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ACCEPTED MANUSCRIPT

APPLICATION OF 2D-HPLC COUPLED WITH PRINCIPAL COMPONENT ANALYSIS TO STUDY AN INDUSTRIAL OPIATE PROCESSING STREAM

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Abstract

Principal component analysis (PCA) loading plots were used to elucidate key differences between two-dimensional high performance liquid chromatography (2D-HPLC) fingerprint data from samples collected from stages along the *Papaver somniferum* industrial process chemistry workflow. Data reduction was completed using a 2D-HPLC peak picking approach as a precursor to chemometric analysis. Using comparisons of the final stages of product extraction as an example, PCA analysis of characteristic 2D-HPLC fingerprints accounted for 84.9% of variation between the two sample sets measured in triplicate, with 64.7% explained by PC1. Loadings plots of PC1 on each sample set identified where the significant changes were occurring and normalised bubble plots provided an indication of the relative importance of each of these changes. These findings highlight 2D-HPLC with appropriate chemometric analysis as a useful tool for the exploration of bioactive molecules within biomass.

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