

Supplementary Table 1. Discriminating variables for cirrhosis and controls with VIP values larger than 2 based on the dataset of RP column

Var ID	Tr	mass	VIP
771	15.493	523.365	8.187
769	12.849	519.334	6.888
736	9.952	463.276	6.038
723	10.422	431.303	5.613
173	5.985	529.128	5.096
720	8.447	429.288	4.844
793	8.541	584.263	4.794
709	8.446	411.277	4.754
327	8.448	465.308	4.238
247	10.273	898.629	4.160
361	2.616	99.069	3.971
51	6.085	206.058	3.962
796	5.446	600.258	3.617
87	6.085	302.116	3.598
435	10.400	449.314	3.527
225	6.005	645.143	3.433
50	9.202	206.058	3.432
848	13.318	990.665	3.400
779	12.990	543.333	3.368
222	9.877	632.249	3.124
113	5.246	357.195	2.894
710	8.904	413.293	2.866
343	10.172	582.247	2.841
167	6.083	518.140	2.806
326	8.282	461.260	2.783
766	13.338	517.315	2.735
99	9.202	320.126	2.678
650	10.377	338.260	2.489
839	17.955	805.559	2.399
98	6.085	320.126	2.350
86	9.202	302.116	2.323
254	1.087	102.046	2.226
328	8.282	479.271	2.221
576	19.125	264.245	2.146
432	9.612	447.298	2.125
496	11.562	118.078	2.079
499	17.025	122.109	2.066
83	6.006	289.106	2.024
583	7.817	273.271	2.004

All the above variables were enrolled in the result of combined dataset.

Var ID: Variable ID. Tr: retention time. VIP: Variable importance in the projection.

Supplementary Table 2 Discriminating variables for cirrhosis and controls with VIP values larger than 2 based on the dataset of HILIC column

Var ID	Tr	mass	VIP
h174	8.536	471.300	4.974
h76	10.785	203.120	4.478
h152	8.532	413.290	4.299
h172	1.352	463.280	4.112
h95	8.164	253.990	4.067
h220	1.862	580.230	4.058
h15	8.623	103.100	4.014
h551	5.104	142.070	3.953
h428	6.367	137.050	3.953
h257	8.638	779.550	3.909
h344	9.398	543.330	3.759
h568	1.146	206.060	3.461
h483	3.321	461.260	3.072
h163	8.544	431.300	3.030
h264	8.592	803.540	2.998
h240	9.233	700.550	2.933
h221	8.779	584.260	2.853
h224	10.605	590.310	2.760
h695	8.603	757.560	2.751
h330	9.309	411.280	2.675
h102	8.179	268.010	2.675
h33	4.574	125.010	2.594
h122	1.992	326.190	2.549
h331	9.306	429.290	2.541
h176	8.164	472.000	2.535
h188	9.473	495.330	2.511
h247	8.710	729.530	2.451
h385	8.575	765.570	2.413
h485	3.322	479.270	2.389
h169	8.135	457.990	2.371
h591	9.582	302.120	2.351
h89	8.130	239.980	2.287
h569	9.580	206.060	2.241
h252	8.686	755.550	2.233
h355	2.673	614.240	2.229
h267	8.556	827.540	2.221
h655	5.232	546.330	2.208
h590	1.153	302.120	2.197
h150	8.168	404.010	2.181
h395	8.602	791.580	2.177

h85	10.718	228.150	2.134
h198	9.488	517.320	2.130
h445*	1.584	268.080	2.117
h514*	8.709	731.550	2.086
h123*	1.709	329.330	2.062
h229*	8.175	622.020	2.034

(*): Did not appear in the result of combined dataset.

Var ID: Variable ID. Tr: retention time. VIP: Variable importance in the projection.

Supplementary Table 3 Discriminating variables for cirrhosis and controls with VIP values larger than 2 based on the combined dataset of two columns

Var ID	Tr	mass	VIP
771	15.493	523.365	8.564
769	12.849	519.334	7.205
736	9.952	463.276	6.317
723	10.422	431.303	5.871
173	5.985	529.128	5.331
720	8.447	429.288	5.067
793	8.541	584.263	5.015
709	8.446	411.277	4.974
h174	8.536	471.3	4.685
327	8.448	465.308	4.433
247	10.273	898.629	4.352
h76	10.785	203.12	4.218
361	2.616	99.0685	4.154
51	6.085	206.058	4.144
h152	8.532	413.29	4.049
h172	1.352	463.28	3.874
h95	8.164	253.99	3.831
h220	1.862	580.23	3.822
796	5.446	600.258	3.783
h15	8.623	103.1	3.781
87	6.085	302.116	3.764
h551	5.104	142.07	3.724
h428	6.367	137.05	3.723
435	10.4	449.314	3.690
h257	8.638	779.55	3.682
225	6.005	645.143	3.592
50	9.202	206.058	3.590
848	13.318	990.665	3.556
h344	9.398	543.33	3.541
779	12.99	543.333	3.523
222	9.877	632.249	3.268
h568	1.146	206.06	3.261

113	5.246	357.195	3.027
710	8.904	413.293	2.998
343	10.172	582.247	2.972
167	6.083	518.14	2.935
326	8.282	461.26	2.912
h483	3.321	461.26	2.894
766	13.338	517.315	2.861
h163	8.544	431.3	2.854
h264	8.592	803.54	2.824
99	9.202	320.126	2.802
h240	9.233	700.55	2.763
h221	8.779	584.26	2.688
650	10.377	338.26	2.604
h224	10.605	590.31	2.600
h695	8.603	757.56	2.592
h330	9.309	411.28	2.520
h102	8.179	268.01	2.520
839	17.955	805.559	2.510
98	6.085	320.126	2.458
h33	4.574	125.01	2.444
86	9.202	302.116	2.431
h122	1.992	326.19	2.401
h331	9.306	429.29	2.394
h176	8.164	472	2.388
h188	9.473	495.33	2.365
254	1.087	102.046	2.329
328	8.282	479.271	2.324
h247	8.71	729.53	2.309
h385	8.575	765.57	2.273
h485	3.322	479.27	2.251
576	19.125	264.245	2.245
h169	8.135	457.99	2.234
432	9.612	447.298	2.223
h591	9.582	302.12	2.214
496	11.562	118.078	2.175
499	17.025	122.109	2.161
h89	8.13	239.98	2.155
83	6.006	289.106	2.117
h569	9.58	206.06	2.111
h252	8.686	755.55	2.103
h355	2.673	614.24	2.099
583	7.817	273.271	2.096
h267	8.556	827.54	2.092
h655	5.232	546.33	2.080

h590	1.153	302.12	2.069
788 *	13.14	567.332	2.069
h150	8.168	404.01	2.054
h395	8.602	791.58	2.051
448*	13	581.241	2.036
715*	12.943	425.35	2.029
h85	10.718	228.15	2.010
h198	9.488	517.32	2.006
394*	5.636	282.101	2.004
453*	9.942	632.248	2.001

(*) Variables did not appeared in the result of RP column.

Var ID: Variable ID. Tr: retention time. VIP: Variable importance in the projection.

Supplementary Table 4 Discriminating variables for HCC and controls with VIP values larger than 2 based on the dataset of RP column

Var ID	Tr	mass	VIP
769	12.849	519.334	8.922
361	2.616	99.069	8.590
771	15.493	523.365	8.526
834	20.550	781.560	4.801
793	8.541	584.263	4.377
629	8.015	317.296	4.253
496	11.562	118.078	4.206
839	17.955	805.559	3.991
848	13.318	990.665	3.984
407	11.108	329.335	3.949
809	20.691	636.298	3.828
549	0.774	225.945	3.751
18	1.087	136.039	3.729
766	13.338	517.315	3.347
658	9.663	345.325	3.245
599	5.484	285.194	3.166
688	11.288	373.357	3.103
624	6.885	313.225	3.079
669	12.304	356.271	2.985
795	22.356	595.590	2.872
614	9.467	301.301	2.768
576	19.125	264.245	2.754
583	7.817	273.271	2.693
833	17.089	779.543	2.668
788	13.140	567.332	2.659
721	0.770	429.907	2.274
603	8.103	289.262	2.270
779	12.990	543.333	2.204

649	22.709	337.335	2.169
504	1.246	131.073	2.115
778	11.951	541.316	2.073
563*	6.334	245.236	2.015

(*): Variables did not appear in the results of combined dataset.

Var ID: Variable ID. Tr: retention time. VIP: Variable importance in the projection.

Supplementary Table 5 Discriminating variables for HCC and controls with VIP values larger than 2 based on the dataset of HILIC column

Var ID	Tr	mass	VIP
h428	6.367	137.050	7.604
h33	4.574	125.010	6.656
h264	8.592	803.540	5.372
h344	9.398	543.330	5.307
h140	4.579	375.040	4.589
h459	1.340	317.290	4.040
h445	1.584	268.080	3.797
h138	2.044	373.360	3.405
h134	2.157	361.320	3.319
h198	9.488	517.320	3.152
h107	9.745	285.190	3.147
h188	9.473	495.330	3.073
h257	8.638	779.550	3.061
h19	1.559	109.030	2.919
h191	4.589	500.060	2.718
h17	8.150	103.980	2.709
h216	9.404	567.330	2.692
h89	8.130	239.980	2.690
h537	6.362	93.057	2.546
h356	4.584	625.070	2.383
h699	8.603	793.600	2.380
h439	8.068	225.960	2.369
h240	9.233	700.550	2.352
h378	8.711	733.560	2.331
h324	1.928	356.270	2.331
h14	9.639	102.050	2.326
h380	8.635	741.570	2.319
h15	8.623	103.100	2.316
h93	1.312	245.240	2.284
h101	2.240	261.230	2.266
h85	10.718	228.150	2.213
h76	10.785	203.120	2.200
h514	8.709	731.550	2.181
h57	10.746	161.110	2.148

h695	8.603	757.560	2.144
h129	1.345	345.320	2.112
h489	9.389	523.360	2.108
h526	8.581	815.580	2.107
h147	1.339	399.370	2.038
h256*	8.632	767.580	2.022

(*): Variables did not appear in the results of combined dataset

Var ID: Variable ID. Tr: retention time. VIP: Variable importance in the projection.

Supplementary Table 6 Discriminating variables for HCC and controls with VIP values larger than 2 based on the dataset of two columns

Var ID	Tr	mass	VIP
769	12.849	519.334	8.774
361	2.616	99.0685	8.447
771	15.493	523.365	8.384
h428	6.367	137.05	7.476
h33	4.574	125.01	6.544
h264	8.592	803.54	5.281
h344	9.398	543.33	5.218
834	20.55	781.56	4.721
h140	4.579	375.04	4.512
793	8.541	584.263	4.304
629	8.015	317.296	4.183
496	11.562	118.078	4.136
h459	1.34	317.29	3.972
839	17.955	805.559	3.925
848	13.318	990.665	3.918
407	11.108	329.335	3.883
809	20.691	636.298	3.764
h445	1.584	268.08	3.733
549	0.774	225.945	3.688
18	1.087	136.039	3.667
h138	2.044	373.36	3.348
766	13.338	517.315	3.292
h134	2.157	361.32	3.263
658	9.663	345.325	3.191
599	5.484	285.194	3.114
h198	9.488	517.32	3.099
h107	9.745	285.19	3.095
688	11.288	373.357	3.051
624	6.885	313.225	3.028
h188	9.473	495.33	3.021
h257	8.638	779.55	3.009
669	12.304	356.271	2.936

h19	1.559	109.03	2.870
795	22.356	595.59	2.824
614	9.467	301.301	2.722
576	19.125	264.245	2.708
h191	4.589	500.06	2.672
h17	8.15	103.98	2.663
583	7.817	273.271	2.648
h216	9.404	567.33	2.646
h89	8.13	239.98	2.645
833	17.089	779.543	2.624
788	13.14	567.332	2.615
h537	6.362	93.057	2.503
h356	4.584	625.07	2.343
h699	8.603	793.6	2.340
h439	8.068	225.96	2.329
h240	9.233	700.55	2.313
h378	8.711	733.56	2.291
h324	1.928	356.27	2.291
h14	9.639	102.05	2.287
h380	8.635	741.57	2.280
h15	8.623	103.1	2.277
h93	1.312	245.24	2.245
721	0.77	429.907	2.236
603	8.103	289.262	2.232
h101	2.24	261.23	2.228
h85	10.718	228.15	2.176
779	12.99	543.333	2.167
h76	10.785	203.12	2.163
h514	8.709	731.55	2.145
649	22.709	337.335	2.133
h57	10.746	161.11	2.112
h695	8.603	757.56	2.108
504	1.246	131.073	2.080
h129	1.345	345.32	2.076
h489	9.389	523.36	2.073
h526	8.581	815.58	2.071
778	11.951	541.316	2.038
h147	1.339	399.37	2.003

Var ID: Variable ID. Tr: retention time. VIP: Variable importance in the projection.