Computer aided molecular design with combined molecular modeling and group contribution - DTU Orbit (07/01/2019)

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Computer-aided molecular design (CAMD) provides a means for determining molecules or mixtures of molecules (CAMMD) having a desirable set of physicochemical properties. The application range of CAMD is restricted due to limitations on the complexity of the generated molecular structures and on the availability of suitable models for property prediction. A new CAMD methodology that addresses this issue by combining molecular modeling techniques with a traditional CAMD approach is presented. The new method includes a new molecular/atomic structure generation algorithm, a large collection of property estimation methods, and, a link to molecular modelling tools. Application of the new CAMD method is highlighted through two industrial examples. (C) 1999 Elsevier Science B.V. All rights reserved.

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