

Abstract

Croat. Chem. Acta., 78, 141-149 (2005)

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Binary substructure descriptors for organic compounds.

Organic chemical structures are represented by binary vectors that contain information about presence or absence of 1365 substructures. The guiding ideas for selecting this set of substructures are described and examples are given.

Software SubMat has been developed for a fast and flexible computation of binary substructure descriptors from molecular structures.

Examples from structure similarity searches demonstrate the performance of representing organic chemical structures by the described set of substructures.