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Near infra red spectroscopy as a multivariate process analytical tool for predicting pharmaceutical co-crystal concentration

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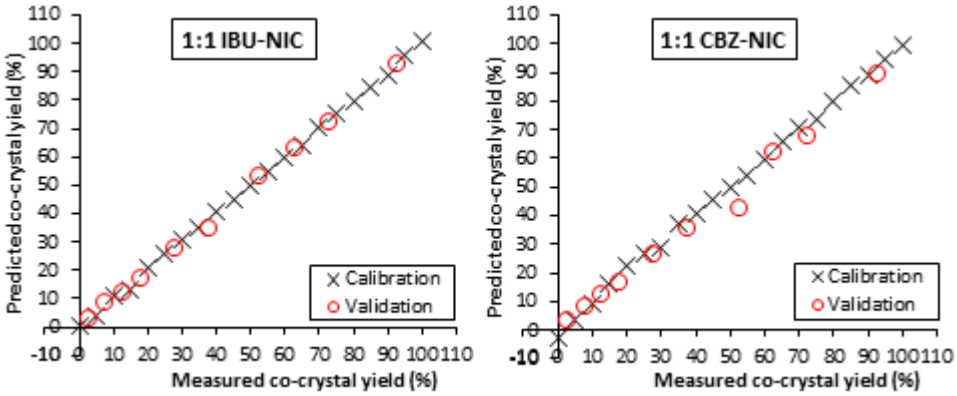
Graphical abstract



Hgihlights

- NIR spectroscopy can distinguish between the API, co-former and the co-crystal form
- Linear PLS regression models for two pharmaceutical co-crystals were made
- The co-crystals were 1:1 carbamazepine-nicotinamide and 1:1 ibuprofen-nicotinamide
- Different regions of the NIR spectra and varying levels of chemometrics were tried
- Both models can be used to predict the respective co-crystal concentration

Abstract

The use of near infra red spectroscopy to predict the concentration of two pharmaceutical co-crystals; 1:1 ibuprofen - nicotinamide (IBU-NIC) and 1:1 carbamazepine – nicotinamide (CBZ-NIC) has been evaluated. A Partial Least Squares (PLS) regression model was developed for both co-crystal pairs using sets of standard samples to create calibration and validation data sets with which to build and validate the models. Parameters such as the root mean square error of calibration (RMSEC), root mean square error of prediction (RMSEP) and correlation coefficient were used to assess the