

Table S1: Protons and Chemical Shift (in ppm) for the lipid constituents and headgroups identified in HDL lipid extract by NMR and selected signals for Lipid Quantification

Lipid constituents and headgroups	¹ H NMR signal assignment	Chemical Shift (ppm)	Quantification of lipids from selected well-resolved NMR signals
Cholesterol molecule	C ₁₈ H ₃	0.68	Total Cholesterol, FC, CE
	C ₂₆ H ₃ , C ₂₇ H ₃ , C ₂₁ H	0.87	
	C ₁₉ H ₃	1.00	
	C ₃ H	3.40	
	C ₆ H	5.36	
Glycerol backbone	C ₁ H ^u and C ₃ H ^u of glycerol backbone of TG and DAGPLs	4.16	TG
	C ₁ H ^d and C ₃ H ^d of glycerol backbone of TG	4.32	
	C ₁ H ^d and C ₃ H ^d of glycerol backbone of DAGPLs	4.40	Ether GPLs Total Diacyl glycerophospholipids (DAGPLs)
	C ₂ H of glycerol backbone in ether glycerophospholipids	5.15	
	C ₂ H of glycerol backbone in total DAGPLs	5.18	
	C ₂ H of glycerol backbone in TG	5.22	
Sphingosine moiety	-CH ₂ -CH=CHCHOH	5.40	Total SLs
	-CH ₂ -CH=CHCHOH	5.70	
Head-group and substituent	-CH ₂ -CH ₂ -N ⁺ (CH ₃) ₃ (choline)	3.20	Total choline-containing PLs (PC, SM, LPC)
	-CH ₂ -CH ₂ -N ⁺ (CH ₃) ₃	3.59	
	-CH ₂ -CH ₂ -N ⁺ (CH ₃) ₃	4.24	PE PLA (ether GPLs)
	-CH ₂ -CH ₂ -NH ₃ ⁺ (ethanolamine)	3.10	
	-OCH=CHCH ₂	5.90	
Fatty acid chains	ω-CH ₃ (methyl) in fatty acyl chains	0.88	AA (20:4 ω-6) + EPA (20:5 ω-3) UFA Total FA DHA (22:6 ω-3) LA (18:2 ω-6) PUFA
	ω-CH ₃ (methyl) of total omega-3 FA	0.95	
	-(CH ₂) _n - (methylene) in fatty acyl chains	1.30	
	-CO-CH ₂ -CH ₂ - (β-methylene) in the fatty acyl chains	1.59	
	β-CH ₂ (β-methylene) of the sum of AA+EPA	1.67	
	-CH ₂ -CH= (allylic) in fatty acyl chains	2.04	
	-CO-CH ₂ (α-methylene) in the fatty acyl chains	2.30	
	α and β CH ₂ (methylene) of DHA	2.38	
	-CH=CH-CH ₂ -CH=CH- of linoleic acid	2.75	
	-(CH=CH-CH ₂ -CH=CH) _n , n > 1 in the fatty acyl chains	2.80	
	-CH=CH- in the fatty acyl chains	5.36	

Key AA, arachidonic acid; CE, cholesteryl ester; DAGPLs, Diacyl glycerophospholipids; DHA, docosahexaenoic acid; EPA, eicosapentaenoic acid; FA, fatty acids; FC, free cholesterol; GPLs, glycerophospholipids; LA, Linoleic acid; LPC, lysophosphatidylcholine; PC, phosphatidylcholine; PE, phosphatidylethanolamine; PLA, plasmalogens; PUFA, polyunsaturated fatty acids; SLs, Sphingolipids; SM, sphingomyelin; TG, triglycerides; UFA, Unsaturated fatty acids.