

Supplemental Information

Table S1. Potential biomarkers in the subtypes diagnosed by WM stages (A) and CM syndrome types (B).

(A)

metabolites	Rt, s	VIP	Healthy ^a	Pre-clinic ^a	NPDR ^a	PDR ^a
unknown	555.8	8.05	5.0±1.8	4.9±1.5	4.6±1.2	4.2±1.1
phosphate	626.42	4.93	1.1±0.26	0.87±0.11	0.83±0.11	0.86±0.11
unknown	1351.82	4.28	1.7±0.29	1.8±0.45	1.7±0.33	1.6±0.34
glucose*	1073.18	3.32	0.44±0.27	1.5±0.20	1.4±0.21	1.6±0.27
β-hydroxybutyric acid*	520.58	2.70	0.086±0.036	0.14±0.094	0.19±0.16	0.14±0.074
trans-oleic acid	1238.6	2.45	0.49±0.15	0.54±0.20	0.52±0.23	0.45±0.23
unknown	859.22	2.39	0.085±0.034	0.10±0.044	0.11±0.054	0.16±0.11
stearic acid*	1251.8	2.21	0.77±0.096	0.83±0.099	0.79±0.10	0.78±0.10
linoleic acid	1235.6	2.20	0.25±0.062	0.27±0.091	0.23±0.096	0.21±0.091
pyruvic acid*	454.22	2.06	0.084±0.034	0.084±0.037	0.073±0.025	0.099±0.039
stearic acid derivative	1506.2	1.72	0.15±0.027	0.15±0.027	0.13±0.020	0.14±0.026
L-aspartic acid*	782.42	1.59	0.046±0.019	0.056±0.021	0.068±0.022	0.079±0.032
unknown	770.78	1.51	0.052±0.025	0.054±0.026	0.043±0.021	0.034±0.017
citric acid*	1023.98	1.38	0.088±0.031	0.14±0.029	0.15±0.035	0.13±0.040
unknown	765.62	1.25	0.040±0.013	0.047±0.014	0.039±0.015	0.033±0.0071
unknown	822.2	1.19	0.042±0.017	0.039±0.014	0.033±0.009	0.028±0.0070
arachidonic acid*	1316.18	1.11	0.035±0.014	0.038±0.012	0.037±0.015	0.029±0.013
unknown	515.0	1.03	0.045±0.021	0.033±0.020	0.029±0.017	0.039±0.024
methylmaleic acid	533.0	1.02	0.10±0.055	0.064±0.030	0.076±0.036	0.075±0.046

(B)

metabolites	Rt, s	VIP	Healthy ^a	non-Yang deficiency ^a	Yang deficiency ^a
unknown	555.8	8.62	5.0±1.8	4.8±1.4	4.2±1.0
unknown	1351.82	4.47	1.7±0.29	1.8±0.41	1.6±0.31
phosphate	626.42	4.22	1.1±0.26	0.84±0.11	0.86±0.11
glycerol*	622.58	3.10	0.25±0.080	0.28±0.19	0.22±0.07
L-aspartic acid*	782.42	2.18	0.046±0.019	0.061±0.022	0.076±0.029
pyruvic acid*	454.22	1.82	0.084±0.034	0.074±0.032	0.097±0.035
unknown	1368.02	1.48	0.046±0.027	0.048±0.028	0.034±0.026
unknown	959.6	1.46	0.019±0.0073	0.024±0.011	0.032±0.012
cholesterol*	1662.62	1.42	0.48±0.13	0.44±0.068	0.46±0.084
unknown	932.42	1.31	0.040±0.014	0.056±0.018	0.062±0.015
unknown	770.78	1.28	0.052±0.025	0.048±0.025	0.038±0.019
unknown	822.2	1.26	0.042±0.017	0.036±0.012	0.030±0.007
unknown	1320.38	1.23	0.047±0.022	0.054±0.024	0.044±0.018
unknown	515.0	1.18	0.045±0.021	0.029±0.019	0.037±0.022
unknown	1113.62	1.18	0.021±0.0088	0.026±0.0096	0.031±0.0092
stearic acid derivative	1506.2	1.11	0.15±0.027	0.14±0.025	0.14±0.025

^a The relative concentration of the potential biomarkers in each subtypes were shown as ‘average peak area (related to the internal standard) ±standard deviation.

*: confirmed by the standards.