

Supplementary Materials

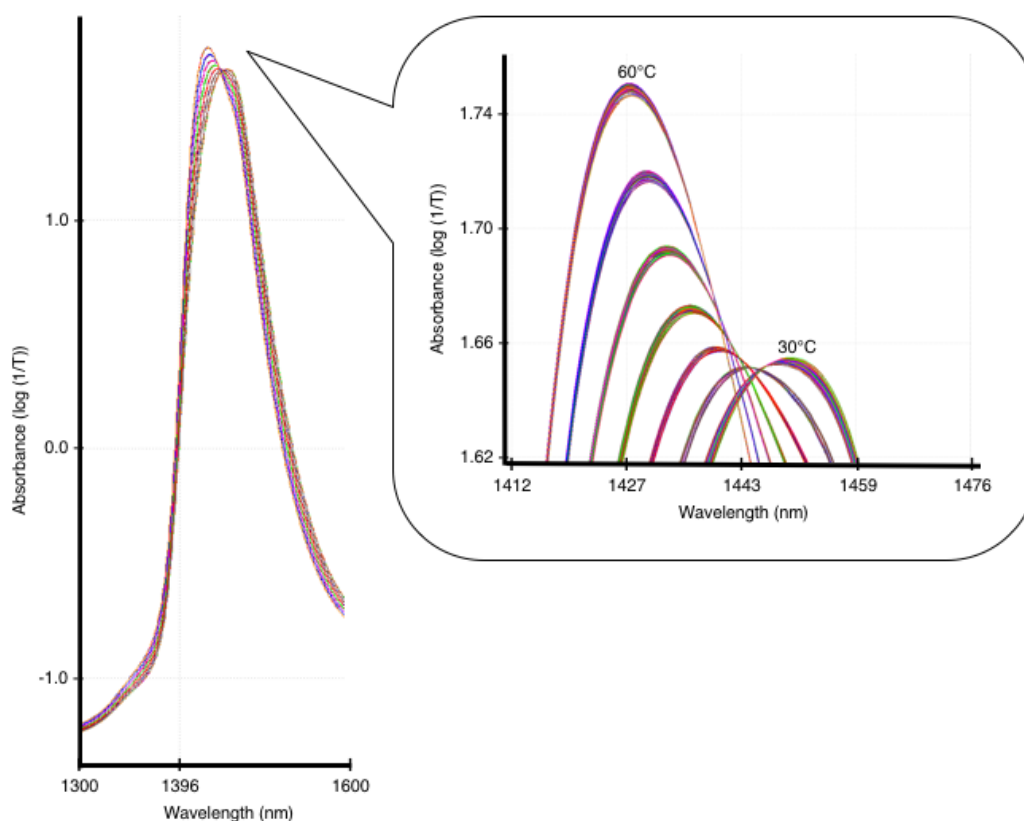


Figure S1. The SNV transformed NIR absorbance spectra of nine different waters at different temperatures in the 1300 – 1600 nm region (left). The magnified view of the same spectra around 1440 nm shows the peak shift to the left (blue shift) as a result of the temperature perturbation in 5 °C increments (right). To explore in detail complex spectral changes occurring as a result of increasing temperature and especially whether this approach helps in the discrimination between waters, preliminary assessment of NIR absorbance spectra of waters obtained at different temperatures (Figure S1) showed typical features of temperature influence: blue shift with the increasing temperature and an isosbestic point around 1442 nm.

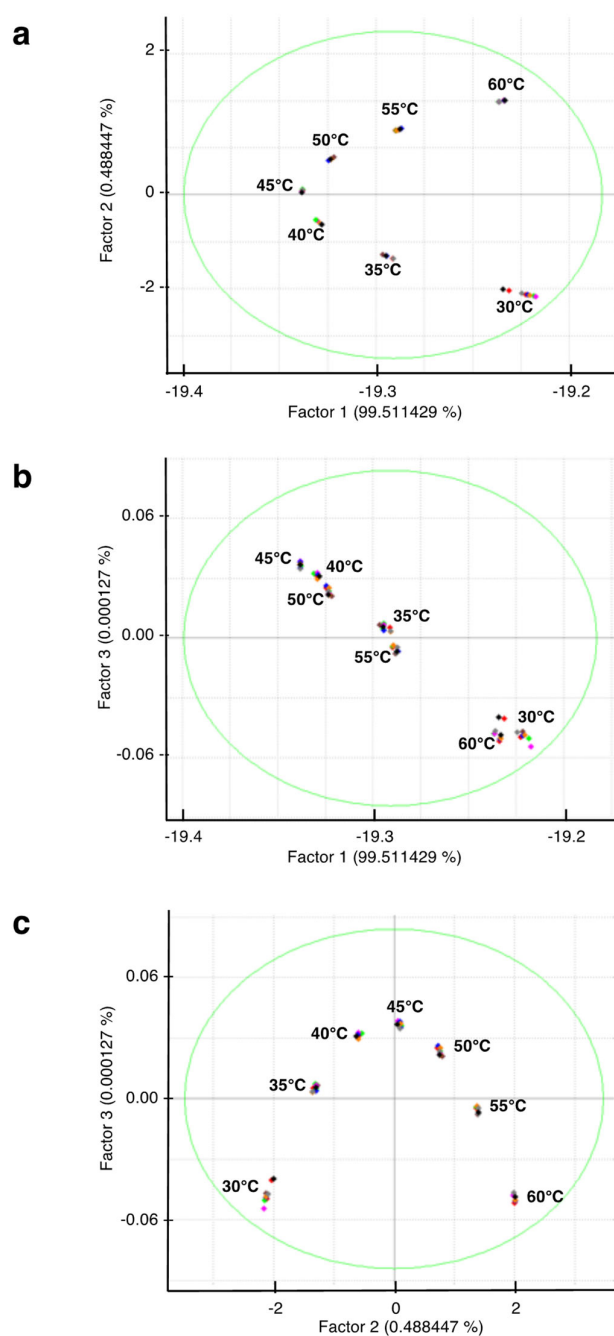


Figure S2. Principal component analysis (PCA) of nine different waters under temperature perturbation. The average spectral data at the given temperature are transformed using the SNV, smoothed using Savitzky Golay filter (25pts) and validated by leave-one-out step method. Spectral data, presented on score plots of (A) factor1 (PC1) vs. factor 2 (PC2), (B) factor 1 (PC1) vs. factor 3 (PC3) and (C) factor 2 (PC2) vs. factor 3 (PC3), reveal dominant influence of temperature. The percentage in brackets by near factors in the figure were explained by the total variance.

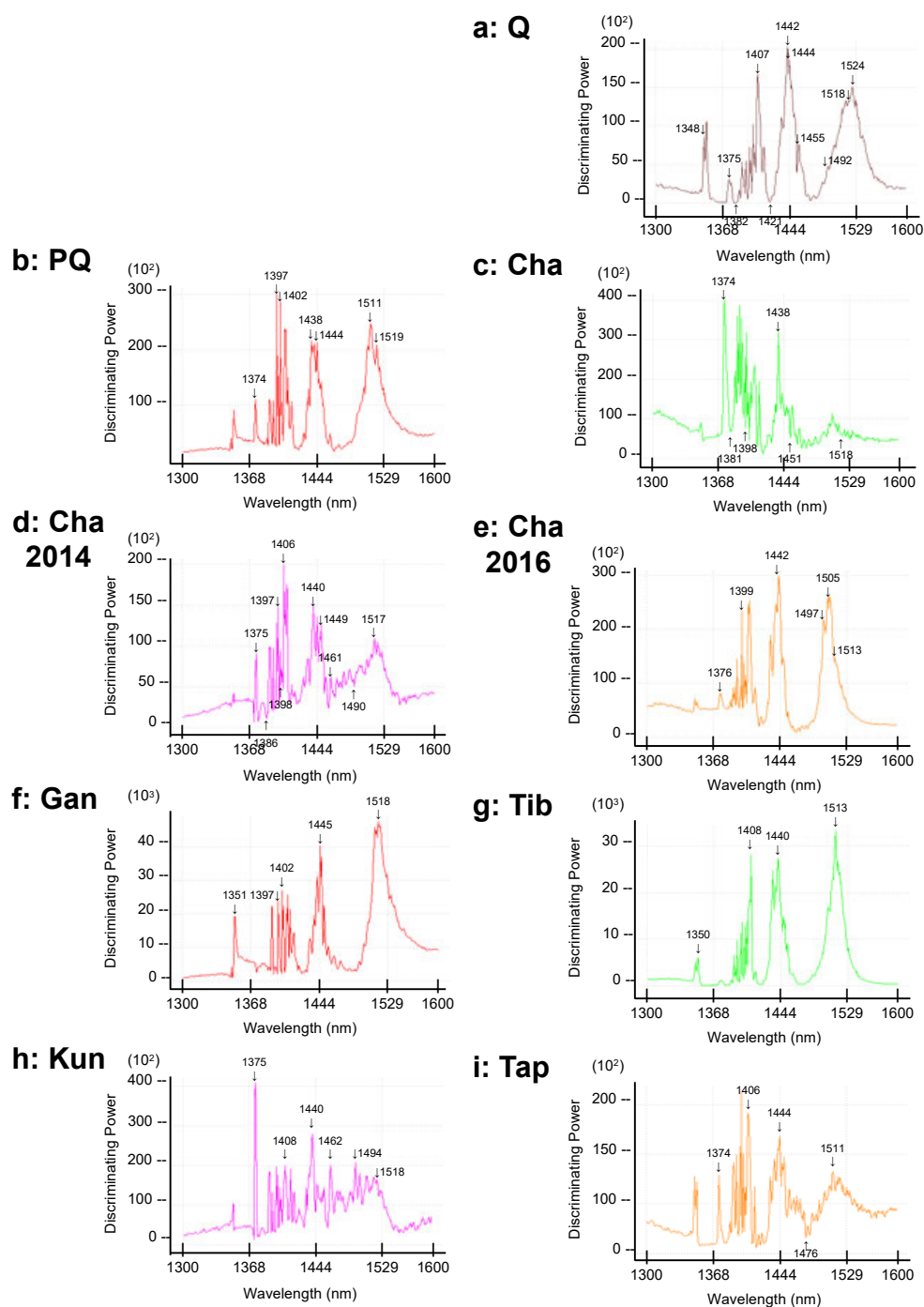


Figure S3. The discriminating powers of SIMCA indicate regions, which had highest discriminatory power for different stages of temperature perturbation (A: Q, B: PQ, C: Cha, D: Cha2014, E: Cha2016, F: Gan, G: Tib, H: Kun, and I: Tap). The gray bars show the regions from which specific wavelengths were selected for displaying the water absorbance spectral pattern in aquagrams. Spectra data transformed the snv and subtracted average Q at all temperatures.

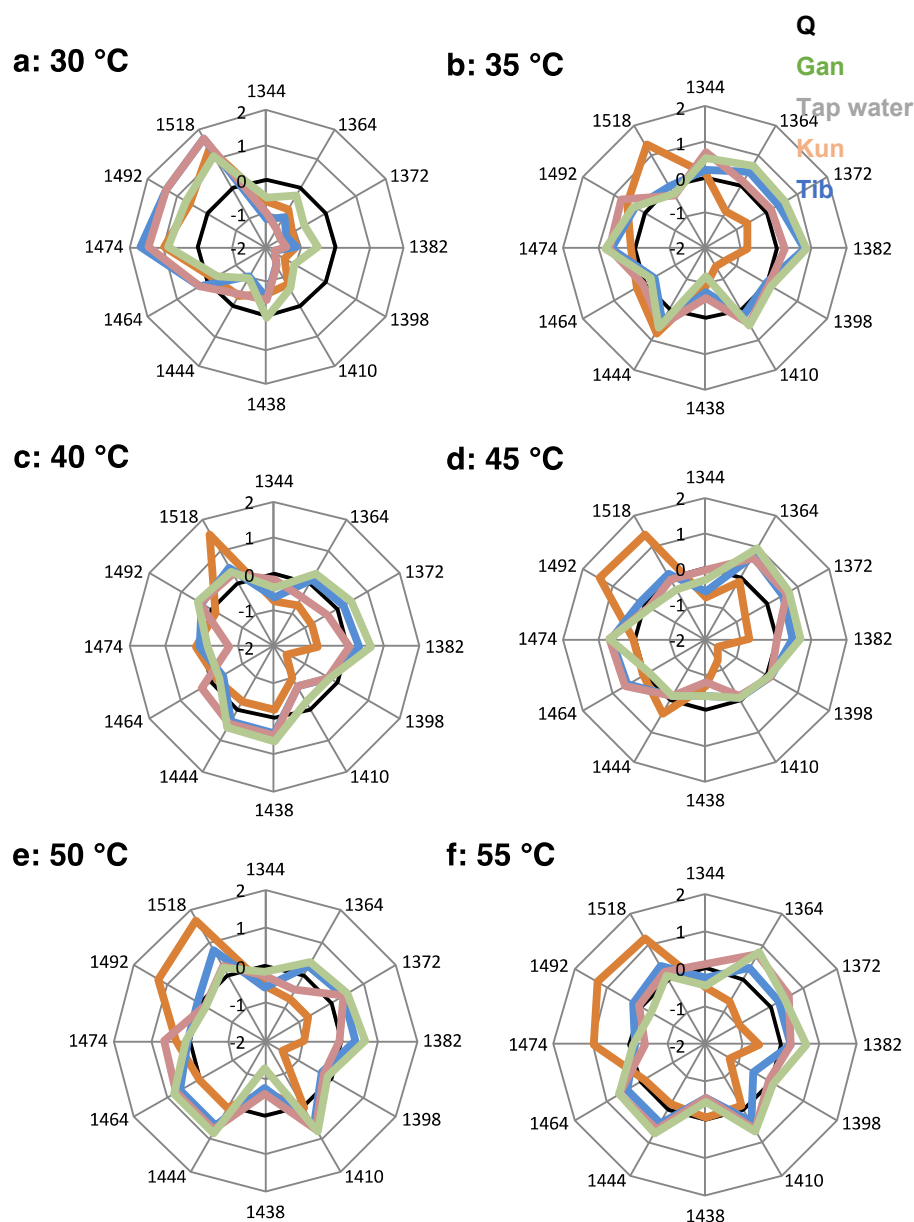


Figure S4. The aquagrams displaying the water absorbance spectral pattern of all analyzed waters under temperature perturbation: (a, 30°C; b, 35°C; c, 40°C; d, 45°C; e, 50°C; and f, 55°C). Normalized absorbance presented at radial axes is calculated as follows: an average of pure water at all temperatures was subtracted from the averaged spectra of each water at a specific temperature and SNV transformed. Different color of the lines represents different waters (Gan: orange, Tib: blue, Kun: pink, and Tap: green). Since all waters are being compared to the pure water, central zero line corresponds to the spectrum of pure water averaged across all temperatures (Q: black). Spectral data are SNV transformed and average Q across all temperatures is subtracted.

(%)	30°C	35°C	45°C	55°C
Q	83	89	94	82
PQ	78	89	78	67
Cha	89	100	100	100
Cha2014	100	100	100	78
Cha2016	67	89	89	67
Gan	89	89	100	89
Tib	89	100	100	89
Kun	78	89	89	78
Tap	78	100	100	78

Table S1. The percentage indicates that the accurate number exactly classified to each mineral water depends on the temperature. The exactly predicted number of misclassification/total number of experiments was calculated.