THEORETICAL STUDY ON ENVIRONMENTAL BEHAVIOR AND POTENTIAL TOXICITY OF PERSISTENT ORGANIC POLLUTANTS

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Introduction

With the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) came into force in the European Union on Jun 1, 2007, *in silico* methods such as virtual high-throughput screening, quantitative structure-activity relationship ((Q)SAR), and read-cross become indispensable technique in risk assessment of chemicals[1]. Simultaneously, the predominant role of computational toxicology in realizing the promise of the Toxicity Testing in the 21st Century has been stressed[2,3]. Researchers in the field of persistent organic pollutants (POPs) also participate in the related investigation and share rich experience in both theoretical principles and its diverse methodologies[4]. ,

Theoretical Method

In recent years, along with the development of computer technology, molecular biology, and computational chemistry, theoretical study has become an important research area in exploring environmental behavior and potential toxicity of persistent organic pollutants. Generally, computational methods such as homology modeling, molecule docking and molecular dynamics simulations are adopted in elucidating biochemical interaction between POPs and protein receptors or nucleic acids. Quantum chemical calculation is applied in finding the underlying reaction mechanism of specific environmental processes. In addition, work of developing practical tools have been done to fill the gap.

Case Study

Theoretical study on POPs environmental behavior and potential toxicity of organic chemicals has already become an active research field. High level quantum chemical calculation was successfully used in clarifying the generation mechanism of different dioxin compounds by various precursors including chlorophenols[5]. Quantitative structure-photoinduced toxicity relationship was discovered and established based on DFT-calculated descriptors[6]. Induced fit conformational changes based upon proof-of-principle calculations on both human estrogen receptor α and p53 was explored[7,8]. Nevertheless, the application of theoretical simulation to POPs study requires additional efforts to obtain more robust and informative methods.

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