

2012.11.15-16.
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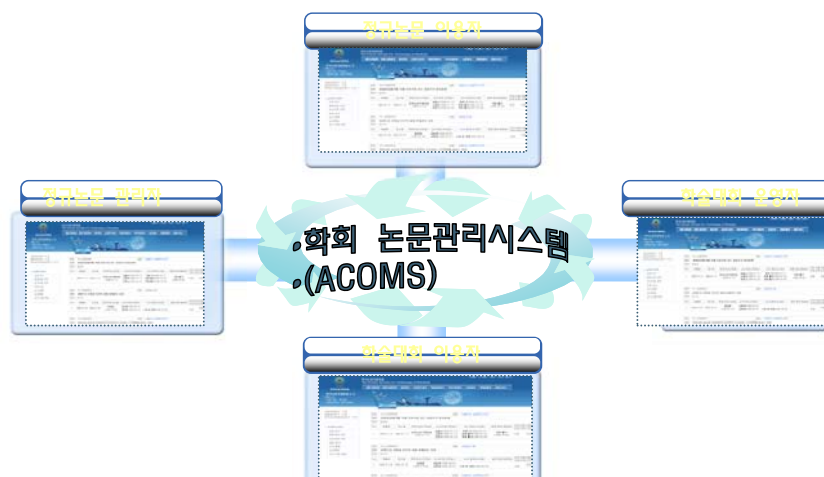
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이승호, 이성광



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- 논문투고, 심사관리, 사용자관리 등의 업무를 웹 기반으로 온라인상에서 관리하는 시스템
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- 이용자 : 편집위원장, 편집위원, 심사위원, 논문저자(투고자)
- 관리자 : 학회(시스템) 관리자



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- 2013년 1월부터 전면 시행
- 논문 심사 강화
 - 논문심사자 3인을 원칙으로 함. (최소 심사 2인)
 - **Accept, Minor revision(수정후가), Major revision(수정후재심사), Reject**
 - Reject 2명 이상 또는 reject 1명 + major revision 1명 이상 : 자동 reject
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- 빨라진 논문 심사 과정
 - 논문심사자 초대 응답시한 : 1주일
 - 논문심사자 심사기간 : 2주
 - 논문제출 후 판정 시한 : 30~60일
- Graphic abstract 추가
 - 분석과학지 표지로 선정 예정

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*** Title**

Prediction and analysis of acute fish toxicity of pesticides to the rainbow trout using 2D-QSAR

*** Abstract (250 word limit)**

statistical parameters between the experimental and predicted pLC50. After preprocessing, population based forward selection were used to select the best subsets of descriptors in the learning methods including 5-fold cross-validation procedure. The support vector machine model was used as the best model (R2CV= 0.677, RMSECV=0.887, MSECV=0.674) and also correctly classified 87% for the training set according to EU regulation criteria. The MLR model could describe the structural characteristics of toxic chemicals and interaction with lipid membrane of fish. All the developed models were validated by 5 fold cross-validation and Y-scrambling test.

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Title

- Prediction and analysis of acute fish toxicity of pesticides to the rainbow trout using 2D-QSAR

Abstract

- The acute toxicity in the rainbow trout (*Oncorhynchus mykiss*) was analyzed and predicted using quantitative structure-activity relationships (QSAR). The aquatic toxicity, 96h LC50 (median lethal concentration) of 275 organic pesticides, was obtained from EU-funded project Demetra. Prediction models were derived from 558 2D molecular descriptors, calculated in PreADMET. The linear (multiple linear regression) and non-linear (support vector machine and artificial neural network) learning methods were optimized by taking into account the statistical parameters between the experimental and predicted pLC50. After preprocessing, population based forward selection were used to select the best subsets of descriptors in the learning methods including 5-fold cross-validation procedure. The support vector machine model was used as the best model (R2CV= 0.677, RMSECV=0.887, MSECv=0.674) and also correctly classified 87% for the training set according to EU regulation criteria. The MLR model could describe the structural characteristics of toxic chemicals and interaction with lipid membrane of fish. All the developed models were validated by 5 fold cross-validation and Y-scrambling test.

Keywords

- pesticide, QSAR, acute fish toxicity, rainbow trout, cross-validation

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Seungho Lee acoms-noreply@kisti.re.kr 도메인: hnu.kr

Sung에게 ▾

Prof. Sung Kwang Lee께서

2012-11-09에 Analytical Science & Technology로 논문이 투고되었음을 알려드립니다.

제목: Prediction and analysis of acute fish toxicity of pesticides to the rainbow trout using 2D-QSAR

저자: In Sik Song; Ji Young Cha; Sung Kwang Lee;

투고하신 논문의 번호는 #Anal. Sci. Technol.-008이며, 현재 peer-review 과정에 들어갔습니다.

투고하신 논문의 진행상황을 확인하기려면, 다음의 URL로 가셔서 'Submissions under Review'를 클릭하시면 됩니다.

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Seungho Lee

[Anal.Sci.Technol] Reviewer Invitation for Anal. Sci. Technol.-008

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Seungho Lee acoms-noreply@kisti.re.kr 도메인: hnu.kr

20:11 (1분 전) ☆



Sung에게 ▾

안녕하세요. Prof. Sung Kwang Lee,

Analytical Science & Technology(분석과학)의 편집위원께서 Anal. Sci. Technol.-008논문에 대한 심사를 귀하께 의뢰하게 되었습니다. 본 투고논문의 논문심사에 동의해 주시면 매우 감사하겠습니다.
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Our editor would like to ask you to review the manuscript submitted for publication in the Analytical Science & Technology. We would greatly appreciate it if you agree to be the reviewer of this manuscript.

- Manuscript No: Anal. Sci. Technol.-008
- Title: Prediction and analysis of acute fish toxicity of pesticides to the rainbow trout using 2D-QSAR
- Author: In Sik Song; Ji Young Cha; Sung Kwang Lee;
- Date Reviewer Invited: 2012-11-09
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Date : 2012-11-14
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To : Seunggho Lee <slee@hannam.kr>
Subject : Anal. Sci. Technol.: MS #Anal. Sci. Technol.-008 Reviewer's Recommendation Letter

Dear Seunggho Lee:

I have completed my review of the manuscript, referenced below.

MS #Anal. Sci. Technol.-008
'Prediction and analysis of acute fish toxicity of pesticides to the rainbow trout using 2D-QSAR.'

Sincerely yours,

Body :

Comments to Author
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