



Advances in Molecular Similarity, Volume 2

R. Carbó-Dorca, P.G. Mezey

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This volume highlights some of the advances in molecular similarity. Molecular similarity research is a dynamic field where the rapid transfer of ideas and methodologies from the theoretical, quantum chemical and mathematical chemistry disciplines to efficient algorithms and computer programs used in industrially important applications is especially evident. These applications often serve as motivating factors toward new advances in the fundamental and theoretical fields, and the combination of intellectual challenge and practical utility provides mutual advantages to theoreticians and experimentalists. The aim of this volume is to present an overview of the current methodologies of molecular similarity studies, and to point out new challenges, unsolved problems, and areas where important new advances can be expected.

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