

**Table S1.** Correlations of the top 5 metabolites correlations with MDS and each of the food groups assessed in the 14-item MD score.

Food group	Citric Acid			Mannose			Pyruvic Acid			Myo-Inositol			Betaine		
	r	p	Q	r	p	Q	r	p	Q	r	p	Q	r	p	Q
MD score	0.28**	0.001	0.26	-0.20*	0.02	0.63	-0.02**	0.008	0.56	-0.18*	0.03	0.63	0.19*	0.02	0.63
Fruit (Fr)	0.15	0.07	0.80	-0.27**	0.002	0.31	-0.23**	0.007	0.56	-0.16	0.06	0.88	0.05	0.55	0.91
Fruit Juice (J)	0.18*	0.03	0.70	-0.10	0.23	0.90	-0.05	0.56	0.91	-0.01	0.85	0.98	0.19*	0.03	0.64
Fruit and Fruit Juice (FJ)	0.22*	0.02	0.63	-0.27**	0.002	0.31	-0.19*	0.02	0.63	-0.11	0.18	0.73	0.15	0.07	0.81
Vegetables (V)	0.02	0.83	0.97	-0.02	0.79	0.97	-0.06	0.50	0.91	-0.12	0.15	0.88	0.06	0.44	0.91
Fr & J & V combined (FJV)	0.20*	0.02	0.63	-0.23**	0.007	0.31	-0.15	0.07	0.80	-0.16	0.06	0.71	0.20*	0.02	0.63
Red meat (RM)	-0.06	0.48	0.91	0.09	0.25	0.90	0.13	0.11	0.86	0.10	0.24	0.90	-0.01	0.90	0.99
Chicken and Turkey (CT)	0.04	0.06	0.93	-0.14	0.10	0.86	-0.11	0.19	0.90	0.06	0.95	0.99	0.02	0.79	0.97
Fish (F)	0.13	0.12	0.86	-0.02	0.78	0.97	-0.32**	<.0001	0.18	-0.14	0.10	0.83	0.12	0.14	0.88
Nuts (N)	0.06	0.52	0.91	0.02	0.84	0.98	-0.13	0.13	0.88	-0.15	0.09	0.83	0.04	0.68	0.95
Processed meat (PM)	-0.02	0.79	0.97	-0.004	0.96	0.99	0.22**	0.009	0.59	0.18*	0.03	0.63	-0.02	0.85	0.98
Legumes	0.11	0.19	0.90	-0.06	0.46	0.91	0.02	0.77	0.97	0.02	0.81	0.97	0.10	0.13	0.86
Alcohol (A)	0.02	0.82	0.97	0.09	0.27	0.90	-0.09	0.28	0.90	0.02	0.82	0.97	0.07	0.41	0.91
Olive spreads (OS)	0.07	0.40	0.90	-0.12	0.14	0.88	-0.19*	0.02	0.63	-0.021*	0.01	0.63	0.05	0.54	0.91
Olive / Rapeseed oil (OR)	0.11	0.21	0.90	-0.07	0.35	0.90	-0.09	0.31	0.90	-0.05	0.54	0.91	0.09	0.29	0.90

Sweet foods (S)	-0.19*	0.03	0.63	-0.03	0.64	0.93	-0.15	0.06	0.73	0.11	0.22	0.90	-0.11	0.21	0.90
Sweet foods & drinks (SD) (SD)	-0.19*	0.03	0.63	-0.13	0.12	0.86	-0.005	0.58	0.91	0.03	0.69	0.95	-0.08	0.33	0.90
Whole grain cereals (C)	0.03	0.74	0.96	-0.21*	0.015	0.63	-0.09	0.30	0.90	-0.04	0.67	0.95	0.05	0.53	0.91

Spearman’s rank correlation coefficients (r) and false discovery rates (Q) were obtained for the top five discriminant metabolites to indicate those significantly correlated with the 14-item MD score. Individual food group correlations coefficients and its false discovery rates were also identified for citric acid: (J, FJ, FJV, S and SD); mannose: (Fr, FJ, FJV, and C); pyruvic acid: (Fr, FJ, F, PM and OS) and *Myo*-inositol (PM and OS) and Betaine: (J and FJV). Significance is indicated as \* $P < 0.05$ , \*\* $P < 0.01$ .

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**Table S2.** Baseline characteristics of study participants.

Variable	Low MDS	High MDS	P-value
Age (years) Mean (SD)	56.13 (9.37)	60.54 (7.88)	0.12
Blood Pressure: Systolic (mmHg) Mean (SD)	122.02 (15.98)	132.84 (17.74)	0.04*
Blood Pressure: Diastolic (mmHg) Mean (SD)	66.72 (9.22)	73.57 (8.29)	0.02*
BMI (kg/m <sup>2</sup> ) Mean (SD)	30.23 (5.14)	29.77 (6.81)	0.79
Smokers %	26.66	0	
Sex: Male %	77.78	92.31	
Sex: Female %	22.22	7.69	

Patients general characteristics measured at baseline (n=58). Mean age was 56.13 for the low MDS group and 60.54 for the high MDS group. Mean BMI was 30.23 kg/m<sup>2</sup> for the low MDS group and 29.77 for the high MDS with no significant differences in BMI between the two groups. Mean BMI of 30.23 and 29.77 indicate that most patients were obese and overweight respectively.

**Table S3.** Assigned MDS scores listed by group.

Low MDS (n = 64)						High MDS Group (n = 73)					
MDS	0	1	2	3	4	5	6	7	8	9	10
Samples (n)	n=3	n=9	n=15	n=15	n=22	n=18	n=21	n=10	n=16	n=6	n=2

Table shows the number of individuals assigned each Mediterranean diet score (MDS). Groups were divided at the median. Group 1 (0-4): Low MDS; Group 2 (5-10): High MDS.

**Table S4.** Performance of multivariate modelling of metabolomic data.

Measure	1 component	2 components	3 components
Accuracy	0.546	0.646	0.694
R2	0.219	0.319	0.389
Q2	-0.006	0.055	0.039

Cross validation of the PLS-DA multivariate model as performed using Metaboanalyst 4.0.

Table S5. Food group-to-Food group correlations within the study cohort.

Food group		Fruit	Fruit Juice	Legumes	Red meat	Proc. meat	Fish	Nuts	Alcohol	Sweets & Carbonated Drinks	Olive spread	Olive/Rapeseed Oil	Chicken & Turkey	Cereals (WG)	Sweets
Vegetables	r	0.22*	0.04	-0.11	0.01	-0.37***	0.19*	0.21*	0.16	-0.21*	0.08	0.17*	-0.04	-0.07	-0.18*
	p-value	0.01	0.67	0.19	0.93	7.5E-06	0.027	.013	0.06	0.01	0.37	0.048	0.60	0.43	0.03
Fruit	r		0.19*	0.08	-0.12	-0.36***	0.46**	0.16	-0.12	-0.38**	0.33**	0.28**	0.24***	.18*	-0.36**
	p-value		0.02	0.35	0.15	1.3E-5	1.9E-08	0.06	0.14	4.5E-06	7.4E-5	0.001	0.05	0.03	1.4 E-5
Fruit juice	r			0.24**	0-.05	-0.07	0.18*	0.23**	-0.19*	0.01	0.25**	0.08	0.19*	0.13	-0.07
	p-value			0.005	0.51	0.38	0.04	0.006	0.03	0.91	0.003	0.35	0.026	0.13	0.42
Legumes	r				0.23**	0.23**	0.04	0.15	0.16	-0.01	-0.01	0.12	0.03	0.17	-0.10
	p-value				0.006	0.006	0.62	0.08	0.06	0.88	0.88	0.14	0.73	0.05	0.24
Red meat	r					0.26**	-0.19*	-0.20*	0.20*	0.08	-0.09	0.15	-0.10	0.07	0.04
	p-value					0.003	0.030	0.019	0.02	0.30	0.31	0.07	0.22	0.41	0.62
Processed meat	r						-0.34**	-0.26**	-0.03	0.18*	-0.09	-0.07	0.02	0.13	0.12
	p-value						4.8x10 <sup>-5</sup>	0.002	0.76	0.037	0.26	0.44	0.86	0.13	0.15
Fish	r							0.12	0.05	-0.26**	0.27**	0.17*	-0.04	0.12	-0.14*
	p-value							0.15	0.54	0.002	0.002	0.048	0.67	0.15	0.036
Nuts	r								0.04	-0.01	0.11	-0.01	0.13	0.03	-0.05
	p-value								0.43	0.89	0.18	0.92	0.13	0.71	0.53

Alcohol	r	-0.12	-0.20*	0.12	-0.20*	-0.02	-0.14
	p-value	0.16	0.019	0.14	0.023	0.81	0.10
Sweets & Drinks	r	-0.13	-0.12	-0.02	0.01	0.84**	
	p-value	0.11	0.17	0.78	0.88	3.94E-38	
Olive spread	r	0.18***	0.16	0.22***	-0.13		
	p-value	0.003	0.06	0.01	0.11		

Spearman's rank correlation coefficients were obtained with significance is indicated as \*P < 0.05 and \*\*P < 0.01

Table S6. Correlations of all 59 metabolites against each food group scored within the MDS.

Metabolites		Fruit incl. juice	Fruit excl. juice	Fruit Juice	Vegetables	Fruit, Fruit Juice & Vegetables	Legume s	Olive/ rapeseed oil	Olive spreads	Nuts	Fish	Red meat	Process ed meat	Chicken & turkey	Cereals	Alcohol	Sweets & Drinks	Sweets
1-Methylhistidine	r	0.060	-0.029	0.118	-0.015	0.083	0.098	0.059	0.096	0.054	0.009	0.028	0.137	0.056	0.108	-0.063	0.040	0.086
	p	0.488	0.739	0.170	0.860	0.339	0.256	0.498	0.268	0.531	0.918	0.746	0.113	0.517	0.210	0.468	0.643	0.318
2-Hydroxybutyric acid	r	-0.075	-0.015	-0.063	-0.129	-0.121	-0.010	-0.030	-.229**	-0.039	-.170*	0.052	0.164	0.134	-0.082	-0.117	0.048	-0.013
	p	0.385	0.865	0.467	0.134	0.159	0.906	0.725	0.007	0.649	0.048	0.547	0.056	0.120	0.344	0.175	0.575	0.885
Acetic acid	r	0.164	0.128	0.119	0.134	.175*	.229**	.291**	0.116	0.097	0.099	0.007	0.080	0.037	0.079	0.086	0.069	0.095
	p	0.057	0.136	0.168	0.120	0.041	0.007	0.001	0.178	0.264	0.252	0.934	0.352	0.667	0.360	0.317	0.427	0.269
Betaine	r	0.151	0.051	.183*	0.066	.181*	0.139	0.091	0.053	0.035	0.126	-0.009	0.015	0.023	0.053	0.070	-0.083	-0.108
	p	0.079	0.556	0.033	0.445	0.035	0.105	0.292	0.540	0.688	0.143	0.920	0.859	0.792	0.538	0.418	0.335	0.212
Acetoacetate	r	-0.049	-0.011	-0.017	0.073	-0.015	0.030	0.168	-0.037	-0.022	0.023	0.141	0.065	0.066	-0.027	0.059	-0.039	-0.086
	p	0.575	0.903	0.841	0.400	0.860	0.729	0.050	0.672	0.796	0.791	0.101	0.450	0.444	0.752	0.492	0.656	0.320
Carnitine	r	-0.044	-0.120	0.075	-0.011	-0.023	0.095	-0.011	-0.101	-0.107	-0.072	0.102	0.146	0.036	-0.088	0.062	0.003	0.003
	p	0.612	0.165	0.382	0.900	0.788	0.273	0.896	0.240	0.216	0.404	0.239	0.091	0.680	0.307	0.473	0.977	0.976
Creatine	r	0.035	0.048	0.010	-0.014	0.037	0.040	0.063	-0.082	-0.004	-0.023	0.079	0.074	0.098	-0.014	-0.090	0.010	-0.049
	p	0.688	0.577	0.907	0.869	0.667	0.646	0.468	0.345	0.963	0.791	0.358	0.392	0.255	0.869	0.297	0.912	0.568

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Dimethylamine	r	-0.094	-0.166	0.052	-0.053	-0.068	0.055	-0.066	-0.142	-0.079	-0.056	0.056	0.104	-0.053	0.081	0.121	0.134	0.060
	p	0.275	0.053	0.550	0.536	0.432	0.523	0.448	0.099	0.363	0.519	0.514	0.228	0.540	0.347	0.159	0.121	0.487
Dimethylglycine	r	-0.160	-0.078	-.182*	0.008	-.199*	0.009	0.004	-0.108	0.003	-0.040	0.051	-0.033	-0.145	-.188*	-0.071	-0.045	-0.091
	p	0.062	0.365	0.034	0.925	0.020	0.916	0.967	0.212	0.976	0.641	0.559	0.703	0.091	0.029	0.411	0.605	0.293
Citrate	r	.208*	0.153	.174*	0.019	.190*	0.113	0.109	0.072	0.056	0.135	-0.061	-0.023	0.043	0.029	0.020	-.186*	-.189*
	p	0.015	0.075	0.043	0.828	0.027	0.190	0.206	0.402	0.517	0.117	0.483	0.790	0.623	0.736	0.819	0.030	0.027
Choline	r	0.013	-0.071	0.130	0.021	0.019	0.080	0.075	-0.080	-0.064	-0.051	0.149	.258**	0.095	0.000	-0.037	0.052	-0.016
	p	0.876	0.412	0.132	0.812	0.824	0.354	0.388	0.356	0.461	0.552	0.083	0.002	0.270	0.996	0.666	0.551	0.853
Ethanol	r	-0.010	0.051	-0.080	-0.034	0.008	-0.014	0.114	0.049	-0.055	0.034	0.039	0.011	0.128	-0.055	-0.021	-0.091	-0.145
	p	0.907	0.556	0.356	0.694	0.924	0.874	0.188	0.572	0.524	0.695	0.649	0.899	0.137	0.522	0.809	0.294	0.091
L- Proline	r	0.010	-0.055	0.077	-0.009	0.039	0.121	-0.014	0.002	-0.008	0.056	0.107	0.041	-0.080	0.042	-0.060	-0.016	-0.077
	p	0.906	0.525	0.372	0.916	0.652	0.160	0.867	0.979	0.930	0.517	0.213	0.634	0.356	0.629	0.487	0.857	0.374
L-Threonine	r	-0.049	-0.059	-0.004	-0.093	-0.078	-0.112	0.001	-0.062	-0.048	0.003	-0.162	-0.077	0.063	-0.106	0.035	0.057	0.102
	p	0.570	0.493	0.965	0.280	0.370	0.196	0.993	0.476	0.582	0.972	0.060	0.373	0.468	0.220	0.683	0.507	0.235
L-Asparagine	r	0.038	-0.018	0.123	0.036	0.069	0.045	0.034	0.042	-0.037	0.078	-0.005	0.115	0.025	-0.023	-0.029	-0.113	-0.087
	p	0.663	0.831	0.155	0.680	0.422	0.605	0.693	0.627	0.671	0.370	0.953	0.181	0.772	0.793	0.736	0.189	0.313
D-Glucose	r	0.100	0.013	0.165	-0.057	0.091	0.033	0.059	-0.006	-0.063	-0.107	0.162	0.047	0.063	0.043	-0.113	0.021	-0.053
	p	0.247	0.881	0.054	0.513	0.293	0.703	0.494	0.949	0.467	0.216	0.059	0.589	0.469	0.622	0.190	0.809	0.537
Glycine	r	-0.071	-0.163	0.091	0.058	-0.034	0.023	-0.007	-0.080	.210*	0.003	-0.033	-0.070	-.238**	-0.063	.178*	-0.046	-0.073
	p	0.415	0.057	0.290	0.501	0.699	0.794	0.934	0.352	0.014	0.977	0.706	0.419	0.005	0.464	0.039	0.592	0.396
Glycerol	r	-0.086	-.187*	0.123	0.021	-0.055	0.061	-0.028	-0.120	.175*	0.011	-0.021	-0.028	-.220*	-0.047	.185*	-0.013	-0.036
	p	0.320	0.030	0.153	0.806	0.523	0.477	0.745	0.162	0.041	0.894	0.810	0.742	0.010	0.589	0.031	0.882	0.680
Fumaric acid	r	0.093	0.004	0.148	-0.134	0.051	0.047	0.034	-0.103	-0.001	0.031	-0.085	0.157	0.112	0.032	0.004	0.051	0.009
	p	0.282	0.964	0.085	0.121	0.554	0.585	0.690	0.233	0.994	0.719	0.326	0.068	0.195	0.712	0.963	0.555	0.919
Formate	r	0.009	-0.026	0.093	0.084	0.040	0.084	0.123	-0.083	0.049	0.005	0.035	0.057	0.065	0.013	-0.031	0.018	0.008
	p	0.914	0.767	0.282	0.332	0.645	0.329	0.155	0.339	0.574	0.952	0.683	0.513	0.455	0.883	0.723	0.839	0.927
L-Glutamic acid	r	-0.090	-0.150	0.014	0.040	-0.010	0.048	-0.065	-0.034	-.190*	-0.129	0.127	.190*	-0.089	0.038	-0.006	0.027	-0.060
	p	0.297	0.082	0.872	0.644	0.908	0.578	0.449	0.275	0.027	0.135	0.142	0.026	0.304	0.661	0.941	0.759	0.490
Hypoxanthine	r	0.045	0.055	0.039	0.115	0.086	-0.089	0.093	0.018	0.003	0.038	0.061	-0.081	0.001	-0.021	-0.084	0.106	0.153
	p	0.607	0.527	0.654	0.183	0.317	0.304	0.280	0.831	0.974	0.662	0.482	0.348	0.995	0.813	0.331	0.221	0.076
Tyrosine	r	0.102	0.081	0.104	0.084	0.147	0.113	0.001	0.104	0.064	0.073	0.063	0.069	0.072	.170*	0.005	-0.110	-0.138
	p	0.237	0.348	0.228	0.332	0.087	0.191	0.993	0.230	0.461	0.400	0.467	0.422	0.404	0.048	0.951	0.204	0.110
L-Phenylalanine	r	-0.032	-0.087	0.101	0.096	0.017	0.077	0.033	-.187*	-0.059	-0.078	0.102	0.149	0.060	0.012	-0.067	0.007	-0.029
	p	0.708	0.314	0.243	0.268	0.844	0.372	0.701	0.030	0.498	0.364	0.237	0.084	0.485	0.892	0.440	0.932	0.737
LAlanine	r	-0.013	-0.070	0.051	0.045	0.037	0.058	-0.032	0.089	-0.009	0.014	0.065	0.109	-0.060	0.070	-0.035	-0.022	-0.031
	p	0.876	0.418	0.555	0.605	0.670	0.503	0.710	0.305	0.914	0.869	0.454	0.208	0.488	0.418	0.682	0.797	0.718
Mannose	r	-.257**	-.254**	-0.103	-0.023	-.252**	-0.064	-0.079	-0.125	0.017	-0.023	0.098	-0.004	-0.140	-.209*	0.095	-0.133	-0.039
	p	0.002	0.003	0.234	0.793	0.003	0.462	0.358	0.146	0.840	0.789	0.255	0.964	0.103	0.015	0.272	0.121	0.649
Isoleucine	r	0.046	-0.043	0.127	0.016	0.077	-0.024	0.042	0.012	-0.149	-0.054	0.046	0.093	0.028	0.010	-0.162	0.006	-0.063
	p	0.596	0.618	0.140	0.853	0.372	0.781	0.626	0.890	0.084	0.532	0.592	0.283	0.749	0.904	0.060	0.944	0.469
L-Histidine	r	0.076	-0.056	0.155	-0.029	0.029	-0.016	-0.160	-0.029	-.203*	0.099	-0.048	0.042	0.038	-0.081	-0.087	-0.022	-0.088
	p	0.379	0.516	0.071	0.739	0.741	0.857	0.062	0.741	0.018	0.249	0.576	0.628	0.660	0.348	0.312	0.796	0.309
L-Lysine	r	0.014	-0.080	0.148	0.054	0.035	0.114	-0.020	-0.058	0.025	0.016	0.123	0.015	0.026	0.028	-0.027	0.026	0.016
	p	0.868	0.356	0.086	0.535	0.686	0.186	0.816	0.502	0.775	0.853	0.152	0.859	0.768	0.745	0.753	0.763	0.856
L-Serine	r	-.213*	-.184*	-0.075	-0.047	-.220**	-0.089	-0.083	-0.020	-0.126	-0.023	0.033	0.051	-0.053	-0.108	-0.017	0.016	0.095
	p	0.013	0.032	0.387	0.588	0.010	0.305	0.337	0.819	0.144	0.791	0.699	0.559	0.543	0.212	0.845	0.850	0.273
L-Lactic acid	r	-0.058	-0.150	0.098	0.012	-0.004	0.028	0.033	-0.131	-0.143	-0.149	0.103	.250**	0.003	0.065	-0.040	-0.050	-0.083
	p	0.503	0.080	0.256	0.888	0.960	0.745	0.702	0.129	0.096	0.083	0.235	0.003	0.973	0.452	0.640	0.566	0.338
Aspartate	r	-0.142	-.189*	0.045	-0.072	-0.121	0.035	-0.071	-.178*	-0.059	-0.004	-0.055	0.125	-0.019	-0.063	-0.072	0.055	0.047
	p	0.100	0.028	0.599	0.405	0.159	0.682	0.411	0.038	0.495	0.964	0.526	0.147	0.828	0.467	0.402	0.522	0.583
Myo-inositol	r	-0.122	-0.163	-0.016	-0.123	-0.161	0.021	-0.052	-.210*	-0.146	-0.140	0.100	.186*	0.005	-0.037	0.019	0.034	0.106
	p	0.157	0.059	0.854	0.153	0.061	0.810	0.547	0.014	0.091	0.105	0.249	0.030	0.956	0.671	0.826	0.695	0.220
L-Ornithine	r	0.004	-0.021	0.036	0.084	0.033	0.121	0.062	-0.061	0.088	0.063	-0.032	-0.049	0.060	0.075	-0.087	-0.054	-0.089

	p	0.964	0.810	0.682	0.329	0.706	0.162	0.471	0.479	0.306	0.465	0.710	0.572	0.484	0.388	0.314	0.529	0.306
	r	-.192*	-.222**	-0.049	-0.058	-0.152	0.025	-0.086	-.192*	-0.128	-0.30**	0.134	.224**	-0.111	-0.088	-0.093	-0.047	-0.156
Pyruvate	p	0.025	0.009	0.568	0.505	0.077	0.776	0.317	0.025	0.137	0.000	0.119	0.009	0.199	0.308	0.282	0.588	0.069
	r	0.039	0.005	0.076	0.138	0.104	0.046	0.134	-0.037	-0.036	0.095	0.038	0.090	0.036	0.099	0.073	-0.009	0.007
Succinate	p	0.650	0.953	0.379	0.110	0.228	0.592	0.121	0.669	0.676	0.270	0.661	0.299	0.680	0.252	0.399	0.913	0.932
	r	0.024	-0.049	0.104	0.126	0.096	0.045	0.105	0.005	0.007	0.126	-0.021	0.031	-0.023	0.132	0.116	-0.034	-0.025
Pyroglutamic acid	p	0.778	0.572	0.229	0.145	0.266	0.600	0.225	0.949	0.935	0.144	0.804	0.722	0.793	0.125	0.181	0.691	0.769
	r	-0.002	-0.079	0.134	-0.024	0.015	-0.041	-0.049	-0.063	0.054	0.052	-.208*	-0.006	0.010	-0.048	-0.110	0.095	0.134
Sarcosine	p	0.985	0.362	0.119	0.781	0.858	0.638	0.569	0.465	0.529	0.548	0.015	0.946	0.905	0.576	0.203	0.272	0.120
	r	0.002	0.037	-0.082	0.095	0.053	-0.100	0.086	0.067	0.036	0.093	-0.121	-0.004	0.107	0.027	-0.066	0.058	0.098
Xanthine	p	0.986	0.673	0.343	0.269	0.541	0.249	0.322	0.438	0.676	0.282	0.162	0.964	0.215	0.757	0.446	0.502	0.257
	r	0.036	0.026	0.061	0.132	0.124	-0.019	0.039	0.030	-0.115	-0.026	-0.076	0.105	0.121	-0.145	-0.084	-0.105	-0.135
Urea	p	0.678	0.763	0.481	0.126	0.151	0.823	0.652	0.733	0.181	0.761	0.378	0.222	0.162	0.091	0.333	0.224	0.116
	r	-0.073	-0.057	0.024	-0.027	-0.067	0.060	0.168	-0.044	-0.001	0.027	0.106	0.074	0.004	-0.004	0.060	-0.034	-0.064
3-Hydroxybutyric acid	p	0.397	0.509	0.778	0.758	0.439	0.489	0.051	0.614	0.990	0.758	0.221	0.390	0.961	0.965	0.489	0.694	0.456
	r	-0.021	-.180*	.198*	0.029	-0.014	0.162	-0.029	-0.043	-0.030	-0.136	0.061	0.094	-0.086	0.059	0.124	0.022	-0.031
3-Methylhistidine	p	0.811	0.036	0.021	0.740	0.875	0.060	0.737	0.621	0.732	0.115	0.482	0.274	0.318	0.495	0.151	0.797	0.720
	r	-0.067	-0.023	-0.076	0.166	0.000	-0.024	0.006	-0.051	-0.039	0.067	-0.020	0.022	-0.099	-0.074	-0.051	-0.059	0.007
L-Arginine	p	0.441	0.791	0.379	0.054	0.997	0.779	0.949	0.555	0.649	0.438	0.813	0.803	0.252	0.393	0.557	0.497	0.932
	r	0.068	-0.031	0.139	0.028	0.114	0.100	-0.023	0.027	0.002	0.052	0.044	0.097	0.045	-0.005	-0.097	0.017	-0.081
Creatinine	p	0.429	0.716	0.106	0.751	0.186	0.245	0.794	0.753	0.982	0.546	0.614	0.260	0.599	0.951	0.263	0.846	0.348
	r	0.049	0.017	0.032	.303**	.175*	-0.089	0.122	-0.030	-0.051	0.012	-0.090	-0.035	0.014	-0.105	0.083	-.199*	-0.127
L-Glutamine	p	0.574	0.848	0.715	0.000	0.041	0.302	0.157	0.731	0.553	0.889	0.299	0.683	0.868	0.225	0.335	0.020	0.139
	r	-0.013	-0.077	0.099	0.046	0.035	0.056	0.065	-0.096	-0.121	-0.056	0.061	0.128	0.063	0.002	-0.085	0.035	-0.005
L-Leucine	p	0.878	0.375	0.252	0.595	0.690	0.516	0.451	0.265	0.161	0.516	0.477	0.138	0.469	0.978	0.323	0.687	0.957
	r	0.089	-0.026	.185*	-0.109	0.058	0.132	0.023	0.068	0.003	0.133	0.019	0.054	0.056	0.069	-0.120	-0.043	-0.104
Malonate	p	0.305	0.763	0.031	0.208	0.499	0.126	0.789	0.429	0.972	0.122	0.822	0.531	0.515	0.422	0.165	0.623	0.229
	r	0.007	-0.050	0.112	0.133	0.057	0.104	0.118	-0.076	-0.013	-0.030	0.100	0.099	0.065	0.060	-0.034	-0.003	-0.023
Methionine	p	0.931	0.563	0.195	0.121	0.512	0.229	0.172	0.377	0.880	0.727	0.247	0.251	0.451	0.491	0.694	0.974	0.789
	r	0.040	-0.021	0.077	-0.108	0.015	-0.063	0.077	0.004	-0.034	0.013	-0.121	0.109	.196*	-0.095	-0.137	0.092	0.107
Hippuric acid	p	0.642	0.806	0.371	0.212	0.860	0.468	0.371	0.960	0.697	0.881	0.162	0.208	0.022	0.274	0.113	0.288	0.213
	r	-0.096	-.173*	0.072	0.048	-0.062	-0.085	0.010	-0.104	-0.166	-0.086	-0.053	0.017	-0.152	-0.084	-0.075	-0.039	-0.001
Isovaleric acid	p	0.265	0.044	0.402	0.582	0.475	0.327	0.906	0.226	0.053	0.317	0.542	0.841	0.077	0.328	0.384	0.654	0.986
	r	0.008	0.002	0.038	0.035	0.011	-.196*	-0.063	-0.020	0.016	0.099	-.270**	-0.123	0.132	-0.155	-0.077	0.059	0.078
3-Hydroxyisovalericacid	p	0.930	0.986	0.659	0.689	0.900	0.022	0.470	0.817	0.849	0.252	0.002	0.155	0.125	0.072	0.373	0.495	0.364
	r	-0.111	-0.029	-0.098	-0.062	-0.158	-0.002	0.075	-0.055	0.002	-0.066	0.113	.175*	0.091	-0.052	0.073	-0.026	-0.032
Isopropyl alcohol	p	0.199	0.734	0.254	0.470	0.066	0.982	0.383	0.528	0.979	0.445	0.189	0.041	0.291	0.546	0.397	0.763	0.715
	r	0.083	-0.020	.197*	0.020	0.106	0.125	-0.019	-0.011	-0.002	0.000	0.081	0.094	0.008	0.088	-0.044	-0.028	-0.047
Valine	p	0.340	0.817	0.022	0.813	0.219	0.147	0.830	0.901	0.982	0.998	0.350	0.279	0.927	0.306	0.609	0.749	0.585
	r	-0.135	-0.051	-0.078	0.079	-0.098	-0.160	0.154	-0.140	-0.098	-0.002	0.012	0.011	0.060	-0.106	-0.054	0.083	0.060
Tryptophan	p	0.117	0.557	0.364	0.360	0.255	0.063	0.073	0.104	0.254	0.982	0.886	0.896	0.487	0.218	0.532	0.340	0.486
	r	0.017	-0.044	0.161	0.011	0.035	0.111	0.153	-0.094	0.099	0.083	0.103	0.077	0.077	0.061	0.109	-0.024	-0.051
Acetone	p	0.845	0.611	0.062	0.895	0.689	0.199	0.075	0.276	0.252	0.339	0.234	0.372	0.375	0.478	0.204	0.785	0.556
	r	0.006	0.004	0.042	0.088	0.070	-0.082	0.091	0.019	-0.050	-0.097	0.016	0.163	0.103	-0.110	-0.088	-.181*	-.213*
Isobutyric acid	p	0.949	0.966	0.626	0.310	0.417	0.346	0.292	0.827	0.561	0.263	0.849	0.058	0.231	0.203	0.307	0.035	0.013
	r	0.040	0.062	-0.027	0.076	0.054	0.110	0.139	-0.134	0.011	-0.042	0.147	0.037	0.071	-0.067	-0.064	0.002	-0.090
Methanol	p	0.647	0.471	0.756	0.377	0.532	0.203	0.107	0.120	0.896	0.631	0.087	0.668	0.412	0.435	0.462	0.983	0.298
	r	0.060	0.060	0.083	0.091	0.089	0.001	0.079	-0.045	0.005	-0.056	-0.002	0.121	-0.002	-0.116	-0.029	0.006	-0.008
Propyleneglycol	p	0.486	0.487	0.339	0.294	0.301	0.993	0.364	0.601	0.954	0.518	0.980	0.159	0.982	0.178	0.740	0.947	0.929
	r	-0.081	-0.113	0.015	.193*	0.010	-0.059	0.060	0.023	0.050	0.017	0.050	-0.069	0.015	-0.105	0.079	-0.050	-0.063
Dimethylsulfone	p	0.349	0.192	0.866	0.024	0.905	0.496	0.485	0.793	0.563	0.848	0.562	0.425	0.859	0.224	0.363	0.561	0.468

**Table S7.** 14-point criteria used to measure adherence to MD on the MEDDINI study.14 POINT MEDITERRANEAN DIET SCORE (MDS).

Questions.		Criteria for 1 point
1.	Do you use olive oil or rapeseed oil as your main cooking fat?	Yes
2.	Do you use olive or rapeseed oil-based spreads (e.g. Golden olive, Olivio, Bertolli)?	Yes ≥ 4 tbsp oil / day
3.	How much olive/ rapeseed oil do you consume in a given day? Including oil used for frying, salads, out-of-house meals etc (in tablespoons) How much olive or rapeseed oil-based spread do you consume in a given day? (in teaspoons)	and/or 3 tsp spread/ day
4.	How many portions of fruit (including natural fruit juices) do you consume per day? (1 portion = 1 apple/banana (80g), small glass juice (150ml)	≥ 2 portions/ day
5.	How many vegetable servings do you consume per day? Including raw/ cooked vegetables, salad but not including potatoes (1 serving: 3 tablespoons/80g)	≥ 3 portions/ day
6.	How many servings of legumes (peas, beans and lentils including kidney beans, baked beans, chickpeas, red lentils etc) do you consume per week? (1 serving :3 tablespoons/ 80g)	≥ 3 servings/ week
7.	How many servings of red meat including beef, pork, lamb and minced beef do you consume per week? (1 serving: medium portion/ 100–150 g)	≤ 2 servings /week
8.	How many servings of processed meat including ham, bacon, sausages, meat pies and other meat products etc.) do you consume per week? (1 serving: medium portion/ 100–150 g)	≤ 1 serving / week
9.	How many servings of chicken/ turkey do you consume per week? (1 serving: medium portion/ 100-150g)	2 servings /week
10.	How many servings of fish (tuna, cod, haddock, salmon, mackerel, herring, and sardines etc, including tinned varieties, excluding crumbed or battered fish) or shellfish do you consume per week? (1 serving: 1 fillet/small fish or 140g)	≥ 3 servings /week
11.	Do you preferentially consume wholegrain bread and/ or cereal and/ or rice and/ or pasta instead of non-wholegrain (white) varieties?	Yes
12.	How many servings of natural nuts do you consume per week? (1 serving: 1 small handful/ 30 g)	≥ 3 servings /week
13.	How many times per week do you consume sweet foods (including biscuits, buns, pastries, chocolate, sweets, sweet or carbonated drinks or desserts)?	≤ 3 times/ week
14.	How often would you consume up to 3 small glasses of wine or equivalent other alcoholic beverages per week? (1 small glass:125ml)	1–3 glasses or equivalent ≥ 3 days/ week