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QbD-steered development and validation of an RP-HPLC method for quantification of ferulic acid: Rational application of chemometric tools

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Abstract: The present work describes the systematic development of a simple, rapid, sensitive, robust, effective and cost-effective reversed-phase high performance liquid chromatographic method for quantitative analysis of ferulic acid using analytical quality by design paradigms. Initially, apt wavelength for the analysis of ferulic acid was selected employing principal component analysis as the chemometric tool. An Ishikawa fishbone diagram was constructed to delineate various plausible variables influencing analytical target profile, viz. peak area, theoretical plate count, retention time and peak tailing as the critical analytical attributes. Risk assessment using risk estimation matrix and factor screening studies employing Taguchi design aided in demarcating two critical method parameters, viz. mobile phase ratio and flow rate affecting critical analytical attributes. Subsequently, the optimum operational conditions of the liquid chromatographic method were delineated using face-centred composite design. Multicollinearity among the chosen factors for optimization was analyzed by the magnitude of variance inflation factor optimized analytical design space, providing optimum method performance, was earmarked using numerical and graphical optimization and corroborated using Monte Carlo simulations. Validation, as per the ICH Q2(R1) guidelines, ratified the efficiency and sensitivity of the developed novel analytical method of ferulic acid in the mobile phase and the human plasma matrix. The optimal method used a mobile phase, comprising of acetonitrile: water (47:53% v/v, pH adjusted to 3.0 with glacial acetic acid), at a flow rate of 0.8 mL·min−1, at a λmax of 322 nm using a C18 column. Use of principal component analysis unearthed the suitable wavelength for analysis, while analytical quality by design approach, along with Monte Carlo simulations, facilitated the identification of influential variables in obtaining the “best plausible” validated chromatographic solution for efficient quantification of ferulic acid.

Key words: Bioanalytical methodPrincipal Component Analysis (PCA)Design of Experiments (DoE)Monte Carlo simulationsAnalytical Quality by design (AQbD)

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