

634 **Supplementary Tables**

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636 **Supplementary Table 1.** Features (Host characteristics and dietary habits) used in Dataset 1.

Host Characteristics	Dietary Habits
Age	Whether you drink milk (Yes/No)
Race	Whether you eat yogurt (Yes/No)
Height (cm)	Whether you eat cheese (Yes/No)
Weight (kg)	Quantity of eating vegetables
Whether currently exercise on a fairly regular basis (Yes/No)	Quantity of eating fruit
Whether you smoke(d) cigarettes (Yes/No)	Frequency of eating eggs
Whether you drink (drank) alcohol (Yes/No)	Quantity of eating eggs in a day
Whether you are currently taking any probiotics supplements (Yes/No)	Frequency of eating steak
Whether you have you taken any probiotics in the past 12 months (Yes/No)	Quantity of eating steak in a day
BMI	Frequency of eating pork chops
Whether you have used antibiotics in the past 12 months (Yes/No)	Quantity of eating pork chops in a day
Whether you are currently taking any gastric acid lowering medications (Yes/No)	Frequency of eating cookies
Whether you have you taken any gastric acid lowering medications in the past 12 months (Yes/No)	Quantity of eating cookies in a day
Frequency of bicycling or swimming	Frequency of eating chocolate candy
Time in bicycling or swimming for each time	Quantity of eating chocolate candy in a day
Frequency of heavy work	Frequency of eating cold cereals
Time in heavy work for each time	Quantity of eating cold cereals in a day
	Quantity of drinking water in a day
	Frequency of drinking milky coffee
	Quantity of drinking milky coffee in a day
	Frequency of drinking non-milky coffee
	Quantity of drinking non-milky coffee in a day
	Frequency of drinking hot tea
	Quantity of drinking hot tea in a day
	Frequency of eating pickles
	Quantity of eating pickles in a day
	Frequency of taking folic acid
	Frequency of taking fiber supplements
	Frequency of taking calcium
	Quantity of taking calcium in a day
	Frequency of taking fat oil
	Number of meals in a day
	How much eating fried fish, fish sticks, fish sandwich, breaded fillets (g)

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639 **Supplementary Table 2.** Features (Host characteristics and dietary habits) used in Dataset 2.

Host Characteristics	Dietary Habits
Age	Whether you drink milk (Yes/No)
Gender	Whether you eat yogurt (Yes/No)
Race	Whether you eat cheese (Yes/No)
Height (cm)	
Weight (kg)	
Whether currently exercise on a fairly regular basis (Yes/No)	
Whether you smoke(d) cigarettes (Yes/No)	
Whether you drink (drank) alcohol (Yes/No)	
Whether you are currently taking any probiotics supplements (Yes/No)	
Whether you have you taken any probiotics in the past 12 months (Yes/No)	
BMI	

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Supplementary Table 3. Hyperparameters Tuning.

Hyperparameters	Values
Dropout	0.1, 0.3, 0.5, 0.7
Number of epochs	1000, 1500, 2000, 2500, 3000
Average number of edges per node that are retained including self-connections (k)	2, 5, 10

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Supplementary Table 4. Important factors associated with blood acetic acids.

Gut Microbiotas		Host Characteristics		Dietary Features	
Dataset 1	Dataset 2	Dataset 1	Dataset 2	Dataset 1	Dataset 2
Subdoligranulum_unclassified	Bacteroides_intestinalis	Weight (kg)	Gender	Frequency of eating pickles	Whether you eat yogurt
Ruminococcus_torques	candidate_division_TM7_single_cell_isolate_TM7b	Time in bicycling or swimming for each time	Race	Frequency of eating steak	Whether you drink milk
Oscillibacter_unclassified	Atopobium_vaginae	Whether you have you taken any probiotics in the past 12 months (Yes/No)	Height (cm)	Frequency of taking fat oil	Whether you eat cheese
Bacteroides_uniformis	Weissella_confusa	Height (cm)	Weight (kg)	Quantity of eating eggs in a day	
Clostridium_asparagiforme	Lachnospiraceae_bacterium_2_1_46FAA	Whether you have used antibiotics in the past 12 months (Yes/No)	Whether you have you taken any probiotics in the past 12 months (Yes/No)	Quantity of eating cold cereals in a day	
Ruminococcus_sp_5_1_39BFAA	Bombyx_mori_nucleopolyhedrovirus				
Rothia_mucilaginosa	Streptococcus_mutans				
Prevotella_copri	Faecalibacterium_prausnitzii				
Roseburia_intestinalis	Clostridium_sp_HGF2				
Bacteroides_thetaiotaomicron	Ruminococcus_obeum				
Desulfovibrio_piger	Bordetella_unclassified				
Alistipes_unclassified	Anaerococcus_vaginalis				
Bifidobacterium_catenulatum	Alistipes_sp_HGB5				
Lactobacillus_salivarius	Avian_carcinoma_virus				
Clostridium_leptum	New_World_begomovirus_associated_satellite_DNA				
Acidaminococcus_sp_BV3L6	Sapporo_virus				

Erysipelotrichaceae_bacterium_6_1_45	Bifidobacterium_breve
Bacteroides_fragilis	Gemella_sanguinis
Parabacteroides_merdae	Fusobacterium_necrophorum
Alistipes_senegalensis	Culex_flavivirus
Mitsuokella_unclassified	Anaerotruncus_colihominis
Bacteroides_caccae	Lachnospiraceae_bacterium_5_1_63FAA
Turcibacter_unclassified	Bacteroides_cellulosilyticus
Bacteroides_sp_4_3_47FAA	Porphyromonas_asaccharolytica
Blautia_hansenii	Alistipes_finegoldii
Clostridium_clostridioforme	Facklamia_unclassified
Rhodococcus_erythropolis	Staphylococcus_phage_phiETA3
Clostridium_citroniae	Cupriavidus_unclassified
Ruminococcus_albus	Chicory_yellow_mottle_virus_large_satellite_RNA
Bacteroides_eggertii	Erysipelotrichaceae_bacterium_21_3
	Gemella_unclassified
	Porphyromonas_uenonis
	Classical_swine_fever_virus
	Eubacterium_infirmum
	Enterovirus_B
	Escherichia_unclassified
	Eubacterium_sp_3_1_31
	Coprobacillus_unclassified

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Bovine_viral_diarrhea_virus_2

Fusobacterium_nucleatum

Coprobacter_fastidiosus

Coprobacillus_sp_D6

Clostridiales_bacterium_1_7_47FAA

Ruminococcus_sp_JC304

Bacteroides_dorei

Mycoplasma_hominis

Actinomyces_urogenitalis

Bovine_viral_diarrhea_virus_3

Royal_Farm_virus

Prevotella_timonensis

Pseudomonas_thermotolerans

Coprococcus_sp_ART55_1

Bacteroides_pectinophilus

Blautia_hydrogenotrophica

Dorea_unclassified

Collinsella_aerofaciens

Sutterella_wadsworthensis

Eubacterium_biforme

Clostridiales_bacterium_BV3C26

Clostridium_sp_KLE_1755

Melon_aphid_borne_yell

ows_virus
Veillonella_dispar
Bacteroides_salysersiae
Clostridium_bartlettii
Lachnospiraceae_bacteri
um_9_1_43BFAA
Campylobacter_ureolyti
cus
Lactobacillus_antri
Montana_myotis_leukoe
ncephalitis_virus
Entamoeba_dispar
Leuconostoc_gelidum
Caulobacter_unclassified
Fusobacterium_periodon
ticum
Coriobacteriaceae_bacte
rium_BV3Ac1
Cardiobacterium_valvar
um
Bacteroides_fragilis
Bifidobacterium_pseudo
longum
Porphyromonas_bennoni
s
Orthohepadnavirus_uncl
assified
Ruminococcus_gnavus
Alistipes_sp_AP11
Enterovirus_D
Lactobacillus_mucosae
Streptococcus_macedoni
cus
**Bacteroides_thetaiota
micron**
Coprobacillus_sp_29_1

Chicken_anemia_virus
Lachnospiraceae_bacteri
um_1_4_56FAA
Eggerthella_lenta
Cetobacterium_somerae
Circovirus_like_genome
_SAR_A
Granulicatella_elegans
Ruminococcus_flavefaci
ens
Parascardovia_denticole
ns
Pseudomonas_phage_M
P38
Bilophila_unclassified
Actinomyces_viscosus
Actinomyces_naeslundii
Streptococcus_agalactiae
Salmon_pancreas_diseas
e_virus
C2likevirus_unclassified

Note: Top 30 gut microbiota species in dataset 1; top 100 gut microbiota species in dataset 2. Top 5 host characteristics features and top 5 dietary features in datasets 1 and 2.

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Supplementary Table 5. Important factors associated with blood butyric acids.

Gut Microbiotas		Host Characteristics		Dietary Features	
Dataset 1	Dataset 2	Dataset 1	Dataset 2	Dataset 1	Dataset 2
Ruminococcus_torques	Ruminococcaceae_bacterium_D16	Weight (kg)	Gender	Frequency of eating pickles	Whether you eat yogurt
Subdoligranulum_unclassified	Nilaparvata_lugens_honeydew_virus_2	Whether you have you taken any probiotics in the past 12 months (Yes/No)	Race	Quantity of eating cold cereals in a day	Whether you drink milk
Roseburia_intestinalis	Bordetella_unclassified	Whether you are currently taking any gastric acid lowering medications (Yes/No)	Weight (kg)	Quantity of eating chocolate candy in a day	Whether you eat cheese
Oscillibacter_unclassified	Providencia_unclassified	Height (cm)	BMI	Frequency of eating steak	
Bifidobacterium_catenulatum	Weissella_confusa	Whether you have used antibiotics in the past 12 months (Yes/No)	Whether you have you taken any probiotics in the past 12 months (Yes/No)	Quantity of eating steak in a day	
Bacteroides_thetaiotaomicron	Coprococcus_sp_ART55_1				
Parabacteroides_merdae	Coriobacteriaceae_bacterium_BV3Ac1				
Turicibacter_unclassified	Eubacterium_infirmum				
Bacteroides_cacciae	Corynebacterium_durum				
Bacteroides_uniformis	Apoi_virus				
Prevotella_copri	Alistipes_finegoldii				
Rothia_mucilaginososa	Plectrovirus_unclassified				
Erysipelotrichaceae_bacterium_6_1_45	Actinomyces_turicensis				
Erysipelotrichaceae_bacterium_6_1_45	Anaerostipes_caccae				
Blautia_hansenii	Alistipes_indistinctus				
Ruminococcus_spp_5_1_39BFAA	Parabacteroides_johnsonii				

Alistipes_senegalensis	Erysipelotrichaceae_bacterium_21_3
Desulfovibrio_piger	Eggerthella_unclassified
Bacteroides_vulgaris	Lactobacillus_animalis
Veillonella_unclassified	Lactobacillus_vaginalis
Streptococcus_salivarius	Campylobacter_ureolyticus
Lactobacillus_plantarum	Atopobium_parvulum
Rhodococcus_erythropolis	Enterococcus_casseliflavus
Eubacterium_limosum	Leuconostoc_pseudomenteroides
Faecalibacterium_prausnitzii	Megasphaera_micronuciformis
Ruminococcus_albus	Desulfovibrio_terminidis
Oscillibacter_sp_KLE_1745	Enterococcus_avium
Propionibacterium_freudenreichii	Peptostreptococcus_unclassified
Clostridium_amaragiforme	Lachnospiraceae_bacterium_5_1_63FAA
Weissella_unclassified	Clostridium_sp_HGF2
	Quail_picornavirus_QPV1_HUN_2010
	Leuconostoc_carnosum
	Dialister_succinatiphilus
	Prevotella_bergensis
	Actinobacillus_unclassified
	Ruminococcus_obeum
	Bifidobacterium_pseudotenulatum
	Alistipes_sp_AP11

Collinsella_stercoris
Porphyromonas_uenonis
Streptococcus_tigurinus
Turicibacter_sanguinis
Actinomyces_massiliensis
Bacteroides_intestinalis
Anaerostipes_sp_3_2_56F
AA
Cupriavidus_unclassified
Weissella_paramesenteroides
Holdemania_unclassified
Clostridium_hathewayi
Streptococcus_salivarius
Chicory_yellow_mottle_virus_large_satellite_RNA
Leuconostoc_mesenteroides
Odoribacter_splanchnicus
Culex_flavivirus
Clostridiales_bacterium_BV3C26
Blautia_hydrogenotrophica
Clostridiaceae_bacterium_JC118
Clostridium_glycolicum
Clostridium_sp_KLE_1755
Bifidobacterium_pseudolongum
Collinsella_aerofaciens
Veillonella_unclassified
Leuconostoc_inhae
Dysgonomonas_unclassifi

ed

Okra_yellow_crinkle_Cam

eroon_alphasatellite

Streptococcus_australis

Lactobacillus_helveticus

Bovine_viral_diarrhea_vir

us_2

Rhodopseudomonas_palus

tris

Bacteroides_pectinophilus

Bacteroides_coprocola

Passion_fruit_woodiness_

virus

Slackia_unclassified

Prevotella_timonensis

Bombyx_mori_nucleopoly

hedrovirus

Hepatitis_C_virus

Fusobacterium_necrophor

um

Anaerococcus_vaginalis

Avian_carcinoma_virus

Clostridium_bifermentans

Gastropod_associated_circ

ular_ssDNA_virus

Actinomyces_urogenitalis

Olsenella_unclassified

Bilophila_wadsworthia

Hafnia_alvei

Oat_blue_dwarf_virus

Dorea_formicigenerans

Akkermansia_muciniphila

Hepatitis_A_virus

Streptococcus_mutans

Lactobacillus_salivarius
Lactobacillus_casei_parac
asei
Pepper_vein_yellows_viru
s
**Oscillibacter_sp_KLE_1
745**
Bacteroidales_bacterium_
ph8
Mycoplasma_hominis
Ruminococcus_bromii
Pseudomonas_thermotoler
ans
Cardiobacterium_valvaru
m
Lindernia_anagallis_yello
w_vein_virus_satellite_D
NA_beta

Note: Top 30 gut microbiota species in dataset 1 ; top 100 gut microbiota species in dataset 2. Top 5 host characteristics features and top 5 dietary features in datasets 1 and 2.

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Supplementary Table 6. Important factors associated with blood hexanoic acids.

Gut Microbiotas		Host Characteristics		Dietary Features	
Dataset 1	Dataset 2	Dataset 1	Dataset 2	Dataset 1	Dataset 2
Subdoligranulum_unclassified	Ruminococcus_bromii	Weight (kg)	Consent_Age	Quantity of eating steak in a day	Whether you eat yogurt
Ruminococcus_torques	Erysipelotrichaceae_bacterium_21_3	Frequency of heavy work	Gender	Quantity of eating eggs in a day	Whether you drink milk
Oscillibacter_unclassified	Faecalibacterium_prausnitzii	Height (cm)	Height (cm)	Frequency of eating steak	Whether you eat cheese
Alistipes_unclassified	Lachnospiraceae_bacterium_5_1_63FAA	Exercise_Regular	Race	Frequency of eating pickles	
Clostridium_asparagiforme	Ruminococcaceae_bacterium_D16	Time in heavy work for each time	Whether you have you taken any probiotics in the past 12 months (Yes/No)	Frequency of taking fat oil	
Bacteroides_uniformis	Desulfovibrio_termitidis				
Desulfovibrio_piger	Collinsella_stercoris				
Rothia_mucilaginosa	Coriobacteriaceae_bacterium_BV3Ac1				
Ruminococcus_sp_5_1_39BFAA	candidate_division_TM7_single_cell_isolate_TM7b				
Clostridium_leptum	Lactobacillus_phage_PL_1				
Bacteroides_thetaiotaomicron	Clostridium_sp_HGF2				
Roseburia_intestinalis	Dorea_formicigenerans				
Lactobacillus_salivarius	Classical_swine_fever_virus				
Prevotella_copri	Solobacterium_moorei				
Clostridium_citroniae	Lactobacillus_casei_paracasei				
Bacteroides_nordii	Gemella_unclassified				
Faecalibacterium_prausnitzii	Actinomyces_naeslundii				
Parabacteroides_unclassified	Turicibacter_sanguinis				
Bifidobacterium_cate	Lactobacillus_saerimneri				

nulatum

Bacteroides_sp_4_3_47FAA	Ruminococcus_obeum
Clostridium_bolteae	Bordetella_unclassified
Clostridium_clostridioforme	Lindernia_anagallis_yellow_vein_virus_satellite_DNA_beta
Acidaminococcus_sp_BV3L6	Enterovirus_B
Erysipelotrichaceae_bacterium_6_1_45	Lachnospiraceae_bacterium_4_1_37FAA
Paraprevotella_clara	Clostridiaceae_bacterium_JC118
Bacteroides_fragilis	Roseburia_inulinivorans
Bacteroides_dorei	Weissella_confusa
Leuconostoc_gelidum	Acidaminococcus_sp_BV3L6
Bacteroides_eggerthii	Ruminococcus_sp_JC304
Blautia_hansenii	Clostridium_bifermentans
	Chicory_yellow_mottle_virus_large_satellite_RNA
	Campylobacter_ureolyticus
	Oat_blue_dwarf_virus
	Streptococcus_vestibularis
	Coriobacteriaceae_bacterium_phi
	I
	Enterobacteria_phage_SfV
	Facklamia_unclassified
	Actinomyces_viscosus
	Ruminococcus_champanellensis
	Actinomyces_massiliensis
	Lactobacillus_animalis
	Anaerostipes_caccae
	Quail_picornavirus_QPV1_HUN_2010
	West_Nile_virus

Atopobium_vaginae
Lactococcus_lactis
Bacteroides_intestinalis
Sida_yellow_vein_Vietnam_virus_satellite_DNA_beta
Streptococcus_parasanguinis
Enterococcus_avium
Rothia_dentocariosa
Bovine_rhinitis_B_virus
Weissella_paramesenteroides
Bovine_viral_diarrhea_virus_2
Barbel_circovirus
Parvimonas_unclassified
Dysgonomonas_unclassified
Ruminococcus_sp_5_1_39BFA
A
Fusobacterium_mortiferum
Gastropod_associated_circular_sDNA_virus
Parascardovia_denticolens
Erysipelotrichaceae_bacterium_5_2_54FAA
Lactobacillus_vaginalis
Neisseria_flavescens
Phascolarctobacterium_succinatutens
Entamoeba_dispar
Circovirus_like_genome_SAR_A
Sutterella_wadsworthensis
Human_cosavirus_B
Providencia_unclassified
Leuconostoc_carnosum
Peptostreptococcus_anaerobius

Kelp_fly_virus
Fusobacterium_necrophorum
Hepatitis_GB_virus_B
Pennisetum_mosaic_virus
Gemella_haemolysans
Blautia_hydrogenotrophica
Bacteroides_cellulosilyticus
Eubacterium_infirmum
Bilophila_wadsworthia
Petunia_vein_clearing_virus
Porphyromonas_asaccharolytica
Clostridiales_bacterium_BV3C2
6
Holdemania_unclassified
Lactococcus_phage_jm2
Klebsiella_phage_KP36
Plectrovirus_unclassified
Bifidobacterium_breve
Parabacteroides_sp_20_3
Okra_yellow_crinkle_Cameroon
_alphasatellite
Border_disease_virus
Melon_aphid_borne_yellows_virus
Oligella_urethralis
Lactobacillus_antri
Candidatus_Zinderia_insecticola
Haemophilus_sputorum
Malvastrum_leaf_curl_Philippines_betasatellite
Weissella_cibaria
Actinomyces_urogenitalis

651 Note: Top 30 gut microbiota species in dataset 1 ; top 100 gut microbiota species in dataset 2. Top 5 host characteristics features and top 5 dietary features in
652 datasets 1 and 2.
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Supplementary Table 7. Important factors associated with blood 2-methylbutyric acids.

Gut Microbiotas		Host Characteristics		Dietary Features	
Dataset 1	Dataset 2	Dataset 1	Dataset 2	Dataset 1	Dataset 2
Subdoligranulum_unclassified	candidate_division_TM7_singlé_cell_isolate_TM7b	Weight (kg)	Race	Frequency of eating steak	Whether you drink milk
Ruminococcus_torques	Ruminococcus_obeum	Time in bicycling or swimming for each time	Gender	Frequency of eating pickles	Whether you eat yogurt
Bacteroides_uniformis	Weissella_confusa	Height (cm)	BMI	Quantity of eating eggs in a day	Whether you eat cheese
Bifidobacterium_catenulatum	Lactobacillus_phage_PL_1	Age	Whether you have taken any probiotics in the past 12 months (Yes/No)	Frequency of taking fat oil	
Oscillibacter_unclassified	Faecalibacterium_prausnitzii	Race	Weight (kg)	Quantity of eating steak in a day	
Clostridium_asparagiforme	Bovine_viral_diarrhea_virus_2				
Ruminococcus_albus	Anaerostipes_unclassified				
Alistipes_senegalensis	Coriobacteriaceae_bacterium_BV3Ac1				
Alistipes_unclassified	Okra_yellow_crinkle_Cameroon_alphasatellite				
Roseburia_intestinalis	Klebsiella_phage_KP36				
Veillonella_unclassified	Candidatus_Zinderia_insecticola				
Faecalibacterium_prausnitzii	Bordetella_unclassified				
Bacteroides_thetaiotaomicron	Cardiobacterium_valvarum				
Prevotella_copri	Eubacterium_siraeum				
Rothia_mucilaginosa	Zinnia_leaf_curl_virus_associated_DNA_beta				
Acidaminococcus_sp_BV3L6	Granulicella_unclassified				
Clostridium_leptum	Bifidobacterium_pseudolongum				
Desulfovibrio_piger	Clostridium_sp_KLE_1755				

Erysipelotrichaceae_	Ruminococcus_champanell
bacterium_6_1_45	ensis
Ruminococcus_sp_5_	Orthohepadnavirus_unclass
1_39BFAA	ified
Lactobacillus_salivari	Campylobacter_ureolyticus
us	
Clostridium_scindens	Parabacteroides_sp_20_3
Weissella_unclassifie	Streptococcus_agalactiae
d	
Paraprevotella_clara	Dysgonomonas_mossii
Bacteroides_eggerthii	Dorea_formicigenerans
Bacteroides_fragilis	Alloprevotella_tannerae
Bacteroides_sp_4_3_	Aggregatibacter_segnis
47FAA	
Roseburia_hominis	Borrelia_duttonii
Bacteroides_nordii	Granulicatella_unclassified
Bacteroides_caccae	Holdemania_sp_AP2
	Gemella_haemolysans
	Enterobacteria_phage_SfV
	Streptococcus_vestibularis
	Sapporo_virus
	Streptococcus_mutans
	Anaerotruncus_colihominis
	Erysipelotrichaceae_bacteri
	um_21_3
	Coprobacter_fastidiosus
	Eubacterium_ramulus
	Haemophilus_pittmaniae
	Olsenella_unclassified
	Alistipes_sp_HGB5
	Actinomyces_urogenitalis
	Lachnospiraceae_bacterium
	_5_1_63FAA
	Alloprevotella_unclassified

Pseudomonas_phage_MP3
8
Lactobacillus_crispatus
Prevotella_amnii
Bacteroides_coprocola
Anaerococcus_vaginalis
Enterococcus_hirae
Eubacterium_biforme
Barbel_circovirus
Cetobacterium_somerae
Butyrivibrio_crossotus
Peptostreptococcus_anaero
bius
Bovine_viral_diarrhea_viru
s_3
Pediococcus_lolii
Helicobasidium_mompa_e
ndornavirus_1
Culex_flavivirus
Leuconostoc_gasicomitatu
m
Oligella_urethralis
Bacteroides_dorei
Bovine_rhinitis_B_virus
Brachyspira_unclassified
Streptococcus_gordonii
Abiotrophia_defectiva
Lachnospiraceae_bacterium
_4_1_37FAA
Alistipes_finegoldii
Desulfovibrio_terminidis
Lachnospiraceae_bacterium
_9_1_43BFAA
Clostridium_bifermentans

Entamoeba_dispar
Lachnospiraceae_bacterium
_8_1_57FAA
Infectious_flacherie_virus
Bifidobacterium_breve
Lactobacillus_fermentum
Lactobacillus_gasseri
Rothia_mucilaginosa
Pseudomonas_aeruginosa
Bacteroides_fragilis
Clostridium_sp_HGF2
Apoi_virus
Staphylococcus_phage_phi
ETA3
Turicibacter_sanguinis
Lactobacillus_saerimneri
**Erysipelotrichaceae_bacte
rium_6_1_45**
Sepik_virus
Porphyromonas_asaccharol
ytica
Clostridium_difficile
Streptococcus_macedonicu
s
Gastropod_associated_circ
ular_ssDNA_virus
Subdoligranulum_variabile
Hippeastrum_mosaic_virus
Prevotella_bergensis
Colombian_datura_virus
Dorea_unclassified
Royal_Farm_virus
Enterovirus_B

Blautia_hydrogenotrophica

654 Note: Top 30 gut microbiota species in dataset 1 ; top 100 gut microbiota species in dataset 2. Top 5 host characteristics features and top 5 dietary features in
655 datasets 1 and 2.
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Supplementary Table 8. Important factors associated with blood valeric acids.

Gut Microbiotas		Host Characteristics		Dietary Features	
Dataset 1	Dataset 2	Dataset 1	Dataset 2	Dataset 1	Dataset 2
Subdoligranulum_unclassified	Ruminococcus_obeum	Weight (kg)	Gender	Frequency of eating pickles	Whether you drink milk
Ruminococcus_torques	Weissella_confusa	Whether you have you taken any gastric acid lowering medications in the past 12 months (Yes/No)	Race	Quantity of eating chocolate candy in a day	Whether you eat yogurt
Oscillibacter_unclassified	Epsilon15likevirus_unclassified	Whether you have you taken any probiotics in the past 12 months (Yes/No)	Height (cm)	Quantity of eating fruit	Whether you eat cheese
Rothia_mucilaginosa	Faecalibacterium_prausnitzii	Time in heavy work for each time	Weight (kg)	Quantity of eating cold cereals in a day	
Alistipes_unclassified	Classical_swine_fever_virus	Frequency of bicycling or swimming	BMI	Frequency of eating steak	
Desulfovibrio_piger	Campylobacter_ureolyticus				
Clostridium_asparagiforme	Desulfovibrio_terminidis				
Bacteroides_thetaiotaomicron	Clostridium_sp_HGF2				
Bacteroides_uniformis	Bovine_rhinitis_B_virus				
Bacteroides_nordii	C2likevirus_unclassified				
Clostridium_bolteae	candidate_division_TM7_single_cell_isolate_TM7b				
Parabacteroides_unclassified	Eubacterium_sp_3_1_31				
Bacteroides_dorei	Corynebacterium_propinquum				
Clostridium_citroniae	Gemella_unclassified				
Collinsella_unclassified	Prevotella_bergensis				
Clostridium_clostridioforme	Neisseria_flavescens				
Bacteroides_fragilis	Cyclovirus_NGchicken15_NGA_2009				

Faecalibacterium_prausnitzii	Okra_yellow_crinkle_Cameroon_alphasatellite
Clostridium_leptum	Alloprevotella_unclassified
Eubacterium_ramulus	Lachnospiraceae_bacterium_5_1_63FAA
Bacteroides_sp_4_3_47FAA	Peptostreptococcus_anaerobius
Actinomyces_viscosus	Bacteroides_vulgatus
Ruminococcus_sp_5_1_39BFAA	Actinomyces_urogenitalis
Parabacteroides_merdae	Ruminococcus_champanelensis
Leuconostoc_gelidum	Lactobacillus_phage_PL_1
Prevotella_copri	Gastropod_associated_circular_ssDNA_virus
Lactobacillus_salivarius	Lactobacillus_antri
Escherichia_unclassified	Corynebacterium_jeikeium
Bacteroides_eggerthii	Coprococcus_comes
Erysipelotrichaceae_bacterium_6_1_45	Bordetella_unclassified
	Rhodospirillum_unclassified
	Neisseria_unclassified
	Streptococcus_parasanguinis
	JC_polyomavirus
	Prevotella_bivia
	Lachnospiraceae_bacterium_4_1_37FAA
	Pseudomonas_alcaligenes
	Bilophila_wadsworthia
	Pseudomonas_phage_MP38

Parabacteroides_sp_20_3
Stomatobaculum_longum
Lactobacillus_saerimneri
Slow_bee_paralysis_virus
Parvimonas_unclassified
Providencia_unclassified
Enterovirus_B
Megasphaera_genomosp_t
ype_1
Alistipes_putredinis
Cetobacterium_somerae
Pepper_vein_yellows_virus
s
Actinobacillus_unclassified
d
Clostridiales_bacterium_1
_7_47FAA
Alistipes_sp_HGB5
Porphyromonas_uenonis
Eubacterium_cylindroides
Bifidobacterium_longum
Enterobacter_cloacae
Enterobacteria_phage_HK
225
Bifidobacterium_breve
Bacteroides_coprocola
Streptococcus_gordonii
Atopobium_parvulum
Blautia_producta
Atopobium_vaginae
Bean_common_mosaic_necrosis_virus
Melon_aphid_borne_yellows_virus

Morganella_morganii
Streptococcus_mutans
Pestivirus_strain_Aydin_0
4_TR
Streptococcus_tigurinus
Lachnospiraceae_bacteriu
m_8_1_57FAA
Rothia_dentocariosa
Bacteroides_cellulosilyticu
s
Clostridium_sp_KLE_175
5
Solobacterium_moorei
Porphyromonas_asaccharo
lytica
Leuconostoc_gelidum
Veillonella_unclassified
Clostridium_difficile
Orthohepadnavirus_unclas
sified
Clostridium_hathewayi
Hippeastrum_mosaic_viru
s
Streptococcus_gallolyticus
Eubacterium_dolichum
Collinsella_stercoris
Alloprevotella_tannerae
Acidaminococcus_sp_D21
Dorea_unclassified
Fusobacterium_nucleatum
Candida_glabrata
Anaerotruncus_colihomini
s
Anaerococcus_prevotii

Lactobacillus_sakei
Coprobacillus_unclassified
Hepatitis_GB_virus_B
Helicobasidium_mompa_e
ndornavirus_1
Fig_fleck_associated_virus
Prevotella_timonensis
Cardiobacterium_valvaru
m
Collinsella_aerofaciens

658 Note: Top 30 gut microbiota species in dataset 1 ; top 100 gut microbiota species in dataset 2. Top 5 host characteristics features and top 5 dietary features in
659 datasets 1 and 2.
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Supplementary Table 9. Important factors associated with blood propionic acids.

Gut Microbiotas		Host Characteristics		Dietary Features	
Dataset 1	Dataset 2	Dataset 1	Dataset 2	Dataset 1	Dataset 2
Subdoligranulum_unclassified	Weissella_confusa	Whether you have you taken any probiotics in the past 12 months (Yes/No)	Gender	Frequency of eating pickles	Whether you eat yogurt
Ruminococcus_torques	Ruminococcaceae_bacterium_D16	Weight (kg)	Race	Frequency of eating steak	Whether you drink milk
Oscillibacter_unclassified	Desulfovibrio_terminidis	Whether you have used antibiotics in the past 12 months (Yes/No)	BMI	Quantity of eating steak in a day	Whether you eat cheese
Bacteroides_uniformis	Ruminococcus_obeum	Age	Consent_Age	Frequency of drinking non-milky coffee	
Roseburia_intestinalis	Lachnospiraceae_bacterium_5_1_6_3FAA	Height (cm)	Weight (kg)	Quantity of eating chocolate candy in a day	
Bacteroides_thetaiotaomicron	Providencia_unclassified				
Bifidobacterium_catenulatum	Cyclovirus_NGchicken15_NGA_2009				
Rothia_mucilaginosa	Enterovirus_B				
Alistipes_unclassified	Porphyromonas_uenonis				
Desulfovibrio_piger	Turicibacter_sanguinis				
Prevotella_copri	Lactococcus_garvieae				
Ruminococcus_sp_5_1_39_BFAA	Ruminococcus_champanellensis				
Clostridium_asparagiforme	Classical_swine_fever_virus				
Blautia_hansenii	Prevotella_nanceiensis				
Faecalibacterium_prausnitzii	Culex_flavivirus				
Acidaminococcus_sp_BV3_L6	Epsilon15likevirus_unclassified				
Turicibacter_unclassified	Enterobacteria_phage_HK225				
Parabacteroides_merdae	Bordetella_unclassified				
Erysipelotrichaceae_bacterium_6_1_45	Actinobacillus_unclassified				

Bacteroides_caccae	Prevotella_bergensis
Lactobacillus_salivarius	Olsenella_unclassified
Ruminococcus_albus	Faecalibacterium_prausnitzii
Clostridium_citroniae	Melon_aphid_borne_yellows_virus
Alistipes_senegalensis	Peptostreptococcus_anaerobius
Bacteroides_nordii	Streptococcus_galloyticus
Bacteroides_eggerthii	Collinsella_aerofaciens
Bacteroides_sp_4_3_47FA	Hafnia_alvei
A	
Clostridium_leptum	Streptococcus_mutans
Veillonella_unclassified	candidate_division_TM7_single_cell_isolate_TM7b
Bacteroides_vulgatus	Dorea_formicigenerans
	Eubacterium_sp_3_1_31
	Parabacteroides_johnsonii
	Odoribacter_splanchnicus
	Lactobacillus_helveticus
	Bacteroides_phage_B124_14
	Clostridium_hathewayi
	Clostridium_bifermentans
	Corynebacterium_jeikeium
	Bacteroides_pectinophilus
	Blautia_hydrogenotrophica
	Eubacterium_ramulus
	Enterobacteriaceae_bacterium_9_2_54FAA
	Gastropod_associated_circular_ssDNA_virus
	Lactobacillus_phage_PL_1
	Fig_fleck_associated_virus
	Hippeastrum_mosaic_virus
	Streptococcus_gordonii
	Anaerotruncus_colihominis

Clostridium_sp_HGF2
Colombian_datura_virus
Streptococcus_salivarius
C2likevirus_unclassified
Hepatitis_GB_virus_B
Streptococcus_tigurinus
Plectrovirus_unclassified
Campylobacter_ureolyticus
Avian_carcinoma_virus
Chlorobium_phaeobacteroides
Coriobacteriaceae_bacterium_BV3
Ac1
Clostridium_nexile
Clostridium_difficile
Gemella_unclassified
Weissella_paramesenteroides
Actinomyces_turicensis
Stomatobaculum_longum
Chicory_yellow_mottle_virus_large_satellite_RNA
Okra_yellow_crinkle_Cameroon_alpha_satellite
Prevotella_buccalis
Lachnospiraceae_bacterium_8_1_5
7FAA
Bilophila_wadsworthia
Mobiluncus_curtisii
Corynebacterium_amycolatum
Veillonella_unclassified
Lachnospiraceae_bacterium_7_1_5
8FAA
Collinsella_stercoris
Pestivirus_strain_Aydin_04_TR

Ruminococcus_lactaris
Anaerococcus_prevotii
Bacteroides_ovatus
Clostridium_perfringens
Alistipes_indistinctus
Actinomyces_urogenitalis
Bifidobacterium_pseudolongum
Bifidobacterium_longum
Neisseria_flavescens
Parabacteroides_sp_20_3
Facklamia_unclassified
Erysipelotrichaceae_bacterium_21_3
Streptococcus_phage_ALQ13_2
Human_cosavirus_B
Parsnip_yellow_fleck_virus
Bovine_rhinitis_B_virus
Sida_yellow_vein_Vietnam_virus_satellite_DNA_beta
Leuconostoc_mesenteroides
Ruminococcus_bromii
Alistipes_sp_HGB5
Roseburia_inulinivorans
Clostridiales_bacterium_BV3C26
Candida_glabrata
Slackia_unclassified

662 Note: Top 30 gut microbiota species in dataset 1 ; top 100 gut microbiota species in dataset 2. Top 5 host characteristics features and top 5 dietary features in
663 datasets 1 and 2.

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Supplementary Table 10. Important factors associated with blood isobutyric acids.

Gut Microbiotas		Host Characteristics		Dietary Features	
Dataset 1	Dataset 2	Dataset 1	Dataset 2	Dataset 1	Dataset 2
Subdoligranulum_unclassified	candidate_division_TM7_sing le_cell_isolate_TM7b	Height (cm)	Race	Frequency of eating pickles	Whether you drink milk
Ruminococcus_torques	Weissella_confusa	Weight (kg)	Gender	Quantity of eating steak in a day	Whether you eat yogurt
Oscillibacter_unclassified	Ruminococcus_obeum	Time in bicycling or swimming for each time	Height (cm)	Frequency of eating steak	Whether you eat cheese
Bacteroides_uniformis	Streptococcus_mutans	Age	Whether you have you taken any probiotics in the past 12 months (Yes/No)	Quantity of eating eggs in a day	
Clostridium_asparagiforme	Campylobacter_ureolyticus	Time in heavy work for each time	BMI	Frequency of drinking non-milky coffee	
Alistipes_unclassified	Clostridium_sp_HGF2				
Rothia_mucilaginosa	Corynebacterium_jeikeium				
Bacteroides_thetaiotaomicron	Eubacterium_sp_3_1_31				
Faecalibacterium_prausnitzii	Desulfovibrio_terminidis				
Bifidobacterium_catenulatum	Bifidobacterium_longum				
Roseburia_intestinalis	Bacteroides_vulgatus				
Desulfovibrio_piger	Faecalibacterium_prausnitzii				
Clostridium_leptum	Epsilon15likevirus_unclassified				
Ruminococcus_albus	Ruminococcus_champanellensis				
Ruminococcus_sp_5_1_39BFAA	Bacteroides_coprocola				
Prevotella_copri	Bordetella_unclassified				
Alistipes_senegalensis	Providencia_unclassified				

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Lactobacillus_salivarius	Classical_swine_fever_virus
Bacteroides_eggertshii	Bovine_rhinitis_B_virus
Erysipelotrichaceae_bacterium_6_1_45	Cetobacterium_somerae
Acidaminococcus_spp_BV3L6	Okra_yellow_crinkle_Cameroon_alphasatellite
Bacteroides_nordii	Lactobacillus_phage_PL_1
Veillonella_unclassified	Enterobacteria_phage_SfV
Bacteroides_sp_4_3_47FAA	Parabacteroides_sp_20_3
Bacteroides_caccae	Cyclovirus_NGchicken15_NGA_2009
Clostridium_citroniae	Prevotella_bergensis
Blautia_hansenii	Rhodospirillum_unclassified
Clostridium_boltea	Enterobacteria_phage_HK225
Bacteroides_fragilis	C2likevirus_unclassified
Roseburia_inulinivorans	Pseudomonas_alcaligenes
	Neisseria_flavescens
	Corynebacterium_propinquum
	Coriobacteriaceae_bacterium_BV3Ac1
	Peptostreptococcus_anaerobius
	Eubacterium_siraeum
	Bilophila_wadsworthia
	Circovirus_like_genome_SAR_A
	Bifidobacterium_pseudolongum
	Clostridium_hathewayi

Alistipes_sp_HGB5
Leuconostoc_gasicomitatum
Enterovirus_B
Melon_aphid_borne_yellows_
virus
Anaerotruncus_colihominis
Eubacterium_cylindroides
Bifidobacterium_breve
Dysgonomonas_unclassified
Fusobacterium_nucleatum
JC_polyomavirus
Prevotella_buccalis
Cardiobacterium_valvarum
Actinobacillus_unclassified
Erysipelotrichaceae_bacterium
_21_3
Lactobacillus_antri
Facklamia_unclassified
Lachnospiraceae_bacterium_5
_1_63FAA
Prevotella_bivia
Gemella_haemolysans
Clostridium_difficile
Solobacterium_moorei
Pepper_vein_yellows_virus
Veillonella_unclassified
Eubacterium_ramulus
Turicibacter_sanguinis
Prevotella_timonensis
Lindernia_anagallis_yellow_v
ein_virus_satellite_DNA_beta
Enterococcus_casseliflavus
Royal_Farm_virus

Collinsella_stercoris
Human_cosavirus_B
Megasphaera_unclassified
Atopobium_parvulum
Clostridium_amosum
Atopobium_vaginae
Fig_fleck_associated_virus
Marvinbryantia_formatexigen
s
Collinsella_aerofaciens
Acidaminococcus_sp_D21
Eubacterium_dolichum
Leuconostoc_gelidum
Haemophilus_pittmaniae
Prevotella_nanceiensis
Dorea_unclassified
Lactococcus_raffinolactis
Clostridium_bolteae
Helicobasidium_mompa_endo
navirus_1
Lactobacillus_sakei
Lactobacillus_vaginalis
Porphyromonas_uenonis
Pestivirus_strain_Aydin_04_T
R
Anaerostipes_unclassified
Eggerthella_sp_1_3_56FAA
Oligella_urethralis
Lachnospiraceae_bacterium_8
_1_57FAA
Halomonas_unclassified
Actinomyces_turicensis
Gastropod_associated_circular

_ssDNA_virus

Streptococcus_vestibularis

Hippeastrum_mosaic_virus

Eubacterium_brachy

666 Note: Top 30 gut microbiota species in dataset 1 ; top 100 gut microbiota species in dataset 2. Top 5 host characteristics features and top 5 dietary features in
667 datasets 1 and 2.

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Supplementary Table 11. Important factors associated with blood isovaleric acids.

Gut Microbiotas		Host Characteristics		Dietary Features	
Dataset 1	Dataset 2	Dataset 1	Dataset 2	Dataset 1	Dataset 2
Subdoligranulum_unclassified	Desulfovibrio_termitidis	Height (cm)	Gender	Frequency of eating pickles	Whether you eat yogurt
Ruminococcus_torques	Ruminococcaceae_bacterium_D16	Weight (kg)	Race	Frequency of eating steak	Whether you drink milk
Oscillibacter_unclassified	Lactobacillus_phage_PL_1	Time in bicycling or swimming for each time	Height (cm)	Frequency of drinking non-milky coffee	Whether you eat cheese
Bacteroides_uniformis	Bovine_viral_diarrhea_virus_2	Time in heavy work for each time	Weight (kg)	Quantity of eating steak in a day	
Rothia_mucilaginosa	Lachnospiraceae_bacterium_5_1_63FAA	Whether you have you taken any probiotics in the past 12 months (Yes/No)	BMI	Quantity of eating chocolate candy in a day	
Clostridium_asparagiforme	Clostridium_sp_KLE_1755				
Bifidobacterium_catenulatum	Lactobacillus_saerimneri				
Bacteroides_thetaiotaomicron	Alloprevotella_tannerae				
Roseburia_intestinalis	Okra_yellow_crinkle_Cameroon_alphasatellite				
Alistipes_unclassified	Dorea_formicigenerans				
Desulfovibrio_piger	Ruminococcus_obeum				
Faecalibacterium_prausnitzii	Porphyromonas_asaccharolytica				
Bacteroides_nordii	Turicibacter_sanguinis				
Prevotella_copri	Peptostreptococcus_unclassified				
Acidaminococcus_sp_BV3L6	Alloprevotella_unclassified				
Ruminococcus_albus	Eubacterium_ramulus				
Alistipes_senegalensis	Bacteroides_ovatus				
Clostridium_leptum	Coriobacteriaceae_bacterium_BV3Ac1				
Ruminococcus_sp_5_1_39BFAA	Avian_carcinoma_virus				
Bacteroides_eggerth	Weissella_confusa				

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Veillonella_unclassified	Fig_fleck_associated_virus
Parabacteroides_merdae	Streptococcus_salivarius
Bacteroides_caccae	Ruminococcus_champanellensis
Erysipelotrichaceae_bacterium_6_1_45	Faecalibacterium_prausnitzii
Clostridium_citroniae	Slow_bee_paralysis_virus
Blautia_hansanii	Olsenella_unclassified
Bacteroides_sp_4_3_47FAA	Klebsiella_pneumoniae
Lactobacillus_salivarius	Pestivirus_strain_Aydin_04_TR
Bacteroides_fragilis	Enterococcus_avium
Weissella_unclassified	Culex_flavivirus
	Campylobacter_ureolyticus
	candidate_division_TM7_single_cell_isolate_TM7b
	Apoi_virus
	Odoribacter_unclassified
	Barbel_circovirus
	Enterobacteria_phage_SfV
	Lactococcus_lactis
	Weissella_unclassified
	Lactobacillus_delbrueckii
	Holdemania_unclassified
	Actinomyces_urogenitalis
	Clostridium_sp_HGF2
	Bilophila_wadsworthia
	Aggregatibacter_segnis
	Actinobacillus_unclassified

Valsa_ceratosperma_hypovirus_1

Bacteroides_eggerthii

Campylobacter_conciscus

Proteus_mirabilis

Nilaparvata_lugens_honeydew_virus_2

Zinnia_leaf_curl_virus_associated_DNA_beta

Orthohepadnavirus_unclassified

Klebsiella_phage_KP36

Collinsella_stercoris

Hippeastrum_mosaic_virus

Pseudomonas_phage_MP38

Anaerostipes_unclassified

Oligella_urethralis

Bifidobacterium_pseudolongum

Coprobacillus_unclassified

Candidatus_Zinderia_insecticola

Porphyromonas_uenonis

Collinsella_aerofaciens

Phascolarctobacterium_succinatutens

Parabacteroides_johnsonii

Clostridium_bifermentans

Bacteroides_sp_1_1_30

Holdemania_sp_AP2

Bovine_viral_diarrhea_virus_3

Granulicatella_unclassified

Cardiobacterium_valvarum

Lachnospiraceae_bacterium_8_1_57FAA

Blautia_producta

Escherichia_sp_TW09276
Akkermansia_muciniphila
Streptococcus_peroris
Lindernia_anagallis_yellow_vein
_virus_satellite_DNA_beta
Corynebacterium_amycolatum
Butyrivibrio_crossotus
Hepatitis_C_virus
Stomatobaculum_longum
Alistipes_finegoldii
Sapporo_virus
Human_adenovirus_B
Peptostreptococcus_anaerobius
Actinomyces_naeslundii
Collinsella_intestinalis
Parabacteroides_sp_20_3
Corynebacterium_durum
Colombian_datura_virus
Bacteroides_fragilis
Bordetella_unclassified
Anaerostipes_caccae
Lactobacillus_gasseri
Eubacterium_siraeum
Gastropod_associated_circular_s
sDNA_virus
Anaerotruncus_colihominis
Barnesiella_intestinihominis
Mobiluncus_curtisii
Leuconostoc_inhae

670 Note: Top 30 gut microbiota species in dataset 1 ; top 100 gut microbiota species in dataset 2. Top 5 host characteristics features and top 5 dietary features in
671 datasets 1 and 2.
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