

Supporting Information

J. Chem. Metrol. X:X (202X) XX-XX

¹H NMR spectroscopy-based serum metabolomics analysis of iron deficiency anemia

Metin Demirel^{1,2*}, Ayse Zehra Gul¹, Fatmanur Koktasoglu¹, Halime Agac¹, Ahmet Ceyhan Goren³, Cumali Karatoprak⁴ and Sahabettin Selek¹

¹*Department of Medical Biochemistry, Bezmialem Vakif University Faculty of Medicine, Istanbul, Türkiye*

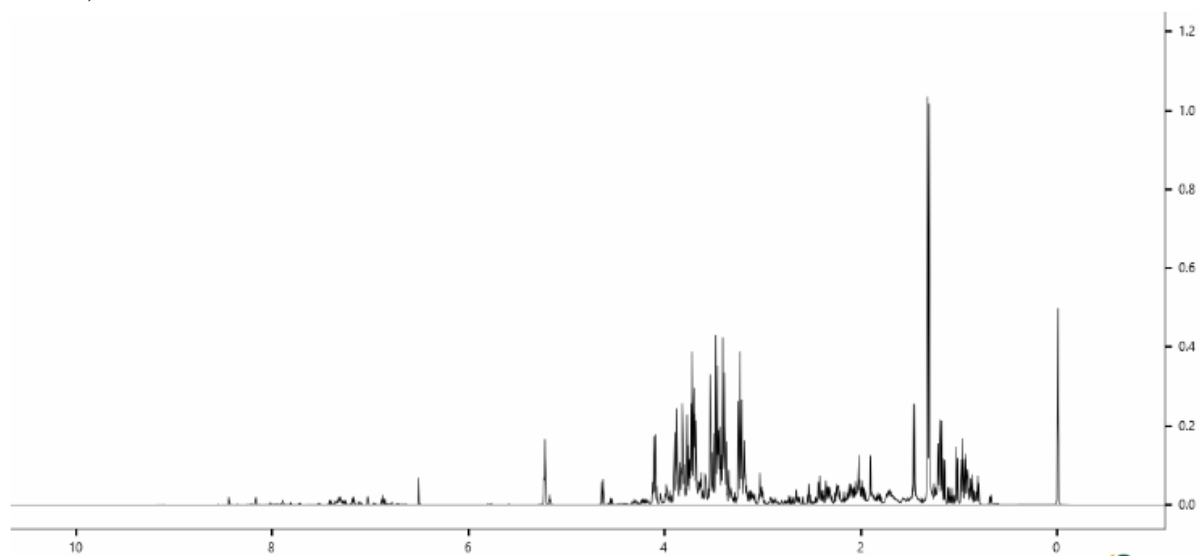
²*Health Sciences Institute, Bezmialem Vakif University, Istanbul, Türkiye*

³*Department of Chemistry, Gebze Technical University, Kocaeli, Türkiye*

⁴*Department of Internal Medicine, Bezmialem Vakif University Faculty of Medicine, Istanbul, Türkiye*

Table of Contents	Page
Figure S1: Typical representation of ¹ H NMR (NOESY and CPMG sequence) spectra	2
Figure S2: Typical representation of ¹ H NMR (NOESY and CPMG sequence) spectra A) Typical representation of ¹ H NMR NOESY of Control Serum B) CPMG sequence) spectra for a control serum CPMG) control: healthy individual	3
Table S1: Demographic and clinical laboratory analysis	4

A) IDA Serum-NOESY



B) IDA serum- CPMG

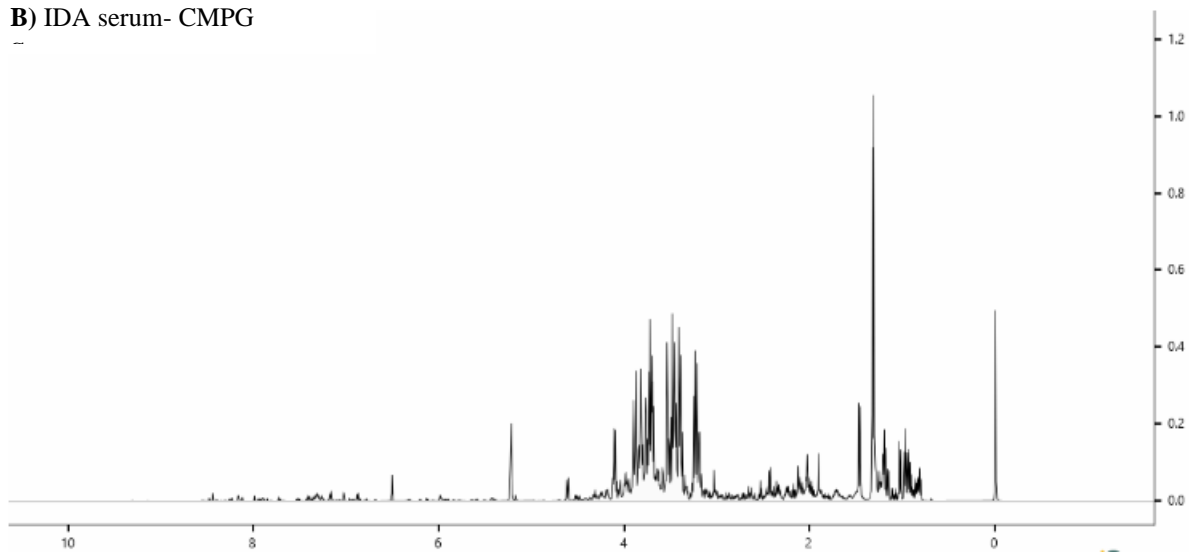


Figure S1: Typical representation of 1H NMR (NOESY and CPMG sequence) spectra **A)** IDA Serum-NOESY Sequence **B)** IDA serum- CPMG Sequence

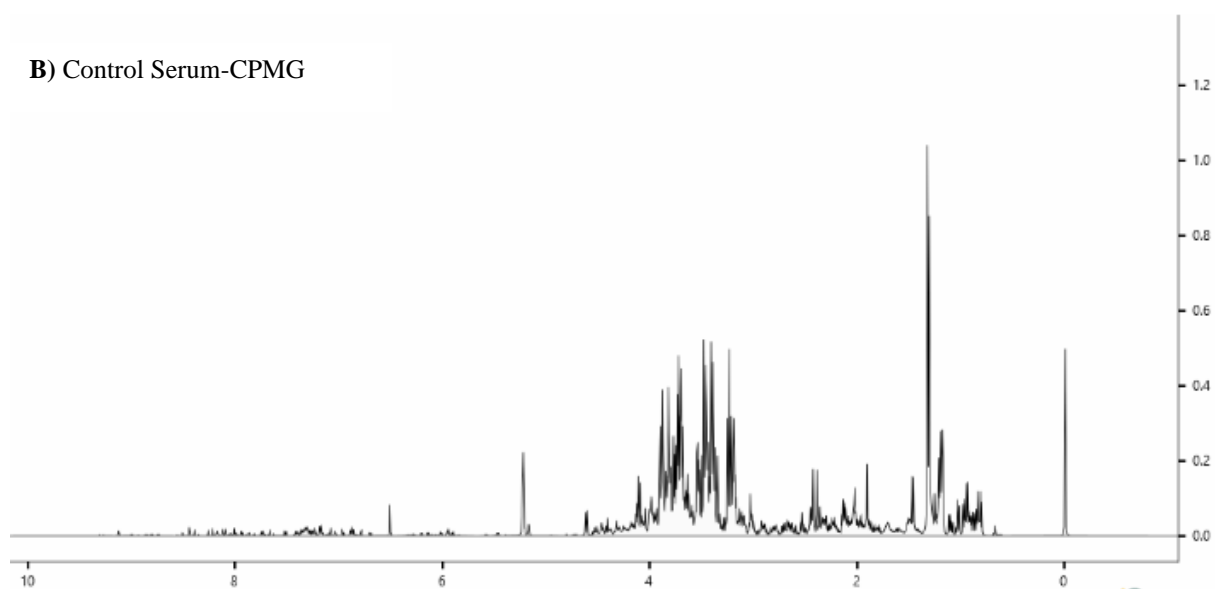
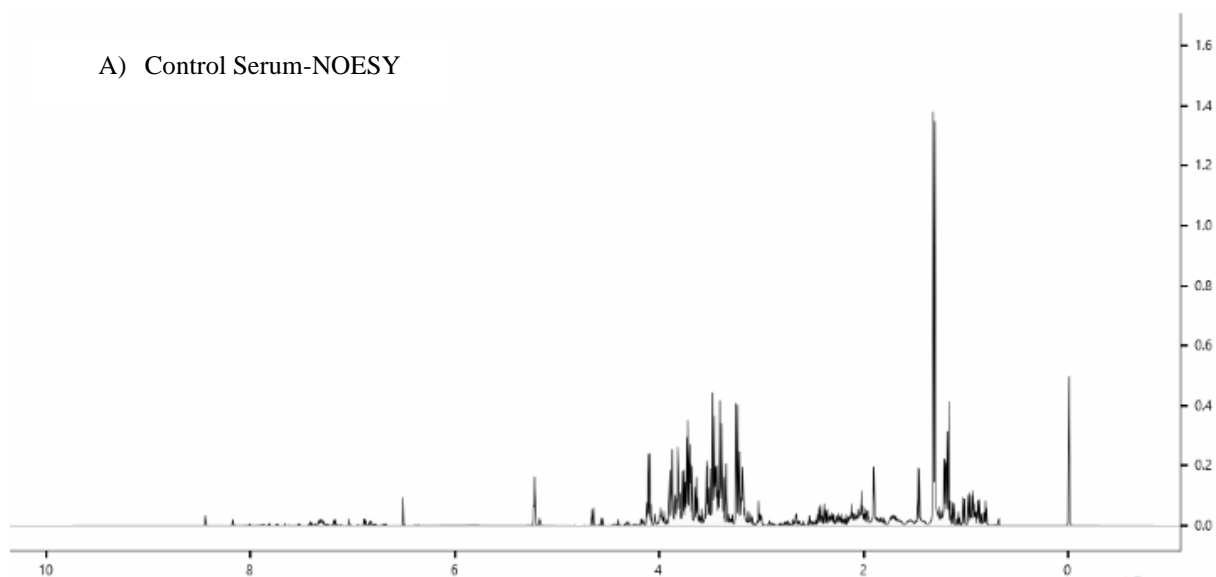


Figure S2: Typical representation of ¹H NMR (NOESY and CPMG sequence) spectra **A)** Typical representation of ¹H NMR NOESY of Control Serum **B)** CPMG sequence) spectra for a control serum CPMG) control: healthy individual

Table S1: Demographic and clinical laboratory analysis (Characteristics of individuals were shown as mean \pm standard deviation for continuous variables and as median (Md) with quartiles (pct) for discontinuous parameters (ns: nonsignificant; * $p < 0.001$ level of significance)).

	Iron Deficiency Anemia (Mean \pm SD; Median with 25 th -75 th percentiles)	Control (Mean \pm SD; Median with 25 th -75 th percentiles)	<i>p</i> Value
Age (year)	40 (Md); 33-49 (pct)	38 (Md); 27.5-49.5 (pct)	ns
BMI (kg/m²)	24.4 \pm 3.4	24.5 \pm 5.0	ns
Fasting glucose (mg/dL)	89.7 \pm 8.6	88.9 \pm 9	ns
Albumin (g/dL)	4.54 \pm 0.5	4.67 \pm 0.3	ns
Creatinine (mg/dL)	0.84 \pm 0.2	0.85 \pm 0.2	ns
Urea (mg/dL)	25.5 (Md); 18-33 (pct)	24 (Md); 18.8-28.5 (pct)	ns
Total protein (g/dL)	7.98 \pm 0.8	7.74 \pm 0.4	ns
Hemoglobin (mg/dL)	9.72 \pm 1.9	13.56 \pm 1.5	0.001*
Hematocrit (%)	31.44 \pm 5.3	40.66 \pm 3.8	0.001*
MCV (fL)	73.68 \pm 8.7	87.42 \pm 5.7	0.001*
RDW (%)	15.42 \pm 2.3	12.79 \pm 0.9	0.001*
Iron (μg/dL)	22 (Md); 14.5-29.5 (pct)	87 (Md); 71.5- 111.5 (pct)	0.001*
Ferritin (μg/dL)	3.2 (Md); 1.8-6.7 (pct)	38.1 (Md); 18.8-71.3 (pct)	0.001*
UIBC (μg/dL)	362.4 \pm 59.4	216.7 \pm 61	0.001*
TIBC (μg/dL)	387.49 \pm 61	311.27 \pm 51.1	0.001*