

Figure S1. PCA for GCA (blue circles) and healthy controls (red triangles) using the metabolomics data. (A) PCA score plot in the positive ion modes. (B) PCA score plot in the negative ion modes. PCA, principal component analysis; GCA, gastric cardia adenocarcinoma.

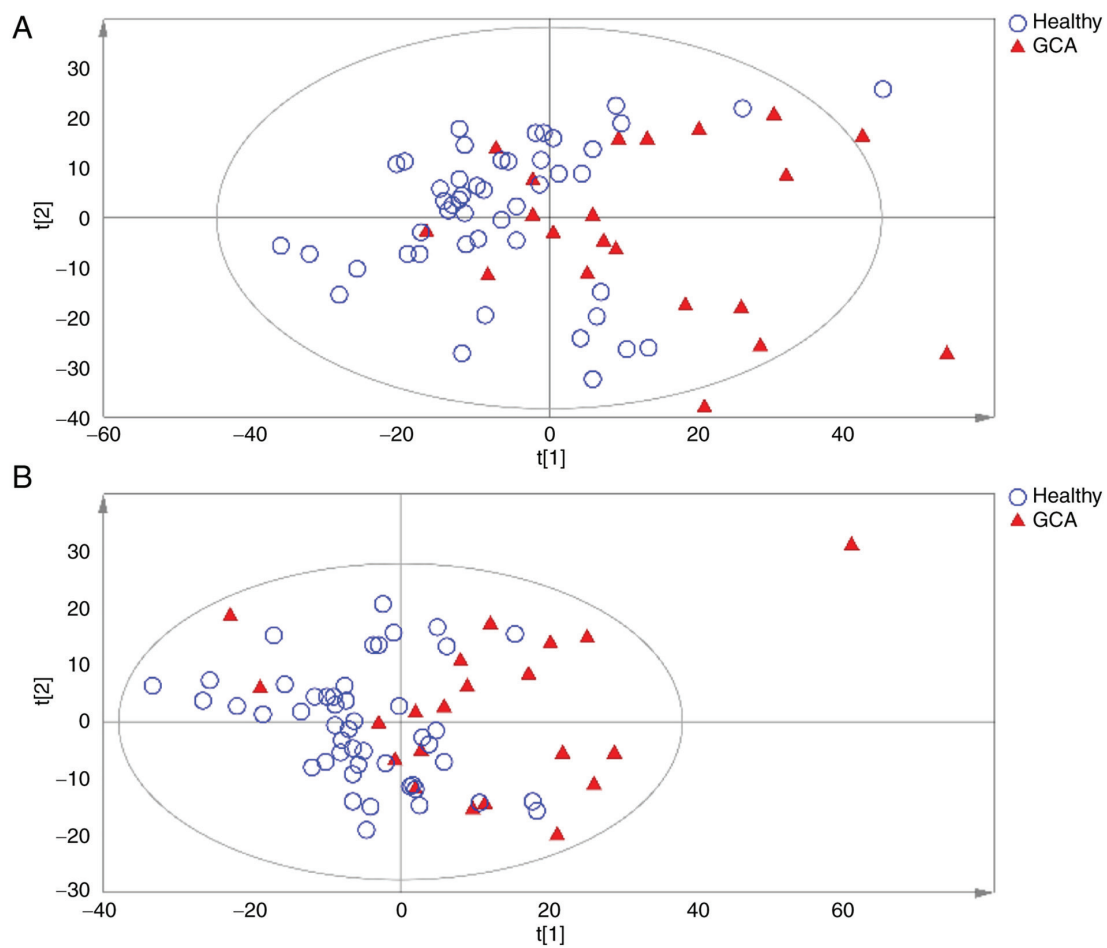


Table SI. Results of the precision analysis of the instrument (retention time).

Peak name	Retention time, min						Mean, min	% RSD
	1	2	3	4	5	6		
S1	1.980	1.977	1.977	1.980	1.975	1.978	1.978	0.100
S2	8.233	8.237	8.237	8.232	8.238	8.235	8.235	0.029
S3	11.484	11.487	11.488	11.491	11.491	11.492	11.489	0.026
S4	11.716	11.723	11.718	11.724	11.721	11.723	11.721	0.028
S5	12.008	12.012	12.011	12.012	12.017	12.011	12.012	0.024
S6	12.255	12.261	12.255	12.259	12.260	12.259	12.258	0.022
S7	12.451	12.452	12.450	12.453	12.454	12.455	12.453	0.016
S8	12.861	12.867	12.860	12.866	12.870	12.867	12.865	0.029
S9	13.221	13.221	13.220	13.222	13.223	13.223	13.222	0.008
S10	13.956	13.955	13.954	13.959	13.956	13.957	13.956	0.013
S11	14.482	14.484	14.483	14.479	14.483	14.481	14.482	0.012

RSD, relative standard deviation.

Table SII. Results of the precision analysis of the instrument (intensity).

Peak name	Intensity, counts per sec						Mean	% RSD
	1	2	3	4	5	6		
S1	32228.1	32856.1	33537.3	33190.6	31364.7	38069.6	33541.1	7.000
S2	58552.8	54558.6	55847.1	53468.2	54998.5	65344.3	57128.2	7.658
S3	130624.8	149033.8	132065.4	133668.2	133072.2	130147.9	134768.7	5.283
S4	566037.3	503198.8	519923.9	523825.9	509432.1	519010.4	523571.4	4.230
S5	138161.8	152078.2	156990.2	161438.5	150562.4	167058.5	154381.6	6.479
S6	589463.6	570000.4	564297.5	634577.8	585366.4	526944.0	578441.6	6.109
S7	187075.7	188730.9	181997.6	196783.8	189871.3	180183.0	187440.4	3.177
S8	73978.0	69358.2	68168.6	74703.6	69776.9	69120.8	70851.0	3.901
S9	310312.7	301192.0	289606.0	302301.8	263634.1	285055.9	292017.1	5.699
S10	61673.5	68952.5	68250.9	60942.3	61613.6	60957.6	63731.7	5.949
S11	381781.6	423654.4	412149.6	393056.8	399326.4	436527.3	407749.3	4.980

RSD, relative standard deviation.

Table SIII. Results of the sample stability analysis (retention time).

Peak name	Retention time, min						Mean, min	% RSD
	0 h	2 h	4 h	8 h	12 h	24 h		
S1	1.980	1.975	1.969	1.982	1.983	1.981	1.978	0.281
S2	8.230	8.230	8.234	8.232	8.231	8.222	8.230	0.049
S3	11.484	11.491	11.496	11.494	11.492	11.493	11.492	0.035
S4	11.716	11.721	11.724	11.713	11.712	11.708	11.716	0.051
S5	12.008	12.017	12.015	12.012	12.007	12.013	12.012	0.032
S6	12.255	12.260	12.261	12.260	12.241	12.249	12.254	0.065
S7	12.451	12.454	12.456	12.450	12.451	12.445	12.451	0.031
S8	12.861	12.870	12.866	12.865	12.861	12.862	12.864	0.027
S9	13.221	13.223	13.222	13.220	13.220	13.213	13.220	0.028
S10	13.956	13.956	13.956	13.956	13.959	13.952	13.956	0.018
S11	14.482	14.483	14.482	14.482	14.483	14.484	14.483	0.004

RSD, relative standard deviation.

Table SIV. Result of the sample stability analysis (intensity).

Peak name	Intensity, counts per sec						Mean	% RSD
	0 h	2 h	4 h	8 h	12 h	24 h		
S1	32228.1	31364.7	29133.3	30138.1	30828.3	29654.8	30557.9	3.741
S2	257880.7	240274.9	217965.6	238923.3	258552.8	261895.5	245915.5	6.853
S3	130624.8	133072.2	120553.7	121890.5	122462.3	121283.3	124981.1	4.331
S4	566037.3	509432.1	500257.8	502631.3	513912.9	515689.0	517993.4	4.692
S5	138161.8	150562.4	145973.7	142638.5	147837.5	142495.1	144611.5	3.056
S6	589463.6	585366.4	586339.0	576251.9	583310.9	571178.5	581985.1	1.185
S7	187075.7	189871.3	190653.8	187230.5	178045.0	187590.8	186744.5	2.416
S8	73978.0	69776.9	70959.3	70253.8	70053.3	70319.3	70890.1	2.204
S9	310312.7	263634.1	276403.3	271835.0	273641.4	271085.4	277818.6	5.931
S10	61673.5	61613.6	75017.8	73918.6	73092.4	70725.8	69340.3	8.836
S11	381781.6	399326.4	412071.9	410374.7	402618.3	408614.3	402464.5	2.790

RSD, relative standard deviation.

Table SV. Receiver operating characteristic analysis results of 27 biomarkers and the combined model.

Type	Metabolite	AUC	Standard error	95% CI		Sensitivity	Specificity
				Lower	Upper		
Phospholipids	Phosphorylcholine ^a	0.913	0.035	0.843	0.982	0.854	1.000
	LysoPE (20:0/0:0)	0.864	0.051	0.764	0.965	0.875	0.714
	LysoPC (14:0)	0.837	0.054	0.731	0.944	0.813	0.762
	LysoPE (0:0/20:0)	0.832	0.052	0.730	0.934	0.688	0.952
	LysoPE [18:2(9Z,12Z)/0:0]	0.829	0.059	0.713	0.946	0.854	0.762
	PC [14:1(9Z)/18:1(9Z)]	0.814	0.055	0.707	0.922	0.771	0.714
	LysoPC (16:1(9Z))	0.788	0.067	0.657	0.919	0.875	0.667
	LysoPE (18:0/0:0)	0.759	0.072	0.617	0.901	0.896	0.619
	LysoPC (15:0)	0.744	0.061	0.625	0.863	0.563	0.857
	Glucosylsphingosine	0.743	0.076	0.595	0.891	0.833	0.667
	PC (13:0/0:0)	0.732	0.062	0.611	0.853	0.563	0.810
	LysoPE (16:0/0:0)	0.731	0.062	0.610	0.852	0.729	0.714
	LysoPC (18:1(9Z))	0.715	0.080	0.559	0.871	0.938	0.571
	Amino acids	N-Acetyl-L-aspartic acid	0.842	0.053	0.738	0.946	0.708
L-Acetylcarnitine ^a		0.803	0.054	0.698	0.907	0.762	0.708
Decanoylcarnitine		0.840	0.056	0.730	0.950	0.792	0.905
L-Tryptophan		0.793	0.066	0.664	0.921	0.771	0.762
Selenohomocysteine		0.737	0.064	0.613	0.862	0.714	0.708
Unsaturated fatty acids	L-Valine	0.731	0.064	0.606	0.856	0.667	0.750
	Arachidonic acid ^a	0.887	0.050	0.789	0.985	0.905	0.833
	Eicosapentaenoic acid	0.870	0.048	0.775	0.965	0.857	0.875
	Linoleic acid	0.779	0.063	0.656	0.902	0.714	0.812
	Oleic acid	0.774	0.069	0.640	0.908	0.524	0.937
	Palmitic acid	0.722	0.072	0.581	0.863	0.524	0.975
Cholic acids	Glycocholic acid ^a	0.808	0.056	0.697	0.918	0.729	0.810
	Cholic acid	0.768	0.058	0.654	0.882	0.750	0.667
	Glycoursodeoxycholic acid	0.768	0.057	0.656	0.880	0.500	0.952
Combined indicator	Four metabolites model ^a	0.990	0.008	0.000	1.000	0.979	0.952

^aThe four metabolites model comprised phosphorylcholine, L-acetylcarnitine, arachidonic acid and glycocholic acid. CI, confidence interval; AUC, area under the curve; PC, phosphatidylcholine; LysoPC, lysophosphatidylcholine; LysoPE, lysophosphatidylethanolamine.