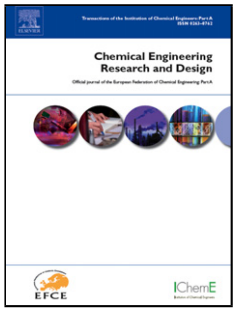

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Computer-aided molecular design: An introduction and review of tools, applications, and solution techniques

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Abstract

This article provides an introduction to and review of the field of computer-aided molecular design (CAMD). It is intended to be approachable for the absolute beginner as well as useful to the seasoned CAMD practitioner. We begin by discussing various quantitative structure-property relationships (QSPRs) which have been demonstrated to work well with CAMD problems. The methods discussed in this article are: (1) group contribution methods; (2) topological indices; and (3) signature descriptors. Next, we present general optimization formulations for various forms of the CAMD problem. Common design constraints are discussed and structural feasibility constraints are provided for the three types of QSPRs addressed. We then detail useful techniques for approaching CAMD optimization problems, including decomposition methods, heuristic approaches, and mathematical programming strategies. Finally, we discuss many applications that have been addressed using CAMD.

Keywords: Computer-aided mixture design; Computer-aided molecular design; Integrated product and process design; Group contribution; Topological indices; Signature descriptors