

Supplementary Information

Near-Infrared Combined with Mid-Infrared Spectroscopic Detection of Low-Molecular Weight Proteins in Human Serum Using Glycine as a Model Protein

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Spectral Analysis of spiked serum samples: ATR spectroscopy

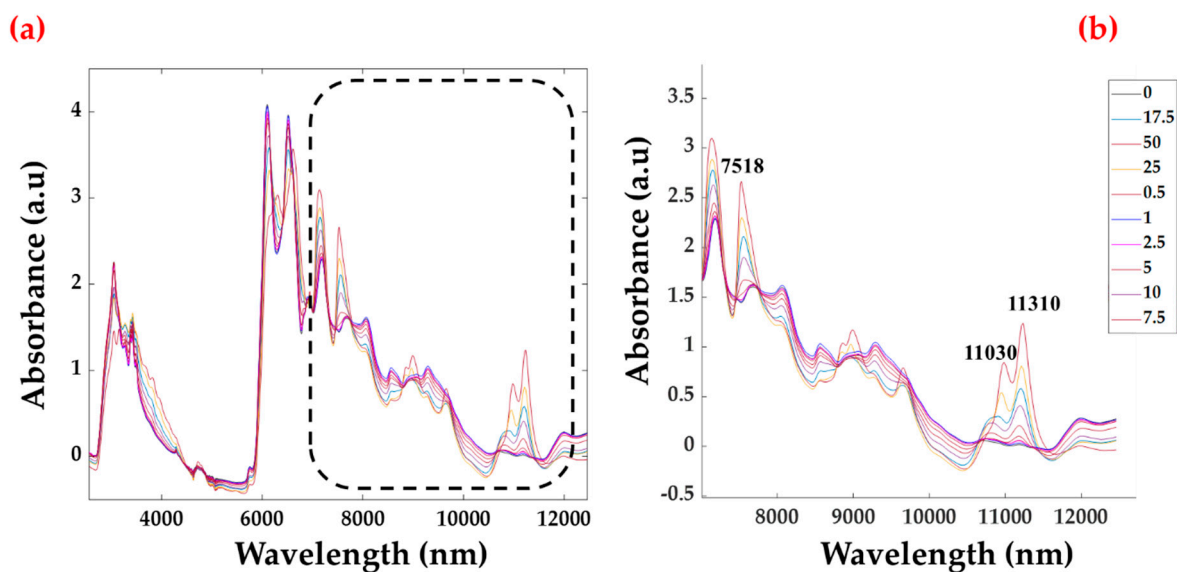
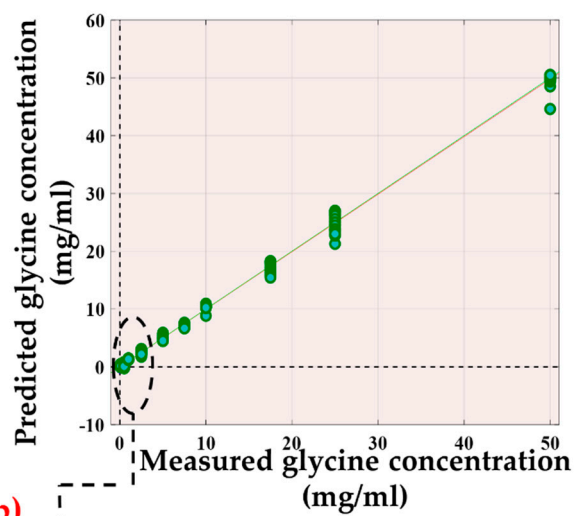
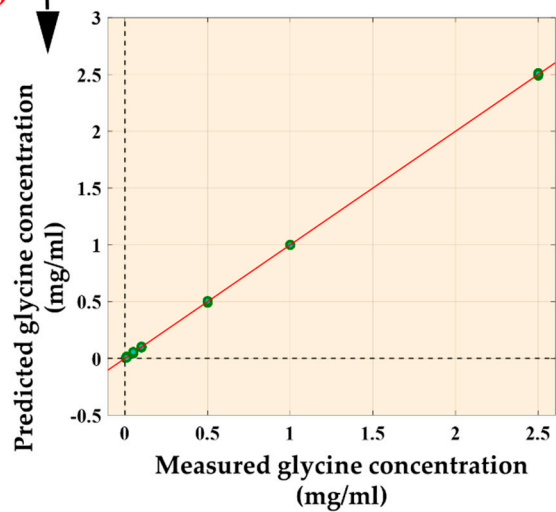


Figure S1. **a)** Baseline corrected raw spectra of glycine spiked human plasma samples. The concentration of glycine is ranging from 0 – 50 mg/ml. **b)** magnified view of 12000 – 7000 nm region where major contribution from glycine is observed.

(a)



(b)



(c)

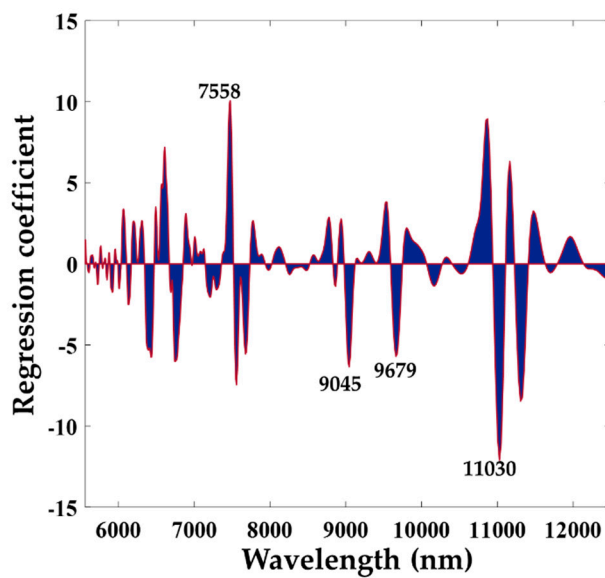


Figure S2. PLS – regression plot and its associated regression vector in the 12500 – 5555 nm region.

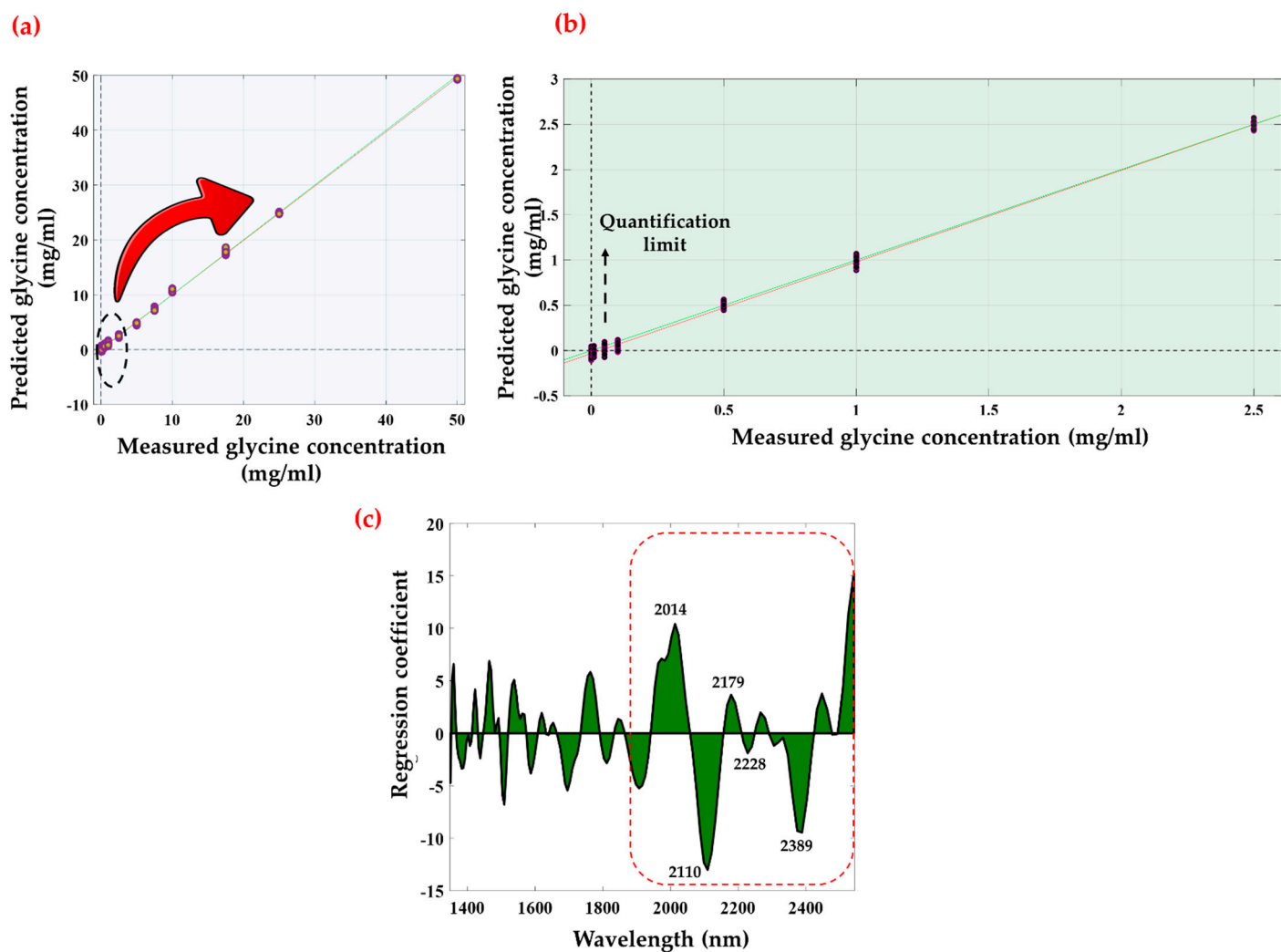


Figure S3. PLS – regression plot and its associated regression vector in the 2500 – 1350 nm region.

Table S1. Major band positions observed from the NIR and MIR spectra.

Band	Band Assignment
906 cm^{-1}	CH_2 rocking from glycine
1036 cm^{-1}	C–N stretching from glycine
1111 cm^{-1}	N–H ₃ rocking from glycine
1330 cm^{-1}	C H ₂ wagging from glycine
1414 cm^{-1}	O–C=O symmetric stretching from glycine from glycine
2055 nm	N–H stretch/amide Ib combination band
2110 nm	(N–H + C–H) combination band from glycine
2180 nm	N–H bend second overtone, C–H stretch/C=O stretch combination

	and C=O stretch/amide IIIb combination mode
2204 nm	combinations of (C-H and C-H) stretching modes from glycine
2375 nm	combinations of (C-H and C-H) stretching modes from glycine

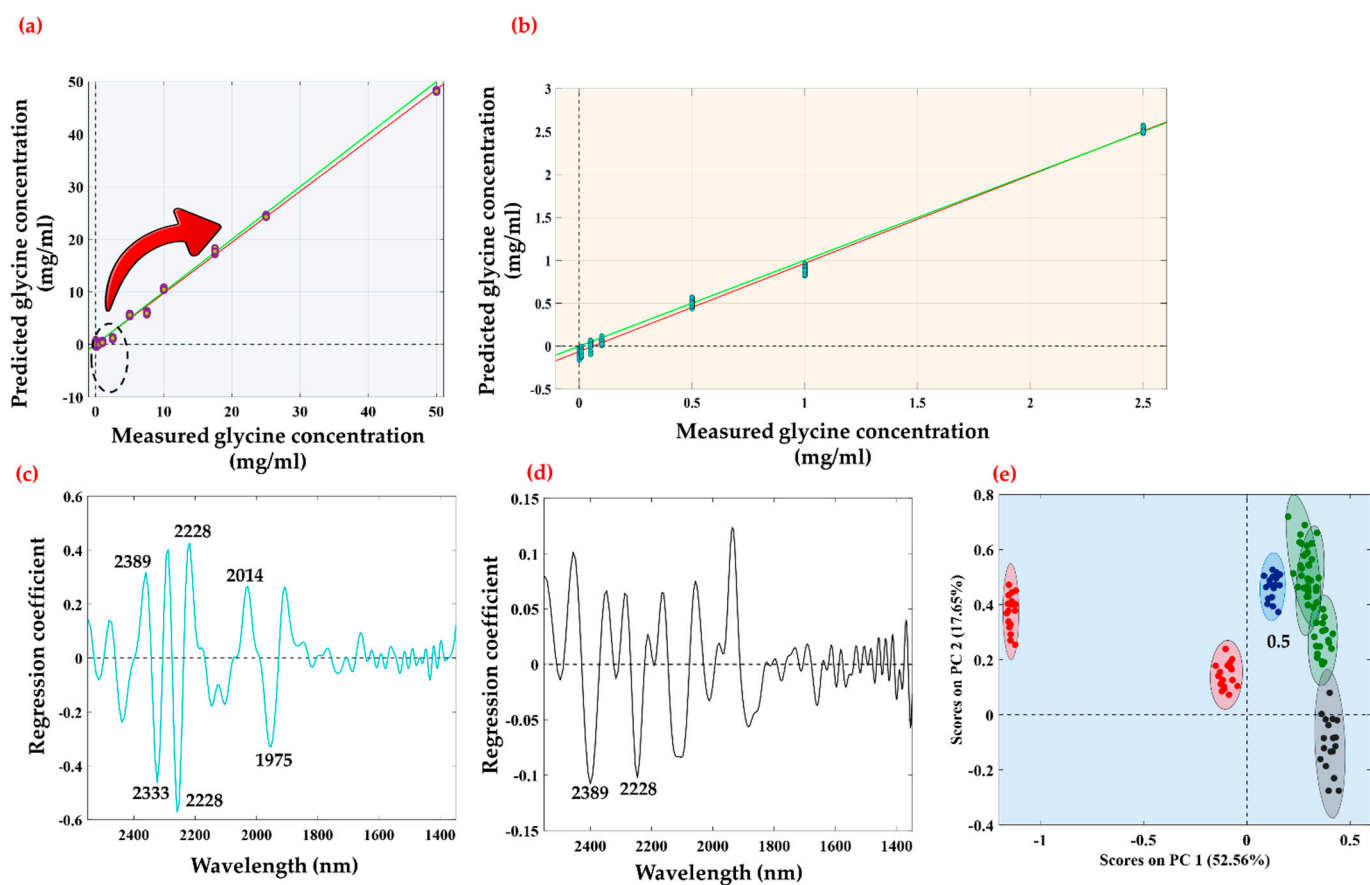


Figure S4. PCR predicted model of glycine spiked serum samples and it's a) regression plot of entire range between 0 (control) – 50 mg/mL region b) remodelled 0 – 2.5 mg/mL c) corresponding regression coefficient/vector for 0 – 50 mg/mL d) 0 – 2.5 mg/mL over 2500 – 2000 nm region. e) corresponding PC scores plot.

Table S2. Values associated with the LoB and LoD calculation from the regression statistics.

Method	Mean_{blank}	SD_{blank}	LoB	SD_{low concentration}	LoD
ATR	-0.187	0.132	0.030	0.142	0.265
NIR	-0.032	0.129	0.181	0.0288	0.228
Combined ATR - NIR	-0.217	0.1536	0.0354	0.0821	0.170