

## **Abstract**

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### **Substructure isomorphism matrix**

A substructure isomorphism matrix  $n \times p$  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  $n \times n$  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.