

Supplementary Table S1. Grouping of fatty acids, dimethyl acetals (DMAs, derivatives of plasmalogen phospholipid alkenyl chains), their sums, and derived ratios based on hierarchical clustering. Group 4 consists of 2 subgroups that were fused for biological reasons (short saturated fatty acids).

<u>Group 1</u>		<u>Group 2</u>		<u>Group 3</u>	
16:1n-5	CHEBI:35464	22:1n-7	CHEBI:180035	16:1n-9	CHEBI:35465
22:1n-9	CHEBI:28792	20:4n-6	CHEBI:15843	18:3n-3	CHEBI:27432
22:0	CHEBI:28941	Sum DMA		18:1n-9	CHEBI:16196
24:1n-9	CHEBI:44247	DMA 18:0		Sum MUFA	
22:1n-11	CHEBI:32428	20:3n-6	CHEBI:53486	14:1n-5	CHEBI:27781
18:3n-6	CHEBI:28661	18:0	CHEBI:28842	16:1n-7	CHEBI:28716
24:0	CHEBI:28866	20:0	CHEBI:28822	18:1n-7	CHEBI:50464
		18:2n-6	CHEBI:17351	17:1n-8	CHEBI:84328
		22:4n-6	CHEBI:53487	UFA/SFA ratio	
		Sum PUFA			
		Sum n-6 PUFA			
		20:5n-3	CHEBI:28364		
		Sum n-3 PUFA			
		22:5n-3	CHEBI:53488		
		22:6n-3	CHEBI:28125		
<u>Group 4</u>		<u>Group 5</u>			
15:0 iso	CHEBI:39250	18:1n-5	CHEBI:82617		
15:0 anteiso	CHEBI:39251	n-3/n-6 PUFA ratio			
DMA 16:0		20:1n-9	CHEBI:32425		
14:0	CHEBI:28875	17:0 anteiso	CHEBI:84874		
15:0	CHEBI:42504	17:0 iso	CHEBI:70850		
16:0	CHEBI:15756	17:0	CHEBI:32365		
Sum SFA					

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