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# Computational Toxicology for Environmental Criteria/Benchmarks of Emerging Contaminants

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## **Message from the Guest Editors**

Dear Colleagues,

The rapid development of computational toxicology is bridging the data gap and providing effective solutions for the comprehensive assessment of hazards.

This Special Issue invites contributions from diverse computational toxicological modeling studies pertaining environmental criteria/benchmarks to and risk assessments. We strongly encourage submissions on all relevant topics including the virtual screening of preferential controlled pollutants, quantitative structureactivity relationships (OSARs), simulations of toxicological mechanisms, the modeling of internal and external exposure, interspecies differences, and environmental impacts on the bioavailability of emerging pollutants, as well as their environmental geochemical behaviors. The scope of research also includes new approaches for environmental criterion development, uncertainty analysis in risk assessments, and life cycle risk assessments. Further, contributions originating from meta-analyses based on the present datasets are also embraced for inclusion in this Special Issue.

Dr. Yunsong Mu Dr. Jing Liu Dr. Huiming Cao *Guest Editors* 







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## Message from the Editor-in-Chief

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