Introduction to Calculator Plugins

ChemAxon’s Calculator Plugins provide solutions to a wide range of problems at all levels of chemical modeling. Implemented calculations and property predictions can efficiently calculate physico-chemical properties and molecular descriptors even for large compound libraries.

Calculator Plugins has many attractive features like trainable physico-chemical property prediction, a wide selection of life-science-related chemical descriptors, modeling in 2D and 3D, and many others. All these features come with nice GUIs, making them powerful cheminformatics tools.

To get started as a user with the Calculator Plugins, look at the User's Guide. However, if you want to develop your own plugin, have a look at our Developer's Guide pages. You can also find the scientific models behind the plugins here.

Some of the most frequently asked questions are discussed on this page. If you get stuck, don't hesitate to ask for help.