Abstract

In this presented work chemometric method for the characterization of isotopologues of Gabapentin is carried out along with separation of residual solvents. Spectroscopy and multivariate data analysis form a powerful combination for obtaining both quantitative and qualitative information and it is shown how spectroscopic techniques in combination with chemometric data evaluation can be used to obtain rapid, simple and efficient analytical methods. Chemometric tools used in the study are multivariate analysis along with isotopic dilution mass spectrometry, parallel factor analysis (PARAFAC) and design of experimental (DoE). The analytical techniques used are gas chromatographic mass spectroscopy (GC-MS), head space gas chromatography (HS-GC), ultra-performance liquid chromatography with diode array detection (UPLC-DAD). Chapter 1 introduces basic terminology and statistics used throughout the study. Chapter 2 and chapter 3 describes quantification of Gabapentin and its deuterated analogs by GC-MS. Chapter 2 describes development and validation of GC-MS method for the quantification of Gabapentin. Chapter 3 describes multivariate isotopic dilution mass spectrometric analysis of Gabapentin and its deuterated analogues. Chapter 4 is studies of effect of chromatographic parameters like injection port temperature, carrier gas flow and head space extractor parameters like incubation temperature, and incubation time on the separation of residual solvents. Chapter 5 and chapter 6 is about chromatographic separation of Gabapentin and its deuterated isotopologues. Chapter 5 describes methodology used for the detection of isotopologues of Gabapentin by PDA detector using PARAFAC data decomposition after UPLC separation. Chapter 6 describes optimization of UPLC parameters by two level full factorial design for the separation of deuterated isotopologues of Gabapentin.