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# Integration of Fuzzy Analytic Hierarchy Process into Multi-objective Computer Aided Molecular Design

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## HIGHLIGHTS

- Novel methodology for multiobjective molecular design
- Integrate Fuzzy Analytic Hierarchy Process in molecular design
- Consideration of different classes of property targets in molecular design
- Application example in solvent design for oil extraction

## Abstract

In this paper, a novel Computer Aided Molecular Design (CAMD) framework is developed to solve multi-objective molecular design problems. CAMD can be formulated as a multi-objective optimisation problem when there are multiple target properties to be optimised simultaneously. A major obstacle faced by multi-objective CAMD problems is the difficulty in assigning weighting factors to the target properties, since the relative importance of these factors is not always defined. It is particularly difficult to compare target properties which belong to different categories, such as physicochemical, safety, health and environmental

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