

## INTISARI

Kreatin sebagai zat ergogenik mampu meningkatkan performa olahraga serta berkhasiat dalam terapi penyakit neurodegeneratif. Berbagai teknik spektroskopi hingga kromatografi telah diterapkan dalam analisis kreatin. Namun demikian, metode kromatografi memerlukan solvent organik dan waktu yang lebih lama. Pengembangan spektroskopi FTIR kombinasi kemometrika dipilih dengan pertimbangan proses yang mudah, cepat, serta pendekatan *green chemistry* untuk mencapai SDGs 13 yaitu *climate action*. Penelitian ini bertujuan untuk penetapan kadar kreatin monohidrat pada sediaan *floating tablet*. Target kedepannya, penelitian ini dapat diterapkan dalam analisis rutin keseragaman kadar sediaan pada proses produksi di industri farmasi.

Pendekatan kemometrika dilakukan dengan kalibrasi multivariat model PCR dan PLS yang didesain menggunakan bantuan *software TQ Analyst*. Validasi metode dilakukan dengan mengevaluasi parameter statistik berupa  $R^2$ , RMSEC, RMSEP, RMSECV. Koleksi data spektra FTIR dilakukan dengan *Software Thermo Scientific™ OMNIC™ Series*. Visualisasi dan pemrosesan spektra dikerjakan dengan *software Origin 2023*.

Hasil pemindaian spektra dioptimasi melalui aspek pemilihan daerah *wavenumber* serta jenis spektra. Berdasarkan hasil parameter validasi dipilih model PLS pada spektra normal dengan *wavenumber*  $1650\text{-}1350\text{ cm}^{-1}$ . Model ini memberikan hasil  $R^2$  untuk kalibrasi, validasi, dan *cross-validation* sebesar 0,9983; 0,9985; 0,9977 serta nilai RMSEC, RMSEP, dan RMSECV yaitu 1,74; 1,72; 2,07. Penerapan metode ini untuk penetapan kadar kreatin monohidrat dalam sediaan *floating tablet* memberikan hasil konsentrasi sebesar  $99,99 \pm 1,04\%$  yang telah memenuhi persyaratan kadar kreatin pada monografi USP 44.

**Kata kunci:** kreatin monohidrat, *floating tablet*, FTIR, kemometrika

## ABSTRACT

*Creatine as an ergogenic substance can improve sports performance and treat neurodegenerative diseases. Various spectroscopic to chromatographic techniques have been applied in the analysis of creatine. However, the chromatographic method requires organic solvents and a longer time. The development of FTIR spectroscopy with chemometrics was chosen because of an easy and fast process with consideration of the green chemistry approach to achieve SDGs 13 (climate action). This study aims to determine the levels of creatine monohydrate in floating tablet preparations. This research can be applied in the routine analysis of dosage uniformity in production processes in the pharmaceutical industry.*

*The chemometric approach was carried out by multivariate calibration of the PCR and PLS models which were designed using TQ Analyst software. Method validation was carried out by evaluating the statistical parameters of  $R^2$ , RMSEC, RMSEP, and RMSECV. FTIR spectral data collection was performed with the Thermo Scientific™ OMNIC™ Series Software. Spectral visualization and processing were done with the Origin 2023 software.*

*The results of the spectral scanning are optimized through the aspect of wavenumber area and the type of spectra. Based on the results, the PLS model was selected in the normal spectra with a wavenumber of  $1650\text{-}1350\text{ cm}^{-1}$ . This model gives  $R^2$  results for calibration, validation, and cross-validation of 0.9983; 0.9985; 0.9977 and the RMSEC, RMSEP, and RMSECV values are 1.74; 1.72; 2.07. The application of this method for determining creatine monohydrate content in floating tablet gave a concentration of  $99.99 \pm 1.04\%$  which met the requirements for creatine levels in USP 44 monograph.*

**Keywords:** *creatine monohydrate, floating tablet, FTIR, chemometrics*