Abstract

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Substructure isomorphism matrix.

A substructure isomorphism matrix n x p contains binary elements describing which of the given p query structures (substructures) are part of the given n target structures (molecular structures). Such a matrix can be used to investigate the diversity of the target structures and allows the characterization and comparison of structural libraries.

A quadratic substructure isomorphism matrix n x n is obtained if the same structures are used as molecular structures and as substructures; this matrix contains full information about the topological hierarchy of the n structures. A hierarchical arrangement of chemical structures is useful for the evaluation of results obtained from searches in structure databases.