

Supplementary Materials

Analysis of oxidized 1-palmitoyl-2-arachidonoyl-sn-glycero-3 phosphocholine products in uremic patients by LC-ESI/MS

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Table S2: Proposed structures of the long-chain ox-PAPC products

Proposed structures of the short-chain ox-PAPC products

m/z	Name	ion	m/z	Name	ion
478	1-palmitoyl-3-phosphatidylcholine	[M+H] ⁺	622	1-palmitoyl-2-(4-hexenedioic acid)-GPC	[M+H] ⁺
496	1-palmitoyl-2-hydroxy-sn-glycero-3-phosphocholine	[M+H] ⁺	632	1-palmitoyl-2-(pentanedioic acid)-GPC	[M+Na] ⁺
594	1-palmitoyl-2-(5-oxo-pentanoic acid)-GPC	[M+H] ⁺	636	1-palmitoyl-2-(4-hydroxy-7-oxo-5-heptenoic acid)-GPC	[M+H] ⁺
610	1-palmitoyl-2-(pentanedioic acid)-GPC	[M+H] ⁺	650	1-palmitoyl-2-(5-hydroxy-8-oxo-6-octenoic acid)-GPC	[M+H] ⁺
616	1-palmitoyl-2-(5-oxo-pentanoic acid)-GPC	[M+Na] ⁺	666	1-palmitoyl-2-(5-hydroxy-6-octendioic acid)-GPC	[M+H] ⁺
620	1-palmitoyl-2-(7-oxo-5-heptenoic acid)-GPC	[M+H] ⁺	690	1-palmitoyl-2-(5-hydroxy-6,8-undecedioic acid)-GPC	[M+H] ⁺

Proposed structures of the long-chain ox-PAPC products

m/z	Name	ion	m/z	Name	ion
820.5	1-palmitoyl-2-(hydroxy-eicosatetraenoic acid)-GPC	[M+Na] ⁺	850.5	1-palmitoyl-2-(hydroxy-hydroperoxide-eicosatetraenoic acid)-GPC	[M+Na] ⁺
828.5	1-palmitoyl-2-(D2/E2-isoprostanes)-GPC	[M+H] ⁺	852.5	1-palmitoyl-2-(hydroxy-hydroperoxide-eicosatetraenoic acid)-GPC	[M+Na] ⁺
836.5	1-palmitoyl-2-(hydroperoxide-eicosatetraenoic acid)-GPC	[M+Na] ⁺	868.5	1-palmitoyl-2-(di-hydroperoxide-eicosatetraenoic acid)-GPC	[M+Na] ⁺
846.5	PAPC_5-epoxy_8-E/D-IsoP_14-epoxy 1-palmitoyl-2-(di-hydroperoxide-eicosatetraenoic acid)-GPC	[M+H] ⁺	884.5	1-palmitoyl-2-(hydroxy-di-hydroperoxide-eicosatetraenoic acid)-GPC	[M+Na] ⁺
			900.5	1-palmitoyl-2-(tri-hydroperoxide-eicosatetraenoic acid)-GPC	[M+H] ⁺

References

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