Supplementary Information

Qualitative and quantitative analysis of metronidazole formulations using a low-cost near infrared transmission spectrophotometer and chemometric tools

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Table S1 Raw validation data of the quantitative method

Series	Concentration level (mg mL^{-1})	Introduced concentration (mg mL^{-1})	Predicted concentration (mg mL^{-1})
Series 1	50	48.9	47.2
	50	52.0	50.6
	50	50.4	48.0
	75	75.5	74.2
	75	76.3	75.3
	75	75.9	75.6
	90	90.5	90.9
	90	90.1	90.8
	90	90.3	90.3
	100	102.7	103.1
	100	101.4	102.0
	100	102.1	101.9
	125	124.6	124.0
	125	124.7	124.0
	125	124.6	121.2
Series 2	50	50.4	49.5
	50	49.3	48.9
	50	49.8	48.3
	75	76.1	77.0
	75	75.8	76.1
	75	76.0	75.7
	90	91.3	92.5
	90	91.2	92.4
	90	91.2	92.0
	100	100.6	101.5
	100	101.3	102.0
	100	100.9	101.6
	125	124.9	124.8
	125	123.8	123.2
	125	124.3	123.1
Series 3	50	51.6	51.8
	50	51.6	52.6
	50	52.4	51.8
	75	76.2	76.2
	75	76.2	76.8
	75	74.4	75.2
	90	88.8	87.3
	90	88.8	88.1
	90	89.9	89.2
	100	100.3	101.2
	100	100.3	101.9
	100	103.8	104.2

125	125.4	124.8
125	125.4	124.2
125	127.4	125.8

Table S2 Results of the quantitative analysis of metronidazole tablets using the validated PLS model

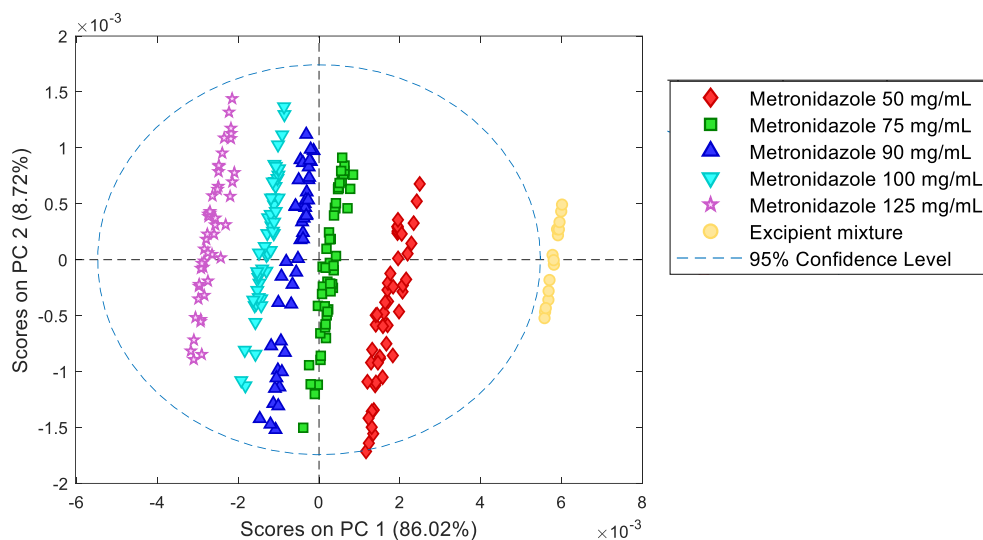| Brand name	Dosage (mg)	Number of tested batches	Metronidazole content (%) range
Flagyl®	500	03	95,4 – 100,6
Flagyl®	250	02	98,2 – 99,0
Nidazol®	500	02	98,6 – 99,8
Metronidazole Africure	500	03	96,3 – 99,0
Metronidazole Africure	250	02	92,4 – 95,1
Metronidazole Humanwell	500	06	97,2 – 99,4
Metronidazole Tongmei	500	02	101,0 – 102,0

Fig. S1 PC1-PC2 score plot of the preprocessed spectra of metronidazole calibration samples and excipient mixture
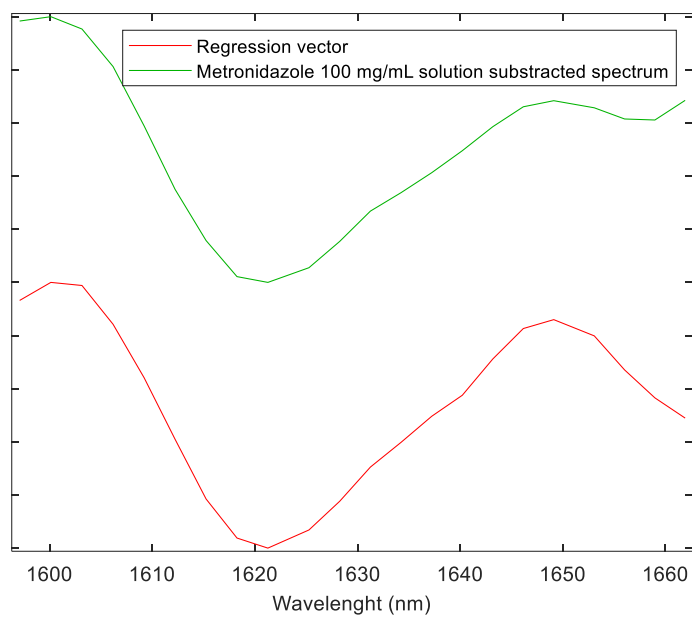

Fig. S2 Regression vector presented with the spectrum of 100 mg mL^{-1} metronidazole solution. The spectral range and preprocessing are those utilized in the PLS model. To visualize the metronidazole bands, the preprocessed spectrum of 1M HCl was subtracted from the metronidazole solution spectrum. The spectra are offset to improve visual discernibility.
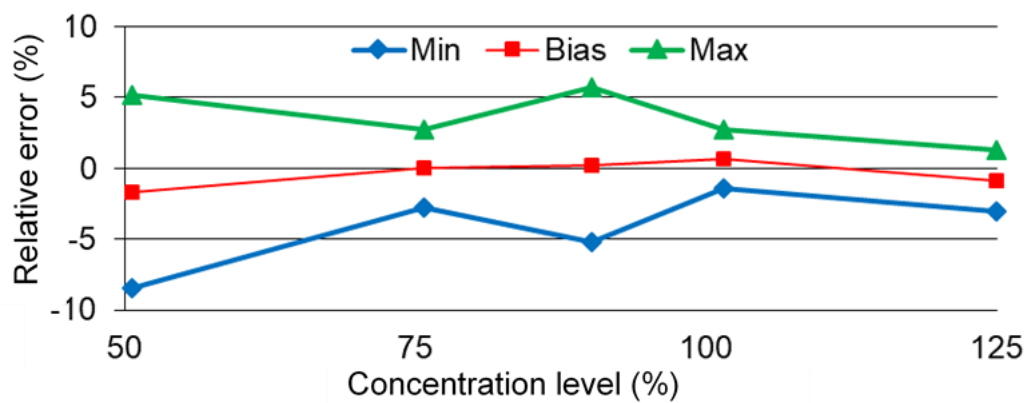
Fig. S3. Accuracy profile of the quantitative method