

Supplementary Table 1. Genus, Strain, and Biosample ID for the Bacterial Genomes

Genus	Strain	Biosample ID NCBI
<i>Bacteroides</i>	<i>Bacteroides cellulosilyticus</i> CL02T12C19	SAMN00630422
<i>Bacteroides</i>	<i>Bacteroides dorei</i> 5_1_36/D4	SAMN00012892
<i>Bacteroides</i>	<i>Bacteroides finegoldii</i> CL09T03C10	SAMN00627907
<i>Bacteroides</i>	<i>Bacteroides fragilis</i> CL03T12C07	SAMN16451179
<i>Bacteroides</i>	<i>Bacteroides ovatus</i> 3_8_47FAA	SAMN02463791
<i>Bacteroides</i>	<i>Bacteroides tethaoitamicron</i> VPI 5482	Sequencing
<i>Bacteroides</i>	<i>Bacteroides vulgatus</i> ATCC 8482	SAMN02604309
<i>Bifidobacterium</i>	<i>Bifidobacterium adolescentis</i> ATCC 15703	SAMD00061080
<i>Bifidobacterium</i>	<i>Bifidobacterium longum</i> PT8	Sequencing
<i>Clostridium</i>	<i>Clostridium</i> sp. 7_2_43FAA	SAMN02463700
<i>Clostridium</i>	<i>Clostridium</i> sp. HGF2	SAMN00116782
<i>Clostridium</i>	<i>Clostridium</i> sp. M62/1	SAMN02415619
<i>Lachnospirillum</i>	<i>Clostridium symbiosum</i> WAL14673	SAMN00110774
<i>Escherichia</i>	<i>Escherichia coli</i> K-12 MG1655	SAMD00019998
<i>Flavonifractor</i>	<i>Flavonifractor plautii</i> 1_3_50AFAA	SAMN00103468
<i>Enterocloster</i>	<i>Lachnospirillum clostridioforme</i> 2_1_49FAA	SAMN00016629
<i>Lactobacillus</i>	<i>Lactobacillus paracasei</i> M38	Sequencing
<i>Lactobacillus</i>	<i>Lactobacillus plantarum</i> ATCC 8014	SAMN02463698
<i>Mediterraneibacter</i>	<i>Ruminococcus gnavus</i> CC55_001C	SAMN01162086

Supplementary Table 2. Exchange reactions employed for simulating the mZMB medium by the metabolic models.

Reaction	Metabolite	Global ID	Flux
EX_4abz_m	4abz_m	EX_4abz(e)	1.000000
EX_ala_L_m	ala_L_m	EX_ala_L(e)	0.251762
EX_asn_L_m	asn_L_m	EX_asn_L(e)	0.225000
EX_asp_L_m	asp_L_m	EX_asp_L(e)	0.571946
EX_cys_L_m	cys_L_m	EX_cys_L(e)	0.035089
EX_gln_L_m	gln_L_m	EX_gln_L(e)	0.820199
EX_glu_L_m	glu_L_m	EX_glu_L(e)	0.820199
EX_gly_m	gly_m	EX_gly(e)	0.157022
EX_h2o_m	h2o_m	EX_h2o(e)	1000.000000
EX_xan_m	xan_m	EX_xan(e)	1.000000
EX_arg_L_m	arg_L_m	EX_arg_L(e)	0.290359
EX_thymd_m	thymd_m	EX_thymd(e)	1.00
EX_gthox_m	gthox_m	EX_gthox(e)	1.00
EX_inost_m	EX_inost_m	EX_inost(e)	1.000000
EX_pnto_R_m	pnto_R_m	EX_pnto_R(e)	1.00
EX_pro_L_m	pro_L_m	EX_pro_L(e)	0.758794
EX_pydx_m	pydx_m	EX_pydx(e)	1.00
EX_sheme_m	sheme_m	EX_sheme(e)	1.00
EX_thm_m	thm_m	EX_thm(e)	1.00
EX_thr_L_m	thr_L_m	EX_thr_L(e)	0.342992
EX_tyr_L_m	tyr_L_m	EX_tyr_L(e)	0.163163
EX_val_L_m	val_L_m	EX_val_L(e)	0.483347
EX_zn2_m	zn2_m	EX_zn2(e)	1.00
EX_h2s_m	h2s_m	EX_h2s(e)	1.00
EX_ribflv_m	ribflv_m	EX_ribflv(e)	1.00
EX_ser_L_m	ser_L_m	EX_ser_L(e)	0.445627
EX_ura_m	ura_m	EX_ura(e)	1.00
EX_trp_L_m	trp_L_m	EX_trp_L(e)	0.092108
EX_ni2_m	EX_ni2_m	EX_ni2(e)	1.000000
EX_h_m	h_m	EX_h(e)	1000.000000
EX_ile_L_m	ile_L_m	EX_ile_L(e)	0.392994
EX_leu_L_m	leu_L_m	EX_leu_L(e)	0.669318
EX_lys_L_m	lys_L_m	EX_lys_L(e)	0.571069
EX_met_L_m	met_L_m	EX_met_L(e)	0.206146
EX_phe_L_m	phe_L_m	EX_phe_L(e)	0.358782
EX_pheme_m	pheme_m	EX_pheme(e)	1.00
EX_pi_m	pi_m	EX_pi(e)	1.00
EX_mn2_m	mn2_m	EX_mn2(e)	1.00
EX_na1_m	na1_m	EX_na1(e)	1.00
EX_nac_m	nac_m	EX_nac(e)	1.00
EX_btn_m	btn_m	EX_btn(e)	1.00
EX_ade_m	ade_m	EX_ade(e)	1.00
EX_mobd_m	mobd_m	EX_mobd(e)	1.00
EX_nh4_m	EX_nh4_m	EX_nh4_m	1.00
EX_ca2_m	ca2_m	EX_ca2(e)	1
EX_cl_m	cl_m	EX_cl(e)	1.00
EX_cobalt2_m	cobalt2_m	EX_cobalt2(e)	1.00
EX_fe2_m	fe2_m	EX_fe2(e)	1.00
EX_fe3_m	fe3_m	EX_fe3(e)	1.00
EX_gua_m	gua_m	EX_gua(e)	1.00
EX_k_m	k_m	EX_k(e)	1.00
EX_mg2_m	mg2_m	EX_mg2(e)	1.00

Supplementary Table 3. Bacteria selected for ML model training

Code	Genus	Species
49FAA	<i>Enterocloster</i>	<i>Lachnoclostridium clostridioforme</i> 2_1_49FAA
50AFAA	<i>Flavonifractor</i>	<i>Flavonifractor plautii</i> 1_3_50AFAA
ado_ATCC	<i>Bifidobacterium</i>	<i>Bifidobacterium adolescentis</i> ATCC 15703
CC55	<i>Mediterraneibacter</i>	<i>Ruminococcus gnavus</i> CC55_001C
CL02T12c19	<i>Bacteroides</i>	<i>Bacteroides cellulosilyticus</i> CL02T12C19
Cl03	<i>Bacteroides</i>	<i>Bacteroides fragilis</i> CL03T12C07
CL09T03C10	<i>Bacteroides</i>	<i>Bacteroides fingoldii</i> CL09T03C10
D4A	<i>Bacteroides</i>	<i>Bacteroides dorei</i> 5_1_36/D4
Eco3	<i>Escherichia</i>	<i>Escherichia coli</i> K-12 MG1655
plant_ATCC	<i>Lactiplantibacillus</i>	<i>Lactobacillus plantarum</i> ATCC 8014
tet2	<i>Bacteroides</i>	<i>Bacteroides tethaoitamicron</i> VPI 5482
vul_ATCC	<i>Bacteroides</i>	<i>Bacteroides vulgatus</i> ATCC 8482
w14673	<i>Lachnoclostridium</i>	<i>Clostridium symbiosum</i> WAL14673