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## ACCEPTED MANUSCRIPT

Selective determination of caffeine and trigonelline in aqueous extract of green coffee beans by FT-MIR ATR spectroscopy

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## ABSTRACT

A non-destructive, fast, simple and reliable Fourier transform mid-infrared attenuated total reflectance spectroscopy (FT-MIR-ATR) method for the selective determination of caffeine and trigonelline in the aqueous extract of green coffee beans was developed and validated. The calibration curves were linear in the range 2000–7000 mg/L for caffeine and trigonelline with  $R^2 \ge 0.9997$ . The limits of detection (LOD) were 140 and 100 mg/L and the limits of quantification (LOQ) were 470 and 330 mg/L for caffeine and trigonelline, respectively. The precision (% RSD) was 3.0% and 4.3% for caffeine and trigonelline, respectively. The developed method was applied to three samples of green coffee beans to determine the two alkaloids. The amount of caffeine and trigonelline in the green coffee beans were found in the range 0.97–1.04% (*w/w*) and 0.93–0.96% (*w/w*), respectively. The accuracy of the developed analytical method was evaluated by spiking standard caffeine and trigonelline to green coffee beans and the average recoveries were  $93\pm5\%$  and  $98\pm4\%$ , respectively. Therefore, the developed FT-MIR-ATR methods can be used for direct determination of the two alkaloids in the green coffee beans.

Keywords: caffeine; trigonelline; green coffee beans; FT-MIR-ATR

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