ChemCorrect™
Organic Interference Identification Software

PICARRO

The **Picarro ChemCorrect software** is available for all Picarro L21x0-*i* water isotope analyzers. It is a unique software program that performs two functions:

1. Measures baseline shifts and other characteristics to detect organics that can skew isotopic ratio readings. It flags compromised samples, providing unparalleled confidence in sample fidelity, and by extension, sample analysis.
2. Provides a data processing program that automatically collects the data from known standards, generates a calibration curve and applies a correction to unknown samples to provide corrected values.

ChemCorrect should be used by all scientists that are studying the isotopes of water that may contain organic material. Various methodologies can be applied to running such samples. Please see our Application Note AN040: Accurate Water Stable Isotope Analysis of Organic Contaminated Water.

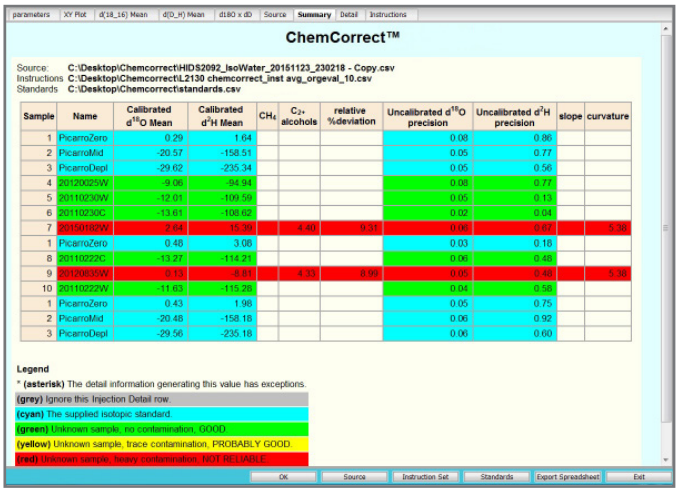
The software program compares a number of features in the spectra from the samples and the standards, applies a statistical test to see if the samples are different from the standards, and assigns flags based on the statistical differences. These flags alert the user to artifacts, potentially from contamination, that may affect the accuracy of your results.

ChemCorrect	
Provides easy-to-interpret, color-coded outputs for each water sample	Yes
Easy import of standard Picarro data files	Yes
Easy import of other data files in .csv (requires correct format)	Yes
Full data processing, including calibration correction	Yes
Flexible methods; number and placement of standards, number of injections, excluded injections pre sample	Yes
Results displayed graphically for all samples	Yes
Results can be easily exported to Excel for further processing	Yes
Evaluates spectral features from small organic molecules	Yes
Evaluates baseline skew, tilt and level for larger organic molecules	Yes
Fully automated organics flagging, no training samples required	Yes

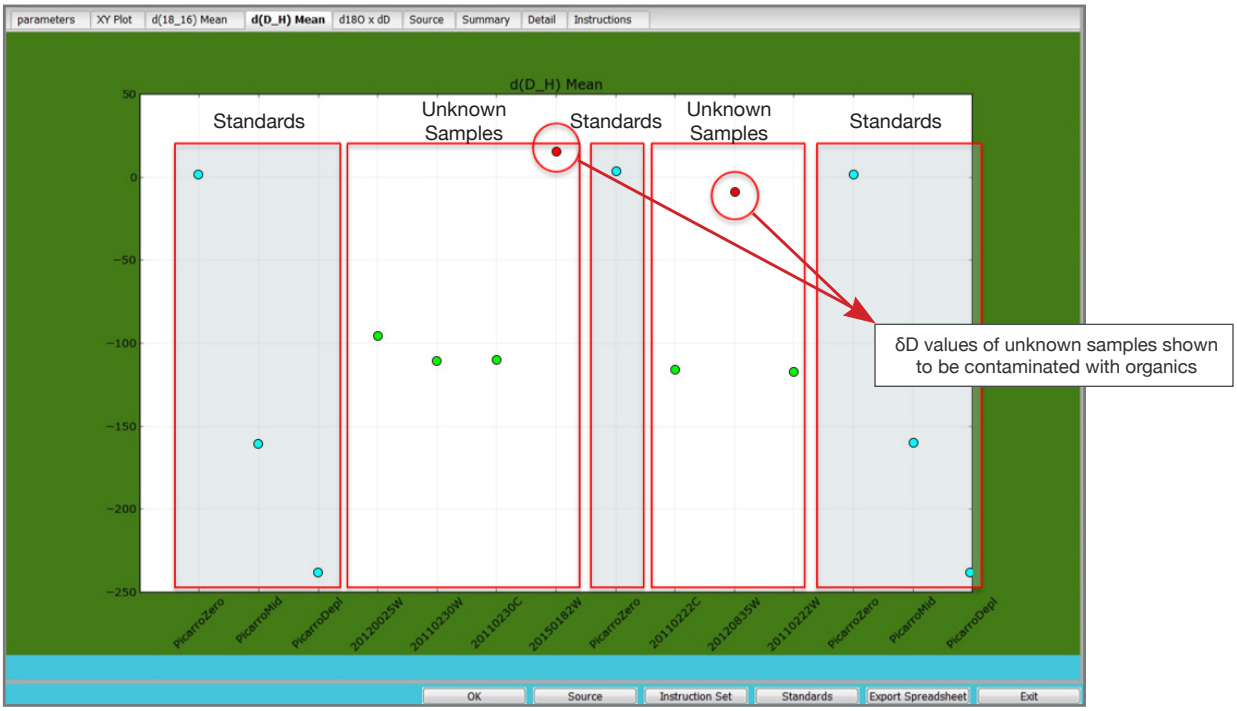
ChemCorrect Software Platform

The ChemCorrect software platform derives statistical data from spectral parameters acquired from each sample as part of the process of converting raw ring-down data into the highly accurate, temperature and pressure controlled spectral curves from which all Picarro concentration and isotope data are calculated. During data acquisition, the analyzer calculates residual fits of the raw data points to the final spectral output, as well as fundamental baseline characteristics such as the slope and curvature to assess data quality.

The software flags these indicators if they deviate from the thresholds set in ChemCorrect, coding the samples with red, yellow and green flags.



ChemCorrect color-coded output summary. Cyan indicates that the sample is a standard as specified by the user. Green indicates that the sample analysis is valid and does not present any signs of organic contamination. Yellow indicates that the sample contains trace amounts of organics and isotope values are slightly shifted. Red indicates that the sample analysis is highly compromised by organic contamination.



Example of ChemCorrect graphical display of δD values show standards (Picarro Zero, Mid and Depleted) in blue, and samples color-coded to represent organic contamination.

LIT CODE: ChemC-DS31-V2.0-210127

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