

Amir Hashim et al., *BiolImpacts*, 2021, 11(1), 33-43

doi: [10.34172/bi.2021.05](https://doi.org/10.34172/bi.2021.05)

<http://bi.tbzmed.ac.ir/>

Global metabolomics profiling of colorectal cancer in Malaysian patients

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Supplementary file 1

Table S1. LCMS/QTOF intensity readings for the 11 identified differential metabolites in normal healthy controls.

Compound	A02	A03	A04	A07	A08	A09	A10	A11	A12	B01
Methionine	0.939837	0.954792	0.379128	0.283476	-0.73946	-0.05553	-17.2338	-16.1613	-1.19253	-0.27766
Acetylcarnitine	-0.25718	-0.39982	-1.08159	-1.7455	-1.70545	-1.21752	-1.23084	0.498238	15.47497	-0.59527
LysoPE	2.415915	0.115127	2.019341	2.780739	1.455385	1.265194	6.064514	7.060195	21.68113	1.698626
LysoPC	0.279353	-0.02513	0.645247	1.127947	0.125347	1.067127	5.374449	5.494617	21.33356	0.004461
Uric acid	0.938346	0.863342	0.424258	0.218883	-0.20885	-18.5859	-18.5086	-17.4361	-2.46734	0.140946
Pipecolic acid	0.572307	0.28064	0.203773	0.729171	0.126668	0.065019	1.574855	2.373339	17.54675	0.127002
Tyrosine	0.251606	0.435033	-0.33036	-0.05913	-1.17484	-0.24227	-20.4736	-19.4011	-4.43233	-0.72115
5-Oxoproline	0.170375	0.19751	-18.3361	-0.62214	-1.79241	-0.59683	-18.2811	-17.2085	-2.23982	-0.40577
Hypoxanthine	0.058626	-0.23791	0.139814	-0.06819	-0.37824	-0.61579	-17.314	-16.2414	-1.27271	-0.80691
Xanthine	-0.70039	-15.0444	-14.547	-0.71126	-14.7365	-1.05825	-17.3786	-16.3935	-16.3858	-15.0539
Citric acid	-0.7552	-1.48348	-0.98232	-2.18712	-2.20837	-1.21089	-2.72515	-1.21969	-0.62205	-1.07384

Compound	B02	B03	B04	B05	B06	B07	B09	B10	B11	B12
Methionine	-0.01816	-1.19253	0.171526	-1.19253	-1.19253	-0.76475	0.091221	-17.3488	-17.0041	-5.03465
Acetylcarnitine	-0.64324	-6.37668	-1.61899	-6.37668	-6.37668	-21.1041	-1.17621	-0.36974	-0.50399	11.76412
LysoPE	1.386852	0	2.414848	0	0	2.929154	2.714359	5.851688	6.385513	18.49313
LysoPC	0.080528	0	0.612581	0	0	0.174278	1.017227	5.409569	5.790896	17.59501
Uric acid	0.597829	-2.46734	-18.6125	-2.46734	-2.46734	-17.1947	0.363372	-18.6236	-18.2789	-6.30946
Pipecolic acid	0.170245	-0.41041	0.611472	-0.41041	-0.41041	-15.1378	0.427959	1.272952	1.944434	13.70103
Tyrosine	-0.08593	13.75202	-0.53287	-4.43233	-4.43233	0.387224	0.175765	-20.5886	-20.2439	-8.27445
5-Oxoproline	-0.44108	14.13914	-0.12602	14.70023	14.57103	-16.9672	-0.92452	-18.3961	-18.0514	-6.08194
Hypoxanthine	-17.3435	16.32364	0.057854	15.05875	-1.27271	-16.0001	-0.69056	-17.429	-17.0843	-5.11483
Xanthine	3.436826	1.019513	-14.8447	5.38325	3.888167	16.47467	-0.76628	-16.6423	-17.2323	-16.3946
Citric acid	-1.6895	1.41724	-1.96781	4.836589	2.953364	-3.52089	-2.12718	-0.55964	-1.05097	-0.48874

Compound	C01	C02	C04	C06	C07	C08	C09	C10	C11	C12
Methionine	0.288908	-0.63947	-1.19253	-1.19253	-0.46289	1.044411	0.449908	0.758239	-15.3555	-15.1653
Acetylcarnitine	-1.48139	-2.01932	-6.37668	-6.37668	-21.5787	-0.32112	-0.60641	-0.07723	1.260469	1.460697
LysoPE	0.136597	2.197487	0	0	2.745554	-14.6552	-15.5783	4.908103	8.045706	8.310926
LysoPC	-0.04553	0.898941	0	0	0.799391	-14.6552	1.990923	3.383918	7.586657	7.175063
Uric acid	0.332503	0.421918	-2.46734	-2.46734	0.748223	1.93222	0.764401	1.376871	-16.6303	-16.4401
Pipecolic acid	0.159181	-16.8674	-0.41041	-0.41041	0.695191	1.615171	-15.9887	-15.6529	-14.5734	3.745514
Tyrosine	0.169875	-0.78025	-4.43233	-4.43233	0.005013	-19.0876	0.427975	0.728141	-18.5953	-18.4051
5-Oxoproline	0.003806	-1.01848	-2.23982	-2.23982	-0.37732	0.31495	0.142653	0.515841	-16.4028	-16.2126
Hypoxanthine	-0.01277	-1.20999	-1.27271	-1.27271	-16.4748	0.815779	0.755722	1.424882	-15.4357	-15.2455
Xanthine	-15.0084	-0.38962	16.09408	-11.3648	-1.64337	0	0.081944	-0.41022	-17.7977	-17.6194
Citric acid	-1.5884	-2.54918	17.15392	4.426892	-1.2953	15.73068	-1.54395	-1.71026	-2.08562	-1.76076

Compound	C03	C05	D01	D02	D04	D06	D07	D09	D10	D11
Methionine	-1.19253	-1.19253	-0.34289	0.318425	-1.19253	-1.19253	-1.19253	0.734274	-0.54163	-16.4054
Acetylcarnitine	-6.37668	-6.37668	-2.16817	-0.42153	-6.37668	-6.37668	-6.37668	-0.22369	-1.2822	0.200723
LysoPE	0	0	1.184795	3.014463	0	0	0	3.129793	2.034315	6.344944
LysoPC	0	0	-1.10959	1.636389	0	0	0	1.751202	1.232576	5.829676
Uric acid	-2.46734	-2.46734	-0.3202	0.389245	-2.46734	-2.46734	-2.46734	0.328748	-0.40647	-17.6802
Pipecolic acid	-0.41041	-0.41041	-0.06292	0.57133	-0.41041	-0.41041	-0.41041	-15.7817	-17.0507	2.216151
Tyrosine	-4.43233	-4.43233	-0.77333	-0.15496	-4.43233	-4.43233	-4.43233	0.519486	-0.71897	-19.6452
5-Oxoproline	13.93914	-2.23982	-0.86322	0.309764	13.2028	-2.23982	-2.23982	0.118966	-0.62231	-17.4527
Hypoxanthine	-1.27271	-1.27271	-0.64853	0.01277	-1.27271	-1.27271	-1.27271	0.774551	-0.58278	-16.4856
Xanthine	0	-14.9179	-14.9085	-0.27406	0	-0.02936	0.061715	0	-1.96003	0
Citric acid	-3.52089	1.682149	-1.54155	0.09727	16.81851	0.30861	-18.7187	13.09107	-1.56615	-3.52089

Compound	D12	DO3	DO5	E01	E02	E03	E04	E05	E06	E08
Methionine	-15.8402	-1.19253	-1.19253	-0.29614	-0.00745	14.86928	-4.55975	-1.19253	-16.8803	-15.4767
Acetylcarnitine	0.69134	-6.37668	-6.37668	-1.82738	-0.27851	-6.37668	12.0377	15.25067	0.054145	0.219247
LysoPE	7.186951	0	0	-16.3715	0.817972	0	-3.36722	0	-15.6877	-14.2842
LysoPC	5.78158	0	0	0.031206	-0.26003	0	16.40037	20.52036	4.459282	5.945543
Uric acid	-17.115	-2.46734	-2.46734	-0.32599	0.563527	-2.46734	-5.83456	-2.46734	-18.1551	-16.7515
Pipelicolic acid	-15.0581	-0.41041	-0.41041	-0.00831	0.512977	-0.41041	13.53241	17.03616	1.118949	3.180669
Tyrosine	-19.08	-4.43233	-4.43233	-0.66313	-0.18095	-4.43233	-7.79955	-4.43233	-20.1201	1.176741
5-Oxoproline	-16.8875	13.42127	-2.23982	-0.60942	-0.06299	14.68312	-5.60704	-2.23982	-17.9276	1.214965
Hypoxanthine	-15.9204	-1.27271	-1.27271	-0.35175	-1.2249	14.48124	-4.63993	-1.27271	-16.9604	-15.5569
Xanthine	-15.4165	15.19256	0	-15.2482	0	-0.16808	-17.9567	-18.137	-18.7448	-19.0127
Citric acid	-0.09727	16.80402	16.64008	-1.90972	13.98628	-0.74038	-1.85093	-3.51349	-3.3835	-3.8509

Table B: LCMS/QTOF intensity readings for the 11 identified differential metabolites in colorectal patients.

Compound	C181	C187	C190	C194	C200	C273	C288	C289	C298	C330
Methionine	13.41624	14.29697	15.04859	13.28187	0.211723	-1.19253	14.92334	13.35044	13.9034	1.760199
Acetylcarnitine	13.29178	13.69093	14.3324	12.49465	-0.70884	16.10717	12.70555	12.50529	13.67567	0.859902
LysoPE	0	0	0	0	1.018355	20.43334	0	0	0	-14.5847
LysoPC	0	0	0	0	-0.07396	0	0	0	0	-14.5847
Uric acid	14.87426	15.17857	15.25892	13.58841	0.863674	-2.46734	13.88651	14.88682	-2.46734	0.478961
Pipelicolic acid	-0.41041	-0.41041	15.07815	-0.41041	0.406342	-0.41041	-0.41041	-0.41041	-0.41041	2.17308
Tyrosine	13.22622	13.52718	14.68103	12.70999	-0.00501	-4.43233	13.874	12.75306	13.73674	0.954625
5-Oxoproline	-2.23982	15.0236	-2.23982	12.44499	0.375818	-2.23982	15.471	13.77016	-2.23982	1.657205
Hypoxanthine	13.2722	16.08451	14.5066	12.67639	0.981828	-1.27271	14.08375	-1.27271	17.27772	2.057726
Xanthine	3.746219	5.042977	15.91485	13.93138	3.849494	0	0	4.247788	-14.0155	0
Citric acid	5.777569	4.983871	15.92267	15.64035	1.083953	-3.52089	15.57789	4.728128	1.388138	13.56608

Compound	C335	C341	C353	C354	C358	C372	C373	C379	C380	C388
Methionine	0.628776	-0.42612	-1.19253	14.3764	13.50752	13.16728	15.70975	0.73321	0.635217	-1.17703
Acetylcarnitine	-1.20429	-2.2012	16.09324	13.02026	12.49412	13.19617	15.65208	-0.05414	-0.13228	-0.08588
LysoPE	-0.22793	-16.2681	0	0	0	0	0	-15.4748	-15.0064	-15.4944
LysoPC	-15.6623	0.224083	0	0	0	0	0	0.090118	1.677884	-15.4944
Uric acid	0.794704	-0.14095	-2.46734	14.12966	14.73565	13.56556	15.97128	1.211024	0.904102	0.768686
Pipecolic acid	-0.04463	-0.0476	16.91077	-0.41041	-0.41041	-0.41041	15.8646	0.882184	0.772335	0.165318
Tyrosine	0.141529	-0.40724	-4.43233	13.22726	12.26156	12.52585	15.25263	0.470189	0.634651	-0.55605
5-Oxoproline	-0.27909	-0.64402	-2.23982	13.59751	14.09641	14.13427	15.70967	1.822232	0.7213	-0.5451
Hypoxanthine	0.064988	-17.5408	19.96642	13.36482	15.72376	12.2912	17.52545	3.55724	1.499454	-0.02467
Xanthine	-15.5948	-1.22942	-10.4086	14.89121	0	0	3.836943	15.40245	-10.3155	-10.1139
Citric acid	-2.39265	-3.60967	5.727039	15.26661	14.31541	14.86824	3.796709	13.31105	3.223976	3.484183

Compound	C396	C398	C401	C404	C414	C418	C420	C431	C434	C437
Methionine	-0.02249	1.89247	14.88318	16.20381	16.55495	14.68793	14.45762	0.668318	17.2657	14.23042
Acetylcarnitine	-0.25585	0.96634	13.82709	12.77578	15.61458	14.06048	13.18706	0.632602	14.84685	12.86953
LysoPE	1.44346	-13.9164	0	0	0	0	0	-14.9802	0	0
LysoPC	0.158643	-13.9164	0	0	0	0	0	0.002811	0	0
Uric acid	0.364347	1.028956	15.47462	-2.46734	-2.46734	14.8206	14.02422	1.098414	13.8184	-2.46734
Pipecolic acid	0.067337	1.741258	-0.41041	-0.41041	16.78589	-0.41041	-0.41041	1.568198	16.56255	-0.41041
Tyrosine	-0.50514	1.601004	14.37913	-4.43233	16.26447	14.38386	14.24128	0.683806	16.45187	13.54978
5-Oxoproline	0.148748	2.943988	15.10017	15.00274	17.15963	14.95253	15.28677	2.649568	18.64796	14.8478
Hypoxanthine	1.767304	3.949158	15.87474	14.35346	-1.27271	16.70155	15.68395	2.033979	20.71756	16.11061
Xanthine	0	14.42476	0.516785	17.84465	14.16349	4.616601	-0.41122	14.59852	17.64147	15.72393
Citric acid	12.93984	12.82526	0.802177	14.79413	12.77673	5.755894	-1.09368	12.26426	15.43636	13.94889

Compound	C438	C445	C449	C450	C459	C467	C469	C474	C476	C482
Methionine	13.19184	15.09741	-1.19253	0.007452	14.95208	14.0689	-1.19253	-1.19253	-0.04541	-0.36769
Acetylcarnitine	-6.37668	13.60549	15.39855	-0.13921	13.7823	12.6316	15.87351	16.02099	0.265836	-1.25593
LysoPE	0	0	0	-15.5663	0	0	0	0	1.79615	2.522778
LysoPC	0	0	0	-15.5663	0	0	0	0	-0.87815	1.008295
Uric acid	-2.46734	14.31584	-2.46734	0.923309	14.84528	12.94026	-2.46734	-2.46734	0.354087	0.258849
Pipecolic acid	-0.41041	-0.41041	17.37063	0.008307	-0.41041	-0.41041	17.50268	-0.41041	1.219674	0.148643
Tyrosine	13.1568	13.70684	15.53402	-0.32417	14.42045	13.35659	15.23206	-4.43233	1.041077	-0.35575
5-Oxoproline	13.69671	15.00795	-2.23982	0.442635	15.18455	14.86652	-2.23982	-2.23982	-0.00381	-0.42072
Hypoxanthine	-1.27271	15.86889	-1.27271	1.898755	17.76941	16.65653	-1.27271	-1.27271	1.970247	1.771185
Xanthine	14.89031	15.48564	-16.7677	9.185621	6.65139	4.601765	-16.5671	-10.9812	14.86424	-0.44895
Citric acid	-3.52089	-3.52089	-1.13494	-13.5862	4.146317	-15.2497	-2.6644	-14.5021	13.24431	-1.24324

Compound	C483	C484	C485	C488	C497	C498	C500	C501	C503	C507
Methionine	2.560803	1.407015	-1.19253	14.20871	14.00041	12.89641	13.10995	-1.19253	1.257127	-1.19253
Acetylcarnitine	0.669562	0.662065	15.26133	12.87932	11.59832	11.62795	11.43066	15.35454	-0.28964	14.06737
LysoPE	-14.3773	3.912405	0	0	0	-3.68113	-3.59512	0	0.970167	0
LysoPC	-14.3773	-0.45623	0	0	0	12.73504	11.50283	0	-0.24274	0
Uric acid	-16.8446	0.522264	-2.46734	12.76328	11.98168	12.4221	12.01271	-2.46734	-17.4448	-2.46734
Pipecolic acid	1.602168	1.563609	-0.41041	-0.41041	-0.41041	-4.09154	13.28081	-0.41041	1.08979	16.42405
Tyrosine	1.536948	1.12267	-4.43233	13.64179	13.48411	12.62825	12.61736	15.40807	0.902862	15.26931
5-Oxoproline	1.212556	2.84674	-2.23982	14.30601	13.38203	13.41919	12.8825	-2.23982	0.577881	-2.23982
Hypoxanthine	1.449518	1.778832	19.22808	16.37382	17.37713	-4.95384	14.71762	20.28928	3.355714	-1.27271
Xanthine	0	5.02523	-12.6812	15.63793	1.88006	13.87489	15.32938	-16.2946	14.5205	-16.6249
Citric acid	13.55732	3.838162	3.127121	15.39177	1.254246	13.76254	12.7832	-3.09319	11.25796	-3.90534

Note: Codes refer to individual subjects

Table S2. Prediction of new samples (20 CRC and 20 Normal) using 11 panel of biomarkers.

Normal			Cancer		
A01v	0.92	1	C325v	0.77667	0
A02v	0.73333	1	C511v	0.75	0
A03v	0.85667	0	C547v	0.87667	0
A04v	0.86667	1	C552v	0.81333	0
A05v	0.70667	1	C569v	0.52667	0
A06v	0.71333	1	C570v	0.63333	0
A07v	0.82333	1	C584v	0.54667	0
A07vv	0.92	1	C603v	0.87667	0
A08v	0.85	0	C647v	0.94667	0
A09v	0.83	1	C656v	0.82667	0
A10v	0.72667	1	C658v	0.69333	1
A11v	0.74333	1	C660v	0.89667	0
A12v	0.71	1	C662v	0.85333	0

B01v	0.76	1	C663v	0.74	0
B02v	0.51	0	C666v	0.59667	0
B03v	0.67333	1	C667v	0.67333	1
B04v	0.89333	1	C668v	0.68	0
B05v	0.79333	1	C669v	0.84	1
B06v	0.84	1	C678v	0.74	0
B07v	0.89	0	C679v	0.65667	1

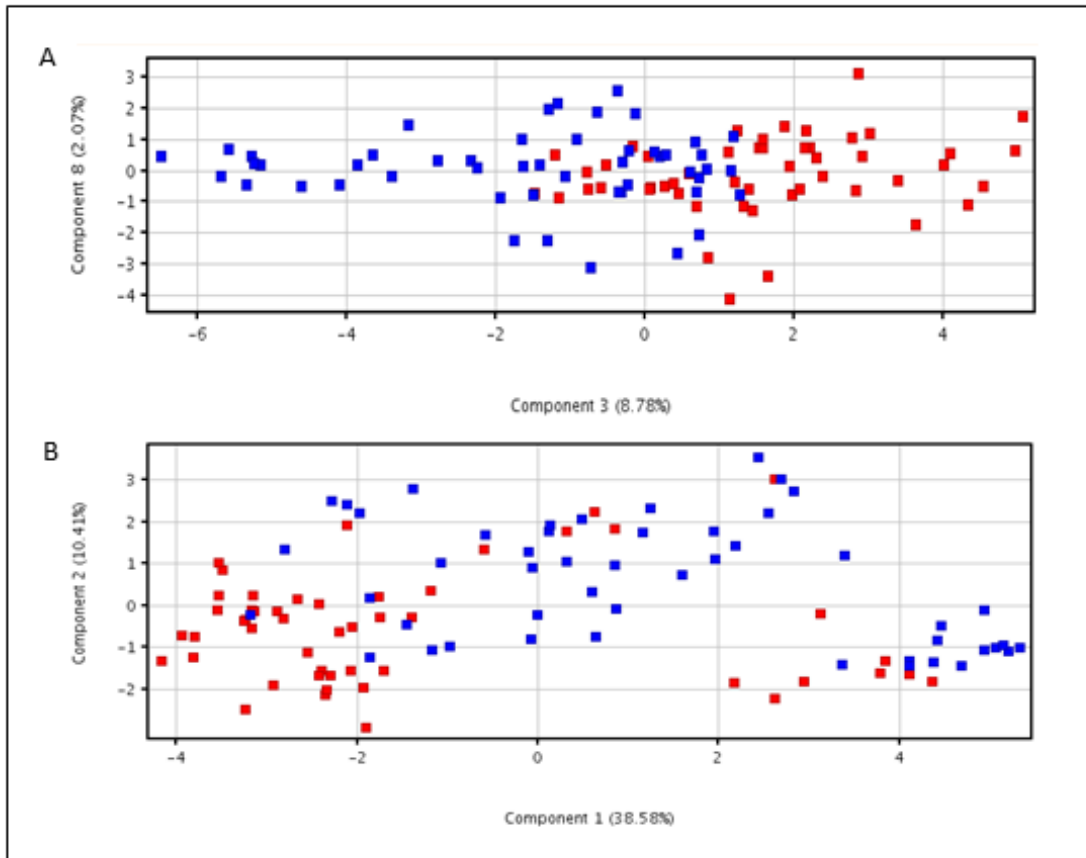


Fig. S1. A) 2D-PCA Score Plot for Patients and Healthy Volunteers in Positive Ion Mode.

B) 2D-PCA Score Plot for Patients and Healthy Volunteers in Negative Ion Mode.

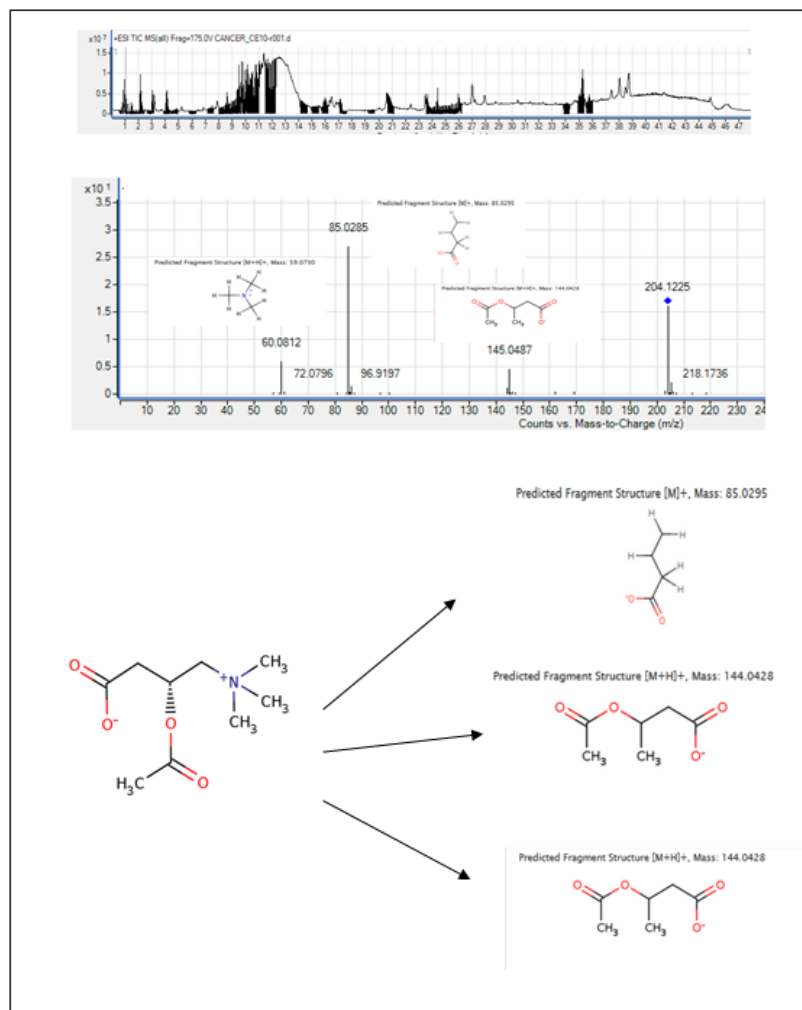


Fig. S2. Full chromatogram of CRC pooled samples with fragmented ions of acetylcarnitine.