

Supplementary Table 1. Lipid species and classes

Lipid Species	Group	Class (Full name)	Class (Abbreviation)
Sph(d18:1)	sphingolipids	Sphingosine	Sph
Sph(d18:2)	sphingolipids	Sphingosine	Sph
S1P(d16:1)	sphingolipids	Sphingosine-1-phosphate	S1P
S1P(d18:0)	sphingolipids	Sphingosine-1-phosphate	S1P
S1P(d18:1)	sphingolipids	Sphingosine-1-phosphate	S1P
S1P(d18:2)	sphingolipids	Sphingosine-1-phosphate	S1P
dhCer(d18:0/16:0)	sphingolipids	Dihydroceramide	dhCer
dhCer(d18:0/18:0)	sphingolipids	Dihydroceramide	dhCer
dhCer(d18:0/20:0)	sphingolipids	Dihydroceramide	dhCer
dhCer(d18:0/22:0)	sphingolipids	Dihydroceramide	dhCer
dhCer(d18:0/24:0)	sphingolipids	Dihydroceramide	dhCer
dhCer(d18:0/24:1)	sphingolipids	Dihydroceramide	dhCer
Cer(d16:1/16:0)	sphingolipids	Ceramide	Cer(d)
Cer(d16:1/18:0)	sphingolipids	Ceramide	Cer(d)
Cer(d16:1/20:0)	sphingolipids	Ceramide	Cer(d)
Cer(d16:1/22:0)	sphingolipids	Ceramide	Cer(d)
Cer(d16:1/23:0)	sphingolipids	Ceramide	Cer(d)
Cer(d16:1/24:0)	sphingolipids	Ceramide	Cer(d)
Cer(d16:1/24:1)	sphingolipids	Ceramide	Cer(d)
Cer(d17:1/16:0)	sphingolipids	Ceramide	Cer(d)
Cer(d17:1/18:0)	sphingolipids	Ceramide	Cer(d)
Cer(d17:1/20:0)	sphingolipids	Ceramide	Cer(d)
Cer(d17:1/22:0)	sphingolipids	Ceramide	Cer(d)
Cer(d17:1/23:0)	sphingolipids	Ceramide	Cer(d)
Cer(d17:1/24:0)	sphingolipids	Ceramide	Cer(d)
Cer(d17:1/24:1)	sphingolipids	Ceramide	Cer(d)
Cer(d18:1/14:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:1/16:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:1/18:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:1/19:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:1/20:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:1/21:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:1/22:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:1/23:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:1/24:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:1/24:1)	sphingolipids	Ceramide	Cer(d)
Cer(d18:1/26:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:2/14:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:2/16:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:2/18:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:2/20:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:2/21:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:2/22:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:2/23:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:2/24:0)	sphingolipids	Ceramide	Cer(d)
Cer(d18:2/24:1)	sphingolipids	Ceramide	Cer(d)
Cer(d18:2/26:0)	sphingolipids	Ceramide	Cer(d)
Cer(d19:1/16:0)	sphingolipids	Ceramide	Cer(d)
Cer(d19:1/18:0)	sphingolipids	Ceramide	Cer(d)
Cer(d19:1/20:0)	sphingolipids	Ceramide	Cer(d)
Cer(d19:1/22:0)	sphingolipids	Ceramide	Cer(d)
Cer(d19:1/23:0)	sphingolipids	Ceramide	Cer(d)
Cer(d19:1/24:0)	sphingolipids	Ceramide	Cer(d)
Cer(d19:1/24:1)	sphingolipids	Ceramide	Cer(d)
Cer(d19:1/26:0)	sphingolipids	Ceramide	Cer(d)
Cer(d20:1/22:0)	sphingolipids	Ceramide	Cer(d)
Cer(d20:1/23:0)	sphingolipids	Ceramide	Cer(d)
Cer(d20:1/24:0)	sphingolipids	Ceramide	Cer(d)
Cer(d20:1/24:1)	sphingolipids	Ceramide	Cer(d)
Cer(m18:0/20:0)	sphingolipids	Deoxyceramide	Cer(m)
Cer(m18:0/22:0)	sphingolipids	Deoxyceramide	Cer(m)

Cer(m18:0/23:0)	sphingolipids	Deoxyceramide	Cer(m)
Cer(m18:0/24:0)	sphingolipids	Deoxyceramide	Cer(m)
Cer(m18:0/24:1)	sphingolipids	Deoxyceramide	Cer(m)
Cer(m18:1/18:0)	sphingolipids	Deoxyceramide	Cer(m)
Cer(m18:1/20:0)	sphingolipids	Deoxyceramide	Cer(m)
Cer(m18:1/22:0)	sphingolipids	Deoxyceramide	Cer(m)
Cer(m18:1/23:0)	sphingolipids	Deoxyceramide	Cer(m)
Cer(m18:1/24:0)	sphingolipids	Deoxyceramide	Cer(m)
Cer(m18:1/24:1)	sphingolipids	Deoxyceramide	Cer(m)
Cer1P(d18:1/16:0)	sphingolipids	Ceramide-1-phosphate	C1P
HexCer(d16:1/18:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d16:1/20:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d16:1/22:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d16:1/24:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d18:1/16:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d18:1/18:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d18:1/20:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d18:1/22:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d18:1/24:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d18:1/24:1)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d18:2/18:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d18:2/20:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d18:2/22:0)	sphingolipids	Monohexosylceramide	HexCer
HexCer(d18:2/24:0)	sphingolipids	Monohexosylceramide	HexCer
Hex2Cer(d16:1/16:0)	sphingolipids	Dihexosylceramide	Hex2Cer
Hex2Cer(d16:1/24:1)	sphingolipids	Dihexosylceramide	Hex2Cer
Hex2Cer(d18:1/16:0)	sphingolipids	Dihexosylceramide	Hex2Cer
Hex2Cer(d18:1/20:0)	sphingolipids	Dihexosylceramide	Hex2Cer
Hex2Cer(d18:1/22:0)	sphingolipids	Dihexosylceramide	Hex2Cer
Hex2Cer(d18:1/24:0)	sphingolipids	Dihexosylceramide	Hex2Cer
Hex2Cer(d18:1/24:1)	sphingolipids	Dihexosylceramide	Hex2Cer
Hex2Cer(d18:2/16:0)	sphingolipids	Dihexosylceramide	Hex2Cer
Hex2Cer(d18:2/24:1)	sphingolipids	Dihexosylceramide	Hex2Cer
Hex3Cer(d18:1/16:0)	sphingolipids	Trihexosylceramide	Hex3Cer
Hex3Cer(d18:1/18:0)	sphingolipids	Trihexosylceramide	Hex3Cer
Hex3Cer(d18:1/20:0)	sphingolipids	Trihexosylceramide	Hex3Cer
Hex3Cer(d18:1/22:0)	sphingolipids	Trihexosylceramide	Hex3Cer
Hex3Cer(d18:1/24:0)	sphingolipids	Trihexosylceramide	Hex3Cer
Hex3Cer(d18:1/24:1)	sphingolipids	Trihexosylceramide	Hex3Cer
GM3(d18:1/16:0)	sphingolipids	GM3 ganglioside	GM3
GM3(d18:1/18:0)	sphingolipids	GM3 ganglioside	GM3
GM3(d18:1/20:0)	sphingolipids	GM3 ganglioside	GM3
GM3(d18:1/22:0)	sphingolipids	GM3 ganglioside	GM3
GM3(d18:1/24:0)	sphingolipids	GM3 ganglioside	GM3
GM3(d18:1/24:1)	sphingolipids	GM3 ganglioside	GM3
GM1(d18:1/16:0)	sphingolipids	GM1 ganglioside	GM1
SHexCer(d18:1/16:0(OH))	sphingolipids	Sulfatide	SHexCer
SHexCer(d18:1/16:0)	sphingolipids	Sulfatide	SHexCer
SHexCer(d18:1/24:0(OH))	sphingolipids	Sulfatide	SHexCer
SHexCer(d18:1/24:0)	sphingolipids	Sulfatide	SHexCer
SHexCer(d18:1/24:1(OH))	sphingolipids	Sulfatide	SHexCer
SHexCer(d18:1/24:1)	sphingolipids	Sulfatide	SHexCer
SM(34:3)	sphingolipids	Sphingomyelin	SM
SM(35:2) (b)	sphingolipids	Sphingomyelin	SM
SM(37:1)	sphingolipids	Sphingomyelin	SM
SM(37:2)	sphingolipids	Sphingomyelin	SM
SM(38:3) (a)	sphingolipids	Sphingomyelin	SM
SM(38:3) (b)	sphingolipids	Sphingomyelin	SM
SM(40:3) (a)	sphingolipids	Sphingomyelin	SM
SM(40:3) (b)	sphingolipids	Sphingomyelin	SM
SM(41:0)	sphingolipids	Sphingomyelin	SM
SM(41:1) (a)	sphingolipids	Sphingomyelin	SM
SM(43:1)	sphingolipids	Sphingomyelin	SM

SM(43:2) (b)	sphingolipids	Sphingomyelin	SM
SM(43:2) (c)	sphingolipids	Sphingomyelin	SM
SM(44:1)	sphingolipids	Sphingomyelin	SM
SM(44:2)	sphingolipids	Sphingomyelin	SM
SM(44:3)	sphingolipids	Sphingomyelin	SM
SM(d16:1/19:0)	sphingolipids	Sphingomyelin	SM
SM(d16:1/23:0) & SM(d17:1/22:0)	sphingolipids	Sphingomyelin	SM
SM(d16:1/24:1)	sphingolipids	Sphingomyelin	SM
SM(d17:1/14:0)	sphingolipids	Sphingomyelin	SM
SM(d17:1/16:0)	sphingolipids	Sphingomyelin	SM
SM(d17:1/24:1)	sphingolipids	Sphingomyelin	SM
SM(d18:0/14:0)	sphingolipids	Sphingomyelin	SM
SM(d18:0/16:0)	sphingolipids	Sphingomyelin	SM
SM(d18:0/22:0)	sphingolipids	Sphingomyelin	SM
SM(d18:1/14:0) & SM(d16:1/16:0)	sphingolipids	Sphingomyelin	SM
SM(d18:1/16:0)	sphingolipids	Sphingomyelin	SM
SM(d18:1/17:0) & SM(d17:1/18:0)	sphingolipids	Sphingomyelin	SM
SM(d18:1/18:0) & SM(d16:1/20:0)	sphingolipids	Sphingomyelin	SM
SM(d18:1/20:0) & SM(d16:1/22:0)	sphingolipids	Sphingomyelin	SM
SM(d18:1/22:0) & SM(d16:1/24:0)	sphingolipids	Sphingomyelin	SM
SM(d18:1/23:0) & SM(d17:1/24:0)	sphingolipids	Sphingomyelin	SM
SM(d18:1/24:0)	sphingolipids	Sphingomyelin	SM
SM(d18:1/24:1)	sphingolipids	Sphingomyelin	SM
SM(d18:2/14:0)	sphingolipids	Sphingomyelin	SM
SM(d18:2/16:0)	sphingolipids	Sphingomyelin	SM
SM(d18:2/17:0)	sphingolipids	Sphingomyelin	SM
SM(d18:2/18:0)	sphingolipids	Sphingomyelin	SM
SM(d18:2/18:1)	sphingolipids	Sphingomyelin	SM
SM(d18:2/20:0)	sphingolipids	Sphingomyelin	SM
SM(d18:2/22:0)	sphingolipids	Sphingomyelin	SM
SM(d18:2/23:0)	sphingolipids	Sphingomyelin	SM
SM(d18:2/24:0)	sphingolipids	Sphingomyelin	SM
SM(d19:1/24:1)	sphingolipids	Sphingomyelin	SM
PA(34:1)	glycerophospholipids	Phosphatidic acid	PA
PA(36:1)	glycerophospholipids	Phosphatidic acid	PA
PA(36:2)	glycerophospholipids	Phosphatidic acid	PA
PA(36:3)	glycerophospholipids	Phosphatidic acid	PA
PA(36:4)	glycerophospholipids	Phosphatidic acid	PA
PA(40:6)	glycerophospholipids	Phosphatidic acid	PA
PC(14:0_16:0)	glycerophospholipids	Phosphatidylcholine	PC
PC(14:0_20:4)	glycerophospholipids	Phosphatidylcholine	PC
PC(14:0_22:6)	glycerophospholipids	Phosphatidylcholine	PC
PC(15-MHDA_18:1)	glycerophospholipids	Phosphatidylcholine	PC
PC(15-MHDA_18:2)	glycerophospholipids	Phosphatidylcholine	PC
PC(15-MHDA_20:4)	glycerophospholipids	Phosphatidylcholine	PC
PC(15-MHDA_22:6)	glycerophospholipids	Phosphatidylcholine	PC
PC(15:0_20:3)	glycerophospholipids	Phosphatidylcholine	PC
PC(15:0_20:4)	glycerophospholipids	Phosphatidylcholine	PC
PC(15:0_22:6)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:0_16:0)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:0_18:0)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:0_18:1)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:0_18:2)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:0_18:3) (a)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:0_18:3) (b)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:0_20:3) (a)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:0_20:3) (b)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:0_20:4)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:0_20:5)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:0_22:6)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:1_18:2)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:1_20:4)	glycerophospholipids	Phosphatidylcholine	PC
PC(16:1_22:6)	glycerophospholipids	Phosphatidylcholine	PC











PIP1(38:4)	glycerophospholipids	Phosphatidylinositol monophosphate	PIP1
LPI(18:0) [sn1]	glycerophospholipids	Lysophosphatidylinositol	LPI
LPI(18:0) [sn2]	glycerophospholipids	Lysophosphatidylinositol	LPI
LPI(18:1) [sn1]	glycerophospholipids	Lysophosphatidylinositol	LPI
LPI(18:1) [sn2]	glycerophospholipids	Lysophosphatidylinositol	LPI
LPI(18:2) [sn1]	glycerophospholipids	Lysophosphatidylinositol	LPI
LPI(18:2) [sn2]	glycerophospholipids	Lysophosphatidylinositol	LPI
LPI(20:4) [sn1]	glycerophospholipids	Lysophosphatidylinositol	LPI
LPI(20:4) [sn2]	glycerophospholipids	Lysophosphatidylinositol	LPI
PS(36:1)	glycerophospholipids	Phosphatidylserine	PS
PS(36:2)	glycerophospholipids	Phosphatidylserine	PS
PS(38:3)	glycerophospholipids	Phosphatidylserine	PS
PS(38:4)	glycerophospholipids	Phosphatidylserine	PS
PS(40:5)	glycerophospholipids	Phosphatidylserine	PS
PS(40:6)	glycerophospholipids	Phosphatidylserine	PS
PG(34:1)	glycerophospholipids	Phosphatidylglycerol	PG
PG(36:1)	glycerophospholipids	Phosphatidylglycerol	PG
PG(36:2)	glycerophospholipids	Phosphatidylglycerol	PG
CE(14:0)	Neutral/Other	Cholesteryl ester	CE
CE(15:0)	Neutral/Other	Cholesteryl ester	CE
CE(16:0)	Neutral/Other	Cholesteryl ester	CE
CE(16:1)	Neutral/Other	Cholesteryl ester	CE
CE(16:2)	Neutral/Other	Cholesteryl ester	CE
CE(17:0)	Neutral/Other	Cholesteryl ester	CE
CE(17:1)	Neutral/Other	Cholesteryl ester	CE
CE(18:0)	Neutral/Other	Cholesteryl ester	CE
CE(18:1)	Neutral/Other	Cholesteryl ester	CE
CE(18:2)	Neutral/Other	Cholesteryl ester	CE
CE(18:3)	Neutral/Other	Cholesteryl ester	CE
CE(20:0)	Neutral/Other	Cholesteryl ester	CE
CE(20:1)	Neutral/Other	Cholesteryl ester	CE
CE(20:2)	Neutral/Other	Cholesteryl ester	CE
CE(20:3)	Neutral/Other	Cholesteryl ester	CE
CE(20:4)	Neutral/Other	Cholesteryl ester	CE
CE(20:5)	Neutral/Other	Cholesteryl ester	CE
CE(22:0)	Neutral/Other	Cholesteryl ester	CE
CE(22:1)	Neutral/Other	Cholesteryl ester	CE
CE(22:4)	Neutral/Other	Cholesteryl ester	CE
CE(22:5)	Neutral/Other	Cholesteryl ester	CE
CE(22:6)	Neutral/Other	Cholesteryl ester	CE
CE(24:0)	Neutral/Other	Cholesteryl ester	CE
CE(24:1)	Neutral/Other	Cholesteryl ester	CE
CE(24:4)	Neutral/Other	Cholesteryl ester	CE
CE(24:5)	Neutral/Other	Cholesteryl ester	CE
CE(24:6)	Neutral/Other	Cholesteryl ester	CE
COH	Neutral/Other	Free Cholesterol	COH
DE(16:0)	Neutral/Other	Dehydrocholesterol ester	DE
DE(18:1)	Neutral/Other	Dehydrocholesterol ester	DE
DE(18:2)	Neutral/Other	Dehydrocholesterol ester	DE
DE(20:4)	Neutral/Other	Dehydrocholesterol ester	DE
DE(20:5)	Neutral/Other	Dehydrocholesterol ester	DE
DE(22:6)	Neutral/Other	Dehydrocholesterol ester	DE
deDE(18:2)	Neutral/Other	Dehydrodemosterol ester	deDE
deDE(20:4)	Neutral/Other	Dehydrodemosterol ester	deDE
methyl-CE(18:0)	Neutral/Other	Methyl-cholesteryl ester	methyl-CE
methyl-CE(18:1)	Neutral/Other	Methyl-cholesteryl ester	methyl-CE
methyl-CE(18:2)	Neutral/Other	Methyl-cholesteryl ester	methyl-CE
methyl-CE(20:4)	Neutral/Other	Methyl-cholesteryl ester	methyl-CE
methyl-CE(22:6)	Neutral/Other	Methyl-cholesteryl ester	methyl-CE
methyl-DE(18:1)	Neutral/Other	Methyl-dehydrocholesteryl ester	methyl-DE
methyl-DE(18:2)	Neutral/Other	Methyl-dehydrocholesteryl ester	methyl-DE
dimethyl-CE(18:1)	Neutral/Other	Dimethyl-cholesteryl ester	dimethyl-CE
dimethyl-CE(18:2)	Neutral/Other	Dimethyl-cholesteryl ester	dimethyl-CE

dimethyl-CE(20:4)	Neutral/Other	Dimethyl-cholesteryl ester	dimethyl-CE
dimethyl-CE(22:6)	Neutral/Other	Dimethyl-cholesteryl ester	dimethyl-CE
FA(14:0)	Neutral/Other	Free fatty acid	FFA
FA(16:0)	Neutral/Other	Free fatty acid	FFA
FA(16:1)	Neutral/Other	Free fatty acid	FFA
FA(17:0)	Neutral/Other	Free fatty acid	FFA
FA(17:1)	Neutral/Other	Free fatty acid	FFA
FA(18:0)	Neutral/Other	Free fatty acid	FFA
FA(18:1)	Neutral/Other	Free fatty acid	FFA
FA(18:2)	Neutral/Other	Free fatty acid	FFA
FA(18:3)	Neutral/Other	Free fatty acid	FFA
FA(20:2)	Neutral/Other	Free fatty acid	FFA
FA(20:3)	Neutral/Other	Free fatty acid	FFA
FA(20:4)	Neutral/Other	Free fatty acid	FFA
FA(20:5)	Neutral/Other	Free fatty acid	FFA
FA(22:4)	Neutral/Other	Free fatty acid	FFA
FA(22:5)	Neutral/Other	Free fatty acid	FFA
FA(22:6)	Neutral/Other	Free fatty acid	FFA
AC(12:0)	Neutral/Other	Acylcarnitine	AC
AC(12:1)	Neutral/Other	Acylcarnitine	AC
AC(13:0)	Neutral/Other	Acylcarnitine	AC
AC(14:0)	Neutral/Other	Acylcarnitine	AC
AC(14:1)	Neutral/Other	Acylcarnitine	AC
AC(14:2)	Neutral/Other	Acylcarnitine	AC
AC(15:0) (a)	Neutral/Other	Acylcarnitine	AC
AC(15:0) (b)	Neutral/Other	Acylcarnitine	AC
AC(16:0)	Neutral/Other	Acylcarnitine	AC
AC(16:1)	Neutral/Other	Acylcarnitine	AC
AC(17:0) (a)	Neutral/Other	Acylcarnitine	AC
AC(17:0) (b)	Neutral/Other	Acylcarnitine	AC
AC(18:0)	Neutral/Other	Acylcarnitine	AC
AC(18:1)	Neutral/Other	Acylcarnitine	AC
AC(18:2)	Neutral/Other	Acylcarnitine	AC
AC(18:3)	Neutral/Other	Acylcarnitine	AC
AC(20:3) (a)	Neutral/Other	Acylcarnitine	AC
AC(20:3) (b)	Neutral/Other	Acylcarnitine	AC
AC(20:4)	Neutral/Other	Acylcarnitine	AC
AC(20:5)	Neutral/Other	Acylcarnitine	AC
AC(22:5)	Neutral/Other	Acylcarnitine	AC
AC(22:6)	Neutral/Other	Acylcarnitine	AC
AC(24:0)	Neutral/Other	Acylcarnitine	AC
AC(24:1)	Neutral/Other	Acylcarnitine	AC
AC(26:0)	Neutral/Other	Acylcarnitine	AC
AC(26:1)	Neutral/Other	Acylcarnitine	AC
AC(14:0)-OH	Neutral/Other	Hydroxylated acylcarnitine	AC-OH
AC(14:1)-OH	Neutral/Other	Hydroxylated acylcarnitine	AC-OH
AC(16:0)-OH	Neutral/Other	Hydroxylated acylcarnitine	AC-OH
AC(16:1)-OH	Neutral/Other	Hydroxylated acylcarnitine	AC-OH
AC(18:0)-OH	Neutral/Other	Hydroxylated acylcarnitine	AC-OH
AC(18:1)-OH	Neutral/Other	Hydroxylated acylcarnitine	AC-OH
AC(20:3)-OH	Neutral/Other	Hydroxylated acylcarnitine	AC-OH
AC(22:5)-OH	Neutral/Other	Hydroxylated acylcarnitine	AC-OH
AC(24:1)-OH	Neutral/Other	Hydroxylated acylcarnitine	AC-OH
CA	Neutral/Other	Bile acid	BA
dxCA	Neutral/Other	Bile acid	BA
DG(14:0_16:0)	Neutral/Other	Diacylglycerol	DG
DG(14:0_18:2)	Neutral/Other	Diacylglycerol	DG
DG(16:0_16:0)	Neutral/Other	Diacylglycerol	DG
DG(16:0_16:1)	Neutral/Other	Diacylglycerol	DG
DG(16:0_18:1)	Neutral/Other	Diacylglycerol	DG
DG(16:0_18:2)	Neutral/Other	Diacylglycerol	DG
DG(16:0_20:4)	Neutral/Other	Diacylglycerol	DG
DG(16:0_22:5)	Neutral/Other	Diacylglycerol	DG





Supplementary Table 2. Association of lipid species with baseline A/T/N biomarkers

Lipid Species	A: Amyloid PET (AV45) uptake				T: CSF pTau				N1: Hippocampal volume				N2: FDG uptake				
	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	
				(BH)				(BH)				(BH)				(BH)	
SM(4:1)	-0.148	-0.224	-0.073	0.000	0.034	-0.054	0.120	0.012	0.110	0.333	0.095	0.045	0.146	0.000	0.007	0.087	0.016
LPC(0-24:1)	0.134	0.065	0.202	0.000	0.034	0.053	-0.009	0.115	0.095	0.311	-0.033	-0.081	0.016	0.186	0.484	-0.113	-0.177
LPC(0-24:2)	0.134	0.067	0.202	0.000	0.034	0.052	-0.009	0.114	0.095	0.311	-0.050	-0.097	-0.004	0.034	0.209	-0.053	-0.117
SM(d18:1/23:0) & SM(d17:1/24:0)	-0.163	-0.254	-0.071	0.001	0.044	-0.046	-0.126	0.034	0.256	0.492	0.113	0.051	0.175	0.000	0.009	0.063	-0.022
LPC(18:2) [sn1]	0.133	0.061	0.204	0.000	0.044	0.069	0.005	0.132	0.035	0.196	0.009	-0.040	0.057	0.722	0.887	-0.012	-0.079
LPC(18:2) [sn2]	0.127	0.056	0.198	0.000	0.044	0.052	-0.012	0.116	0.108	0.331	0.013	-0.034	0.060	0.587	0.811	-0.005	-0.071
LPC(19:1) (b)	0.121	0.054	0.189	0.000	0.044	0.070	0.009	0.131	0.025	0.169	-0.018	-0.067	0.031	0.465	0.732	-0.087	-0.150
LPC(0-22:1)	0.124	0.057	0.191	0.000	0.044	0.059	-0.002	0.120	0.058	0.254	-0.029	-0.079	0.020	0.246	0.562	-0.106	-0.169
PE(0-18:0/22:6)	0.139	0.062	0.208	0.000	0.044	-0.102	-0.165	-0.058	0.002	0.042	0.073	0.027	0.121	0.003	0.046	0.038	-0.029
PE(20:1/20:4)	-0.114	-0.180	-0.047	0.001	0.060	-0.075	-0.134	-0.016	0.102	0.110	0.044	0.000	0.088	0.050	0.252	0.036	-0.026
LPC(20:1) [sn1]	0.113	0.044	0.181	0.001	0.084	0.021	-0.041	0.082	0.516	0.709	0.023	-0.027	0.073	0.359	0.668	-0.033	-0.098
LPC(20:2) [sn1]	0.113	0.044	0.182	0.001	0.084	0.053	-0.009	0.116	0.092	0.310	0.012	-0.038	0.062	0.629	0.829	-0.022	-0.087
HexCer(d18:1/24:1)	0.116	0.045	0.187	0.001	0.085	0.001	-0.063	0.064	0.981	0.985	-0.009	-0.056	0.038	0.703	0.875	-0.051	-0.117
HexCer(d18:1/16:0)	0.113	0.039	0.187	0.003	0.088	0.056	-0.009	0.122	0.094	0.310	-0.020	-0.070	0.030	0.434	0.715	-0.077	-0.146
Cer(d18:2/24:1)	0.113	0.040	0.186	0.002	0.088	0.018	-0.049	0.084	0.600	0.778	-0.043	-0.094	0.007	0.092	0.346	-0.093	-0.162
PC(16:1_18:2)	0.138	0.050	0.227	0.002	0.088	0.128	0.049	0.206	0.001	0.037	-0.078	-0.138	-0.017	0.012	0.114	-0.141	-0.222
LPC(18:1) [sn1]	0.113	0.042	0.183	0.002	0.088	0.060	-0.003	0.122	0.062	0.264	-0.021	-0.075	0.033	0.452	0.728	-0.081	-0.146
LPC(18:1) [sn2]	0.109	0.038	0.181	0.003	0.088	0.061	-0.001	0.124	0.056	0.254	-0.020	-0.072	0.033	0.461	0.730	-0.058	-0.124
LPC(19:1) (c)	0.108	0.039	0.177	0.002	0.088	0.055	-0.007	0.117	0.080	0.292	-0.006	-0.051	0.039	0.795	0.914	-0.012	-0.076
LPC(0-20:1)	0.100	0.035	0.165	0.003	0.088	0.058	-0.002	0.117	0.057	0.254	-0.047	-0.101	0.007	0.086	0.332	-0.124	-0.186
LPC(16:0) [sn1]	0.114	0.042	0.169	0.002	0.088	0.110	0.048	0.173	0.001	0.026	-0.075	-0.127	0.024	0.044	0.057	-0.121	-0.185
PE(0-18:0/22:5)	-0.111	-0.181	-0.041	0.002	0.088	0.003	-0.060	0.067	0.921	0.939	0.008	-0.040	0.056	0.741	0.892	0.016	-0.049
PE(0-38:5) (b)	-0.110	-0.181	-0.039	0.003	0.088	-0.046	-0.109	0.018	0.158	0.395	0.019	-0.029	0.067	0.430	0.714	0.019	-0.047
DE(20:4)	-0.149	-0.244	-0.053	0.002	0.088	-0.035	-0.120	0.050	0.417	0.620	0.035	-0.026	0.096	0.260	0.577	0.041	-0.047
LPC(19:1) (a)	0.102	0.035	0.170	0.003	0.093	0.058	-0.003	0.119	0.063	0.268	0.002	-0.046	0.049	0.951	0.979	-0.053	-0.117
LFE(18:2) [sn2]	0.103	0.034	0.172	0.003	0.097	0.085	0.023	0.147	0.007	0.093	-0.035	-0.082	0.012	0.140	0.424	-0.038	-0.103
HexCer(d18:2/24:1)	0.113	0.036	0.191	0.004	0.102	0.027	-0.041	0.096	0.433	0.633	-0.004	-0.054	0.046	0.878	0.953	-0.014	-0.086
LPC(18:3) [sn1] & LPC(18:3) [sn2] (b)	0.098	0.031	0.165	0.004	0.102	0.070	0.010	0.130	0.022	0.154	-0.018	-0.062	0.027	0.437	0.718	-0.019	-0.081
LPC(18:3) [sn2] (a)	0.098	0.031	0.165	0.004	0.102	0.086	0.026	0.146	0.005	0.077	-0.021	-0.067	0.024	0.357	0.667	-0.042	-0.105
LPC(19:0) [sn1] (b)	0.106	0.034	0.177	0.004	0.102	0.037	-0.027	0.101	0.254	0.492	0.022	-0.030	0.074	0.399	0.691	-0.013	-0.079
PE(0-18:0/20:4)	-0.098	-0.165	-0.031	0.004	0.102	-0.017	-0.078	0.044	0.581	0.765	0.049	0.004	0.095	0.035	0.210	-0.002	-0.065
LFE(18:2) [sn1]	0.100	0.032	0.169	0.004	0.102	0.079	0.018	0.141	0.012	0.107	-0.038	-0.085	0.009	0.112	0.381	-0.038	-0.103
SM(d16:0/22:0)	0.114	0.047	0.181	0.003	0.093	0.077	0.016	0.133	0.119	0.323	0.027	-0.027	0.125	0.020	0.089	0.064	-0.049
LPC(18:3) [sn1] [104_sn1]	0.095	0.029	0.162	0.005	0.109	0.077	0.017	0.136	0.011	0.106	-0.015	-0.060	0.029	0.494	0.749	-0.024	-0.086
LPC(17:1) [sn1] [104_sn1]	0.097	0.029	0.165	0.005	0.109	0.082	0.021	0.143	0.008	0.096	-0.025	-0.074	0.024	0.323	0.635	-0.099	-0.162
LPC(17:1) [sn1] & LPC(17:1) [sn2] (b)	0.097	0.029	0.165	0.005	0.109	0.065	0.005	0.126	0.035	0.196	-0.028	-0.074	0.017	0.223	0.534	-0.082	-0.144
LPC(P-18:1)	0.097	0.028	0.166	0.006	0.114	0.069	0.008	0.129	0.027	0.175	-0.022	-0.079	0.035	0.458	0.730	-0.097	-0.159
TG(50:3) [NL-14:0]	0.121	0.035	0.207	0.006	0.114	0.107	0.024	0.190	0.011	0.106	-0.079	-0.143	-0.015	0.016	0.137	-0.083	-0.168
TG(54:6) [NL-22:6]	-0.101	-0.173	-0.029	0.006	0.114	-0.086	-0.151	-0.021	0.009	0.099	0.022	-0.026	0.071	0.372	0.673	0.020	-0.048
LPC(19:0) [sn1] & LPC(19:0) [sn2] (b)	0.100	0.028	0.171	0.007	0.119	0.018	-0.047	0.082	0.592	0.773	0.024	-0.025	0.074	0.336	0.644	-0.002	-0.068
TG(56:7) [NL-22:6]	-0.097	-0.167	-0.027	0.007	0.119	-0.093	-0.155	-0.031	0.003	0.060	0.046	-0.001	0.093	0.053	0.259	0.021	-0.044
GM3(d18:1/24:1)	0.104	0.029	0.178	0.007	0.120	0.015	-0.052	0.081	0.670	0.826	-0.034	-0.087	0.020	0.214	0.524	-0.143	-0.214
LPC(0-18:1)	0.089	0.025	0.154	0.007	0.121	0.044	-0.016	0.103	0.153	0.385	0.011	-0.042	0.065	0.673	0.858	-0.079	-0.140
PE(P-15:0/22:4) (b)	-0.095	-0.164	-0.026	0.007	0.123	-0.107	-0.168	-0.046	0.001	0.026	0.065	0.019	0.111	0.005	0.065	0.040	-0.024
LPC(22:5) [sn1] (n3) & LPC(22:5) [sn2] (n6)	-0.087	-0.155	-0.019	0.012	0.124	0.099	0.030	0.151	0.033	0.060	-0.060	-0.107	-0.013	0.012	0.114	-0.046	-0.109
SM(44:1)	-0.105	-0.182	-0.027	0.008	0.129	-0.062	-0.131	0.007	0.078	0.289	0.101	0.050	0.152	0.000	0.004	0.113	0.041
PE(P-19:0/20:4) (a)	-0.091	-0.158	-0.024	0.008	0.129	-0.051	-0.111	0.008	0.092	0.310	0.040	-0.004	0.085	0.078	0.317	-0.015	-0.047
LPC(18:3) [sn1] (b)	0.091	0.023	0.158	0.009	0.135	0.079	0.019	0.139	0.010	0.100	-0.015	-0.060	0.029	0.503	0.757	-0.029	-0.092
Cer(d17:1/24:1)	0.095	0.024	0.167	0.009	0.139	0.051	-0.014	0.115	0.124	0.353	-0.025	-0.073	0.023	0.305	0.622	-0.079	-0.145
SM(18:2/24:0)	-0.112	-0.196	-0.027	0.009	0.139	-0.049	-0.125	0.026	0.201	0.443	0.120	0.064	0.176	0.000	0.001	0.126	0.047
LPC(P-18:0)	0.091	0.022	0.160	0.009	0.139	0.038	-0.023	0.100	0.222	0.465	-0.019	-0.071	0.033	0.476	0.737	-0.070	-0.135
Cer(d18:1/24:1)	0.095	0.022	0.167	0.011	0.150	0.034	-0.032	0.101	0.308	0.541	-0.044	-0.094	0.007	0.090	0.340	-0.138	-0.207
LPC(0-20:0)	0.089	0.021	0.157	0.011	0.150	0.049	-0.013	0.111	0.120	0.346	-0.028	-0.077	0.021	0.268	0.588	-0.085	-0.150
DE(20:5)	-0.101	-0.179	-0.023	0.011	0.152	-0.125	-0.195	-0.056	0.000	0.021	0.057	0.006	0.108	0.029	0.192	0.078	0.006
LPC(16:0) [sn2]	0.095	0.022	0.168	0.011	0.152	0.042	-0.024	0.108	0.215	0.456	-0.046	-0.098	0.006	0.081	0.324	-0.073	-0.142
DE(22:6)	-0.103	-0.183	-0.023	0.012	0.156	-0.108	-0.176	-0.040	0.002	0.042	0.057	0.006	0.107	0.028	0.185	0.061	-0.010
PE(P-20:1/22:6)	-0.087	-0.155	-0.019	0.012	0.158												

LPC(P-20.0)	0.070	0.002	0.139	0.044	0.254	0.033	-0.029	0.095	0.294	0.528	-0.023	-0.071	0.026	0.362	0.669	-0.083	-0.147	-0.019	0.011	0.090
LMC(22.0) [sn2]	0.072	0.002	0.143	0.045	0.255	-0.003	-0.067	0.060	0.914	0.964	0.026	-0.021	0.073	0.276	0.596	0.042	-0.023	0.107	0.201	0.407
SM(43:1)	-0.075	-0.149	-0.001	0.046	0.257	-0.025	-0.091	0.041	0.457	0.656	0.102	0.052	0.151	0.000	0.020	0.061	-0.009	0.130	0.087	0.273
LPC(16.0) [sn1]	0.074	0.001	0.146	0.046	0.257	0.034	-0.030	0.099	0.296	0.528	-0.019	-0.075	0.037	0.504	0.757	-0.066	-0.133	0.001	0.055	0.213
PEI(0.38:5) (a)	-0.070	-0.140	-0.001	0.046	0.257	-0.014	-0.076	0.048	0.698	0.815	0.045	-0.002	0.092	0.062	0.284	0.006	-0.058	0.071	0.849	0.916
PEI(18.0:18:1)	-0.072	-0.143	-0.001	0.046	0.258	-0.062	-0.125	0.001	0.055	0.253	0.095	0.048	0.143	0.002	0.003	0.059	0.006	0.124	0.075	0.259
SM(d18:1/22.0) & SM(d16:1/24.0)	-0.091	-0.180	-0.001	0.047	0.259	-0.019	-0.098	0.060	0.641	0.799	0.095	0.034	0.156	0.002	0.028	0.035	-0.050	0.119	0.422	0.642
HexCer(d16:1/22.0)	0.070	0.001	0.139	0.048	0.260	0.068	0.007	0.128	0.209	0.182	-0.017	-0.062	0.029	0.471	0.737	-0.004	-0.068	0.059	0.891	0.944
LPC(15-MHDA) [sn1] & LPC(17.0) [sn2]	0.068	0.000	0.136	0.049	0.260	0.034	-0.027	0.094	0.274	0.509	-0.004	-0.052	0.045	0.879	0.953	-0.052	-0.115	0.011	0.103	0.287
LPC(O-22.0)	0.071	0.000	0.142	0.049	0.260	0.026	-0.037	0.090	0.416	0.620	-0.007	-0.056	0.042	0.783	0.910	-0.059	-0.144	-0.013	0.019	0.125
LPC(20:3) [sn1]	0.071	0.000	0.142	0.049	0.260	0.078	0.016	0.140	0.014	0.116	0.024	-0.025	0.073	0.343	0.650	-0.008	-0.073	0.057	0.806	0.899
TG(52:4) [NL-16:1]	0.073	0.000	0.145	0.049	0.260	0.070	0.003	0.137	0.041	0.215	-0.045	-0.103	0.012	0.122	0.393	-0.083	-0.152	-0.013	0.020	0.128
TC(O-52:1) [NL-18:1]	-0.071	-0.142	0.000	0.050	0.262	-0.043	-0.107	0.022	0.194	0.429	-0.106	0.057	0.155	0.000	0.001	0.004	-0.062	0.071	0.901	0.948
Cer(d18:2/21:0)	0.074	0.000	0.148	0.051	0.264	0.080	0.015	0.144	0.016	0.131	-0.034	-0.083	0.014	0.167	0.458	-0.094	-0.161	-0.028	0.005	0.065
PC(O-18:1)	0.089	0.000	0.178	0.051	0.264	0.034	-0.045	0.113	0.394	0.602	0.050	-0.012	0.111	0.111	0.381	-0.033	-0.114	0.048	0.427	0.644
SHexCer(d18:1/24:0)(OH)	0.073	-0.001	0.147	0.053	0.264	-0.015	-0.081	0.051	0.655	0.812	0.009	-0.040	0.057	0.721	0.887	-0.011	-0.079	0.057	0.751	0.870
PC(O-34:4)	-0.068	-0.137	0.001	0.053	0.264	-0.021	-0.082	0.040	0.500	0.693	0.021	-0.025	0.067	0.367	0.672	-0.024	-0.084	0.029	0.971	1.010
LPC(22:0) [sn1]	0.071	-0.001	0.142	0.052	0.264	0.000	-0.064	0.063	0.992	0.994	0.021	-0.027	0.069	0.385	0.768	0.024	-0.041	0.089	0.471	0.685
PEI(18:0/20:3) (b)	-0.070	-0.140	0.001	0.052	0.264	-0.010	-0.072	0.051	0.741	0.871	0.047	0.000	0.095	0.051	0.256	-0.016	-0.080	0.049	0.629	0.806
TG(54:7) [NL-22:6]	-0.077	-0.154	0.000	0.051	0.264	-0.070	-0.138	-0.001	0.047	0.225	0.016	-0.035	0.067	0.541	0.779	-0.017	-0.089	0.054	0.632	0.806
TG(48:3) [NL-16:1]	0.096	0.001	0.193	0.052	0.264	0.153	0.066	0.240	0.001	0.026	-0.127	-0.195	-0.059	0.000	0.008	-0.185	-0.275	-0.095	0.000	0.011
HexCer(d18:1/22:0)	0.077	-0.001	0.155	0.054	0.266	0.072	0.003	0.142	0.042	0.215	-0.011	-0.062	0.041	0.687	0.868	-0.048	-0.120	0.025	0.198	0.403
LPC(26:0) [sn1]	0.083	-0.001	0.168	0.054	0.266	0.002	-0.073	0.076	0.961	0.980	-0.003	-0.057	0.051	0.913	0.964	-0.024	-0.100	0.051	0.526	0.725
HexCer(d16:1/16:0)	0.066	-0.002	0.133	0.055	0.271	0.051	-0.009	0.111	0.093	0.310	-0.038	-0.082	0.006	0.093	0.346	-0.044	-0.106	0.018	0.166	0.371
PI(18:0_22:5) (n6)	-0.066	-0.134	0.002	0.056	0.272	0.015	-0.045	0.076	0.619	0.783	0.024	-0.020	0.069	0.285	0.602	-0.033	-0.096	0.029	0.299	0.519
AC(20:3) (a)	0.064	-0.002	0.129	0.056	0.272	0.044	-0.014	0.103	0.138	0.372	-0.005	-0.048	0.038	0.820	0.925	-0.006	-0.067	0.054	0.833	0.911
HexCer(d18:1/16:0)	0.067	-0.002	0.136	0.057	0.274	-0.006	-0.067	0.055	0.849	0.938	-0.009	-0.055	0.037	0.689	0.868	-0.031	-0.095	0.033	0.484	0.574
TG(O-52:1) [NL-16:0]	-0.071	-0.144	0.002	0.057	0.274	-0.032	-0.097	0.034	0.347	0.575	0.084	0.032	0.136	0.001	0.027	-0.010	-0.079	0.059	0.784	0.884
TC(18:0_18:1)	-0.114	-0.232	0.004	0.059	0.274	-0.103	-0.233	-0.003	0.044	0.216	0.020	-0.029	0.079	0.390	0.596	-0.075	-0.181	0.031	0.164	0.371
LPC(18:1) [sn1]	-0.064	-0.131	0.003	0.060	0.282	-0.002	-0.060	0.057	0.956	0.980	0.034	-0.011	0.080	0.133	0.417	-0.008	-0.070	0.053	0.794	0.891
PEI(17:0/20:4) (b)	-0.064	-0.131	0.003	0.060	0.282	-0.036	-0.095	0.023	0.235	0.480	0.062	-0.017	0.107	0.006	0.078	-0.001	-0.063	0.060	0.963	0.977
LPE(18:0) [sn1]	0.075	-0.003	0.153	0.061	0.282	0.018	-0.051	0.088	0.607	0.778	-0.041	-0.096	0.014	0.141	0.424	-0.080	-0.153	-0.008	0.030	0.159
HexCer(d18:2/16:0)	0.067	-0.005	0.139	0.067	0.311	0.029	-0.034	0.093	0.363	0.580	-0.026	-0.073	0.021	0.282	0.601	-0.051	-0.117	0.015	0.132	0.333
PE(O-36:5)	-0.065	-0.135	0.005	0.068	0.311	-0.078	-0.141	-0.015	0.015	0.121	0.021	-0.026	0.067	0.386	0.678	0.036	-0.029	0.100	0.278	0.489
PC(O-34:1)	0.061	-0.007	0.169	0.070	0.317	0.043	-0.036	0.122	0.283	0.518	0.026	-0.036	0.089	0.405	0.695	-0.045	-0.127	0.036	0.274	0.483
TC(O-16:0/20:4)	-0.084	-0.133	0.005	0.070	0.317	-0.033	-0.094	0.028	0.290	0.525	0.044	-0.002	0.091	0.058	0.270	-0.019	-0.083	0.044	0.549	0.739
TG(50:2) [NL-14:0]	0.069	-0.006	0.144	0.070	0.317	0.048	-0.023	0.120	0.185	0.426	-0.029	-0.084	0.025	0.294	0.616	-0.035	-0.109	0.038	0.346	0.572
TG(50:4) [NL-18:3]	0.090	-0.008	0.187	0.071	0.317	0.122	0.033	0.212	0.007	0.093	-0.083	-0.152	-0.014	0.019	0.151	-0.147	-0.240	-0.054	0.002	0.041
HexCer(d18:1/22:0)	0.069	-0.006	0.145	0.073	0.322	0.017	-0.049	0.084	0.605	0.778	0.018	-0.032	0.068	0.476	0.737	-0.016	-0.085	0.054	0.655	0.816
PEI(16:0/20:5)	-0.064	-0.135	0.006	0.072	0.322	-0.091	-0.155	-0.028	0.005	0.073	0.042	-0.005	0.089	0.080	0.322	0.056	-0.009	0.120	0.093	0.278
TC(O-52:2) [NL-17:1]	-0.065	-0.137	0.006	0.074	0.326	-0.068	-0.132	-0.003	0.040	0.210	0.138	-0.089	0.187	0.000	0.000	0.068	0.000	0.135	0.050	0.254
LPE(18:0) [sn2]	0.070	-0.007	0.148	0.076	0.327	0.009	-0.060	0.078	0.793	0.907	-0.034	-0.088	0.020	0.214	0.524	-0.063	-0.135	0.010	0.089	0.275
PEI(16:0/20:3) (b)	-0.063	-0.133	0.006	0.075	0.327	-0.003	-0.065	0.059	0.923	0.964	0.057	0.011	0.104	0.016	0.137	-0.005	-0.068	0.059	0.883	0.937
AC(15:0) (a)	-0.060	-0.127	0.006	0.076	0.327	-0.029	-0.089	0.031	0.343	0.572	0.008	-0.036	0.051	0.730	0.887	-0.020	-0.081	0.041	0.525	0.725
TG(54:5) [NL-18:3]	0.066	-0.007	0.138	0.076	0.327	0.046	-0.022	0.114	0.181	0.425	0.002	-0.053	0.057	0.943	0.973	-0.031	-0.102	0.039	0.383	0.610
PC(18:1_22:6) (a)	0.063	-0.007	0.133	0.077	0.329	0.023	-0.086	0.039	0.464	0.661	0.029	-0.019	0.077	0.233	0.546	0.008	-0.057	0.073	0.805	0.899
GM3(d18:1/18:0)	-0.068	-0.144	0.008	0.080	0.331	-0.029	-0.096	0.038	0.392	0.600	0.002	-0.050	0.054	0.930	0.969	-0.042	-0.113	0.029	0.246	0.457
PEI(18:0/22:5) (n6)	-0.062	-0.131	0.007	0.079	0.331	0.032	-0.030	0.094	0.306	0.541	0.025	-0.022	0.072	0.297	0.616	-0.039	-0.103	0.025	0.233	0.444
AC(13:0)	-0.061	-0.128	0.007	0.080	0.331	-0.069	-0.129	-0.009	0.025	0.169	0.040	-0.004	0.085	0.077	0.317	0.006	-0.056	0.068	0.853	0.918
TG(54:2) [NL-20:1]	-0.089	-0.187	0.010	0.079	0.331	-0.008	-0.096	0.080	0.853	0.939	0.055	-0.013	0.123	0.111	0.381	-0.018	-0.111	0.074	0.699	0.840
DG(18:1_18:3)	0.090	-0.100	0.191	0.078	0.331	0.017	-0.072	0.106	0.709	0.853	-0.027	-0.095	0.040	0.426	0.713	-0.085	-0.177	0.007	0.070	0.250
PEI(18:1/20:5) (a)	-0.063	-0.135	0.008	0.082	0.335	-0.108	-0.173	-0.043	0.001	0.034	0.052	0.004	0.100	0.034	0.209	0.078	0.011	0.144	0.022	0.134
TG(O-54:3) [NL-17:1]	-0.061	-0.130	0.008	0.081	0.335	-0.044	-0.096	0.037	0.156	0.392	0.114	-0.066	0.162	0.000	0.000	0.010	-0.055	0.074	0.771	0.875
CE(24:1)	0.075	0.010	0.160	0.082	0.337	-0.006	-0.079	0.067	0.875	0.946	-0.009	-0.063	0.045	0.742	0.892	-0.107	-0.184	-0.030	0.007	0.073
SIP(d18:1)	0.057	-0.008	0.122	0.086	0.338	0.055	-0.003	0.113	0.064	0.268	-0.025	-0.071	0.021	0.292	0.612	-0.043	-0.103	0.018	0.167	0.372
HexCer(d16:1/24:0)	0.062	-0.009	0.133	0.086	0.338	0.019	-0.042	0.080	0.538	0.729	-0.031	-0.077	0.016	0.195	0.497	-0.015	-0.048	0.07		

AC(26:0)	-0.050	-0.121	0.022	0.172	0.491	-0.033	-0.097	0.031	0.308	0.541	0.055	0.008	0.102	0.021	0.158	0.065	-0.001	0.131	0.054	0.212
DG(18:1;18:2)	0.072	-0.032	0.176	0.173	0.492	-0.025	-0.117	0.066	0.588	0.770	-0.029	-0.101	0.042	0.423	0.111	-0.073	-0.167	0.022	0.132	0.333
PE(38:5) (b)	-0.061	-0.149	0.027	0.177	0.495	0.006	-0.073	0.084	0.889	0.954	-0.073	-0.133	-0.013	0.017	0.142	-0.082	-0.163	-0.001	0.407	0.200
PE(16:0;20:3)	-0.048	-0.118	0.022	0.177	0.495	-0.001	-0.064	0.061	0.973	0.982	0.017	-0.032	0.066	0.505	0.757	-0.031	-0.096	0.033	0.342	0.569
Ac(24:1)-OH	-0.047	-0.114	0.021	0.177	0.495	-0.033	-0.094	0.021	0.975	0.510	0.012	-0.033	0.058	0.590	0.811	-0.012	-0.074	0.050	0.700	0.846
LPC(52:0) [NL-22:4]	-0.047	-0.115	0.021	0.176	0.495	-0.065	-0.136	0.004	0.036	0.197	0.037	-0.009	0.082	0.816	0.388	0.001	0.063	0.065	0.978	0.964
SM(d16:1/23:0) & SM(d17:1/22:0)	-0.056	-0.139	0.026	0.181	0.495	0.032	-0.040	0.105	0.384	0.592	0.059	0.004	0.114	0.036	0.211	0.053	-0.024	0.131	0.177	0.382
GM3(d18:1/22:0)	0.053	-0.024	0.130	0.179	0.495	0.070	0.001	0.140	0.046	0.224	-0.031	-0.087	0.026	0.286	0.604	-0.142	-0.215	-0.070	0.000	0.012
PS(38:3)	0.044	-0.020	0.107	0.181	0.495	0.022	-0.035	0.079	0.453	0.653	0.007	-0.037	0.050	0.768	0.902	0.067	0.008	0.126	0.026	0.152
AC(18:0)-OH	-0.045	-0.111	0.021	0.179	0.495	0.024	-0.035	0.084	0.426	0.628	-0.017	-0.062	0.029	0.474	0.737	-0.097	-0.158	-0.036	0.002	0.041
AC(22:5)-OH	-0.047	-0.115	0.022	0.180	0.495	-0.070	-0.130	-0.009	0.025	0.169	0.048	0.003	0.093	0.039	0.220	0.040	-0.023	0.104	0.210	0.419
TG(50:3) [NL-16:1]	0.058	-0.027	0.144	0.180	0.495	0.132	0.054	0.210	0.001	0.033	-0.107	-0.168	-0.045	0.001	0.016	-0.145	-0.227	-0.062	0.001	0.025
LPC(20:3) [sm2]	0.050	-0.024	0.123	0.183	0.497	0.068	0.005	0.132	0.036	0.196	0.028	-0.020	0.077	0.252	0.572	0.016	-0.051	0.083	0.635	0.808
deDE(20:4)	0.047	-0.022	0.116	0.183	0.497	0.060	-0.002	0.122	0.057	0.254	-0.110	-0.155	-0.065	0.000	0.000	-0.116	-0.179	-0.053	0.000	0.017
Cer(d17:1;21:0)	0.050	-0.024	0.124	0.185	0.501	0.037	-0.029	0.102	0.269	0.506	0.020	-0.028	0.069	0.416	0.705	0.024	-0.044	0.092	0.488	0.696
LPC(18:0) [sm1]	0.049	-0.024	0.122	0.187	0.503	0.014	-0.050	0.079	0.662	0.818	-0.006	-0.058	0.047	0.832	0.929	-0.054	-0.121	0.013	0.117	0.310
PC(16:0;16:0)	-0.051	-0.126	0.025	0.188	0.504	0.012	-0.056	0.079	0.734	0.868	-0.023	-0.074	0.027	0.365	0.672	-0.029	-0.099	0.041	0.145	0.460
LPC(22:4) [sm2]	0.047	-0.023	0.117	0.189	0.506	0.115	0.053	0.177	0.000	0.019	-0.043	-0.092	0.004	0.084	0.246	-0.088	-0.153	0.022	0.099	0.064
TG(50:2) [NL-16:0]	-0.048	-0.120	0.024	0.190	0.507	0.017	-0.048	0.082	0.612	0.782	0.028	-0.022	0.078	0.276	0.596	-0.041	-0.108	0.027	0.236	0.446
CE(2:0)	0.053	-0.027	0.133	0.191	0.508	0.036	-0.034	0.107	0.313	0.545	0.003	-0.049	0.056	0.802	0.961	-0.016	-0.089	0.057	0.667	0.823
CA	-0.042	-0.106	0.022	0.195	0.515	-0.012	-0.069	0.046	0.687	0.836	0.061	0.019	0.104	0.004	0.057	0.064	0.024	0.143	0.006	0.065
Cer(d18:1;21:0)	0.049	-0.026	0.124	0.197	0.516	0.075	0.008	0.142	0.229	0.182	-0.058	-0.110	-0.007	0.027	0.185	-0.119	-0.188	-0.051	0.001	0.027
DG(14:0;18:2)	0.067	-0.035	0.168	0.197	0.516	0.052	-0.039	0.142	0.262	0.493	-0.084	-0.152	-0.015	0.016	0.137	-0.098	-0.191	-0.005	0.038	0.182
TG(56:7) [NL-20:5]	-0.045	-0.114	0.023	0.196	0.516	-0.041	-0.102	0.021	0.193	0.429	0.033	-0.013	0.078	0.160	0.454	0.018	-0.045	0.082	0.577	0.759
LPC(20:4) [sm2]	0.046	-0.024	0.117	0.198	0.516	0.053	-0.009	0.115	0.093	0.310	-0.005	-0.053	0.042	0.822	0.925	-0.080	-0.145	-0.015	0.017	0.115
dhCer(d18:0/24:0)	-0.051	-0.130	0.027	0.199	0.517	-0.029	-0.098	0.039	0.403	0.610	0.050	-0.001	0.101	0.057	0.270	0.062	-0.010	0.134	0.090	0.277
LPE(22:6) [sm2]	0.048	-0.025	0.121	0.200	0.517	-0.038	-0.103	0.028	0.257	0.492	-0.009	-0.061	0.042	0.731	0.887	0.042	-0.025	0.109	0.216	0.422
TG(52:4) [NL-18:2]	0.048	-0.026	0.122	0.201	0.520	0.080	0.010	0.149	0.025	0.169	-0.045	-0.101	0.012	0.121	0.375	-0.043	-0.116	0.027	0.240	0.451
PC(14:0;16:0)	-0.059	-0.151	0.034	0.214	0.526	0.043	-0.038	0.125	0.295	0.528	-0.032	-0.095	0.031	0.314	0.428	-0.067	-0.153	0.019	0.125	0.325
PC(38:5) (a)	0.048	-0.026	0.122	0.205	0.521	0.085	0.021	0.148	0.009	0.099	-0.048	-0.099	0.003	0.066	0.298	-0.068	-0.135	-0.001	0.047	0.208
LPC(18:0;22:6)	-0.046	-0.116	0.025	0.203	0.521	-0.079	-0.141	-0.016	0.014	0.116	0.044	-0.003	0.091	0.068	0.294	0.028	-0.037	0.093	0.391	0.615
PE(16:0;22:5) (ns)	-0.047	-0.119	0.025	0.203	0.521	0.057	-0.005	0.120	0.073	0.285	0.044	-0.009	0.096	0.101	0.364	-0.062	-0.128	0.003	0.062	0.234
PI(18:0;20:3) (a)	0.042	-0.023	0.108	0.205	0.521	-0.001	-0.060	0.058	0.962	0.980	0.008	-0.035	0.052	0.707	0.875	0.054	-0.007	0.115	0.083	0.269
PI(20:0;20:4)	0.044	-0.024	0.111	0.206	0.521	0.032	-0.028	0.093	0.296	0.528	0.016	-0.029	0.061	0.484	0.739	0.040	-0.022	0.103	0.208	0.415
TG(50:1) [NL-18:1]	-0.044	-0.113	0.024	0.206	0.521	-0.074	-0.135	-0.012	0.019	0.141	0.106	0.060	0.151	0.000	0.000	0.022	-0.042	0.085	0.501	0.701
PC(10:40:5)	0.046	-0.026	0.108	0.209	0.525	0.085	0.021	0.149	0.009	0.099	-0.025	-0.077	0.028	0.356	0.667	-0.124	-0.190	-0.058	0.000	0.017
Cer(m18:0/20:0)	-0.054	-0.138	0.030	0.211	0.528	-0.013	-0.087	0.060	0.728	0.864	0.000	-0.056	0.057	0.988	0.994	-0.068	-0.144	0.009	0.083	0.269
PC(16:0;20:3)	0.046	-0.026	0.118	0.211	0.528	0.073	0.011	0.136	0.022	0.152	0.008	-0.043	0.059	0.759	0.900	-0.060	-0.126	0.006	0.075	0.259
PE(16:0;22:5) (ns)	-0.047	-0.122	0.027	0.212	0.528	-0.008	-0.074	0.057	0.802	0.912	0.044	-0.006	0.094	0.082	0.325	0.017	-0.051	0.085	0.619	0.799
Cer(m18:1;18:0)	-0.050	-0.128	0.029	0.213	0.528	-0.025	-0.095	0.044	0.475	0.669	-0.010	-0.061	0.041	0.703	0.875	-0.025	-0.096	0.046	0.487	0.696
PC(14:0;16:0)	-0.059	-0.151	0.034	0.214	0.526	0.043	-0.038	0.125	0.295	0.528	-0.032	-0.095	0.031	0.314	0.428	-0.067	-0.153	0.019	0.125	0.325
LPC(14:0) [sm1]	0.045	-0.027	0.117	0.216	0.529	0.049	-0.015	0.113	0.130	0.360	-0.055	-0.102	-0.007	0.025	0.177	-0.057	-0.124	0.009	0.092	0.278
LPE(16:20:0)	0.043	-0.025	0.110	0.215	0.529	0.036	-0.024	0.096	0.236	0.480	-0.020	-0.064	0.024	0.370	0.672	-0.012	-0.074	0.050	0.701	0.840
TG(50:2) [NL-16:0]	-0.045	-0.116	0.026	0.216	0.529	-0.058	-0.122	0.006	0.075	0.286	0.133	-0.084	0.181	0.000	0.000	0.054	-0.013	0.121	0.112	0.302
Cer(d19:1;24:1)	0.041	-0.024	0.107	0.218	0.530	0.027	-0.031	0.086	0.363	0.580	-0.009	-0.052	0.035	0.699	0.875	-0.071	-0.132	-0.011	0.021	0.129
PC(32:2)	0.052	-0.032	0.136	0.222	0.530	0.085	0.010	0.161	0.027	0.175	-0.064	-0.120	-0.007	0.027	0.185	-0.093	-0.171	-0.014	0.020	0.128
PC(16:0;18:1)	0.065	-0.039	0.169	0.220	0.530	0.100	-0.082	0.101	0.836	0.932	0.027	-0.043	0.096	0.450	0.728	-0.042	-0.135	0.052	0.381	0.610
PE(16:0;16:0)	0.049	-0.030	0.127	0.223	0.530	0.040	-0.030	0.111	0.257	0.492	-0.024	-0.077	0.029	0.379	0.678	-0.052	-0.125	0.021	0.165	0.371
LPC(19:0) (a) [sm1] [104_sm1]	0.044	-0.027	0.115	0.224	0.530	0.005	-0.058	0.068	0.700	0.944	0.037	-0.111	0.086	0.129	0.407	-0.002	-0.067	0.063	0.958	0.977
LPC(15:0) [sm1]	0.043	-0.026	0.111	0.226	0.530	0.033	-0.028	0.095	0.286	0.521	-0.013	-0.059	0.033	0.583	0.810	-0.026	-0.090	0.037	0.418	0.640
PE(16:0;22:4)	-0.044	-0.115	0.027	0.225	0.530	0.041	-0.022	0.105	0.204	0.446	0.008	-0.041	0.056	0.756	0.899	-0.061	-0.127	0.005	0.072	0.253
PE(18:1;20:4) (a)	-0.044	-0.113	0.026	0.218	0.530	-0.037	-0.098	0.024	0.236	0.480	0.087	-0.041	0.133	0.000	0.000	0.011	-0.052	0.075	0.727	0.855
AC(20:3) (b)	0.040	-0.025	0.105	0.225	0.530	0.054	-0.004	0.113	0.067	0.272	-0.015	-0.058	0.028	0.488	0.742	-0.039	-0.099	0.021	0.201	0.406
TG(50:2) [NL-18:1]	0.049	-0.030	0.128	0.220	0.530	0.070	-0.003	0.143	0.060	0.259	-0.058	-0.114	-0.001	0.045	0.243	-0.063	-0.140	0.013	0.105	0.292
TG(52:3) [NL-16:1]	0.042	-0.026	0.110	0.225	0.530	0.065	0.002	0.128	0.042	0.215	-0.016	-0.068	0.036	0.545	0.779	-0.069	-0.134	-0.003	0.039	0.183
PC(34:2) +OH	0.048	-0.029	0.125	0.223	0.530	-0.053	-0.120	0.013	0.116	0.344	0.001	-0.048	0.050	0.967	0.985	-0.027	-0.097	0.043	0.446	0.661
SM(40:3) (a)	0.051	-0																		

TG(50:3) [NL:14:1]	0.040	-0.040	0.121	0.325	0.613	0.078	0.004	0.151	0.038	0.204	-0.045	-0.105	0.015	0.145	0.427	-0.106	-0.182	-0.030	0.006	0.069
TG(48:2) [NL:18:2]	0.044	-0.043	0.130	0.324	0.613	0.070	-0.011	0.151	0.090	0.310	-0.060	-0.122	0.001	0.054	0.263	-0.075	-0.160	0.010	0.083	0.269
Cer(d16:1/23:0)	0.037	-0.037	0.111	0.327	0.613	0.052	-0.013	0.118	0.117	0.344	-0.014	-0.063	0.034	0.567	0.797	-0.017	-0.085	0.050	0.620	0.800
CE(24:5)	-0.041	-0.123	0.041	0.326	0.613	-0.013	-0.085	0.059	0.726	0.864	0.028	-0.025	0.081	0.298	0.616	0.054	-0.021	0.129	0.159	0.359
SIP(18:2)	0.033	-0.034	0.101	0.329	0.615	0.076	0.006	0.125	0.031	0.188	0.015	-0.021	0.061	0.529	0.778	-0.012	-0.073	0.050	0.709	0.894
PE(24:4)	0.042	-0.043	0.127	0.329	0.615	0.056	-0.019	0.130	0.145	0.380	0.000	-0.055	0.056	0.593	0.994	-0.057	-0.135	0.021	0.154	0.359
PI(17:0_22:6)	-0.039	-0.117	0.040	0.331	0.615	-0.096	-0.166	-0.025	0.008	0.095	-0.033	-0.020	0.086	0.218	0.530	-0.028	-0.045	0.100	0.451	0.666
PI(38:5) (a)	0.039	-0.040	0.117	0.330	0.615	0.117	0.046	0.187	0.001	0.096	-0.009	-0.062	0.044	0.743	0.892	-0.047	-0.119	0.026	0.208	0.415
AC(16:0)-OH	-0.032	-0.098	0.033	0.335	0.621	0.004	-0.055	0.063	0.898	0.960	-0.025	-0.069	0.019	0.270	0.588	-0.102	-0.162	-0.041	0.001	0.028
DG(18:0_18:2)	-0.055	-0.167	0.057	0.336	0.621	-0.054	-0.149	0.042	0.272	0.507	-0.055	-0.132	0.022	0.161	0.454	-0.092	-0.192	0.008	0.700	0.250
PCP(35:2) (a)	0.037	-0.039	0.113	0.340	0.628	0.050	-0.016	0.116	0.136	0.369	0.039	-0.010	0.089	0.120	0.391	-0.008	-0.077	0.062	0.824	0.909
Cer(d18:1/19:0)	0.032	-0.035	0.098	0.352	0.630	-0.002	-0.062	0.058	0.948	0.977	-0.002	-0.046	0.043	0.941	0.973	-0.005	-0.067	0.057	0.868	0.929
SM(d17:1/24:1)	0.037	-0.040	0.114	0.346	0.630	0.004	-0.064	0.072	0.906	0.960	0.036	-0.015	0.087	0.165	0.457	-0.063	-0.135	0.008	0.082	0.269
PC(16:0_20:5)	-0.035	-0.109	0.039	0.352	0.630	-0.046	-0.113	0.020	0.170	0.407	-0.015	-0.064	0.034	0.553	0.783	-0.068	-0.077	0.061	0.818	0.907
PA(36:3)	0.033	-0.036	0.101	0.349	0.630	-0.003	-0.063	0.056	0.917	0.964	0.015	-0.030	0.060	0.515	0.768	0.065	0.003	0.127	0.040	0.185
PCP(18:0/22:6)	-0.037	-0.115	0.040	0.347	0.630	-0.101	-0.169	-0.033	0.004	0.060	0.075	-0.024	0.126	0.004	0.057	0.016	-0.054	0.086	0.651	0.816
PCP(35:2) (b)	0.036	-0.039	0.111	0.348	0.630	0.004	-0.064	0.087	0.524	0.716	0.037	-0.013	0.089	0.146	0.429	-0.022	-0.078	0.033	0.233	0.279
LPC(15:0) [sn2]	0.033	-0.036	0.101	0.351	0.630	0.034	-0.027	0.095	0.219	0.514	-0.017	-0.063	0.029	0.458	0.730	-0.025	-0.098	0.038	0.334	0.651
PI(16:0_16:1)	-0.036	-0.112	0.040	0.351	0.630	0.064	-0.004	0.132	0.066	0.272	-0.035	-0.085	0.016	0.180	0.479	-0.058	-0.129	0.013	0.111	0.301
PI(18:0_22:4)	-0.038	-0.118	0.041	0.344	0.630	0.068	-0.002	0.138	0.056	0.254	-0.029	-0.084	0.026	0.298	0.616	-0.060	-0.134	0.014	0.110	0.301
PEP(16:0/20:3) (a)	-0.033	-0.102	0.035	0.344	0.630	-0.105	-0.075	0.045	0.617	0.783	0.054	-0.009	0.099	0.019	0.154	0.045	-0.017	0.108	0.155	0.359
FA(17:0)	-0.031	-0.095	0.034	0.347	0.630	0.007	-0.050	0.065	0.804	0.913	0.000	-0.043	0.043	0.993	0.994	-0.087	-0.146	-0.027	0.004	0.057
AC(22:6)	-0.032	-0.100	0.036	0.350	0.630	-0.087	-0.148	-0.026	0.005	0.077	0.037	-0.010	0.084	0.124	0.397	-0.057	-0.006	0.121	0.077	0.264
COH	0.042	-0.045	0.129	0.344	0.630	-0.003	-0.077	0.071	0.935	0.970	0.007	-0.054	0.068	0.823	0.925	-0.100	-0.180	-0.020	0.014	0.104
AC(12:1)	-0.031	-0.096	0.034	0.354	0.631	0.045	-0.014	0.104	0.132	0.362	-0.009	-0.054	0.035	0.676	0.860	-0.068	-0.129	-0.008	0.027	0.153
PE(18:1_18:2)	0.033	-0.037	0.104	0.355	0.631	0.029	-0.036	0.095	0.376	0.586	0.016	-0.033	0.065	0.520	0.773	0.019	-0.048	0.087	0.573	0.758
SM(43:2) (c)	-0.040	-0.125	0.045	0.357	0.633	-0.054	-0.129	0.021	0.160	0.397	0.093	-0.038	0.149	0.001	0.021	0.050	-0.029	0.129	0.212	0.422
LPC(26:0) [sn2]	0.039	-0.044	0.123	0.357	0.633	-0.018	-0.091	0.055	0.629	0.789	0.007	-0.046	0.061	0.790	0.912	0.073	-0.001	0.148	0.053	0.212
Cer(d18:1/22:0)	0.037	-0.043	0.118	0.359	0.633	0.021	-0.035	0.138	0.067	0.275	-0.010	-0.065	0.045	0.932	0.887	-0.014	-0.073	0.045	0.651	0.816
PC(36:4) [+OH]	-0.033	-0.102	0.037	0.360	0.635	0.021	-0.041	0.083	0.512	0.705	-0.002	-0.050	0.045	0.926	0.968	-0.102	-0.166	-0.037	0.002	0.041
SIP(d16:1)	0.031	-0.037	0.099	0.369	0.641	0.079	0.019	0.139	0.010	0.100	-0.012	-0.057	0.032	0.591	0.811	-0.004	-0.066	0.058	0.906	0.948
PC(15-MHDA_18:2)	0.035	-0.042	0.112	0.372	0.641	0.056	-0.012	0.125	0.108	0.331	0.020	-0.032	0.072	0.459	0.730	-0.045	-0.116	0.026	0.215	0.422
PE(18:0_20:3) (b)	-0.036	-0.114	0.042	0.365	0.641	0.006	-0.063	0.076	0.857	0.940	-0.045	-0.097	0.008	0.095	0.346	-0.062	-0.155	-0.009	0.027	0.153
PE(18:1_22:6) (b)	-0.036	-0.114	0.043	0.369	0.641	0.020	-0.048	0.088	0.570	0.754	-0.025	-0.081	0.031	0.384	0.678	-0.062	-0.131	0.008	0.082	0.269
PEP(20:0/22:6)	-0.034	-0.107	0.040	0.370	0.641	-0.130	-0.195	-0.064	0.000	0.016	0.057	0.009	0.105	0.021	0.158	0.021	-0.046	0.088	0.534	0.729
LPEP(18:1)	0.030	-0.036	0.096	0.370	0.641	0.049	-0.010	0.107	0.104	0.327	0.028	-0.023	0.078	0.281	0.601	-0.028	-0.089	0.033	0.368	0.597
AC(20:3)-OH	0.030	-0.036	0.097	0.367	0.641	0.046	-0.012	0.105	0.122	0.351	-0.006	-0.050	0.039	0.803	0.918	-0.023	-0.085	0.038	0.454	0.668
DG(16:0_20:4)	-0.041	-0.132	0.050	0.372	0.641	-0.088	-0.089	0.073	0.845	0.937	-0.001	-0.063	0.060	0.962	0.983	-0.075	-0.160	0.010	0.088	0.269
TG(56:7) [NL:22:5]	-0.034	-0.107	0.040	0.371	0.641	0.011	-0.056	0.079	0.742	0.871	-0.024	-0.076	0.028	0.364	0.671	-0.055	-0.125	0.015	0.122	0.322
PC(18:0_22:4)	-0.034	-0.110	0.041	0.373	0.642	0.090	0.023	0.137	0.008	0.096	-0.036	-0.089	0.016	0.177	0.476	-0.071	-0.142	0.000	0.050	0.204
Sph(d18:1)	0.029	-0.035	0.092	0.379	0.645	0.021	-0.036	0.079	0.466	0.642	-0.005	-0.047	0.038	0.835	0.956	-0.014	-0.073	0.045	0.651	0.816
SM(44:3)	0.038	-0.047	0.123	0.380	0.651	0.005	-0.069	0.079	0.890	0.954	-0.012	-0.067	0.042	0.659	0.849	-0.031	-0.109	0.047	0.440	0.657
TG(56:6) [NL:22:5]	-0.033	-0.106	0.041	0.381	0.652	0.004	-0.062	0.070	0.904	0.960	-0.012	-0.063	0.038	0.635	0.843	-0.022	-0.091	0.048	0.543	0.733
PS(36:1)	0.028	-0.035	0.092	0.383	0.654	0.034	-0.023	0.091	0.240	0.482	-0.004	-0.046	0.038	0.842	0.932	0.019	-0.039	0.078	0.516	0.717
Cer(d18:2/16:0)	0.035	-0.045	0.115	0.389	0.658	0.038	-0.033	0.109	0.298	0.529	-0.026	-0.081	0.029	0.350	0.660	-0.050	-0.124	0.024	0.184	0.389
PC(18:0/18:1)	0.035	-0.044	0.114	0.388	0.658	0.062	-0.009	0.132	0.085	0.302	-0.005	-0.062	0.053	0.866	0.946	-0.078	-0.152	-0.004	0.039	0.183
CE(16:2)	0.043	-0.054	0.140	0.387	0.658	0.090	0.008	0.172	0.031	0.188	-0.051	-0.113	0.011	0.105	0.368	-0.053	-0.136	0.031	0.214	0.422
SM(d18:1/20:0) & SM(d16:1/22:0)	-0.038	-0.125	0.049	0.391	0.660	0.044	-0.033	0.120	0.261	0.493	0.058	-0.001	0.117	0.053	0.259	0.036	-0.046	0.119	0.384	0.611
PC(18:0/22:6)	-0.032	-0.105	0.041	0.392	0.660	-0.034	-0.099	0.031	0.308	0.541	0.032	-0.019	0.083	0.223	0.534	-0.055	-0.122	0.012	0.108	0.298
CE(22:1)	0.034	-0.044	0.113	0.392	0.660	-0.024	-0.092	0.044	0.488	0.682	0.001	-0.049	0.052	0.954	0.980	-0.074	-0.146	-0.002	0.045	0.194
TG(48:1) [NL:16:1]	-0.033	-0.111	0.044	0.394	0.660	0.040	-0.030	0.111	0.260	0.493	-0.042	-0.095	0.012	0.128	0.407	-0.054	-0.128	0.020	0.152	0.358
TG(54:4) [NL:17:1]	-0.030	-0.098	0.038	0.394	0.660	-0.029	-0.089	0.032	0.352	0.576	0.106	-0.058	0.154	0.000	0.001	0.012	-0.051	0.075	0.716	0.845
PE(16:0_18:1)	-0.034	-0.105	0.113	0.397	0.662	0.071	-0.032	0.140	0.043	0.217	-0.008	-0.064	0.047	0.746	0.902	-0.057	-0.130	0.015	0.123	0.322
PEP(18:1/20:3) (a)	-0.030	-0.101	0.040	0.397	0.662	0.005	-0.057	0.067	0.867	0.943	0.087	-0.040	0.135	0.000	0.008	0.044	-0.021	0.108	0.181	0.386
FA(18:1)	-0.029	-0.096	0.038	0.398	0.662	-0.040	-0.100	0.020	0.189	0.426	0.007	-0.038	0.051	0.772	0.902	-0.055	-0.117	0.007	0.084	0.270
PEP(18:1/20:3) (b)	-0.029	-0.098	0.039	0.401	0.665	0.025	-0.036	0.086	0.414	0.617	0.049	-0.001	0.098	0.055	0.264	-0.028	-0.091	0.035	0.387	0.611
TG(48:2) [NL:1																				

FA(20:4)	0.020	-0.046	0.086	0.547	0.774	0.027	-0.032	0.085	0.374	0.584	-0.024	-0.069	0.021	0.288	0.606	-0.054	-0.114	0.007	0.081	0.268
Ubiquinone	-0.020	-0.087	0.046	0.548	0.774	0.021	-0.038	0.080	0.490	0.684	-0.005	-0.051	0.041	0.845	0.934	-0.002	-0.063	0.060	0.960	0.977
SM(d16:1/24:1)	0.024	-0.056	0.104	0.551	0.775	-0.014	-0.085	0.056	0.688	0.836	0.014	-0.039	0.067	0.603	0.815	-0.077	-0.151	-0.004	0.030	0.183
HexCer(d18:1/18:0)	0.020	-0.046	0.087	0.554	0.775	0.033	-0.028	0.093	0.289	0.525	-0.036	-0.082	0.009	0.121	0.331	-0.037	-0.099	0.026	0.252	0.461
PA(36:2)	0.022	-0.049	0.099	0.551	0.775	0.001	-0.061	0.063	0.974	0.982	0.027	-0.018	0.073	0.244	0.560	0.045	-0.020	0.109	0.173	0.378
PC(15:0_16:0)	0.024	-0.056	0.105	0.554	0.775	0.055	-0.018	0.127	0.139	0.372	-0.060	-0.115	0.005	0.033	0.209	-0.097	-0.172	-0.023	0.011	0.089
PC(40:8)	0.026	-0.061	0.114	0.555	0.775	0.014	-0.060	0.088	0.707	0.851	0.036	-0.022	0.094	0.225	0.534	-0.054	-0.132	0.023	0.167	0.372
TG(50:2) [NL:18:1]	-0.020	-0.085	0.046	0.553	0.775	-0.039	-0.097	0.019	0.191	0.428	0.030	-0.014	0.074	0.185	0.483	-0.041	-0.101	0.020	0.188	0.394
Cer(d17:1/16:0)	0.020	-0.048	0.089	0.563	0.784	0.035	-0.026	0.096	0.257	0.492	0.027	-0.018	0.073	0.236	0.549	0.007	-0.056	0.070	0.829	0.909
Cer(d18:1/18:0)	-0.021	-0.092	0.050	0.563	0.784	0.021	-0.043	0.085	0.529	0.719	-0.036	-0.084	0.012	0.147	0.429	-0.076	-0.142	-0.010	0.024	0.144
PA(36:4)	0.020	-0.049	0.090	0.567	0.785	-0.050	-0.110	0.010	0.105	0.328	0.030	-0.015	0.074	0.192	0.494	0.064	0.002	0.127	0.044	0.194
PC(15:0_22:6)	-0.021	-0.095	0.052	0.565	0.785	-0.073	-0.138	-0.008	0.208	0.182	0.038	-0.011	0.087	0.129	0.407	-0.003	-0.070	0.065	0.940	0.969
FA(18:0)	0.019	-0.046	0.084	0.567	0.785	-0.023	-0.081	0.035	0.441	0.641	-0.002	-0.045	0.041	0.927	0.968	-0.051	-0.111	0.008	0.091	0.278
Cer(d19:1/23:0)	0.020	-0.049	0.088	0.575	0.788	0.038	-0.022	0.099	0.217	0.457	0.010	-0.035	0.056	0.651	0.848	-0.037	-0.099	0.026	0.252	0.461
PC(32:1)	0.023	-0.058	0.105	0.574	0.788	0.097	0.025	0.169	0.008	0.096	-0.084	-0.139	-0.029	0.003	0.045	-0.117	-0.193	-0.042	0.002	0.041
PC(15-MHDA_18:1)	0.021	-0.051	0.092	0.575	0.788	0.039	-0.025	0.103	0.229	0.475	-0.011	-0.060	0.038	0.658	0.849	-0.064	-0.130	-0.002	0.059	0.227
PCP(20:0/18:2)	0.027	-0.066	0.119	0.572	0.788	0.005	-0.074	0.084	0.905	0.960	0.051	-0.005	0.112	0.344	0.546	0.000	-0.083	0.092	0.765	0.977
PC(15:0_20:3)	0.022	-0.054	0.098	0.575	0.788	0.074	0.006	0.142	0.038	0.194	0.018	-0.035	0.070	0.511	0.765	-0.006	-0.076	0.065	0.878	0.934
TG(48:3) [NL:18:3]	0.025	-0.062	0.112	0.575	0.788	0.064	-0.016	0.144	0.117	0.344	-0.039	-0.099	0.021	0.205	0.510	-0.061	-0.145	0.022	0.151	0.358
Cer(d18:1/14:0)	0.020	-0.052	0.092	0.585	0.789	0.041	-0.023	0.106	0.206	0.450	-0.011	-0.059	0.037	0.665	0.854	-0.045	-0.111	0.021	0.185	0.390
Cer(d18:1/24:0)	0.023	-0.059	0.105	0.580	0.789	0.009	-0.063	0.081	0.807	0.914	0.031	-0.025	0.086	0.277	0.596	-0.009	-0.083	0.066	0.822	0.909
PC(32:2)	0.022	-0.055	0.099	0.584	0.789	0.070	0.001	0.139	0.046	0.225	-0.009	-0.062	0.043	0.725	0.887	-0.036	-0.108	0.036	0.325	0.551
PE(16:0_20:3)	0.022	-0.056	0.100	0.581	0.789	0.084	0.014	0.154	0.019	0.141	-0.048	-0.104	0.008	0.095	0.346	-0.046	-0.118	0.027	0.219	0.426
PI(15-MHDA_20:4) & PI(17:0_20:4)	0.021	-0.054	0.097	0.578	0.789	0.095	0.028	0.162	0.006	0.077	-0.008	-0.060	0.043	0.746	0.894	-0.065	-0.136	0.005	0.069	0.249
dxcA	0.018	-0.047	0.083	0.581	0.789	0.061	0.004	0.119	0.037	0.198	-0.021	-0.064	0.022	0.339	0.648	-0.051	-0.110	0.009	0.097	0.281
DG(16:1_18:1)	0.031	-0.079	0.140	0.582	0.789	0.062	-0.032	0.155	0.197	0.435	-0.088	-0.162	-0.015	0.018	0.148	-0.164	-0.260	-0.067	0.001	0.028
DG(18:1_20:3)	-0.023	-0.106	0.060	0.585	0.789	0.016	-0.058	0.089	0.677	0.830	0.018	-0.038	0.074	0.538	0.779	-0.059	-0.136	0.018	0.135	0.335
CE(22:6) [+OH]	0.019	-0.050	0.088	0.582	0.789	-0.080	-0.141	-0.019	0.010	0.100	-0.002	-0.051	0.047	0.936	0.972	-0.067	-0.130	-0.005	0.036	0.177
FA(18:2)	-0.018	-0.085	0.048	0.588	0.791	-0.037	-0.074	0.043	0.581	0.725	-0.001	-0.045	0.043	0.962	0.985	-0.045	-0.106	0.017	0.156	0.359
methyI-CE(18:1)	-0.020	-0.094	0.053	0.592	0.793	-0.030	-0.097	0.036	0.370	0.583	0.063	-0.014	0.112	0.012	0.114	0.044	-0.024	0.112	0.208	0.415
TG(54:3) [NL:18:2]	0.021	-0.055	0.096	0.591	0.793	0.041	-0.029	0.112	0.248	0.492	-0.013	-0.049	0.043	0.653	0.848	-0.016	-0.090	0.058	0.674	0.824
PCP(18:0/18:2)	0.023	-0.062	0.109	0.593	0.793	0.029	-0.044	0.103	0.432	0.633	0.036	-0.021	0.093	0.218	0.530	-0.028	-0.105	0.049	0.473	0.686
SM(38:3) (a)	0.019	-0.052	0.091	0.595	0.795	0.058	-0.006	0.123	0.074	0.286	-0.023	-0.072	0.025	0.345	0.653	-0.075	-0.142	-0.009	0.027	0.152
PE(20:0_20:4)	0.020	-0.054	0.094	0.597	0.796	0.020	-0.046	0.087	0.553	0.742	-0.021	-0.070	0.029	0.414	0.705	-0.029	-0.040	0.098	0.415	0.640
PE(16:0_18:3) (a)	0.021	-0.057	0.098	0.599	0.797	0.060	-0.010	0.130	0.091	0.310	-0.041	-0.094	0.013	0.135	0.417	-0.062	-0.134	0.011	0.095	0.278
HexCer(d18:2/18:0)	0.018	-0.051	0.088	0.605	0.803	0.010	-0.053	0.072	0.765	0.885	-0.020	-0.066	0.027	0.402	0.691	-0.047	-0.112	0.017	0.149	0.357
TG(51:2) [NL:15:0]	0.021	-0.059	0.101	0.605	0.803	0.037	-0.037	0.111	0.330	0.564	-0.016	-0.073	0.042	0.596	0.811	-0.025	-0.102	0.052	0.529	0.727
SM(37:1)	-0.019	-0.092	0.054	0.609	0.804	0.037	-0.027	0.102	0.258	0.493	0.033	-0.015	0.082	0.179	0.479	-0.021	-0.047	0.089	0.539	0.729
Cer(d18:2/18:0)	-0.019	-0.093	0.055	0.608	0.804	0.006	-0.060	0.071	0.867	0.943	-0.017	-0.067	0.032	0.492	0.747	-0.018	-0.086	0.051	0.613	0.796
CE(14:0)	0.018	-0.051	0.087	0.611	0.805	0.028	-0.033	0.090	0.370	0.583	-0.029	-0.075	0.016	0.209	0.517	-0.034	-0.097	0.030	0.299	0.519
PC(36:0)	-0.017	-0.081	0.048	0.614	0.806	0.018	-0.039	0.075	0.537	0.729	-0.010	-0.052	0.033	0.655	0.848	-0.011	-0.071	0.048	0.705	0.940
PC(16:0_22:6)	-0.019	-0.093	0.055	0.617	0.809	-0.084	-0.149	-0.020	0.011	0.106	0.040	-0.100	0.089	0.116	0.388	-0.007	-0.075	0.061	0.837	0.912
LFPE-16:0	0.017	-0.049	0.082	0.619	0.809	-0.017	-0.075	0.041	0.574	0.757	0.030	-0.104	0.074	0.177	0.476	0.025	-0.035	0.085	0.419	0.640
DG(16:0_16:1)	-0.026	-0.127	0.076	0.619	0.809	0.070	-0.018	0.158	0.120	0.346	-0.078	-0.147	-0.009	0.026	0.181	-0.144	-0.236	-0.051	0.002	0.041
TG(48:2) [NL:16:1]	0.021	-0.063	0.106	0.617	0.809	0.092	0.016	0.168	0.018	0.140	-0.074	-0.133	-0.015	0.014	0.125	-0.114	-0.194	-0.035	0.005	0.061
PCP(17:0/20:4) (b)	-0.018	-0.088	0.053	0.621	0.809	0.015	-0.047	0.077	0.631	0.790	0.053	0.006	0.099	0.027	0.185	-0.027	-0.091	0.037	0.408	0.632
PE(18:1_18:1)	-0.018	-0.089	0.053	0.621	0.809	-0.014	-0.079	0.051	0.681	0.831	0.049	0.001	0.097	0.047	0.243	-0.046	-0.222	0.113	0.184	0.389
Cer(d16:1/18:0)	-0.018	-0.092	0.055	0.623	0.810	0.024	-0.040	0.089	0.460	0.659	-0.003	-0.051	0.046	0.918	0.964	-0.011	-0.079	0.056	0.740	0.863
SM(d18:2/17:0)	-0.021	-0.105	0.063	0.624	0.810	0.043	-0.030	0.116	0.251	0.492	0.029	-0.028	0.086	0.320	0.635	-0.069	-0.145	0.008	0.077	0.264
PC(20:0_20:4)	0.018	-0.055	0.091	0.626	0.811	0.044	-0.021	0.109	0.186	0.426	0.007	-0.042	0.055	0.789	0.912	-0.011	-0.079	0.058	0.762	0.874
PE(18:0/18:3)	-0.017	-0.088	0.053	0.628	0.812	0.018	-0.044	0.081	0.563	0.746	0.039	-0.008	0.086	0.102	0.364	-0.024	-0.040	0.089	0.465	0.678
AC(22:5)	0.016	-0.050	0.083	0.630	0.813	-0.005	-0.064	0.055	0.878	0.947	0.005	-0.039	0.049	0.812	0.925	0.009	-0.052	0.070	0.771	0.875
PCP(20:0/20:4)	-0.017	-0.087	0.053	0.634	0.814	-0.031	-0.093	0.031	0.332	0.546	0.019	-0.027	0.065	0.427	0.717	-0.048	-0.112	0.016	0.143	0.349
AC(18:0)	0.017	-0.052	0.085	0.634	0.814	0.034	-0.028	0.096	0.285	0.520	-0.032	-0.080	0.015	0.183	0.482	-0.098	-0.162	-0.033	0.003	0.049
TG(52:2) [NL:16:0]	-0.019	-0.099	0.040	0.633	0.814	0.051	-0.024	0.126	0.184	0.425	0.010	-0.051	0.071	0.757	0.899	-0.048	-0.128	0.031	0.234	0.444
SM(d18:0/16:0)	-0.019	-0.097	0.059	0.636	0.816	-0.048	-0.118	0.022	0.181	0.425	0.086	0.033	0.139	0.001	0.027	0.074	0.002	0.147	0.405	0.194
SM(d18:2/14:0)	0.024	-0.076	0.124	0.644	0.824	0.														

PA(40:6)	0.007	-0.060	0.074	0.841	0.947	0.023	-0.035	0.081	0.434	0.633	-0.009	-0.052	0.034	0.669	0.855	-0.004	-0.064	0.057	0.908	0.948
PC(18:0/22:5)	-0.009	-0.093	0.075	0.837	0.947	0.013	-0.060	0.086	0.727	0.864	0.017	-0.038	0.073	0.544	0.779	-0.046	-0.121	0.028	0.225	0.435
AC(24:1)	0.007	-0.060	0.074	0.840	0.947	-0.015	-0.076	0.046	0.622	0.783	0.011	-0.037	0.058	0.666	0.854	-0.060	-0.124	0.003	0.062	0.234
CE(20:4)	0.011	-0.096	0.118	0.839	0.947	0.077	-0.018	0.172	0.110	0.333	-0.014	-0.084	0.055	0.683	0.864	-0.115	-0.212	-0.018	0.020	0.128
Gx9(d18:1/20:0)	0.006	-0.059	0.071	0.845	0.947	0.025	-0.034	0.084	0.411	0.617	-0.003	-0.052	0.046	0.903	0.961	-0.051	-0.112	0.010	0.101	0.284
PC(35:0) (a)	0.007	-0.067	0.081	0.847	0.947	0.051	-0.015	0.117	0.128	0.358	-0.020	-0.070	0.031	0.443	0.722	-0.059	-0.128	0.009	0.089	0.275
SM(d19:1/24:1)	0.007	-0.060	0.073	0.848	0.947	-0.006	-0.065	0.054	0.851	0.928	0.042	-0.002	0.085	0.062	0.283	-0.023	-0.084	0.039	0.473	0.686
PC(44:12)	-0.007	-0.076	0.063	0.849	0.947	-0.068	-0.131	-0.006	0.032	0.188	0.031	-0.016	0.077	0.193	0.495	-0.029	-0.093	0.035	0.377	0.604
PI(16:0_20:3) (b)	0.008	-0.071	0.086	0.848	0.947	0.081	0.012	0.151	0.022	0.152	-0.041	-0.095	0.013	0.133	0.413	-0.100	-0.153	-0.007	0.031	0.162
TG(51:2) [NL:17:1]	0.009	-0.078	0.095	0.845	0.947	0.082	0.014	0.160	0.040	0.210	-0.025	-0.086	0.036	0.421	0.709	-0.086	-0.189	-0.024	0.012	0.090
PC(33:1)	0.008	-0.073	0.089	0.852	0.949	0.070	-0.002	0.142	0.058	0.254	-0.032	-0.088	0.023	0.257	0.574	-0.075	-0.150	0.001	0.052	0.207
PC(18:0_18:2)	0.008	-0.073	0.089	0.851	0.949	0.035	-0.039	0.109	0.350	0.576	0.015	-0.043	0.073	0.622	0.826	0.013	-0.064	0.089	0.741	0.863
Cer(d16:1/16:0)	-0.007	-0.078	0.064	0.854	0.949	0.017	-0.046	0.080	0.602	0.778	-0.034	-0.080	0.013	0.155	0.446	-0.036	-0.101	0.029	0.274	0.483
Cer(d19:1/18:0)	0.006	-0.060	0.072	0.856	0.949	0.029	-0.029	0.088	0.324	0.557	-0.008	-0.051	0.036	0.734	0.887	-0.065	-0.125	-0.004	0.036	0.180
PEIP-18:1/22:5) (a)	-0.007	-0.079	0.066	0.857	0.950	0.038	-0.025	0.102	0.238	0.481	-0.037	-0.014	0.088	0.155	0.446	0.010	-0.056	0.076	0.767	0.874
PEO-18:1/18:2)	-0.006	-0.077	0.065	0.868	0.959	-0.010	-0.073	0.053	0.759	0.885	0.065	0.018	0.112	0.007	0.081	0.047	-0.018	0.112	0.156	0.359
PEIP-18:1/18:2) (a)	0.006	-0.066	0.078	0.868	0.959	0.004	-0.059	0.057	0.905	0.960	0.073	0.026	0.121	0.003	0.044	0.078	0.012	0.143	0.020	0.128
TG(50:2) [NL:16:1]	0.007	-0.071	0.084	0.870	0.960	0.066	-0.006	0.137	0.072	0.282	-0.056	-0.111	0.000	0.048	0.245	-0.077	-0.152	-0.002	0.044	0.194
PC(36:6) (a)	0.006	-0.071	0.083	0.876	0.961	0.007	-0.062	0.075	0.849	0.928	-0.031	-0.082	0.020	0.227	0.537	-0.040	-0.111	0.031	0.267	0.475
PC(14:0_20:4)	0.007	-0.076	0.089	0.877	0.961	0.064	-0.009	0.136	0.085	0.302	-0.039	-0.094	0.016	0.163	0.454	-0.100	-0.176	-0.024	0.010	0.089
PEIP-18:1/18:2) (b)	-0.005	-0.073	0.062	0.876	0.961	0.064	0.004	0.125	0.036	0.197	0.019	-0.033	0.070	0.479	0.737	-0.043	-0.106	0.019	0.174	0.379
LP(18:2) [sn2]	0.005	-0.062	0.072	0.875	0.961	0.064	0.005	0.124	0.033	0.190	-0.015	-0.060	0.030	0.524	0.773	-0.023	-0.085	0.039	0.462	0.676
TG(56:7) [NL:20:4]	-0.005	-0.071	0.061	0.877	0.961	0.043	-0.015	0.102	0.146	0.381	0.029	-0.018	0.075	0.224	0.534	-0.034	-0.095	0.028	0.287	0.504
OG(18:2_20:4)	0.006	-0.076	0.089	0.879	0.961	0.013	-0.060	0.085	0.736	0.868	0.001	-0.055	0.056	0.982	0.992	-0.072	-0.148	0.004	0.063	0.238
PC(38:4) (b)	-0.006	-0.086	0.074	0.881	0.961	0.014	0.055	0.193	0.000	0.021	-0.036	-0.094	0.023	0.233	0.546	-0.068	-0.141	0.005	0.067	0.248
TG(50:2) [NL:18:2]	-0.005	-0.072	0.062	0.881	0.961	-0.021	-0.082	0.040	0.493	0.686	0.063	0.017	0.110	0.007	0.083	0.010	-0.053	0.073	0.756	0.874
TG(50:3) [NL:18:3]	0.006	-0.075	0.087	0.884	0.961	0.046	-0.030	0.122	0.238	0.481	-0.015	-0.073	0.043	0.620	0.825	-0.039	-0.120	0.041	0.342	0.569
Cer(m18:1/24:1)	-0.005	-0.085	0.074	0.893	0.965	-0.040	-0.110	0.030	0.262	0.493	-0.019	-0.071	0.033	0.471	0.737	-0.064	-0.137	0.008	0.081	0.268
SM(d18:2/16:0)	-0.007	-0.110	0.096	0.892	0.965	0.024	-0.066	0.114	0.602	0.778	0.004	-0.065	0.073	0.909	0.962	-0.083	-0.177	0.011	0.085	0.270
PC(16:0_20:3) (a)	0.006	-0.082	0.094	0.895	0.965	0.105	0.030	0.179	0.006	0.080	0.003	-0.062	0.068	0.917	0.964	-0.041	-0.120	0.038	0.313	0.528
PC(38:7) (c)	0.006	-0.075	0.086	0.890	0.965	-0.008	-0.075	0.060	0.822	0.922	-0.007	-0.064	0.051	0.815	0.925	-0.099	-0.169	-0.029	0.006	0.065
PCIP-17:0/20:4) (a)	0.005	-0.065	0.075	0.891	0.965	0.044	-0.018	0.106	0.163	0.398	0.035	-0.012	0.082	0.141	0.424	-0.048	-0.112	0.017	0.146	0.353
TG(54:4) [NL:18:2]	0.004	-0.062	0.071	0.895	0.965	-0.016	-0.076	0.044	0.605	0.778	0.077	0.029	0.124	0.001	0.027	0.028	-0.034	0.090	0.373	0.603
TG(48:2) [NL:14:1]	0.006	-0.078	0.089	0.891	0.965	0.069	-0.007	0.146	0.074	0.286	-0.054	-0.113	0.005	0.072	0.302	-0.089	-0.168	-0.009	0.029	0.154
PC(34:5)	-0.005	-0.079	0.069	0.897	0.965	-0.024	-0.090	0.042	0.475	0.669	-0.023	-0.072	0.026	0.360	0.668	-0.022	-0.090	0.047	0.537	0.729
PS(36:2)	-0.004	-0.068	0.060	0.901	0.968	0.073	0.017	0.130	0.011	0.106	-0.042	-0.088	0.003	0.068	0.294	-0.026	-0.086	0.033	0.382	0.610
PC(18:0/20:4)	0.004	-0.065	0.074	0.904	0.970	0.084	0.022	0.147	0.008	0.095	0.003	-0.045	0.052	0.889	0.955	-0.092	-0.157	-0.027	0.006	0.065
AC(14:0)	-0.004	-0.069	0.061	0.910	0.975	0.049	-0.009	0.107	0.097	0.312	-0.039	-0.082	0.004	0.076	0.313	-0.088	-0.148	-0.028	0.004	0.056
PC(16:0_20:3) (b)	-0.004	-0.082	0.073	0.911	0.975	0.087	0.018	0.156	0.014	0.116	-0.053	-0.108	0.002	0.058	0.270	-0.065	-0.138	0.008	0.080	0.268
LPC(20:5) [sn1]	0.004	-0.066	0.074	0.919	0.976	-0.030	-0.093	0.033	0.347	0.575	-0.013	-0.059	0.034	0.591	0.811	0.003	-0.061	0.068	0.921	0.958
PEIP-16:0/18:3)	-0.004	-0.074	0.067	0.914	0.976	-0.009	-0.070	0.053	0.786	0.902	0.063	0.017	0.109	0.007	0.082	0.038	-0.026	0.102	0.248	0.459
CE(15:0)	0.004	-0.070	0.078	0.917	0.976	0.026	-0.041	0.092	0.454	0.654	0.001	-0.049	0.050	0.976	0.990	-0.029	-0.041	0.098	0.419	0.640
AC(18:1)	0.004	-0.061	0.068	0.915	0.976	0.028	-0.030	0.087	0.340	0.572	-0.028	-0.074	0.019	0.240	0.553	-0.048	-0.143	-0.021	0.008	0.082
CE(18:2) [+OH]	0.004	-0.073	0.081	0.919	0.976	0.002	-0.065	0.069	0.946	0.977	0.047	-0.004	0.098	0.071	0.302	-0.004	-0.074	0.065	0.902	0.948
PC(18:1_22:6) (b)	0.003	-0.064	0.071	0.921	0.977	0.042	-0.017	0.101	0.162	0.398	-0.020	-0.075	0.034	0.462	0.730	-0.073	-0.134	-0.012	0.019	0.125
HexCer(d18:1/20:0)	-0.004	-0.079	0.072	0.926	0.977	0.031	-0.037	0.099	0.370	0.583	-0.016	-0.068	0.036	0.540	0.779	-0.094	-0.124	0.016	0.129	0.331
PC(16:0/20:4)	-0.004	-0.077	0.072	0.923	0.977	0.033	-0.034	0.099	0.330	0.566	0.038	-0.013	0.090	0.144	0.427	-0.054	-0.162	-0.025	0.008	0.078
AC(17:0) (a)	-0.003	-0.068	0.062	0.926	0.977	0.048	-0.010	0.106	0.107	0.331	-0.025	-0.068	0.018	0.256	0.573	-0.083	-0.143	-0.023	0.007	0.073
TG(52:2) [NL:18:2]	-0.004	-0.086	0.079	0.926	0.977	0.023	-0.054	0.099	0.562	0.746	-0.042	-0.101	0.018	0.168	0.458	-0.064	-0.145	0.017	0.124	0.323
PI(15-MHDA_18:2) & PI(17:0_18:2)	0.003	-0.073	0.080	0.930	0.979	0.081	0.013	0.150	0.019	0.143	-0.015	-0.067	0.036	0.552	0.783	-0.074	-0.145	-0.003	0.040	0.185
SM(d16:1/19:0)	-0.003	-0.073	0.068	0.940	0.979	0.027	-0.036	0.090	0.403	0.610	0.025	-0.023	0.073	0.308	0.623	-0.056	-0.122	0.010	0.094	0.278
SM(d18:1/16:0)	-0.004	-0.098	0.091	0.940	0.981	0.004	-0.077	0.085	0.921	0.964	0.028	-0.040	0.097	0.421	0.709	-0.117	-0.203	-0.031	0.008	0.079
PC(18:2_20:5)	0.003	-0.073	0.078	0.943	0.981	-0.032	-0.100	0.036	0.352	0.576	0.015	-0.035	0.065	0.553	0.783	0.015	-0.055	0.085	0.672	0.824
PCIP-15:0/20:4) (b)	-0.003	-0.070	0.064	0.935	0.981	0.009	-0.050	0.067	0.774	0.894	0.063	0.020	0.107	0.004	0.057	0.039	-0.022	0.100	0.215	0.422
PC(39:5) (a)	-0.003	-0.074	0.068	0.938	0.981	-0.062	-0.125	0.002	0.056	0.254	-0.018	-0.065	0.030	0.461	0.730	-0.021	-0.045	0.086	0.539	0.729
PE(15-MHDA_22:6)	0.003	-0.073	0.079	0.940	0.981	-0.055	-0.123	0.014	0.116	0.344	0.004	-0.047	0.054	0.885	0.954	-0.011				

Supplementary Table 3. Associations of lipid classes with baseline A/T/N biomarkers

Lipid classes	A: Amyloid PET (AV45) uptake					T: CSF pTau					N1: Hippocampal volume					N2: FDG uptake				
	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)
LPC(O)	0.121	0.053	0.189	0.001	0.024	0.056	-0.006	0.118	0.076	0.414	-0.033	-0.085	0.019	0.211	0.649	-0.111	-0.175	-0.047	0.001	0.011
LPC	0.119	0.047	0.192	0.001	0.030	0.064	-0.001	0.128	0.054	0.414	-0.012	-0.064	0.039	0.638	0.889	-0.055	-0.122	0.012	0.110	0.224
LPC(P)	0.096	0.027	0.165	0.006	0.047	0.049	-0.012	0.111	0.115	0.414	-0.009	-0.061	0.043	0.734	0.916	-0.080	-0.144	-0.017	0.013	0.071
LPE	0.104	0.030	0.178	0.006	0.047	0.060	-0.006	0.127	0.074	0.414	-0.044	-0.095	0.006	0.086	0.360	-0.070	-0.139	0.000	0.048	0.137
Hex2Cer	0.115	0.035	0.194	0.005	0.047	0.062	-0.009	0.132	0.085	0.414	-0.030	-0.009	0.022	0.254	0.649	-0.055	-0.129	0.019	0.146	0.269
DE	-0.127	-0.213	-0.041	0.004	0.047	-0.077	-0.153	-0.002	0.045	0.414	0.029	-0.026	0.084	0.299	0.687	0.055	-0.023	0.133	0.170	0.300
PE(O)	-0.095	-0.169	-0.022	0.011	0.073	-0.051	-0.117	0.014	0.126	0.414	0.064	0.014	0.113	0.012	0.094	0.014	-0.054	0.082	0.689	0.754
HexCer	0.089	0.015	0.163	0.018	0.106	0.024	-0.041	0.090	0.465	0.684	-0.016	-0.065	0.033	0.515	0.845	-0.018	-0.086	0.051	0.609	0.700
GM1	0.079	0.007	0.150	0.030	0.148	0.003	-0.059	0.065	0.921	0.935	-0.056	-0.103	-0.009	0.020	0.135	-0.085	-0.151	-0.020	0.011	0.071
PE(P)	-0.082	-0.158	-0.007	0.032	0.148	-0.031	-0.096	0.035	0.361	0.594	0.091	0.040	0.142	0.001	0.008	0.022	-0.046	0.090	0.528	0.639
deDE	0.077	0.002	0.152	0.045	0.174	0.070	0.004	0.136	0.038	0.414	-0.149	-0.197	-0.102	0.000	0.000	-0.140	-0.208	-0.073	0.000	0.002
dhCer	-0.081	-0.160	-0.002	0.045	0.174	-0.038	-0.108	0.031	0.279	0.584	0.034	-0.018	0.086	0.199	0.649	0.007	-0.065	0.080	0.848	0.907
OxSpecies	0.064	-0.008	0.135	0.082	0.500	-0.010	-0.074	0.053	0.752	0.805	0.009	-0.040	0.058	0.725	0.916	-0.052	-0.117	0.013	0.117	0.224
GM3	0.058	-0.026	0.143	0.174	0.500	0.043	-0.032	0.117	0.262	0.574	-0.029	-0.091	0.033	0.355	0.743	-0.136	-0.213	-0.058	0.001	0.011
dimethyl-CE	-0.052	-0.126	0.022	0.167	0.500	-0.055	-0.122	0.011	0.105	0.414	0.082	0.032	0.131	0.001	0.014	0.083	0.015	0.151	0.017	0.078
TG(O) [NL]	-0.051	-0.123	0.020	0.157	0.500	-0.050	-0.114	0.014	0.125	0.414	0.119	0.070	0.169	0.000	0.000	0.017	-0.050	0.083	0.626	0.703
S1P	0.044	-0.022	0.110	0.194	0.525	0.071	0.012	0.130	0.018	0.414	-0.016	-0.062	0.030	0.497	0.845	-0.022	-0.083	0.040	0.490	0.633
methyl-DE	-0.045	-0.121	0.031	0.244	0.565	-0.019	-0.088	0.050	0.591	0.718	0.074	0.023	0.124	0.004	0.039	0.097	0.027	0.168	0.007	0.071
SHexCer	0.050	-0.034	0.134	0.246	0.565	-0.023	-0.097	0.051	0.543	0.718	0.003	-0.051	0.058	0.904	0.970	-0.069	-0.145	0.008	0.079	0.191
LPI	-0.042	-0.111	0.028	0.240	0.565	0.038	-0.023	0.098	0.224	0.531	0.004	-0.044	0.051	0.878	0.970	-0.030	-0.094	0.034	0.350	0.520
DG	-0.066	-0.193	0.061	0.309	0.592	-0.051	-0.158	0.055	0.343	0.585	-0.031	-0.114	0.052	0.465	0.822	-0.125	-0.235	-0.015	0.026	0.085
AC-OH	-0.035	-0.100	0.031	0.298	0.592	0.008	-0.050	0.067	0.781	0.817	-0.012	-0.056	0.032	0.590	0.876	-0.070	-0.130	-0.009	0.024	0.085
Cer(d)	0.042	-0.036	0.120	0.292	0.592	0.047	-0.023	0.117	0.184	0.498	-0.013	-0.066	0.040	0.638	0.889	-0.060	-0.132	0.013	0.105	0.224
SM	-0.052	-0.147	0.044	0.291	0.592	0.024	-0.060	0.107	0.577	0.718	0.073	0.006	0.140	0.032	0.164	-0.037	-0.126	0.052	0.414	0.577
COH	0.042	-0.045	0.129	0.344	0.633	-0.003	-0.077	0.071	0.935	0.935	0.007	-0.054	0.068	0.823	0.970	-0.100	-0.180	-0.020	0.014	0.071
Cer(m)	-0.040	-0.125	0.046	0.361	0.639	-0.026	-0.100	0.048	0.490	0.684	0.003	-0.053	0.059	0.925	0.970	-0.038	-0.115	0.039	0.337	0.517
PC(O)	0.032	-0.053	0.118	0.460	0.707	0.046	-0.028	0.120	0.220	0.531	0.033	-0.027	0.093	0.285	0.687	-0.081	-0.158	-0.004	0.040	0.124
FFA	-0.025	-0.093	0.042	0.461	0.707	-0.013	-0.073	0.048	0.683	0.786	0.000	-0.044	0.045	0.995	0.995	-0.058	-0.120	0.004	0.068	0.173
PIP1	0.027	-0.038	0.092	0.416	0.707	0.050	-0.008	0.108	0.093	0.414	0.012	-0.031	0.056	0.578	0.876	0.003	-0.057	0.063	0.930	0.972
LPE(P)	0.025	-0.042	0.092	0.458	0.707	0.016	-0.043	0.076	0.587	0.718	0.019	-0.028	0.066	0.424	0.780	0.001	-0.061	0.062	0.986	0.986
CE	0.037	-0.072	0.145	0.510	0.711	0.067	-0.026	0.160	0.156	0.447	-0.012	-0.086	0.063	0.757	0.916	-0.123	-0.221	-0.025	0.014	0.071
PC	0.035	-0.067	0.136	0.504	0.711	0.078	-0.009	0.165	0.077	0.414	-0.022	-0.095	0.050	0.547	0.867	-0.108	-0.199	-0.017	0.020	0.085
Sph	0.022	-0.041	0.086	0.494	0.711	-0.023	-0.079	0.034	0.435	0.667	0.007	-0.036	0.050	0.746	0.916	0.020	-0.039	0.079	0.509	0.633
Ubiquinone	-0.020	-0.087	0.046	0.548	0.741	0.021	-0.038	0.080	0.490	0.684	-0.005	-0.051	0.041	0.845	0.970	-0.002	-0.063	0.060	0.960	0.982
PA	0.019	-0.053	0.092	0.602	0.785	-0.010	-0.074	0.053	0.751	0.805	0.024	-0.023	0.070	0.317	0.693	0.057	-0.009	0.123	0.089	0.204
PI	-0.022	-0.107	0.063	0.614	0.785	0.063	-0.013	0.139	0.103	0.414	-0.002	-0.061	0.057	0.952	0.973	-0.064	-0.143	0.015	0.112	0.224
BA	-0.014	-0.078	0.051	0.671	0.835	0.030	-0.028	0.087	0.311	0.585	0.025	-0.018	0.068	0.252	0.649	0.020	-0.039	0.080	0.505	0.633
methyl-CE	-0.012	-0.086	0.061	0.745	0.865	-0.012	-0.078	0.055	0.735	0.805	0.055	0.005	0.104	0.031	0.164	0.034	-0.034	0.103	0.327	0.517
C1P	0.014	-0.072	0.100	0.752	0.865	0.037	-0.039	0.113	0.343	0.585	0.003	-0.059	0.059	0.928	0.970	-0.039	-0.116	0.038	0.324	0.517
PS	0.012	-0.052	0.076	0.721	0.865	0.025	-0.032	0.082	0.391	0.621	-0.009	-0.051	0.033	0.686	0.916	0.017	-0.042	0.076	0.567	0.668
PE	-0.013	-0.102	0.077	0.783	0.878	0.044	-0.038	0.125	0.292	0.584	-0.039	-0.101	0.023	0.219	0.649	-0.053	-0.137	0.030	0.210	0.358
TG [NL]	-0.013	-0.117	0.092	0.810	0.887	0.070	-0.025	0.164	0.148	0.447	-0.053	-0.128	0.022	0.169	0.649	-0.116	-0.216	-0.016	0.024	0.085
Hex3Cer	-0.008	-0.100	0.083	0.861	0.922	0.022	-0.059	0.103	0.593	0.718	-0.026	-0.089	0.037	0.416	0.780	-0.113	-0.195	-0.030	0.008	0.071
AC	0.003	-0.063	0.070	0.924	0.945	0.029	-0.031	0.089	0.340	0.585	-0.019	-0.064	0.025	0.390	0.780	-0.062	-0.124	0.000	0.051	0.137
PG	-0.005	-0.109	0.099	0.922	0.945	-0.057	-0.149	0.036	0.231	0.531	-0.042	-0.111	0.027	0.236	0.649	-0.037	-0.131	0.058	0.447	0.604
PC(P)	0.001	-0.089	0.091	0.981	0.981	0.016	-0.060	0.093	0.673	0.786	0.054	-0.005	0.114	0.074	0.340	-0.037	-0.116	0.042	0.364	0.523

Supplementary Table 4. Lipid species in modules identified with WGCNA

Module	Number of Lipid species	Lipid species
M1	28	PE(15-MHDA_18:1), PE(15-MHDA_18:2), PE(15-MHDA_20:4), PE(16:0_16:1), PE(16:0_18:1), PE(16:0_18:2), PE(16:0_18:3) (a), PE(16:0_18:3) (b), PE(16:0_20:3), PE(16:0_20:4), PE(16:1_18:2), PE(16:1_20:4), PE(17:0_18:1), PE(17:0_18:2), PE(17:0_20:4), PE(18:0_18:1), PE(18:0_18:2), PE(18:0_20:3) (a), PE(18:0_20:3) (b), PE(18:0_20:4), PE(18:0_22:4), PE(18:0_22:5) (n3), PE(18:0_22:5) (n6), PE(18:1_18:1), PE(18:1_18:2), PE(20:0_20:4), PE(38:5) (a), PE(38:5) (b)
M2	60	PE(16:0_16:0), PG(34:1), PG(36:1), PG(36:2), CE(20:4), DE(20:4), DG(14:0_16:0), DG(14:0_18:2), DG(16:0_16:0), DG(16:0_16:1), DG(16:0_18:1), DG(16:1_18:1), DG(18:0_18:1), DG(18:0_18:2), DG(18:1_18:1), TG(48:0) [NL-16:0], TG(48:0) [NL-18:0], TG(48:1) [NL-16:1], TG(48:1) [NL-18:1], TG(48:2) [NL-14:0], TG(48:2) [NL-14:1], TG(48:2) [NL-16:1], TG(48:2) [NL-18:2], TG(48:3) [NL-14:0], TG(48:3) [NL-16:1], TG(48:3) [NL-18:3], TG(49:1) [NL-16:1], TG(49:1) [NL-17:1], TG(50:0) [NL-18:0], TG(50:1) [NL-14:0], TG(50:1) [NL-16:0], TG(50:1) [NL-18:1], TG(50:2) [NL-14:0], TG(50:2) [NL-16:1], TG(50:2) [NL-18:1], TG(50:2) [NL-18:2], TG(50:3) [NL-14:0], TG(50:3) [NL-14:1], TG(50:3) [NL-16:1], TG(50:3) [NL-18:2], TG(50:3) [NL-18:3], TG(50:4) [NL-14:0], TG(50:4) [NL-18:3], TG(50:4) [NL-20:4], TG(51:0) [NL-16:0], TG(51:1) [NL-17:0], TG(51:2) [NL-15:0], TG(51:2) [NL-17:0], TG(51:2) [NL-17:1], TG(52:1) [NL-18:0], TG(52:1) [NL-18:1], TG(52:2) [NL-16:0], TG(52:2) [NL-18:2], TG(52:4) [NL-18:3], TG(53:2) [NL-17:1], TG(53:2) [NL-18:1], TG(54:0) [NL-18:0], TG(54:1) [NL-18:1], TG(54:2) [NL-18:0], TG(54:2) [NL-20:1]
M3	48	LPC(15-MHDA) [sn1] [104_sn1], LPC(15-MHDA) [sn1] & LPC(17:0) [sn2], LPC(15-MHDA) [sn2], LPC(15:0) [sn1], LPC(15:0) [sn2], LPC(16:0) [sn1], LPC(16:0) [sn2], LPC(16:1) [sn1], LPC(16:1) [sn2], LPC(17:0) [sn1], LPC(17:1) (a) [sn1] [104_sn1], LPC(17:1) [sn1] (a) & LPC(17:1) [sn2] (b), LPC(17:1) [sn1] (b), LPC(17:1) [sn2] (a), LPC(18:0) [sn1], LPC(18:0) [sn2], LPC(18:1) [sn1], LPC(18:1) [sn2], LPC(19:0) (a) [sn1] [104_sn1], LPC(19:0) [sn1] (a) & LPC(19:0) [sn2] (b), LPC(19:0) [sn1] (b), LPC(19:0) [sn2] (a), LPC(19:1) (a), LPC(19:1) (b), LPC(19:1) (c), LPC(20:1) [sn1], LPC(20:1) [sn2], LPC(20:2) [sn1], LPC(20:2) [sn2], LPC(22:1) [sn1], LPC(22:1) [sn2], LPC(O-16:0), LPC(O-18:0), LPC(O-18:1), LPC(P-16:0), LPC(P-17:0) (a), LPC(P-17:0) (b), LPC(P-18:0), LPC(P-18:1), LPE(16:0) [sn1], LPE(16:0) [sn2], LPE(18:0) [sn1], LPE(18:0) [sn2], LPE(P-16:0), LPE(P-18:0), LPE(P-18:1), LPE(P-20:0), AC(24:1)-OH
M4	5	PC(18:0_22:5) (n3) & PC(20:1_20:4), PC(39:5) (b), LPC(22:5) (n3) [sn1] [104_sn1], LPC(22:5) [sn1] (a) & LPC(22:5) [sn2] (n6), LPC(22:5) [sn2] (n3)
M5	14	FA(14:0), FA(16:0), FA(16:1), FA(17:0), FA(17:1), FA(18:0), FA(18:1), FA(18:2), FA(18:3), FA(20:2), FA(20:3), FA(20:4), FA(22:4), FA(22:5)
M6	11	PC(15-MHDA_20:4), PC(15:0_20:4), PC(16:0_20:4), PC(16:1_20:4), PC(17:0_20:4), PC(18:0_20:4), PC(38:5) (a), TG(56:6) [NL-20:4], TG(56:7) [NL-20:4], CE(20:4) [+OH], PC(36:4) [+OH]
M7	11	PC(20:0_20:4), LPC(20:0) [sn1], LPC(20:0) [sn2], LPC(22:0) [sn1], LPC(22:0) [sn2], LPC(24:0) [sn1], LPC(24:0) [sn2], LPC(26:0) [sn1], LPC(26:0) [sn2], PI(20:0_20:4), AC(24:0)
M8	8	PE(P-16:0/20:4), PE(P-17:0/20:4) (b), PE(P-18:0/20:4), PE(P-18:1/20:4) (a), PE(P-19:0/20:4) (a), PE(P-19:0/20:4) (b), PE(P-20:0/20:4), PE(P-20:1/20:4)
M9	9	SHexCer(d18:1/24:0(OH)), SM(d16:1/23:0) & SM(d17:1/22:0), SM(d18:1/20:0) & SM(d16:1/22:0), SM(d18:1/22:0) & SM(d16:1/24:0), SM(d18:1/23:0) & SM(d17:1/24:0), SM(d18:1/24:0), SM(d18:2/22:0), SM(d18:2/23:0), SM(d18:2/24:0)
M10	11	PC(O-32:1), PC(O-32:2), PC(O-34:4), PC(O-35:4), PC(P-15:0/20:4) (a), PC(P-15:0/20:4) (b), PC(P-17:0/20:4) (a), PC(P-17:0/20:4) (b), PE(P-15:0/20:4) (a), PE(P-15:0/20:4) (b), PE(P-17:0/20:4) (a)
M11	5	AC(18:2), AC(18:3), AC(20:3) (a), AC(20:3) (b), AC(20:4)
M12	11	methyl-CE(18:0), methyl-CE(18:1), methyl-CE(18:2), methyl-CE(20:4), methyl-CE(22:6), methyl-DE(18:1), methyl-DE(18:2), dimethyl-CE(18:1), dimethyl-CE(18:2), dimethyl-CE(20:4), dimethyl-CE(22:6)
M13	11	CE(18:0), CE(20:0), CE(20:1), CE(20:2), CE(22:0), CE(22:1), CE(24:0), CE(24:1), CE(24:4), CE(24:5), CE(18:2) [+OH]
M14	5	PI(38:5) (b), PI(15-MHDA_18:2) & PI(17:0_18:2), PI(16:0_20:3) (a), PI(18:1_18:2), PI(36:2)
M15	31	PE(O-16:0/18:2), PE(O-16:0/20:3), PE(O-16:0/20:4), PE(O-18:0/20:4), PE(O-18:0/22:5), PE(O-18:1/18:2), PE(O-34:1), PE(O-38:5) (a), PE(P-16:0/18:1), PE(P-16:0/18:2), PE(P-16:0/18:3), PE(P-16:0/20:3) (a), PE(P-16:0/20:3) (b), PE(P-16:0/22:5) (n3), PE(P-18:0/18:1), PE(P-18:0/18:2), PE(P-18:0/18:3), PE(P-18:0/20:3) (a), PE(P-18:0/20:3) (b), PE(P-18:0/22:5) (n3), PE(P-18:1/18:1) (a), PE(P-18:1/18:1) (b), PE(P-18:1/18:2) (a), PE(P-18:1/18:2) (b), PE(P-18:1/18:3), PE(P-18:1/20:3) (a), PE(P-18:1/20:3) (b), PE(P-18:1/20:4) (b), PE(P-18:1/22:5) (a), PE(P-20:0/18:1), PE(P-20:0/18:2)
M16	19	TG(O-50:1) [NL-15:0], TG(O-50:1) [NL-16:0], TG(O-50:1) [NL-17:1], TG(O-50:1) [NL-18:1], TG(O-50:2) [NL-18:1], TG(O-50:2) [NL-18:2], TG(O-50:3) [NL-18:2], TG(O-52:0) [NL-16:0], TG(O-52:1) [NL-16:0], TG(O-52:1) [NL-18:1], TG(O-52:2) [NL-16:0], TG(O-52:2) [NL-17:1], TG(O-52:2) [NL-18:1], TG(O-54:2) [NL-17:1], TG(O-54:2) [NL-18:1], TG(O-54:3) [NL-17:1], TG(O-54:3) [NL-18:1], TG(O-54:4) [NL-17:1], TG(O-54:4) [NL-18:2]
M17	12	Cer(d19:1/16:0), Cer(d19:1/18:0), Cer(d19:1/20:0), Cer(d19:1/22:0), Cer(d19:1/23:0), Cer(d19:1/24:0), Cer(d19:1/24:1), Cer(d19:1/26:0), Cer(d20:1/22:0), Cer(d20:1/23:0)
M18	5	Cer(d20:1/24:0), Cer(d20:1/24:1)
M18	5	CE(16:2), CE(18:3), DE(18:2), deDE(18:2), deDE(20:4)

M19	14	HexCer(d16:1/18:0), HexCer(d16:1/20:0), HexCer(d16:1/22:0), HexCer(d16:1/24:0), HexCer(d18:1/16:0), HexCer(d18:1/18:0), HexCer(d18:1/20:0), HexCer(d18:1/22:0), HexCer(d18:1/24:0), HexCer(d18:1/24:1), HexCer(d18:2/18:0), HexCer(d18:2/20:0), HexCer(d18:2/22:0), HexCer(d18:2/24:0)
M20	6	LPI(18:1) [sn1], LPI(18:1) [sn2], LPI(18:2) [sn1], LPI(18:2) [sn2], LPI(20:4) [sn1], LPI(20:4) [sn2] PC(18:0_22:4), PC(18:0_22:5) (n6), PC(38:4) (b), LPC(20:4) [sn1], LPC(20:4) [sn2], LPC(22:4) [sn1], LPC(22:4) [sn2], LPC(22:5) [sn1] (n6), LPE(20:4) [sn1], LPE(20:4) [sn2], PI(18:0_22:4), PI(18:0_22:5) (n6)
M21	12	PE(15-MHDA_22:6), PE(16:0_22:6), PE(17:0_22:6), PE(18:0_22:6), PE(18:1_22:6) (a), PE(18:1_22:6) (b)
M22	6	(b)
M23	12	SM(34:3), SM(37:2), SM(38:3) (a), SM(38:3) (b), SM(40:3) (a), SM(40:3) (b), SM(d18:1/18:0) & SM(d16:1/20:0), SM(d18:2/16:0), SM(d18:2/17:0), SM(d18:2/18:0), SM(d18:2/18:1), SM(d18:2/20:0) PC(14:0_22:6), PC(16:0_20:5), PC(18:2_20:5), PC(34:5), PC(35:5), PC(36:6) (a), PC(38:5) (b), PC(O-36:5), PC(P-16:0/20:5), LPC(20:5) [sn1], LPC(20:5) [sn2], PE(16:0_20:5), PE(O-36:5), PE(P-15:0/22:6) (a), PE(P-16:0/20:5), PE(P-18:0/20:5), PE(P-18:1/20:5) (a), PE(P-18:1/20:5) (b), LPE(22:6) [sn1], LPE(22:6) [sn2], CE(20:5), DE(20:5), FA(20:5)
M24	23	
M25	7	AC(15:0) (b), AC(16:0), AC(17:0) (a), AC(17:0) (b), AC(18:0), AC(24:1), AC(26:1) AC(12:0), AC(12:1), AC(14:0), AC(14:1), AC(14:2), AC(16:1), AC(18:1), AC(14:0)-OH, AC(14:1)-OH,
M26	14	AC(16:0)-OH, AC(16:1)-OH, AC(18:0)-OH, AC(18:1)-OH, AC(20:3)-OH Cer(m18:0/20:0), Cer(m18:0/22:0), Cer(m18:0/23:0), Cer(m18:0/24:0), Cer(m18:0/24:1), Cer(m18:1/18:0), Cer(m18:1/20:0), Cer(m18:1/22:0), Cer(m18:1/23:0), Cer(m18:1/24:0),
M27	11	Cer(m18:1/24:1)
M28	7	SM(37:1), SM(41:1) (a), SM(43:1), SM(44:1), SM(d16:1/19:0), SM(d18:1/17:0) & SM(d17:1/18:0), SM(d19:1/24:1)
M29	10	DG(16:0_20:4), DG(18:0_20:4), DG(18:1_20:3), DG(18:1_20:4), DG(18:2_20:4), TG(52:5) [NL-20:4], TG(54:4) [NL-20:3], TG(54:5) [NL-20:4], TG(54:6) [NL-20:4], TG(56:8) [NL-20:4] PC(14:0_16:0), PC(14:0_20:4), PC(16:0_18:1), PC(16:0_18:3) (b), PC(16:0_20:3) (b), PC(18:0_18:1), PC(28:0), PC(32:1), PC(32:2), LPC(14:0) [sn1], LPC(14:0) [sn2], PI(15-MHDA_18:1) & PI(17:0_18:1), PI(15-MHDA_20:4) & PI(17:0_20:4), PI(16:0_16:1), PI(16:0_20:3) (b), PI(16:0_20:4), PI(16:0/16:0), PI(18:0_18:1), PI(18:0_20:3) (b), PI(18:0_20:4), PI(34:0), PI(34:1), PI(38:5) (a), CE(14:0), CE(16:1), PC(34:2) [+OH]
M30	26	
M31	7	PC(16:0_20:3) (a), PC(18:0_20:3), PC(18:1_20:3), PC(40:7) (a), LPC(20:3) [sn1], LPC(20:3) [sn2], CE(20:3)
M32	20	S1P(d16:1), Cer(d16:1/16:0), Cer(d16:1/22:0), Cer(d16:1/23:0), Cer(d16:1/24:0), Cer(d16:1/24:1), Cer(d17:1/22:0), Cer(d17:1/23:0), Cer(d17:1/24:0), Cer(d17:1/24:1), Cer(d18:1/22:0), Cer(d18:1/23:0), Cer(d18:1/24:0), Cer(d18:1/24:1), Cer(d18:1/26:0), Cer(d18:2/22:0), Cer(d18:2/23:0), Cer(d18:2/24:0), Cer(d18:2/24:1), Cer(d18:2/26:0)
M33	30	PS(40:5), PS(40:6), FA(22:6), AC(13:0), AC(15:0) (a), AC(20:5), AC(22:5), AC(22:6), AC(22:5)-OH, DG(16:0_22:5), DG(16:0_22:6), DG(18:1_20:5), DG(18:1_22:5), DG(18:1_22:6), DG(18:2_22:6), TG(52:5) [NL-20:5], TG(54:6) [NL-20:5], TG(54:6) [NL-22:6], TG(54:7) [NL-20:5], TG(54:7) [NL-22:6], TG(56:6) [NL-22:5], TG(56:7) [NL-20:5], TG(56:7) [NL-22:5], TG(56:7) [NL-22:6], TG(56:8) [NL-20:5], TG(56:8) [NL-22:6], TG(56:9) [NL-22:6], TG(58:10) [NL-22:6], TG(58:8) [NL-22:6], TG(58:9) [NL-22:6] LPC(18:2) [sn1], LPC(18:2) [sn2], LPC(18:3) (a) [sn1] [104_sn1], LPC(18:3) [sn1] (a) & LPC(18:3) [sn2] (b), LPC(18:3) [sn1] (b), LPC(18:3) [sn2] (a), LPE(18:1) [sn1], LPE(18:1) [sn2], LPE(18:2) [sn1], LPE(18:2) [sn2], LPC(18:2) [+OH]
M34	11	
M35	10	PC(O-16:0/20:4), PC(O-18:0/20:4), PC(O-38:5), PC(O-40:5), PC(P-16:0/20:4), PC(P-18:0/20:4), PC(P-18:0/22:5), PC(P-20:0/20:4), PC(P-38:5) (a), PC(P-38:5) (b)
M36	14	DG(16:0_18:2), DG(18:1_18:2), DG(18:1_18:3), DG(18:2_18:2), TG(52:3) [NL-16:1], TG(52:3) [NL-18:2], TG(52:4) [NL-16:1], TG(52:4) [NL-18:2], TG(52:5) [NL-18:3], TG(54:3) [NL-18:1], TG(54:3) [NL-18:2], TG(54:4) [NL-18:2], TG(54:5) [NL-18:3], TG(54:6) [NL-18:3]
M37	8	dhCer(d18:0/16:0), dhCer(d18:0/18:0), dhCer(d18:0/20:0), dhCer(d18:0/22:0), dhCer(d18:0/24:0), dhCer(d18:0/24:1), SM(41:0), SM(d18:0/22:0)
M38	10	Hex2Cer(d16:1/16:0), Hex2Cer(d16:1/24:1), Hex2Cer(d18:1/16:0), Hex2Cer(d18:1/20:0), Hex2Cer(d18:1/22:0), Hex2Cer(d18:1/24:0), Hex2Cer(d18:1/24:1), Hex2Cer(d18:2/16:0), Hex2Cer(d18:2/24:1), GM1(d18:1/16:0)
M39	8	LPC(O-20:0), LPC(O-20:1), LPC(O-22:0), LPC(O-22:1), LPC(O-24:0), LPC(O-24:1), LPC(O-24:2), LPC(P-20:0)
M40	10	Sph(d18:1), S1P(d18:0), S1P(d18:1), S1P(d18:2), PS(36:1), PS(36:2), PS(38:3), PS(38:4), LPC(20:4) [+OH], LPC(22:6) [+OH]
M41	19	Cer(d17:1/16:0), Cer(d18:1/14:0), Cer(d18:2/14:0), SM(d17:1/14:0), SM(d17:1/16:0), SM(d18:0/14:0), SM(d18:1/14:0) & SM(d16:1/16:0), SM(d18:2/14:0), PC(15-MHDA_18:1), PC(17:0_18:1), PC(31:0) (a), PC(31:0) (b), PC(33:0) (a), PC(33:0) (b), PC(33:1), PC(P-16:0/14:0), CE(15:0), CE(17:0), CE(17:1)

	<p>Cer(d18:1/16:0), Cer(d18:2/16:0), Cer1P(d18:1/16:0), Hex3Cer(d18:1/16:0), Hex3Cer(d18:1/18:0), Hex3Cer(d18:1/20:0), Hex3Cer(d18:1/22:0), Hex3Cer(d18:1/24:0), Hex3Cer(d18:1/24:1), GM3(d18:1/16:0), GM3(d18:1/18:0), GM3(d18:1/22:0), GM3(d18:1/24:0), GM3(d18:1/24:1), SHexCer(d18:1/16:0(OH)), SHexCer(d18:1/16:0), SHexCer(d18:1/24:1(OH)), SM(35:2) (b), SM(d18:0/16:0), SM(d18:1/16:0), PC(15-MHDA_18:2), PC(15:0_20:3), PC(16:0_16:0), PC(16:0_18:0), PC(16:0_18:2), PC(16:0_18:3) (a), PC(16:1_18:2), PC(17:0_18:2), PC(17:1_18:2), PC(18:0_18:2), PC(18:1_18:1), PC(18:1_18:2), PC(18:2_18:2), PC(33:2), PC(38:2), PC(38:6) (a), PC(40:8), PC(O-16:0/16:0), PC(O-16:0/20:3), PC(O-18:0/18:1), PC(O-18:0/18:2), PC(O-18:1/18:1), PC(O-18:1/18:2), PC(O-34:1), PC(O-34:2), PC(O-36:0), PC(P-16:0/16:0), PC(P-16:0/16:1), PC(P-16:0/18:0), PC(P-16:0/18:1), PC(P-16:0/18:2), PC(P-16:0/18:3), PC(P-18:0/18:2), PC(P-18:1/18:1), PC(P-35:2) (a), PC(P-35:2) (b), PC(P-36:3), PI(18:0_20:2), CE(16:0), CE(18:1),</p>
M42	62 CE(18:2), COH
M43	9 PE(O-16:0/22:4), PE(P-16:0/22:4), PE(P-16:0/22:5) (n6), PE(P-18:0/22:4), PE(P-18:0/22:5) (n6), PE(P-18:1/22:4), PE(P-18:1/22:5) (b), CE(22:4), CE(22:5)
M44	11 Cer(d16:1/18:0), Cer(d16:1/20:0), Cer(d17:1/18:0), Cer(d17:1/20:0), Cer(d18:1/18:0), Cer(d18:1/19:0), Cer(d18:1/20:0), Cer(d18:1/21:0), Cer(d18:2/18:0), Cer(d18:2/20:0), Cer(d18:2/21:0)
M45	39 PC(15-MHDA_22:6), PC(15:0_22:6), PC(16:0_22:6), PC(16:1_22:6), PC(17:0_22:6), PC(18:0_22:6), PC(18:1_22:6) (a), PC(18:1_22:6) (b), PC(38:7) (c), PC(39:5) (a), PC(44:12), PC(O-16:0/22:6), PC(O-18:0/22:6), PC(P-16:0/22:6), PC(P-18:0/22:6), PC(P-18:1/22:6), LPC(22:6) [sn1], LPC(22:6) [sn2], PE(O-16:0/22:6), PE(O-18:0/22:6), PE(O-18:1/22:6), PE(O-38:5) (b), PE(P-15:0/22:6) (b), PE(P-16:0/22:6), PE(P-17:0/22:6) (a), PE(P-17:0/22:6) (b), PE(P-18:0/22:6), PE(P-18:1/22:6) (a), PE(P-18:1/22:6) (b), PE(P-20:0/22:6), PE(P-20:1/22:6), PI(18:0_22:5) (n3), PI(18:0_22:6), PI(37:6),
M46	8 SHexCer(d18:1/24:1), SM(43:2) (b), SM(43:2) (c), SM(44:2), SM(44:3), SM(d16:1/24:1), SM(d17:1/24:1), SM(d18:1/24:1)

Supplementary Table 5. Associations of lipid correlation network modules with baseline A/T/N biomarkers

Lipid modu	A: Amyloid PET (AV45) uptake					T: CSF pTau					N1: Hippocampal volume					N2: FDG uptake				
	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)
M39	0.122	0.053	0.192	0.001	0.026	0.053	-0.010	0.116	0.100	0.229	-0.037	-0.088	0.013	0.149	0.395	-0.110	-0.175	-0.045	0.001	0.042
M34	0.112	0.043	0.180	0.001	0.033	0.079	0.018	0.141	0.011	0.102	-0.014	-0.060	0.033	0.559	0.857	-0.027	-0.092	0.037	0.403	0.530
M3	0.104	0.033	0.174	0.004	0.047	0.048	-0.015	0.111	0.135	0.239	-0.009	-0.061	0.043	0.723	0.890	-0.065	-0.131	0.000	0.051	0.148
M38	0.118	0.038	0.198	0.004	0.047	0.058	-0.012	0.129	0.104	0.229	-0.036	-0.088	0.017	0.181	0.438	-0.063	-0.137	0.011	0.097	0.235
M37	-0.108	-0.188	-0.028	0.008	0.075	-0.049	-0.119	0.021	0.171	0.271	0.058	0.005	0.111	0.031	0.128	0.032	-0.042	0.106	0.396	0.530
M8	-0.090	-0.160	-0.020	0.012	0.090	-0.059	-0.121	0.002	0.060	0.188	0.068	0.022	0.114	0.004	0.035	0.008	-0.056	0.072	0.808	0.909
M19	0.089	0.015	0.163	0.018	0.121	0.024	-0.041	0.090	0.465	0.578	-0.016	-0.065	0.033	0.515	0.816	-0.018	-0.086	0.051	0.609	0.737
M11	0.066	0.001	0.132	0.047	0.271	0.055	-0.004	0.113	0.068	0.196	-0.024	-0.068	0.020	0.279	0.569	-0.033	-0.094	0.028	0.286	0.454
M4	0.070	-0.001	0.141	0.055	0.279	0.070	0.008	0.133	0.028	0.143	-0.059	-0.107	-0.012	0.015	0.069	-0.033	-0.099	0.032	0.318	0.488
M36	0.083	-0.005	0.170	0.064	0.292	0.056	-0.024	0.137	0.169	0.271	-0.028	-0.094	0.039	0.412	0.702	-0.066	-0.150	0.018	0.121	0.266
M9	-0.088	-0.188	0.012	0.085	0.292	-0.001	-0.088	0.087	0.984	0.984	0.103	0.036	0.171	0.003	0.032	0.069	-0.025	0.163	0.148	0.310
M7	0.068	-0.008	0.144	0.081	0.292	-0.006	-0.074	0.062	0.859	0.919	0.028	-0.022	0.078	0.274	0.569	0.042	-0.027	0.111	0.236	0.402
M32	0.071	-0.010	0.151	0.085	0.292	0.056	-0.016	0.127	0.125	0.239	-0.011	-0.065	0.043	0.682	0.871	-0.042	-0.115	0.032	0.270	0.443
M33	-0.063	-0.136	0.010	0.089	0.292	-0.079	-0.143	-0.014	0.018	0.135	0.030	-0.019	0.078	0.232	0.533	0.008	-0.059	0.076	0.810	0.909
M42	0.090	-0.022	0.203	0.115	0.352	0.083	-0.011	0.178	0.083	0.214	0.018	-0.064	0.100	0.666	0.871	-0.125	-0.223	-0.028	0.012	0.079
M15	-0.056	-0.131	0.019	0.143	0.410	-0.008	-0.074	0.059	0.821	0.910	0.079	0.027	0.130	0.003	0.032	0.029	-0.039	0.098	0.402	0.530
M16	-0.051	-0.123	0.020	0.157	0.412	-0.050	-0.114	0.014	0.125	0.239	0.119	0.070	0.169	0.000	0.000	0.017	-0.050	0.083	0.626	0.739
M40	0.046	-0.018	0.109	0.161	0.412	0.055	-0.003	0.112	0.061	0.188	-0.016	-0.059	0.028	0.479	0.787	-0.001	-0.060	0.058	0.976	0.983
M18	0.070	-0.040	0.181	0.211	0.477	0.112	0.017	0.207	0.021	0.135	-0.138	-0.205	-0.071	0.000	0.001	-0.100	-0.196	-0.005	0.039	0.139
M10	-0.046	-0.116	0.025	0.202	0.477	0.001	-0.060	0.063	0.966	0.984	0.058	0.012	0.105	0.014	0.069	-0.004	-0.068	0.060	0.895	0.980
M45	-0.049	-0.126	0.029	0.218	0.477	-0.105	-0.173	-0.038	0.002	0.053	0.069	0.017	0.121	0.009	0.054	0.002	-0.068	0.072	0.952	0.983
M20	-0.039	-0.107	0.029	0.260	0.543	0.046	-0.014	0.105	0.135	0.239	0.007	-0.040	0.054	0.775	0.891	-0.045	-0.108	0.018	0.160	0.317
M21	0.035	-0.040	0.109	0.361	0.554	0.113	0.047	0.178	0.001	0.036	-0.041	-0.094	0.011	0.123	0.378	-0.101	-0.170	-0.031	0.005	0.077
M43	-0.037	-0.111	0.037	0.331	0.554	0.091	0.025	0.156	0.007	0.080	0.000	-0.054	0.054	0.996	0.996	-0.083	-0.152	-0.014	0.018	0.104
M12	-0.036	-0.111	0.039	0.345	0.554	-0.032	-0.100	0.036	0.356	0.468	0.073	0.023	0.123	0.005	0.035	0.070	0.001	0.140	0.047	0.146
M13	0.053	-0.046	0.151	0.293	0.554	0.023	-0.062	0.108	0.594	0.683	0.011	-0.053	0.075	0.741	0.890	-0.081	-0.170	0.009	0.077	0.197
M27	-0.040	-0.125	0.046	0.361	0.554	-0.026	-0.100	0.048	0.490	0.593	0.003	-0.053	0.059	0.925	0.967	-0.038	-0.115	0.039	0.337	0.493
M24	-0.037	-0.111	0.037	0.326	0.554	-0.066	-0.133	0.001	0.053	0.188	0.013	-0.037	0.062	0.616	0.864	0.022	-0.047	0.091	0.534	0.682
M28	-0.034	-0.106	0.038	0.351	0.554	-0.002	-0.065	0.062	0.962	0.984	0.064	0.016	0.112	0.009	0.054	0.019	-0.049	0.087	0.583	0.725
M22	-0.041	-0.122	0.040	0.324	0.554	-0.077	-0.150	-0.004	0.038	0.174	0.014	-0.041	0.069	0.620	0.864	-0.001	-0.076	0.074	0.983	0.983
M14	0.032	-0.046	0.110	0.417	0.619	0.102	0.032	0.171	0.004	0.064	-0.012	-0.067	0.043	0.676	0.871	-0.077	-0.148	-0.005	0.036	0.136
M5	-0.024	-0.091	0.043	0.487	0.700	-0.007	-0.067	0.054	0.831	0.910	-0.003	-0.048	0.041	0.886	0.948	-0.063	-0.125	-0.001	0.048	0.146
M26	-0.020	-0.085	0.045	0.549	0.765	0.030	-0.028	0.089	0.309	0.431	-0.021	-0.065	0.023	0.339	0.624	-0.080	-0.141	-0.019	0.010	0.077
M23	-0.023	-0.110	0.064	0.600	0.812	0.072	-0.002	0.146	0.057	0.188	0.005	-0.058	0.068	0.867	0.948	-0.102	-0.179	-0.024	0.010	0.077
M29	-0.022	-0.113	0.068	0.628	0.826	0.038	-0.042	0.118	0.354	0.468	0.000	-0.063	0.062	0.990	0.996	-0.081	-0.166	0.004	0.061	0.166
M31	0.019	-0.063	0.101	0.655	0.837	0.081	0.010	0.151	0.026	0.143	0.042	-0.015	0.100	0.150	0.395	-0.001	-0.077	0.074	0.971	0.983
M41	0.015	-0.068	0.097	0.724	0.900	0.054	-0.019	0.127	0.144	0.246	-0.015	-0.070	0.041	0.604	0.864	-0.050	-0.126	0.026	0.196	0.347
M44	0.012	-0.063	0.087	0.748	0.905	0.042	-0.025	0.109	0.219	0.324	-0.024	-0.074	0.027	0.362	0.641	-0.049	-0.119	0.020	0.165	0.317
M35	-0.006	-0.086	0.074	0.887	0.913	0.055	-0.014	0.125	0.118	0.239	0.031	-0.026	0.087	0.284	0.569	-0.098	-0.170	-0.026	0.008	0.077
M6	-0.010	-0.086	0.065	0.788	0.913	0.058	-0.008	0.124	0.084	0.214	-0.008	-0.060	0.044	0.755	0.890	-0.095	-0.165	-0.026	0.007	0.077
M2	-0.009	-0.116	0.097	0.862	0.913	0.062	-0.034	0.159	0.204	0.313	-0.067	-0.142	0.008	0.081	0.294	-0.116	-0.218	-0.015	0.025	0.114
M30	0.006	-0.080	0.092	0.890	0.913	0.079	0.003	0.155	0.042	0.174	-0.046	-0.105	0.013	0.123	0.378	-0.093	-0.173	-0.013	0.023	0.114
M25	-0.006	-0.073	0.062	0.868	0.913	0.023	-0.037	0.084	0.451	0.576	-0.023	-0.068	0.022	0.319	0.612	-0.069	-0.132	-0.007	0.030	0.127
M17	0.006	-0.062	0.075	0.855	0.913	0.017	-0.044	0.078	0.585	0.683	0.005	-0.041	0.051	0.832	0.934	-0.052	-0.115	0.011	0.106	0.244
M1	-0.006	-0.093	0.081	0.893	0.913	0.066	-0.014	0.145	0.105	0.229	-0.044	-0.105	0.017	0.155	0.395	-0.057	-0.139	0.025	0.174	0.320
M46	0.002	-0.086	0.089	0.968	0.968	-0.045	-0.121	0.032	0.251	0.361	0.050	-0.007	0.108	0.083	0.294	-0.039	-0.121	0.042	0.343	0.493

Supplementary Table 6. Associations of lipid species with longitudinal A/T/N biomarkers

Lipid Species	A: Amyloid PET (AV45) uptake					T: CSF pTau					N1: Hippocampal volume					N2: FDG uptake				
	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)
deDE(20:4)	-0.002	-0.024	0.020	0.859	0.981	0.008	-0.006	0.023	0.255	0.506	-0.026	-0.037	-0.015	0.000	0.004	-0.048	-0.077	-0.019	0.001	0.018
PI(38:5) (b)	-0.017	-0.039	0.005	0.136	0.903	-0.009	-0.023	0.005	0.222	0.482	-0.024	-0.035	-0.013	0.000	0.005	-0.058	-0.084	-0.031	0.000	0.004
PC(18:1_22:6) (b)	-0.002	-0.024	0.021	0.890	0.981	-0.009	-0.023	0.005	0.231	0.488	-0.023	-0.034	-0.012	0.000	0.008	-0.067	-0.094	-0.040	0.000	0.001
deDE(18:2)	0.000	-0.022	0.023	0.975	0.995	-0.007	-0.021	0.007	0.314	0.557	-0.022	-0.032	-0.011	0.000	0.013	-0.049	-0.077	-0.022	0.000	0.010
GM3(d18:1/22:0)	0.000	-0.022	0.021	0.976	0.995	-0.007	-0.021	0.007	0.336	0.574	-0.021	-0.032	-0.011	0.000	0.018	-0.056	-0.083	-0.028	0.000	0.005
AC(18:2)	-0.008	-0.030	0.014	0.496	0.922	-0.007	-0.021	0.007	0.315	0.557	-0.021	-0.031	-0.010	0.000	0.020	-0.026	-0.053	0.001	0.064	0.184
LPC(O-24:2)	-0.013	-0.035	0.009	0.262	0.903	-0.016	-0.030	-0.003	0.020	0.273	-0.020	-0.031	-0.009	0.000	0.022	-0.036	-0.063	-0.008	0.012	0.066
LPC(O-22:1)	-0.004	-0.026	0.018	0.693	0.964	-0.022	-0.036	-0.008	0.002	0.259	-0.020	-0.031	-0.009	0.000	0.022	-0.044	-0.071	-0.017	0.002	0.022
GM3(d18:1/16:0)	-0.001	-0.023	0.021	0.949	0.995	-0.007	-0.021	0.008	0.352	0.592	-0.020	-0.031	-0.009	0.000	0.022	-0.057	-0.084	-0.030	0.000	0.004
GM3(d18:1/20:0)	-0.007	-0.029	0.015	0.527	0.922	-0.009	-0.023	0.006	0.240	0.495	-0.020	-0.031	-0.009	0.000	0.030	-0.052	-0.080	-0.024	0.000	0.008
LPC(O-20:1)	-0.004	-0.026	0.018	0.716	0.964	-0.019	-0.033	-0.005	0.007	0.259	-0.019	-0.030	-0.009	0.000	0.030	-0.039	-0.066	-0.011	0.006	0.047
AC(18:1)	0.002	-0.020	0.024	0.841	0.981	-0.016	-0.030	-0.002	0.024	0.285	-0.019	-0.030	-0.008	0.001	0.030	-0.051	-0.078	-0.024	0.000	0.008
Hex3Cer(d18:1/20:0)	0.002	-0.020	0.024	0.858	0.981	0.007	-0.007	0.021	0.332	0.572	-0.019	-0.030	-0.008	0.001	0.030	-0.038	-0.066	-0.010	0.007	0.049
LPC(O-24:1)	-0.011	-0.033	0.011	0.330	0.922	-0.026	-0.040	-0.013	0.000	0.092	-0.018	-0.029	-0.008	0.001	0.043	-0.043	-0.070	-0.016	0.002	0.025
HexCer(d18:1/20:0)	0.006	-0.016	0.028	0.575	0.933	-0.012	-0.026	0.002	0.093	0.359	-0.018	-0.029	-0.008	0.001	0.043	-0.040	-0.068	-0.013	0.004	0.042
PE(P-15:0/22:6) (b)	-0.005	-0.028	0.017	0.647	0.960	0.001	-0.013	0.015	0.881	0.934	0.018	0.007	0.029	0.001	0.051	0.008	-0.019	0.036	0.551	0.730
SM(d18:2/18:1)	-0.003	-0.025	0.019	0.766	0.969	0.001	-0.013	0.015	0.915	0.951	-0.018	-0.029	-0.007	0.001	0.059	-0.055	-0.081	-0.028	0.000	0.005
PE(P-15:0/22:6) (a)	-0.001	-0.024	0.022	0.929	0.995	-0.006	-0.019	0.008	0.429	0.661	0.017	0.006	0.028	0.002	0.076	0.012	-0.015	0.039	0.396	0.611
LPC(18:1) [sn1]	-0.006	-0.028	0.016	0.574	0.933	-0.016	-0.029	-0.002	0.026	0.285	-0.017	-0.028	-0.006	0.002	0.081	-0.037	-0.065	-0.010	0.007	0.049
LPC(18:1) [sn2]	-0.004	-0.026	0.018	0.724	0.964	-0.017	-0.031	-0.004	0.012	0.273	-0.017	-0.028	-0.006	0.002	0.081	-0.041	-0.068	-0.014	0.003	0.037
LPC(O-18:0)	-0.012	-0.034	0.010	0.275	0.903	-0.011	-0.025	0.003	0.125	0.385	-0.017	-0.027	-0.006	0.002	0.083	-0.036	-0.063	-0.008	0.011	0.063
AC(20:4)	-0.009	-0.031	0.013	0.444	0.922	-0.009	-0.022	0.005	0.193	0.454	-0.017	-0.027	-0.006	0.002	0.083	-0.027	-0.054	-0.001	0.046	0.155
GM3(d18:1/24:1)	-0.015	-0.037	0.007	0.185	0.903	-0.021	-0.036	-0.007	0.003	0.259	-0.017	-0.027	-0.006	0.003	0.084	-0.058	-0.086	-0.031	0.000	0.004
LPC(20:2) [sn1]	-0.012	-0.034	0.010	0.281	0.903	-0.011	-0.025	0.003	0.111	0.380	-0.016	-0.027	-0.006	0.003	0.084	-0.021	-0.048	0.005	0.118	0.293
Hex3Cer(d18:1/16:0)	-0.006	-0.028	0.016	0.574	0.933	-0.012	-0.026	0.002	0.107	0.375	-0.017	-0.027	-0.006	0.003	0.084	-0.060	-0.086	-0.033	0.000	0.004
AC(18:3)	0.002	-0.020	0.024	0.842	0.981	-0.002	-0.016	0.012	0.792	0.891	-0.016	-0.027	-0.006	0.003	0.084	-0.018	-0.045	0.010	0.205	0.416
PI(16:0_20:3) (a)	-0.019	-0.041	0.003	0.089	0.903	-0.008	-0.022	0.006	0.279	0.524	-0.016	-0.027	-0.005	0.003	0.090	-0.035	-0.062	-0.008	0.010	0.061
LPC(P-20:0)	-0.009	-0.031	0.013	0.444	0.922	-0.008	-0.022	0.006	0.282	0.527	-0.016	-0.027	-0.005	0.003	0.090	-0.026	-0.053	0.001	0.063	0.184
LPC(O-20:0)	-0.010	-0.032	0.012	0.374	0.922	-0.017	-0.031	-0.003	0.016	0.273	-0.016	-0.027	-0.005	0.004	0.092	-0.038	-0.066	-0.011	0.007	0.048
AC(20:3) (a)	-0.017	-0.038	0.005	0.139	0.903	-0.014	-0.028	-0.001	0.035	0.298	-0.016	-0.027	-0.005	0.004	0.097	-0.026	-0.053	0.001	0.061	0.183
HexCer(d18:1/18:0)	-0.011	-0.034	0.011	0.317	0.922	-0.012	-0.026	0.002	0.081	0.356	-0.016	-0.026	-0.005	0.004	0.097	-0.056	-0.083	-0.028	0.000	0.005
PI(18:1_18:2)	0.000	-0.022	0.022	0.973	0.995	0.006	-0.008	0.019	0.435	0.666	-0.016	-0.027	-0.005	0.004	0.097	-0.013	-0.040	0.014	0.353	0.572
AC(20:3) (b)	-0.010	-0.032	0.012	0.360	0.922	-0.016	-0.029	-0.003	0.018	0.273	-0.015	-0.026	-0.004	0.006	0.119	-0.041	-0.066	-0.015	0.002	0.025
Cer(d18:2/20:0)	-0.009	-0.031	0.013	0.405	0.922	-0.012	-0.026	0.002	0.092	0.356	-0.015	-0.026	-0.004	0.006	0.119	-0.043	-0.071	-0.016	0.002	0.026
GM3(d18:1/24:0)	0.007	-0.015	0.029	0.528	0.922	-0.001	-0.015	0.013	0.867	0.932	-0.015	-0.026	-0.004	0.006	0.119	-0.039	-0.067	-0.012	0.005	0.045
LPC(20:1) [sn1]	0.007	-0.015	0.029	0.536	0.923	-0.011	-0.025	0.003	0.137	0.401	-0.015	-0.026	-0.004	0.006	0.119	-0.025	-0.052	0.003	0.079	0.217
AC(18:0)	-0.006	-0.028	0.016	0.616	0.950	-0.020	-0.034	-0.007	0.004	0.259	-0.015	-0.026	-0.005	0.005	0.119	-0.054	-0.081	-0.027	0.000	0.005
LPC(O-18:1)	-0.004	-0.025	0.018	0.744	0.964	-0.012	-0.026	0.002	0.084	0.356	-0.015	-0.026	-0.004	0.006	0.119	-0.026	-0.053	0.001	0.057	0.173
GM1(d18:1/16:0)	0.003	-0.020	0.025	0.823	0.980	-0.018	-0.032	-0.003	0.015	0.273	-0.015	-0.026	-0.005	0.005	0.119	-0.060	-0.089	-0.032	0.000	0.004
LPC(P-18:1)	-0.007	-0.029	0.015	0.526	0.922	-0.012	-0.025	0.002	0.099	0.366	-0.015	-0.026	-0.004	0.007	0.120	-0.024	-0.051	0.003	0.081	0.221
LPC(19:1) (b)	-0.006	-0.028	0.016	0.597	0.950	-0.010	-0.024	0.003	0.141	0.406	-0.015	-0.026	-0.004	0.006	0.120	-0.040	-0.068	-0.013	0.004	0.041
DE(18:1)	0.001	-0.021	0.023	0.935	0.995	-0.003	-0.016	0.011	0.717	0.855	-0.015	-0.026	-0.004	0.007	0.120	-0.040	-0.068	-0.012	0.006	0.047
SM(40:3) (b)	-0.013	-0.036	0.009	0.234	0.903	-0.009	-0.023	0.005	0.216	0.477	-0.015	-0.026	-0.004	0.007	0.127	-0.054	-0.081	-0.028	0.000	0.005
PE(P-15:0/20:4) (b)	-0.012	-0.034	0.010	0.293	0.903	-0.005	-0.019	0.008	0.458	0.682	0.014	0.004	0.025	0.008	0.127	0.009	-0.018	0.036	0.524	0.714
PE(18:1_22:6) (b)	-0.008	-0.030	0.014	0.484	0.922	-0.013	-0.027	0.001	0.071	0.349	-0.015	-0.026	-0.004	0.008	0.127	-0.036	-0.063	-0.008	0.012	0.066
SM(d18:0/22:0)	0.009	-0.013	0.031	0.424	0.922	0.011	-0.003	0.025	0.122	0.385	0.015	0.004	0.025	0.008	0.127	0.008	-0.019	0.036	0.566	0.742
PE(16:0_20:3)	-0.014	-0.036	0.008	0.199	0.903	-0.015	-0.029	-0.001	0.031	0.291	-0.015	-0.025	-0.004	0.008	0.128	-0.026	-0.054	0.001	0.063	0.184
Hex3Cer(d18:1/20:0)	-0.003	-0.025	0.019	0.778	0.973	-0.008	-0.022	0.006	0.263	0.514	-0.015	-0.025	-0.004	0.008	0.128	-0.046	-0.073	-0.018	0.001	0.019
PC(18:1_22:6) (a)	0.011	-0.011	0.033	0.337	0.922	-0.013	-0.027	0.001	0.060	0.327	-0.014	-0.025	-0.004	0.009	0.139	-0.045	-0.072	-0.018	0.001	0.020

TG(52:4) [NL-16:1]	-0.011	-0.033	0.011	0.324	0.922	-0.016	-0.030	-0.002	0.021	0.273	-0.014	-0.025	-0.003	0.010	0.139	-0.044	-0.071	-0.016	0.002	0.025
LPC(O-22:0)	-0.005	-0.028	0.017	0.629	0.954	-0.015	-0.029	-0.001	0.040	0.305	-0.014	-0.025	-0.004	0.009	0.139	-0.033	-0.061	-0.005	0.020	0.092
SM(35:2) (b)	-0.005	-0.027	0.017	0.660	0.960	-0.006	-0.020	0.008	0.413	0.646	-0.014	-0.025	-0.004	0.009	0.139	-0.051	-0.078	-0.025	0.000	0.006
AC(16:1)	0.000	-0.022	0.022	0.986	0.996	-0.011	-0.025	0.002	0.108	0.377	-0.014	-0.025	-0.003	0.010	0.146	-0.046	-0.074	-0.019	0.001	0.017
TG(O-50:1) [NL-18:1]	-0.010	-0.032	0.011	0.351	0.922	-0.003	-0.016	0.011	0.703	0.846	0.014	0.003	0.025	0.011	0.150	0.028	0.000	0.056	0.047	0.156
LPE(18:2) [sn2]	-0.024	-0.046	-0.002	0.030	0.903	-0.012	-0.026	0.002	0.087	0.356	-0.014	-0.025	-0.003	0.012	0.156	-0.021	-0.049	0.006	0.134	0.320
TG(O-54:2) [NL-17:1]	-0.017	-0.039	0.006	0.146	0.903	-0.008	-0.022	0.005	0.218	0.477	0.014	0.003	0.025	0.012	0.156	0.016	-0.011	0.043	0.242	0.456
PC(O-18:0/18:2)	-0.011	-0.033	0.011	0.326	0.922	-0.008	-0.022	0.006	0.246	0.501	-0.014	-0.025	-0.003	0.012	0.156	-0.037	-0.064	-0.010	0.007	0.049
PC(38:5) (a)	-0.004	-0.026	0.018	0.715	0.964	-0.005	-0.019	0.008	0.439	0.667	-0.014	-0.024	-0.003	0.012	0.156	-0.056	-0.083	-0.028	0.000	0.005
Cer(d18:1/20:0)	-0.021	-0.043	0.000	0.054	0.903	-0.014	-0.028	0.000	0.053	0.317	-0.014	-0.024	-0.003	0.013	0.166	-0.039	-0.066	-0.011	0.006	0.048
LPC(20:0) [sn1]	0.013	-0.009	0.034	0.261	0.903	-0.003	-0.018	0.011	0.633	0.803	-0.014	-0.024	-0.003	0.014	0.167	-0.010	-0.038	0.018	0.472	0.665
PS(36:2)	-0.010	-0.032	0.012	0.379	0.922	-0.016	-0.030	-0.002	0.024	0.285	-0.014	-0.024	-0.003	0.014	0.167	-0.018	-0.045	0.009	0.197	0.409
PC(38:7) (c)	-0.004	-0.026	0.018	0.725	0.964	-0.013	-0.027	0.001	0.073	0.350	-0.014	-0.025	-0.003	0.014	0.167	-0.051	-0.079	-0.024	0.000	0.008
CE(16:2)	0.004	-0.018	0.026	0.739	0.964	-0.003	-0.016	0.011	0.712	0.853	-0.013	-0.024	-0.003	0.014	0.167	-0.032	-0.058	-0.005	0.021	0.093
LPE(18:2) [sn1]	-0.021	-0.042	0.001	0.066	0.903	-0.011	-0.024	0.003	0.122	0.385	-0.014	-0.024	-0.003	0.015	0.169	-0.026	-0.054	0.001	0.064	0.184
PE(P-15:0/20:4) (a)	-0.020	-0.043	0.002	0.074	0.903	-0.009	-0.023	0.005	0.201	0.463	0.013	0.003	0.024	0.015	0.169	0.008	-0.018	0.035	0.548	0.729
Hex2Cer(d18:1/16:0)	-0.006	-0.028	0.016	0.613	0.950	-0.005	-0.019	0.009	0.471	0.689	-0.013	-0.024	-0.003	0.015	0.169	-0.049	-0.075	-0.022	0.000	0.010
PC(18:1_18:2)	0.002	-0.020	0.024	0.884	0.981	-0.008	-0.022	0.005	0.232	0.488	-0.013	-0.024	-0.003	0.015	0.169	-0.025	-0.052	0.002	0.072	0.201
PC(O-35:4)	-0.019	-0.040	0.003	0.092	0.903	-0.002	-0.016	0.012	0.769	0.881	0.013	0.003	0.024	0.015	0.170	0.007	-0.020	0.034	0.625	0.790
LPC(20:1) [sn2]	0.015	-0.007	0.037	0.177	0.903	-0.005	-0.019	0.009	0.513	0.724	-0.013	-0.024	-0.002	0.016	0.171	-0.026	-0.054	0.001	0.060	0.179
CE(22:5)	-0.003	-0.025	0.019	0.780	0.973	0.003	-0.011	0.016	0.700	0.846	-0.013	-0.024	-0.002	0.016	0.171	-0.038	-0.065	-0.011	0.006	0.047
PE(P-17:0/22:6) (a)	-0.007	-0.029	0.016	0.568	0.933	-0.009	-0.023	0.005	0.216	0.477	0.013	0.002	0.024	0.017	0.174	0.011	-0.017	0.038	0.446	0.652
dhCer(d18:0/24:0)	0.000	-0.022	0.023	0.965	0.995	0.009	-0.005	0.023	0.227	0.488	0.013	0.002	0.024	0.016	0.174	0.014	-0.014	0.041	0.326	0.544
Hex2Cer(d18:1/22:0)	0.004	-0.018	0.026	0.747	0.964	0.004	-0.010	0.018	0.622	0.792	-0.013	-0.024	-0.002	0.018	0.181	-0.027	-0.054	0.000	0.051	0.168
SM(34:3)	-0.003	-0.025	0.020	0.817	0.980	-0.001	-0.015	0.013	0.842	0.925	-0.013	-0.024	-0.002	0.018	0.181	-0.050	-0.076	-0.023	0.000	0.008
Cer(d18:2/21:0)	-0.003	-0.025	0.019	0.810	0.980	-0.009	-0.022	0.005	0.197	0.458	-0.013	-0.024	-0.002	0.018	0.181	-0.040	-0.068	-0.012	0.006	0.047
Hex3Cer(d18:1/18:0)	-0.009	-0.031	0.012	0.397	0.922	-0.007	-0.021	0.006	0.296	0.540	-0.013	-0.024	-0.002	0.019	0.186	-0.044	-0.071	-0.017	0.002	0.022
DE(18:2)	0.009	-0.013	0.032	0.400	0.922	0.010	-0.003	0.024	0.126	0.385	-0.013	-0.023	-0.002	0.019	0.186	-0.006	-0.034	0.022	0.676	0.824
Hex2Cer(d18:2/16:0)	-0.006	-0.028	0.016	0.602	0.950	0.003	-0.011	0.017	0.687	0.840	-0.013	-0.024	-0.002	0.019	0.186	-0.024	-0.051	0.004	0.093	0.244
PE(P-17:0/20:4) (a)	-0.006	-0.028	0.017	0.624	0.954	-0.004	-0.018	0.010	0.584	0.763	0.013	0.002	0.023	0.020	0.186	0.011	-0.016	0.038	0.428	0.638
LPC(16:1) [sn1]	-0.018	-0.040	0.004	0.109	0.903	-0.012	-0.026	0.001	0.081	0.356	-0.013	-0.023	-0.002	0.020	0.186	-0.038	-0.064	-0.011	0.006	0.047
HexCer(d16:1/20:0)	-0.002	-0.024	0.020	0.862	0.981	-0.013	-0.027	0.000	0.056	0.317	-0.013	-0.023	-0.002	0.020	0.186	-0.032	-0.059	-0.004	0.024	0.105
Cer(d18:1/16:0)	-0.013	-0.035	0.009	0.235	0.903	-0.013	-0.027	0.001	0.066	0.338	-0.013	-0.024	-0.002	0.020	0.186	-0.039	-0.067	-0.012	0.005	0.046
CE(22:4)	-0.009	-0.031	0.013	0.411	0.922	0.000	-0.013	0.014	0.957	0.976	-0.013	-0.023	-0.002	0.021	0.192	-0.038	-0.065	-0.011	0.006	0.048
PC(16:0_18:3) (a)	-0.014	-0.036	0.008	0.211	0.903	-0.007	-0.022	0.007	0.317	0.557	-0.013	-0.023	-0.002	0.023	0.193	-0.029	-0.056	-0.002	0.036	0.134
LPC(20:2) [sn2]	-0.013	-0.035	0.009	0.237	0.903	-0.012	-0.026	0.002	0.085	0.356	-0.013	-0.023	-0.002	0.023	0.193	-0.015	-0.042	0.012	0.276	0.500
LPC(22:5) [sn1] (n3) & LPC(22:5) [sn2] (n6)	-0.009	-0.031	0.013	0.403	0.922	-0.014	-0.027	0.000	0.052	0.317	-0.012	-0.023	-0.002	0.022	0.193	-0.040	-0.068	-0.013	0.004	0.043
PE(P-16:0/20:4)	-0.005	-0.027	0.017	0.657	0.960	0.009	-0.005	0.024	0.198	0.460	0.013	0.002	0.023	0.022	0.193	-0.002	-0.030	0.026	0.879	0.948
CE(18:2)	-0.003	-0.026	0.019	0.756	0.969	-0.004	-0.018	0.010	0.537	0.740	-0.013	-0.023	-0.002	0.022	0.193	-0.047	-0.075	-0.019	0.001	0.017
PE(P-19:0/20:4) (a)	-0.010	-0.032	0.012	0.363	0.922	-0.007	-0.020	0.007	0.355	0.595	0.012	0.002	0.023	0.023	0.194	0.011	-0.016	0.038	0.422	0.635
LPC(P-18:0)	-0.008	-0.030	0.014	0.481	0.922	-0.010	-0.024	0.004	0.159	0.432	-0.012	-0.023	-0.002	0.024	0.195	-0.029	-0.056	-0.001	0.040	0.144
PC(P-15:0/20:4) (b)	-0.004	-0.026	0.018	0.716	0.964	-0.003	-0.017	0.011	0.689	0.840	0.012	0.002	0.023	0.023	0.195	0.018	-0.010	0.045	0.206	0.417
CE(20:2)	-0.014	-0.036	0.008	0.205	0.903	-0.002	-0.016	0.012	0.780	0.884	-0.012	-0.023	-0.002	0.024	0.197	-0.032	-0.059	-0.005	0.019	0.089
SM(41:0)	0.016	-0.005	0.038	0.141	0.903	0.000	-0.014	0.014	0.985	0.989	0.012	0.002	0.023	0.025	0.198	-0.002	-0.029	0.025	0.883	0.948
HexCer(d18:2/22:0)	0.012	-0.010	0.034	0.273	0.903	0.006	-0.008	0.019	0.437	0.667	-0.012	-0.023	-0.002	0.025	0.201	-0.013	-0.040	0.015	0.370	0.590
SM(d18:2/20:0)	-0.003	-0.025	0.019	0.782	0.973	-0.001	-0.015	0.013	0.854	0.929	-0.012	-0.023	-0.001	0.026	0.201	-0.055	-0.082	-0.028	0.000	0.005
AC(14:2)	0.003	-0.019	0.025	0.791	0.973	0.000	-0.014	0.013	0.946	0.972	-0.012	-0.023	-0.001	0.026	0.201	-0.035	-0.063	-0.007	0.015	0.076
LPC(19:0) [sn1] (b)	-0.001	-0.023	0.021	0.901	0.985	-0.013	-0.027	0.000	0.057	0.317	-0.012	-0.023	-0.001	0.026	0.201	-0.019	-0.047	0.008	0.169	0.373
PA(36:2)	-0.006	-0.028	0.017	0.625	0.954	-0.007	-0.021	0.007	0.302	0.546	-0.012	-0.023	-0.001	0.027	0.206	0.001	-0.027	0.029	0.933	0.964
TG(54:4) [NL-18:2]	0.005	-0.016	0.027	0.623	0.954	-0.008	-0.022	0.006	0.280	0.524	-0.012	-0.023	-0.001	0.028	0.212	-0.020	-0.047	0.008	0.159	0.359
PE(P-19:0/20:4) (b)	-0.008	-0.030	0.015	0.493	0.922	-0.001	-0.015	0.013	0.919	0.953	0.012	0.001	0.023	0.030	0.223	0.006	-0.021	0.034	0.664	0.815
PE(P-17:0/20:4) (b)	-0.009	-0.031	0.013	0.413	0.922	0.002	-0.012	0.016	0.751	0.877	0.012	0.001	0.023	0.030	0.225	-0.007	-0.034	0.021	0.632	0.794
PE(P-18:1/22:4)	-0.012	-0.034	0.010	0.271	0.903	-0.002	-0.016	0.012	0.781	0.884	-0.012	-0.023	-0.001	0.031	0.226	-0.037	-0.063	-0.010	0.006	0.048
PE(P-16:0/18:1)	-0.006	-0.028	0.016	0.594	0.950	-0.004	-0.018	0.011	0.624	0.793	0.012	0.001	0.023	0.031	0.226	-0.006	-0.034	0.021	0.660	0.814

LPC(20:0) [sn2]	0.016	-0.006	0.038	0.162	0.903	-0.001	-0.015	0.013	0.890	0.939	-0.012	-0.022	-0.001	0.034	0.242	-0.009	-0.036	0.019	0.541	0.725
TG(O-50:1) [NL-15:0]	-0.011	-0.033	0.010	0.309	0.907	-0.003	-0.016	0.011	0.703	0.846	0.012	0.001	0.022	0.034	0.242	0.013	-0.015	0.040	0.359	0.577
SM(38:3) (a)	-0.010	-0.032	0.012	0.369	0.922	-0.004	-0.018	0.010	0.607	0.777	-0.012	-0.022	-0.001	0.035	0.244	-0.051	-0.077	-0.024	0.000	0.008
SM(38:3) (b)	-0.012	-0.034	0.010	0.299	0.903	-0.012	-0.026	0.002	0.090	0.356	-0.012	-0.022	-0.001	0.037	0.253	-0.049	-0.075	-0.023	0.000	0.008
Cer(d18:1/21:0)	-0.014	-0.036	0.008	0.225	0.903	-0.008	-0.022	0.006	0.258	0.509	-0.012	-0.022	-0.001	0.036	0.253	-0.046	-0.073	-0.018	0.001	0.018
LPC(17:0) [sn1]	-0.004	-0.026	0.018	0.709	0.964	-0.013	-0.027	0.001	0.064	0.338	-0.011	-0.022	-0.001	0.037	0.253	-0.033	-0.061	-0.006	0.017	0.085
Cer(d18:2/24:1)	-0.007	-0.029	0.015	0.517	0.922	-0.017	-0.031	-0.004	0.014	0.273	-0.012	-0.022	-0.001	0.037	0.253	-0.031	-0.059	-0.004	0.027	0.110
AC(12:1)	-0.005	-0.027	0.017	0.675	0.964	-0.005	-0.018	0.009	0.501	0.719	-0.011	-0.022	-0.001	0.038	0.253	-0.048	-0.076	-0.020	0.001	0.014
PE(38:5) (a)	-0.013	-0.035	0.009	0.259	0.903	-0.014	-0.028	0.000	0.054	0.317	-0.011	-0.022	-0.001	0.038	0.255	-0.034	-0.062	-0.006	0.018	0.087
TG(54:5) [NL-18:3]	-0.005	-0.027	0.017	0.643	0.960	-0.012	-0.026	0.001	0.081	0.356	-0.011	-0.022	-0.001	0.040	0.266	-0.012	-0.039	0.015	0.392	0.609
GM3(d18:1/18:0)	-0.018	-0.040	0.004	0.114	0.903	-0.009	-0.022	0.005	0.225	0.486	-0.011	-0.022	0.000	0.042	0.267	-0.056	-0.083	-0.028	0.000	0.005
LPE(16:0) [sn2]	-0.017	-0.039	0.005	0.125	0.903	-0.017	-0.030	-0.003	0.014	0.273	-0.011	-0.022	0.000	0.041	0.267	-0.031	-0.058	-0.004	0.025	0.106
PI(38:5) (a)	-0.016	-0.038	0.006	0.155	0.903	-0.006	-0.019	0.008	0.431	0.663	-0.011	-0.022	0.000	0.043	0.267	-0.027	-0.055	0.000	0.053	0.170
TG(O-50:1) [NL-16:0]	-0.013	-0.035	0.008	0.228	0.903	-0.006	-0.019	0.008	0.419	0.650	0.011	0.000	0.022	0.042	0.267	0.018	-0.010	0.046	0.211	0.420
PC(O-40:5)	-0.008	-0.031	0.014	0.456	0.922	-0.009	-0.023	0.005	0.218	0.477	-0.011	-0.022	0.000	0.042	0.267	-0.052	-0.079	-0.026	0.000	0.006
LPE(P-20:0)	0.005	-0.017	0.027	0.629	0.954	-0.013	-0.027	0.001	0.062	0.333	-0.011	-0.022	0.000	0.041	0.267	-0.023	-0.051	0.005	0.107	0.272
PC(18:1_18:1)	-0.004	-0.026	0.018	0.706	0.964	-0.018	-0.032	-0.004	0.013	0.273	-0.011	-0.022	0.000	0.042	0.267	-0.032	-0.059	-0.005	0.020	0.092
TG(O-52:1) [NL-18:1]	-0.013	-0.035	0.008	0.225	0.903	-0.008	-0.022	0.005	0.239	0.495	0.011	0.000	0.022	0.043	0.268	0.018	-0.009	0.046	0.189	0.401
PC(O-18:0/18:1)	-0.012	-0.034	0.010	0.290	0.903	-0.012	-0.026	0.002	0.081	0.356	-0.011	-0.022	0.000	0.048	0.270	-0.051	-0.078	-0.024	0.000	0.008
LPC(O-16:0)	-0.012	-0.033	0.010	0.280	0.903	-0.010	-0.024	0.004	0.153	0.424	-0.011	-0.022	0.000	0.047	0.270	-0.021	-0.049	0.006	0.124	0.301
HexCer(d18:1/22:0)	0.015	-0.007	0.037	0.184	0.903	0.001	-0.013	0.015	0.862	0.930	-0.011	-0.022	0.000	0.049	0.270	-0.020	-0.048	0.008	0.155	0.352
LPC(16:0) [sn1]	-0.014	-0.036	0.007	0.198	0.903	-0.017	-0.031	-0.003	0.014	0.273	-0.011	-0.022	0.000	0.051	0.270	-0.019	-0.046	0.008	0.168	0.373
PC(O-34:4)	-0.015	-0.037	0.007	0.183	0.903	-0.004	-0.018	0.010	0.616	0.787	0.011	0.000	0.021	0.048	0.270	0.010	-0.017	0.037	0.466	0.664
LPC(18:3) [sn2] (a)	-0.012	-0.034	0.010	0.295	0.903	-0.009	-0.023	0.005	0.220	0.479	-0.011	-0.022	0.000	0.047	0.270	-0.010	-0.037	0.018	0.481	0.675
LPC(16:0) [sn2]	-0.015	-0.037	0.007	0.175	0.903	-0.012	-0.026	0.002	0.089	0.356	-0.011	-0.022	0.000	0.047	0.270	-0.005	-0.032	0.022	0.698	0.842
HexCer(d18:1/24:1)	0.008	-0.014	0.030	0.463	0.922	-0.015	-0.028	-0.001	0.034	0.298	-0.011	-0.022	0.000	0.047	0.270	-0.029	-0.057	-0.001	0.040	0.142
TG(O-52:2) [NL-17:1]	-0.008	-0.029	0.014	0.495	0.922	-0.005	-0.019	0.008	0.453	0.678	0.011	0.000	0.021	0.049	0.270	0.021	-0.007	0.048	0.141	0.330
PE(P-16:0/20:5)	0.011	-0.011	0.033	0.336	0.922	-0.006	-0.020	0.008	0.416	0.649	0.011	0.000	0.022	0.047	0.270	0.001	-0.027	0.028	0.961	0.971
LPC(22:5) (n3) [sn1] [104_sn1]	-0.006	-0.028	0.016	0.617	0.950	-0.015	-0.029	-0.001	0.032	0.298	-0.011	-0.022	0.000	0.048	0.270	-0.039	-0.067	-0.011	0.006	0.048
LPC(22:5) [sn2] (n3)	-0.005	-0.027	0.017	0.657	0.960	-0.014	-0.028	-0.001	0.042	0.306	-0.011	-0.021	0.000	0.051	0.270	-0.037	-0.065	-0.010	0.008	0.050
TG(54:6) [NL-22:6]	-0.005	-0.027	0.017	0.652	0.960	-0.011	-0.025	0.003	0.119	0.385	0.011	0.000	0.022	0.051	0.270	0.013	-0.015	0.041	0.366	0.586
DG(18:1_22:6)	0.004	-0.018	0.026	0.735	0.964	-0.012	-0.026	0.002	0.086	0.356	0.011	0.000	0.022	0.049	0.270	0.009	-0.019	0.038	0.508	0.702
TG(56:7) [NL-22:6]	0.005	-0.017	0.027	0.668	0.964	-0.014	-0.028	0.000	0.051	0.317	0.011	0.000	0.022	0.047	0.270	0.007	-0.021	0.035	0.640	0.801
PE(P-18:1/20:4) (a)	-0.003	-0.025	0.019	0.794	0.974	0.008	-0.006	0.022	0.272	0.521	0.011	0.000	0.022	0.046	0.270	-0.003	-0.031	0.025	0.826	0.923
AC(24:1)	0.002	-0.020	0.024	0.848	0.981	-0.010	-0.024	0.004	0.172	0.438	-0.011	-0.022	0.000	0.049	0.270	-0.020	-0.047	0.006	0.135	0.320
LPC(18:2) [+OH]	0.001	-0.021	0.024	0.898	0.983	-0.010	-0.024	0.004	0.163	0.432	-0.011	-0.022	0.000	0.051	0.270	-0.002	-0.030	0.026	0.900	0.952
HexCer(d18:1/24:0)	0.001	-0.021	0.023	0.913	0.987	0.000	-0.013	0.014	0.956	0.976	-0.011	-0.022	0.000	0.044	0.270	-0.021	-0.048	0.007	0.142	0.330
LPE(P-18:1)	-0.001	-0.022	0.021	0.962	0.995	-0.001	-0.016	0.013	0.856	0.929	-0.011	-0.021	0.000	0.051	0.270	-0.031	-0.058	-0.004	0.026	0.107
PE(O-36:5)	0.001	-0.022	0.023	0.964	0.995	-0.009	-0.023	0.005	0.212	0.475	0.011	0.000	0.021	0.051	0.270	0.004	-0.024	0.031	0.793	0.904
TG(52:4) [NL-18:2]	-0.012	-0.034	0.010	0.276	0.903	-0.007	-0.021	0.007	0.301	0.546	-0.011	-0.021	0.000	0.053	0.274	-0.023	-0.050	0.005	0.108	0.274
LPC(18:0) [sn1]	-0.005	-0.027	0.017	0.649	0.960	-0.009	-0.023	0.004	0.180	0.450	-0.011	-0.021	0.000	0.052	0.274	-0.027	-0.054	0.001	0.056	0.173
PC(16:1_18:2)	-0.013	-0.035	0.009	0.253	0.903	-0.008	-0.022	0.006	0.267	0.520	-0.011	-0.021	0.000	0.053	0.275	-0.032	-0.059	-0.006	0.018	0.086
dhCer(d18:0/20:0)	-0.007	-0.029	0.015	0.543	0.929	0.001	-0.013	0.014	0.938	0.969	0.011	0.000	0.021	0.054	0.278	-0.002	-0.030	0.025	0.881	0.948
AC(14:1)	0.005	-0.017	0.027	0.629	0.954	-0.006	-0.020	0.007	0.358	0.598	-0.011	-0.021	0.000	0.055	0.280	-0.046	-0.073	-0.018	0.001	0.020
HexCer(d18:2/18:0)	0.002	-0.020	0.024	0.861	0.981	-0.017	-0.031	-0.003	0.017	0.273	-0.011	-0.021	0.000	0.056	0.282	-0.034	-0.062	-0.006	0.017	0.084
PE(P-16:0/22:6)	0.002	-0.021	0.024	0.882	0.981	0.000	-0.014	0.015	0.962	0.979	0.011	0.000	0.021	0.056	0.283	0.002	-0.026	0.030	0.878	0.948
Cer(d18:2/22:0)	-0.004	-0.026	0.018	0.730	0.964	-0.003	-0.017	0.012	0.698	0.845	-0.011	-0.021	0.000	0.057	0.284	-0.016	-0.044	0.012	0.259	0.477
dhCer(d18:0/22:0)	0.001	-0.021	0.023	0.914	0.987	0.009	-0.005	0.023	0.213	0.475	0.010	0.000	0.021	0.058	0.287	0.013	-0.014	0.040	0.358	0.577
PE(P-18:1/20:5) (a)	0.013	-0.009	0.035	0.250	0.903	-0.008	-0.022	0.006	0.269	0.520	0.010	0.000	0.021	0.060	0.292	-0.009	-0.036	0.019	0.532	0.719
PE(P-18:1/18:2) (b)	-0.008	-0.030	0.014	0.474	0.922	0.001	-0.013	0.015	0.906	0.944	-0.010	-0.021	0.000	0.060	0.292	-0.034	-0.060	-0.007	0.014	0.072
LPC(18:0) [sn2]	-0.003	-0.025	0.019	0.781	0.973	-0.009	-0.022	0.005	0.226	0.487	-0.010	-0.021	0.000	0.061	0.292	-0.025	-0.052	0.003	0.077	0.215
PC(P-16:0/22:6)	-0.001	-0.023	0.022	0.961	0.995	-0.007	-0.021	0.007	0.340	0.578	0.010	0.000	0.021	0.060	0.292	-0.001	-0.029	0.026	0.924	0.964
Cer1P(d18:1/16:0)	-0.004	-0.025	0.018	0.747	0.964	-0.001	-0.015	0.013	0.898	0.942	-0.010	-0.021	0.000	0.061	0.293	-0.025	-0.053	0.003	0.078	0.216
SM(44:3)	-0.008	-0.030	0.015	0.500	0.922	-0.008	-0.022	0.006	0.256	0.507	-0.010	-0.021	0.000	0.062	0.294	-0.039	-0.066	-0.012	0.004	0.042
TG(52:3) [NL-16:1]	0.003	-0.018	0.025	0.757	0.969	-0.019	-0.033	-0.006	0.006	0.259	-0.010	-0.021	0.001	0.062	0.294	-0.053	-0.080	-0.025	0.000	0.008

AC(18:1)-OH	0.002	-0.020	0.024	0.878	0.981	-0.008	-0.022	0.005	0.240	0.495	-0.010	-0.021	0.001	0.063	0.294	-0.041	-0.068	-0.013	0.004	0.038
PC(40:8)	-0.002	-0.024	0.021	0.874	0.981	-0.009	-0.023	0.005	0.232	0.488	-0.010	-0.021	0.001	0.064	0.300	-0.026	-0.054	0.001	0.060	0.181
LPE(18:1) [sn1]	-0.013	-0.035	0.009	0.263	0.903	-0.015	-0.028	-0.001	0.038	0.301	-0.010	-0.021	0.001	0.067	0.309	-0.019	-0.047	0.008	0.174	0.378
Hex3Cer(d18:1/22:0)	0.001	-0.021	0.023	0.948	0.995	-0.004	-0.018	0.010	0.607	0.777	-0.010	-0.021	0.001	0.067	0.309	-0.045	-0.072	-0.018	0.001	0.018
Cer(d18:1/18:0)	-0.026	-0.048	-0.005	0.017	0.903	-0.013	-0.027	0.000	0.056	0.317	-0.010	-0.021	0.001	0.068	0.310	-0.049	-0.076	-0.022	0.001	0.011
PC(O-18:1/18:1)	0.000	-0.022	0.022	1.000	1.000	-0.011	-0.025	0.003	0.129	0.390	-0.010	-0.021	0.001	0.068	0.310	-0.036	-0.063	-0.009	0.009	0.056
PE(P-18:0/20:4)	-0.006	-0.028	0.016	0.568	0.933	0.006	-0.008	0.021	0.400	0.638	0.010	-0.001	0.021	0.069	0.312	-0.002	-0.030	0.026	0.887	0.948
HexCer(d16:1/22:0)	0.009	-0.013	0.032	0.404	0.922	-0.009	-0.023	0.004	0.186	0.453	-0.010	-0.021	0.001	0.069	0.312	-0.011	-0.039	0.016	0.417	0.631
AC(12:0)	-0.002	-0.024	0.021	0.891	0.981	-0.007	-0.021	0.007	0.304	0.546	-0.010	-0.021	0.001	0.070	0.312	-0.050	-0.079	-0.022	0.000	0.010
LPC(15-MHDA) [sn1] & LPC(17:0) [sn2]	-0.003	-0.025	0.019	0.791	0.973	-0.015	-0.029	-0.001	0.037	0.301	-0.010	-0.021	0.001	0.071	0.317	-0.036	-0.063	-0.008	0.011	0.064
LPE(18:0) [sn1]	-0.018	-0.040	0.004	0.111	0.903	-0.012	-0.026	0.001	0.073	0.350	-0.010	-0.021	0.001	0.072	0.319	-0.021	-0.049	0.006	0.127	0.309
PC(P-16:0/20:5)	0.008	-0.014	0.030	0.481	0.922	-0.009	-0.023	0.005	0.219	0.477	0.010	-0.001	0.021	0.073	0.319	0.003	-0.025	0.031	0.837	0.928
S1P(d18:0)	-0.005	-0.027	0.017	0.676	0.964	-0.010	-0.024	0.004	0.145	0.406	-0.010	-0.020	0.001	0.073	0.319	-0.022	-0.050	0.006	0.119	0.293
PE(P-17:0/22:6) (b)	-0.002	-0.024	0.021	0.879	0.981	-0.002	-0.017	0.012	0.749	0.877	0.010	-0.001	0.021	0.073	0.319	-0.003	-0.032	0.025	0.826	0.923
PE(P-16:0/20:3) (a)	-0.010	-0.033	0.012	0.356	0.922	-0.005	-0.019	0.009	0.465	0.686	0.010	-0.001	0.021	0.074	0.320	-0.014	-0.042	0.013	0.303	0.526
AC(16:0)	-0.014	-0.036	0.008	0.211	0.903	-0.015	-0.029	-0.002	0.030	0.289	-0.010	-0.020	0.001	0.075	0.323	-0.048	-0.075	-0.022	0.000	0.010
PC(38:4) (b)	-0.016	-0.037	0.006	0.157	0.903	-0.003	-0.017	0.011	0.640	0.807	-0.010	-0.021	0.001	0.076	0.323	-0.039	-0.066	-0.013	0.004	0.042
LPC(22:4) [sn1]	-0.011	-0.033	0.010	0.300	0.903	-0.004	-0.018	0.010	0.566	0.748	-0.010	-0.020	0.001	0.076	0.323	-0.018	-0.045	0.010	0.208	0.419
AC(14:0)	-0.003	-0.025	0.019	0.791	0.973	-0.013	-0.027	0.000	0.057	0.317	-0.010	-0.020	0.001	0.076	0.323	-0.046	-0.074	-0.019	0.001	0.017
LPE(18:1) [sn2]	-0.013	-0.035	0.009	0.263	0.903	-0.013	-0.027	0.000	0.055	0.317	-0.010	-0.021	0.001	0.077	0.324	-0.020	-0.048	0.007	0.149	0.340
Cer(d18:2/16:0)	-0.003	-0.025	0.019	0.770	0.973	-0.006	-0.021	0.008	0.368	0.603	-0.010	-0.021	0.001	0.078	0.325	-0.033	-0.061	-0.006	0.018	0.086
TG(O-50:3) [NL-18:2]	-0.030	-0.052	-0.009	0.006	0.903	0.010	-0.003	0.024	0.138	0.403	0.010	-0.001	0.020	0.078	0.326	0.020	-0.006	0.047	0.133	0.318
Cer(d18:1/24:1)	-0.020	-0.042	0.002	0.070	0.903	-0.019	-0.033	-0.006	0.006	0.259	-0.010	-0.020	0.001	0.079	0.328	-0.040	-0.067	-0.012	0.005	0.044
LPC(22:0) [sn2]	0.012	-0.009	0.034	0.266	0.903	0.005	-0.009	0.018	0.521	0.727	-0.010	-0.020	0.001	0.080	0.328	0.004	-0.023	0.031	0.768	0.892
Cer(d18:2/18:0)	-0.015	-0.037	0.007	0.181	0.903	-0.010	-0.023	0.004	0.162	0.432	-0.010	-0.020	0.001	0.081	0.330	-0.044	-0.072	-0.017	0.002	0.023
dxCA	-0.013	-0.036	0.009	0.250	0.903	0.001	-0.013	0.014	0.941	0.971	-0.010	-0.021	0.001	0.082	0.333	-0.015	-0.042	0.012	0.279	0.503
PE(18:1_18:2)	-0.005	-0.027	0.017	0.649	0.960	-0.012	-0.026	0.001	0.080	0.356	-0.010	-0.020	0.001	0.083	0.337	-0.005	-0.033	0.023	0.728	0.863
PE(P-18:0/22:6)	0.003	-0.019	0.025	0.798	0.975	-0.004	-0.019	0.010	0.544	0.745	0.010	-0.001	0.020	0.086	0.345	-0.003	-0.031	0.025	0.815	0.918
SM(d18:2/18:0)	-0.014	-0.036	0.008	0.208	0.903	-0.005	-0.019	0.008	0.448	0.673	-0.009	-0.020	0.001	0.087	0.346	-0.050	-0.077	-0.023	0.000	0.008
LPE(20:4) [sn2]	-0.016	-0.038	0.006	0.164	0.903	-0.010	-0.024	0.004	0.159	0.432	-0.009	-0.020	0.001	0.090	0.346	-0.043	-0.070	-0.015	0.003	0.030
PC(16:0_20:3) (a)	-0.012	-0.034	0.010	0.276	0.903	-0.011	-0.025	0.003	0.119	0.385	-0.009	-0.020	0.001	0.089	0.346	-0.037	-0.064	-0.011	0.006	0.048
LPC(22:0) [sn1]	0.014	-0.008	0.036	0.216	0.903	0.002	-0.012	0.016	0.769	0.881	-0.009	-0.020	0.001	0.090	0.346	0.008	-0.020	0.035	0.590	0.756
HexCer(d16:1/18:0)	-0.009	-0.032	0.013	0.411	0.922	-0.010	-0.023	0.004	0.162	0.432	-0.009	-0.020	0.001	0.089	0.346	-0.034	-0.062	-0.007	0.014	0.074
PE(P-18:0/20:5)	0.010	-0.012	0.033	0.363	0.922	-0.008	-0.023	0.006	0.246	0.501	0.009	-0.001	0.020	0.089	0.346	-0.005	-0.032	0.023	0.748	0.882
PC(O-36:0)	-0.006	-0.028	0.016	0.590	0.948	-0.008	-0.022	0.006	0.274	0.521	-0.009	-0.020	0.001	0.089	0.346	-0.044	-0.071	-0.017	0.001	0.021
TG(O-52:2) [NL-18:1]	-0.005	-0.026	0.017	0.674	0.964	-0.004	-0.018	0.010	0.554	0.748	0.009	-0.001	0.020	0.089	0.346	0.018	-0.010	0.046	0.203	0.416
TG(54:6) [NL-18:3]	-0.001	-0.023	0.021	0.897	0.983	-0.005	-0.018	0.009	0.519	0.727	-0.009	-0.020	0.001	0.087	0.346	-0.002	-0.029	0.026	0.905	0.954
LPC(19:1) (a)	-0.005	-0.027	0.018	0.687	0.964	-0.010	-0.024	0.004	0.148	0.410	-0.009	-0.020	0.001	0.091	0.347	-0.028	-0.056	-0.001	0.044	0.150
DG(16:0_22:6)	-0.003	-0.026	0.019	0.762	0.969	-0.011	-0.025	0.003	0.115	0.382	0.009	-0.002	0.020	0.092	0.350	0.009	-0.018	0.037	0.513	0.706
DG(18:2_22:6)	0.003	-0.019	0.025	0.782	0.973	-0.008	-0.022	0.006	0.280	0.524	0.009	-0.002	0.020	0.093	0.351	0.008	-0.020	0.036	0.568	0.743
LPC(19:0) [sn1] (a) & LPC(19:0) [sn2] (b)	0.003	-0.019	0.025	0.760	0.969	-0.010	-0.024	0.004	0.165	0.432	-0.009	-0.020	0.002	0.094	0.354	-0.019	-0.046	0.008	0.172	0.376
LPC(20:4) [+OH]	0.006	-0.016	0.029	0.571	0.933	-0.002	-0.015	0.012	0.819	0.907	-0.009	-0.020	0.002	0.095	0.355	-0.021	-0.048	0.006	0.134	0.320
CE(16:0)	-0.002	-0.024	0.020	0.847	0.981	-0.004	-0.018	0.010	0.548	0.747	-0.009	-0.020	0.002	0.095	0.355	-0.038	-0.065	-0.010	0.007	0.049
PE(P-20:1/20:4)	0.004	-0.019	0.026	0.756	0.969	0.001	-0.012	0.015	0.871	0.932	0.009	-0.002	0.020	0.096	0.356	0.016	-0.011	0.043	0.252	0.465
HexCer(d18:2/24:0)	0.013	-0.009	0.035	0.243	0.903	-0.003	-0.017	0.011	0.686	0.840	-0.009	-0.020	0.002	0.097	0.358	-0.012	-0.040	0.015	0.376	0.592
LPE(20:4) [sn1]	-0.019	-0.041	0.003	0.095	0.903	-0.010	-0.024	0.004	0.157	0.432	-0.009	-0.020	0.002	0.109	0.389	-0.038	-0.065	-0.010	0.008	0.053
LPC(O-24:0)	-0.012	-0.034	0.010	0.284	0.903	-0.021	-0.035	-0.007	0.004	0.259	-0.009	-0.020	0.002	0.107	0.389	-0.036	-0.064	-0.009	0.010	0.062
LPE(18:0) [sn2]	-0.011	-0.033	0.010	0.304	0.903	-0.010	-0.024	0.003	0.143	0.406	-0.009	-0.020	0.002	0.109	0.389	-0.018	-0.045	0.010	0.202	0.416
PC(P-15:0/20:4) (a)	-0.007	-0.029	0.015	0.529	0.922	-0.007	-0.021	0.007	0.317	0.557	0.009	-0.002	0.019	0.108	0.389	0.021	-0.006	0.048	0.131	0.317
Cer(d20:1/23:0)	-0.007	-0.029	0.015	0.527	0.922	-0.006	-0.020	0.008	0.395	0.634	0.009	-0.002	0.020	0.110	0.389	-0.014	-0.041	0.013	0.314	0.537
SHexCer(d18:1/24:1(OH))	0.005	-0.017	0.027	0.667	0.964	-0.005	-0.019	0.009	0.493	0.710	-0.009	-0.020	0.002	0.109	0.389	-0.017	-0.046	0.011	0.239	0.452
PC(O-16:0/22:6)	-0.002	-0.024	0.020	0.851	0.981	-0.008	-0.022	0.006	0.285	0.530	0.009	-0.002	0.020	0.108	0.389	-0.008	-0.036	0.020	0.573	0.745
PC(16:1_22:6)	0.001	-0.021	0.023	0.942	0.995	-0.012	-0.026	0.002	0.085	0.356	-0.009	-0.020	0.002	0.106	0.389	-0.038	-0.065	-0.011	0.007	0.048
PC(38:6) (a)	0.001	-0.021	0.024	0.912	0.987	-0.006	-0.020	0.008	0.391	0.632	-0.009	-0.020	0.002	0.111	0.391	-0.025	-0.052	0.003	0.079	0.218

TG(54:0) [NL-18:0]	-0.024	-0.046	-0.002	0.030	0.903	-0.016	-0.029	-0.002	0.021	0.273	0.009	-0.002	0.019	0.115	0.403	0.014	-0.014	0.042	0.322	0.540
Cer(d18:2/14:0)	-0.005	-0.027	0.017	0.679	0.964	-0.007	-0.021	0.007	0.330	0.572	-0.009	-0.020	0.002	0.115	0.404	-0.042	-0.070	-0.015	0.003	0.032
Sph(d18:2)	0.012	-0.010	0.034	0.287	0.903	-0.007	-0.021	0.007	0.304	0.546	0.009	-0.002	0.020	0.119	0.404	0.015	-0.010	0.041	0.245	0.458
TG(50:0) [NL-18:0]	-0.024	-0.046	-0.002	0.032	0.903	-0.012	-0.026	0.001	0.070	0.348	0.008	-0.002	0.019	0.118	0.404	0.012	-0.015	0.040	0.381	0.596
PI(34:0)	-0.019	-0.041	0.004	0.101	0.903	-0.004	-0.019	0.010	0.555	0.748	0.009	-0.002	0.019	0.118	0.404	-0.011	-0.038	0.016	0.432	0.640
TG(51:0) [NL-16:0]	-0.023	-0.044	-0.001	0.044	0.903	-0.012	-0.026	0.001	0.069	0.347	0.009	-0.002	0.019	0.116	0.404	0.009	-0.018	0.037	0.518	0.709
TG(O-52:2) [NL-16:0]	-0.009	-0.030	0.013	0.436	0.922	-0.003	-0.017	0.011	0.655	0.817	0.009	-0.002	0.019	0.118	0.404	0.021	-0.007	0.049	0.138	0.325
PC(O-18:1/18:2)	-0.002	-0.024	0.020	0.847	0.981	-0.002	-0.016	0.012	0.746	0.876	-0.009	-0.020	0.002	0.118	0.404	-0.025	-0.053	0.002	0.069	0.195
SM(d18:1/16:0)	-0.010	-0.031	0.012	0.396	0.922	-0.007	-0.021	0.007	0.332	0.572	-0.009	-0.020	0.002	0.119	0.404	-0.050	-0.077	-0.023	0.000	0.008
TG(O-50:2) [NL-18:2]	-0.013	-0.035	0.009	0.247	0.903	0.002	-0.012	0.016	0.781	0.884	0.009	-0.002	0.019	0.121	0.405	0.025	-0.003	0.053	0.078	0.216
PI(16:0/16:0)	-0.019	-0.041	0.003	0.096	0.903	0.001	-0.013	0.014	0.944	0.971	0.009	-0.002	0.019	0.121	0.405	0.002	-0.025	0.029	0.901	0.952
PC(17:1_18:2)	-0.005	-0.027	0.018	0.689	0.964	-0.013	-0.026	0.001	0.076	0.356	-0.009	-0.019	0.002	0.120	0.405	-0.029	-0.056	-0.003	0.032	0.127
LPE(16:0) [sn1]	-0.017	-0.039	0.005	0.129	0.903	-0.017	-0.030	-0.003	0.015	0.273	-0.008	-0.019	0.002	0.122	0.406	-0.027	-0.054	0.001	0.055	0.173
TG(56:8) [NL-22:6]	0.000	-0.022	0.023	0.965	0.995	-0.011	-0.025	0.003	0.132	0.395	0.009	-0.002	0.019	0.124	0.411	0.010	-0.018	0.038	0.468	0.665
LPC(22:4) [sn2]	-0.012	-0.034	0.009	0.269	0.903	-0.004	-0.018	0.010	0.560	0.748	-0.008	-0.019	0.002	0.129	0.426	-0.019	-0.046	0.009	0.181	0.387
LPC(17:1) (a) [sn1] [104_sn1]	-0.014	-0.036	0.008	0.229	0.903	-0.019	-0.032	-0.005	0.007	0.259	-0.008	-0.019	0.002	0.131	0.429	-0.030	-0.057	-0.003	0.032	0.127
PC(16:0_18:0)	-0.010	-0.032	0.012	0.385	0.922	-0.008	-0.022	0.006	0.247	0.501	-0.008	-0.019	0.002	0.131	0.429	-0.040	-0.067	-0.013	0.003	0.037
Cer(d17:1/16:0)	-0.004	-0.026	0.019	0.736	0.964	-0.001	-0.015	0.013	0.880	0.934	-0.008	-0.019	0.003	0.133	0.432	-0.010	-0.038	0.017	0.469	0.665
PI(16:0_20:3) (b)	-0.014	-0.036	0.008	0.227	0.903	-0.014	-0.028	0.000	0.050	0.317	-0.008	-0.019	0.003	0.138	0.442	-0.027	-0.054	0.000	0.054	0.172
TG(50:3) [NL-14:0]	-0.014	-0.036	0.007	0.196	0.903	-0.015	-0.029	-0.002	0.027	0.285	-0.008	-0.019	0.003	0.141	0.442	-0.023	-0.052	0.005	0.105	0.269
LPC(18:3) (a) [sn1] [104_sn1]	-0.013	-0.035	0.010	0.270	0.903	-0.007	-0.021	0.007	0.301	0.546	-0.008	-0.019	0.003	0.139	0.442	-0.002	-0.030	0.025	0.880	0.948
TG(53:2) [NL-17:1]	-0.017	-0.038	0.005	0.133	0.903	-0.016	-0.029	-0.002	0.022	0.273	0.008	-0.003	0.019	0.138	0.442	0.000	-0.028	0.027	0.993	0.996
S1P(d18:1)	-0.010	-0.032	0.012	0.388	0.922	-0.015	-0.029	-0.001	0.040	0.305	-0.008	-0.019	0.003	0.141	0.442	-0.027	-0.054	0.000	0.052	0.170
CE(20:4) [+OH]	-0.005	-0.027	0.018	0.686	0.964	-0.004	-0.018	0.010	0.564	0.748	-0.008	-0.019	0.003	0.139	0.442	-0.020	-0.048	0.008	0.169	0.373
FA(20:4)	0.001	-0.021	0.023	0.912	0.987	-0.004	-0.018	0.010	0.583	0.763	-0.008	-0.019	0.003	0.139	0.442	-0.015	-0.042	0.013	0.299	0.523
PA(36:3)	0.000	-0.021	0.022	0.968	0.995	-0.007	-0.021	0.008	0.366	0.602	-0.008	-0.019	0.003	0.140	0.442	-0.008	-0.035	0.020	0.583	0.753
PE(O-16:0/22:6)	0.000	-0.022	0.022	0.997	0.999	0.001	-0.013	0.016	0.872	0.932	0.008	-0.003	0.019	0.137	0.442	-0.001	-0.029	0.027	0.931	0.964
TG(O-50:2) [NL-18:1]	-0.002	-0.024	0.020	0.842	0.981	-0.010	-0.024	0.004	0.172	0.438	0.008	-0.003	0.019	0.143	0.447	-0.001	-0.030	0.027	0.925	0.964
TG(54:1) [NL-18:1]	-0.021	-0.042	0.001	0.065	0.903	-0.013	-0.027	0.000	0.055	0.317	0.008	-0.003	0.019	0.144	0.448	0.012	-0.016	0.040	0.404	0.620
TG(58:8) [NL-22:6]	0.007	-0.015	0.029	0.559	0.933	-0.011	-0.025	0.003	0.133	0.395	0.008	-0.003	0.019	0.146	0.451	0.004	-0.024	0.032	0.793	0.904
PC(O-16:0/20:3)	-0.007	-0.029	0.015	0.518	0.922	-0.008	-0.022	0.006	0.254	0.506	-0.008	-0.019	0.003	0.150	0.457	-0.039	-0.065	-0.012	0.005	0.044
PC(18:1_20:3)	-0.009	-0.031	0.013	0.413	0.922	-0.010	-0.024	0.003	0.142	0.406	-0.008	-0.019	0.003	0.150	0.457	-0.034	-0.061	-0.007	0.014	0.074
Cer(d17:1/24:1)	-0.010	-0.032	0.012	0.364	0.922	-0.017	-0.031	-0.003	0.018	0.273	-0.008	-0.019	0.003	0.149	0.457	-0.029	-0.057	-0.002	0.038	0.138
PE(P-18:1/18:1) (a)	0.010	-0.012	0.033	0.363	0.922	0.002	-0.012	0.016	0.793	0.891	0.008	-0.003	0.019	0.149	0.457	-0.008	-0.036	0.020	0.562	0.739
DE(22:6)	0.010	-0.012	0.032	0.368	0.922	0.004	-0.010	0.018	0.566	0.748	-0.008	-0.019	0.003	0.152	0.461	-0.024	-0.051	0.004	0.099	0.256
TG(O-52:0) [NL-16:0]	-0.023	-0.045	-0.002	0.035	0.903	-0.009	-0.022	0.004	0.190	0.454	0.008	-0.003	0.018	0.156	0.463	0.008	-0.019	0.035	0.552	0.730
PC(16:1_20:4)	-0.009	-0.031	0.013	0.421	0.922	-0.003	-0.017	0.011	0.696	0.845	-0.008	-0.019	0.003	0.157	0.463	-0.032	-0.060	-0.005	0.023	0.099
PC(P-16:0/20:4)	-0.010	-0.032	0.012	0.389	0.922	0.001	-0.013	0.015	0.845	0.927	0.008	-0.003	0.019	0.157	0.463	-0.002	-0.030	0.025	0.860	0.937
dhCer(d18:0/16:0)	-0.008	-0.030	0.014	0.479	0.922	-0.003	-0.017	0.011	0.651	0.815	0.008	-0.003	0.018	0.154	0.463	0.001	-0.026	0.029	0.932	0.964
PE(P-18:1/22:6) (b)	0.004	-0.018	0.026	0.734	0.964	-0.006	-0.020	0.009	0.435	0.666	-0.008	-0.019	0.003	0.155	0.463	-0.036	-0.062	-0.009	0.008	0.053
PC(18:2_18:2)	-0.004	-0.026	0.018	0.742	0.964	-0.001	-0.015	0.013	0.855	0.929	-0.008	-0.019	0.003	0.154	0.463	-0.003	-0.031	0.024	0.815	0.918
PC(P-17:0/20:4) (b)	-0.003	-0.025	0.019	0.812	0.980	-0.002	-0.016	0.012	0.778	0.884	0.008	-0.003	0.018	0.155	0.463	-0.001	-0.028	0.026	0.942	0.966
LPC(18:2) [sn1]	-0.008	-0.030	0.014	0.476	0.922	-0.008	-0.022	0.005	0.241	0.495	-0.008	-0.019	0.003	0.159	0.466	-0.014	-0.042	0.014	0.330	0.547
PIP1(38:4)	-0.006	-0.028	0.016	0.601	0.950	-0.007	-0.021	0.006	0.290	0.536	-0.008	-0.018	0.003	0.159	0.466	-0.035	-0.062	-0.008	0.011	0.062
TG(50:3) [NL-14:1]	-0.012	-0.034	0.010	0.278	0.903	-0.017	-0.031	-0.004	0.012	0.273	-0.008	-0.019	0.003	0.160	0.466	-0.033	-0.061	-0.005	0.023	0.101
CE(18:2) [+OH]	-0.008	-0.030	0.014	0.468	0.922	-0.012	-0.026	0.002	0.089	0.356	-0.008	-0.019	0.003	0.162	0.472	-0.017	-0.045	0.010	0.225	0.434
PC(P-18:1/18:1)	-0.003	-0.025	0.019	0.779	0.973	-0.008	-0.022	0.005	0.236	0.493	-0.008	-0.019	0.003	0.164	0.474	-0.035	-0.062	-0.008	0.012	0.066
PI(18:0_20:4)	-0.019	-0.041	0.002	0.077	0.903	-0.014	-0.027	0.000	0.055	0.317	-0.008	-0.018	0.003	0.165	0.475	-0.040	-0.067	-0.013	0.004	0.038
TG(O-52:1) [NL-16:0]	-0.015	-0.036	0.007	0.177	0.903	-0.007	-0.020	0.007	0.337	0.574	0.008	-0.003	0.018	0.165	0.475	0.009	-0.018	0.036	0.529	0.718
PE(P-18:1/22:6) (a)	0.012	-0.010	0.034	0.286	0.903	-0.003	-0.018	0.011	0.682	0.840	0.008	-0.003	0.018	0.167	0.477	-0.009	-0.037	0.019	0.536	0.720
TG(51:1) [NL-17:0]	-0.024	-0.045	-0.002	0.033	0.903	-0.015	-0.029	-0.001	0.031	0.291	0.007	-0.003	0.018	0.169	0.482	-0.001	-0.029	0.027	0.954	0.969
SM(40:3) (a)	-0.010	-0.032	0.012	0.389	0.922	-0.007	-0.021	0.006	0.293	0.536	-0.008	-0.018	0.003	0.172	0.484	-0.045	-0.071	-0.018	0.001	0.018
SHexCer(d18:1/16:0(OH))	-0.007	-0.029	0.015	0.533	0.923	0.001	-0.013	0.015	0.889	0.939	-0.008	-0.018	0.003	0.172	0.484	-0.032	-0.060	-0.004	0.025	0.106
DG(18:2_18:2)	-0.006	-0.028	0.016	0.576	0.933	-0.002	-0.016	0.012	0.779	0.884	-0.008	-0.018	0.003	0.171	0.484	-0.012	-0.039	0.015	0.394	0.609

LPC(18:3) [sn1] (a) & LPC(18:3) [sn2] (b)	-0.013	-0.035	0.010	0.261	0.903	-0.004	-0.018	0.010	0.561	0.748	-0.007	-0.018	0.003	0.174	0.487	-0.001	-0.028	0.026	0.941	0.966
TG(52:3) [NL-18:2]	-0.010	-0.031	0.011	0.367	0.922	-0.012	-0.026	0.002	0.092	0.356	-0.007	-0.018	0.003	0.174	0.487	-0.027	-0.055	0.001	0.057	0.174
TG(52:4) [NL-18:3]	-0.019	-0.041	0.002	0.081	0.903	-0.015	-0.029	-0.002	0.028	0.285	-0.007	-0.018	0.003	0.180	0.487	-0.022	-0.050	0.006	0.123	0.300
TG(52:1) [NL-18:0]	-0.018	-0.040	0.004	0.108	0.903	-0.013	-0.027	0.000	0.057	0.317	0.007	-0.003	0.018	0.179	0.487	0.006	-0.021	0.034	0.657	0.814
PS(40:5)	0.017	-0.005	0.039	0.131	0.903	-0.013	-0.027	0.000	0.058	0.319	-0.007	-0.018	0.003	0.179	0.487	-0.004	-0.032	0.024	0.778	0.894
PE(O-16:0/20:4)	-0.008	-0.030	0.014	0.452	0.922	0.002	-0.012	0.016	0.742	0.874	0.007	-0.003	0.018	0.179	0.487	-0.002	-0.030	0.026	0.886	0.948
PI(36:2)	-0.007	-0.028	0.015	0.547	0.929	0.000	-0.015	0.014	0.948	0.972	-0.007	-0.018	0.003	0.178	0.487	-0.018	-0.045	0.009	0.191	0.402
PE(P-18:1/18:1) (b)	-0.006	-0.029	0.016	0.576	0.933	0.004	-0.010	0.018	0.587	0.764	-0.007	-0.018	0.003	0.178	0.487	-0.032	-0.058	-0.005	0.019	0.090
TG(54:7) [NL-22:6]	-0.005	-0.027	0.018	0.689	0.964	-0.015	-0.029	-0.001	0.037	0.301	0.008	-0.003	0.018	0.176	0.487	0.004	-0.024	0.032	0.767	0.892
AC(22:5)	0.003	-0.019	0.025	0.798	0.975	-0.015	-0.029	-0.002	0.029	0.289	-0.007	-0.018	0.003	0.177	0.487	-0.011	-0.038	0.016	0.417	0.631
PE(15-MHDA_18:1)	-0.015	-0.037	0.008	0.203	0.903	-0.014	-0.028	0.000	0.045	0.306	0.007	-0.004	0.018	0.187	0.499	-0.019	-0.047	0.009	0.188	0.401
PE(16:1_18:2)	-0.021	-0.043	0.001	0.063	0.903	-0.013	-0.026	0.001	0.073	0.350	-0.007	-0.018	0.004	0.189	0.499	-0.017	-0.044	0.010	0.205	0.416
LPC(18:3) [sn1] (b)	-0.016	-0.038	0.007	0.173	0.903	-0.008	-0.022	0.006	0.263	0.514	-0.007	-0.018	0.004	0.189	0.499	0.002	-0.026	0.029	0.914	0.959
LPC(P-16:0)	-0.010	-0.032	0.012	0.369	0.922	-0.007	-0.021	0.007	0.324	0.563	-0.007	-0.018	0.004	0.187	0.499	-0.015	-0.042	0.012	0.284	0.509
PE(P-16:0/20:3) (b)	-0.009	-0.031	0.013	0.426	0.922	-0.001	-0.015	0.013	0.879	0.934	0.007	-0.004	0.018	0.186	0.499	-0.010	-0.038	0.017	0.456	0.660
PC(O-36:5)	0.010	-0.012	0.032	0.381	0.922	-0.009	-0.023	0.005	0.194	0.454	0.007	-0.004	0.018	0.187	0.499	-0.002	-0.029	0.026	0.910	0.956
PE(O-38:5) (a)	-0.007	-0.029	0.016	0.560	0.933	0.007	-0.007	0.021	0.309	0.550	0.007	-0.004	0.018	0.188	0.499	-0.009	-0.037	0.019	0.529	0.718
PE(O-38:5) (b)	-0.002	-0.025	0.020	0.826	0.981	-0.004	-0.018	0.010	0.586	0.763	0.007	-0.003	0.018	0.186	0.499	-0.013	-0.040	0.014	0.343	0.563
HexCer(d18:1/24:0)	0.012	-0.010	0.034	0.285	0.903	-0.001	-0.015	0.012	0.859	0.929	-0.007	-0.018	0.004	0.191	0.501	-0.014	-0.042	0.013	0.304	0.527
Cer(d18:2/23:0)	-0.009	-0.031	0.013	0.431	0.922	-0.005	-0.019	0.009	0.512	0.724	-0.007	-0.018	0.004	0.191	0.501	-0.022	-0.050	0.005	0.110	0.276
TG(O-50:1) [NL-17:1]	-0.007	-0.029	0.014	0.512	0.922	-0.006	-0.020	0.008	0.393	0.633	0.007	-0.004	0.018	0.194	0.505	0.019	-0.008	0.047	0.173	0.378
PE(16:1_20:4)	-0.022	-0.044	0.000	0.053	0.903	-0.010	-0.024	0.003	0.142	0.406	-0.007	-0.018	0.004	0.194	0.505	-0.014	-0.041	0.013	0.306	0.527
Cer(m18:1/23:0)	-0.016	-0.038	0.006	0.166	0.903	-0.008	-0.022	0.006	0.251	0.503	0.007	-0.004	0.018	0.196	0.509	0.001	-0.026	0.029	0.925	0.964
dhCer(d18:0/24:1)	-0.009	-0.031	0.013	0.422	0.922	-0.006	-0.020	0.007	0.363	0.601	0.007	-0.004	0.018	0.197	0.509	-0.011	-0.038	0.017	0.447	0.652
PE(P-18:0/18:1)	0.000	-0.022	0.022	0.985	0.996	0.002	-0.012	0.016	0.805	0.898	0.007	-0.004	0.018	0.198	0.510	-0.004	-0.032	0.023	0.761	0.891
PC(20:0_20:4)	0.008	-0.014	0.030	0.495	0.922	0.009	-0.005	0.022	0.215	0.476	-0.007	-0.018	0.004	0.200	0.511	-0.018	-0.046	0.009	0.191	0.402
SM(d18:2/22:0)	0.004	-0.018	0.026	0.728	0.964	0.004	-0.009	0.018	0.534	0.738	-0.007	-0.018	0.004	0.201	0.511	-0.029	-0.055	-0.002	0.037	0.134
Hex2Cer(d16:1/16:0)	-0.002	-0.024	0.021	0.883	0.981	-0.002	-0.016	0.012	0.775	0.884	-0.007	-0.018	0.004	0.200	0.511	-0.020	-0.047	0.008	0.162	0.362
Cer(d16:1/20:0)	-0.015	-0.037	0.007	0.187	0.903	-0.013	-0.026	0.001	0.071	0.349	-0.007	-0.018	0.004	0.202	0.512	-0.026	-0.054	0.001	0.064	0.184
PC(O-34:1)	-0.009	-0.031	0.013	0.445	0.922	-0.012	-0.026	0.002	0.097	0.361	-0.007	-0.018	0.004	0.202	0.512	-0.035	-0.062	-0.008	0.012	0.067
PC(O-16:0/16:0)	-0.016	-0.038	0.006	0.149	0.903	-0.011	-0.025	0.003	0.114	0.382	-0.007	-0.018	0.004	0.205	0.516	-0.033	-0.060	-0.006	0.017	0.085
PI(18:0_20:3) (a)	-0.022	-0.044	0.000	0.054	0.903	-0.016	-0.030	-0.003	0.021	0.273	-0.007	-0.018	0.004	0.209	0.524	-0.035	-0.063	-0.008	0.013	0.068
PE(16:0_18:3) (a)	-0.019	-0.041	0.003	0.097	0.903	-0.007	-0.021	0.007	0.312	0.555	-0.007	-0.018	0.004	0.209	0.524	-0.011	-0.038	0.016	0.423	0.635
SHexCer(d18:1/16:0)	-0.009	-0.031	0.013	0.442	0.922	-0.011	-0.025	0.003	0.124	0.385	-0.007	-0.018	0.004	0.212	0.528	-0.025	-0.052	0.003	0.078	0.217
PI(18:0_20:2)	-0.020	-0.041	0.002	0.073	0.903	-0.017	-0.032	-0.003	0.016	0.273	-0.007	-0.018	0.004	0.212	0.528	-0.027	-0.053	0.000	0.047	0.157
TG(50:4) [NL-14:0]	-0.014	-0.036	0.008	0.213	0.903	-0.009	-0.023	0.005	0.192	0.454	-0.007	-0.018	0.004	0.213	0.529	-0.005	-0.032	0.023	0.750	0.882
FA(18:3)	0.001	-0.021	0.023	0.937	0.995	0.003	-0.011	0.017	0.701	0.846	-0.007	-0.018	0.004	0.215	0.531	-0.009	-0.037	0.019	0.545	0.728
Cer(d19:1/20:0)	-0.001	-0.023	0.021	0.959	0.995	-0.008	-0.022	0.006	0.278	0.524	-0.007	-0.018	0.004	0.216	0.532	-0.039	-0.068	-0.011	0.006	0.048
TG(52:5) [NL-18:3]	-0.012	-0.034	0.010	0.280	0.903	-0.006	-0.020	0.008	0.396	0.634	-0.007	-0.017	0.004	0.221	0.539	-0.007	-0.035	0.020	0.605	0.768
PE(O-18:0/20:4)	-0.008	-0.030	0.014	0.463	0.922	0.005	-0.009	0.019	0.495	0.711	0.007	-0.004	0.017	0.221	0.539	0.008	-0.019	0.035	0.570	0.745
AC(22:5)-OH	0.003	-0.019	0.025	0.808	0.980	-0.007	-0.020	0.007	0.350	0.592	0.007	-0.004	0.018	0.220	0.539	0.005	-0.022	0.033	0.703	0.845
Hex3Cer(d18:1/24:0)	-0.001	-0.023	0.021	0.946	0.995	-0.004	-0.018	0.010	0.565	0.748	-0.007	-0.017	0.004	0.220	0.539	-0.028	-0.055	-0.001	0.045	0.153
LPC(16:1) [sn2]	-0.014	-0.036	0.008	0.217	0.903	-0.010	-0.023	0.004	0.166	0.432	-0.007	-0.017	0.004	0.222	0.539	-0.026	-0.053	0.001	0.056	0.173
Cer(d18:1/22:0)	-0.012	-0.034	0.010	0.290	0.903	-0.001	-0.015	0.013	0.885	0.938	-0.007	-0.017	0.004	0.229	0.551	-0.018	-0.045	0.009	0.189	0.401
SHexCer(d18:1/24:0(OH))	-0.011	-0.034	0.011	0.323	0.922	0.004	-0.010	0.018	0.563	0.748	-0.007	-0.017	0.004	0.229	0.551	-0.023	-0.051	0.006	0.116	0.289
CE(20:4)	0.008	-0.014	0.030	0.482	0.922	0.014	0.000	0.028	0.044	0.306	-0.007	-0.017	0.004	0.231	0.552	-0.018	-0.046	0.010	0.209	0.419
CE(18:3)	0.003	-0.019	0.025	0.794	0.974	0.004	-0.009	0.018	0.539	0.742	-0.007	-0.017	0.004	0.230	0.552	-0.016	-0.044	0.011	0.239	0.452
LPC(15-MHDA) [sn1] [104_sn1]	-0.007	-0.029	0.015	0.546	0.929	-0.014	-0.028	-0.001	0.041	0.306	-0.007	-0.017	0.004	0.232	0.552	-0.031	-0.059	-0.003	0.028	0.112
PC(P-16:0/18:0)	-0.012	-0.034	0.010	0.286	0.903	-0.006	-0.020	0.008	0.372	0.608	-0.007	-0.017	0.004	0.233	0.555	-0.037	-0.063	-0.010	0.007	0.049
PE(O-18:0/22:6)	0.000	-0.023	0.022	0.987	0.996	-0.001	-0.016	0.013	0.847	0.927	0.007	-0.004	0.017	0.235	0.557	0.002	-0.026	0.030	0.896	0.952
Cer(d17:1/20:0)	-0.014	-0.036	0.008	0.214	0.903	-0.014	-0.028	0.000	0.053	0.317	-0.006	-0.017	0.004	0.240	0.562	-0.035	-0.063	-0.007	0.014	0.074
PG(34:1)	-0.015	-0.037	0.007	0.188	0.903	-0.020	-0.034	-0.007	0.004	0.259	-0.006	-0.017	0.004	0.240	0.562	-0.017	-0.045	0.011	0.225	0.434
LPC(17:1) [sn1] (a) & LPC(17:1) [sn2] (b)	-0.008	-0.031	0.014	0.454	0.922	-0.018	-0.031	-0.004	0.010	0.270	-0.006	-0.017	0.004	0.240	0.562	-0.028	-0.055	-0.001	0.043	0.149
DE(16:0)	0.009	-0.013	0.031	0.418	0.922	0.016	0.003	0.030	0.021	0.273	-0.006	-0.017	0.004	0.238	0.562	-0.017	-0.043	0.010	0.210	0.420

PE(P-18:1/22:5) (a)	0.004	-0.018	0.026	0.730	0.964	0.000	-0.015	0.014	0.966	0.980	-0.007	-0.017	0.004	0.244	0.565	-0.049	-0.076	-0.022	0.000	0.009
SM(43:1)	0.004	-0.018	0.026	0.708	0.964	-0.004	-0.018	0.010	0.588	0.764	0.006	-0.004	0.017	0.244	0.565	-0.018	-0.045	0.009	0.195	0.408
PE(P-20:0/18:1)	-0.004	-0.026	0.018	0.744	0.964	-0.005	-0.020	0.009	0.445	0.672	0.006	-0.004	0.017	0.244	0.565	-0.002	-0.030	0.025	0.872	0.944
CE(22:6) [+OH]	-0.001	-0.023	0.022	0.956	0.995	-0.011	-0.024	0.003	0.120	0.385	-0.007	-0.018	0.005	0.244	0.565	-0.015	-0.043	0.013	0.287	0.509
TG(52:1) [NL-18:1]	-0.020	-0.042	0.002	0.074	0.903	-0.014	-0.027	0.000	0.051	0.317	0.006	-0.004	0.017	0.250	0.565	0.004	-0.024	0.032	0.789	0.904
TG(O-54:2) [NL-18:1]	-0.007	-0.029	0.015	0.515	0.922	-0.004	-0.018	0.009	0.542	0.743	0.006	-0.004	0.017	0.246	0.565	0.005	-0.022	0.033	0.706	0.845
SM(d18:2/17:0)	-0.003	-0.025	0.019	0.766	0.969	-0.003	-0.017	0.011	0.668	0.829	-0.006	-0.017	0.004	0.247	0.565	-0.048	-0.074	-0.021	0.001	0.012
CE(24:1)	-0.003	-0.026	0.019	0.786	0.973	-0.002	-0.015	0.012	0.814	0.903	-0.006	-0.017	0.004	0.249	0.565	-0.027	-0.055	0.000	0.047	0.156
PI(20:0_20:4)	-0.003	-0.025	0.019	0.791	0.973	0.001	-0.013	0.015	0.899	0.942	-0.006	-0.017	0.004	0.247	0.565	-0.010	-0.039	0.018	0.478	0.672
AC(16:1)-OH	-0.003	-0.025	0.019	0.813	0.980	-0.010	-0.024	0.004	0.145	0.406	-0.006	-0.017	0.004	0.250	0.565	-0.036	-0.063	-0.008	0.011	0.063
LPC(19:0) (a) [sn1] [104_sn1]	0.002	-0.021	0.024	0.889	0.981	-0.009	-0.022	0.005	0.231	0.488	-0.006	-0.017	0.004	0.249	0.565	-0.015	-0.042	0.013	0.294	0.518
Hex3Cer(d18:1/24:1)	-0.005	-0.028	0.017	0.629	0.954	-0.007	-0.022	0.007	0.307	0.549	-0.006	-0.017	0.004	0.252	0.568	-0.040	-0.068	-0.012	0.005	0.044
Sph(d18:1)	0.006	-0.016	0.028	0.609	0.950	-0.006	-0.020	0.009	0.449	0.673	-0.006	-0.017	0.005	0.253	0.568	0.006	-0.022	0.034	0.681	0.827
DG(18:1_20:5)	-0.004	-0.026	0.018	0.729	0.964	-0.011	-0.025	0.003	0.122	0.385	0.006	-0.005	0.017	0.254	0.569	-0.002	-0.030	0.026	0.894	0.952
PC(P-17:0/20:4) (a)	-0.002	-0.024	0.020	0.871	0.981	-0.007	-0.020	0.007	0.357	0.598	0.006	-0.004	0.017	0.255	0.569	0.002	-0.025	0.029	0.888	0.948
PE(P-16:0/18:2)	-0.012	-0.034	0.011	0.306	0.903	0.002	-0.012	0.016	0.804	0.898	0.006	-0.005	0.017	0.258	0.572	-0.003	-0.031	0.024	0.812	0.917
TG(52:5) [NL-20:5]	-0.007	-0.029	0.015	0.545	0.929	-0.009	-0.023	0.004	0.179	0.450	0.006	-0.005	0.017	0.257	0.572	0.005	-0.023	0.033	0.720	0.854
TG(58:10) [NL-22:6]	0.006	-0.016	0.028	0.609	0.950	-0.006	-0.020	0.008	0.367	0.603	0.006	-0.005	0.017	0.262	0.581	0.020	-0.007	0.048	0.151	0.345
LPC(22:5) [sn1] (n6)	-0.012	-0.034	0.009	0.270	0.903	-0.003	-0.017	0.011	0.672	0.831	-0.006	-0.017	0.005	0.263	0.581	-0.011	-0.038	0.016	0.428	0.638
SM(d18:1/23:0) & SM(d17:1/24:0)	-0.004	-0.026	0.018	0.738	0.964	0.000	-0.014	0.013	0.948	0.972	0.006	-0.005	0.017	0.264	0.582	-0.016	-0.042	0.011	0.249	0.464
HexCer(d18:1/16:0)	0.011	-0.012	0.033	0.349	0.922	-0.004	-0.018	0.010	0.594	0.767	-0.006	-0.017	0.005	0.267	0.586	-0.037	-0.065	-0.010	0.008	0.051
LPC(18:2) [sn2]	-0.002	-0.025	0.020	0.839	0.981	-0.003	-0.017	0.011	0.650	0.814	-0.006	-0.017	0.005	0.268	0.587	-0.006	-0.034	0.022	0.668	0.818
S1P(d18:2)	-0.009	-0.031	0.013	0.429	0.922	0.002	-0.011	0.016	0.733	0.870	-0.006	-0.017	0.005	0.270	0.588	-0.017	-0.044	0.010	0.214	0.422
PE(17:0_18:2)	-0.011	-0.033	0.011	0.320	0.922	-0.016	-0.029	-0.002	0.026	0.285	-0.006	-0.017	0.005	0.271	0.588	-0.013	-0.040	0.015	0.367	0.586
PC(18:0_18:2)	-0.007	-0.029	0.015	0.530	0.922	-0.009	-0.023	0.005	0.206	0.467	-0.006	-0.017	0.005	0.271	0.588	-0.036	-0.064	-0.009	0.010	0.061
PC(16:0_18:3) (b)	-0.021	-0.043	0.001	0.065	0.903	-0.009	-0.023	0.005	0.203	0.465	-0.006	-0.017	0.005	0.273	0.588	-0.035	-0.062	-0.007	0.013	0.070
TG(48:0) [NL-16:0]	-0.023	-0.045	-0.001	0.041	0.903	-0.005	-0.019	0.009	0.471	0.689	0.006	-0.005	0.017	0.273	0.588	0.013	-0.014	0.041	0.337	0.554
LPC(24:0) [sn1]	0.011	-0.011	0.033	0.321	0.922	0.002	-0.012	0.016	0.749	0.877	-0.006	-0.017	0.005	0.273	0.588	0.005	-0.023	0.033	0.710	0.847
PC(18:0_22:5) (n3) & PC(20:1_20:4)	-0.007	-0.029	0.015	0.520	0.922	-0.010	-0.024	0.003	0.145	0.406	-0.006	-0.017	0.005	0.275	0.589	-0.055	-0.082	-0.027	0.000	0.006
LPC(P-17:0) (a)	-0.003	-0.025	0.019	0.766	0.969	-0.010	-0.024	0.003	0.142	0.406	-0.006	-0.017	0.005	0.275	0.589	-0.020	-0.047	0.008	0.159	0.358
AC(13:0)	0.011	-0.011	0.033	0.326	0.922	-0.012	-0.025	0.002	0.097	0.361	0.006	-0.005	0.017	0.277	0.590	0.010	-0.018	0.038	0.484	0.676
LPC(15-MHDA) [sn2]	-0.006	-0.028	0.017	0.614	0.950	-0.014	-0.028	0.000	0.051	0.317	-0.006	-0.017	0.005	0.279	0.590	-0.030	-0.058	-0.002	0.034	0.132
CE(20:3)	0.003	-0.019	0.025	0.813	0.980	-0.002	-0.015	0.012	0.817	0.905	-0.006	-0.017	0.005	0.279	0.590	-0.039	-0.067	-0.011	0.006	0.048
SHexCer(d18:1/24:1)	-0.001	-0.023	0.021	0.910	0.987	-0.006	-0.020	0.007	0.364	0.602	-0.006	-0.017	0.005	0.279	0.590	-0.024	-0.052	0.003	0.081	0.220
TG(48:0) [NL-18:0]	-0.021	-0.043	0.001	0.062	0.903	-0.009	-0.022	0.004	0.190	0.454	0.006	-0.005	0.017	0.284	0.594	0.010	-0.018	0.037	0.502	0.699
Cer(d16:1/24:1)	-0.011	-0.033	0.011	0.334	0.922	-0.019	-0.033	-0.005	0.008	0.265	-0.006	-0.017	0.005	0.284	0.594	-0.024	-0.052	0.004	0.088	0.236
TG(56:7) [NL-20:5]	0.006	-0.016	0.028	0.615	0.950	-0.010	-0.024	0.004	0.158	0.432	0.006	-0.005	0.017	0.282	0.594	-0.003	-0.031	0.025	0.827	0.923
PC(35:5)	0.004	-0.018	0.026	0.723	0.964	-0.008	-0.022	0.005	0.236	0.493	0.006	-0.005	0.017	0.284	0.594	-0.012	-0.040	0.016	0.400	0.617
TG(50:3) [NL-18:2]	-0.018	-0.039	0.004	0.112	0.903	-0.014	-0.028	-0.001	0.040	0.306	-0.006	-0.016	0.005	0.290	0.597	-0.029	-0.057	-0.001	0.045	0.153
PE(16:0_18:3) (b)	-0.026	-0.048	-0.004	0.022	0.903	-0.008	-0.022	0.005	0.224	0.485	-0.006	-0.017	0.005	0.289	0.597	-0.010	-0.037	0.017	0.460	0.663
LPC(19:1) (c)	-0.006	-0.029	0.016	0.589	0.948	-0.011	-0.025	0.002	0.096	0.361	-0.006	-0.017	0.005	0.290	0.597	-0.029	-0.056	-0.002	0.039	0.139
FA(17:1)	-0.004	-0.027	0.019	0.738	0.964	0.004	-0.010	0.018	0.560	0.748	0.006	-0.005	0.017	0.288	0.597	0.013	-0.014	0.040	0.335	0.553
LPI(18:2) [sn2]	-0.004	-0.027	0.018	0.691	0.964	0.006	-0.008	0.020	0.373	0.608	-0.006	-0.017	0.005	0.289	0.597	-0.010	-0.037	0.017	0.461	0.664
Hex2Cer(d18:2/24:1)	0.002	-0.021	0.024	0.886	0.981	0.000	-0.014	0.014	0.998	0.998	-0.006	-0.017	0.005	0.288	0.597	-0.024	-0.052	0.004	0.091	0.241
PE(P-16:0/22:5) (n3)	-0.015	-0.037	0.007	0.189	0.903	0.006	-0.009	0.020	0.445	0.672	0.006	-0.005	0.017	0.293	0.598	-0.024	-0.052	0.003	0.086	0.230
TG(58:9) [NL-22:6]	0.008	-0.014	0.030	0.472	0.922	-0.010	-0.024	0.004	0.161	0.432	0.006	-0.005	0.017	0.292	0.598	0.013	-0.015	0.041	0.359	0.577
PE(18:0_22:6)	-0.005	-0.027	0.017	0.652	0.960	-0.011	-0.025	0.002	0.109	0.379	0.006	-0.005	0.017	0.294	0.598	-0.003	-0.031	0.024	0.804	0.910
PE(O-34:1)	0.001	-0.021	0.024	0.908	0.987	0.005	-0.009	0.019	0.506	0.722	0.006	-0.005	0.017	0.294	0.598	-0.003	-0.030	0.025	0.850	0.933
Cer(d17:1/18:0)	-0.013	-0.036	0.009	0.238	0.903	-0.008	-0.022	0.006	0.248	0.501	-0.006	-0.016	0.005	0.295	0.598	-0.037	-0.065	-0.010	0.008	0.053
PE(16:0_16:0)	-0.023	-0.045	-0.002	0.036	0.903	-0.008	-0.021	0.006	0.249	0.501	-0.006	-0.016	0.005	0.298	0.598	-0.008	-0.035	0.019	0.552	0.730
Cer(d20:1/22:0)	-0.009	-0.030	0.013	0.440	0.922	0.003	-0.011	0.017	0.673	0.831	0.006	-0.005	0.016	0.296	0.598	-0.007	-0.034	0.020	0.601	0.765
Hex2Cer(d18:1/24:1)	-0.005	-0.027	0.017	0.654	0.960	-0.008	-0.022	0.006	0.239	0.495	-0.006	-0.017	0.005	0.298	0.598	-0.024	-0.051	0.004	0.096	0.250
PC(39:5) (b)	-0.002	-0.024	0.021	0.863	0.981	-0.015	-0.028	-0.001	0.033	0.298	-0.006	-0.016	0.005	0.297	0.598	-0.051	-0.078	-0.024	0.000	0.008
HexCer(d18:2/20:0)	0.000	-0.022	0.022	0.993	0.997	-0.006	-0.020	0.008	0.411	0.646	-0.006	-0.017	0.005	0.299	0.598	-0.018	-0.046	0.010	0.204	0.416

Cer(m18:1/24:0)	-0.017	-0.039	0.005	0.126	0.903	-0.006	-0.020	0.008	0.405	0.643	0.006	-0.005	0.016	0.304	0.605	0.003	-0.024	0.031	0.819	0.920
TG(5:4:3) [NL-18:1]	0.006	-0.016	0.027	0.616	0.950	-0.014	-0.028	0.000	0.048	0.317	-0.006	-0.016	0.005	0.304	0.605	-0.017	-0.045	0.010	0.216	0.425
TG(5:6:9) [NL-22:6]	0.003	-0.019	0.025	0.783	0.973	-0.009	-0.023	0.005	0.186	0.453	0.006	-0.005	0.017	0.306	0.605	0.014	-0.014	0.041	0.337	0.554
PE(18:1_22:6) (a)	-0.003	-0.024	0.019	0.820	0.980	-0.014	-0.028	0.000	0.044	0.306	-0.006	-0.016	0.005	0.305	0.605	-0.010	-0.038	0.018	0.471	0.665
CE(18:1)	0.000	-0.022	0.022	0.976	0.995	-0.015	-0.029	-0.002	0.030	0.289	-0.006	-0.017	0.005	0.307	0.605	-0.032	-0.059	-0.004	0.025	0.105
LPC(26:0) [sn1]	0.000	-0.023	0.022	0.973	0.995	-0.009	-0.023	0.005	0.214	0.476	-0.006	-0.017	0.005	0.308	0.605	-0.029	-0.056	-0.001	0.042	0.147
FA(18:2)	0.000	-0.022	0.022	0.998	0.999	0.005	-0.009	0.018	0.511	0.724	-0.006	-0.017	0.005	0.307	0.605	-0.007	-0.034	0.021	0.636	0.798
TG(50:3) [NL-16:1]	-0.021	-0.043	0.001	0.059	0.903	-0.017	-0.031	-0.004	0.014	0.273	-0.006	-0.016	0.005	0.309	0.606	-0.030	-0.058	-0.003	0.032	0.126
DG(18:0_18:1)	-0.017	-0.038	0.005	0.136	0.903	-0.015	-0.029	-0.002	0.026	0.285	0.006	-0.005	0.016	0.311	0.609	-0.003	-0.031	0.025	0.853	0.933
PE(P-18:0/20:3) (a)	-0.009	-0.031	0.014	0.449	0.922	-0.004	-0.018	0.010	0.566	0.748	0.006	-0.005	0.016	0.313	0.610	-0.015	-0.042	0.012	0.275	0.499
PS(38:3)	-0.002	-0.024	0.020	0.880	0.981	-0.001	-0.015	0.012	0.857	0.929	0.006	-0.005	0.016	0.314	0.611	0.018	-0.009	0.046	0.181	0.387
SM(d18:1/18:0) & SM(d16:1/20:0)	-0.017	-0.039	0.005	0.129	0.903	-0.008	-0.021	0.006	0.276	0.524	-0.006	-0.016	0.005	0.316	0.613	-0.047	-0.075	-0.020	0.001	0.014
PE(P-20:0/18:2)	-0.003	-0.025	0.019	0.813	0.980	0.001	-0.013	0.015	0.936	0.968	-0.006	-0.016	0.005	0.317	0.613	-0.014	-0.042	0.013	0.297	0.521
PI(16:0_16:1)	-0.017	-0.039	0.005	0.135	0.903	-0.001	-0.015	0.013	0.914	0.951	0.005	-0.005	0.016	0.321	0.616	-0.004	-0.031	0.023	0.774	0.893
Cer(m18:1/22:0)	-0.014	-0.036	0.008	0.219	0.903	-0.008	-0.022	0.006	0.291	0.536	0.005	-0.005	0.016	0.320	0.616	0.004	-0.024	0.031	0.796	0.905
PE(P-20:1/22:6)	0.004	-0.018	0.027	0.696	0.964	-0.010	-0.023	0.004	0.180	0.450	0.005	-0.005	0.016	0.321	0.616	0.007	-0.020	0.035	0.606	0.769
SM(d18:1/20:0) & SM(d16:1/22:0)	0.000	-0.022	0.022	0.989	0.996	-0.003	-0.017	0.011	0.675	0.833	-0.005	-0.016	0.005	0.322	0.616	-0.026	-0.053	0.001	0.063	0.184
TG(48:3) [NL-16:1]	-0.021	-0.043	0.001	0.066	0.903	-0.014	-0.028	-0.001	0.041	0.306	-0.005	-0.016	0.005	0.324	0.620	-0.017	-0.045	0.010	0.214	0.422
AC(24:0)	0.008	-0.014	0.030	0.503	0.922	0.009	-0.005	0.023	0.191	0.454	0.005	-0.005	0.016	0.326	0.620	0.014	-0.013	0.042	0.301	0.524
LPC(17:1) [sn2] (a)	-0.015	-0.037	0.007	0.193	0.903	-0.018	-0.032	-0.005	0.008	0.263	-0.005	-0.016	0.005	0.328	0.621	-0.027	-0.054	0.001	0.055	0.173
TG(49:1) [NL-17:1]	-0.019	-0.041	0.003	0.087	0.903	-0.011	-0.024	0.003	0.117	0.385	0.005	-0.005	0.016	0.327	0.621	0.000	-0.027	0.027	0.997	0.997
AC(26:0)	-0.002	-0.024	0.020	0.890	0.981	0.005	-0.009	0.019	0.516	0.727	0.005	-0.005	0.016	0.329	0.621	0.003	-0.025	0.030	0.836	0.928
PC(O-32:1)	-0.010	-0.032	0.012	0.391	0.922	-0.006	-0.020	0.008	0.373	0.608	0.005	-0.005	0.016	0.330	0.623	-0.022	-0.050	0.005	0.116	0.289
COH	-0.005	-0.027	0.017	0.644	0.960	-0.003	-0.017	0.011	0.666	0.829	-0.005	-0.016	0.006	0.332	0.625	-0.040	-0.067	-0.013	0.004	0.038
dhCer(d18:0/18:0)	-0.026	-0.048	-0.004	0.022	0.903	0.002	-0.011	0.016	0.735	0.870	0.005	-0.005	0.016	0.338	0.634	-0.036	-0.063	-0.009	0.009	0.054
Cer(d18:2/24:0)	0.001	-0.021	0.023	0.944	0.995	0.001	-0.013	0.016	0.864	0.930	-0.005	-0.016	0.006	0.339	0.636	-0.008	-0.036	0.020	0.565	0.742
DG(18:1_18:3)	-0.011	-0.033	0.011	0.343	0.922	-0.009	-0.023	0.005	0.194	0.454	-0.005	-0.016	0.006	0.343	0.641	-0.013	-0.040	0.015	0.372	0.590
PC(P-18:0/18:2)	-0.006	-0.028	0.016	0.572	0.933	-0.004	-0.018	0.010	0.552	0.748	-0.005	-0.016	0.006	0.344	0.642	-0.021	-0.047	0.006	0.133	0.318
TG(5:4:6) [NL-20:5]	0.000	-0.023	0.022	0.976	0.995	-0.013	-0.027	0.001	0.066	0.338	0.005	-0.006	0.016	0.346	0.643	0.002	-0.026	0.030	0.901	0.952
DG(16:0_16:0)	-0.014	-0.036	0.008	0.211	0.903	-0.012	-0.026	0.001	0.082	0.356	0.005	-0.006	0.016	0.350	0.648	0.014	-0.014	0.041	0.324	0.541
Cer(d18:1/14:0)	-0.001	-0.023	0.021	0.933	0.995	-0.005	-0.020	0.009	0.464	0.686	-0.005	-0.016	0.006	0.350	0.648	-0.029	-0.057	-0.001	0.046	0.155
methyl-CE(18:2)	0.013	-0.009	0.035	0.249	0.903	0.003	-0.011	0.017	0.694	0.845	-0.005	-0.016	0.006	0.353	0.649	-0.011	-0.039	0.016	0.421	0.634
TG(50:4) [NL-18:3]	-0.022	-0.044	0.000	0.047	0.903	-0.012	-0.026	0.001	0.076	0.356	-0.005	-0.016	0.006	0.352	0.649	-0.011	-0.039	0.017	0.429	0.638
TG(5:4:3) [NL-18:2]	-0.006	-0.027	0.016	0.602	0.950	-0.011	-0.025	0.003	0.117	0.385	-0.005	-0.016	0.006	0.354	0.649	0.001	-0.027	0.029	0.945	0.966
FA(16:1)	0.003	-0.019	0.025	0.777	0.973	-0.002	-0.016	0.012	0.764	0.881	-0.005	-0.016	0.006	0.355	0.650	-0.014	-0.042	0.014	0.316	0.537
PC(38:2)	-0.009	-0.031	0.013	0.423	0.922	-0.005	-0.019	0.009	0.478	0.696	-0.005	-0.016	0.006	0.358	0.654	-0.029	-0.056	-0.002	0.033	0.127
Cer(m18:0/24:0)	-0.014	-0.036	0.008	0.204	0.903	-0.003	-0.017	0.011	0.719	0.856	0.005	-0.006	0.016	0.360	0.656	0.004	-0.024	0.031	0.791	0.904
PC(16:0_20:5)	0.007	-0.015	0.029	0.521	0.922	-0.012	-0.025	0.002	0.105	0.373	0.005	-0.006	0.016	0.361	0.656	-0.011	-0.039	0.017	0.440	0.644
PC(17:0_18:2)	-0.008	-0.030	0.013	0.455	0.922	-0.011	-0.025	0.003	0.122	0.385	-0.005	-0.016	0.006	0.364	0.660	-0.034	-0.061	-0.007	0.014	0.074
AC(17:0) (b)	-0.007	-0.029	0.016	0.555	0.933	-0.015	-0.028	-0.001	0.036	0.301	-0.005	-0.016	0.006	0.365	0.660	-0.034	-0.061	-0.008	0.012	0.068
PE(P-18:1/20:4) (b)	-0.006	-0.028	0.016	0.583	0.940	0.002	-0.012	0.016	0.755	0.879	-0.005	-0.016	0.006	0.366	0.661	-0.031	-0.058	-0.005	0.022	0.097
TG(48:1) [NL-16:1]	-0.021	-0.043	0.001	0.058	0.903	-0.009	-0.023	0.004	0.186	0.453	0.005	-0.006	0.016	0.368	0.661	0.004	-0.023	0.032	0.768	0.892
PE(P-18:1/20:3) (a)	-0.009	-0.031	0.013	0.432	0.922	-0.003	-0.017	0.011	0.634	0.803	0.005	-0.006	0.016	0.368	0.661	-0.019	-0.045	0.008	0.175	0.378
SM(41:1) (a)	0.001	-0.021	0.023	0.911	0.987	-0.004	-0.018	0.010	0.558	0.748	0.005	-0.006	0.016	0.369	0.661	-0.017	-0.044	0.010	0.211	0.420
PC(38:5) (b)	0.002	-0.021	0.024	0.892	0.981	-0.012	-0.026	0.002	0.091	0.356	-0.005	-0.016	0.006	0.370	0.661	-0.047	-0.074	-0.020	0.001	0.014
AC(15:0) (a)	0.008	-0.014	0.030	0.473	0.922	-0.015	-0.029	-0.001	0.031	0.291	0.005	-0.006	0.016	0.371	0.662	-0.004	-0.032	0.023	0.749	0.882
LPC(22:1) [sn1]	0.011	-0.011	0.033	0.331	0.922	-0.011	-0.024	0.003	0.136	0.399	-0.005	-0.016	0.006	0.374	0.665	-0.009	-0.036	0.019	0.543	0.726
Cer(m18:1/18:0)	-0.022	-0.044	-0.001	0.045	0.903	-0.009	-0.023	0.004	0.180	0.450	0.005	-0.006	0.016	0.375	0.666	-0.016	-0.043	0.011	0.251	0.465
PC(31:0) (a)	-0.017	-0.040	0.005	0.129	0.903	-0.009	-0.022	0.005	0.212	0.475	0.005	-0.006	0.016	0.379	0.671	-0.020	-0.048	0.007	0.145	0.335
PE(P-18:0/22:5) (n3)	-0.009	-0.031	0.013	0.427	0.922	0.004	-0.010	0.019	0.540	0.743	0.005	-0.006	0.016	0.380	0.671	-0.030	-0.057	-0.002	0.035	0.132
SM(44:1)	0.012	-0.011	0.034	0.303	0.903	-0.005	-0.019	0.009	0.486	0.704	0.005	-0.006	0.016	0.391	0.680	-0.024	-0.051	0.004	0.093	0.244
Cer(m18:0/23:0)	-0.015	-0.037	0.008	0.198	0.903	-0.006	-0.020	0.008	0.399	0.638	0.005	-0.006	0.015	0.393	0.680	-0.011	-0.039	0.016	0.427	0.638
DG(18:1_18:2)	-0.008	-0.030	0.014	0.478	0.922	-0.010	-0.024	0.003	0.147	0.408	-0.005	-0.015	0.006	0.388	0.680	-0.017	-0.045	0.010	0.222	0.430
PE(O-18:1/22:6)	0.009	-0.013	0.031	0.415	0.922	-0.001	-0.015	0.013	0.864	0.930	0.005	-0.006	0.015	0.393	0.680	-0.004	-0.032	0.023	0.762	0.891

CE(15:0)	0.007	-0.015	0.029	0.534	0.923	-0.006	-0.019	0.008	0.413	0.646	-0.005	-0.015	0.006	0.388	0.680	-0.037	-0.065	-0.009	0.009	0.055
PE(P-18:0/20:3) (b)	-0.006	-0.028	0.016	0.577	0.933	0.000	-0.014	0.015	0.981	0.989	0.005	-0.006	0.016	0.392	0.680	-0.018	-0.045	0.010	0.204	0.416
PC(P-16:0/18:1)	-0.004	-0.026	0.018	0.708	0.964	-0.008	-0.022	0.006	0.248	0.501	-0.005	-0.016	0.006	0.391	0.680	-0.032	-0.059	-0.005	0.022	0.098
TG(56:7) [NL-20:4]	-0.004	-0.026	0.018	0.723	0.964	0.005	-0.009	0.019	0.520	0.727	-0.005	-0.015	0.006	0.392	0.680	-0.003	-0.031	0.025	0.860	0.937
CE(22:0)	-0.003	-0.025	0.020	0.818	0.980	0.010	-0.004	0.023	0.162	0.432	-0.005	-0.016	0.006	0.392	0.680	-0.009	-0.035	0.018	0.507	0.702
Cer(d18:1/23:0)	-0.012	-0.034	0.010	0.275	0.903	-0.007	-0.021	0.007	0.353	0.592	-0.005	-0.015	0.006	0.395	0.680	-0.023	-0.050	0.004	0.094	0.246
DE(20:4)	0.016	-0.006	0.038	0.150	0.903	0.019	0.005	0.032	0.007	0.263	-0.005	-0.015	0.006	0.395	0.680	0.001	-0.027	0.029	0.945	0.966
PI(15-MHDA_18:2) & PI(17:0_18:2)	-0.014	-0.036	0.008	0.216	0.903	0.004	-0.010	0.018	0.599	0.771	-0.005	-0.015	0.006	0.398	0.684	-0.021	-0.047	0.006	0.130	0.315
Cer(d19:1/18:0)	-0.006	-0.028	0.016	0.568	0.933	-0.009	-0.023	0.005	0.211	0.475	-0.005	-0.015	0.006	0.400	0.685	-0.043	-0.070	-0.016	0.002	0.024
DE(20:5)	0.013	-0.010	0.035	0.268	0.903	-0.004	-0.018	0.010	0.555	0.748	0.005	-0.006	0.015	0.402	0.687	-0.008	-0.035	0.020	0.590	0.756
PE(38:5) (b)	-0.010	-0.032	0.013	0.399	0.922	-0.016	-0.030	-0.003	0.019	0.273	-0.005	-0.015	0.006	0.402	0.687	-0.024	-0.051	0.004	0.088	0.236
TG(54:5) [NL-20:4]	-0.015	-0.037	0.007	0.178	0.903	-0.007	-0.021	0.006	0.285	0.530	0.004	-0.006	0.015	0.417	0.708	-0.001	-0.029	0.027	0.932	0.964
DG(18:1_20:3)	-0.011	-0.033	0.011	0.324	0.922	-0.011	-0.025	0.002	0.106	0.373	0.004	-0.006	0.015	0.417	0.708	-0.014	-0.042	0.015	0.346	0.564
PG(36:1)	-0.020	-0.042	0.002	0.069	0.903	-0.014	-0.028	-0.001	0.038	0.301	0.004	-0.006	0.015	0.418	0.709	0.010	-0.017	0.038	0.466	0.664
DG(14:0_18:2)	-0.017	-0.040	0.005	0.121	0.903	-0.009	-0.023	0.004	0.176	0.446	-0.004	-0.015	0.006	0.420	0.709	-0.014	-0.042	0.014	0.315	0.537
FA(20:2)	-0.009	-0.031	0.014	0.449	0.922	0.000	-0.014	0.014	0.982	0.989	-0.005	-0.016	0.007	0.421	0.709	-0.010	-0.038	0.017	0.462	0.664
PC(P-16:0/18:3)	-0.009	-0.031	0.013	0.423	0.922	-0.005	-0.019	0.009	0.448	0.673	-0.004	-0.015	0.006	0.423	0.709	-0.008	-0.035	0.020	0.583	0.753
CE(20:1)	0.005	-0.017	0.027	0.649	0.960	-0.001	-0.015	0.013	0.860	0.929	-0.004	-0.015	0.006	0.422	0.709	-0.026	-0.054	0.002	0.066	0.189
PC(34:5)	0.001	-0.022	0.023	0.951	0.995	-0.006	-0.020	0.008	0.406	0.643	0.004	-0.006	0.015	0.422	0.709	-0.004	-0.032	0.024	0.770	0.892
AC(24:1)-OH	0.015	-0.007	0.037	0.172	0.903	-0.012	-0.026	0.001	0.071	0.350	-0.004	-0.015	0.006	0.424	0.710	0.007	-0.020	0.034	0.613	0.775
TG(O-54:3) [NL-17:1]	-0.007	-0.029	0.014	0.501	0.922	-0.005	-0.019	0.009	0.471	0.689	0.004	-0.006	0.015	0.426	0.711	0.003	-0.025	0.031	0.836	0.928
CE(24:0)	-0.001	-0.023	0.022	0.944	0.995	0.011	-0.003	0.024	0.127	0.385	-0.004	-0.015	0.006	0.427	0.711	-0.010	-0.037	0.017	0.463	0.664
PC(16:0_20:3) (b)	-0.016	-0.038	0.007	0.168	0.903	-0.011	-0.025	0.002	0.101	0.368	-0.004	-0.015	0.006	0.429	0.712	-0.044	-0.071	-0.017	0.002	0.022
Ubiquinone	0.007	-0.015	0.029	0.511	0.922	-0.004	-0.018	0.010	0.577	0.759	-0.004	-0.015	0.006	0.431	0.713	-0.010	-0.038	0.017	0.464	0.664
LPI(18:0) [sn1]	-0.010	-0.032	0.012	0.360	0.922	-0.002	-0.017	0.013	0.812	0.902	0.004	-0.007	0.015	0.431	0.713	-0.001	-0.029	0.027	0.941	0.966
PC(16:0_16:0)	-0.014	-0.036	0.008	0.222	0.903	-0.009	-0.023	0.005	0.203	0.464	-0.004	-0.015	0.007	0.435	0.715	-0.029	-0.056	-0.002	0.035	0.133
LPE(P-16:0)	-0.009	-0.031	0.013	0.426	0.922	-0.006	-0.020	0.009	0.438	0.667	-0.004	-0.015	0.006	0.434	0.715	-0.016	-0.044	0.012	0.275	0.499
PE(18:0_18:1)	-0.007	-0.029	0.015	0.548	0.929	-0.012	-0.025	0.002	0.095	0.360	0.004	-0.006	0.015	0.434	0.715	0.015	-0.012	0.043	0.280	0.505
TG(50:1) [NL-18:1]	-0.022	-0.043	0.000	0.052	0.903	-0.011	-0.025	0.003	0.122	0.385	0.004	-0.006	0.015	0.438	0.719	-0.002	-0.030	0.026	0.884	0.948
PC(17:0_18:1)	-0.015	-0.036	0.007	0.193	0.903	-0.018	-0.032	-0.004	0.010	0.270	-0.004	-0.015	0.007	0.441	0.720	-0.048	-0.075	-0.021	0.001	0.012
PE(16:0_18:2)	-0.017	-0.038	0.005	0.133	0.903	-0.012	-0.025	0.002	0.104	0.372	-0.004	-0.015	0.007	0.441	0.720	-0.011	-0.039	0.016	0.425	0.636
PE(P-18:1/22:5) (b)	-0.004	-0.026	0.018	0.722	0.964	0.004	-0.010	0.018	0.549	0.747	-0.004	-0.015	0.007	0.444	0.723	-0.005	-0.032	0.021	0.698	0.842
SM(d18:0/16:0)	0.007	-0.015	0.029	0.547	0.929	-0.002	-0.016	0.012	0.810	0.902	-0.004	-0.015	0.007	0.445	0.723	-0.028	-0.055	-0.001	0.042	0.147
SM(d18:1/24:0)	0.003	-0.019	0.025	0.805	0.980	0.006	-0.008	0.020	0.418	0.649	0.004	-0.007	0.015	0.446	0.723	-0.008	-0.035	0.019	0.575	0.746
Cer(m18:0/22:0)	-0.014	-0.036	0.008	0.225	0.903	-0.003	-0.017	0.011	0.640	0.807	0.004	-0.007	0.015	0.450	0.727	-0.007	-0.034	0.021	0.629	0.793
PC(O-32:2)	-0.013	-0.035	0.009	0.253	0.903	-0.006	-0.020	0.008	0.423	0.655	0.004	-0.007	0.015	0.450	0.727	-0.003	-0.031	0.024	0.802	0.910
PC(O-16:0/20:4)	-0.007	-0.029	0.014	0.512	0.922	0.003	-0.011	0.017	0.633	0.803	0.004	-0.007	0.015	0.452	0.727	-0.016	-0.043	0.012	0.262	0.482
Cer(d18:2/26:0)	0.004	-0.019	0.026	0.745	0.964	0.002	-0.012	0.016	0.804	0.898	-0.004	-0.015	0.007	0.452	0.727	-0.022	-0.050	0.005	0.112	0.278
Cer(d16:1/18:0)	-0.012	-0.034	0.009	0.267	0.903	-0.014	-0.027	0.000	0.052	0.317	-0.004	-0.015	0.007	0.455	0.727	-0.033	-0.061	-0.006	0.018	0.087
AC(18:0)-OH	0.000	-0.022	0.022	0.989	0.996	-0.008	-0.021	0.006	0.278	0.524	-0.004	-0.015	0.007	0.454	0.727	-0.032	-0.060	-0.005	0.021	0.093
TG(50:1) [NL-16:0]	-0.019	-0.041	0.002	0.082	0.903	-0.009	-0.023	0.004	0.181	0.450	0.004	-0.007	0.015	0.458	0.731	0.001	-0.027	0.029	0.964	0.973
AC(26:1)	0.001	-0.021	0.023	0.949	0.995	-0.001	-0.015	0.013	0.857	0.929	-0.004	-0.015	0.007	0.460	0.733	-0.016	-0.043	0.011	0.237	0.450
PC(18:0_20:3)	-0.010	-0.032	0.011	0.347	0.922	-0.006	-0.019	0.008	0.418	0.649	0.004	-0.007	0.015	0.462	0.734	-0.020	-0.047	0.007	0.145	0.335
Cer(d17:1/22:0)	-0.007	-0.029	0.015	0.524	0.922	-0.002	-0.016	0.012	0.753	0.879	-0.004	-0.015	0.007	0.468	0.741	-0.016	-0.044	0.011	0.245	0.458
LPC(20:4) [sn1]	-0.005	-0.027	0.017	0.645	0.960	-0.002	-0.016	0.012	0.730	0.868	-0.004	-0.015	0.007	0.471	0.741	-0.014	-0.042	0.014	0.323	0.541
SM(d18:2/16:0)	-0.002	-0.024	0.020	0.871	0.981	0.005	-0.009	0.019	0.462	0.686	-0.004	-0.015	0.007	0.470	0.741	-0.027	-0.053	0.000	0.053	0.171
PC(18:0_22:6)	0.001	-0.021	0.024	0.895	0.983	-0.008	-0.022	0.006	0.251	0.503	0.004	-0.007	0.015	0.469	0.741	-0.025	-0.053	0.003	0.083	0.224
PE(17:0_22:6)	0.001	-0.021	0.023	0.920	0.990	-0.014	-0.028	-0.001	0.038	0.302	0.004	-0.007	0.015	0.467	0.741	-0.004	-0.031	0.024	0.793	0.904
PC(P-16:0/16:1)	-0.009	-0.031	0.014	0.449	0.922	-0.013	-0.027	0.001	0.066	0.338	-0.004	-0.015	0.007	0.475	0.746	-0.029	-0.056	-0.002	0.034	0.132
CE(22:1)	0.011	-0.011	0.033	0.342	0.922	0.001	-0.013	0.014	0.942	0.971	0.004	-0.007	0.015	0.476	0.746	-0.013	-0.041	0.014	0.335	0.553
PC(15:0_20:3)	-0.013	-0.035	0.009	0.265	0.903	-0.008	-0.021	0.006	0.269	0.520	-0.004	-0.015	0.007	0.478	0.747	-0.032	-0.059	-0.006	0.018	0.087
Cer(d16:1/16:0)	-0.003	-0.025	0.020	0.822	0.980	-0.008	-0.022	0.006	0.252	0.503	-0.004	-0.015	0.007	0.480	0.749	-0.014	-0.042	0.013	0.306	0.527
PC(O-18:0/22:6)	-0.008	-0.030	0.015	0.504	0.922	-0.015	-0.029	-0.001	0.043	0.306	-0.004	-0.015	0.007	0.484	0.752	-0.037	-0.065	-0.010	0.007	0.049
PC(O-38:5)	0.004	-0.018	0.026	0.723	0.964	0.004	-0.009	0.018	0.528	0.735	-0.004	-0.015	0.007	0.483	0.752	-0.030	-0.056	-0.003	0.032	0.126

LPC(P-17:0) (b)	-0.011	-0.033	0.011	0.330	0.922	-0.007	-0.021	0.007	0.307	0.549	-0.004	-0.014	0.007	0.487	0.756	-0.018	-0.045	0.009	0.195	0.408
TG(O-54:3) [NL-18:1]	0.001	-0.021	0.023	0.946	0.995	-0.002	-0.016	0.012	0.766	0.881	0.004	-0.007	0.014	0.490	0.758	0.006	-0.021	0.034	0.647	0.807
TG(48:3) [NL-14:0]	-0.020	-0.042	0.002	0.077	0.903	-0.012	-0.026	0.002	0.083	0.356	-0.004	-0.014	0.007	0.494	0.759	-0.011	-0.039	0.016	0.420	0.634
LPC(24:0) [sn2]	0.013	-0.009	0.035	0.241	0.903	0.002	-0.012	0.016	0.739	0.873	-0.004	-0.015	0.007	0.495	0.759	0.009	-0.019	0.036	0.549	0.729
LPC(22:1) [sn2]	0.015	-0.006	0.037	0.164	0.903	-0.008	-0.022	0.005	0.232	0.488	-0.004	-0.015	0.007	0.493	0.759	-0.005	-0.032	0.023	0.740	0.874
SM(d18:2/14:0)	0.001	-0.021	0.023	0.914	0.987	-0.001	-0.015	0.013	0.899	0.942	-0.004	-0.015	0.007	0.495	0.759	-0.036	-0.063	-0.009	0.008	0.053
PE(15-MHDA_18:2)	-0.012	-0.034	0.010	0.292	0.903	-0.017	-0.031	-0.003	0.017	0.273	-0.004	-0.015	0.007	0.496	0.760	-0.030	-0.057	-0.002	0.036	0.134
LPC(20:5) [sn2]	0.008	-0.014	0.030	0.482	0.922	-0.011	-0.025	0.003	0.121	0.385	0.004	-0.007	0.015	0.498	0.761	-0.005	-0.033	0.022	0.713	0.847
Cer(d18:1/19:0)	-0.018	-0.040	0.005	0.124	0.903	-0.008	-0.021	0.006	0.273	0.521	-0.004	-0.015	0.007	0.500	0.762	-0.028	-0.055	0.000	0.049	0.161
PC(33:0) (b)	-0.012	-0.034	0.010	0.285	0.903	-0.009	-0.022	0.005	0.231	0.488	-0.004	-0.014	0.007	0.505	0.767	-0.047	-0.074	-0.019	0.001	0.016
DG(16:0_18:2)	-0.014	-0.036	0.008	0.205	0.903	-0.008	-0.022	0.005	0.230	0.488	-0.004	-0.014	0.007	0.510	0.767	-0.009	-0.036	0.019	0.534	0.719
DG(18:1_20:4)	-0.016	-0.038	0.006	0.155	0.903	-0.006	-0.020	0.008	0.386	0.626	0.004	-0.007	0.014	0.509	0.767	-0.003	-0.031	0.025	0.835	0.928
PC(P-16:0/14:0)	-0.007	-0.029	0.016	0.557	0.933	-0.007	-0.021	0.007	0.337	0.574	0.004	-0.007	0.014	0.509	0.767	-0.030	-0.057	-0.002	0.035	0.132
SM(d18:2/24:0)	0.007	-0.015	0.029	0.554	0.933	0.004	-0.010	0.018	0.555	0.748	-0.004	-0.015	0.007	0.508	0.767	-0.019	-0.046	0.008	0.161	0.360
PC(36:4) [+OH]	-0.005	-0.027	0.017	0.633	0.958	0.005	-0.008	0.019	0.432	0.663	0.004	-0.007	0.014	0.508	0.767	-0.003	-0.031	0.024	0.803	0.910
methyl-CE(18:0)	-0.002	-0.025	0.021	0.856	0.981	0.003	-0.011	0.016	0.698	0.845	-0.004	-0.015	0.007	0.511	0.767	-0.013	-0.040	0.014	0.344	0.563
SM(d16:1/19:0)	-0.001	-0.024	0.021	0.928	0.995	-0.009	-0.023	0.005	0.190	0.454	-0.004	-0.014	0.007	0.508	0.767	-0.044	-0.071	-0.016	0.002	0.024
FA(22:5)	-0.003	-0.025	0.019	0.806	0.980	0.002	-0.011	0.016	0.742	0.874	0.004	-0.007	0.015	0.512	0.767	0.004	-0.024	0.031	0.795	0.905
TG(54:6) [NL-20:4]	-0.014	-0.036	0.008	0.217	0.903	-0.002	-0.016	0.012	0.778	0.884	-0.004	-0.014	0.007	0.513	0.768	-0.006	-0.034	0.022	0.675	0.823
AC(22:6)	0.010	-0.012	0.032	0.376	0.922	-0.009	-0.023	0.005	0.212	0.475	0.004	-0.007	0.014	0.514	0.768	0.001	-0.027	0.028	0.954	0.969
TG(48:1) [NL-18:1]	-0.019	-0.041	0.003	0.083	0.903	-0.012	-0.026	0.001	0.081	0.356	0.004	-0.007	0.014	0.518	0.771	-0.003	-0.031	0.025	0.847	0.933
PC(P-18:0/22:6)	-0.002	-0.025	0.020	0.830	0.981	-0.010	-0.024	0.004	0.171	0.438	0.004	-0.007	0.014	0.519	0.771	-0.015	-0.042	0.012	0.281	0.505
PE(P-20:0/20:4)	-0.001	-0.023	0.021	0.939	0.995	0.001	-0.013	0.015	0.877	0.934	0.003	-0.007	0.014	0.528	0.782	-0.022	-0.049	0.006	0.131	0.315
PC(P-38:5) (b)	0.001	-0.021	0.023	0.958	0.995	-0.011	-0.025	0.003	0.126	0.385	-0.003	-0.014	0.007	0.528	0.782	-0.028	-0.055	-0.002	0.038	0.138
PI(18:0_22:5) (n3)	-0.013	-0.035	0.009	0.232	0.903	-0.010	-0.024	0.004	0.164	0.432	-0.003	-0.014	0.007	0.529	0.782	-0.035	-0.062	-0.008	0.013	0.069
Cer(m18:0/24:1)	-0.019	-0.040	0.003	0.096	0.903	-0.013	-0.027	0.000	0.059	0.323	0.003	-0.007	0.014	0.537	0.791	-0.017	-0.044	0.010	0.230	0.439
PC(P-16:0/16:0)	-0.012	-0.034	0.010	0.305	0.903	-0.010	-0.024	0.003	0.144	0.406	-0.003	-0.014	0.007	0.538	0.791	-0.014	-0.042	0.013	0.306	0.527
Cer(d19:1/26:0)	0.001	-0.022	0.024	0.928	0.995	-0.001	-0.016	0.014	0.892	0.940	0.003	-0.007	0.014	0.537	0.791	-0.004	-0.032	0.024	0.777	0.894
TG(54:4) [NL-20:3]	-0.014	-0.035	0.008	0.220	0.903	-0.014	-0.028	0.000	0.046	0.306	0.003	-0.007	0.014	0.540	0.791	-0.012	-0.040	0.016	0.405	0.620
PE(16:0_16:1)	-0.021	-0.043	0.001	0.066	0.903	-0.009	-0.023	0.004	0.187	0.454	0.003	-0.007	0.014	0.544	0.791	-0.012	-0.040	0.015	0.381	0.596
PE(P-16:0/22:4)	-0.023	-0.044	-0.001	0.044	0.903	0.008	-0.006	0.022	0.269	0.520	0.003	-0.007	0.014	0.543	0.791	-0.008	-0.035	0.020	0.574	0.745
AC(16:0)-OH	-0.007	-0.029	0.015	0.520	0.922	-0.009	-0.022	0.005	0.213	0.475	-0.003	-0.014	0.007	0.543	0.791	-0.033	-0.060	-0.006	0.017	0.084
PE(O-16:0/18:2)	-0.009	-0.031	0.014	0.451	0.922	0.003	-0.011	0.017	0.644	0.809	0.003	-0.007	0.014	0.541	0.791	-0.006	-0.033	0.021	0.659	0.814
Hex2Cer(d16:1/24:1)	-0.003	-0.025	0.020	0.814	0.980	-0.004	-0.018	0.009	0.530	0.735	-0.003	-0.014	0.007	0.545	0.792	-0.006	-0.034	0.021	0.658	0.814
PC(18:0_22:5) (n6)	-0.010	-0.032	0.012	0.386	0.922	0.002	-0.012	0.016	0.787	0.889	-0.003	-0.014	0.007	0.547	0.792	-0.014	-0.041	0.013	0.298	0.522
DG(18:1_22:5)	-0.006	-0.028	0.016	0.611	0.950	-0.016	-0.029	-0.002	0.025	0.285	0.003	-0.007	0.014	0.548	0.792	-0.014	-0.042	0.014	0.315	0.537
TG(56:6) [NL-22:5]	-0.008	-0.029	0.014	0.501	0.922	-0.019	-0.033	-0.006	0.005	0.259	0.003	-0.007	0.014	0.550	0.794	-0.019	-0.047	0.009	0.178	0.383
Cer(d16:1/22:0)	-0.005	-0.027	0.017	0.666	0.964	-0.007	-0.022	0.007	0.295	0.539	-0.003	-0.014	0.008	0.552	0.795	0.005	-0.022	0.033	0.702	0.845
SM(44:2)	-0.002	-0.024	0.020	0.872	0.981	-0.012	-0.026	0.002	0.087	0.356	0.003	-0.007	0.014	0.555	0.797	-0.031	-0.058	-0.004	0.025	0.106
FA(22:4)	-0.004	-0.026	0.018	0.718	0.964	0.004	-0.010	0.018	0.545	0.745	-0.003	-0.014	0.008	0.558	0.801	-0.012	-0.040	0.015	0.381	0.596
LPC(20:5) [sn1]	0.008	-0.015	0.030	0.497	0.922	-0.012	-0.026	0.002	0.102	0.368	0.003	-0.008	0.014	0.565	0.810	-0.004	-0.032	0.024	0.777	0.894
SM(43:2) (c)	0.002	-0.020	0.024	0.865	0.981	-0.009	-0.023	0.004	0.170	0.437	0.003	-0.008	0.014	0.566	0.810	-0.023	-0.050	0.003	0.084	0.226
PC(O-34:2)	-0.006	-0.028	0.016	0.612	0.950	0.003	-0.011	0.017	0.687	0.840	-0.003	-0.014	0.008	0.568	0.810	-0.014	-0.041	0.013	0.317	0.537
TG(O-54:4) [NL-17:1]	-0.015	-0.036	0.007	0.190	0.903	-0.001	-0.016	0.013	0.836	0.919	0.003	-0.008	0.014	0.573	0.813	0.018	-0.010	0.046	0.208	0.419
PC(40:7) (a)	-0.010	-0.032	0.012	0.386	0.922	-0.005	-0.018	0.009	0.521	0.727	-0.003	-0.014	0.008	0.574	0.813	-0.022	-0.050	0.005	0.109	0.276
FA(22:6)	0.003	-0.019	0.025	0.816	0.980	-0.006	-0.020	0.007	0.361	0.599	0.003	-0.008	0.014	0.573	0.813	0.003	-0.025	0.031	0.837	0.928
CA	-0.001	-0.023	0.021	0.917	0.988	0.002	-0.012	0.016	0.760	0.881	0.003	-0.008	0.014	0.574	0.813	0.009	-0.018	0.037	0.507	0.702
TG(54:2) [NL-18:0]	-0.012	-0.033	0.010	0.289	0.903	-0.014	-0.028	0.000	0.044	0.306	0.003	-0.008	0.014	0.580	0.817	-0.001	-0.029	0.027	0.927	0.964
CE(18:0)	-0.006	-0.028	0.016	0.604	0.950	-0.002	-0.016	0.012	0.793	0.891	-0.003	-0.014	0.008	0.580	0.817	-0.041	-0.069	-0.014	0.003	0.035
CE(24:4)	0.002	-0.021	0.024	0.879	0.981	0.010	-0.004	0.023	0.163	0.432	-0.003	-0.014	0.008	0.578	0.817	-0.011	-0.039	0.016	0.408	0.623
LPC(22:6) [sn1]	0.001	-0.022	0.023	0.955	0.995	-0.015	-0.029	-0.001	0.034	0.298	-0.003	-0.014	0.008	0.581	0.817	-0.020	-0.048	0.008	0.155	0.352
PC(15:0_20:4)	-0.006	-0.027	0.016	0.613	0.950	0.000	-0.014	0.014	0.984	0.989	0.003	-0.008	0.014	0.583	0.817	-0.030	-0.057	-0.002	0.035	0.133
TG(51:2) [NL-15:0]	-0.012	-0.034	0.010	0.296	0.903	-0.019	-0.033	-0.006	0.006	0.259	-0.003	-0.014	0.008	0.586	0.820	-0.028	-0.056	0.000	0.053	0.170
PE(36:0)	-0.016	-0.038	0.005	0.140	0.903	-0.009	-0.023	0.004	0.185	0.453	-0.003	-0.014	0.008	0.588	0.820	-0.003	-0.031	0.025	0.840	0.928
PC(P-18:0/20:4)	-0.009	-0.031	0.012	0.398	0.922	0.002	-0.012	0.016	0.745	0.875	0.003	-0.008	0.014	0.588	0.820	-0.014	-0.041	0.013	0.320	0.539

PI(18:0_18:1)	-0.008	-0.030	0.014	0.456	0.922	-0.012	-0.027	0.002	0.083	0.356	-0.003	-0.014	0.008	0.591	0.821	-0.020	-0.047	0.007	0.147	0.337
TG(5:3:2) [NL-18:1]	-0.011	-0.033	0.011	0.339	0.922	-0.020	-0.033	-0.006	0.004	0.259	0.003	-0.008	0.014	0.592	0.821	-0.014	-0.042	0.014	0.317	0.537
SM(d18:1/17:0) & SM(d17:1/18:0)	-0.002	-0.024	0.021	0.882	0.981	-0.005	-0.019	0.009	0.510	0.724	-0.003	-0.014	0.008	0.592	0.821	-0.048	-0.075	-0.021	0.001	0.013
LPC(20:4) [sn2]	-0.005	-0.027	0.017	0.659	0.960	-0.002	-0.016	0.012	0.827	0.913	-0.003	-0.014	0.008	0.595	0.823	-0.015	-0.043	0.013	0.285	0.509
PC(33:0) (a)	-0.015	-0.037	0.007	0.184	0.903	-0.012	-0.026	0.002	0.092	0.356	0.003	-0.008	0.014	0.599	0.825	-0.034	-0.061	-0.006	0.016	0.080
Cer(m18:1/24:1)	-0.018	-0.040	0.004	0.113	0.903	-0.012	-0.026	0.002	0.082	0.356	0.003	-0.008	0.014	0.599	0.825	-0.004	-0.031	0.023	0.774	0.893
SHexCer(d18:1/24:0)	0.002	-0.020	0.025	0.839	0.981	-0.015	-0.028	-0.001	0.041	0.306	0.003	-0.008	0.014	0.600	0.825	-0.009	-0.037	0.020	0.548	0.729
AC(14:1)-OH	0.001	-0.021	0.023	0.946	0.995	-0.002	-0.015	0.011	0.770	0.881	-0.003	-0.014	0.008	0.600	0.825	-0.024	-0.052	0.004	0.091	0.241
TG(5:6:8) [NL-20:4]	-0.012	-0.034	0.010	0.295	0.903	0.006	-0.008	0.020	0.425	0.657	-0.003	-0.014	0.008	0.604	0.828	0.009	-0.019	0.037	0.530	0.718
LPE(P-18:0)	-0.008	-0.030	0.014	0.490	0.922	-0.004	-0.018	0.010	0.590	0.764	-0.003	-0.014	0.008	0.603	0.828	-0.020	-0.047	0.008	0.159	0.358
PC(32:2)	-0.019	-0.041	0.003	0.092	0.903	-0.004	-0.018	0.010	0.599	0.771	-0.003	-0.014	0.008	0.617	0.830	-0.013	-0.040	0.014	0.358	0.577
DG(16:0_20:4)	-0.020	-0.042	0.002	0.070	0.903	-0.006	-0.019	0.008	0.404	0.643	0.003	-0.008	0.013	0.618	0.830	0.003	-0.024	0.031	0.818	0.920
PA(34:1)	-0.012	-0.034	0.010	0.299	0.903	-0.020	-0.034	-0.006	0.005	0.259	-0.003	-0.014	0.008	0.619	0.830	-0.002	-0.029	0.026	0.897	0.952
PC(16:0_18:2)	-0.007	-0.029	0.015	0.520	0.922	-0.012	-0.026	0.002	0.104	0.372	-0.003	-0.014	0.008	0.619	0.830	-0.034	-0.061	-0.006	0.016	0.080
AC(20:3)-OH	-0.007	-0.029	0.015	0.523	0.922	0.004	-0.010	0.018	0.583	0.763	-0.003	-0.014	0.008	0.614	0.830	-0.017	-0.043	0.010	0.219	0.429
Cer(d19:1/24:0)	0.008	-0.014	0.031	0.465	0.922	-0.001	-0.015	0.013	0.870	0.932	0.003	-0.008	0.014	0.613	0.830	-0.010	-0.037	0.018	0.483	0.676
PE(P-18:0/22:5) (n6)	-0.007	-0.029	0.015	0.515	0.922	0.007	-0.007	0.021	0.336	0.574	0.003	-0.008	0.013	0.610	0.830	0.009	-0.018	0.035	0.520	0.709
TG(5:4:7) [NL-20:5]	-0.007	-0.030	0.015	0.523	0.922	-0.009	-0.023	0.004	0.185	0.453	0.003	-0.008	0.014	0.614	0.830	0.005	-0.022	0.033	0.706	0.845
LPC(19:0) [sn2] (a)	0.005	-0.017	0.027	0.651	0.960	-0.007	-0.021	0.007	0.316	0.557	-0.003	-0.014	0.008	0.610	0.830	-0.008	-0.035	0.020	0.588	0.756
PC(17:0_22:6)	0.005	-0.018	0.027	0.690	0.964	-0.014	-0.029	0.000	0.046	0.306	-0.003	-0.014	0.008	0.609	0.830	-0.039	-0.067	-0.012	0.005	0.047
SM(d19:1/24:1)	0.005	-0.018	0.027	0.676	0.964	-0.012	-0.026	0.002	0.097	0.361	0.003	-0.008	0.013	0.616	0.830	-0.026	-0.054	0.001	0.063	0.184
PC(15-MHDA_22:6)	0.002	-0.020	0.025	0.845	0.981	-0.015	-0.029	-0.001	0.037	0.301	0.003	-0.008	0.014	0.620	0.830	-0.037	-0.065	-0.009	0.010	0.059
SM(37:1)	0.000	-0.023	0.022	0.975	0.995	-0.006	-0.020	0.008	0.411	0.646	-0.003	-0.013	0.008	0.612	0.830	-0.042	-0.069	-0.014	0.003	0.035
LPC(14:0) [sn2]	-0.012	-0.034	0.011	0.311	0.910	-0.010	-0.023	0.004	0.167	0.433	-0.003	-0.013	0.008	0.622	0.831	-0.017	-0.045	0.010	0.220	0.429
PC(14:0_16:0)	-0.017	-0.039	0.005	0.123	0.903	-0.009	-0.023	0.004	0.184	0.453	-0.003	-0.013	0.008	0.626	0.831	-0.026	-0.054	0.001	0.058	0.177
PI(34:1)	-0.012	-0.034	0.010	0.296	0.903	-0.005	-0.019	0.009	0.505	0.722	0.003	-0.008	0.014	0.630	0.831	-0.008	-0.035	0.020	0.587	0.756
methyl-DE(18:2)	0.015	-0.007	0.037	0.188	0.903	0.004	-0.010	0.018	0.584	0.763	-0.003	-0.014	0.008	0.625	0.831	0.000	-0.027	0.028	0.974	0.982
LPC(15:0) [sn1]	-0.011	-0.033	0.012	0.348	0.922	-0.011	-0.025	0.003	0.114	0.382	-0.003	-0.013	0.008	0.629	0.831	-0.027	-0.054	0.001	0.060	0.179
PC(28:0)	-0.009	-0.031	0.013	0.418	0.922	-0.007	-0.021	0.007	0.318	0.557	-0.003	-0.013	0.008	0.630	0.831	-0.026	-0.053	0.001	0.061	0.183
HexCer(d16:1/24:0)	0.009	-0.013	0.031	0.424	0.922	-0.002	-0.016	0.012	0.766	0.881	-0.003	-0.014	0.008	0.627	0.831	0.006	-0.022	0.033	0.694	0.840
PS(40:6)	0.008	-0.014	0.031	0.456	0.922	-0.017	-0.031	-0.003	0.020	0.273	0.003	-0.008	0.014	0.630	0.831	0.003	-0.025	0.031	0.842	0.928
PC(P-18:0/22:5)	-0.010	-0.032	0.013	0.401	0.922	-0.008	-0.022	0.006	0.259	0.509	-0.003	-0.013	0.008	0.638	0.835	-0.038	-0.065	-0.012	0.005	0.044
PS(38:4)	0.009	-0.014	0.031	0.440	0.922	-0.010	-0.024	0.003	0.132	0.395	-0.003	-0.013	0.008	0.637	0.835	-0.010	-0.038	0.017	0.453	0.657
FA(18:0)	-0.005	-0.027	0.018	0.680	0.964	-0.002	-0.015	0.011	0.766	0.881	0.003	-0.008	0.013	0.637	0.835	0.008	-0.017	0.034	0.535	0.719
CE(20:0)	-0.003	-0.026	0.019	0.764	0.969	0.007	-0.006	0.021	0.303	0.546	-0.003	-0.013	0.008	0.635	0.835	-0.012	-0.039	0.015	0.380	0.596
S1P(d16:1)	0.000	-0.023	0.022	0.980	0.995	-0.006	-0.020	0.008	0.384	0.624	-0.003	-0.013	0.008	0.639	0.835	-0.010	-0.038	0.018	0.471	0.665
PI(37:6)	0.005	-0.017	0.028	0.638	0.960	-0.010	-0.024	0.004	0.177	0.447	0.003	-0.008	0.013	0.642	0.837	-0.038	-0.067	-0.010	0.007	0.049
FA(16:0)	-0.004	-0.026	0.019	0.753	0.969	0.003	-0.011	0.016	0.717	0.855	0.003	-0.008	0.013	0.644	0.837	0.000	-0.027	0.027	0.988	0.992
PE(P-18:1/18:3)	0.000	-0.022	0.023	0.979	0.995	-0.002	-0.016	0.012	0.765	0.881	-0.003	-0.013	0.008	0.644	0.837	-0.005	-0.032	0.022	0.737	0.872
CE(22:6)	0.008	-0.014	0.030	0.494	0.922	-0.003	-0.016	0.011	0.715	0.855	-0.002	-0.013	0.008	0.650	0.841	-0.029	-0.057	-0.001	0.042	0.147
PS(36:1)	-0.007	-0.029	0.015	0.548	0.929	-0.014	-0.028	0.000	0.045	0.306	0.003	-0.008	0.013	0.650	0.841	-0.001	-0.029	0.026	0.928	0.964
SM(d17:1/14:0)	-0.004	-0.027	0.018	0.709	0.964	-0.005	-0.019	0.009	0.466	0.686	-0.002	-0.013	0.008	0.649	0.841	-0.033	-0.060	-0.005	0.021	0.093
LPC(20:3) [sn1]	-0.012	-0.034	0.010	0.291	0.903	-0.012	-0.025	0.002	0.092	0.356	-0.002	-0.013	0.008	0.653	0.842	-0.019	-0.046	0.009	0.180	0.386
CE(24:6)	0.004	-0.018	0.026	0.740	0.964	-0.005	-0.019	0.009	0.480	0.697	-0.003	-0.014	0.008	0.652	0.842	-0.006	-0.034	0.021	0.656	0.814
PC(O-18:0/20:4)	-0.009	-0.031	0.013	0.403	0.922	0.000	-0.014	0.014	0.997	0.998	-0.002	-0.013	0.008	0.658	0.846	-0.033	-0.060	-0.006	0.016	0.080
PC(18:0_18:1)	-0.010	-0.032	0.012	0.364	0.922	-0.015	-0.029	-0.001	0.034	0.298	-0.002	-0.013	0.008	0.658	0.846	-0.032	-0.060	-0.005	0.022	0.097
PE(18:0_22:5) (n3)	-0.012	-0.034	0.009	0.262	0.903	-0.014	-0.027	0.000	0.052	0.317	-0.002	-0.013	0.008	0.662	0.847	-0.021	-0.048	0.007	0.141	0.330
TG(50:1) [NL-14:0]	-0.016	-0.038	0.006	0.163	0.903	-0.010	-0.024	0.003	0.134	0.396	0.002	-0.008	0.013	0.663	0.847	0.003	-0.026	0.031	0.862	0.937
Cer(d18:1/24:0)	-0.002	-0.024	0.020	0.881	0.981	0.003	-0.011	0.017	0.670	0.803	-0.002	-0.013	0.008	0.661	0.847	-0.007	-0.034	0.021	0.639	0.800
Cer(m18:0/20:0)	-0.018	-0.040	0.004	0.105	0.903	-0.013	-0.027	0.001	0.062	0.332	0.002	-0.008	0.013	0.666	0.850	-0.012	-0.040	0.015	0.373	0.590
LPC(17:1) [sn1] (b)	-0.012	-0.035	0.011	0.300	0.903	-0.012	-0.026	0.002	0.084	0.356	-0.002	-0.013	0.008	0.675	0.853	-0.031	-0.059	-0.003	0.029	0.118
PE(P-18:0/22:4)	-0.013	-0.035	0.009	0.241	0.903	0.008	-0.006	0.022	0.274	0.521	-0.002	-0.013	0.008	0.675	0.853	-0.015	-0.042	0.012	0.287	0.509
TG(48:2) [NL-14:0]	-0.019	-0.041	0.003	0.092	0.903	-0.013	-0.026	0.001	0.069	0.347	-0.002	-0.013	0.008	0.674	0.853	-0.009	-0.037	0.019	0.519	0.709
PE(17:0_20:4)	-0.010	-0.032	0.012	0.372	0.922	-0.013	-0.027	0.001	0.072	0.350	-0.002	-0.013	0.008	0.676	0.853	-0.029	-0.057	-0.001	0.042	0.147

SM(d17:1/16:0)	-0.004	-0.026	0.018	0.738	0.964	0.000	-0.014	0.014	0.957	0.976	-0.002	-0.013	0.009	0.675	0.853	-0.028	-0.056	-0.001	0.044	0.150
LPC(22:6) [+OH]	0.002	-0.021	0.024	0.883	0.981	-0.005	-0.020	0.009	0.445	0.672	-0.002	-0.013	0.009	0.677	0.853	-0.001	-0.029	0.027	0.943	0.966
LPI(20:4) [sn1]	-0.001	-0.023	0.021	0.961	0.995	-0.002	-0.016	0.013	0.826	0.913	0.002	-0.008	0.013	0.677	0.853	0.006	-0.021	0.033	0.669	0.818
SM(d16:1/23:0) & SM(d17:1/22:0)	0.000	-0.022	0.022	0.990	0.996	-0.001	-0.015	0.013	0.904	0.943	0.002	-0.008	0.013	0.670	0.853	-0.014	-0.041	0.013	0.318	0.538
DG(16:1_18:1)	-0.018	-0.040	0.004	0.107	0.903	-0.016	-0.030	-0.003	0.020	0.273	-0.002	-0.013	0.008	0.681	0.855	-0.029	-0.056	-0.001	0.042	0.147
CE(20:5)	0.015	-0.007	0.037	0.192	0.903	0.001	-0.013	0.015	0.875	0.934	0.002	-0.008	0.013	0.681	0.855	-0.010	-0.038	0.018	0.475	0.668
methyl-DE(18:1)	0.016	-0.006	0.038	0.159	0.903	-0.001	-0.015	0.013	0.852	0.929	0.002	-0.009	0.013	0.684	0.855	0.003	-0.025	0.030	0.839	0.928
dimethyl-CE(18:1)	0.011	-0.011	0.033	0.329	0.922	-0.005	-0.019	0.009	0.466	0.686	0.002	-0.009	0.013	0.683	0.855	-0.016	-0.044	0.012	0.260	0.479
PE(O-18:1/18:2)	-0.004	-0.027	0.018	0.699	0.964	0.008	-0.006	0.022	0.290	0.536	0.002	-0.009	0.013	0.685	0.855	-0.007	-0.035	0.020	0.603	0.767
PE(18:0_18:2)	-0.013	-0.035	0.009	0.243	0.903	-0.012	-0.026	0.002	0.095	0.360	-0.002	-0.013	0.009	0.689	0.858	0.000	-0.027	0.028	0.979	0.985
methyl-CE(20:4)	0.013	-0.010	0.035	0.268	0.903	0.009	-0.006	0.023	0.233	0.490	0.002	-0.009	0.013	0.694	0.863	-0.006	-0.033	0.022	0.685	0.830
PE(15-MHDA_20:4)	-0.015	-0.037	0.007	0.176	0.903	-0.010	-0.024	0.004	0.145	0.406	0.002	-0.009	0.013	0.695	0.864	-0.020	-0.048	0.007	0.146	0.337
PI(38:6)	-0.006	-0.028	0.016	0.601	0.950	-0.012	-0.026	0.002	0.092	0.356	-0.002	-0.013	0.009	0.697	0.864	-0.017	-0.045	0.010	0.220	0.430
CE(17:1)	-0.005	-0.027	0.017	0.652	0.960	-0.008	-0.022	0.005	0.241	0.495	-0.002	-0.013	0.009	0.704	0.872	-0.038	-0.066	-0.011	0.007	0.048
PC(18:0_22:4)	-0.015	-0.037	0.006	0.162	0.903	0.001	-0.013	0.015	0.903	0.943	-0.002	-0.013	0.009	0.707	0.873	-0.019	-0.046	0.008	0.164	0.366
LPE(22:6) [sn1]	-0.011	-0.033	0.012	0.346	0.922	-0.012	-0.026	0.001	0.082	0.356	-0.002	-0.013	0.009	0.707	0.873	-0.012	-0.040	0.015	0.372	0.590
PC(33:2)	-0.010	-0.032	0.012	0.383	0.922	-0.007	-0.021	0.007	0.347	0.589	-0.002	-0.013	0.009	0.710	0.873	-0.031	-0.058	-0.004	0.026	0.107
PE(18:1_18:1)	0.000	-0.022	0.022	0.988	0.996	-0.013	-0.027	0.000	0.059	0.323	-0.002	-0.013	0.009	0.710	0.873	0.009	-0.019	0.037	0.512	0.706
LPC(26:0) [sn2]	0.006	-0.016	0.029	0.569	0.933	-0.007	-0.021	0.007	0.322	0.560	-0.002	-0.013	0.009	0.715	0.878	-0.009	-0.037	0.018	0.517	0.709
PE(P-18:1/20:5) (b)	0.008	-0.014	0.030	0.475	0.922	-0.008	-0.022	0.006	0.292	0.536	0.002	-0.009	0.013	0.722	0.885	-0.022	-0.049	0.006	0.119	0.293
DG(18:0_20:4)	-0.017	-0.039	0.005	0.124	0.903	-0.013	-0.027	0.000	0.053	0.317	0.002	-0.009	0.013	0.726	0.888	-0.001	-0.029	0.027	0.948	0.968
TG(52:5) [NL-20:4]	-0.020	-0.042	0.002	0.076	0.903	-0.006	-0.020	0.007	0.351	0.592	0.002	-0.009	0.012	0.739	0.892	-0.002	-0.030	0.026	0.901	0.952
LPI(18:1) [sn2]	0.012	-0.010	0.034	0.287	0.903	0.001	-0.013	0.014	0.903	0.943	-0.002	-0.013	0.009	0.734	0.892	-0.002	-0.028	0.025	0.908	0.955
CE(14:0)	-0.009	-0.031	0.014	0.450	0.922	-0.013	-0.027	0.001	0.065	0.338	-0.002	-0.013	0.009	0.738	0.892	-0.021	-0.049	0.007	0.137	0.323
DG(16:0_22:5)	-0.011	-0.033	0.011	0.333	0.922	-0.015	-0.028	-0.002	0.028	0.285	-0.002	-0.013	0.009	0.735	0.892	-0.017	-0.044	0.011	0.229	0.430
FA(20:5)	0.010	-0.012	0.032	0.371	0.922	-0.013	-0.027	0.001	0.066	0.338	0.002	-0.009	0.013	0.738	0.892	-0.001	-0.028	0.027	0.957	0.970
Cer(d17:1/23:0)	-0.007	-0.029	0.015	0.536	0.923	-0.005	-0.020	0.009	0.450	0.674	-0.002	-0.013	0.009	0.739	0.892	-0.017	-0.044	0.010	0.225	0.434
PC(36:6) (a)	0.004	-0.019	0.026	0.744	0.964	-0.009	-0.023	0.005	0.199	0.460	-0.002	-0.013	0.009	0.740	0.892	-0.019	-0.046	0.008	0.175	0.378
PC(15:0_22:6)	0.001	-0.021	0.023	0.942	0.995	-0.012	-0.026	0.002	0.100	0.366	0.002	-0.009	0.013	0.732	0.892	-0.026	-0.055	0.002	0.065	0.186
FA(18:1)	-0.001	-0.023	0.022	0.944	0.995	0.001	-0.013	0.015	0.872	0.932	-0.002	-0.013	0.009	0.740	0.892	-0.017	-0.045	0.011	0.231	0.440
Cer(d18:1/26:0)	-0.012	-0.035	0.010	0.286	0.903	0.005	-0.009	0.019	0.503	0.720	-0.002	-0.013	0.009	0.743	0.893	-0.015	-0.043	0.012	0.270	0.495
PE(15-MHDA_22:6)	-0.007	-0.030	0.015	0.520	0.922	-0.014	-0.028	0.000	0.044	0.306	0.002	-0.009	0.013	0.742	0.893	-0.014	-0.042	0.014	0.327	0.545
LPI(18:0) [sn2]	-0.010	-0.032	0.012	0.371	0.922	-0.005	-0.019	0.010	0.530	0.735	-0.002	-0.013	0.009	0.745	0.894	-0.002	-0.029	0.026	0.896	0.952
TG(48:2) [NL-18:2]	-0.022	-0.043	0.000	0.051	0.903	-0.010	-0.024	0.003	0.142	0.406	-0.002	-0.012	0.009	0.748	0.896	-0.005	-0.034	0.023	0.707	0.845
PI(18:0_22:4)	-0.026	-0.047	-0.004	0.020	0.903	-0.012	-0.026	0.002	0.103	0.371	-0.002	-0.013	0.009	0.750	0.897	-0.019	-0.046	0.008	0.167	0.371
TG(56:8) [NL-20:5]	0.003	-0.019	0.025	0.785	0.973	-0.007	-0.021	0.007	0.331	0.572	0.002	-0.009	0.013	0.751	0.898	0.003	-0.025	0.030	0.853	0.933
PE(P-18:1/20:3) (b)	-0.012	-0.034	0.010	0.304	0.903	-0.004	-0.018	0.010	0.576	0.758	-0.002	-0.013	0.009	0.753	0.898	-0.031	-0.057	-0.004	0.025	0.106
PC(44:12)	0.009	-0.013	0.031	0.413	0.922	-0.008	-0.022	0.006	0.273	0.521	0.002	-0.009	0.013	0.758	0.902	0.003	-0.026	0.031	0.851	0.933
TG(54:2) [NL-20:1]	-0.009	-0.031	0.013	0.406	0.922	-0.017	-0.031	-0.004	0.014	0.273	0.002	-0.009	0.012	0.765	0.909	-0.007	-0.035	0.021	0.632	0.794
PE(O-18:0/22:5)	-0.008	-0.030	0.014	0.491	0.922	0.003	-0.011	0.017	0.646	0.811	0.002	-0.009	0.012	0.771	0.915	-0.020	-0.047	0.007	0.141	0.330
PA(40:6)	0.000	-0.021	0.022	0.984	0.996	-0.007	-0.022	0.007	0.318	0.557	-0.002	-0.012	0.009	0.774	0.917	-0.007	-0.036	0.023	0.657	0.814
LPC(15:0) [sn2]	-0.011	-0.033	0.011	0.335	0.922	-0.011	-0.025	0.002	0.100	0.366	-0.002	-0.012	0.009	0.777	0.919	-0.027	-0.055	0.001	0.055	0.173
LPI(20:4) [sn2]	-0.010	-0.032	0.012	0.363	0.922	-0.003	-0.017	0.011	0.684	0.840	0.002	-0.009	0.012	0.779	0.921	-0.010	-0.037	0.018	0.486	0.678
FA(17:0)	-0.005	-0.027	0.018	0.694	0.964	-0.006	-0.021	0.009	0.409	0.645	-0.002	-0.013	0.010	0.781	0.921	0.001	-0.027	0.029	0.958	0.970
TG(50:4) [NL-20:4]	-0.020	-0.042	0.002	0.075	0.903	-0.008	-0.021	0.006	0.273	0.521	0.001	-0.009	0.012	0.783	0.921	0.006	-0.022	0.034	0.682	0.827
SM(d18:2/23:0)	0.002	-0.020	0.024	0.854	0.981	0.000	-0.014	0.014	0.996	0.998	-0.002	-0.012	0.009	0.783	0.921	-0.024	-0.051	0.003	0.081	0.221
PC(16:0_22:6)	0.002	-0.020	0.024	0.867	0.981	-0.013	-0.027	0.002	0.084	0.356	0.002	-0.009	0.012	0.786	0.922	-0.023	-0.052	0.005	0.102	0.261
Cer(d19:1/16:0)	0.001	-0.021	0.024	0.902	0.985	-0.006	-0.020	0.008	0.390	0.631	-0.001	-0.012	0.009	0.789	0.925	-0.016	-0.044	0.012	0.272	0.498
TG(51:2) [NL-17:1]	-0.017	-0.039	0.005	0.126	0.903	-0.019	-0.033	-0.005	0.006	0.259	0.001	-0.009	0.012	0.792	0.925	-0.023	-0.051	0.004	0.099	0.256
CE(24:5)	0.003	-0.019	0.025	0.777	0.973	-0.001	-0.015	0.012	0.832	0.917	-0.001	-0.012	0.009	0.791	0.925	-0.013	-0.041	0.014	0.352	0.572
Cer(d19:1/22:0)	0.004	-0.018	0.027	0.708	0.964	-0.004	-0.018	0.009	0.532	0.737	-0.001	-0.012	0.009	0.794	0.926	-0.027	-0.055	0.000	0.048	0.157
TG(48:2) [NL-16:1]	-0.021	-0.044	0.001	0.057	0.903	-0.015	-0.028	-0.001	0.036	0.301	-0.001	-0.012	0.009	0.795	0.927	-0.016	-0.044	0.011	0.243	0.457
DG(14:0_16:0)	-0.015	-0.037	0.007	0.186	0.903	-0.011	-0.024	0.003	0.121	0.385	0.001	-0.009	0.012	0.797	0.927	0.006	-0.021	0.033	0.661	0.814
Cer(d19:1/24:1)	-0.002	-0.025	0.020	0.857	0.981	-0.017	-0.031	-0.003	0.018	0.273	-0.001	-0.012	0.009	0.801	0.930	-0.030	-0.057	-0.002	0.035	0.132

PE(O-16:0/22:4)	-0.016	-0.038	0.006	0.163	0.903	0.009	-0.005	0.023	0.194	0.454	0.001	-0.009	0.012	0.807	0.932	-0.006	-0.033	0.021	0.669	0.818
SM(d16:1/24:1)	-0.004	-0.027	0.018	0.694	0.964	-0.012	-0.026	0.002	0.089	0.356	0.001	-0.009	0.012	0.805	0.932	-0.027	-0.055	0.001	0.057	0.173
PE(P-20:0/22:6)	0.004	-0.019	0.026	0.747	0.964	-0.012	-0.026	0.003	0.112	0.382	0.001	-0.010	0.012	0.806	0.932	-0.026	-0.054	0.002	0.069	0.195
TG(52:2) [NL-18:2]	-0.025	-0.046	-0.004	0.023	0.903	-0.007	-0.021	0.006	0.293	0.536	0.001	-0.009	0.012	0.810	0.934	0.005	-0.022	0.033	0.712	0.847
PE(16:0_22:6)	-0.002	-0.024	0.020	0.848	0.981	-0.012	-0.026	0.001	0.075	0.355	0.001	-0.009	0.012	0.809	0.934	-0.012	-0.040	0.016	0.406	0.620
dimethyl-CE(18:2)	0.012	-0.010	0.034	0.287	0.903	0.002	-0.012	0.016	0.771	0.881	-0.001	-0.012	0.010	0.814	0.935	-0.011	-0.038	0.017	0.456	0.660
SM(43:2) (b)	-0.007	-0.029	0.015	0.561	0.933	-0.015	-0.029	-0.001	0.034	0.298	0.001	-0.009	0.012	0.813	0.935	-0.038	-0.065	-0.011	0.007	0.048
Cer(d20:1/24:1)	-0.012	-0.034	0.010	0.273	0.903	-0.012	-0.026	0.002	0.089	0.356	0.001	-0.010	0.012	0.817	0.937	-0.023	-0.050	0.005	0.107	0.272
PC(31:0) (b)	-0.008	-0.030	0.014	0.491	0.922	-0.007	-0.021	0.007	0.320	0.559	0.001	-0.009	0.012	0.821	0.940	-0.036	-0.063	-0.008	0.011	0.064
CE(16:1)	-0.008	-0.030	0.015	0.505	0.922	-0.011	-0.024	0.003	0.127	0.385	-0.001	-0.012	0.010	0.824	0.940	-0.018	-0.045	0.010	0.209	0.419
TG(50:2) [NL-14:0]	-0.002	-0.024	0.020	0.853	0.981	-0.017	-0.031	-0.003	0.015	0.273	-0.001	-0.012	0.010	0.825	0.940	-0.016	-0.045	0.013	0.276	0.500
TG(56:6) [NL-20:4]	-0.002	-0.024	0.020	0.850	0.981	0.002	-0.012	0.016	0.807	0.899	0.001	-0.010	0.012	0.823	0.940	-0.004	-0.032	0.024	0.771	0.892
PE(P-18:0/18:2)	-0.008	-0.030	0.014	0.500	0.922	0.004	-0.010	0.018	0.570	0.752	-0.001	-0.012	0.010	0.827	0.941	-0.008	-0.035	0.019	0.571	0.745
FA(14:0)	0.008	-0.014	0.030	0.460	0.922	0.001	-0.013	0.015	0.891	0.939	-0.001	-0.012	0.010	0.829	0.942	-0.012	-0.040	0.016	0.401	0.617
PI(18:0_20:3) (b)	-0.016	-0.038	0.007	0.170	0.903	-0.026	-0.040	-0.012	0.000	0.092	-0.001	-0.012	0.010	0.832	0.943	-0.038	-0.066	-0.011	0.007	0.048
PI(15-MHDA_18:1) & PI(17:0_18:1)	-0.013	-0.035	0.009	0.259	0.903	-0.011	-0.025	0.003	0.134	0.396	-0.001	-0.012	0.010	0.831	0.943	-0.015	-0.042	0.013	0.296	0.520
dimethyl-CE(20:4)	0.012	-0.011	0.034	0.305	0.903	0.005	-0.009	0.019	0.458	0.682	-0.001	-0.012	0.010	0.837	0.944	-0.017	-0.045	0.010	0.214	0.422
Cer(m18:1/20:0)	-0.021	-0.043	0.001	0.064	0.903	-0.010	-0.023	0.004	0.161	0.432	0.001	-0.010	0.012	0.838	0.944	-0.011	-0.038	0.016	0.432	0.640
TG(48:3) [NL-18:3]	-0.020	-0.042	0.002	0.071	0.903	-0.009	-0.023	0.004	0.182	0.452	-0.001	-0.012	0.010	0.837	0.944	0.002	-0.026	0.030	0.870	0.943
LPC(22:6) [sn2]	0.003	-0.019	0.026	0.765	0.969	-0.014	-0.028	0.000	0.045	0.306	-0.001	-0.012	0.010	0.837	0.944	-0.014	-0.042	0.014	0.321	0.540
PC(34:2) [+OH]	-0.013	-0.035	0.009	0.248	0.903	-0.002	-0.016	0.011	0.766	0.881	0.001	-0.010	0.012	0.844	0.948	0.004	-0.023	0.032	0.762	0.891
PC(P-18:1/22:6)	0.002	-0.020	0.024	0.871	0.981	-0.012	-0.026	0.002	0.088	0.356	-0.001	-0.012	0.010	0.843	0.948	-0.028	-0.055	-0.001	0.044	0.150
PE(20:0_20:4)	-0.016	-0.038	0.007	0.167	0.903	-0.005	-0.018	0.009	0.512	0.724	0.001	-0.010	0.012	0.851	0.954	0.011	-0.016	0.038	0.439	0.644
PC(32:1)	-0.020	-0.042	0.002	0.075	0.903	-0.011	-0.025	0.003	0.113	0.382	-0.001	-0.012	0.010	0.860	0.962	-0.027	-0.054	0.001	0.056	0.173
DG(18:2_20:4)	-0.015	-0.037	0.007	0.183	0.903	0.002	-0.012	0.016	0.790	0.891	-0.001	-0.012	0.010	0.862	0.962	-0.001	-0.029	0.026	0.920	0.963
LPE(22:6) [sn2]	-0.010	-0.032	0.013	0.402	0.922	-0.012	-0.025	0.002	0.088	0.356	-0.001	-0.012	0.010	0.862	0.962	-0.011	-0.039	0.016	0.412	0.628
SM(d18:1/24:1)	-0.012	-0.034	0.010	0.298	0.903	-0.011	-0.025	0.003	0.125	0.385	-0.001	-0.012	0.010	0.884	0.964	-0.029	-0.056	-0.001	0.041	0.146
SM(37:2)	-0.012	-0.034	0.010	0.292	0.903	0.000	-0.015	0.014	0.950	0.972	0.001	-0.010	0.012	0.883	0.964	-0.016	-0.043	0.011	0.243	0.456
PI(16:0_20:4)	-0.024	-0.046	-0.002	0.033	0.903	-0.004	-0.018	0.010	0.554	0.748	-0.001	-0.012	0.010	0.878	0.964	-0.015	-0.042	0.013	0.294	0.518
TG(51:2) [NL-17:0]	-0.019	-0.041	0.002	0.082	0.903	-0.016	-0.029	-0.002	0.023	0.285	0.001	-0.010	0.011	0.895	0.964	-0.012	-0.040	0.016	0.392	0.609
DG(16:0_16:1)	-0.020	-0.043	0.002	0.071	0.903	-0.011	-0.025	0.002	0.110	0.380	-0.001	-0.011	0.010	0.895	0.964	-0.011	-0.038	0.016	0.434	0.641
methyl-CE(22:6)	0.018	-0.005	0.040	0.120	0.903	0.000	-0.013	0.014	0.973	0.983	-0.001	-0.011	0.010	0.892	0.964	-0.009	-0.037	0.019	0.535	0.719
Cer(d16:1/23:0)	-0.012	-0.034	0.010	0.291	0.903	-0.011	-0.025	0.003	0.114	0.382	-0.001	-0.012	0.010	0.887	0.964	-0.007	-0.035	0.020	0.601	0.765
dimethyl-CE(22:6)	0.014	-0.009	0.036	0.231	0.903	0.000	-0.014	0.014	0.963	0.979	0.001	-0.010	0.012	0.891	0.964	-0.005	-0.033	0.022	0.708	0.845
PG(36:2)	-0.019	-0.041	0.004	0.102	0.903	-0.009	-0.023	0.004	0.166	0.432	-0.001	-0.012	0.010	0.883	0.964	0.004	-0.024	0.032	0.770	0.892
PC(16:0_18:1)	-0.011	-0.032	0.011	0.348	0.922	-0.012	-0.026	0.002	0.095	0.360	-0.001	-0.012	0.010	0.888	0.964	-0.039	-0.067	-0.011	0.006	0.048
CE(17:0)	-0.009	-0.031	0.013	0.437	0.922	-0.006	-0.020	0.007	0.359	0.598	-0.001	-0.012	0.010	0.869	0.964	-0.038	-0.065	-0.011	0.007	0.048
PC(15-MHDA_18:2)	-0.009	-0.031	0.013	0.413	0.922	-0.013	-0.027	0.001	0.065	0.338	-0.001	-0.012	0.010	0.889	0.964	-0.031	-0.058	-0.004	0.027	0.111
TG(52:2) [NL-16:0]	-0.008	-0.030	0.014	0.466	0.922	-0.020	-0.033	-0.006	0.006	0.259	-0.001	-0.012	0.010	0.892	0.964	-0.030	-0.058	-0.002	0.036	0.134
PC(P-35:2) (b)	-0.008	-0.030	0.014	0.481	0.922	-0.005	-0.018	0.009	0.509	0.724	-0.001	-0.012	0.010	0.878	0.964	-0.010	-0.037	0.016	0.447	0.652
AC(17:0) (a)	-0.006	-0.028	0.016	0.612	0.950	-0.017	-0.031	-0.004	0.012	0.273	-0.001	-0.012	0.010	0.878	0.964	-0.031	-0.057	-0.004	0.025	0.106
PE(P-18:0/18:3)	-0.006	-0.028	0.017	0.627	0.954	-0.002	-0.016	0.012	0.768	0.881	-0.001	-0.012	0.010	0.888	0.964	-0.007	-0.035	0.022	0.651	0.811
SM(d17:1/24:1)	-0.005	-0.027	0.017	0.653	0.960	-0.014	-0.028	0.000	0.046	0.306	-0.001	-0.011	0.010	0.893	0.964	-0.033	-0.060	-0.005	0.020	0.091
PE(16:0_20:5)	-0.004	-0.026	0.018	0.714	0.964	-0.016	-0.030	-0.002	0.022	0.273	0.001	-0.010	0.012	0.886	0.964	-0.009	-0.037	0.018	0.508	0.702
TG(O-54:4) [NL-18:2]	-0.004	-0.026	0.018	0.732	0.964	0.011	-0.003	0.024	0.130	0.390	0.001	-0.010	0.012	0.877	0.964	0.008	-0.020	0.035	0.574	0.745
FA(20:3)	-0.004	-0.026	0.018	0.707	0.964	0.000	-0.014	0.014	0.972	0.983	-0.001	-0.012	0.010	0.891	0.964	-0.003	-0.030	0.025	0.853	0.933
PC(14:0_22:6)	-0.003	-0.026	0.019	0.786	0.973	-0.011	-0.025	0.002	0.106	0.373	-0.001	-0.012	0.010	0.892	0.964	-0.018	-0.046	0.009	0.197	0.409
PC(16:0_20:4)	0.002	-0.020	0.024	0.864	0.981	-0.001	-0.015	0.013	0.898	0.942	-0.001	-0.012	0.010	0.889	0.964	-0.032	-0.060	-0.003	0.030	0.120
PE(P-18:1/18:2) (a)	-0.002	-0.025	0.020	0.839	0.981	0.005	-0.009	0.019	0.459	0.682	0.001	-0.010	0.012	0.887	0.964	-0.014	-0.041	0.014	0.332	0.550
LPI(18:1) [sn1]	0.002	-0.020	0.024	0.881	0.981	-0.014	-0.028	0.000	0.054	0.317	-0.001	-0.012	0.010	0.869	0.964	0.012	-0.015	0.039	0.383	0.598
TG(48:2) [NL-14:1]	-0.020	-0.042	0.003	0.083	0.903	-0.017	-0.030	-0.003	0.017	0.273	-0.001	-0.011	0.010	0.903	0.969	-0.017	-0.045	0.010	0.222	0.430
PC(P-38:5) (a)	-0.004	-0.026	0.018	0.727	0.964	-0.003	-0.017	0.011	0.643	0.809	-0.001	-0.012	0.010	0.902	0.969	-0.025	-0.052	0.002	0.071	0.200
TG(56:7) [NL-22:5]	-0.005	-0.027	0.017	0.669	0.964	-0.011	-0.025	0.003	0.113	0.382	-0.001	-0.011	0.010	0.903	0.969	-0.015	-0.043	0.013	0.288	0.509
PC(33:1)	-0.017	-0.039	0.005	0.139	0.903	-0.016	-0.029	-0.002	0.028	0.285	-0.001	-0.012	0.010	0.906	0.971	-0.039	-0.067	-0.012	0.005	0.044

PI(15-MHDA_20:4) & PI(17:0_20:4)	-0.025	-0.047	-0.004	0.023	0.903	-0.009	-0.023	0.005	0.192	0.454	-0.001	-0.011	0.010	0.910	0.972	-0.029	-0.057	-0.002	0.037	0.136
PC(P-16:0/18:2)	-0.010	-0.032	0.012	0.387	0.922	-0.002	-0.016	0.012	0.800	0.897	0.001	-0.010	0.011	0.909	0.972	-0.012	-0.039	0.015	0.388	0.604
LPC(20:3) [sn2]	-0.012	-0.033	0.010	0.299	0.903	-0.011	-0.024	0.003	0.124	0.385	-0.001	-0.011	0.010	0.921	0.975	-0.013	-0.040	0.014	0.345	0.564
PE(18:0_22:5) (n6)	-0.013	-0.034	0.009	0.258	0.903	-0.005	-0.019	0.009	0.488	0.705	-0.001	-0.011	0.010	0.922	0.975	0.001	-0.026	0.028	0.945	0.966
TG(49:1) [NL-16:1]	-0.019	-0.041	0.003	0.096	0.903	-0.006	-0.019	0.008	0.407	0.643	-0.001	-0.011	0.010	0.923	0.975	0.001	-0.026	0.028	0.950	0.968
AC(14:0)-OH	-0.006	-0.029	0.016	0.565	0.933	-0.006	-0.020	0.007	0.366	0.602	-0.001	-0.011	0.010	0.920	0.975	-0.019	-0.046	0.008	0.171	0.376
PC(P-35:2) (a)	-0.005	-0.027	0.017	0.657	0.960	-0.010	-0.024	0.004	0.168	0.433	0.001	-0.010	0.011	0.917	0.975	-0.007	-0.035	0.020	0.593	0.758
AC(15:0) (b)	-0.004	-0.026	0.018	0.714	0.964	-0.010	-0.023	0.004	0.163	0.432	0.001	-0.010	0.011	0.920	0.975	-0.032	-0.059	-0.005	0.019	0.089
SM(d18:1/22:0) & SM(d16:1/24:0)	0.004	-0.018	0.026	0.733	0.964	0.006	-0.008	0.020	0.395	0.634	0.001	-0.010	0.011	0.917	0.975	-0.017	-0.043	0.010	0.229	0.439
SM(d18:0/14:0)	0.002	-0.020	0.024	0.864	0.981	-0.004	-0.017	0.010	0.600	0.771	-0.001	-0.011	0.010	0.921	0.975	-0.030	-0.057	-0.002	0.035	0.132
PE(18:0_22:4)	-0.018	-0.039	0.004	0.114	0.903	-0.004	-0.018	0.010	0.590	0.764	0.001	-0.010	0.011	0.926	0.976	-0.002	-0.030	0.025	0.868	0.942
PA(36:4)	-0.002	-0.024	0.020	0.879	0.981	-0.003	-0.017	0.011	0.696	0.845	-0.001	-0.011	0.010	0.925	0.976	0.024	-0.004	0.051	0.091	0.241
PC(39:5) (a)	0.009	-0.013	0.032	0.415	0.922	-0.009	-0.023	0.005	0.195	0.455	0.000	-0.010	0.011	0.928	0.976	-0.042	-0.070	-0.014	0.004	0.038
Cer(d17:1/24:0)	-0.005	-0.028	0.017	0.636	0.960	0.002	-0.012	0.017	0.735	0.870	0.000	-0.011	0.010	0.929	0.976	-0.003	-0.031	0.024	0.821	0.921
PC(P-36:3)	-0.007	-0.028	0.015	0.559	0.933	-0.005	-0.019	0.009	0.479	0.696	0.000	-0.011	0.010	0.933	0.979	-0.022	-0.049	0.005	0.111	0.277
TG(50:2) [NL-16:1]	-0.020	-0.041	0.002	0.079	0.903	-0.017	-0.030	-0.003	0.015	0.273	0.000	-0.011	0.010	0.939	0.980	-0.027	-0.055	0.001	0.056	0.173
PE(18:0_20:3) (a)	-0.013	-0.035	0.009	0.242	0.903	-0.012	-0.026	0.002	0.083	0.356	0.000	-0.011	0.010	0.938	0.980	-0.011	-0.038	0.016	0.438	0.644
TG(50:3) [NL-18:3]	-0.024	-0.045	-0.002	0.034	0.903	-0.010	-0.023	0.004	0.166	0.432	0.000	-0.010	0.011	0.936	0.980	0.002	-0.026	0.029	0.906	0.954
PI(18:0_22:5) (n6)	-0.009	-0.031	0.012	0.397	0.922	-0.019	-0.033	-0.005	0.007	0.259	0.000	-0.011	0.010	0.937	0.980	-0.006	-0.033	0.021	0.662	0.814
PE(O-16:0/20:3)	-0.017	-0.039	0.005	0.127	0.903	-0.005	-0.019	0.009	0.477	0.696	0.000	-0.011	0.010	0.941	0.980	-0.016	-0.042	0.011	0.249	0.464
PE(17:0_18:1)	-0.009	-0.031	0.013	0.441	0.922	-0.016	-0.030	-0.003	0.018	0.273	0.000	-0.010	0.011	0.944	0.982	-0.008	-0.036	0.019	0.556	0.734
TG(50:2) [NL-18:1]	-0.019	-0.041	0.003	0.084	0.903	-0.019	-0.033	-0.005	0.006	0.259	0.000	-0.011	0.010	0.952	0.984	-0.027	-0.055	0.002	0.065	0.186
LPC(14:0) [sn1]	-0.015	-0.037	0.008	0.203	0.903	-0.009	-0.023	0.005	0.205	0.466	0.000	-0.011	0.010	0.951	0.984	-0.013	-0.040	0.014	0.353	0.572
PC(14:0_20:4)	-0.013	-0.036	0.009	0.243	0.903	0.000	-0.014	0.014	0.985	0.989	0.000	-0.011	0.011	0.966	0.984	-0.011	-0.038	0.017	0.449	0.653
PE(16:0_18:1)	-0.014	-0.036	0.008	0.224	0.903	-0.012	-0.026	0.002	0.089	0.356	0.000	-0.011	0.011	0.965	0.984	-0.010	-0.038	0.017	0.466	0.664
DG(16:0_18:1)	-0.015	-0.037	0.007	0.170	0.903	-0.015	-0.029	-0.002	0.026	0.285	0.000	-0.010	0.011	0.963	0.984	-0.009	-0.037	0.019	0.519	0.709
DG(18:0_18:2)	-0.015	-0.037	0.007	0.180	0.903	-0.011	-0.024	0.003	0.116	0.384	0.000	-0.011	0.010	0.965	0.984	0.002	-0.025	0.030	0.862	0.937
PA(36:1)	0.012	-0.010	0.034	0.276	0.903	-0.019	-0.033	-0.005	0.010	0.270	0.000	-0.011	0.011	0.963	0.984	-0.001	-0.031	0.029	0.941	0.966
PC(15-MHDA_18:1)	-0.011	-0.033	0.012	0.353	0.922	-0.019	-0.032	-0.005	0.009	0.268	0.000	-0.011	0.011	0.963	0.984	-0.039	-0.066	-0.011	0.006	0.048
Cer(d20:1/24:0)	-0.008	-0.030	0.014	0.498	0.922	-0.004	-0.018	0.010	0.563	0.748	0.000	-0.011	0.011	0.962	0.984	-0.012	-0.040	0.015	0.374	0.592
methyl-CE(18:1)	0.009	-0.013	0.032	0.414	0.922	0.000	-0.014	0.014	0.970	0.983	0.000	-0.010	0.011	0.952	0.984	-0.012	-0.039	0.016	0.414	0.629
Cer(d16:1/24:0)	-0.007	-0.030	0.015	0.514	0.922	-0.005	-0.019	0.009	0.519	0.727	0.000	-0.011	0.011	0.954	0.984	0.001	-0.026	0.029	0.918	0.962
PI(39:6)	-0.007	-0.029	0.015	0.551	0.931	-0.015	-0.029	-0.002	0.030	0.289	0.000	-0.010	0.011	0.954	0.984	-0.014	-0.042	0.014	0.317	0.537
SM(d18:1/14:0) & SM(d16:1/16:0)	-0.006	-0.028	0.016	0.596	0.950	-0.003	-0.017	0.011	0.707	0.849	0.000	-0.011	0.011	0.957	0.984	-0.027	-0.054	0.001	0.056	0.173
AC(20:5)	0.004	-0.018	0.026	0.712	0.964	-0.009	-0.023	0.004	0.189	0.454	0.000	-0.011	0.011	0.967	0.984	-0.004	-0.031	0.023	0.762	0.891
PC(15-MHDA_20:4)	-0.003	-0.025	0.019	0.819	0.980	-0.007	-0.021	0.007	0.333	0.572	0.000	-0.011	0.010	0.950	0.984	-0.040	-0.067	-0.013	0.004	0.042
PC(17:0_20:4)	-0.001	-0.023	0.021	0.945	0.995	-0.004	-0.018	0.010	0.617	0.787	0.000	-0.010	0.011	0.961	0.984	-0.035	-0.063	-0.008	0.013	0.069
PE(18:0_20:4)	-0.011	-0.033	0.010	0.304	0.903	-0.008	-0.022	0.006	0.248	0.501	0.000	-0.011	0.011	0.977	0.990	-0.011	-0.039	0.017	0.435	0.641
PC(18:2_20:5)	0.008	-0.014	0.031	0.470	0.922	-0.009	-0.023	0.005	0.201	0.463	0.000	-0.011	0.011	0.977	0.990	-0.001	-0.028	0.027	0.958	0.970
LPI(18:2) [sn1]	0.000	-0.022	0.021	0.969	0.995	0.008	-0.006	0.022	0.263	0.514	0.000	-0.011	0.011	0.977	0.990	0.015	-0.012	0.042	0.286	0.509
PE(18:0_20:3) (b)	-0.018	-0.040	0.004	0.103	0.903	-0.020	-0.034	-0.007	0.004	0.259	0.000	-0.011	0.011	0.979	0.990	-0.019	-0.047	0.009	0.177	0.382
PC(18:0_20:4)	-0.002	-0.024	0.020	0.861	0.981	0.003	-0.011	0.017	0.687	0.840	0.000	-0.011	0.011	0.979	0.990	-0.023	-0.051	0.005	0.106	0.271
PI(18:0_22:6)	-0.009	-0.031	0.013	0.442	0.922	-0.016	-0.030	-0.002	0.026	0.285	0.000	-0.011	0.011	0.981	0.990	-0.018	-0.046	0.010	0.200	0.416
DG(18:1_18:1)	-0.008	-0.029	0.014	0.503	0.922	-0.018	-0.031	-0.004	0.011	0.273	0.000	-0.011	0.011	0.986	0.994	-0.018	-0.046	0.010	0.204	0.416
PE(16:0_20:4)	-0.013	-0.035	0.008	0.230	0.903	-0.011	-0.025	0.003	0.123	0.385	0.000	-0.011	0.011	0.995	0.998	-0.018	-0.046	0.010	0.205	0.416
TG(50:2) [NL-18:2]	-0.021	-0.043	0.000	0.051	0.903	-0.005	-0.019	0.009	0.489	0.706	0.000	-0.011	0.010	0.994	0.998	0.000	-0.027	0.028	0.980	0.985
PC(P-20:0/20:4)	-0.008	-0.030	0.014	0.492	0.922	-0.001	-0.014	0.013	0.920	0.953	0.000	-0.011	0.011	0.996	0.998	-0.031	-0.058	-0.004	0.024	0.105
PE(P-16:0/22:5) (n6)	-0.009	-0.031	0.013	0.423	0.922	0.003	-0.011	0.017	0.667	0.829	0.000	-0.011	0.011	0.998	0.998	0.000	-0.026	0.026	0.995	0.996
Cer(d19:1/23:0)	0.004	-0.019	0.026	0.741	0.964	-0.008	-0.022	0.006	0.256	0.507	0.000	-0.011	0.011	0.996	0.998	-0.026	-0.053	0.001	0.063	0.184
PE(P-16:0/18:3)	-0.004	-0.026	0.018	0.718	0.964	0.001	-0.013	0.016	0.855	0.929	0.000	-0.011	0.011	0.997	0.998	0.008	-0.020	0.036	0.588	0.756

Supplementary Table 7. Associations of lipid classes with longitudinal A/T/N biomarkers

Lipid classes	A: Amyloid PET (AV45) uptake					T: CSF pTau					N1: Hippocampal volume					N2: FDG uptake				
	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)
GM3	-0.007	-0.029	0.015	0.543	0.901	-0.011	-0.026	0.003	0.116	0.382	-0.022	-0.032	-0.011	0.000	0.002	-0.065	-0.092	-0.038	0.000	0.000
GM1	0.003	-0.020	0.025	0.823	0.901	-0.018	-0.032	-0.003	0.015	0.221	-0.015	-0.026	-0.005	0.005	0.063	-0.060	-0.089	-0.032	0.000	0.001
deDE	-0.001	-0.024	0.022	0.929	0.929	0.000	-0.014	0.015	0.952	0.973	-0.027	-0.038	-0.016	0.000	0.000	-0.057	-0.086	-0.029	0.000	0.001
Hex3Cer	-0.005	-0.027	0.017	0.681	0.901	-0.008	-0.022	0.006	0.261	0.512	-0.013	-0.024	-0.002	0.021	0.138	-0.050	-0.077	-0.023	0.000	0.004
PC	-0.011	-0.033	0.012	0.352	0.901	-0.013	-0.027	0.001	0.063	0.241	-0.006	-0.017	0.005	0.296	0.524	-0.045	-0.072	-0.018	0.001	0.011
AC	-0.003	-0.025	0.019	0.798	0.901	-0.014	-0.028	-0.001	0.041	0.224	-0.013	-0.023	-0.002	0.020	0.138	-0.044	-0.070	-0.017	0.002	0.012
SM	-0.003	-0.025	0.019	0.763	0.901	-0.006	-0.019	0.008	0.437	0.669	-0.004	-0.015	0.007	0.466	0.650	-0.042	-0.069	-0.016	0.002	0.013
LPC(O)	-0.010	-0.032	0.012	0.365	0.901	-0.020	-0.033	-0.006	0.006	0.221	-0.019	-0.029	-0.008	0.001	0.011	-0.041	-0.068	-0.013	0.004	0.019
COH	-0.005	-0.027	0.017	0.644	0.901	-0.003	-0.017	0.011	0.666	0.901	-0.005	-0.016	0.006	0.332	0.566	-0.040	-0.067	-0.013	0.004	0.019
CE	-0.002	-0.024	0.021	0.895	0.919	-0.002	-0.015	0.012	0.798	0.973	-0.008	-0.019	0.003	0.139	0.343	-0.039	-0.066	-0.012	0.005	0.025
PC(O)	-0.010	-0.032	0.012	0.360	0.901	-0.008	-0.022	0.006	0.274	0.512	-0.005	-0.015	0.006	0.408	0.608	-0.036	-0.062	-0.009	0.009	0.038
PIP1	-0.006	-0.028	0.016	0.601	0.901	-0.007	-0.021	0.006	0.290	0.512	-0.008	-0.018	0.003	0.159	0.366	-0.035	-0.062	-0.008	0.011	0.040
Cer(d)	-0.011	-0.033	0.011	0.342	0.901	-0.011	-0.025	0.003	0.134	0.412	-0.007	-0.018	0.004	0.208	0.415	-0.034	-0.061	-0.006	0.016	0.058
Hex2Cer	-0.002	-0.024	0.020	0.877	0.919	-0.001	-0.015	0.013	0.881	0.973	-0.012	-0.023	-0.002	0.024	0.138	-0.032	-0.059	-0.005	0.022	0.068
AC-OH	-0.003	-0.025	0.019	0.802	0.901	-0.007	-0.021	0.006	0.300	0.512	-0.005	-0.015	0.006	0.409	0.608	-0.032	-0.060	-0.005	0.022	0.068
HexCer	0.008	-0.014	0.030	0.467	0.901	-0.008	-0.022	0.005	0.230	0.495	-0.013	-0.024	-0.003	0.016	0.138	-0.031	-0.058	-0.003	0.028	0.079
LPE	-0.020	-0.042	0.002	0.078	0.901	-0.016	-0.029	-0.002	0.024	0.221	-0.012	-0.023	-0.001	0.030	0.153	-0.030	-0.058	-0.003	0.029	0.079
PI	-0.020	-0.042	0.002	0.077	0.901	-0.012	-0.026	0.002	0.099	0.351	-0.005	-0.016	0.006	0.354	0.582	-0.029	-0.056	-0.002	0.035	0.088
LPC	-0.007	-0.029	0.015	0.557	0.901	-0.014	-0.027	0.000	0.050	0.232	-0.011	-0.022	-0.001	0.041	0.170	-0.028	-0.055	0.000	0.048	0.114
SHexCer	-0.005	-0.027	0.018	0.679	0.901	-0.007	-0.021	0.007	0.346	0.562	-0.007	-0.018	0.004	0.200	0.415	-0.028	-0.056	0.000	0.050	0.114
LPE(P)	-0.004	-0.026	0.018	0.717	0.901	-0.007	-0.021	0.008	0.355	0.562	-0.008	-0.019	0.003	0.139	0.343	-0.026	-0.053	0.002	0.067	0.147
C1P	-0.004	-0.025	0.018	0.747	0.901	-0.001	-0.015	0.013	0.898	0.973	-0.010	-0.021	0.000	0.061	0.216	-0.025	-0.053	0.003	0.078	0.163
LPC(P)	-0.009	-0.031	0.013	0.424	0.901	-0.010	-0.024	0.004	0.162	0.467	-0.011	-0.022	0.000	0.048	0.182	-0.024	-0.051	0.003	0.087	0.174
S1P	-0.007	-0.029	0.015	0.514	0.901	-0.008	-0.022	0.006	0.237	0.495	-0.008	-0.019	0.003	0.142	0.343	-0.023	-0.050	0.004	0.098	0.187
PC(P)	-0.007	-0.029	0.015	0.534	0.901	-0.008	-0.022	0.006	0.280	0.512	0.001	-0.010	0.012	0.852	0.945	-0.020	-0.047	0.007	0.152	0.279
DE	0.013	-0.009	0.035	0.240	0.901	0.009	-0.004	0.023	0.178	0.482	-0.009	-0.020	0.002	0.094	0.281	-0.020	-0.048	0.008	0.159	0.282
TG(O) [NL]	-0.012	-0.034	0.009	0.264	0.901	-0.004	-0.018	0.009	0.544	0.807	0.010	-0.001	0.020	0.079	0.260	0.017	-0.011	0.044	0.240	0.409
OxSpecies	-0.005	-0.027	0.018	0.692	0.901	-0.009	-0.023	0.005	0.203	0.491	-0.009	-0.020	0.002	0.098	0.281	-0.016	-0.044	0.012	0.250	0.411
PE	-0.016	-0.037	0.006	0.166	0.901	-0.015	-0.029	-0.001	0.032	0.224	-0.003	-0.014	0.008	0.582	0.765	-0.015	-0.043	0.012	0.282	0.448
Sph	0.011	-0.011	0.033	0.317	0.901	-0.009	-0.022	0.005	0.229	0.495	0.001	-0.010	0.012	0.791	0.933	0.014	-0.013	0.041	0.308	0.472
PE(P)	-0.007	-0.029	0.015	0.528	0.901	0.000	-0.015	0.014	0.951	0.973	0.007	-0.004	0.018	0.201	0.415	-0.013	-0.041	0.014	0.329	0.474
dimethyl-CE	0.013	-0.009	0.036	0.241	0.901	0.001	-0.013	0.015	0.923	0.973	0.000	-0.011	0.011	0.981	0.981	-0.014	-0.041	0.014	0.327	0.474
methyl-CE	0.012	-0.010	0.035	0.279	0.901	0.003	-0.011	0.017	0.646	0.900	-0.002	-0.012	0.009	0.763	0.923	-0.012	-0.040	0.016	0.392	0.547
Ubiquinone	0.007	-0.015	0.029	0.511	0.901	-0.004	-0.018	0.010	0.577	0.830	-0.004	-0.015	0.006	0.431	0.620	-0.010	-0.038	0.017	0.464	0.628
TG [NL]	-0.019	-0.041	0.002	0.083	0.901	-0.016	-0.029	-0.002	0.023	0.221	0.001	-0.010	0.011	0.896	0.958	-0.009	-0.037	0.019	0.539	0.708
DG	-0.015	-0.037	0.007	0.188	0.901	-0.013	-0.027	0.000	0.059	0.241	0.001	-0.009	0.012	0.829	0.945	-0.008	-0.035	0.020	0.592	0.757
PE(O)	-0.006	-0.029	0.016	0.571	0.901	0.002	-0.012	0.016	0.754	0.964	0.006	-0.004	0.017	0.237	0.454	-0.007	-0.034	0.020	0.625	0.777
Cer(m)	-0.018	-0.040	0.004	0.102	0.901	-0.009	-0.023	0.005	0.199	0.491	0.005	-0.006	0.015	0.401	0.608	-0.006	-0.034	0.021	0.646	0.782
FFA	-0.001	-0.024	0.021	0.899	0.919	0.000	-0.014	0.014	1.000	1.000	-0.002	-0.013	0.009	0.762	0.923	-0.006	-0.033	0.022	0.675	0.797
dhCer	-0.009	-0.032	0.013	0.403	0.901	0.002	-0.011	0.016	0.753	0.964	0.011	0.001	0.022	0.038	0.170	-0.003	-0.031	0.024	0.806	0.904
BA	-0.008	-0.031	0.014	0.461	0.901	0.002	-0.012	0.015	0.820	0.973	-0.004	-0.015	0.007	0.497	0.672	-0.003	-0.031	0.024	0.814	0.904
PS	0.003	-0.019	0.025	0.796	0.901	-0.015	-0.028	-0.001	0.035	0.224	-0.003	-0.014	0.008	0.614	0.785	-0.003	-0.031	0.024	0.826	0.904
PA	-0.003	-0.025	0.019	0.809	0.901	-0.014	-0.028	0.000	0.044	0.224	-0.006	-0.017	0.005	0.258	0.474	0.002	-0.025	0.030	0.860	0.920
LPI	-0.003	-0.025	0.018	0.759	0.901	-0.001	-0.016	0.013	0.843	0.973	0.000	-0.011	0.010	0.943	0.981	0.002	-0.025	0.029	0.890	0.921
methyl-DE	0.016	-0.006	0.039	0.151	0.901	0.001	-0.013	0.015	0.852	0.973	0.000	-0.011	0.011	0.965	0.981	0.002	-0.026	0.029	0.901	0.921
PG	-0.020	-0.042	0.002	0.080	0.901	-0.016	-0.029	-0.002	0.021	0.221	-0.001	-0.012	0.010	0.863	0.945	-0.001	-0.029	0.027	0.956	0.956

Supplementary Table 8. Associations of lipid correlation network modules with longitudinal A/T/N biomarkers

Lipid modules	A: Amyloid PET (AV45) uptake					T: CSF pTau					N1: Hippocampal volume					N2: FDG uptake				
	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)	Beta	95% CI (Lower)	95% CI (Upper)	Pvalue	Pvalue(BH)
M23	-0.010	-0.032	0.012	0.378	0.900	-0.004	-0.018	0.009	0.536	0.782	-0.011	-0.022	0.000	0.041	0.147	-0.053	-0.079	-0.026	0.000	0.005
M4	-0.007	-0.029	0.015	0.557	0.900	-0.015	-0.029	-0.001	0.030	0.270	-0.011	-0.021	0.000	0.055	0.168	-0.049	-0.076	-0.021	0.001	0.012
M42	-0.009	-0.031	0.013	0.417	0.900	-0.011	-0.025	0.003	0.129	0.340	-0.011	-0.022	0.000	0.041	0.147	-0.045	-0.071	-0.018	0.001	0.014
M44	-0.017	-0.039	0.004	0.119	0.900	-0.013	-0.027	0.001	0.061	0.309	-0.011	-0.022	0.000	0.048	0.159	-0.046	-0.073	-0.018	0.001	0.014
M39	-0.010	-0.032	0.012	0.387	0.900	-0.021	-0.034	-0.007	0.004	0.164	-0.019	-0.030	-0.008	0.001	0.008	-0.042	-0.070	-0.015	0.002	0.014
M26	-0.001	-0.024	0.021	0.894	0.935	-0.008	-0.022	0.005	0.233	0.465	-0.010	-0.020	0.001	0.074	0.213	-0.044	-0.071	-0.016	0.002	0.014
M25	-0.006	-0.028	0.016	0.578	0.900	-0.016	-0.030	-0.002	0.024	0.270	-0.008	-0.019	0.003	0.150	0.346	-0.042	-0.069	-0.015	0.002	0.014
M41	-0.009	-0.031	0.013	0.428	0.900	-0.010	-0.023	0.004	0.171	0.414	-0.002	-0.013	0.009	0.714	0.906	-0.043	-0.070	-0.015	0.002	0.014
M18	0.005	-0.018	0.027	0.688	0.935	0.003	-0.010	0.017	0.627	0.849	-0.019	-0.030	-0.009	0.000	0.008	-0.037	-0.064	-0.009	0.009	0.040
M38	-0.001	-0.024	0.021	0.901	0.935	-0.003	-0.017	0.011	0.696	0.873	-0.013	-0.024	-0.002	0.016	0.113	-0.036	-0.064	-0.009	0.010	0.040
M28	0.003	-0.019	0.025	0.792	0.935	-0.008	-0.022	0.006	0.276	0.497	0.002	-0.009	0.012	0.760	0.906	-0.037	-0.064	-0.009	0.009	0.040
M46	-0.005	-0.028	0.017	0.627	0.931	-0.013	-0.026	0.001	0.068	0.312	-0.001	-0.012	0.010	0.863	0.906	-0.035	-0.063	-0.008	0.011	0.041
M11	-0.010	-0.032	0.012	0.380	0.900	-0.012	-0.025	0.002	0.091	0.340	-0.020	-0.031	-0.009	0.000	0.008	-0.032	-0.059	-0.006	0.018	0.060
M14	-0.013	-0.035	0.009	0.243	0.900	-0.002	-0.016	0.012	0.804	0.902	-0.016	-0.026	-0.005	0.005	0.056	-0.032	-0.059	-0.006	0.018	0.060
M6	-0.004	-0.026	0.018	0.723	0.935	-0.001	-0.015	0.013	0.863	0.922	-0.003	-0.014	0.008	0.581	0.835	-0.033	-0.061	-0.005	0.020	0.063
M19	0.008	-0.014	0.030	0.467	0.900	-0.008	-0.022	0.005	0.230	0.465	-0.013	-0.024	-0.003	0.016	0.113	-0.031	-0.058	-0.003	0.028	0.075
M35	-0.007	-0.029	0.015	0.531	0.900	-0.002	-0.016	0.012	0.761	0.898	-0.001	-0.012	0.010	0.867	0.906	-0.030	-0.057	-0.004	0.027	0.075
M3	-0.008	-0.030	0.014	0.485	0.900	-0.015	-0.028	-0.001	0.038	0.270	-0.012	-0.023	-0.001	0.031	0.144	-0.030	-0.057	-0.003	0.030	0.077
M31	-0.010	-0.032	0.011	0.351	0.900	-0.009	-0.023	0.004	0.188	0.433	-0.004	-0.015	0.007	0.456	0.724	-0.030	-0.057	-0.003	0.032	0.079
M30	-0.020	-0.042	0.003	0.083	0.900	-0.011	-0.025	0.003	0.119	0.340	-0.002	-0.013	0.009	0.749	0.906	-0.027	-0.054	0.001	0.055	0.125
M17	-0.002	-0.025	0.020	0.831	0.935	-0.008	-0.022	0.006	0.278	0.497	0.000	-0.010	0.011	0.936	0.936	-0.027	-0.054	0.001	0.057	0.125
M21	-0.015	-0.037	0.006	0.163	0.900	-0.006	-0.020	0.008	0.412	0.654	-0.007	-0.018	0.004	0.192	0.420	-0.026	-0.053	0.001	0.060	0.126
M45	0.001	-0.021	0.024	0.896	0.935	-0.011	-0.026	0.003	0.120	0.340	0.002	-0.009	0.013	0.743	0.906	-0.025	-0.053	0.003	0.077	0.154
M13	-0.002	-0.024	0.021	0.876	0.935	0.003	-0.011	0.016	0.708	0.873	-0.005	-0.016	0.006	0.359	0.636	-0.023	-0.050	0.004	0.089	0.171
M9	0.001	-0.021	0.023	0.914	0.935	0.003	-0.011	0.016	0.721	0.873	-0.001	-0.012	0.010	0.824	0.906	-0.022	-0.049	0.005	0.109	0.201
M36	-0.007	-0.029	0.014	0.509	0.900	-0.011	-0.025	0.003	0.116	0.340	-0.009	-0.020	0.001	0.088	0.226	-0.020	-0.048	0.008	0.155	0.274
M32	-0.009	-0.031	0.013	0.430	0.900	-0.008	-0.022	0.006	0.281	0.497	-0.006	-0.017	0.005	0.291	0.558	-0.020	-0.047	0.008	0.163	0.278
M15	-0.008	-0.030	0.014	0.481	0.900	0.001	-0.013	0.015	0.857	0.922	0.003	-0.008	0.014	0.546	0.835	-0.017	-0.045	0.010	0.207	0.340
M43	-0.013	-0.035	0.009	0.258	0.900	0.005	-0.008	0.019	0.448	0.688	-0.004	-0.015	0.007	0.442	0.724	-0.016	-0.043	0.010	0.227	0.359
M16	-0.012	-0.034	0.009	0.264	0.900	-0.004	-0.018	0.009	0.544	0.782	0.010	-0.001	0.020	0.079	0.214	0.017	-0.011	0.044	0.240	0.368
M40	-0.003	-0.025	0.019	0.789	0.935	-0.011	-0.025	0.003	0.113	0.340	-0.007	-0.018	0.004	0.213	0.446	-0.014	-0.042	0.013	0.300	0.435
M1	-0.016	-0.038	0.006	0.143	0.900	-0.014	-0.028	0.000	0.045	0.270	-0.003	-0.014	0.008	0.572	0.835	-0.015	-0.042	0.013	0.302	0.435
M22	-0.004	-0.026	0.018	0.711	0.935	-0.014	-0.028	-0.001	0.041	0.270	-0.001	-0.012	0.010	0.842	0.906	-0.014	-0.042	0.014	0.330	0.461
M34	-0.014	-0.037	0.008	0.202	0.900	-0.010	-0.024	0.003	0.133	0.340	-0.011	-0.022	0.000	0.042	0.147	-0.013	-0.040	0.015	0.356	0.482
M24	0.007	-0.016	0.029	0.563	0.900	-0.011	-0.025	0.003	0.125	0.340	0.005	-0.006	0.016	0.341	0.627	-0.010	-0.038	0.018	0.477	0.610
M12	0.014	-0.008	0.037	0.212	0.900	0.002	-0.012	0.016	0.784	0.901	-0.001	-0.012	0.010	0.899	0.919	-0.010	-0.038	0.017	0.467	0.610
M10	-0.012	-0.034	0.010	0.291	0.900	-0.006	-0.020	0.008	0.395	0.649	0.013	0.002	0.023	0.020	0.113	0.008	-0.019	0.035	0.544	0.676
M27	-0.018	-0.040	0.004	0.102	0.900	-0.009	-0.023	0.005	0.199	0.436	0.005	-0.006	0.015	0.401	0.684	-0.006	-0.034	0.021	0.646	0.747
M2	-0.021	-0.043	0.001	0.057	0.900	-0.015	-0.029	-0.002	0.026	0.270	0.001	-0.010	0.012	0.843	0.906	-0.007	-0.035	0.021	0.617	0.747
M5	-0.002	-0.024	0.020	0.852	0.935	0.001	-0.013	0.015	0.894	0.922	-0.002	-0.013	0.009	0.711	0.906	-0.006	-0.034	0.021	0.649	0.747
M7	0.012	-0.010	0.034	0.296	0.900	0.001	-0.013	0.015	0.902	0.922	-0.008	-0.019	0.003	0.133	0.323	-0.005	-0.032	0.023	0.748	0.839
M33	0.001	-0.021	0.024	0.909	0.935	-0.014	-0.028	0.000	0.047	0.270	0.007	-0.004	0.018	0.229	0.458	0.003	-0.024	0.031	0.808	0.871
M29	-0.017	-0.039	0.005	0.125	0.900	-0.007	-0.020	0.007	0.341	0.582	0.002	-0.009	0.012	0.755	0.906	-0.003	-0.031	0.025	0.831	0.871
M20	-0.001	-0.023	0.021	0.946	0.946	-0.001	-0.015	0.013	0.937	0.937	-0.001	-0.012	0.010	0.864	0.906	0.003	-0.024	0.030	0.833	0.871
M37	-0.003	-0.025	0.019	0.794	0.935	0.004	-0.010	0.017	0.610	0.849	0.013	0.002	0.024	0.018	0.113	-0.001	-0.028	0.026	0.929	0.949
M8	-0.006	-0.028	0.016	0.587	0.900	0.003	-0.011	0.017	0.651	0.856	0.012	0.002	0.023	0.024	0.121	0.000	-0.028	0.027	0.984	0.984

Supplementary Table 9. Cross-sectional and longitudinal associations between plasmalogen subtypes and AD biomarkers

	Baseline A/T/N biomarkers								longitudinal A/T/N biomarkers							
	A		T		N1		N2		A		T		N1		N2	
	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p
Omega3 Plasmalogen	-0.081 (-0.158,-0.004)	0.04	-0.113 (-0.181,-0.045)	0.001	0.086 (0.035,0.137)	0.001	0.042 (-0.028,0.111)	0.238	0.003 (-0.02,0.025)	0.81	-0.007 (-0.022,0.007)	0.319	0.009 (-0.002,0.019)	0.117	-0.013 (-0.041,0.015)	0.361
Omega6 Plasmalogen	-0.067 (-0.139,0.006)	0.071	0.01 (-0.054,0.073)	0.758	0.058 (0.009,0.108)	0.02	-0.028 (-0.094,0.038)	0.413	-0.01 (-0.032,0.012)	0.368	0.001 (-0.013,0.015)	0.901	0.009 (-0.002,0.019)	0.112	-0.004 (-0.031,0.024)	0.799

Supplementary Table 10. Indices-based analysis of plasma lipidomics profile in relation to AD biomarkers

	Baseline A/T/N biomarkers								longitudinal A/T/N biomarkers							
	A		T		N1		N2		A		T		N1		N2	
	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p	Beta(95%CI)	p
Omega3 index surrogate	-0.062 (-0.132,0.008)	0.084	-0.12 (-0.183,-0.057)	<0.001	0.038 (-0.009,0.085)	0.116	0.053 (-0.013,0.118)	0.113	0.014 (-0.008,0.036)	0.228	-0.004 (-0.017,0.01)	0.616	0.008 (-0.003,0.018)	0.176	0.001 (-0.027,0.029)	0.934
CERT2	0.034 (-0.036,0.105)	0.334	0.008 (-0.056,0.071)	0.814	-0.029 (-0.077,0.018)	0.227	-0.093 (-0.159,-0.028)	0.005	-0.033 (-0.055,-0.011)	0.003	-0.017 (-0.031,-0.003)	0.018	-0.009 (-0.019,0.002)	0.119	-0.031 (-0.059,-0.003)	0.029

## Supplementary code

```
library(tidyverse)
library(data.table)
library(ADNIMERGE)
library(Hmisc)
library(lmerTest)
library(broom.mixed)
library(DT)
library(future.apply)
library(furrr)
library(mergeutils)

csf <- upennbiomk9 %>%
  mutate_if(is.character, list(~na_if(as.character(.), ""))) %>% filter(!is.na(PTAU)) %>%
  mutate(VISCODE = as.character(VISCODE)) %>%
  mutate(PTAU = PTAU %>% as.numeric()) %>%
  mutate(PTAU_log=log10(PTAU)) %>%
  select(RID, VISCODE, PTAU_log)

bmi <- read.csv("../data/BMI_IU.csv") %>%
  rowwise() %>%
  mutate(RID=str_split(RID_visit, pattern="_")[[1]][1] %>% as.integer(),
         VISCODE = str_split(RID_visit, pattern="_")[[1]][2]) %>%
  select(RID, VISCODE, BMI)

lipid <- read.csv("../data/clinical_lipids.csv") %>%
  rowwise() %>%
  mutate(RID=str_split(RID_visit, pattern="_")[[1]][1] %>% as.integer(), VISCODE =
str_split(RID_visit, pattern="_")[[1]][2]) %>%
  select(RID, VISCODE, hdl, chol, trig)

fdg <- read.csv("../data/adni_fdg_IU.csv") %>%
```

```

select(RID, contains("Mean")) %>%
pivot_longer(cols = -RID, names_to = "VISCODE0", values_to="FDG") %>%
mutate(VISCODE = str_split(VISCODE0, pattern="_", simplify=T)[,1] %>% tolower(),
       region = str_split(VISCODE0, pattern="_", simplify=T)[,3]) %>%
select(RID, VISCODE, region, FDG) %>% filter(!is.na(FDG)) %>%
pivot_wider(names_from=region , values_from = FDG) %>%
merge(., adnimerge %>% select(RID,VISCODE,FDG), by=c("RID","VISCODE"))

mri <- read.csv("../data/adni_freesurfer_IU.csv") %>%
pivot_longer(cols = -RID, names_to="VISCODE0", values_to="measurement") %>%
filter(!is.na(measurement)) %>%
mutate(VISCODE = str_split(VISCODE0, pattern="_", simplify=T)[,1] %>% tolower())
%>%
rowwise %>%
mutate(region = paste(tail(str_split(VISCODE0, pattern="_")[[1]], -1), collapse="_" )
%>%
ungroup %>%
filter(region %in% c("ICV", "Mag", "HippVol")) %>%
pivot_wider(id_cols= c("RID","VISCODE"), names_from = "region", values_from =
"measurement")

av45 <- read.csv("../data/AV45_IU.csv") %>%
select(RID, contains("FBP_WC_GlCtx"), -contains("CL")) %>%
pivot_longer(names_to = "VISCODE", values_to = "AV45", values_drop_na = TRUE, cols
= (-RID)) %>%
mutate(VISCODE=tolower(str_remove(VISCODE, "_FBP_WC_GlCtx")), AV45 =
log10(AV45))

metadata <- adnimerge %>%
select(RID, VISCODE, EXAMDATE, AGE, PTGENDER, PTEDUCAT ,APOE4) %>%
mutate(APOE_bin = ifelse(APOE4==0,0,1)) %>%
rename(age_bl = AGE) %>%
filter(VISCODE=="bl") %>%
select(-c(VISCODE, EXAMDATE))

```

```

age_time <- adnimerge %>%
  select(RID, VISCODE, AGE, Years.bl) %>%
  mutate(age = AGE + Years.bl) %>%
  select(-AGE)

# baseline phenotypes
fdg_bl <- fdg %>% filter(VISCODE=='bl') %>% select(-VISCODE)
mri_bl <- mri %>% filter(VISCODE=='bl') %>% select(-VISCODE)
csf_bl <- csf %>% filter(VISCODE=="bl") %>% select(-VISCODE)
av45_bl <- av45 %>% filter(VISCODE=="bl") %>% select(-VISCODE)

# Lipid classes information (supplementary table 1)
lipids <- read.csv("../data/lipid_species_revised.csv") %>%
  mutate(group = factor(group, levels = c("sphingolipids", "glycerophospholipids",
"Neutral/Other")),
         class=as.factor(class),
         abbr = as.factor(abbr),
         species = as.factor(species))

pheno_df <- data.frame(rbind(data.frame(modality = "MRI", phenotype="HippVol"),
                             cbind(modality = "CSF", phenotype="PTAU_log"),
                             cbind(modality = "FDG", phenotype="Temporal"),
                             cbind(modality = "AV45", phenotype="AV45")))

# Lipidomics DB call
mlab <- fread("../data/MeikleLab_Lipidomics.csv") %>%
  select(1:10, all_of(lipids$species))
mlab_log <- mlab %>%
  mutate(across("SPH.D18.1.":"PC.36.4....OH.", log10)) %>%
  as.data.table
mlab_log_duprm <- mlab_log %>%
  distinct(RID, VISCODE2, .keep_all=TRUE) %>% #duplicate removal
  select(-VISCODE) %>%

```

```

rename(VISCODE = VISCODE2)

# fasting data
fasting <- read.csv("../data/Fasting.csv") %>%
  rowwise() %>%
  mutate(RID=str_split(RID_visit, pattern="_")[[1]][1] %>% as.integer(), VISCODE =
str_split(RID_visit, pattern="_")[[1]][2]) %>%
  select(RID, VISCODE, fast)
# lipidomics + fasting + clinical lipids data
mlab_df <- merge(mlab_log_duprm, fasting, by=c("RID","VISCODE"), sort=F) %>%
  merge(lipid, by=c("RID","VISCODE"), all.x=T) %>%
  rename(BIFAST = fast)# fasting status data merge
mlab_rids <- mlab_df$RID %>% unique

#####
##### baseline species-level cross-sectional analysis #####
#####

mlab_anal_cross <- mlab_df %>% filter(VISCODE=="bl") %>%
  merge(metadata, by="RID", all.x=T) %>%
  merge(age_time, by=c("RID","VISCODE"), all.x=T) %>%
  merge(fdg_bl, by="RID", all.x=TRUE) %>%
  merge(mri_bl, by="RID", all.x=TRUE) %>%
  merge(csf_bl, by="RID", all.x=TRUE) %>%
  merge(bmi, by=c("RID","VISCODE"), all.x=TRUE) %>%
  merge(av45_bl, by="RID", all.x=TRUE)

mlab_metabolites <- lipids$species %>% as.character

mlab_grid_cross <- expand.grid(pheno_df$phenotype, mlab_metabolites) %>%
  set_names(c("phenotype","metabolite")) %>%
  merge(pheno_df, by="phenotype") %>%
  distinct_at(c("phenotype", "metabolite","modality")) %>%

```

```

rowwise() %>%

  mutate(formu_bl = ifelse(str_detect(modality,"MRI"), glue::glue("{phenotype} ~
{metabolite} + age_bl + PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST +
statin + omega3 + PTEDUCAT + ICV + Mag"),

                ifelse(modality=="Cog", glue::glue("{phenotype} ~ {metabolite} +
age_bl + PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3
+ PTEDUCAT"),

                glue::glue("{phenotype} ~ {metabolite} + age_bl + PTGENDER +
APOE_bin + trig + hdl + chol + BMI + BIFAST+ statin + omega3" )))

  formu_sex_int = ifelse(modality == "MRI", glue::glue("{phenotype} ~ {metabolite}
*PTGENDER + age_bl + APOE_bin + trig + hdl + chol + BMI + BIFAST+ statin + omega3
+ PTEDUCAT + ICV + Mag"),

                        ifelse(modality == "Cog", glue::glue("{phenotype} ~ {metabolite}
*PTGENDER + age_bl + APOE_bin + trig + hdl + chol + BMI + BIFAST+ statin + omega3
+ PTEDUCAT"),

                        glue::glue("{phenotype} ~ {metabolite}*PTGENDER + age_bl +
APOE_bin + trig + hdl + chol + BMI + BIFAST+ statin + omega3"))),

  formu_apoe_int = ifelse(modality == "MRI", glue::glue("{phenotype} ~ {metabolite}
*APOE_bin + age_bl + PTGENDER + trig + hdl + chol + BMI + BIFAST+ statin + omega3
+ PTEDUCAT + ICV + Mag"),

                          ifelse(modality == "Cog", glue::glue("{phenotype} ~ {metabolite}
*APOE_bin + age_bl + PTGENDER + trig + hdl + chol + BMI + BIFAST+ statin + omega3
+ PTEDUCAT"),

                          glue::glue("{phenotype} ~ {metabolite}*APOE_bin + age_bl +
PTGENDER + trig + hdl + chol + BMI + BIFAST+ statin + omega3")))) %>%

  ungroup()

assoc_anal_cross <- function(modality, phenotype, metabolite, formu_bl, formu_sex_int,
formu_apoe_int, df){

  model_bl <- lm(formula(formu_bl), data=df) %>% jtools::summ(scale=TRUE,
transform.response = TRUE, confint=TRUE) %>% .$coeftable %>% data.frame

  pval <- model_bl[2,1:5] %>% set_names(c("b", "CIlow", "CIhigh", "T_value", "pval"))

  model_sex_int <- lm(formula(formu_sex_int), data=df) %>% jtools::summ(scale=TRUE,
transform.response = TRUE, confint=TRUE) %>% .$coeftable %>% data.frame %>%
rownames_to_column("term")

  p_sex_int <- model_sex_int %>% filter(str_detect(term, ":PTGENDER")) %>% .[1,2:6]
%>% set_names(c("b_sex_int", "CIlow_sex_int", "CIhigh_sex_int", "T_sex_int", "p_sex_int"))

  model_apoe_int <- lm(formula(formu_apoe_int), data=df) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .$coeftable
%>% data.frame %>% rownames_to_column("term")

  p_apoe_int <- model_apoe_int %>% filter(str_detect(term, ":APOE")) %>% .[1,2:6] %>%
set_names(c("b_apoe_int", "CIlow_apoe_int", "CIhigh_apoe_int", "T_apoe_int", "p_apoe_int"))

```

```

}

plan(multisession)
mlab_result_cross <-
  future_pmap_dfr(mlab_grid_cross, ~assoc_anal_cross(..3,..1,..2,..4,..5, ..6,
df=mlab_anal_cross), .progress=T) %>%
  group_by(phenotype) %>%
  mutate(p.fdr = p.adjust(pval, "BH"),
         p.male.fdr = p.adjust(p_male,"BH"),
         p.female.fdr=p.adjust(p_female,"BH")) %>%
  ungroup()

#####
##### baseline class-level analysis #####
#####

classes <- lipids$abbr %>% unique %>% as.character()

mlab_cross_pca <- mlab_anal_cross %>% filter(VISCODE=="bl")
for(i in seq_along(classes)){
  species_interest <- lipids %>% filter(abbr == classes[i]) %>% pull(species)
  mlab_sub <- mlab_cross_pca %>% select(all_of(species_interest))
  prc <- psych::principal(mlab_sub)
  tempdf <- prc$scores %>% data.frame %>% set_names(paste("class",classes[i],sep="_"))
  mlab_cross_pca <- cbind(mlab_cross_pca, tempdf)
}

classcols <- grep(names(mlab_cross_pca), pattern = "class", value = TRUE)
phenocols <- pheno_df$phenotype

mlab_grid_cross_pca <- expand.grid(phenocols, classcols) %>%

```

```

set_names("phenotype", "classes") %>%
merge(pheno_df, by = "phenotype") %>%

mutate(formu = ifelse(str_detect(modality,"MRI"), glue::glue("{phenotype} ~ `{classes}`
+ age_bl + PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin +
omega3 + PTEDUCAT + ICV + Mag"),

ifelse(modality=="Cog", glue::glue("{phenotype} ~ `{classes}` + age_bl +
PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3 +
PTEDUCAT"),

glue::glue("{phenotype} ~ `{classes}` + age_bl + PTGENDER +
APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3" ) ),

formu.sex.int = ifelse(str_detect(modality,"MRI"), glue::glue("{phenotype} ~
`{classes}`*PTGENDER + age_bl + APOE_bin + trig + hdl + chol + BMI + BIFAST+ statin
+ omega3 + PTEDUCAT + ICV + Mag"),

ifelse(modality=="Cog", glue::glue("{phenotype} ~ `{classes}
`*PTGENDER + age_bl + APOE_bin + trig + hdl + chol + BMI + BIFAST+ statin + omega3
+ PTEDUCAT"),

glue::glue("{phenotype} ~ `{classes}`*PTGENDER + age_bl +
APOE_bin + trig + hdl + chol + BMI + BIFAST+ statin + omega3" ) ),

formu.apoe.int = ifelse(str_detect(modality,"MRI"), glue::glue("{phenotype} ~
`{classes}`*APOE_bin + age_bl + PTGENDER + trig + hdl + chol + BMI + BIFAST+ statin
+ omega3 + PTEDUCAT + ICV + Mag"),

ifelse(modality=="Cog", glue::glue("{phenotype} ~ `{classes}
`*APOE_bin + age_bl + PTGENDER + trig + hdl + chol + BMI + BIFAST+ statin + omega3
+ PTEDUCAT"),

glue::glue("{phenotype} ~ `{classes}`*APOE_bin + age_bl +
PTGENDER + trig + hdl + chol + BMI + BIFAST+ statin + omega3" ) )))

assoc_anal_cross_pca <- function(phenotype, classes, formu, formu.sex.int,
formu.apoe.int, df){

model_bl <- lm(formu, data=df)

coeffs <- model_bl %>% jtools::summ(scale=TRUE, transform.response = TRUE,
confint=TRUE) %>% .$coeftable

pval <- coeffs[2,c(1,2,3,5)] %>% t() %>% data.frame %>%
set_names(c("Beta", "CIlow", "CIhigh", "pval"))

model_sex_int <- lm(formu.sex.int, data=df)

coeffs_sex_int <- model_sex_int %>% jtools::summ(scale=TRUE, transform.response =
TRUE, confint=TRUE) %>% .$coeftable %>% as.data.frame

pval_sex_int <- coeffs_sex_int %>% select(1,2,3,5) %>% filter(.,grepl(":", rownames(.)))
%>% `rownames<-`( NULL ) %>%
set_names(c("Beta_sint", "CIlow_sint", "CIhigh_sint", "pval_sint"))

```

```

model_apoe_int <- lm(formu.apoe.int, data=df)

coeffs_apoe_int <- model_apoe_int %>% jtools::summ(scale=TRUE, transform.response
= TRUE, confint=TRUE) %>% .$coefstable %>% as.data.frame

pval_apoe_int <- coeffs_apoe_int %>% select(1,2,3,5) %>% filter(.,grepl(":",
rownames(.))) %>% `rownames<-` ( NULL ) %>%
set_names(c("Beta_aint", "CIlow_aint", "CIhigh_aint", "pval_aint"))

return(data.frame(phenotype, classes, pval, pval_sex_int, pval_apoe_int))
}

```

```

mlab_result_cross_pca <- future_pmap_dfr(mlab_grid_cross_pca,
~assoc_anal_cross_pca(..1,..2,..4, ..5, ..6, df = mlab_cross_pca))

```

```

#####
# baseline metabolite - longitudinal phenotype association analysis #
#####

```

```

mlab_bl <- mlab_df %>%
filter(VISCODE=="bl") %>%
select(-c(VID, COHORT, SAMPLE.ID, VISCODE))

```

```

mri_multi <- mri %>% group_by(RID) %>% filter(n()>=2) %>% ungroup
csf_multi <- csf %>% group_by(RID) %>% filter(n()>=2) %>% ungroup
fdg_multi <- fdg %>% group_by(RID) %>% filter(n()>=2) %>% ungroup
cog_multi <- cognition %>% group_by(RID) %>% filter(n()>=2) %>% ungroup
av45_multi <- av45 %>% group_by(RID) %>% filter(n()>=2) %>% ungroup
bmi_bl <- bmi %>% filter(VISCODE=="bl") %>% select(-VISCODE)

```

```

pheno_long <- multimerge(list(csf_multi, mri_multi, fdg_multi, av45_multi, age_time),
by=list(c("RID", "VISCODE")))

```

```

mlab_bl_met_long_phen <- multimerge(list(pheno_long, metadata, mlab_bl, bmi_bl),
by="RID") %>%

```

```

filter(complete.cases(Years.bl, PTGENDER, APOE4, BMI, trig, chol, hdl, PTEDUCAT,
BIFAST))

```

```

assoc_bl_met_long_phen <- function(modality, phenotype, metabolite, formu,
formu_sex_int, formu_apoe_int, df){

  modelsummary <- lmer(formula(formu), data=df, na.action=na.exclude) %>%

  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coeftable %>% data.frame %>% rownames_to_column("term")

  pval <- modelsummary %>% filter(str_detect(term,":Years.bl")) %>% select(Est.,
X2.5.,X97.5., p) %>% set_names(c("b", "CIlow","CIhigh","pval"))

  summary_sex_int <- lmer(formula(formu_sex_int), data=df, na.action=na.exclude) %>%

  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coeftable %>% data.frame %>% rownames_to_column("term")

  pval_sex_int <- summary_sex_int %>% filter(str_detect(term,":Years.bl:PTGENDER"))
%>% select(Est., X2.5.,X97.5., p) %>%
set_names(c("b_sex_int","CIlow_sex_int","CIhigh_sex_int","p_sex_int"))

  summary_apoe_int <- lmer(formula(formu_apoe_int), data=df, na.action=na.exclude)
%>%

  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coeftable %>% data.frame %>% rownames_to_column("term")

  pval_apoe_int <- summary_apoe_int %>% filter(str_detect(term,":Years.bl:APOE_bin"))
%>% select(Est., X2.5.,X97.5., p) %>%
set_names(c("b_apoe_int","CIlow_apoe_int","CIhigh_apoe_int","p_apoe_int"))

  return(data.frame(modality, phenotype, metabolite, pval,pval_sex_int,pval_apoe_int))
}

grid_bl_met_long_phen <- expand.grid(c("HippVol", "PTAU_log", "Temporal", "AV45"),
mlab_metabolites) %>%

set_names(c("phenotype","metabolite")) %>%

merge(pheno_df, by="phenotype") %>%

distinct_at(c("phenotype", "metabolite","modality")) %>%

rowwise() %>%

mutate(formu = ifelse(modality == "MRI", glue::glue("{phenotype} ~ {metabolite}
*Years.bl + age_bl + PTGENDER + APOE_bin + BMI + trig + chol + hdl + PTEDUCAT +
scale(ICV) + factor(Mag) + BIFAST + statin + omega3 + (Years.bl|RID)"),

glue::glue("{phenotype} ~ {metabolite}*Years.bl + age_bl + PTGENDER +
APOE_bin + BMI + trig + chol + hdl+ BIFAST + statin + omega3 + (Years.bl|RID)")),

```

```
formu_sex_int = ifelse(modality == "MRI", glue::glue("{phenotype} ~ {metabolite}
*Years.bl*PTGENDER + age_bl + APOE_bin + BMI + trig + chol + hdl + PTEDUCAT +
scale(ICV) + factor(Mag) + BIFAST + statin + omega3 + (Years.bl|RID)"),
```

```
glue::glue("{phenotype} ~ {metabolite}*Years.bl*PTGENDER +
age_bl + APOE_bin + BMI + trig + chol + hdl+ BIFAST + statin + omega3 + (Years.bl|
RID)")),
```

```
formu_apoe_int = ifelse(modality == "MRI", glue::glue("{phenotype} ~
{metabolite}*Years.bl*APOE_bin + age_bl + PTGENDER + BMI + trig + chol + hdl +
PTEDUCAT + scale(ICV) + factor(Mag) + BIFAST + statin + omega3 + (Years.bl|RID)"),
```

```
glue::glue("{phenotype} ~ {metabolite}*Years.bl*APOE_bin + age_bl
+ PTGENDER + BMI + trig + chol + hdl+ BIFAST + statin + omega3 + (Years.bl|RID)"))
%>%
```

```
ungroup()
```

```
plan(multisession)
```

```
pval_bl_met_long_phen <- future_pmap_dfr(grid_bl_met_long_phen,
~assoc_bl_met_long_phen(..3,..1,..2,..4,..5,..6,df=mlab_bl_met_long_phen), .progress=T)
```

```
mlab_result_bl_longi <- pval_bl_met_long_phen %>%
```

```
group_by(phenotype) %>%
```

```
mutate(p.fdr = p.adjust(pval, "BH")) %>%
```

```
ungroup()
```

```
#####
```

```
#### longitudinal class level analysis (baseline lipid class PC1 - longitudinal
phenotype)####
```

```
#####
```

```
classcols <- grep(names(mlab_cross_pca), pattern = "class", value = TRUE)
```

```
phenocols <- c("HippVol","PTAU_log","Temporal", "AV45")
```

```
mlab_bl_longi_pca <-merge(mlab_bl_met_long_phen, mlab_cross_pca %>%
select(RID,contains("class_")), by="RID", sort=F)
```

```
mlab_grid_bl_longi_pca <- expand.grid(phenocols, classcols) %>%
```

```
set_names("phenotype", "classes") %>%
```

```

merge(pheno_df, by = "phenotype") %>%

  mutate(formu = ifelse(modality == "MRI", glue::glue("{phenotype} ~ `{classes}
`*Years.bl + age_bl + PTGENDER + APOE_bin + BMI + trig + chol + hdl + PTEDUCAT +
scale(ICV) + factor(Mag) + BIFAST + statin + omega3 + (Years.bl|RID)"),

  ifelse(modality=="Cog", glue::glue("{phenotype} ~ `{classes}`*Years.bl +
age_bl + PTGENDER + APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3
+ PTEDUCAT + (Years.bl|RID)"),

  glue::glue("{phenotype} ~ `{classes}`*Years.bl + age_bl +
PTGENDER + APOE_bin + BMI + trig + chol + hdl+ BIFAST + statin + omega3 +
(Years.bl|RID)"))),

  formu.sex = ifelse(modality == "MRI", glue::glue("{phenotype} ~ `{classes}
`*Years.bl*PTGENDER + age_bl + APOE_bin + BMI + trig + chol + hdl + PTEDUCAT +
scale(ICV) + factor(Mag) + BIFAST + statin + omega3 + (Years.bl|RID)"),

  ifelse(modality=="Cog", glue::glue("{phenotype} ~ `{classes}
`*Years.bl*PTGENDER + age_bl + APOE_bin + BMI + trig + chol + hdl + BIFAST + statin
+ omega3 + PTEDUCAT + (Years.bl|RID)"),

  glue::glue("{phenotype} ~ `{classes}`*Years.bl*PTGENDER +
age_bl + APOE_bin + BMI + trig + chol + hdl+ BIFAST + statin + omega3 + (Years.bl|
RID)"))),

  formu.apoe = ifelse(modality == "MRI", glue::glue("{phenotype} ~ `{classes}
`*Years.bl*APOE_bin + age_bl + PTGENDER + BMI + trig + chol + hdl + PTEDUCAT +
scale(ICV) + factor(Mag) + BIFAST + statin + omega3 + (Years.bl|RID)"),

  ifelse(modality=="Cog", glue::glue("{phenotype} ~ `{classes}
`*Years.bl*APOE_bin + age_bl + PTGENDER + BMI + trig + chol + hdl + BIFAST + statin
+ omega3 + PTEDUCAT + (Years.bl|RID)"),

  glue::glue("{phenotype} ~ `{classes}`*Years.bl*APOE_bin + age_bl
+ PTGENDER + BMI + trig + chol + hdl+ BIFAST + statin + omega3 + (Years.bl|RID)"))))

assoc_anal_bl_longi_pca <- function(phenotype, classes, formu, formu.sex, formu.apoe, df)
{

  model_bl <- lmer(formu, data=df, na.action=na.exclude, control=lmerControl(optimizer
= "Nelder_Mead"))

  coeffs <- model_bl %>% jtools::summ(scale=TRUE, transform.response = TRUE,
confint=TRUE) %>% .$coefstable %>% data.frame

  pval <- coeffs %>% select(1,2,3,6) %>% filter(.,grepl(":", rownames(.))) %>%
set_names(c("Beta", "CIlow", "CIhigh", "pval"))

  summary_sex_int <- lmer(formu.sex, data=df, na.action=na.exclude,
control=lmerControl(optimizer = "Nelder_Mead")) %>%

  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefstable %>% data.frame %>% rownames_to_column("term")

```

```

  pval_sex_int <- summary_sex_int %>% filter(str_detect(term,":Years.bl:PTGENDER"))
%>% select(Est., X2.5.,X97.5., p) %>%
set_names(c("b_sex_int","CIlow_sex_int","CIhigh_sex_int","p_sex_int"))

```

```

  summary_apoe_int <- lmer(formu.apoe, data=df, na.action=na.exclude,
control=lmerControl(optimizer = "Nelder_Mead")) %>%

```

```

  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coeftable %>% data.frame %>% rownames_to_column("term")

```

```

  pval_apoe_int <- summary_apoe_int %>% filter(str_detect(term,":Years.bl:APOE_bin"))
%>% select(Est., X2.5.,X97.5., p) %>%
set_names(c("b_apoe_int","CIlow_apoe_int","CIhigh_apoe_int","p_apoe_int"))

```

```

  return(data.frame(phenotype, classes, pval,pval_sex_int, pval_apoe_int))
}

```

```

plan(multisession)

```

```

mlab_result_bl_longi_pca <- future_pmap_dfr(mlab_grid_bl_longi_pca,
~assoc_anal_bl_longi_pca(..1,..2,..4,..5,..6,df = mlab_bl_longi_pca))

```

```

mlab_grid_bl_longi_species <- merge(grid_bl_met_long_phen %>% select(modality,
metabolite, phenotype, formu),

```

```

      lipids %>% select(species, abbr), by.x = "metabolite", by.y
="species", sort=FALSE) %>%

```

```

  mutate(abbr = factor(abbr, levels= classes))

```

```

assoc_anal_bl_longi_pca_species <- function(species, phenotype, classes, formu, df){

```

```

  model_bl <- lmer(formu, data=df, na.action=na.exclude, control=lmerControl(optimizer
= "Nelder_Mead"))

```

```

  coeffs <- model_bl %>% jtools::summ(scale=TRUE, transform.response = TRUE,
confint=TRUE) %>% .$coeftable %>% data.frame

```

```

  pval <- coeffs %>% select(1,2,3,6) %>% filter(.,grepl(":", rownames(.))) %>%
set_names(c("Beta","CIlow","CIhigh","pval"))

```

```

  return(data.frame(phenotype,classes,species,pval))
}

```

```

#####

```

```

##### WGCNA analysis #####

```

```

#####

```

```

library(WGCNA)

#### data ####
lipid_metabolites <- lipids$species
datLipid <- mlab_anal_cross %>% select(RID, all_of(lipid_metabolites)) %>%
column_to_rownames("RID")

#### power selection ####
options(stringsAsFactors = FALSE)
powers = c(c(1:10), seq(from = 12, to=20, by=2))
sft = pickSoftThreshold(datLipid, powerVector = powers, verbose = 5)
sizeGrWindow(9, 5)
par(mfrow = c(1,2));
cex1 = 0.9;
# Scale-free topology fit index as a function of the soft-thresholding power
plot(sft$fitIndices[,1], -sign(sft$fitIndices[,3])*sft$fitIndices[,2],
      xlab="Soft Threshold (power)",ylab="Scale Free Topology Model Fit,signed
R^2",type="n",
      main = paste("Scale independence"));
text(sft$fitIndices[,1], -sign(sft$fitIndices[,3])*sft$fitIndices[,2],
      labels=powers,cex=cex1,col="red");
# this line corresponds to using an R^2 cut-off of h
abline(h=0.80,col="red")
# Mean connectivity as a function of the soft-thresholding power
plot(sft$fitIndices[,1], sft$fitIndices[,5],
      xlab="Soft Threshold (power)",ylab="Mean Connectivity", type="n",
      main = paste("Mean connectivity"))
text(sft$fitIndices[,1], sft$fitIndices[,5], labels=powers, cex=cex1,col="red")

#### module generation ####
net = blockwiseModules(datLipid, power = 7,
                      TOMType = "signed",
                      corType = "bicor",
                      minModuleSize = 5,

```

```

    deepSplit =4,
    reassignThreshold = 0, mergeCutHeight = 0.25,
    numericLabels = FALSE, pamRespectsDendro = FALSE,
    verbose = 3)

# removing grey module & converting to numbers

membership <- net$colors %>% as.data.frame() %>% set_names("Module") %>%
filter(Module != "grey") %>% mutate(Module_num =
paste0("M",as.numeric(as.factor(Module))))

membership_convert <- membership %>% distinct

#####

##### Module -baseline phenotype analysis #####

#####

mlab_me_cross <- merge(mlab_anal_cross %>% data.frame, net$MEs, by.x="RID",
by.y="row.names")

phenos <- c("AV45", "PTAU_log", "HippVol", "Temporal")
menames <- names(net$MEs)[1:46]

mlab_me_grid <- expand.grid(phenos, menames) %>%
  set_names(c("phenotype", "ME_metabolite")) %>%
  merge(pheno_df, by="phenotype") %>%
  distinct_at(c("phenotype", "ME_metabolite", "modality")) %>%
  rowwise() %>%

  mutate(formu_bl = ifelse(str_detect(modality, "MRI"), glue::glue("{phenotype} ~
{ME_metabolite} + age_bl + PTGENDER + APOE_bin + BIFAST + BMI + hdl + chol + trig
+ statin + omega3 + PTEDUCAT + ICV + factor(Mag)"),
          ifelse(modality=="Cog", glue::glue("{phenotype} ~ {ME_metabolite} +
age_bl + PTGENDER + APOE_bin + BIFAST + BMI + hdl + chol + trig + statin + omega3
+ PTEDUCAT"),

```

```

      glue::glue("{phenotype} ~ {ME_metabolite} + age_bl + PTGENDER
+ APOE_bin + BIFAST + BMI + hdl + chol + trig + statin + omega3" )),
      formu_sex_int = ifelse(modality == "MRI", glue::glue("{phenotype} ~
{ME_metabolite}*PTGENDER + age_bl + APOE_bin + trig + hdl + chol + statin + omega3
+ BMI + BIFAST + PTEDUCAT + ICV + factor(Mag)"),
      ifelse(modality == "Cog", glue::glue("{phenotype} ~ {ME_metabolite}
*PTGENDER + age_bl + APOE_bin + trig + hdl + chol + statin + omega3 + BMI + BIFAST
+ PTEDUCAT"),
      glue::glue("{phenotype} ~ {ME_metabolite}*PTGENDER +
age_bl + APOE_bin + trig + hdl + chol + statin + omega3 + BMI + BIFAST" )),
      formu_apoe_int = ifelse(modality == "MRI", glue::glue("{phenotype} ~
{ME_metabolite}*APOE_bin + age_bl + PTGENDER + trig + hdl + chol + statin + omega3
+ BMI + BIFAST + PTEDUCAT + ICV + factor(Mag)"),
      ifelse(modality == "Cog", glue::glue("{phenotype} ~
{ME_metabolite}*APOE_bin + age_bl + PTGENDER + trig + hdl + chol + statin + omega3
+ BMI + BIFAST + PTEDUCAT"),
      glue::glue("{phenotype} ~ {ME_metabolite}*APOE_bin + age_bl
+ PTGENDER + trig + hdl + chol + statin + omega3 + BMI + BIFAST" )),) %>%
ungroup()

```

```

assoc_me_cross <- function(modality, phenotype, me_metabolite, formu_bl, formu_sex_int,
formu_apoe_int, df){
  model_bl <- lm(formula(formu_bl), data=df) %>% jtools::summ(scale=TRUE,
transform.response = TRUE, confint=TRUE) %>% .$coefstable %>% data.frame
  pval <- model_bl[2,1:5] %>% set_names(c("b", "CIlow", "CIhigh", "T_value", "pval"))
  model_sex_int <- lm(formula(formu_sex_int), data=df) %>% jtools::summ(scale=TRUE,
transform.response = TRUE, confint=TRUE) %>% .$coefstable %>% data.frame %>%
rownames_to_column("term")
  p_sex_int <- model_sex_int %>% filter(str_detect(term, ":PTGENDER")) %>% .[1,2:6]
%>% set_names(c("b_sex_int", "CIlow_sex_int", "CIhigh_sex_int", "T_sex_int", "p_sex_int"))
  model_apoe_int <- lm(formula(formu_apoe_int), data=df) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .$coefstable
%>% data.frame %>% rownames_to_column("term")
  p_apoe_int <- model_apoe_int %>% filter(str_detect(term, ":APOE")) %>% .[1,2:6] %>%
set_names(c("b_apoe_int", "CIlow_apoe_int", "CIhigh_apoe_int", "T_apoe_int", "p_apoe_int"))
  return(data.frame(modality, phenotype, me_metabolite, pval, p_sex_int, p_apoe_int))
}

```

```
plan(multisession)
```

```
mlab_me_result_cross <-
```

```

future_pmap_dfr(mlab_me_grid, ~assoc_me_cross(..3,..1,..2,..4,..5,..6,df=mlab_me_cross),
.progress=T) %>%
  group_by(phenotype) %>%
  mutate(p.fdr = p.adjust(pval, "BH"),
         p.sex.int.fdr = p.adjust(p_sex_int, "BH"),
         p.e4.int.fdr = p.adjust(p_apoe_int, "BH")) %>%
  ungroup()

me_result_df <- mlab_me_result_cross %>% filter(p.fdr < 0.05) %>% rowwise() %>%
  mutate(n_metabolites = sum(paste("ME",net$colors,sep="") == me_metabolite)) %>%
  ungroup %>%
  mutate(Module = str_remove(me_metabolite, "ME")) %>% arrange(phenotype,p.fdr)
%>%
  mutate(p.sexint.fdr = p.adjust(p_sex_int,"BH"),
         p.apoeint.fdr = p.adjust(p_apoe_int,"BH")) %>%
  mutate_if(is.numeric, ~signif(.x,2)) %>%
  ungroup %>%
  select(phenotype, Module, n_metabolites, T_value, p.fdr,p.sexint.fdr,p.apoeint.fdr)

datatable(me_result_df)

```

```

#####
####   module - longitudinal phenotype   #####
#####

```

```

mlab_bl_ME_long_phen <- merge(mlab_bl_met_long_phen, net$MEs, by.x="RID",
by.y="row.names")

assoc_bl_ME_long_phen <- function(modality, phenotype, module,formu, formu_sex_int,
formu_apoe_int, df){

  modelsummary <- lmer(formula(formu), data=df, na.action=na.exclude,
control=lmerControl(optimizer = "Nelder_Mead")) %>%

  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefstable %>% data.frame %>% rownames_to_column("term")

```

```

    pval <- modelsummary %>% filter(str_detect(term,":Years.bl")) %>% select(Est.,
X2.5.,X97.5., t.val., p) %>% set_names(c("estimate", "CIlow","CIhigh","T_value", "pval"))

    model_sex_int <- lmer(formula(formu_sex_int), data=df, na.action=na.exclude,
control=lmerControl(optimizer = "Nelder_Mead")) %>%

    jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coeftable %>% data.frame %>% rownames_to_column("term")

    p_sex_int <- model_sex_int %>% filter(str_count(term, ":")==2) %>% select(Est.,
X2.5.,X97.5., p) %>%
set_names(c("b_sex_int","CIlow_sex_int","CIhigh_sex_int","p_sex_int"))

    model_apoe_int <- lmer(formula(formu_apoe_int), data=df, na.action=na.exclude,
control=lmerControl(optimizer = "Nelder_Mead")) %>%

    jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coeftable %>% data.frame %>% rownames_to_column("term")

    p_apoe_int <- model_apoe_int %>% filter(str_count(term, ":")==2) %>% select(Est.,
X2.5.,X97.5., p) %>%
set_names(c("b_apoe_int","CIlow_apoe_int","CIhigh_apoe_int","p_apoe_int"))

    return(data.frame(modality, phenotype, module, pval,p_sex_int,p_apoe_int))
}

grid_bl_ME_long_phen <- expand.grid(phenos, menames) %>%
set_names(c("phenotype","module")) %>%
merge(pheno_df, by="phenotype") %>%
distinct_at(c("phenotype", "module","modality")) %>%
rowwise() %>%

mutate(formu = ifelse(modality == "MRI", glue::glue("{phenotype} ~ {module}*Years.bl
+ age_bl + PTGENDER + APOE_bin + BMI + trig + chol + statin + omega3 + hdl +
PTEDUCAT + scale(ICV) + factor(Mag) + BIFAST + (Years.bl|RID)"),

ifelse(modality=="Cog", glue::glue("{phenotype} ~ {module}*Years.bl +
age_bl + PTGENDER + APOE_bin + BMI + trig + chol + statin + omega3 + hdl + BIFAST
+ PTEDUCAT + (Years.bl|RID)"),

glue::glue("{phenotype} ~ {module}*Years.bl + age_bl + PTGENDER
+ APOE_bin + BMI + trig + chol + statin + omega3 + hdl+ BIFAST + (Years.bl|RID)")),

formu_sex_int = ifelse(modality == "MRI", glue::glue("{phenotype} ~ {module}
*PTGENDER*Years.bl + age_bl + APOE_bin + trig + hdl + chol + statin + omega3 + BMI
+ BIFAST + PTEDUCAT + scale(ICV) + factor(Mag) + (Years.bl|RID)"),

```

```
      ifelse(modality == "Cog", glue::glue("{phenotype} ~ {module}
*PTGENDER*Years.bl + age_bl + APOE_bin + trig + hdl + chol + statin + omega3 + BMI
+ BIFAST + PTEDUCAT + (Years.bl|RID)"),
```

```
      glue::glue("{phenotype} ~ {module}*PTGENDER*Years.bl +
age_bl + APOE_bin + trig + hdl + chol + statin + omega3 + BMI + BIFAST + (Years.bl|
RID)"))),
```

```
      formu_apoe_int = ifelse(modality == "MRI", glue::glue("{phenotype} ~ {module}
*APOE_bin*Years.bl + age_bl + PTGENDER + trig + hdl + chol + statin + omega3 + BMI
+ BIFAST + PTEDUCAT + scale(ICV) + factor(Mag) + (Years.bl|RID)"),
```

```
      ifelse(modality == "Cog", glue::glue("{phenotype} ~ {module}
*APOE_bin*Years.bl + age_bl + PTGENDER + trig + hdl + chol + statin + omega3 + BMI
+ BIFAST + PTEDUCAT + (Years.bl|RID)"),
```

```
      glue::glue("{phenotype} ~ {module}*APOE_bin*Years.bl +
age_bl + PTGENDER + trig + hdl + chol + statin + omega3 + BMI + BIFAST + (Years.bl|
RID)")))) %>%
```

```
  ungroup()
```

```
  plan(multisession)
```

```
  pval_bl_ME_long_phen <- future_pmap_dfr(grid_bl_ME_long_phen,
~assoc_bl_ME_long_phen(..3,..1,..2,..4,..5,..6,df=mlab_bl_ME_long_phen), .progress=T)
```

```
  mlab_result_bl_ME_longi <- pval_bl_ME_long_phen %>%
```

```
    group_by(phenotype) %>%
```

```
    mutate(p.fdr = p.adjust(pval, "BH"),
```

```
  ) %>%
```

```
  ungroup()
```

```
#####
```

```
### Plasmalogen - omega3, omega6 analysis ###
```

```
#####
```

```
# cross-sectional
```

```
omega3 <- lipids %>% filter(plasmalogen_omega == "omega3") %>% pull(species)
```

```
omega6 <- lipids %>% filter(plasmalogen_omega == "omega6") %>% pull(species)
```

```
omega3prc <- mlab_cross_pca %>% select(all_of(omega3)) %>% psych::principal()
```

```
omega6prc <- mlab_cross_pca %>% select(all_of(omega6)) %>% psych::principal()
```

```
omegapca <- cbind(omega3prc$scores %>% data.frame %>% set_names("omega3pc"),
omega6prc$scores %>% data.frame %>% set_names("omega6pc"))
```

```
mlab_cross_pca_omega <- cbind(mlab_cross_pca, omegapca)
```

```
o3_A <- lm(mlab_cross_pca_omega, formula = AV45 ~ omega3pc + age_bl + PTGENDER
+ APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .$coefstable
%>% data.frame %>% .[,2,]
```

```
o6_A <- lm(mlab_cross_pca_omega, formula = AV45 ~ omega6pc + age_bl + PTGENDER
+ APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefstable%>% data.frame %>% .[,2,]
```

```
o3_T<-lm(mlab_cross_pca_omega, formula = PTAU_log ~ omega3pc + age_bl +
PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefstable%>% data.frame %>% .[,2,]
```

```
o6_T <-lm(mlab_cross_pca_omega, formula = PTAU_log ~ omega6pc + age_bl +
PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefstable%>% data.frame %>% .[,2,]
```

```
o3_N1<-lm(mlab_cross_pca_omega, formula = HippVol ~ omega3pc + age_bl +
PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3 +
PTEDUCAT + ICV + Mag) %>% jtools::summ(scale=TRUE, transform.response = TRUE,
confint=TRUE) %>% .$coefstable%>% data.frame %>% .[,2,]
```

```
o6_N1 <-lm(mlab_cross_pca_omega, formula = HippVol ~ omega6pc + age_bl +
PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3 +
PTEDUCAT + ICV + Mag) %>% jtools::summ(scale=TRUE, transform.response = TRUE,
confint=TRUE) %>% .$coefstable%>% data.frame %>% .[,2,]
```

```
o3_N2<-lm(mlab_cross_pca_omega, formula = Temporal ~ omega3pc + age_bl +
PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefstable%>% data.frame %>% .[,2,]
```

```
o6_N2<-lm(mlab_cross_pca_omega, formula = Temporal ~ omega6pc + age_bl +
PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefstable%>% data.frame %>% .[,2,]
```

```
omegatable <- function(df){
```

```
df%>% round(3) %>% mutate(`Beta(95%CI)` = paste0(Est., "(", X2.5., ", ", X97.5., ")"))
%>% select(6,5)
```

```

}

omegareults <- rbind(
  cbind(o3_A %>% omegatable, o3_T %>% omegatable, o3_N1 %>% omegatable, o3_N2
%>% omegatable),
  cbind(o6_A %>% omegatable, o6_T %>% omegatable, o6_N1 %>% omegatable, o6_N2
%>% omegatable)
) %>% `row.names<-`(c("Omega3 Plasmalogen", "Omega6 Plasmalogen"))

# longitudinal
mlab_longi_pca_omega <- merge(mlab_bl_longi_pca, mlab_cross_pca_omega %>%
select(RID, omega3pc, omega6pc), by="RID")

o3_AL <- lmer(formula = AV45~ omega3pc*Years.bl + age_bl + PTGENDER + APOE_bin
+ BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),
data=mlab_longi_pca_omega, na.action=na.exclude, control=lmerControl(optimizer =
"Nelder_Mead")) %>%

jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefstable %>% as.data.frame %>% slice(n())

o3_TL <- lmer(formula = PTAU_log~ omega3pc*Years.bl + age_bl + PTGENDER +
APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),
data=mlab_longi_pca_omega, na.action=na.exclude, control=lmerControl(optimizer =
"Nelder_Mead")) %>%

jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefstable %>% as.data.frame %>% slice(n())

o3_N1L <- lmer(formula = HippVol~ omega3pc*Years.bl + age_bl + PTGENDER +
APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3 + scale(ICV) +
factor(Mag) + PTEDUCAT + (Years.bl|RID), data=mlab_longi_pca_omega,
na.action=na.exclude, control=lmerControl(optimizer = "Nelder_Mead")) %>%

jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefstable %>% as.data.frame %>% slice(n())

o3_N2L <- lmer(formula = Temporal~ omega3pc*Years.bl + age_bl + PTGENDER +
APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),
data=mlab_longi_pca_omega, na.action=na.exclude, control=lmerControl(optimizer =
"Nelder_Mead")) %>%

jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefstable %>% as.data.frame %>% slice(n())

o6_AL <- lmer(formula = AV45~ omega6pc*Years.bl + age_bl + PTGENDER + APOE_bin
+ BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),

```

```
data=mlab_longi_pca_omega, na.action=na.exclude, control=lmerControl(optimizer = "Nelder_Mead")) %>%
```

```
  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .  
  $coefstable %>% as.data.frame %>% slice(n())
```

```
  o6_TL <- lmer(formula = PTAU_log ~ omega6pc*Years.bl + age_bl + PTGENDER +  
  APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),  
  data=mlab_longi_pca_omega, na.action=na.exclude, control=lmerControl(optimizer =  
  "Nelder_Mead")) %>%
```

```
  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .  
  $coefstable %>% as.data.frame %>% slice(n())
```

```
  o6_N1L <- lmer(formula = HippVol ~ omega6pc*Years.bl + age_bl + PTGENDER +  
  APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3 + scale(ICV) +  
  factor(Mag) + PTEDUCAT + (Years.bl|RID), data=mlab_longi_pca_omega,  
  na.action=na.exclude, control=lmerControl(optimizer = "Nelder_Mead")) %>%
```

```
  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .  
  $coefstable %>% as.data.frame %>% slice(n())
```

```
  o6_N2L <- lmer(formula = Temporal ~ omega6pc*Years.bl + age_bl + PTGENDER +  
  APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),  
  data=mlab_longi_pca_omega, na.action=na.exclude, control=lmerControl(optimizer =  
  "Nelder_Mead")) %>%
```

```
  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .  
  $coefstable %>% as.data.frame %>% slice(n())
```

```
  omegatable_longi <- function(df){  
    df %>% round(3) %>% mutate(`Beta(95%CI)` = paste0(Est., "(", `2.5%`, ", ", `97.5%`, ")"))  
    %>% select(7,6)  
  }
```

```
  omegaresults_long <- rbind(  
    cbind(o3_AL %>% omegatable_longi, o3_TL %>% omegatable_longi, o3_N1L %>%  
    omegatable_longi, o3_N2L %>% omegatable_longi),  
    cbind(o6_AL %>% omegatable_longi, o6_TL %>% omegatable_longi, o6_N1L %>%  
    omegatable_longi, o6_N2L %>% omegatable_longi)  
  ) %>% `row.names` <- `c("Omega3 Plasmalogen", "Omega6 Plasmalogen")
```

```
#####
```

```
### Omega 3 index analysis ###
```

```
#####
```

```

species_names <- lipids %>% filter(group=="glycerophospholipids") %>% pull(species)
omega3_species <- species_names[grepl("20.5|22.6", species_names) | (grepl("22.5",
species_names) & !grepl("N6", species_names))]

##### O3 index - percent omega3 method - divided by total phospholipids #####

# cross-sectional
mlab_cross_pca_omega <- mlab_cross_pca %>%
  rowwise() %>%
  mutate(
    PL_total = sum(c_across(all_of(species_names))),
    omega3_total = sum(c_across(all_of(omega3_species))),
    omega3_index = (omega3_total / PL_total) * 100
  ) %>%
  ungroup()

o3i_A <- lm(mlab_cross_pca_omega, formula = AV45 ~ omega3_index + age_bl +
PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .$coefable
%>% data.frame %>% .[,2,]

o3i_T<-lm(mlab_cross_pca_omega, formula = PTAU_log ~ omega3_index + age_bl +
PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefable%>% data.frame %>% .[,2,]

o3i_N1<-lm(mlab_cross_pca_omega, formula = HippVol ~ omega3_index + age_bl +
PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3 + ICV +
Mag) %>% jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefable%>% data.frame %>% .[,2,]

o3i_N2<-lm(mlab_cross_pca_omega, formula = Temporal ~ omega3_index + age_bl +
PTGENDER + APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefable%>% data.frame %>% .[,2,]

# longitudinal
mlab_longi_pca_omega_index <- merge(mlab_bl_longi_pca, mlab_cross_pca_omega %>%
select(RID, omega3_index), by="RID")

o3i_AL <- lmer(formula = AV45~ omega3_index*Years.bl + age_bl + PTGENDER +
APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),

```

```
data=mlab_longi_pca_omega_index, na.action=na.exclude, control=lmerControl(optimizer = "Nelder_Mead")) %>%
```

```
  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .  
  $coefable %>% as.data.frame %>% slice(n())
```

```
  o3i_TL <- lmer(formula = PTAU_log~ omega3_index*Years.bl + age_bl + PTGENDER +  
  APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),  
  data=mlab_longi_pca_omega_index, na.action=na.exclude, control=lmerControl(optimizer = "Nelder_Mead")) %>%
```

```
  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .  
  $coefable %>% as.data.frame %>% slice(n())
```

```
  o3i_N1L <- lmer(formula = HippVol~ omega3_index*Years.bl + age_bl + PTGENDER +  
  APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3 + scale(ICV) +  
  factor(Mag) + PTEDUCAT + (Years.bl|RID), data=mlab_longi_pca_omega_index,  
  na.action=na.exclude, control=lmerControl(optimizer = "Nelder_Mead")) %>%
```

```
  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .  
  $coefable %>% as.data.frame %>% slice(n())
```

```
  o3i_N2L <- lmer(formula = Temporal~ omega3_index*Years.bl + age_bl + PTGENDER +  
  APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),  
  data=mlab_longi_pca_omega_index, na.action=na.exclude, control=lmerControl(optimizer = "Nelder_Mead")) %>%
```

```
  jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .  
  $coefable %>% as.data.frame %>% slice(n())
```

```
#####
```

```
#### ceramide index - cert2 ###
```

```
#####
```

```
mlab_cross_pca_cer <- mlab_cross_pca %>%
```

```
  mutate(cer_ratio1 = CER.D18.1.24.1./CER.D18.1.24.0.,
```

```
    cer_ratio2 = CER.D18.1.16.0./PC.38.5...A.,
```

```
    cer_ratio3 = CER.D18.1.18.0./PC.14.0_22.6.) %>%
```

```
  mutate(cer_quart1 = ntile(cer_ratio1,4)-1,
```

```
    cer_quart2 = ntile(cer_ratio2,4)-1,
```

```
    cer_quart3 = ntile(cer_ratio3,4)-1,
```

```
    pc_quart1 = ntile(PC.16.0_16.0.,4)-1
```

```
  ) %>%
```

```
  mutate(cert2 =cer_quart1 + cer_quart2 + cer_quart3 +pc_quart1)
```

```
cert2_A <- lm(mlab_cross_pca_cer, formula = AV45 ~ cert2 + age_bl + PTGENDER +
APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .$coefable
%>% data.frame %>% .[,2,]
```

```
cert2_T <- lm(mlab_cross_pca_cer, formula = PTAU_log ~ cert2 + age_bl + PTGENDER +
APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .$coefable
%>% data.frame %>% .[,2,]
```

```
cert2_N1 <- lm(mlab_cross_pca_cer, formula = HippVol ~ cert2 + age_bl + PTGENDER +
APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3 + ICV + Mag) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .$coefable
%>% data.frame %>% .[,2,]
```

```
cert2_N2 <- lm(mlab_cross_pca_cer, formula = Temporal ~ cert2 + age_bl + PTGENDER +
APOE_bin + trig + hdl + chol + BMI + BIFAST + statin + omega3) %>%
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .$coefable
%>% data.frame %>% .[,2,]
```

```
ceramide_results <- cbind(cert2_A %>% omegatable, cert2_T %>% omegatable, cert2_N1
%>% omegatable, cert2_N2 %>% omegatable)
```

```
knitr::kable(ceramide_results) %>% kableExtra::kable_styling() %>%
kableExtra::add_header_above(c(" " =1, "A" = 2, "T" = 2, "N1"=2, "N2"=2))
```

```
mlab_longi_pca_cer <- merge(mlab_bl_longi_pca,mlab_cross_pca_cer %>% select(RID,
cert2), by="RID" )
```

```
cert2_AL <- lmer(formula = AV45~ cert2*Years.bl + age_bl + PTGENDER + APOE_bin +
BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),
data=mlab_longi_pca_cer, na.action=na.exclude, control=lmerControl(optimizer =
"Nelder_Mead")) %>%
```

```
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .
$coefable%>% as.data.frame %>% slice(n())
```

```
cert2_TL <- lmer(formula = PTAU_log~ cert2*Years.bl + age_bl + PTGENDER + APOE_bin
+ BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),
data=mlab_longi_pca_cer, na.action=na.exclude, control=lmerControl(optimizer =
"Nelder_Mead")) %>%
```

```
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .$coefable
%>% as.data.frame %>% slice(n())
```

```
cert2_N1L <-lmer(formula = HippVol~ cert2*Years.bl + age_bl + PTGENDER + APOE_bin
+ BMI + trig + chol + hdl + BIFAST + statin + omega3 + scale(ICV) + factor(Mag) +
PTEDUCAT + (Years.bl|RID), data=mlab_longi_pca_cer, na.action=na.exclude,
control=lmerControl(optimizer = "Nelder_Mead")) %>%
```

```
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .$coefable  
%>% as.data.frame %>% slice(n())
```

```
cert2_N2L <- lmer(formula = Temporal~ cert2*Years.bl + age_bl + PTGENDER +  
APOE_bin + BMI + trig + chol + hdl + BIFAST + statin + omega3 + (Years.bl|RID),  
data=mlab_longi_pca_cer, na.action=na.exclude, control=lmerControl(optimizer =  
"Nelder_Mead")) %>%
```

```
jtools::summ(scale=TRUE, transform.response = TRUE, confint=TRUE) %>% .$coefable  
%>% as.data.frame %>% slice(n())
```

```
ceramide_results_longi <- cbind(cert2_AL %>% omegatable_longi, cert2_TL %>%  
omegatable_longi, cert2_N1L %>% omegatable_longi, cert2_N2L %>% omegatable_longi)
```

```
knitr::kable(ceramide_results_longi) %>% kableExtra::kable_styling() %>%  
kableExtra::add_header_above(c(" " = 1, "A" = 2, "T" = 2, "N1" = 2, "N2" = 2))
```