

目 次

1 序言

于海瀛,尉小旋

综述

2 溴系阻燃剂毒理效应的计算模拟预测与环境风险评估进展

李斐,王晓晴,刘佳琳,孟祥敬,吉成龙,吴惠丰

14 卤代有机污染物抑制甲状腺激素代谢酶活性的研究进展

耿利鸣,马广才,尉小旋,于海瀛

23 微塑料对环境中有机污染物吸附解吸的研究进展

王一飞,李森,于海瀛,马广才,尉小旋

31 多溴联苯醚分布特征及环境风险研究进展

王磊,陶秀成,万锐

43 欧盟健康风险评估技术概述

李潍,于相毅,史薇,毛岩,张效伟,于红霞

54 农用地土壤重金属生态安全阈值确定方法的研究进展

窦韦强,安毅,秦莉,徐震,王苗苗,林大松,曾庆楠,夏晴

专论

65 ·Cl 引发 3 种环状含有 NH 结构有机化合物的大气转化机制及动力学

刘聪,马芳芳,付自豪,谢宏彬,陈景文

73 细胞色素 P450 酶催化烟草特异性亚硝胺 N'-亚硝基新烟草碱和 N'-亚硝基假木贼碱代谢活化的分子机制研究

倪君秀,徐婷,温家乐,徐小琴,于海瀛,尉小旋,马广才

83 基于 PBPK 模型评价三氯乙烯的职业暴露健康风险

刘远,王中钰,陈景文,乔显亮

92 十溴二苯乙烷对部分血糖内分泌干扰的计算机辅助理论研究

张天庆,杨秀榕,曾凡刚,张严

104 全氟辛烷磺酸在大连区域环境多介质中的归趋模拟

谷晓悦,丁光辉,刘全斌,李婉然,薛欢欢

113 水中典型光敏剂引发金雀异黄酮三线态敏化光降解机理

杨晨,张思玉,雷蕾,韩雅琦,孔宇,张雪娇,赵青,李海波,李英华

121 有机磷农药对蛋白核小球藻的毒性相互作用研究

曾莎莎,梁延鹏,覃礼堂,莫凌云,曾鸿鸽

130 2 种经典模型对抗生素与重金属锌的蛋白核小球藻时间依赖联合毒性作用的评估比较

王滔,张瑾,卞志强,姜慧,申慧彦

140 抗生素与三唑类杀菌剂混合物对羊角月牙藻的长期毒性相互作用研究

农琼媛,覃礼堂,莫凌云,刘勇安,梁延鹏

150 氨基甲酸酯类农药对蛋白核小球藻联合毒性作用特点及机制

卞志强,张瑾,王滔,徐晨茗,陶梦婷

- 163 构建有机化合物斑马鱼雌激素干扰效应的二元分类模型
王园宁, 刘会会, 杨先海
- 170 构建基于 GHS 标准的黑头呆鱼(*Pimephales promelas*)急性毒性二元分类模型
王雅琪, 刘会会, 杨先海
- 175 卤代肉桂酸对羊角月牙藻的急性毒性及 3D-QSAR 研究
李敏, 殷茂娇, 朱娟娟, 马海军
- 183 基于形态修正的描述符构建可电离化合物对大型溞急性毒性的 QSAR 模型
席越, 杨先海, 张红雨, 刘会会
- 192 取代苯酚类化合物抑藻活性的 CoMFA 模型
唐自强, 冯长君

CONTENTS

- 1 Preface
Yu Haiying, Wei Xiaoxuan
- 2 Advances in Computational Simulation and Environmental Risk Assessment on the Toxicological Effects of Brominated Flame Retardants
Li Fei, Wang Xiaoqing, Liu Jialin, Meng Xiangjing, Ji Chenglong, Wu Huifeng
- 14 Inhibition of Metabolic Activities of Thyroid Hormones by Halogenated Organic Contaminants
Geng Liming, Ma Guangcai, Wei Xiaoxuan, Yu Haiying
- 23 Research Progress on the Adsorption and Desorption between Microplastics and Environmental Organic Pollutants
Wang Yifei, Li Miao, Yu Haiying, Ma Guangcai, Wei Xiaoxuan
- 31 Research Progress in Distribution Characteristics and Environmental Risk of Polybrominated Diphenyl Ethers
Wang Lei, Tao Xiucheng, Wan Rui
- 43 Overview of EU Human Health Risk Assessment Technology
Li Wei, Yu Xiangyi, Shi Wei, Mao Yan, Zhang Xiaowei, Yu Hongxia
- 54 Research Progress in Determination Methods of Ecological Safety Thresholds for Heavy Metals in Agricultural Land
Dou Weiqiang, An Yi, Qin Li, Xu Zhen, Wang Miaomiao, Lin Dasong, Zeng Qingnan, Xia Qing
- 65 Atmospheric Transformation Mechanism and Kinetics of Three Cyclic NH-containing Compounds Initiated by \cdot Cl
Liu Cong, Ma Fangfang, Fu Zihao, Xie Hongbin, Chen Jingwen
- 73 Mechanistic Insight into Cytochrome P450-catalyzed Activation of Tobacco-specific N'-Nitrosoanatabine and N'-Nitrosoanabasine
Ni Junxiu, Xu Ting, Wen Jiale, Xu Xiaoqin, Yu Haiying, Wei Xiaoxuan, Ma Guangcai
- 83 Health Risk Assessment of Occupational Exposure to Trichloroethylene Based on PBPK Model
Liu Yuan, Wang Zhongyu, Chen Jingwen, Qiao Xianliang
- 92 Computer-aided Theoretical Study of Endocrine Disrupting of Some Blood Glucose by DBDPE
Zhang Tianqing, Yang Xiurong, Zeng Fangang, Zhang Yan
- 104 Simulating the Fate of Perfluorooctane Sulfonate (PFOS) in Environmental Multimedia of Dalian Area
Gu Xiaoyue, Ding Guanghui, Liu Quanbin, Li Wanran, Xue Huanhuan
- 113 Triplet-sensitized Photodegradation Mechanism of Genistein Induced by Typical Photosensitizers in Water
Yang Chen, Zhang Siyu, Lei Lei, Han Yaqi, Kong Yu, Zhang Xuejiao, Zhao Qing, Li Haibo, Li Yinghua
- 121 Toxicological Interactions of Organophosphorus Pesticides Mixtures to *Chlorella pyrenoidosa*
Zeng Shasha, Liang Yanpeng, Qin Litang, Mo Lingyun, Zeng Honghu
- 130 Comparative Evaluation on the Time-dependent Joint Toxicity of Antibiotics and Heavy Metal Zinc towards *Chlorella pyrenoidosa* between Two Classical Model
Wang Tao, Zhang Jin, Bian Zhiqiang, Jiang Hui, Shen Huiyan
- 140 The Toxic Interactions of Long-term Effects Involving Antibiotics and Triazole Fungicides on *Selenastrum capricornutum*
Nong Qiongyuan, Qin Litang, Mo Lingyun, Liu Yongan, Liang Yanpeng
- 150 Time-dependent Joint Toxicity Characteristics and Mechanisms of Five Carbamate Pesticides towards *Chlorella pyrenoidosa*
Bian Zhiqiang, Zhang Jin, Wang Tao, Xu Chenming, Tao Mengting

- 163 Development of Binary Classification Models for Predicting Estrogenic Activity of Organic Compounds on Zebrafish
Wang Yuanning, Liu Huihui, Yang Xianhai
- 170 Development of GHS-based Binary Classification Models for Predicting Acute Toxicity of Fathead Minnow (*Pimephales promelas*)
Wang Yaqi, Liu Huihui, Yang Xianhai
- 175 Acute Toxicity and 3D-QSAR Studies on Halogenated Cinnamic Acids to Microalga *Selenastrum capricornutum*
Li Min, Yin Maojiao, Zhu Juanjuan, Ma Haijun
- 183 Development of Acute Toxicity of *Daphnia magna* QSAR Models for Ionogenic Organic Chemicals Based on Chemical Form Adjusted Descriptors
Xi Yue, Yang Xianhai, Zhang Hongyu, Liu Huihui
- 192 CoMFA Model for Inhibitory Activity of Chlorinated Phenolic Compounds to *Dunaliella salina*
Tang Ziqiang, Feng Changjun