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Isfahan University of Medical Sciences

Application of factorial design in preparation of PCEC copolymers

L. Barghi[1,*], H. Valizadeh[2], D. Asgari[2], J. Barar[2]

[1]Faculty of Pharmacy, Tabriz University of Medical Sciences, Tabriz, Iran. 2. Student Research Committee, Tabriz University of Medical Sciences, Tabriz, Iran.
[2]Faculty of Pharmacy, Tabriz University of Medical Sciences, Tabriz, Iran. 2. Research Center for Pharmaceutical Nanotechnology, Tabriz University of Medical Sciences, Tabriz, Iran.

Background and Aims: Polycaprolactone (PCL) is a biodegradable polyester and has attracted attention in controlled drug delivery due to its non-toxicity. It has been reported that the biodegradability of PCL can be enhanced by copolymerization with other copolymers such as PEG. The purpose of this study was to prepare PCEC copolymers by using factorial design.
Methods: The composition of copolymers was designed using full factorial methodology. Molecular weight (Mw) of PEG (5 levels) and Mass ratio of epsilon-caprolactone/PEG (3 levels) were selected as input factors. Molecular weight of synthesized copolymers was the output factor. The PCL-PEG-PCL copolymers were prepared by ring opening polymerization. Formation of copolymers was confirmed by FT-IR spectroscopy as well as H-NMR. The Mw of PCL-PEG-PCL copolymers was calculated from HNMR spectra. The thermal behavior of copolymers was characterized on differential scanning calorimeter.
Results: Starting from PEG polymers with different molecular weight and varying the initial CL/PEG mass ratio, copolymers with different Mw, composition and average length of the blocks were obtained. According to the obtained results, the observed Mw of copolymers ranged from 1522 to 9264. Obtained data were analyzed to fit the following polynomial equation Y (Mw copolymer), where numerical values are constant regression coefficient and A & B are molecular weight of PEG and weight ratio of Cl/PEG respectively ($Y=1.98225A+1430.26B-1286.48$, $r=0.96$, p-value<0.001, MPE= 22.43). Data of training set were used to assess the performance of the proposed model in forecasting Mw of testing set. Average percent error for prediction of Mw was 14.05%.
Conclusions: Considering the low percent error, it might be concluded that this model has a good predictive power in the studied rang of variables and they have the ability of generalization to Unknown cases.

Keywords: Caprolactone; Factorial design; Ring opening polymerization