

12-months metabolic changes among gender dysphoric individuals under cross-sex hormone treatment: a targeted metabolomics study

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Supplement table 1

Metabolite	Commonly used name	Attached Synonyms	Attached HMDB_ID	Attached KEGG_ID	Class
Ac-Orn	Acetylorithine	(2S)-2-acetamido-5-a	HMDB03357	C00437	Amino Acids and Derivatives
		dimethylamino-methylidene)amino-pentanoate, 2-Amino-5-(amino-dimethylamino-methylidene)amino-pentanoic acid, ADMA, Asymmetric dimethylarginine, Dimethyl-L-arginine, N(Omega), N(omega)-dimethyl-L-arginine, NG, NG-Dimethyl-L-arginine, NG, NG-dimethylarginine, NG-dimethylarginine, Nomega, Nomega'-Dimethyl-L-arginine			
	Asymmetric dimethylarginine	2-Amino-5-(amino-dimethylamino-methylidene)amino-pentanoate, 2-Amino-5-(amino-dimethylamino-methylidene)amino-pentanoic acid, ADMA, Asymmetric dimethylarginine, Dimethyl-L-arginine, N(Omega),	HMDB01539	C03626	Amino Acids and Derivatives
ADMA	Asymmetric dimethylarginine	N(omega)-dimethyl-L-	HMDB01539	C03626	Amino Acids and Derivatives

Supplement table 1

Ala		Carboxyethylamine, 3-Amino-Propanoate, 3-Amino-Propanoic acid, 3- Aminopropanoate, 3- Aminopropanoic acid, 3- Aminopropionate, 3- Aminopropionic acid, Abufene, B-Alanine, b-Aminopropanoate, b-Aminopropanoic acid, b- Aminopropionate, b- Aminopropionic acid, beta Alanine, beta- Alanine, beta- Aminopropanoate, beta-Aminopropanoic acid, beta- Aminopropionate, beta-Aminopropionic acid, Omega- Aminopropionate, Omega- Aminopropionic acid			
	beta-Alanine	(2S)-2- Aminopropanoate,	HMDB00056	C00099	Amino Acids and Derivatives
	L-Alanine	(2S)-2- Aminopropanoic	HMDB00161	C00041	Amino Acids and Derivatives
	D-Alanine	acid, (S)-(+)-Alanine,	HMDB01310	C00133	Amino Acids and Derivatives
	beta-Alanine	(S)-2-amino-	HMDB00056	C00099	Amino Acids and Derivatives
	L-Alanine		HMDB00161	C00041	Amino Acids and Derivatives
	D-Alanine		HMDB01310	C00133	Amino Acids and Derivatives

Supplement table 1

		(+/-)-2-Aminoadipic acid, 2-Aminoadipate, 2-Aminoadipic acid, a-Aminoadipate, a-Aminoadipic acid, alpha-Amino-adipic acid, alpha-Aminoadipate, alpha-Aminoadipic acid, Aminoadipate, DL-2-Aminoadipate, DL-2-Aminoadipic acid, DL-2-Aminohexanedioate, DL-2-Aminohexanedioic acid, DL-a-Aminoadipate, DL-a-Aminoadipic acid, DL-alpha-Aminoadipate, DL-alpha-Aminoadipic acid, L-2-Aminoadipate, L-2-Aminoadipic acid, L-2-Aminohexanedioate, L-2-Aminohexanedioic acid, L-alpha-Aminoadipate, L-alpha-Aminoadipic acid			
alpha-AAA	L-2-Aminoadipic acid L-2-Aminoadipic acid	Aminoadipate, L-alpha-Aminoadipic	HMDB00510 HMDB00510	C00956 C00956	Amino Acids and Derivatives Amino Acids and Derivatives

Supplement table 1

Arg	L-Arginine D-Arginine L-Arginine D-Arginine	[[aminoiminomethyl) amino]-Pentanoate, (S)-2-amino-5-[[aminoiminomethyl) amino]-Pentanoic acid, (S)-2-Amino-5-[[aminoiminomethyl) amino]pentanoate, (S)-2-Amino-5-[[aminoiminomethyl) amino]pentanoic acid, 2-Amino-5-guanidinovalerate, 2-Amino-5-guanidinovaleric acid, 5-[[Aminoiminomethyl) amino]-L-Norvaline, Arginine, L-(+)-Arginine, L- α -Amino-D-guanidinovalerate, L- α -Amino-D-guanidinovaleric acid, L- α -Amino- δ - δ -guanidinovalerate, L- α -Amino- δ - δ -guanidinovaleric acid, N5-(aminoiminomethyl)-L-Ornithine D-2-Amino-5-	HMDB00517 HMDB03416 HMDB00517 HMDB03416	C00062 C00792 C00062 C00792	Amino Acids and Derivatives Amino Acids and Derivatives Amino Acids and Derivatives Amino Acids and Derivatives
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Supplement table 1

Asn		4-Diamino-4-oxobutanoate, (S)-2,			
		4-Diamino-4-oxobutanoic acid, (S)-			
		Asparagine, 2-Aminosuccinamate,			
		2-Aminosuccinamic acid, a-Aminosuccinamate,			
	a-Aminosuccinamic acid, Agedoite, alpha				
	Amminosuccinamate, alpha				
	Amminosuccinamic acid, alpha-				
	Aminosuccinamate, alpha-				
	Aminosuccinamic acid, Altheine, Asn,				
	Asparagine, Asparagine acid,				
	Asparamide, Aspartamate,				
	Aspartamic acid, Aspartic acid amide,				
	Aspartic acid b-amide, Aspartic acid				
	beta amide, B2, 4-(S)-				
	diamino-4-oxo-	HMDB00168	C00152	Amino Acids and Derivatives	
	D-Asparagine	HMDB33780	C01905	Amino Acids and Derivatives	
	L-Asparagine	HMDB00168	C00152	Amino Acids and Derivatives	
	D-Asparagine	HMDB33780	C01905	Amino Acids and Derivatives	
		utanoate, B2, 4-(S)-			
		diamino-4-oxo-			
		utanoic acid, Crystal			

Supplement table 1

Asp	L-Aspartic acid D-Aspartic acid L-Aspartic acid D-Aspartic acid	(+)-Aspartic acid, (2S)-Aspartate, (2S)- Aspartic acid, (L)- Aspartate, (L)- Aspartic acid, (R)-2- aminosuccinate, (S)- (+)-Aspartate, (S)-(+)- Aspartic acid, (S)-2- aminosuccinate, (S)- 2-aminosuccinic acid, (S)-amino- Butanedioate, (S)- amino-Butanedioic acid, (S)- Aminobutanedioate, (S)- Aminobutanedioic acid, (S)-Aspartate, (S)-Aspartic acid, 2- Amino-3- methylsuccinate, 2- Amino-3- methylsuccinic acid, 2-Aminosuccinate, 2- Aminosuccinic acid, alpha- Aminosuccinate, alpha-Aminosuccinic acid, Aminosuccinate, Asparagate, Asparagic acid,	HMDB00191 HMDB06483 HMDB00191 HMDB06483	C00049 C00402 C00049 C00402	Amino Acids and Derivatives Amino Acids and Derivatives Amino Acids and Derivatives Amino Acids and Derivatives
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Supplement table 1

C0	L-Carnitine D-Carnitine	(trimethylammonio)butyrate, (-)-carnitine, (R)-(3-Carboxy-2-hydroxypropyl)trimethylammonium hydroxide, (R)-carnitine, (S)-carnitine, 1-Carnitine, 3-Carboxy-2-hydroxy-N, N, N-trimethyl-1-propanaminium, 3-Hydroxy-4-trimethylammoniobutanoate, 3-Hydroxy-4-trimethylammoniobutanoic acid, Bicarnesine, Carniking, Carniking 50, Carnilean, Carnipass, Carnipass 20, Carnitene, Carnitine, Carnitor, D-Carnitine, delta-Carnitine, DL-carnitine, gamma-Trimethyl-ammonium-beta-hydroxybutirate, gamma-Trimethyl-beta-hydroxybutyrobetaine, gamma-Trimethyl-hydroxybutyrobetaine	HMDB00062 HMDB00062	C15025 C15025	Alkylamines Alkylamines
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Supplement table 1

		Decanoyl-L-carnitine, Decanoylcarnitine Decanoyl-L-carnitine, Decanoylcarnitine	HMDB00651 HMDB00651 HMDB00651		Fatty Acid Esters Fatty Acid Esters Fatty Acid Esters
C10	Decanoylcarnitine Decanoyl-L-carnitine Decanoylcarnitine	Decanoyl-L-carnitine, Decanoylcarnitine Decanoyl-L-carnitine, Decanoylcarnitine	HMDB00651 HMDB00651 HMDB00651		Fatty Acid Esters Fatty Acid Esters Fatty Acid Esters
	C10:1		HMDB13205		Fatty Acid Esters
	C10:2				

Supplement table 1

		(-)-Lauroylcarnitine, (R)- Dodecanoylcarnitine, Dodecanoyl-L- carnitine, L-Carnitine dodecanoyl ester, Lauroyl-L(-)-carnitin, Lauroyl-L-carnitine, Lauroylcarnitine (-)-Lauroylcarnitine, (R)- Dodecanoylcarnitine, Dodecanoyl-L- carnitine, L-Carnitine dodecanoyl ester, Lauroyl-L(-)-carnitin, Lauroyl-L-carnitine, Lauroylcarnitine (-)-Lauroylcarnitine, (R)- Dodecanoylcarnitine, Dodecanoyl-L- carnitine, L-Carnitine dodecanoyl ester, Lauroyl-L(-)-carnitin, Lauroyl-L-carnitine, Lauroylcarnitine			
C12	Dodecanoylcarnitine Dodecanoyl-L- carnitine Dodecanoylcarnitine	dodecanoyl ester, Lauroyl-L(-)-carnitin, Lauroyl-L-carnitine, Lauroylcarnitine	HMDB02250 HMDB02250 HMDB02250		Fatty Acid Esters Fatty Acid Esters Fatty Acid Esters
C12-DC	Dodecanedioylcarniti ne Dodecanedioylcarniti ne	Dodecanedioyl-L- carnitine Dodecanedioyl-L- carnitine	HMDB13327 HMDB13327		Carboxylic Acids and Derivatives Carboxylic Acids and Derivatives
C12:1	C12:1				

Supplement table 1

C14	C14	(-)-Myristoylcarnitine,	HMDB05066		Fatty Acid Esters
	cis-5-Tetradecenoylcarnitine				
C14:1	cis-5-Tetradecenoylcarnitine		HMDB02014		Fatty Acid Esters
C14:1-OH	C14:1-OH	3-Hydroxy-5(Z)-tetrad	HMDB13330		Hydroxy Acids and Derivatives
C14:2	C14:2	(3E, 5E)-tetradecadie	HMDB13331		Fatty Acid Esters
C14:2-OH	C14:2-OH				

Supplement table 1

		<p>palmitoylcarnitine, (3S)-3-hexadecanoyloxy-4-(trimethylammonio)butanoate, (3S)-3-hexadecanoyloxy-4-(trimethylammonio)butanoic acid, (3S)-3-palmitoyloxy-4-(trimethylammonio)butanoate, (3S)-3-palmitoyloxy-4-(trimethylammonio)butanoic acid, 3-Carboxy-N, N, N-trimethyl-2-[(1-oxohexadecyl)oxy]-1-Propanaminium, D-Palmitoylcarnitine, Hexadecanoyl-L-carnitine, Hexadecenoyl carnitine, L(-)-Palmitoylcarnitine, L-Carnitine palmitoyl ester, L-Palmitoyl-L-carnitine, Palmitoyl D-carnitine, Palmitoyl(-)-carnitine, Palmitoyl-L-carnitine, Palmitoyl-L-carnitine (+)-</p>			
C16	L-Palmitoylcarnitine D-Palmitoylcarnitine L-Palmitoylcarnitine Palmitoylcarnitine		HMDB00222 HMDB00222 HMDB00222 HMDB00222	C02990 C02990 C02990 C02990	Fatty Acid Esters Fatty Acid Esters Fatty Acid Esters Fatty Acid Esters
C16-OH	C16-OH				

Supplement table 1

		(2E)-Hexadecenoyl-carnitine, trans-2-Hexadecenoyl-carnitine			
	trans-Hexadec-2-enoyl carnitine	(2E)-Hexadecenoyl-carnitine, trans-2-Hexadecenoyl-carnitine	HMDB06317		Fatty Acid Esters
C16:1	trans-Hexadec-2-enoyl carnitine		HMDB06317		Fatty Acid Esters
C16:1-OH	C16:1-OH	3-Hydroxy-(9Z)-hexadecanoic acid	HMDB13333		Hydroxy Acids and Derivatives
C16:2	C16:2	(Z, Z)9, 12-hexadecadienoic acid	HMDB13334		Fatty Acid Esters
C16:2-OH	C16:2-OH	3-Hydroxy-9(Z), 12(Z)-hexadecadienoic acid	HMDB13335		Hydroxy Acids and Derivatives

Supplement table 1

C18	Stearoylcarnitine Stearoylcarnitine	(R)-3-carboxy-N, N, N-trimethyl-2-[(1-oxooctadecyl)oxy]-1-Propanaminium inner salt, (R)-Stearoylcarnitine, Acylcarnitine C18:0, L-(3-Carboxy-2-hydroxypropyl)trimethyl-Ammonium stearate hydroxide inner salt, L-Stearic acid ester with (3-carboxy-2-hydroxypropyl)trimethylammonium hydroxide inner salt, L-Stearoylcarnitine, Octadecanoyl-L-carnitine, Octadecanoylcarnitine, Stearoyl-L-carnitine, Stearoylcarnitine (-)-Stearoylcarnitine, (R)-3-carboxy-N, N, N-trimethyl-2-[(1-oxooctadecyl)oxy]-1-Propanaminium inner salt, (R)-Stearoylcarnitine, Acylcarnitine C18:0,	HMDB00848 HMDB00848		Fatty Acid Esters Fatty Acid Esters
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Supplement table 1

		(Z)-(+)-3-carboxy-N, N, N-trimethyl-2-((1- oxo-9- octadecenyl)oxy)-1- Propanaminium,	HMDB05065		Fatty Acid Esters
	Oleoylcarnitine	Acylcarnitine C18:1,	HMDB06464		Fatty Acid Esters
	Elaidic carnitine	Oleoyl-L-carnitine,	HMDB06464		Fatty Acid Esters
C18:1	Oleoylcarnitine	Oleoylcarnitine	HMDB06464		Fatty Acid Esters
C18:1-OH	C18:1-OH	3-Hydroxy-11(Z)-octadecenoic acid	HMDB13339		Hydroxy Acids and Derivatives
C18:2	Linoelaidylcarnitine	Acylcarnitine C18:2	HMDB06461		Fatty Acid Esters

Supplement table 1

C2	Acetyl-L-carnitine Acetylcarnitine	(+-)-Acetylcarnitine, (-)-Acetylcarnitine, (R)-Acetylcarnitine, Acetyl-carnitine , Acetyl-L(-)-carnitine, Acetyl-L-carnitine, Acetylcarnitine, ALCAR, L-Acetylcarnitine, L-Carnitine acetyl ester, L-O-Acetylcarnitine, Levocarnitine acetyl, Nicetile, O-Acetyl-L-carnitine, O-Acetylcarnitine (+-)-Acetylcarnitine, (-)-Acetylcarnitine, (R)-Acetylcarnitine, Acetyl-carnitine , Acetyl-L(-)-carnitine, Acetyl-L-carnitine, Acetylcarnitine, ALCAR, L-Acetylcarnitine, L-Carnitine acetyl ester, L-O-Acetylcarnitine, Levocarnitine acetyl, Nicetile, O-Acetyl-L-carnitine, O-Acetylcarnitine	HMDB00201 HMDB00201	C02571 C02571	Fatty Acid Esters Fatty Acid Esters
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Supplement table 1

C3		Propionylcarnitine chloride, (3-carboxy-2-hydroxypropyl)trimethyl-hydroxide Ammonium inner salt, 3-Carboxy-N, N, N-trimethyl-2-(1-oxopropoxy)-1-propanaminium inner salt, L-Propionylcarnitine, O-Propanoylcarnitine, O-Propionylcarnitine, Propionyl carnitine, Propionyl-carnitine, Propionyl-L-carnitine (+/-)-Propionylcarnitine chloride, (3-carboxy-2-hydroxypropyl)trimethyl-hydroxide Ammonium inner salt, 3-Carboxy-N, N, N-trimethyl-2-(1-oxopropoxy)-1-propanaminium inner salt, L-			
	Propionylcarnitine	Propionylcarnitine, O-	HMDB00824	C03017	Fatty Acid Esters
	Propionyl-L-carnitine	Propanoylcarnitine,	HMDB00824	C03017	Fatty Acid Esters
	Propionylcarnitine	O-Propionylcarnitine,	HMDB00824	C03017	Fatty Acid Esters

Supplement table 1

		Carboxyacetyl)oxy]-4-hydroxy-N, N, N-trimethyl-4-oxo-1-Butanaminium inner salt, 3-Carboxy-2-[(carboxyacetyl)oxy]-N, N, N-trimethyl-1-Propanaminium inner salt, Malonyl-L-carnitine		
		2-[(2-Carboxyacetyl)oxy]-4-hydroxy-N, N, N-trimethyl-4-oxo-1-Butanaminium inner salt, 3-Carboxy-2-[(carboxyacetyl)oxy]-N, N, N-trimethyl-1-Propanaminium inner salt, Malonyl-L-carnitine		
	Malonylcarnitine	2-[(2-Carboxyacetyl)oxy]-4-hydroxy-N, N, N-trimethyl-4-oxo-1-Butanaminium inner salt, 3-Carboxy-2-[(carboxyacetyl)oxy]-N, N, N-trimethyl-1-Propanaminium inner salt, Malonyl-L-carnitine	HMDB02095	Fatty Acid Esters
	Hydroxybutyrylcarnitine	2-[(2-Carboxyacetyl)oxy]-4-hydroxy-N, N, N-trimethyl-4-oxo-1-Butanaminium inner salt, 3-Carboxy-2-[(carboxyacetyl)oxy]-N, N, N-trimethyl-1-Propanaminium inner salt, Malonyl-L-carnitine	HMDB13127	Fatty Acid Esters
	Malonyl-D-carnitine	2-[(2-Carboxyacetyl)oxy]-4-hydroxy-N, N, N-trimethyl-4-oxo-1-Butanaminium inner salt, 3-Carboxy-2-[(carboxyacetyl)oxy]-N, N, N-trimethyl-1-Propanaminium inner salt, Malonyl-L-carnitine	HMDB02095	Fatty Acid Esters
	Malonyl-L-carnitine	2-[(2-Carboxyacetyl)oxy]-4-hydroxy-N, N, N-trimethyl-4-oxo-1-Butanaminium inner salt, 3-Carboxy-2-[(carboxyacetyl)oxy]-N, N, N-trimethyl-1-Propanaminium inner salt, Malonyl-L-carnitine	HMDB02095	Fatty Acid Esters
	Malonylcarnitine	2-[(2-Carboxyacetyl)oxy]-4-hydroxy-N, N, N-trimethyl-4-oxo-1-Butanaminium inner salt, 3-Carboxy-2-[(carboxyacetyl)oxy]-N, N, N-trimethyl-1-Propanaminium inner salt, Malonyl-L-carnitine	HMDB02095	Fatty Acid Esters
	Hydroxybutyrylcarnitine	2-[(2-Carboxyacetyl)oxy]-4-hydroxy-N, N, N-trimethyl-4-oxo-1-Butanaminium inner salt, 3-Carboxy-2-[(carboxyacetyl)oxy]-N, N, N-trimethyl-1-Propanaminium inner salt, Malonyl-L-carnitine	HMDB02095	Fatty Acid Esters
C3-DC (C4-OH)		2-[(2-Carboxyacetyl)oxy]-4-hydroxy-N, N, N-trimethyl-4-oxo-1-Butanaminium inner salt, 3-Carboxy-2-[(carboxyacetyl)oxy]-N, N, N-trimethyl-1-Propanaminium inner salt, Malonyl-L-carnitine	HMDB13127	Fatty Acid Esters
C3-OH	Hydroxypropionylcarnitine	Hydroxypropionyl-L-carnitine	HMDB13125	Fatty Acid Esters
C3:1	C3:1	Propenoyl-L-carnitine	HMDB13124	Fatty Acid Esters

Supplement table 1

		carnitine, Isobutyryl-L-carnitine, L-Isobutyric acid ester with (3-carboxy-2-hydroxypropyl)trimethylammonium hydroxide inner salt (3-carboxy-2-hydroxypropyl)trimethyl-L-butyrate, (R)-3-carboxy-N, N, N-trimethyl-2-(1-oxobutoxy)-1-Propanaminium, Butyryl-L-carnitine, Ester with (3-carboxy-2-hydroxypropyl)trimethylammonium L-Butyric acid, Ester with L-(3-carboxy-2-hydroxypropyl)trimethylammonium Butyric acid, L-Carnitine butyryl ester, N-Butyryl-L(-)-carnitine, O-Butanoylcarnitine	HMDB00736 HMDB02013 HMDB00736 HMDB00736 HMDB02013 HMDB02013	C02862	Fatty Acid Esters Fatty Acid Esters Fatty Acid Esters Fatty Acid Esters Fatty Acid Esters Fatty Acid Esters
C4	Isobutyryl-L-carnitine Butyrylcarnitine Isobutyryl-L-carnitine Isobutyrylcarnitine Butyryl-L-carnitine Butyrylcarnitine	Isobutyryl-L(-)-carnitine, Isobutyryl-L-carnitine, L-Isobutyric acid ester with (3-	HMDB02013 HMDB02013	C02862 C02862	Fatty Acid Esters Fatty Acid Esters
C4:1	Butenyl-L-carnitine	Butenyl-L-carnitine	HMDB13126		Fatty Acid Esters

Supplement table 1

		Isovaleryl L-carnitine, Isovalerylcarnitine Pentanoylcarnitine, Valeryl-L-carnitine			
		(2- methylbutyryl)carnitin e, 2- Methylbutyroylcarniti ne, L-2- Methylbutyrate (3- carboxy-2- hydroxypropyl)trimet hyl-hydroxide Ammonium inner salt, Methylbutyroyl- carnitine			
	Isovalerylcarnitine	Isovaleryl L-carnitine,	HMDB00688		Fatty Acid Esters
	Valerylcarnitine	Isovalerylcarnitine	HMDB13128		Fatty Acid Esters
	Pivaloylcarnitine	Isovaleryl L-carnitine,	HMDB41993		Fatty Acid Esters
	2- Methylbutyrylcarnitin e	Isovalerylcarnitine	HMDB00378		Fatty Acid Esters
	Isovalery-L-carnitine	Pentanoylcarnitine,	HMDB00688		Fatty Acid Esters
	Isovalerylcarnitine	Valeryl-L-carnitine	HMDB00688		Fatty Acid Esters
	Valeryl-L-carnitine	Pentanoylcarnitine,	HMDB13128		Fatty Acid Esters
C5	Valerylcarnitine	Valeryl-L-carnitine	HMDB13128		Fatty Acid Esters
C5-DC (C6-OH)	C5-DC (C6-OH)		HMDB13130		Fatty Acid Esters
C5-M-DC	Methylglutaryl-L-carni	3-Methylglutaryl-carniti	HMDB00552		Fatty Acid Esters
C5-OH (C3-DC-M)	C5-OH (C3-DC-M)		HMDB13132		Alkylamines
	Tiglylcarnitine	Tiglyl-L-carnitine	HMDB02366		Fatty Acid Esters
C5:1	Tiglylcarnitine	Tiglyl-L-carnitine	HMDB02366		Fatty Acid Esters
C5:1-DC	Glutaconylcarnitine	Glutaconyl-L-carnitine	HMDB13129		Fatty Acid Esters

Supplement table 1

		Hexanoate, Hexanoic acid, Hexanoic acid ester with (3-carboxy-2- hydroxypropyl)trimet hylammonium hydroxide inner salt, Hexanoyl DL- carnitine, Hexanoyl- D, L-carnitine, Hexanoylcarnitine (R)-3-carboxy-N, N, N-trimethyl-2-[(1- oxohexyl)oxy]-1- Propanaminium inner salt, (R)- Caproylcarnitine, Hexanoate, Hexanoic acid, Hexanoic acid ester with L-(3-carboxy-2- hydroxypropyl)trimet hylammonium hydroxide inner salt, Hexanoyl-L-carnitine, L-Carnitine hexanoyl ester, L-Hexanoate, L-Hexanoic acid, L- Hexanoic acid ester with (3-carboxy-2- hydroxypropyl)trimet hylammonium			
C6 (C4:1-DC)	Hexanoylcarnitine (Fumaryl carnitine) L-Hexanoylcarnitine Hexanoylcarnitine (Fumaryl carnitine) L-Hexanoylcarnitine	Hexanoic acid ester with L-(3-carboxy-2- hydroxypropyl)trimet hylammonium	HMDB00705 HMDB00756 HMDB00705 HMDB00756		Fatty Acid Esters Fatty Acid Esters Fatty Acid Esters Fatty Acid Esters
C6:1	C6:1	Hexenoyl-L-carnitine	HMDB13161		Fatty Acid Esters
C7-DC	Pimelylcarnitine	Heptanedioylcarnitine	HMDB13328		Carboxylic Acids and Derivatives

Supplement table 1

		(-)-Octanoylcarnitine, L-Carnitine octanoyl ester, L-O-Octanoylcarnitine, L-Octanoylcarnitine, Octanoate, Octanoic acid, Octanoic acid ester with L-(3-carboxy-2-hydroxypropyl)trimethylammonium hydroxide inner salt, Octanoyl-L-carnitine, Octanoylcarnitine (-)-Octanoylcarnitine, L-Carnitine octanoyl ester, L-O-Octanoylcarnitine, L-Octanoylcarnitine, Octanoate, Octanoic acid, Octanoic acid ester with L-(3-carboxy-2-hydroxypropyl)trimethylammonium hydroxide inner salt, Octanoyl-L-carnitine, Octanoylcarnitine			
C8	Octanoyl-L-carnitine Octanoylcarnitine	Octanoyl-L-carnitine, Octanoylcarnitine	HMDB00791 HMDB00791	C02838 C02838	Fatty Acid Esters Fatty Acid Esters
C9	2,6 Dimethylheptanoyl	2, 6-Dimethylheptanoyl	HMDB06320		Fatty Acid Esters

Supplement table 1

		b-Alanylhistidine, beta-Alanyl-L- histidine, beta- Alanylhistidine, Carnosine, Igotine, Karnozin, Karnozzn, L-Carnosine, N-(3- Aminopropanoyl)histi dine, N-(b-Alanyl)-L- histidine, N-b-Alanyl- L-Histidine, N-beta- Alanyl-L-Histidine, Sevitin			
		b-Alanyl-L-histidine, b-Alanylhistidine, beta-Alanyl-L- histidine, beta- Alanylhistidine, Carnosine, Igotine, Karnozin, Karnozzn, L-Carnosine, N-(3- Aminopropanoyl)histi dine, N-(b-Alanyl)-L- histidine, N-b-Alanyl- L-Histidine, N-beta- Alanyl-L-Histidine, Sevitin			
	Carnosine	b-Alanyl-L-histidine,	HMDB00033	C00386	Peptidomimetics
	L-Carnosine	b-Alanylhistidine,	HMDB00033	C00386	Peptidomimetics
	Carnosine	beta-Alanyl-L-	HMDB00033	C00386	Peptidomimetics
	L-Carnosine	histidine, beta-	HMDB00033	C00386	Peptidomimetics
Carnosine	L-Carnosine	Alanylhistidine,	HMDB00033	C00386	Peptidomimetics

Supplement table 1

	Citrulline L-Citrulline L-Citrulline	(2S)-2-amino-5-(carba	HMDB00904 HMDB00904 HMDB00904	C00327 C00327 C00327	Amino Acids and Derivatives Amino Acids and Derivatives Amino Acids and Derivatives
Cit					

Supplement table 1

		1-Methylglycocyanamide, 1-Methylhydantoin-2-imide, 2-Amino-1-methyl-1, 5-dihydroimidazol-4-one, 2-Amino-1-methylimidazolin-4-one, Creatine anhydride, Creatinine			
		1-Methylglycocyanamide, 1-Methylhydantoin-2-imide, 2-Amino-1-methyl-1, 5-dihydroimidazol-4-one, 2-Amino-1-methylimidazolin-4-one, Creatine anhydride, Creatinine			
		1-Methylglycocyanamide, 1-Methylhydantoin-2-imide, 2-Amino-1-methyl-1, 5-dihydroimidazol-4-one, 2-Amino-1-methylimidazolin-4-one, Creatine anhydride, Creatinine	HMDB00562	C00791	Lactams
Creatinine	Creatinine	one, Creatine anhydride, Creatinine	HMDB00562	C00791	Lactams
	Creatinine	one, Creatine anhydride, Creatinine	HMDB00562	C00791	Lactams

Supplement table 1

DOPA	L-Dihydroxyphenylalanine Dihydroxyphenylalanine	(-)-3-(3, 4-dihydroxyphenyl)	HMDB00181 HMDB00609	C00355 C00355	Amino Acids and Derivatives Amino Acids and Derivatives
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Supplement table 1

		Dihydroxyphenyl)ethylamine, 3, 4- Dihydroxyphenethylamine, 3, 4- Dihydroxyphenylethylamine, 3- Hydroxytyramine, 4-(2-Aminoethyl)-1, 2-benzenediol, 4-(2-Aminoethyl)- Pyrocatechol, 4-(2-Aminoethyl)catechol, 4-(2-Aminoethyl)pyrocatechol, a-(3, 4-Dihydroxyphenyl)-b-aminoethane, alpha-(3, 4-Dihydroxyphenyl)-beta-aminoethane, Deoxyepinephrine, Dopamin, Dopamine, Dopaminum, Dopastat, Dophamine, Dynatra, Hydroxytyramin, Hydroxytyramine, Intropin, Oxytyramine, Revivan	HMDB00073 HMDB00073 HMDB00073	C03758 C03758 C03758	Phenols and Derivatives Phenols and Derivatives Phenols and Derivatives
Dopamine	Dopamine Dopamine Dopamine				

Supplement table 1

Gln		oxopentanoate, (2S)-2, 5-diamino-5-oxopentanoic acid, (2S)-2-amino-4-carbamoylbutanoate, (2S)-2-amino-4-carbamoylbutanoic acid, (S)-2, 5-Diamino-5-oxopentanoate, (S)-2, 5-Diamino-5-oxopentanoic acid, 2-Aminoglutaramic acid, Cebrogen, gamma-Glutamine, Glavamin, Glumin, Glutamic acid 5-amide, Glutamic acid amide, Glutamine, L-(+)-Glutamine, L-2-Aminoglutaramic acid, L-2-Aminoglutaramidic acid, L-Glutamic acid 5-amide, L-Glutamic acid gamma-amide, L-Glutamid, L-Glutamide, L-Glutamin, L-Glutamine, L-Glutaminsaeure-5-amid, Levoglutamid,	HMDB00641	C00064	Amino Acids and Derivatives
	L-Glutamine		HMDB03423	C00819	Amino Acids and Derivatives
	D-Glutamine		HMDB00641	C00064	Amino Acids and Derivatives
	D-Glutamine		HMDB03423	C00819	Amino Acids and Derivatives

Supplement table 1

Glu		Aminopentanedioate, (2S)-2-			
		Aminopentanedioic acid, (S)-(+)-			
		Glutamate, (S)-(+)-			
		Glutamic acid, (S)-2-			
		Aminopentanedioate, (S)-2-			
		Aminopentanedioic acid, (S)-			
		Glutamate, (S)-			
		Glutamic acid, 1-			
		Amino-propane-1, 3-			
		dicarboxylate, 1-			
		Amino-propane-1, 3-			
		dicarboxylic acid, 1-			
		Aminopropane-1, 3-			
		dicarboxylate, 1-			
		Aminopropane-1, 3-			
		dicarboxylic acid, 2-			
		Aminoglutarate, 2-			
		Aminoglutamic acid, 2-			
		Aminopentanedioate, 2-			
		Aminopentanedioic acid, a-			
		Aminoglutarate, a-			
		Aminoglutamic acid, a-			
		Glutamate, a-			
		Glutamic acid,			
	L-Glutamic acid	Aciglut, alpha-	HMDB00148	C00025	Amino Acids and Derivatives
	D-Glutamic acid	Aminoglutarate,	HMDB03339	C00217	Amino Acids and Derivatives
	L-Glutamic acid	alpha-Aminoglutamic acid,	HMDB00148	C00025	Amino Acids and Derivatives
	D-Glutamic acid	alpha-	HMDB03339	C00217	Amino Acids and Derivatives

Supplement table 1

Gly	Glycine Glycine	2-Aminoacetate, 2-Aminoacetic acid, Aciport, Amino-Acetate, Amino-Acetic acid, Aminoacetate, Aminoacetic acid, Aminoethanoate, Aminoethanoic acid, Glicoamin, Glycocol, Glycolixir, Glycosthene, Gyn-Hydralin, Padil 2-Aminoacetate, 2-Aminoacetic acid, Aciport, Amino-Acetate, Amino-Acetic acid, Aminoacetate, Aminoacetic acid, Aminoethanoate, Aminoethanoic acid, Glicoamin, Glycocol, Glycolixir, Glycosthene, Gyn-Hydralin, Padil	HMDB00123 HMDB00123	C00037 C00037	Amino Acids and Derivatives Amino Acids and Derivatives
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Supplement table 1

		Glucose, Anhydrous dextrose, Cerelose, Cerelose 2001, Clearsweet 95, Clintose L, Corn sugar, CPC hydrate, D(+)-Glucose, Dextropur, Dextrose, Dextrosol, Glucodin, Glucolin, Glucose, Goldsugar, Grape sugar, Meritose, Staleydex 111, Staleydex 95M, Tabfine 097(HS), Vadex			
	D-Glucose	(+)-Galactose, 5abp,	HMDB00122	C00031	Monosaccharides
	D-Galactose	8abp, alpha D-	HMDB00143	C00984	Monosaccharides
	D-Galactose	Galactose, alpha-D-	HMDB00143	C00984	Monosaccharides
	D-Mannose	Galactopyranose,	HMDB00169	C00159	Monosaccharides
	Beta-D-Glucose	alpha-D-Galactose,	HMDB00516	C00221	Monosaccharides
	D-Fructose	D-(+)-Galactose, D-	HMDB00660	C02336	Monosaccharides
	D-Fructose	Galactose, D-	HMDB00660	C02336	Monosaccharides
	L-Sorbose	Hexose, GAL,	HMDB01266	C08356	Monosaccharides
	Alpha-D-Glucose	Galactose,	HMDB03345	C00267	Monosaccharides
	D-Tagatose	Galactose (NF),	HMDB03418	C00795	Monosaccharides
	Beta-D-Galactose	GLA, GLC, Hexose	HMDB03449	C00962	Monosaccharides
	L-Gulose	(+)-Galactose, 5abp,	HMDB12326	C15923	Monosaccharides
	L-Gulose	8abp, alpha D-	HMDB12326	C15923	Monosaccharides
	L-Galactose	Galactose, alpha-D-	HMDB33704	C01825	Monosaccharides
	D-Glucose	Galactopyranose,	HMDB00122	C00031	Monosaccharides
	D-Galactose	alpha-D-Galactose,	HMDB00143	C00984	Monosaccharides
	D-Mannose	D-(+)-Galactose, D-	HMDB00169	C00159	Monosaccharides
	Beta-D-Glucose	Galactose, D-	HMDB00516	C00221	Monosaccharides
	D-Fructose	Hexose, GAL,	HMDB00660	C02336	Monosaccharides
	Alpha-D-Glucose	Galactose,	HMDB03345	C00267	Monosaccharides
	D-Tagatose	Galactose, alpha-D-	HMDB03418	C00795	Monosaccharides
	Beta-D-Galactose	Galactopyranose,	HMDB03449	C00962	Monosaccharides
H1	L-Gulose	alpha-D-Galactose,	HMDB12326	C15923	Monosaccharides

Supplement table 1

His	L-Histidine L-Histidine	alanine, (S)-2-Amino-3-(4-imidazolyl)propionate, (S)-4-(2-Amino-2-carboxyethyl)imidazole, (S)-alpha-Amino-1H-imidazole-4-propanoate, (S)-alpha-Amino-1H-imidazole-4-propanoic acid, (S)-alpha-Amino-1H-imidazole-4-propanoate, (S)-alpha-Amino-1H-imidazole-4-propanoic acid, (S)-alpha-Amino-1H-imidazole-4-propionate, (S)-alpha-Amino-1H-imidazole-4-propionic acid, (S)-Histidine, (S)1H-Imidazole-4-alanine, 3-(1H-Imidazol-4-yl)-L-Alanine, Amino-1H-imidazole-4-propanoate, Amino-1H-imidazole-4-propanoic acid, Amino-4-imidazolepropionate,	HMDB00177 HMDB00177	C00135 C00135	Amino Acids and Derivatives Amino Acids and Derivatives
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Supplement table 1

		ethanamine, 2-(1H-Imidazol-4-yl)ethanamine, 2-(1H-Imidazol-4-yl)ethylamine, 2-(1H-Imidazol-5-yl)ethanamine, 2-(1H-Imidazol-5-yl)ethylamine, 2-(4-Imidazolyl)ethanamine, 2-(4-Imidazolyl)ethylamine, 2-Imidazol-4-yl-Ethylamine, 2-Imidazol-4-ylethylamine, 4-(2-Aminoethyl)-1H-imidazole, 4-(2-Aminoethyl)imidazole, 4-Imidazoleethylamine, 5-Imidazoleethylamine, b-Imidazolyl-4-ethylamine, beta-Aminoethylglyoxaline, beta-Aminoethylimidazole, beta-Aminoethylglyoxaline, beta-Imidazolyl-4-ethylamine, Eramin,			
	Histamine	Aminothethylglyoxaline, beta-Imidazolyl-4-ethylamine, Eramin,	HMDB00870	C00388	Azoles
	Histamine		HMDB00870	C00388	Azoles
Histamine	Histamine		HMDB00870	C00388	Azoles

Supplement table 1

Ile	L-Isoleucine L-Isoleucine Allo-L-Isoleucine	(2S, 3S)-2-amino-3-m	HMDB00172 HMDB00172 HMDB00557	C00407 C00407	Amino Acids and Derivatives Amino Acids and Derivatives Amino Acids and Derivatives
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Supplement table 1

Kynurenine	L-Kynurenine L-Kynurenine	diamino-3-hydroxy- gamma-oxo- Benzenebutanoate, (alphaS)-alpha, 2- diamino-3-hydroxy- gamma-oxo- Benzenebutanoic acid, (S)-alpha, 2- diamino-3-hydroxy- gamma-oxo- Benzenebutanoate, (S)-alpha, 2-diamino- 3-hydroxy-gamma- oxo- Benzenebutanoic acid, 3-(3- Hydroxyanthraniloyl)- L-alanine, 3- Anthraniloyl-Alanine, 3-Anthraniloyl-L- alanine, 3- Anthraniloylalanine, 3- Hydroxy-L- kynurenine, alpha, 2- Diamino-gamma-oxo- Benzenebutanoate, alpha, 2-Diamino- gamma-oxo- Benzenebutanoic acid, DL-Kynurenine, DL-Kynureninefree base, Kynurenin,	HMDB00684 HMDB00684	C00328 C00328	Amino Acids and Derivatives Amino Acids and Derivatives
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Supplement table 1

		methylpentanoate, (2S)-2-Amino-4-methylpentanoic acid, (S)-(+)-Leucine, (S)-2-Amino-4-methylpentanoate, (S)-2-Amino-4-methylpentanoic acid, (S)-2-Amino-4-methylvalerate, (S)-2-Amino-4-methylvaleric acid, (S)-Leucine, 4-Methyl-L-Norvaline, L-(+)-Leucine, L-alpha-Aminoisocaproate, L-alpha-Aminoisocaproic acid, L-alpha-Aminoisocaproate, L-alpha-Aminoisocaproic acid, Leu, Leucine			
	L-Leucine	beta-Leucine, L-beta-Leucine	HMDB00687	C00123	Amino Acids and Derivatives
	beta-Leucine		HMDB03640	C02486	Amino Acids and Derivatives
	D-beta-Leucine	beta-2-Amino-4-	HMDB03640	C02486	Amino Acids and Derivatives
	L-beta-Leucine	methylvaleric acid,	HMDB03640	C02486	Amino Acids and Derivatives
	D-Leucine	beta-Leucine, L-beta-	HMDB13773	C01570	Amino Acids and Derivatives
	L-Leucine	Leucine	HMDB00687	C00123	Amino Acids and Derivatives
	D-beta-Leucine	beta-2-Amino-4-	HMDB03640	C02486	Amino Acids and Derivatives
Leu	L-beta-Leucine	methylvaleric acid,	HMDB03640	C02486	Amino Acids and Derivatives

Supplement table 1

		diamino-Hexanoate, (S)-2, 6-diamino- Hexanoic acid, (S)-2, 6-Diaminohexanoate, (S)-2, 6- Diaminohexanoic acid, (S)-a, e- Diaminocaproate, (S)- a, e-Diaminocaproic acid, (S)-Lysine, 2, 6- Diaminohexanoate, 2, 6- Diaminohexanoic acid, 6-Amino- Aminutrin, 6-Amino-L- Norleucine, a-Lysine, alpha-Lysine, Aminutrin, h-Lys-oh, L-(+)-Lysine, L-2, 6- Diaminohexanoate, L- 2, 6-Diaminohexanoic acid, L-2, 6- Diaminocaproate, L- 2, 6-Diaminocaproic acid, L-Lys, Lys, Lysine, Lysine acid D-2, 6- Diaminohexanoate, D-2, 6- Diaminohexanoic acid			
Lys	L-Lysine	(+)-S-Lysine, (S)-2, 6-	HMDB00182	C00047	Amino Acids and Derivatives
	D-Lysine	Diaminohexanoic	HMDB03405	C00739	Amino Acids and Derivatives
	L-Lysine	acid	HMDB00182	C00047	Amino Acids and Derivatives
	D-Lysine	(+)-S-Lysine, (S)-2, 6-	HMDB03405	C00739	Amino Acids and Derivatives

Supplement table 1

Met	L-Methionine L-Methionine	(2S)-2-amino-4-(meth	HMDB00696 HMDB00696	C00073 C00073	Amino Acids and Derivatives Amino Acids and Derivatives
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Supplement table 1

Met-SO	L-Methionine sulfoxide L-Methionine sulfoxide	2-Amino-4-(methylsulfinyl)-Butanoate, 2-Amino-4-(methylsulfinyl)-Butanoic acid, alpha-Amino-gamma-(methylsulfinyl)-Butyric acid, DL-Methionine sulfoxide, L-Methionine (S)-S-oxide, L-Methionine R-oxide, L-Methionine sulfoxide, Met-SO, S-Oxide-methionine 2-Amino-4-(methylsulfinyl)-Butanoate, 2-Amino-4-(methylsulfinyl)-Butanoic acid, alpha-Amino-gamma-(methylsulfinyl)-Butyric acid, DL-Methionine sulfoxide, L-Methionine (S)-S-oxide, L-Methionine R-oxide, L-Methionine sulfoxide, Met-SO, S-Oxide-methionine	HMDB02005 HMDB02005	Amino Acids and Derivatives Amino Acids and Derivatives
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Supplement table 1

Nitro-Tyr	3-Nitrotyrosine 3-Nitrotyrosine	3-Nitrotyrosine, 5- Nitrotyrosine, m- Nitrotyrosine 3-Nitrotyrosine, 5- Nitrotyrosine, m- Nitrotyrosine	HMDB01904 HMDB01904		Amino Acids and Derivatives Amino Acids and Derivatives
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Supplement table 1

		pyrrolidinecarboxylic acid, (2S, 4R)-4-hydroxypyrrolidine-2-carboxylic acid, (4R)-4-hydroxy-L-proline, 4-Hydroxy-2-pyrrolidinecarboxylic acid, 4-Hydroxy-L-proline, 4-L-Hydroxyproline, delta-Hydroxyproline, Hydroxiproline, Hydroxy-L-proline, Hydroxy-proline, Hydroxyproline, L-4-Hydroxyproline, L-Hydroxyproline, L-Threo-4-hydroxyproline, LS-hydroxyproline, Oxaceprol, trans-4-Hydroxy-L-proline, trans-4-			
	4-Hydroxyproline	trans-4-			
	3-Hydroxy-L-proline	Hydroxyproline,			
	4-Hydroxy-L-proline	Trans-	HMDB00725	C01157	Amino Acids and Derivatives
	cis-4-Hydroxy-L-proline	hydroxyproline,	HMDB02113	C04397	Amino Acids and Derivatives
	4-Hydroxy-L-proline	Trans-L-	HMDB06055	C01015	Amino Acids and Derivatives
	4-Hydroxy-L-proline	hydroxyproline	HMDB06055	C01015	Amino Acids and Derivatives
	4-Hydroxyproline	Procollagen trans-3-	HMDB00725	C01157	Amino Acids and Derivatives
	3-Hydroxy-L-proline	hydroxy-L-proline	HMDB00725	C01157	Amino Acids and Derivatives
	cis-4-Hydroxy-L-proline	(2S)-4-	HMDB02113	C04397	Amino Acids and Derivatives
OH-Pro		hydroxypyrrolidine-2-	HMDB06055	C01015	Amino Acids and Derivatives

Supplement table 1

		2, 5-Diaminopentanoate, (S)-2, 5-Diaminopentanoic acid, (S)-a, D-Diaminovalerate, (S)-a, D-Diaminovaleric acid, (S)-Ornithine, 5-Amino-L-Norvaline, L-(-)-Ornithine, L-Ornithine (+)-S-Ornithine, (S)-2, 5-Diaminopentanoate, (S)-2, 5-Diaminopentanoic acid, (S)-a, D-Diaminovalerate, (S)-a, D-Diaminovaleric acid, (S)-Ornithine, 5-Amino-L-Norvaline, L-(-)-Ornithine, L-Ornithine (2R)-2, 5-diaminopentanoate, (2R)-2, 5-diaminopentanoic acid, (R)-ornithine, Ornithine (+)-S-Ornithine, (S)-2, 5-Diaminopentanoate,			
Orn	Ornithine L-Ornithine D-Ornithine L-Ornithine D-Ornithine		HMDB00214 HMDB00214 HMDB03374 HMDB00214 HMDB03374	C00077 C00077 C00515 C00077 C00515	Amino Acids and Derivatives Amino Acids and Derivatives Amino Acids and Derivatives Amino Acids and Derivatives Amino Acids and Derivatives
PC aa C26:0	PC aa C26:0				
PC aa C28:1	PC aa C28:1				

Supplement table 1

		<p>palmitoyl-sn-glycero-3-phosphocholine, GPCho(14:0/16:0), GPCho(30:0), Lecithin, PC aa C30:0, PC(14:0/16:0), PC(30:0), Phosphatidylcholine(14:0/16:0), Phosphatidylcholine(30:0)</p> <p>1, 2-Dipentadecanoyl-rac-glycero-3-phosphocholine, GPCho(15:0/15:0), GPCho(30:0), Lecithin, PC aa C30:0, PC(15:0/15:0), PC(30:0), Phosphatidylcholine(15:0/15:0), Phosphatidylcholine(30:0)</p> <p>1-Palmitoyl-2-myristoyl-sn-glycero-3-phosphocholine, GPCho(16:0/14:0), GPCho(30:0), Lecithin, PC aa C30:0,</p>			
	PC(14:0/16:0)		HMDB07869	C00157	Glycerophospholipids
	PC(15:0/15:0)		HMDB07934	C00157	Glycerophospholipids
	PC(16:0/14:0)		HMDB07965	C00157	Glycerophospholipids
	PC(14:0/16:0)		HMDB07869	C00157	Glycerophospholipids
	PC(15:0/15:0)		HMDB07934	C00157	Glycerophospholipids
PC aa C30:0	PC(16:0/14:0)		HMDB07965	C00157	Glycerophospholipids
PC aa C30:2	PC aa C30:2				

Supplement table 1

	PC(16:0/16:0)		HMDB00564	C00157	Glycerophospholipids
	PC(14:0/18:0)		HMDB07871	C00157	Glycerophospholipids
	PC(18:0/14:0)		HMDB08031	C00157	Glycerophospholipids
	PC(16:0/16:0)		HMDB00564	C00157	Glycerophospholipids
	PC(14:0/18:0)		HMDB07871	C00157	Glycerophospholipids
PC aa C32:0	PC(18:0/14:0)	(R)-4-hydroxy-N, N, N	HMDB08031	C00157	Glycerophospholipids

Supplement table 1

		vaccenoyl-sn-glycero-3-phosphocholine, GPCho(14:0/18:1), GPCho(14:0/18:1n7), GPCho(14:0/18:1w7), GPCho(32:1), Lecithin, PC aa C32:1, PC(14:0/18:1), PC(14:0/18:1n7), PC(14:0/18:1w7), PC(32:1), Phosphatidylcholine(14:0/18:1), Phosphatidylcholine(14:0/18:1n7), Phosphatidylcholine(14:0/18:1w7), Phosphatidylcholine(32:1)			
	PC(14:0/18:1(11Z))	1-Myristoyl-2-oleoyl-sn-glycero-3-phosphocholine, GPCho(14:0/18:1), GPCho(14:0/18:1n9),	HMDB07872	C00157	Glycerophospholipids
	PC(14:0/18:1(9Z))	GPCho(14:0/18:1w9),	HMDB07873	C00157	Glycerophospholipids
	PC(16:0/16:1(9Z))	, GPCho(32:1),	HMDB07969	C00157	Glycerophospholipids
	PC(18:1(9Z)/14:0)	Lecithin, PC aa	HMDB08097	C00157	Glycerophospholipids
	PC(14:0/18:1(11Z))	C32:1,	HMDB07872	C00157	Glycerophospholipids
	PC(14:0/18:1(9Z))	PC(14:0/18:1),	HMDB07873	C00157	Glycerophospholipids
	PC(16:0/16:1(9Z))	PC(14:0/18:1n9),	HMDB07969	C00157	Glycerophospholipids
PC aa C32:1	PC(18:1(9Z)/14:0)	PC(14:0/18:1w9),	HMDB08097	C00157	Glycerophospholipids

Supplement table 1

		linoleoyl-sn-glycero-3-phosphocholine, GPCho(14:0/18:2), GPCho(14:0/18:2n6), GPCho(14:0/18:2w6), GPCho(32:2), Lecithin, PC aa C32:2, PC(14:0/18:2), PC(14:0/18:2n6), PC(14:0/18:2w6), PC(32:2), Phosphatidylcholine(14:0/18:2), Phosphatidylcholine(14:0/18:2n6), Phosphatidylcholine(14:0/18:2w6), Phosphatidylcholine(32:2)			
	PC(14:0/18:2(9Z,12Z))	GPCho(16:1n7/16:1n7),			
	PC(16:1(9Z)/16:1(9Z))	GPCho(16:1w7/16:1w7), GPCho(32:2),			
	PC(14:0/18:2(9Z,12Z))	Lecithin, PC aa C32:2,	HMDB07874	C00157	Glycerophospholipids
	PC(16:1(9Z)/16:1(9Z))	PC(16:1/16:1),	HMDB08002	C00157	Glycerophospholipids
PC aa C32:2		PC(16:1n7/16:1n7),	HMDB07874	C00157	Glycerophospholipids
			HMDB08002	C00157	Glycerophospholipids

Supplement table 1

PC aa C32:3	PC(14:0/18:3(9Z,12Z,15Z)) PC(14:0/18:3(9Z,12Z,15Z))	linolenoyl-sn-glycero-3-phosphocholine, 1-Myristoyl-2-alpha-linolenoyl-sn-glycero-3-phosphocholine, GPCho(14:0/18:3), GPCho(14:0/18:3n3), GPCho(14:0/18:3w3), GPCho(32:3), Lecithin, PC aa C32:3, PC(14:0/18:3), PC(14:0/18:3n3), PC(14:0/18:3w3), PC(32:3), Phosphatidylcholine(14:0/18:3), Phosphatidylcholine(14:0/18:3n3), Phosphatidylcholine(14:0/18:3w3), Phosphatidylcholine(32:3) 1-Myristoyl-2-alpha-linolenoyl-sn-glycero-3-phosphocholine, 1-Myristoyl-2-alpha-linolenoyl-sn-glycero-3-phosphocholine, GPCho(14:0/18:3), GPCho(14:0/18:3n3), GPCho(14:0/18:3w3)	HMDB07876 HMDB07876	C00157 C00157	Glycerophospholipids Glycerophospholipids
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Supplement table 1

		vaccenoyl-sn-glycero-3-phosphocholine, GPCho(16:0/18:1), GPCho(16:0/18:1n7), GPCho(16:0/18:1w7), GPCho(34:1), Lecithin, PC aa C34:1, PC(16:0/18:1), PC(16:0/18:1n7), PC(16:0/18:1w7), PC(34:1), Phosphatidylcholine(16:0/18:1), Phosphatidylcholine(16:0/18:1n7), Phosphatidylcholine(16:0/18:1w7), Phosphatidylcholine(34:1)			
	PC(16:0/18:1(11Z))	1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine,	HMDB07971	C00157	Glycerophospholipids
	PC(16:0/18:1(9Z))	GPCho(16:0/18:1),	HMDB07972	C00157	Glycerophospholipids
	PC(16:1(9Z)/18:0)	GPCho(16:0/18:1n9),	HMDB08003	C00157	Glycerophospholipids
	PC(18:0/16:1(9Z))	GPCho(16:0/18:1w9)	HMDB08035	C00157	Glycerophospholipids
	PC(18:1(9Z)/16:0)	, GPCho(34:1),	HMDB08100	C00157	Glycerophospholipids
	PC(16:0/18:1(11Z))	Lecithin, PC aa	HMDB07971	C00157	Glycerophospholipids
	PC(16:0/18:1(9Z))	C34:1,	HMDB07972	C00157	Glycerophospholipids
	PC(16:1(9Z)/18:0)	PC(16:0/18:1),	HMDB08003	C00157	Glycerophospholipids
	PC(18:0/16:1(9Z))	PC(16:0/18:1n9),	HMDB08035	C00157	Glycerophospholipids
PC aa C34:1	PC(18:1(9Z)/16:0)	PC(16:0/18:1w9),	HMDB08100	C00157	Glycerophospholipids

Supplement table 1

		linoleoyl-sn-glycero-3-phosphocholine, GPCho(16:0/18:2), GPCho(16:0/18:2n6), GPCho(16:0/18:2w6), GPCho(34:2), Lecithin, PC aa C34:2, PC(16:0/18:2), PC(16:0/18:2n6), PC(16:0/18:2w6), PC(34:2),			
	PC(16:0/18:2(9Z,12Z))	Phosphatidylcholine(16:0/18:2),			
	PC(16:1(9Z)/18:1(11Z))	Phosphatidylcholine(16:0/18:2n6),			
	PC(16:1(9Z)/18:1(9Z))	Phosphatidylcholine(16:0/18:2w6),			
	PC(18:1(9Z)/16:1(9Z))	Phosphatidylcholine(34:2)			
	PC(18:2(9Z,12Z)/16:0)	1-Palmitoleoyl-2-vaccenoyl-sn-glycero-			
	PC(16:0/18:2(9Z,12Z))	3-phosphocholine, HMDB07973		C00157	Glycerophospholipids
		GPCho(16:1/18:1), HMDB08004		C00157	Glycerophospholipids
	PC(16:1(9Z)/18:1(11Z))	GPCho(16:1n7/18:1n7), HMDB08005		C00157	Glycerophospholipids
		7), HMDB08101		C00157	Glycerophospholipids
	PC(16:1(9Z)/18:1(9Z))	GPCho(16:1w7/18:1w7), GPCho(34:2), HMDB08133		C00157	Glycerophospholipids
		HMDB07973		C00157	Glycerophospholipids
	PC(18:1(9Z)/16:1(9Z))	Lecithin, PC aa C34:2, HMDB08004		C00157	Glycerophospholipids
		HMDB08005		C00157	Glycerophospholipids
	PC(18:2(9Z,12Z)/16:0)	PC(16:1/18:1), HMDB08101		C00157	Glycerophospholipids
PC aa C34:2		PC(16:1n7/18:1n7), HMDB08133		C00157	Glycerophospholipids

Supplement table 1

		linolenoyl-sn-glycero-3-phosphocholine, 1-Palmitoyl-2-gamma-linolenoyl-sn-glycero-3-phosphocholine, GPCho(16:0/18:3), GPCho(16:0/18:3n6), GPCho(16:0/18:3w6), GPCho(34:3), Lecithin, PC aa C34:3, PC(16:0/18:3), PC(16:0/18:3n6), PC(16:0/18:3w6), PC(34:3), Phosphatidylcholine(16:0/18:3), Phosphatidylcholine(16:0/18:3n6), Phosphatidylcholine(16:0/18:3w6), Phosphatidylcholine(34:3)			
	PC(16:0/18:3(6Z,9Z,12Z))	1-Palmitoyl-2-alpha-linolenoyl-sn-glycero-3-phosphocholine, 1-Palmitoyl-2-alpha-linolenoyl-sn-glycero-3-phosphocholine,	HMDB07974	C00157	Glycerophospholipids
	PC(16:0/18:3(9Z,12Z,15Z))	GPCho(16:0/18:3), GPCho(16:0/18:3n3), GPCho(16:0/18:3w3)	HMDB07975	C00157	Glycerophospholipids
	PC(16:1(9Z)/18:2(9Z,12Z))		HMDB08006	C00157	Glycerophospholipids
	PC(16:0/18:3(6Z,9Z,12Z))		HMDB07974	C00157	Glycerophospholipids
	PC(16:0/18:3(9Z,12Z,15Z))		HMDB07975	C00157	Glycerophospholipids
PC aa C34:3	PC(16:1(9Z)/18:2(9Z,12Z))		HMDB08006	C00157	Glycerophospholipids

Supplement table 1

PC aa C34:4	<p>PC(14:0/20:4(5Z,8Z,11Z,14Z))</p> <p>PC(16:0/18:4(6Z,9Z,12Z,15Z))</p> <p>PC(14:0/20:4(5Z,8Z,11Z,14Z))</p> <p>PC(16:0/18:4(6Z,9Z,12Z,15Z))</p>	<p>arachidonoyl-sn-glycero-3-phosphocholine, GPCho(14:0/20:4), GPCho(14:0/20:4n6), GPCho(14:0/20:4w6), GPCho(34:4), Lecithin, PC aa C34:4, PC(14:0/20:4), PC(14:0/20:4n6), PC(14:0/20:4w6), PC(34:4), Phosphatidylcholine(14:0/20:4), Phosphatidylcholine(14:0/20:4n6), Phosphatidylcholine(14:0/20:4w6), Phosphatidylcholine(34:4)</p> <p>1-Palmitoyl-2-stearidonoyl-sn-glycero-3-phosphocholine, GPCho(16:0/18:4), GPCho(16:0/18:4n3), GPCho(16:0/18:4w3), GPCho(34:4), Lecithin, PC aa C34:4, PC(16:0/18:4),</p>	<p>HMDB07883</p> <p>HMDB07976</p> <p>HMDB07883</p> <p>HMDB07976</p>	<p>C00157</p> <p>C00157</p> <p>C00157</p> <p>C00157</p>	<p>Glycerophospholipids</p> <p>Glycerophospholipids</p> <p>Glycerophospholipids</p> <p>Glycerophospholipids</p>
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Supplement table 1

		behenoyl-sn-glycero-3-phosphocholine, GPCho(14:0/22:0), GPCho(36:0), Lecithin, PC aa C36:0, PC(14:0/22:0), PC(36:0), Phosphatidylcholine(14:0/22:0), Phosphatidylcholine(36:0)			
		1-Palmitoyl-2-arachidonyl-sn-glycero-3-phosphocholine, GPCho(16:0/20:0), GPCho(36:0), Lecithin, PC aa C36:0, PC(16:0/20:0), PC(36:0),			
	PC(14:0/22:0)	Phosphatidylcholine(HMDB07886	C00157	Glycerophospholipids
	PC(16:0/20:0)	16:0/20:0),	HMDB07977	C00157	Glycerophospholipids
	PC(18:0/18:0)	Phosphatidylcholine(HMDB08036	C00157	Glycerophospholipids
	PC(20:0/16:0)	36:0)	HMDB08265	C00157	Glycerophospholipids
	PC(22:0/14:0)	1, 2-Distearoyl-rac-	HMDB08525	C00157	Glycerophospholipids
	PC(14:0/22:0)	glycero-3-	HMDB07886	C00157	Glycerophospholipids
	PC(16:0/20:0)	phosphocholine,	HMDB07977	C00157	Glycerophospholipids
	PC(18:0/18:0)	GPCho(18:0/18:0),	HMDB08036	C00157	Glycerophospholipids
	PC(20:0/16:0)	GPCho(36:0),	HMDB08265	C00157	Glycerophospholipids
PC aa C36:0	PC(22:0/14:0)	Lecithin, PC aa	HMDB08525	C00157	Glycerophospholipids

Supplement table 1

		vaccenoyl-sn-glycero-3-phosphocholine, GPCho(18:0/18:1), GPCho(18:0/18:1n7), GPCho(18:0/18:1w7), GPCho(36:1), Lecithin, PC aa C36:1, PC(18:0/18:1), PC(18:0/18:1n7), PC(18:0/18:1w7), PC(36:1), Phosphatidylcholine(18:0/18:1), Phosphatidylcholine(18:0/18:1n7), Phosphatidylcholine(18:0/18:1w7), Phosphatidylcholine(36:1)			
	PC(18:0/18:1(11Z))	1-Stearoyl-2-oleoyl-sn-glycero-3-phosphocholine, GPCho(18:0/18:1), GPCho(18:0/18:1n9),	HMDB08037	C00157	Glycerophospholipids
	PC(18:0/18:1(9Z))	GPCho(18:0/18:1w9),	HMDB08038	C00157	Glycerophospholipids
	PC(18:1(11Z)/18:0)	, GPCho(36:1),	HMDB08069	C00157	Glycerophospholipids
	PC(18:1(9Z)/18:0)	Lecithin, PC aa	HMDB08102	C00157	Glycerophospholipids
	PC(18:0/18:1(11Z))	C36:1,	HMDB08037	C00157	Glycerophospholipids
	PC(18:0/18:1(9Z))	PC(18:0/18:1),	HMDB08038	C00157	Glycerophospholipids
	PC(18:1(11Z)/18:0)	PC(18:0/18:1n9),	HMDB08069	C00157	Glycerophospholipids
PC aa C36:1	PC(18:1(9Z)/18:0)	PC(18:0/18:1w9),	HMDB08102	C00157	Glycerophospholipids

Supplement table 1

		sn-glycero-3-phosphocholine, GPCho(18:0/18:2), GPCho(18:0/18:2n6), GPCho(18:0/18:2w6), GPCho(36:2), Lecithin, PC aa C36:2, PC(18:0/18:2), PC(18:0/18:2n6), PC(18:0/18:2w6), PC(36:2), Phosphatidylcholine(18:0/18:2), Phosphatidylcholine(18:0/18:2n6), Phosphatidylcholine(18:0/18:2w6), Phosphatidylcholine(36:2))			
	PC(18:0/18:2(9Z,12Z))	1, 2-Divaccenoyl-rac-glycero-3-phosphocholine,			
	PC(18:1(11Z)/18:1(1Z))	GPCho(18:1/18:1),			
	PC(18:2(9Z,12Z)/18:0)	GPCho(18:1n7/18:1n7),	HMDB08039	C00157	Glycerophospholipids
	PC(18:1(9Z)/18:1(9Z))	GPCho(18:1w7/18:1w7), GPCho(36:2),	HMDB08070	C00157	Glycerophospholipids
	PC(18:0/18:2(9Z,12Z))	Lecithin, PC aa C36:2,	HMDB08135	C00157	Glycerophospholipids
	PC(18:1(11Z)/18:1(1Z))	PC(18:1/18:1),	HMDB00593	C00157	Glycerophospholipids
	PC(18:2(9Z,12Z)/18:0)	PC(18:1n7/18:1n7),	HMDB08039	C00157	Glycerophospholipids
PC aa C36:2			HMDB08070	C00157	Glycerophospholipids
			HMDB08135	C00157	Glycerophospholipids

Supplement table 1

		meadoyl-sn-glycero-3-phosphocholine, GPCho(16:0/20:3), GPCho(16:0/20:3n9), GPCho(16:0/20:3w9), GPCho(36:3), Lecithin, PC aa C36:3, PC(16:0/20:3), PC(16:0/20:3n9), PC(16:0/20:3w9), PC(36:3), Phosphatidylcholine(16:0/20:3), Phosphatidylcholine(16:0/20:3n9), Phosphatidylcholine(16:0/20:3w9), Phosphatidylcholine(36:3)			
	PC(16:0/20:3(5Z,8Z,11Z))	Phosphatidylcholine(16:0/20:3w9),			
	PC(16:0/20:3(8Z,11Z,14Z))	Phosphatidylcholine(36:3)			
	PC(18:0/18:3(6Z,9Z,12Z))	1-Palmitoyl-2-homog-linolenoyl-sn-glycero-3-phosphocholine, 1-Palmitoyl-2-homogamma-linolenoyl-sn-glycero-3-phosphocholine,	HMDB07980	C00157	Glycerophospholipids
	PC(18:1(9Z)/18:2(9Z,12Z))	phosphocholine, 1-Palmitoyl-2-homogamma-linolenoyl-sn-glycero-3-phosphocholine,	HMDB07981	C00157	Glycerophospholipids
	PC(16:0/20:3(5Z,8Z,11Z))	GPCho(16:0/20:3), GPCho(16:0/20:3n6), GPCho(16:0/20:3w6), GPCho(36:3),	HMDB08040	C00157	Glycerophospholipids
	PC(16:0/20:3(8Z,11Z,14Z))		HMDB08105	C00157	Glycerophospholipids
	PC(18:0/18:3(6Z,9Z,12Z))		HMDB07980	C00157	Glycerophospholipids
	PC(18:1(9Z)/18:2(9Z,12Z))		HMDB07981	C00157	Glycerophospholipids
PC aa C36:3			HMDB08040	C00157	Glycerophospholipids
			HMDB08105	C00157	Glycerophospholipids

Supplement table 1

PC aa C36:4	PC(16:0/20:4(5Z,8Z,11Z,14Z))	arachidonoyl-sn-glycero-3-phosphocholine,			
	PC(18:0/18:4(6Z,9Z,12Z,15Z))	GPCho(16:0/20:4),			
	PC(18:1(9Z)/18:3(6Z,9Z,12Z))	GPCho(16:0/20:4n6),			
	PC(18:1(9Z)/18:3(9Z,12Z,15Z))	GPCho(16:0/20:4w6),			
	PC(18:2(9Z,12Z)/18:2(9Z,12Z))	, GPCho(36:4),			
	PC(18:3(6Z,9Z,12Z)/18:1(9Z))	Lecithin, PC aa			
	PC(18:3(9Z,12Z,15Z)/18:1(9Z))	C36:4,			
	PC(20:4(5Z,8Z,11Z,14Z)/16:0)	PC(16:0/20:4),			
	PC(16:0/20:4(5Z,8Z,11Z,14Z))	PC(16:0/20:4n6),	HMDB07982	C00157	Glycerophospholipids
	PC(18:0/18:4(6Z,9Z,12Z,15Z))	PC(16:0/20:4w6),	HMDB08042	C00157	Glycerophospholipids
	PC(18:1(9Z)/18:3(6Z,9Z,12Z))	Phosphatidylcholine(16:0/20:4),	HMDB08106	C00157	Glycerophospholipids
	PC(18:1(9Z)/18:3(6Z,9Z,12Z))	Phosphatidylcholine(16:0/20:4n6),	HMDB08107	C00157	Glycerophospholipids
	PC(18:1(9Z)/18:3(9Z,12Z,15Z))	Phosphatidylcholine(16:0/20:4w6),	HMDB08138	C00157	Glycerophospholipids
	PC(18:1(9Z)/18:3(9Z,12Z,15Z))	36:4)	HMDB08170	C00157	Glycerophospholipids
	PC(18:1(9Z)/18:3(9Z,12Z,15Z))	1-Stearoyl-2-stearidonoyl-sn-glycero-3-phosphocholine,	HMDB08203	C00157	Glycerophospholipids
	PC(18:2(9Z,12Z)/18:2(9Z,12Z))	GPCho(18:0/18:4),	HMDB08429	C00157	Glycerophospholipids
	PC(18:3(6Z,9Z,12Z)/18:1(9Z))	GPCho(18:0/18:4n3),	HMDB07982	C00157	Glycerophospholipids
PC(18:3(9Z,12Z,15Z)/18:1(9Z))	GPCho(18:0/18:4w3),	HMDB08042	C00157	Glycerophospholipids	
PC(20:4(5Z,8Z,11Z,14Z)/16:0)	GPCho(18:0/18:4w3),	HMDB08106	C00157	Glycerophospholipids	
	, GPCho(36:4),	HMDB08107	C00157	Glycerophospholipids	
	Lecithin, PC aa	HMDB08138	C00157	Glycerophospholipids	
	C36:4,	HMDB08170	C00157	Glycerophospholipids	
	PC(18:0/18:4),	HMDB08203	C00157	Glycerophospholipids	
		HMDB08429	C00157	Glycerophospholipids	

Supplement table 1

		eicosapentaenoyl-sn-glycero-3-phosphocholine, GPCho(16:0/20:5), GPCho(16:0/20:5n3), GPCho(16:0/20:5w3), GPCho(36:5), Lecithin, PC aa C36:5, PC(16:0/20:5), PC(16:0/20:5n3), PC(16:0/20:5w3), PC(36:5), Phosphatidylcholine(16:0/20:5), Phosphatidylcholine(16:0/20:5n3), Phosphatidylcholine(16:0/20:5w3), Phosphatidylcholine(36:5)			
	PC(16:0/20:5(5Z,8Z,11Z,14Z,17Z))	1-Palmitoleoyl-2-arachidonoyl-sn-glycero-3-phosphocholine, GPCho(16:1/20:4),			
	PC(16:1(9Z)/20:4(5Z,8Z,11Z,14Z))	GPCho(16:1n7/20:4n6),			
	PC(16:0/20:5(5Z,8Z,11Z,14Z,17Z))	GPCho(16:1w7/20:4w6), GPCho(36:5),	HMDB07984	C00157	Glycerophospholipids
	PC(16:1(9Z)/20:4(5Z,8Z,11Z,14Z))	Lecithin, PC aa C36:5,	HMDB08015	C00157	Glycerophospholipids
PC aa C36:5			HMDB07984	C00157	Glycerophospholipids
			HMDB08015	C00157	Glycerophospholipids

Supplement table 1

PC aa C36:6	<p>PC(14:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))</p> <p>PC(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))</p> <p>PC(14:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))</p> <p>PC(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))</p>	<p>docosahexaenoyl-sn-glycero-3-phosphocholine, GPCho(14:0/22:6), GPCho(14:0/22:6n3), GPCho(14:0/22:6w3), GPCho(36:6), Lecithin, PC aa C36:6, PC(14:0/22:6), PC(14:0/22:6n3), PC(14:0/22:6w3), PC(36:6), Phosphatidylcholine(14:0/22:6), Phosphatidylcholine(14:0/22:6n3), Phosphatidylcholine(14:0/22:6w3), Phosphatidylcholine(36:6)</p> <p>1, 2-Dia-linolenoyl-rac-glycero-3-phosphocholine, GPCho(18:3/18:3), GPCho(18:3n3/18:3n3), GPCho(18:3w3/18:3w3), GPCho(36:6), Lecithin, PC aa C36:6, PC(18:3/18:3),</p>	<p>HMDB07892</p> <p>HMDB08206</p> <p>HMDB07892</p> <p>HMDB08206</p>	<p>C00157</p> <p>C00157</p> <p>C00157</p> <p>C00157</p>	<p>Glycerophospholipids</p> <p>Glycerophospholipids</p> <p>Glycerophospholipids</p> <p>Glycerophospholipids</p>
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Supplement table 1

		lignoceroyl-sn-glycero-3-phosphocholine, GPCho(14:0/24:0), GPCho(38:0), Lecithin, PC aa C38:0, PC(14:0/24:0), PC(38:0), Phosphatidylcholine(14:0/24:0), Phosphatidylcholine(38:0)			
		1-Palmitoyl-2-behenoyl-sn-glycero-3-phosphocholine, GPCho(16:0/22:0), GPCho(38:0), Lecithin, PC aa C38:0,			
	PC(14:0/24:0)	PC(16:0/22:0),	HMDB07893	C00157	Glycerophospholipids
	PC(16:0/22:0)	PC(38:0),	HMDB07985	C00157	Glycerophospholipids
	PC(18:0/20:0)	Phosphatidylcholine(HMDB08043	C00157	Glycerophospholipids
	PC(20:0/18:0)	16:0/22:0),	HMDB08267	C00157	Glycerophospholipids
	PC(22:0/16:0)	Phosphatidylcholine(HMDB08528	C00157	Glycerophospholipids
	PC(24:0/14:0)	38:0)	HMDB08755	C00157	Glycerophospholipids
	PC(14:0/24:0)	1-Stearoyl-2-	HMDB07893	C00157	Glycerophospholipids
	PC(16:0/22:0)	arachidonyl-sn-	HMDB07985	C00157	Glycerophospholipids
	PC(18:0/20:0)	glycero-3-	HMDB08043	C00157	Glycerophospholipids
	PC(20:0/18:0)	phosphocholine,	HMDB08267	C00157	Glycerophospholipids
	PC(22:0/16:0)	GPCho(18:0/20:0),	HMDB08528	C00157	Glycerophospholipids
PC aa C38:0	PC(24:0/14:0)	GPCho(38:0),	HMDB08755	C00157	Glycerophospholipids

Supplement table 1

		nervonoyl-sn-glycero-3-phosphocholine, GPCho(14:0/24:1), GPCho(14:0/24:1n9), GPCho(14:0/24:1w9), GPCho(38:1), Lecithin, PC aa C38:1, PC(14:0/24:1), PC(14:0/24:1n9), PC(14:0/24:1w9), PC(38:1), Phosphatidylcholine(14:0/24:1), Phosphatidylcholine(14:0/24:1n9), Phosphatidylcholine(14:0/24:1w9), Phosphatidylcholine(38:1)			
	PC(14:0/24:1(15Z))	1-Palmitoyl-2-erucoyl-	HMDB07894	C00157	Glycerophospholipids
	PC(16:0/22:1(13Z))	sn-glycero-3-	HMDB07986	C00157	Glycerophospholipids
	PC(18:0/20:1(11Z))	phosphocholine,	HMDB08044	C00157	Glycerophospholipids
	PC(18:1(9Z)/20:0)	GPCho(16:0/22:1),	HMDB08109	C00157	Glycerophospholipids
	PC(20:0/18:1(11Z))	GPCho(16:0/22:1n9),	HMDB08268	C00157	Glycerophospholipids
	PC(20:0/18:1(9Z))	GPCho(16:0/22:1w9)	HMDB08269	C00157	Glycerophospholipids
	PC(14:0/24:1(15Z))	, GPCho(38:1),	HMDB07894	C00157	Glycerophospholipids
	PC(16:0/22:1(13Z))	Lecithin, PC aa	HMDB07986	C00157	Glycerophospholipids
	PC(18:0/20:1(11Z))	C38:1,	HMDB08044	C00157	Glycerophospholipids
	PC(18:1(9Z)/20:0)	PC(16:0/22:1),	HMDB08109	C00157	Glycerophospholipids
	PC(20:0/18:1(11Z))	PC(16:0/22:1n9),	HMDB08268	C00157	Glycerophospholipids
PC aa C38:1	PC(20:0/18:1(9Z))	PC(16:0/22:1w9),	HMDB08269	C00157	Glycerophospholipids

Supplement table 1

PC aa C38:3	<p>PC(18:0/20:3(5Z,8Z,11Z))</p> <p>PC(18:0/20:3(8Z,11Z,14Z))</p> <p>PC(18:0/20:3(5Z,8Z,11Z))</p> <p>PC(18:0/20:3(8Z,11Z,14Z))</p>	<p>sn-glycero-3-phosphocholine, GPCho(18:0/20:3), GPCho(18:0/20:3n9), GPCho(18:0/20:3w9), GPCho(38:3), Lecithin, PC aa C38:3, PC(18:0/20:3), PC(18:0/20:3n9), PC(18:0/20:3w9), PC(38:3), Phosphatidylcholine(18:0/20:3), Phosphatidylcholine(18:0/20:3n9), Phosphatidylcholine(18:0/20:3w9), Phosphatidylcholine(38:3)</p> <p>1-Stearoyl-2-homo-g-linolenoyl-sn-glycero-3-phosphocholine, 1-Stearoyl-2-homo-gamma-linolenoyl-sn-glycero-3-phosphocholine, GPCho(18:0/20:3), GPCho(18:0/20:3n6), GPCho(18:0/20:3w6), GPCho(38:3), Lecithin, PC aa</p>	<p>HMDB08046</p> <p>HMDB08047</p> <p>HMDB08046</p> <p>HMDB08047</p>	<p>C00157</p> <p>C00157</p> <p>C00157</p> <p>C00157</p>	<p>Glycerophospholipids</p> <p>Glycerophospholipids</p> <p>Glycerophospholipids</p> <p>Glycerophospholipids</p>
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Supplement table 1

		adrenoyl-sn-glycero-3-phosphocholine, GPCho(16:0/22:4), GPCho(16:0/22:4n6), GPCho(16:0/22:4w6), GPCho(38:4), Lecithin, PC aa C38:4, PC(16:0/22:4), PC(16:0/22:4n6), PC(16:0/22:4w6), PC(38:4), Phosphatidylcholine(16:0/22:4), Phosphatidylcholine(16:0/22:4n6), Phosphatidylcholine(16:0/22:4w6), Phosphatidylcholine(38:4)			
	PC(16:0/22:4(7Z,10Z,13Z,16Z))	1-Stearoyl-2-arachidonoyl-sn-glycero-3-phosphocholine,			
	PC(18:0/20:4(5Z,8Z,11Z,14Z))	GPCho(18:0/20:4),			
	PC(18:1(9Z)/20:3(5Z,8Z,11Z))	GPCho(18:0/20:4n6),	HMDB07988	C00157	Glycerophospholipids
	PC(16:0/22:4(7Z,10Z,13Z,16Z))	GPCho(18:0/20:4w6), GPCho(38:4),	HMDB08048	C00157	Glycerophospholipids
	PC(18:0/20:4(5Z,8Z,11Z,14Z))	Lecithin, PC aa C38:4,	HMDB08112	C00157	Glycerophospholipids
	PC(18:1(9Z)/20:3(5Z,8Z,11Z))	PC(18:0/20:4),	HMDB07988	C00157	Glycerophospholipids
PC aa C38:4		PC(18:0/20:4n6),	HMDB08048	C00157	Glycerophospholipids
			HMDB08112	C00157	Glycerophospholipids

Supplement table 1

		docosapentaenoyl-sn-glycero-3-phosphocholine, 1-Palmitoyl-2- osbondoyl-sn-glycero-3-phosphocholine, GPCho(16:0/22:5), GPCho(16:0/22:5n6), GPCho(16:0/22:5w6), GPCho(38:5), Lecithin, PC aa C38:5, PC(16:0/22:5), PC(16:0/22:5n6), PC(16:0/22:5w6), PC(38:5), Phosphatidylcholine(16:0/22:5), Phosphatidylcholine(16:0/22:5n6), Phosphatidylcholine(16:0/22:5w6), Phosphatidylcholine(38:5)			
	PC(16:0/22:5(4Z,7Z,10Z,13Z,16Z))				
	PC(16:0/22:5(7Z,10Z,13Z,16Z,19Z))				
	PC(18:0/20:5(5Z,8Z,11Z,14Z,17Z))				
	PC(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))				
	PC(16:0/22:5(4Z,7Z,10Z,13Z,16Z))	1-Palmitoyl-2-	HMDB07989	C00157	Glycerophospholipids
	PC(16:0/22:5(7Z,10Z,13Z,16Z,19Z))	docosapentaenoyl-sn-glycero-3-	HMDB07990	C00157	Glycerophospholipids
	PC(18:0/20:5(5Z,8Z,11Z,14Z,17Z))	phosphocholine,	HMDB08050	C00157	Glycerophospholipids
	PC(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))	GPCho(16:0/22:5),	HMDB08114	C00157	Glycerophospholipids
		GPCho(16:0/22:5n3),	HMDB07989	C00157	Glycerophospholipids
		GPCho(16:0/22:5w3),	HMDB07990	C00157	Glycerophospholipids
		, GPCho(38:5),	HMDB08050	C00157	Glycerophospholipids
PC aa C38:5			HMDB08114	C00157	Glycerophospholipids

Supplement table 1

		docosahexaenoyl-sn-glycero-3-phosphocholine, GPCho(16:0/22:6), GPCho(16:0/22:6n3), GPCho(16:0/22:6w3), GPCho(38:6), Lecithin, PC aa C38:6, PC(16:0/22:6), PC(16:0/22:6n3), PC(16:0/22:6w3), PC(38:6), Phosphatidylcholine(16:0/22:6), Phosphatidylcholine(16:0/22:6n3), Phosphatidylcholine(16:0/22:6w3), Phosphatidylcholine(38:6) 1-Vaccenoyl-2-eicosapentaenoyl-sn-glycero-3-phosphocholine, GPCho(18:1/20:5), GPCho(18:1n7/20:5n3), GPCho(18:1w7/20:5w3), GPCho(38:6), Lecithin, PC aa C38:6,			
	PC(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))				
	PC(18:1(11Z)/20:5(5Z,8Z,11Z,14Z,17Z))				
	PC(18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))				
	PC(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))				
	PC(20:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))				
	PC(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))				
	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:0)				
	PC(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))		HMDB07991	C00157	Glycerophospholipids
	PC(18:1(11Z)/20:5(5Z,8Z,11Z,14Z,17Z))		HMDB08083	C00157	Glycerophospholipids
	PC(18:1(11Z)/20:5(5Z,8Z,11Z,14Z,17Z))		HMDB08116	C00157	Glycerophospholipids
	PC(18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))		HMDB08147	C00157	Glycerophospholipids
	PC(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))		HMDB08434	C00157	Glycerophospholipids
	PC(20:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))		HMDB08499	C00157	Glycerophospholipids
	PC(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))		HMDB08725	C00157	Glycerophospholipids
	PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:0)		HMDB07991	C00157	Glycerophospholipids
	PC(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))		HMDB08083	C00157	Glycerophospholipids
	PC(18:1(11Z)/20:5(5Z,8Z,11Z,14Z,17Z))		HMDB08116	C00157	Glycerophospholipids
	PC(18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))		HMDB08147	C00157	Glycerophospholipids
	PC(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))		HMDB08434	C00157	Glycerophospholipids
	PC(20:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))		HMDB08499	C00157	Glycerophospholipids
	PC(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))		HMDB08725	C00157	Glycerophospholipids
PC aa C38:6			HMDB08725	C00157	Glycerophospholipids

Supplement table 1

		nervonoyl-sn-glycero-3-phosphocholine, GPCho(16:0/24:1), GPCho(16:0/24:1n9), GPCho(16:0/24:1w9), GPCho(40:1), Lecithin, PC aa C40:1, PC(16:0/24:1), PC(16:0/24:1n9), PC(16:0/24:1w9), PC(40:1), Phosphatidylcholine(16:0/24:1), Phosphatidylcholine(16:0/24:1n9), Phosphatidylcholine(16:0/24:1w9), Phosphatidylcholine(40:1)			
	PC(16:0/24:1(15Z))	1-Stearoyl-2-erucoyl-sn-glycero-3-phosphocholine,	HMDB07993	C00157	Glycerophospholipids
	PC(18:0/22:1(13Z))	GPCho(18:0/22:1),	HMDB08052	C00157	Glycerophospholipids
	PC(18:1(11Z)/22:0)	GPCho(18:0/22:1n9),	HMDB08084	C00157	Glycerophospholipids
	PC(18:1(9Z)/22:0)	GPCho(18:0/22:1w9)	HMDB08117	C00157	Glycerophospholipids
	PC(20:0/20:1(11Z))	, GPCho(40:1),	HMDB08275	C00157	Glycerophospholipids
	PC(16:0/24:1(15Z))	Lecithin, PC aa	HMDB07993	C00157	Glycerophospholipids
	PC(18:0/22:1(13Z))	C40:1,	HMDB08052	C00157	Glycerophospholipids
	PC(18:1(11Z)/22:0)	PC(18:0/22:1),	HMDB08084	C00157	Glycerophospholipids
	PC(18:1(9Z)/22:0)	PC(18:0/22:1n9),	HMDB08117	C00157	Glycerophospholipids
PC aa C40:1	PC(20:0/20:1(11Z))	PC(18:0/22:1w9),	HMDB08275	C00157	Glycerophospholipids

Supplement table 1

		eicosadienoyl-sn-glycero-3-phosphocholine, GPCho(20:0/20:2), GPCho(20:0/20:2n6), GPCho(20:0/20:2w6), GPCho(40:2), Lecithin, PC aa C40:2, PC(20:0/20:2), PC(20:0/20:2n6), PC(20:0/20:2w6), PC(40:2), Phosphatidylcholine(20:0/20:2), Phosphatidylcholine(20:0/20:2n6), Phosphatidylcholine(20:0/20:2w6), Phosphatidylcholine(40:2)			
	PC(20:0/20:2(11Z,14Z))	1, 2-Dieicosenoyl-rac-glycero-3-phosphocholine, GPCho(20:1/20:1), GPCho(20:1n9/20:1n9), GPCho(20:1w9/20:1w9), GPCho(40:2), Lecithin, PC aa C40:2,	HMDB08276	C00157	Glycerophospholipids
	PC(20:1(11Z)/20:1(1Z))		HMDB08308	C00157	Glycerophospholipids
	PC(20:0/20:2(11Z,14Z))		HMDB08276	C00157	Glycerophospholipids
PC aa C40:2	PC(20:1(11Z)/20:1(1Z))	PC(20:1/20:1),	HMDB08308	C00157	Glycerophospholipids
PC aa C40:3					

Supplement table 1

		adrenoyl-sn-glycero-3-phosphocholine, GPCho(18:0/22:4), GPCho(18:0/22:4n6), GPCho(18:0/22:4w6), GPCho(40:4), Lecithin, PC aa C40:4, PC(18:0/22:4), PC(18:0/22:4n6), PC(18:0/22:4w6), PC(40:4), Phosphatidylcholine(18:0/22:4), Phosphatidylcholine(18:0/22:4n6), Phosphatidylcholine(18:0/22:4w6), Phosphatidylcholine(40:4)			
	PC(18:0/22:4(7Z,10Z,13Z,16Z))	1-Arachidonoyl-2-arachidonoyl-sn-glycero-3-phosphocholine,			
	PC(20:0/20:4(5Z,8Z,11Z,14Z))	GPCho(20:0/20:4),			
	PC(22:4(7Z,10Z,13Z,16Z)/18:0)	GPCho(20:0/20:4n6),			
	PC(18:0/22:4(7Z,10Z,13Z,16Z))	GPCho(20:0/20:4w6), GPCho(40:4),	HMDB08054	C00157	Glycerophospholipids
	PC(20:0/20:4(5Z,8Z,11Z,14Z))	Lecithin, PC aa C40:4,	HMDB08279	C00157	Glycerophospholipids
	PC(22:4(7Z,10Z,13Z,16Z)/18:0)	PC(20:0/20:4),	HMDB08628	C00157	Glycerophospholipids
PC aa C40:4		PC(20:0/20:4n6),	HMDB08054	C00157	Glycerophospholipids
			HMDB08279	C00157	Glycerophospholipids
			HMDB08628	C00157	Glycerophospholipids

Supplement table 1

		docosapentaenoyl-sn-glycero-3-phosphocholine, 1-Stearoyl-2- osbondoyl -sn-glycero-3-phosphocholine, GPCho(18:0/22:5), GPCho(18:0/22:5n6), GPCho(18:0/22:5w6), GPCho(40:5), Lecithin, PC(18:0/22:5), PC(18:0/22:5n6), PC(18:0/22:5w6), PC(40:5), Phosphatidylcholine(18:0/22:5), Phosphatidylcholine(18:0/22:5n6), Phosphatidylcholine(18:0/22:5w6), Phosphatidylcholine(40:5)			
	PC(18:0/22:5(4Z,7Z,10Z,13Z,16Z))	1-Stearoyl-2-			
	PC(18:0/22:5(7Z,10Z,13Z,16Z,19Z))	docosapentaenoyl-sn-glycero-3-			
	PC(18:1(9Z)/22:4(7Z,10Z,13Z,16Z))	phosphocholine,	HMDB08055	C00157	Glycerophospholipids
	PC(18:0/22:5(4Z,7Z,10Z,13Z,16Z))	GPCho(18:0/22:5),	HMDB08056	C00157	Glycerophospholipids
	PC(18:0/22:5(7Z,10Z,13Z,16Z,19Z))	GPCho(18:0/22:5n3),	HMDB08120	C00157	Glycerophospholipids
	PC(18:1(9Z)/22:4(7Z,10Z,13Z,16Z))	GPCho(18:0/22:5w3),	HMDB08055	C00157	Glycerophospholipids
		, GPCho(40:5),	HMDB08056	C00157	Glycerophospholipids
PC aa C40:5		Lecithin,	HMDB08120	C00157	Glycerophospholipids

Supplement table 1

		docosahexaenoyl-sn-glycero-3-phosphocholine, GPCho(18:0/22:6), GPCho(18:0/22:6n3), GPCho(18:0/22:6w3), GPCho(40:6), Lecithin, PC aa C40:6, PC(18:0/22:6), PC(18:0/22:6n3), PC(18:0/22:6w3), PC(40:6), Phosphatidylcholine(18:0/22:6), Phosphatidylcholine(18:0/22:6n3), Phosphatidylcholine(18:0/22:6w3), Phosphatidylcholine(40:6)			
	PC(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	1-Vaccenoyl-2-			
	PC(18:1(11Z)/22:5(7Z,10Z,13Z,16Z,19Z))	docosapentaenoyl-sn-glycero-3-			
	PC(18:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))	phosphocholine, GPCho(18:1/22:5),			
	PC(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	GPCho(18:1n7/22:5n3),	HMDB08057	C00157	Glycerophospholipids
	PC(18:1(11Z)/22:5(7Z,10Z,13Z,16Z,19Z))	GPCho(18:1w7/22:5w3), GPCho(40:6),	HMDB08089	C00157	Glycerophospholipids
	PC(18:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))	Lecithin, PC aa C40:6,	HMDB08122	C00157	Glycerophospholipids
PC aa C40:6			HMDB08057	C00157	Glycerophospholipids
			HMDB08089	C00157	Glycerophospholipids
			HMDB08122	C00157	Glycerophospholipids

Supplement table 1

		lignoceroyl-sn-glycero-3-phosphocholine, GPCho(18:0/24:0), GPCho(42:0), Lecithin, PC aa C42:0, PC(18:0/24:0), PC(42:0), Phosphatidylcholine(18:0/24:0), Phosphatidylcholine(42:0)			
		1-Arachidonyl-2-behenoyl-sn-glycero-3-phosphocholine, GPCho(20:0/22:0), GPCho(42:0), Lecithin, PC aa C42:0, PC(20:0/22:0), PC(42:0), Phosphatidylcholine(20:0/22:0), Phosphatidylcholine(42:0)			
	PC(18:0/24:0)	Phosphatidylcholine(42:0)	HMDB08058	C00157	Glycerophospholipids
	PC(20:0/22:0)	1-Behenoyl-2-arachidonyl-sn-glycero-3-phosphocholine,	HMDB08282	C00157	Glycerophospholipids
	PC(22:0/20:0)	GPCho(22:0/20:0),	HMDB08537	C00157	Glycerophospholipids
	PC(24:0/18:0)	GPCho(42:0),	HMDB08760	C00157	Glycerophospholipids
	PC(18:0/24:0)	Lecithin, PC aa C42:0,	HMDB08058	C00157	Glycerophospholipids
	PC(20:0/22:0)	PC(20:0/22:0),	HMDB08282	C00157	Glycerophospholipids
	PC(22:0/20:0)	PC(42:0),	HMDB08537	C00157	Glycerophospholipids
PC aa C42:0	PC(24:0/18:0)	Phosphatidylcholine(20:0/22:0),	HMDB08760	C00157	Glycerophospholipids

Supplement table 1

		nervonoyl-sn-glycero-3-phosphocholine, GPCho(18:0/24:1), GPCho(18:0/24:1n9), GPCho(18:0/24:1w9), GPCho(42:1), Lecithin, PC aa C42:1, PC(18:0/24:1), PC(18:0/24:1n9), PC(18:0/24:1w9), PC(42:1), Phosphatidylcholine(18:0/24:1), Phosphatidylcholine(18:0/24:1n9), Phosphatidylcholine(18:0/24:1w9), Phosphatidylcholine(42:1)			
	PC(18:0/24:1(15Z))	glycero-3-	HMDB08059	C00157	Glycerophospholipids
	PC(18:1(9Z)/24:0)	phosphocholine,	HMDB08124	C00157	Glycerophospholipids
	PC(20:0/22:1(13Z))	GPCho(18:1/24:0),	HMDB08283	C00157	Glycerophospholipids
	PC(22:0/20:1(11Z))	GPCho(18:1n9/24:0),	HMDB08538	C00157	Glycerophospholipids
	PC(24:0/18:1(9Z))	GPCho(18:1w9/24:0)	HMDB08762	C00157	Glycerophospholipids
	PC(18:0/24:1(15Z))	, GPCho(42:1),	HMDB08059	C00157	Glycerophospholipids
	PC(18:1(9Z)/24:0)	Lecithin, PC aa	HMDB08124	C00157	Glycerophospholipids
	PC(20:0/22:1(13Z))	C42:1,	HMDB08283	C00157	Glycerophospholipids
	PC(22:0/20:1(11Z))	PC(18:1/24:0),	HMDB08538	C00157	Glycerophospholipids
PC aa C42:1	PC(24:0/18:1(9Z))	PC(18:1n9/24:0),	HMDB08762	C00157	Glycerophospholipids
PC aa C42:2	PC aa C42:2	1-Erucoyl-2-eicosenoyl-	HMDB08570		Glycerophospholipids
PC aa C42:4	PC aa C42:4	1-Erucoyl-2-meadoyl-	HMDB08572		Glycerophospholipids

Supplement table 1

PC aa C42:5	<p>PC(20:0/22:5(7Z,10Z,13Z,16Z,19Z))</p> <p>PC(20:0/22:5(7Z,10Z,13Z,16Z,19Z))</p>	<p>docosapentaenoyl-sn-glycero-3-phosphocholine, GPCho(20:0/22:5), GPCho(20:0/22:5n3), GPCho(20:0/22:5w3), GPCho(42:5), Lecithin, PC aa C42:5, PC(20:0/22:5), PC(20:0/22:5n3), PC(20:0/22:5w3), PC(42:5), Phosphatidylcholine(20:0/22:5), Phosphatidylcholine(20:0/22:5n3), Phosphatidylcholine(20:0/22:5w3), Phosphatidylcholine(42:5)</p> <p>1-Arachidonyl-2-docosapentaenoyl-sn-glycero-3-phosphocholine, GPCho(20:0/22:5), GPCho(20:0/22:5n3), GPCho(20:0/22:5w3), GPCho(42:5), Lecithin, PC aa C42:5, PC(20:0/22:5),</p>	<p>HMDB08287</p> <p>HMDB08287</p>	<p>C00157</p> <p>C00157</p>	<p>Glycerophospholipids</p> <p>Glycerophospholipids</p>
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Supplement table 1

PC aa C42:6	PC(20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)) PC(20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	docosahexaenoyl-sn-glycero-3-phosphocholine, GPCho(20:0/22:6), GPCho(20:0/22:6n3), GPCho(20:0/22:6w3), GPCho(42:6), Lecithin, PC aa C42:6, PC(20:0/22:6), PC(20:0/22:6n3), PC(20:0/22:6w3), PC(42:6), Phosphatidylcholine(20:0/22:6), Phosphatidylcholine(20:0/22:6n3), Phosphatidylcholine(20:0/22:6w3), Phosphatidylcholine(42:6) 1-Arachidonyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine, GPCho(20:0/22:6), GPCho(20:0/22:6n3), GPCho(20:0/22:6w3), GPCho(42:6), Lecithin, PC aa C42:6, PC(20:0/22:6),	HMDB08288 HMDB08288	C00157 C00157	Glycerophospholipids Glycerophospholipids
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Supplement table 1

PC ae C30:0	PC(o-14:0/16:0) PC(o-14:0/16:0)	1-Myristyl-2-palmitoyl- sn-glycero-3- phosphocholine, GPCho(14:0/16:0), GPCho(30:0), Lecithin, PC ae C30:0, PC(14:0/16:0), PC(30:0), PC(O- 30:0), Phosphatidylcholine(14:0/16:0), Phosphatidylcholine(30:0) 1-Myristyl-2-palmitoyl- sn-glycero-3- phosphocholine, GPCho(14:0/16:0), GPCho(30:0), Lecithin, PC ae C30:0, PC(14:0/16:0), PC(30:0), PC(O- 30:0), Phosphatidylcholine(14:0/16:0), Phosphatidylcholine(30:0)	HMDB13341 HMDB13341		Glycerophospholipids Glycerophospholipids
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Supplement table 1

		<p>palmitoleoyl-sn-glycero-3-phosphocholine, GPCho(14:0/16:1), GPCho(14:0/16:1n7), GPCho(14:0/16:1w7), GPCho(30:1), Lecithin, PC ae C30:1, PC(14:0/16:1), PC(14:0/16:1n7), PC(14:0/16:1w7), PC(30:1), PC(O-30:1), Phosphatidylcholine(14:0/16:1), Phosphatidylcholine(14:0/16:1n7), Phosphatidylcholine(14:0/16:1w7), Phosphatidylcholine(30:1)</p> <p>1-Myristyl-2-palmitoleoyl-sn-glycero-3-phosphocholine, GPCho(14:0/16:1), GPCho(14:0/16:1n7), GPCho(14:0/16:1w7), GPCho(30:1), Lecithin, PC ae C30:1,</p>			
PC ae C30:1	PC(o-14:0/16:1(9Z)) PC(o-14:0/16:1(9Z))		HMDB13402 HMDB13402		Glycerophospholipids Glycerophospholipids
PC ae C30:2	PC ae C30:2				
PC ae C32:1	PC ae C32:1				
PC ae C32:2	PC ae C32:2				

Supplement table 1

		1-Palmityl-2-stearoyl-sn-glycero-3-phosphocholine, GPCho(16:0/18:0), GPCho(34:0), Lecithin, PC ae C34:0, PC(16:0/18:0), PC(34:0), PC(O-34:0), Phosphatidylcholine(16:0/18:0), Phosphatidylcholine(34:0)			
		1-Palmityl-2-stearoyl-sn-glycero-3-phosphocholine, GPCho(16:0/18:0), GPCho(34:0), Lecithin, PC ae C34:0, PC(16:0/18:0), PC(34:0), PC(O-34:0), Phosphatidylcholine(16:0/18:0), Phosphatidylcholine(34:0)			
PC ae C34:0	PC(o-16:0/18:0) PC(o-16:0/18:0)	Phosphatidylcholine(34:0)	HMDB13405 HMDB13405		Glycerophospholipids Glycerophospholipids
PC ae C34:1	PC ae C34:1				

Supplement table 1

PC ae C34:2	PC(O-16:0/18:2(9Z,12Z)) PC(O-16:0/18:2(9Z,12Z))	12Z-octadecadienoyl)-sn-glycero-3-phosphocholine, 2-(9Z, 12Z-Octadecadienoyl)-1-hexadecyl-sn-glycero-3-phosphocholine, PC ae C34:2, PC(16:0e/18:2(9Z, 12Z)), PC(O-34:2), [(2R)-3-hexadecoxy-2-[(9Z, 12Z)-octadeca-9, 12-dienoyl]oxypropyl] 2-trimethylazaniumylethyl phosphate 1-Hexadecyl-2-(9Z, 12Z-octadecadienoyl)-sn-glycero-3-phosphocholine, 2-(9Z, 12Z-Octadecadienoyl)-1-hexadecyl-sn-glycero-3-phosphocholine, PC ae C34:2, PC(16:0e/18:2(9Z, 12Z)), PC(O-34:2), [(2R)-3-hexadecoxy-2-[(9Z, 12Z)-octadeca-9, 12-	HMDB11151 HMDB11151		Glycerophospholipids Glycerophospholipids
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Supplement table 1

PC ae C34:3	<p>PC(P-16:0/18:2(9Z,12Z)) PC(P-16:0/18:2(9Z,12Z))</p>	<p>linoleoyl-sn-glycero-3-phosphocholine, GPCho(16:0/18:2), GPCho(16:0/18:2n6), GPCho(16:0/18:2w6) , GPCho(34:2), Lecithin, PC aa C34:2, PC(16:0/18:2), PC(16:0/18:2n6), PC(16:0/18:2w6), PC(34:2), Phosphatidylcholine(16:0/18:2), Phosphatidylcholine(16:0/18:2n6), Phosphatidylcholine(16:0/18:2w6), Phosphatidylcholine(34:2) 1-(1-Enyl-palmitoyl)-2-linoleoyl-sn-glycero-3-phosphocholine, GPCho(16:0/18:2), GPCho(16:0/18:2n6), GPCho(16:0/18:2w6) , GPCho(34:2), Lecithin, PC aa C34:2, PC(16:0/18:2), PC(16:0/18:2n6), PC(16:0/18:2w6),</p>	<p>HMDB11211 HMDB11211</p>		<p>Glycerophospholipids Glycerophospholipids</p>
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Supplement table 1

		arachidonyl-sn-glycero-3-phosphocholine, GPCho(16:0/20:0), GPCho(36:0), Lecithin, PC ae C36:0, PC(16:0/20:0), PC(36:0), PC(O-36:0), Phosphatidylcholine(16:0/20:0), Phosphatidylcholine(36:0) 1-Stearyl-2-stearoyl-sn-glycero-3-phosphocholine, GPCho(18:0/18:0), GPCho(36:0), Lecithin, PC ae C36:0, PC(18:0/18:0), PC(36:0), PC(O-36:0), Phosphatidylcholine(18:0/18:0), Phosphatidylcholine(36:0)			
	PC(o-16:0/20:0)	1-Palmityl-2-	HMDB13406		Glycerophospholipids
	PC(o-18:0/18:0)	arachidonyl-sn-	HMDB13417		Glycerophospholipids
	PC(o-16:0/20:0)	glycero-3-	HMDB13406		Glycerophospholipids
PC ae C36:0	PC(o-18:0/18:0)	phosphocholine,	HMDB13417		Glycerophospholipids
PC ae C36:1	PC ae C36:1	1-Oleyl-2-stearoyl-sn-	HMDB13427		Glycerophospholipids

Supplement table 1

		oleoyl-sn-glycero-3-phosphocholine, GPCho(18:0/18:1), GPCho(18:0/18:1n9), GPCho(18:0/18:1w9), GPCho(36:1), Lecithin, PC aa C36:1, PC(18:0/18:1), PC(18:0/18:1n9), PC(18:0/18:1w9), PC(36:1), Phosphatidylcholine(18:0/18:1), Phosphatidylcholine(18:0/18:1n9), Phosphatidylcholine(18:0/18:1w9), Phosphatidylcholine(36:1)			
PC ae C36:2	PC(P-18:0/18:1(9Z)) PC(P-18:0/18:1(9Z))	1-(1-Enyl-stearoyl)-2-oleoyl-sn-glycero-3-phosphocholine, GPCho(18:0/18:1), GPCho(18:0/18:1n9), GPCho(18:0/18:1w9), GPCho(36:1), Lecithin, PC aa C36:1, PC(18:0/18:1), PC(18:0/18:1n9), PC(18:0/18:1w9),	HMDB11243 HMDB11243		Glycerophospholipids Glycerophospholipids
PC ae C36:3	PC ae C36:3	1-Oleoyl-2-linoleoyl-sn-	HMDB13429		Glycerophospholipids
PC ae C36:4	PC ae C36:4	1-Linoleyl 2-linoleoyl-s	HMDB13435		Glycerophospholipids

Supplement table 1

PC ae C36:5	PC(P-16:0/20:4(5Z,8Z,11Z,14Z)) PC(P-16:0/20:4(5Z,8Z,11Z,14Z))	Phosphatidylcholine(dm16:0/20:4(5Z, 8Z, 11Z, 14Z)) Phosphatidylcholine(dm16:0/20:4(5Z, 8Z, 11Z, 14Z))	HMDB11220 HMDB11220		Glycerophospholipids Glycerophospholipids
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Supplement table 1

		behenoyl-sn-glycero-3-phosphocholine, GPCho(16:0/22:0), GPCho(38:0), Lecithin, PC ae C38:0, PC(16:0/22:0), PC(38:0), PC(O-38:0), Phosphatidylcholine(16:0/22:0), Phosphatidylcholine(38:0) 1-Stearyl-2-arachidonyl-sn-glycero-3-phosphocholine, GPCho(18:0/20:0), GPCho(38:0), Lecithin, PC ae C38:0, PC(18:0/20:0), PC(38:0), PC(O-38:0), Phosphatidylcholine(18:0/20:0), Phosphatidylcholine(38:0)			
PC ae C38:0	PC(o-16:0/22:0) PC(o-18:0/20:0) PC(o-16:0/22:0) PC(o-18:0/20:0)	1-Palmityl-2-behenoyl-sn-glycero-3-phosphocholine, GPCho(16:0/22:0),	HMDB13408 HMDB13419 HMDB13408 HMDB13419		Glycerophospholipids Glycerophospholipids Glycerophospholipids Glycerophospholipids
PC ae C38:1	PC ae C38:1	1-Oleyl-2-arachidonyl-	HMDB13430		Glycerophospholipids
PC ae C38:2	PC ae C38:2	1-Oleyl-2-eicosenoyl-	HMDB13431		Glycerophospholipids
PC ae C38:3	PC ae C38:3	1-Arachidyl-2-g-linole-	HMDB13439		Glycerophospholipids

Supplement table 1

PC ae C38:4	PC(o-18:0/20:4(8Z,11Z,14Z,17Z)) PC(o-18:0/20:4(8Z,11Z,14Z,17Z))	1-Stearyl-2-eicsoatetraenoyl-sn-glycero-3-phosphocholine, 1-Stearyl-2-eicsoic acid, GPCho(18:0/20:4), GPCho(18:0/20:4n3), GPCho(18:0/20:4w3), GPCho(38:4), Lecithin, PC ae C38:4, PC(18:0/20:4), PC(18:0/20:4n3), PC(18:0/20:4w3), PC(38:4), PC(O-38:4), Phosphatidylcholine(18:0/20:4), Phosphatidylcholine(18:0/20:4n3), Phosphatidylcholine(18:0/20:4w3), Phosphatidylcholine(38:4) 1-Stearyl-2-eicsoate, 1-Stearyl-2-eicsoatetraenoyl-sn-glycero-3-phosphocholine, 1-Stearyl-2-eicsoic acid,	HMDB13420 HMDB13420		Glycerophospholipids Glycerophospholipids
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Supplement table 1

PC ae C38:5	PC(o-18:1(9Z)/20:4(8Z,11Z,14Z,17Z)) PC(o-18:1(9Z)/20:4(8Z,11Z,14Z,17Z))	Oleyl-2-eicsoatetraenoyl-sn-glycero-3-phosphocholine, 1-Oleyl-2-eicsoic acid, GPCho(18:1/20:4), GPCho(18:1n9/20:4n3), GPCho(18:1w9/20:4w3), GPCho(38:5), Lecithin, PC ae C38:5, PC(18:1/20:4), PC(18:1n9/20:4n3), PC(18:1w9/20:4w3), PC(38:5), PC(O-38:5), Phosphatidylcholine(18:1/20:4), Phosphatidylcholine(18:1n9/20:4n3), Phosphatidylcholine(18:1w9/20:4w3), Phosphatidylcholine(38:5) 1-Oleyl-2-eicsoate, 1-Oleyl-2-eicsoatetraenoyl-sn-glycero-3-phosphocholine, 1-Oleyl-2-eicsoic acid, GPCho(18:1/20:4),	HMDB13432 HMDB13432		Glycerophospholipids Glycerophospholipids
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Supplement table 1

PC ae C38:6	<p>PC(o-16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))</p> <p>PC(o-16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))</p>	<p>docosahexaenoyl-sn-glycero-3-phosphocholine, GPCho(16:0/22:6), GPCho(16:0/22:6n3), GPCho(16:0/22:6w3), GPCho(38:6), Lecithin, PC ae C38:6, PC(16:0/22:6), PC(16:0/22:6n3), PC(16:0/22:6w3), PC(38:6), PC(O-38:6), Phosphatidylcholine(16:0/22:6), Phosphatidylcholine(16:0/22:6n3), Phosphatidylcholine(16:0/22:6w3), Phosphatidylcholine(38:6)</p> <p>1-Palmityl-2-docosahexaenoyl-sn-glycero-3-phosphocholine, GPCho(16:0/22:6), GPCho(16:0/22:6n3), GPCho(16:0/22:6w3), GPCho(38:6), Lecithin, PC ae C38:6,</p>	<p>HMDB13409</p> <p>HMDB13409</p>		<p>Glycerophospholipids</p> <p>Glycerophospholipids</p>
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Supplement table 1

		1-Stearyl-2-behenoyl-sn-glycero-3-phosphocholine, GPCho(18:0/22:0), GPCho(40:0), Lecithin, PC ae C40:0, PC(18:0/22:0), PC(40:0), PC(O-40:0), Phosphatidylcholine(18:0/22:0), Phosphatidylcholine(40:0)			
		1-Stearyl-2-behenoyl-sn-glycero-3-phosphocholine, GPCho(18:0/22:0), GPCho(40:0), Lecithin, PC ae C40:0, PC(18:0/22:0), PC(40:0), PC(O-40:0), Phosphatidylcholine(18:0/22:0), Phosphatidylcholine(40:0)			
PC ae C40:0	PC(o-18:0/22:0) PC(o-18:0/22:0)	Phosphatidylcholine(40:0)	HMDB13421 HMDB13421		Glycerophospholipids Glycerophospholipids
PC ae C40:1	PC ae C40:1	1-Oleyl-2-behenoyl-sn-glycero-3-phosphocholine	HMDB13433		Glycerophospholipids
PC ae C40:2	PC ae C40:2	1-Linoleyl-2-behenoyl-sn-glycero-3-phosphocholine	HMDB13437		Glycerophospholipids
PC ae C40:3	PC ae C40:3	1-Behenyl-2-g-linolenyl-sn-glycero-3-phosphocholine	HMDB13445		Glycerophospholipids
PC ae C40:4	PC ae C40:4	1-Arachidyl-2-eicsoatyl-sn-glycero-3-phosphocholine	HMDB13442		Glycerophospholipids
PC ae C40:5	PC ae C40:5	1-Eicosenyl-2-eicsoatyl-sn-glycero-3-phosphocholine	HMDB13444		Glycerophospholipids

Supplement table 1

PC ae C40:6	<p>PC(o-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))</p> <p>PC(o-18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))</p>	<p>docosahexaenoyl-sn-glycero-3-phosphocholine, GPCho(18:0/22:6), GPCho(18:0/22:6n3), GPCho(18:0/22:6w3), GPCho(40:6), Lecithin, PC ae C40:6, PC(18:0/22:6), PC(18:0/22:6n3), PC(18:0/22:6w3), PC(40:6), PC(O-40:6), Phosphatidylcholine(18:0/22:6), Phosphatidylcholine(18:0/22:6n3), Phosphatidylcholine(18:0/22:6w3), Phosphatidylcholine(40:6)</p> <p>1-Stearyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine, GPCho(18:0/22:6), GPCho(18:0/22:6n3), GPCho(18:0/22:6w3), GPCho(40:6), Lecithin, PC ae C40:6,</p>	<p>HMDB13422</p> <p>HMDB13422</p>		<p>Glycerophospholipids</p> <p>Glycerophospholipids</p>
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Supplement table 1

		1-Arachidyl-2-behenoyl-sn-glycero-3-phosphocholine, GPCho(20:0/22:0), GPCho(42:0), Lecithin, PC ae C42:0, PC(20:0/22:0), PC(42:0), PC(O-42:0), Phosphatidylcholine(20:0/22:0), Phosphatidylcholine(42:0)			
		1-Arachidyl-2-behenoyl-sn-glycero-3-phosphocholine, GPCho(20:0/22:0), GPCho(42:0), Lecithin, PC ae C42:0, PC(20:0/22:0), PC(42:0), PC(O-42:0), Phosphatidylcholine(20:0/22:0), Phosphatidylcholine(42:0)			
PC ae C42:0	PC(o-20:0/22:0) PC(o-20:0/22:0)	Phosphatidylcholine(42:0)	HMDB13443 HMDB13443		Glycerophospholipids Glycerophospholipids
PC ae C42:1	PC ae C42:1	1-Oleyl-2-lignoceroyl-s	HMDB13434		Glycerophospholipids
PC ae C42:2	PC ae C42:2	1-Linoleyl-2-lignocero	HMDB13438		Glycerophospholipids
PC ae C42:3	PC ae C42:3	1-Lignoceryl-2-a-linole	HMDB13459		Glycerophospholipids
PC ae C42:4	PC ae C42:4	1-Behenyl-2-eicsoate,	HMDB13448		Glycerophospholipids
PC ae C42:5	PC ae C42:5	1-Erucyl-2-eicsoate, 1	HMDB13451		Glycerophospholipids
PC ae C44:3	PC ae C44:3	1-Behenyl-2-(10Z, 13Z	HMDB13449		Glycerophospholipids
PC ae C44:4	PC ae C44:4	1-Erucyl-2-(10Z, 13Z,	HMDB13453		Glycerophospholipids

Supplement table 1

PC ae C44:5	PC ae C44:5	1-Docosadienyl-2-(10	HMDB13456		Glycerophospholipids
PC ae C44:6	PC ae C44:6	1-Docosatrienyl-2-(10	HMDB13457		Glycerophospholipids
		Aminoethyl)benzene, 1-Amino-1- phenylethane, 1- Fenylethylamin, 1- Phenyl-1- ethanamine, 1- Phenylethanamine, 1- Phenylethylamine, a- Aminoethylbenzene, a- Methylbenzenemetha namine, a- Methylbenzylamine, a-Phenethylamine, a- Phenylethylamine, alpha- Aminoethylbenzene, alpha- Methylbenzenemetha namine, alpha- Methylbenzylamine, alpha- Phenethylamine, alpha- Phenylethylamine, Sumine 2079 (2- Aminoethyl)benzene, (2- Aminoethyl)polystyre ne, 1-Amino-2- phenylethane, 1-			
PEA	1-Phenylethylamine 2-Phenylethylamine 1-Phenylethylamine 2-Phenylethylamine		HMDB02017 HMDB12275 HMDB02017 HMDB12275	C02455 C05332 C02455 C05332	Phenylmethyamines Phenethylamines Phenylmethyamines Phenethylamines

Supplement table 1

		Phenylalanine, (L)- Phenylalanine, (S)-(-)- Phenylalanine, (S)-2- amino-3- phenylpropanoate, (S)-2-amino-3- phenylpropanoic acid, (S)-2-Amino-3- phenylpropionate, (S)- 2-Amino-3- phenylpropionic acid, (S)-alpha-Amino- benzenepropanoate, (S)-alpha-Amino- benzenepropanoic acid, (S)-alpha- Amino-beta- phenylpropionate, (S)- alpha-Amino-beta- phenylpropionic acid, (S)-alpha- Aminobenzenepropa noate, (S)-alpha- Aminobenzenepropa noic acid, (S)-alpha- Aminohydrocinnamat e, (S)-alpha- Aminohydrocinnamic acid, (S)- Phenylalanine, 3- Phenyl-L-alanine, alpha-			
Phe	L-Phenylalanine L-Phenylalanine		HMDB00159 HMDB00159	C00079 C00079	Amino Acids and Derivatives Amino Acids and Derivatives

Supplement table 1

Pro		Pyrrolidinecarboxylate, (-)-2-			
		Pyrrolidinecarboxylic acid, (-)-Proline, (S)-(-)-Proline, (S)-(-)-Pyrrolidine-2-carboxylate, (S)-(-)-Pyrrolidine-2-carboxylic acid, (S)-2-Carboxypyrrolidine, (S)-2-			
		Pyrralidinecarboxylate, (S)-2-			
		Pyrralidinecarboxylic acid, (S)-2-			
		Pyrrolidinecarboxylate, (S)-2-			
		Pyrrolidinecarboxylic acid, (S)-Proline, 2-			
	L-Proline	Pyrrolidinecarboxylate, (R)-	HMDB00162	C00148	Amino Acids and Derivatives
	D-Proline	pyrrolidine-2-	HMDB03411	C00763	Amino Acids and Derivatives
L-Proline	carboxylic acid, D-	HMDB00162	C00148	Amino Acids and Derivatives	
D-Proline	Prolin, D-Proline, R)-	HMDB03411	C00763	Amino Acids and Derivatives	

Supplement table 1

		1, 4-Butylenediamine, 1, 4-Diaminobutane, 1, 4-Tetramethylenediamine, Butylenediamine, Putrescin, Tetramethyldiamine, Tetramethylenediamine			
		1, 4-Butanediamine, 1, 4-Butylenediamine, 1, 4-Diaminobutane, 1, 4-Tetramethylenediamine, Butylenediamine, Putrescin, Tetramethyldiamine, Tetramethylenediamine			
		1, 4-Butanediamine, 1, 4-Butylenediamine, 1, 4-Diaminobutane, 1, 4-Tetramethylenediamine, Butylenediamine, Putrescin, Tetramethyldiamine, Tetramethylenediamine			
Putrescine	Putrescine	Tetramethyldiamine, Tetramethylenediamine	HMDB01414	C00134	Alkylamines
	Putrescine	Tetramethylenediamine	HMDB01414	C00134	Alkylamines
	Putrescine	Tetramethylenediamine	HMDB01414	C00134	Alkylamines

Supplement table 1

		<p>dimethylarginine, N(G1), N(G2)- Dimethylarginine, N, N'-Dimethylarginine, N5- ((methylamino)(methylimino)methyl)-L- Ornithine, N5-(N, N'-dimethylamidino)-L- Ornithine, N5-[bis(methylamino)methylene]-L-Ornithine, NG, N'G-Dimethyl-L-arginine, NG, N'G-dimethylarginine, NG, NG'-dimethylarginine, SDMA Guanidino-N(1), N(2)-dimethylarginine, N(G1), N(G2)- Dimethylarginine, N, N'-Dimethylarginine, N5- ((methylamino)(methylimino)methyl)-L- Ornithine, N5-(N, N'-dimethylamidino)-L- Ornithine, N5-[bis(methylamino)methylene]-L-Ornithine, NG, N'G-Dimethyl-L-</p>			
SDMA	Symmetric dimethylarginine Symmetric dimethylarginine		HMDB03334 HMDB03334		Amino Acids and Derivatives Amino Acids and Derivatives
SM (OH) C14:1	SM (OH) C14:1				
SM (OH) C16:1	SM (OH) C16:1				
SM (OH) C22:1	SM (OH) C22:1				

Supplement table 1

SM (OH) C22:2	SM (OH) C22:2				
SM (OH) C24:1	SM (OH) C24:1				
SM C16:0	SM C16:0	C16 Sphingomyelin, N	HMDB10169		Sphingolipids
SM C16:1	Sphingomyelin with ac		HMDB29216		Sphingolipids
SM C18:0	SM C18:0	N-(Octadecanoyl)-sph	HMDB01348		Sphingolipids
		N-(11Z-Octadecenoyl)-sphing-4-enine-1-phosphocholine, SPH(d18:1/18:1(11Z)), Sphingomyelin, Sphingomyelin (d18:1/18:1(11Z))			
	C18:1;11Z-enoyl Sphingomyelin	C18:1 Sphingomyelin, N-(9Z-Octadecenoyl)-sphing-4-enine-1-phosphocholine, SPH(d18:1/18:1(11Z)), Sphingomyelin, Sphingomyelin (d18:1/18:1(11Z))	HMDB12100 HMDB12101	C00550 C00550	Sphingolipids Sphingolipids
SM C18:1	C18:1;9Z-enoyl Sphingomyelin				
SM C20:2	SM C20:2				
SM C22:3	SM C22:3				
SM C24:0	SM C24:0				
		C24:1 Sphingomyelin, N-(15Z-Tetracosenoyl)-sphing-4-enine-1-phosphocholine			
	C24:1 Sphingomyelin, N-(15Z-Tetracosenoyl)-sphing-4-enine-1-phosphocholine				
SM C24:1	SM(d18:1/24:1(15Z)) SM(d18:1/24:1(15Z))		HMDB12107 HMDB12107	C00550 C00550	Sphingolipids Sphingolipids

Supplement table 1

SM C26:0	SM C26:0	N-(Hexacosanoyl)-sph	HMDB11698		Sphingolipids
		C26:1 Sphingomyelin, N- (Tricosanoyl)-sphing- 4-enine-1- phosphocholine, Sphingomyelin			
	SM(d18:0/26:1(17Z))	C26:1 Sphingomyelin, N- (Tricosanoyl)-sphing- 4-enine-1- phosphocholine,	HMDB13461	C00550	Sphingolipids
SM C26:1	SM(d18:0/26:1(17Z))	Sphingomyelin	HMDB13461	C00550	Sphingolipids

Supplement table 1

		amino-3-hydroxy-Propanoate, (S)-2-amino-3-hydroxy-Propanoic acid, (S)-2-Amino-3-hydroxypropanoate, (S)-2-Amino-3-hydroxypropanoic acid, (S)- α -Amino- β -hydroxypropionate, (S)- α -Amino- β -hydroxypropionic acid, (S)- α -Amino- β -hydroxypropionate, (S)- α -Amino- β -hydroxypropionic acid, (S)- β -Amino-3-hydroxypropionate, (S)- β -Amino-3-hydroxypropionic acid, (S)-Serine, 2-Amino-3-hydroxypropanoate, 2-Amino-3-hydroxypropanoic acid, 3-Hydroxy-L-			
Ser	L-Serine D-Serine L-Serine D-Serine	hydroxypropanoate, hydroxypropanoic acid, 3-Hydroxy-L-	HMDB00187 HMDB03406 HMDB00187 HMDB03406	C00065 C00740 C00065 C00740	Amino Acids and Derivatives Amino Acids and Derivatives Amino Acids and Derivatives Amino Acids and Derivatives

Supplement table 1

Serotonin	Serotonin Serotonin Serotonin	indol-5-ol, 3-(2-Aminoethyl)indol-5-ol, 3-(b-Aminoethyl)-5-hydroxyindole, 5-HT, 5-HTA, 5-Hydroxy-3-(b-aminoethyl)indole, 5-Hydroxy-tryptamine, 5-Hydroxytryptamine, 5-Hydroxytryptamine, 5-Hydroxytryptamine, Antemovis, DS substance, Enteramin, Enteramine 3-(2-Aminoethyl)-1H-indol-5-ol, 3-(2-Aminoethyl)indol-5-ol, 3-(b-Aminoethyl)-5-hydroxyindole, 5-HT, 5-HTA, 5-Hydroxy-3-(b-aminoethyl)indole, 5-Hydroxy-tryptamine, 5-Hydroxytryptamine, 5-Hydroxytryptamine, Antemovis, DS substance, Enteramin,	HMDB00259 HMDB00259 HMDB00259	C00780 C00780 C00780	Indoles Indoles Indoles
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Supplement table 1

Spermidine	Spermidine Spermidine Spermidine	Triazadecane, 1, 8-Diamino-4-azaooctane, 4-Azaooctamethylenediamine, 4-Azaooctane-1, 8-diamine, Aminopropylbutandiamine, N-(3-Aminopropyl)-1, 4-butane-diamine, N-(3-Aminopropyl)-1, 4-butanediamine, N-(3-Aminopropyl)-1, 4-diamino-butane, N-(3-Aminopropyl)-1, 4-diaminobutane, N-(3-Aminopropyl)-4-aminobutylamine, N-(4-Aminobutyl)-1, 3-diaminopropane, N-(gamma-Aminopropyl)tetramethylenediamine, SPD, Spermidin, Spermidine 1, 5, 10-Triazadecane, 1, 8-Diamino-4-azaooctane, 4-Azaooctamethylenediamine, 4-Azaooctane-1, 8-diamine,	HMDB01257 HMDB01257 HMDB01257	C00315 C00315 C00315	Alkylamines Alkylamines Alkylamines
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Supplement table 1

		Tetraazatetradecane, 4, 9-Diaza-1, 12- dodecanediamine, 4, 9- Diazadodecamethyle nediamine, 4, 9- Diazadodecane-1, 12- diamine, Diaminopropyl- tetramethylenediami ne, Diaminopropyltetram ethylenediamine, Gerontine, Musculamine, N, N'- Bis(3-aminopropyl)- 1, 4-Butanediamine, N, N'-Bis(3- aminopropyl)-1, 4- tetramethylenediami ne, N, N'-Bis(3- aminopropyl)butane- 1, 4-diamine, N1, N4- bis(3-aminopropyl)-1, 4-butanediamine, Neuridine, Spermin, Spermine, Spermine dihydrate, Spermine puriss, SPM			
	Spermine	1, 5, 10, 14-	HMDB01256	C00750	Alkylamines
	Spermine	Tetraazatetradecane,	HMDB01256	C00750	Alkylamines
Spermine	Spermine	4, 9-Diaza-1, 12-	HMDB01256	C00750	Alkylamines

Supplement table 1

		sulfonate, 1- Aminoethane-2- sulfonic acid, 2- Aminoethanesulfonat e, 2- Aminoethanesulfonic acid, 2- Aminoethylsulfonate, 2-Aminoethylsulfonic acid, 2- Sulfoethylamine, Aminoethylsulfonate, Aminoethylsulfonic acid, b- Aminoethylsulfonate, b-Aminoethylsulfonic acid, beta- Aminoethylsulfonate, beta- Aminoethylsulfonic acid, Taurine 1-Aminoethane-2- sulfonate, 1- Aminoethane-2- sulfonic acid, 2- Aminoethanesulfonat e, 2- Aminoethanesulfonic acid, 2- Aminoethylsulfonate, 2-Aminoethylsulfonic acid, 2-			
Taurine	Taurine	Aminoethylsulfonate,	HMDB00251	C00245	Sulfonic Acids and Derivatives
	Taurine	2-Aminoethylsulfonic	HMDB00251	C00245	Sulfonic Acids and Derivatives
	Taurine	acid, 2-	HMDB00251	C00245	Sulfonic Acids and Derivatives

Supplement table 1

		Threonine, (2S, 3R)-2-Amino-3-hydroxybutyrate, (2S, 3R)-2-Amino-3-hydroxybutyric acid, (R-(R*, S*))-2-Amino-3-hydroxybutanoate, (R-(R*, S*))-2-Amino-3-hydroxybutanoic acid, (S)-Threonine, 2-Amino-3-hydroxybutanoate, 2-Amino-3-hydroxybutanoic acid, 2-Amino-3-hydroxybutyrate, 2-Amino-3-hydroxybutyric acid, L-(-)-Threonine, L-2-Amino-3-hydroxybutyrate, L-2-Amino-3-hydroxybutyric acid, L-alpha-Amino-beta-hydroxybutyrate, L-alpha-Amino-beta-hydroxybutyric acid, Threonin, Threonine,			
	L-Threonine	[R-(R*, S*)]-2-amino-	HMDB00167	C00188	Amino Acids and Derivatives
	L-Allothreonine	3-hydroxy-Butanoate,	HMDB04041	C05519	Amino Acids and Derivatives
	L-Threonine	[R-(R*, S*)]-2-amino-	HMDB00167	C00188	Amino Acids and Derivatives
Thr	L-Allothreonine	3-hydroxy-Butanoic	HMDB04041	C05519	Amino Acids and Derivatives

Supplement table 1

	L-Tryptophan		HMDB00929	C00078	Amino Acids and Derivatives
	D-Tryptophan		HMDB13609	C00525	Amino Acids and Derivatives
	L-Tryptophan		HMDB00929	C00078	Amino Acids and Derivatives
Trp	D-Tryptophan	(-)-tryptophan, (2S)-2-	HMDB13609	C00525	Amino Acids and Derivatives

Supplement table 1

		hydroxyhydrocinnamate, (-)- α -Amino-p-hydroxyhydrocinnamic acid, (-)- α -Amino-p-hydroxyhydrocinnamate, (-)- α -Amino-p-hydroxyhydrocinnamic acid, (S)-(-)-Tyrosine, (S)-2-Amino-3-(p-hydroxyphenyl)propionate, (S)-2-Amino-3-(p-hydroxyphenyl)propionic acid, (S)-3-(p-Hydroxyphenyl)alanine, (S)- α -amino-4-hydroxy-Benzenepropanoate, (S)- α -amino-4-hydroxy-Benzenepropanoic acid, (S)- α -Amino-4-hydroxybenzenepropanoate, (S)- α -Amino-4-hydroxybenzenepropanoic acid, (S)- α -amino-4-hydroxy-Benzenepropanoate,			
Tyr	L-Tyrosine L-Tyrosine		HMDB00158 HMDB00158	C00082 C00082	Amino Acids and Derivatives Amino Acids and Derivatives

Supplement table 1

Val	L-Valine L-Valine	methylbutanoate, (2S)-2-Amino-3-methylbutanoic acid, (S)-2-amino-3-methyl-Butanoate, (S)-2-amino-3-methyl-Butanoic acid, (S)-2-Amino-3-methylbutanoate, (S)-2-Amino-3-methylbutanoic acid, (S)-2-Amino-3-methylbutyrate, (S)-2-Amino-3-methylbutyric acid, (S)-a-Amino-b-methylbutyrate, (S)-a-Amino-b-methylbutyric acid, (S)-alpha-Amino-beta-methylbutyrate, (S)-alpha-Amino-beta-methylbutyric acid, (S)-Valine, 2-Amino-3-methylbutanoate, 2-Amino-3-methylbutanoic acid, 2-Amino-3-methylbutyrate, 2-Amino-3-methylbutyric acid, L-	HMDB00883 HMDB00883	C00183 C00183	Amino Acids and Derivatives Amino Acids and Derivatives
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Supplement table 1

		1-Myristoyl-glycero-3-phosphocholine, LPC(14:0), LPC(14:0/0:0), LyPC(14:0), LyPC(14:0/0:0), lysoPC a C14:0, LysoPC(14:0), LysoPC(14:0/0:0), Lysophosphatidylcholine(14:0), Lysophosphatidylcholine(14:0/0:0)			
		1-Myristoyl-glycero-3-phosphocholine, LPC(14:0), LPC(14:0/0:0), LyPC(14:0), LyPC(14:0/0:0), lysoPC a C14:0, LysoPC(14:0), LysoPC(14:0/0:0), Lysophosphatidylcholine(14:0), Lysophosphatidylcholine(14:0/0:0)			
lysoPC a C14:0	LysoPC(14:0)	Lysophosphatidylcholine(14:0/0:0)	HMDB10379	C04230	Glycerophospholipids
	LysoPC(14:0)	Lysophosphatidylcholine(14:0/0:0)	HMDB10379	C04230	Glycerophospholipids

Supplement table 1

		1-Palmitoyl-glycero-3-phosphocholine, 1-Palmitoyl-lysophosphatidylcholine, LPC(16:0), LPC(16:0/0:0), LyPC(16:0), LyPC(16:0/0:0), lysoPC a C16:0, LysoPC(16:0), LysoPC(16:0/0:0), Lysophosphatidylcholine(16:0), Lysophosphatidylcholine(16:0/0:0)			
		1-Palmitoyl-glycero-3-phosphocholine, 1-Palmitoyl-lysophosphatidylcholine, LPC(16:0), LPC(16:0/0:0), LyPC(16:0), LyPC(16:0/0:0), lysoPC a C16:0, LysoPC(16:0), LysoPC(16:0/0:0), Lysophosphatidylcholine(16:0),			
lysoPC a C16:0	LysoPC(16:0) LysoPC(16:0)	Lysophosphatidylcholine(16:0/0:0)	HMDB10382 HMDB10382	C04230 C04230	Glycerophospholipids Glycerophospholipids

Supplement table 1

		glycero-3-phosphocholine, LPC(16:1), LPC(16:1/0:0), LPC(16:1n7/0:0), LPC(16:1w7/0:0), LyPC(16:1), LyPC(16:1/0:0), LyPC(16:1n7/0:0), LyPC(16:1w7/0:0), lysoPC a C16:1, LysoPC(16:1), LysoPC(16:1/0:0), LysoPC(16:1n7/0:0), LysoPC(16:1w7/0:0), Lysophosphatidylcholine(16:1), Lysophosphatidylcholine(16:1/0:0), Lysophosphatidylcholine(16:1n7/0:0), Lysophosphatidylcholine(16:1w7/0:0) 1-Palmitoleoyl-glycero-3-phosphocholine, LPC(16:1), LPC(16:1/0:0), LPC(16:1n7/0:0), LPC(16:1w7/0:0), LyPC(16:1), LyPC(16:1/0:0),			
lysoPC a C16:1	LysoPC(16:1(9Z)) LysoPC(16:1(9Z))	LyPC(16:1), LyPC(16:1/0:0),	HMDB10383 HMDB10383	C04230 C04230	Glycerophospholipids Glycerophospholipids

Supplement table 1

		1-Heptadecanoyl-glycero-3-phosphocholine, LPC(17:0), LPC(17:0/0:0), LyPC(17:0), LyPC(17:0/0:0), lysoPC a C17:0, LysoPC(17:0), LysoPC(17:0/0:0), Lysophosphatidylcholine(17:0), Lysophosphatidylcholine(17:0/0:0)			
		1-Heptadecanoyl-glycero-3-phosphocholine, LPC(17:0), LPC(17:0/0:0), LyPC(17:0), LyPC(17:0/0:0), lysoPC a C17:0, LysoPC(17:0), LysoPC(17:0/0:0), Lysophosphatidylcholine(17:0),			
lysoPC a C17:0	LysoPC(17:0)	Lysophosphatidylcholine(17:0/0:0)	HMDB12108	C04230	Glycerophospholipids
	LysoPC(17:0)		HMDB12108	C04230	Glycerophospholipids

Supplement table 1

		phosphocholine, LPC(18:0), LPC(18:0/0:0), LyPC(18:0), LyPC(18:0/0:0), lysoPC a C18:0, LysoPC(18:0), LysoPC(18:0/0:0), Lysophosphatidylchol ine(18:0), Lysophosphatidylchol ine(18:0/0:0) 1-Hydroxy-2- Octadecanoyl-sn- glycero-3- phosphocholine, 1- Hydroxy-2-stearoyl- sn-glycero-3- phosphocholine, Lysophosphatidylchol ine, Stearoyl lysophosphatidylcholi ne 1-Stearoyl-glycero-3- phosphocholine, LPC(18:0), LPC(18:0/0:0), LyPC(18:0), LyPC(18:0/0:0), lysoPC a C18:0, LysoPC(18:0), LysoPC(18:0/0:0),			
lysoPC a C18:0	LysoPC(18:0) LysoPC(0:0/18:0) LysoPC(18:0) LysoPC(0:0/18:0)		HMDB10384 HMDB11128 HMDB10384 HMDB11128	C04230 C04230	Glycerophospholipids Glycerophospholipids Glycerophospholipids Glycerophospholipids

Supplement table 1

		sn-glycero-3-phosphocholine, 1-Oleoyl-sn-glycero-3-phosphocholine, 1-Oleoylglycerophosphocholine, 3-Oleoyl-rac-glycerol-1-phosphorylcholine, Choline phosphate (ester) 3-ester with 1-monoolein, Choline phosphate 3-ester with 1-monoolein, GPCCho(18:1(9Z)/0:0) [rac], LPC(18:1n9/0:0), LPC(18:1w9/0:0), LyPC(18:1), LyPC(18:1/0:0), LyPC(18:1w9/0:0), lysoPC a C18:1, LysoPC(18:1), LysoPC(18:1n9/0:0), LysoPC(18:1w9/0:0), Lysophosphatidylcholine(18:1), Lysophosphatidylcholine(18:1/0:0),			
	LysoPC(18:1(9Z))	Lysophosphatidylcholine(18:1n9/0:0),	HMDB02815	C04230	Glycerophospholipids
	LysoPC(18:1(11Z))	Lysophosphatidylcholine(18:1w9/0:0),	HMDB10385	C04230	Glycerophospholipids
	LysoPC(18:1(9Z))	Lysophosphatidylcholine(18:1n9/0:0),	HMDB02815	C04230	Glycerophospholipids
lysoPC a C18:1	LysoPC(18:1(11Z))	Lysophosphatidylcholine(18:1w9/0:0),	HMDB10385	C04230	Glycerophospholipids

Supplement table 1

		phosphocholine, LPC(18:2), LPC(18:2/0:0), LPC(18:2n6/0:0), LPC(18:2w6/0:0), LyPC(18:2), LyPC(18:2/0:0), LyPC(18:2n6/0:0), LyPC(18:2w6/0:0), lysoPC a C18:2, LysoPC(18:2), LysoPC(18:2/0:0), LysoPC(18:2n6/0:0), LysoPC(18:2w6/0:0), Lysophosphatidylchol ine(18:2), Lysophosphatidylchol ine(18:2/0:0), Lysophosphatidylchol ine(18:2n6/0:0), Lysophosphatidylchol ine(18:2w6/0:0) 1-Linoleoyl-glycero-3- phosphocholine, LPC(18:2), LPC(18:2/0:0), LPC(18:2n6/0:0), LPC(18:2w6/0:0), LyPC(18:2), LyPC(18:2/0:0), LyPC(18:2n6/0:0), LyPC(18:2w6/0:0),			
lysoPC a C18:2	LysoPC(18:2(9Z,12Z)) LysoPC(18:2(9Z,12Z))		HMDB10386 HMDB10386	C04230 C04230	Glycerophospholipids Glycerophospholipids

Supplement table 1

		phosphocholine, LPC(20:3), LPC(20:3/0:0), LPC(20:3n9/0:0), LPC(20:3w9/0:0), LyPC(20:3), LyPC(20:3/0:0), LyPC(20:3n9/0:0), LyPC(20:3w9/0:0), lysoPC a C20:3, LysoPC(20:3), LysoPC(20:3/0:0), LysoPC(20:3n9/0:0), LysoPC(20:3w9/0:0), Lysophosphatidylchol ine(20:3), Lysophosphatidylchol ine(20:3/0:0), Lysophosphatidylchol ine(20:3n9/0:0), Lysophosphatidylchol ine(20:3w9/0:0) 1-Homo-g-linolenoyl- glycero-3-			
	LysoPC(20:3(5Z,8Z,1 1Z))	phosphocholine, 1- Homo-gamma-			
	LysoPC(20:3(8Z,11Z, 14Z))	linolenoyl-glycero-3-			
	LysoPC(20:3(5Z,8Z,1 1Z))	phosphocholine, LPC(20:3),	HMDB10393	C04230	Glycerophospholipids
	LysoPC(20:3(8Z,11Z, 14Z))	LPC(20:3/0:0), LPC(20:3n6/0:0), LPC(20:3w6/0:0),	HMDB10394 HMDB10393 HMDB10394	C04230 C04230 C04230	Glycerophospholipids Glycerophospholipids Glycerophospholipids
lysoPC a C20:3					

Supplement table 1

		glycero-3-phosphocholine, LPC(20:4), LPC(20:4/0:0), LPC(20:4n6/0:0), LPC(20:4w6/0:0), LyPC(20:4), LyPC(20:4/0:0), LyPC(20:4n6/0:0), LyPC(20:4w6/0:0), lysoPC a C20:4, LysoPC(20:4), LysoPC(20:4/0:0), LysoPC(20:4n6/0:0), LysoPC(20:4w6/0:0), Lysophosphatidylcholine(20:4), Lysophosphatidylcholine(20:4/0:0), Lysophosphatidylcholine(20:4n6/0:0), Lysophosphatidylcholine(20:4w6/0:0)			
	LysoPC(20:4(5Z,8Z,11Z,14Z))	Eicsoatetraenoyl-glycero-3-phosphocholine, 1-Eicsoate, 1-			
	LysoPC(20:4(8Z,11Z,14Z,17Z))	Eicsoic acid,			
	LysoPC(20:4(5Z,8Z,11Z,14Z))	LPC(20:4),	HMDB10395	C04230	Glycerophospholipids
	LysoPC(20:4(8Z,11Z,14Z,17Z))	LPC(20:4/0:0),	HMDB10396	C04230	Glycerophospholipids
		LPC(20:4n3/0:0),	HMDB10395	C04230	Glycerophospholipids
lysoPC a C20:4		LPC(20:4w3/0:0),	HMDB10396	C04230	Glycerophospholipids

Supplement table 1

		1-Lignoceroyl-glycero-3-phosphocholine, LPC(24:0), LPC(24:0/0:0), LyPC(24:0), LyPC(24:0/0:0), lysoPC a C24:0, LysoPC(24:0), LysoPC(24:0/0:0), Lysophosphatidylcholine(24:0), Lysophosphatidylcholine(24:0/0:0)			
		1-Lignoceroyl-glycero-3-phosphocholine, LPC(24:0), LPC(24:0/0:0), LyPC(24:0), LyPC(24:0/0:0), lysoPC a C24:0, LysoPC(24:0), LysoPC(24:0/0:0), Lysophosphatidylcholine(24:0),			
lysoPC a C24:0	LysoPC(24:0)	Lysophosphatidylcholine(24:0/0:0)	HMDB10405	C04230	Glycerophospholipids
	LysoPC(24:0)		HMDB10405	C04230	Glycerophospholipids
lysoPC a C26:0	lysoPC a C26:0	lysoPC a C26:0	HMDB29205		Glycerophospholipids
lysoPC a C26:1	lysoPC a C26:1	lysoPC a C26:1	HMDB29220		Glycerophospholipids
lysoPC a C28:0	lysoPC a C28:0	lysoPC a C28:0	HMDB29206		Glycerophospholipids
lysoPC a C28:1	lysoPC a C28:1	lysoPC a C28:1	HMDB29221		Glycerophospholipids