

Figure S1. MS/MS fragmentation of CL species with m/z 1529.9 from irradiated lung.

Two overlapping signals corresponding to molecular species of oxidized CL (CL-C_{18:1}/C_{18:2-OOH}/C_{18:1}/C_{22:6}, and CL-C_{18:2}/C_{20:4-OH}/C_{20:4-OH}/C_{18:1}) along with several non-oxidized CL were detected in MS/MS spectrum of CL molecular ion with m/z 1529.9. CL-C_{18:1}/C_{18:2-OOH}/C_{18:2}/C_{22:6} ions [a₁]⁻ and [b₁]⁻ with m/z 729.5 and m/z 743.5, respectively corresponding to C_{18:1}/C_{18:2-OOH}-PA and C_{18:1}/C_{22:6}-PA were formed during fragmentation of the molecular ion with m/z 1529.9. Additionally characteristic daughter ions [a₁+56]⁻ (m/z 785.8), [a₁+136]⁻ (m/z 865.6), and [b₁+136]⁻ (m/z 879.8) were detected on MS/MS spectrum as well. CL-C_{18:2}/C_{20:4-OH}/C_{20:4-OH}/C_{18:1}: [a₃]⁻ and [b₃]⁻ ions with m/z 735.4 and m/z 737.6 corresponding to C_{18:2}/C_{20:4-OOH}-PA and C_{20:4-OH}/C_{18:1}⁻ PA as well as additional ions with m/z 793.8 ([a₃+56]⁻), m/z 871.6 ([a₃+136]⁻) and m/z 873.5 ([b₃+136]⁻) were formed after fragmentation of molecular ion with m/z 1529.9. In addition, molecular ions of C_{18:1} (m/z 281.3), C_{18:2} (m/z 279.3), C_{18:2-OOH} (m/z 311.3), C_{20:4-OH} (m/z 319.3), and C_{22:6} (m/z 327.3) were present in MS/MS spectrum. Parts of MS² spectrum of the molecular ion with m/z 1529.8 are shown in the ranges of m/z 270 – 340 (a) in the range of m/z 720 – 800 (b) and in the range of m/z 860 – 890 (c).

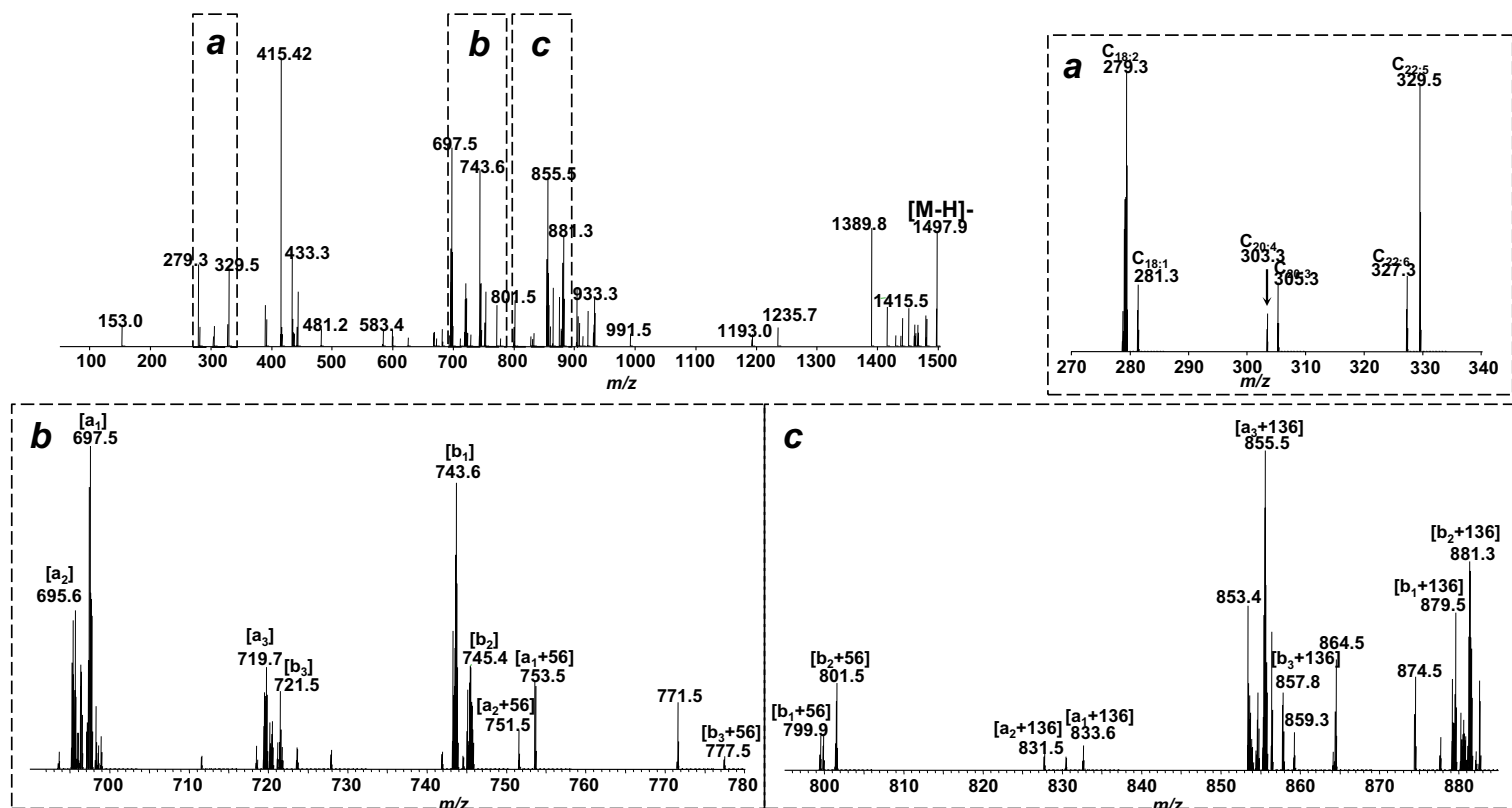


Figure S2. MS/MS fragmentation of CL species with m/z 1497.9 from control lung.

Four overlapping molecular species of CL ($\text{CL-C}_{18:1}/\text{C}_{18:2}/\text{C}_{18:2}/\text{C}_{22:6}$, $\text{CL-C}_{18:2}/\text{C}_{18:2}/\text{C}_{18:2}/\text{C}_{22:5}$, $\text{CL-C}_{18:2}/\text{C}_{20:4}/\text{C}_{20:3}/\text{C}_{18:2}$, and $\text{CL-C}_{18:2}/\text{C}_{20:4}/\text{C}_{20:4}/\text{C}_{18:1}$) were detected in MS/MS spectrum of CL molecular ion with m/z 1497.9. $\text{CL-C}_{18:1}/\text{C}_{18:2}/\text{C}_{18:2}/\text{C}_{22:6}$ ions $[\text{a}_1]^-$ and $[\text{b}_1]^-$ with m/z 697.7 and m/z 743.5, respectively corresponding to $\text{C}_{18:1}/\text{C}_{18:2}$ -PA and $\text{C}_{18:2}/\text{C}_{22:6}$ -PA were formed during fragmentation of the molecular ion with m/z 1497.9. Additionally characteristic daughter ions $[\text{a}_1+56]^-$ (m/z 753.7), $[\text{a}_1+136]^-$ (m/z 833.6), $[\text{b}_1+56]^-$ (m/z 799.9), and $[\text{b}_1+136]^-$ (m/z 879.6) were detected on MS/MS spectrum as well. $\text{CL-C}_{18:2}/\text{C}_{18:2}/\text{C}_{18:2}/\text{C}_{22:5}$: Fragmentation analysis revealed the presence of $[\text{a}_2]^-$ and $[\text{b}_2]^-$ ions with m/z 695.5 and m/z 745.8 mainly corresponding to $\text{C}_{18:2}/\text{C}_{18:2}$ -PA and $\text{C}_{18:2}/\text{C}_{22:5}$ -PA. Daughter ions with m/z 751.7 ($[\text{a}_2+56]^-$); m/z 831.5 ($[\text{a}_2+136]^-$); m/z 801.6 ($[\text{a}_2+56]^-$ and 881.3 ($[\text{b}_2+136]^-$) were additionally detected on MS/MS spectrum. $\text{CL-C}_{18:2}/\text{C}_{20:4}/\text{C}_{20:3}/\text{C}_{18:2}$ and $\text{CL-C}_{18:2}/\text{C}_{20:4}/\text{C}_{20:4}/\text{C}_{18:1}$: $[\text{a}_3]^-$ and $[\text{b}_3]^-$ ions with m/z 719.3 and 721.6 corresponding to $\text{C}_{18:2}/\text{C}_{20:4}$ -PA and $\text{C}_{20:3}/\text{C}_{18:2}$ -PA or $\text{C}_{20:4}/\text{C}_{18:1}$ -PA as well as addition ions with m/z 855.5 ($[\text{a}_3+136]^-$), m/z 777.5 ($[\text{b}_3+56]^-$) and m/z 857.5 ($[\text{b}_3+136]^-$) were formed after fragmentation of molecular ion with m/z 1497.9. Molecular ions with m/z 415.5 and m/z 417.5 were formed during fragmentation of the molecular ion with m/z 1497.9 as well and corresponding to ions $[\text{a}]^-$ and $[\text{b}]^-$ without one fatty acid residue. In addition, molecular ions of $\text{C}_{18:1}$ (m/z 281.3), $\text{C}_{18:2}$ (m/z 279.3), $\text{C}_{22:5}$ (m/z 329.3), $\text{C}_{20:4}$ (m/z 303.3), $\text{C}_{20:3}$ (m/z 305.3) and $\text{C}_{22:6}$ (m/z 327.3) were presented in MS² spectrum as well. Parts of MS/MS spectrum of molecular ion with m/z 1497.9 shown in the range of m/z 270 – 340 (a) in the range of m/z 690 – 780 (b) and in the range of m/z 790–890 (c).

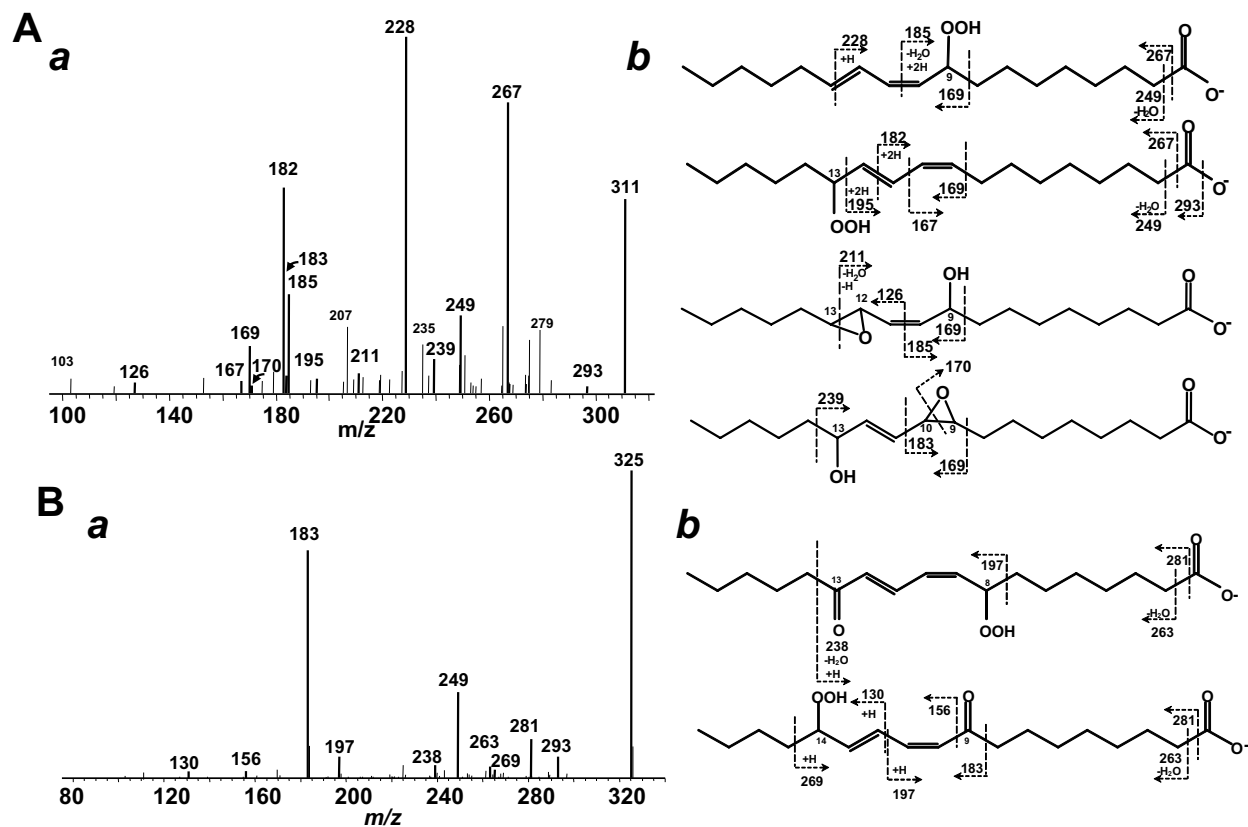


Figure S3. Identification of oxygenated fatty acids in CL obtained from the lung of mice exposed to TBI.

A –Typical MS/MS spectrum of oxygenated $C_{18:2}$ with m/z 311 (**a**) after CL hydrolysis by phospholipase A_2 . Fragmentation pattern of molecular ion with m/z 311 (**b**). **B** –Typical MS/MS spectrum of oxygenated $C_{18:2}$ with m/z 325 (**a**) after CL hydrolysis by phospholipase A_2 . Fragmentation pattern of molecular ion with m/z 325 (**b**).

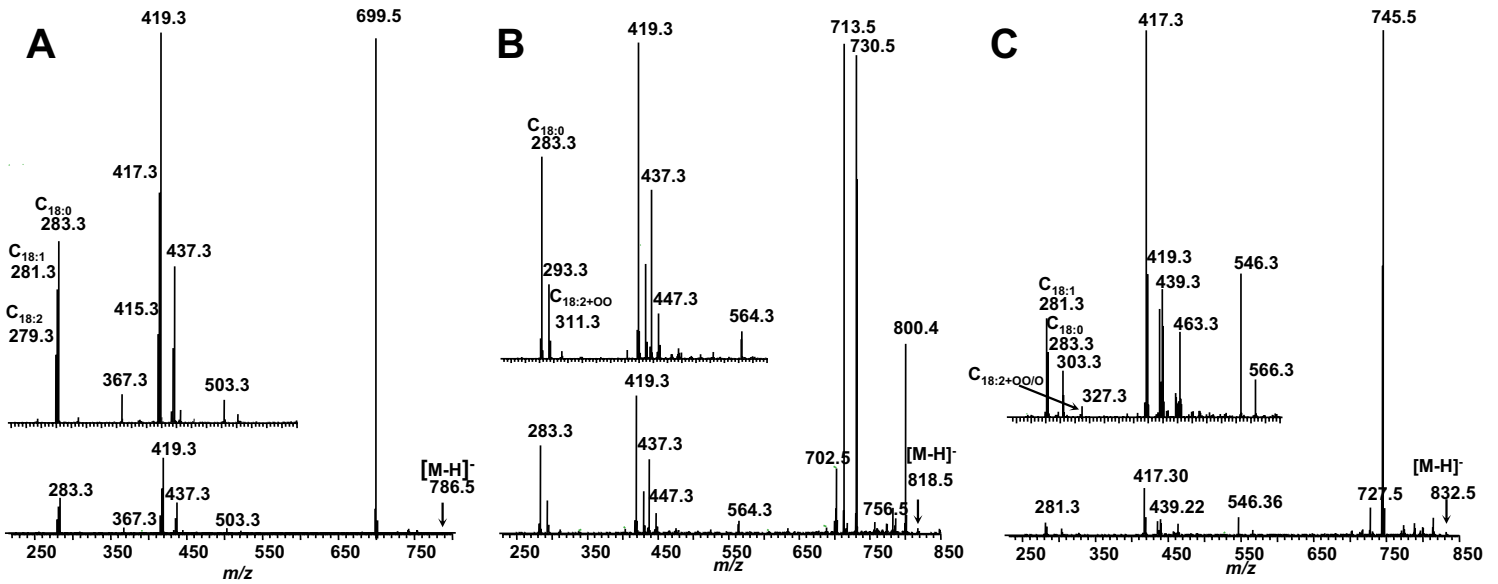


Figure S4. Identification of oxidized PS molecular species from the lung of mice exposed to TBI.

A – Negative ion ESI-MS/MS spectra of PS species with m/z 786.5 from control lung. **B** – MS/MS fragmentation of oxidized PS molecular species with m/z 818.5 from the lung of mice exposed to TBI at the dose of 10Gy. **C** – MS/MS fragmentation of oxidized PS molecular species with m/z 832.5 from the lung of mice exposed to TBI at the dose of 10Gy. Part of MS/MS spectra in the range of m/z 200 – 600 for the respective molecular ions is shown as an inserts. The loss of serine group of PS with m/z 786.5, m/z 818.5 and m/z 832.5 yielded the fragments with m/z 699.5, m/z 731.5 and m/z 745.6, respectively. Product ions with m/z 419.3 originated from fragments with m/z 699.5, m/z 731.5 and m/z 745.6 after loss of $C_{18:2}$, mono-hydroperoxy- $C_{18:2}$ or mono-hydroxy/mono-epoxy- $C_{18:2}$ and mono-hydroperoxy/mono-oxo- $C_{18:2}$, respectively. Molecular ions with m/z 283.3, m/z 281.3 and m/z 279.3 corresponding to $C_{18:0}$, $C_{18:1}$ and $C_{18:2}$ acids, respectively were also formed during fragmentation of parent ion with m/z 786.7. Fragmentation of oxidized molecular species of PS with m/z 818.5 and 832.5 revealed formation of additional ions with m/z 311.3 and m/z 325 corresponding to mono-hydroperoxy- $C_{18:2}$ or mono-hydroxy/mono-epoxy- $C_{18:2}$ and mono-hydroperoxy/mono-oxo- $C_{18:2}$, respectively. Daughter ions with m/z 281.3 and m/z 327.3 were present in spectrum of molecular ions with m/z 832.5 and correspond to non-oxidized PS $C_{18:1}/C_{22:6}$. Thus, the molecular ion at m/z 786.5 corresponds to molecular species of PS $C_{18:0}/C_{18:2}$ whereas the molecular ions with m/z 818.5 and m/z 832.5 correspond to molecular species of oxidized PS $C_{18:0}/$ mono-hydroperoxy- $C_{18:2}$ or $C_{18:0}/$ mono-hydroxy/monio-epoxy- $C_{18:2}$ and $C_{18:0}/$ mono-hydroperoxy/mono-oxo- $C_{18:2}$.