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A SINGLE MCR-ALS MODEL FOR DRUG ANALYSIS IN DIFFERENT FORMULATIONS: APPLICATION ON DIAZEPAM COMMERCIAL PREPARATIONS

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Highlights

- MCR-ALS modelling was used to quantify diazepam in 30 commercial liquid formulations.
- MCR calibration was run on the UV-vis data of the commercial DZP samples.
- This model was optimized by appropriate selection of the most useful wavelengths.
- The predictive performance of the MCR model was compared with PLSR.

ABSTRACT

A multivariate curve resolution - alternating least squares (MCR-ALS) analysis was used to quantify diazepam (DZP) in thirty commercial liquid formulations. MCR calibration was run on the UV spectrophotometric data of the commercial DZP samples over the range 200-400 nm, allowing the resolution of the drug signal and then the excipients contained in all the formulations. A single model MCR for the determination of the drug in all samples was then built through the adoption of the correlation constraint. This model was optimized by an appropriate selection of the most useful wavelength ranges and then validated on external samples. DZP concentrations in the pharmaceutical formulations were measured by HPLC-DAD analysis. The performance of the MCR model was compared with that from application of classical partial least squares regression (PLSR). The results, in terms of error of prediction, were very satisfactory, reaching a relative error below of 1.66% against 2.56%, respectively.

Keywords: *Diazepam; Multivariate curve resolution; Partial least squares regression; UV spectrophotometry; Pharmaceutical analysis; HPLC.*

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