" Near-infrared spectroscopy is a type of molecular vibration spectroscopy. Temperature variations cause changes in molecular vibrations such as O-H and inter molecular forces such as hydrogen bonding" which lead to absorption spectral intensity and peaks changes" affecting the prediction accuracy of minor components such as blood glucose. To address the impact of temperature perturbation on spectral detection and modeling analysis" a method of temperature perturbation discrimination based on aquaphotomics and two-trace two-dimensional correlation spectroscopy" 2T2D-COS" was proposed. The 2T2D-COS analysis was applied to diffuse reflectance spectra of simulated solutions under temperature perturbation and varying glucose concentrations. Spectral features induced by changes in temperature and glucose concentration were successfully extracted" revealing distinct water spectral patterns under different perturbations. Quantitative analysis shows that temperature changes of 0. 1 °C is equivalent to glucose concentration changes of 45 mg/dL in terms of intensity. A temperature perturbation outliers discrimination model was further established based on raw spectra" water spectral features" and 2T2D-COS asynchronous spectra. The accuracy rates of the model based on 2T2D-COS asynchronous spectra is 95. 83%. After removing outliers" the root mean square error of glucose concentration prediction is reduced by 51. 89%. This work provides a foundation for improving the accuracy of in vivo blood glucose detection using near-infrared spectroscopy.

" near-infrared spectroscopy" two-trace two-dimensional correlation analysis" aquaphotomics" temperature

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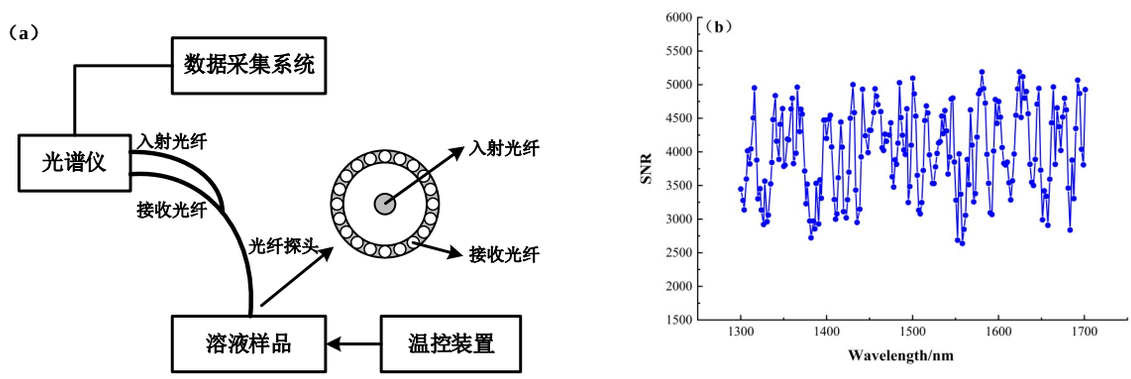

“ 1“ “ “ “ “ “ “ “ “ “ “ “ “ “ “ “ a“ “ “ “ “ “ “ “ “ “ “ “ “ “ “ b“ “ “ “ “ “ “

Fig. 1“ Schematic diagram of the near-infrared diffuse reflectance spectroscopy detection system: (a) schematic diagram of the diffuse reflectance spectroscopy detection system; (b) evaluation of instrument signal-to-noise ratio

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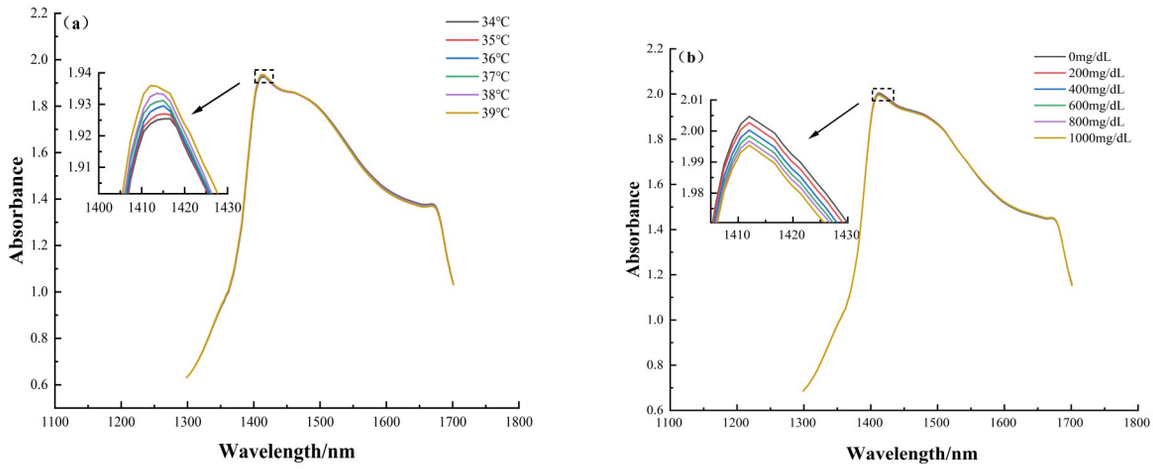
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35℃
36℃
37℃
38℃
39℃
Absorbance
Wavelength/nm
(b)
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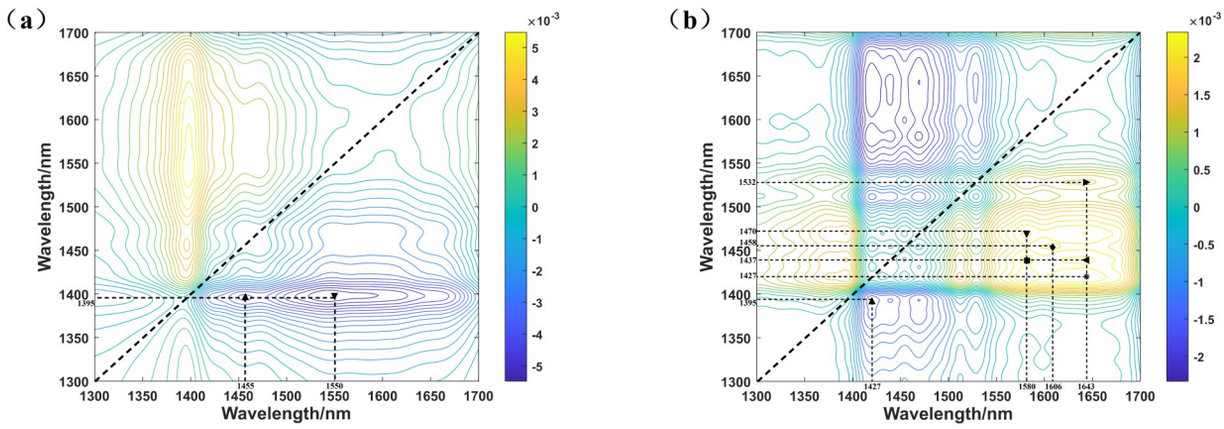
1000mg/dL
Absorbance
Wavelength/nm

“ 2“ “ “ “ “ “ “ “ “



“ 3“ “ “ “ “ “ “ “ “ “ “ “ “ “ “ “ “ “ 2T2D-COS“ “ “ “ “ a“ “ “ “ “ (“ “ “ “ “ “ 0 mg/dL“ “ “ “ “ “ 36 “ “ “ “ “ “ 37 “ “ 1 455 nm“ 1 395 nm“ “ “ 1 550 nm“ 1 395 nm“ “ “ b“ “ “ “ “ “ “ “ “ “ 36 “ “ “ “ “ “ “ “ “ “ “ 0 mg/dL“ “ “ “ “ “ “ “ “ “ “ 200 mg/dL“ “ 1 427 nm“ 1 395 nm“ “ “ 1 580 nm“ 1 478 nm“ “ “ 1 580 nm“ 1 437 nm“ “ “ 1 606 nm“ 1 458 nm“ “ “ 1 643 nm“ 1 532 nm“ “ “ 1 643 nm“ 1 532 nm“ “ “ 1 643 nm“ 1 427 nm“ “

Fig. 3“ 2T2D-COS asynchronous spectra of tissue phantom solution under different temperatures and glucose concentrations: (a)different temperatures (Glucose concentration: 0 mg/dL, Reference spectrum: 36 , Sample spectrum: 37 . “ 1 455 nm“ 1 395 nm“ “ “ 1 550 nm“ 1 395 nm“ “ ; (b)different glucose concentrations (Temperature: 36 , Reference spectrum: 0 mg/dL, Sample spectrum: 200 mg/dL. “ 1 427 nm“ 1 395 nm“ “ “ 1 580 nm“ 1 478 nm“ “ “ 1 580 nm“ 1 437 nm“ “ “ 1 606 nm“ 1 458 nm“ “ “ 1 643 nm“ 1 532 nm“ “ “ 1 643 nm“ 1 532 nm“ “ “ 1 643 nm“ 1 427 nm“ “

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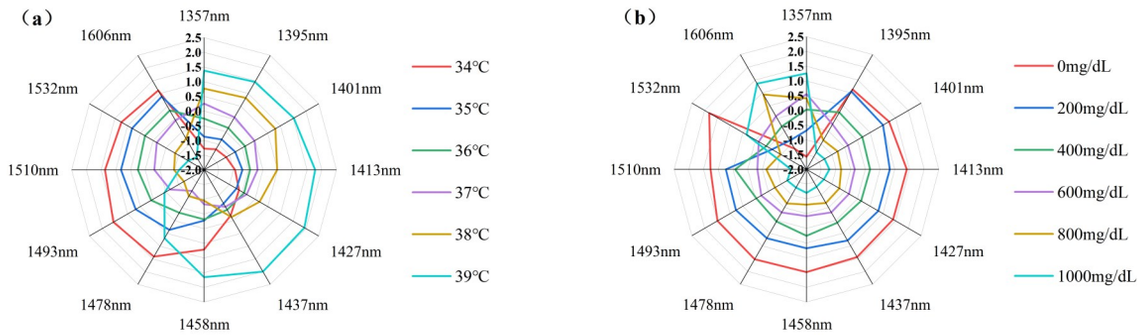
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34°C
35°C
36°C
37°C
38°C
39°C
(b)
0mg/dL
200mg/dL
400mg/dL
600mg/dL
800mg/dL
1000mg/dL

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