User-Friendly Cloud System for Functional Chemical Synthesis Route Development

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In recent years, the development of functional chemicals has increasingly required the use of Process Informatics to accelerate the entire workflow—from synthesis route design to production process construction. At the outset of this approach, the first step involves designing synthetic routes using AI, followed by the refinement and selection of optimal routes through quantum chemical simulations. It is also essential that these processes can be performed not only by experts in organic chemistry but also by non-specialists. To address these challenges, we are developing a user-friendly cloud system for route development. This system is offered as a SaaS platform and can be accessed through the internet. The system enables users to input target chemical structures, select from multiple route-generation engines such as AIPHOS/KOSP/TOSP, choose various reaction knowledge bases or transforms, and evaluate candidate routes based on multiple scoring criteria, including precursor availability and cost. This facilitates the generation of diverse, multi-step synthetic routes. In addition, the platform is designed to seamlessly integrate quantum chemical simulations for route screening. In this presentation, we will demonstrate these features, screen examples, and case studies on route development for functional chemicals such as PPAR α / δ dual agonists and integrase inhibitors.