Original Paper

Computational approach to the prediction of blood-brain partitioning of basic drug candidates using mixed micellar liquid chromatography

Arshadi S (Ph.D)*[1]

[1]**Assistant Professor, Department of Chemistry, Payame Noor University, Tehran, Iran.**

Abstract

Background and Objective: The blood–brain barrier (BBB) is considered to be the main barrier to drug transport into the central nervous system. In this study, the capability of biopartitioning micellar chromatography (BMC) using the mixed micellar system of Brij-35/sodium dodecyl sulfate (Brij-35/SDS, 85:15 mol/mol) has been studied to predict pharmacokinetic parameter (BBB penetration ability) of 14 basic drugs.

Methods: In this descriptive-analytical study, the potential of BMC using mixed micellar system (Brij-35/SDS, 85:15 mol/mol) in 0.04 M at physiological pH 7.4 was evaluated to predict pharmacokinetic parameter (BBB penetration ability) of 14 basic drugs. The regression model for the prediction of blood-brain distribution coefficient is derived from the multiple linear regression analysis using the training set in mixed micellar mobile phase. Also, the predictive ability of model was evaluated for a prediction set of 5 compounds (Chlorpromazine, Mianserin, Propranolol, Cimetidine, and Thioridazine). The fair R2 indicates good stability and predictive ability of the developed model for the drugs not included in modeling.

Results: The relationship between the BMC retention data of 14 basic drugs and their log BB parameter showed a good statistically model (R2=0.822, F=25.42, SE=0.225, R2CV=0.781).

Conclusion: This study points out the usefulness of mixed micellar solution of Brij-35/SDS, 85:15 (mol/mol) in BMC as a high-throughput primary screening tool that can provide key information about the blood-brain distribution of basic drugs in a simple and economical way.

Keywords: Blood–brain barrier, Sodium dodecyl sulfate, Polyoxyethylene (23) lauryl ether (Brij-35), Biopartitioning micellar chromatography

*** Corresponding Author: Arshadi S (Ph.D), E-mail: chemistry_arshadi@pnu.ac.ir**

Received 15 Aug 2015 **Revised** 15 Feb 2016 **Accepted** 19 Apr 2016

Cite this article as: Arshadi S. [Computational approach to the prediction of blood-brain partitioning of basic drug candidates using mixed micellar liquid chromatography]. J Gorgan Uni Med Sci. Spring 2017; 19(1): 96-102. [Article in Persian]