생체발광을 이용한 독성농도(EC_{50})의 QSAR 모델

QSAR Modeling of Toxicant Concentrations(EC_{50}) on the Use of Bioluminescence

이용제 · 정성제 · 1)전억한
경희대학교 생명과학부 식품가공학과,

Lee, Yong-Je, Seong-Je Jung, and Uck-Han Chun[1]
Department of Food Technology and Science, Institute of Life Science, Kyung Hee University, Suwon, 440-701, Korea

Abstract

Concern for the effects of toxic chemicals on the environment leads the search for better bioassay test organisms and test procedures. *Photobacterium phosphoreum* was used successfully as a test organism, and the luminometer detection technique was an effective and simple method for determining the concentration of toxic chemicals. With EC_{50} a total of 14 chlorine substituted phenols, benzenes and ethanes were used for the experiments. The test results showed that the toxicity to *P. phosphoreum* increased in the order of phenol > benzene > ethane and the toxicity also increased with the number of chlorine substitution. Quantitative structure activity relationship (QSAR) model can be used to predict EC_{50} to save time and endeavor. Correlation was well established with the QSAR parameters, such as log P, log S and solvatochromic parameter($Vi/100$, π^*, βm and αm). The QSAR modeling was used with multi-regression analysis and mono-regression analysis. These analyses resulted in the following QSAR : log EC_{50} = 2.48 + 0.914 log S (n=9, R^2=85.5%, RE = 0.378), log EC_{50} = 0.35 - 4.48 $Vi/100$ + 2.84π^* + 9.46βm - 4.48αm (n = 14, R^2 = 98.2%, RE = 0.102), log EC_{50} = 2.64 - 1.66 log P (n = 5, R^2 = 98.8%, RE = 0.16), log EC50 = 3.44 - 1.09 log P (n = 9, R^2 = 80.8%, RE =0.207).

Key Word : *Photobacterium phosphoreum*, EC_{50},
Quantitative Structure Activity Relationship(QSAR), bioluminescence

1 Corresponding Author : Department of Food Technology and Science, Institute of Life Science, Kyung Hee University, Suwon 440-701, Korea
Tel : 0331-201-2626, Fax : 0331-204-8116
e-mail : uhchun@nms.kyunghee.ac.kr