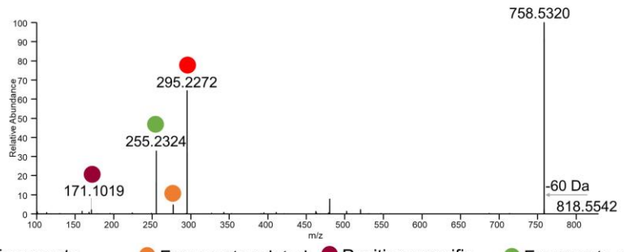
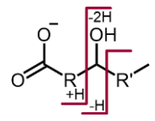
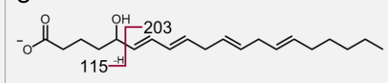
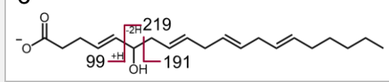
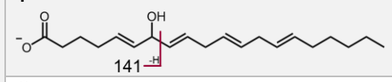
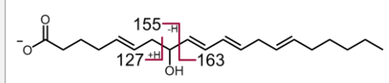
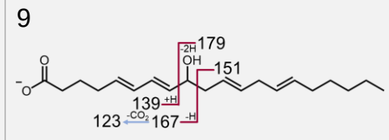
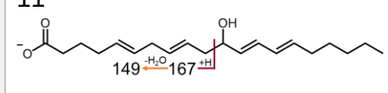
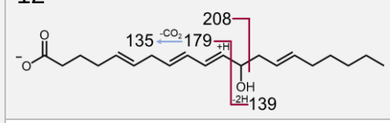
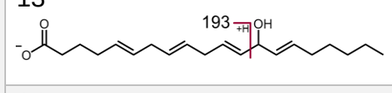
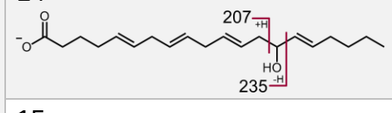
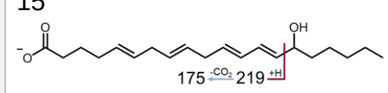
Full-length oxygenated: <OH>

[M+HCOO]$^-$ adducts (precursors)

Precursor	Chemical Formula & *m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula & *m/z*	Pos.-specific fragmentation	Chemical Formula	*m/z*
PC(16:0/18:1<OH>)	$C_{43}H_{83}O_{11}NP$ 820.5709	PC (16:0/FA<OH>)  **FA fragmentation pattern:** 	**FA(18:1<OH>)** H_2O loss CO_2 loss H_2O&CO_2 loss	**$C_{18}H_{33}O_3$** **297.2435** $C_{18}H_{31}O_2$ 279.2330 $C_{17}H_{33}O$ 253.2536 $C_{17}H_{31}$ 235.2431	9 	$C_8H_{13}O_2$ $C_{10}H_{19}O$ **$C_9H_{15}O_3$**	141.0921 155.1441 **171.1027**
PC(16:0/18:2<OH>)	$C_{43}H_{81}O_{11}NP$ 818.5553		**FA(18:2<OH>)** H_2O loss CO_2 loss H_2O&CO_2 loss	**$C_{18}H_{31}O_3$** **295.2279** $C_{18}H_{29}O_2$ 277.2173 $C_{17}H_{31}O$ 251.2380 $C_{17}H_{29}$ 233.2275	9 	C_9H_{15} $C_{10}H_{15}O$ **$C_9H_{15}O_3$**	123.1179 151.1128 **171.1027**
					10 	$C_9H_{15}O$ $C_9H_{15}O_2$ $C_{10}H_{15}O_3$	139.1128 155.1078 183.1027
					11 	C_7H_{13} $C_8H_{13}O$ $C_{10}H_{17}O_2$ $C_{11}H_{17}O_3$	97.1023 125.0972 169.1234 197.1183
					12 	C_6H_{11} **$C_{11}H_{19}O_2$** $C_{12}H_{19}O_3$	83.0866 **183.1391** 211.1340
					13 	**$C_{12}H_{19}O_2$**	**195.1391**
					14 	$C_{13}H_{21}O_2$	209.1547

Full-length oxygenated: <OH> (continued)

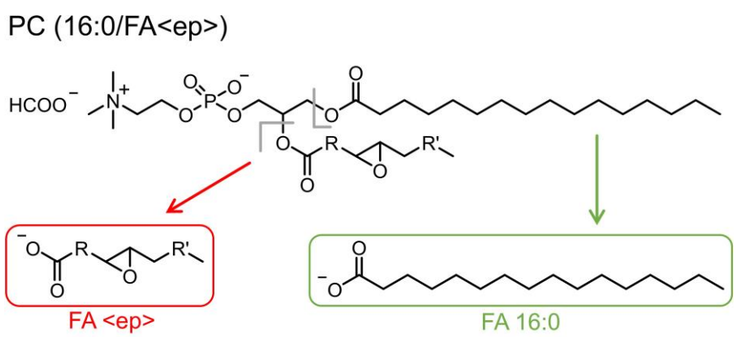
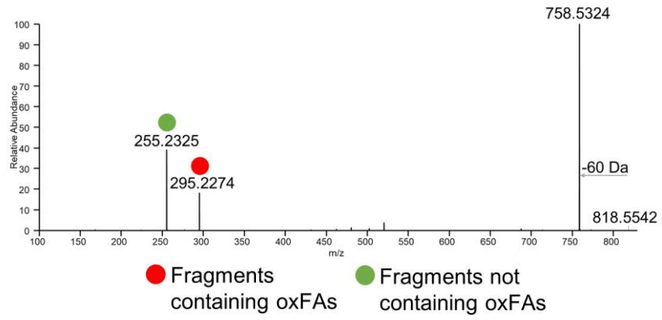
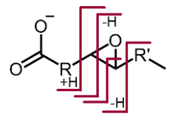
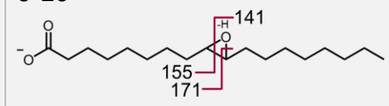
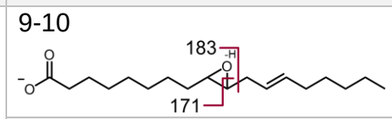
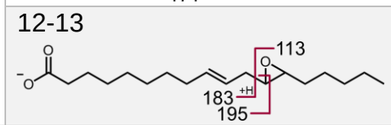
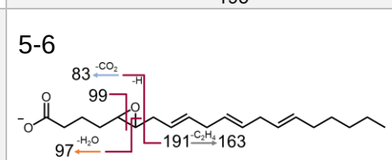
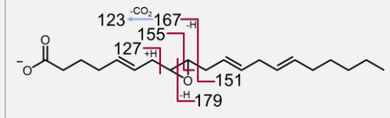
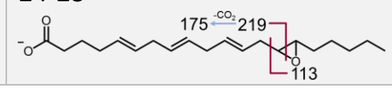
[M+HCOO]$^-$ adducts

Precursor	Chemical Formula & *m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula & *m/z*	Pos.-specific fragmentation	Chemical Formula	*m/z*
PC(16:0/20:4<OH>)	$C_{45}H_{81}O_{11}NP$ 842.5553	PC (16:0/FA<OH>)   **FA fragmentation pattern:**  	**FA(20:4<OH>)** H_2O loss CO_2 loss H_2O&CO_2 loss	**$C_{20}H_{31}O_3$** **319.2279** $C_{20}H_{29}O_2$ 301.2173 $C_{19}H_{31}O$ 275.2380 $C_{19}H_{29}$ 257.2275	5  	**$C_5H_7O_3$** $C_{15}H_{23}$	**115.0401** 203.1805[5]
					6  	$C_5H_7O_2$ $C_{14}H_{23}$ $C_{15}H_{23}O$	99.0452 191.1805 219.1754
					7  	$C_7H_9O_3$	141.0557
					8  	$C_7H_{11}O_2$ **$C_8H_{11}O_3$** **$C_{12}H_{19}$**	127.0765 **155.0714** **163.1492**
					9  	**$C_8H_{11}O$** $C_8H_{11}O_2$ $C_{11}H_{19}$ $C_9H_{11}O_3$ **$C_{12}H_{19}O$**	**123.0815** 139.0765 151.1492 167.0714 **179.1441**
					11  	$C_{10}H_{13}O$ **$C_{10}H_{15}O_2$**	149.0972 **167.1078**
					12  	$C_{10}H_{15}$ $C_9H_{15}O$ **$C_{11}H_{15}O_2$** $C_{12}H_{16}O_3$	135.1179 139.1128 **179.1078** 208.1105[6]
					13  	$C_{12}H_{17}O_2$	193.1234
					14  	**$C_{13}H_{19}O_2$** $C_{14}H_{19}O_3$	**207.1391** 235.1340
					15  	**$C_{13}H_{19}$** **$C_{14}H_{19}O_2$**	**175.1492** **219.1391**

[5] The signal is not OH{5}-specific (can be found in the spectra of other isomers, but less intense)
[6] The signal should correspond to an anion-radical that is the unique case for position 12.

Full-length oxygenated: <ep>

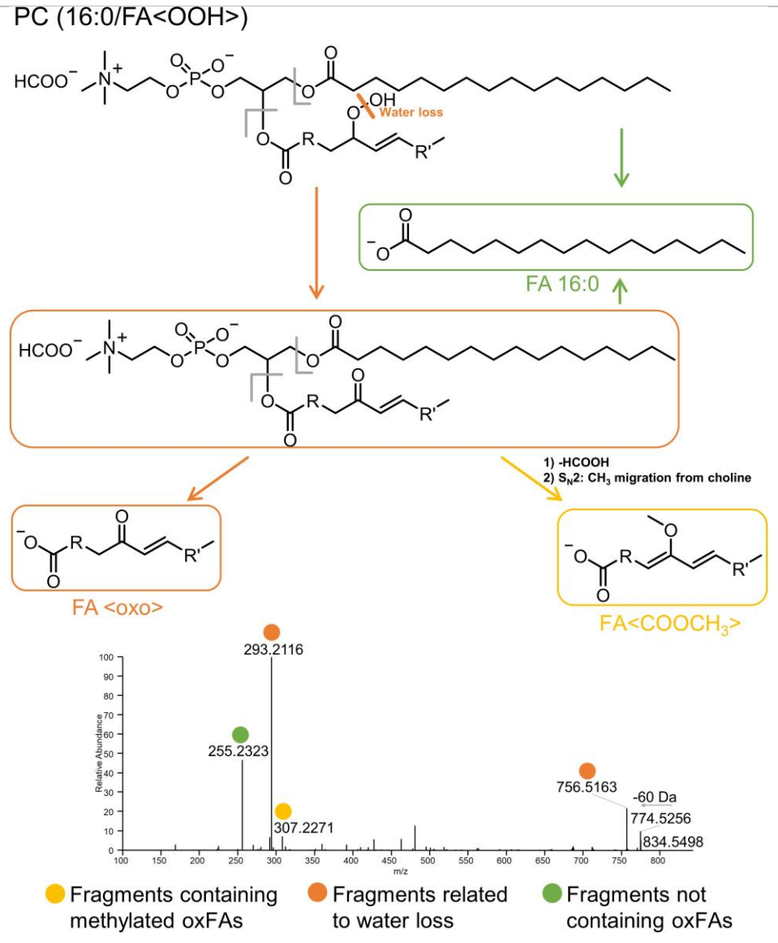
$[M+HCOO]^-$ adducts

Precursor	Chemical Formula & *m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula & *m/z*	Pos.-specific fragmentation	Chemical Formula	*m/z*
PC(16:0/18:0<ep>)	$C_{43}H_{83}O_{11}NP$ 820.5709	PC (16:0/FA<ep>)   Fragments containing oxFAs Fragments not containing oxFAs **FA fragmentation pattern:** 	**FA(18:0<ep>)** H_2O loss	**$C_{18}H_{33}O_3$** **297.2435** $C_{18}H_{31}O_2$ 279.2330	9-10  	$C_9H_{17}O$ $C_9H_{15}O_2$ **$C_9H_{15}O_3$**	141.1285 155.1078 **171.1027**
PC(16:0/18:1<ep>)	$C_{43}H_{81}O_{11}NP$ 818.5553		**FA(18:1<ep>)** H_2O loss	**$C_{18}H_{31}O_3$** **295.2279** $C_{18}H_{29}O_2$ 277.2173	9-10  	**$C_9H_{15}O_3$** $C_{10}H_{15}O_3$	**171.1027** 183.1027
					12-13  	$C_7H_{13}O$ **$C_{11}H_{19}O_2$** **$C_{12}H_{19}O_2$**	113.0972 **183.1391** **195.1391**
PC(16:0/20:3<ep>)	$C_{45}H_{81}O_{11}NP$ 842.5553		**FA(20:3<ep>)** H_2O loss $H_2O\&CO_2$ loss	**$C_{20}H_{31}O_3$** **319.2279** $C_{20}H_{29}O_2$ 301.2173 $C_{19}H_{29}$ 257.2275	5-6  	C_5H_7O $C_5H_5O_2$ $C_5H_7O_2$ **$C_{12}H_{19}$** **$C_{14}H_{23}$**	83.0502 97.0295 99.0452 **163.1492** **191.1805**
					8-9  	**$C_7H_{11}O_2$** **$C_8H_{11}O$** **$C_{11}H_{19}$** **$C_8H_{11}O_3$** **$C_9H_{11}O_3$** **$C_{12}H_{19}O$**	**127.0765**[7] **123.0815** **151.1492** **155.0714** **167.0714** **179.1441**
					11-12  	**$C_{10}H_{15}O_2$** **$C_{11}H_{15}O_2$** $C_{12}H_{15}O_3$	**167.1078** **179.1078** 208.1104[8]
					14-15  	$C_7H_{13}O$ **$C_{13}H_{19}$** **$C_{14}H_{19}O_2$**	113.0972 **175.1492** **219.1391**

[7] The abundances of fragments do not differ much, so it is difficult to choose the major one.
[8] The signal should correspond to an anion-radical that is the unique case for position 12.

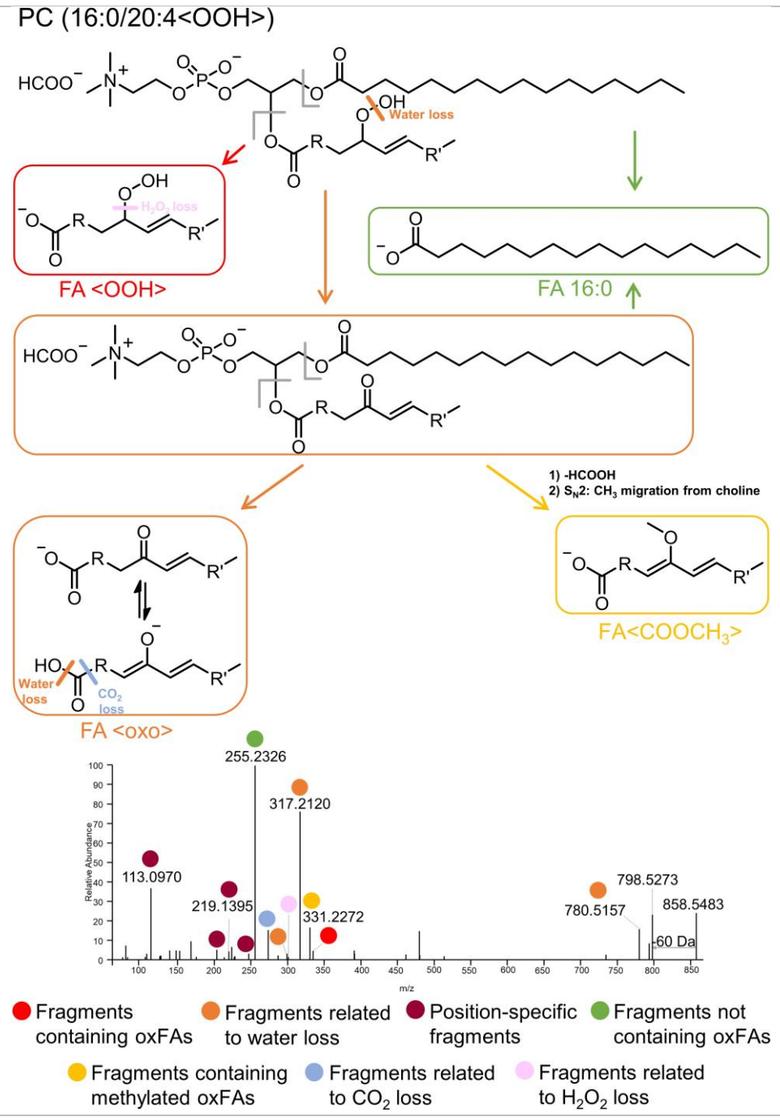
Full-length oxygenated: <OOH>

[M+HCOO]$^-$ adducts

Precursor	Chemical Formula & *m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula & *m/z*	Pos.-specific fragmentation
PC(16:0/18:1<OOH>)	$C_{43}H_{83}O_{12}NP$ 836.5658		FA(18:1<OOH>) **H_2O loss** Methylation H_2O&CO_2 loss 2H_2O loss H_2O_2 loss	$C_{18}H_{33}O_4$ 313.2384 **$C_{18}H_{31}O_3$** **295.2279** $C_{19}H_{33}O_3$ 309.2435 $C_{17}H_{31}O$ 251.2380 $C_{18}H_{29}O_2$ 277.2173 $C_{18}H_{27}O_2$ 275.2016	
PC(16:0/18:2<OOH>)	$C_{43}H_{81}O_{12}NP$ 834.5502		FA(18:2<OOH>) **H_2O loss** Methylation H_2O&CO_2 loss 2H_2O loss H_2O_2 loss	$C_{18}H_{31}O_4$ 311.2228 **$C_{18}H_{29}O_3$** **293.2122** $C_{19}H_{31}O_3$ 307.2279 $C_{17}H_{29}O$ 249.2224 $C_{18}H_{27}O_2$ 275.2016 $C_{18}H_{29}O_2$ 277.2173	See above (Full-length oxygenated: <oxo>)

Full-length oxygenated: <OOH> (continued)

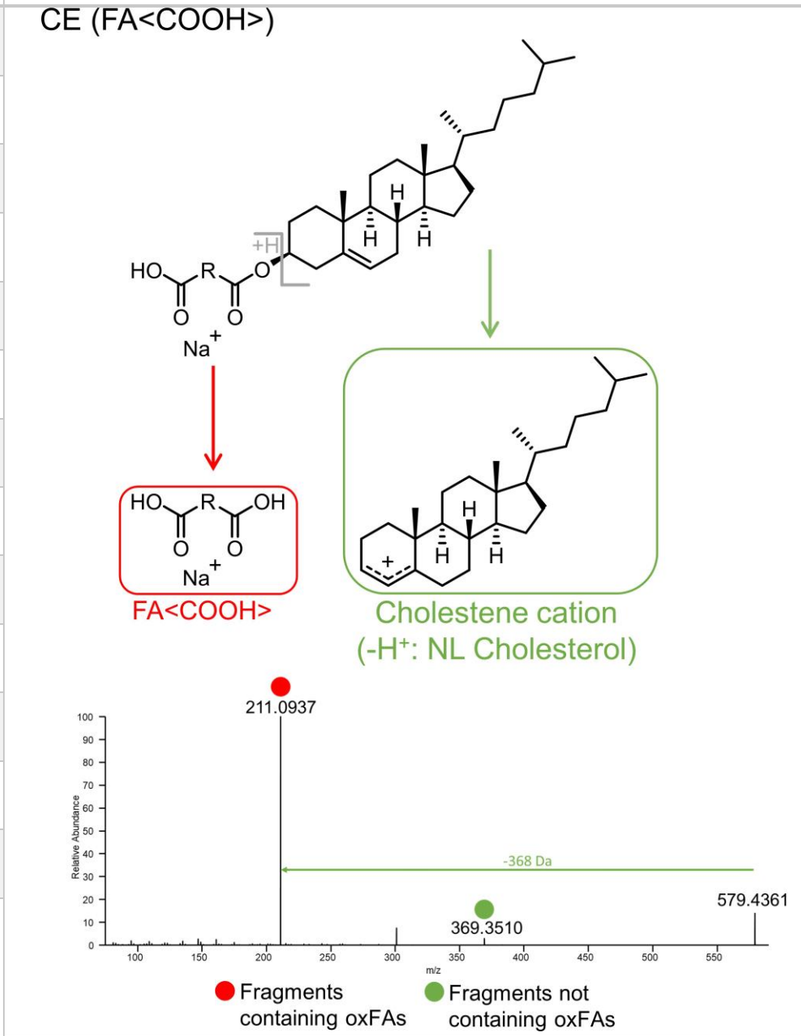
[M+HCOO]$^-$ adducts

Precursor	Chemical Formula & *m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula & *m/z*	Pos.-specific fragmentation
PC(16:0/20:4<OOH>)	$C_{45}H_{81}O_{12}NP$ 858.5502		FA(20:4<OOH>) **H_2O loss** Methylation H_2O&CO_2 loss $2H_2O$ loss H_2O_2 loss	$C_{20}H_{31}O_4$ 335.2228 **$C_{20}H_{29}O_3$** **317.2122** $C_{21}H_{31}O_3$ 331.2279 $C_{19}H_{29}O$ 273.2224 $C_{20}H_{27}O_2$ 299.2017 $C_{20}H_{29}O_2$ 301.2173	See above (Full-length oxygenated: <oxo>)

CHOLESTERYL ESTERS

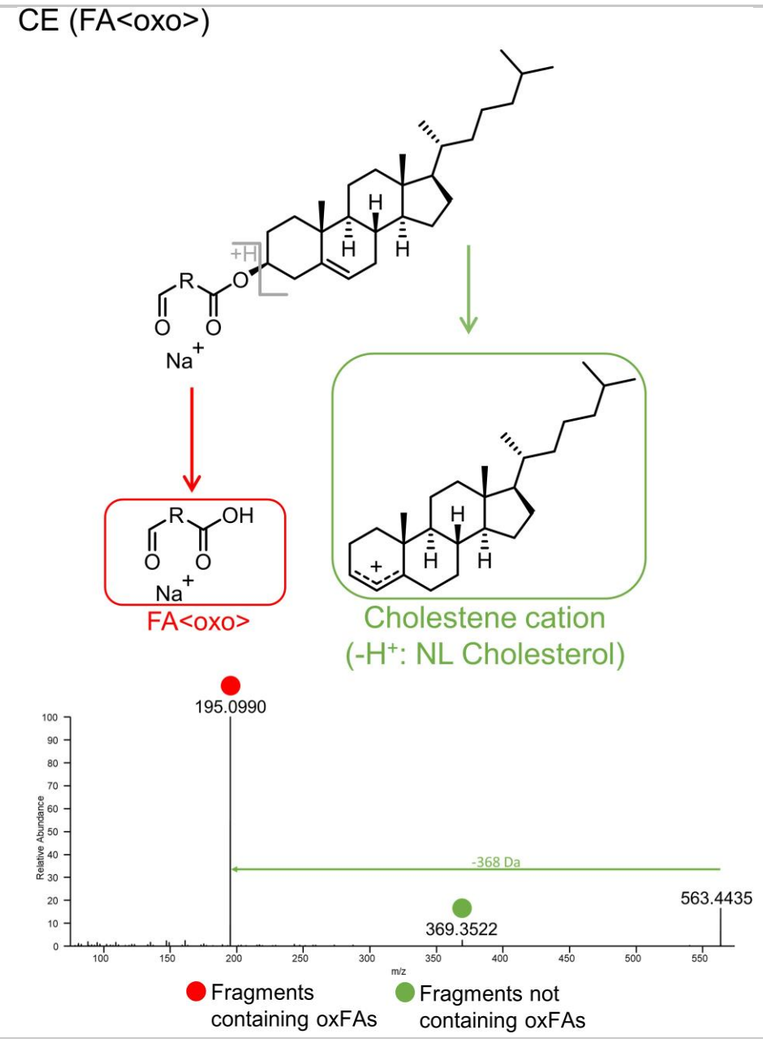
Oxidatively truncated: <COOH>

$[M+Na]^+$ adducts

Mod. position	Precursor	Chemical Formula	*m/z*	MS^2 Fragmentation	Mod./pos.-specific fragment	Chemical Formula	*m/z*
4	CE(4:0<COOH>)	$C_{31}H_{50}O_4Na$	509.3601		FA(4:0<COOH>)	$C_4H_6O_4Na$	141.0158
5	CE(5:0<COOH>)	$C_{32}H_{52}O_4Na$	523.3758		FA(5:0<COOH>)	$C_5H_8O_4Na$	155.0315
7	CE(7:0<COOH>)	$C_{34}H_{56}O_4Na$	551.4071		FA(7:0<COOH>)	$C_7H_{12}O_4Na$	183.0628
8	CE(8:0<COOH>)	$C_{35}H_{58}O_4Na$	565.4227		FA(8:0<COOH>)	$C_8H_{14}O_4Na$	197.0784
9	CE(9:0<COOH>)	$C_{36}H_{60}O_4Na$	579.4384		FA(9:0<COOH>)	$C_9H_{16}O_4Na$	211.0941
10	CE(10:0<COOH>)	$C_{37}H_{62}O_4Na$	593.4540		FA(10:0<COOH>)	$C_{10}H_{18}O_4Na$	225.1097
	CE(10:1<COOH>)	$C_{37}H_{60}O_4Na$	591.4384		FA(10:1<COOH>)	$C_{10}H_{16}O_4Na$	223.0941
11	CE(11:1<COOH>)	$C_{38}H_{62}O_4Na$	605.4540		FA(11:1<COOH>)	$C_{11}H_{18}O_4Na$	237.1097
	CE(11:2<COOH>)	$C_{38}H_{60}O_4Na$	603.4384		FA(11:2<COOH>)	$C_{11}H_{16}O_4Na$	235.0941
12	CE(12:1<COOH>)	$C_{39}H_{64}O_4Na$	619.4697		FA(12:1<COOH>)	$C_{12}H_{20}O_4Na$	251.1254
	CE(12:2<COOH>)	$C_{39}H_{62}O_4Na$	617.4540		FA(12:2<COOH>)	$C_{12}H_{18}O_4Na$	249.1097
13	CE(13:2<COOH>)	$C_{40}H_{64}O_4Na$	631.4697		FA(13:2<COOH>)	$C_{13}H_{20}O_4Na$	263.1254
	CE(13:3<COOH>)	$C_{40}H_{62}O_4Na$	629.4540		FA(13:3<COOH>)	$C_{13}H_{18}O_4Na$	261.1097
14	CE(14:3<COOH>)	$C_{41}H_{64}O_4Na$	643.4697		FA(14:3<COOH>)	$C_{14}H_{20}O_4Na$	275.1254

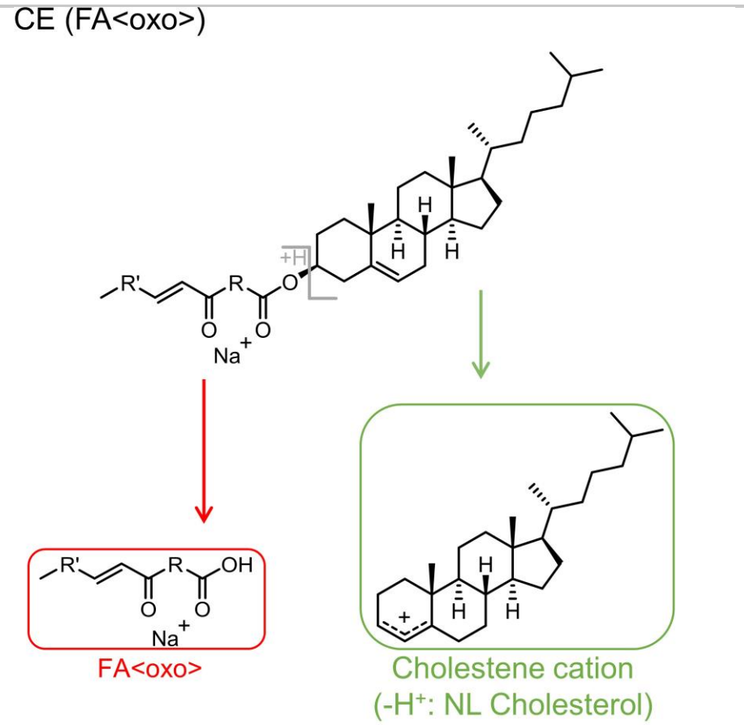
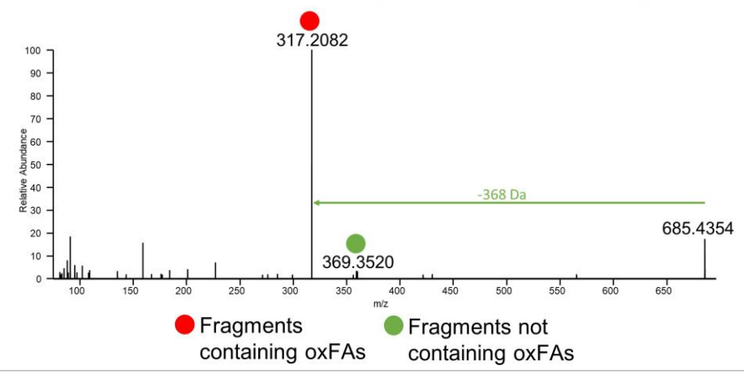
Oxidatively truncated: <oxo>

$[M+Na]^+$ adducts

Mod. position	Precursor	Chemical Formula	*m/z*	MS² Fragmentation	Mod./pos.-specific fragment	Chemical Formula	*m/z*
4	CE(4:0<oxo>)	$C_{31}H_{50}O_3Na$	493.3652		FA(4:0<oxo>)	$C_4H_6O_3Na$	125.0209
5	CE(5:0<oxo>)	$C_{32}H_{52}O_3Na$	507.3809		FA(5:0<oxo>)	$C_5H_8O_3Na$	139.0366
7	CE(7:0<oxo>)	$C_{34}H_{56}O_3Na$	535.4122		FA(7:0<oxo>)	$C_7H_{12}O_3Na$	167.0679
8	CE(8:0<oxo>)	$C_{35}H_{58}O_3Na$	549.4278		FA(8:0<oxo>)	$C_8H_{14}O_3Na$	181.0835
9	CE(9:0<oxo>)	$C_{36}H_{60}O_3Na$	563.4435		FA(9:0<oxo>)	$C_9H_{16}O_3Na$	195.0992
10	CE(10:0<oxo>)	$C_{37}H_{62}O_3Na$	577.4591		FA(10:0<oxo>)	$C_{10}H_{18}O_3Na$	209.1148
	CE(10:1<oxo>)	$C_{37}H_{60}O_3Na$	575.4435		FA(10:1<oxo>)	$C_{10}H_{16}O_3Na$	207.0992
11	CE(11:1<oxo>)	$C_{38}H_{62}O_3Na$	589.4591		FA(11:1<oxo>)	$C_{11}H_{18}O_3Na$	221.1148
	CE(11:2<oxo>)	$C_{38}H_{60}O_3Na$	587.4435		FA(11:2<oxo>)	$C_{11}H_{16}O_3Na$	219.0992
12	CE(12:1<oxo>)	$C_{39}H_{64}O_3Na$	603.4748		FA(12:1<oxo>)	$C_{12}H_{20}O_3Na$	235.1305
	CE(12:2<oxo>)	$C_{39}H_{62}O_3Na$	601.4591		FA(12:2<oxo>)	$C_{12}H_{18}O_3Na$	233.1148
13	CE(13:2<oxo>)	$C_{40}H_{64}O_3Na$	615.4748		FA(13:2<oxo>)	$C_{13}H_{20}O_3Na$	247.1305
	CE(13:3<oxo>)	$C_{40}H_{62}O_3Na$	613.4591		FA(13:3<oxo>)	$C_{13}H_{18}O_3Na$	245.1148
14	CE(14:3<oxo>)	$C_{41}H_{64}O_3Na$	627.4748		FA(14:3<oxo>)	$C_{14}H_{20}O_3Na$	259.1305

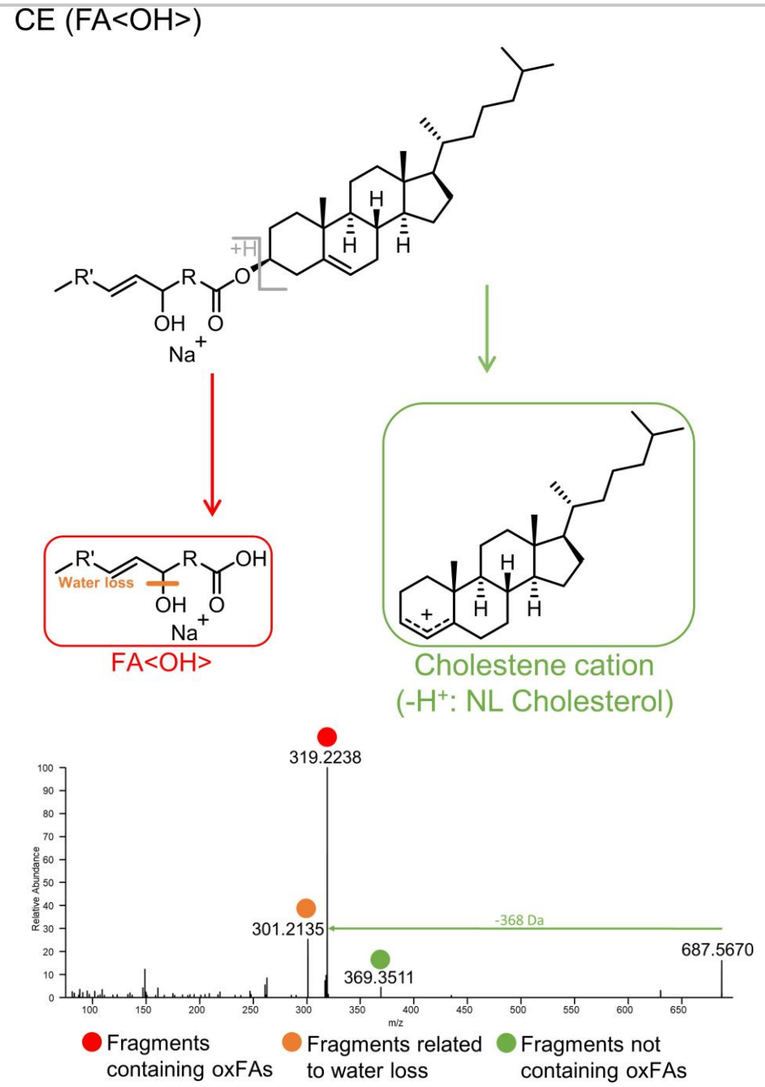
Full-length oxygenated: <oxo>

$[M+Na]^+$ adducts

Precursor	Chemical Formula	*m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula	*m/z*
CE(18:1)<oxo>	$C_{45}H_{76}O_3Na$	687.5687		FA(18:1)<oxo>	$C_{18}H_{32}O_3Na$	319.2244
CE(18:2)<oxo>	$C_{45}H_{74}O_3Na$	685.5530		FA(18:2)<oxo>	$C_{18}H_{30}O_3Na$	317.2087
CE(20:4)<oxo>	$C_{47}H_{74}O_3Na$	709.5530		FA(20:4)<oxo>	$C_{20}H_{30}O_3Na$	341.2087

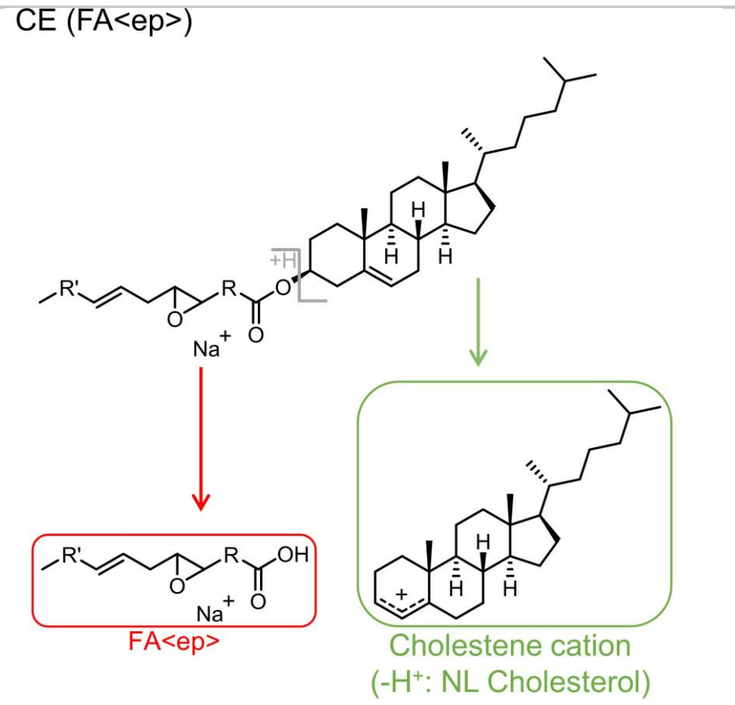
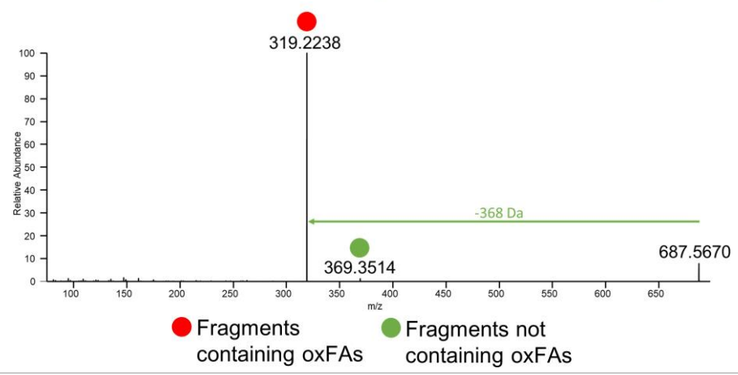
Full-length oxygenated: <OH>

$[M+Na]^+$ adducts

Precursor	Chemical Formula	*m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula	*m/z*
CE(18:1<OH>)	$C_{45}H_{78}O_3Na$	689.5843		**FA(18:1<OH>)** H_2O loss	**$C_{18}H_{34}O_3Na$** $C_{18}H_{32}O_2Na$	**321.2400** 303.2295
CE(18:2<OH>)	$C_{45}H_{76}O_3Na$	687.5687		**FA(18:2<OH>)** H_2O loss	**$C_{18}H_{32}O_3Na$** $C_{18}H_{30}O_2Na$	**319.2244** 301.2138
CE(20:4<OH>)	$C_{47}H_{76}O_3Na$	711.5687		**FA(20:4<OH>)** H_2O loss	**$C_{20}H_{32}O_3Na$** $C_{20}H_{30}O_2Na$	**343.2244** 325.2138

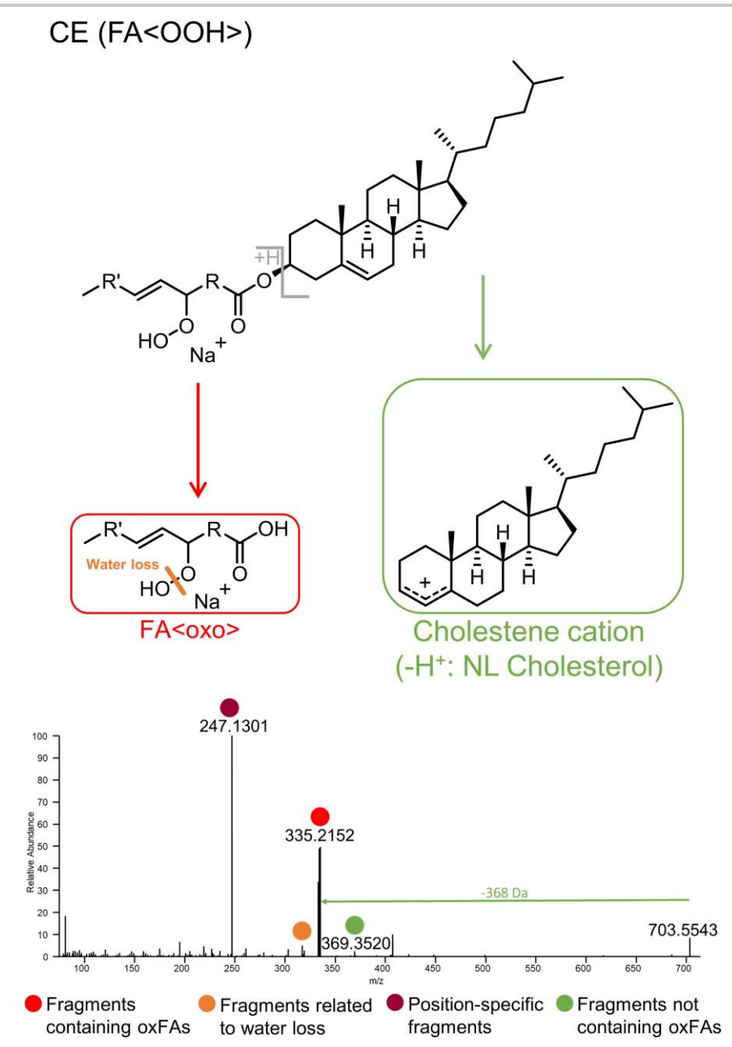
Full-length oxygenated: <ep>

$[M+Na]^+$ adducts

Precursor	Chemical Formula	*m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula	*m/z*
CE(18:0<ep>)	$C_{45}H_{78}O_3Na$	689.5843		FA(18:0<ep>)	$C_{18}H_{34}O_3Na$	321.2400
CE(18:1<ep>)	$C_{45}H_{76}O_3Na$	687.5687		FA(18:1<ep>)	$C_{18}H_{32}O_3Na$	319.2244
CE(20:3<ep>)	$C_{47}H_{76}O_3Na$	711.5687		FA(20:3<ep>)	$C_{20}H_{32}O_3Na$	343.2244

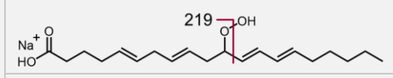
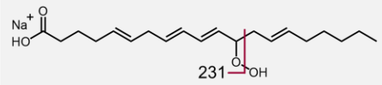
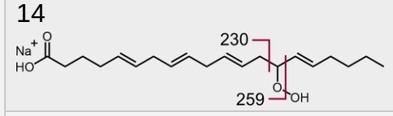
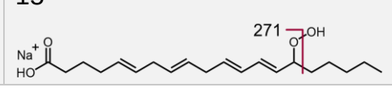
Full-length oxygenated: <OOH>

$[M+Na]^+$ adducts

Precursor	Chemical Formula & *m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula & *m/z*	Pos.-specific fragment	Chemical Formula	*m/z*
CE(18:1<OOH>)	$C_{45}H_{78}O_4Na$ 705.5792		**FA(18:1<OOH>)** H_2O loss	**$C_{18}H_{34}O_4Na$** **337.2349** $C_{18}H_{32}O_3Na$ 319.2244	9 195 OH 193 OH	$C_9H_{16}O_3Na$ $C_9H_{14}O_3Na$	195.0992 193.0835
CE(18:2<OOH>)	$C_{45}H_{76}O_4Na$ 703.5636		**FA(18:2<OOH>)** H_2O loss	**$C_{18}H_{32}O_4Na$** **335.2193** $C_{18}H_{30}O_3Na$ 317.2087	9 195 OH 10 207 OH 11 221 OH 12 206 235 OH 13 247 OH	$C_9H_{16}O_3Na$ $C_{10}H_{16}O_3Na$ $C_{11}H_{18}O_3Na$ $C_{11}H_{19}O_2Na$ $C_{12}H_{20}O_3Na$ $C_{13}H_{20}O_3Na$	195.0992 207.0992 221.1148 206.1277[10] 235.1305 247.1305
CE(20:4<OOH>)	$C_{47}H_{76}O_4Na$ 727.5636	**FA fragmentation pattern:**	**FA(20:4<OOH>)** H_2O loss	**$C_{20}H_{32}O_4Na$** **359.2193** $C_{20}H_{30}O_3Na$ 341.2087	5 139 OH 6 151 OH 8 179 OH 9 191 OH	$C_5H_8O_3Na$ $C_6H_8O_3Na$ $C_8H_{12}O_3Na$ $C_9H_{12}O_3Na$	139.0366 151.0366 179.0679 191.0679

Full-length oxygenated: <OOH> (continued)

$[M+Na]^+$ adducts

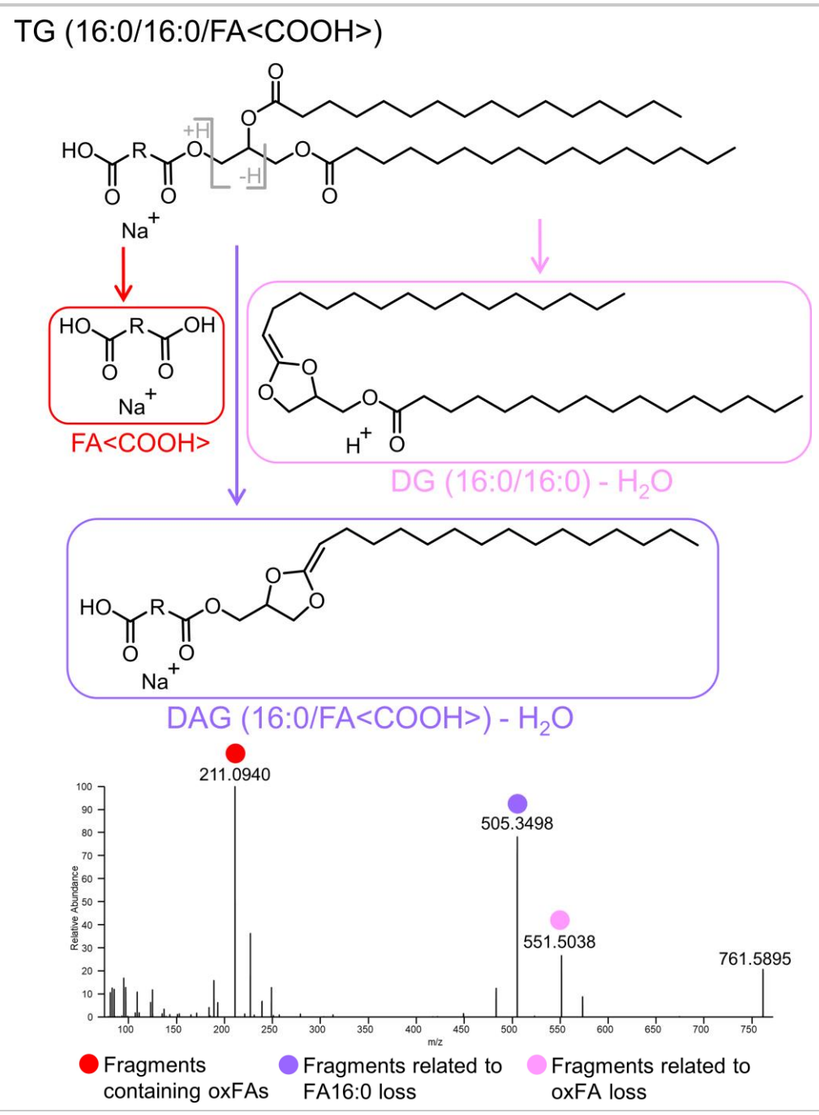
Precursor	Chemical Formula & *m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula & *m/z*	Pos.-specific fragment	Chemical Formula	*m/z*
CE(20:4<OOH>)	$C_{47}H_{76}O_4Na$ 727.5636		**FA(20:4<OOH>)** H_2O loss	**$C_{20}H_{32}O_4Na$ 359.2193** $C_{20}H_{30}O_3Na$ 341.2087	11 	$C_{11}H_{16}O_3Na$	219.0992
					12 	$C_{12}H_{16}O_3Na$	231.0992
					14 	$C_{13}H_{19}O_2Na$ $C_{14}H_{20}O_3Na$	230.1277[9] 259.1305
					15 	$C_{15}H_{20}O_3Na$	271.1305

[9] See *Ito, J., Mizuochi, S., Nakagawa, K., Kato, S., Miyazawa, T., 2015. Tandem Mass Spectrometry Analysis of Linoleic and Arachidonic Acid Hydroperoxides via Promotion of Alkali Metal Adduct Formation. Anal. Chem. 87, 4980–4987.*

TRIACYLGLYCEROLS

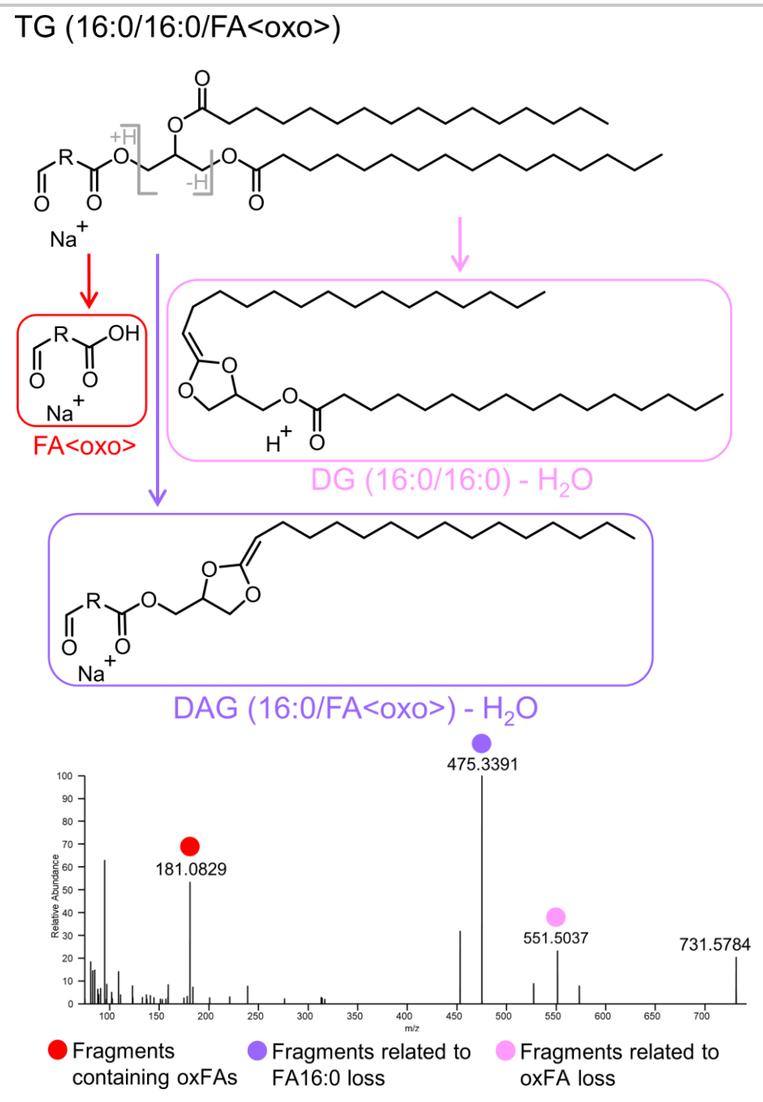
Oxidatively truncated: <COOH>

$[M+Na]^+$ adducts

Mod. position	Precursor	Chemical Formula	*m/z*	MS^2 Fragmentation	Mod./pos.-specific fragment	Chemical Formula	*m/z*
4	TG(16:0/16:0/4:0<COOH>)	$C_{39}H_{72}O_8Na$	691.5119		FA(4:0<COOH>)	$C_4H_6O_4Na$	141.0158
5	TG(16:0/16:0/5:0<COOH>)	$C_{40}H_{74}O_8Na$	705.5276		FA(5:0<COOH>)	$C_5H_8O_4Na$	155.0315
7	TG(16:0/16:0/7:0<COOH>)	$C_{42}H_{78}O_8Na$	733.5589		FA(7:0<COOH>)	$C_7H_{12}O_4Na$	183.0628
8	TG(16:0/16:0/8:0<COOH>)	$C_{43}H_{80}O_8Na$	747.5745		FA(8:0<COOH>)	$C_8H_{14}O_4Na$	197.0784
9	TG(16:0/16:0/9:0<COOH>)	$C_{44}H_{82}O_8Na$	761.5902		FA(9:0<COOH>)	$C_9H_{16}O_4Na$	211.0941
10	TG(16:0/16:0/10:0<COOH>)	$C_{45}H_{84}O_8Na$	775.6058		FA(10:0<COOH>)	$C_{10}H_{18}O_4Na$	225.1097
	TG(16:0/16:0/10:1<COOH>)	$C_{45}H_{82}O_8Na$	773.5902		FA(10:1<COOH>)	$C_{10}H_{16}O_4Na$	223.0941
11	TG(16:0/16:0/11:1<COOH>)	$C_{46}H_{84}O_8Na$	787.6058		FA(11:1<COOH>)	$C_{11}H_{18}O_4Na$	237.1097
	TG(16:0/16:0/11:2<COOH>)	$C_{46}H_{82}O_8Na$	785.5902		FA(11:2<COOH>)	$C_{11}H_{16}O_4Na$	235.0941
12	TG(16:0/16:0/12:1<COOH>)	$C_{47}H_{86}O_8Na$	801.6215		FA(12:1<COOH>)	$C_{12}H_{20}O_4Na$	251.1254
	TG(16:0/16:0/12:2<COOH>)	$C_{47}H_{84}O_8Na$	799.6058		FA(12:2<COOH>)	$C_{12}H_{18}O_4Na$	249.1097
13	TG(16:0/16:0/13:2<COOH>)	$C_{48}H_{86}O_8Na$	813.6215		FA(13:2<COOH>)	$C_{13}H_{20}O_4Na$	263.1254
	TG(16:0/16:0/13:3<COOH>)	$C_{48}H_{84}O_8Na$	811.6058		FA(13:3<COOH>)	$C_{13}H_{18}O_4Na$	261.1097
14	TG(16:0/16:0/14:3<COOH>)	$C_{49}H_{86}O_8Na$	825.6215		FA(14:3<COOH>)	$C_{14}H_{20}O_4Na$	275.1254

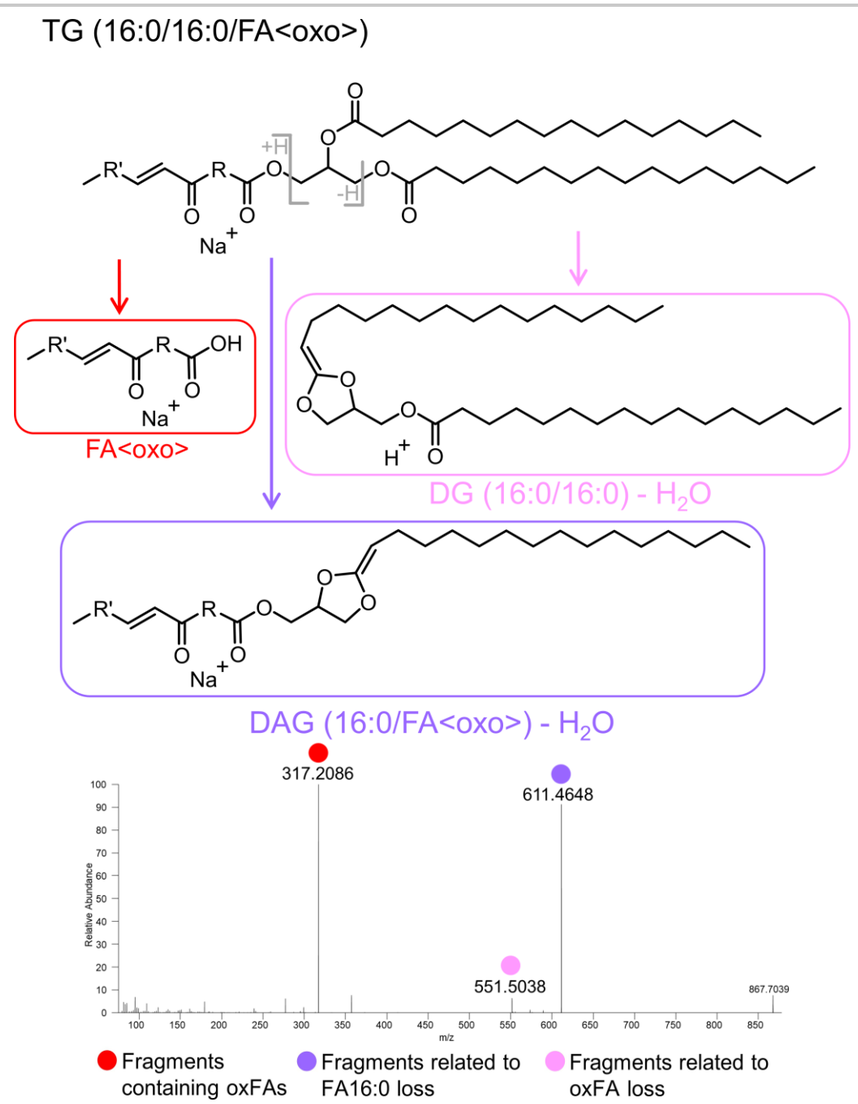
Oxidatively truncated: <oxo>

$[M+Na]^+$ adducts

Mod. position	Precursor	Chemical Formula	*m/z*	MS² Fragmentation	Mod./pos.-specific fragment	Chemical Formula	*m/z*
4	TG(16:0/16:0/4:0<oxo>)	$C_{39}H_{72}O_7Na$	675.5170		FA(4:0<oxo>)	$C_4H_6O_3Na$	125.0209
5	TG(16:0/16:0/5:0<oxo>)	$C_{40}H_{74}O_7Na$	689.5327		FA(5:0<oxo>)	$C_5H_8O_3Na$	139.0366
7	TG(16:0/16:0/7:0<oxo>)	$C_{42}H_{78}O_7Na$	717.5640		FA(7:0<oxo>)	$C_7H_{12}O_3Na$	167.0679
8	TG(16:0/16:0/8:0<oxo>)	$C_{43}H_{80}O_7Na$	731.5796		FA(8:0<oxo>)	$C_8H_{14}O_3Na$	181.0835
9	TG(16:0/16:0/9:0<oxo>)	$C_{44}H_{82}O_7Na$	745.5953		FA(9:0<oxo>)	$C_9H_{16}O_3Na$	195.0992
10	TG(16:0/16:0/10:0<oxo>)	$C_{45}H_{84}O_7Na$	759.6109		FA(10:0<oxo>)	$C_{10}H_{18}O_3Na$	209.1148
	TG(16:0/16:0/10:1<oxo>)	$C_{45}H_{82}O_7Na$	757.5953		FA(10:1<oxo>)	$C_{10}H_{16}O_3Na$	207.0992
11	TG(16:0/16:0/11:1<oxo>)	$C_{46}H_{84}O_7Na$	771.6109		FA(11:1<oxo>)	$C_{11}H_{18}O_3Na$	221.1148
	TG(16:0/16:0/11:2<oxo>)	$C_{46}H_{82}O_7Na$	769.5953		FA(11:2<oxo>)	$C_{11}H_{16}O_3Na$	219.0992
12	TG(16:0/16:0/12:1<oxo>)	$C_{47}H_{86}O_7Na$	785.6266		FA(12:1<oxo>)	$C_{12}H_{20}O_3Na$	235.1305
	TG(16:0/16:0/12:2<oxo>)	$C_{47}H_{84}O_7Na$	783.6109		FA(12:2<oxo>)	$C_{12}H_{18}O_3Na$	233.1148
13	TG(16:0/16:0/13:2<oxo>)	$C_{48}H_{86}O_7Na$	797.6266		FA(13:2<oxo>)	$C_{13}H_{20}O_3Na$	247.1305
	TG(16:0/16:0/13:3<oxo>)	$C_{48}H_{84}O_7Na$	795.6109		FA(13:3<oxo>)	$C_{13}H_{18}O_3Na$	245.1148
14	TG(16:0/16:0/14:3<oxo>)	$C_{49}H_{86}O_7Na$	809.6266		FA(14:3<oxo>)	$C_{14}H_{20}O_3Na$	259.1305

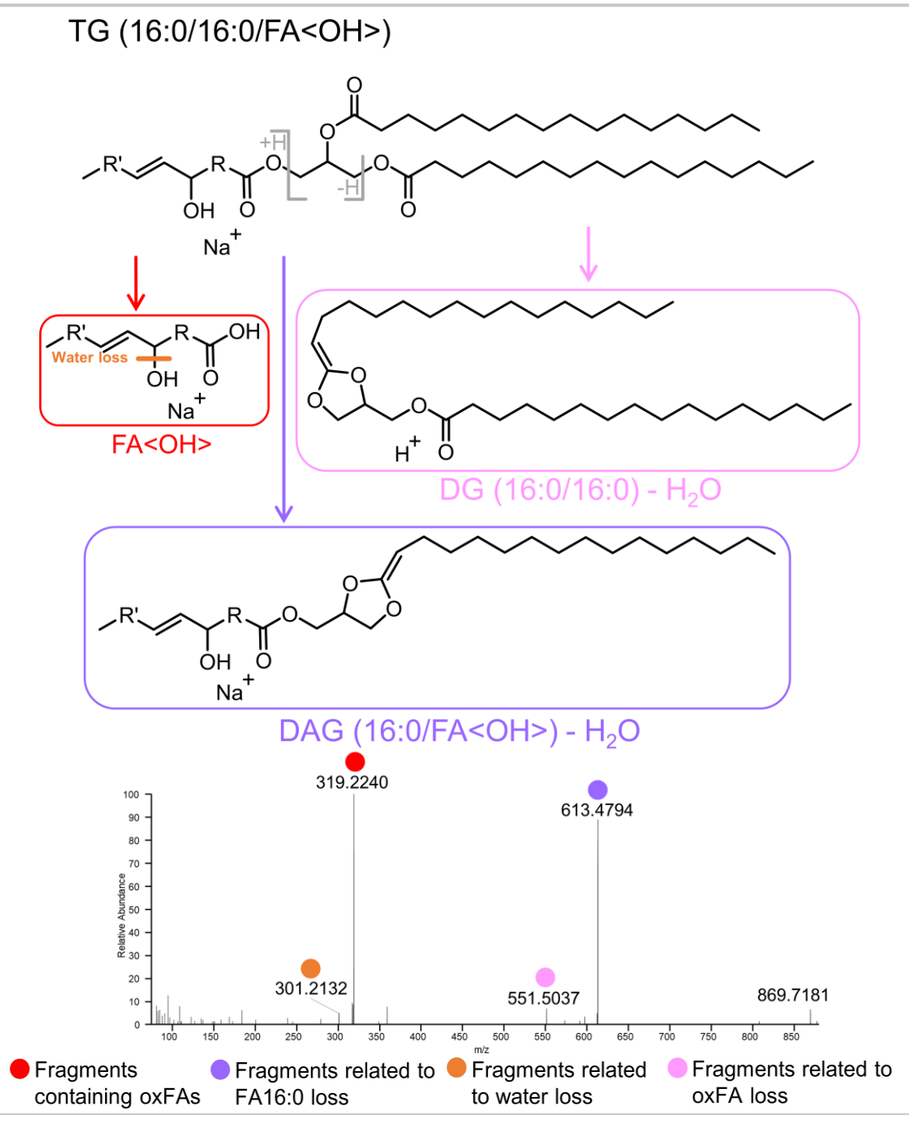
Full-length oxygenated: <oxo>

$[M+Na]^+$ adducts

Precursor	Chemical Formula	*m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula	*m/z*
TG(16:0/16:0/18:1<oxo>)	$C_{53}H_{98}O_7Na$	869.7205		FA(18:1<oxo>)	$C_{18}H_{32}O_3Na$	319.2244
TG(16:0/16:0/18:2<oxo>)	$C_{53}H_{96}O_7Na$	867.7048		FA(18:2<oxo>)	$C_{18}H_{30}O_3Na$	317.2087
TG(16:0/16:0/20:4<oxo>)	$C_{55}H_{96}O_7Na$	891.7048		FA(20:4<oxo>)	$C_{20}H_{30}O_3Na$	341.2087

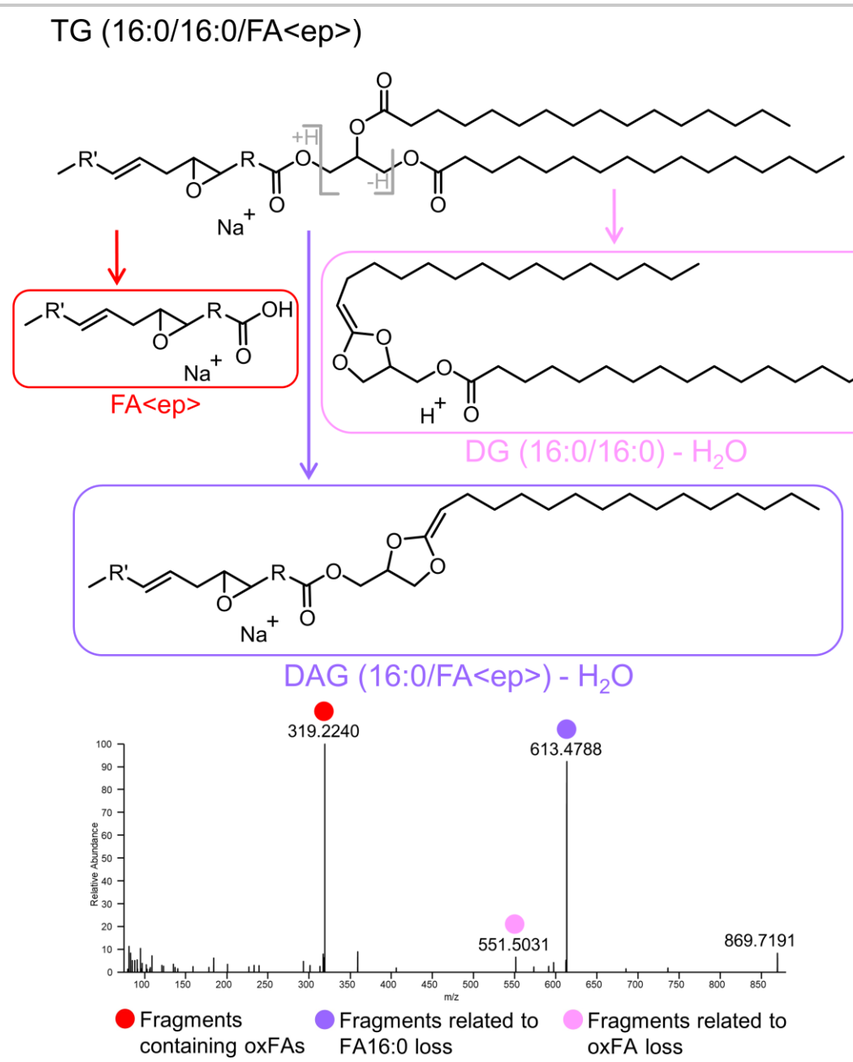
Full-length oxygenated: <OH>

$[M+Na]^+$ adducts

Precursor	Chemical Formula	*m/z*	MS² Fragmentation	Mod.-specific fragment	Chemical Formula	*m/z*
TG(16:0/16:0/18:1<OH>)	$C_{53}H_{100}O_7Na$	871.7361		**FA(18:1<OH>)** H_2O loss	**$C_{18}H_{34}O_3Na$** $C_{18}H_{32}O_2Na$	**321.2400** 303.2295
TG(16:0/16:0/18:2<OH>)	$C_{53}H_{98}O_7Na$	869.7205		**FA(18:2<OH>)** H_2O loss	**$C_{18}H_{32}O_3Na$** $C_{18}H_{30}O_2Na$	**319.2244** 301.2138
TG(16:0/16:0/20:4<OH>)	$C_{55}H_{98}O_7Na$	893.7205		**FA(20:4<OH>)** H_2O loss	**$C_{20}H_{32}O_3Na$** $C_{20}H_{30}O_2Na$	**343.2244** 325.2138

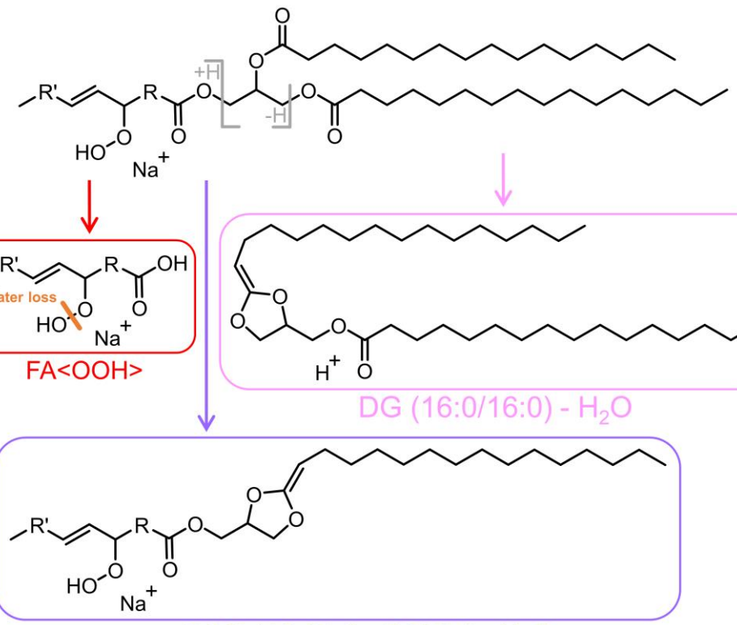
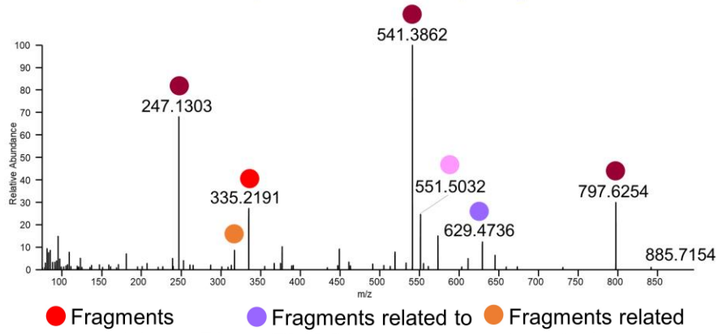
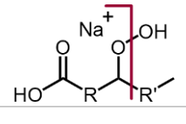
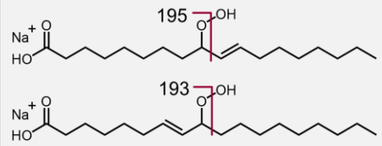
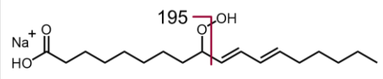
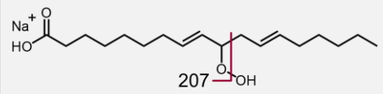
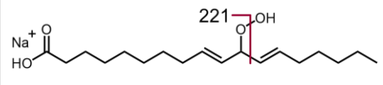
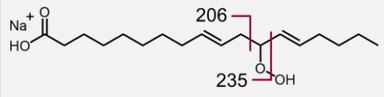
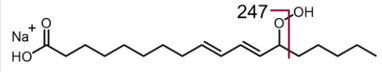
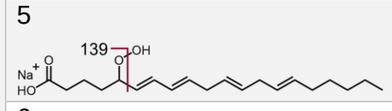
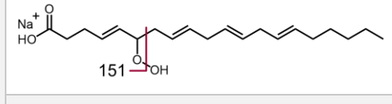
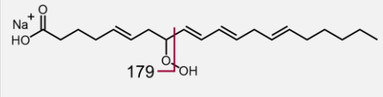
Full-length oxygenated: <ep>

$[M+Na]^+$ adducts

Precursor	Chemical Formula	*m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula	*m/z*
TG(16:0/16:0/18:0<ep>)	$C_{53}H_{100}O_7Na$	871.7361		FA(18:0<ep>)	$C_{18}H_{34}O_3Na$	321.2400
TG(16:0/16:0/18:1<ep>)	$C_{53}H_{98}O_7Na$	869.7205		FA(18:1<ep>)	$C_{18}H_{32}O_3Na$	319.2244
TG(16:0/16:0/20:3<ep>)	$C_{55}H_{98}O_7Na$	893.7205		FA(20:3<ep>)	$C_{20}H_{32}O_3Na$	343.2244

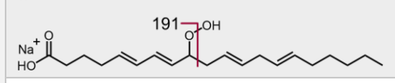
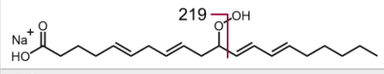
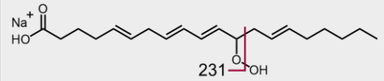
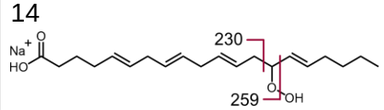
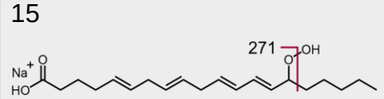
Full-length oxygenated: <OOH>

$[M+Na]^+$ adducts

Precursor	Chemical Formula & *m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula & *m/z*	Pos.-specific fragment	Chemical Formula	*m/z*
TG(16:0/16:0/18:1<OOH>)	$C_{53}H_{100}O_8Na$ 887.7310	TG (16:0/16:0/FA<OOH>)   **FA fragmentation pattern:**  	**FA(18:1<OOH>)** H_2O loss	**$C_{18}H_{34}O_4Na$ 337.2349** $C_{18}H_{32}O_3Na$ 319.2244	9  	$C_9H_{16}O_3Na$ $C_9H_{14}O_3Na$	195.0992 193.0835
TG(16:0/16:0/18:2<OOH>)	$C_{53}H_{98}O_8Na$ 885.7154		**FA(18:2<OOH>)** H_2O loss	**$C_{18}H_{32}O_4Na$ 335.2193** $C_{18}H_{30}O_3Na$ 317.2087	9  	$C_9H_{16}O_3Na$	195.0992
					10  	$C_{10}H_{16}O_3Na$	207.0992
					11  	$C_{11}H_{18}O_3Na$	221.1148
					12  	$C_{11}H_{19}O_2Na$ $C_{12}H_{20}O_3Na$	206.1277[11] 235.1305
					13  	$C_{13}H_{20}O_3Na$	247.1305
TG(16:0/16:0/20:4<OOH>)	$C_{55}H_{98}O_8Na$ 909.7154		**FA(20:4<OOH>)** H_2O loss	**$C_{20}H_{32}O_4Na$ 359.2193** $C_{20}H_{30}O_3Na$ 341.2087	5  	$C_5H_8O_3Na$	139.0366
					6  	$C_6H_8O_3Na$	151.0366
					8  	$C_8H_{12}O_3Na$	179.0679

Full-length oxygenated: <OOH> (continued)

$[M+Na]^+$ adducts

Precursor	Chemical Formula & *m/z*	MS^2 Fragmentation	Mod.-specific fragment	Chemical Formula & *m/z*	Pos.-specific fragment	Chemical Formula	*m/z*
TG(16:0/16:0/20:4<OOH>)	$C_{55}H_{98}O_8Na$ 909.7154		**FA(20:4<OOH>)** H_2O loss	**$C_{20}H_{30}O_3Na$ 359.2193** $C_{20}H_{32}O_4Na$ 341.2087	9 	$C_9H_{12}O_3Na$	191.0679
					11 	$C_{11}H_{16}O_3Na$	219.0992
					12 	$C_{12}H_{16}O_3Na$	231.0992
					14 	$C_{13}H_{19}O_2Na$ $C_{14}H_{20}O_3Na$	230.1277[10] 259.1305
					15 	$C_{15}H_{20}O_3Na$	271.1305

[10] See *Ito, J., Mizuochi, S., Nakagawa, K., Kato, S., Miyazawa, T., 2015. Tandem Mass Spectrometry Analysis of Linoleic and Arachidonic Acid Hydroperoxides via Promotion of Alkali Metal Adduct Formation. Anal. Chem. 87, 4980–4987.*

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- Murphy, R.C., 2015. Tandem mass spectrometry of lipids: molecular analysis of complex lipids, New developments in mass spectrometry. Royal Society of Chemistry, Cambridge.
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- Levison, B.S., 2013. Quantification of fatty acid oxidation products using online high-performance liquid chromatography tandem mass spectrometry. Free Radic. Biol. Med. 12. https://doi.org/10.1016/j.freeradbiomed.2013.03.001

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- Garscha, U., Nilsson, T., Oliw, E.H., 2008. Enantiomeric separation and analysis of unsaturated hydroperoxy fatty acids by chiral column chromatography-mass spectrometry. J. Chromatogr. B 872, 90–98. https://doi.org/10.1016/j.jchromb.2008.07.013

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- Garscha, U., Oliw, E.H., 2007. Steric analysis of 8-hydroxy- and 10-hydroxyoctadecadienoic acids and dihydroxyoctadecadienoic acids formed from 8R-hydroperoxyoctadecadienoic acid by hydroperoxide isomerases. Anal. Biochem. 367, 238–246. https://doi.org/10.1016/j.ab.2007.04.045

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Characteristic ions in MS/MS of the regioisomeric FA(18:2<OH>), FA(20:4<OH>), FA(20:3<ep>) in PC-esterified forms (negative ion mode):

- Aoyagi, R., Ikeda, K., Isobe, Y., Arita, M., 2017. Comprehensive analyses of oxidized phospholipids using a measured MS/MS spectra library. J. Lipid Res. 58, 2229–2237. https://doi.org/10.1194/jlr.D077123 (see also MS/MS in *.msp format: http://prime.psc.riken.jp/compms/msdial/download/msp/MSMS-Neg-RikenOxPLs.msp)

Characteristic ions in MS/MS of the regioisomeric FA(20:4<OH>) in PC-esterified forms (negative ion mode):

- Mazaleuskaya, L.L., Salamatipour, A., Sarantopoulou, D., Weng, L., FitzGerald, G.A., Blair, I.A., Mesaros, C., 2018. Analysis of HETEs in human whole blood by chiral UHPLC-ECAPCI/HRMS. J. Lipid Res. 59, 564–575. https://doi.org/10.1194/jlr.D081414

MS/MS of the regioisomeric FA(20:4<OH>) in FFA and PE-esterified forms (negative ion mode; see supplementary files there):

- Slatter, D.A., Aldrovandi, M., O'Connor, A., Allen, S.M., Brasher, C.J., Murphy, R.C., Mecklemann, S., Ravi, S., Darley-Usmar, V., O'Donnell, V.B., 2016. Mapping the Human Platelet Lipidome Reveals Cytosolic Phospholipase A2 as a Regulator of Mitochondrial Bioenergetics during Activation. Cell Metab. 23, 930–944. https://doi.org/10.1016/j.cmet.2016.04.001

LIPIDMAPS MS/MS spectra

(negative ionization mode, CE 30V)
https://www.lipidmaps.org/resources/standards/index.php?lipid_category=FA

Name / LIPIDMAPS ID
FA(18:1<ep{9-10}>) / LMFA02000037
FA(18:1<ep{12-13}>) / LMFA02000038
FA(18:2<oxo{13}>) / LMFA02000016
FA(18:2<OH{9}>) / LMFA02000036, LMFA02000188
FA(18:2<OH{13}>) / LMFA02000035, LMFA02000228
FA(18:2<OOH{9}>) / LMFA02000012
FA(18:2<OOH{13}>) / LMFA02000034
FA(20:3<ep{5-6}>) / LMFA03080002
FA(20:3<ep{8-9}>) / LMFA03080003
FA(20:3<ep{11-12}>) / LMFA03080004
FA(20:3<ep{14-15}>) / LMFA03080005
FA(20:4<oxo{5}>) / LMFA03060011
FA(20:4<oxo{12}>) / LMFA03060019
FA(20:4<OH{5}>) / LMFA03060002
FA(20:4<OH{8}>) / LMFA03060006
FA(20:4<OH{9}>) / LMFA03060089
FA(20:4<OH{11}>) / LMFA03060003
FA(20:4<OH{12}>) / LMFA03060007, LMFA03060008
FA(20:4<OH{15}>) / LMFA03060001
FA(20:4<OOH{5}>) / LMFA03060012
FA(20:4<OOH{12}>) / LMFA03060013
FA(20:4<OOH{15}>) / LMFA03060014

METLIN MS/MS spectra

(negative ion mode, CE 10, 20V)
https://metlin.scripps.edu/landing_page.php?pgcontent=mainPage

Name / METLIN ID

FA(18:0<ep{9-10}>) / 36008
FA(18:1<ep{9-10}>) / 43441
FA(18:1<ep{12-13}>) / 43442
FA(18:2<OH{9}>) / 35487, 45660, 45662
FA(18:2<OH{13}>) / 35490, 45665, 45667
FA(18:2<oxo{9}>) / 35860
FA(18:2<oxo{13}>) / 36023
FA(18:2<OOH{9}>) / 36019, 64785
FA(18:2<OOH{13}>) / 36036, 64784
FA(20:4<OH{5}>) / 36336, 45646, 45684
FA(20:4<OH{8}>) / 36286, 3840, 45730
FA(20:4<OH{9}>) / 36290, 45649, 45650
FA(20:4<OH{11}>) / 36337, 3838, 45056
FA(20:4<OH{12}>) / 3841, 45054, 45653
FA(20:4<OH{15}>) / 3836, 45651
FA(20:4<oxo{5}>) / 3844
FA(20:4<oxo{12}>) / 36285
FA(20:4<OOH{5}>) / 36281
FA(20:4<OOH{12}>) / 3845
FA(20:4<OOH{15}>) / 3846