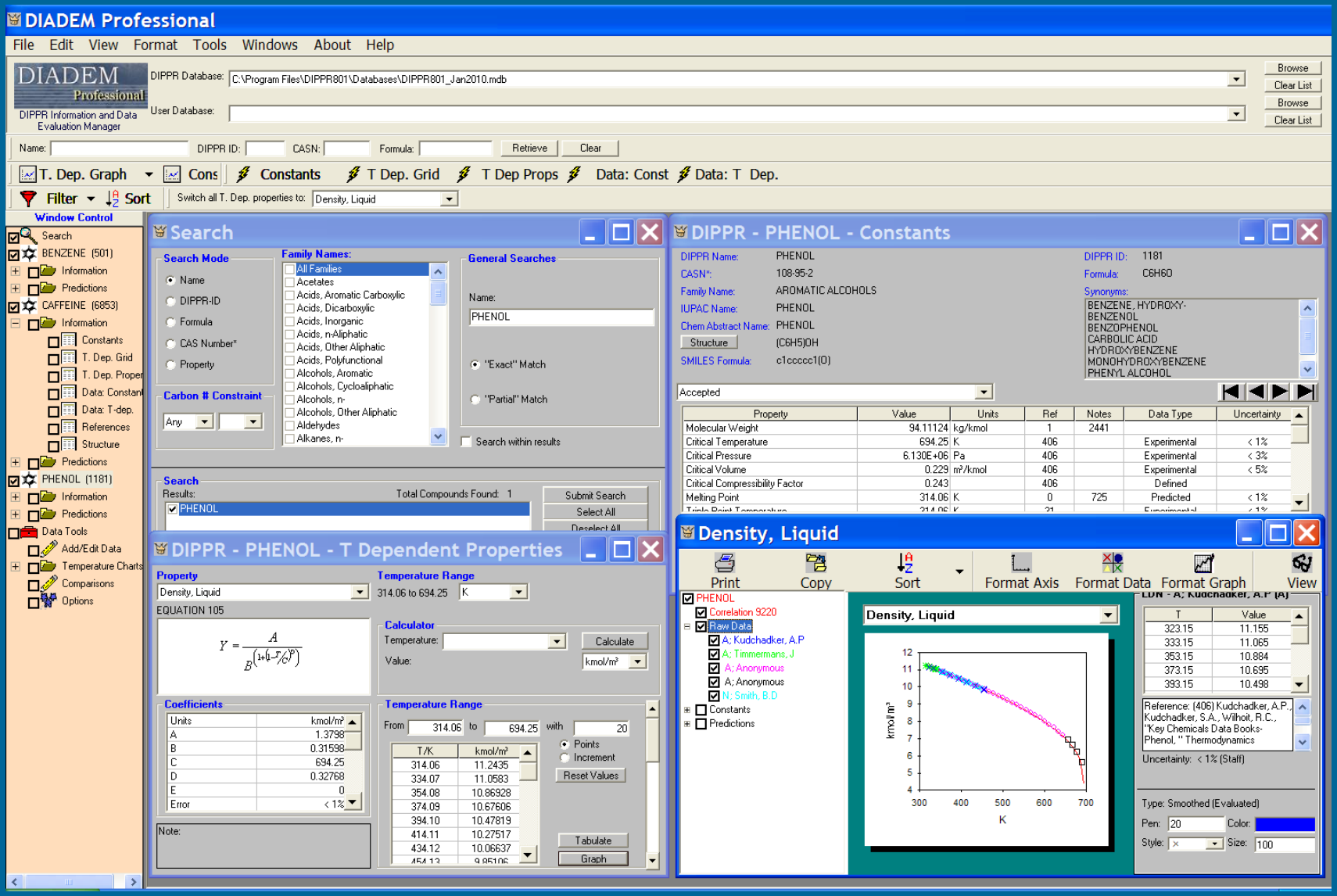
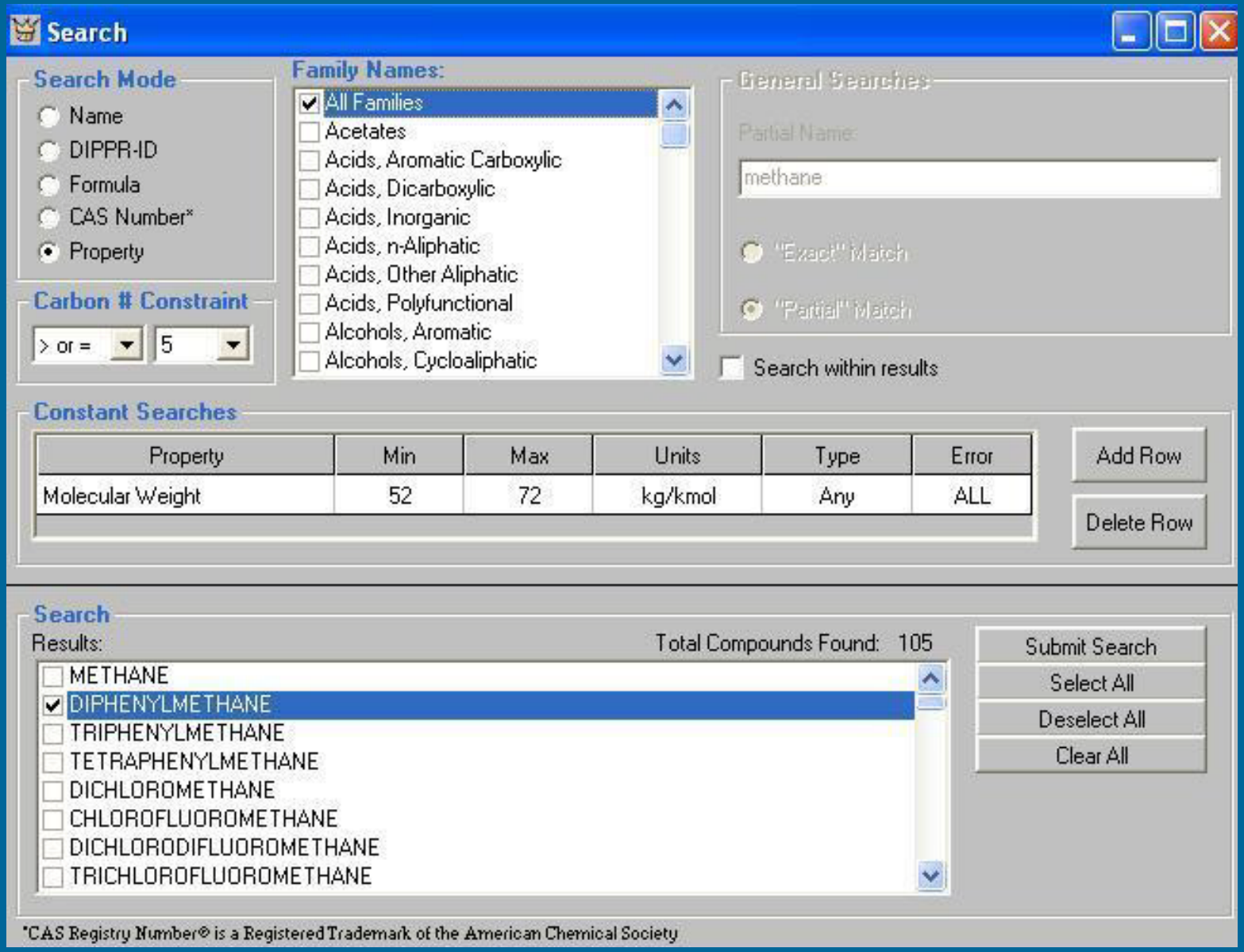
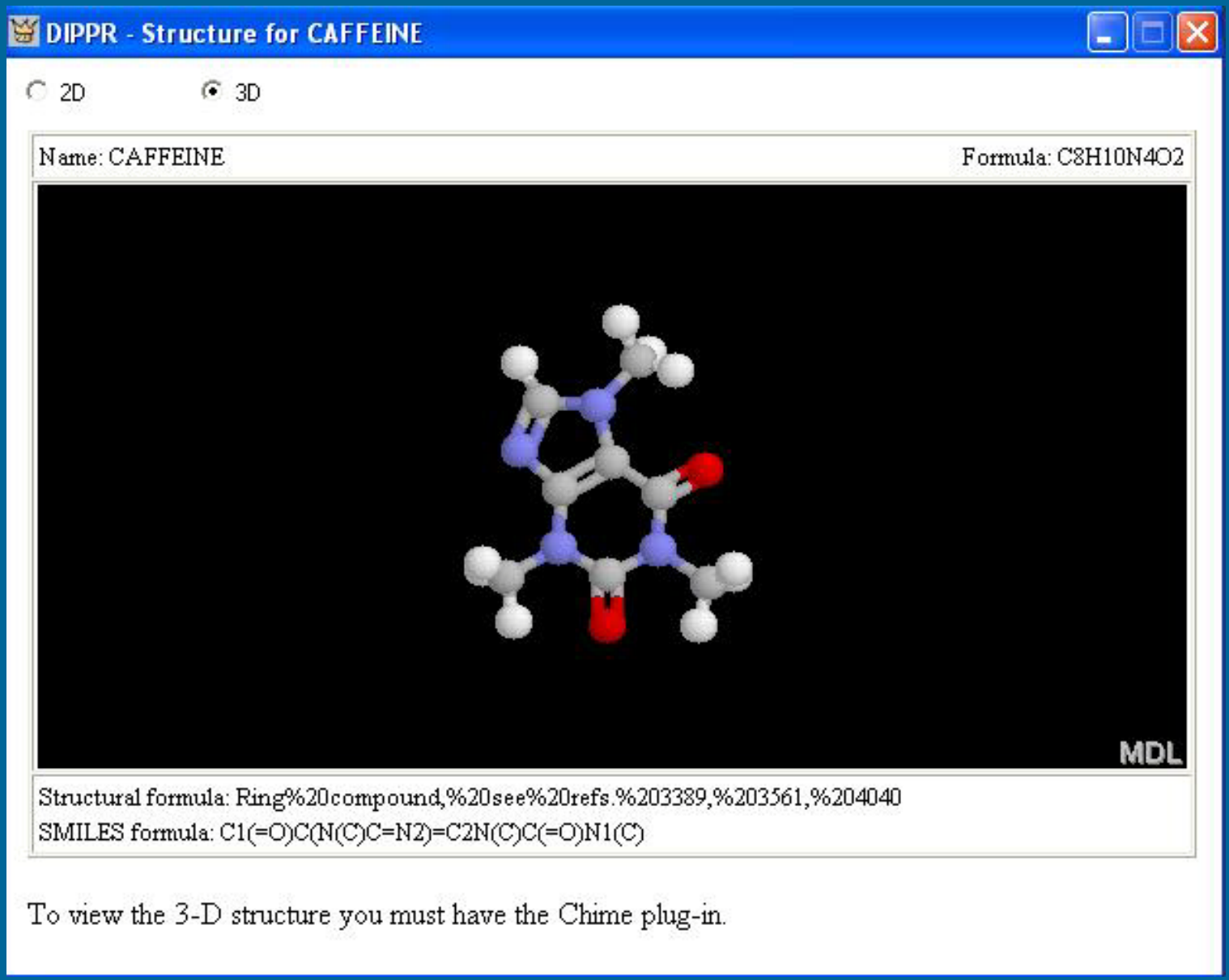


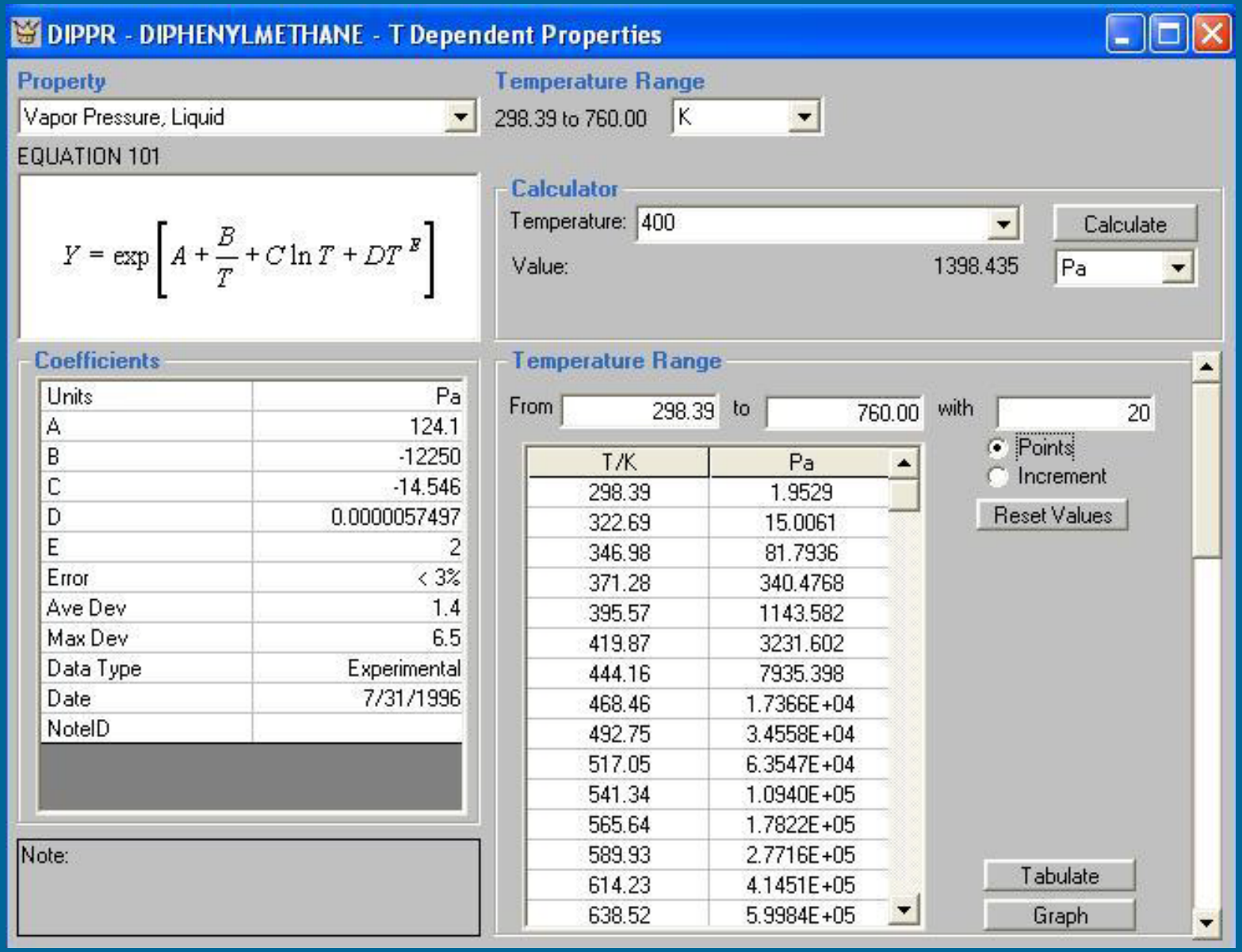
DIADEM is the official interface for the DIPPR® 801 database. Using DIADEM, users can view 2D and 3D images of compounds, plot constant and temperature dependent data and correlations, predict values for compounds using a variety of prediction methods, plus thousands of other options.



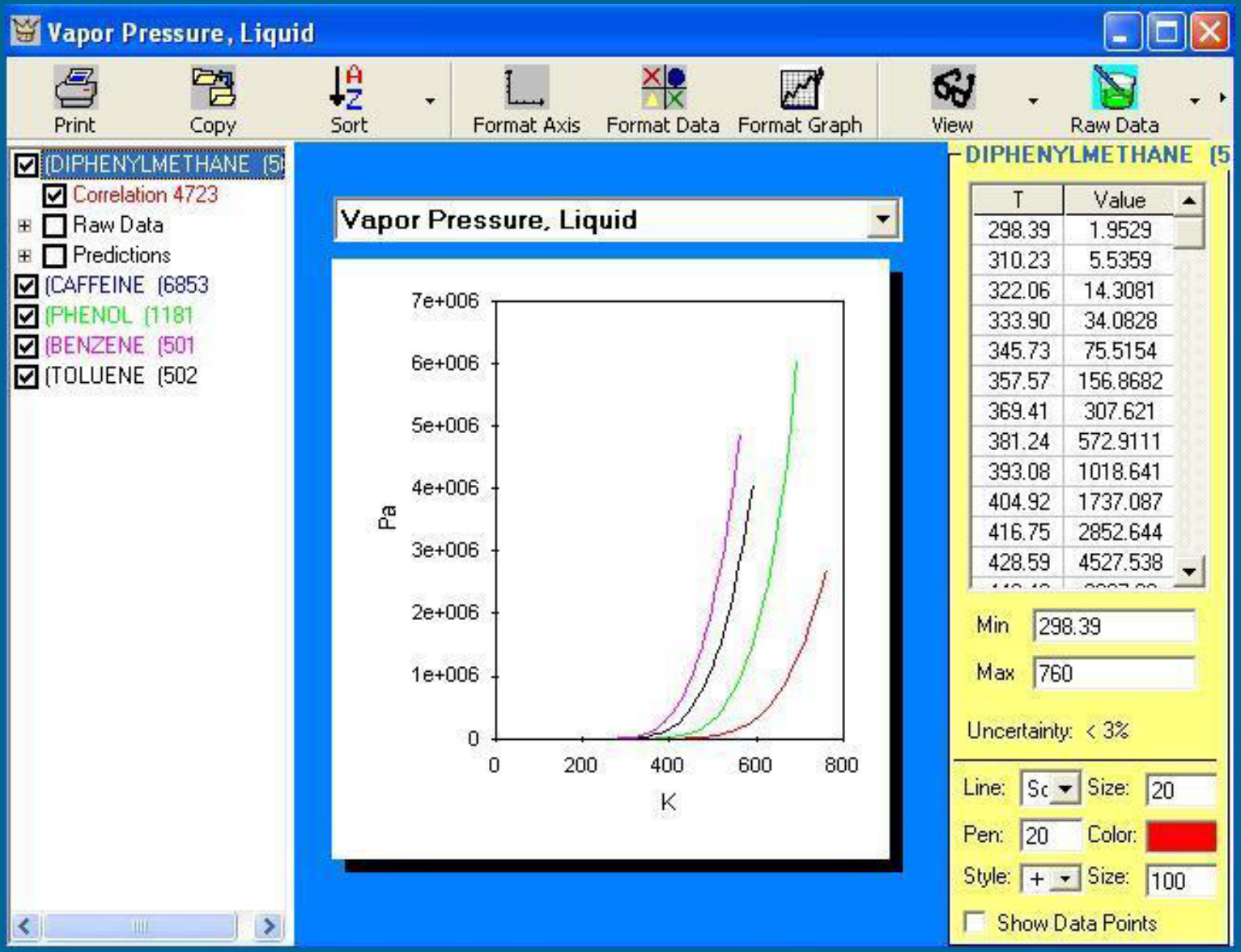
DIADEM's search capabilities include searching by compound name, formula, CAS #, carbon constraints, as well as by user-defined property criteria as is shown here.



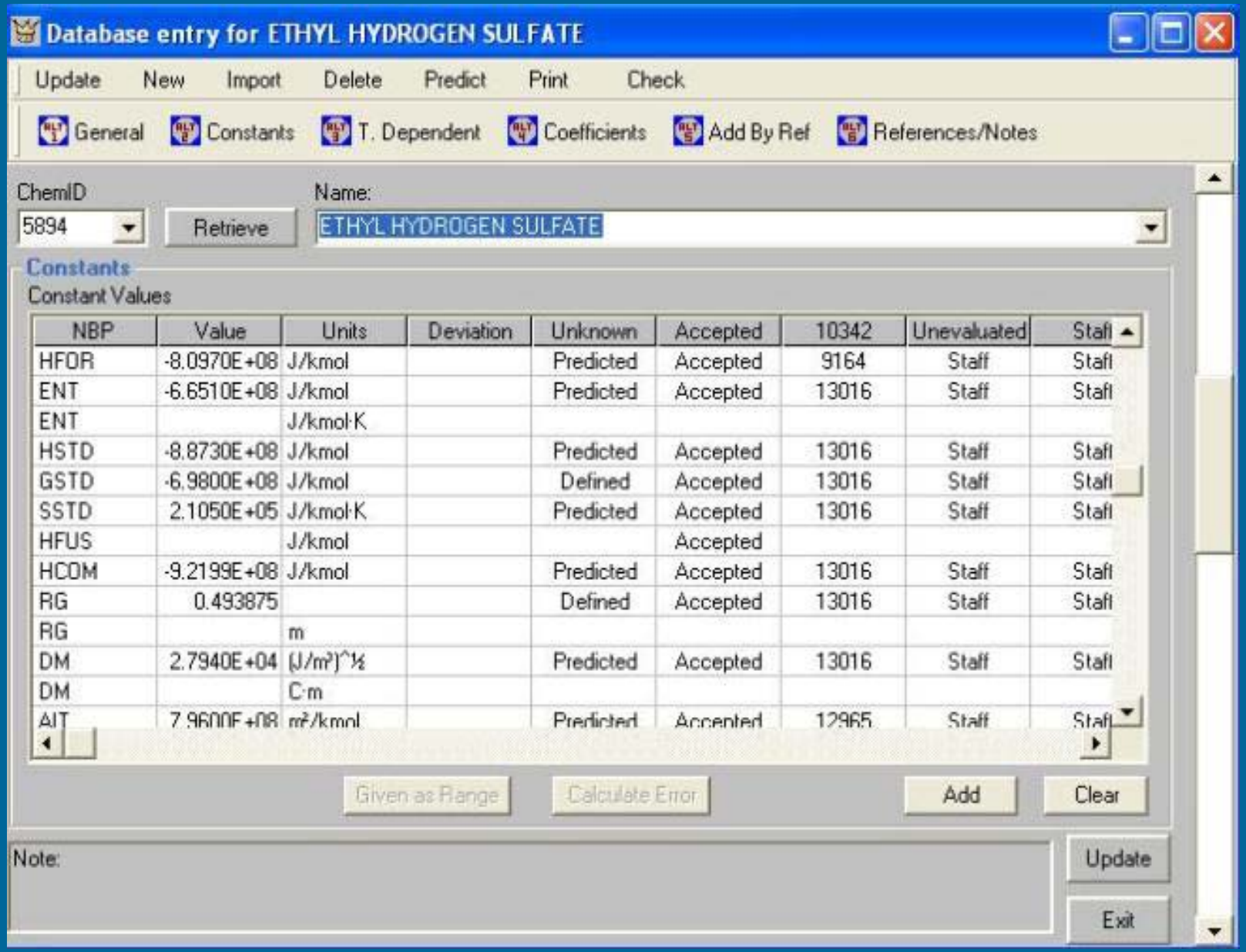
Users can view compound structures in 2- or 3-D and can rotate the compound in 3-D for viewing at many different angles.



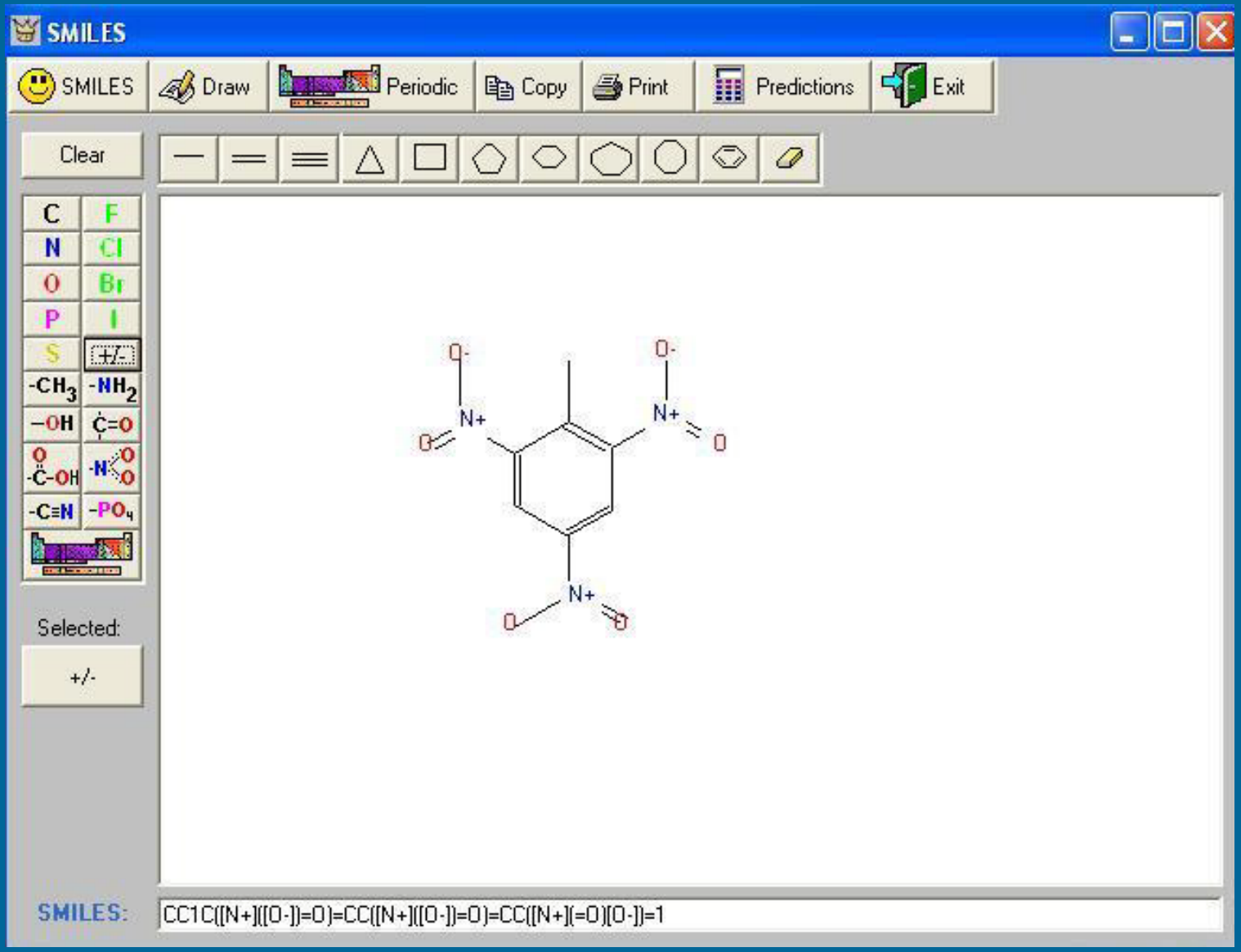
Users can calculate temperature dependent property values at a specific temperature or over a range of temperatures.



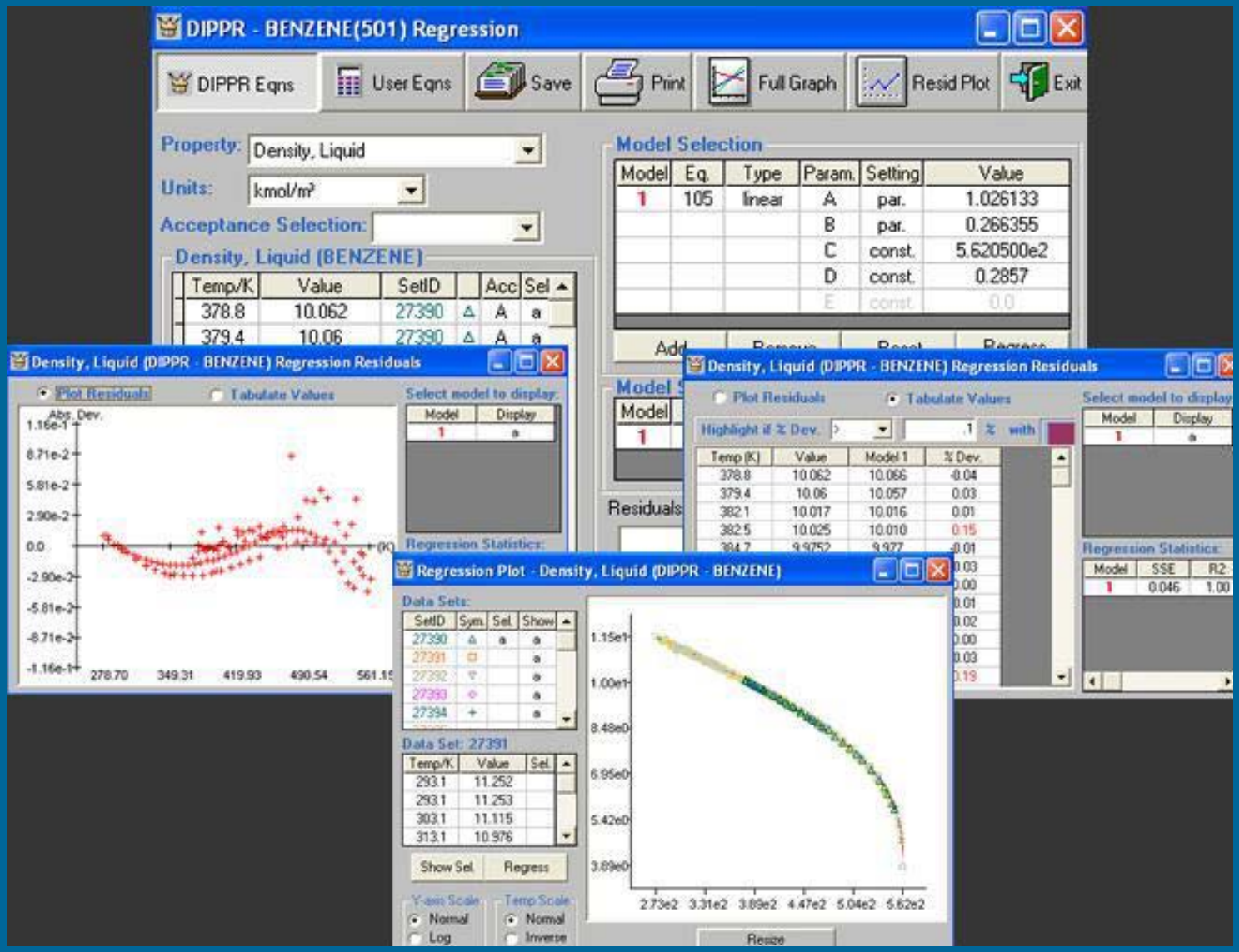
Use DIADEM to simultaneously plot data for multiple compounds for any of the properties in the DIPPR® 801 database. Plots can simultaneously include correlations, raw data, and predicted values.



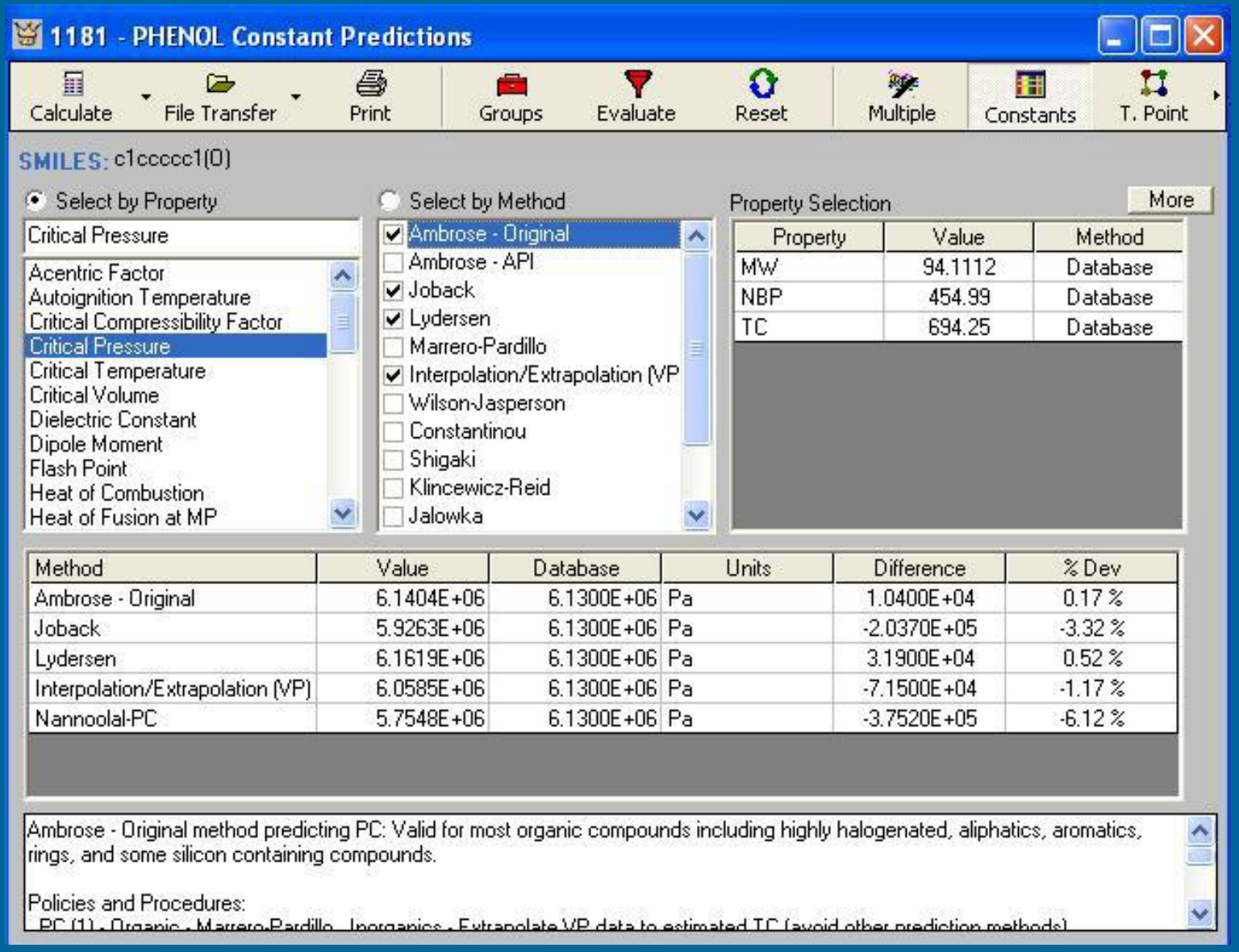
DIADEM enables users to create and maintain a database for user compounds and data. Then, the user's data can be easily compared to DIPPR® 801 data.



Draw a compound's structure and DIADEM will output a SMILES formula, or enter a SMILES formula and DIADEM will draw the structure.



DIADEM's regression package contains linear and nonlinear capabilities and allows regression of user equations. Data points used in the regression can be selected using the interactive regression graph. Residuals can be viewed in graphical or tabular form, with user-specified deviations highlighted.



DIADEM's prediction package allows users to select published predictive methods to estimate a properties for ANY compound, even those not included in the DIPPR® 801 database.