Supplementary Table 1. Food groupings used in factor analysis

Food Group	Example of the Food Group
Rice	Rice, rice flour
Wheat flour and products	Noodle, bread, bun, flour, steamed twisted roll
Whole grains	Brown rice, millet, sorghum, black rice
Tubers	Potatoes, sweet potatoes
Pork	Pork, pork ribs, pork fat
Beef and lamb	Beef, lamb
Poultry	Chicken, duck, goose
Organ meats	Liver, kidney, blood, large intestine
Freshwater fish	Carp, squid, grass carp, chub, catfish
Marine fish	Hair tail, yellow croaker, squid, herring, striped bass
Shrimps, crabs, and mussels	Shrimp, crab, scallop, oyster
Seaweed	Fresh or dried seaweed
Milk	Cow milk, goat milk
Dairy products	Yogurt, cheese
Eggs	Egg, duck egg, goose egg
Beans and bean products	Broad bean, soy, tofu, dried tofu, soy milk
Fruits	Apple, pear, orange, banana, grape, peach, watermelon, cherry, jujube
Vegetables	Spinach, cabbage, Chinese cabbage, celery, rape, oil wheat, western lettuce, chives, tomato, cucumber, carrot, winter melon, onion, green paper, broccoli, mushroom
Nuts	Peanut, walnut, sesame, cashew, almond, sunflower seed, pistachio
Pastry and candy	Jelly, jam, chocolate, honey, sugar, candy, mooncake
Fried foods	Chips, French fries, fritters
Sweat Beverages	Carbonated drinks, sweet tea, soft drinks, fruit juice
Alcohol	Beer, rice wine, white wine
Tea	Green tea, black tea, oolong tea, dark tea

Supplementary Table 2. Factor loadings of foods in the dominant dietary patterns from food frequency questionnaires in all participants

Dietary Patterns	Food	Factor Loading Coefficient	Variance Explained (%)
Meat pattern			11.28
	Freshwater fish	0.756	
	Marine fish	0.747	
	Poultry	0.508	
	Organ meats	0.493	
	Beef and lamb	0.458	
	Shrimps, crabs, and mussels	0.374	
	Seaweed	0.231	
	Pork	0.220	
	Alcohol	0.216	
	Beans and bean products	0.209	
Protein–sweets pattern			6.42
	Pastry and candy	0.627	
	Milk	0.528	
	Fruits	0.418	
	Nuts	0.388	
	Dairy products	0.363	
	Seaweed	0.350	
	Fried foods	0.334	
	Poultry	0.226	
	Eggs	0.212	
Traditional Chinese pattern			5.55
	Vegetables	0.683	
	Whole grains	0.563	
	Wheat flour and products	0.538	
	Beans and bean products	0.327	
	Pork	0.292	
	Alcohol	0.262	
	Eggs	0.236	
Rice and tuber pattern			5.28
	Rice	0.708	
	Tubers	0.501	
	Whole grains	-0.357	
	Fried foods	0.324	
	Dairy products	-0.307	
	Sweat Beverages	0.283	
	Vegetables	0.242	
	Pastry and candy	0.216	

*Bold values reflect factor loadings above 0.2 or below -0.2.

Supplementary Table 3. Stratified analysis of the association between meat pattern and MetS

Characteristic	Tertile 1	Tertile 2	Tertile 3	*P* for interaction
Sex				**0.035**
Male	1	1.09 (0.64, 1.86)	1.17 (0.70, 1.96)	
Female	1	**1.47 (1.12, 1.93)**	1.34 (0.98, 1.83)	
Age (years)				**<0.001**
≤60	1	1.26 (0.85, 1.85)	1.20 (0.80, 1.78)	
>60	1	**1.40 (1.03, 1.91)**	**1.48 (1.04, 2.11)**	
Ethnicity				0.349
Han	1	**1.37 (1.02, 1.84)**	1.27 (0.93, 1.76)	
Mongolian	1	1.33 (0.88, 2.01)	1.47 (0.93, 2.33)	
Marital status				**0.019**
Married	1	1.23 (0.95, 1.59)	1.27 (0.69, 1.67)	
Others	1	**2.41 (1.23, 4.73)**	1.85 (0.81, 4.21)	
Education status				0.333
Middle school or below	1	**1.67 (1.15, 2.41)**	1.18 (0.77, 1.80)	
Middle school above	1	1.20 (0.87, 1.65)	1.38 (0.99, 1.93)	
Annual income (yuan)				0.346
<10, 000	1	**1.44 (1.05, 1.98)**	1.13 (0.79, 1.63)	
≥10, 000	1	1.30 (0.89, 1.90)	**1.55 (1.05, 2.28)**	
Smoking status				0.061
Yes	1	1.15 (0.71, 1.87)	1.36 (0.83, 2.23)	
No	1	**1.41 (1.07, 1.87)**	1.31 (0.96, 1.78)	
Physical activity				**0.013**
Light or below	1	1.26 (0.82, 1.93)	1.37 (0.87, 2.13)	
Moderate or vigorous	1	**1.37 (1.03, 1.83)**	1.31 (0.95, 1.82)	
Family history of diabetes				**0.005**
Yes	1	1.08 (0.22, 5.37)	5.28 (0.83, 33.66)	
No	1	**1.41 (1.10, 1.79)**	1.28 (0.98, 1.67)	
Family history of hypertension				**0.005**
Yes	1	1.38 (0.79, 2.42)	**2.00 (1.09, 3.69)**	
No	1	**1.35 (1.04, 1.77)**	1.26 (0.94, 1.68)	
Overweight				**<0.001**
BMI≥24	1	**1.42 (1.08, 1.87)**	1.32 (0.98, 1.78)	
BMI<24	**1**	**1.06 (0.64, 1.75)**	**1.26 (0.73, 2.18)**	

Adjust for Age (<60, ≥60); Sex (Female, Male); Ehnicity (Han, Mongolian); Marital status (Married, others); Education status (Middle school or below, Middle school above); Annual income (yuan) (<10, 000, ≥10, 000); Smoking status (Yes, No); Moderate physical inactivity (Light or below, Moderate or vigorous); Family history of diabetes (Yes, No); Family history of hypertension (Yes, No), Energy intake (kcal/d), BMI (kg/m^2), and other dietary patterns.

Supplementary Table 4. Stratified analysis of the association between protein-sweets pattern and MetS

Characteristic	Tertile 1	Tertile 2	Tertile 3	*P* for interaction
Sex				0.706
Male	1	1.19 (0.74, 1.91)	0.99 (0.56, 1.75)	
Female	1	0.82 (0.62, 1.09)	**0.63 (0.44, 0.90)**	
Age (years)				**0.004**
≤60	1	0.94 (0.66, 1.34)	**0.58 (0.36, 0.91)**	
>60	1	0.80 (0.58, 1.11)	0.77 (0.52, 1.14)	
Ethnicity				0.744
Han	1	0.91 (0.68, 1.21)	**0.64 (0.44, 0.93)**	
Mongolian	1	0.75 (0.48, 1.15)	0.66 (0.40, 1.11)	
Marital status				0.202
Married	1	0.88 (0.69, 1.15)	**0.72 (0.53, 0.99)**	
Others	1	0.59 (0.29, 1.21)	**0.29 (0.12, 0.73)**	
Education status				0.197
Middle school or below	1	0.78 (0.54, 1.14)	**0.60 (0.37, 0.97)**	
Middle school above	1	0.87 (0.64, 1.19)	**0.68 (0.47, 0.992)**	
Annual income (yuan)				0.229
<10, 000	1	0.84 (0.60, 1.16)	0.73 (0.48, 1.10)	
≥10, 000	1	0.89 (0.62, 1.26)	**0.62 (0.40, 0.95)**	
Smoking status				0.179
Yes	1	1.02 (0.65, 1.62)	0.96 (0.56, 1.65)	
No	1	0.81 (0.61, 1.07)	**0.60 (0.42, 0.85)**	
Physical activity				**<0.001**
Light or below	1	0.84 (0.56, 1.26)	0.71 (0.42, 1.23)	
Moderate or vigorous	1	0.85 (0.64, 1.15)	**0.64 (0.45, 0.92)**	
Family history of diabetes				**0.007**
Yes	1	1.05 (0.21, 5.13)	0.82 (0.09, 7.43)	
No	1	0.86 (0.67, 1.09)	**0.65 (0.48, 0.88)**	
Family history of hypertension				0.082
Yes	1	0.77 (0.45, 1.32)	0.51 (0.26, 1.01)	
No	1	0.88 (0.68, 1.15)	**0.71 (0.51, 0.985)**	
Overweight				**<0.001**
BMI≥24	1	0.82 (0.62, 1.07)	**0.65 (0.46, 0.91)**	
BMI<24	1	1.03 (0.62, 1.70)	0.86 (0.45, 1.61)	

Adjust for Age (<60, ≥60); Sex (Female, Male); Ehnicity (Han, Mongolian); Marital status (Married, others); Education status (Middle school or below, Middle school above); Annual income (yuan) (<10, 000, ≥10, 000); Smoking status (Yes, No); Moderate physical inactivity (Light or below, Moderate or vigorous); Family history of diabetes (Yes, No); Family history of hypertension (Yes, No), Energy intake (kcal/d), BMI (kg/m^2), and other dietary patterns.

Supplementary Table 5. Stratified analysis of the association between traditional Chinese pattern and MetS

Characteristic	Tertile 1	Tertile 2	Tertile 3	*P* for interaction
Sex				**0.014**
Male	1	1.22 (0.72, 2.08)	1.25 (0.65, 2.41)	
Female	1	**1.37 (1.02, 1.82)**	**1.68 (1.12, 2.54)**	
Age (years)				**<0.001**
≤60	1	**1.56 (1.06, 2.31)**	**1.81 (1.07, 3.05)**	
>60	1	1.12 (0.80, 1.57)	1.28 (0.81, 2.02)	
Ethnicity				0.509
Han	1	1.10 (0.81, 1.50)	**1.68 (1.11, 2.54)**	
Mongolian	1	1.66 (0.74, 2.43)	1.34 (0.74, 2.43)	
Marital status				**0.017**
Married	1	**1.31 (1.001, 1.71)**	**1.60 (1.11, 2.30)**	
Others	1	0.85 (0.41, 1.77)	1.09 (0.42, 2.86)	
Education status				0.360
Middle school or below	1	1.31 (0.88, 1.93)	1.25 (0.71, 2.19)	
Middle school above	1	1.29 (0.93, 1.79)	**1.74 (1.13, 2.67)**	
Annual income (yuan)				0.964
<10, 000	1	1.36 (0.96, 1.91)	**1.79 (1.11, 2.87)**	
≥10, 000	1	1.18 (0.81, 1.72)	1.34 (0.82, 2.21)	
Smoking status				0.100
Yes	1	0.83 (0.52, 1.35)	1.26 (0.69, 2.31)	
No	1	**1.53 (1.14, 2.06)**	**1.66 (1.10, 2.51)**	
Physical activity				**0.011**
Light or below	1	1.23 (0.80, 1.88)	1.59 (0.84, 3.01)	
Moderate or vigorous	1	1.31 (0.96, 1.79)	**1.52 (1.01, 2.28)**	
Family history of diabetes				**0.003**
Yes	1	4.83 (0.87, 26.78)	**10.60 (1.20, 93.66)**	
No	1	1.22 (0.95, 1.58)	**1.42 (1.01, 2.01)**	
Family history of hypertension				**0.006**
Yes	1	0.89 (0.49, 1.60)	1.36 (0.62, 2.96)	
No	1	**1.37 (1.04, 1.81)**	**1.58 (1.08, 2.31)**	
Overweight				**<0.001**
BMI≥24	1	1.29 (0.97, 1.72)	**1.52 (1.03, 2.25)**	
BMI<24	1	1.37 (0.80, 2.33)	1.81 (0.89, 3.71)	

Adjust for Age (<60, ≥60); Sex (Female, Male); Ehnicity (Han, Mongolian); Marital status (Married, others); Education status (Middle school or below, Middle school above); Annual income (yuan) (<10, 000, ≥10, 000); Smoking status (Yes, No); Moderate physical inactivity (Light or below, Moderate or vigorous); Family history of diabetes (Yes, No); Family history of hypertension (Yes, No), Energy intake (kcal/d), BMI (kg/m^2), and other dietary patterns.

Supplementary Table 6. Stratified analysis of the association between rice and tuber pattern and MetS

Characteristic	Tertile 1	Tertile 2	Tertile 3	*P* for interaction
Sex				0.949
Male	1.00	0.73 (0.45, 1.17)	**0.51 (0.32, 0.82)**	
Female	1.00	0.82 (0.63, 1.07)	**0.72 (0.53, 0.98)**	
Age (years)				0.176
≤60	1.00	0.97 (0.68, 1.38)	0.77 (0.53, 1.12)	
>60	1.00	**0.70 (0.52, 0.94)**	**0.57 (0.41, 0.80)**	
Ethnicity				0.746
Han	1.00	**0.74 (0.56, 0.98)**	**0.61 (0.45, 0.83)**	
Mongolian	1.00	0.90 (0.61, 1.32)	0.70 (0.46, 1.07)	
Marital status				0.255
Married	1.00	**0.77 (0.60, 0.97)**	**0.65 (0.50, 0.85)**	
Others	1.00	0.98 (0.50 1.95)	0.60 (0.29, 1.26)	
Education status				0.070
Middle school or below	1.00	0.82 (0.57, 1.18)	0.70 (0.47, 1.04)	
Middle school above	1.00	0.77 (0.57, 1.03)	**0.61 (0.45, 0.84)**	
Annual income (yuan)				0.255
<10, 000	1.00	0.74 (0.54, 1.01)	**0.65 (0.46, 0.92)**	
≥10, 000	1.00	0.85 (0.60, 1.19)	**0.67 (0.47, 0.96)**	
Smoking status				0.968
Yes	1.00	0.68 (0.44, 1.06)	**0.58 (0.37, 0.91)**	
No	1.00	0.84 (0.65, 1.11)	**0.67 (0.50, 0.90)**	
Physical activity				**<0.001**
Light or below	1.00	0.87 (0.59, 1.27)	0.74 (0.47, 1.15)	
Moderate or vigorous	1.00	0.76 (0.57, 1.01)	**0.62 (0.46, 0.83)**	
Family history of diabetes				0.159
Yes	1.00	**0.12 (0.03, 0.53)**	0.42 (0.10, 1.79)	
No	1.00	0.85 (0.68, 1.07)	**0.67 (0.52, 0.86)**	
Family history of hypertension				0.283
Yes	1.00	**0.48 (0.29, 0.80)**	**0.41 (0.23, 0.72)**	
No	1.00	0.90 (0.69, 1.16)	**0.73 (0.55, 0.96)**	
Overweight				**<0.001**
BMI≥24	1.00	0.90 (0.70, 1.17)	**0.70 (0.53, 0.93)**	
BMI<24	1.00	**0.60 (0.37, 0.96)**	**0.54 (0.32, 0.91)**	

Adjust for Age (<60, ≥60); Sex (Female, Male); Ehnicity (Han, Mongolian); Marital status (Married, others); Education status (Middle school or below, Middle school above); Annual income (yuan) (<10, 000, ≥10, 000); Smoking status (Yes, No); Moderate physical inactivity (Light or below, Moderate or vigorous); Family history of diabetes (Yes, No); Family history of hypertension (Yes, No), Energy intake (kcal/d), BMI (kg/m^2), and other dietary patterns.

Supplementary Table 7. Characteristics of the study population for metabolomics analysis

Characteristic	Non-MetS（n=200）	MetS（n=200）	*P*
Sex			0.096
Male	49（24.50）	64（32.00）	
Female	151（75.50）	136（68.00）	
Age (years)			0.416
≤60	86（43.00）	78（39.00）	
>60	114（57.00）	122（61.00）	
Ethnicity			**<0.001**
Han	169（84.50）	126（63.00）	
Mongolian	31（15.50）	74（37.00）	
Marital status			0.330
Married	166（83.00）	173（86.50）	
Others	34（17.00）	27（13.50）	
Education status			0.919
Middle school or below	82（50.31）	81（49.69）	
Middle school above	118（49.79）	119（50.21）	
Annual income (yuan)			**0.035**
<10, 000	119（54.84）	98（45.16）	
≥10, 000	81（44.26）	102（55.74）	
Smoking status			0.208
Yes	57（28.50）	46（23.00）	
No	143（71.50）	154（77.00）	
Physical activity			0.078
Light or below	50（43.10）	66（56.90）	
Moderate or vigorous	150（52.82）	134（47.18）	
Family history of diabetes			0.359
Yes	12（6.00）	8（4.00）	
No	188（94.00）	192（96.00）	
Family history of hypertension			0.711
Yes	40（20.00）	43（21.50）	
No	160（80.00）	157（78.50）	
Energy intake (kcal/d)	1583.26±628.82	1686.92±687.27	0.097
BMI (kg/m^2)	25.90±3.18	26.95±3.13	0.807

Supplementary Table 8. Differential metabolites between meat pattern groups (Tertile 1 vs. Tertile 3)

Metabolites Name	Formula	Class_I	FC	log2FC	*P* value	FDR	VIP	Regulation (T1 vs T3)
Phe-Pro	C14 H18 N2 O3	Organic acids and derivatives	1.277	0.352	<0.001	<0.001	3.286	up
N-Acetyl-L-carnosine	C11 H16 N4 O4		1.359	0.443	<0.001	<0.001	3.224	up
5,8-dihydroxy-10-methyl-5,8,9,10-tetrahydro-2H-oxecin-2-one	C10 H14 O4		1.550	0.632	<0.001	0.005	2.743	up
methyl 2-(2-acetyl-4,5-dimethoxyphenyl)acetate	C13 H16 O5		1.394	0.480	<0.001	0.008	2.621	up
3-(3,4,5-trimethoxyphenyl)propanoic acid	C12 H16 O5		1.537	0.620	<0.001	0.012	2.525	up
(2E)-4-Hydroxy-3,7-dimethyl-2,6-octadien-1-yl beta-D-glucopyranoside	C16 H28 O7		1.563	0.644	<0.001	0.022	2.540	up
N-(2-methyl-5-nitrophenyl)-N-(methylsulfonyl)methanesulfonamide	C9 H12 N2 O6 S2		1.376	0.461	<0.001	0.023	2.296	up
5-Phenylvaleric Acid	C11 H14 O2	Lipids and lipid-like molecules	1.413	0.499	<0.001	0.024	2.538	up
Etiocholanolone	C19 H30 O2	Lipids and lipid-like molecules	1.286	0.363	<0.001	0.031	2.293	up
LPA 16:1	C19 H37 O7 P	Lipids and lipid-like molecules	0.732	-0.451	<0.001	0.036	2.316	down
ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	C10 H14 N2 O2 S		1.908	0.932	<0.001	0.036	2.312	up
Testosterone	C19 H28 O2	Lipids and lipid-like molecules	1.276	0.352	<0.001	0.037	2.207	up
N1-(3-amino-4-chlorophenyl)-2-[2,4-di(tert-pentyl)phenoxy]acetamide	C24 H33 Cl N2 O2		1.295	0.372	<0.001	0.037	2.196	up
Biochanin A	C16 H12 O5	Phenylpropanoids and polyketides	1.387	0.471	<0.001	0.037	2.366	up
LPA 18:3	C21 H37 O7 P	Lipids and lipid-like molecules	0.802	-0.318	0.001	0.043	2.239	down
Testosterone sulfate	C19 H28 O5 S	Lipids and lipid-like molecules	1.309	0.388	0.001	0.076	2.035	up
Mesterolone	C20 H32 O2	Lipids and lipid-like molecules	1.297	0.375	0.002	0.096	1.851	up
trans-4-Hydroxy-L-proline	C5 H9 N O3	Organic acids and derivatives	1.213	0.279	0.002	0.114	1.935	up
1,3-Dimethyluric acid	C7 H8 N4 O3	Organoheterocyclic compounds	1.353	0.436	0.003	0.124	1.874	up
Desoxycortone	C21 H30 O3	Lipids and lipid-like molecules	1.233	0.303	0.003	0.130	1.795	up
Jasmonic acid	C12 H18 O3	Lipids and lipid-like molecules	1.546	0.628	0.003	0.134	2.047	up
N1-[6-hydroxy-2-(2-pyridyl)pyrimidin-4-yl]acetamide	C11 H10 N4 O2		1.772	0.825	0.004	0.134	1.910	up
3-(5,7-dimethoxy-4-oxo-4H-chromen-2-yl)propanoic acid	C14 H14 O6		1.357	0.441	0.004	0.135	2.033	up
ACar 13:0	C20 H40 N O4	Lipids and lipid-like molecules	1.211	0.276	0.004	0.137	1.918	up
Isorhapontigenin	C15 H14 O4	Phenylpropanoids and polyketides	0.062	-4.017	0.004	0.141	1.548	down

4-Hydroxyisoleucine	C6 H13 N O3	Organic acids and derivatives	0.721	-0.472	0.005	0.147	1.956	down
Prunin	C21 H22 O10	Phenylpropanoids and polyketides	0.186	-2.428	0.005	0.148	1.590	down
Pantethine	C22 H42 N4 O8 S2	Organic acids and derivatives	3.756	1.909	0.006	0.164	2.218	up
(+/-)5(6)-EET	C20 H32 O3	Lipids and lipid-like molecules	1.288	0.365	0.007	0.176	1.695	up
9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one	C8 H10 N4 O3		1.339	0.421	0.008	0.191	1.740	up
4-amino-2-(2,4-dimethoxyanilino)-5-pyrimidinecarbonitrile	C13 H13 N5 O2		1.831	0.873	0.009	0.197	2.057	up
N-[1-(4-methoxy-2-oxo-2H-pyran-6-yl)-2-methylbutyl]acetamide	C13 H19 N O4		0.031	-5.002	0.009	0.199	1.401	down
Oxoamide	C10 H12 N2 O2	Organic oxygen compounds	1.366	0.450	0.009	0.201	1.645	up
Theophylline	C7 H8 N4 O2	Organoheterocyclic compounds	1.218	0.284	0.011	0.212	1.741	up
Quinoline-4-carboxylic acid	C10 H7 N O2	Organoheterocyclic compounds	1.283	0.359	0.011	0.216	1.803	up
Temazepam	C16 H13 Cl N2 O2	Organoheterocyclic compounds	0.731	-0.452	0.012	0.221	1.706	down
Allantoin	C4 H6 N4 O3	Organoheterocyclic compounds	1.281	0.358	0.012	0.222	1.777	up
Piperine	C17 H19 N O3	Alkaloids and derivatives	1.291	0.368	0.013	0.235	1.646	up
LPE 20:3	C25 H46 N O7 P	Lipids and lipid-like molecules	0.829	-0.270	0.015	0.250	1.696	down
PC (16:1/17:2)	C41 H76 N O8 P	Lipids and lipid-like molecules	1.253	0.326	0.016	0.258	1.753	up
8(S),15(S)-DiHETE	C20 H32 O4	Lipids and lipid-like molecules	3.125	1.644	0.019	0.273	1.514	up
1,2-di(3,4-dimethoxyphenyl)diaz-1-ene	C16 H18 N2 O4		0.774	-0.369	0.019	0.276	1.357	down
N'1-[1-(2-hydroxyphenyl)ethylidene]-3-methoxybenzene-1-carbohydrazide	C16 H16 N2 O3		0.387	-1.371	0.019	0.276	1.511	down
15-epi Prostaglandin A1	C20 H32 O4	Lipids and lipid-like molecules	0.577	-0.793	0.020	0.280	1.613	down
Kahweol	C20 H26 O3	Organoheterocyclic compounds	1.206	0.270	0.020	0.286	1.609	up
Meclocycline	C22 H21 Cl N2 O8	Phenylpropanoids and polyketides	0.395	-1.341	0.021	0.286	1.543	down
Sorbic acid	C6 H8 O2	Lipids and lipid-like molecules	0.732	-0.451	0.021	0.289	1.488	down
All-Trans-13,14-Dihydroretinol	C20 H32 O		1.450	0.536	0.022	0.292	1.500	up
Spermidine	C7 H19 N3	Organic nitrogen compounds	1.330	0.412	0.023	0.300	1.537	up
PC (15:1/18:2)	C41 H76 N O8 P	Lipids and lipid-like molecules	1.225	0.292	0.025	0.309	1.453	up
4-(allyloxy)-1,2-dihydroquinolin-2-one	C12 H11 N O2		0.701	-0.512	0.025	0.311	1.481	down
Ibuprofen metabolite B	C13 H16 O4	Phenylpropanoids and polyketides	0.593	-0.755	0.027	0.326	1.427	down
tetranor-12(R)-HETE	C16 H26 O3		2.443	1.289	0.028	0.331	1.389	up
FAHFA (16:1/18:3)	C34 H58 O4	Lipids and lipid-like molecules	0.806	-0.311	0.029	0.335	1.377	down
Ranitidine N-oxide	C13 H22 N4 O4 S	Organoheterocyclic compounds	1.307	0.387	0.030	0.338	1.748	up

3-Methylamino-L-alanine	C4 H10 N2 O2	Organic acids and derivatives	0.499	-1.003	0.030	0.340	1.174	down
Daidzein	C15 H10 O4	Phenylpropanoids and polyketides	0.763	-0.390	0.031	0.340	1.289	down
Riboflavin-5-phosphate	C17 H21 N4 O9 P	Nucleosides, nucleotides, and analogues	0.652	-0.617	0.032	0.345	1.391	down
ACar 15:0	C22 H44 N O4	Lipids and lipid-like molecules	1.278	0.354	0.033	0.348	1.517	up
15-keto Prostaglandin E1	C20 H32 O5	Lipids and lipid-like molecules	1.938	0.954	0.034	0.354	1.871	up
4-oxo-4,5,6,7-tetrahydrobenzo[b]furan-3-carboxylic acid	C9 H8 O4		0.466	-1.102	0.034	0.358	1.592	down
Pipecolic acid	C6 H11 N O2	Organic acids and derivatives	0.742	-0.430	0.036	0.367	1.359	down
Caffeine	C8 H10 N4 O2	Organoheterocyclic compounds	1.204	0.268	0.037	0.371	1.567	up
Tetrahydroaldosterone	C21 H32 O5	Organoheterocyclic compounds	0.633	-0.659	0.038	0.377	1.567	down
2-hydroxy-3,6-diphenylcyclohexyl acetate	C20 H22 O3		1.205	0.269	0.038	0.377	1.686	up
PC (18:5e/4:0)	C30 H52 N O7 P	Lipids and lipid-like molecules	0.783	-0.352	0.043	0.395	1.457	down
LPC 17:2	C25 H48 N O7 P	Lipids and lipid-like molecules	1.204	0.268	0.044	0.395	1.354	up
4-amino-1-(2-furylmethyl)-6-hydroxy-1,2-dihydropyrimidine-2-thione	C9 H9 N3 O2 S		0.748	-0.418	0.044	0.396	1.253	down
Ethyl-beta-glucuronide	C8 H14 O7	Organic oxygen compounds	2.044	1.032	0.044	0.398	1.418	up
N-Lauroylsarcosine	C15 H29 N O3	Organic acids and derivatives	0.525	-0.930	0.049	0.415	1.258	down
Indoxyl sulfate	C8 H7 N O4 S	Organic acids and derivatives	1.256	0.329	0.049	0.415	1.290	up
LPE 18:3	C23 H42 N O7 P	Lipids and lipid-like molecules	0.829	-0.271	0.050	0.416	1.488	down

Differential metabolites were screened by partial least squares-discriminant analysis (PLS-DA) combined with univariate statistics; VIP: Variable Importance in the Projection from the first component of the PLS-DA model, indicating the metabolite's contribution to group discrimination; FC (Fold Change): The ratio of the average abundance of all biological replicates in the Tertile 3 group to that in the Tertile 1 group (T3/T1); An FC > 1 indicates up-regulation in the Tertile 3 group; *P*-value was calculated by Student's t-test to assess the significance of the difference; The screening thresholds were set as follows: VIP > 1.0, FC > 1.2 or FC < 0.833, and *P*-value < 0.05.

Supplementary Table 9. Differential metabolites between protein-sweets pattern groups (Tertile 1 vs. Tertile 3)

Metabolites Name	Formula	Class_I	FC	log2FC	*P* value	FDR	VIP	Regulation (T1 vs T3)
N-Acetylvaline	C7 H13 N O3	Organic acids and derivatives	2.118	1.083	<0.001	0.026	2.682	up
6-(4-methoxyphenyl)pyrimidine-2,4-diamine	C11 H12 N4 O		0.833	-0.263	0.001	0.082	2.199	down
LPC 17:0	C25 H52 N O7 P	Lipids and lipid-like molecules	1.270	0.345	0.002	0.083	2.673	up
ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	C10 H14 N2 O2 S		1.691	0.758	0.002	0.092	2.278	up
Sebacic acid	C10 H18 O4	Lipids and lipid-like molecules	0.820	-0.287	0.002	0.106	2.228	down
N2-Acetyl-L-ornithine	C7 H14 N2 O3	Organic acids and derivatives	0.721	-0.472	0.002	0.111	2.211	down
Pentadecanoic Acid	C15 H30 O2	Lipids and lipid-like molecules	1.227	0.296	0.003	0.119	2.394	up
Tetrahydroaldosterone	C21 H32 O5	Organoheterocyclic compounds	0.380	-1.394	0.004	0.134	1.909	down
15-epi Prostaglandin A1	C20 H32 O4	Lipids and lipid-like molecules	0.424	-1.237	0.005	0.158	1.906	down
11-dehydro Thromboxane B2	C20 H32 O6	Lipids and lipid-like molecules	0.741	-0.432	0.006	0.165	2.072	down
bicyclo[2.2.2]oct-2-en-1-yl 4-methylbenzene-1-sulfonate	C15 H18 O3 S		0.790	-0.340	0.006	0.168	1.904	down
4-Phenyl-3-buten-2-one	C10 H10 O	Benzenoids	0.812	-0.301	0.008	0.184	2.066	down
Ochratoxin A	C20 H18 Cl N O6	Phenylpropanoids and polyketides	0.555	-0.849	0.009	0.199	1.938	down
Δ17-6-keto prostaglandin F1α	C20 H32 O6	Lipids and lipid-like molecules	0.635	-0.655	0.010	0.201	1.686	down
Methyl EudesMate	C11 H14 O5	Benzenoids	0.449	-1.156	0.013	0.235	1.601	down
Lysope 14:0	C19 H40 N O7 P	Lipids and lipid-like molecules	1.379	0.464	0.014	0.244	2.109	up
11β-Hydroxyandrosterone	C19 H30 O3	Lipids and lipid-like molecules	0.396	-1.338	0.015	0.249	1.695	down
4-decyl-3-hydroxy-5-oxooxolane-2,3-dicarboxylic acid	C16 H26 O7		0.326	-1.619	0.015	0.250	1.924	down
Hydrocortisone acetate	C23 H32 O6	Lipids and lipid-like molecules	0.721	-0.473	0.017	0.258	1.669	down
(2S)-2-(2-hydroxypropan-2-yl)-2H,3H,7H-furo[3,2-g]chromen-7-one	C14 H14 O4		1.205	0.269	0.017	0.259	1.639	up
Quercetin-3β-D-glucoside	C21 H20 O12	Phenylpropanoids and polyketides	0.736	-0.443	0.018	0.270	1.894	down
LPC 12:0	C20 H42 N O7 P	Lipids and lipid-like molecules	1.310	0.389	0.023	0.300	1.880	up
PA (2:0/18:2)	C23 H41 O8 P	Lipids and lipid-like molecules	0.689	-0.538	0.024	0.303	1.830	down
13-Hpotre(R)	C18 H30 O4		0.670	-0.577	0.024	0.303	1.620	down
Prostaglandin K2	C20 H30 O5	Lipids and lipid-like molecules	0.696	-0.523	0.026	0.317	1.706	down
Cafestol	C20 H28 O3	Organoheterocyclic compounds	0.545	-0.876	0.027	0.323	1.476	down
N~5~-(pyridin-2-ylmethyl)-1H-1,2,4-triazole-3,5-diamine	C8 H10 N6		0.799	-0.323	0.028	0.329	1.749	down
Orotic Acid	C5 H4 N2 O4	Organoheterocyclic compounds	1.202	0.266	0.030	0.339	2.349	up

PC (16:1/17:2)	C41 H76 N O8 P	Lipids and lipid-like molecules	1.239	0.310	0.033	0.347	1.578	up
Adenylyl Sulfate	C10 H14 N5 O10 P S		0.310	-1.692	0.034	0.354	1.567	down
Prunin	C21 H22 O10	Phenylpropanoids and polyketides	0.214	-2.225	0.036	0.364	1.684	down
Kanamycin	C18 H36 N4 O11	Organic oxygen compounds	0.542	-0.883	0.036	0.367	1.357	down
4'-Hydroxydiclofenac	C14 H11 Cl2 N O3	Benzenoids	0.370	-1.436	0.037	0.374	1.538	down
PC (18:5e/4:0)	C30 H52 N O7 P	Lipids and lipid-like molecules	0.793	-0.334	0.038	0.379	1.500	down
6-Aminonicotinamide	C6 H7 N3 O	Organoheterocyclic compounds	1.349	0.432	0.040	0.385	1.463	up
N1-(3-amino-4-chlorophenyl)-2-[2,4-di(tert-pentyl)phenoxy]acetamide	C24 H33 Cl N2 O2		1.216	0.282	0.041	0.385	1.475	up
N1-(4-cyclohexylphenyl)-2-[(4-methylphenyl)thio]acetamide	C21 H25 N O S		0.802	-0.318	0.041	0.388	1.883	down
Ranitidine N-oxide	C13 H22 N4 O4 S	Organoheterocyclic compounds	1.261	0.335	0.041	0.388	1.500	up
12-Oxo phytodienoic acid	C18 H28 O3	Lipids and lipid-like molecules	0.704	-0.506	0.042	0.389	1.520	down
2-chloro-6-(4-methoxyphenoxy)benzonitrile	C14 H10 Cl N O2		0.262	-1.933	0.044	0.396	1.407	down
4-amino-1-(2-furylmethyl)-6-hydroxy-1,2-dihydropyrimidine-2-thione	C9 H9 N3 O2 S		0.687	-0.543	0.044	0.398	1.411	down
Norephedrine	C9 H13 N O	Benzenoids	0.781	-0.357	0.044	0.398	1.614	down
Acetaminophen glucuronide	C14 H17 N O8	Organic oxygen compounds	0.290	-1.786	0.045	0.399	1.446	down
Neopterin	C9 H11 N5 O4	Organoheterocyclic compounds	1.299	0.377	0.046	0.401	1.743	up
O-Desmethylnaproxen	C13 H12 O3	Benzenoids	0.724	-0.465	0.046	0.402	1.593	down
N-[1-(4-methoxy-2-oxo-2H-pyran-6-yl)-2-methylbutyl]acetamide	C13 H19 N O4		0.109	-3.192	0.046	0.402	1.622	down
1,7-bis(4-hydroxyphenyl)heptan-3-one	C19 H22 O3		1.340	0.422	0.046	0.402	1.456	up
3-(1-cyano-1,2-dihydroisoquinolin-2-yl)-3-oxopropyl propionate	C16 H16 N2 O3		0.810	-0.303	0.046	0.402	1.670	down
3-Indoleacrylic acid	C11 H9 N O2	Organic acids and derivatives	1.263	0.337	0.047	0.402	1.647	up
3-Hydroxysebacic acid	C10 H18 O5	Organic acids and derivatives	0.825	-0.278	0.049	0.415	1.389	down
ethyl 1-(3-nitro-2-thienyl)piperidine-4-carboxylate	C12 H16 N2 O4 S		0.675	-0.568	0.049	0.415	1.713	down

Differential metabolites were screened by partial least squares-discriminant analysis (PLS-DA) combined with univariate statistics; VIP: Variable Importance in the Projection from the first component of the PLS-DA model, indicating the metabolite's contribution to group discrimination; FC (Fold Change): The ratio of the average abundance of all biological replicates in the Tertile 3 group to that in the Tertile 1 group (T3/T1); An FC > 1 indicates up-regulation in the Tertile 3 group; *P*-value was calculated by Student's t-test to assess the significance of the difference; The screening thresholds were set as follows: VIP > 1.0, FC > 1.2 or FC < 0.833, and *P*-value < 0.05.

Supplementary Table 10. Differential metabolites between traditional Chinese pattern groups (Tertile 1 vs. Tertile 3)

Metabolites Name	Formula	Class_I	FC	log2FC	*P* value	FDR	VIP	Regulation (T1 vs T3)
4-Methylphenol	C7 H8 O	Benzenoids	0.699	-0.516	<0.001	0.031	3.001	down
2-(14,15-Epoxyeicosatrienoyl) glycerol	C23 H38 O5	Lipids and lipid-like molecules	0.619	-0.692	<0.001	0.035	2.672	down
ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	C10 H14 N2 O2 S		1.952	0.965	0.001	0.073	2.581	up
aminoimidazole carboxamide ribonucleotide	C9 H15 N4 O8 P		0.783	-0.354	0.002	0.103	2.590	down
Isobutyryl carnitine	C11 H21 N O4	Lipids and lipid-like molecules	1.301	0.379	0.004	0.134	2.245	up
4-Methylcatechol	C7 H8 O2	Benzenoids	0.785	-0.350	0.004	0.144	2.413	down
(2,6-dimethylmorpholino)(1-methyl-5-nitro-1H-pyrazol-4-yl)methanone	C11 H16 N4 O4		0.779	-0.361	0.005	0.147	2.485	down
3-(5,7-dimethoxy-4-oxo-4H-chromen-2-yl)propanoic acid	C14 H14 O6		0.817	-0.291	0.007	0.173	1.955	down
Xanthurenic acid	C10 H7 N O4	Organoheterocyclic compounds	0.785	-0.348	0.007	0.177	2.608	down
23-Nordeoxycholic acid	C23 H38 O4		0.756	-0.404	0.008	0.190	2.053	down
Dehydrocholic acid	C24 H34 O5	Lipids and lipid-like molecules	0.798	-0.325	0.008	0.191	2.239	down
4-benzyl-N-(3,5-dichlorophenyl)-1,4-diazepane-1-carboxamide	C19 H21 Cl2 N3 O		0.472	-1.084	0.010	0.204	2.020	down
FAHFA (20:4/20:3)	C40 H64 O4	Lipids and lipid-like molecules	1.225	0.293	0.011	0.212	1.867	up
4-Hydroxyisoleucine	C6 H13 N O3	Organic acids and derivatives	0.799	-0.324	0.012	0.228	1.834	down
Ergosterol peroxide	C28 H44 O3	Lipids and lipid-like molecules	0.787	-0.346	0.014	0.245	1.797	down
Apocynin	C9 H10 O3	Organic oxygen compounds	0.810	-0.304	0.017	0.263	1.890	down
Riboflavin-5-phosphate	C17 H21 N4 O9 P	Nucleosides, nucleotides, and analogues	0.582	-0.781	0.019	0.276	1.830	down
FAHFA (22:4/18:0)	C40 H70 O4	Lipids and lipid-like molecules	1.223	0.290	0.019	0.276	2.043	up
2-[(3S)-1-(2-Thienylmethyl)-3-pyrrolidinyl]-1,3-benzothiazole	C16 H16 N2 S2	Organoheterocyclic compounds	0.545	-0.875	0.020	0.283	1.663	down
Monoolein	C21 H40 O4	Lipids and lipid-like molecules	1.206	0.270	0.023	0.300	2.109	up
Methyl indole-3-acetate	C11 H11 N O2	Organoheterocyclic compounds	0.508	-0.978	0.023	0.300	1.623	down
2-(tert-butyl)-1,3-thiazolane-4-carboxylic acid	C8 H15 N O2 S		0.779	-0.361	0.032	0.345	1.570	down
Methyl EudesMate	C11 H14 O5	Benzenoids	0.234	-2.096	0.032	0.345	1.407	down
1,2-di(3,4-dimethoxyphenyl)diaz-1-ene	C16 H18 N2 O4		0.722	-0.470	0.034	0.358	1.450	down
6-(3-hydroxybutan-2-yl)-5-(hydroxymethyl)-4-methoxy-2H-pyran-2-one	C11 H16 O5		0.704	-0.507	0.035	0.361	1.308	down
Neohesperidin	C28 H34 O15	Phenylpropanoids and polyketides	0.794	-0.332	0.039	0.381	2.214	down
PC (20:5/20:5)	C48 H76 N O8 P	Lipids and lipid-like molecules	1.319	0.400	0.039	0.381	1.845	up

5-Hydroxyindole	C8 H7 N O	Organoheterocyclic compounds	0.761	-0.393	0.039	0.381	1.853	down
3-methoxy-2-phenyl-4H-furo[2,3-h]chromen-4-one	C18 H12 O4		0.589	-0.764	0.039	0.381	1.488	down
Pyroglutamic acid	C5 H7 N O3	Organic acids and derivatives	0.811	-0.302	0.045	0.398	1.754	down

Differential metabolites were screened by partial least squares-discriminant analysis (PLS-DA) combined with univariate statistics; VIP: Variable Importance in the Projection from the first component of the PLS-DA model, indicating the metabolite's contribution to group discrimination; FC (Fold Change): The ratio of the average abundance of all biological replicates in the Tertile 3 group to that in the Tertile 1 group (T3/T1); An FC > 1 indicates up-regulation in the Tertile 3 group; *P*-value was calculated by Student's t-test to assess the significance of the difference; The screening thresholds were set as follows: VIP > 1.0, FC > 1.2 or FC < 0.833, and *P*-value < 0.05.

Supplementary Table 11. Differential metabolites between rice and tuber pattern groups (Tertile 1 vs. Tertile 3)

Metabolites Name	Formula	Class_I	FC	log2FC	*P* value	FDR	VIP	Regulation (T1 vs T3)
N-Acetyl-L-carnosine	C11 H16 N4 O4		1.337	0.419	<0.001	<0.001	2.788	up
Phe-Pro	C14 H18 N2 O3	Organic acids and derivatives	1.271	0.346	<0.001	<0.001	2.880	up
Testosterone	C19 H28 O2	Lipids and lipid-like molecules	1.379	0.463	<0.001	0.001	2.629	up
trans-4-Hydroxy-L-proline	C5 H9 N O3	Organic acids and derivatives	1.382	0.466	<0.001	0.003	2.452	up
1-(2-furyl)pentane-1,4-dione	C9 H10 O3		1.312	0.392	<0.001	0.006	2.413	up
Kaempferol	C15 H10 O6	Phenylpropanoids and polyketides	1.217	0.284	<0.001	0.024	2.062	up
N1-(3-amino-4-chlorophenyl)-2-[2,4-di(tert-pentyl)phenoxy]acetamide	C24 H33 Cl N2 O2		1.336	0.418	<0.001	0.026	1.968	up
5-(2,5-dihydroxyhexyl)oxolan-2-one	C10 H18 O4		1.318	0.399	<0.001	0.035	1.937	up
(2S)-2-(2-hydroxypropan-2-yl)-2H,3H,7H-furo[3,2-g]chromen-7-one	C14 H14 O4		1.353	0.436	0.001	0.038	2.088	up
ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	C10 H14 N2 O2 S		1.630	0.705	0.001	0.047	1.873	up
3-(5,7-dimethoxy-4-oxo-4H-chromen-2-yl)propanoic acid	C14 H14 O6		0.699	-0.517	0.001	0.076	2.285	down
Mupirocin	C26 H44 O9	Lipids and lipid-like molecules	1.251	0.323	0.002	0.082	1.631	up
LPC 17:0	C25 H52 N O7 P	Lipids and lipid-like molecules	0.794	-0.333	0.002	0.084	2.161	down
Methionine	C5 H11 N O2 S	Organic acids and derivatives	1.331	0.413	0.002	0.106	1.721	up
2-[(butylamino)(imino)methyl]-1-oxohydrazinium-1-olate	C5 H12 N4 O2		1.241	0.311	0.002	0.106	1.783	up
1,3-Dimethyluric acid	C7 H8 N4 O3	Organoheterocyclic compounds	1.754	0.811	0.003	0.120	1.644	up
7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-decahydronaphthalen-1-ol	C15 H28 O2		0.796	-0.329	0.003	0.124	1.554	down
N-benzyl-2-(6-methoxy-2-naphthyl)propanamide	C21 H21 N O2		1.262	0.336	0.003	0.124	1.964	up
2-Hydroxycaproic acid	C6 H12 O3	Lipids and lipid-like molecules	1.226	0.294	0.003	0.129	1.817	up
Capryloylglycine	C10 H19 N O3	Organic acids and derivatives	1.212	0.277	0.003	0.134	1.607	up
N-(2-Furoyl)glycine	C7 H7 N O4	Organic acids and derivatives	1.636	0.711	0.004	0.134	1.660	up
Oleoyl ethylamide	C20 H39 N O	Lipids and lipid-like molecules	0.659	-0.603	0.004	0.134	1.462	down
3-Hydroxysebacic acid	C10 H18 O5	Organic acids and derivatives	0.782	-0.355	0.005	0.147	1.508	down
Enrofloxacin	C19 H22 F N3 O3	Organoheterocyclic compounds	1.367	0.451	0.005	0.147	1.925	up
FAHFA (20:4/20:3)	C40 H64 O4	Lipids and lipid-like molecules	0.818	-0.289	0.005	0.151	1.790	down
Allantoin	C4 H6 N4 O3	Organoheterocyclic compounds	1.249	0.321	0.005	0.154	1.559	up
Deoxycholic acid	C24 H40 O4	Lipids and lipid-like molecules	1.420	0.506	0.005	0.155	1.543	up
Spiculisporic Acid	C17 H28 O6	Organic acids and derivatives	1.278	0.354	0.005	0.158	1.661	up

1-Methyluric acid	C6 H6 N4 O3	Organoheterocyclic compounds	1.417	0.503	0.005	0.159	1.592	up
2-(4-methylphenyl)-5-(3,4,5-trimethoxyphenyl)-2H-1,2,3,4-tetraazole	C17 H18 N4 O3		1.205	0.269	0.006	0.164	1.886	up
alpha-Benzylsuccinic acid	C11 H12 O4	Phenylpropanoids and polyketides	1.217	0.284	0.006	0.166	1.799	up
6-Aminonicotinamide	C6 H7 N3 O	Organoheterocyclic compounds	1.449	0.535	0.007	0.174	1.552	up
Hexadecanamide	C16 H33 N O	Lipids and lipid-like molecules	0.762	-0.393	0.007	0.178	1.356	down
Pregnenolone	C21 H32 O2	Lipids and lipid-like molecules	0.832	-0.265	0.008	0.183	1.538	down
1-Methylxanthine	C6 H6 N4 O2	Organoheterocyclic compounds	1.284	0.361	0.008	0.184	1.592	up
Ochratoxin A	C20 H18 Cl N O6	Phenylpropanoids and polyketides	1.750	0.807	0.008	0.193	2.140	up
8-Aminooctanoic acid	C8 H17 N O2	Organic acids and derivatives	1.223	0.290	0.008	0.196	1.443	up
N-Tetradecanamide	C14 H29 N O	Lipids and lipid-like molecules	0.793	-0.335	0.009	0.199	1.316	down
(±)9(10)-DiHOME	C18 H34 O4		1.312	0.392	0.009	0.199	1.548	up
1-(5H-dibenzo[b,f]azepin-5-yl)ethan-1-one	C16 H13 N O		1.207	0.271	0.009	0.199	1.827	up
Stearamide	C18 H37 N O	Organic acids and derivatives	0.803	-0.317	0.009	0.201	1.347	down
PC (3:0/16:2)	C27 H50 N O8 P	Lipids and lipid-like molecules	0.633	-0.660	0.011	0.212	1.244	down
Theophylline	C7 H8 N4 O2	Organoheterocyclic compounds	1.637	0.711	0.011	0.213	1.390	up
Oleamide	C18 H35 N O	Lipids and lipid-like molecules	0.807	-0.309	0.013	0.234	1.288	down
FAHFA (22:4/18:0)	C40 H70 O4	Lipids and lipid-like molecules	0.789	-0.342	0.013	0.235	1.362	down
Hydroxyproline	C5 H9 N O3	Organic acids and derivatives	1.550	0.632	0.014	0.244	1.619	up
3-amino-1H-pyrazolo[4,3-c]pyridine-4,6-diol	C6 H6 N4 O2		1.349	0.431	0.015	0.249	1.392	up
6-benzyl-4-oxo-1,4-dihydropyridine-3-carboxamide	C13 H12 N2 O2		1.677	0.746	0.015	0.249	1.421	up
2-hydroxy-3,6-diphenylcyclohexyl acetate	C20 H22 O3		1.234	0.304	0.015	0.251	1.436	up
Terephthalic Acid	C8 H6 O4	Organic acids and derivatives	1.471	0.557	0.016	0.252	1.485	up
Chenodeoxycholic Acid	C24 H40 O4	Lipids and lipid-like molecules	1.373	0.457	0.016	0.253	1.339	up
(+/-)5(6)-EET Ethanolamide	C22 H37 N O3	Organic nitrogen compounds	1.332	0.414	0.017	0.260	1.741	up
9-Methyluric acid	C6 H6 N4 O3	Organoheterocyclic compounds	1.295	0.373	0.020	0.283	1.637	up
Homocystine	C8 H16 N2 O4 S2	Organic acids and derivatives	1.779	0.831	0.020	0.283	1.611	up
Diacetoxyscirpenol	C19 H26 O7	Lipids and lipid-like molecules	1.231	0.300	0.021	0.289	1.465	up
Arachidonoyl amide	C20 H33 N O	Lipids and lipid-like molecules	0.747	-0.422	0.023	0.300	1.159	down
Caffeine	C8 H10 N4 O2	Organoheterocyclic compounds	1.439	0.525	0.025	0.310	1.270	up
Linoleoyl ethanolamide	C20 H37 N O2	Organic nitrogen compounds	1.784	0.835	0.025	0.313	1.652	up

Maltol	C6 H6 O3	Organoheterocyclic compounds	0.740	-0.434	0.027	0.322	1.190	down
FAHFA (16:1/18:3)	C34 H58 O4	Lipids and lipid-like molecules	0.807	-0.310	0.028	0.330	1.380	down
Testosterone sulfate	C19 H28 O5 S	Lipids and lipid-like molecules	1.204	0.268	0.032	0.346	1.166	up
23-Norcholic acid	C23 H38 O5		1.204	0.268	0.033	0.347	1.270	up
Genistein	C15 H10 O5	Phenylpropanoids and polyketides	1.306	0.385	0.034	0.354	1.196	up
All-Trans-13,14-Dihydroretinol	C20 H32 O		1.216	0.282	0.034	0.354	1.106	up
Ginsenoside Rg3	C42 H72 O13	Lipids and lipid-like molecules	1.473	0.559	0.037	0.371	1.352	up
methyl 2-(2-acetyl-4,5-dimethoxyphenyl)acetate	C13 H16 O5		0.797	-0.328	0.039	0.380	1.974	down
1,7-Dimethyluric acid	C7 H8 N4 O3	Organoheterocyclic compounds	1.344	0.427	0.040	0.385	1.218	up
Benzamide	C7 H7 N O	Benzenoids	1.230	0.299	0.040	0.385	1.162	up
Glutamine	C5 H10 N2 O3	Organic acids and derivatives	0.809	-0.305	0.041	0.388	1.771	down
N1-phenyl-4-benzoylpiperidine-1-carboxamide	C19 H20 N2 O2		0.230	-2.122	0.042	0.389	1.247	down
Norfloxacin	C16 H18 F N3 O3	Organoheterocyclic compounds	1.434	0.520	0.042	0.389	1.230	up
Paracetamol	C8 H9 N O2	Benzenoids	3.352	1.745	0.044	0.396	1.372	up
Betulin	C30 H50 O2	Lipids and lipid-like molecules	1.927	0.946	0.044	0.396	1.293	up
16,16-Dimethyl prostaglandin A1	C22 H36 O4	Lipids and lipid-like molecules	1.323	0.404	0.046	0.402	1.207	up
β-Cortolone	C21 H34 O5	Lipids and lipid-like molecules	0.597	-0.745	0.049	0.415	1.242	down

Differential metabolites were screened by partial least squares-discriminant analysis (PLS-DA) combined with univariate statistics; VIP: Variable Importance in the Projection from the first component of the PLS-DA model, indicating the metabolite's contribution to group discrimination; FC (Fold Change): The ratio of the average abundance of all biological replicates in the Tertile 3 group to that in the Tertile 1 group (T3/T1); An FC > 1 indicates up-regulation in the Tertile 3 group; *P*-value was calculated by Student's t-test to assess the significance of the difference; The screening thresholds were set as follows: VIP > 1.0, FC > 1.2 or FC < 0.833, and *P*-value < 0.05.

Supplementary Table 12. Differential metabolites between MetS groups (Non-MetS vs. MetS)

Metabolites Name	Formula	Class_I	FC	log2FC	*P* value	FDR	VIP	Regulation (T1 vs T3)
Monoolein	C21 H40 O4	Lipids and lipid-like molecules	1.725	0.787	<0.001	<0.001	3.621	up
MAG (18:3)	C21 H36 O4	Lipids and lipid-like molecules	1.671	0.741	<0.001	<0.001	3.449	up
6-Sialyllactose	C23 H39 N O19	Organic oxygen compounds	1.267	0.341	<0.001	<0.001	3.053	up
N-lactoyl-phenylalanine	C12 H15 N O4	Organic acids and derivatives	1.238	0.308	<0.001	<0.001	3.054	up
6-Deoxy-D-glucose	C6 H12 O5	Organic oxygen compounds	0.742	-0.431	<0.001	<0.001	2.976	down
2-Thio-acetyl MAGE	C21 H42 O3 S	Organic acids and derivatives	1.365	0.449	<0.001	<0.001	2.975	up
5-(2,5-dihydroxyhexyl)oxolan-2-one	C10 H18 O4		0.758	-0.399	<0.001	<0.001	2.927	down
2,4-dihydroxyheptadec-16-en-1-yl acetate	C19 H36 O4		1.379	0.464	<0.001	<0.001	2.806	up
4-Hydroxyisoleucine	C6 H13 N O3	Organic acids and derivatives	0.713	-0.488	<0.001	<0.001	2.761	down
Pipecolic acid	C6 H11 N O2	Organic acids and derivatives	0.705	-0.504	<0.001	<0.001	2.694	down
Sorbic acid	C6 H8 O2	Lipids and lipid-like molecules	0.700	-0.515	<0.001	<0.001	2.659	down
Myristic Acid	C14 H28 O2	Lipids and lipid-like molecules	1.213	0.279	<0.001	0.003	2.649	up
PC (5:0/13:1)	C26 H50 N O8 P	Lipids and lipid-like molecules	0.786	-0.347	<0.001	0.003	2.392	down
L-Cysteine-glutathione gisulfide	C13 H22 N4 O8 S2		0.804	-0.315	<0.001	0.005	2.330	down
Lysine Butyrate	C10 H22 N2 O4	Organic acids and derivatives	0.796	-0.329	<0.001	0.014	2.258	down
DL-Norvaline	C5 H11 N O2	Organic acids and derivatives	0.798	-0.325	<0.001	0.015	2.248	down
2-[(butylamino)(imino)methyl]-1-oxohydrazinium-1-olate	C5 H12 N4 O2		0.807	-0.309	<0.001	0.021	2.083	down
Lysope 14:0	C19 H40 N O7 P	Lipids and lipid-like molecules	1.252	0.324	<0.001	0.023	2.064	up
LPC 12:0	C20 H42 N O7 P	Lipids and lipid-like molecules	1.232	0.301	<0.001	0.028	1.998	up
N1-(1H-1,2,4-triazol-3-yl)-2-hydroxybenzamide	C9 H8 N4 O2		1.577	0.657	<0.001	0.030	2.003	up
2-[6-(1H-benzo[d]imidazol-2-yl)-2-pyridyl]-1H-benzo[d]imidazole	C19 H13 N5		1.220	0.287	0.001	0.047	1.893	up
MAG (18:2)	C21 H38 O4	Lipids and lipid-like molecules	1.281	0.358	0.001	0.048	1.947	up
N-(2-methyl-5-nitrophenyl)-N-(methylsulfonyl)methanesulfonamide	C9 H12 N2 O6 S2		0.768	-0.381	0.001	0.055	1.978	down
LPC 14:1	C22 H44 N O7 P	Lipids and lipid-like molecules	1.226	0.294	0.001	0.063	1.973	up
Calcium D-Panthotenate	C18 H32 Ca N2 O10	Organic acids and derivatives	0.420	-1.251	0.002	0.082	1.908	down
L-Leucyl-L-Alanine	C9 H18 N2 O3	Organic acids and derivatives	0.805	-0.312	0.002	0.111	1.734	down
D-Panthenol	C9 H19 N O4	Organic oxygen compounds	0.772	-0.373	0.002	0.114	1.767	down
Ala-Leu	C9 H18 N2 O3	Organic acids and derivatives	0.794	-0.333	0.003	0.134	1.646	down

Glycocholic acid	C26 H43 N O6	Lipids and lipid-like molecules	1.215	0.281	0.004	0.134	1.641	up
4-(2-chloro-6-fluorobenzyl)-3,5-dimethyl-4-prop-2-ynyl-4H-pyrazole	C15 H14 Cl F N2		1.240	0.310	0.005	0.147	1.697	up
Panthenol	C9 H19 N O4	Lipids and lipid-like molecules	0.785	-0.349	0.005	0.147	1.645	down
LPE 16:1	C21 H42 N O7 P	Lipids and lipid-like molecules	1.236	0.306	0.005	0.158	1.667	up
Chenodeoxycholic acid-3-beta-D-glucuronide	C30 H48 O10		1.349	0.432	0.006	0.160	1.576	up
Heptadecanoic acid	C17 H34 O2	Lipids and lipid-like molecules	0.680	-0.556	0.006	0.164	1.721	down
Norbutorphanol	C16 H21 N O2	Benzenoids	0.828	-0.272	0.006	0.164	1.559	down
ILK	C18 H36 N4 O4		1.414	0.500	0.007	0.175	1.551	up
Cinchophen	C16 H11 N O2		0.562	-0.832	0.007	0.176	1.536	down
Pantethine	C22 H42 N4 O8 S2	Organic acids and derivatives	4.744	2.246	0.007	0.176	1.567	up
Cholic acid	C24 H40 O5	Lipids and lipid-like molecules	1.385	0.469	0.008	0.183	1.517	up
Pyridoxamine	C8 H12 N2 O2	Organoheterocyclic compounds	1.436	0.522	0.008	0.184	1.770	up
Avobenzone	C20 H22 O3		0.664	-0.591	0.008	0.191	1.473	down
Chenodeoxycholic Acid	C24 H40 O4	Lipids and lipid-like molecules	1.428	0.514	0.009	0.197	1.468	up
Coniferyl alcohol	C10 H12 O3	Benzenoids	0.820	-0.286	0.009	0.199	2.026	down
(±)13-HODE	C18 H32 O3		1.214	0.280	0.010	0.205	1.519	up
6-chloro-3-[(dimethylamino)methylidene]chroman-4-one	C12 H12 Cl N O2		1.888	0.917	0.010	0.205	1.706	up
6-Keto-prostaglandin f1alpha	C20 H34 O6	Lipids and lipid-like molecules	0.780	-0.358	0.011	0.210	1.431	down
23-Norcholic acid	C23 H38 O5		1.222	0.290	0.011	0.216	1.446	up
N1-morpholinocarbonyl-4-methylbenzene-1-sulfonamide	C12 H16 N2 O4 S		1.936	0.953	0.011	0.216	1.416	up
Taurochenodeoxycholic Acid (sodium salt)	C26 H45 N O6 S		1.226	0.294	0.012	0.221	1.425	up
Thromboxane B2	C20 H34 O6	Lipids and lipid-like molecules	0.818	-0.291	0.012	0.228	1.413	down
Deoxycholic acid	C24 H40 O4	Lipids and lipid-like molecules	1.485	0.571	0.015	0.250	1.356	up
3-Methoxycinnamic acid	C10 H10 O3	Phenylpropanoids and polyketides	0.778	-0.362	0.017	0.263	1.320	down
4-Methoxycinnamic acid	C10 H10 O3	Phenylpropanoids and polyketides	0.755	-0.405	0.018	0.266	1.316	down
Heroin-d3	C21 H20 [2]H3 N O5		0.695	-0.524	0.018	0.270	1.416	down
N-Acetylneuraminic acid	C11 H19 N O9	Organic oxygen compounds	1.441	0.527	0.022	0.292	1.372	up
3-(2-propynylsulfanyl)-5-[4-(trifluoromethyl)phenyl]-4H-1,2,4-triazole	C12 H8 F3 N3 S		0.645	-0.632	0.028	0.327	1.225	down
N'-(benzoyloxy)-2-(2,2-dichlorocyclopropyl)ethanimidamide	C12 H12 Cl2 N2 O2		0.746	-0.422	0.029	0.333	1.237	down
1-(7-methoxy-2-oxo-2H-chromen-8-yl)-3-methyl-2-oxobutyl acetate	C17 H18 O6		0.554	-0.852	0.030	0.339	1.250	down

(S)-Equol	C15 H14 O3	Phenylpropanoids and polyketides	1.267	0.341	0.031	0.341	1.517	up
Paracetamol	C8 H9 N O2	Benzenoids	2.443	1.289	0.031	0.343	1.387	up
Noroxycodone-d3	C17 H16 [2]H3 N O4		0.812	-0.300	0.032	0.345	1.277	down
Pyridoxine O-Glucoside	C14 H21 N O8	Organoheterocyclic compounds	1.291	0.368	0.035	0.361	1.289	up
PC (3:0/16:2)	C27 H50 N O8 P	Lipids and lipid-like molecules	1.352	0.435	0.039	0.381	1.161	up
12-Oxo phytodienoic acid	C18 H28 O3	Lipids and lipid-like molecules	0.789	-0.341	0.041	0.388	1.135	down
Kynurenic acid O-hexside	C16 H17 N O8	Organoheterocyclic compounds	1.259	0.332	0.042	0.389	1.137	up
1-(4-benzhydrylpiperidino)-2,2,2-trichloroethan-1-one	C20 H20 Cl3 N O		1.647	0.719	0.043	0.390	1.139	up
L-threo-3-Phenylserine	C9 H11 N O3	Organic acids and derivatives	4.158	2.056	0.043	0.392	1.210	up
13-Hpotre(R)	C18 H30 O4		0.791	-0.338	0.044	0.396	1.189	down
Glutathione	C10 H17 N3 O6 S	Organic acids and derivatives	0.606	-0.723	0.045	0.399	1.142	down
4-[1-(dimethylamino)ethylidene]-2-phenyl-1,3-oxazol-5(4H)-one	C13 H14 N2 O2		0.677	-0.562	0.049	0.415	1.090	down
L-Adrenaline	C9 H13 N O3	Benzenoids	0.695	-0.524	0.050	0.416	1.167	down

Differential metabolites were screened by partial least squares-discriminant analysis (PLS-DA) combined with univariate statistics; VIP: Variable Importance in the Projection from the first component of the PLS-DA model, indicating the metabolite's contribution to group discrimination; FC (Fold Change): The ratio of the average abundance of all biological replicates in the MetS group to that in the Non-MetS group (MetS/Non- MetS); An FC > 1 indicates up-regulation in the MetS group; *P*-value was calculated by Student's t-test to assess the significance of the difference; The screening thresholds were set as follows: VIP > 1.0, FC > 1.2 or FC < 0.833, and *P*-value < 0.05.

Supplementary Table 13. Feature metabolites selected by LASSO regression and their coefficients for association with different dietary patterns

Dietary patterns	Metabolites	Coefficients
Meat pattern		
	N-Acetyl-L-carnosine	0.16755
	5,8-dihydroxy-10-methyl-5,8,9,10-tetrahydro-2H-oxecin-2-one	0.03112
	methyl 2-(2-acetyl-4,5-dimethoxyphenyl)acetate	0.00808
	Biochanin A	0.03846
	N1-[6-hydroxy-2-(2-pyridyl)pyrimidin-4-yl]acetamide	0.07872
	3-(5,7-dimethoxy-4-oxo-4H-chromen-2-yl)propanoic acid	0.01347
	4-Hydroxyisoleucine	-0.00729
	PC (15:1/18:2)	0.00336
	LPE 20:3	-0.01227
Protein-sweets pattern		
	N-Acetylvaline	0.0239
	6-(4-methoxyphenyl)pyrimidine-2,4-diamine	-0.01718
	LPC 17:0	0.04138
	Sebacic acid	-0.04483
	N2-Acetyl-L-ornithine	-0.05944
	4-Phenyl-3-buten-2-one	-0.0333
	LPC 12:0	0.0594
	Δ17-6-keto prostaglandin F1α	-0.04533
	Quercetin-3β-D-glucoside	-0.13513
	4-decyl-3-hydroxy-5-oxooxolane-2,3-dicarboxylic acid	-0.02494
	(2S)-2-(2-hydroxypropan-2-yl)-2H,3H,7H-furo[3,2-g]chromen-7-one	0.04897
	PA (2:0/18:2)	-0.01204
	13-Hpotre(R)	-0.04291
	Orotic Acid	0.09636
	PC (16:1/17:2)	0.02542
	Adenylyl Sulfate	-0.01688
	6-Aminonicotinamide	0.02526
	2-chloro-6-(4-methoxyphenoxy)benzonitrile	-0.05903
	O-Desmethylnaproxen	-0.03739
	1,7-bis(4-hydroxyphenyl)heptan-3-one	0.12507
	11-dehydro Thromboxane B2	-0.04301
Traditional Chinese pattern		
	ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	0.13406
	aminoimidazole carboxamide ribonucleotide	-0.07802
	3-(5,7-dimethoxy-4-oxo-4H-chromen-2-yl)propanoic acid	-0.03672
	23-Nordeoxycholic acid	-0.02224
	Dehydrocholic acid	-0.00014
	4-Hydroxyisoleucine	-0.07569

	Apocynin	-0.02632
	FAHFA (22:4/18:0)	0.01286
	PC (20:5/20:5)	0.00584
Rice and tuber pattern		
	N-Acetyl-L-carnosine	0.01783
	trans-4-Hydroxy-L-proline	0.03903
	1-(2-furyl)pentane-1,4-dione	0.08374
	5-(2,5-dihydroxyhexyl)oxolan-2-one	0.13918
	(2S)-2-(2-hydroxypropan-2-yl)-2H,3H,7H-furo[3,2-g]chromen-7-one	0.033
	LPC 17:0	-0.02283
	N-(2-Furoyl)glycine	0.26812
	2-(4-methylphenyl)-5-(3,4,5-trimethoxyphenyl)-2H-1,2,3,4-tetraazole	0.01654
	6-Aminonicotinamide	0.06881
	1-(5H-dibenzo[b,f]azepin-5-yl)ethan-1-one	0.13352
	FAHFA (22:4/18:0)	-0.03708
	Glutamine	-0.01445
	Paracetamol	0.17755

Metabolites included in the LASSO regression were those with $P < 0.05$ in the initial differential metabolite analysis.

Supplementary Table 14. Feature metabolites selected by LASSO regression and their coefficients for association with MetS

Metabolites	Coefficients
Monoolein	0.13171
MAG (18:3)	0.47816
6-Sialyllactose	0.20183
N-lactoyl-phenylalanine	0.25718
6-Deoxy-D-glucose	-0.07096
4-Hydroxyisoleucine	-0.18205
PC (5:0/13:1)	-0.39631
L-Cysteine-glutathione gisulfide	-0.04811
Lysine Butyrate	-0.09671
Lysope 14:0	0.13305
2-[6-(1H-benzo[d]imidazol-2-yl)-2-pyridyl]-1H-benzo[d]imidazole	0.17267
N-(2-methyl-5-nitrophenyl)-N-(methylsulfonyl)methanesulfonamide	-0.20263
Calcium D-Panthotenate	-0.16118
L-Leucyl-L-Alanine	-0.20073
D-Panthenol	-0.08047
4-(2-chloro-6-fluorobenzyl)-3,5-dimethyl-4-prop-2-ynyl-4H-pyrazole	0.10462
Chenodeoxycholic acid-3-beta-D-glucuronide	0.15552
Heptadecanoic acid	0.12549
Norbutorphanol	-0.10142
Pyridoxamine	0.11910
Coniferyl alcohol	-0.16044
6-chloro-3-[(dimethylamino)methylidene]chroman-4-one	0.14959
N1-morpholinocarbonyl-4-methylbenzene-1-sulfonamide	0.05893
Taurochenodeoxycholic Acid (sodium salt)	0.07410
Thromboxane B2	-0.02960
3-Methoxycinnamic acid	-0.36390
Heroin-d3	-4.43602
3-(2-propynylsulfanyl)-5-[4-(trifluoromethyl)phenyl]-4H-1,2,4-triazole	-0.08211
(S)-Equol	0.03967
Paracetamol	0.22266
Noroxycodone-d3	-0.05022
Pyridoxine O-Glucoside	0.18100
PC (3:0/16:2)	0.10378
12-Oxo phytodienoic acid	-0.06206
L-Adrenaline	-0.11086

Metabolites included in the LASSO regression were those with $P < 0.05$ in the initial differential metabolite analysis.

Supplementary Table 15. Feature metabolites selected by LASSO regression and their coefficients for association with different dietary patterns in the sensitivity analysis

Dietary patterns	Metabolites	Coefficients
Meat pattern		
	N-Acetyl-L-carnosine	0.25723
	N1-[6-hydroxy-2-(2-pyridyl)pyrimidin-4-yl]acetamide	0.18466
	5-Phenylvaleric Acid	0.14057
	Desoxycortone	0.07347
	Phe-Pro	0.05429
	(2E)-4-Hydroxy-3,7-dimethyl-2,6-octadien-1-yl beta-D-glucopyranoside	0.0534
	methyl 2-(2-acetyl-4,5-dimethoxyphenyl)acetate	0.05132
	3-(5,7-dimethoxy-4-oxo-4H-chromen-2-yl)propanoic acid	0.04473
	5,8-dihydroxy-10-methyl-5,8,9,10-tetrahydro-2H-oxecin-2-one	0.00468
	LPA 18:3	-0.05146
	4-Hydroxyisoleucine	-0.11078
Protein-sweets pattern		
	LPC 17:0	0.09385
	ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	0.09085
	N-Acetylvaline	0.06467
	11-dehydro Thromboxane B2	-0.03855
	Ochratoxin A	-0.00305
	Tetrahydroaldosterone	-0.00665
	6-(4-methoxyphenyl)pyrimidine-2,4-diamine	-0.06949
	15-epi Prostaglandin A1	-0.07013
	4-Phenyl-3-buten-2-one	-0.07675
	Sebacic acid	-0.10566
	N2-Acetyl-L-ornithine	-0.14746
Traditional Chinese pattern		
	ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	0.18199
	Isobutyryl carnitine	0.01787
	2-(14,15-Epoxyeicosatrienoyl) glycerol	-0.00862
	Dehydrocholic acid	-0.02636
	23-Nordeoxycholic acid	-0.03302
	3-(5,7-dimethoxy-4-oxo-4H-chromen-2-yl)propanoic acid	-0.05336
	aminoimidazole carboxamide ribonucleotide	-0.18148
Rice and tuber pattern		
	N-(2-Furoyl)glycine	0.41025
	1-(5H-dibenzo[b,f]azepin-5-yl)ethan-1-one	0.24039

5-(2,5-dihydroxyhexyl)oxolan-2-one	0.18681
6-Aminonicotinamide	0.13926
Testosterone	0.10441
(2S)-2-(2-hydroxypropan-2-yl)-2H,3H,7H-furo[3,2-g]chromen-7-one	0.09213
trans-4-Hydroxy-L-proline	0.06481
2-(4-methylphenyl)-5-(3,4,5-trimethoxyphenyl)-2H-1,2,3,4-tetraazole	0.06439
1-(2-furyl)pentane-1,4-dione	0.05055
Deoxycholic acid	0.04059
Ochratoxin A	0.0288
ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	0.0248
Phe-Pro	0.02363
Kaempferol	0.00824
(±)9(10)-DiHOME	0.00258
3-(5,7-dimethoxy-4-oxo-4H-chromen-2-yl)propanoic acid	-0.06255
3-Hydroxysebacic acid	-0.08303
LPC 17:0	-0.10754
7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-decahydronaphthalen-1-ol	-0.12394

Metabolites included in the LASSO regression were those with *FDR* < 0.2 in the initial differential metabolite analysis.

Supplementary Table 16. Feature metabolites selected by LASSO regression and their coefficients for association with MetS in the sensitivity analysis

Metabolites	Coefficients
Monoolein	0.40161
N-lactoyl-phenylalanine	0.30589
MAG (18:3)	0.28887
2-[6-(1H-benzo[d]imidazol-2-yl)-2-pyridyl]-1H-benzo[d]imidazole	0.22389
Pyridoxamine	0.20243
6-Sialyllactose	0.16228
Chenodeoxycholic acid-3-beta-D-glucuronide	0.13227
Lysope 14:0	0.08609
4-(2-chloro-6-fluorobenzyl)-3,5-dimethyl-4-prop-2-ynyl-4H-pyrazole	0.07501
2-Thio-acetyl MAGE	0.03185
Lysine Butyrate	-0.05389
Norbutorphanol	-0.08563
L-Cysteine-glutathione gisulfide	-0.09006
Cinchophen	-0.15708
Ala-Leu	-0.16938
4-Hydroxyisoleucine	-0.18871
Heptadecanoic acid	-0.20625
6-Deoxy-D-glucose	-0.21219
D-Panthenol	-0.24779
N-(2-methyl-5-nitrophenyl)-N-(methylsulfonyl)methanesulfonamide	-0.2518
Coniferyl alcohol	-0.35989
Calcium D-Panthotenate	-0.42304
PC (5:0/13:1)	-0.45331

Metabolites included in the LASSO regression were those with *FDR* < 0.2 in the initial differential metabolite analysis.

Supplementary Table 17. Associations between metabolic signatures of dietary patterns, metabolic risk score, and MetS in the sensitivity analysis

	Tertile 1	Tertile 2	Tertile 3	*P* for trend
	OR (95% CI)	OR (95% CI)	OR (95% CI)	
Metabolic risk score	1.00	**4.61 (2.66, 8.23)**	**25.74 (13.77, 50.42)**	**<0.001**
Metabolic signature of meat pattern	1.00	1.50 (0.93, 2.44)	**1.23 (1.006, 1.50)**	0.199
Metabolic signature of protein-sweets pattern	1.00	0.85 (0.52, 1.37)	1.42 (0.88, 2.30)	0.160
Metabolic signature of traditional Chinese pattern	1.00	0.96 (0.59, 1.55)	1.05 (0.65, 1.69)	0.854
Metabolic signature of rice and tuber pattern	1.00	0.87 (0.54, 1.41)	0.96 (0.59, 1.55)	0.854

This sensitivity analysis used a metabolite selection threshold of *FDR* < 0.2 for inclusion in the LASSO regression models.

Supplementary Table 18. Differential metabolites between MetS groups (Non-MetS vs. MetS) using a stricter QC threshold (CV <25%)

Metabolites Name	Formula	Class_I	FC	log2FC	*P* value	VIP	Regulation (T1 vs T3)
Monoolein	C21 H40 O4	Lipids and lipid-like molecules	1.725204968	0.786767776	2.37257E-11	3.621990651	up
MAG (18:3)	C21 H36 O4	Lipids and lipid-like molecules	1.671306293	0.740976154	2.62266E-10	3.452956418	up
6-Sialyllactose	C23 H39 N O19	Organic oxygen compounds	1.266569995	0.340926808	2.21546E-08	3.050816567	up
N-lactoyl-phenylalanine	C12 H15 N O4	Organic acids and derivatives	1.238064227	0.30808616	2.49469E-08	3.053133736	up
6-Deoxy-D-glucose	C6 H12 O5	Organic oxygen compounds	0.741545706	-0.431392477	5.84806E-08	2.972748076	down
2-Thio-acetyl MAGE	C21 H42 O3 S	Organic acids and derivatives	1.365265183	0.449181201	6.77245E-08	2.997817195	up
5-(2,5-dihydroxyhexyl)oxolan-2-one	C10 H18 O4		0.758472174	-0.398831842	8.94203E-08	2.925106465	down
2,4-dihydroxyheptadec-16-en-1-yl acetate	C19 H36 O4		1.37914362	0.463772702	4.62321E-07	2.79944175	up
4-Hydroxyisoleucine	C6 H13 N O3	Organic acids and derivatives	0.71287173	-0.488285586	5.48972E-07	2.762332074	down
Pipecolic acid	C6 H11 N O2	Organic acids and derivatives	0.705143651	-0.504010903	8.76768E-07	2.69253679	down
Sorbic acid	C6 H8 O2	Lipids and lipid-like molecules	0.699732598	-0.515124391	1.22527E-06	2.657934115	down
Myristic Acid	C14 H28 O2	Lipids and lipid-like molecules	1.21341546	0.279073598	1.03745E-05	2.57523233	up
PC (5:0/13:1)	C26 H50 N O8 P	Lipids and lipid-like molecules	0.786446337	-0.346579768	1.57971E-05	2.382232624	down
L-Cysteine-glutathione gisulfide	C13 H22 N4 O8 S2		0.804060375	-0.31462426	2.29101E-05	2.327628594	down
Lysine Butyrate	C10 H22 N2 O4	Organic acids and derivatives	0.796329696	-0.328562236	8.39999E-05	2.265963953	down
DL-Norvaline	C5 H11 N O2	Organic acids and derivatives	0.798252973	-0.325082074	9.72118E-05	2.258173357	down
2-[(butylamino)(imino)methyl]-1-oxohydrazinium-1-olate	C5 H12 N4 O2		0.80709547	-0.309188758	0.000158039	2.081708872	down
Lysope 14:0	C19 H40 N O7 P	Lipids and lipid-like molecules	1.252172172	0.324432945	0.000197781	2.055968264	up
LPC 12:0	C20 H42 N O7 P	Lipids and lipid-like molecules	1.232173156	0.301205011	0.000294961	1.995772703	up
N1-(1H-1,2,4-triazol-3-yl)-2-hydroxybenzamide	C9 H8 N4 O2		1.577049135	0.65722761	0.000320404	1.998071174	up
2-[6-(1H-benzo[d]imidazol-2-yl)-2-pyridyl]-1H-benzo[d]imidazole	C19 H13 N5		1.219760432	0.286597822	0.000675326	1.882013414	up
MAG (18:2)	C21 H38 O4	Lipids and lipid-like molecules	1.281350669	0.357665354	0.000704865	1.93466774	up
N-(2-methyl-5-nitrophenyl)-N-(methylsulfonyl)methanesulfonamide	C9 H12 N2 O6 S2		0.768034078	-0.38075777	0.000826499	1.969931645	down
LPC 14:1	C22 H44 N O7 P	Lipids and lipid-like molecules	1.225973258	0.29392751	0.001026736	2.017414125	up
Calcium D-Panthotenate	C18 H32 Ca N2 O10	Organic acids and derivatives	0.42021909	-1.250786392	0.001515093	1.931575455	down
L-Leucyl-L-Alanine	C9 H18 N2 O3	Organic acids and derivatives	0.805334727	-0.31233955	0.002332984	1.746760858	down

D-Panthenol	C9 H19 N O4	Organic oxygen compounds	0.77202193	-0.373286265	0.002493148	1.748612033	down
Ala-Leu	C9 H18 N2 O3	Organic acids and derivatives	0.793747405	-0.333248124	0.003408956	1.656425819	down
Glycocholic acid	C26 H43 N O6	Lipids and lipid-like molecules	1.214841514	0.280768115	0.003634144	1.662771659	up
4-(2-chloro-6-fluorobenzyl)-3,5-dimethyl-4-prop-2-ynyl-4H-pyrazole	C15 H14 Cl F N2		1.239502836	0.309761573	0.004563485	1.701621076	up
Panthenol	C9 H19 N O4	Lipids and lipid-like molecules	0.785036377	-0.349168588	0.004710359	1.62188313	down
LPE 16:1	C21 H42 N O7 P	Lipids and lipid-like molecules	1.236422646	0.306171984	0.005388935	1.698244966	up
Chenodeoxycholic acid-3-beta-D-glucuronide	C30 H48 O10		1.348703751	0.431573488	0.005535453	1.579537016	up
Heptadecanoic acid	C17 H34 O2	Lipids and lipid-like molecules	0.68027188	-0.55581664	0.005856847	1.72267408	down
Norbutorphanol	C16 H21 N O2	Benzenoids	0.828332823	-0.271717537	0.005913871	1.552398421	down
ILK	C18 H36 N4 O4		1.414174713	0.499960367	0.006827124	1.546741045	up
Cinchophen	C16 H11 N O2		0.561741288	-0.832022251	0.006923959	1.523587216	down
Pantethine	C22 H42 N4 O8 S2	Organic acids and derivatives	4.744329798	2.246204301	0.007003102	1.59061042	up
Cholic acid	C24 H40 O5	Lipids and lipid-like molecules	1.384513786	0.46937942	0.007532594	1.512222179	up
Pyridoxamine	C8 H12 N2 O2	Organoheterocyclic compounds	1.435513405	0.521566803	0.0076865	1.802310761	up
Avobenzone	C20 H22 O3		0.663800986	-0.591177323	0.008246649	1.468095125	down
Chenodeoxycholic Acid	C24 H40 O4	Lipids and lipid-like molecules	1.428107676	0.514104759	0.008594368	1.461744223	up
Coniferyl alcohol	C10 H12 O3	Benzenoids	0.819948459	-0.286394868	0.009088278	1.96553579	down
(±)13-HODE	C18 H32 O3		1.213937513	0.279694162	0.009954849	1.478409131	up
6-chloro-3-[(dimethylamino)methylidene]chroman-4-one	C12 H12 Cl N O2		1.888150443	0.91697372	0.010082285	1.722073546	up
6-Keto-prostaglandin f1alpha	C20 H34 O6	Lipids and lipid-like molecules	0.780210615	-0.358064468	0.010560779	1.429355687	down
23-Norcholic acid	C23 H38 O5		1.222437429	0.289760622	0.011097391	1.43789619	up
N1-morpholinocarbonyl-4-methylbenzene-1-sulfonamide	C12 H16 N2 O4 S		1.936406861	0.953382111	0.011112626	1.42432866	up
Taurochenodeoxycholic Acid (sodium salt)	C26 H45 N O6 S		1.225934449	0.29388184	0.011557101	1.449941698	up
Thromboxane B2	C20 H34 O6	Lipids and lipid-like molecules	0.817613087	-0.290509806	0.012218179	1.40640829	down
Deoxycholic acid	C24 H40 O4	Lipids and lipid-like molecules	1.485315234	0.570769152	0.015027141	1.35175934	up
3-Methoxycinnamic acid	C10 H10 O3	Phenylpropanoids and polyketides	0.777832614	-0.362468367	0.01725312	1.320857253	down
4-Methoxycinnamic acid	C10 H10 O3	Phenylpropanoids and polyketides	0.755011516	-0.405429445	0.017589172	1.316439991	down
Heroin-d3	C21 H20 [2]H3 N O5		0.695204668	-0.524490327	0.018184624	1.400817956	down
N-Acetylneuraminic acid	C11 H19 N O9	Organic oxygen compounds	1.440648688	0.526718568	0.021549286	1.37946998	up
3-(2-propynylsulfanyl)-5-[4-(trifluoromethyl)phenyl]-4H-1,2,4-triazole	C12 H8 F3 N3 S		0.645490828	-0.631531498	0.027560009	1.225707095	down

N'-(benzoyloxy)-2-(2,2-dichlorocyclopropyl)ethanimidamide	C12 H12 Cl2 N2 O2		0.746363379	-0.422049893	0.028681556	1.222440697	down
1-(7-methoxy-2-oxo-2H-chromen-8-yl)-3-methyl-2-oxobutyl acetate	C17 H18 O6		0.5539455	-0.852184051	0.030193806	1.249620847	down
(S)-Equol	C15 H14 O3	Phenylpropanoids and polyketides	1.266821357	0.341213094	0.030824418	1.552293099	up
Paracetamol	C8 H9 N O2	Benzenoids	2.44312645	1.288728536	0.031214772	1.382641467	up
Noroxycodone-d3	C17 H16 [2]H3 N O4		0.81248838	-0.299580915	0.031927703	1.243241598	down
Pyridoxine O-Glucoside	C14 H21 N O8	Organoheterocyclic compounds	1.290840179	0.368310389	0.034993231	1.319257431	up
12-Oxo phytodienoic acid	C18 H28 O3	Lipids and lipid-like molecules	0.789289771	-0.341373043	0.041321746	1.13431993	down
Kynurenic acid O-hexside	C16 H17 N O8	Organoheterocyclic compounds	1.258908383	0.332173295	0.042093283	1.137064413	up
1-(4-benzhydrylpiperidino)-2,2,2-trichloroethan-1-one	C20 H20 Cl3 N O		1.646500227	0.71940271	0.042521028	1.133806424	up
L-threo-3-Phenylserine	C9 H11 N O3	Organic acids and derivatives	4.157553752	2.055734916	0.042892566	1.199355765	up
13-Hpotre(R)	C18 H30 O4		0.790968601	-0.33830767	0.044058469	1.196780029	down
Glutathione	C10 H17 N3 O6 S	Organic acids and derivatives	0.605742851	-0.723222621	0.045346921	1.155890835	down
4-[1-(dimethylamino)ethylidene]-2-phenyl-1,3-oxazol-5(4H)-one	C13 H14 N2 O2		0.677297462	-0.562138506	0.049446591	1.09008591	down
L-Adrenaline	C9 H13 N O3	Benzenoids	0.695293603	-0.524305778	0.049695625	1.191656894	down

Differential metabolites were screened by partial least squares-discriminant analysis (PLS-DA) combined with univariate statistics; VIP: Variable Importance in the Projection from the first component of the PLS-DA model, indicating the metabolite's contribution to group discrimination; FC (Fold Change): The ratio of the average abundance of all biological replicates in the Tertile 3 group to that in the Tertile 1 group (T3/T1); An FC > 1 indicates up-regulation in the Tertile 3 group; *P*-value was calculated by Student's t-test to assess the significance of the difference; The screening thresholds were set as follows: VIP > 1.0, FC > 1.2 or FC < 0.833, and *P*-value < 0.05.

Supplementary Table 19. Differential metabolites between meat pattern groups (Tertile 1 vs. Tertile 3) using a stricter QC threshold (CV <25%)

Metabolites Name	Formula	Class_I	FC	log2FC	*P* value	VIP	Regulation (T1 vs T3)
Phe-Pro	C14 H18 N2 O3	Organic acids and derivatives	1.276725076	0.352447895	5.47121E-07	3.320974431	up
N-Acetyl-L-carnosine	C11 H16 N4 O4		1.359407553	0.442978043	7.28836E-07	3.268668046	up
5,8-dihydroxy-10-methyl-5,8,9,10-tetrahydro-2H-oxecin-2-one	C10 H14 O4		1.550029398	0.632295578	2.47974E-05	2.776805842	up
methyl 2-(2-acetyl-4,5-dimethoxyphenyl)acetate	C13 H16 O5		1.394342621	0.479585107	4.30238E-05	2.664317594	up
3-(3,4,5-trimethoxyphenyl)propanoic acid	C12 H16 O5		1.53705675	0.620170432	7.38656E-05	2.553135323	up
(2E)-4-Hydroxy-3,7-dimethyl-2,6-octadien-1-yl beta-D-glucopyranoside	C16 H28 O7		1.563181431	0.644485235	0.000181345	2.566669282	up
N-(2-methyl-5-nitrophenyl)-N-(methylsulfonyl)methanesulfonamide	C9 H12 N2 O6 S2		1.376435415	0.460936918	0.000196186	2.303283161	up
5-Phenylvaleric Acid	C11 H14 O2	Lipids and lipid-like molecules	1.413243761	0.499010328	0.000219646	2.568078945	up
Etiocholanolone	C19 H30 O2	Lipids and lipid-like molecules	1.285934848	0.36281755	0.000331155	2.311759195	up
ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	C10 H14 N2 O2 S		1.907885202	0.931974367	0.000460477	2.335449895	up
Testosterone	C19 H28 O2	Lipids and lipid-like molecules	1.276151592	0.351799715	0.000478208	2.232326497	up
N1-(3-amino-4-chlorophenyl)-2-[2,4-di(tert-pentyl)phenoxy]acetamide	C24 H33 Cl N2 O2		1.294523766	0.372421451	0.000478237	2.224696393	up
Testosterone sulfate	C19 H28 O5 S	Lipids and lipid-like molecules	1.308553084	0.387972452	0.001298316	2.056156189	up
Mesterolone	C20 H32 O2	Lipids and lipid-like molecules	1.296608755	0.37474322	0.00191656	1.871885921	up
trans-4-Hydroxy-L-proline	C5 H9 N O3	Organic acids and derivatives	1.213124359	0.278727451	0.002477721	1.959023181	up
1,3-Dimethyluric acid	C7 H8 N4 O3	Organoheterocyclic compounds	1.352670334	0.435810276	0.002885205	1.892333947	up
Desoxycortone	C21 H30 O3	Lipids and lipid-like molecules	1.233489368	0.30274528	0.00320654	1.813995497	up
Jasmonic acid	C12 H18 O3	Lipids and lipid-like molecules	1.545857626	0.628407453	0.003491266	2.065242761	up
N1-[6-hydroxy-2-(2-pyridyl)pyrimidin-4-yl]acetamide	C11 H10 N4 O2		1.771783436	0.825202275	0.003790215	1.937185465	up
3-(5,7-dimethoxy-4-oxo-4H-chromen-2-yl)propanoic acid	C14 H14 O6		1.357194901	0.440627915	0.003882763	2.050343696	up
ACar 13:0	C20 H40 N O4	Lipids and lipid-like molecules	1.211093403	0.276310134	0.004010829	1.940800929	up
Isorhapontigenin	C15 H14 O4	Phenylpropanoids and polyketides	0.06175847	-4.017219186	0.004159407	1.556905636	down
4-Hydroxyisoleucine	C6 H13 N O3	Organic acids and derivatives	0.721153498	-0.471621724	0.004614468	1.951100592	down
Prunin	C21 H22 O10	Phenylpropanoids and polyketides	0.185766331	-2.428439048	0.004831405	1.597495114	down
Pantethine	C22 H42 N4 O8 S2	Organic acids and derivatives	3.75637173	1.909339839	0.005913081	2.218043702	up
(+/-)5(6)-EET	C20 H32 O3	Lipids and lipid-like molecules	1.287790625	0.364898052	0.006874078	1.710563785	up
9-[(2-hydroxyethoxy)methyl]-1,9-dihydro-6H-purin-6-one	C8 H10 N4 O3		1.339049422	0.421209209	0.008138066	1.762506947	up
N-[1-(4-methoxy-2-oxo-2H-pyran-6-yl)-2-methylbutyl]acetamide	C13 H19 N O4		0.031209134	-5.001887877	0.009031778	1.398112757	down

Theophylline	C7 H8 N4 O2	Organoheterocyclic compounds	1.217782254	0.284256195	0.010737006	1.7484517	up
Quinoline-4-carboxylic acid	C10 H7 N O2	Organoheterocyclic compounds	1.282617911	0.359091459	0.011154228	1.784361389	up
Temazepam	C16 H13 Cl N2 O2	Organoheterocyclic compounds	0.731147383	-0.451765845	0.011590928	1.705001093	down
Allantoin	C4 H6 N4 O3	Organoheterocyclic compounds	1.281452589	0.357780103	0.011816693	1.761890999	up
Piperine	C17 H19 N O3	Alkaloids and derivatives	1.290792984	0.368257641	0.013028803	1.664084866	up
LPE 20:3	C25 H46 N O7 P	Lipids and lipid-like molecules	0.82945671	-0.269761407	0.014987704	1.739226711	down
8(S),15(S)-DiHETE	C20 H32 O4	Lipids and lipid-like molecules	3.125218324	1.643956978	0.01857204	1.521679955	up
1,2-di(3,4-dimethoxyphenyl)diaz-1-ene	C16 H18 N2 O4		0.774073697	-0.369457167	0.018950366	1.388393605	down
15-epi Prostaglandin A1	C20 H32 O4	Lipids and lipid-like molecules	0.577144947	-0.792994405	0.019568189	1.623688506	down
Kahweol	C20 H26 O3	Organoheterocyclic compounds	1.205687871	0.269856469	0.020464775	1.647790723	up
Meclocycline	C22 H21 Cl N2 O8	Phenylpropanoids and polyketides	0.394755217	-1.340969764	0.020536885	1.544977837	down
Sorbic acid	C6 H8 O2	Lipids and lipid-like molecules	0.7316017	-0.450869668	0.020834328	1.488924513	down
All-Trans-13,14-Dihydroretinol	C20 H32 O		1.449800527	0.535854419	0.021550051	1.507523703	up
Spermidine	C7 H19 N3	Organic nitrogen compounds	1.330082062	0.411515258	0.022573189	1.561166987	up
4-(allyloxy)-1,2-dihydroquinolin-2-one	C12 H11 N O2		0.701206817	-0.512088072	0.025115389	1.513019659	down
Ibuprofen metabolite B	C13 H16 O4	Phenylpropanoids and polyketides	0.592605117	-0.75485701	0.027202027	1.431876188	down
tetranor-12(R)-HETE	C16 H26 O3		2.442974535	1.288638826	0.028442578	1.394003957	up
FAHFA (16:1/18:3)	C34 H58 O4	Lipids and lipid-like molecules	0.805954181	-0.311230273	0.029046864	1.379623148	down
3-Methylamino-L-alanine	C4 H10 N2 O2	Organic acids and derivatives	0.499026852	-1.002810649	0.030432	1.186078413	down
Daidzein	C15 H10 O4	Phenylpropanoids and polyketides	0.763106026	-0.390044575	0.030539909	1.299141301	down
Riboflavin-5-phosphate	C17 H21 N4 O9 P	Nucleosides, nucleotides, and analogues	0.652099217	-0.616836607	0.031583776	1.412769724	down
ACar 15:0	C22 H44 N O4	Lipids and lipid-like molecules	1.27778108	0.353640683	0.032829108	1.532238726	up
15-keto Prostaglandin E1	C20 H32 O5	Lipids and lipid-like molecules	1.937823531	0.954437197	0.033579122	1.886808888	up
Pipecolic acid	C6 H11 N O2	Organic acids and derivatives	0.742480831	-0.429574316	0.036111255	1.364188427	down
Caffeine	C8 H10 N4 O2	Organoheterocyclic compounds	1.20446088	0.268387537	0.037006978	1.578772366	up
Tetrahydroaldosterone	C21 H32 O5	Organoheterocyclic compounds	0.63336627	-0.658888055	0.037907288	1.551830658	down
2-hydroxy-3,6-diphenylcyclohexyl acetate	C20 H22 O3		1.205301348	0.269393892	0.03794944	1.599552384	up
PC (18:5e/4:0)	C30 H52 N O7 P	Lipids and lipid-like molecules	0.783404531	-0.352170622	0.043395173	1.385916747	down
4-amino-1-(2-furylmethyl)-6-hydroxy-1,2-dihydropyrimidine-2-thione	C9 H9 N3 O2 S		0.748202549	-0.418499214	0.043841223	1.262786817	down
Ethyl-beta-glucuronide	C8 H14 O7	Organic oxygen compounds	2.044182799	1.031524213	0.044372936	1.433139022	up

N-Lauroylsarcosine	C15 H29 N O3	Organic acids and derivatives	0.524733846	-0.930342245	0.049150557	1.270250769	down
Indoxyl sulfate	C8 H7 N O4 S	Organic acids and derivatives	1.255839985	0.328652653	0.049466969	1.303407099	up
LPE 18:3	C23 H42 N O7 P	Lipids and lipid-like molecules	0.82900108	-0.270554113	0.049746217	1.548460955	down

Differential metabolites were screened by partial least squares-discriminant analysis (PLS-DA) combined with univariate statistics; VIP: Variable Importance in the Projection from the first component of the PLS-DA model, indicating the metabolite's contribution to group discrimination; FC (Fold Change): The ratio of the average abundance of all biological replicates in the Tertile 3 group to that in the Tertile 1 group (T3/T1); An FC > 1 indicates up-regulation in the Tertile 3 group; *P*-value was calculated by Student's t-test to assess the significance of the difference; The screening thresholds were set as follows: VIP > 1.0, FC > 1.2 or FC < 0.833, and *P*-value < 0.05.

Supplementary Table 20. Differential metabolites between protein-sweets pattern groups (Tertile 1 vs. Tertile 3) using a stricter QC threshold (CV <25%)

Metabolites Name	Formula	Class_I	FC	log2FC	*P* value	VIP	Regulation (T1 vs T3)
N-Acetylvaline	C7 H13 N O3	Organic acids and derivatives	2.118457909	1.083014464	0.000248224	2.696464016	up
6-(4-methoxyphenyl)pyrimidine-2,4-diamine	C11 H12 N4 O		0.833316642	-0.263063302	0.001495957	2.208644798	down
LPC 17:0	C25 H52 N O7 P	Lipids and lipid-like molecules	1.270168351	0.345019728	0.001551428	2.705089996	up
ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	C10 H14 N2 O2 S		1.690604581	0.757539264	0.001744162	2.296215741	up
Sebacic acid	C10 H18 O4	Lipids and lipid-like molecules	0.819774883	-0.286700308	0.002204491	2.232023123	down
N2-Acetyl-L-ornithine	C7 H14 N2 O3	Organic acids and derivatives	0.721057709	-0.471813366	0.00236046	2.230077327	down
Pentadecanoic Acid	C15 H30 O2	Lipids and lipid-like molecules	1.227344579	0.295540345	0.002633516	2.42215628	up
Tetrahydroaldosterone	C21 H32 O5	Organoheterocyclic compounds	0.380394396	-1.394432103	0.003730843	1.914488295	down
15-epi Prostaglandin A1	C20 H32 O4	Lipids and lipid-like molecules	0.424326397	-1.236753666	0.005436272	1.907455001	down
11-dehydro Thromboxane B2	C20 H32 O6	Lipids and lipid-like molecules	0.741197624	-0.432069839	0.005971799	2.083877997	down
4-Phenyl-3-buten-2-one	C10 H10 O	Benzenoids	0.811928503	-0.300575403	0.00770729	2.079566217	down
Ochratoxin A	C20 H18 Cl N O6	Phenylpropanoids and polyketides	0.555069016	-0.84926093	0.008952546	1.953726778	down
Δ17-6-keto prostaglandin F1α	C20 H32 O6	Lipids and lipid-like molecules	0.634999607	-0.655172396	0.009602792	1.692713027	down
Methyl EudesMate	C11 H14 O5	Benzenoids	0.44884312	-1.155716815	0.013043076	1.607093433	down
Lysope 14:0	C19 H40 N O7 P	Lipids and lipid-like molecules	1.37902604	0.4636497	0.014087101	2.124740697	up
11β-Hydroxyandrosterone	C19 H30 O3	Lipids and lipid-like molecules	0.395514572	-1.338197244	0.01472949	1.676062724	down
4-decyl-3-hydroxy-5-oxooxolane-2,3-dicarboxylic acid	C16 H26 O7		0.325555663	-1.619023862	0.015062712	1.936478715	down
Hydrocortisone acetate	C23 H32 O6	Lipids and lipid-like molecules	0.720566591	-0.472796332	0.016523366	1.678726458	down
(2S)-2-(2-hydroxypropan-2-yl)-2H,3H,7H-furo[3,2-g]chromen-7-one	C14 H14 O4		1.205336615	0.269436104	0.016664251	1.647701202	up
Quercetin-3β-D-glucoside	C21 H20 O12	Phenylpropanoids and polyketides	0.73559379	-0.443018795	0.018206169	1.907465763	down
LPC 12:0	C20 H42 N O7 P	Lipids and lipid-like molecules	1.309888828	0.389444373	0.02267867	1.907132892	up
PA (2:0/18:2)	C23 H41 O8 P	Lipids and lipid-like molecules	0.688723968	-0.53800221	0.023650451	1.844720712	down
13-Hpotre(R)	C18 H30 O4		0.670422509	-0.576857507	0.023795631	1.627570466	down
Prostaglandin K2	C20 H30 O5	Lipids and lipid-like molecules	0.695797098	-0.523261434	0.025958679	1.714180965	down
Cafestol	C20 H28 O3	Organoheterocyclic compounds	0.544987294	-0.875705499	0.026690624	1.471902768	down
N~5~-(pyridin-2-ylmethyl)-1H-1,2,4-triazole-3,5-diamine	C8 H10 N6		0.799463049	-0.322896741	0.028076796	1.762419676	down
Adenylyl Sulfate	C10 H14 N5 O10 P S		0.309587292	-1.691581842	0.033612024	1.570710005	down
Prunin	C21 H22 O10	Phenylpropanoids and polyketides	0.213963171	-2.224565603	0.035640021	1.695303879	down

Kanamycin	C18 H36 N4 O11	Organic oxygen compounds	0.542203569	-0.883093485	0.036171691	1.354398391	down
4'-Hydroxydiclofenac	C14 H11 Cl2 N O3	Benzenoids	0.369522042	-1.436267671	0.037378237	1.546772304	down
PC (18:5e/4:0)	C30 H52 N O7 P	Lipids and lipid-like molecules	0.793408672	-0.333863929	0.038420965	1.473415974	down
6-Aminonicotinamide	C6 H7 N3 O	Organoheterocyclic compounds	1.348990754	0.43188046	0.040433911	1.476988196	up
N1-(3-amino-4-chlorophenyl)-2-[2,4-di(tert-pentyl)phenoxy]acetamide	C24 H33 Cl N2 O2		1.215919079	0.282047219	0.040509359	1.484784324	up
N1-(4-cyclohexylphenyl)-2-[(4-methylphenyl)thio]acetamide	C21 H25 N O S		0.802193815	-0.317977251	0.041129513	1.847754281	down
12-Oxo phytodienoic acid	C18 H28 O3	Lipids and lipid-like molecules	0.704069434	-0.506210383	0.042190472	1.523663447	down
2-chloro-6-(4-methoxyphenoxy)benzonitrile	C14 H10 Cl N O2		0.261865016	-1.933104762	0.043790971	1.416469569	down
4-amino-1-(2-furylmethyl)-6-hydroxy-1,2-dihydropyrimidine-2-thione	C9 H9 N3 O2 S		0.68656863	-0.542524155	0.044426155	1.419906676	down
Norephedrine	C9 H13 N O	Benzenoids	0.780715592	-0.357131012	0.044481766	1.619637407	down
Acetaminophen glucuronide	C14 H17 N O8	Organic oxygen compounds	0.290047781	-1.785637515	0.045351921	1.449445928	down
Neopterin	C9 H11 N5 O4	Organoheterocyclic compounds	1.298856963	0.377242562	0.045681709	1.712772063	up
N-[1-(4-methoxy-2-oxo-2H-pyran-6-yl)-2-methylbutyl]acetamide	C13 H19 N O4		0.109418444	-3.192072154	0.04603876	1.634987523	down
1,7-bis(4-hydroxyphenyl)heptan-3-one	C19 H22 O3		1.340183914	0.422430995	0.046084825	1.488408366	up
3-(1-cyano-1,2-dihydroisoquinolin-2-yl)-3-oxopropyl propionate	C16 H16 N2 O3		0.810488969	-0.303135544	0.046451673	1.616456337	down
3-Indoleacrylic acid	C11 H9 N O2	Organic acids and derivatives	1.262919029	0.336762145	0.046540414	1.63437775	up
3-Hydroxysebacic acid	C10 H18 O5	Organic acids and derivatives	0.824905559	-0.277699136	0.049146563	1.379155222	down
ethyl 1-(3-nitro-2-thienyl)piperidine-4-carboxylate	C12 H16 N2 O4 S		0.674731577	-0.567614415	0.049436874	1.71271963	down

Differential metabolites were screened by partial least squares-discriminant analysis (PLS-DA) combined with univariate statistics; VIP: Variable Importance in the Projection from the first component of the PLS-DA model, indicating the metabolite's contribution to group discrimination; FC (Fold Change): The ratio of the average abundance of all biological replicates in the Tertile 3 group to that in the Tertile 1 group (T3/T1); An FC > 1 indicates up-regulation in the Tertile 3 group; *P*-value was calculated by Student's t-test to assess the significance of the difference; The screening thresholds were set as follows: VIP > 1.0, FC > 1.2 or FC < 0.833, and *P*-value < 0.05.

Supplementary Table 21. Differential metabolites between traditional Chinese pattern groups (Tertile 1 vs. Tertile 3) using a stricter QC threshold (CV <25%)

Metabolites Name	Formula	Class_I	FC	log2FC	*P* value	VIP	Regulation (T1 vs T3)
4-Methylphenol	C7 H8 O	Benzenoids	0.699080731	-0.516469024	0.000340732	2.9734445	down
2-(14,15-Epoxyeicosatrienoyl) glycerol	C23 H38 O5	Lipids and lipid-like molecules	0.619096016	-0.69176492	0.000405498	2.643309713	down
ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	C10 H14 N2 O2 S		1.951998204	0.964951725	0.001234598	2.55288445	up
aminoimidazole carboxamide ribonucleotide	C9 H15 N4 O8 P		0.78257833	-0.353692932	0.00210168	2.572151192	down
Isobutyryl carnitine	C11 H21 N O4	Lipids and lipid-like molecules	1.300880303	0.379488223	0.003760014	2.25861175	up
4-Methylcatechol	C7 H8 O2	Benzenoids	0.784571791	-0.35002263	0.004386101	2.383571735	down
(2,6-dimethylmorpholino)(1-methyl-5-nitro-1H-pyrazol-4-yl)methanone	C11 H16 N4 O4		0.778814436	-0.360648469	0.004599754	2.465505521	down
3-(5,7-dimethoxy-4-oxo-4H-chromen-2-yl)propanoic acid	C14 H14 O6		0.817188729	-0.291258789	0.006546645	1.966464812	down
23-Nordeoxycholic acid	C23 H38 O4		0.755857616	-0.403813601	0.008026894	2.052431716	down
Dehydrocholic acid	C24 H34 O5	Lipids and lipid-like molecules	0.798216551	-0.325147901	0.008178175	2.215880885	down
FAHFA (20:4/20:3)	C40 H64 O4	Lipids and lipid-like molecules	1.225438189	0.293297717	0.010682963	1.850728282	up
4-Hydroxyisoleucine	C6 H13 N O3	Organic acids and derivatives	0.799067106	-0.323611428	0.012236499	1.833465436	down
Ergosterol peroxide	C28 H44 O3	Lipids and lipid-like molecules	0.786842202	-0.345853756	0.014186797	1.795851805	down
Apocynin	C9 H10 O3	Organic oxygen compounds	0.809822696	-0.304322019	0.017323174	1.871232344	down
Riboflavin-5-phosphate	C17 H21 N4 O9 P	Nucleosides, nucleotides, and analogues	0.581967629	-0.780989188	0.018950644	1.821795803	down
2-[(3S)-1-(2-Thienylmethyl)-3-pyrrolidinyl]-1,3-benzothiazole	C16 H16 N2 S2	Organoheterocyclic compounds	0.545271055	-0.874954521	0.020012633	1.661886362	down
Monoolein	C21 H40 O4	Lipids and lipid-like molecules	1.205660685	0.269823939	0.023111613	1.99602774	up
Methyl indole-3-acetate	C11 H11 N O2	Organoheterocyclic compounds	0.507653083	-0.978085162	0.023184493	1.62433769	down
2-(tert-butyl)-1,3-thiazolane-4-carboxylic acid	C8 H15 N O2 S		0.778714634	-0.360833357	0.031803382	1.557041958	down
Methyl EudesMate	C11 H14 O5	Benzenoids	0.233881907	-2.096147837	0.031890063	1.414054148	down
1,2-di(3,4-dimethoxyphenyl)diaz-1-ene	C16 H18 N2 O4		0.722012935	-0.469903411	0.034450296	1.455865526	down
6-(3-hydroxybutan-2-yl)-5-(hydroxymethyl)-4-methoxy-2H-pyran-2-one	C11 H16 O5		0.70390817	-0.506540863	0.034834818	1.310732683	down
Neohesperidin	C28 H34 O15	Phenylpropanoids and polyketides	0.794302479	-0.33223959	0.039208434	2.162788908	down
PC (20:5/20:5)	C48 H76 N O8 P	Lipids and lipid-like molecules	1.319251191	0.399719286	0.039372292	1.852451839	up
5-Hydroxyindole	C8 H7 N O	Organoheterocyclic compounds	0.761300337	-0.393462379	0.039378411	1.858441665	down
3-methoxy-2-phenyl-4H-furo[2,3-h]chromen-4-one	C18 H12 O4		0.588677004	-0.764451824	0.039432071	1.493596758	down
Pyroglutamic acid	C5 H7 N O3	Organic acids and derivatives	0.811072355	-0.302097473	0.044634837	1.735887688	down

Differential metabolites were screened by partial least squares-discriminant analysis (PLS-DA) combined with univariate statistics; VIP: Variable Importance in the Projection from the first component of the PLS-DA model, indicating the metabolite's contribution to group discrimination; FC (Fold Change): The ratio of the average abundance of all biological replicates in the Tertile 3 group to that in the Tertile 1 group (T3/T1); An FC > 1 indicates up-regulation in the Tertile 3 group; *P*-value was calculated by Student's t-test to assess the significance of the difference; The screening thresholds were set as follows: VIP > 1.0, FC > 1.2 or FC < 0.833, and *P*-value < 0.05.

Supplementary Table 22. Differential metabolites between rice and tuber pattern (Tertile 1 vs. Tertile 3) using a stricter QC threshold (CV <25%)

Metabolites Name	Formula	Class_I	FC	log2FC	*P* value	VIP	Regulation (T1 vs T3)
N-Acetyl-L-carnosine	C11 H16 N4 O4		1.336569949	0.418535342	1.97966E-07	2.805220257	up
Phe-Pro	C14 H18 N2 O3	Organic acids and derivatives	1.271242453	0.346239209	2.11678E-07	2.893061625	up
Testosterone	C19 H28 O2	Lipids and lipid-like molecules	1.378676579	0.463284058	3.06708E-06	2.647088376	up
trans-4-Hydroxy-L-proline	C5 H9 N O3	Organic acids and derivatives	1.381620562	0.466361459	1.11756E-05	2.461393314	up
1-(2-furyl)pentane-1,4-dione	C9 H10 O3		1.31209607	0.391873357	3.15096E-05	2.424391953	up
N1-(3-amino-4-chlorophenyl)-2-[2,4-di(tert-pentyl)phenoxy]acetamide	C24 H33 Cl N2 O2		1.336149792	0.418081754	0.000263989	1.980686836	up
5-(2,5-dihydroxyhexyl)oxolan-2-one	C10 H18 O4		1.318241116	0.398614274	0.000421962	1.952332412	up
(2S)-2-(2-hydroxypropan-2-yl)-2H,3H,7H-furo[3,2-g]chromen-7-one	C14 H14 O4		1.352761068	0.435907045	0.000509643	2.095488612	up
ethyl 2-cyano-3-(tetrahydro-3-thiophenylamino)acrylate	C10 H14 N2 O2 S		1.629989108	0.704862324	0.000692164	1.880864475	up
3-(5,7-dimethoxy-4-oxo-4H-chromen-2-yl)propanoic acid	C14 H14 O6		0.698882648	-0.516877867	0.001333032	2.236873872	down
Mupirocin	C26 H44 O9	Lipids and lipid-like molecules	1.250764132	0.322809753	0.001501559	1.649417651	up
LPC 17:0	C25 H52 N O7 P	Lipids and lipid-like molecules	0.793761314	-0.333222844	0.001589939	2.110422838	down
Methionine	C5 H11 N O2 S	Organic acids and derivatives	1.33106737	0.412583593	0.002191122	1.728403882	up
2-[(butylamino)(imino)methyl]-1-oxohydrazinium-1-olate	C5 H12 N4 O2		1.240986842	0.311487819	0.002227746	1.789354541	up
1,3-Dimethyluric acid	C7 H8 N4 O3	Organoheterocyclic compounds	1.753890774	0.810558905	0.002722903	1.657906009	up
7-(2-hydroxypropan-2-yl)-1,4a-dimethyl-decahydronaphthalen-1-ol	C15 H28 O2		0.795892707	-0.329354139	0.002868931	1.551128206	down
N-benzyl-2-(6-methoxy-2-naphthyl)propanamide	C21 H21 N O2		1.261908674	0.335607505	0.00289766	1.982067919	up
2-Hydroxycaproic acid	C6 H12 O3	Lipids and lipid-like molecules	1.225729086	0.293640145	0.003115594	1.819184662	up
Capryloylglycine	C10 H19 N O3	Organic acids and derivatives	1.211565998	0.276872995	0.003396491	1.608836601	up
N-(2-Furoyl)glycine	C7 H7 N O4	Organic acids and derivatives	1.636443738	0.710564002	0.003711436	1.663606324	up
Oleoyl ethylamide	C20 H39 N O	Lipids and lipid-like molecules	0.658547085	-0.602641502	0.003712097	1.472479652	down
3-Hydroxysebacic acid	C10 H18 O5	Organic acids and derivatives	0.781766222	-0.355190843	0.004699139	1.538093967	down
Enrofloxacin	C19 H22 F N3 O3	Organoheterocyclic compounds	1.366882076	0.450888783	0.004744319	1.920689333	up
FAHFA (20:4/20:3)	C40 H64 O4	Lipids and lipid-like molecules	0.818244974	-0.289395259	0.005000905	1.839162206	down
Allantoin	C4 H6 N4 O3	Organoheterocyclic compounds	1.249453965	0.321297747	0.005116877	1.567596117	up
Deoxycholic acid	C24 H40 O4	Lipids and lipid-like molecules	1.420338255	0.50623455	0.005210241	1.556570898	up
Spiculisporic Acid	C17 H28 O6	Organic acids and derivatives	1.277982406	0.353867975	0.005365007	1.660573289	up
1-Methyluric acid	C6 H6 N4 O3	Organoheterocyclic compounds	1.417457249	0.503305224	0.005475959	1.611859042	up

2-(4-methylphenyl)-5-(3,4,5-trimethoxyphenyl)-2H-1,2,3,4-tetraazole	C17 H18 N4 O3		1.20512285	0.269180222	0.005805017	1.856905996	up
alpha-Benzylsuccinic acid	C11 H12 O4	Phenylpropanoids and polyketides	1.217244504	0.283618987	0.006046962	1.804911822	up
6-Aminonicotinamide	C6 H7 N3 O	Organoheterocyclic compounds	1.448603754	0.534663019	0.006647797	1.564676808	up
Hexadecanamide	C16 H33 N O	Lipids and lipid-like molecules	0.761680368	-0.392742383	0.007233422	1.362378643	down
Pregnenolone	C21 H32 O2	Lipids and lipid-like molecules	0.832194945	-0.265006569	0.00753725	1.572025284	down
1-Methylxanthine	C6 H6 N4 O2	Organoheterocyclic compounds	1.284318779	0.361003336	0.00767593	1.602793868	up
Ochratoxin A	C20 H18 Cl N O6	Phenylpropanoids and polyketides	1.749966472	0.807327282	0.008350006	2.063305141	up
8-Aminooctanoic acid	C8 H17 N O2	Organic acids and derivatives	1.222573472	0.289921168	0.008496382	1.449070911	up
N-Tetradecanamide	C14 H29 N O	Lipids and lipid-like molecules	0.792903871	-0.334782126	0.00880652	1.322089959	down
(±)9(10)-DiHOME	C18 H34 O4		1.312319123	0.39211859	0.00896047	1.566255072	up
1-(5H-dibenzo[b,f]azepin-5-yl)ethan-1-one	C16 H13 N O		1.207018722	0.271448054	0.009012712	1.834012035	up
Stearamide	C18 H37 N O	Organic acids and derivatives	0.802518051	-0.317394252	0.009449957	1.354457391	down
Theophylline	C7 H8 N4 O2	Organoheterocyclic compounds	1.637403996	0.711410321	0.010847405	1.397669415	up
Oleamide	C18 H35 N O	Lipids and lipid-like molecules	0.807212474	-0.308979625	0.012792547	1.291520895	down
Hydroxyproline	C5 H9 N O3	Organic acids and derivatives	1.54978377	0.632066941	0.014082806	1.64708003	up
3-amino-1H-pyrazolo[4,3-c]pyridine-4,6-diol	C6 H6 N4 O2		1.348608528	0.431471626	0.014767611	1.402248109	up
2-hydroxy-3,6-diphenylcyclohexyl acetate	C20 H22 O3		1.234276608	0.303665746	0.015382921	1.408788594	up
Terephthalic Acid	C8 H6 O4	Organic acids and derivatives	1.471156451	0.556950679	0.015503713	1.471240872	up
Chenodeoxycholic Acid	C24 H40 O4	Lipids and lipid-like molecules	1.372542186	0.456850493	0.015629821	1.346474963	up
(+/-)5(6)-EET Ethanolamide	C22 H37 N O3	Organic nitrogen compounds	1.332431287	0.414061135	0.016968132	1.762605985	up
9-Methyluric acid	C6 H6 N4 O3	Organoheterocyclic compounds	1.295490575	0.37349852	0.019852685	1.625994243	up
Homocystine	C8 H16 N2 O4 S2	Organic acids and derivatives	1.779483652	0.831458679	0.020071863	1.613084686	up
Arachidonoyl amide	C20 H33 N O	Lipids and lipid-like molecules	0.746608744	-0.42157569	0.02318912	1.160081892	down
Caffeine	C8 H10 N4 O2	Organoheterocyclic compounds	1.43923112	0.525298287	0.02494997	1.279992202	up
Linoleoyl ethanolamide	C20 H37 N O2	Organic nitrogen compounds	1.784054016	0.835159297	0.025440754	1.655849693	up
Maltol	C6 H6 O3	Organoheterocyclic compounds	0.740287822	-0.433841799	0.026538179	1.209689338	down
FAHFA (16:1/18:3)	C34 H58 O4	Lipids and lipid-like molecules	0.806705745	-0.309885564	0.028185973	1.269147052	down
Testosterone sulfate	C19 H28 O5 S	Lipids and lipid-like molecules	1.204254841	0.268140723	0.032228567	1.163618551	up
23-Norcholic acid	C23 H38 O5		1.204030441	0.267871868	0.032641696	1.263825985	up
Genistein	C15 H10 O5	Phenylpropanoids and polyketides	1.305924187	0.385071146	0.033564439	1.198223424	up

All-Trans-13,14-Dihydroretinol	C20 H32 O		1.215635787	0.281711052	0.033644744	1.112147434	up
Ginsenoside Rg3	C42 H72 O13	Lipids and lipid-like molecules	1.473029515	0.558786338	0.036890195	1.360307349	up
methyl 2-(2-acetyl-4,5-dimethoxyphenyl)acetate	C13 H16 O5		0.79684379	-0.327631163	0.038596262	1.870033819	down
1,7-Dimethyluric acid	C7 H8 N4 O3	Organoheterocyclic compounds	1.344147443	0.4266914	0.040172857	1.221911245	up
Benzamide	C7 H7 N O	Benzenoids	1.230240278	0.298940116	0.040314882	1.169885829	up
Glutamine	C5 H10 N2 O3	Organic acids and derivatives	0.809257247	-0.305329715	0.041015521	1.730812667	down
N1-phenyl-4-benzoylpiperidine-1-carboxamide	C19 H20 N2 O2		0.229649204	-2.12249631	0.041820225	1.206478885	down
Norfloxacin	C16 H18 F N3 O3	Organoheterocyclic compounds	1.43393979	0.519984448	0.042172753	1.224744935	up
Paracetamol	C8 H9 N O2	Benzenoids	3.351854732	1.744959625	0.043863328	1.354673639	up
Betulin	C30 H50 O2	Lipids and lipid-like molecules	1.926751803	0.946170741	0.043963848	1.301149213	up
16,16-Dimethyl prostaglandin A1	C22 H36 O4	Lipids and lipid-like molecules	1.323021408	0.403836406	0.046417769	1.214224279	up

Differential metabolites were screened by partial least squares-discriminant analysis (PLS-DA) combined with univariate statistics; VIP: Variable Importance in the Projection from the first component of the PLS-DA model, indicating the metabolite's contribution to group discrimination; FC (Fold Change): The ratio of the average abundance of all biological replicates in the Tertile 3 group to that in the Tertile 1 group (T3/T1); An FC > 1 indicates up-regulation in the Tertile 3 group; *P*-value was calculated by Student's t-test to assess the significance of the difference; The screening thresholds were set as follows: VIP > 1.0, FC > 1.2 or FC < 0.833, and *P*-value < 0.05.

Supplementary Table 23. Characteristics of metabolomics study participants in the Training and Testing Sets

Characteristic	Training set（n=280）	Testng set（n=120）	*P*
Sex			0.094
Male	86（30.71）	27（22.50）	
Female	194（69.29）	93（77.50）	
Age (years)			0.534
≤60	112（40.00）	52（43.33）	
>60	168（60.00）	68（56.67）	
Ethnicity			0.385
Han	203（72.59）	92（76.67）	
Mongolian	77（27.50）	28（23.33）	
Marital status			0.154
Married	242（86.43）	97（80.83）	
Others	38（13.57）	23（19.17）	
Education status			0.176
Middle school or below	108（38.57）	55（45.83）	
Middle school above	172（61.43）	65（54.17）	
Annual income (yuan)			0.810
<10, 000	153（54.64）	64（53.33）	
≥10, 000	127（45.36）	56（46.67）	
Smoking status			0.469
Yes	75（26.79）	28（23.33）	
No	205（73.21）	92（76.67）	
Physical activity			0.442
Light or below	78（27.86）	38（31.67）	
Moderate or vigorous	202（72.14）	82（68.33）	
Family history of diabetes			1.000
Yes	14（5.00）	6（5.00）	
No	266（95.00）	114（95.00）	
Family history of hypertension			0.112
Yes	64（22.86）	19（15.83）	
No	216（77.14）	101（84.17）	
Energy intake (kcal/d)	1669.01±683.45	1669.01±597.02	0.387
BMI (kg/m^2)	26.44±2.33	26.26±3.13	0.800

Supplementary Table 24. Performance comparison of MetS risk assessment models based on machine learning for dietary patterns and their metabolite biomarkers

Model	Training Set			Testing Set		
	Accuracy（95%CI）	Sensitivity	Specificity	Accuracy（95%CI）	Sensitivity	Specificity
Logistic Regression	0.696 (0.639, 0.750)	0.693	0.700	0.633 (0.541, 0.719)	0.600	0.667
Random Forest	0.999 (0.987, 0.999)	0.999	0.999	0.633 (0.575, 0.719)	0.633	0.633
KNN	0.999 (0.987, 0.999)	0.999	0.999	0.633 (0.541, 0.719)	0.533	0.733
SVM	0.746 (0.691, 0.796)	0.750	0.743	0.675 (0.584, 0.758)	0.667	0.683
XGBoost	0.999 (0.987, 0.999)	0.999	0.999	0.625 (0.532, 0.712)	0. 667	0.583
LightGBM	0.961 (0.931, 0.980)	0.971	0.950	0.650 (0.558, 0.735)	0.717	0. 583

Supplementary Table 25. Performance comparison of MetS risk assessment models based on machine learning for dietary patterns and MetS metabolite biomarkers

Model	Training Set			Testing Set		
	Accuracy（95%CI）	Sensitivity	Specificity	Accuracy（95%CI）	Sensitivity	Specificity
Logistic Regression	0.800 (0.748, 0.845)	0.771	0.829	0.708 (0.618, 0.788)	0.733	0.683
Random Forest	0.999 (0.987, 0.999)	0.999	0.999	0.692 (0.601, 0.773)	0.717	0.667
KNN	0.939 (0.905, 0.964)	0.907	0.971	0.700 (0.610, 0.780)	0.550	0.850
SVM	0.782 (0.729, 0.829)	0.729	0.836	0.708 (0.618, 0.788)	0.717	0.700
XGBoost	0.996 (0.980, 0.999)	0.993	0.999	0.717 (0.627, 0.795)	0.683	0.750
LightGBM	0.986 (0.964, 0.996)	0.999	0.971	0.692 (0.601, 0.773)	0.733	0.650

Supplementary Table 26. Performance comparison of MetS risk assessment models based on machine learning for dietary patterns and their metabolite biomarkers in the sensitivity analysis

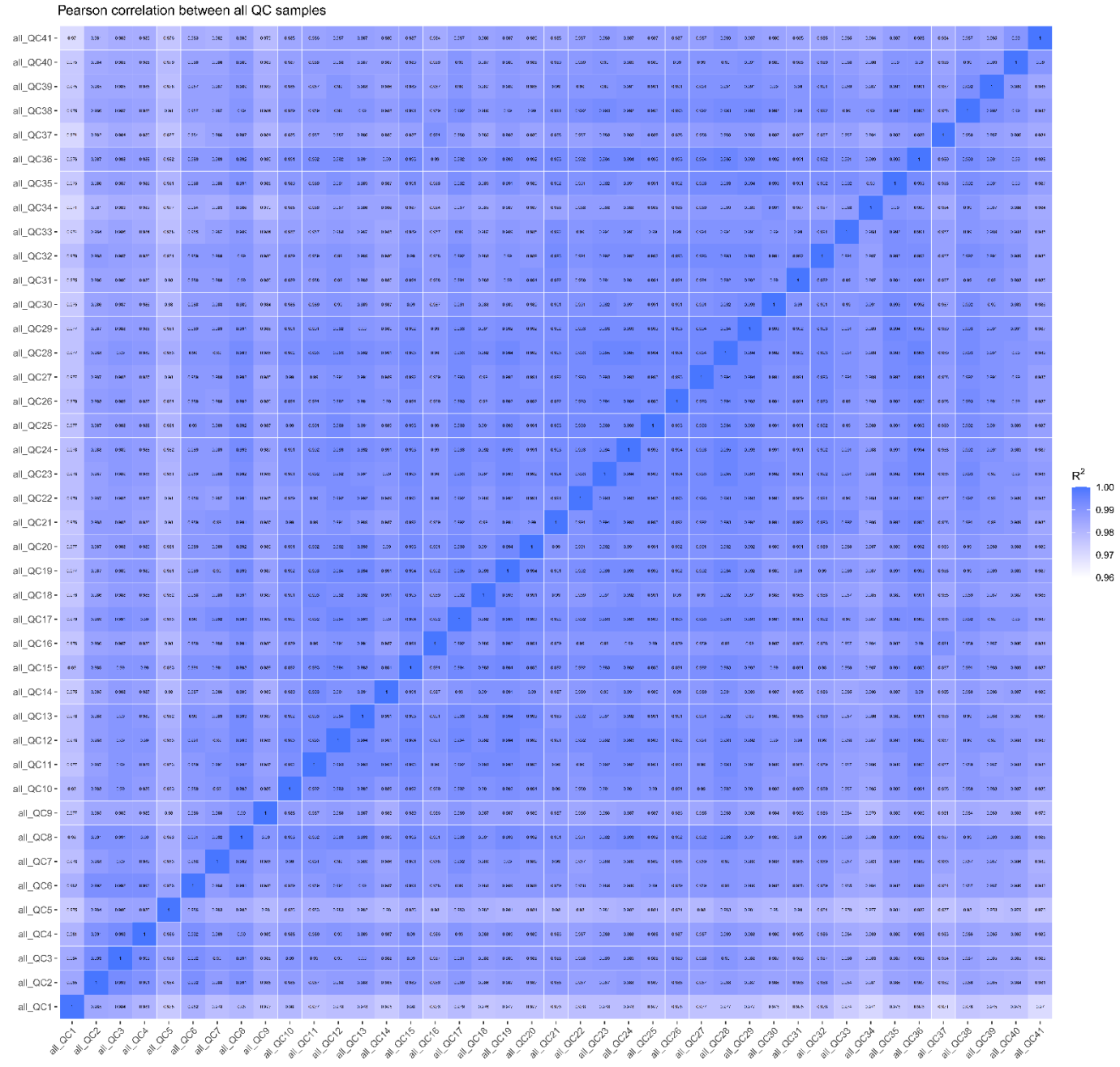
Model	Training Set			Testing Set		
	Accuracy（95%CI）	Sensitivity	Specificity	Accuracy（95%CI）	Sensitivity	Specificity
Logistic Regression	0.696 (0.639, 0.750)	0.693	0.7	0.633 (0.541, 0.719)	0.6	0.667
Random Forest	0.999 (0.987, 0.999)	0.999	0.999	0.633 (0.575, 0.719)	0.633	0.633
KNN	0.999 (0.987, 0.999)	0.999	0.999	0.633 (0.541, 0.719)	0.533	0.733
SVM	0.746 (0.691, 0.796)	0.75	0.743	0.675 (0.584, 0.758)	0.667	0.683
XGBoost	0.999 (0.987, 0.999)	0.999	0.999	0.625 (0.532, 0.712)	0.667	0.583
LightGBM	0.961 (0.931, 0.980)	0.971	0.95	0.650 (0.558, 0.735)	0.717	0.583

This sensitivity analysis used a metabolite selection threshold of *FDR* < 0.2 for inclusion in the LASSO regression models.

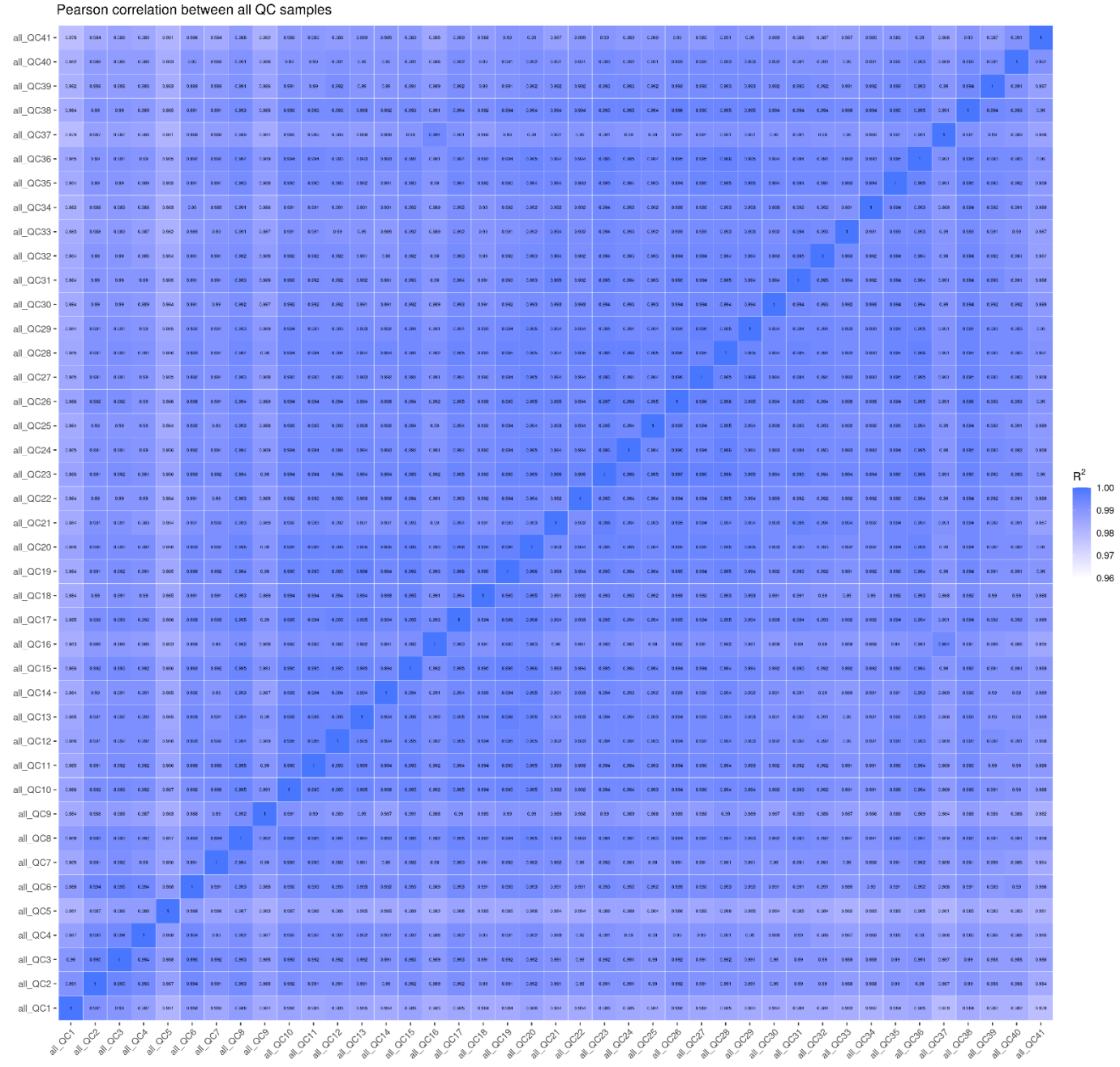
Supplementary Table 27. Performance comparison of MetS risk assessment models based on machine learning for dietary patterns and their metabolite biomarkers in the sensitivity analysis

Model	Training Set			Testing Set		
	Accuracy（95%CI）	Sensitivity	Specificity	Accuracy（95%CI）	Sensitivity	Specificity
Logistic Regression	0.800 (0.748, 0.845)	0.771	0.829	0.708 (0.618, 0.788)	0.733	0.683
Random Forest	0.999 (0.987, 0.999)	0.999	0.999	0.692 (0.601, 0.773)	0.717	0.667
KNN	0.939 (0.905, 0.964)	0.907	0.971	0.700 (0.610, 0.780)	0.55	0.85
SVM	0.782 (0.729, 0.829)	0.729	0.836	0.708 (0.618, 0.788)	0.717	0.7
XGBoost	0.996 (0.980, 0.999)	0.993	0.999	0.717 (0.627, 0.795)	0.683	0.75
LightGBM	0.986 (0.964, 0.996)	0.999	0.971	0.692 (0.601, 0.773)	0.733	0.65

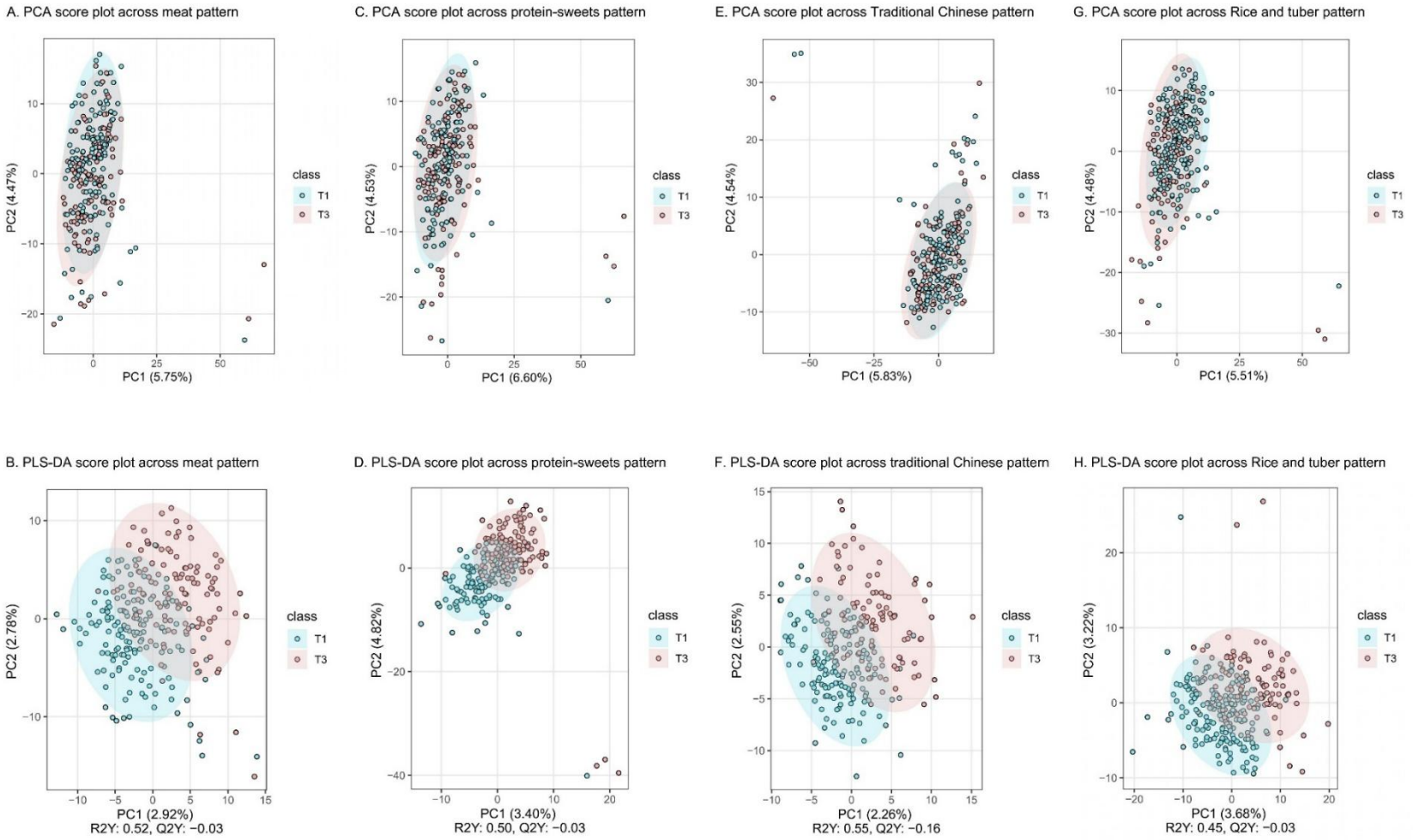
This sensitivity analysis used a metabolite selection threshold of *FDR* < 0.2 for inclusion in the LASSO regression models.



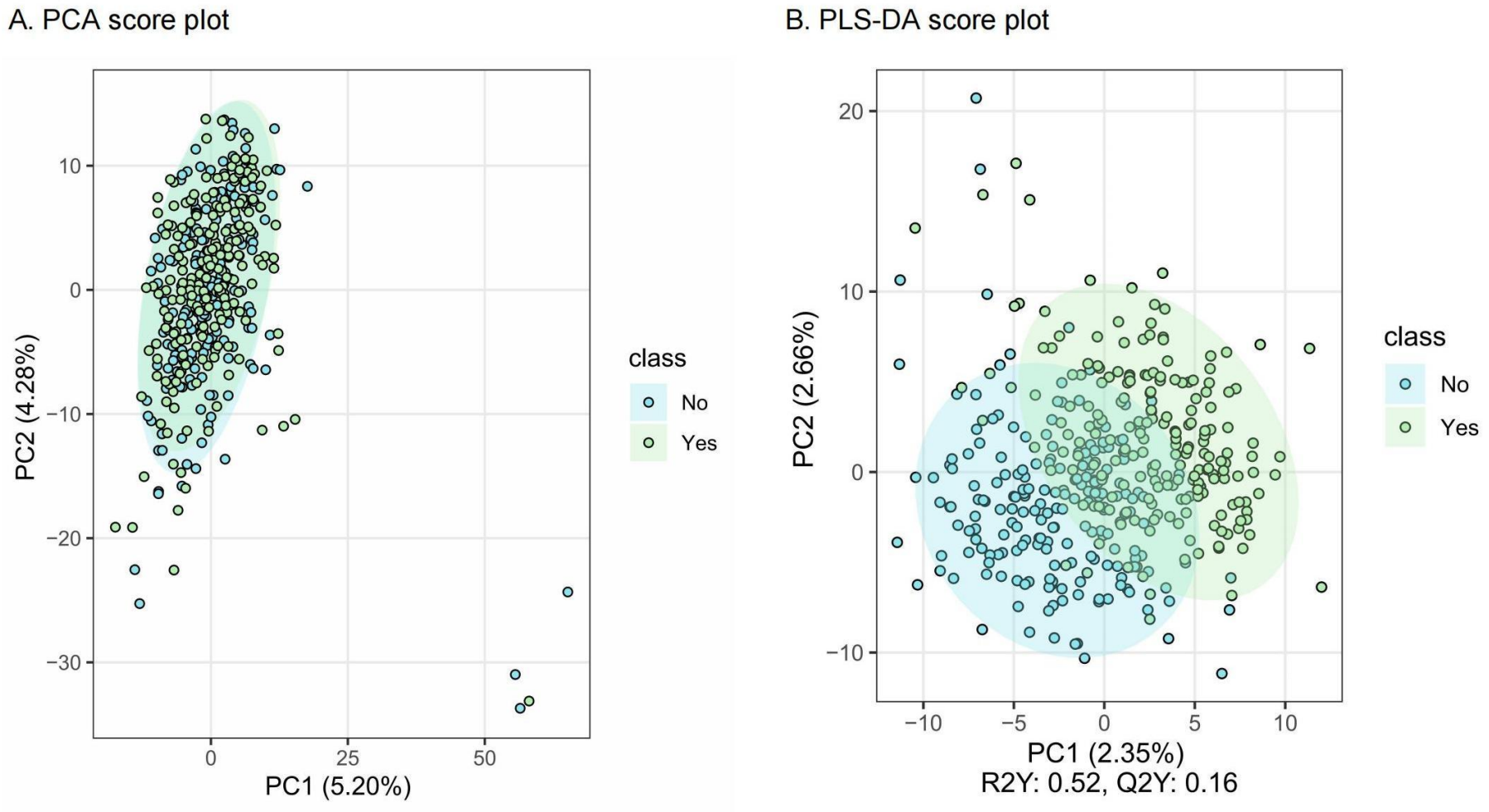
Supplementary Figure 1. Pearson correlation heatmaps of QC samples



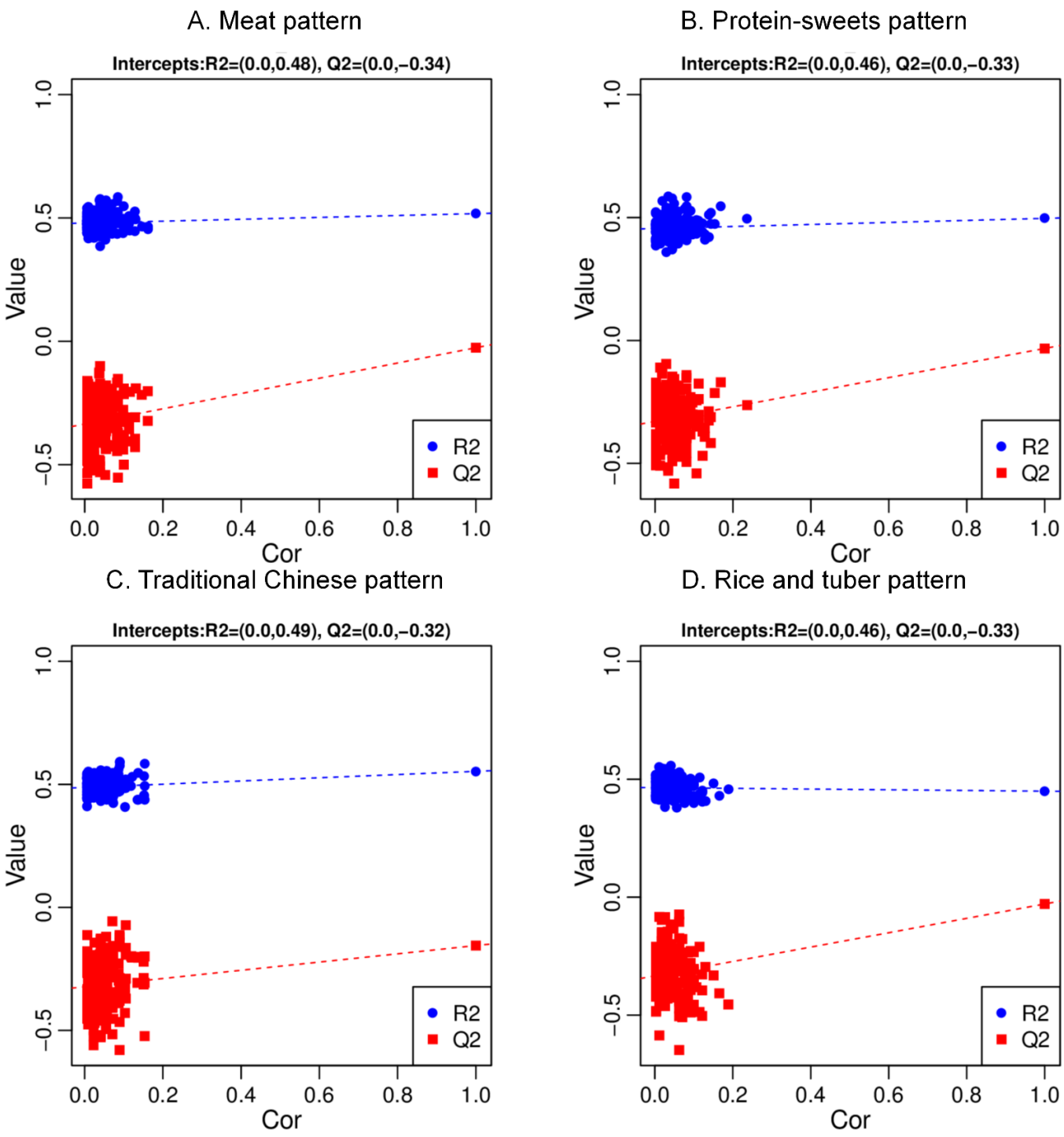
Supplementary Figure 2. Pearson correlation heatmaps of QC samples using a stricter QC threshold (CV <25%)



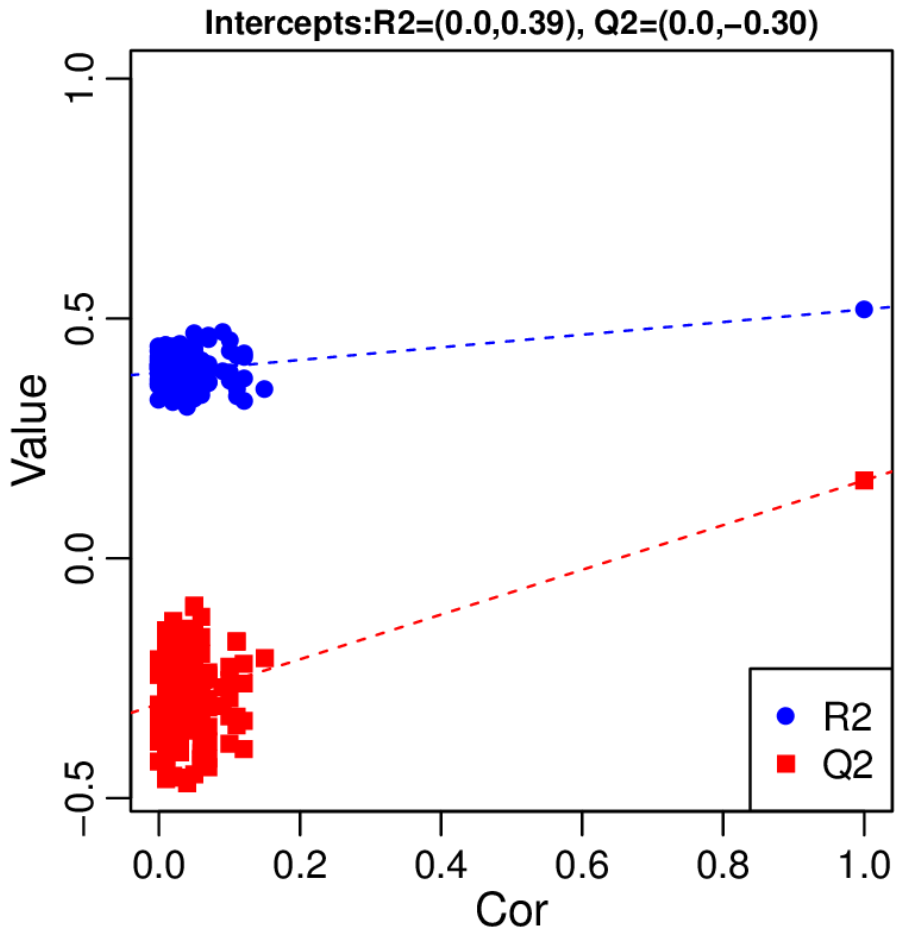
Supplementary Figure 3. Multivariate analysis of metabolite profiles across different dietary patterns groups



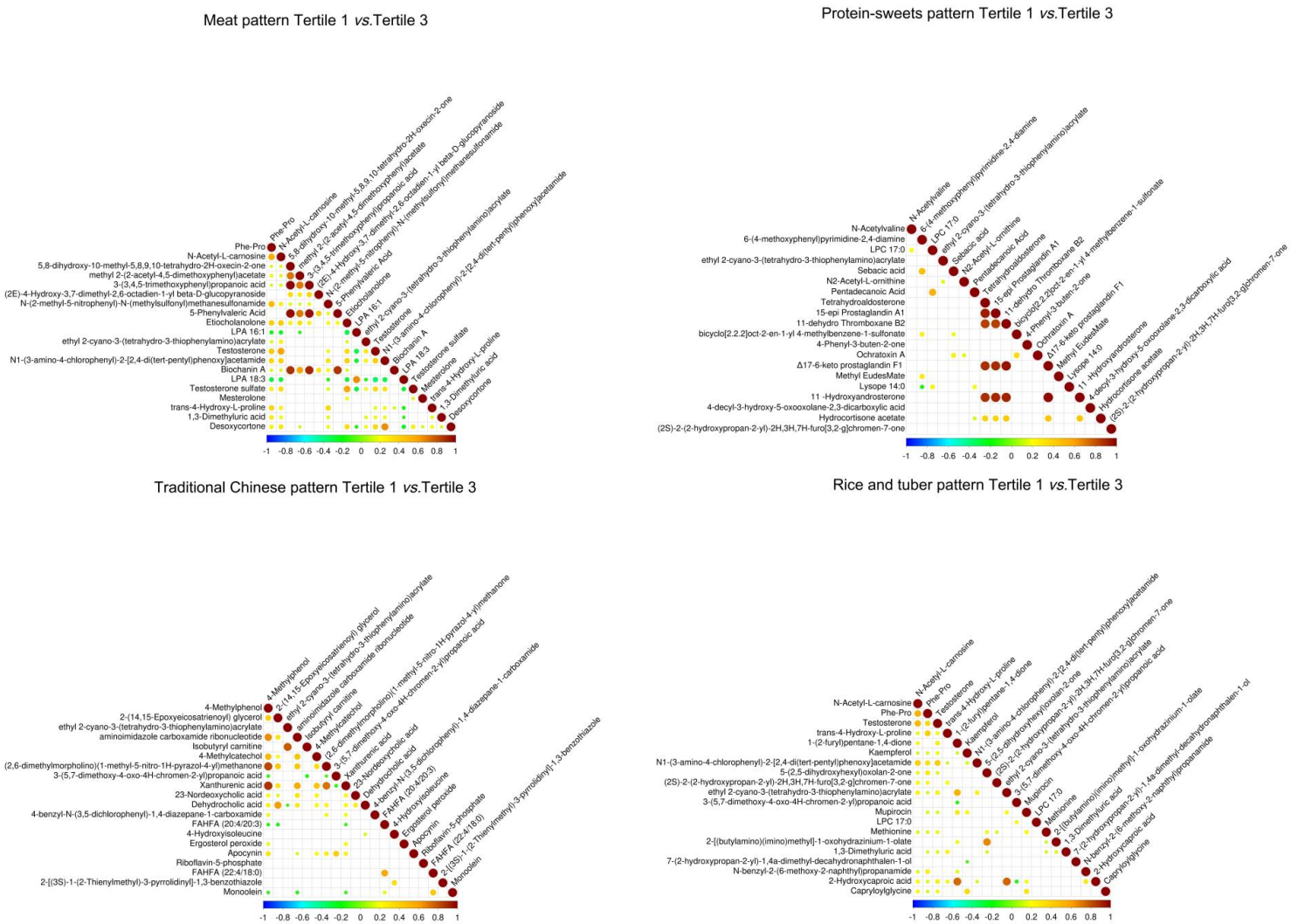
Supplementary Figure 4. Multivariate analysis of metabolite profiles across MetS groups



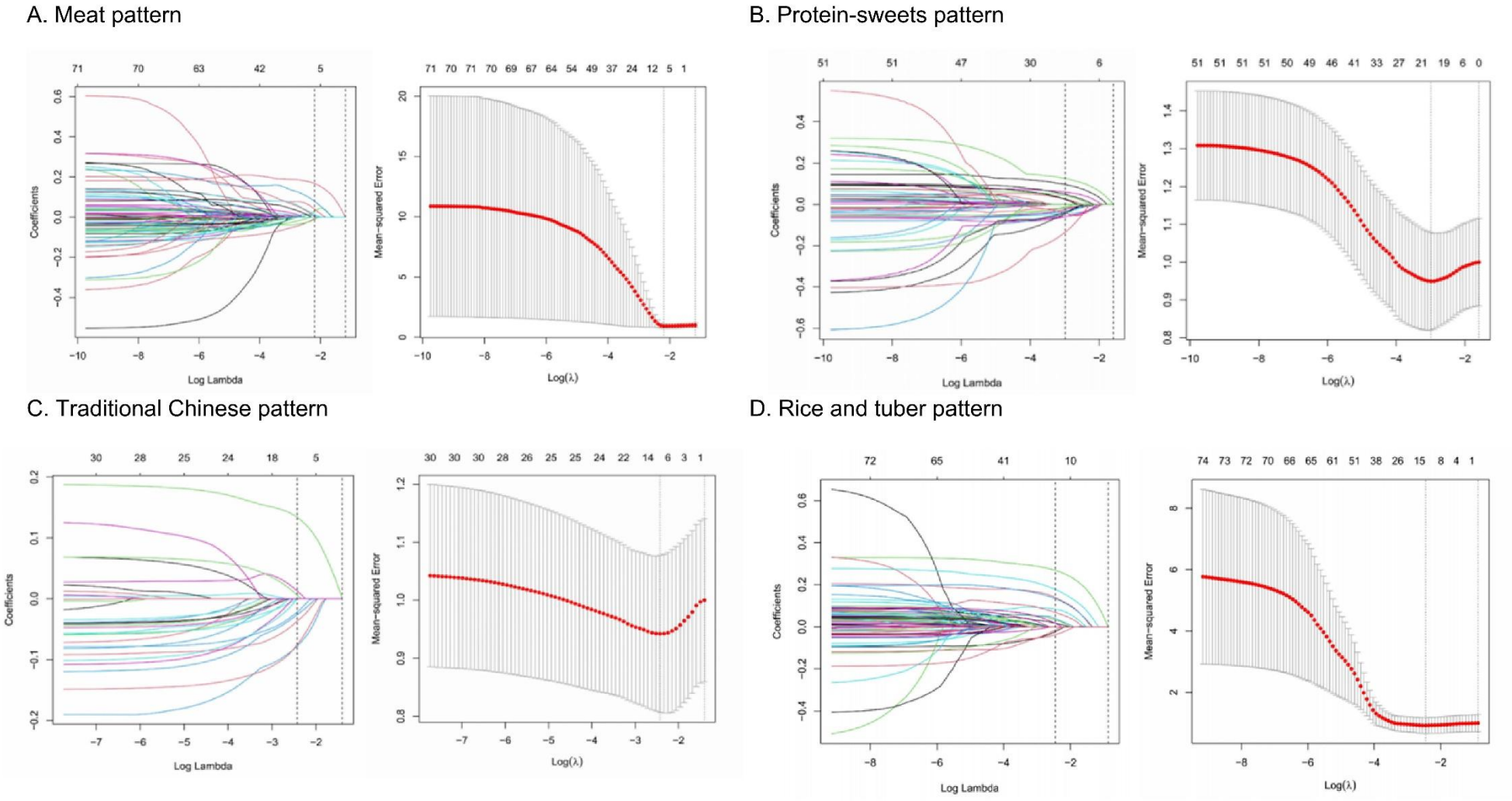
Supplementary Figure 5. PLS-DA permutation test plots for model validation in Dietary patterns



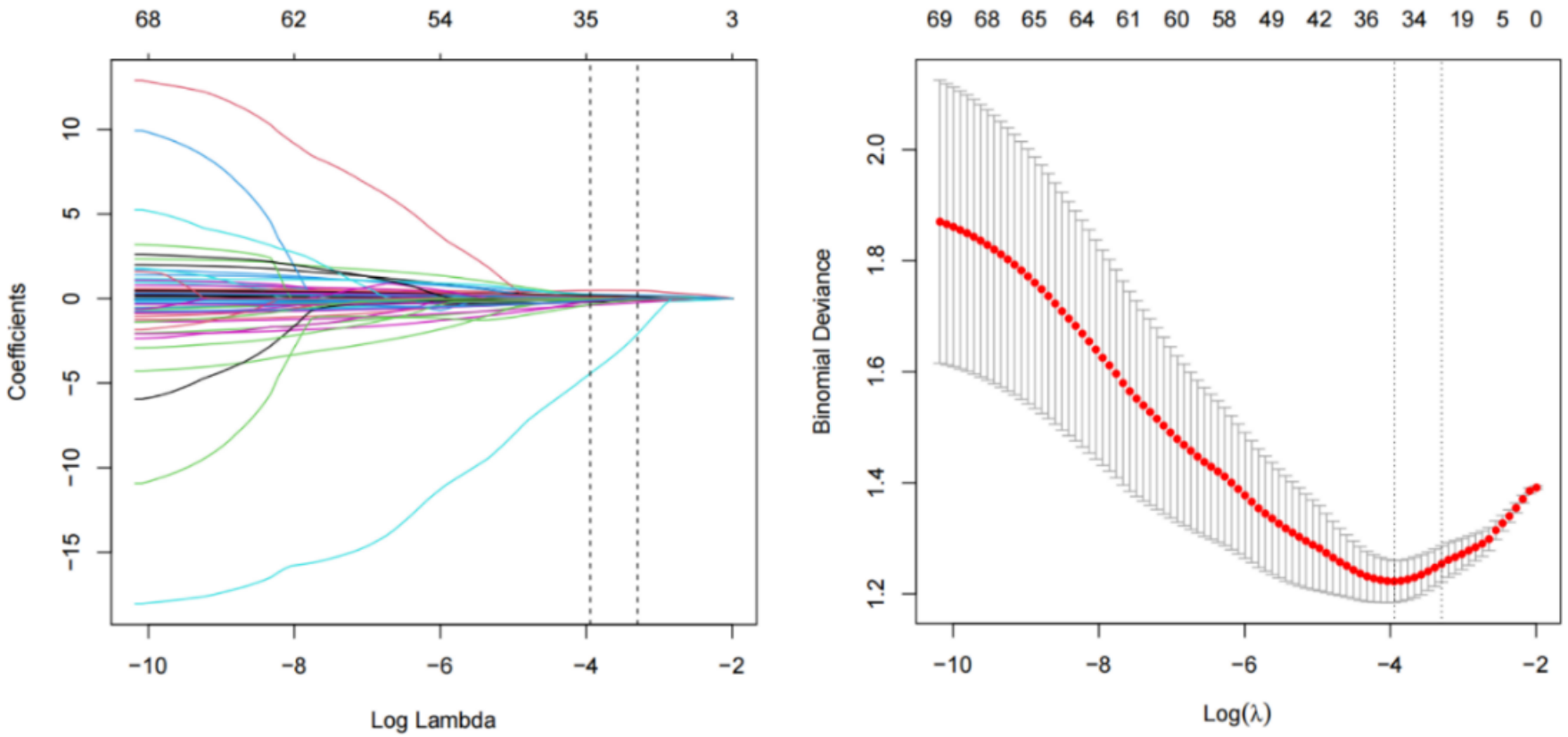
Supplementary Figure 6. PLS-DA permutation test plots for model validation in MetS



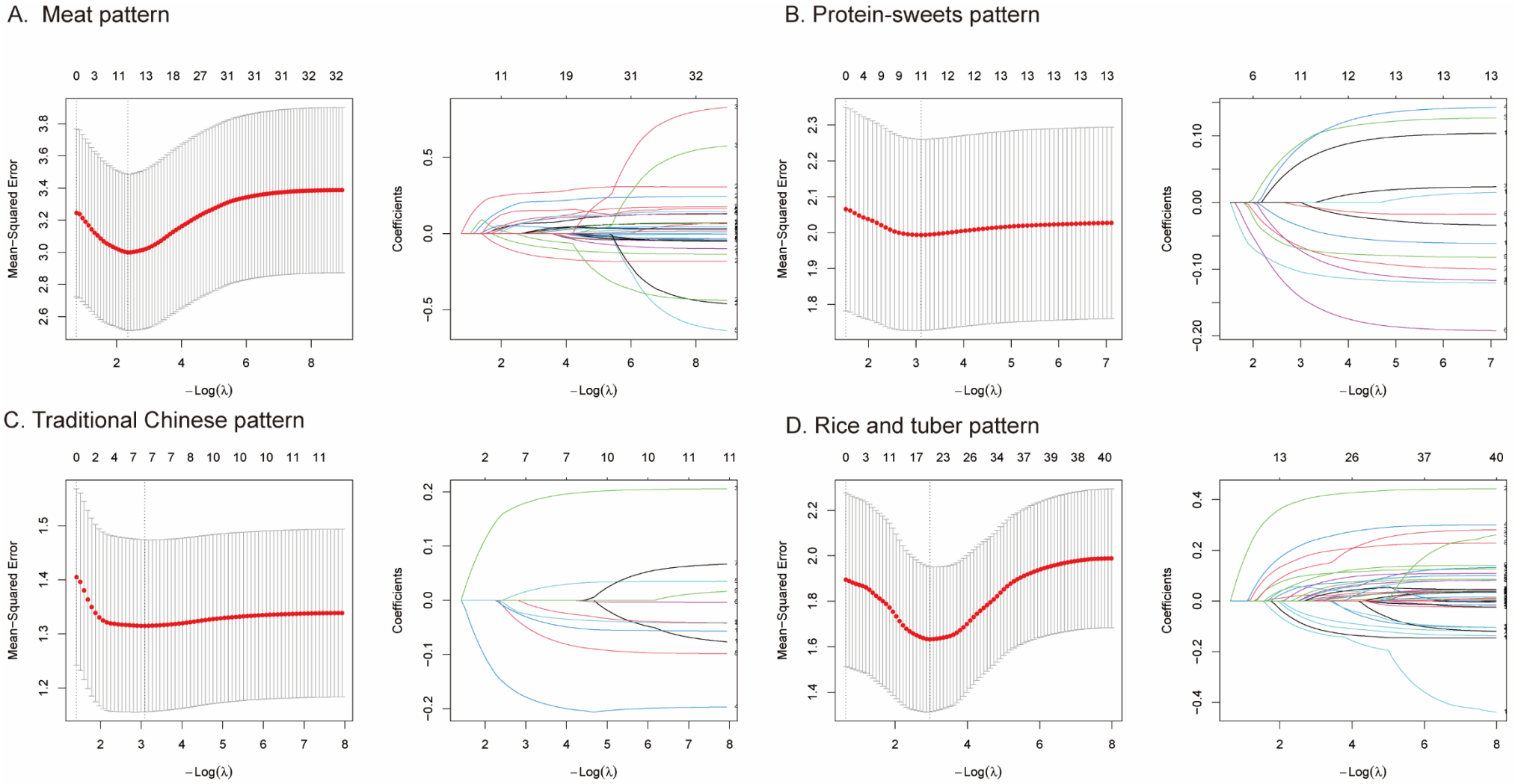
Supplementary Figure 7. Correlation analysis among differential metabolites across four dietary patterns



Supplementary Figure 8. A combined plot of LASSO regression for identifying feature metabolites associated with dietary patterns

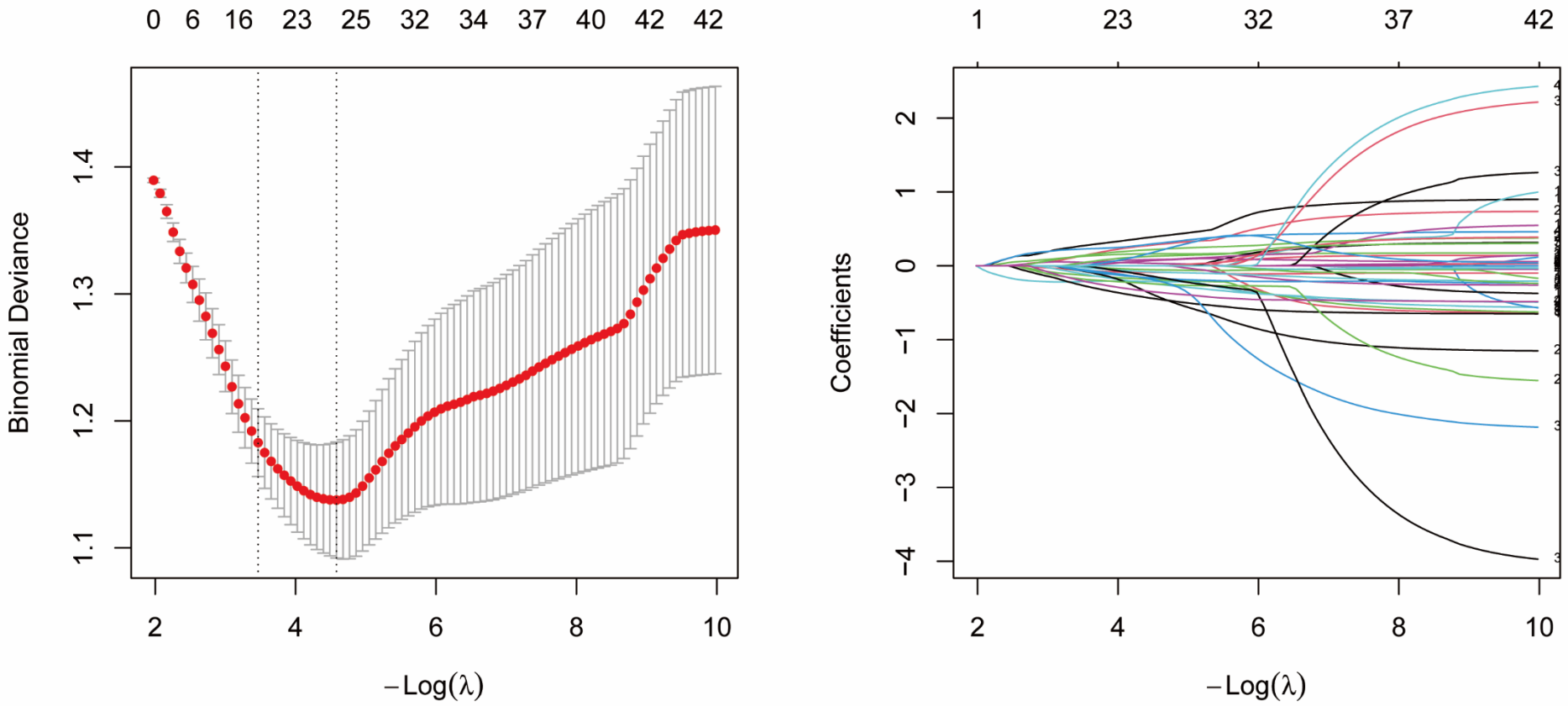


Supplementary Figure 9. A combined plot of LASSO regression for identifying feature metabolites associated with MetS



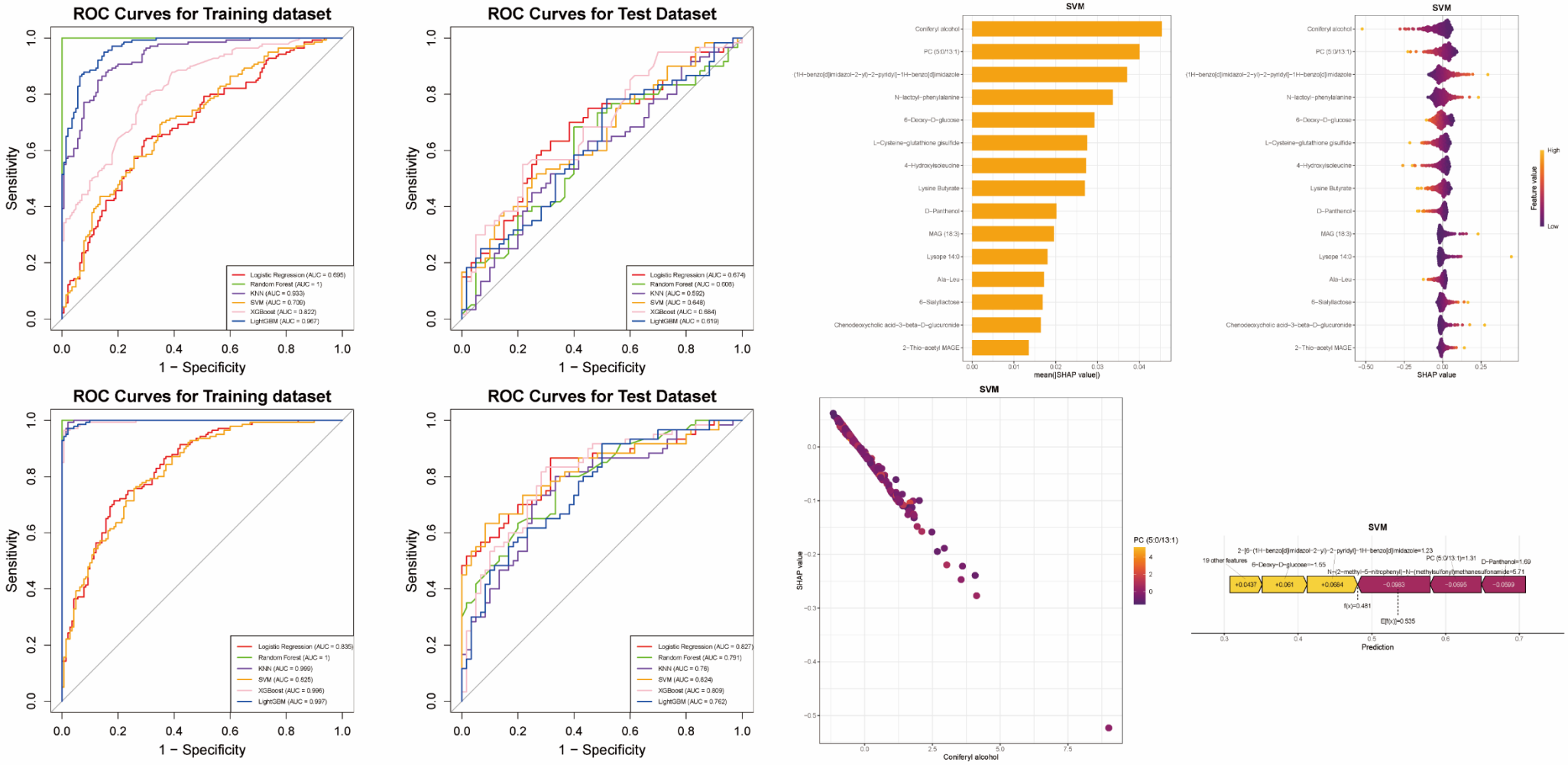
Supplementary Figure 10. A combined plot of LASSO regression for identifying feature metabolites associated with dietary patterns in the sensitivity analysis

This sensitivity analysis used a metabolite selection threshold of *FDR* < 0.2 for inclusion in the LASSO regression models.



Supplementary Figure 11. A combined plot of LASSO regression for identifying feature metabolites associated with MetS in the sensitivity analysis

This sensitivity analysis used a metabolite selection threshold of *FDR* < 0.2 for inclusion in the LASSO regression models.



Supplementary Figure 12. Development, evaluation, and interpretation of MetS risk assessment models based on dietary patterns and metabolites in the sensitivity analysis.

ROC curves of the model utilizing dietary patterns and their key metabolites in the (A) training and (B) testing sets. ROC curves of the model utilizing dietary patterns and MetS metabolic biomarkers in the (C) training and (D) testing sets. (E-H) SHAP plots for interpreting the best-performing model. (E) Bar chart of the top 15 features. (F) Beeswarm plot of the top 15 features. (G) Scatter plots depicting the association between the top two features and the SHAP value. (H) Force plot for a single participant.

Supplementary Data

Supplementary Data S1. Detailed information and identification levels of all 1,328 detected metabolites

Supplementary Data S2. Detailed information and identification levels of all 1,178 detected metabolites using a stricter QC threshold (CV <25%)