以密閉式藻類毒性試驗方法評估芳香醛(苯甲醛)之毒性與結構-活性關係之研究

學生：蔡定裕　　指導教授：陳重元

國立交通大學環境工程研究所

摘　要

此篇研究以 20 種芳香醛(苯甲醛)針對月芽藻 (*Pseudokirchneriellasubcapitata*)所進行之 48 小時密閉式毒性試驗。實驗所得到之結果，將利用藻細胞的數量變化 (Final yield)做為觀測終點，藉由 Probit 模式求出半致死濃度 (50% Effect concentration，EC_{50})，將其毒性試驗後所得到的log(1/EC_{50})，與其物化參數(包括 log Kow 和 E_{LUMO})進行回歸分析，找出毒性方程式。

其結果顯示三種苯甲醛(苯甲醛、香草醛及 3,4-二烴基苯甲醛)會與藻種行歧化作用(dismutation)。此作用會造成苯甲醛轉化為苯甲酸之過程中行耗氧作用，因而減少溶氧產生量並降低其毒性。 而在不同烴基苯甲醛之毒性中，以 5-溴-2-烴基其毒性最毒。除了 3-溴-4-烴基苯甲醛之外，其他位於對位(*para*-)之烴基苯甲醛其毒性皆比鄰位(*ortho*-)低。

針對低影響濃度(NOEC、LOEC、EC_{10}、NEC)進行敏感性之比較，其結果: NOEC > EC_{10} > NEC > LOEC。在本研究之三種反應終點當中對於苯甲醛類之敏感性最高者為細胞密度變化量，其次為溶氧產生量，而敏感性最差之反應終點為生長率。與其他生物種進行比較可以發現本研究之藻類其敏感性最高、其他依序為鱒魚、水蚤、海洋性發光菌，敏感性最差者為纖毛蟲。

另一方面，由結果亦可發現在烴基苯甲醛中，其毒性易高對於其他苯甲醛類。再將 8 種烴基苯甲醛利用 logKow 進行 QSAR 之回歸分析，可以發現有一個 outlier (2,5-dihydroxybenzaldehyde)，若將此點去除後再進行迴歸即可得到較好之 QSAR 模式。而以反應終點為生長率所建立之 QSAR 模式有較精確之預測能力。

關鍵字: 月芽藻、QSAR、苯甲醛、半影響濃度(EC_{50})

The Study of Toxicity Assessment of Aromatic Aldehydes (Benzaldehydes) Using a Closed-System Algal Test and The Quantitative Structure-Activity Relationships

Student: Din-Yu Tsai Advisor: Chung-Yuan Chen

Institute of Environmental Engineering

National Chiao Tung University

Abstract

The objective of this study is to study the toxic effect of aromatic aldehydes (benzaldehyde) on *Pseudokirchneriella subcapitata* using a closed system test. The effects of benzaldehydes were evaluated by three kinds of response endpoints, i.e., cell density, algal growth rate, and the dissolved oxygen production. Median effective concentratons (EC_{50}s) were estimated using the Probit model with a test duration of 48hr. The quantitative structure-activity relationships (QSARs) were established based on the 1-octanol/water partition coefficient ($logK_{ow}$) and an electronic parameters-Lowest unoccupied molecular orbit (E_{LUMO}).

The result shows that the algae would make three types of benzaldehydes (benzaldehdye、vanillin and 3,4-dihydroxybenzaldehyde) into benzoic acid, and this reaction is called the dismutation. Special attention should be paid to that the oxygen produced by algae and toxicity of benzaldehydes will be decreased in the dismutation. The highest toxicity in different kinds of hydroxyl-benzaldehydes is 5-bromo-2-hydroxybenzaldehyde. In addition, the toxicity of *para*-hydroxy-benzaldehydes is lower than that of *ortho*-hydroxy- benzalde-hydes, exept 3-bromo-4-hydroxybenzaldehyde.

The results also reveal that the value of the lower effect concentration (EC_{10}、LOEC、NOEC and NEC) of the benzaldehydes is NOEC <EC_{10}<

NEC<LOEC. This demonstrates that the relative sensitivity is NOEC >EC_{10}> NEC>LOEC. Besides, the experiment results (EC_{50}) are compared with literature data derived by various toxicity tests. The order of the relative sensitivity is then obtained as follows : algae(Final yield)>algae(DO production)>algae(Grwoth rate)>*Fathead minnow*>*Daphnia magna*> Microtox >*Tetrahymena pyriformis*.

On the other hand, the toxicity of hydroxy-benzaldehydes is demonstrated to be higher than that of other benzaldehydes, and a single parameter ($logK_{ow}$) is used to estabilish QSAR of the hydroxy-benzaldehydes, except the one outlier (2,5-dihydroxybenzaldehyde).[$log(1/EC_{50})$G.R = 0.8457X - 0.34 96, R^2 = 0.9152, n=7]

Keyword: *Pesudokirchneriella subcapitata*, QSAR, Benzaldehyde, Median effective concentration (EC_{50})