Multivariate statistical analysis characterization of newly synthesized hydantoins

Tatjana Djaković-Sekulić and Zagorka Lozanov-Crvenković

University of Novi Sad, Serbia

Abstract

Several multivariate statistical analyzes were performed in a quantitative structure-retention relationship study (QSRR) in order to correlate the retention of 18 newly synthesized hydantoins with potential biological activity and their molecular characteristics.

Hydantoins are a class of antiepileptic drugs used in the treatment of epilepsy. Among the investigated compounds two of them are well known. The first one is phenytoin, widely used drug in the treatment for the most common forms of epilepsy. The second is nirvanol, quite toxic significant metabolite of mephenytoin, also commonly used anticonvulsant drug.

Principal component analysis (PCA) followed by partial least squares (PLS) was performed to identify the most important factors, to quantify their influences, and to select descriptors that best describe the compounds investigated. Further, the best multiple linear regression (MLR) models were formed. High agreement between experimental and predicted relative retention, obtained in the validation procedure, indicated the good quality of the derived QSRR models.

Keywords

Hydantoins, Quantitative structure-retention relationship, Principal component analysis, Partial least squares, Multiple linear regression.

References

[1] Kaliszan, R. (1997). *Structure and Retention in Chromatographiy: A Chemometric Approach.* Amsterdam: Harwood Academic Publishers.

[2] Puzyn, T., J. Leszczynski and M.T.D. Cronin, (Eds) (2010). *Recent Advances in QSAR Studies. Methods and Applications.* Haildelberg: Springer.