

Supplementary material S2. Microbiota metabolite modifications and microbiota variation in several pathologies. *Gut microbiota-metabolite correlation +/-

Ref., Sample size, Biosample	Gut microbiota taxa modification	Metabolite modifications	*	Health status
[103] Northern Finland Birth Cohort <i>n</i> = 12,058; microbiome <i>n</i> = 563; metabolome <i>n</i> = 340 Faeces	<i>Blautia</i>	N-Acetilalanine, Ursodeoxycholate, N6,N6,N6-Trimethyllysine, 7-	+	NW
	<i>Ruminococcus</i>	Methylguanine, Isoursodeoxycholate, Deoxycholate, N-Propionylalanine	+	OW
	<i>Blautia</i>	Cholate sulfate, Dihomo-linolenate (20:3n3 or n6), 5α-Androstan-3α,17α-diol disulfate, Homocitrulline, Androsterone sulfate, Palmitoylcarnitine (C16), Propionylglutamine, Isoursodeoxycholate, 5α-Androstan-3α,17β-diol monosulfate, Deoxycholate, 2-Acetamidobutanoate, Phytosphingosine, N-Propionylalanine, Oleoylcarnitine (C18:1), Oleoyl ethanolamide, Glycodeoxycholate, N6-Carboxymethyllysine	+	OW
	<i>Roseburia</i>	Bilirubin (E,Z or Z,E), I-Urobilinogen, D-Urobilin, Stearoyl ethanolamide, N1-Methyl-2-pyridone-5-carboxamide, 7-Methylguanine, Carnosine, 2-Hydroxyadipate, Thymidine	+	OW
	<i>Oscillospira</i>	Nicotinate, Pantothenate	+	OW
	<i>Eggerthella</i>	Cholate sulfate	+	OW
	<i>Haemophilus</i>	5α-Androstan-3β,17β-diol monosulfate, Pregnenolone steroid monosulfate, Pregnenolone sulfate	+	OW
	<i>Veillonella</i>	Ribonate	+	OW
		Arabonate/xylonate	+	OW
[104] <i>n</i> = 33; OB/NoPCOS <i>n</i> = 15; OB/PCOS <i>n</i> = 18 Faeces	<i>Parabacteroides</i>	Teasterone	+	OB/PCOS
	<i>Veillonella</i>	Arachidonic acid, 8,11,14-Eicosatrienoic acid, Docosahexaenoic acid, Adrenic acid	+	
	<i>Lachnospira</i>	Taurocholic acid	-	
		Arachidonic acid, 8,11,14-Eicosatrienoic acid, Docosahexaenoic acid, Adrenic acid	+	
		Taurocholic acid	-	
	<i>Fusobacterium</i>	Teasterone	-	
	<i>Lachnoclostridium</i>	Teasterone	-	
	<i>Eubacterium coprostanoligenes</i> group	Teasterone	+	

	<i>Ruminococcaceae</i> UCG-002	Teasterone	+	
	<i>Erysipelotrichaceae</i> UCG-003	Dehydroepiandrosterone-sulfate	-	
	<i>Lachnospiraceae</i> NK4A136 group	Teasterone	+	
	norank <i>Muribaculaceae</i>	Dehydroepiandrosterone-sulfate	+	
[105]	<i>Akkermansia</i>	Indolepropionate	+	LH
<i>n</i> = 1280; LH <i>n</i> =	<i>Barnesiella</i>	Valine	+	LH
633; ObH <i>n</i> = 494; <i>Clostridium</i> IV		Tyrosine	+	LH
ObT2D <i>n</i> = 153		Isovalerate, Glutamine, Oxalate	-	LH
<i>n</i> = 400; LH <i>n</i> =	<i>Clostridium</i> XIVa	Phenylalanine, Glycylvaline	+	LH
228; ObH <i>n</i> = 145;		Glutamine, 3-Phenylpropionate, Inosine	-	LH
ObT2D <i>n</i> = 27	<i>Prevotella</i>	3-Phenylpropionate	+	LH
subset	<i>Intestimonas</i>	N1-Methyl-2-pyridone-5-carboxamide	+	LH
Serum	<i>Barnesiella</i>	Docosapentaenoate	-	LH
	<i>Butyricicoccus</i>	1-Stearoyl-GPE (18:0)	+	LH
	<i>Anaerovorax</i>	2-Methylbutyrylcarnitine	+	LH
		Adrenate (22:4n6), Epiandrosterone sulfate	-	ObH
	<i>Parabacteroides</i>	Indolepropionate, 1-Linoleoyl-GPC (18:2), 1-Dihomo-linoleoyl-GPC (20:2)	+	ObH
		10-Heptadecenoate (17:1n7)	-	LH
	<i>Ruminococcus</i>	Gamma-CEHC	+	ObH
		1-Arachidonoyl-GPI (20:4)	-	LH
	<i>Odoribacter</i>	Indolepropionate, 3-Phenylpropionate	+	ObH
		Glycylvaline	-	LH
	<i>Butyricimonas</i>	3-Phenylpropionate, 2-Linoleoyl-GPC (18:2), 1-Linoleoyl-GPC (18:2)	+	ObH
	<i>Oscillibacter</i>	Citrulline, 1-Oleoyl-GPC (18:1), Cinnamoylglycine	+	ObH
	<i>Anaerotruncus</i>	1-Linoleoyl-GPC (18:2)	+	ObH
[106]	<i>Fusobacterium varium</i>	Leucine, Glutamate	+	OB MLGs
<i>n</i> = 151; LC <i>n</i> = 79;	<i>Fusobacterium ulcerans</i>	Leucine, Glutamate	+	OB MLGs
OB <i>n</i> = 72	<i>Ruminococcus torques</i>	Glutamate, Phenylalanine	+	OB MLGs
	<i>Dorea longicatena</i>	Phenylalanine, Glutamate	+	OB MLGs

Serum		Glutamine	-	OB MLGs
	<i>Eubacterium hallii</i>	Glutamate	+	OB MLGs
	<i>Ruminococcus spp.</i>	Glutamate	+	OB MLGs
		Glutamine	-	OB MLGs
	<i>Coprococcus comes</i>	Glutamate	+	OB MLGs
		Glutamine	-	OB MLGs
	<i>Lachnospiraceae bacterium</i>	Leucine, Glutamate, Phenylalanine	+	OB MLGs
	<i>Bacteroides spp.</i>	Valine, Leucine, Isoleucine, Phenylalanine, Tyrosine, Glutamate	-	Control MLGs
	<i>Veillonella spp.</i>	Glutamate	-	Control MLGs
	<i>Haemophilus parainfluenzae</i>	Glutamate	-	Control MLGs
	<i>Bacteroides thetaiotaomicron</i>	Valine, Leucine, Phenylalanine, Tyrosine, Glutamate	-	Control MLGs
	<i>Bacteroides ovatus</i>	Valine, Phenylalanine, Tyrosine, Glutamate	-	Control MLGs
	<i>Bacteroides intestinalis</i>	Valine, Leucine, Isoleucine, Phenylalanine, Tyrosine, Glutamate	-	Control MLGs
	<i>Holdemania filiformis</i>	Valine, Leucine	-	Control MLGs
	<i>Faecalibacterium prausnitzii</i>	Valine, Leucine, Isoleucine, Phenylalanine, Glutamate	-	Control MLGs
	<i>Clostridiales bacterium</i>	Valine, Isoleucine, Phenylalanine, Tyrosine, Glutamate	-	Control MLGs
	<i>Anaerotruncus colihominis</i>	Valine, Leucine, Isoleucine, Phenylalanine	-	Control MLGs
	<i>Bacteroides uniformis</i>	Valine, Leucine, Phenylalanine, Tyrosine	-	Control MLGs
	<i>Klebsiella pneumoniae</i>	Glutamate	-	Control MLGs
	<i>Dialister invisus</i>	Valine, Phenylalanine, Glutamate	-	Control MLGs
	<i>Alistipes spp.</i>	Tyrosine	-	Control MLGs
	<i>Alistipes putredinis</i>	Valine, Leucine	-	Control MLGs
	<i>Bacteroides xylanisolvens</i>	Valine	-	Control MLGs
	<i>Akkermansia muciniphila</i>	Phenylalanine	-	Control MLGs
	<i>Odoribacter splanchnicus</i>	Phenylalanine	-	Control MLGs
	<i>Alistipes shahii</i>	Tyrosine	-	Control MLGs
[107] <i>n</i> = 16; NW <i>n</i> = 8; OB <i>n</i> = 8 Faeces	Enterococcaceae	Octadecenoic acid (Diet), N-Acetyl-DOPA(Gut-Brain)	+	ND, ↓ OB
	Enterobacteriaceae	Octadecenoic acid (Diet)	+	ND
		Ascorbic acid (Diet)	-	ND
	Christensenellaceae	Azelaic acid (Diet), Suberic acid (Diet)	+	ND, ↓ OB

Succinivibrionaceae	Suberic acid (Diet)	+	↓ OB
Coriobacteriaceae	Deoxycholic acid (Liver)	+	↑ OB
Propionibacteriaceae	Urobilin (Liver), Deoxycholic acid (Liver)	+	ND, ↑ OB
Synergistaceae	Deoxycholic acid (Liver)	+	↑ OB
Erysipelotrichaceae	Dimethyl-2-oxoglutarate (Gut-Endogen)	+	↓ OB
	Ascorbic acid (Diet)	-	ND
Ruminococcaceae	Dimethyl-2-oxoglutarate (Gut-Endogen)	+	↓ OB
	Tripeptide (Diet)	-	↑ OB
Prevotellaceae	Ascorbic acid (Diet)	+	ND
Clostridiaceae	Hydroxyhexadecanedioic acid (Diet)	+	ND
Rhodobacteraceae	Hydroxyhexadecanedioic acid (Diet), Azelaic acid (Diet)	+	ND, ND
Desulfovibrionaceae	Hydroxyhexadecanedioic acid (Diet), Azelaic acid (Diet)	+	ND, ND
Streptococcaceae	N-Acetyl-DOPA (Gut-Brain)	-	↓ OB
Porphyromonadaceae	Hydroxyphenyl propionic acid (Diet), Tripeptide (Diet), 12-ketodeoxycholic acid (Liver)	+	ND, ↑ OB, ↑ OB
DeFluviitaleaceae	Hydroxyphenyl propionic acid (Diet), Tripeptide (Diet), 12-ketodeoxycholic acid (Liver)	+	ND, ↑ OB, ↑ OB
Staphylococcaceae	Homovanillic acid (Gut-Brain)	+	ND
Alcaligenaceae	Rosmarinic acid (Diet), Quinic acid (Diet), Homovanillic acid (Gut-Brain)	+	ND, ND, ND
Helicobacteraceae	Homovanillic acid (Gut-Brain)	+	ND
Bacteroidaceae	Quinic acid (Diet), Tripeptide (Diet), Homovanillic acid (Gut-Brain)	+	ND, ↑ OB, ND
	Dimethyl-2-oxoglutarate (Gut-Endogen), Suberic acid (Diet), Urobilin (Liver)	-	↓ OB, ↓ OB, ND
U. m. of Clostridiales order	Dimethyl-2-oxoglutarate (Gut-Endogen), N-Acetyl-DOPA (Gut-Brain)	+	↓ OB, ↓ OB
U. m. of Bacteroidales order	Hydroxyphenyl propionic acid (Diet), Tripeptide (Diet), 12-ketodeoxycholic acid (Liver)	+	ND, ↑ OB, ↑ OB
Tenericutes	Suberic acid (Diet)	+	↓ OB
Firmicutes	Dimethyl-2-oxoglutarate (Gut-Endogen)	+	↓ OB

		Quinic acid (Diet), Tripeptide (Diet), Urobilin (Liver)	-	ND, ↑ OB, ND
Bacteroidetes		Tripeptide (Diet)	+	↑ OB
		Dimethyl-2-oxoglutarate (Gut-Endogen), Suberic acid (Diet)	-	↓ OB, ↓ OB
[108] <i>n</i> = 100; HC <i>n</i> = 35; T2D+ <i>n</i> = 49; T2D- <i>n</i> = 16 Faeces	<i>Enhydrobacter</i>	LDL cholesterol	+	T2D+
	<i>Acinetobacter</i>			
	<i>Pseudomonas</i>			
	<i>Aeromonas</i>			
	<i>Providencia</i>			
	M5			
	<i>Akkermansia</i>	HDL cholesterol	+	HC
	MM12			
	<i>Sarcina</i>	Cholic acid	-	HC
	Mollicutes			
	Tenericutes			
	MM13			
	<i>Solibacillus</i>	Acetate, Glycoursodeoxycholic acid, Chenodeoxyglycocholate	-	HC
	<i>Oligella</i>			
	<i>Epulopiscium</i>			
	<i>Parapusillimonas</i>			
	<i>Psychrobacter</i>			
	<i>Flavobacterium</i>			
	MM14			
	<i>Shuttleworthia</i>	Palmitoylcarnitine, Diacylglycerol (15:0/18:3), Diacylglycerol (15:0/20:3)	+	T2D+
	<i>Peptoniphilus</i>			
	<i>Atopobium</i>			
	<i>Anaerococcus</i>			
	MM15			
	<i>Allisonella</i>	Lysophosphatidylcholine (18:2), Phosphatidylcholine (16:0/17:0)	+	T2D+
	<i>Ochrobactrum</i>			
	<i>Butyricicoccus</i>			
	<i>Anaerostipes</i>			

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	<i>Ruminococcus toques</i> group			
	MM16			
	<i>Veillonella</i>	Linolenic acid, Lysophosphatidylcholine (18:2)	+	T2D+
	<i>Weissella</i>			
	<i>Pseudobutyrvibrio</i>			
	<i>Streptococcus</i>	Butyrate	-	
	<i>Prevotellaceae</i> UCG-003			
	MM19			
	<i>Blautia</i>	HDL cholesterol	-	T2D-
	<i>Marvinbryantia</i>			
	<i>Lachnospiraceae</i> NK4A136 group			
	MM32			
	<i>Morganella</i>	Acetate, Butyrate, Glycocholic acid, Cholic acid	-	HC
	<i>Campylobacter</i>			
	MM34			
	<i>Lactococcus</i>	Palmitoylcarnitine, Lysophosphatidylcholine (18:2),	+	T2D+
	<i>Prevotella</i>	Phosphatidylcholine (16:0/17:0)		
	MM35			
	<i>Eubacterium oxidoreducens</i> group	Glycoursodeoxycholic acid, Chenodeoxyglycocholate, Glycocholic-		HC
	<i>Prevotellaceae</i> NK3B31 group	acid		
	MM38			
	<i>Neisseria</i>	Cholic acid	+	T2D+
	MM40			
[109] <i>n</i> = 60; NGT <i>n</i> = 20; T2D <i>n</i> = 20; IGR <i>n</i> = 20 Faeces	<i>Blautia</i>	PA (O-16:0/12:0), 24-Nor-9,11-seco-11-acetoxy-3,6- dihydroxycholest-7,22-dien-9-one, Matricin, 8Z-Decen-4,6-diynoic acid, Docosanedioic acid, Methyl, Ikarisoside	-	T2D vs. IGR
	<i>Coproccoccus</i> 3	Matricin, (6S)-Dehydrovomifoliol	-	T2D vs. IGR
	<i>Lactobacillaceae</i>	14,15-HxA3-D (11S), Cytochalasin, Tanariflavanone	-	T2D vs. IGR
	<i>Subdoligranulum</i>	PA (O-16:0/12:0), 24-Nor-9,11-seco-11-acetoxy-3,6- dihydroxycholest-7,22-dien-9-one, Tanariflavanone	-	T2D vs. IGR

<i>Prebotella</i> 9	PA (O-16:0/12:0), 24-Nor-9,11-seco-11-acetoxy-3,6-dihydroxycholest-7,22-dien-9-one	+	T2D vs. IGR
<i>Bacteroides</i>	PI (O-20:0/18:0), 3Z,6Z,9Z,12Z,15Z,19Z,22Z,25Z,28Z-Hentriacontanonaene, 10Z-Pentacosene, SM (d18:1/25:0), TG (13:0/17:1(9Z)/17:1(9Z))[iso3], GlcCer (d18:1/20:0), SM (d18:1/24:0), GlcCer (d18:2/23:0), TG (15:0/15:0/15:0), 1 α ,25-Dihydroxy-22-oxavitamin, 3-O-(β -D-glucopyranosyl-(1 \rightarrow 6)- β -D-glucopytanosyl), Diamino-pimelic acid	+	T2D vs. IGR
<i>Fusicatenibater</i>	24-Nor-9,11-seco-11-acetoxy-3,6-dihydroxycholest-7,22-dien-9-one -	-	T2D vs. IGR
<i>Faecalibacterium</i>	17-Oxo-octadecanoic	+	T2D vs. IGR
	PA (O-16:0/12:0), 24-Nor-9,11-seco-11-acetoxy-3,6-dihydroxycholest-7,22-dien-9-one, PC (O-12:0/O-2:0)	-	T2D vs. IGR
<i>Dorea</i>	26,26,26,27,27,27-Hexafluoro-25-hydroxy-23,23,24,24-tetrahydrovitamin	-	T2D vs. IGR
<i>Rummicococcus torques</i> group	LysoPC (15:0), 17-Oxo-octadecanoic	+	T2D vs. IGR
<i>Lachnospiraceae</i> NK4A136 group	(3S)-3',7-Dihydroxy-2',4',5',8-tetramethoxyisoflavan	+	T2D vs. IGR
	1 α ,25-Dihydroxy-22-oxavitamin	-	T2D vs. IGR
<i>Butyricicoccus</i>	PI (O-20:0/18:0), 3Z,6Z,9Z,12Z,15Z,19Z,22Z,25Z,28Z-Hentriacontanonaene, GalNAc β 1-4Gal β 1-4Glc β -Cer(d18:1/24:1(15Z)), TG (15:0/15:0/15:0), SM(d18:1/24:0), PG (O-20:0/21:0), 10Z-Pentacosene, 21-Methyl-8Z-pentatriacontene, (6S)-Dehydrovomifoliol	+	IGR vs. NGT
<i>Bacteroides</i>	γ -Glutamylglutamine, L-Lysine, MGDG (20:5(5Z,8Z,11Z,14Z,17Z)/18:3(9Z,12Z,15Z))	+	IGR vs. NGT
<i>Lachnoclostridium</i>	L-Lysine	+	IGR vs. NGT
<i>Roseburia</i>	1 α ,25-Dihydroxy-22-oxavitamin	+	IGR vs. NGT
<i>Faecalibacterium</i>	L-Tyrosine, DL-2-hydroxy, 21-Methyl-8Z-pentatriacontene	+	IGR vs. NGT
<i>Blautia</i>	5 α -Cholestane-3 α ,7 α ,12 α ,23,25-pentol	+	IGR vs. NGT
<i>Coproccoccus</i> 1	L-Lysine, Scillaren	+	IGR vs. NGT
<i>Fusicatenibacter</i>	γ -Glutamylglutamine, L-Tyrosine, L-Lysine	+	IGR vs. NGT

<i>Subdoligranulum</i>	7-Dehydro-desmosterol, 24-Keto-25dehydrocholesterol, Simvastatin, 5a-Cholestane-3a,7a,12a,23,25-pentol, (22S)-1a,22,25-Trihydroxy-23,24-tetradecahydro-24a-homo-20-epivitamin, PA (14:1/(9Z)/0:0), Manoalide, PA (17:0/21:0), Teasterone, Hippuristanolide	+	IGR vs. NGT
<i>Collinsella</i>	Afrormosin, PG (P-16:0/15:0)	+	IGR vs. NGT
<i>Ruminococcus torques</i> group	2-Methyl-tridecanedioic, 27-Nor-campestan-3β,4β,5a,6a,7β,8β,14a,15a,24-nonol, LysoPC (14:1(9Z))	+	IGR vs. NGT
<i>Eubacterium hallii</i> group	L-Tyrosine, L-Lysine	+	IGR vs. NGT
<i>Eubacterium rectale</i> group	L-Lysine, Dodecanedioic, (+)-Cucurbitic acid	+	IGR vs. NGT
<i>Eubacterium coprostanoligenes</i> group	7-Dehydro-desmosterol, 24-Keto-25dehydrocholesterol, Simvastatin, 5a-Cholestane-3a,7a,16a,26-tetrol, 5a-Cholestane-3a,7a,12a,23,25-pentol, Scillaren, PA (14:1/(9Z)/0:0), Manoalide, PA (17:0/21:0), Hippuristanolide	+	IGR vs. NGT
<i>Lachnospiraceae</i> UCG-004	1a,25-Dihydroxy-22-oxavitamin	+	IGR vs. NGT
<i>Lachnospiraceae</i> NC2004 group	L-Lysine, DL-2-hydroxy, Enkephalin, Ptilosteroid, 7E,9E,11-Dodecatrienyl, Hexacosanoic, Hexacosanedioic, Artonin, Viscutin	+	IGR vs. NGT
<i>Lachnospiraceae</i> ND3007 group	L-Lysine	+	IGR vs. NGT
<i>Lachnospiraceae</i> NK4A136 group	L-Tyrosine, 7-Dehydro-desmosterol, 24-Keto-25dehydrocholesterol, Simvastatin, 5a-Cholestane-3a,7a,16a,26-tetrol, 5a-Cholestane-3a,7a,12a,23,25-pentol, Scillaren	+	IGR vs. NGT
<i>Bifidobacterium</i>	Cristacarpin	+	T2D vs. NGT
<i>Bacteroides</i>	12,13-Dihydroxy-11-methoxy-9-octadecenoic acid, Cer (d18:0/h 17:0)	+	T2D vs. NGT
<i>Parabacteroides</i>	12,13-Dihydroxy-11-methoxy-9-octadecenoic acid, Cer (d18:0/h 17:0)	+	T2D vs. NGT
<i>Intestinibacter</i>	12,13-Dihydroxy-11-methoxy-9-octadecenoic acid	+	T2D vs. NGT
<i>Subdoligranulum</i>	12,13-Dihydroxy-11-methoxy-9-octadecenoic acid, Cer (d18:0/h 17:0)	+	T2D vs. NGT
<i>Fusicatenibacter</i>	12,13-Dihydroxy-11-methoxy-9-octadecenoic acid	+	T2D vs. NGT
<i>Ruminococcaceae</i> UCG-005	Piceid, γ-Glutamylglutamine	+	T2D vs. NGT

	<i>Lachnospiraceae</i> NK4A136 group	Cristacarpin, 24-Keto-25dehydrocholesterol, 5a-Cholestane-3a,7a,12a,23,25-pentol	+	T2D vs. NGT
[110] <i>n</i> = 9180; <i>n</i> = 759 HCHS/SOL participants Serum	<i>Ruminococcus, Flavonifractor, Faecalitalea,</i>	Indolepropionate	+, -, +, ↓ T2D	
	<i>Lachnoclostridium, Faecalibacterium,</i>		-, +, +,	
	<i>Subdoligranulum, Clostridium,</i>		+, +, +,	
	<i>Lachnoanaerobaculum, Intestinimonas,</i>		-, +, +,	
	<i>Erysipelatoclostridium, Cellulomonas,</i>		+, +, +,	
	<i>Eubacterium, Fournierella, Dorea,</i>		-, +, +,	
	<i>Butyrivibrio, Eggerthella,</i>		+, -, +,	
	<i>Pseudoflavonifractor, Bifidobacterium,</i>			
	<i>Porphyromonas, Parabacteroides, Bittarella,</i>	Indoleacetate	ND	ND
	<i>Cellulomonas, Fournierella,</i>			
[111] <i>n</i> = 69; HC <i>n</i> = 40; Pseudomonadaceae Non-PN SBS <i>n</i> = 5; SBS I <i>n</i> = 10; Staphylococcaceae SBS II <i>n</i> = 14 Faeces and serum	<i>Methanobrevibacter, Anaerostipes,</i>			
	<i>Catenibacterium</i>			
	<i>Faecalitalea, Pseudoflavonifractor,</i>	Indoxyl sulfate	ND	ND
	<i>Parabacteroides, Alistipes, Akkermansia,</i>			
	<i>Faecalicatena, Intestinibacter, Odoribacter,</i>			
	<i>Gordonibacter, Sanguibacteroides,</i>			
	<i>Anaerotruncus</i>			
		2-Pentyl furan, Nonanal, Dodecanoic acid, Decanoic acid,	+	SBS
		Chenodeoxycholic acid, Deoxycholic acid		
		Pentanoic acid, Butanoic acid, Lithocholic acid	-	HC
Enterococcaceae		2-Pentyl furan, Hexanal, Octanal, Decanoic acid, Taurocholic acid,	+	SBS
		Chenodeoxycholic acid, Deoxycholic acid		
		γ-Undecalactone, Geranyl acetone, Butanoic acid	-	HC
		2-Pentyl furan, Hexanal, Octanal, Nonanal, Decanoic acid,	+	SBS
		Chenodeoxycholic acid, Deoxycholic acid		
		Indole, γ-Undecalactone, Geranyl acetone, Pentanoic acid,	-	HC
		Butanoic acid, Lithocholic acid		
		2-Pentyl furan, Hexanal, Octanal, Nonanal, Taurocholic acid,	+	SBS
Fusobacteriaceae		Chenodeoxycholic acid, Deoxycholic acid		

Enterobacteriaceae	γ-Undecalactone, Geranyl acetone, Pentanoic acid, Butanoic acid	-	HC
	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid, Cholic acid, Glycocholic acid, Glycochenodeoxycholic acid	+	SBS
Lactobacillaceae	γ-Undecalactone, p-Cresol, 1-Nonanol, Pentanoic acid, Butanoic acid, Lithocholic acid	-	HC
	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid, Cholic acid	+	SBS
Streptococcaceae	Indole, γ-Undecalactone, Geranyl acetone, p-Cresol, 1-Nonanol, Pentanoic acid, Butanoic acid, Lithocholic acid	-	HC
	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid, Glycochenodeoxycholic acid	+	SBS
Clostridiaceae	Indole, γ-Undecalactone, Geranyl acetone, p-Cresol, 1-Nonanol, Pentanoic acid, Butanoic acid, Lithocholic acid	-	HC
	Butanoic acid, 1-Nonanol	+	HC
Coriobacteriaceae	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Chenodeoxycholic acid, Deoxycholic acid, Glycodeoxycholic acid	-	SBS
	Pentanoic acid, p-Cresol, Lithocholic acid	+	HC
Rikenellaceae	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Phenol, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid	-	SBS
	Butanoic acid, Pentanoic acid, 1-Nonanol, p-Cresol, Geranyl acetone, γ-Undecalactone, Indole, Lithocholic acid	+	HC
	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Phenol, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid, Glycochenodeoxycholic acid	-	SBS

Ruminococcaceae	Butanoic acid, Pentanoic acid, 1-Nonanol, p-Cresol, Geranyl acetone, γ -Undecalactone, Lithocholic acid	+	HC
	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid, Cholic acid, Glycocholic acid, Glycochenodeoxycholic acid	-	SBS
Barnesiellaceae	Butanoic acid, Pentanoic acid, 1-Nonanol, p-Cresol, Geranyl acetone, γ -Undecalactone, Indole, Lithocholic acid	+	HC
	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid, Cholic acid, Glycocholic acid, Glycochenodeoxycholic acid	-	SBS
Odoribacteraceae	Butanoic acid, Pentanoic acid, 1-Nonanol, p-Cresol, Geranyl acetone, γ -Undecalactone, Lithocholic acid	+	HC
	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid, Cholic acid, Glycochenodeoxycholic acid	-	SBS
Porphyromonadaceae	Butanoic acid, Pentanoic acid, 1-Nonanol, p-Cresol, Lithocholic acid	+	HC
	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Chenodeoxycholic acid, Deoxycholic acid	-	SBS
Paraprevotellaceae	Butanoic acid, Pentanoic acid, 1-Nonanol, p-Cresol, γ -Undecalactone, Lithocholic acid	+	HC
	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid	-	SBS
Prevotellaceae	Butanoic acid, Pentanoic acid, 1-Nonanol, p-Cresol, Geranyl acetone, Lithocholic acid	+	HC
	2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Chenodeoxycholic acid, Deoxycholic acid, Glycochenodeoxycholic acid	-	SBS

S24 7		Butanoic acid, p-Cresol, Geranyl acetone, Lithocholic acid	+	HC
		2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Chenodeoxycholic acid, Deoxycholic acid, Cholic acid	-	SBS
Alcaligenaceae		Butanoic acid, Pentanoic acid, 1-Nonanol, p-Cresol, γ-Undecalactone, Indole	+	HC
		Dodecanoic acid, Decanoic acid, Taurocholic acid, Chenodeoxycholic acid, Glycocholic acid	-	SBS
Bacteroidaceae		Butanoic acid, Pentanoic acid, 1-Nonanol, p-Cresol, γ-Undecalactone, Indole, Lithocholic acid	+	HC
		2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid, Glycocholic acid, Glycochenodeoxycholic acid	-	SBS
Lachnospiraceae		Butanoic acid, Pentanoic acid, 1-Nonanol, p-Cresol, Geranyl acetone, γ-Undecalactone, Indole, Lithocholic acid	+	HC
		2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid, Glycocholic acid, Glycochenodeoxycholic acid	-	SBS
Clostridiales		Butanoic acid, Pentanoic acid, 1-Nonanol, p-Cresol, Geranyl acetone, γ-Undecalactone, Lithocholic acid	+	HC
		2-Pentyl furan, Hexanal, Octanal, Nonanal, Dodecanoic acid, Decanoic acid, Phenol, Taurocholic acid, Chenodeoxycholic acid, Deoxycholic acid, Glycochenodeoxycholic acid	-	SBS
[112] n = 155; Non-IBD n=34; CD n = 68; UC n = 53 Faeces	<i>Eubacterium ventriosum</i>	Urobilin, 4-Methylcatechol	+	non-IBD
		Eicosatrienoic acid	-	IBD:CD
	<i>Coproccoccus catus</i>	Urobilin	+	Non-IBD
		Eicosatrienoic acid	-	IBD:CD
	<i>Roseburia hominis</i>	Urobilin, Dodecanedioic acid	+	Non -IBD
		Eicosatrienoic acid	-	IBD:CD
	<i>Dorea longicatena</i>	Urobilin	+	Non -IBD
	<i>Eubacterium hallii</i>	Urobilin, 3-Methyladipate-pimelate	+	Non -IBD

	Linoleoyl ethanolamide, Docosapentaenoic acid, Eicosatrienoic acid	-	IBD:CD
<i>Eubacterium siraeum</i>	C14 carnitine, C3-DC-CH3 carnitine	-	IBD:CD+UC
	Dodecanedioic acid	+	Non -IBD
<i>Alistipes shahii</i>	N-Acetylputrescine, Phytosphingosine	-	IBD:CD
	Urobilin	+	Non -IBD
<i>Alistipes putredinis</i>	C3-DC-CH3 carnitine	-	IBD:CD+UC
	Urobilin	+	Non -IBD
<i>Alistipes finegoldii</i>	Taurine	-	IBD:CD
	5 α -Cholesterol	+	Non -IBD
<i>Roseburia inulinivorans</i>	Cholate, Chenodeoxycholate	-	IBD:CD
	Urobilin, 4-Methylcatechol, Cholestenone	+	Non -IBD
<i>Roseburia intestinalis</i>	2-Hydroxyphenethylamine, Linoleoyl ethanolamide, Eicosatrienoic acid	-	IBD:CD
	Urobilin, Hydrocinnamic acid	+	Non -IBD
	Linoleoyl ethanolamide	-	IBD:CD
<i>Faecalibacterium prausnitzii</i>	C14 carnitine	-	IBD:CD+UC
	Urobilin	+	Non -IBD
<i>Eubacterium aligens</i>	2-Hydroxyphenethylamine	-	IBD:CD
	Linoleoyl ethanolamide, Palmitoylethanolamide, Docosapentaenoic acid, Eicosatrienoic acid	-	IBD:CD
<i>Bacteroidales bacterium ph8</i>	Urobilin	+	Non -IBD
	C3-DC-CH3 carnitine	-	IBD:CD+UC
<i>Alistipes indistinctus</i>	Dodecanedioic acid	+	Non -IBD
<i>Alistipes senegalensis</i>	Linoleoyl ethanolamide, C18:0 CE	-	IBD:CD
<i>Ruminococcus callidus</i>	Caproic acid	+	Non -IBD
<i>Holdemania filiformis</i>	Urobilin, Cholestenone	+	Non -IBD
	C14 carnitine	-	IBD:CD+UC
<i>Gordonibacter pamelaee</i>	Pipecolic acid	+	Non -IBD
	Cholate, Chenodeoxycholate	-	IBD:CD
<i>Lachnospiraceae bacterium</i>	Urobilin, Pipecolic acid, 2-Hydroxyhexadecanoate, Cholestenone	+	Non -IBD

	<i>Adlercreutzia equolifaciens</i>	ADMA, Cholate	-	IBD:CD
		Urobilin, Cholestenone, 5α-Cholesterol, 3-Methyladipate-pimelate+		Non -IBD
		2-Hydroxyphenethylamine, N-Acetylputrescine, ADMA, Cholate, -		IBD:CD
		Chenodeoxycholate		
	<i>Alistipes onderdonkii</i>	C14 carnitine	-	IBD:CD+UC
		Urobilin, 2-Hydroxyhexadecanoate, Cholestenone, 5α-	+	Non -IBD
		Cholesterol, Dodecanedioic acid, 3-Methyladipate-pimelate,		
		Undecanedionate, Azelaic acid		
		Taurine	-	IBD:CD
		C14 carnitine	-	IBD:CD+UC
	<i>Blautia producta</i>	Docosapentaenoic acid, Eicosatrienoic acid	+	IBD:CD
	<i>Lactobacillus gasseri</i>	Taurine	+	IBD:CD
		Carnosol	-	Non -IBD
	<i>Enterococcus faecium</i>	2-Hydroxyphenethylamine	+	IBD:CD
	<i>Lachnospiraceae bacterium</i>	Docosapentaenoic acid	+	IBD:CD
	<i>Clostridium clostridioforme</i>	Docosapentaenoic acid, Eicosatrienoic acid	+	IBD:CD
		Carnosol, Urobilin	-	Non -IBD
	<i>Roseburia gnavus</i>	Docosapentaenoic acid, Eicosatrienoic acid	+	IBD:CD
		Caprylic acid, 5α-Cholesterol, Caproic acid	-	Non -IBD
[113]	<i>Clostridium</i>	Glycine, Homocysteine	+	IBS
<i>n</i> = 30; HC <i>n</i> = 15;	<i>Lachnospira</i>	Homocysteine	+	
IBS <i>n</i> = 15	<i>Haemophilus</i>	Homocysteine	+	
Faeces	<i>Corynebacterium</i>	Homocysteine	-	
	<i>Lachnospiraceae</i>	Homocysteine	-	
[114]	<i>Ruminococcus gnavus</i> group	Glycoprotein acetyls	+	Steatosis
<i>n</i> = 1355; No-				
Steatosis <i>n</i> = 883;				
Steatosis <i>n</i> = 472				
Serum				
[115]	<i>Gemmiger formicilis</i>	Lithocholic acid	+	NAFLD

n = 68; HC *n* = 36;
NAFLD *n* = 32

	7-Dehydrocholic acid, 3-Dehydrocholic acid, Cholic acid, Chenodeoxycholic acid, 12-Dehydrocholic acid, 3 β -cholic acid, β Muricholic acid, Allocholic acid, 6-Keto-Lithocholic acid, Ursodeoxycholic acid, Taurohyocholic acid, Tauroursodeoxycholic acid, Chenodeoxycholic acid-3Gln, Taurocholic acid, Glycocholic acid, Glycochenodeoxycholic acid, 6,7-Diketolithocholic acid	-
<i>Ruminococcus bicirculans</i>	7,12-Diketolithocholic acid, 7-Ketolithocholic acid, Lithocholic acid, Hyodeoxycholic acid, Nordeoxycholic acid	+
<i>Neglecta timonensis</i>	7,12-Diketolithocholic acid, 7-Ketolithocholic acid, Lithocholic acid, Glycolithocholic acid, β Deoxycholic acid, Nordeoxycholic acid	+
	7-Dehydrocholic acid, 3-Dehydrocholic acid, Cholic acid, Chenodeoxycholic acid, 12-Dehydrocholic acid, Taurohyocholic acid, Chenodeoxycholic acid-3Gln, Taurocholic acid	-
<i>Oscillibacter sp.</i>	7,12-Diketolithocholic acid, 7-Ketolithocholic acid, Lithocholic acid, Glycolithocholic acid, Dehydrocholic acid, β Deoxycholic acid, Hyodeoxycholic acid, Nordeoxycholic acid	+
	3-Dehydrocholic acid, Cholic acid, Chenodeoxycholic acid, Murocholic acid, Taurocholic acid	-
<i>Enterobacter cloacae</i>	Chenodeoxycholic acid-3Gln	+
	7,12-Diketolithocholic acid, Hyodeoxycholic acid	-
<i>Escherichia coli</i>	Glycocholic acid	+
	7,12-Diketolithocholic acid, 7-Ketolithocholic acid, Lithocholic acid, β Deoxycholic acid, Hyodeoxycholic acid, Nordeoxycholic acid	-
<i>Eubacterium sp.</i>	7,12-Diketolithocholic acid	+
	Glycolithocholic acid-3S, Chenodeoxycholic acid-3Gln, Taurodeoxycholic acid	-
<i>Bacteroides intestinalis</i>	Taurolithocholic acid, 6,7-Diketolithocholic acid	+

	<i>Akkermansia muciniphila</i>	7,12-Diketolithocholic acid, 7-Ketolithocholic acid, Lithocholic acid, Glycolithocholic acid, Deoxycholic acid, Dehydrocholic acid, β Deoxycholic acid, Glycodeoxycholic acid, α Muricholic acid	-	
	<i>Eubacterium</i> sp.	7,12-Diketolithocholic acid, 7-Ketolithocholic acid, Lithocholic acid	+	
[116]	<i>Ruminococcus</i>	2-Butanone	-	NAFLD
<i>n</i> = 115; HC <i>n</i> =54;	<i>Coprococcus</i>	4-Methyl-2-pentanone	-	HC
OB <i>n</i> = 8; NAFLD	<i>Streptococcus</i>	2-Butanone	-	NAFLD
<i>n</i> = 27; NASH <i>n</i> =	<i>Blautia</i>	4-Methyl-2-pentanone	-	HC
26		4-Methyl-2-pentanone	+	NAFLD
Faeces				
[117]	<i>Faecalibacterium</i>	Steroids, Phosphatidylethanolamine, Phosphatidylcholine, Ceramides, Glycerophospholipid, Potassium chloride	+	CAD -
<i>n</i> = 201; HC <i>n</i> =	<i>Roseburia</i>			
40; CAD <i>n</i> = 161	<i>Oscillibacter</i>	Fatty acyls, Carboxylic acids, Benzene/derivatives, Prenol lipids, Glycerolipids, Amino acids (L-Leucine)	-	CAD +
Serum	Lachnospiraceae (CAG4)			
	<i>Clostridium</i> IV	Potassium chloride, Addictives/ingredients	-	CAD -
	<i>Alistipes</i>			
	<i>Butyricimonas</i>			
	Clostridiales (CAG5)			
	<i>Escherichia/Shigella</i>	Phosphatidylethanolamine, Phosphatidylcholine	-	CAD -
	<i>Bacteroides</i>			
	<i>Dialister</i>			
	Lactobacillaceae			
	<i>Eggerthella</i>			
	<i>Clostridium</i> IV, XIVa, XIVb, XVIII			
	<i>Flavonifractor</i>			
	<i>Coprobacillus</i>			
	Erysipelotrichaceae incertae sedis			

(CAG9)			
<i>Butyricimonas</i>	Fatty acyls, Carboxylic acids, Glycerolipids	+	CAD +
<i>Bacteroides</i>			
<i>Barnesiella</i>			
<i>Coprobacar</i>	Addictives/ingredients	-	CAD -
<i>Alistipes</i>			
(CAG13)			
<i>Ruminococcus 2</i>	Prenol lipids	-	CAD +
<i>Dorea</i>			
<i>Blautia</i>			
<i>Clostridium XVIII</i>			
Lachnospiracea incertae sedis			
(CAG14)			
<i>Anaerostipes</i>	Sphingolipids, Phosphatidylethanolamine, Addictives/ingredients	+	CAD -
<i>Blautia</i>			
Lactobacillaceae			
<i>Fusicatenibacter</i>	Benzene/derivatives, Glycerolipids	-	CAD +
<i>Clostridium XIVa</i>			
<i>Gemella</i>			
<i>Bifidobacterium</i>			
<i>Saccharibacteria genera incertae sedis</i>	Taurine	-	CAD -
(CAG15)			
<i>Roseburia</i>	Addictives/ingredients	+	CAD -
<i>Clostridium XIVb</i>			
<i>Parasutterella</i>	Fatty acyls, Carboxylic acids, Benzene/derivatives, Prenol lipids, Glycerolipids	-	CAD +
<i>Butyricicoccus</i>			
Lachnospiracea incertae sedis	Taurine	-	CAD -
(CAG16)			
<i>Oscillibacter</i>	Fatty acyl carnitines, Addictives/ingredients	-	CAD -
<i>Clostridium IV</i>			

	(CAG19)			
	<i>Oscillibacter</i>	Benzene/derivatives	+	CAD +
	<i>Clostridium IV, XIVa</i>			
	(CAG23)	Fatty acyl carnitines, Potassium chloride, Addictives/ingredients	-	CAD -
[118] <i>n</i> = 196; HC <i>n</i> = 41; pHT <i>n</i> = 56; HT <i>n</i> = 99 <i>n</i> = 124; HC <i>n</i> = 30; pHT <i>n</i> = 31; HT <i>n</i> = 63 subset Serum	<i>Butyricicoccus</i>	PA (12:0/0:0), Hippurin-1	+	HT/HC
		LysoPC (18:2)	-	HC
	<i>Intestinimonas</i>	Na-Acetyl-L-arginine, S-Carboxymethyl-L-cysteine, Hippurin-1	+	HT/HC/HC
		LysoPC (18:2)	-	HC
	<i>Ruminococcus</i>	Trichloroethanol glucuronide	+	HC
		PA (12:0/0:0), 3-Keto stearic acid, LysoPC (18:2), PS(O-18:0/0:0)	-	HT/HT/HC/HC
	<i>Paenibacillus</i>	9,10-Dichloro-octadecanoic acid, Petunidin 3-rhamnoside 5-glucoside, Hippurin-1	+	HT/HT/HC
		Trichloroethanol glucuronide	-	HC
	<i>Lachnoclostridium</i>	PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid, Petunidin 3-rhamnoside 5-glucoside, 3-Keto stearic acid, Pyridine	+	HT/HT/HT/HT/HC
		Trichloroethanol glucuronide	-	HC
	<i>Butyrivibrio</i>	Petunidin 3-rhamnoside 5-glucoside	+	HT
	<i>Faecalibacterium</i>	Petunidin 3-rhamnoside 5-glucoside, 3-Keto stearic acid	+	HT/HT
	<i>Enterococcus</i>	9,10-Dichloro-octadecanoic acid	+	HT
	<i>Coprococcus</i>	Na-Acetyl-L-arginine, Petunidin 3-rhamnoside 5-glucoside	+	HT/HT
	<i>Flavonifractor</i>	3-Keto stearic acid	-	HT
	<i>Blautia</i>	PS (O-18:0/0:0)	+	HC
		PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid, 3-Keto stearic acid	-	HT/HT/HT
	<i>Bifidobacterium</i>	Trichloroethanol glucuronide	+	HC
		PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid, 3-Keto stearic acid	-	HT/HT/HT
	<i>Subdoligranulum</i>	LysoPC(18:2), Trichloroethanol glucuronide	+	HC/HC
		PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid, Petunidin 3-rhamnoside 5-glucoside	-	HT/HT/HT
	<i>Marvinbryantia</i>	S-Carboxymethyl-L-cysteine, Trichloroethanol glucuronide	+	HC/HC

	PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid, Petunidin 3-rhamnoside 5-glucoside	-	HT/HT/HT
<i>Holdemania</i>	Na-Acetyl-L-arginine, Pyridine, S-Carboxymethyl-L-cysteine, PS (O-18:0/0:0)	+	HT/HC/HC/HC
	PA (12:0/0:0)	-	HT
<i>Robinsoniella</i>	Na-Acetyl-L-arginine, Pyridine, PS(O-18:0/0:0), Trichloroethanol glucuronide	+	HT/HC/HC/HC
<i>Veillonella</i>	3-Keto stearic acid, LysoPC(22:5), Pyridine	+	HT/HC/HC
	PA (12:0/0:0)	-	HT
<i>Clostridium</i>	9,10-Dichloro-octadecanoic acid	-	HT
<i>Oribacterium</i>	Pyridine	+	HC
	PA (12:0/0:0), Na-Acetyl-L-arginine, 3-Keto stearic acid, PS (O-18:0/0:0)	-	HT/HT/HT/HC
<i>Bilophila</i>	Pyridine	+	HC
	Na-Acetyl-L-arginine, 3-Keto stearic acid	-	HT/HT
<i>Akkermansia</i>	PA (12:0/0:0), Pyridine, Trichloroethanol glucuronide	+	HT/HC/HC
	Na-Acetyl-L-arginine	-	HT
<i>Pyramidobacter</i>	LysoPC (22:5), Hippurin-1	+	HC/HC
	PA (12:0/0:0), Pyridine	-	HT/HC
<i>Tyzzerella</i>	LysoPC (18:2)	+	HC
	Petunidin 3-rhamnoside 5-glucoside, 3-Keto stearic acid, Pyridine	-	HT/HT/HC
<i>Roseburia</i>	LysoPC (22:5), S-Carboxymethyl-L-cysteine, Hippurin-1	+	HC/HC/HC
	PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid, Na-Acetyl-L-arginine	-	HT/HT/HT
<i>Ruminiclostridium</i>	LysoPC (22:5), LysoPC (18:2), Hippurin-1	+	HC/HC/HC
	Na-Acetyl-L-arginine, Trichloroethanol glucuronide	-	HT/HC
<i>Oscillibacter</i>	PA (12:0/0:0)	+	HT
	Na-Acetyl-L-arginine, LysoPC (22:5), S-Carboxymethyl-L-cysteine	-	HT/HC/HC
<i>Treponema</i>	PA (12:0/0:0)	+	HT
	LysoPC (22:5), Pyridine, LysoPC (18:2)	-	HC/HC/HC
<i>Peptoclostridium</i>	PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid	+	HT/HT

	S-Carboxymethyl-L-cysteine, Trichloroethanol glucuronide, Hippurin-1	-	HC/HC/HC
<i>Anaerotruncus</i>	PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid, PS (O-18:0/0:0), Hippurin-1	-	HT/HT/HC/HC
<i>Eggerthella</i>	3-Keto stearic acid, LysoPC (22:5)	+	HT/HC
	PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid, Hippurin-1	-	HT/HT/HC
<i>Acidiphilium</i>	PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid, 3-Keto stearic acid, LysoPC(18:2), PS(O-18:0/0:0), Trichloroethanol glucuronide	+	HT/HT/HT/HC/HC/HC
	Na-Acetyl-L-arginine, Petunidin 3-rhamnoside 5-glucoside	-	HT/HT
<i>Klebsiella</i>	9,10-Dichloro-octadecanoic acid, S-Carboxymethyl-L-cysteine	+	HT/HC
	Hippurin-1	-	HC
<i>Azospirillum</i>	Na-Acetyl-L-arginine	+	HT
	Hippurin-1	-	HC
<i>Prevotella</i>	PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid	+	HT/HT
	3-Keto stearic acid, LysoPC (22:5), Trichloroethanol glucuronide	-	HT/HC/HC
<i>Dorea</i>	PA (12:0/0:0), 3-Keto stearic acid	+	HT/HT
	9,10-Dichloro-octadecanoic acid, Trichloroethanol glucuronide	-	HT/HC
<i>Acidaminococcus</i>	PA (12:0/0:0)	+	HT
	Trichloroethanol glucuronide	-	HC
<i>Enterobacter</i>	PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid, Petunidin 3-rhamnoside 5-glucoside	+	HT/HT/HT
	3-Keto stearic acid	-	HT
<i>Streptococcus</i>	Hippurin-1	+	HC
	Na-Acetyl-L-arginine, LysoPC (18:2)	-	HT/HC
<i>Porphyromonas</i>	9,10-Dichloro-octadecanoic acid, LysoPC (22:5), Pyridine, Hippurin-1	+	HT/HC/HC/HC
	PS (O-18:0/0:0)	-	HC
<i>Coprobacillus</i>	Petunidin 3-rhamnoside 5-glucoside	+	HT
	9,10-Dichloro-octadecanoic acid, LysoPC (22:5), S-Carboxymethyl-L-cysteine	-	HT/HC/HC
<i>Actinomyces</i>	3-Keto stearic acid	+	HT

<i>Desulfovibrio</i>	PA (12:0/0:0), 9,10-Dichloro-octadecanoic acid, LysoPC (22:5),	-	HT/HT/HC/HC
	Pyridine		
	3-Keto stearic acid	+	HT
	Pyridine, Trichloroethanol glucuronide, Hippurin-1	-	HC/HC/HC

CAD: coronary artery disease; CAG: co-abundance group; CD: Crohn's disease; HC: healthy control; HCHS/SOL: Hispanic Community Health Study/Study of Latinos; HT: hypertension; IBD: irritable bowel disease; IBS: irritable bowel syndrome; IGR: impaired glucose regulation; LC: lean control; LH: lean healthy; MLGs: metagenomic linkage groups; MM: microbial modules; NAFLD: non-alcoholic fatty liver disease; NASH: non-alcoholic steatohepatitis; ND: not determined; NGT: normal glucose tolerance; Non-PN SBS: parenteral nutrition-independent short bowel syndrome; NW: normal weight; OB: obese; ObH: obese healthy; OW: overweight; PCOS: polycystic ovary syndrome; p-HT: pre-hypertension; SBS I: parenteral nutrition-dependent short bowel syndrome I; SBS II: parenteral nutrition-dependent short bowel syndrome II; T2D: type 2 diabetes; T2D+: diabetes with chronic complications; T2D-: diabetes without chronic complications; UC: ulcerative colitis.