

Article

Exploring Serum NMR-Based Metabolomic Fingerprint of Colorectal Cancer Patients: Effects of Surgery and Possible Associations with Cancer Relapse

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Table S1. Data completeness for the different metabolites quantified in the serum samples analyzed via NMR. LOQ = limit of quantification.

Metabolite	Levels outside the measurable range (%)	LOQ (mmol/L)	95% Range (mmol/L)
Alanine	0	< 0.02	0.64 - 0.29
Creatine	0	< 0.01	≤ 0.07
Creatinine	0	< 0.01	0.14 - 0.06
Glutamine	0	< 0.02	0.83 - 0.3
Glycine	0	< 0.01	0.44 - 0.17
Histidine	0	< 0.02	0.16 - 0.07
Isoleucine	0	< 0.03	0.11 - 0.03
Leucine	0	< 0.01	0.2 - 0.07
N,N-Dimethylglycine	1.2	< 0.01	≤ 0.01
Phenylalanine	0	< 0.03	≤ 0.07
Tyrosine	0	< 0.03	≤ 0.08
Valine	0	< 0.03	0.35 - 0.15
Acetic acid	0	< 0.01	≤ 0.06
Citric acid	0	< 0.03	≤ 0.21
Formic acid	0	< 0.02	≤ 0.03
Lactic acid	0	< 0.03	7.14 - 2.23
Succinic acid	4.8	< 0.01	≤ 0.01
3-Hydroxybutyric acid	20.2	< 0.02	≤ 0.26
Acetoacetic acid	10.7	< 0.01	≤ 0.02
Acetone	0	< 0.01	≤ 0.06
Pyruvic acid	8.3	< 0.03	≤ 0.07
Glucose	0	< 0.54	6.08 - 1.73
Dimethyl sulfone	0	< 0.01	≤ 0.02

Table S2. Correlation between clinical data and metabolites. Correlation coefficients and p-values are reported in table.

Metabolite	pT		N		GRADE		STAGE		LOCALIZATION		SEX		ECOG PS	
	r	p	r	p	r	p	r	p	r	p	r	p	r	p
Alanine	-0.151	0.203	0.069	0.592	-0.074	0.547	0.042	0.738	-0.097	0.384	0.049	0.663	-0.129	0.365
Creatine	0.061	0.619	0.131	0.300	0.191	0.103	0.027	0.835	-0.098	0.381	-0.280	0.011	0.139	0.295
Creatinine	-0.047	0.691	0.141	0.231	0.067	0.581	0.248	0.093	0.034	0.762	0.385	3.566·10 ⁻⁰⁴	0.104	0.434
Glutamine	-0.103	0.394	-0.034	0.809	-0.151	0.210	-0.167	0.159	-0.035	0.755	-0.225	0.042	0.072	0.604
Glycine	-0.226	0.048	-0.028	0.830	-0.027	0.829	-0.191	0.119	-0.137	0.220	-0.319	0.003	-0.061	0.667
Histidine	-0.322	0.003	-0.070	0.601	-0.179	0.134	-0.236	0.050	-0.071	0.529	0.124	0.269	-0.110	0.462
Isoleucine	0.071	0.563	0.157	0.217	-0.015	0.905	0.292	0.015	0.102	0.362	0.250	0.024	-0.253	0.098
Leucine	0.065	0.595	0.084	0.526	-0.162	0.176	0.060	0.637	0.116	0.298	0.223	0.045	-0.248	0.063
N,N-Dimethylglycine	0.063	0.605	-0.026	0.845	0.093	0.447	0.075	0.542	-0.029	0.795	0.171	0.125	0.263	0.034
Phenylalanine	0.066	0.591	0.071	0.597	0.022	0.861	0.162	0.177	-0.040	0.722	0.142	0.204	-0.142	0.293
Tyrosine	-0.178	0.134	-0.390	0.001	-0.117	0.336	-0.291	0.008	0.021	0.853	-0.096	0.391	-0.234	0.092
Valine	0.026	0.831	0.056	0.675	-0.102	0.406	0.104	0.397	0.073	0.513	0.160	0.151	-0.372	0.002
Acetic acid	0.029	0.816	-0.116	0.555	0.096	0.425	-0.013	0.908	0.188	0.091	0.141	0.208	-0.442	0.571
Citric acid	-0.010	0.934	0.179	0.157	-0.223	0.055	0.110	0.378	-0.032	0.777	-0.013	0.910	-0.002	0.991
Formic acid	0.154	0.205	0.174	0.174	0.153	0.200	0.196	0.139	-0.045	0.687	0.232	0.036	-0.096	0.458
Lactic acid	0.019	0.879	0.112	0.387	0.075	0.536	0.145	0.251	0.134	0.230	0.161	0.148	-0.087	0.514
Succinic acid	0.139	0.250	0.052	0.685	0.008	0.946	0.139	0.268	0.139	0.212	-0.005	0.964	0.122	0.363
3-Hydroxybutyric acid	0.104	0.394	0.097	0.442	-0.033	0.787	0.164	0.216	0.044	0.693	0.010	0.932	0.170	0.187
Acetoacetic acid	0.001	0.994	0.024	0.847	0.007	0.954	0.073	0.568	0.115	0.302	-0.027	0.807	0.144	0.268
Acetone	0.035	0.780	0.002	0.989	-0.029	0.814	0.123	0.356	0.218	0.049	0.048	0.668	-0.163	0.357
Pyruvic acid	-0.043	0.722	0.016	0.905	0.156	0.196	0.020	0.875	-0.032	0.778	0.013	0.910	0.027	0.850
Glucose	-0.097	0.420	0.114	0.372	-0.125	0.301	0.113	0.362	-0.049	0.661	-0.033	0.766	0.049	0.714
Dimethylsulfone	-0.183	0.115	0.130	0.267	0.044	0.717	0.165	0.247	0.081	0.467	0.063	0.575	0.262	0.025
Triglycerides	-0.029	0.808	-0.038	0.762	-0.053	0.668	0.106	0.406	0.119	0.288	0.139	0.212	-0.419	0.002
Cholesterol	-0.131	0.280	-0.085	0.511	0.176	0.138	-0.095	0.444	0.268	0.015	-0.441	3.359·10 ⁻⁰⁵	-0.407	0.001
LDL Cholesterol	-0.032	0.795	-0.033	0.798	0.201	0.085	-0.059	0.635	0.293	0.008	-0.363	0.001	-0.327	0.014
HDL Cholesterol	-0.071	0.561	-0.068	0.597	0.149	0.217	-0.193	0.113	-0.111	0.323	-0.554	6.733·10 ⁻⁰⁸	-0.021	0.884
Apo-A1	-0.152	0.206	-0.207	0.102	0.027	0.826	-0.292	0.010	-0.066	0.553	-0.541	1.530·10 ⁻⁰⁷	-0.181	0.189
Apo-A2	-0.118	0.333	-0.201	0.123	0.006	0.963	-0.232	0.049	0.062	0.581	-0.370	0.001	-0.342	0.008
Apo-B100	0.009	0.942	-0.018	0.890	0.226	0.050	0.024	0.845	0.356	0.001	-0.317	0.004	-0.369	0.003

ECOG PS: Eastern Cooperative Oncology Group Performance Status; pT: primary tumor size; N: regional lymph nodes

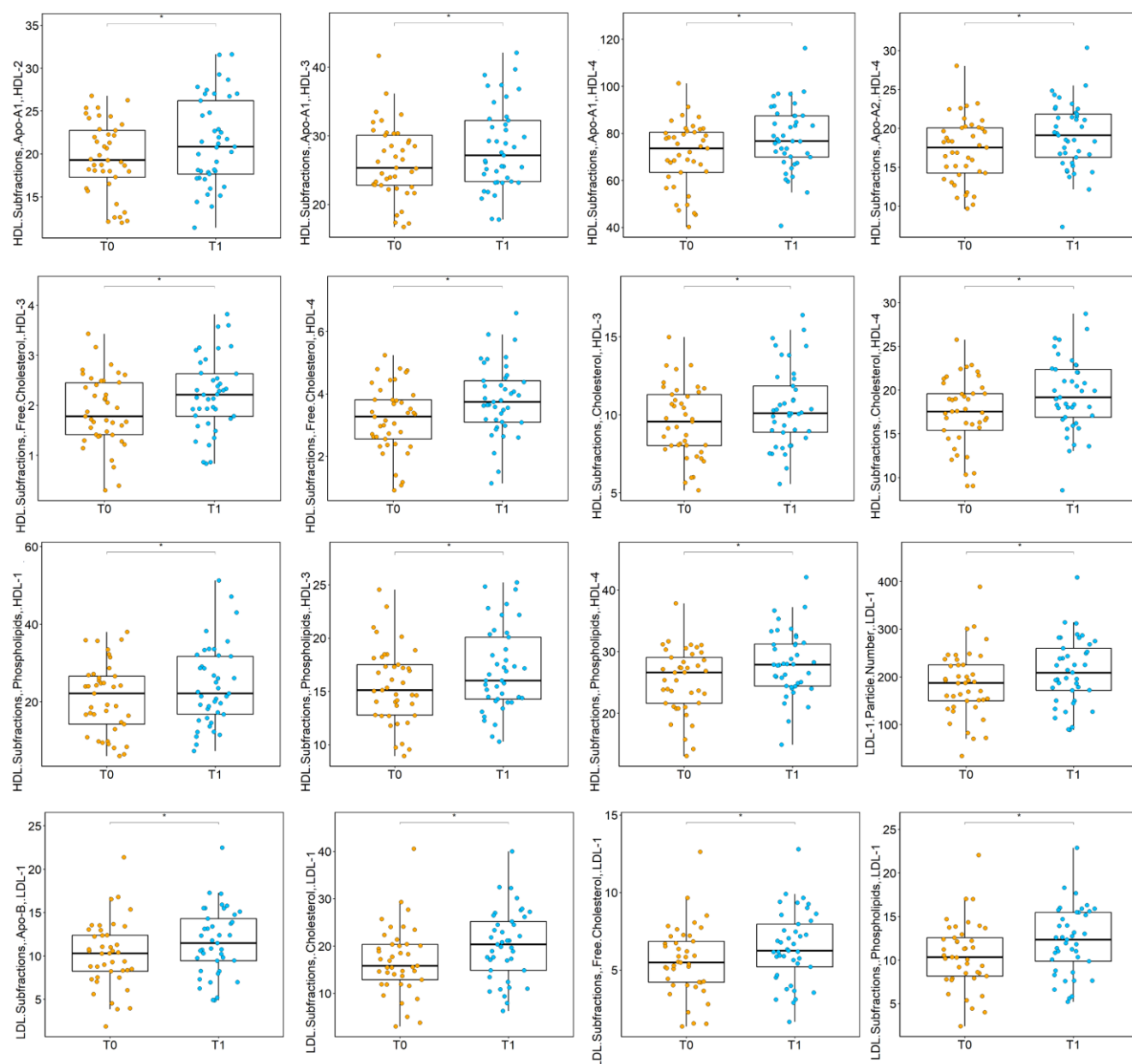


Figure S1. Boxplots of the statistically significant lipoproteins-related parameters discriminating of CRC patients at t0 (orange) and t1 (turquoise); p -values obtained using Wilcoxon signed-rank test and adjusted for FDR are reported. *** $p < 0.001$; ** $p < 0.01$; * $p < 0.05$.