Journal of Hydrology 672 (2026) 135401

Contents lists available at ScienceDirect

Journal of Hydrology

journal homepage: www.elsevier.com/locate/jhydrol

Research papers

Online screening tool for precipitation stable isotopes records: hybrid distance / density based outlier filtering approach via interactive web application

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ARTICLE INFO

This manuscript was handled by Marco Borga, Editor-in-Chief, with the assistance of Daniele Penna, Associate Editor

Keywords:
Precipitation stable isotopes
δ^2H
δ^{18}O
d-excess
Outlier detection
Slovenia

ABSTRACT

The ratio between the heavy and light stable isotopes in precipitation is an effective tool for addressing questions in e.g., hydrology, climatology, biogeochemistry etc., but only if spatiotemporally sufficient data is available from precipitation monitoring networks. However, when data from multiple sources are gathered into large databases these can contain errors severely impacting research outcomes. The most common practices for stable isotopic database filtering apply static thresholds, not accounting for the spatially dynamically changing nature of the variable. We propose a distance-based outlier detection approach in the form of an online tool. The IsoQC App is developed to identify likely-outliers or inconsistent data points by deriving adjustable elevation-corrected average isotope values for nearby stations within an adjustable search radius ($0 < R \leq 500$ km). The IsoQC is showcased on the records of the precipitation stable isotope network of Slovenia and its vicinity. It enables an objective and reproducible analysis of spatial and temporal patterns of nearby precipitation stable isotopic records by employing thresholds for dissimilarity between regional averages and individual station records in a dynamic graphical user interface. The interactive nature of the application allows users to explore spatial and temporal variations in precipitation isotope compositions, identify anomalous data points, and empirically assess regional isotope patterns in real time. The developed IsoQC tool is freely available at https://sapps.geochem.hu/isoqc/

1. Introduction

The ratio of heavy to light stable isotopes in the water molecule ($^{18}O/^{16}O$;$^2H/^1H$) serves as a key tool in environmental isotope geochemistry, including hydrology, climatology, biogeochemistry etc. (Coplen et al., 2000). The stable isotopic composition of oxygen and hydrogen is conventionally expressed as δ values (δ^2H and δ^{18}O respectively) reported in per mille (‰) (Coplen, 1994). The stable isotopic composition of hydrogen and oxygen in precipitation (δ_p) offers insights into the origin of water vapor, the conditions attained during condensation, and precipitation (Aggarwal et al., 2016; Dansgaard, 1964). These variations make precipitation stable isotopes valuable natural tracers in water cycle studies (Bowen and Good, 2015; Fórizs, 2003) and have ignited the establishment of a Global Network of Isotopes in Precipitation (GNIP) (IAEA, 2019) and a few national networks collecting monthly composite precipitation samples and then determining and archiving their δ^2H and δ^{18}O values; such as the Austrian Network for Isotopes in Precipitation (ANIP) (Hager and Foelsche, 2015), the Chinese Network for Isotopes in Precipitation (Liu et al., 2014), the Australian Water Isotopes Network (Hollins et al., 2018) or the research platform like Slovenian Network for Isotopes in Precipitation (SLONIP) (Vreča et al., 2022). The mission of precipitation isotope monitoring networks is to provide basic isotope data for the use of environmental isotopes in hydro(geo)logical investigations (Rozanski

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https://doi.org/10.1016/j.jhydrol.2026.135401
Received 29 April 2025; Received in revised form 14 March 2026; Accepted 24 March 2026
Available online 25 March 2026

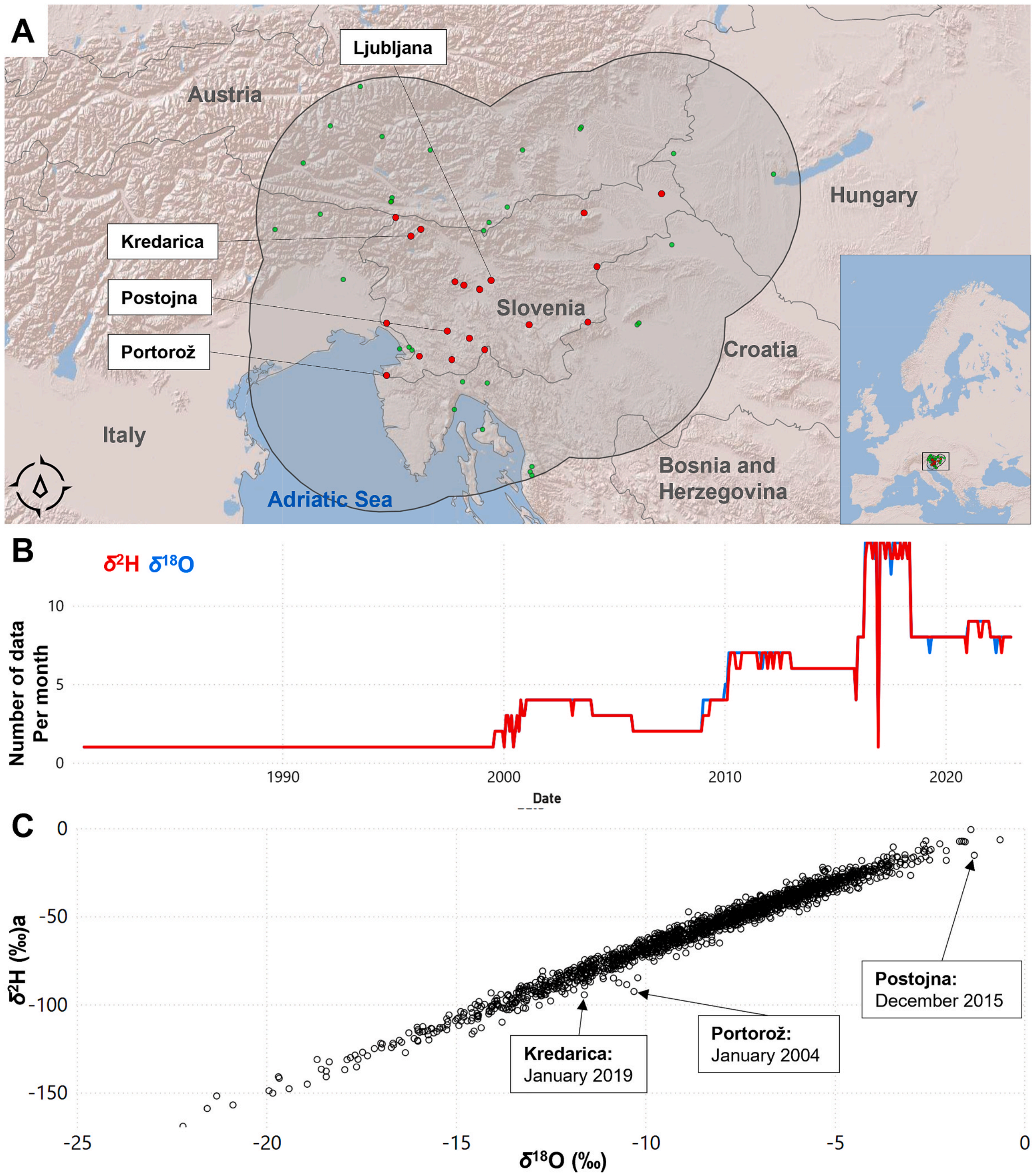

Fig. 1. Study area, monitoring sites and available raw data. Map of Slovenia and their δ_p monitoring sites (red dots) (A). For details on the Slovenian stations please see Table A1. Number of monthly Slovenian δ_p records obtained for the period 1981–2024 (B). $\delta - \delta$ cross plot of all of monthly δ_p records (C) with the selected anomalies annotated and listed under the station name for the Slovenian data. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

et al., 1993) within the scope of water resources inventory, planning and development (IAEA, 2019).

An outlier is "an observation which deviates so much from other observations as to arouse suspicions that it was generated by a different mechanism" (Hawkins, 1980b). Outlier detection is the most fundamental step in preprocessing data, since they can significantly bias experimental results and lead to misinterpretation. Outliers have existed for as long as data has been collected. As early as the 18th century, Bernoulli (1777) was intrigued by the notion: "discarding any values that seemed discordant and behaving as if the remaining observations constituted the entire sample". Since then, the treatment of outliers has remained a central issue in all scientific disciplines that rely on data (Barnett and Lewis, 1974; Hawkins, 1980a; Pearson and Sekar, 1936).

In hydrology, outlier detection has been a topic of debate for decades (Bárdossy and Kundzewicz, 1990; Hu, 1987; Kirk and McCuen, 2008), yet in isotope-hydrology, it has not received the required attention. Although a plethora of tools and approaches exist that could be adopted for this subdiscipline (e.g. Angiulli et al. (2006); Knorr et al. (2000)), it is essential to account for the mechanism(s) by which outliers are believed to be generated so that, despite appearances, they can be correctly classified within the distribution under study (Hawkins, 1980b).

Isotope hydrological research studies extracting δ_p time series from on-line databases typically do not entertain the possibility of erroneous δ_p records or lack the documentation of database screening. While some outliers may be removed upon database compilation (IAEA, 1992), many potential outliers still remain undetected since such datasets are not rigorously and systematically screened for errors (Erdélyi et al., 2024). In the few positive examples, the secondary isotopic parameter so-called deuterium excess or d-excess — calculated as $d = \delta^2H - 8 \times \delta^{18}O$ (Dansgaard, 1964) — was applied for outlier screening. An early example proposed that d-excess values < 3‰ should be handled with caution (Harvey, 2005). Later studies removed all δ_p values corresponding to d-excess values outside the range of −10‰ to +30‰ (Bowen et al., 2018), while some applied even wider thresholds, keeping δ_p values corresponding to d-excess between −30‰ and +50‰ (Nelson et al., 2021). It is unquestionable that δ_p related to such d-excess are unreliable; however, δ_p with less striking d-excess values may also be indicative of outlying data. This can practically be considered as an analogue to a density-based outlier detection approach (Boniol et al., 2023; Smiti, 2020), but lacking the spatial aspect.

In the case of the Tibetan Network for Isotopes in Precipitation, a static threshold was used to find outliers based on the $\delta^{18}O$ variable. $\delta^{18}O$ records which were > 5‰ and strongly deviated from surrounding data were considered as aberrant (Yao et al., 2013). Nevertheless, the study does not clarify the criteria for defining "deviation from surrounding" data, rendering the approach irreproducible. This last example highlights the importance of the 'spatial aspect' in outlier detection of isotope hydrological data.

Errors during sample collection, storage, handling, analysis and/or data entry (e.g., retyping or copying) can impact stable isotope composition values in the database, producing similar effects as natural variations (Coplen and Qi, 2009; Nigro et al., 2024); see Sect. 2.2 for additional details. These data errors can result in extreme values that are indistinguishable from natural variations when inspecting data from only a single station. Therefore, the simultaneous examination of δ_p time series from nearby stations is essential for differentiating isotopic signals associated with small-scale natural effects from possible database errors. Such database errors may appear only at a single station and may not be reproducible at neighboring stations, even those just a few kilometers apart. This is the fundamental idea behind distance-based outlier detection procedures (Muhr and Affenzeller, 2022; Smiti, 2020).

The efforts toward a distance-based outlier detection approach in precipitation stable isotopic databases have only recently emerged, integrating local Moran I statistics (Moran, 1950) and a predefined threshold for d-excess (Erdélyi et al., 2023). A more advanced distance- and density-based approach was introduced using the ANIP as an example, yet it remained heavily dependent on expert judgment and the assessment of monitoring data within quasi-subjectively defined spatial domains (Erdélyi et al., 2024). These works addressed the problem of outlier detection in isotope hydrology, but required extensive manual effort and included an element of subjectivity in the decision-making process. Therefore, there is a clear need for discipline-specific tools tailored to the particular characteristics of isotope hydrology while minimizing reliance on subjective assessments.

The aim of the present study is to introduce a newly developed online tool, the Isotope Quality Control Application, IsoQC App for short, for preprocessing meteoric water stable isotopic data collected at uniform sampling frequency across multiple locations to identify possible database inconsistencies. The proposed tool supports the standardized quality control of isotope records across different databases and facilitates harmonious interoperability based on FAIR data principles (Wilkinson et al., 2016). The online app was tested on data collected since 1981 in Slovenia and its neighboring countries.

2. Materials and methods

2.1. Monthly precipitation stable isotope records from Slovenia and its surroundings

Systematic measurements of the stable isotopic composition (i.e. δ^2H and $\delta^{18}O$) of precipitation were commenced in 1972 in Slovenia at three stations (Gospodarič and Habič, 1976). However, the gathered data were not archived properly, and are thus unavailable. In the past decades, stable isotopes have been monitored at more than 30 different locations in Slovenia but many of them, especially those which operated only for a relatively short period, reported only aggregated values, or essential metadata (e.g. geographical coordinates) remains unpublished (Vreča et al., 2018; Vreča and Malenšek, 2016). The main types of missing information were identified in the past as: a lack of information about sampling (e.g. sampling period, sampling frequency, sample treatment and sample storage), and methods (e.g. type of collector, instrumentation, quality control, measurement uncertainty) (Vreča and Malenšek, 2016). Only a few stations have been in operation for more than four years and the data from 8 stations are being included into the publicly available SLONIP research platform (Vreča et al., 2022). Note that three sites - Ljubljana, Kozina, and Portorož - provided data to the GNIP (IAEA, 2019) but only until 2003.

To test the IsoQC App, monthly δ_p values (1718 δ^2H data and 1797 $\delta^{18}O$ data) were acquired from 19 stations in Slovenia from the period of 1981–2022 (Table A1). The main source was the SLONIP research platform (Vreča et al., 2022) whereas additional monthly composite precipitation δ^2H and/or $\delta^{18}O$ data were retrieved from the Jožef Stefan Institute (IJS) archive (unpublished data). Additional monthly composite precipitation δ^2H and/or $\delta^{18}O$ data were collected from research papers (Domínguez-Villar, 2018; Gačnik et al., 2026; Koren Pepelnik et al., 2025, 2026; Krklec et al., 2018; Rusjan et al., 2019) and doctoral dissertations (Doctor, 2002; Mali, 2006; Zavadlav, 2013) (Fig. 1, Table A1).

The fewest data ($N = 12$) were available from Sela na Krasu (Doctor 2002), while most data were available at Ljubljana recording 476 $\delta^{18}O$ and 473 δ^2H measurements between May 1981 and December 2022 (Table A1). The time when most stations were providing data in parallel was between 2016 and 2018 (Fig. 1B).

It is expected that the δ_p monitoring stations closer to each other should provide more similar observations, regardless of national borders (Hatvani et al., 2021). Thus, besides the precipitation stable isotope records available from within the national borders of Slovenia, additional records were gathered from the neighboring countries along the border and used in the screening process to validate the regional (dis) agreement of potentially erroneous data spotted in the Slovenian set of precipitation stable isotope data. Specifically, those stations were considered from neighboring countries that operated between 1981 and 2022 and were located within 90 km of at least one Slovenian station. The final selection area corresponds to the union of all 90 km radius circles centered on the Slovenian stations, that is, the cumulative coverage of these overlapping circular buffers, ensuring that all stations within this merged region are considered (Fig. 1A). These included mainly GNIP ($N = 6$) (IAEA, 2019) and ANIP ($N = 12$) stations, complemented with additional ones from Hungary ($N = 2$) (Kern et al., 2020), and Croatia ($N = 8$) (Karlović and Marković, 2020; Krajcar Bronić et al., 2020; Mance et al., 2022; Paar et al., 2019).

2.2. Methodology

Stable isotope ratios in precipitation are primarily determined by kinetic and equilibrium isotopic fractionation associated with the processes of evaporation and condensation, and atmospheric transport in the global water cycle (Dansgaard, 1964; Eriksson, 1965). Considering that these physical processes (such as atmospheric circulation, topography, and air temperature) controlling δ_p variations are characterized by considerable spatial autocorrelation (Di Cecco and Gouhier, 2018; Eshel et al., 2022), notable spatial associations among nearby δ_p variations can reasonably be assumed. Hence, a distance-based outlier screening approach was followed when developing the IsoQC App, the foundations of which were laid down previously (Erdélyi et al., 2024; Kracht et al., 2014). It is also an important requirement that the outliers

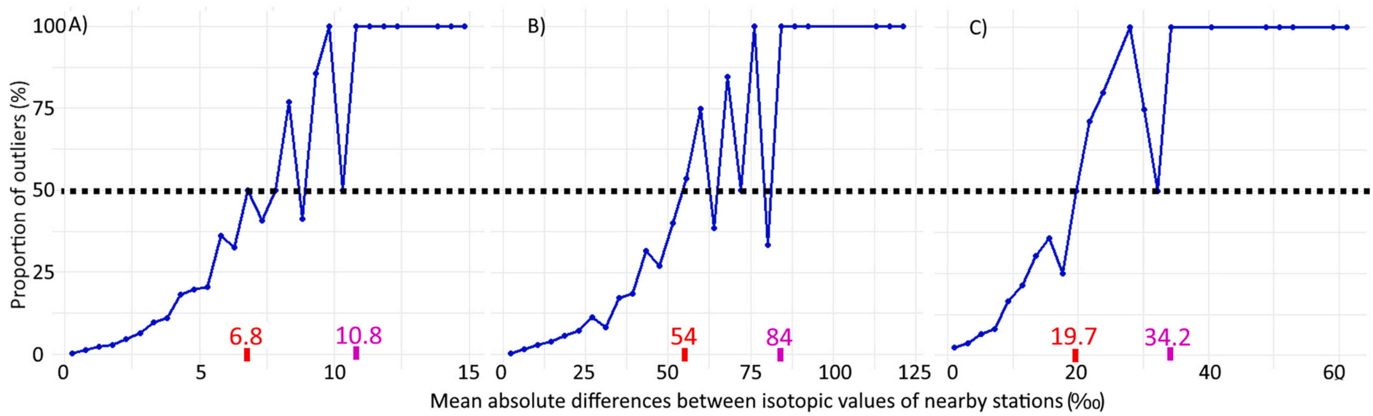

Fig. 2. Mean absolute difference vs. proportion of outliers for δ^{18}O (A), δ^2H (B) and d-excess (C). The blue line illustrates how the number of cases classified as likely outliers increases with the difference in X. The black dashed line indicates the 50% level above which more cases are considered as outliers than not. The red values mark the smallest mean absolute differences corresponding to the 50% level. These are the default thresholds in the IsoQC app and also used in the present study. The purple values mark the mean absolute differences corresponding to the 100%-level. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

are not to be explored individually, but the dataset with all of its discordant values is investigated as a whole (Pearson and Sekar, 1936), together with its neighboring observations, a criterion that is met by our suggested approach. Two main types of potential outliers are considered here from a persistence point of view: potential point anomalies (isolated erroneous data points) and interval/collective anomalies (sequences of points sustaining a deviation over time) (Boniol et al., 2023; Erdélyi et al., 2024).

2.2.1. Elevation effect

The strongest driver of the isotopic composition of precipitation at short distances stems from the adiabatic cooling of the air masses as they ascend on a mountain. This is accompanied by the rainout of the excess moisture (Gonfiantini et al., 2001) which results in a gradual depletion of ^{18}O and ^{2}H isotopes as elevation increases (Dansgaard, 1964). Thus, when comparing the stable isotopic compositions of meteoric water samples from stations operating in diverse relief conditions, the correction for altitude effect is a necessity. To standardize the meteoric stable isotope values across different altitudes, the tool enables an elevation correction (Eqs. (1a) & (1b)) based on defined lapse rates:

$$\delta^{18}O_{corr,i} = \delta^{18}\mathrm{O}_i + g_{\delta^{18}\mathrm{O}} \times \frac{(h_i - h_f)}{1000} \tag{1a}$$

$$\delta^2\mathrm{H}_{\mathrm{corr,\,i}} = \delta^2\mathrm{H}_i + g_{\delta^2\mathrm{H}} \times \frac{(h_i - h_f)}{1000} \tag{1b}$$

where: $\delta^{18}\mathrm{O}_{\mathrm{corr,i}}$, $\delta^2\mathrm{H}_{\mathrm{corr,i}}$ are the elevation-corrected isotopic values at station i, $\delta^{18}\mathrm{O}_\mathrm{i}$, $\delta^2\mathrm{H}_\mathrm{i}$ are the observed isotopic values at station i, $g\delta^{18}_{\mathrm{O}}$, $g^{2}_{\delta\mathrm{H}}$ are the user-defined elevation correction coefficients (‰ km^{-1}), h_i is the altitude of station i, and h_f is the altitude of the focal station.

Under different geographical and topographical conditions, the regional isotopic elevation effects were reported ranging from −1.7 to −5.0‰ km^{-1} for δ^{18}O in precipitation (Poage and Chamberlain, 2001). In the regions from which the example data are derived from (Fig. 1A), the 'altitude' effect was documented to be −1.2‰ km^{-1} for δ^{18}O and −7.9‰ km^{-1} for δ^2H (Kern et al., 2020). The latter values are set as defaults in the IsoQC App. However, these are adjustable and should be modified for each region of interest accordingly.

2.2.2. Distance-based outlier detection

The core of the IsoQC App lies in dynamically determining a search radius, a subset of the whole (called outlier detection solving set) is formed. It is a fundamental requirement that the solving set includes a sufficient number of points that permits the detection of the outliers based on only a subset of the complete dataset (Angiulli et al., 2006). Therefore, in the IsoQC App the solving set is dynamically determined by selecting a so-called focal station and determining its 'nearby' stations. A station is considered 'nearby' if it lies within an adjustable radius R. The distance matrix is computed pairwise using geodesic distance (Vincenty, 1975) with the geosphere::distGeo() (Hijmans et al., 2017) in R (R Core Team, 2019) function (Eq. (2)) between the locations, i.e. considered the curvature of the Earth using the WGS84 ellipsoid.

In the IsoQC App, R is set to 90 km by default, chosen based on the semivariogram ranges of precipitation stable isotope records of the Alpine realm (Kern et al., 2015) and Iberian Peninsula (Hatvani et al., 2020). The adjustable R is maximized in 500 km to avoid the "accidental" comparison of very remote sites. The mean elevation-corrected isotopic values of nearby stations at the same time step are computed as follows. For each station i, the mean isotopic values of the nearby stations i) (within R) are computed for the same time step t:

$$\overline{\mathrm{X}}_{i,\,t} = \frac{1}{N_{i,\,t}} \sum_{j \in S_{i,t}} \mathrm{X}_{j,\,t} \tag{2}$$

where X represents the δ^{18}O, δ^2H, or d-excess values, t is the specific time step (in the present study month), $\mathrm{S}_{i,t}$ is the set of nearby stations for station i that also have data available at time t, $N_{i,t}$ is the number of nearby stations for station i that also have observations at time t. Note, the data of the focal station (i) are not included when calculating $\overline{\mathrm{X}}_{i,t}$. Ultimately the difference between $\overline{\mathrm{X}}_{i,t}$ and $\delta^{18}\mathrm{O}_{i,t}$, $\delta^2\mathrm{H}_{i,t}$, or d-excess$_{i,t}$ values are calculated denoted as $D_{i,t}$, guiding the screening procedure. The core of the approach is similar to that developed for outlier detection in large scale ambient air quality datasets (Kracht and Gerboles, 2013; Kracht and Gerboles, 2015; Kracht et al., 2014). Nevertheless, it specifically incorporates isotope hydrological concepts, such as the d-excess and correction for the isotopic altitude effect.

The data filtering exercise of Erdélyi et al. (2024) on the ANIP provided the foundation for determining the preliminary threshold(s) to separate the δ^{18}O, δ^2H and d-excess values into outliers and normal data and use the experience gathered to indicate whether $X_{i,t}$ belong to normal data or potential outlier from the perspective of the focal station's time series compared to the solving set. For each of the variables, $\overline{\mathrm{X}}_{i,t}$ were grouped into 31 uniform bins and plotted along with the ratio of corresponding cases classified as outliers in the particular bin. This helps to see how the proportion of outliers increases as the mean absolute difference between the nearby stations' values increase (Fig. 2). This allowed to determine an empirical threshold for all three parameters, above which more records (> 50%) are considered as outliers than

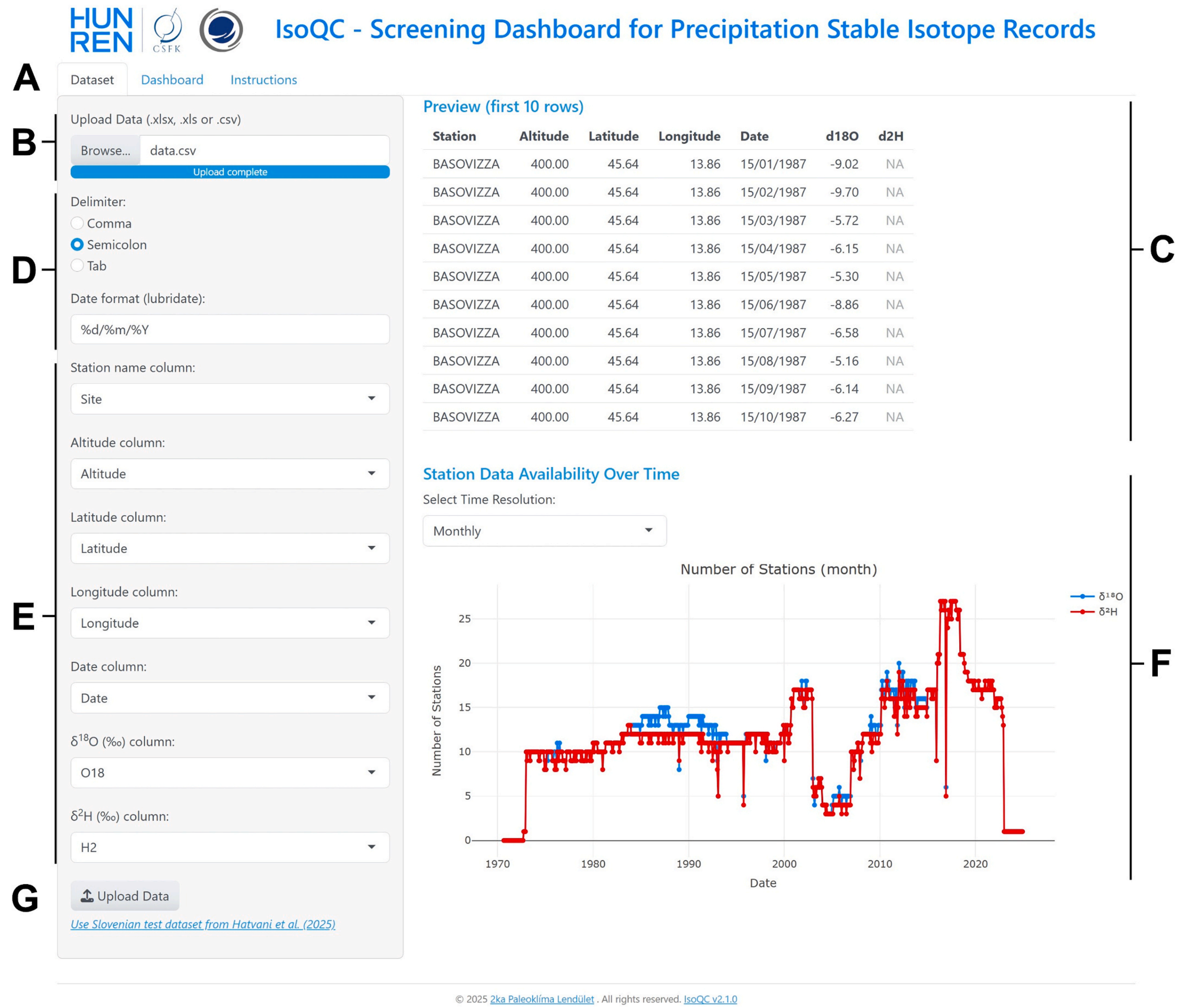

Fig. 3. Landing page of the IsoQC App (A) where the data upload can be carried out (B). After successful file upload, in case of CSV files, the delimiter and date format selector appear (C) and the required column should be paired between the app and the file in the column mapping window (D). Upload can be executed with the 'Upload Data' button (E). Further extensive description can be seen in Sect. 3.1.

not on the example of the ANIP (Fig. 2). To be on the safe side this was 6.8, 54 and 19.7‰ for δ^{18}O (Fig. 2A), δ^{2}H (Fig. 2B) and d-excess (Fig. 2C), respectively. A δ_p value corresponding to such a mean absolute difference is considered a *likely-outlier*. Although the proportion of outliers vs. non-outliers does not increase monotonically, the trend is clear, and a critical threshold is reached at a given mean absolute difference above which all cases are outliers ($p = 1$) (Fig. 2 purple ticks).

3. Features and requirements

The graphical user interface contains a Dataset-, Dashboard- and an Instructions tab. The Instructions tab shows a step-by-step guide of the tool with the excerpt of the input requirements and the functionality of the app, so users would not have to open this paper to obtain information on the tool's usage. The dataset investigated in this study is available in Table S1 and can be used to reproduce the results and figures, as well as to test the application. It also serves as the template for creating the User's own dataset to be explored with the IsoQC App.

3.1. *Data upload and input requirements –dataset tab*

The IsoQC App allows users to upload their own datasets to analyze stable isotope records from regularly collected precipitation samples, e.g. daily, weekly, monthly, annual. The data upload module (Fig. 3A) supports MS Excel (.xlsx,.xls) and CSV (.csv) with a maximum file size limit of 500 MB. To ensure proper functionality, the uploaded data must contain specific columns: *Station* (measurement station name or identifier), *Date* (observation date in a standard format such as DD/MM/YYYY), *Altitude (in meters)*, *Longitude*, *Latitude* (geographic coordinates in decimal degrees), δ^{18}O (‰) and δ^{2}H (‰) values. Date values should be properly formatted in the case of MS Excel files, and if necessary, users can manually specify the date format and delimiter before finalizing the upload in the case of CSV files (Fig. 3D). Longitude and latitude must be within valid geographic ranges, and missing values are allowed, though rows where both δ^{18}O and δ^{2}H are missing will be automatically excluded. For further specifics, see Appendix Sect. 1. The file should not contain extra header rows, with only the first row dedicated to column names.

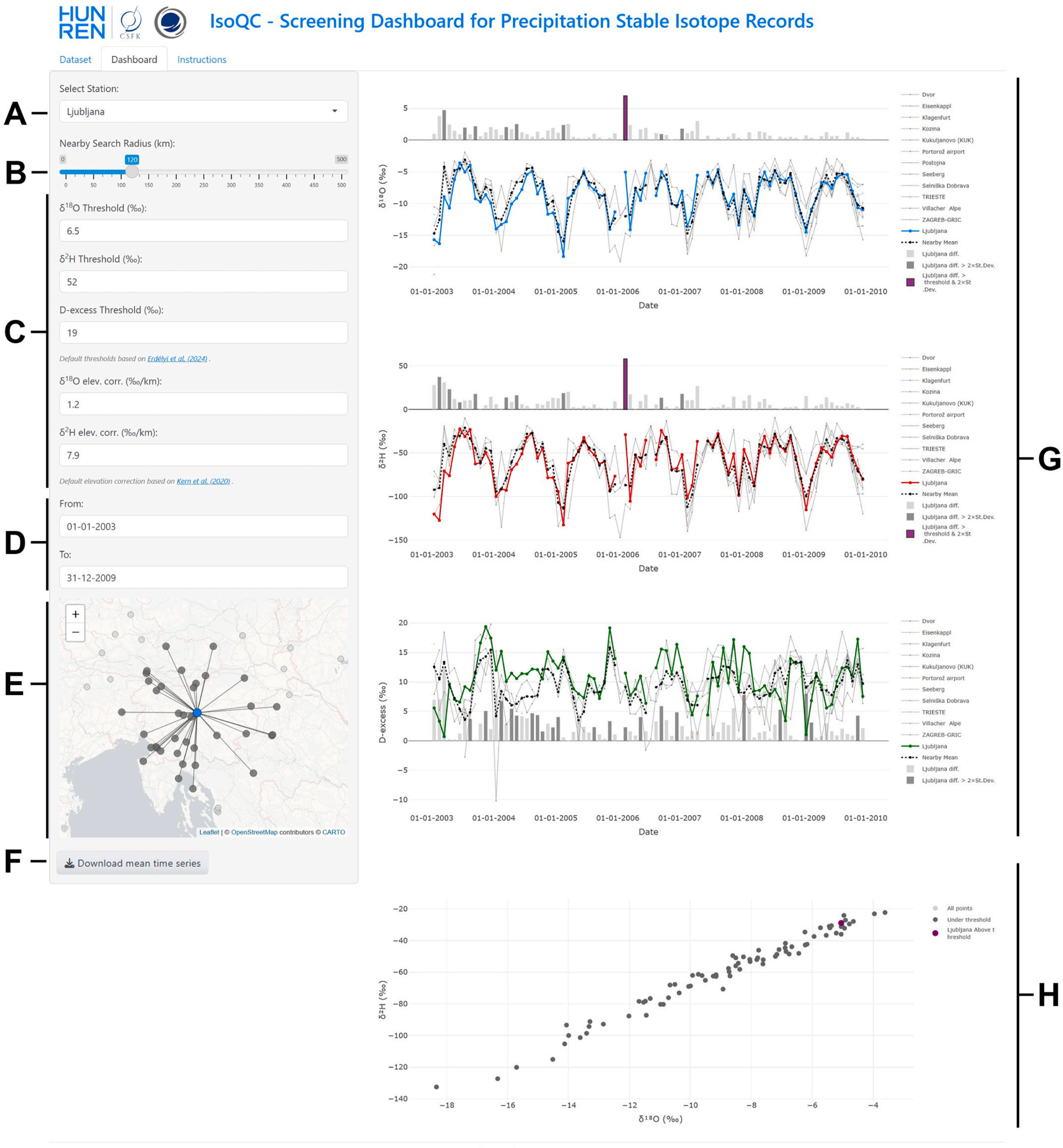

Fig. 4. Screenshot of the main graphical user interface of the IsoQC app with precipitation stable isotopic data from Slovenia. Further extensive description can be seen in Sect. 3.2.

The upload process begins with file selection via the file input widget (Fig. 3B). The application generates a preview of the first ten rows (Fig. 3C), allowing users to verify the structure before proceeding. After loading the file, a column mapping dialog appears (Fig. 3E), enabling users to match their dataset's columns to the required variables. This mapping feature ensures that datasets with different column names can still be processed correctly. Once mapping is confirmed, station availability is plotted (Fig. 3F) and the dataset can be uploaded by pressing the 'Upload Data' button (Fig. 3G), and users can proceed with data visualization and analysis; see Sect. 3.2.

3.2. *Functionality – dashboard tab*

The Dashboard tab includes a sidebar panel for user input and an embedded map, while the main panel presents the interactive plots. The sidebar panel allows users to select a specific measurement station from

Fig. 5. Time series for the Portorož station (01.2001–12.2010) from the IsoQC app, displaying δ^{18}O (top, blue), δ^2H (middle, red), and d-excess (bottom, green) values. The solid-colored line represents data from the selected focal station, while the thick black dashed line indicates the mean values of nearby stations. Grey hairlines represent individual time series from neighboring stations within the defined search radius ($R = 110$ km). Bars in the background highlight the difference of the elevation-corrected δ_p and raw d-excess values between the nearby stations and the focal station, with purple bars marking $D_{i,t}$ values exceeding user-defined thresholds and dark grey bars showing those difference values which are larger than two times the st. dev. of the data in the solving set for a particular month. Dataset . (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
Source: SLONIP platform. For further information see Sect. 3.2

a dropdown list (Fig. 4A), and to change the search radius ($0 < R \leq 500$ km, default 90 km) to include or exclude stations in the solving set (Fig. 4B). Increasing the default search radius can be feasible over plain terrains with homogenous hydrometeorological conditions, while decreasing the default search radius can be necessary over rugged reliefs where hydrometeorological conditions could change considerably over short distances. Additionally, users can adjust the default $\overline{X}_{i,t}$ values for δ^{18}O, δ^2H, and d-excess (Fig. 4C) and can also apply elevation corrections to isotope values tailored for their area of interest or even set it to zero to work with the original data, if needed (Fig. 4C).

The sidebar panel also includes a date selector (Fig. 4D) which ensures that only data within the selected period is displayed in the main plots and calculations. The interactive Leaflet map (Fig. 4E) shows the selected focal station, nearby stations, and other available stations. Hovering over these elements provides additional information, such as the exact distance (in km) between a given station of the solving set and the selected focal station.

Below the map, a 'Download mean time series' button allows users to download the regional mean time series shown in the main panel (Fig. 4F). These regional mean values obtained via the IsoQC app are recommended to be used for imputation when a complete time series is required (Gačnik et al., 2026; Kern and Hatvani, 2025). Since regional means are only calculated if a numeric value is present at the focal station, users are advised to temporally fill in the gap at a given point in time with a dummy value in order to obtain the altitude-corrected regional mean of nearby stations. For details on possible error messages see Appendix Sect. 2.

The main panel (Fig. 4G) provides a suite of interactive graphs for visualizing isotope time series. The first three plots display time series line diagrams of the data for δ^{18}O, δ^2H, and d-excess, comparing the

Fig. 6. Time series for the Ljubljana station (01.2003–12.2009) from the IsoQC app, displaying δ^{18}O (top, blue), δ^{2}H (middle, red), and d-excess (bottom, green) values. Dataset . (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
Source: SLONIP platform. The search radius was set to 120 km to select the solving set. For a detailed description of the figure elements see the caption of Fig. 5

selected focal station's values to the mean of nearby stations (thick black dashed line). In the time series plots, missing data points are explicitly visualized by interruptions in the line graphs, where gaps appear instead of continuous connections, ensuring that periods of missing observations are clearly distinguishable. In addition, a barplot of $D_{i,t}$ is included, highlighting in purple the deviations exceeding the user-defined thresholds.

Based on experiences gained during the testing of the IsoQC app, the default thresholds were found suitable for up to ~ 10% changes of the search radius. However, in the case of very different R values, the thresholds should be fine-tuned; according to our test, the threshold corresponding to δ^{18}O increases by 0.04, while for δ^{2}H it increases by 0.4 per 10 km significantly ($\alpha = 0.01$). For d-excess, however, no significant change was observed, thus, the default value can be retained. In addition, to provide the user with a more detailed picture of the data at hand, the internal variability of the solving set around a focal station is considered by calculating 2 × st. dev of $X_{j,t}$ and highlighting the corresponding $D_{i,t}$ values with dark grey (Figs. 5–8). If $S_{i,t}$ contains only a sole station, this option is not available. However, by increasing R, as soon as the elements in $S_{i,t} \geq 2$, it automatically becomes available again. When a particular $D_{i,t}$ exceeds the user defined threshold, but it lies inside 2 × st. dev of $X_{j,t}$, this is indicated by a purple bar without a black outline. In such cases the user is advised to examine the particular record and even consider reducing the R, to probably reduce the variance of the solving set.

The notion that the two primary isotopic parameters (δ^{18}O and δ^{2}H) have a strong linear relationship is a classical concept of isotope hydrology (Gat, 2005). Thus, deviations from this strong covariance may indicate suspicious δ^{18}O and δ^{2}H pairs (e.g. Fig. 1C). To detect likely-outliers, the cross plot between δ^{18}O and δ^{2}H ($\delta - \delta$ plot) for precipitation is derived as the last panel of the IsoQC dashboard (Fig. 4H) which helps distinguishing data points (marked in purple) that exceed the defined thresholds.

Clicking on station markers on the map updates the plots accordingly, and all visual elements dynamically respond to user inputs, making the tool highly adaptable for exploratory data analysis and quality control in isotope hydrology studies.

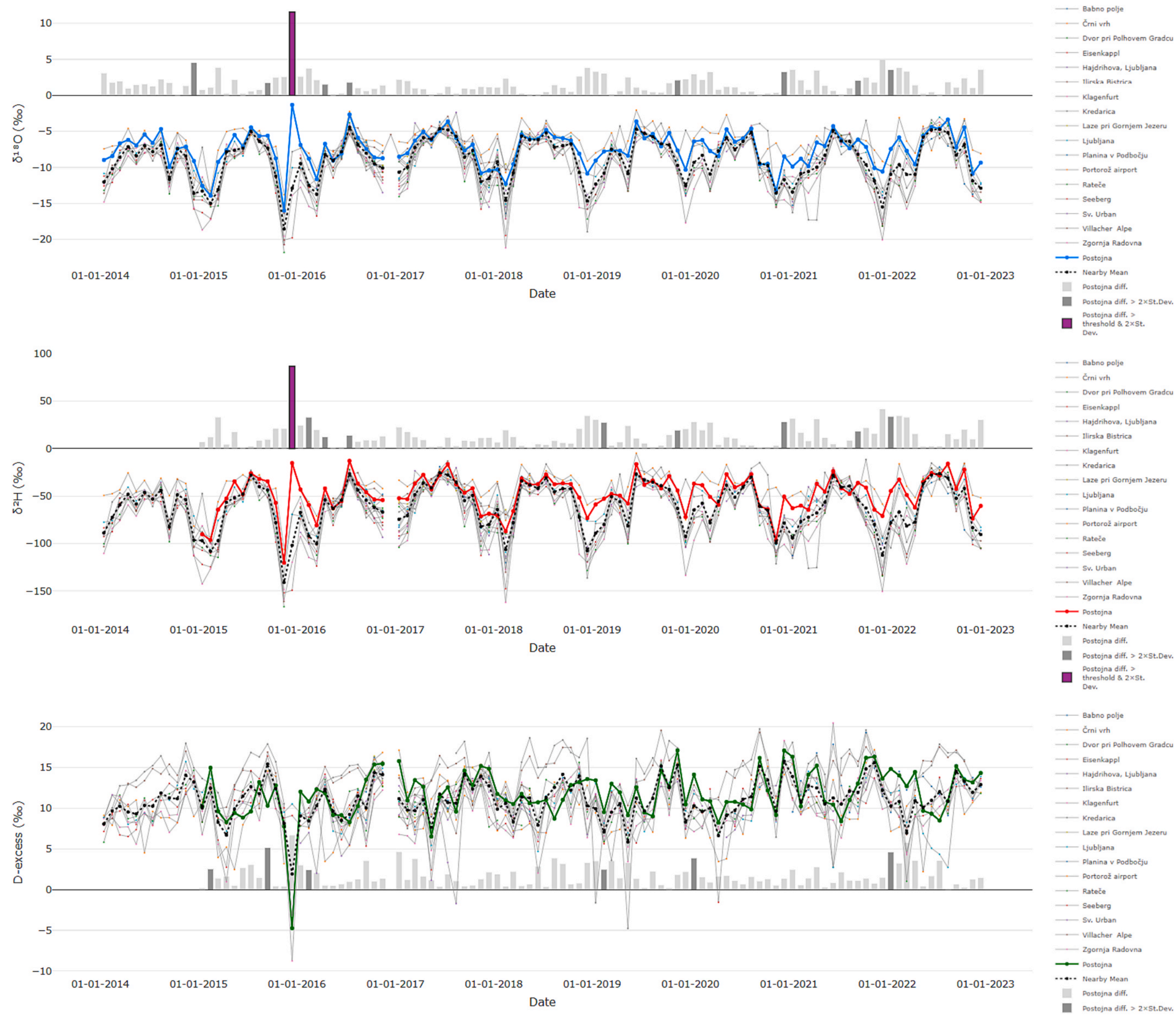

Fig. 7. Time series for the Postojna station (01.2014–12.2022) from the IsoQC app, displaying δ^{18}O (top, blue), δ^{2}H (middle, red), and d-excess (bottom, green) values. Dataset . (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
Source: (Domínguez-Villar et al., 2018; Krklec et al., 2018) and unpublished data from the IJS archive. Default search radius (90 km) was used to select the solving set. For a detailed description of the figure elements see the caption of Fig. 5

4. Showcasing on the Slovenian precipitation stable isotopic database

When assessing the precipitation stable isotopic data from Slovenia, potentially inconsistent values were detected at four stations, namely Portorož, Ljubljana, Postojna and Kredarica. These sites nicely mirror the isotope hydrological diversity of Central Europe from the Alpine areas across the Mediterranean to continental regions (Fig. 1A). Default threshold values were applied in each example while the search radius was fine tuned in certain cases as described below.

At the **Portorož** station, in 01.2004 an unusually low d-excess value was recorded (d-excess = −10.2‰). It was already marked as potentially biased data caused by secondary evaporation (Vreča et al., 2011). Unfortunately, for this particular t, the default $R = 90$ km left the solving set ($S_{i,t}$) empty. Therefore, R was increased to have at least one neighboring station. With $R = 110$ km, the $D_{i,t}$ for d-excess suggests the value is a likely-outlier (Fig. 5). The screening process via IsoQC reinforces earlier observations (Vreča et al., 2011), thus it should be discarded in isotope hydrological analyses.

At the **Ljubljana** station, a likely-outlier was observed in 02.2006 (the δ_p values are higher than the regional average while d-excess follows the regional pattern) which was not found as problematic when the station data was assessed in isolation, years before (Vreča et al., 2008). However, the default $R = 100$ km left the solving set ($S_{i,t}$) with a sole neighboring station for this particular period. Therefore, for further confirmation, R was extended by 20 km to increase the elements of the $S_{i,t}$ to $N = 3$. Consequently, 02.2006 was confirmed to be a likely outlier (Fig. 6) with $D_{i,t}$ above the chosen threshold and substantially larger than even 2 × st. dev. of the data in the solving set.

At the **Postojna** station, a single likely-outlier (12.2015) was detected via the IsoQC app based on the $D_{i,t}$ values exceeding the predetermined threshold and 2 × st. dev. of the solving set using default search radius for δ_p, while the d-excess followed the regional pattern (Fig. 7). The amount of precipitation was unusually low at Postojna (< 1

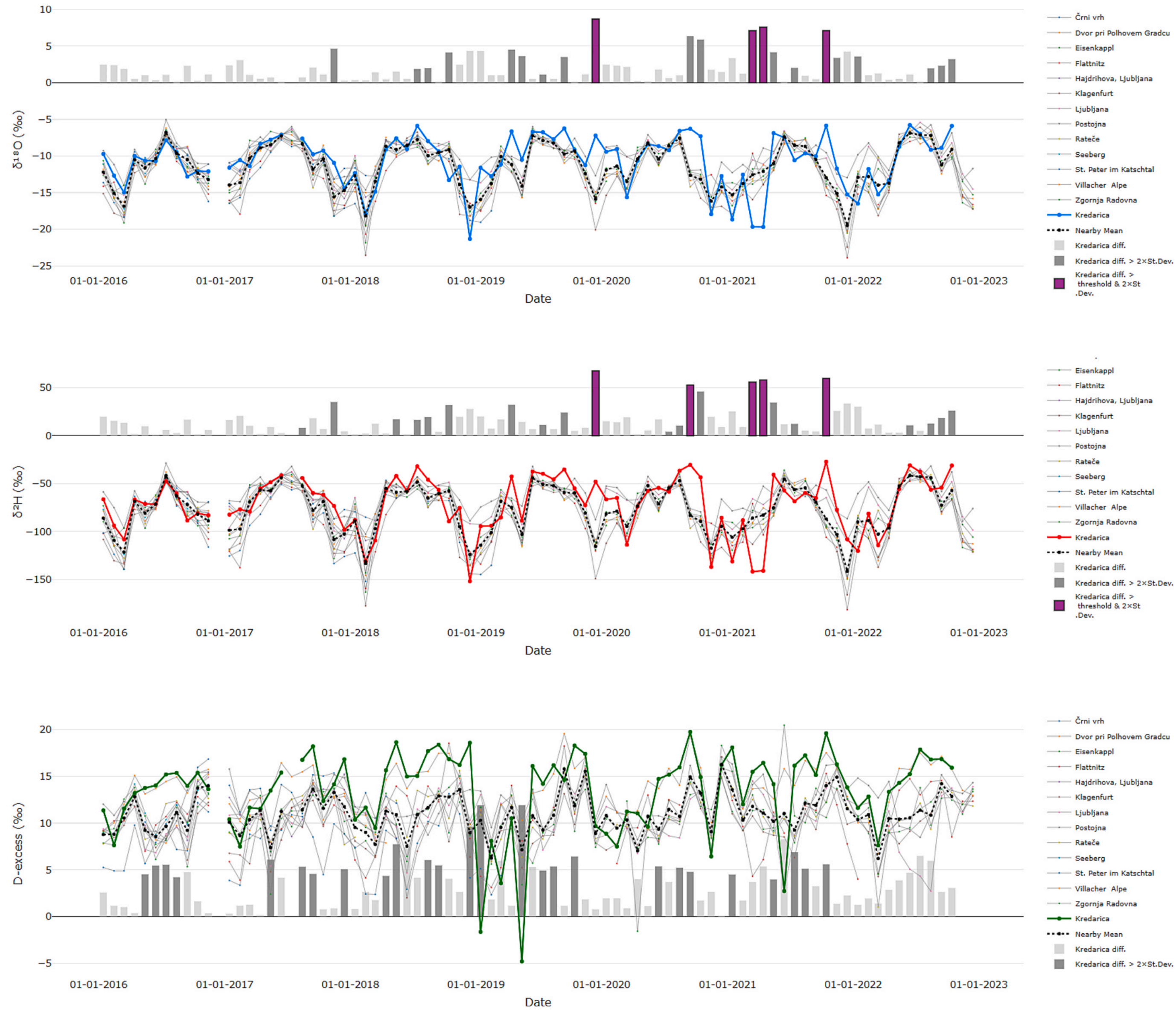

Fig. 8. Time series visualization from the IsoQC app, displaying δ^{18}O (top, blue), δ^{2}H (middle, red), and d-excess (bottom, green) values for the Kredarica station (01.2016–12.2022). Dataset . (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
Source: SLONIP platform. The search radius was set to 80 km to select the solving set. For a detailed description of the figure elements see the caption of Fig. 5

mm) in the given month making the evaporation-proof storage of such samples challenging (Nigro et al., 2024). The anomalies, such as the above δ_p example, and d-excess being far below the usual range, resemble secondary evaporation effect (Cappa et al., 2003). In the meanwhile, the same pattern is reflected in two neighboring stations (Kredarica, Klagenfurt) situated within the 100 km surroundings of Postojna where precipitation amount was also small (e.g. Kredarica 1.4 mm). Although the δ_p values of the 12.2015 Postojna sample seem extreme (Fig. 7), it falls in line with data reported from nearby stations arguing for similar regional isotope hydrometeorological conditions. Therefore, we suggest keeping the 12.2015 extreme values of the Postojna record, especially since the corresponding small amount of precipitation renders the influence of these extreme values negligible if amount-weighted isotopic parameters are to be the final output (Vreča et al., 2007).

At the **Kredarica** station, the data between 2019 and 2022 were frequently inconsistent with its neighbors when screened via the IsoQC App using the default settings. The neighboring stations are mostly under 1000 m, however, the Villacher Alps station (elevation: 2164 m) represents a comparable environment. To get a climatologically more appropriate solving set, the search radius was reduced to 80 km which still left a sufficiently abundant set ($N = 6$) for comparison for 2019–2022 (Fig. 8).

In January and May 2019, both primary water isotope time series show more positive, and d-excess shows unusually negative values compared to their neighbors. Nevertheless, the $D_{i,t}$ values do not exceed the default thresholds, but do exceed 2 × st. dev. for d-excess (Fig. 8) raising suspicion and suggesting a secondary evaporation effect due to unspecified local phenomena. For this reason, the data are flagged with a comment, but no further correction is applied, as the high internal variability during these months does not justify a specific intervention.

In 12.2019, both primary isotopic parameters should be marked as likely-outliers, despite the d-excess value being in harmony with its neighbors. In 09.2020, $D_{i,t}$ of δ^{2}H exceeds, while δ^{18}O is slightly below the threshold; thus, these values should be marked as likely outliers. In the meanwhile, in October of the same year a very similar patterns emerges, and internal variability raises alarms even though spatial inconsistency is not so stark. In March, April and October 2021, the $D_{i,t}$

values exceeded the default thresholds whereas in the intervening period, frequent mismatches —in all cases still surpassing 2 × st. dev— were observed (Fig. 8). According to the data provider, sample collection was not performed according to prescribed protocol in the 2021–2022 period and the monthly sample composite was not collected appropriately. Both primary (Fig. 8A and B) and secondary (Fig. 8C) isotopic parameters are consistent with the neighbors in January and February 2021, suggesting that inappropriate sampling has been started only from March 2021. Therefore, the data from 03.2021 to 01.2022 should not be considered for further isotope hydrology applications. These δ_p values should each be tagged as "random/incomplete collection". Note that from February 2022 onwards, the data once again meet the IsoQC screening criteria and can be considered reliable.

5. Conclusions and outlook

A distance-based outlier detection approach was developed to support the objective and reproducible screening of water stable isotope datasets as a fundamental step prior to isotope hydrological applications. The IsoQC app compares primary (δ^{18}O, δ^2H) and secondary (d-excess) isotopic records across multiple monitoring stations within an adjustable search radius, enhances the ability to distinguish between true natural variations and possible anomalies arising from sampling, measurement or data entry errors.

The IsoQC app, when employed on the selected Slovenian and neighboring precipitation isotope dataset, demonstrated its efficacy in identifying likely outliers, such as point errors (e.g. Portorož, 01.2004) and an interval error (Kredarica 03.2021 – 01.2022), and even in verifying the natural extreme character of unusual values, which may appear as outliers when explored in isolation (e.g. Postojna, 12.2015). Argumentation for the validity of an extreme value instead of flagging it as a likely-outlier in a database should involve careful inspection of local conditions—particularly precipitation amount—during the sampling and synoptic situations.

Likely outliers are flagged when the deviation of a given station's elevation-corrected isotope value from the mean of its neighboring stations ($\overline{X}_{i,t}$) exceeds predefined thresholds. The presented examples underscore the necessity of neighboring station comparisons in evaluating the consistency of isotope records.

While IsoQC app is fine-tuned for screening monthly precipitation stable isotope records, there are no methodological or technical limitations preventing its application to other water stable isotopic datasets, including groundwater, soil water, and lake water, provided that the datasets are comparable in temporal sampling resolution/frequency. The interactive data upload functionality allows users to work with their own datasets. Moreover, the ability to dynamically adjust the solving set and apply elevation corrections provides flexibility across different hydrological and climatological settings.

6. Code availability

The source code of the IsoQC App is available on GitHub at https://github.com/erdelyidani/IsoQC.

CRediT authorship contribution statement

István Gábor Hatvani: Writing – review & editing, Writing – original draft, Software, Methodology, Investigation, Formal analysis, Conceptualization. **Dániel Erdélyi:** Writing – review & editing, Writing – original draft, Visualization, Software, Methodology, Investigation, Formal analysis, Conceptualization. **Polona Vreča:** Writing – review & editing, Writing – original draft, Supervision, Resources, Investigation, Funding acquisition, Formal analysis, Data curation. **Sonja Lojen:** Writing – review & editing, Resources, Investigation, Formal analysis, Data curation. **Klara Žagar:** Writing – review & editing, Resources, Investigation, Formal analysis. **Jan Gačnik:** Writing – review & editing, Investigation, Formal analysis. **Zoltán Kern:** Writing – review & editing, Writing – original draft, Supervision, Methodology, Investigation, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This is contribution no. 96 of the 2ka Palæoclimatology Research Group. The Cost Action 19120 WATSON is acknowledged for the intriguing discussions and project SNN 143868 for additional support. On behalf of project 'Machine learning prediction of precipitation stable isotopes' we thank for the usage of HUN-REN Cloud (https://science-cloud.hu/) which helped us achieve the results published in this paper.

Funding

The research leading to these results received funding from Slovenian Research and Innovation Agency under Grant Agreements P1-0143, J6-3141, J6-50214, N1-0054, N1-0309, from EU Partnership Agriculture of Data and IAEA under Grant Agreements F31006, F33024, F33031, RER7013, RER7017 and SLO7001.

Appendix

1. Input File Format and Structure Requirements

Mandatory Columns (case-sensitive names are not required, as mapping is performed after upload):

- o **Station**: Name or identifier of the measurement station (text).
- o **Date**: Observation date.
- o **Longitude**: Geographic longitude of the station (decimal degrees, EPSG:4326).
- o **Latitude**: Geographic latitude of the station (decimal degrees, EPSG:4326).
- o **Altitude**: Elevation of the station (in meters above sea level).
- o **δ^{18}O (‰)**: Measured oxygen isotope ratio (numerical).
- o **δ^2H (‰)**: Measured hydrogen isotope ratio (numerical).

Data Formatting Considerations:

- o Date values should be **properly formatted as dates** (DD/MM/YYYY).

- Longitude and latitude should be **in decimal degrees** and within the valid geographic range (−180 to 180 for longitude, −90 to 90 for latitude).
- **Missing values are allowed**, but rows where both $\delta^{18}O$ and $\delta^{2}H$ are missing will be automatically excluded from the dataset.

2. **Error messages**

The general error message is '**Error:** An error has occurred. Check your logs or contact the app author for clarification', if (i) an unsupported, (ii) incorrectly formatted file is being uploaded, or (iii) such a selection is made in the Dashboard tab which results in no data.

Table A1
Basic geographical information of precipitation stable isotope monitoring stations operating in Slovenia between May 1981 and December 2022. Latitude and longitude are in WGS84 projection, EPSG: 4326. Data collected from published papers, SLONIP platform (https://slonip.ijs.si/) and IJS archive.

Station	Latitude (°)	Longitude (°)	Elevation (m a.s.l.)	No. of monthly data [$\delta^{18}O$; $\delta^{2}H$]	First date (MM-YYYY)	Last date (MM-YYYY)	Ref.
Babno polje	45.64518	14.545	754	23; 23	05–2016	05–2018	Rusjan et al., 2019 and IJS archive
Črni vrh	46.08658	14.25972	785	25;25	05–2016	05–2018	Rusjan et al., 2019 and IJS archive
Dvor	45.8068	14.9637	195	48;44	01–2009	12–2012	Zavadlav 2013 and IJS archive
Dvor pri Polhovem Gradcu	46.06229	14.345	346	23;23	05–2016	04–2018	Rusjan et al., 2019 and IJS archive
Hajdrihova, Ljubljana	46.04162	14.4929	292	24;24	05–2016	05–2018	Rusjan et al., 2019 and IJS archive
Ilirska Bistrica	45.57773	14.24056	439	25;24	05–2016	05–2018	Rusjan et al., 2019 and IJS archive
Kozina	45.60425	13.93194	484	39;39	10–2000	12–2003	SLONIP
Kredarica	46.37878	13.84863	2514	150;150	03–2010	10–2022	SLONIP and IJS archive
Laze pri Gornjem Jezeru	45.72297	14.39889	594	24;24	05–2016	05–2018	Rusjan et al., 2019 and IJS archive
Ljubljana	46.09461	14.59705	282	476; 473	05–1981	12–2022	SLONIP and Gačnik et al., 2026
Murska Sobota	46.65208	16.19128	186	81; 81	01–2016	12–2022	SLONIP and IJS archive (Koren Pepelnik et al., 2025, 2026)
Planina v Podbočju	45.82904	15.50659	678	24;24	01–2021	12–2022	IJS archive
Portorož	45.47531	13.61599	2	35; 35	10–2000	12–2022	SLONIP and Gačnik et al., 2026
Postojna	45.76609	14.19321	533	166;95	01–2009	12–2022	Krklec et al., 2018 and IJS archive
Rateče	46.49709	13.71289	864	147;147	03–2010	12–2022	SLONIP and IJS archive
Sela na Krasu	45.821	13.627	270	12; 12	08–1999	10–2000	Doctor 2002
Selniška Dobrava	46.533	15.467	295	31; 31	01–2001	10–2005	Mali 2006
Sv. Urban	46.18358	15.59075	283	68;68	01–2016	12–2021	Vreča et al. 2024 and SLONIP
Zgornja Radovna	46.42818	13.94272	750	151;151	04–2010	12–2022	SLONIP and IJS archive

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jhydrol.2026.135401.

Data availability

Data used in the study is mostly available from the cited literature and online sources (Table A1), while the yet unpublished part is available in the supplement of the study, see Table S1.

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