

Supporting information

Feasibility of Non-Invasive Measurement of Cardiac Biomarkers Using Mid-Infrared Spectroscopy: Finite Element Analysis and Experimental Validation

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Table S1. Spectral characteristics of common interfering molecules in the mid-infrared region

Interfering Molecule	Amide I Band (~1650 cm ⁻¹)	Amide II Band (~1550 cm ⁻¹)	Other Characteristic Absorptions	Dominant Secondary Structure
Human Serum Albumin	1652 cm ⁻¹ (α -helix)	1545 cm ⁻¹ (N-H bending and C-N stretch)	1235 cm ⁻¹ (Amide III) and ~3300 cm ⁻¹ (N-H stretching)	Predominantly α -helix
Immunoglobulin G	1640 cm ⁻¹ (β -sheet dominant)	1538 cm ⁻¹ (strong β -sheet feature)	1230-1240 cm ⁻¹ (Amide III) and ~3070 cm ⁻¹ (aromatic C-H)	Predominantly β -sheet
Cathepsins (e.g., Cathepsin D)	1635-1650 cm ⁻¹ (mixed α/β)	1520-1550 cm ⁻¹	1210 cm ⁻¹ (proline C-N vibration) and 1315 cm ⁻¹ (tyrosine)	Mixed α/β with notable tertiary structure

Table S2 Comparison of MIR spectral features of cTnI, NT-proBNP, and CRP

Biomarker	Main Absorption Peaks (cm ⁻¹)	Origin of Peaks
cTnI	1650 (Amide I)	β -sheet structure
	1545 (Amide II)	Proline side chain vibration
	1210 (Proline vibration)	
NT-proBNP	1650 (Amide I)	Dominantly α -helical structure
	1550 (Amide II)	Protein backbone modes
	1450 (CH ₂ bending)	
CRP	1645 (Amide I)	Rich in β -sheets and β -turns
	1538 (Amide II)	Carboxylic acid side chains
	1390 (COO ⁻ symmetric stretch)	