Electronic Supplementary Material (ESI) for RSC Advances.

Table S1 Diseases or functions annotation of tentatively identified abnormally expressed metabolites in the T2DM

Diseases or Functions Annotation	p-Value	Activation z-score	Notes	Molecules
Synthesis of reactive oxygen species	0.00000101	0.983	Activation	7
Apoptosis of tumor cell lines	0.00128	0.504		6
Concentration of lipid	0.00253	0.208		6
Synthesis of eicosanoid	0.0000136	1.947		5
Generation of reactive oxygen species	0.0000173	0.984		5
Production of reactive oxygen species	0.000159	1.223		5
Growth of epithelial tissue	0.00107	-0.475	Inhibition	5
Cellular homeostasis	0.0264	-1.578		5
Cell proliferation of tumor cell lines	0.00446	-1.948		6
Synthesis of nucleotide	0.00000364	-1.69		5
Binding of DNA	0.0000222	-1.025		5

Table S2 The AUC data in the classical univariate ROC curve analysis of 33 tentatively identified biomarkers in our experiment.

Name	Compound	Formula	AUC
L-3-Phenyllactic acid	1.35_165.0545m/z	$C_9H_{10}O_3$	1.00000
2-Phenylethanol glucuronide	2.33_299.1148m/z	$C_{14}H_{18}O_7$	1.00000
Cinnamic acid	0.91_147.0442m/z	$C_9H_8O_2$	0.99866
4-Hydroxybenzaldehyde	1.08_121.0283m/z	$C_7H_6O_2$	0.98728
Beta-Leucine	0.81_130.0864m/z	$C_6H_{13}NO_2$	0.98036
Beta-Tyrosine	0.67_180.0650m/z	$C_9H_{11}NO_3$	0.97232
Sorbitol-6-phosphate	1.05_261.0383m/z	$C_6H_{15}O_9P$	0.95536
L-Carnitine	0.50_162.1131m/z	$C_7H_{15}NO_3$	0.93393
SM(d18:0/24:1(15Z))	2.77_815.6941m/z	$C_{47}H_{95}N_2O_6P$	0.84643
Azelaic acid	1.69_187.0965m/z	$C_9H_{16}O_4$	0.84509
LysoPC(15:0)	5.96_482.3258m/z	$C_{23}H4_8NO_7P$	0.84107
Docosahexaenoic acid	6.92_327.2325m/z	$C_{22}H_{32}O_2$	0.83884
LysoPC(18:1(9Z))	4.77_522.3574m/z	$C_{26}H_{52}NO_7P$	0.83326
17a,21-Dihydroxypreg-nenolone	7.27_347.2199m/z	$C_{21}H_{32}O_4$	0.82790
LysoPC(16:0)	4.25_496.3420m/z	$C_{24}H_{50}NO_7P$	0.82522
Inositol cyclic phosphate	3.85_241.0119m/z	$C_6H_{11}O_8P$	0.82299
LysoPC(18:2(9Z,12Z))	3.88_520.3416m/z	$C_{26}H_{50}NO_7P$	0.81183
Gentisate aldehyde	1.86_137.0235m/z	$C_7H_6O_3$	0.80469
LysoPC(16:1(9Z))	3.75_494.3257m/z	$C_{24}H_{48}NO_7P$	0.80126
LysoPC(18:0)	5.64_524.3728m/z	$C_{26}H_{54}NO_7P$	0.79584
LysoPC(14:0)	3.95_466.2943m/z	$C_{22}H_{46}NO_7P$	0.79464
Palmitic acid	4.47_255.2323m/z	$C_{16}H_{32}O_2$	0.75759
Chenodeoxycholic acid	6.53_391.2827m/z	$C_{24}H_{40}O_4$	0.73214
Murocholic acid	6.70_391.2837m/z	$C_{24}H_{40}O_4$	0.71317
Cholesterol sulfate	7.19_465.3097m/z	$C_{27}H_{46}O_4S$	0.71317
Cytidine	0.52_242.0790m/z	$C_9H_{13}N_3O_5$	0.71183
Taurodeoxycholic acid	2.51_498.2876m/z	$C_{26}H_{45}NO_6S$	0.69598
Deoxycholic acid 3-glucuronide	2.75_567.3188m/z	$C_{30}H_{48}O_{10}$	0.68527
Sphingosine 1-phosphate	3.48_378.2398m/z	$C_{18}H_{38}NO_5P$	0.67790
Acetyl-N-formyl-5-methoxykynurenamine	1.24_263.1029m/z	$C_{13}H_{16}N_2O_4$	0.66362
LysoPC(17:0)	6.02_508.3418m/z	$C_{25}H_{52}NO_7P$	0.62165
PC(18:3(6Z,9Z,12Z)/18:1(11Z))	7.92_782.5685m/z	$C_{44}H_{80}NO_8P$	0.60915
14,15-Epoxy-5,8,11-eicosatrienoic acid	4.41_319.2272m/z	$C_{20}H_{32}O_3$	0.59531

Table S3 The basic information of T2DM patient

NO.	Gender	Age	Diagnosis
1	female	59	1.Type 2 diabetes mellitus 2.Hypertension 3.Hyperlipidemia
2	male	80	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy 4.Pulmonary emphysema
3	male	57	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy
4	male	80	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy 4.Cerebral infarction
5	female	79	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy 4.Hyperlipidemia
6	male	60	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy 4.Hyperlipidemia
7	male	80	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy 4.Cerebral infarction
8	female	76	1.Type 2 diabetes mellitus 2.Hypertension
9	female	66	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy
10	female	65	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy 4.Acute cerebrovascular disease
11	female	70	1.Type 2 diabetes mellitus 2.Hypertension 3.Unstable angina

			4.Unexplained edema
12	female	79	1.Type 2 diabetes mellitus 2. Sequel of cerebral infarction 3.Hypertension 4.Coronary atherosclerotic cardiopathy
13	female	75	1.Type 2 diabetes mellitus 2.Hypertension 3.Cerebral infarction 4. Cardiac failure
14	female	63	1.Type 2 diabetes mellitus 2.Hypertension 3.Cerebral infarction 4. Cardiac failure
15	female	66	1.Type 2 diabetes mellitus 2.Hypertension 3.Cerebral infarction 4.Coronary atherosclerotic cardiopathy
16	male	66	1.Type 2 diabetes mellitus 2.Coronary atherosclerotic cardiopathy 3.Hypertension 4.Diabetic peripheral neuropathy 5.Diabetic retinopathy
17	male	63	1.Type 2 diabetes mellitus 2.Hypertension
18	female	69	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy 4.Hyperlipidemia
19	male	56	1.Type 2 diabetes mellitus 2.Hypertension 3.Acute myocardial infarction
20	female	67	1.Type 2 diabetes mellitus 2.Hypertension 3.transient cerebral ischemia
21	female	70	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy 4.Hyperlipidemia
22	female	76	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy

			4.Hyperlipidemia 5.Old cerebral infarction
23	male	65	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Hypertension
24	female	65	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy
25	female	73	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy 4.Cervical spondylosis
26	male	59	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy
27	male	53	1.Type 2 diabetes mellitus 2.Hypertension 3.Coronary atherosclerotic cardiopathy 4.Chronic renal failure 5.Hypothyroidism
28	female	51	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Hypertension 5.Old cerebral infarction
29	male	61	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Cerebral infarction
30	male	79	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Protrusion of lumbar intervertebral disc 5.Unexplained edema
31	female	62	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Cerebral infarction 5.Kidney stone
32	female	54	1.Type 2 diabetes mellitus

			2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Osteoporosis
33	male	80	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Old cerebral infarction 5.Renal insufficiency
34	female	68	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Hypertension 5.Hepatic injury
35	female	73	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Hypertension 5.Unexplained edema
36	female	75	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Hypertension 5.Chronic bronchitis
37	male	78	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Hypertension 5. Benign Prostatic Hyperplasia
38	female	64	1.Type 2 diabetes mellitus 2.Diabetic peripheral neuropathy 3.Hypertension 4.Unstable angina 5.Protrusion of lumbar intervertebral disc
39	female	66	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Hypertension
40	female	80	1.Type 2 diabetes mellitus 2.Hypertension 3.Renal insufficiency
41	female	78	1.Type 2 diabetes mellitus

			2.Hypertension
			3.Stable angina
42	male	73	1.Type 2 diabetes mellitus
			2.Hypertension
			3.Chronic obstructive pulmonary disease
			4.Double pulmonary interstitial lesions
43	female	80	1.Type 2 diabetes mellitus
			2.Hyperlipidemia
			3.Coronary atherosclerotic cardiopathy
			4.Hypertension
			5.Old cerebral infarction
44	female	75	1.Type 2 diabetes mellitus
			2.Hypertension
			3.Chronic bronchitis
			4.Diabetic peripheral neuropathy
			5.Diabetic retinopathy
45	male	76	1.Type 2 diabetes mellitus
			2.Hyperlipidemia
			3.Coronary atherosclerotic cardiopathy
			4.Hypertension
			5.Chronic bronchitis
			6.Cervical spondylosis
46	female	59	1.Type 2 diabetes mellitus
			2.Hyperlipidemia
			3.Coronary atherosclerotic cardiopathy
			4.Hypertension
			5.Old cerebral infarction
47	female	78	1.Type 2 diabetes mellitus
			2.Hyperlipidemia
			3.Coronary atherosclerotic cardiopathy
			4.Hypertension
			5.Diabetic retinopathy
			6. Cataract
48	male	54	1.Type 2 diabetes mellitus
			2.Coronary atherosclerotic cardiopathy
49	male	80	1.Type 2 diabetes mellitus
			2.Coronary atherosclerotic cardiopathy
50	male	60	1.Type 2 diabetes mellitus
			2.Coronary atherosclerotic cardiopathy
51	female	76	1.Type 2 diabetes mellitus
			2.Coronary atherosclerotic cardiopathy

			3.Cerebral infarction
52	female	64	1.Type 2 diabetes mellitus 2.Coronary atherosclerotic cardiopathy 3.Cerebral infarction
53	female	62	1.Type 2 diabetes mellitus 2.Coronary atherosclerotic cardiopathy 3. Nephrotic syndrome
54	male	65	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy
55	female	51	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Reflux esophagitis
56	female	80	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Chronic pyelonephritis
57	female	71	1.Type 2 diabetes mellitus 2.Coronary atherosclerotic cardiopathy 3.Diabetic peripheral neuropathy
58	male	51	1.Type 2 diabetes mellitus 2.Chronic renal failure 3.Coronary atherosclerotic cardiopathy
59	female	58	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Coronary atherosclerotic cardiopathy 4.Old cerebral infarction
60	male	72	1.Type 2 diabetes mellitus 2.Unstable angina
61	male	58	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Chronic obstructive pulmonary disease 4.Dilated cardiomyopathy
62	male	65	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Unstable angina
63	male	67	1.Type 2 diabetes mellitus 2.Coronary atherosclerotic cardiopathy 3.Chronic lymphocytic leukemia 4.Pleural effusion

64	male	80	1.Type 2 diabetes mellitus 2.Hyperlipidemia 3.Renal insufficiency 4. Cardiac failure 5.Hyperuricemia