Pools — metabolites with variable composition

1 Introduction

Here, species are described which are not a single physical entry. They can be seen as pools holding a number of species with a fixed ratio. More precisely it can be seen as a metabolite with a (finite) probability distribution of several similar species — a probabilistic metabolite.

All these species describe lipids with varying fatty acid residues, e.g. PC (phosphatidyl choline). Since the length distribution of these fatty acids is considerably different between different types of lipids (e.g. in PC different from PE, phosphatidyl ethanolamine) different fatty acid distributions are distinguished.

In HepatoNet a number of chemical reactions and transporters are written as processes of pools (e.g. from CDP-diacyl glycerol to PC). The specific fatty acid distribution is carried over from one of these probabilistic metabolite to the other. It is necessary that processes which assume a certain fatty acid distribution are separated from each other (e.g. the PC synthesis pathway is separated from the PE synthesis pathway). These distinguished pathways are described below as "pool areas". Thus, some intermediates must be distinguished (e.g. 1-acyl-phosphate for the PC synthesis is distinguished from the 1-acyl-phosphate for the PE synthesis).

2 VLDL-pools

Although the fatty acid distributions are experimentally determined for lipoprotein particles they can also be used as a rough estimate for other metabolites with fatty acid residues, for instance different Cerebrosides in HepatoNet inherit their fatty acid composition from sphingomyelin in VLDL. This is a reasonable estimate due to the good availability of VLDL for cells — it is a reasonable assumption that the fatty acid distribution does not differ much.

The fatty acid distribution of the different precursors of VLDL are taken from Shorten et al. [SU05].

2.1 VLDL-TG1-pool area

Shorten et al. distinguished the different positions for triacyl glycerol (TG) in VLDL. Thus, each position in TG has its own pool area. This pool describes the first position. Even though the molecule is symmetric the first position is distinguished from the third due to the kinetics of synthesis path [SU05].

Constitution	
fatty acid	per mill
16:0	6440
18:0	823
18:1	1220
18:2	741
20:4	24
total	9248

Involved metabolites	
identfier	name
HC01945_r	VLDL(r)
HC01945_s	VLDL(s)
HC01945_l	VLDL(l)
HC02037_c	1-Acylglycerol-3P-VLDL-TG1-pool(c)
HC02049_c	Phosphatidate-VLDL-TG-pool(c)
HC02055_c	1,2-Diacylglycerol-VLDL-TG-pool(c)
HC02062_r	Triacylglycerol-VLDL-pool(r)
HC02062_c	Triacylglycerol-VLDL-pool(c)
HC02062_l	Triacylglycerol-VLDL-pool(l)
HC02065_c	Fatty-acid-VLDL-TG1-pool(c)
HC02071_c	1-Acylglycerol-VLDL-TG1-pool(c)

Processes defining this pool	
identfier	name
r1198	1220 1-Acylglycerol-3P-ol(c) + 741 1-Acylglycerol-3P-lin(c) + 24 1-Acylglycerol-3P-arach(c) + 6440 1-Acylglycerol-3P-palm(c) + 823 1-Acylglycerol-3P-stea(c) ⇔ 9248 1-Acylglycerol-3P-VLDL-TG1-pool(c)
r1241	6440 Palmitate(c) + 823 Stearate(c) + 741 Linoleate(c) + 24 Arachidonate(c) + 1220 Oleate(c) ⇔ 9248 Fatty-acid-VLDL-TG1-pool(c)

Other involved reactions	
identfier	name
r1083	1 VLDL(r) ⇔ 1 VLDL(s)
r1084	1 VLDL(s) ⇔ 1 VLDL(l)
r1211	1 Phosphatidate-VLDL-TG-pool(c) + 1 CoA(c) ← 1 Acyl-CoA-VLDL-TG2-pool(c) + 1 1-Acylglycerol-3P-VLDL-TG1-pool(c)
r1217	1 Phosphatidate-VLDL-TG-pool(c) + 1 H2O(c) → 1 1,2-Diacylglycerol-VLDL-TG-pool(c) + 1 Pi(c)
r1223	1 Triacylglycerol-VLDL-pool(c) + 1 CoA(c) ← 1 Acyl-CoA-VLDL-TG3-pool(c) + 1 1,2-Diacylglycerol-VLDL-TG-pool(c)
r1224	1 Triacylglycerol-VLDL-pool(c) + 1 H2O(c) → 1 Fatty-acid-VLDL-TG3-pool(c) + 1 1,2-Diacylglycerol-VLDL-TG-pool(c)
r1225	1 H2O(c) + 1 1,2-Diacylglycerol-VLDL-TG-pool(c) → 1 1-Acylglycerol-VLDL-TG1-pool(c) + 1 Fatty-acid-VLDL-TG2-pool(c)
r1231	1 1-Acylglycerol-VLDL-TG1-pool(c) + 1 H2O(c) → 1 Fatty-acid-VLDL-TG1-pool(c) + 1 Glycerol(c)
r1264	1 Triacylglycerol-VLDL-pool(c) ⇔ 1 Triacylglycerol-VLDL-pool(r)
r1265	1 Triacylglycerol-VLDL-pool(l) → 1 Triacylglycerol-VLDL-pool(r)
r1280	1 VLDL(r) ← 7 ApoE(r) + 10385 Triacylglycerol-VLDL-pool(r) + 2165 PC-VLDL-pool(r) + 1645 Cholesterol-ester-pool(r) + 1 PI-pool(r) + 165 2-Lysolecithin-pool(r) + 185 PE-VLDL-pool(r) + 1 ApoB100(r) + 500 Cholesterol(r) + 755 SM-pool(r)
r1281	1 VLDL(l) → 7 ApoE(l) + 10385 Triacylglycerol-VLDL-pool(l) + 2165 PC-VLDL-pool(l) + 1645 Cholesterol-ester-pool(l) + 1 PI-pool(l) + 165 2-Lysolecithin-pool(l) + 185 PE-VLDL-pool(l) + 1 ApoB100(l) + 500 Cholesterol(l) + 755 SM-pool(l)

2.2 VLDL-TG2-pool area

The fatty acid distribution is taken from Shorten et al. [SU05].

Constitution	
fatty acid	per mill
16:0	1200
18:0	384
18:1	4260
18:2	2810
20:4	521
total	9175

Involved metabolites	
identfier	name
HC01945_r	VLDL(r)
HC01945_s	VLDL(s)
HC01945_l	VLDL(l)
HC02043_c	Acyl-CoA-VLDL-TG2-pool(c)
HC02049_c	Phosphatidate-VLDL-TG-pool(c)
HC02055_c	1,2-Diacylglycerol-VLDL-TG-pool(c)
HC02062_r	Triacylglycerol-VLDL-pool(r)
HC02062_c	Triacylglycerol-VLDL-pool(c)
HC02062_l	Triacylglycerol-VLDL-pool(l)
HC02064_c	Fatty-acid-VLDL-TG2-pool(c)

Processes defining this pool	
identfier	name
r1204	1200 Palmitoyl-CoA(c) + 384 Stearoyl-CoA(c) + 4260 Oleoyl-CoA(c) + 521 Arachidonyl-CoA(c) + 2810 Linoleoyl-CoA(c) ⇔ 9175 Acyl-CoA-VLDL-TG2-pool(c)
r1242	1200 Palmitate(c) + 384 Stearate(c) + 2810 Linoleate(c) + 521 Arachidonate(c) + 4260 Oleate(c) ⇔ 9175 Fatty-acid-VLDL-TG2-pool(c)

Other involved reactions	
identfier	name
r1083	1 VLDL(r) ⇔ 1 VLDL(s)
r1084	1 VLDL(s) ⇔ 1 VLDL(l)
r1211	1 Phosphatidate-VLDL-TG-pool(c) + 1 CoA(c) ← 1 Acyl-CoA-VLDL-TG2-pool(c) + 1 1-Acylglycerol-3P-VLDL-TG1-pool(c)
r1217	1 Phosphatidate-VLDL-TG-pool(c) + 1 H2O(c) → 1 1,2-Diacylglycerol-VLDL-TG-pool(c) + 1 Pi(c)
r1223	1 Triacylglycerol-VLDL-pool(c) + 1 CoA(c) ← 1 Acyl-CoA-VLDL-TG3-pool(c) + 1 1,2-Diacylglycerol-VLDL-TG-pool(c)
r1224	1 Triacylglycerol-VLDL-pool(c) + 1 H2O(c) → 1 Fatty-acid-VLDL-TG3-pool(c) + 1 1,2-Diacylglycerol-VLDL-TG-pool(c)
r1225	1 H2O(c) + 1 1,2-Diacylglycerol-VLDL-TG-pool(c) → 1 1-Acylglycerol-VLDL-TG1-pool(c) + 1 Fatty-acid-VLDL-TG2-pool(c)
r1264	1 Triacylglycerol-VLDL-pool(c) ⇔ 1 Triacylglycerol-VLDL-pool(r)
r1265	1 Triacylglycerol-VLDL-pool(l) → 1 Triacylglycerol-VLDL-pool(r)
r1280	1 VLDL(r) ← 7 ApoE(r) + 10385 Triacylglycerol-VLDL-pool(r) + 2165 PC-VLDL-pool(r) + 1645 Cholesterol-ester-pool(r) + 1 PI-pool(r) + 165 2-Lysolecithin-pool(r) + 185 PE-VLDL-pool(r) + 1 ApoB100(r) + 500 Cholesterol(r) + 755 SM-pool(r)
r1281	1 VLDL(l) → 7 ApoE(l) + 10385 Triacylglycerol-VLDL-pool(l) + 2165 PC-VLDL-pool(l) + 1645 Cholesterol-ester-pool(l) + 1 PI-pool(l) + 165 2-Lysolecithin-pool(l) + 185 PE-VLDL-pool(l) + 1 ApoB100(l) + 500 Cholesterol(l) + 755 SM-pool(l)

2.3 VLDL-TG3-pool area

Again, the fatty acid distribution is taken from Shorten et al. [SU05].

Constitution	
fatty acid	per mill
16:0	849
18:0	584
18:1	4570
18:2	2780
20:4	264
total	9047

Involved metabolites	
identfier	name
HC01945_r	VLDL(r)
HC01945_s	VLDL(s)
HC01945_l	VLDL(l)
HC02061_c	Acyl-CoA-VLDL-TG3-pool(c)
HC02062_r	Triacylglycerol-VLDL-pool(r)
HC02062_c	Triacylglycerol-VLDL-pool(c)
HC02062_l	Triacylglycerol-VLDL-pool(l)
HC02063_c	Fatty-acid-VLDL-TG3-pool(c)

Processes defining this pool	
identfier	name
r1205	849 Palmitoyl-CoA(c) + 584 Stearoyl-CoA(c) + 4570 Oleoyl-CoA(c) + 264 Arachidonyl-CoA(c) + 2780 Linoleoyl-CoA(c) ⇔ 9047 Acyl-CoA-VLDL-TG3-pool(c)
r1243	849 Palmitate(c) + 584 Stearate(c) + 2780 Linoleate(c) + 264 Arachidonate(c) + 4570 Oleate(c) ⇔ 9047 Fatty-acid-VLDL-TG3-pool(c)

Other involved reactions	
identfier	name
r1083	1 VLDL(r) ⇔ 1 VLDL(s)
r1084	1 VLDL(s) ⇔ 1 VLDL(l)
r1223	1 Triacylglycerol-VLDL-pool(c) + 1 CoA(c) ← 1 Acyl-CoA-VLDL-TG3-pool(c) + 1 1,2-Diacylglycerol-VLDL-TG-pool(c)
r1224	1 Triacylglycerol-VLDL-pool(c) + 1 H2O(c) → 1 Fatty-acid-VLDL-TG3-pool(c) + 1 1,2-Diacylglycerol-VLDL-TG-pool(c)
r1264	1 Triacylglycerol-VLDL-pool(c) ⇔ 1 Triacylglycerol-VLDL-pool(r)
r1265	1 Triacylglycerol-VLDL-pool(l) → 1 Triacylglycerol-VLDL-pool(r)
r1280	1 VLDL(r) ← 7 ApoE(r) + 10385 Triacylglycerol-VLDL-pool(r) + 2165 PC-VLDL-pool(r) + 1645 Cholesterol-ester-pool(r) + 1 PI-pool(r) + 165 2-Lysolecithin-pool(r) + 185 PE-VLDL-pool(r) + 1 ApoB100(r) + 500 Cholesterol(r) + 755 SM-pool(r)
r1281	1 VLDL(l) → 7 ApoE(l) + 10385 Triacylglycerol-VLDL-pool(l) + 2165 PC-VLDL-pool(l) + 1645 Cholesterol-ester-pool(l) + 1 PI-pool(l) + 165 2-Lysolecithin-pool(l) + 185 PE-VLDL-pool(l) + 1 ApoB100(l) + 500 Cholesterol(l) + 755 SM-pool(l)

2.4 VLDL-PC-pool area

This pool is also used for 2-Lysolecithin. Its fatty acid distribution is taken from Shorten et al. [SU05].

Constitution	
fatty acid	per mill
16:0	3010
18:0	1300
18:1	1170
18:2	2350
20:4	726
total	8556

Involved metabolites	
identfier	name
HC01940_r	HDL(r)
HC01940_s	HDL(s)
HC01940_l	HDL(l)
HC01945_r	VLDL(r)
HC01945_s	VLDL(s)
HC01945_l	VLDL(l)
HC01971_s	LDL(s)
HC01971_l	LDL(l)
HC02000_r	PC-VLDL-pool(r)
HC02000_c	PC-VLDL-pool(c)
HC02000_s	PC-VLDL-pool(s)
HC02000_l	PC-VLDL-pool(l)
HC02016_r	2-Lysolecithin-pool(r)
HC02016_c	2-Lysolecithin-pool(c)
HC02016_l	2-Lysolecithin-pool(l)
HC02038_c	1-Acylglycerol-3P-VLDL-PC-pool(c)
HC02044_c	Acyl-CoA-VLDL-PC-pool(c)
HC02050_c	Phosphatidate-VLDL-PC-pool(c)
HC02056_c	1,2-Diacylglycerol-VLDL-PC-pool(c)
HC02066_r	Fatty-acid-VLDL-PC-pool(r)
HC02066_c	Fatty-acid-VLDL-PC-pool(c)
HC02066_l	Fatty-acid-VLDL-PC-pool(l)
HC02072_c	1-Acylglycerol-VLDL-PC-pool(c)

Processes defining this pool	
identfier	name
r1199	1170 1-Acylglycerol-3P-ol(c) + 2350 1-Acylglycerol-3P-lin(c) + 726 1-Acylglycerol-3P-arach(c) + 3010 1-Acylglycerol-3P-palm(c) + 1300 1-Acylglycerol-3P-stea(c) ⇔ 8556 1-Acylglycerol-3P-VLDL-PC-pool(c)
r1206	3010 Palmitoyl-CoA(c) + 1300 Stearoyl-CoA(c) + 1170 Oleoyl-CoA(c) + 726 Arachidonyl-CoA(c) + 2350 Linoleoyl-CoA(c) ⇔ 8556 Acyl-CoA-VLDL-PC-pool(c)
r1244	3010 Palmitate(r) + 1300 Stearate(r) + 2350 Linoleate(r) + 726 Arachidonate(r) + 1170 Oleate(r) ⇔ 8556 Fatty-acid-VLDL-PC-pool(r)
r1245	3010 Palmitate(c) + 1300 Stearate(c) + 2350 Linoleate(c) + 726 Arachidonate(c) + 1170 Oleate(c) ⇔ 8556 Fatty-acid-VLDL-PC-pool(c)
r1246	3010 Palmitate(l) + 1300 Stearate(l) + 2350 Linoleate(l) + 726 Arachidonate(l) + 1170 Oleate(l) ⇔ 8556 Fatty-acid-VLDL-PC-pool(l)

Other involved reactions	
identfier	name
r0003	1 HDL(r) ← 2 ApoA1(r) + 90 PC-VLDL-pool(r) + 30 PS-VLDL-pool(r) + 20 Cholesterol(r) + 25 PE-VLDL-pool(r) + 75 SM-pool(r)
r0004	1 HDL(l) → 2 ApoA1(l) + 90 PC-VLDL-pool(l) + 30 PS-VLDL-pool(l) + 20 Cholesterol(l) + 25 PE-VLDL-pool(l) + 75 SM-pool(l)
r1053	1 LDL(s) ⇔ 1 LDL(l)
r1083	1 VLDL(r) ⇔ 1 VLDL(s)
r1084	1 VLDL(s) ⇔ 1 VLDL(l)
r1158	1 LDL(l) → 1515 Cholesterol-ester-pool(l) + 1 ApoB100(l) + 680 Cholesterol(l) + 110 CDP-diacylglycerol-VLDL-PI-pool(l) + 425 PC-VLDL-pool(l) + 25 2-Lysolecithin-pool(l) + 160 SM-pool(l) + 30 PE-VLDL-pool(l)
r1160	1 HDL(r) ⇔ 1 HDL(s)
r1161	1 HDL(s) ⇔ 1 HDL(l)
r1212	1 Phosphatidate-VLDL-PC-pool(c) + 1 CoA(c) ← 1 Acyl-CoA-VLDL-PC-pool(c) + 1 1-Acylglycerol-3P-VLDL-PC-pool(c)
r1218	1 Phosphatidate-VLDL-PC-pool(c) + 1 H2O(c) → 1 1,2-Diacylglycerol-VLDL-PC-pool(c) + 1 Pi(c)
r1226	1 H2O(c) + 1 1,2-Diacylglycerol-VLDL-PC-pool(c) → 1 1-Acylglycerol-VLDL-PC-pool(c) + 1 Fatty-acid-VLDL-PC-pool(c)
r1232	1 1-Acylglycerol-VLDL-PC-pool(c) + 1 H2O(c) → 1 Glycerol(c) + 1 Fatty-acid-VLDL-PC-pool(c)
r1237	1 CDP-choline(c) + 1 1,2-Diacylglycerol-VLDL-PC-pool(c) → 1 PC-VLDL-pool(c) + 1 CMP(c)
r1266	1 PC-VLDL-pool(c) ⇔ 1 PC-VLDL-pool(r)
r1267	1 PC-VLDL-pool(l) → 1 PC-VLDL-pool(r)
r1277	1 PC-VLDL-pool(r) + 1 H2O(r) ⇔ 1 2-Lysolecithin-pool(r) + 1 Fatty-acid-VLDL-PC-pool(r)
r1278	1 PC-VLDL-pool(c) + 1 H2O(c) ⇔ 1 2-Lysolecithin-pool(c) + 1 Fatty-acid-VLDL-PC-pool(c)
r1279	1 PC-VLDL-pool(l) + 1 H2O(l) ⇔ 1 2-Lysolecithin-pool(l) + 1 Fatty-acid-VLDL-PC-pool(l)
r1280	1 VLDL(r) ← 7 ApoE(r) + 10385 Triacylglycerol-VLDL-pool(r) + 2165 PC-VLDL-pool(r) + 1645 Cholesterol-ester-pool(r) + 1 PI-pool(r) + 165 2-Lysolecithin-pool(r) + 185 PE-VLDL-pool(r) + 1 ApoB100(r) + 500 Cholesterol(r) + 755 SM-pool(r)
r1281	1 VLDL(l) → 7 ApoE(l) + 10385 Triacylglycerol-VLDL-pool(l) + 2165 PC-VLDL-pool(l) + 1645 Cholesterol-ester-pool(l) + 1 PI-pool(l) + 165 2-Lysolecithin-pool(l) + 185 PE-VLDL-pool(l) + 1 ApoB100(l) + 500 Cholesterol(l) + 755 SM-pool(l)
r1282	1 2-Lysolecithin-pool(c) ⇔ 1 2-Lysolecithin-pool(r)
r1283	1 2-Lysolecithin-pool(l) → 1 2-Lysolecithin-pool(r)
r1369	1 PC-VLDL-pool(c) + 1 H2O(c) → 1 Phosphatidate-VLDL-PC-pool(c) + 1 Choline(c)
r1524	1 PC-VLDL-pool(c) + 1 ATP(c) + 1 H2O(c) → 1 PC-VLDL-pool(s) + 1 ADP(c) + 1 Pi(c)

2.5   VLDL-PE-pool area

Again, the fatty acid distribution is taken from Shorten et al. [SU05].

Constitution	
fatty acid	per mill
16:0	1260
18:0	2010
18:1	628
18:2	1330
20:4	2220
total	7448

Involved metabolites	
identfier	name
HC01940_r	HDL(r)
HC01940_s	HDL(s)
HC01940_l	HDL(l)
HC01945_r	VLDL(r)
HC01945_s	VLDL(s)
HC01945_l	VLDL(l)
HC01971_s	LDL(s)
HC01971_l	LDL(l)
HC02002_r	PE-VLDL-pool(r)
HC02002_b	PE-VLDL-pool(b)
HC02002_c	PE-VLDL-pool(c)
HC02002_l	PE-VLDL-pool(l)
HC02039_c	1-Acylglycerol-3P-VLDL-PE-pool(c)
HC02045_c	Acyl-CoA-VLDL-PE-pool(c)
HC02051_c	Phosphatidate-VLDL-PE-pool(c)
HC02057_c	1,2-Diacylglycerol-VLDL-PE-pool(c)
HC02067_c	Fatty-acid-VLDL-PE-pool(c)
HC02073_c	1-Acylglycerol-VLDL-PE-pool(c)

Processes defining this pool	
identfier	name
r1200	628 1-Acylglycerol-3P-ol(c) + 1330 1-Acylglycerol-3P-lin(c) + 2220 1-Acylglycerol-3P-arach(c) + 1260 1-Acylglycerol-3P-palm(c) + 2010 1-Acylglycerol-3P-stea(c) ⇔ 7448 1-Acylglycerol-3P-VLDL-PE-pool(c)
r1207	1260 Palmitoyl-CoA(c) + 2010 Stearoyl-CoA(c) + 628 Oleoyl-CoA(c) + 2220 Arachidonyl-CoA(c) + 1330 Linoleoyl-CoA(c) ⇔ 7448 Acyl-CoA-VLDL-PE-pool(c)
r1247	1260 Palmitate(c) + 2010 Stearate(c) + 1330 Linoleate(c) + 2220 Arachidonate(c) + 628 Oleate(c) ⇔ 7448 Fatty-acid-VLDL-PE-pool(c)

8

Other involved reactions	
identfier	name
r0003	1 HDL(r) ← 2 ApoA1(r) + 90 PC-VLDL-pool(r) + 30 PS-VLDL-pool(r) + 20 Cholesterol(r) + 25 PE-VLDL-pool(r) + 75 SM-pool(r)
r0004	1 HDL(l) → 2 ApoA1(l) + 90 PC-VLDL-pool(l) + 30 PS-VLDL-pool(l) + 20 Cholesterol(l) + 25 PE-VLDL-pool(l) + 75 SM-pool(l)
r1053	1 LDL(s) ⇔ 1 LDL(l)
r1083	1 VLDL(r) ⇔ 1 VLDL(s)
r1084	1 VLDL(s) ⇔ 1 VLDL(l)
r1158	1 LDL(l) → 1515 Cholesterol-ester-pool(l) + 1 ApoB100(l) + 680 Cholesterol(l) + 110 CDP-diacylglycerol-VLDL-PI-pool(l) + 425 PC-VLDL-pool(l) + 25 2-Lysolecithin-pool(l) + 160 SM-pool(l) + 30 PE-VLDL-pool(l)
r1160	1 HDL(r) ⇔ 1 HDL(s)
r1161	1 HDL(s) ⇔ 1 HDL(l)
r1191	1 PE-VLDL-pool(c) + 1 Serine(c) ⇔ 1 PS-VLDL-pool(c) + 1 Ethanolamine(c)
r1194	1 1,2-Diacylglycerol-VLDL-PE-pool(c) + 1 CDP-ethanolamine(c) → 1 PE-VLDL-pool(c) + 1 CMP(c)
r1213	1 Phosphatidate-VLDL-PE-pool(c) + 1 CoA(c) ← 1 Acyl-CoA-VLDL-PE-pool(c) + 1 1-Acylglycerol-3P-VLDL-PE-pool(c)
r1219	1 Phosphatidate-VLDL-PE-pool(c) + 1 H2O(c) → 1 1,2-Diacylglycerol-VLDL-PE-pool(c) + 1 Pi(c)
r1227	1 H2O(c) + 1 1,2-Diacylglycerol-VLDL-PE-pool(c) → 1 1-Acylglycerol-VLDL-PE-pool(c) + 1 Fatty-acid-VLDL-PE-pool(c)
r1233	1 1-Acylglycerol-VLDL-PE-pool(c) + 1 H2O(c) → 1 Glycerol(c) + 1 Fatty-acid-VLDL-PE-pool(c)
r1268	1 PE-VLDL-pool(c) ⇔ 1 PE-VLDL-pool(r)
r1269	1 PE-VLDL-pool(l) → 1 PE-VLDL-pool(r)
r1280	1 VLDL(r) ← 7 ApoE(r) + 10385 Triacylglycerol-VLDL-pool(r) + 2165 PC-VLDL-pool(r) + 1645 Cholesterol-ester(r) + 1 PI-pool(r) + 165 2-Lysolecithin-pool(r) + 185 PE-VLDL-pool(r) + 1 ApoB100(r) + 500 Cholesterol(r) + 755 SM-pool(r)
r1281	1 VLDL(l) → 7 ApoE(l) + 10385 Triacylglycerol-VLDL-pool(l) + 2165 PC-VLDL-pool(l) + 1645 Cholesterol-ester-pool(l) + 1 PI-pool(l) + 165 2-Lysolecithin-pool(l) + 185 PE-VLDL-pool(l) + 1 ApoB100(l) + 500 Cholesterol(l) + 755 SM-pool(l)
r1371	1 H2O(c) + 1 PE-VLDL-pool(c) → 1 Phosphatidate-VLDL-PE-pool(c) + 1 Ethanolamine(c)
r1509	1 PE-VLDL-pool(c) + 1 ATP(c) + 1 H2O(c) → 1 PE-VLDL-pool(b) + 1 ADP(c) + 1 Pi(c)

2.6   VLDL-PS-pool area

Again, the fatty acid distribution is taken from Shorten et al. [SU05].

Constitution	
fatty acid	per mill
16:0	345
18:0	4820
18:1	332
18:2	181
20:4	2050
total	7728

Involved metabolites	
identfier	name
HC01940_r	HDL(r)
HC01940_s	HDL(s)
HC01940_l	HDL(l)
HC01945_r	VLDL(r)
HC01945_s	VLDL(s)
HC01945_l	VLDL(l)
HC01971_s	LDL(s)
HC01971_l	LDL(l)
HC02006_r	PS-VLDL-pool(r)
HC02006_b	PS-VLDL-pool(b)
HC02006_c	PS-VLDL-pool(c)
HC02006_l	PS-VLDL-pool(l)
HC02040_c	1-Acylglycerol-3P-VLDL-PS-pool(c)
HC02046_c	Acyl-CoA-VLDL-PS-pool(c)
HC02052_c	Phosphatidate-VLDL-PS-pool(c)
HC02058_c	1,2-Diacylglycerol-VLDL-PS-pool(c)
HC02068_c	Fatty-acid-VLDL-PS-pool(c)
HC02074_c	1-Acylglycerol-VLDL-PS-pool(c)
HC02079_c	PE-PS-VLDL-pool(c)

Processes defining this pool	
identfier	name
r1201	332 1-Acylglycerol-3P-ol(c) + 181 1-Acylglycerol-3P-lin(c) + 2050 1-Acylglycerol-3P-arach(c) + 345 1-Acylglycerol-3P-palm(c) + 4820 1-Acylglycerol-3P-stea(c) ⇔ 7728 1-Acylglycerol-3P-VLDL-PS-pool(c)
r1208	345 Palmitoyl-CoA(c) + 4820 Stearoyl-CoA(c) + 332 Oleoyl-CoA(c) + 2050 Arachidonyl-CoA(c) + 181 Linoleoyl-CoA(c) ⇔ 7728 Acyl-CoA-VLDL-PS-pool(c)
r1248	345 Palmitate(c) + 4820 Stearate(c) + 181 Linoleate(c) + 2050 Arachidonate(c) + 332 Oleate(c) ⇔ 7728 Fatty-acid-VLDL-PS-pool(c)

Other involved reactions	
identfier	name
r0003	1 HDL(r) ← 2 ApoA1(r) + 90 PC-VLDL-pool(r) + 30 PS-VLDL-pool(r) + 20 Cholesterol(r) + 25 PE-VLDL-pool(r) + 75 SM-pool(r)
r0004	1 HDL(l) → 2 ApoA1(l) + 90 PC-VLDL-pool(l) + 30 PS-VLDL-pool(l) + 20 Cholesterol(l) + 25 PE-VLDL-pool(l) + 75 SM-pool(l)
r1053	1 LDL(s) ⇔ 1 LDL(l)
r1083	1 VLDL(r) ⇔ 1 VLDL(s)
r1084	1 VLDL(s) ⇔ 1 VLDL(l)
r1158	1 LDL(l) → 1515 Cholesterol-ester-pool(l) + 1 ApoB100(l) + 680 Cholesterol(l) + 110 CDP-diacylglycerol-VLDL-PI-pool(l) + 425 PC-VLDL-pool(l) + 25 2-Lysolecithin-pool(l) + 160 SM-pool(l) + 30 PE-VLDL-pool(l)
r1160	1 HDL(r) ⇔ 1 HDL(s)
r1161	1 HDL(s) ⇔ 1 HDL(l)
r1191	1 PE-VLDL-pool(c) + 1 Serine(c) ⇔ 1 PS-VLDL-pool(c) + 1 Ethanolamine(c)
r1195	1 1,2-Diacylglycerol-VLDL-PS-pool(c) + 1 CDP-ethanolamine(c) → 1 PE-PS-VLDL-pool(c) + 1 CMP(c)
r1214	1 Phosphatidate-VLDL-PS-pool(c) + 1 CoA(c) ← 1 Acyl-CoA-VLDL-PS-pool(c) + 1 1-Acylglycerol-3P-VLDL-PS-pool(c)
r1220	1 Phosphatidate-VLDL-PS-pool(c) + 1 H2O(c) → 1 1,2-Diacylglycerol-VLDL-PS-pool(c) + 1 Pi(c)
r1228	1 H2O(c) + 1 1,2-Diacylglycerol-VLDL-PS-pool(c) → 1 1-Acylglycerol-VLDL-PS-pool(c) + 1 Fatty-acid-VLDL-PS-pool(c)
r1234	1 1-Acylglycerol-VLDL-PS-pool(c) + 1 H2O(c) → 1 Fatty-acid-VLDL-PS-pool(c) + 1 Glycerol(c)
r1270	1 PS-VLDL-pool(b) ⇔ 1 PS-VLDL-pool(c)
r1271	1 PS-VLDL-pool(c) ⇔ 1 PS-VLDL-pool(r)
r1272	1 PS-VLDL-pool(l) → 1 PS-VLDL-pool(r)
r1280	1 VLDL(r) ← 7 ApoE(r) + 10385 Triacylglycerol-VLDL-pool(r) + 2165 PC-VLDL-pool(r) + 1645 Cholesterol-ester-pool(r) + 1 PI-pool(r) + 165 2-Lysolecithin-pool(r) + 185 PE-VLDL-pool(r) + 1 ApoB100(r) + 500 Cholesterol(r) + 755 SM-pool(r)
r1281	1 VLDL(l) → 7 ApoE(l) + 10385 Triacylglycerol-VLDL-pool(l) + 2165 PC-VLDL-pool(l) + 1645 Cholesterol-ester-pool(l) + 1 PI-pool(l) + 165 2-Lysolecithin-pool(l) + 185 PE-VLDL-pool(l) + 1 ApoB100(l) + 500 Cholesterol(l) + 755 SM-pool(l)
r1370	1 PS-VLDL-pool(c) ⇔ 1 PE-PS-VLDL-pool(c) + 1 CO2(c)

2.7 VLDL-PI-pool area

Again, the fatty acid distribution is taken from Shorten et al. [SU05].

Constitution	
fatty acid	per mill
16:0	694
18:0	3640
18:1	1360
18:2	694
20:4	2170
total	8558

Involved metabolites	
identfier	name
HC01945_r	VLDL(r)
HC01945_s	VLDL(s)
HC01945_l	VLDL(l)
HC01971_s	LDL(s)
HC01971_l	LDL(l)
HC02009_r	PI-pool(r)
HC02009_c	PI-pool(c)
HC02009_l	PI-pool(l)
HC02041_c	1-Acylglycerol-3P-VLDL-PI-pool(c)
HC02047_c	Acyl-CoA-VLDL-PI-pool(c)
HC02053_c	Phosphatidate-VLDL-PI-pool(c)
HC02059_c	1,2-Diacylglycerol-VLDL-PI-pool(c)
HC02069_c	Fatty-acid-VLDL-PI-pool(c)
HC02075_c	1-Acylglycerol-VLDL-PI-pool(c)
HC02078_r	CDP-diacylglycerol-VLDL-PI-pool(r)
HC02078_c	CDP-diacylglycerol-VLDL-PI-pool(c)
HC02078_l	CDP-diacylglycerol-VLDL-PI-pool(l)

Processes defining this pool	
identfier	name
r1202	1360 1-Acylglycerol-3P-ol(c) + 694 1-Acylglycerol-3P-lin(c) + 2170 1-Acylglycerol-3P-arach(c) + 694 1-Acylglycerol-3P-palm(c) + 3640 1-Acylglycerol-3P-stea(c) ⇔ 8558 1-Acylglycerol-3P-VLDL-PI-pool(c)
r1209	694 Palmitoyl-CoA(c) + 3640 Stearoyl-CoA(c) + 1360 Oleoyl-CoA(c) + 2170 Arachidonyl-CoA(c) + 694 Linoleoyl-CoA(c) ⇔ 8558 Acyl-CoA-VLDL-PI-pool(c)
r1249	694 Palmitate(c) + 3640 Stearate(c) + 694 Linoleate(c) + 2170 Arachidonate(c) + 1360 Oleate(c) ⇔ 8558 Fatty-acid-VLDL-PI-pool(c)

Other involved reactions	
identfier	name
r1053	1 LDL(s) ⇔ 1 LDL(l)
r1083	1 VLDL(r) ⇔ 1 VLDL(s)
r1084	1 VLDL(s) ⇔ 1 VLDL(l)
r1158	1 LDL(l) → 1515 Cholesterol-ester-pool(l) + 1 ApoB100(l) + 680 Cholesterol(l) + 110 CDP-diacylglycerol-VLDL-PI-pool(l) + 425 PC-VLDL-pool(l) + 25 2-Lysolecithin-pool(l) + 160 SM-pool(l) + 30 PE-VLDL-pool(l)
r1196	1 CDP-diacylglycerol-VLDL-PI-pool(r) + 1 Inositol(r) ⇔ 1 PI-pool(r) + 1 CMP(r)
r1197	1 CDP-diacylglycerol-VLDL-PI-pool(c) + 1 Inositol(c) ⇔ 1 PI-pool(c) + 1 CMP(c)
r1215	1 Phosphatidate-VLDL-PI-pool(c) + 1 CoA(c) ← 1 1-Acylglycerol-3P-VLDL-PI-pool(c) + 1 Acyl-CoA-VLDL-PI-pool(c)
r1221	1 Phosphatidate-VLDL-PI-pool(c) + 1 H2O(c) → 1 1,2-Diacylglycerol-VLDL-PI-pool(c) + 1 Pi(c)
r1229	1 H2O(c) + 1 1,2-Diacylglycerol-VLDL-PI-pool(c) → 1 1-Acylglycerol-VLDL-PI-pool(c) + 1 Fatty-acid-VLDL-PI-pool(c)
r1235	1 1-Acylglycerol-VLDL-PI-pool(c) + 1 H2O(c) → 1 Fatty-acid-VLDL-PI-pool(c) + 1 Glycerol(c)
r1238	1 Phosphatidate-VLDL-PI-pool(c) + 1 CTP(c) ⇔ 1 CDP-diacylglycerol-VLDL-PI-pool(c) + 1 PPi(c)
r1273	1 PI-pool(c) ⇔ 1 PI-pool(r)
r1274	1 PI-pool(l) → 1 PI-pool(r)
r1280	1 VLDL(r) ← 7 ApoE(r) + 10385 Triacylglycerol-VLDL-pool(r) + 2165 PC-VLDL-pool(r) + 1645 Cholesterol-ester-pool(r) + 1 PI-pool(r) + 165 2-Lysolecithin-pool(r) + 185 PE-VLDL-pool(r) + 1 ApoB100(r) + 500 Cholesterol(r) + 755 SM-pool(r)
r1281	1 VLDL(l) → 7 ApoE(l) + 10385 Triacylglycerol-VLDL-pool(l) + 2165 PC-VLDL-pool(l) + 1645 Cholesterol-ester-pool(l) + 1 PI-pool(l) + 165 2-Lysolecithin-pool(l) + 185 PE-VLDL-pool(l) + 1 ApoB100(l) + 500 Cholesterol(l) + 755 SM-pool(l)
r1360	1 CDP-diacylglycerol-VLDL-PI-pool(l) → 1 CDP-diacylglycerol-VLDL-PI-pool(r)
r1372	1 PI-pool(c) + 1 H2O(c) → 1 Inositol-1P(c) + 1 1,2-Diacylglycerol-VLDL-PI-pool(c)

2.8   VLDL-SM-pool area

This pool is also used for the various derivates of cerebrosides. Again, the fatty acid distribution is taken from Shorten et al. [SU05].

Constitution	
fatty acid	per mill
16:0	6260
18:0	1490
18:1	656
18:2	270
20:4	147
total	8823

Involved metabolites	
identfier	name
HC01940_r	HDL(r)
HC01940_s	HDL(s)
HC01940_l	HDL(l)
HC01945_r	VLDL(r)
HC01945_s	VLDL(s)
HC01945_l	VLDL(l)
HC01971_s	LDL(s)
HC01971_l	LDL(l)
HC01990_r	Ceramide-pool(r)
HC01990_c	Ceramide-pool(c)
HC02007_r	SM-pool(r)
HC02007_b	SM-pool(b)
HC02007_c	SM-pool(c)
HC02007_l	SM-pool(l)
HC02008_r	Glucosylceramide-pool(r)
HC02008_c	Glucosylceramide-pool(c)
HC02008_s	Glucosylceramide-pool(s)
HC02042_c	1-Acylglycerol-3P-VLDL-SM-pool(c)
HC02048_c	Acyl-CoA-VLDL-SM-pool(c)
HC02054_c	Phosphatidate-VLDL-SM-pool(c)
HC02060_c	1,2-Diacylglycerol-VLDL-SM-pool(c)
HC02070_c	Fatty-acid-VLDL-SM-pool(c)
HC02076_c	1-Acylglycerol-VLDL-SM-pool(c)
HC02158_c	Dihydroceramide-pool(c)
HC02162_r	LacCer-pool(r)
HC02162_s	LacCer-pool(s)

Processes defining this pool	
identfier	name
r1203	656 1-Acylglycerol-3P-ol(c) + 270 1-Acylglycerol-3P-lin(c) + 147 1-Acylglycerol-3P-arach(c) + 6260 1-Acylglycerol-3P-palm(c) + 1490 1-Acylglycerol-3P-stea(c) ⇔ 8823 1-Acylglycerol-3P-VLDL-SM-pool(c)
r1210	6260 Palmitoyl-CoA(c) + 1490 Stearoyl-CoA(c) + 656 Oleoyl-CoA(c) + 147 Arachidonyl-CoA(c) + 270 Linoleoyl-CoA(c) ⇔ 8823 Acyl-CoA-VLDL-SM-pool(c)
r1250	6260 Palmitate(c) + 1490 Stearate(c) + 270 Linoleate(c) + 147 Arachidonate(c) + 656 Oleate(c) ⇔ 8823 Fatty-acid-VLDL-SM-pool(c)

14

Other involved reactions	
identfier	name
r0003	1 HDL(r) ← 2 ApoA1(r) + 90 PC-VLDL-pool(r) + 30 PS-VLDL-pool(r) + 20 Cholesterol(r) + 25 PE-VLDL-pool(r) + 75 SM-pool(r)
r0004	1 HDL(l) → 2 ApoA1(l) + 90 PC-VLDL-pool(l) + 30 PS-VLDL-pool(l) + 20 Cholesterol(l) + 25 PE-VLDL-pool(l) + 75 SM-pool(l)
r1053	1 LDL(s) ⇔ 1 LDL(l)
r1083	1 VLDL(r) ⇔ 1 VLDL(s)
r1084	1 VLDL(s) ⇔ 1 VLDL(l)
r1158	1 LDL(l) → 1515 Cholesterol-ester-pool(l) + 1 ApoB100(l) + 680 Cholesterol(l) + 110 CDP-diacylglycerol-VLDL-PI-pool(l) + 425 PC-VLDL-pool(l) + 25 2-Lysolecithin-pool(l) + 160 SM-pool(l) + 30 PE-VLDL-pool(l)
r1160	1 HDL(r) ⇔ 1 HDL(s)
r1161	1 HDL(s) ⇔ 1 HDL(l)
r1216	1 CoA(c) + 1 Phosphatidate-VLDL-SM-pool(c) ← 1 Acyl-CoA-VLDL-SM-pool(c) + 1 1-Acylglycerol-3P-VLDL-SM-pool(c)
r1222	1 H2O(c) + 1 Phosphatidate-VLDL-SM-pool(c) → 1 Pi(c) + 1 1,2-Diacylglycerol-VLDL-SM-pool(c)
r1230	1 H2O(c) + 1 1,2-Diacylglycerol-VLDL-SM-pool(c) → 1 1-Acylglycerol-VLDL-SM-pool(c) + 1 Fatty-acid-VLDL-SM-pool(c)
r1236	1 1-Acylglycerol-VLDL-SM-pool(c) + 1 H2O(c) → 1 Fatty-acid-VLDL-SM-pool(c) + 1 Glycerol(c)
r1239	1 Sphingosine(c) + 1 Acyl-CoA-VLDL-SM-pool(c) ⇔ 1 CoA(c) + 1 Ceramide-pool(c)
r1240	1 Ceramide-pool(c) ⇔ 1 Ceramide-pool(r)
r1275	1 SM-pool(c) ⇔ 1 SM-pool(r)
r1276	1 SM-pool(l) → 1 SM-pool(r)
r1280	1 VLDL(r) ← 7 ApoE(r) + 10385 Triacylglycerol-VLDL-pool(r) + 2165 PC-VLDL-pool(r) + 1645 Cholesterol-ester-pool(r) + 1 PI-pool(r) + 165 2-Lysolecithin-pool(r) + 185 PE-VLDL-pool(r) + 1 ApoB100(r) + 500 Cholesterol(r) + 755 SM-pool(r)
r1281	1 VLDL(l) → 7 ApoE(l) + 10385 Triacylglycerol-VLDL-pool(l) + 2165 PC-VLDL-pool(l) + 1645 Cholesterol-ester-pool(l) + 1 PI-pool(l) + 165 2-Lysolecithin-pool(l) + 185 PE-VLDL-pool(l) + 1 ApoB100(l) + 500 Cholesterol(l) + 755 SM-pool(l)
r1404	1 ATP(c) + 1 Ceramide-pool(c) → 1 ADP(c) + 1 Ceramide-1P-pool(c)
r1405	1 UDP-glucose(c) + 1 Ceramide-pool(c) ⇔ 1 UDP(c) + 1 Glucosylceramide-pool(c)
r1406	1 H2O(c) + 1 Glucosylceramide-pool(c) → 1 Glucose(c) + 1 Ceramide-pool(c)
r1407	1 CDP-choline(r) + 1 Ceramide-pool(r) ⇔ 1 CMP(r) + 1 SM-pool(r)
r1408	1 SM-pool(c) + 1 H2O(c) ⇔ 1 Ceramide-pool(c) + 1 Phosphocholine(c)
r1409	1 UDP-galactose(r) + 1 Glucosylceramide-pool(r) ⇔ 1 LacCer-pool(r) + 1 UDP(r)
r1410	1 LacCer-pool(s) + 1 H2O(s) ⇔ 1 Galactose(s) + 1 Glucosylceramide-pool(s)
r1412	1 Sphinganine(c) + 1 Acyl-CoA-VLDL-SM-pool(c) ⇔ 1 Dihydroceramide-pool(c) + 1 CoA(c)
r1413	1 Dihydroceramide-pool(c) + 1 H2O(c) ⇔ 1 Sphinganine(c) + 1 Fatty-acid-VLDL-SM-pool(c)
r1414	1 Dihydroceramide-pool(c) + 1 O2(c) + 1 NADPH(c) ⇔ 2 H2O(c) + 1 Ceramide-pool(c) + 1 NADP+(c)
r1415	1 Ceramide-1P-pool(c) + 1 H2O(c) → 1 Pi(c) + 1 Ceramide-pool(c)
r1416	1 Glucosylceramide-pool(c) ⇔ 1 Glucosylceramide-pool(r)
r1510	1 SM-pool(c) + 1 ATP(c) + 1 H2O(c) → 1 SM-pool(b) + 1 ADP(c) + 1 Pi(c)

2.9 Cholesterol-ester-pool area

The fatty acid distribution is taken from Shorten et al. [SU05].

Constitution	
fatty acid	per mill
16:0	1420
18:0	280
18:1	2050
18:2	4880
20:4	542
total	9172

Involved metabolites	
identfier	name
HC01945_r	VLDL(r)
HC01945_s	VLDL(s)
HC01945_l	VLDL(l)
HC01969_r	Cholesterol-ester-pool(r)
HC01969_l	Cholesterol-ester-pool(l)
HC01971_s	LDL(s)
HC01971_l	LDL(l)

Processes defining this pool	
identfier	name
r1192	2050 Cholesterol-ester-ol(r) + 4880 Cholesterol-ester-lin(r) + 1420 Cholesterol-ester-palm(r) + 280 Cholesterol-ester-stea(r) + 542 Cholesterol-ester-arach(r) ⇔ 9172 Cholesterol-ester-pool(r)
r1193	2050 Cholesterol-ester-ol(l) + 4880 Cholesterol-ester-lin(l) + 1420 Cholesterol-ester-palm(l) + 280 Cholesterol-ester-stea(l) + 542 Cholesterol-ester-arach(l) ⇔ 9172 Cholesterol-ester-pool(l)

Other involved reactions	
identfier	name
r1053	1 LDL(s) ⇔ 1 LDL(l)
r1083	1 VLDL(r) ⇔ 1 VLDL(s)
r1084	1 VLDL(s) ⇔ 1 VLDL(l)
r1158	1 LDL(l) → 1515 Cholesterol-ester-pool(l) + 1 ApoB100(l) + 680 Cholesterol(l) + 110 CDP-diacylglycerol-VLDL-PI-pool(l) + 425 PC-VLDL-pool(l) + 25 2-Lysolecithin-pool(l) + 160 SM-pool(l) + 30 PE-VLDL-pool(l)
r1280	1 VLDL(r) ← 7 ApoE(r) + 10385 Triacylglycerol-VLDL-pool(r) + 2165 PC-VLDL-pool(r) + 1645 Cholesterol-ester-pool(r) + 1 PI-pool(r) + 165 2-Lysolecithin-pool(r) + 185 PE-VLDL-pool(r) + 1 ApoB100(r) + 500 Cholesterol(r) + 755 SM-pool(r)
r1281	1 VLDL(l) → 7 ApoE(l) + 10385 Triacylglycerol-VLDL-pool(l) + 2165 PC-VLDL-pool(l) + 1645 Cholesterol-ester-pool(l) + 1 PI-pool(l) + 165 2-Lysolecithin-pool(l) + 185 PE-VLDL-pool(l) + 1 ApoB100(l) + 500 Cholesterol(l) + 755 SM-pool(l)
r1361	1 Cholesterol-ester-pool(l) → 1 Cholesterol-ester-pool(r)

2.10   VLDL particle

The relations of the different lipid categories have been optained from Swift et al. [SMDL80]. The relative shares of the different phospholipids are from [Phi59] and [VV90].

Involved metabolites	
identfier	name
HC01945_r	VLDL(r)
HC01945_s	VLDL(s)
HC01945_l	VLDL(l)

Processes defining this pool	
identfier	name
r1280	1 VLDL(r) ← 7 ApoE(r) + 10385 Triacylglycerol-VLDL-pool(r) + 2165 PC-VLDL-pool(r) + 1645 Cholesterol-ester-pool(r) + 1 PI-pool(r) + 165 2-Lysolecithin-pool(r) + 185 PE-VLDL-pool(r) + 1 ApoB100(r) + 500 Cholesterol(r) + 755 SM-pool(r)
r1281	1 VLDL(l) → 7 ApoE(l) + 10385 Triacylglycerol-VLDL-pool(l) + 2165 PC-VLDL-pool(l) + 1645 Cholesterol-ester-pool(l) + 1 PI-pool(l) + 165 2-Lysolecithin-pool(l) + 185 PE-VLDL-pool(l) + 1 ApoB100(l) + 500 Cholesterol(l) + 755 SM-pool(l)

Other involved reactions	
identfier	name
r1083	1 VLDL(r) ⇔ 1 VLDL(s)
r1084	1 VLDL(s) ⇔ 1 VLDL(l)

2.11   HDL particle

The relations of the different lipid categories have been optained from Barrans et al. [BJB+96] and Wu et al. [WWZ+07]. The phospholipid composition is obtained from Barrans et al. [BJB+96].

Involved metabolites	
identfier	name
HC01940_r	HDL(r)
HC01940_s	HDL(s)
HC01940_l	HDL(l)

Processes defining this pool	
identfier	name
r0003	1 HDL(r) ← 2 ApoA1(r) + 90 PC-VLDL-pool(r) + 30 PS-VLDL-pool(r) + 20 Cholesterol(r) + 25 PE-VLDL-pool(r) + 75 SM-pool(r)
r0004	1 HDL(l) → 2 ApoA1(l) + 90 PC-VLDL-pool(l) + 30 PS-VLDL-pool(l) + 20 Cholesterol(l) + 25 PE-VLDL-pool(l) + 75 SM-pool(l)

Other involved reactions	
identfier	name
r1160	1 HDL(r) ⇔ 1 HDL(s)
r1161	1 HDL(s) ⇔ 1 HDL(l)

2.12 LDL particle

The composition has been induced from [TSBH04, Phi59, VV90].

Involved metabolites	
identfier	name
HC01971_s	LDL(s)
HC01971_l	LDL(l)

Processes defining this pool	
identfier	name
r1158	1 LDL(l) → 1515 Cholesterol-ester-pool(l) + 1 ApoB100(l) + 680 Cholesterol(l) + 110 CDP-diacylglycerol-VLDL-PI-pool(l) + 425 PC-VLDL-pool(l) + 25 2-Lysolecithin-pool(l) + 160 SM-pool(l) + 30 PE-VLDL-pool(l)
Other involved reactions	
identfier	name
r1053	1 LDL(s) ⇔ 1 LDL(l)

3 Bile-PC-pool area

Fatty acid distribution of PC in bile is measured by van Berge Henegouwen et al. [vBHWR87].

Constitution	
fatty acid	per mill
16:0	4140
16:1	268
18:0	550
18:1	1209
18:2	3283
20:4	564
total	10014

Involved metabolites	
identfier	name
HC02080_b	Bile-PC-pool(b)
HC02080_c	Bile-PC-pool(c)
HC02082_c	Acyl-CoA-Bile-PC-pool(c)
HC02084_c	1-Acylglycerol-3P-Bile-PC-pool(c)
HC02085_c	1,2-Diacylglycerol-Bile-PC-pool(c)
HC02086_c	Phosphatidate-Bile-PC-pool(c)

Processes defining this pool	
identfier	name
r1284	268 1-Acylglycerol-3P-palmn(c) + 1209 1-Acylglycerol-3P-ol(c) + 3283 1-Acylglycerol-3P-lin(c) + 564 1-Acylglycerol-3P-arach(c) + 4140 1-Acylglycerol-3P-palm(c) + 550 1-Acylglycerol-3P-stea(c) ⇔ 10014 1-Acylglycerol-3P-Bile-PC-pool(c)
r1285	4140 Palmitoyl-CoA(c) + 268 (2E)-Hexadecenoyl-CoA(c) + 550 Stearoyl-CoA(c) + 1209 Oleoyl-CoA(c) + 564 Arachidonyl-CoA(c) + 3283 Linoleoyl-CoA(c) ⇔ 10014 Acyl-CoA-Bile-PC-pool(c)

Other involved reactions	
identfier	name
r1286	1 Phosphatidate-Bile-PC-pool(c) + 1 CoA(c) ⇔ 1 Acyl-CoA-Bile-PC-pool(c) + 1 1-Acylglycerol-3P-Bile-PC-pool(c)
r1287	1 Phosphatidate-Bile-PC-pool(c) + 1 H2O(c) → 1 Pi(c) + 1 1,2-Diacylglycerol-Bile-PC-pool(c)
r1288	1 CDP-choline(c) + 1 1,2-Diacylglycerol-Bile-PC-pool(c) → 1 Bile-PC-pool(c) + 1 CMP(c)
r1511	1 Bile-PC-pool(c) + 1 ATP(c) + 1 H2O(c) → 1 Bile-PC-pool(b) + 1 ADP(c) + 1 Pi(c)

4 CL-pool area

Cardiolipin is synthesized in human mitochondria and the respective fatty acid distributions are taken from [Hoc92].

Constitution	
fatty acid	per mill
16:0	43
16:1	47
18:0	19
18:1	138
18:2	738
total	985

Involved metabolites	
identfier	name
HC02087_m	CL-pool(m)
HC02089_c	Acyl-CoA-CL-pool(c)
HC02089_m	Acyl-CoA-CL-pool(m)
HC02091_m	1-Acylglycerol-3P-CL-pool(m)
HC02093_m	Phosphatidate-CL-pool(m)
HC02094_m	CDP-diacylglycerol-CL-pool(m)
HC02095_m	PGP-CL-pool(m)
HC02096_m	PG-CL-pool(m)

Processes defining this pool	
identfier	name
r1305	43 Palmitoyl-CoA(c) + 47 (2E)-Hexadecenoyl-CoA(c) + 19 Stearoyl-CoA(c) + 138 Oleoyl-CoA(c) + 738 Linoleoyl-CoA(c) ⇔ 985 Acyl-CoA-CL-pool(c)

Other involved reactions	
identfier	name
r1306	1 Acyl-CoA-CL-pool(c) ⇔ 1 Acyl-CoA-CL-pool(m)
r1307	1 Acyl-CoA-CL-pool(m) + 1 sn-Glycerol-3P(m) ⇔ 1 CoA(m) + 1 1-Acylglycerol-3P-CL-pool(m)
r1308	1 Phosphatidate-CL-pool(m) + 1 CoA(m) ⇔ 1 Acyl-CoA-CL-pool(m) + 1 1-Acylglycerol-3P-CL-pool(m)
r1309	1 Phosphatidate-CL-pool(m) + 1 CTP(m) ⇔ 1 CDP-diacylglycerol-CL-pool(m) + 1 PPi(m)
r1310	1 CDP-diacylglycerol-CL-pool(m) + 1 sn-Glycerol-3P(m) ⇔ 1 CMP(m) + 1 PGP-CL-pool(m)
r1311	1 PGP-CL-pool(m) + 1 H2O(m) ⇔ 1 PG-CL-pool(m) + 1 Pi(m)
r1312	2 PG-CL-pool(m) ⇔ 1 CL-pool(m) + 1 Pi(m)

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