Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supporting Information

^{1}H NMR-Based Metabolomic Profiling of Diabetes and BMI-Related Changes in the Serum of South-Asian Population

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Figure S1

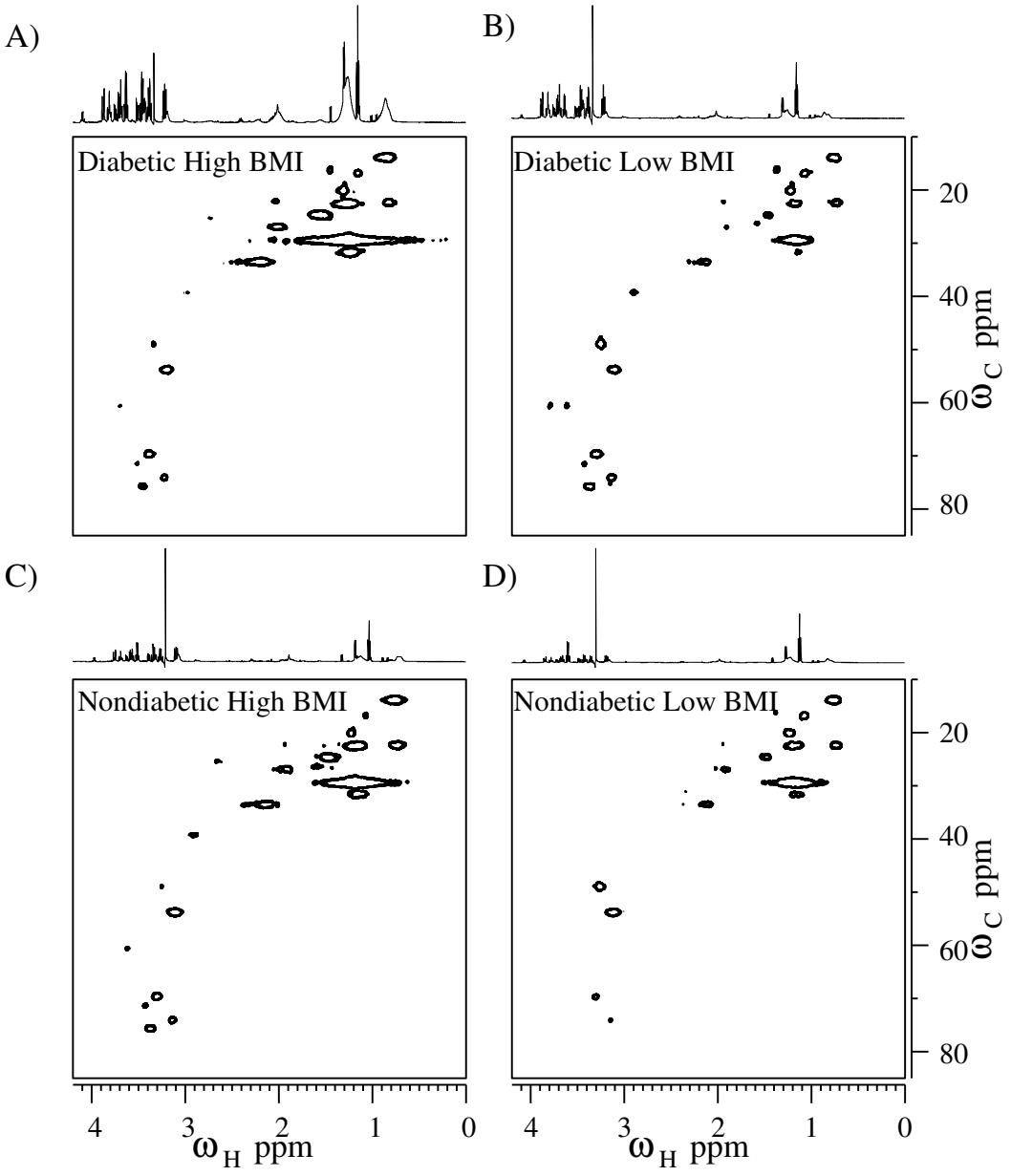

Figure 1: 2D HSQC NMR spectrum of (A) Diabetic-High BMI, (B) Diabetic-Low BMI, (C) Non diabetic-High BMI and (D) Non diabetic-Low BMI subjects, recorded at 600 MHz

Figure S2

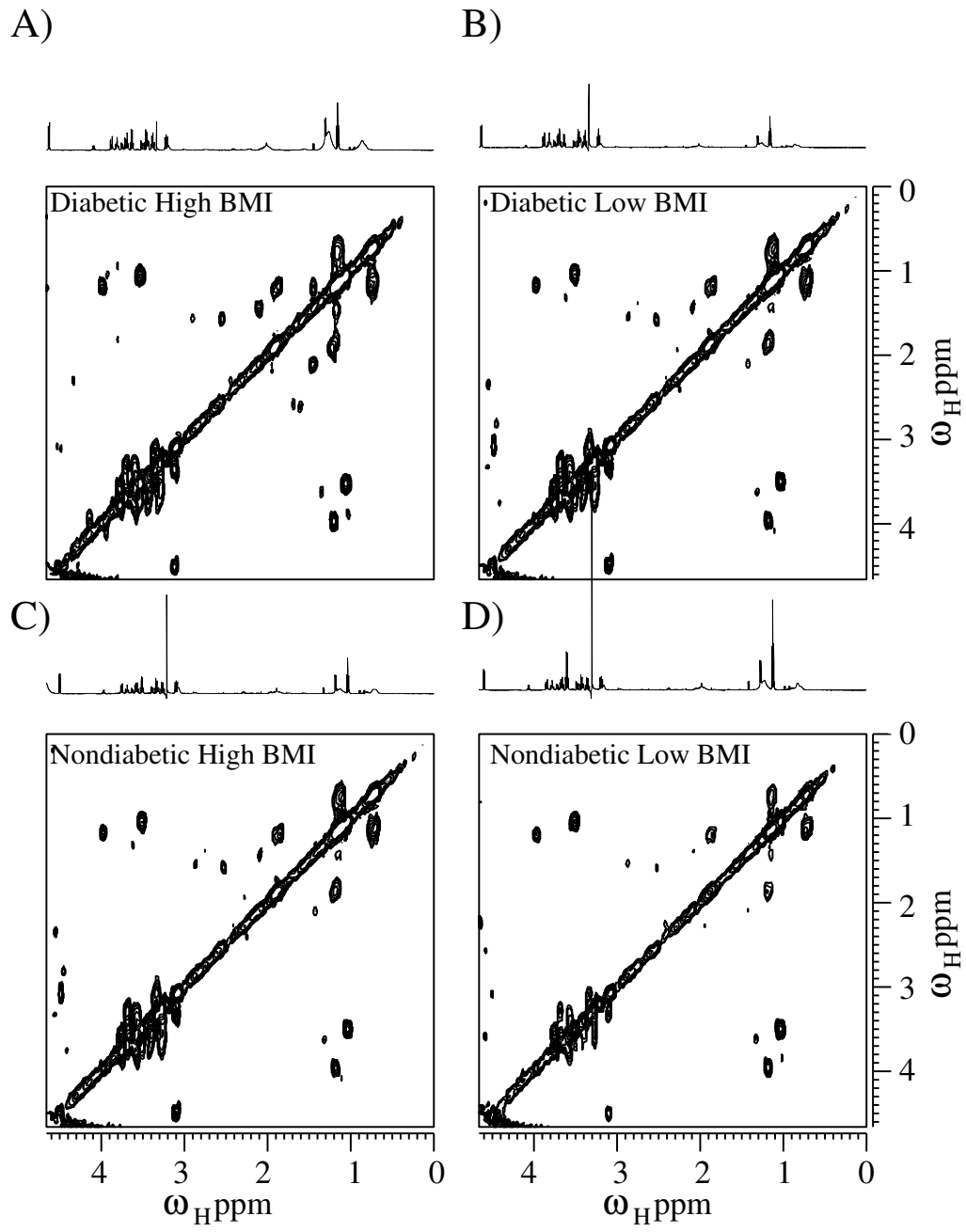

Figure 2: 2D COSY NMR spectrum of (A) Diabetic-High BMI, (B) Diabetic-Low BMI, (C) Non diabetic-High BMI and (D) Non diabetic-Low BMI subjects, recorded at 600 MHz

Table ST1

Metabolite	Chemical shift (ppm)	Identified by	Metabolite	Chemical shift (ppm)	Identified by
Amino acids			**Keto acids**		
Isoleucine	0.94	1D,2D	Ketoleucine	2.12	1D
Valine	0.98	1D, 2D	Pyruvic acid	2.46	1D
Alloisoleucine	1.29	1D	Amino-levulinic acid	2.77	1D
Alanine	1.47	1D	Acetoacetic acid	3.43	1D
Lysine	1.68	1D, 2D	**Lipids**		
Acetylglycine	2.05	1D	Lipid terminal methyl	0.91	1D, 2D
Glutamate	2.12	1D	Lipid backbone methylene groups	1.31	1D, 2D
Ketoleucine	2.13	1D	**Sphingolipids**		
Glutamine	2.14,2.44	1D, 2D	Sphinganine	1.54	1D
Asparagine	2.86	1D, 2D	**Bile acids**		
Creatine	3.03	1D	Chenodeoxycholic acid	1.49	1D
Phenylalaine	3.30	1D, 2D	**Hydroxy acids**		
Proline	3.33	1D	3-hydroxybutyric acid	1.19, 1.20	1D
Glycine	3.54	1D	**Vitamins**		
Threonine	3.58	1D. 2D	Pantothenic acid	3.43	1D, 2D
Leucine	3.73	1D, 2D	**Purines and purine derivatives**		
Serine	3.83	1D	3,7-dimethyluric acid	3.35	1D, 2D
Ureidopropionic acid	3.28	1D	**Fatty acids**		
Tyrosine	6.87, 7.17	1D	Acetic acid	1.91	1D
Histidine	7.05, 7.73	1D, 2D	Isovaleric acid	1.95	1D
Hydroxy acids			**Sugars**		
Lactic acid	1.33, 4.12	1D, 2D	Ribose	2.21	1D
Glycolic acid	3.94	1D	Glycogen	3.71	1D, 2D
Galactonic acid	3.95	1D	Fucose	3.75	1D
Dicarboxylic acids			Galactose	3.85	1D
Oxalacetic acid	2.38	1D	Fructose	3.90	1D
Oxalglutaric acid	2.44	1D	Sucrose	4.22	1D, 2D
Sugar alcohols			beta-glucose	4.63	1D, 2D
Ribitol	3.65	1D	Trehalose	4.64	1D
Sorbitol	3.75	1D, 2D	alpha-glucose	5.14	1D, 2D
Glycerol	3.78	1D, 2D	**Others**		
Arabitol	3.84	1D	Choline	3.19	1D, 2D
			Myoinositol	3.49	1D, 2D

Table 1: List of various metabolites and their NMR chemical shift values and types of NMR experiments used for metabolite fingerprinting of serum samples.

Table ST2

Metabolite	p-value	-log10(p)	FDR	Fisher's LSD
Choline	0.00001167	4.9329	0.00015673	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Proline	0.00001783	4.7486	0.00020960	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
3,7-dimethyl uric acid	0.00002135	4.6707	0.00021093	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Glucose	0.00002468	4.6076	0.00021093	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Pantothenic acid	0.000030465	4.5162	0.00023860	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Glycerol	0.000061967	4.2078	0.00044807	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Histidine	0.0000839	4.0758	0.00056393	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
3-OH butyric acid	0.00065025	3.1869	0.0040749	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Leucine	0.0006964	3.1571	0.0040913	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Sorbitol	0.0043542	2.3611	0.024076	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Myoinositol	0.0049209	2.308	0.025336	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Threonine	0.0051211	2.2906	0.025336	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Isoleucine	0.0096155	2.017	0.044039	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Lysine	0.0098384	2.0071	0.044039	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Saturated fatty acids	0.011722	1.931	0.050084	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Lactate	0.013404	1.8728	0.054782	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Valine	0.024974	1.6025	0.086948	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Phenylalanine	0.029161	1.5352	0.097898	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI
Glutamine	0.045682	1.3403	0.14314	D-HighBMI - ND-LowBMI D-LowBMI - ND-LowBMI

Table 2: Post hoc analysis showing which groups are different given the p value threshold of 0.05, for Diabetic-High BMI, Diabetic-Low BMI and Non diabetic-Low BMI subjects.

Table ST3

Metabolite	p-value	-log10(p)	FDR	Fisher's LSD
Choline	0.00006154	4.2108	0.001919	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
3,7-dimethyl uric acid	0.00008284	4.0818	0.001919	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
Proline	0.00009955	4.0019	0.001919	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
Pantothenic acid	0.0001021	3.9911	0.001919	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
Sorbitol	0.0006173	3.7763	0.002622	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
Glucose	0.0004403	3.3562	0.0059127	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
Glycerol	0.001680	2.7747	0.01754	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
Myoinositol	0.002050	2.6882	0.019274	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
Histidine	0.0031308	2.5043	0.026754	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
Leucine	0.0039119	2.4076	0.029835	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
3-OH butyric acid	0.005139	2.2891	0.034505	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
Threonine	0.0065635	2.1829	0.040789	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
Lysine	0.0069429	2.1585	0.040789	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI
Isoleucine	0.0094388	2.0251	0.052191	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI ND-HighBMI-ND-LowBMI
Saturated fatty acids	0.01303	1.8851	0.068046	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI ND-HighBMI-ND-LowBMI
Lactate	0.017685	1.7524	0.083122	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI ND-HighBMI-ND-LowBMI
Valine	0.035391	1.4511	0.12795	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI ND-HighBMI-ND-LowBMI
Phenylalanine	0.040621	1.3913	0.14142	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI ND-HighBMI-ND-LowBMI
Glutamine	0.047726	1.3212	0.16022	D-HighBMI - ND-HighBMI D-HighBMI - ND-LowBMI

Table 3: Post hoc analysis showing which groups are different given the p value threshold of 0.05, for Diabetic-High BMI, Non diabetic-High BMI and Non diabetic-Low BMI subjects.