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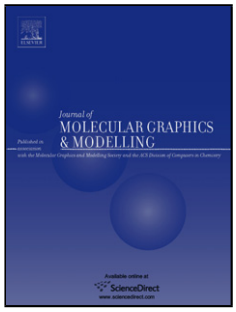

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Wisdom of Crowds for Synthetic Accessibility Evaluation

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Abstract

Synthetic accessibility evaluation is a process to assess the ease of synthesis of compounds. A rapid method for the assessment of synthetic accessibility for a vast number of chemical compounds is expected to bring about a breakthrough in the drug discovery. Although several computational methods have been proposed, the compound evaluation has still been processed by medicinal chemists; however, the low throughput of the human evaluation due to the lack of chemists is a critical issue for handling a large number of compounds. We propose the use of crowdsourcing for addressing this problem, and we conducted experiments to investigate the feasibility of incorporating semi-experts and a statistical aggregation method into the synthetic accessibility evaluation. Our experimental results show that we can obtain accurate synthetic accessibility scores through the statistical aggregation of judgments from semi-experts.

Keywords: Synthetic accessibility, crowdsourcing

1. Introduction

In-silico drug design systems often output novel compounds that are difficult to be synthesized and the synthetic accessibility of each compound must be evaluated. Automatic evaluation methods based on compound synthetic

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