

Topic	Required software Assuming you want to use it with Microsoft Windows, or on Android or iOS
Chemical structure drawing Software	ChemDraw (Microsoft Windows) ACD/ChemSketch (Microsoft Windows or on Android and iOS) Chirys Draw (Android and iOS) KingDraw (Android and iOS).
Explore structures in 3D.	ACD/ChemSketch, Hyperchem, Chemdraw
Structure optimization based on non-electronic structure methods: Molecular Mechanics Methods of Electronic Structure Molecular Dynamics	HyperChem (for Microsoft Windows or on Android and iOS)
The software's for Theoretical Chemistry	Gaussian (Microsoft Windows) HyperChem (Microsoft Windows)
Predicting programs for possible chemical hazards	Chemical Reactivity Worksheet Chemical Safety data sheet
Predict binding mode and approximate binding energy of a compound to a target	Auto Dock (website)
Identify active compounds for a specific target from a chemical library based on docking techniques and on pharmacophore modeling techniques	Virtual Screening
Computational software for the drug discovery in a resource-limited environment	Swiss drug design (website)

Computers In Chemistry

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