Calculator Plugins FAQ

Here you can find some important questions related to Calculator Plugins:

1. How can I reach the plugins?
2. How are plugins used in other tools of ChemAxon?
3. Can I integrate the plugins in my application?
4. Can I train the plugins with my own dataset?
5. Can I combine my in-house application with a ChemAxon tool?

1. Calculator Plugins and their features are available in many ways in ChemAxon's products: directly from MarvinSketch, Instant JChem and Reactor applications, but also from command line, API or via ChemAxon's Chemical Terms language. The calculations can be performed in single or batch mode. Here are some details:

- The plugins are located under the *Calculations* menu in the graphical user interface of MarvinSketch, and under the *Tools* menu in MarvinView.
- They are also available with ChemAxon's applets**.**
- *cxcalc* is a command line tool that offers the same functionalities and enables the user to process molecules in a row.

2. The calculator plugins are used in other tools of ChemAxon as well:

- Calculators are used in the Chemical Terms   language to calculate combinations of properties (like Lipinski's rule of 5) in an easy way. Learn more about it in the Chemical Terms section.
- Plugin calculations can be used for filtering results of database searches in JChem Base, Instant JChem and JChem Cartridge.
- Smart reaction rules can be defined using plugin calculations in Reactor (ChemAxon's virtual reaction processing tool).

3. Plugins can be integrated easily into any Java application**.** For more information on using calculator plugin Java API, please see the chemaxon.marvin.calculation documentation.

4. Some of the calculators (such as $\log P$) can be trained with the user's data via MarvinSketch and the *cxtrain* command line tool.

5. Third-party calculations can be integrated easily into MarvinSketch via the *Services* module of the graphical user interface.

For more information on integrating third-party calculations, see our Setting Services page.