

Maximum of physical properties at a minimum of time

Modules used
MAPS

The discrimination of chemicals with regards to their activity requests the prediction of several properties with a relatively fair accuracy.

In so doing scientists need to have high performance tools that would enable the automatic generation of these of these properties and in some cases the simultaneous execution of other tasks, such as selection criteria before moving to the next step of the chemical selection process.

A similar situation is encountered in other areas, for instance the chemical engineering area where several physical the thermodynamic properties are required.

It becomes obvious that in such a process the number of simulations to be executed becomes very quickly very large. For instance the setup of a single calculation for a small molecule requires not only the creation of the molecular structure but also the setup of the calculation itself through a graphical user interface. Such a procedure requires about 2 to 4 minutes and in order to investigate about 100 molecules one needs to invest a full day simply to setup the calculations.

MAPS offers you an alternative solution which allows not only the fast construction of molecular systems but also the quick setup of production calculations. Indeed MAPS gives access to Python scripting and MAPS automatically generates Python scripts for a given calculation. These scripts can either be executed individually (as exposed in Figure 2) or can be combined in more sophisticated simulation scenarios. MAPS and its scripting capability provide all necessary frameworks for users to develop their own applications and go much beyond standard molecular modeling.

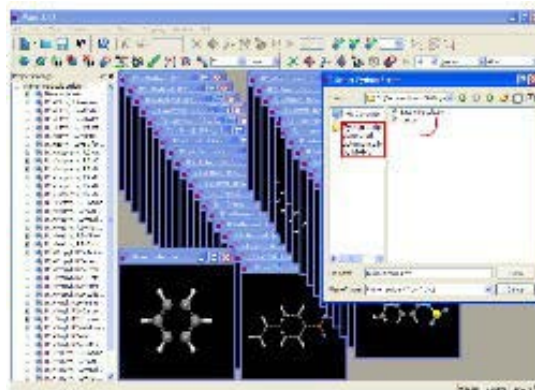


Figure 1: Python embedded in MAPS enables you avoid repetitive tasks and accelerate your R&D. MAPS users can run scripts automatically generated by MAPS or their own sophisticated scenarios

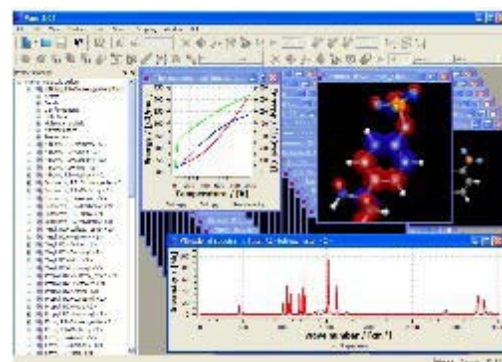


Figure 2: With MAPS the calculation of hundreds of valuable physicochemical properties used for chemicals and processes design and optimization may require only the amount of time that others need to simulate only one system.