# ca1d

NAME
ca1d – Perform a consistency analysis on 1D spectrum

DESCRIPTION
This command starts the *PERCH ACA* module for an automated cost analysis. It calculates a shift prediction based on a given structure proposal and analyses whether the experimentally found signals can be explained by the given structure. A final report is generated including spectra, structure graphics, and a numerical match index.

When *ca1d* is entered or selected from the menu a dialog is shown that asks the user to locate the proposed structure (MOL file) and to specify the predicted spectrum should be stored:
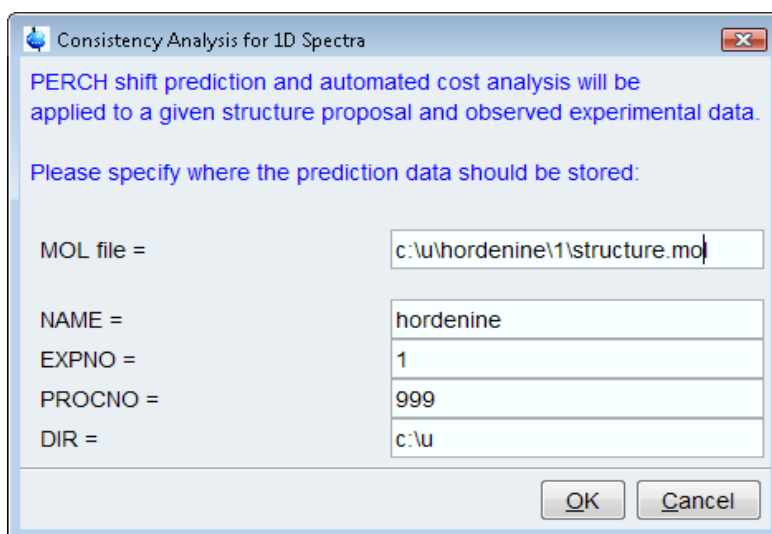

Once the consistency analysis has been started you can follow its operation by observing the messages TopSpin's status line. Please note that the *PERCH ACA* module is started in the background to perform the computing-intensive cost analysis. The command may run a couple of minutes or more to do the required calculations. After a successful run a specific plot layout is generated that documents the results. This layout is stored under the name *ca1d_report.xwp* in the data set that contains the prediction data.

The data window now automatically switches to the 'Plot' tab in order to display this layout.

It shows the original experimental data in the lower half. The spectrum in the upper half includes the predicted data and assigned group labels. Informative panels on the right show the proposed structure, an overview spectrum, numerical results of the cost analysis, and possibly further comments or warnings from the *ca1d* run.
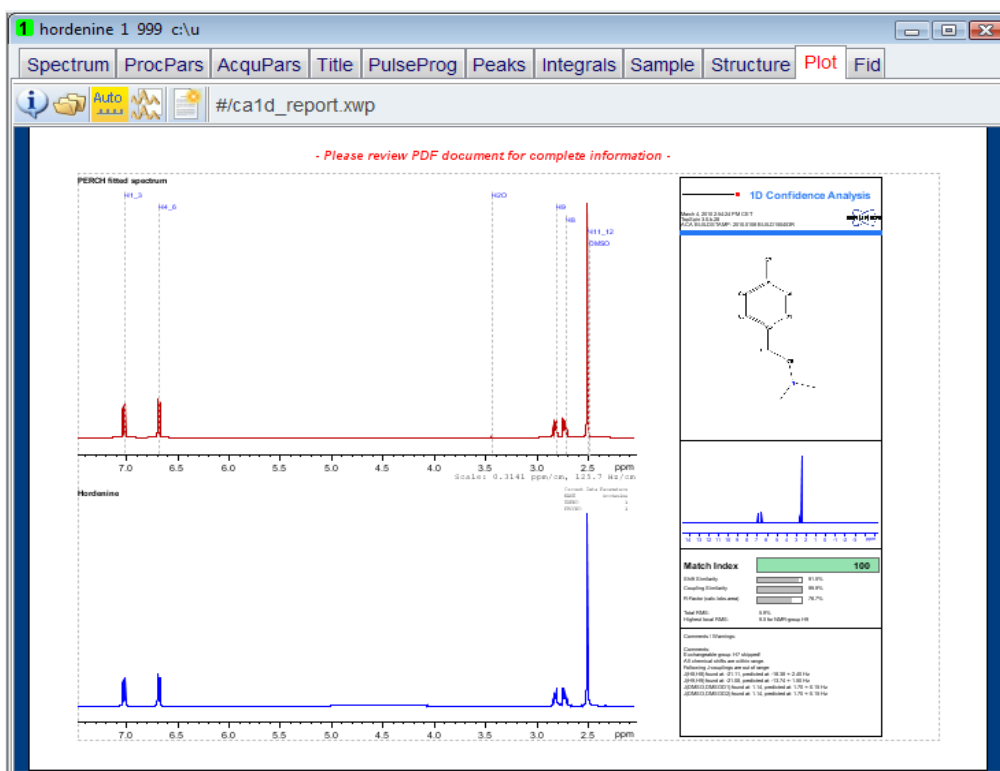
You can print this out by clicking the printer icon in TopSpin's toolbar (as always in the Plot window) . Note that *ca1d* has also created a complete report in the data set in PDF format. The PDF file contains the graphics as well as additional tables for experimental and predicted shifts and couplings:
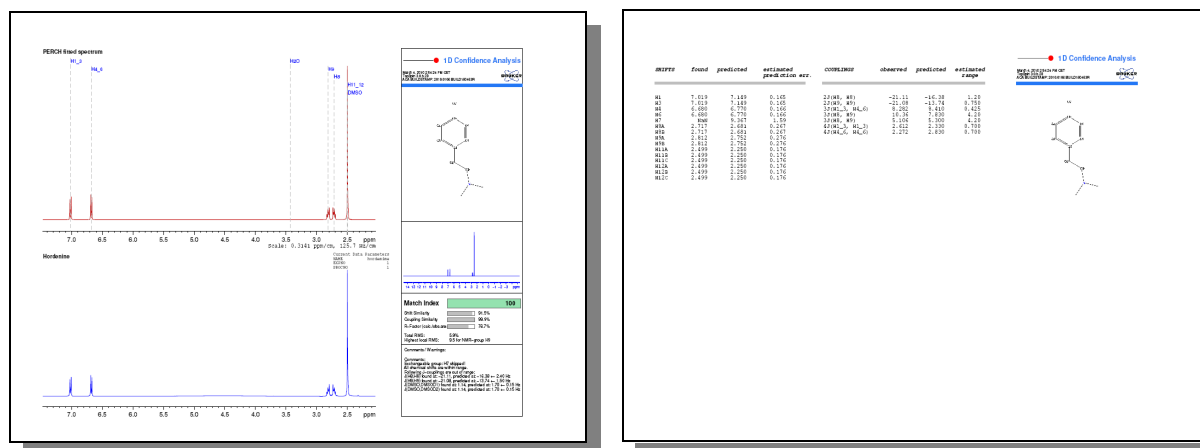
Please note the following preconditions for using ca1d:

- *The PERCH module must be present. Its installation is offered as part of the TopSpin installation procedure. If you have not installed it initially, you can do this at any time later from the TopSpin DVD.*

- *PERCH's functionalities are licensed separately. You may need to get additional license features from Bruker.*