S1 IRMS methodology

The $\delta^2$H and $\delta^{18}$O measurements were done on a Delta+XL isotope ratio mass spectrometer coupled to a high-temperature conversion reactor (HTC) via a ConFloIII. The analysis method is described in Gehre et al. (2004). A daily sequence consisted of the DI1 or DI2 water samples, an in-house reference standard www-j1 (Willi Working Water-Jena1; $\delta^2$H: -66.45 ± 1.0 ‰, $\delta^{18}$O: -9.78 ± 0.10 ‰), an in-house scaling standard BGP-j1 (Brand Greenland Precipitation-Jena1; $\delta^2$H: -187.94 ± 1.0 ‰, $\delta^{18}$O: -24.46 ± 0.10 ‰), and an in-house quality control RWB-j1 (ReinstWasser Brand-Jena1; $\delta^2$H: -1 ± 1.0 ‰, $\delta^{18}$O: 7.8 ± 0.10 ‰). The daily average standard deviation of www-j1 was better than 0.16 ‰ (n = 44) for $\delta^{18}$O, and better than 0.7 ‰ (n = 41) for $\delta^2$H measurements. All in-house standards are regularly calibrated and checked against the international IAEA standards VSMOW2 and SLAP2. Thus the DI1 and DI2 isotope values are given on the VSMOW/SLAP scale.
Figure S1 Boxplots of root mean square error (RMSE) of $\delta^{18}$O, derived from calibrating [H$_2$O]-dependence of $\delta^2$H measurements by each of five fitting methods (i.e., linear, quadratic, cubic, quartic, linear surface fitting methods) for each of four calibration strategies: DI1, DI2, DI1-DI2*1Pair, DI1-DI2*2Pairs. The left-hand figures present boxplots of RMSE of $\delta^3$H measurements by the L2130i, depending on interval length (i.e., the time period used for calibrating [H$_2$O]-dependence). The right-hand figures display boxplots of RMSE of $\delta^{18}$O measurements by the L1102i, depending on interval length. The procedure for assessing [H$_2$O]-dependence uncertainties (= RMSE) is described in section 2.3.
References