

## **computational chemistry**

Computational chemistry is a discipline using mathematical methods for the calculation of molecular properties or for the simulation of molecular behaviour. It also includes, *e.g.*, synthesis planning, database searching, combinatorial library manipulation.

***Source:***

PAC, 1997, 69, 1137 (*Glossary of terms used in computational drug design (IUPAC Recommendations 1997)*) on page 1141