

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(38:7) (c)	glycerophospholipids	Phosphatidylcholine	PC
PC(39:5) (a)	glycerophospholipids	Phosphatidylcholine	PC
PC(39:5) (b)	glycerophospholipids	Phosphatidylcholine	PC
PC(40:7) (a)	glycerophospholipids	Phosphatidylcholine	PC
PC(40:8)	glycerophospholipids	Phosphatidylcholine	PC
PC(44:12)	glycerophospholipids	Phosphatidylcholine	PC
PC(O-16:0/16:0)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-16:0/20:3)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-16:0/20:4)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-16:0/22:6)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-18:0/18:1)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-18:0/18:2)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-18:0/20:4)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-18:0/22:6)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-18:1/18:1)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-18:1/18:2)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-32:1)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-32:2)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-34:1)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-34:2)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-34:4)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-35:4)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-36:0)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-36:5)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-38:5)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(O-40:5)	glycerophospholipids	Alkylphosphatidylcholine	PC(O)
PC(P-15:0/20:4) (a)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-15:0/20:4) (b)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-16:0/14:0)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-16:0/16:0)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-16:0/16:1)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-16:0/18:0)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-16:0/18:1)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-16:0/18:2)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-16:0/18:3)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-16:0/20:4)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-16:0/20:5)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-16:0/22:6)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-17:0/20:4) (a)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-17:0/20:4) (b)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-18:0/18:2)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)

PC(P-18:0/20:4)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-18:0/22:5)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-18:0/22:6)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-18:1/18:1)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-18:1/22:6)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-20:0/20:4)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-35:2) (a)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-35:2) (b)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-36:3)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-38:5) (a)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
PC(P-38:5) (b)	glycerophospholipids	Alkenylphosphatidylcholine (plasmalogen)	PC(P)
LPC(14:0) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(14:0) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(15-MHDA) [sn1] [104_sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(15-MHDA) [sn1] & LPC(17:0) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(15-MHDA) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(15:0) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(15:0) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(16:0) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(16:0) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(16:1) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(16:1) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(17:0) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(17:1) (a) [sn1] [104_sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(17:1) [sn1] (a) & LPC(17:1) [sn2] (b)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(17:1) [sn1] (b)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(17:1) [sn2] (a)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(18:0) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(18:0) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(18:1) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(18:1) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(18:2) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(18:2) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(18:3) (a) [sn1] [104_sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(18:3) [sn1] (a) & LPC(18:3) [sn2] (b)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(18:3) [sn1] (b)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(18:3) [sn2] (a)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(19:0) (a) [sn1] [104_sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(19:0) [sn1] (a) & LPC(19:0) [sn2] (b)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(19:0) [sn1] (b)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(19:0) [sn2] (a)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(19:1) (a)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(19:1) (b)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(19:1) (c)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(20:0) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(20:0) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC

LPC(20:1) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(20:1) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(20:2) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(20:2) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(20:3) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(20:3) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(20:4) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(20:4) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(20:5) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(20:5) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:0) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:0) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:1) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:1) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:4) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:4) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:5) (n3) [sn1] [104_sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:5) [sn1] (n3) & LPC(22:5) [sn2] (n6)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:5) [sn1] (n6)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:5) [sn2] (n3)	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:6) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(22:6) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(24:0) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(24:0) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(26:0) [sn1]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(26:0) [sn2]	glycerophospholipids	Lysophosphatidylcholine	LPC
LPC(O-16:0)	glycerophospholipids	Lysoalkylphosphatidylcholine (lysoplatelet activating factor)	LPC(O)
LPC(O-18:0)	glycerophospholipids	Lysoalkylphosphatidylcholine (lysoplatelet activating factor)	LPC(O)
LPC(O-18:1)	glycerophospholipids	Lysoalkylphosphatidylcholine (lysoplatelet activating factor)	LPC(O)
LPC(O-20:0)	glycerophospholipids	Lysoalkylphosphatidylcholine (lysoplatelet activating factor)	LPC(O)
LPC(O-20:1)	glycerophospholipids	Lysoalkylphosphatidylcholine (lysoplatelet activating factor)	LPC(O)
LPC(O-22:0)	glycerophospholipids	Lysoalkylphosphatidylcholine (lysoplatelet activating factor)	LPC(O)
LPC(O-22:1)	glycerophospholipids	Lysoalkylphosphatidylcholine (lysoplatelet activating factor)	LPC(O)
LPC(O-24:0)	glycerophospholipids	Lysoalkylphosphatidylcholine (lysoplatelet activating factor)	LPC(O)
LPC(O-24:1)	glycerophospholipids	Lysoalkylphosphatidylcholine (lysoplatelet activating factor)	LPC(O)
LPC(O-24:2)	glycerophospholipids	Lysoalkylphosphatidylcholine (lysoplatelet activating factor)	LPC(O)
LPC(P-16:0)	glycerophospholipids	Lysoalkenylphosphatidylcholine (plasmalogen)	LPC(P)
LPC(P-17:0) (a)	glycerophospholipids	Lysoalkenylphosphatidylcholine (plasmalogen)	LPC(P)
LPC(P-17:0) (b)	glycerophospholipids	Lysoalkenylphosphatidylcholine (plasmalogen)	LPC(P)
LPC(P-18:0)	glycerophospholipids	Lysoalkenylphosphatidylcholine (plasmalogen)	LPC(P)
LPC(P-18:1)	glycerophospholipids	Lysoalkenylphosphatidylcholine (plasmalogen)	LPC(P)

LPC(P-20:0)	glycerophospholipids	Lysoalkenylphosphatidylcholine (plasmalogen)	LPC(P)
PE(15-MHDA_18:1)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(15-MHDA_18:2)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(15-MHDA_20:4)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(15-MHDA_22:6)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:0_16:0)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:0_16:1)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:0_18:1)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:0_18:2)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:0_18:3) (a)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:0_18:3) (b)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:0_20:3)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:0_20:4)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:0_20:5)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:0_22:6)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:1_18:2)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(16:1_20:4)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(17:0_18:1)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(17:0_18:2)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(17:0_20:4)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(17:0_22:6)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:0_18:1)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:0_18:2)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:0_20:3) (a)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:0_20:3) (b)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:0_20:4)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:0_22:4)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:0_22:5) (n3)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:0_22:5) (n6)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:0_22:6)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:1_18:1)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:1_18:2)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:1_22:6) (a)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(18:1_22:6) (b)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(20:0_20:4)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(36:0)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(38:5) (a)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(38:5) (b)	glycerophospholipids	Phosphatidylethanolamine	PE
PE(O-16:0/18:2)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-16:0/20:3)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-16:0/20:4)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-16:0/22:4)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-16:0/22:6)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-18:0/20:4)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-18:0/22:5)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-18:0/22:6)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-18:1/18:2)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-18:1/22:6)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-34:1)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-36:5)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-38:5) (a)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(O-38:5) (b)	glycerophospholipids	Alkylphosphatidylethanolamine	PE(O)
PE(P-15:0/20:4) (a)	glycerophospholipids	Alkenylphosphatidylethanolamine (plasmalogen)	PE(P)
PE(P-15:0/20:4) (b)	glycerophospholipids	Alkenylphosphatidylethanolamine (plasmalogen)	PE(P)

LPE(20:4) [sn2]	glycerophospholipids	Lysophosphatidylethanolamine	LPE
LPE(22:6) [sn1]	glycerophospholipids	Lysophosphatidylethanolamine	LPE
LPE(22:6) [sn2]	glycerophospholipids	Lysophosphatidylethanolamine	LPE
LPE(P-16:0)	glycerophospholipids	Lysoalkenylphosphatidylethanolamine (plasmalogen)	LPE(P)
LPE(P-18:0)	glycerophospholipids	Lysoalkenylphosphatidylethanolamine (plasmalogen)	LPE(P)
LPE(P-18:1)	glycerophospholipids	Lysoalkenylphosphatidylethanolamine (plasmalogen)	LPE(P)
LPE(P-20:0)	glycerophospholipids	Lysoalkenylphosphatidylethanolamine (plasmalogen)	LPE(P)
PI(38:5) (b)	glycerophospholipids	Phosphatidylinositol	PI
PI(15-MHDA_18:1) & PI(17:0_18:1)	glycerophospholipids	Phosphatidylinositol	PI
PI(15-MHDA_18:2) & PI(17:0_18:2)	glycerophospholipids	Phosphatidylinositol	PI
PI(15-MHDA_20:4) & PI(17:0_20:4)	glycerophospholipids	Phosphatidylinositol	PI
PI(16:0_16:1)	glycerophospholipids	Phosphatidylinositol	PI
PI(16:0_20:3) (a)	glycerophospholipids	Phosphatidylinositol	PI
PI(16:0_20:3) (b)	glycerophospholipids	Phosphatidylinositol	PI
PI(16:0_20:4)	glycerophospholipids	Phosphatidylinositol	PI
PI(16:0/16:0)	glycerophospholipids	Phosphatidylinositol	PI
PI(18:0_18:1)	glycerophospholipids	Phosphatidylinositol	PI
PI(18:0_20:2)	glycerophospholipids	Phosphatidylinositol	PI
PI(18:0_20:3) (a)	glycerophospholipids	Phosphatidylinositol	PI
PI(18:0_20:3) (b)	glycerophospholipids	Phosphatidylinositol	PI
PI(18:0_20:4)	glycerophospholipids	Phosphatidylinositol	PI
PI(18:0_22:4)	glycerophospholipids	Phosphatidylinositol	PI
PI(18:0_22:5) (n3)	glycerophospholipids	Phosphatidylinositol	PI
PI(18:0_22:5) (n6)	glycerophospholipids	Phosphatidylinositol	PI
PI(18:0_22:6)	glycerophospholipids	Phosphatidylinositol	PI
PI(18:1_18:2)	glycerophospholipids	Phosphatidylinositol	PI
PI(20:0_20:4)	glycerophospholipids	Phosphatidylinositol	PI
PI(34:0)	glycerophospholipids	Phosphatidylinositol	PI
PI(34:1)	glycerophospholipids	Phosphatidylinositol	PI
PI(36:2)	glycerophospholipids	Phosphatidylinositol	PI
PI(37:6)	glycerophospholipids	Phosphatidylinositol	PI
PI(38:5) (a)	glycerophospholipids	Phosphatidylinositol	PI
PI(38:6)	glycerophospholipids	Phosphatidylinositol	PI
PI(39:6)	glycerophospholipids	Phosphatidylinositol	PI
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
DG(16:0_22:6)	Neutral/Other	Diacylglycerol	DG
DG(16:1_18:1)	Neutral/Other	Diacylglycerol	DG
DG(18:0_18:1)	Neutral/Other	Diacylglycerol	DG
DG(18:0_18:2)	Neutral/Other	Diacylglycerol	DG
DG(18:0_20:4)	Neutral/Other	Diacylglycerol	DG
DG(18:1_18:1)	Neutral/Other	Diacylglycerol	DG

DG(18:1_18:2)	Neutral/Other	Diacylglycerol	DG
DG(18:1_18:3)	Neutral/Other	Diacylglycerol	DG
DG(18:1_20:3)	Neutral/Other	Diacylglycerol	DG
DG(18:1_20:4)	Neutral/Other	Diacylglycerol	DG
DG(18:1_20:5)	Neutral/Other	Diacylglycerol	DG
DG(18:1_22:5)	Neutral/Other	Diacylglycerol	DG
DG(18:1_22:6)	Neutral/Other	Diacylglycerol	DG
DG(18:2_18:2)	Neutral/Other	Diacylglycerol	DG
DG(18:2_20:4)	Neutral/Other	Diacylglycerol	DG
DG(18:2_22:6)	Neutral/Other	Diacylglycerol	DG
TG(48:0) [NL-16:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(48:0) [NL-18:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(48:1) [NL-16:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(48:1) [NL-18:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(48:2) [NL-14:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(48:2) [NL-14:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(48:2) [NL-16:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(48:2) [NL-18:2]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(48:3) [NL-14:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(48:3) [NL-16:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(48:3) [NL-18:3]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(49:1) [NL-16:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(49:1) [NL-17:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:0) [NL-18:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:1) [NL-14:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:1) [NL-16:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:1) [NL-18:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:2) [NL-14:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:2) [NL-16:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:2) [NL-18:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:2) [NL-18:2]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:3) [NL-14:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:3) [NL-14:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]

TG(50:3) [NL-16:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:3) [NL-18:2]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:3) [NL-18:3]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:4) [NL-14:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:4) [NL-18:3]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(50:4) [NL-20:4]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(51:0) [NL-16:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(51:1) [NL-17:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(51:2) [NL-15:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(51:2) [NL-17:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(51:2) [NL-17:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:1) [NL-18:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:1) [NL-18:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:2) [NL-16:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:2) [NL-18:2]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:3) [NL-16:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:3) [NL-18:2]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:4) [NL-16:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:4) [NL-18:2]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:4) [NL-18:3]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:5) [NL-18:3]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:5) [NL-20:4]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(52:5) [NL-20:5]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(53:2) [NL-17:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(53:2) [NL-18:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:0) [NL-18:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:1) [NL-18:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:2) [NL-18:0]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]

TG(54:2) [NL-20:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:3) [NL-18:1]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:3) [NL-18:2]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:4) [NL-18:2]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:4) [NL-20:3]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:5) [NL-18:3]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:5) [NL-20:4]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:6) [NL-18:3]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:6) [NL-20:4]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:6) [NL-20:5]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:6) [NL-22:6]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:7) [NL-20:5]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(54:7) [NL-22:6]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(56:6) [NL-20:4]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(56:6) [NL-22:5]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(56:7) [NL-20:4]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(56:7) [NL-20:5]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(56:7) [NL-22:5]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(56:7) [NL-22:6]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(56:8) [NL-20:4]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(56:8) [NL-20:5]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(56:8) [NL-22:6]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(56:9) [NL-22:6]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(58:10) [NL-22:6]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(58:8) [NL-22:6]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(58:9) [NL-22:6]	Neutral/Other	Triacylglycerol (neutral loss, for associations)	TG [NL]
TG(O-50:1) [NL-15:0]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-50:1) [NL-16:0]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]

TG(O-50:1) [NL-17:1]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-50:1) [NL-18:1]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-50:2) [NL-18:1]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-50:2) [NL-18:2]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-50:3) [NL-18:2]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-52:0) [NL-16:0]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-52:1) [NL-16:0]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-52:1) [NL-18:1]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-52:2) [NL-16:0]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-52:2) [NL-17:1]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-52:2) [NL-18:1]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-54:2) [NL-17:1]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-54:2) [NL-18:1]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-54:3) [NL-17:1]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-54:3) [NL-18:1]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-54:4) [NL-17:1]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
TG(O-54:4) [NL-18:2]	Neutral/Other	Alkyldiacylglycerol (neutral loss, for associations)	TG(O) [NL]
Ubiquinone	Neutral/Other	Ubiquinone	Ubiquinone
CE(18:2) [+OH]	Neutral/Other	Oxidised lipids	OxSpecies
CE(20:4) [+OH]	Neutral/Other	Oxidised lipids	OxSpecies
CE(22:6) [+OH]	Neutral/Other	Oxidised lipids	OxSpecies
LPC(18:2) [+OH]	Neutral/Other	Oxidised lipids	OxSpecies
LPC(20:4) [+OH]	Neutral/Other	Oxidised lipids	OxSpecies
LPC(22:6) [+OH]	Neutral/Other	Oxidised lipids	OxSpecies
PC(34:2) [+OH]	Neutral/Other	Oxidised lipids	OxSpecies
PC(36:4) [+OH]	Neutral/Other	Oxidised lipids	OxSpecies