

The impact of oxidative stress on the barrier properties of lipid bilayer models

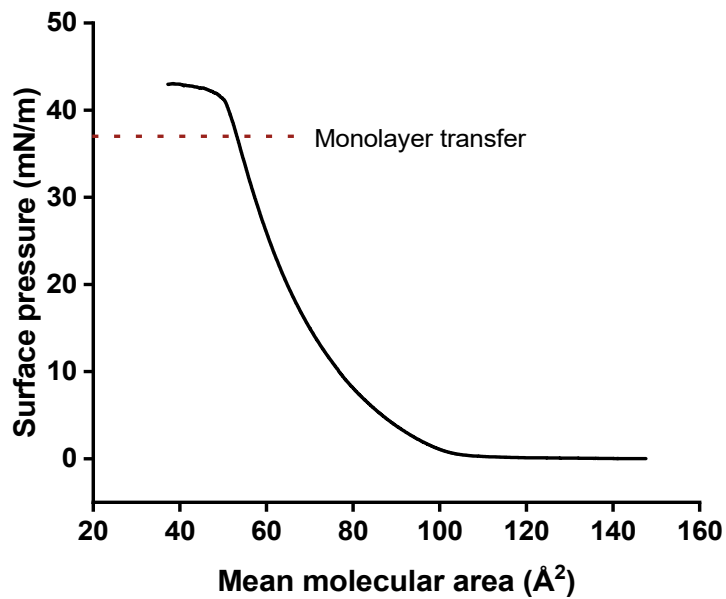


Figure S1. π -A isotherm of DOPE + DOPS + 10% cholesterol obtained on a pure water surface in a nitrogen atmosphere at 22 °C.

Table S1. Target Pressures for the transfer of monolayers with different lipid compositions with Langmuir-Blodgett and Langmuir-Schaefer techniques

Lipid composition	Target pressure (mN/m)
DOPE + DOPS + 10% cholesterol	37
POPC + SM(d18:1/18:0) + 10% cholesterol	37
DOPE + DOPS	38
POPC + SM(d18:1/18:0)	36
POPC	35
SM(d18:1/18:0)	41
DOPE	37
DOPS	38

Table S2. Retention time (RT) analysis of POPC

lipid peroxidation products	Formula neutral	Obs. Mass [M+CH ₃ COO] ⁻	RT [min]
POPC 16:0/18:1;OH,OOH or 16:0/18:0;3O	C ₄₂ H ₈₂ NO ₁₁ P	866.5768	6.77
POPC 16:0/18:0;oxo or Ep	C ₄₂ H ₈₂ NO ₉ P	834.5864	6.90/7.02
POPC 16:0/8:0;oxo	C ₃₂ H ₆₂ NO ₉ P	694.4304	7.33
POPC 16:0/9:0;oxo	C ₃₃ H ₆₄ NO ₉ P	708.4464	7.26
POPC 16:0/9:0;COOH	C ₃₃ H ₆₄ NO ₁₀ P	664.4199 [-H]	8.36/8.50

Table S3. Retention time (RT) analysis of DOPE

lipid peroxidation products	Formula neutral	Obs. Mass [M-H] ⁻	RT [min]
DOPE 18:1/9:0;oxo	C ₃₂ H ₆₀ NO ₉ P	632.3936	6.70
DOPE 18:1/9:0;COOH	C ₃₂ H ₆₀ NO ₁₀ P	634.3727	7.96
DOPE 18:1/18:1;oxo	C ₄₁ H ₇₆ NO ₉ P	756.5177	6.41
DOPE 18:1_0:0	C ₂₃ H ₄₆ NO ₇ P	478.2939	7.57/7.72
DOPE 18:1/18:0;oxo or Ep	C ₄₁ H ₇₈ NO ₉ P	758.5346	6.41/6.53
DOPE 18:1/18:1;oxo(2)	C ₄₁ H ₇₄ NO ₁₀ P	770.4976	6.51

Table S4. Retention time (RT) analysis of DOPS

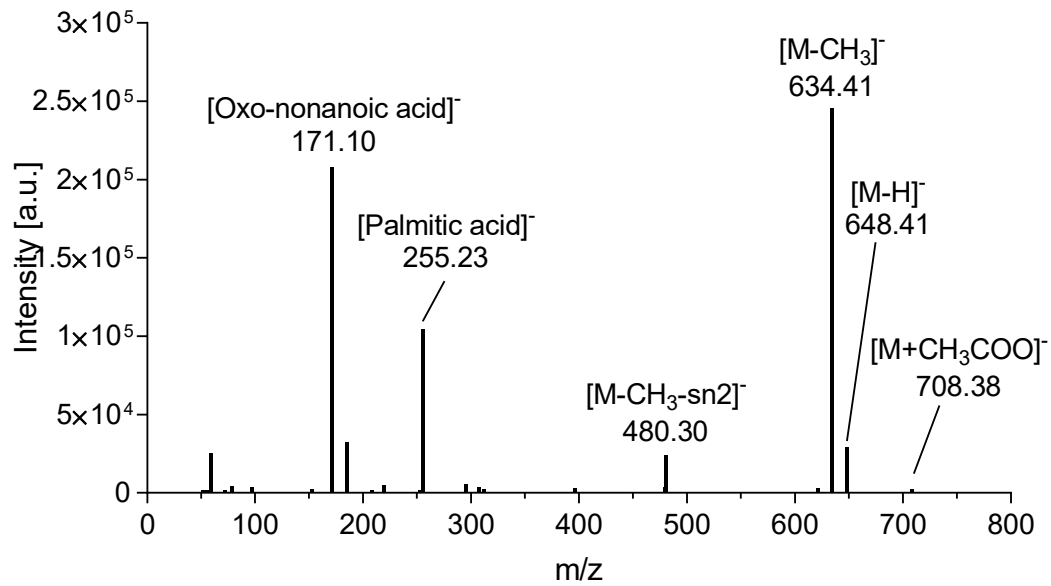
lipid peroxidation products	Formula neutral	Obs. Mass [M-H] ⁻	RT [min]
DOPS 18:1/18:1;GPAA	C ₄₁ H ₇₅ O ₁₀ P	757.4835	6.39
DOPS 18:1/9:0;oxo	C ₃₃ H ₆₀ NO ₁₁ P	676.3836	7.12
DOPS 18:1/18:1;(OOH) ₂ or (OH) ₄ or	C ₄₂ H ₇₈ NO ₁₄ P	850.5082	6.94
DOPS 18:1/18:0;(OH) ₂ ;(oxo) ₂			
DOPS 18:1/18:1;O ₃	C ₄₂ H ₇₈ NO ₁₃ P	834.5135	6.98
DOPS 18:1/18:1;OOH, oxo	C ₄₂ H ₇₆ NO ₁₃ P	832.4982	6.92
DOPS 18:1/18:1;OH, oxo	C ₄₂ H ₇₆ NO ₁₂ P	816.5048	7.00
DOPS 18:1/18:0;oxo or Ep	C ₄₂ H ₇₈ NO ₁₁ P	802.5229	6.84
DOPS 18:1/18:1;oxo	C ₄₂ H ₇₆ NO ₁₁ P	800.5088	6.71

Table S5. Retention time (RT) analysis of SM (d18:1/18:0)

lipid peroxidation products	Formula neutral	Obs. Mass [M+CH ₃ COO] ⁻	RT [min]
SM 18:0/18:1;OH	C ₄₁ H ₈₃ N ₂ O ₇ P	805.6076	7.74
SM 18:0/18:1;oxo	C ₄₁ H ₈₁ N ₂ O ₇ P	803.592	7.57

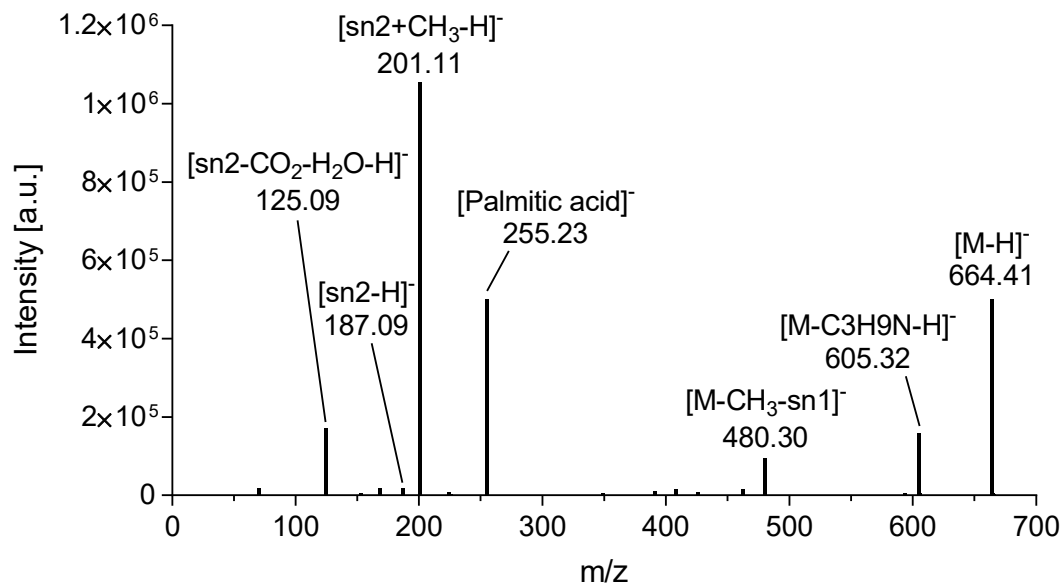
- POPC 16:0/9:0;oxo

PC 16:0/9:0;oxo @ 7.26 min, hcd 21.67



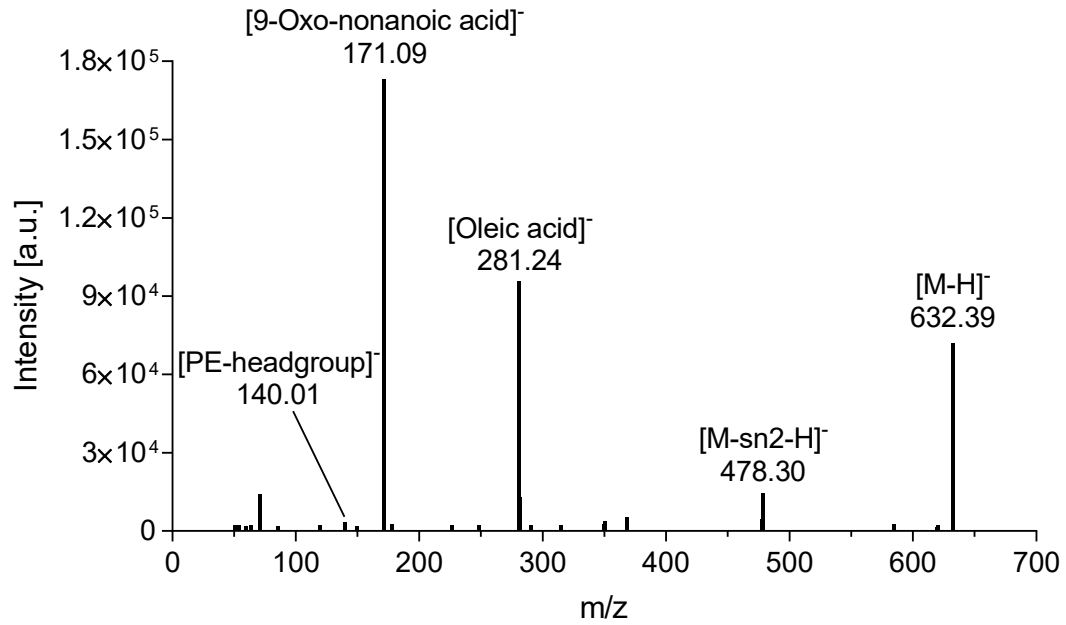
- POPC 16:0/9:0;COOH

PC 16:0/9:0;COOH @ 8.36/8.50, hcd 21.67



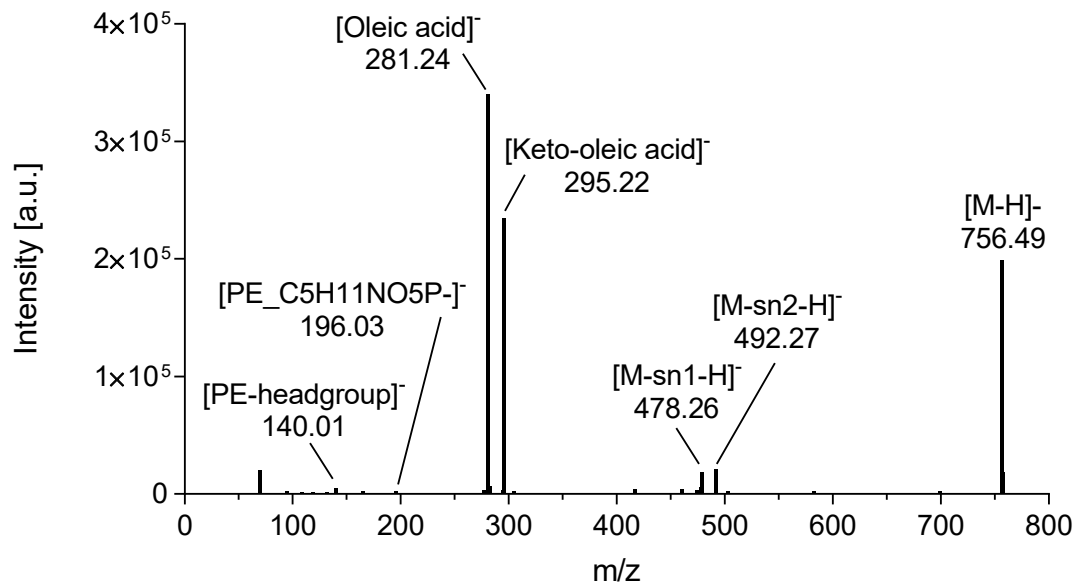
- DOPE 18:1/9:0;oxo

PE 18:1/9:0;oxo @ 6.70 min, hcd 21.67

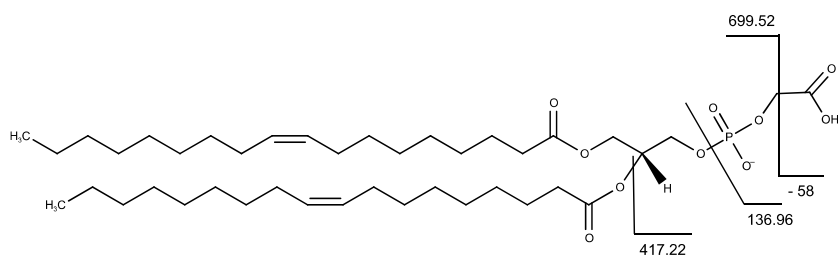


- DOPE 18:1/18:1;oxo

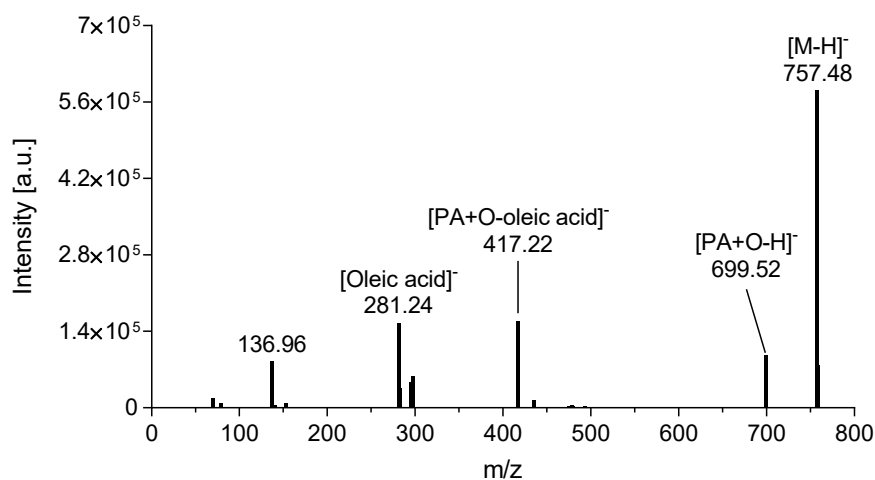
PE 18:1/18:1;oxo @ 6.41 min, hcd 21.67



- DOPS 18:1/18:1;GPAA



PS 18:1/18:1;GPAA @ 6.39 min, hcd 21.67



- DOPS 18:1/18:0;oxo or Ep

PS 18:1/18:0;oxo or Ep @ 6.84 min; hcd 21.67

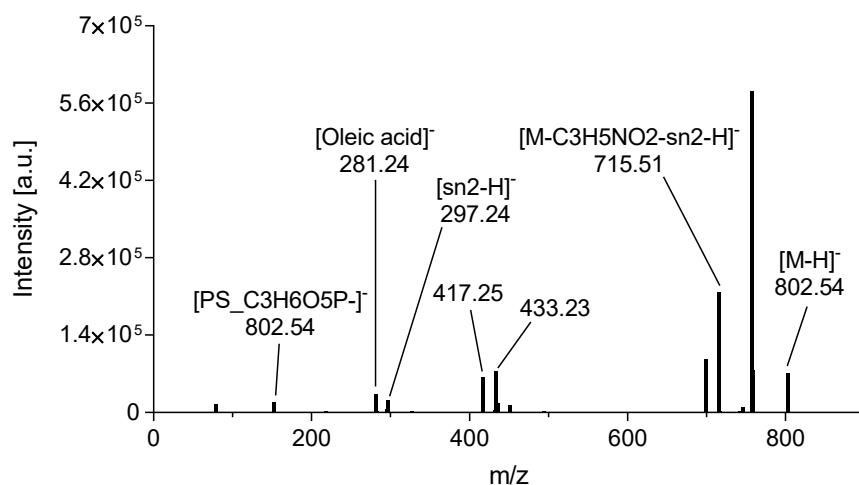


Figure S2. MS² fragmentation pattern of selected LPPs.