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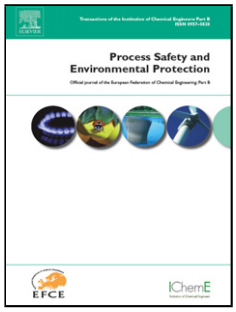

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A Systematic Methodology for Multi-Objective Molecular Design via Analytic Hierarchy Process

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Abstract

This paper presents a novel methodology for solving multi-objective Computer Aided Molecular Design (CAMD) problems. One of the major challenges in multi-objective CAMD problems is the subjectivity involved in assigning the weighting factors to each property that is optimised. It is difficult to define the relative importance of each property in CAMD problems as target properties that belong to different categories cannot be compared on a common scale. It is crucial to solve this issue as distinct solutions will be generated due to different weighting factors of each property. In this work, a systematic framework that combines CAMD and Analytic Hierarchy Process (AHP) is developed to deal with the ambiguities involved in assessing the relative importance weightings

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