



## Supporting Information

for

### **Berberine-loaded polylactic acid nanofiber scaffold as a drug delivery system: The relationship between chemical characteristics, drug-release behavior, and antibacterial efficiency**

Le Thi Le, Hue Thi Nguyen, Liem Thanh Nguyen, Huy Quang Tran  
and Thuy Thi Thu Nguyen

*Beilstein J. Nanotechnol.* **2024**, *15*, 71–82. [doi:10.3762/bjnano.15.7](https://doi.org/10.3762/bjnano.15.7)

## Mathematical models

# 1. Mathematical models

In order to distinguish the release mechanism of BBR from BBR/PLA and BBR NPs/PLA nanofiber scaffolds, the experimental data of BBR release were described by four kinetic models, including the zero-order model, first-order model, Higuchi model, and Ritger–Peppas model.

## 1.1. The zero-order model

The zero-order model is described in Equation (2):

$$\frac{C_t}{C_\infty} = K_0 t, \quad (2)$$

where  $C_\infty$  and  $C_t$  are the concentration of drug release at infinite time and at time  $t$  (hours), respectively.  $K_0$  is the zero-order release constant. This model stands for a drug release system in which the rate of drug release is not dependent on concentration.

## 1.2. The first-order model

The first-order model is described in Equation (3):

$$\frac{C_t}{C_\infty} = 1 - e^{-K_1 t}, \quad (3)$$

where  $K_1$  is the first-order constant. This model expresses a drug release system in which the rate of drug release is concentration dependent.

## 1.3. Higuchi model

The Higuchi model is shown in Equation (4):

$$\frac{C_t}{C_\infty} = K_H t^{\frac{1}{2}}, \quad (4)$$

where  $K_H$  is the Higuchi dissolution constant. This model is used to study the release mechanism of water-soluble and low-soluble drugs loaded into solid matrices. The drug release according to the Higuchi model follows a diffusion process based on Fick's law.

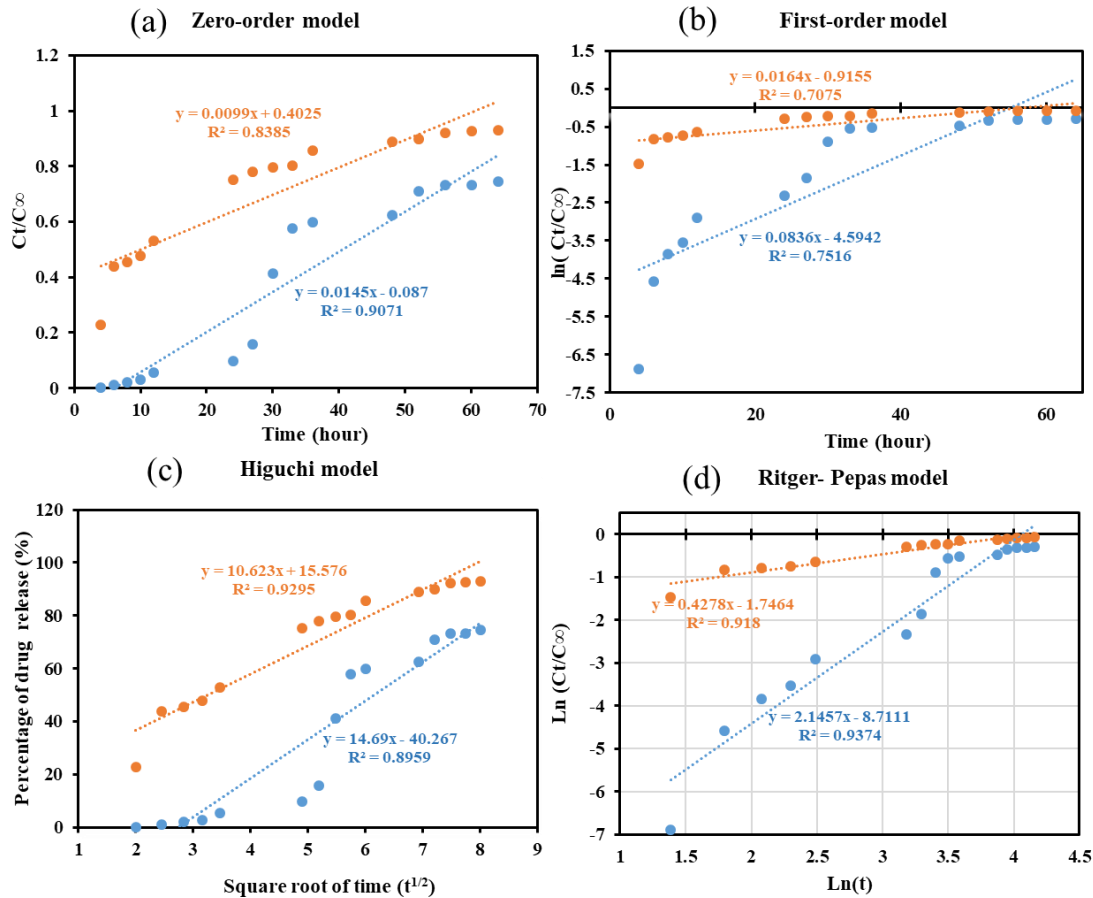
## 1.4. Ritger-Peppas model

The Ritger-Peppas model is represented in Equation (5):

$$\frac{C_t}{C_\infty} = K_R t^n, \quad (5)$$

where  $K_R$  is the Ritger–Peppas kinetic constant,  $n$  is the diffusion exponent indicating the release mechanism of drug from polymer matrices. When  $n \leq 0.5$ , the release mechanism follows a Fickian diffusion.  $0.5 < n < 1.0$  indicates non-Fickian diffusion, including other mechanisms associated with the diffusion. A value of  $n = 1$  represents zero-order release, which is independent of time.

## 2. Results



**Figure S1:** The equations and parameters determined by fitting BBR release data to mathematical models of (a) the zero-order model, (b) the first-order model, (c) the Higuchi model, and (d) the Ritger–Peppas model. The blue curves represent the BBR/PLA nanofiber scaffold and the orange curves represent the BBR NPs/PLA nanofiber scaffold.