Supplementary material 1

1. AMINO ACID METABOLOMICS DETECTION

Reagents and standards

Reagents: Acetonitrile, methanol, n-butanol, and acetyl chloride (chromatographic grade, purchased from CNW Technologies, Germany). Amino Acid Standards: Glycine, alanine, serine, proline, valine, threonine, leucine, isoleucine, asparagine, aspartic acid, glutamine, methionine, phenylalanine, arginine, tyrosine, glutamic acid, lysine, histidine, tryptophan, and cysteine. All standards were sourced from Sigma-Aldrich and Dr. Ehrenstorfer, with purity ≥ 95%. Deuterated Isotope Standards: Glycine-D5, alanine-D4, serine-D3, proline-D3, valine-D8, threonine-D2, leucine-13C, isoleucine-D10, asparagine-D3, aspartic acid-D3, glutamine-13C5, methionine-D3, phenylalanine-D8, arginine-N4, tyrosine-13C6, glutamic acid- 15N, cysteine-D6, lysine-D4, histidine-C6, and tryptophan- D5. All were obtained from Sigma-Aldrich and Dr. Ehrenstorfer, with purity ≥ 95%.

Liquid chromatography and mass spectrometry conditions: Column: CAPCELL PAK ADME column, 150 mm × 2.1 mm, 5 μm. Mobile Phase: A: 2.5 mM ammonium acetate with 0.1% formic acid in water; B: 2.5 mM ammonium acetate with 0.1% formic acid in acetonitrile. Gradient Elution: Conditions detailed in Supplementary Table 1. Column Temperature: 40°C. Injection Volume: 5 μL.

Sample pretreatment: Weigh 0.1 g of sample (accurate to 0.01 g) into a 1.5 mL capped plastic centrifuge tube. Add 1 mL of 90% acetonitrile, vortex to mix, and perform low-temperature ultrasonic extraction for 15 min. Centrifuge at 12,000 rpm for 10 min at 4°C. Transfer the supernatant to a clean nitrogen evaporation tube and dry under a nitrogen stream. Add 100 μL of derivatization reagent to the tube, vortex for 2 min, and derivatize at 50°C for 15 min. Dry again under nitrogen, and then reconstitute with 300 μL of water:acetonitrile (8:2). Filter through a 0.22 μm membrane and prepare for analysis.

Fatty Acid Metabolomics Detection

Reagents and standards: Standards: Palmitoleic acid (C16:1, 99% purity), oleic acid (C18:1, 99% purity), linoleic acid (C18:2, 97% purity), eicosapentaenoic acid (C20:5, 99% purity), eicosenoic acid (C20:1, 99% purity), arachidonic acid (C20:4, 99% purity), docosahexaenoic acid (C22:6, 99% purity), ω3-docosapentaenoic acid (ω3-C22:5, 99% purity), ω6-docosapentaenoic acid (ω6-C22:5, 98% purity), γ-linolenic acid (γ-C18:3, 99% purity), and α-linolenic acid (α-C18:3, 99% purity). All were purchased from Shanghai Anpel Laboratory Technologies Inc. (Shanghai, China). Reagents: Ethyl acetate (chromatographic grade) and formic acid (chromatographic grade) from Dikma (Beijing, China); acetonitrile (chromatographic grade) and n-hexane (chromatographic grade) from Anpel Laboratory Technologies Inc. (Shanghai, China). Ultrapure water was prepared using a Milli-Q system.

Liquid chromatography and mass spectrometry conditions: Column: Waters ACQUITY UPLC® HSS T3 column, 1.8 μm, 2.1 × 50 mm. Column Temperature: 55°C. Mobile Phase: A: 0.05% formic acid in water; B: 0.05% formic acid in acetonitrile. Flow Rate: 0.4 mL/min. Gradient Elution Program: 0.0–1.7 min, 10% B; 1.7–2.0 min, 30% B; 1.8–6.0 min, 50% B; 6.0–6.5 min, 100% B; 6.50–6.51 min, 50% B; 6.51–8.50 min, 10% B. Autosampler Temperature: 10°C. Injection Volume: 1 μL. Ion Source: Electrospray ionization (ESI). Scan Mode: Positive ion scan (ESI+). Data Acquisition: Multiple reaction monitoring (MRM).

Optimized Mass Spectrometry Parameters: ESI source temperature (TEM): 500°C; spray voltage (IS): 5500 V; nebulizer gas (Gas 1): 50 psi; curtain gas (CUR): 40 psi; auxiliary gas (Gas 2): 50 psi.

Sample pretreatment: Transfer serum or calibration working solution into a 1.5 mL centrifuge tube. Add 20 μL of a mixed fatty acid isotope internal standard solution and vortex for 5 min. Add 700 μL of ethyl acetate-acetonitrile solution, vortex at room temperature for 5 min, and centrifuge at 15,000 rpm for 5 min. Transfer 550 μL of the supernatant to a tube and evaporate to dryness under high-purity nitrogen at 35°C. For derivatization, add 200 μL of N,N′-carbonyldiimidazole solution to the residue, vortex for 30 s, and incubate at 25°C for 25 min. Subsequently, add 200 μL of 4-(dimethylamino)-benzylamine solution, vortex for 30 s, and incubate at 70°C for 30 min. Add 400 μL of pre-chilled (-20°C) acetonitrile and analyze the sample.

Bile acid metabolomics detection

Reagents and standards: Bile Acid Standards: Cholic acid (CA), deoxycholic acid (DCA), chenodeoxycholic acid (CDCA), and lithocholic acid (LCA), all purchased from Shanghai Yuanye Bio-Technology Co., Ltd. (Shanghai, China), with purity ≥ 95%. Deuterated Isotope Standards: Cholic acid-d5 (CA-d5), deoxycholic acid-d5 (DCA-d5), chenodeoxycholic acid-d4 (CDCA-d4), and lithocholic acid-d4 (LCA- d4), all sourced from Shanghai Yuanye Bio-Technology Co., Ltd., with purity ≥ 95%.

Liquid chromatography and mass spectrometry conditions: Column: Waters ACQUITY UPLC® HSS T3 column, 50 mm × 2.1 mm, 1.8 μm. Mobile Phase: A: 0.1% formic acid in water; B: methanol. Gradient Elution: Conditions detailed in Supplementary Table S2. Column Temperature: 40°C. Injection Volume: 10 μL.

Sample pretreatment: Transfer 100 μL of sample into a 1.5 mL capped plastic centrifuge tube. Add 400 μL of acetonitrile solution (containing internal standard), vortex for 5 min, and centrifuge at 12,000 rpm for 10 min. Transfer 350 μL of the supernatant to a clean 96-well plate and dry under a nitrogen stream. Reconstitute with 100 μL of water:methanol (1:1), vortex for 2 min, and prepare for analysis.

TMAO metabolomics detection

Reagents and standards: Reagents: Acetonitrile (chromatographic grade,

Sunrise Chemical, USA); methanol (chromatographic grade, Sunrise Chemical, USA); formic acid (chromatographic grade, Dikma, USA); ammonium formate (chromatographic grade, CNW Technologies, Shanghai, China); PBS buffer pH 7.4 (Thermo Fisher Scientific). Ultrapure water was prepared using an ultrapure water system with a resistivity of 18.2 MΩ·cm. Standards: Trimethylamine N-oxide (TMAO, 98.2%), choline (49.0%), creatinine (99.9%), L-carnitine (99.7%), betaine (98.0%), D9-trimethylamine N-oxide (D9-TMAO, 99.1%), D4-choline chloride (99.1%), D3-creatinine (99.8%), and D3-L-carnitine (99.9%), all purchased from Tianjin Alta Scientific Co., Ltd.

Standard solution preparation: Single Standard Stock Solutions: Transfer standard solutions of L-carnitine, betaine, D4-choline, D3-creatinine, and D3-L-carnitine (100 μg/mL) into clean brown vials as individual stock solutions. Accurately weigh 0.010 g of creatinine standard and dissolve in 1% formic acid solution to prepare a 10 mg/mL creatinine stock solution. Dissolve 10 mg of TMAO, 10 mg of choline, and 5 mg of D9-TMAO in 1% formic acid solution to prepare stock solutions of 10 mg/mL, 10 mg/mL, and 5 mg/mL, respectively. Store at -20°C.

Mixed Standard Working Solution: Combine appropriate amounts of TMAO, choline, creatinine, L-carnitine, and betaine single stock solutions to prepare a mixed standard stock solution with final concentrations of 1, 10, 10, 20, 20, and 20 μg/mL, respectively. Dilute this stock solution with 1% formic acid aqueous solution into eight concentration gradient standard series (S1–S8), as detailed in Supplementary Table 3. Mixed Internal Standard Working Solution: Dilute appropriate amounts of single internal standard stock solutions with 1% formic acid aqueous solution to a concentration of 50 ng/mL each.

Mass spectrometry conditions: Mobile Phase Preparation: Phase A: Dissolve 0.252 g of ammonium formate in ultrapure water, filter, dilute with ultrapure water, add 400 μL of formic acid, and adjust to 400 mL to obtain a 10 mmol/L ammonium formate solution with 0.1% formic acid. Prepare fresh daily. Phase B: Add 1 mL of formic acid to acetonitrile and adjust to 1000 mL to obtain a 0.1% formic acid acetonitrile solution.

Ion Source: Electrospray ionization (ESI), positive ion mode. Scan Mode: Multiple reaction monitoring (MRM). Ion Source Temperature: 500°C. Capillary Voltage: 2.5 kV. Cone Voltage: 2.5 V. Desolvation Gas Flow: 150 L/hr. Ion Selection: After identifying parent ions, select the two most intense daughter ions for each target compound, with the strongest used for quantification and the other for qualification. Mass spectrometry parameters (parent ions, daughter ions, collision energies) for the five TMAO-related compounds and their internal standards are listed in Supplementary Table 4.

Supplementary Table 4 Mass Spectrometry Parameters for TMAO Metabolomics

Sample pretreatment: Take 50 μL of blood sample (or mixed standard working solution at eight concentration gradients, S1–S8, as per Supplementary Table 3).

Add 10 μL of mixed internal standard working solution (prepared by diluting single internal standard stock solutions with 1% formic acid aqueous solution to 50 ng/mL each) and mix thoroughly. Add 230 μL of acetonitrile (ACN) to precipitate proteins, vortex for 5 min, and centrifuge at 13,000 × g for 5 min. Transfer 200 μL of the supernatant to a sample vial, add 600 μL of 90% ACN solution for dilution, mix well, and analyze.

Supplementary Table 1 Liquid chromatography elution conditions for amino acid metabolomics detection

Time (minute)	Flow rate (mL/minute)	A%	B%
0.00	0.40	95	5
1.00	0.40	95	5
6.00	0.40	2	98
7.00	0.40	2	98
7.01	0.40	95	5
9.00	0.40	95	5

Ion Source: Electrospray ionization (ESI). Scan Mode: Positive ion scan (ESI+). Capillary Voltage: 0.5 kV. Desolvation Temperature: 1000°C. Desolvation Gas Flow: 500 L/hr. Collision Gas: Argon, flow rate 1.7 mL/min. Mass Spectrometry Scan Mode: Segmented multiple reaction monitoring (MRM).

Supplementary Table 2 Liquid chromatography elution conditions for bile acid metabolomics detection

Time (minute)	Flow rate (mL/minute)	A%	B%
0.00	0.30	50	50
6.00	0.30	10	90
8.50	0.30	10	90
8.51	0.30	50	50
11	0.30	50	50

Ion Source: Electrospray ionization (ESI). Scan Mode: Negative ion MRM. Mass Spectrometry Parameters: Curtain Gas (CUR): 20; Collision Gas (CAD): 8; Ion Spray Voltage (IS): -4500 V; Temperature (TEM): 600°C; Ion Source Gas 1 (GS1): 40; Ion Source Gas 2 (GS2): 40.

Supplementary Table 3 Standard Series Working Solutions for TMAO Metabolomics

Analyte (ng/mL)	S1	S2	S3	S4	S5	S6	S7	S8
TMAO	39.07	78.13	156.25	312.5	625	1250	2500	5000
Free Choline	39.07	78.13	156.25	312.5	625	1250	2500	5000
Creatinine	78.13	156.25	312.5	625	1250	2500	5000	10000
L-Carnitine	78.13	156.25	312.5	625	1250	2500	5000	10000
Betaine	78.13	156.25	312.5	625	1250	2500	5000	10000

Supplementary Table 4 Mass Spectrometry Parameters for TMAO Metabolomics

Compound	CAS Number	Ionization mode	Parent ion (m/z)	daughter ion (m/z)	Collision energy /eV
TMAO	1184-78-7	[M+H]+	76.1	59.2*/58.1	10/10
Choline	123-41-1	[M+H]+	104.2	60.1*/45.2	15/15

Creatinine	60-27-5	[M+H]+	114.1	44.3*/86.2	15/10
L-Carnitine	541-15-1	[M+H]+	162.2	60.3*/103.3	15/15
Betaine	107-43-7	[M+H]+	118.2	58.3*/59.3	15/15
D9-TMAO	1161070-49-0	[M+H]+	85.1	68.2	10
D4-Choline	285979-70-6	[M+H]+	108.2	60.2	15
D3-Creatinine	143827-20-7	[M+H]+	117.1	47.3	15
D3-L-Carnitine	350818-62-1	[M+H]+	165.2	63.3	15

Note: * quantitative ion

2. supplementary-material 2

No.	Gly	Ala	Ser	Pro	Val	Thr	Ile	Glu	Met	His	Phe	Tyr	Trp
1	691.3624617	382.1321301	194.2279037	365.3302788	133.9734982	264.3896071	64.33014409	258.9610818	78.86519	5.595063161	183.2400872	287.0295546	21.81108608
2	277.7339816	236.8662312	160.1624174	176.082776	130.3673849	110.4665044	63.38766486	269.7874314	48.68685075	3.661542923	75.86367214	137.9300734	17.99341397
3	656.3037165	405.6557681	144.1692635	207.4976548	156.7948448	142.3444006	112.5459328	230.5647425	98.65126332	4.5678875	151.424723	194.4473205	6.284301244
4	731.9251365	347.240106	236.1476393	238.851646	190.7456791	283.5993956	106.2914157	184.6934663	42.98823805	1.9458945604537	93.36588171	46.45493681	9.433723436
5	495.2429066	328.3514041	190.9770538	157.9827586	109.884854	147.4844694	64.68030037	219.4935057	62.13792641	5.288347512	117.6649616	203.7859981	12.25996474
6	474.7748768	558.6600108	226.1569405	134.971467	291.8560372	141.0896155	163.4670656	188.5273468	35.48616045	4.258732921	156.8060718	108.7488548	24.66768681
7	397.8051152	433.2616113	265.0756374	232.4737254	195.5249776	237.9709117	105.0844705	191.2436705	227.5889686	3.72824826	109.5734003	150.3721784	15.12692195
8	490.9437858	313.6510315	135.1686969	218.1785807	187.0902687	166.5807589	100.6929938	122.2478233	62.29223913	5.173756123	192.6908106	187.6837022	24.79997062
9	588.5855202	407.9362247	175.7038244	338.9780248	121.3861826	182.9897163	73.65281696	298.9409974	148.3304403	2.582547	158.4818088	222.1336994	13.4029478
10	474.5081257	404.0675579	753.2676582	169.1133936	201.263243	156.3063298	114.5577876	238.4017087	27.44940017	7.281999227	103.7420849	76.48462939	8.73401234
11	578.4940056	450.7651469	204.3130784	381.9976983	156.0653334	196.8014187	86.29541816	259.3732711	59.78721265	2.419695798	110.1697742	107.8678459	8.71601704
12	531.2050753	321.9238669	181.8272427	208.8227221	160.2302323	176.1882555	77.64439277	304.5687458	75.19080491	4.831109822	175.7211696	425.4177659	24.86605132
13	546.8511389	514.0838328	252.9621058	342.188526	172.3083581	214.5124664	106.816917	341.3942527	385.749045	5.1048595	193.6020643	236.9458855	20.56380374
14	524.2889969	429.3922711	212.3782342	332.5381742	183.381165	221.537777	88.35964779	207.1757098	55.49953086	4.509860789	135.019644	246.6438821	31.06279992
15	682.7787398	376.8744248	228.4599622	248.3483453	166.0535191	191.6202569	79.66707326	228.9194856	88.17854031	5.62748131	156.0227919	274.752387	27.53785134
16	327.0456907	394.0635172	239.5535411	248.2488491	234.6699742	148.5912945	118.0737592	242.7251596	296.4925943	2.442188708	304.8958775	188.5601303	25.84298795
17	602.5541495	530.8804184	307.6995279	263.0485972	276.9808249	306.2999077	139.3735991	200.5162816	413.7239126	3.722318897	135.5471578	222.8641481	35.25430908
18	340.3779139	316.6557232	191.4412653	170.0574134	154.3172291	166.1673942	97.41404285	179.8468351	91.22347698	3.378641402	117.2447787	139.8903361	19.6573793
19	542.748568	473.7583339	201.4785647	221.0888126	222.7980425	146.9146659	135.3711977	282.0603688	23.03669325	3.676140758	127.6533083	89.54100668	15.45570953
20	535.6031704	603.3153187	214.4389991	277.888691	127.563256	203.0820601	69.92109476	170.0584521	97.93917968	4.371423047	231.7955082	307.3607815	21.04632259
21	525.0088584	344.065762	163.1291785	188.982194	112.8768666	254.2838314	47.64873828	247.6144744	18.29337846	8.469837587	58.95865367	30.81541476	3.961988052
22	390.0752631	276.9233057	187.2421152	151.8674108	120.6905176	93.59733882	78.76034917	206.1921851	31.44119027	1.314320701	77.27746837	51.00524311	6.459308589
23	376.4860797	408.2197454	216.0011804	229.4494919	211.7798678	206.1367109	124.0826027	252.4694996	62.05917834	5.37667569	134.1603911	214.7151057	22.36213397
24	355.8608632	334.7878084	169.3946176	386.924607	191.7782716	107.1717176	78.8887703	204.7017583	522.0979827	0.661220675	87.68654277	135.7829626	10.60564587
25	372.212868	423.8438615	243.116525	225.239121	140.7964274	125.159587	94.01227415	251.0240673	83.88231352	3.677987	134.5953145	193.7874331	5.884242484
26	899.0753297	681.0386782	347.0938149	576.8303657	386.0987785	260.9774177	174.9820843	159.115742	975.7667382	5.65677578	306.1679278	105.6532645	17.75188522
27	962.3469429	835.3505287	233.3992918	339.2720837	185.508366	253.2370719	97.52588244	200.757867	481.2595671	7.586104666	225.3378231	144.9258513	19.40542062
28	294.0839883	402.5813747	255.8541076	136.6482672	204.2050622	162.1421676	141.3840436	245.1793664	31.56752228	6.617556071	110.6914159	99.26350792	26.45179218
29	737.4180099	780.8831683	308.7326723	340.1002345	233.1929825	216.2075638	164.5615995	377.476908	327.6097111	4.592807425	142.0417701	291.3589602	8.422999706
30	361.2140003	347.2821963	152.730831	243.5311387	121.4886608	17.64783412	53.95273309	211.0028275	28.26874874	2.571990204	128.2611538	73.54889895	15.75661052
31	563.4714933	825.6911801	212.220255	319.1697646	305.5499548	114.3271911	187.6658154	264.5270817	77.72857047	2.221545501	198.7062474	106.4132954	15.55259034
32	430.5025976	762.2653041	127.3692162	336.6552593	169.4268051	165.4189893	98.61984448	181.3339314	69.01591716	8.390467904	165.5861432	163.5926928	24.08329253
33	811.9297322	523.3066761	297.2899906	453.3156866	195.1281255	311.2505457	117.1111916	251.1317619	682.3882448	3.120552978	220.6609359	245.3881561	11.30467143
34	442.4336619	542.1760725	139.6048631	487.8509511	211.377211	205.6613079	170.6746588	457.4095861	66.05029824	1.310808198	97.28412737	50.10508306	4.738394868
35	544.2734781	783.5091589	283.8063739	519.5597151	407.9843769	221.0906229	201.761912	238.4108503	552.7677099	7.279485692	231.179793	244.0520448	0.767530115
36	141.6874917	435.49	189.11	209.6465734	201.9450704	107.5468435	125.7998018	223.9362808	41.56326654	8.794102481	130.257219	111.2263646	60.85302615
37	136.8810444	271.3772028	73.85493387	315.9537914	175.5828425	80.13817999	108.2237173	175.3478896	542.5733195	6.518691589	179.7940553	152.4780065	50.54997062
38	121.6884907	240.5987765	92.39156913	259.0422132	135.7815621	134.1186619	77.38686437	163.8172365	294.7221366	9.017402514	141.9724257	145.6379767	34.22003232
39	133.7979885	563.5973734	105.3156818	373.3866064	290.4016219	71.17583109	152.4278417	311.5838374	189.7006903	8.147019014	92.63314971	73.59205806	10.94785036
40	187.9466498	382.1967112	145.177229	288.2948406	143.4993171	126.988415	96.01722955	249.1036158	122.5951679	2.928488559	191.1329681	149.2332634	46.32501714
41	221.1811642	672.5996184	276.35	318.6529575	271.6526248	139.2364422	196.5123885	279.2030177	188.1514979	11.89825975	173.5713118	151.567443	74.22732837
42	126.3306248	367.8328095	123.535541	250.2224008	204.0784891	105.3807925	141.4209423	101.9820567	120.2843643	10.68211408	143.8028634	124.5546388	39.15931349
43	199.352138	552.0589292	157.5718908	415.4127942	293.210542	191.4182757	203.2240985	162.8191735	857.4737953	8.58163068	136.8913372	203.5846073	88.97096269
44	303.1555881	334.4478617	272.9183557	285.1701989	184.6178831	220.2188969	104.1153465	339.5239584	642.0560954	4.206574283	225.9406441	158.9570065	37.87185388
45	125.5773944	204.0416994	126.499667	168.1850083	202.8682458	125.4198707	122.6502249	208.3683477	33.13906575	5.213438608	104.6676252	87.50066229	74.46895505
46	153.8615292	316.5583679	141.9618898	437.6926962	171.4618438	194.7604516	104.097812	127.8186638	813.7927753	6.056010313	214.3765966	184.573376	31.06312898
47	178.7116691	401.8993714	206.2062518	201.8886042	318.2347418	173.4730524	115.5617519	97.34619044	42.17495476	3.045343216	162.6255221	84.1990452	68.4572275
48	81.52311176	456.3230441	261.7075364	396.1101364	280.1707213	39.7820685	143.2672867	72.17715626	363.5438979	20.5	174.6562746	249.1895524	20.86
49	191.8023178	233.0868223	128.9339614	463.8010944	102.0092616	206.4668402	77.51067317	333.3583566	741.7887876	26.44121818	160.0284524	132.3770076	16.6690334
50	146.8570667	205.315692	104.5466267	165.9646921	110.7987196	129.254995	81.94686285	96.92564399	182.2754842	10.34917821	123.9759671	131.5578122	32.29037313
51	180.4453177	439.5279493	144.2428395	277.5646226	230.2414853	196.2739674	133.1336052	247.1414395	40.02895248	9.013857557	150.1359949	133.1390253	21.657
52	157.1400693	348.7059154	154.6823675	229.2392947	246.8544601	181.1119459	136.6310513	484.1905458	30.3272904	6.374734128	119.1025183	85.1534301	27.38157379
53	193.1280139	667.7645078	184.791179	368.9152263	299.461545	334.9421592	187.9172829	331.6176171	280.5722807	17.54708347	236.0621406	139.4694796	41.10016159
54	119.7430398	357.2300483	78.56627738	339.3757492	246.0342296	108.4482455	154.0000381	74.89883097	47.31402051	13.41263294	173.4637993	118.3449418	56.00039173
55	169.1186892	155.6599506	91.98377581	486.3296708	97.26888604	71.32244795	84.66482427	121.8171685	70.41508612	4.732742507	79.9718506	71.94276726	34.73408579
56	210.5583455	416.6930632	173.6296032	130.1544341	185.5253521	108.7627602	112.5468095	169.2733297	50.66651029	9.118562681	158.253163	85.35647663	61.40493096
57	157.9100839	205.4865866	120.1796555	436.1602536	102.1922749	120.5915044	87.94011688	97.37939237	339.7399303	5.730228811	155.7644228	182.5967493	33.7848154
58	175.8725856	294.8811876	107.3313826	152.5085555	96.26905676	101.5409671	57.94068766	306.7114457	371.5374975	9.616951337	77.3094013	129.220542	65.41080697

No.	Lys	Gln	Leu	Arg	Asp	CA	LCA	CDCA	DCA	C16:1	C18:1	C18:2	C20:5
1	1672.666461	1858.721998	74.4172448	4.755396096	106.4845605	0.378611	0.129619	8.164232	1.965951	35.47244094	117.5886525	81.07142857	5.032894737
2	1174.874102	1220.412008	76.45593505	9.538432836	69.90191586	0.571258	0.018546	2.23097	0.003321	11.77165354	81.34751773	50.57142857	1.907894737
3	265.7394145	387.4593226	127.1511779	6.006745121	57.32242675	0.098044	0.096158	0.445368	0.000574	15.98425197	90.60283688	61.28571429	4.901315789
4	301.7671523	333.2457407	122.5670504	18.41001722	73.47483095	0.049695	0.104712	0.106384	0.000115	13.85826772	52.65957447	25.67857143	6.348684211
5	821.166222	991.888676	77.54288328	11.25467853	50.15030053	0.161472	0.06626	0.629685	0.00583	10.15748031	63.79432624	53.35714286	5.986842105
6	683.1505233	785.814403	180.1589921	3.646613088	76.53215627	0.12401	0.083929	0.095246	0.041424	11.53543307	83.29787234	76.89285714	10.78947368
7	906.5844449	866.6437906	117.0085004	14.92049369	96.70773854	0.921355	0.099593	1.259051	0.022565	10.7480315	66.45390071	70.07142857	3.881578947
8	628.2628771	701.4888471	117.5838225	12.49575201	55.65169046	0.326643	0.075402	2.939487	0.015038	18.8976378	78.04964539	55.03571429	3.125
9	1806.280662	1833.964865	87.48471449	1.970206659	94.0539444	12.22238	0.146474	5.148966	0.010087	11.65354331	93.12056738	67.35714286	4.342105263
10	460.5945003	522.3410879	138.0282458	15.767	406.3985725	0.109746	0.043733	0.173769	0.001139	7.992125984	66.63120567	43.53571429	6.414473684
11	641.688214	912.8864181	98.18068156	34.40060276	55.86292261	0.114974	0.097423	0.531303	0.002039	7.007874016	44.5035461	42.46428571	4.144736842
12	1654.295164	1718.199008	96.1331097	11.83851894	114.6961307	0.200819	0.040654	1.049732	0.010507	6.732283465	89.04255319	83.85714286	3.092105263
13	1162.258636	1357.8961	125.8712739	21.14764638	208.2819684	0.378612	0.046185	6.988234	0.003609	11.33858268	66.27659574	51.25	3.980263158
14	1282.673712	1466.825351	103.4122132	8.912543054	77.83489857	0.190644	0.008023	1.639164	0.015406	1.023622047	6.843971631	3.357142857	0.657894737
15	1393.759625	1343.130893	94.91114584	17.1293341	83.61442524	10.411749	0.087803	1.731714	0.001394	23.46456693	75.88652482	33.89285714	2.927631579
16	997.6736097	1254.073691	132.562743	18.45849598	103.1564989	1.075489	0.016293	6.371898	0.172702	3.700787402	29.96453901	26.03571429	3.552631579
17	619.7127368	932.0424222	169.7672867	17.67944891	99.64887303	0.03851	0.016936	0.179909	0.007787	1.811023622	15.60283688	17.10714286	2.269736842
18	771.7721458	944.7903182	119.3376153	7.09532147	66.51393689	0.168009	0.029674	0.518736	0.00875	11.96850394	82.73049645	45.21428571	2.796052632
19	1215.294719	1345.730824	147.5824503	4.063145809	58.97141247	0.099323	0.047998	0.12586	0.005405	6.377952756	89.04255319	55.32142857	6.348684211
20	1496.956666	1441.146904	84.77159411	14.83498852	75.44387678	0.237007	0.019869	1.67452	0.001002	8.937007874	43.68794326	30.92857143	4.144736842
21	823.083111	1065.788231	53.31764123	15.29718714	89.02145004	27.349583	0.199031	0.300543	0.013779	22.55905512	124.6808511	26.60714286	3.486842105
22	959.0019495	818.9266507	91.56430586	2.973536165	320.5235913	0.210632	0.076361	0.098821	0.000197	11.65354331	92.9787234	32.10714286	5.986842105
23	926.5000342	1247.945946	148.0799726	14.89629736	95.37997746	0.888662	0.015518	2.105981	0.011924	17.75590551	72.76595745	49.5	5.098684211
24	758.7132841	1172.286076	95.74773195	6.908467279	71.83283246	0.319571	0.033056	1.295	0.002134	9.645669291	88.68794326	55.10714286	3.256578947
25	907.2239893	1039.835238	106.0818404	14.73857635	192.055973	0.280789	0.040265	0.451908	0.036964	6.181102362	61.17021277	44.92857143	4.868421053
26	642.7659211	719.1549778	211.7392315	15.20717566	62.59083396	0.055489	0.014761	0.221712	0.000935	1.811023622	20.03546099	19.71428571	4.572368421
27	1072.129352	1230.407834	116.3851109	17.37568886	148.0667919	0.560537	0.028915	0.029814	0.013294	3.070866142	29.18439716	24.60714286	1.644736842
28	1185.19266	1267.308655	140.0229473	34.00341561	51.197145	0.107563	0.026188	0.106049	0.001703	5.196850394	50.78014184	59.10714286	7.861842105
29	2654.436111	3275.185905	175.542464	49.46805396	106.818595	2.721224	0.080303	2.499033	0.031569	14.29133858	94.92907801	82.78571429	5.328947368
30	1635.696525	1506.477181	65.37710605	1.729621125	85.35920361	0.306371	0.009901	3.379532	0.146847	0.905511811	7.127659574	10.42857143	3.519736842
31	1409.124153	1304.414164	216.8026226	38.74575201	41.2947408	0.100255	0.2207	0.290972	0.0013	14.96062992	76.02836879	43.89285714	6.381578947
32	1147.235208	1134.758809	111.707517	16.79259472	58.21968445	0.170138	0.064055	1.815538	0.018184	10.86614173	77.76595745	48.17857143	3.552631579
33	1141.451946	1311.627369	130.1744301	26.27336395	84.46048084	0.479839	0.12509	0.142763	0.001149	25.47244094	126.6312057	94.46428571	4.309210526
34	2938.686675	4006.762607	211.4994282	17.41260046	121.5944403	0.938406	0.008359	4.67978	0.009506	27.32283465	134.822695	57.92857143	6.348684211
35	879.106471	972.2699282	241.0013723	7.531946039	147.4115327	0.594922	0.027783	1.657155	0.017878	4.68503937	39.5035461	23.03571429	3.717105263
36	516.5889696	783.3511119	127.088816	14.82123995	20.95976709	129.0164	13.7341	1904.1911	8.4224	13.31102362	120.5070922	74.51071429	0.430463576
37	636.1323962	756.4938419	108.1723336	10.58272101	29.27547183	1416.2933	27.3266	1308.1534	2.5751	42.22047244	392.6028369	235.1892857	0.533112583
38	750.8546412	675.2548409	75.85957155	14.60990241	46.45450789	85.4174	125.4556	471.0416	11.1401	61.47244094	539.4148936	360.05	0.5
39	3161.49422	266.3003079	148.0777236	22.19213548	64.49244929	66.8351	21.0356	331.3289	20.049	10.96456693	204.7056738	161.375	0.966887417
40	1154.215405	1161.507698	96.18658992	11.77726751	59.90987979	132.5668	15.1273	317.9172	0.7895	14.60629921	234.4751773	174.6392857	0.539735099
41	2467.109891	1800.590968	191.0964016	29.51690586	150.26	3084.7208	46.9526	351.4351	48.4213	20.77559055	321.751773	253.975	0.894039735
42	1124.042924	949.8051317	136.1433255	21.77491389	40	2601.7905	244.3615	2758.8335	2.7976	85.07480315	1082.29078	655.6857143	1.509933775
43	1475.509713	1272.33038	200.3407029	30.19443169	71.24124718	129.972	95.3594	674.5259	6.482	17.33858268	432.212766	310.025	0.642384106
44	1123.008995	1042.12949	104.3731798	10.55401837	72.53444778	10129.3148	202.2126	3371.6257	8.6395	87.86220472	609.2234043	450.6535714	1.082781457
45	588.672994	539.6568936	120.0299611	32.29537887	69.00371901	34.0112	29.8417	100.6095	4.3315	29.43454686	204.4786901	127.4376966	4.847231794
46	620.2668445	574.1424222	99.21220553	21.41871412	72.69722014	348.7131	126.9781	536.4108	6.0102	73.64566929	1015.549645	512.4642857	0.831125828
47	172.4643272	155.4061923	213.4395441	41.51438002	136.3244177	636.3727	86.41	145.9453	4.6415	56.84251969	548.4432624	316.2928571	1.870860927
48	2497.265104	2400.86	163.1	7.557290471	79.22	637.3373	16.4241	586.6909	24.7524	23.12204724	328.535461	214.4642857	0.592715232
49	2909.00879	2398.472152	76.08023938	25.82448335	71.84782119	372.6644	15.3038	92.6467	0.8377	41.1496063	422.4042553	370.2928571	0.632450331
50	1011.927423	829.8893602	78.95471526	20.44761768	214.2069121	4021.1256	225.8174	1780.7197	2.6896	80.77165354	1017.390071	509.9785714	0.778145695
51	363.39	376.89	133.6894107	30.12433984	101.7686702	15.426	81.7217	51.4642	1.4527	23.46850394	310.2695035	213.1821429	2.109271523
52	824.350537	646.8629148	136.3710833	44.07743972	97.69	57.3437	36.556	502.4368	2.9013	70.24015748	649.9751773	304.95	0.993377483
53	1978.914461	1377.339377	182.0304185	20.78200344	198.7332832	176.8155	11.9182	525.6334	28.4359	68.10629921	849.7943262	468.5178571	1.152317881
54	1009.351905	600.9608279	166.3952123	22.31615499	51.29564237	17.3769	268.3945	43.4713	0.2365	39.98818898	379.9432624	143.6	0.629139073
55	793.221561	683.1683886	82.20805062	21.88432836	85.16589031	1024.2136	351.7071	4811.009	27.4677	22.55905512	183.7943262	98.70714286	0.364238411
56	1281.827656	1086.380876	113.0957155	22.73860505	62.32411721	28.1179	24.2182	77.8517	0.0457	10.54724409	46.22340426	26.26785714	0.655629139
57	924.4815651	810.2304482	85.73713502	11.52861653	11.86791886	144.5438	15.9532	642.0502	2.6567	54.86220472	629.9184397	423.6178571	0.758278146
58	1476.739346	1373.885015	57.01124495	28.54380023	131.9738167	152.3442	55.4306	580.1755	5.0694	6.460629921	51.5070922	64.94642857	0.496688742

No.	C20:1	C20:4	C22:6	W3-C22:5	a-C18:3	r-C18:3	W6-C22:5	tlylamine	Choline	Creatinine	L-Carnitine	Betaine
1	0.132450331	0.870967742	0.853658537	0.424242424	0.303030303	1.942446043	1.043165468	0.189517105	21.69511923	63.39367807	28.39838765	46.8206661
2	0.099337748	0.451612903	0.518292683	0.151515152	0.121212121	2.122302158	0.467625899	2.156468421	22.54650673	40.67699298	23.79504753	81.62928729
3	0.198675497	0.451612903	0.945121951	0.363636364	0.151515152	1.654676259	0.467625899	0.0375	52.81914327	130.7207781	97.93898765	57.43303814
4	0.198675497	0.483870968	0.609756098	0.303030303	0.121212121	0.791366906	0.323741007	0.129455263	89.77027692	103.0038026	43.89773951	27.06270424
5	0.165562914	0.290322581	0.914634146	0.393939394	0.181818182	2.769784173	0.791366906	1.929565789	87.16777308	72.86249298	98.98321543	73.41175085
6	0.331125828	0.709677419	1.18902439	0.454545455	0.181818182	0.647482014	0.899280576	2.143709211	72.67457404	75.60491053	57.98317901	30.3580322
7	0.132450331	0.193548387	0.670731707	0.212121212	0.121212121	3.561151079	0.647482014	2.706456579	55.93164904	51.94450439	29.2769963	77.46150678
8	0.132450331	0.64516129	0.670731707	0.303030303	0.181818182	3.417266187	0.611510791	0.026710526	60.25768173	84.60996667	54.3414321	36.38596271
9	0.132450331	0.419354839	1.12804878	0.545454545	0.303030303	2.949640288	0.791366906	1.634547368	29.20655288	57.29351053	33.30626728	51.96838475
10	0.165562914	0.451612903	0.670731707	0.424242424	0.151515152	1.618705036	0.431654676	0.266026316	42.495525	30.42643509	24.15268333	28.67664407
11	0.165562914	0.290322581	0.426829268	0.212121212	0.121212121	2.410071942	0.71942446	0.004778947	84.99564904	54.95897281	111.9472383	69.35667542
12	0.132450331	0.419354839	0.731707317	0.333333333	0.181818182	5.755395683	1.330935252	0.067514474	29.24434038	48.28220351	16.08440123	54.64375339
13	0.132450331	0.419354839	0.792682927	0.242424242	0.151515152	1.510791367	0.107913669	1.641815789	74.805675	72.08895614	45.08142222	95.53932881
14	0.066225166	0.129032258	0.152439024	0.060606061	0.060606061	0.107913669	0.107913669	1.038903947	13.37553568	65.03876316	63.67913333	30.33198051
15	0.231788079	0.483870968	0.792682927	0.333333333	0.121212121	2.302158273	0.539568345	4.491121053	62.09432019	54.25870439	74.30014383	41.48546949
16	0.099337748	0.419354839	0.609756098	0.181818182	0.151515152	1.330935252	0.287769784	0.608419737	49.79571731	47.52927632	81.08509877	53.59844407
17	0.099337748	0.225806452	0.304878049	0.090909091	0.060606061	0.647482014	0.215827338	1.990632895	63.90725865	56.08909298	59.26842716	124.5858975
18	0.099337748	0.838709677	0.731707317	0.272727273	0.212121212	1.115107914	0.107913669	0.042031579	19.42535769	41.08979912	61.14338272	63.69617288
19	0.132450331	0.741935484	0.914634146	0.181818182	0.121212121	1.942446043	0.35971223	2.598260526	86.52861442	62.98197807	22.96315617	37.80919915
20	0.132450331	0.322580645	0.426829268	0.181818182	0.121212121	2.122302158	0.431654676	1.032118421	67.09898942	62.58954211	102.9633833	69.31194746
21	0.132450331	0.548387097	0.396341463	0.151515152	0.121212121	0.827338129	0.251798561	0.292606579	29.77425865	20.12448684	39.25669259	90.67593559
22	0.099337748	0.870967742	0.518292683	0.272727273	0.181818182	0.827338129	0.287769784	0.077757895	42.44645	52.60390088	13.59695062	154.9507364
23	0.132450331	0.387096774	0.853658537	0.363636364	0.212121212	2.374100719	0.107913669	0.037231579	72.31005673	46.22773509	78.62952901	48.40295085
24	0.132450331	0.516129032	0.548780488	0.212121212	0.151515152	2.877697842	0.647482014	0.8674	81.90656154	27.63896754	52.67613704	101.1717042
25	0.132450331	0.580645161	0.945121951	0.272727273	0.151515152	0.35971223	0.503597122	2.018065789	53.44365192	46.17937632	44.25948272	57.25365
26	0.099337748	0.225806452	0.304878049	0.121212121	0.090909091	1.618705036	0.215827338	0.076334211	54.70045192	90.15172018	106.5078704	69.17118729
27	0.099337748	0.290322581	0.274390244	0.121212121	0.060606061	0.971223022	0.287769784	0.062202632	62.21084808	196.9733263	114.6817086	71.37004407
28	0.132450331	0.387096774	0.884146341	0.272727273	0.151515152	2.122302158	0.575539568	11.40156711	86.678175	45.1757807	47.58935864	27.67744322
29	0.198675497	0.580645161	1.280487805	0.575757576	0.303030303	1.079136691	1.18705036	0.453873684	65.22323269	58.29251667	54.46308395	102.0619661
30	0.099337748	0.129032258	0.274390244	0.090909091	0.090909091	0.287769784	0.107913669	0.244672368	52.42048077	68.46021754	51.76188457	5.222057627
31	0.165562914	0.419354839	0.884146341	0.303030303	0.151515152	1.942446043	0.395683453	0.296842105	82.70218173	44.95859211	65.81412284	45.82067203
32	0.165562914	0.903225806	0.579268293	0.212121212	0.121212121	1.834532374	0.503597122	0.501705263	65.17513942	140.2521044	82.01063395	37.86367034
33	0.132450331	0.419354839	0.975609756	0.212121212	0.212121212	3.345323741	0.755395683	1.869481579	63.87734327	65.80185263	46.00333333	86.26712458
34	0.264900662	0.903225806	1.12804878	0.515151515	0.272727273	2.73381295	0.107913669	0.439275	12.26925192	32.64854211	39.23013272	78.13223559
35	0.099337748	0.612903226	0.548780488	0.212121212	0.151515152	0.503597122	0.179856115	2.371461842	23.67833173	53.90564474	93.15815617	135.5581025
36	1.187096774	14.875	2.670731707	0.687878788	2.823741007	0.827338129	0.293939394	2.585584	64.19833981	53.64884513	64.36300124	48.90363504
37	3.2	15.05592105	4.158536585	1.760606061	14.01079137	4.820143885	0.887878788	2.378982667	48.98839417	56.59524248	65.67103789	154.2169282
38	2.606451613	18.70394737	5.390243902	1.257575758	20.92086331	3.892086331	0.996969697	1.510677333	37.3937767	50.4634292	22.48031429	99.10795726
39	1.819354839	19.49671053	3.112804878	1.348484848	8.910071942	3.158273381	0.684848485	4.221533333	41.93757087	159.5462381	45.57502795	113.0974137
40	2.029032258	31.52960526	3.661585366	0.909090909	9.856115108	1.841726619	0.533333333	4.020566667	64.63067961	74.76836549	28.17680435	135.8119034
41	2.532258065	29.81907895	6.344512195	1.839393939	15.27338129	3.31294964	0.884848485	9.675946667	135.1946673	61.39784513	129.3430137	212.1761632
42	11.16774194	53.83223684	8.731707317	3.436363636	45.52877698	11.17985612	1.275757576	0.073464	98.56163301	78.92120088	50.70579689	96.0951641
43	3.577419355	27.04276316	7.167682927	1.818181818	20.04676259	3.064748201	1.145454545	7.274936	58.9655767	62.21238319	58.76972298	90.08400256
44	2.693548387	52.4375	10.64939024	3	24.41366906	8.392086331	2.218181818	1.209745333	53.13292718	87.83986283	31.82068447	207.2248239
45	3.022783668	15.93871484	2.297853891	0.733865746	0.863371466	1.458789205	2.139557501	0.1568	30.7654068	45.03066991	45.40268385	101.4683513
46	4.570967742	32.55592105	8.530487805	2.236363636	22.94604317	5.974820144	1.933333333	0.256412	108.3648243	90.32707788	32.50123665	114.6755214
47	4.790322581	61.60197368	6.704268293	3.139393939	12.58273381	3.384892086	1.036363636	0.073968	120.393433	83.13157522	118.8122236	32.14954701
48	1.332258065	21.71710526	5.762195122	1.36969697	11.88129496	3.244604317	0.9	0.15262	92.25806893	96.97995044	37.9909882	179.6006154
49	2.916129032	13.03289474	3.204268293	1.806060606	28.84532374	5.532374101	0.487878788	0.164402667	31.5545835	99.80028761	62.73751988	193.6350923
50	5.190322581	26.30921053	6.509146341	2.218181818	16.73741007	5.402877698	1.021212121	0.334226667	43.26893301	73.02745487	44.22411242	186.1383701
51	1.661290323	47.33881579	6.030487805	1.236363636	8.769784173	4.089928058	0.6	0.284656	132.7611728	107.1042664	144.9965286	16.46735726
52	4.209677419	39.60526316	5.506097561	1.815151515	12.02517986	2.910071942	0.993939394	0.230270667	96.33013301	84.97306903	43.02035963	75.15908889
53	8.151612903	40.79605263	6.829268293	2.151515152	20.02877698	4.863309353	1.045454545	0.638137333	141.683999	75.16391947	89.19028323	125.9617436
54	3.929032258	19.625	3.082317073	1.818181818	6.323741007	2.215827338	0.518181818	0.370065333	31.69598641	254.1965327	153.7101571	23.12203333
55	1.267741935	16.60197368	2.637195122	0.806060606	5.151079137	1.097122302	0.536363636	0.816568	110.8775806	62.20856195	106.1158211	118.5612094
56	0.438709677	13.72697368	1.795731707	0.475757576	1.172661871	0.669064748	0.354545455	0.249333333	148.4417903	133.3520124	136.3194571	28.34686239
57	2.422580645	24.58552632	5.048780488	1.763636364	26.29856115	5.78057554	0.824242424	0.001956	58.77884757	90.48929823	45.00507329	214.3020342
58	0.406451613	20.78618421	2.076219512	0.466666667	1.852517986	0.705035971	0.272727273	0.289352	122.2397825	93.5408115	48.23273789	98.81105641