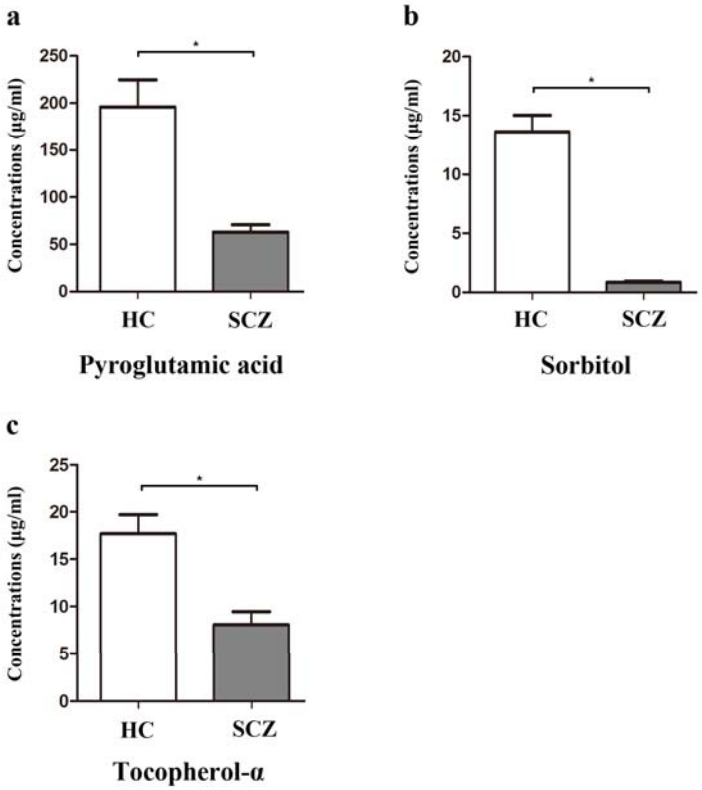
Electronic Supplementary Material (ESI) for Molecular BioSystems.



Supplemental fig.1. (a-c) the concentrations of diagnostic biomarkers in schizophrenia and healthy control groups. * indicates p＜0.001.

Supplemental Table 1. Individual demographic and clinical data of the recruited subjects

Subjects	Training/Test set	Age（years）	Gender	Antipsychotics Use
SZ 01	Training set	29	Male	NO
SZ 02	Training set	37	Female	NO
SZ 03	Training set	41	Male	NO
SZ 04	Training set	56	Female	Olanzapine
SZ 05	Training set	50	Female	Olanzapine
SZ 06	Training set	29	Female	NO
SZ 07	Training set	28	Female	NO
SZ 08	Training set	21	Female	NO
SZ 09	Training set	21	Male	NO
SZ 10	Training set	56	Female	Clozapine, chlorpromazine
SZ 11	Training set	27	Male	Olanzapine
SZ 12	Training set	31	Female	Aripiprazole, quetiapine
SZ 13	Training set	17	Female	NO
SZ 14	Training set	20	Female	NO
SZ 15	Training set	17	Female	NO
SZ 16	Training set	49	Female	NO
SZ 17	Training set	28	Female	NO
SZ 18	Training set	42	Male	Ziprasidone
SZ 19	Training set	26	Female	Aripiprazole, olanzapine
SZ 20	Training set	26	Female	Ziprasidone

SZ 21	Training set	24	Male	Olanzapine
SZ 22	Training set	29	Female	Olanzapine
SZ 23	Training set	44	Female	NO
SZ 24	Training set	30	Male	Olanzapine
SZ 25	Training set	34	Female	Olanzapine, ziprasidone
SZ 26	Training set	42	Male	Olanzapine
SZ 27	Training set	69	Female	NO
SZ 28	Training set	41	Female	Risperidone
SZ 29	Training set	56	Female	Olanzapine
SZ 30	Training set	32	Female	NO
SZ 31	Training set	49	Female	Olanzapine, ziprasidone
SZ 32	Training set	17	Female	NO
SZ 33	Training set	47	Male	NO
SZ 34	Training set	35	Male	Olanzapine
SZ 35	Training set	19	Female	NO
SZ 36	Training set	20	Male	NO
SZ 37	Training set	15	Female	NO
SZ 38	Training set	22	Female	NO
SZ 39	Training set	27	Male	Risperidone
SZ 40	Training set	39	Male	NO
SZ 41	Training set	21	Male	NO
SZ 42	Training set	19	Male	NO
SZ 43	Training set	43	Male	NO

SZ 44	Training set	26	Male	NO
SZ 45	Training set	44	Male	Sulpiride, risperidone
SZ 46	Test set 1	21	Male	Olanzapine
SZ 47	Test set 1	29	Female	Ziprasidone
SZ 48	Test set 1	22	Female	Aripiprazole, olanzapine, paliperidone
SZ 49	Test set 1	22	Female	Olanzapine
SZ 50	Test set 1	20	Female	Risperidone
SZ 51	Test set 1	19	Female	Haloperidol
SZ 52	Test set 1	21	Female	Olanzapine
SZ 53	Test set 1	18	Female	Olanzapine
SZ 54	Test set 1	20	Female	Risperidone
SZ 55	Test set 1	17	Female	Aripiprazole
SZ 56	Test set 1	19	Female	Clozapine
SZ 57	Test set 1	30	Male	Fluoxetine
SZ 58	Test set 1	26	Female	Quetiapine
SZ 59	Test set 1	24	Female	Olanzapine, quetiapine
SZ 60	Test set 1	27	Female	Olanzapine
SZ 61	Test set 1	47	Female	Olanzapine
SZ 62	Test set 1	64	Female	Olanzapine
SZ 63	Test set 1	24	Female	Olanzapine
SZ 64	Test set 1	23	Male	Olanzapine, clozapine
SZ 65	Test set 1	17	Female	Aripiprazole
SZ 66	Test set 1	18	Female	Aripiprazole

SZ 67	Test set 1	21	Male	Aripiprazole
SZ 68	Test set 1	21	Male	Aripiprazole
SZ 69	Test set 1	17	Female	Aripiprazole
SZ 70	Test set 2	37	Female	NO
SZ 71	Test set 2	29	Female	NO
SZ 72	Test set 2	21	Female	NO
SZ 73	Test set 2	49	Female	NO
SZ 74	Test set 2	28	Female	NO
SZ 75	Test set 2	44	Female	NO
SZ 76	Test set 2	22	Female	NO
SZ 77	Test set 2	24	Female	NO
SZ 78	Test set 2	30	Female	NO
SZ 79	Test set 2	40	Female	NO
SZ 80	Test set 2	23	Male	NO
SZ 81	Test set 2	41	Male	NO
SZ 82	Test set 2	21	Male	NO
SZ 83	Test set 2	47	Male	NO
SZ 84	Test set 2	20	Male	NO
SZ 85	Test set 2	19	Male	NO
SZ 86	Test set 2	47	Male	NO
SZ 87	Test set 2	31	Male	NO
SZ 88	Test set 2	40	Male	NO
SZ 89	Test set 2	26	Male	NO
HC 01	Training set	29	Female	NO
HC 02	Training set	30	Female	NO

HC 03	Training set	31	Male	NO
HC 04	Training set	30	Male	NO
HC 05	Training set	19	Female	NO
HC 06	Training set	30	Female	NO
HC 07	Training set	25	Male	NO
HC 08	Training set	31	Male	NO
HC 09	Training set	28	Male	NO
HC 10	Training set	33	Female	NO
HC 11	Training set	28	Male	NO
HC 12	Training set	33	Female	NO
HC 13	Training set	28	Female	NO
HC 14	Training set	29	Male	NO
HC 15	Training set	31	Male	NO
HC 16	Training set	28	Female	NO
HC 17	Training set	30	Male	NO
HC 18	Training set	31	Male	NO
HC 19	Training set	34	Male	NO
HC 20	Training set	45	Male	NO
HC 21	Training set	39	Female	NO
HC 22	Training set	55	Male	NO
HC 23	Training set	39	Male	NO
HC 24	Training set	45	Female	NO
HC 25	Training set	43	Female	NO
HC 26	Training set	33	Female	NO
HC 27	Training set	36	Female	NO

HC 28	Training set	48	Female	NO
HC 29	Training set	58	Female	NO
HC 30	Training set	35	Female	NO
HC 31	Training set	39	Female	NO
HC 32	Training set	40	Female	NO
HC 33	Training set	45	Female	NO
HC 34	Training set	44	Female	NO
HC 35	Training set	43	Female	NO
HC 36	Training set	43	Female	NO
HC 37	Training set	40	Male	NO
HC 38	Training set	32	Male	NO
HC 39	Training set	41	Female	NO
HC 40	Training set	38	Male	NO
HC 41	Training set	36	Female	NO
HC 42	Training set	38	Male	NO
HC 43	Training set	45	Male	NO
HC 44	Training set	41	Male	NO
HC 45	Training set	30	Female	NO
HC 46	Training set	29	Male	NO
HC 47	Training set	46	Female	NO
HC 48	Training set	51	Female	NO
HC 49	Training set	56	Male	NO
HC 50	Training set	52	Female	NO
HC 51	Test set 1	24	Male	NO
HC 52	Test set 1	26	Male	NO

HC 53	Test set 1	26	Female	NO
HC 54	Test set 1	26	Female	NO
HC 55	Test set 1	22	Female	NO
HC 56	Test set 1	24	Male	NO
HC 57	Test set 1	24	Male	NO
HC 58	Test set 1	24	Male	NO
HC 59	Test set 1	24	Male	NO
HC 60	Test set 1	26	Male	NO
HC 61	Test set 1	24	Male	NO
HC 62	Test set 1	26	Male	NO
HC 63	Test set 1	26	Male	NO
HC 64	Test set 1	63	Female	NO
HC 65	Test set 1	24	Male	NO
HC 66	Test set 1	26	Female	NO
HC 67	Test set 1	26	Male	NO
HC 68	Test set 1	34	Male	NO
HC 69	Test set 1	24	Male	NO
HC 70	Test set 1	34	Male	NO
HC 71	Test set 1	55	Male	NO
HC 72	Test set 1	39	Female	NO
HC 73	Test set 1	55	Male	NO
HC 74	Test set 1	59	Male	NO
HC 75	Test set 1	49	Male	NO
HC 76	Test set 1	45	Female	NO
HC 77	Test set 1	48	Female	NO

HC 78	Test set 1	58	Female	NO
HC 79	Test set 1	61	Female	NO
HC 80	Test set 1	67	Female	NO
HC 81	Test set 1	59	Female	NO
HC 82	Test set 1	60	Female	NO
HC 83	Test set 1	58	Female	NO
HC 84	Test set 1	55	Female	NO
HC 85	Test set 1	39	Female	NO
HC 86	Test set 2	30	Female	NO
HC 87	Test set 2	37	Female	NO
HC 88	Test set 2	36	Female	NO
HC 89	Test set 2	36	Female	NO
HC 90	Test set 2	33	Female	NO
HC 91	Test set 2	29	Female	NO
HC 92	Test set 2	39	Female	NO
HC 93	Test set 2	33	Female	NO
HC 94	Test set 2	28	Female	NO
HC 95	Test set 2	38	Female	NO
HC 96	Test set 2	31	Male	NO
HC 97	Test set 2	32	Male	NO
HC 98	Test set 2	28	Male	NO
HC 99	Test set 2	33	Male	NO
HC 100	Test set 2	32	Male	NO
HC 101	Test set 2	34	Male	NO
HC 102	Test set 2	30	Male	NO

HC 103	Test set 2	29	Male	NO
HC 104	Test set 2	34	Male	NO
HC 105	Test set 2	30	Male	NO

Supplemental Table 2. The Mass parameters in SIM mode for quantitative analysis

Metabolites	Retention time (min)	Qualitative ion (m/z)	Quantitative ion (m/z)	Calibration curve equations	R^2
Pyroglutamic acid	11.19	230; 258	156	Y=1.4773X+0.7061	0.9997
Sorbitol	16.01	205; 217	319	Y=1.1503X-0.0782	0.9967
Tocopherol-α	25.12	237; 277	502	Y=0.1348X-0.0126	0.9982

Supplemental Table 3. Quantitative analysis of schizophrenic biomarkers in PBMCs

Samples	Pyroglutamic acid（μg/ml)	Sorbitol（μg/ml)	Tocopherol-α（μg/ml)
HC 86	108.47	3.02	1.78
HC 87	133.95	5.06	23.51
HC 88	111.66	4.57	16.44
HC 89	122.84	9.31	28.35
HC 90	114.19	15.76	11.63
HC 91	300.43	10.52	9.47
HC 92	162.87	15.82	14.12
HC 93	146.35	14.54	13.17
HC 94	72.50	14.82	16.57
HC 95	224.94	13.74	11.09
HC 96	162.23	8.28	26.24
HC 97	114.07	11.41	31.01
HC 98	377.66	26.04	28.07
HC 99	451.96	14.21	4.37
HC 100	433.37	26.59	32.12
HC 101	431.58	13.05	19.96
HC 102	117.21	16.20	19.30
HC 103	143.82	10.24	7.61
HC 104	66.00	19.26	11.01
HC 105	124.04	19.92	27.54
SZ 70	7.34	0.52	2.36

SZ 71	25.97	0.56	5.70
SZ 72	13.08	0.53	1.89
SZ 73	28.31	0.88	6.64
SZ 74	45.59	0.45	0.96
SZ 75	48.89	1.42	8.86
SZ 76	99.12	0.64	0.67
SZ 77	77.17	0.61	9.10
SZ 78	96.67	0.80	12.58
SZ 79	69.04	1.14	21.91
SZ 80	36.60	0.55	3.64
SZ 81	42.93	0.46	2.66
SZ 82	66.90	0.80	2.87
SZ 83	111.79	0.84	9.09
SZ 84	90.43	0.70	9.01
SZ 85	113.15	1.41	21.43
SZ 86	62.04	0.85	16.44
SZ 87	32.34	2.17	5.19
SZ 88	70.79	0.50	10.86
SZ 89	121.29	1.29	9.35