The PAGES CoralHydro2k Seawater $\delta^{18}O$ Database: A FAIR-aligned compilation of seawater $\delta^{18}O$ data to uncover 'hidden' insights from the global ocean

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Abstract. The stable isotope values of seawater ($\delta^{18}O$ and $\delta^{2}H$) provide valuable information on the exchange of water between the ocean, atmosphere, and cryosphere and on ocean mixing processes. As such, observational seawater $\delta^{18}O$ and $\delta^{2}H$ data place powerful constraints on hydrologic changes in the modern ocean. Seawater $\delta^{18}O$ data are also essential for calibrating paleoclimate proxies based on the $\delta^{18}O$ of marine carbonates and are an increasingly critical diagnostic tool for assessing model performance and skill in isotope-enabled climate models. Despite their broad value, no centralized and actively-curated database for this type of data exists, even though a growing number of new seawater $\delta^{18}O$ datasets have been generated over the last decade. As such, many seawater $\delta^{18}O$ datasets remain 'hidden'. To improve the accessibility of seawater $\delta^{18}O$ data for the Earth Science research community, the Past Global Changes (PAGES) CoralHydro2k project has created a new, machine-readable, and metadata-rich database of observational seawater $\delta^{18}O$ data, paired with seawater $\delta^{2}H$ and salinity data, that is compliant with findability, accessibility, interoperability, and reusability (FAIR) standards for digital assets. The data has been collected from public databases and repositories, direct researcher data submissions, scientific papers, and student theses. In total, the PAGES CoralHydro2k Seawater $\delta^{18}O$ Database contains over 18,600 data points with extensive metadata that makes the database suitable for a myriad of research applications. For hidden data, we searched for and included all datasets within the global ocean. For public data, our data collation efforts were focused on the upper 50 m from 35°N to 35°S (to aid in CoralHydro2k's seawater $\delta^{18}O$ reconstruction studies using $\delta^{18}O$ and Sr/Ca in tropical-subtropical coral skeletons). We also provide a set of best practices to the community for reporting seawater isotope data in the future.

Short Summary. The stable isotopic composition of seawater is a valuable tool for studying the global water cycle in the past, present, and future. However, an active repository dedicated to archiving this type of data has been lacking, and many datasets remain hidden from public view. We have created a new database of observational seawater isotope data that is rich in metadata, publicly accessible, and machine readable to increase its availability and usability for a variety of Earth Science applications.

1 Introduction

1.1 Progress and challenges in the synthesis of seawater oxygen isotope data

The stable isotope composition of water ($\delta^{18}O$ and $\delta^{2}H$) provides a powerful tracer of the global water cycle, tracking water as it continuously cycles between the ocean, atmosphere, and land. The isotopic composition of seawater is nearly conservative when no phase change occurs. As water molecules undergo phase changes however, the lighter, more abundant isotope (^{16}O and ^{1}H) is preferentially vaporized during evaporation with respect to the heavier, less abundant isotope (^{18}O and ^{2}H), while the heavy isotope is preferentially condensed during precipitation (Dansgaard, 1964). This partitioning of isotopes based on mass allows the isotope values (where $\delta^{18}O = \left[\frac{\frac{18O}{16O}sample}{\frac{18O}{16O}standard} - 1\right] * 1000$) of water to be used as a tracer of the hydrologic cycle (Dansgaard, 1954; Galewsky et al., 2016; Gat, 1996). In the ocean, the isotope values of seawater ($\delta^{18}O_{sw}$ and $\delta^{2}H_{sw}$) can provide valuable information on an array of processes, including heat and mass exchange with the atmosphere (*via* precipitation and evaporation), large-scale ocean circulation, and freshwater input from rivers and ice sheets (Akhoudas et al., 2021; Benetti et al., 2016; Benway and Mix, 2004; Biddle et al., 2019; Craig and Gordon, 1965; Dee et al., 2023; Frew et al., 2000; Imbrie et al., 1984; Jacobs et al., 1985; Lisiecki and Raymo, 2005; Meredith et al., 1999; Strain and Tan, 1993). $\delta^{18}O_{sw}$ and $\delta^{2}H_{sw}$ values can also provide insight into other ocean tracers such as salinity, since they covary strongly due to the influence of evaporation and precipitation on each of these variables (Craig and Gordon, 1965; LeGrande and Schmidt, 2011). However, because key processes act differentially on salinity as compared to the stable isotope values, $\delta^{18}O_{sw}$ and $\delta^{2}H_{sw}$ provide additional constraints on ocean mixing and the local moisture budget.

Seawater isotope values also create a common unit that uniquely links paleoclimate reconstructions to modern climate observations and isotope-enabled model simulations. Modern $\delta^{18}O_{sw}$ data are essential for the calibration of paleoclimate proxies of past ocean variability based on the $\delta^{18}O$ of marine carbonates such as corals, foraminifera, molluscs, ostracods, and coralline algae. Recent paleoclimate data assimilation efforts such as the Last Millennium Reanalysis project (e.g., Tardif et al., 2019) would greatly benefit from a spatial network of $\delta^{18}O_{sw}$ data to improve quantification of proxy uncertainty and for training the proxy system models that underlie those efforts. Modern $\delta^{2}H_{sw}$ data are used in the calibration of paleoceanographic proxies based on the $\delta^{2}H$ of alkenones and other lipid biomarkers in marine sediments (e.g., Eglinton and

Eglinton, 2008). When used in tandem with $\delta^{18}O$ data (i.e., to calculate d-excess in surface ocean and overlying water vapor), $\delta^{2}H$ data can be used to constrain evaporation parameters (e.g., Benetti et al., 2014). As such, observational and reconstruction efforts based on seawater isotope values enable scientists to better understand the underlying physics that govern the water cycle, and to extend hydroclimate records back to the preindustrial era, thus contextualizing anthropogenic climate change and improving the skill of future climate projections. In modern environments, $\delta^{18}O$ in marine biominerals and $\delta^{2}H$ in lipids can be used to trace plankton and animal movement and provide provenance for ecology, conservation, archaeology, and food forensics studies (Doubleday et al., 2022). Given these wide-ranging applications, seawater isotope data are used in a wide range of fields, including paleo and modern oceanography, atmospheric science, geology, marine biology, archaeology, and geography.

Observational $\delta^{18}O_{sw}$ data can also be used to provide boundary conditions in climate models and to assess model performance and skill. The increasing integration of oxygen isotopes of water in climate models – from models of intermediate complexity to fully coupled Earth System Models (e.g., Blossey et al., 2010; Bong et al., 2024; Bony et al., 2008; Brady et al., 2019; Cauquoin et al., 2019; Dee et al., 2015; Field et al., 2014; Fiorella et al., 2021; Kurita et al., 2011; Lee and Fung, 2008; Noone and Simmonds, 2002; Nusbaumer et al., 2017; Risi et al., 2010, 2020, 2021; Schmidt et al., 2007; Tada et al., 2021; Wei et al., 2018; Werner et al., 2011; Yoshimura et al., 2008) – bolsters the interpretation of modern and paleoclimate observations, while also providing opportunities to test model performance in resolving key features of the hydrologic cycle, e.g., the representation of moisture transport, circulation, and surface water fluxes.

Paralleling recent advances in the numerical simulation of water isotopes, new analytical capabilities have also developed in recent years, including new *in situ* atmospheric measurement techniques and strategies (Finkenbiner et al., 2022; Gupta et al., 2009; Henze et al., 2022), and the development of global atmospheric data products from a variety of remote sensors (e.g., Diekmann et al., 2021; Schneider et al., 2022; Worden et al., 2019). As a result, measurements of water isotopes have become increasingly incorporated in coordinated observing networks and monitoring studies of precipitation and atmospheric water vapor, including the Global Network of Isotopes in Precipitation (www.iaea.org/services/networks/gnip) and the National Ecological Observatory Network (www.neonscience.org/).

However, no such coordinated observing network for seawater $\delta^{18}O$ currently exists. Unlike meteorological observations on land, observations of ocean hydrological properties (e.g., precipitation, evaporation, and salinity) are largely either limited to the past few decades (*via* satellite remote sensing, the ARGO (Wong et al., 2020) and GOOS (Dexter and Summerhayes, 2010) programs, the TAO/TRITON array, and other mooring, drifter, and ship-of-opportunity measurements), or are confined to selected coastal and island locations that have the necessary infrastructure to support sustained *in situ* measurements of ocean surface properties. Furthermore, these ocean observations rarely include $\delta^{18}O_{sw}$ because there is currently no cost-effective, easily deployable instrumentation to measure seawater isotopes *in situ.* Thus, seawater samples must be taken back to a laboratory for isotopic analysis. Despite these structural challenges, a growing number of $\delta^{18}O_{sw}$ datasets have been generated in recent decades due to the accelerated collection of $\delta^{18}O_{sw}$ samples, new instrumentation based on cavity-ring down spectroscopy (CRDS) with reduced analytical costs, the capability to measure both $\delta^{18}O$ and $\delta^{2}H$ in parallel, and new sampling devices that enable long-term seawater sample collections (e.g., Jannasch et al., 2004; Khare et al., 2021).

In recognition of the broad value of $\delta^{18}O_{sw}$ data to the Earth Sciences, a major effort to gather $\delta^{18}O_{sw}$ data occurred in the 1990s (Bigg and Rohling, 2000; Schmidt, 1999; Schmidt et al., 1999) and resulted in the development of the NASA's Goddard Institute for Space Studies (GISS) Global Seawater Oxygen-18 database (https://data.giss.nasa.gov/o18data/), which contains over 26,000 global measurements of $\delta^{18}O_{sw}$ (and some $\delta^{2}H$ data) from the 1950s to 2000s. In 2006, that database was used to construct a global gridded dataset of $\delta^{18}O_{sw}$ and to characterize regional relationships between $\delta^{18}O_{sw}$ and salinity (LeGrande and Schmidt, 2006) and it has subsequently been used in a broad range of studies involving $\delta^{18}O_{sw}$. However, the NASA GISS database is no longer actively updated, with the last $\delta^{18}O_{sw}$ measurement added in 2011. As a result, a growing number of new $\delta^{18}O_{sw}$ datasets published since 2011 remain without an active $\delta^{18}O_{sw}$-specific data repository in which to archive the data. Researchers have instead provided the $\delta^{18}O_{sw}$ data in the supplemental tables of journal articles, or have archived the $\delta^{18}O_{sw}$ data with other geochemical data (e.g., coral $\delta^{18}O$), in data repositories such as the National Centers for Environmental Information (NCEI) for Paleoclimatology (https://www.ncei.noaa.gov/products/paleoclimatology) and PANGAEA (https://www.pangaea.de/). Because these datasets can be difficult to find, non-machine-readable, and/or decentralized, they are not easily accessible to the wide range of research communities that would benefit from this data (see a related review by Chamberlain et al., 2021). Furthermore, many publishers and several funding agencies now require researchers to archive their data in FAIR and public repositories. For these reasons, a comprehensive database of $\delta^{18}O_{sw}$ data that is publicly available and actively maintained is critically needed.

1.2 The PAGES CoralHydro2k Seawater $\delta^{18}O$ Database

CoralHydro2k and its Seawater $\delta^{18}O$ Database started in 2017 as a project in Phase 3 of the Past Global Changes (PAGES) 2k network, a long-running initiative to study past global changes over the last 2000 years and to compile paleoclimate data in publicly available, machine-readable databases (Konecky et al., 2023; PAGES 2k Network Coordinators, 2017; Tierney et al., 2015). The CoralHydro2k project was formed to investigate the variability of hydrology and temperature in the tropical surface ocean during the past 2000 years based on the combination of coral $\delta^{18}O$, which varies with temperature and $\delta^{18}O_{sw}$, and the strontium-to-calcium ratio (Sr/Ca) in corals, which is a temperature proxy. To aid in the calibration and interpretation of the paired coral $\delta^{18}O$ and Sr/Ca records in the database, and derive coral-based reconstructions of seawater $\delta^{18}O$, the CoralHydro2k project started to compile $\delta^{18}O_{sw}$ data.

In recognition of the growing number of $\delta^{18}O_{sw}$ datasets that have been generated during the last two decades, the CoralHydro2k Seawater $\delta^{18}O$ Database project was launched in 2020 to recover 'hidden' $\delta^{18}O_{sw}$ data that were not easily findable. During the past five years, we have integrated these records, along with any associated δ^2H, salinity, and temperature data, with data from public databases and repositories to create a new, centralized, machine-readable, and metadata-rich database that aligns with findability, accessibility, interoperability, and reusability (FAIR) standards (Wilkinson, 2016). Here we provide a detailed description of the PAGES CoralHydro2k Seawater $\delta^{18}O$ Database, highlighting the opportunities and limitations of the current database. We also provide a data submission template with comprehensive metadata for guiding the reporting of seawater isotope data in the future.

2 Methods

2.1 Collaborative model

CoralHydro2k included team members from the Phase 1 PAGES Ocean2k working group (Tierney et al., 2015) and Phase 2 Iso2k working group (Konecky et al., 2020) and many new members, particularly from the coral paleoclimate community. CoralHydro2k continued into Phases 3 and 4 of PAGES 2k, focusing on reconstructing past changes in tropical ocean temperature and hydroclimate using paired Sr/Ca and $\delta^{18}O$ from coral archives over the last 2000 years (Hargreaves et al., 2020; Walter et al., 2023). Recurring calls went out within the international paleoclimate community for working group members, coral experts, and paleo data assimilation experts to join the effort with monthly teleconference meetings and one in-person meeting in 2019 (Hargreaves et al., 2020). As a result, the CoralHydro2k database was produced, a global, actively curated compilation of coral $\delta^{18}O$ and Sr/Ca proxy records of tropical ocean hydrology and temperature for the Common Era (Walter et al., 2022, 2023). A number of sub-projects were developed in conjunction with CoralHydro2k, including a project to develop new proxy system models (PSM) for coral $\delta^{18}O$. The group working on this sub-project realized that the spatial and temporal coverage of observational $\delta^{18}O_{sw}$ data were too sparse to integrate into the PSM framework and that many new $\delta^{18}O_{sw}$ datasets produced during the last few decades are not easily findable or accessible.

CoralHydro2k thus formed a new sub-project in 2020 to compile existing seawater $\delta^{18}O$ data with rich metadata following FAIR standards (Atwood et al., 2024; DeLong et al., 2022). Researchers were invited to submit their data to the CoralHydro2k Seawater $\delta^{18}O$ Database via a Qualtrics survey and accompanying YouTube video that provided instructions on how to submit data.

The workload for assembling the seawater data and metadata was performed by CoralHydro2k members and new members of the Seawater $\delta^{18}O$ Database sub-project. The team was made of volunteer scientists from all academic levels, including undergraduate and graduate students, postdoctoral researchers, and early- to senior-level scientists from several international academic and research institutions. The work was completed remotely in synchronous working sessions and asynchronously across several virtual platforms (Google Suite, Slack, and Zoom). Data discovery, metadata protocols, and compilation were done collaboratively as the project progressed.

2.2 Data curation in the EarthChem Seawater Oxygen Isotopes Community

To facilitate future curation of seawater isotope data by the research community, we established the Seawater Oxygen Isotopes Community (https://www.earthchem.org/communities/seawater-oxygen-isotopes/) in the EarthChem Library (ECL), a data repository that archives, publishes, and provides access to data in the geosciences. The ECL offers a suite of services for data preservation and access, including long-term archiving and data registration with a Digital Object Identifier (DOI). Through the new Seawater Oxygen Isotopes Community, new seawater $\delta^{18}O$ (and $\delta^{2}H$) datasets can be submitted and assigned a DOI, which allows the datasets to be cited and tracked when used by other researchers. The CoralHydro2k members promoted this new database at international conferences in the United States and Europe, in the PAGES newsletter (Atwood et al., 2024), and in Eos, the monthly magazine of the American Geophysical Union (AGU) (DeLong et al., 2022).

2.3 Data aggregation and formatting

The CoralHydro2k Seawater $\delta^{18}O$ Database was designed to be as inclusive and comprehensive as possible in its record-selection criteria to support the project goal of developing a FAIR database of global seawater $\delta^{18}O$ measurements, paired with $\delta^{2}H$ and salinity measurements, and to include as much 'hidden' data as possible. Thus, the Seawater $\delta^{18}O$ Database selection criteria were less restrictive than other PAGES 2k efforts, and the database includes data from peer-reviewed scientific literature, student theses and dissertations, public data repositories, and direct author submission.

For hidden data, we searched for and included datasets spanning all depths and all latitudes across the global ocean. For publicly available data, given the substantial time commitment involved in finding and adding the extensive metadata, we typically only included data from the upper 50 m between 35ºN to 35ºS (to aid in CoralHydro2k's seawater $\delta^{18}O$ reconstruction studies using $\delta^{18}O$ and Sr/Ca in tropical-subtropical shallow-water corals). In subsequent versions of the database, we will target the inclusion of all publicly available datasets.

2.4 Metadata, quality control, and best practices for future data reporting

In alignment with FAIR data principles, the Seawater $\delta^{18}O$ Database contains extensive metadata. 12 metadata fields are required, with an additional 38 optional metadata fields that provide important supporting information on the sampling site, sample collection and storage, isotope analysis method, evaporation and correction flags, and error information. Where available, paired seawater $\delta^{2}H$, salinity, and temperature data are also reported. The full set of required and optional metadata fields in the database are intended to establish a set of best practices for future reporting of seawater isotope data. The Scientific Committee on Oceanic Research (SCOR) working group 171 "Towards best practices for Measuring and Archiving Stable Isotopes in Seawater (MASIS)" further intends to build upon the set of best practices established for the CoralHydro2k

Seawater $\delta^{18}O$ Database. We note that many of the optional metadata fields in the database are essential for proper quality control, inter-comparison, and interpretability across datasets. However, this information was often not reported in the original datasets and publications, and thus this metadata could not be made mandatory without greatly restricting the number of datasets in the database. However, we strongly encourage the inclusion of all metadata fields in this database (required and optional) for future reporting of seawater isotope data. To assist researchers with this process, a blank data submission template (with examples) is provided with the CoralHydro2k Seawater $\delta^{18}O$ Database.

The metadata fields are described in Tables 1–2. The CoralHydro2k Seawater $\delta^{18}O$ Database team implemented several rounds of quality control measures for the data and metadata. Following the Iso2k database procedure (Konecky et al., 2020), each metadata field has an associated quality control certification "Level" from 1 to 5, described below and in Table 1. Level 1 and Level 2 metadata fields constitute 'essential' metadata, and if a dataset lacked one of these fields, it was excluded from the database.

- *Level 1* fields are required for inclusion in the database and they contain standardized vocabularies, according to Table 2. They are recommended as primary fields for filtering and querying records in the database. They were subject to the highest Quality Control (QC) standard. Examples of Level 1 metadata are: "Collection year", "Collection month", "Latitude", "Longitude", and "Depth".
- *Level 2* metadata fields are required for inclusion, but they are not generalizable enough to use standardized vocabularies. They were subject to the highest QC standard and the metadata were obtained from the original publication or data source. An example of Level 2 metadata is "Site name or geographic area".
- *Level 3* metadata fields add important supplementary information related to the seawater $\delta^{18}O$ measurements. They contain standardized vocabularies and can be used as secondary fields for filtering and querying the database; however, they are generally not available for all records and thus not required for inclusion in the database. They were subject to the highest QC standard. Examples of Level 3 metadata are: "Collection day", "$\delta^{18}O$ error", "$\delta^{18}O$ analysis technique", "Water isotope analysis date", "$\delta^{2}H$ value", "Temperature value", and "Salinity value".
- *Level 4* metadata fields also add important supplementary information related to the seawater $\delta^{18}O$ data, but they are not generalizable enough to use standardized vocabularies. They are also generally not available for all records and thus not required for inclusion in the database. They were subject to the highest QC standard. Examples of Level 4 metadata are: "$\delta^{18}O$ correction notes", "$\delta^{18}O$ error notes", "Sample ID", "Publication citation", "Dataset citation", "Cruise ID", "$\delta^{18}O$ analysis location", "Sample collection, processing, and storage notes", and "Water isotope analysis notes".
- *Level 5* metadata fields may be useful to some users of the database, but they are generally not available for all records and thus not required for inclusion in the database. In many cases, these fields contain freeform text with direct quotes from the original publications. During the QC certification process, these fields were checked against the original publication and a quote or summary of the relevant information was provided in the database, but the information provided may not be comprehensive. The Level 5 metadata are: "Location description", "Location type", and "Temperature/salinity notes".

Table 1: Description of all metadata fields in the PAGES CoralHydro2k Seawater $\delta^{18}O$ Database. Bold text indicates required fields in the database (Level 1 and 2).

Level #	Metadata field	Metadata field description	Type	Metadata category
1	CoralHydro2kID*	Unique ID for this database	Text	Entity
1	Collection year	Year of sample collection, YYYY	Numeric	Entity
1	Collection month	Month of sample collection, MM	Numeric	Entity
1	Latitude	Latitude of the sampling site in decimal degrees. South is negative. Decimal degrees N, from -180 to 180	Numeric	Entity
1	Longitude	Longitude of the sampling site in decimal degrees. West is negative. Decimal degrees E, from -180 to 180	Numeric	Entity
1	Depth	Sampling depth, in meters (m) below sea level (no minus sign).	Numeric	Entity
1	$\delta^{18}O$ value	Measured $\delta^{18}O$ value	Numeric	Seawater Data
1	$\delta^{18}O$ correction	Indicates whether a correction has been made to the $\delta^{18}O$ values after the original publication. If the data point has been corrected, "Y" is indicated. If the data has not been corrected, "N" is indicated. If the value of the applied correction is known, this value is indicated in the "$\delta^{18}O$ correction value" (Level 3) metadata field and any accompanying information about how and why the correction was made is indicated in the "$\delta^{18}O$ correction notes" (Level 4) metadata field.	Logic	Seawater Data
1	Evaporation flag	Flag indicating the presence of potential evaporation effects on $\delta^{18}O$ value. "Y" is indicated for cases where authors note that sample evaporation could be a concern or cases where $\delta^{18}O$ data have been corrected for evaporation; "N" otherwise. Further information is provided in the "Sample collection, processing, and storage notes" (Level 4) metadata field.	Logic	Queryable
1	Reference standard	Reference standard used in reporting the $\delta^{18}O$ and $\delta^{2}H$ values (SMOW, VSMOW)	Text	Seawater Data
1	Access date	Date in which the data was downloaded from data repositories, submitted by researchers, or acquired from journal articles (YYYY-MM-DD)	Text	Entity

2	**Site name or geographic area**	**Name of the site or the general area from which the water sample was collected**	**Text**	**Entity**
3	Collection day	Day of sample collection, DD. In some cases, the collection day was not specified in the original publication, only the collection month or a range of dates. In these cases, the midpoint of the date range was selected as the collection day and note is made in the "Collection date notes" (Level 4) metadata field.	Numeric	Entity
3	Collection time	Time of sample collection, in Coordinated Universal Time (UTC) 24-hour format, HH:MM:SS	Text	Entity
3	Water isotope analysis date	Date of water isotope analysis (YYYY-MM-DD)	Text	Entity
3	$\delta^{18}O$ correction value	If a correction was made to the $\delta^{18}O$ value and the correction value is known, the value of the applied correction is indicated in this field. Any accompanying information about how and why the correction was made is reported in the "$\delta^{18}O$ correction notes" (Level 4) metadata field.	Numeric	Seawater Data
3	$\delta^{18}O$ error	Reported error of the $\delta^{18}O$ value. Because many different types of error are reported in the literature, standardization was impossible; therefore, we report the most comprehensive error provided. The type of error along with any supporting information is provided in the "δ18O error notes" (Level 4) metadata field.	Numeric	Seawater Data
3	$\delta^{18}O$ analysis technique	Type of instrument used to make the isotope measurement (isotope ratio mass spectrometry (IRMS), Cavity Ring Down Spectroscopy (CRDS), and off-axis integrated cavity output spectroscopy (ICOS)	Text	Entity
3	$\delta^{2}H$ value	Measured $\delta^{2}H$ value	Numeric	Seawater Data
3	$\delta^{2}H$ correction flag	Indicates whether a correction has been made to the $\delta^{2}H$ value. If the data has been corrected, "Y" is indicated. If the data has not been corrected, "N" is indicated. If the value of the applied correction is known, this value is indicated in the "$\delta^{2}H$ correction value" (Level 3) metadata field and any accompanying information about how and why the correction was made is indicated in the "$\delta^{2}H$ correction notes" (Level 4) metadata field.	Logic	Seawater Data
3	$\delta^{2}H$ correction value	If a correction was made to the $\delta^{2}H$ value and the	Numeric	Seawater

		correction value is known, the value of the applied correction is indicated in this field. Any accompanying information about how and why the correction was made is reported in the “δ^2H correction notes” (Level 4) metadata field.		Data
3	δ^2H error	Reported error of the δ^2H value. Because many different types of error are reported in the literature, standardization was impossible; therefore, we report the most comprehensive error provided.	Numeric	Seawater Data
3	Temperature value	Seawater temperature (degrees Celsius)	Numeric	Seawater Data
3	Temperature error	Reported error of the temperature value (degrees Celsius)	Numeric	Seawater Data
3	Salinity value	Seawater salinity	Numeric	Seawater Data
3	Salinity units	Salinity units (typically "PSU" or "parts per thousand"). Retain original units provided in the publication.	Text	Seawater Data
3	Salinity error	Reported error of the salinity value	Numeric	Seawater Data
4	Collection date notes	A note is made here if the collection day was not specified in the original publication, and only the collection month or a range of dates were specified. In this case the midpoint of the date range was selected as the collection day.	Text	Entity
4	Location notes	A note is made here if the latitude and longitude coordinates are not exact (e.g., some of the NASA GISS database entries have notes stating “A: Position was read off a graph of locations and therefore is not exact"). In these cases, the notes are copied to this metadata field.	Text	Entity
4	Depth notes	If only pressure (and not depth) was reported in the original dataset, a note is made here about how the depth conversion was performed. If a range of depths is provided in the original dataset, the midpoint of the depth range is reported in the “Depth” metadata field (Level 1) and the range is stated here.	Text	Entity
4	$\delta^{18}O$ correction notes	If a correction was made to the $\delta^{18}O$ value, any accompanying information about how and why the correction was made is reported here.	Text	Seawater Data

4	$\delta^{18}O$ error notes	Information about the reported error of the $\delta^{18}O$ value, including the type of error along with any supporting information.	Text	Seawater Data
4	$\delta^{2}H$ correction notes	If a correction was made to the $\delta^{2}H$ value, any accompanying information about how and why the correction was made is reported here.	Text	Seawater Data
4	Sample ID	Unique sample ID provided by original authors.	Text	Queryable
4	$\delta^{18}O$ analysis location	University or institute where the isotope measurements were made.	Text	Entity
4	Publication citation	Citation of the original publication of the data. When the data was obtained from a data repository and no publication citation was found, "NaN" is entered in this field and the relevant citation appears in the "Dataset citation" (Level 4) metadata field.	Text	Entity
4	Publication DOI or URL	DOI or URL of the original publication.	Text	Entity
4	Dataset citation	If the data was obtained from a data repository, the dataset citation is provided here.	Text	Entity
4	Dataset URL	If the data was obtained from a data repository, the dataset URL is provided here.	Text	Entity
4	Dataset ID	If the data was obtained from a data repository, the Dataset ID from that repository is provided here.	Text	Entity
4	Data provenance notes	Indicates the source of the $\delta^{18}O$ data (and $\delta^{2}H$, SST, and SSS data). In some cases, select metadata may have been collected from other data sources, such as the original publication, which is indicated in this field.	Text	Entity
4	Cruise ID	Cruise ID, if applicable.	Text	Entity
4	Station ID	Station ID, if applicable.	Text	Entity
4	Cruise report	Citation of the cruise report, if applicable.	Text	Entity
4	Cruise report URL	Link to the cruise report, if applicable.	Text	Entity
4	Sample collection, processing, and storage notes	Notes on sample collection, sample processing, and sample storage. Sample processing includes any treatments prior to analysis (distillation, filtration, etc). Sample storage includes the type of storage container and any preventative measures taken against evaporation (sample seals, refrigeration, etc).	Text	Entity

4	Water isotope analysis notes	Notes on the isotope analysis methods, including details of any equilibration steps used between the water and CO_2 or H_2 gas, the specific type of instrumentation used for the isotopic analysis, details of the calibration steps and standards used, number of replicate measurements, corrections for instrumental drift and memory effects, and preventative steps taken to minimize salt contamination (e.g., for cavity ring down spectroscopy).	Text	Entity
5	Location type	Type of water body from which the water samples were collected (e.g., open ocean, coastal, bay, lagoon, estuary, enclosed sea, marginal/semi-enclosed sea).	Text	Entity
5	Location description	Description of the sampling location, including a description of the major water masses and currents influencing the region, as well as details on the surface water balance, groundwater or riverine input, upwelling, distance from the coastline, depth and geometry of bay or lagoon, and/or description of co-located coral reef site if applicable.	Text	Entity
5	Temperature/salinity notes	Notes on the sample collection and/or analysis of temperature and salinity.	Text	Entity

*There are four cases in which datasets obtained from the GISS database were not clearly associated with a publication, or the provided reference did not match the dataset. In those cases, the Schmidt et al. (1999) database citation is provided in the "Dataset citation" (Level 4) metadata field and the author letters "SC" are used in the unique CoralHydro2k ID to reference that citation (SC99AO0001, SC99PO0001, SC99IO0001, SC99GI0001). Additional details about the citations and data provenance appear in the "Data provenance notes" (Level 4) metadata field.

**Corrections were applied to the $\delta^{18}O$ data in several datasets in the NASA GISS $\delta^{18}O_{sw}$ database to standardize the data based on deep water masses to correct for changes in standards, different analysis techniques, and other systematic errors. Corrections were also applied to the $\delta^{18}O$ and $\delta^{2}H$ data in the Reverdin et al. (2022) LOCEAN database to account for the effect of salt on the IRMS and CRDS analyses (Benetti et al., 2017b). According to Reverdin et al. (2022): "these corrections could present differences with datasets processed in other institutions without this proposed adjustment of up to 0.10‰ in $\delta^{18}O$ and 0.20‰ in $\delta^{2}H$." The adjusted LOCEAN CRDS $\delta^{18}O$ data thus may be higher (more enriched in heavy isotopes) than other CRDS and IRMS data. Corrections were also applied to some of the samples in the LOCEAN database to adjust for minor evaporation biases, based on the deviation from the expected relationship between d-excess and salinity (see section 2.5 in Reverdin et al. (2022) and Appendix B in Benetti et al. (2017a)). The correction values were reported in the GISS database, but not the LOCEAN database. In the current CoralHydro2k database, all corrections are noted by the $\delta^{18}O$ and $\delta^{2}H$ correction flags and, where available, the values of the corrections are reported in the "$\delta^{18}O$ correction values" and "$\delta^{2}H$ correction values" (Level 3) metadata fields so the user can remove the corrections if desired. Any accompanying information about how and why the correction was made is reported in the "δ^{18}O correction notes" and δ^{2}H correction notes" (Level 4) metadata fields.

Table 2: Standardized controlled vocabulary options for metadata fields in the database.

Metadata Field	Standardized Entries
δ^{18}O correction flag	Y, N
Evaporation flag	Y, N
Reference standard	VSMOW, SMOW
δ^{18}O analysis technique	IRMS, CRDS, ICOS
Salinity units	PSU, PSS-78, PPT, g/L

3 Key characteristics of the seawater δ^{18}O data

3.1 Spatial and temporal coverage of the database

The CoralHydro2k Seawater δ^{18}O Database contains 18,598 data points from 106 datasets (Fig. 1A,B). 53% of the data (9,862 data points) is categorized as "hidden" data (i.e., data not currently available in public databases or public repositories; Fig. 1C,D), and the remaining 47% of the data is from public databases or public repositories (Table 3). 10,407 measurements (56%) are from the sea surface (depth ≤ 5 m; Fig. 1A), 3,693 (20%) are from the mixed layer (between 5–50 m), and 4,498 (24%) are below 50 m. The time span of the database covers 1972 to 2021 (Fig. 2) and the depth range covers the surface to 5,797 m below sea level. The earliest data point in the database was collected in September 1972 and the most recent data point was collected on October 8, 2021. 3,480 data points (19%) were collected before the year 2000, and 15,118 data points (81%) were collected on or after the year 2000 (Fig. 2). Because the addition of public datasets focused on the region between 35ºN and 35ºS, 75% of the measurements in the database are located within the tropical-subtropical region.

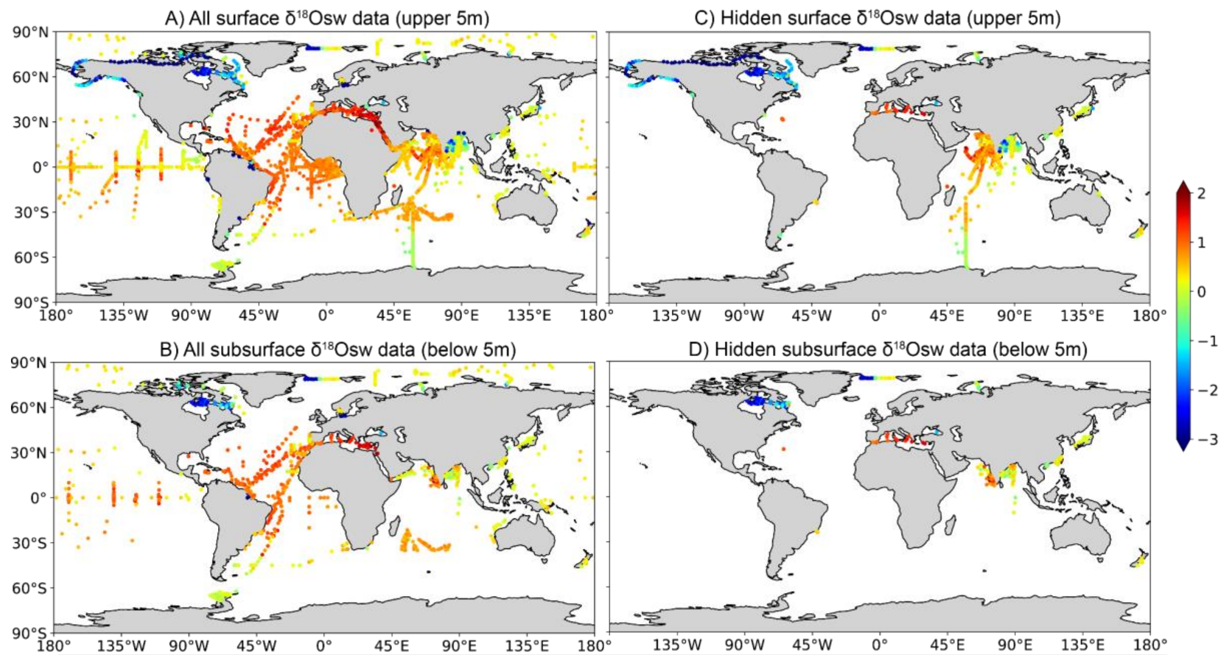

Figure 1: Locations and seawater δ^{18}O values of data in the database: (A) all surface ocean data (upper 5 m of the water column), (B) all subsurface ocean data (below 5 m), (C) the hidden surface ocean data only (upper 5 m), (D) the hidden subsurface ocean data only (below 5 m).

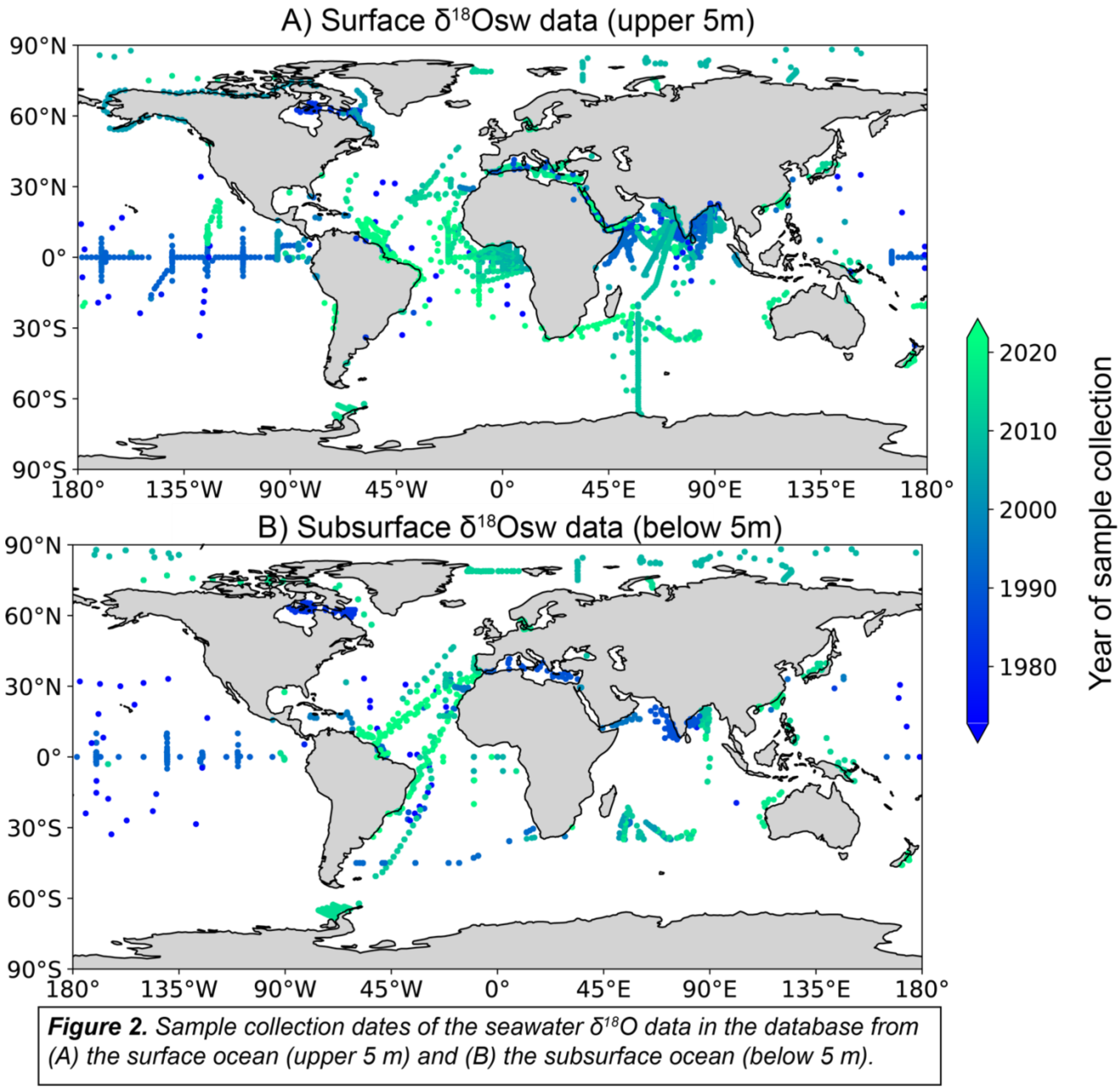

Figure 2: Sample collection dates of the seawater δ^{18}O data in the database from (A) the surface ocean (upper 5 m) and (B) the subsurface ocean (below 5 m).

In addition to δ^{18}O measurements, the database also includes paired δ^{2}H, salinity, and temperature measurements when available. 16,098 data points (87%) have paired salinity values (Fig. 3A), 13,871 data points (75%) have paired temperature values (Fig. 3B), and 9,769 data points (53%) have paired δ^2H measurements (Fig. 3C). 185 measurements have an evaporation flag (Fig. 3D), which allows the user to filter out samples that may be influenced by post-collection evaporation from the database.

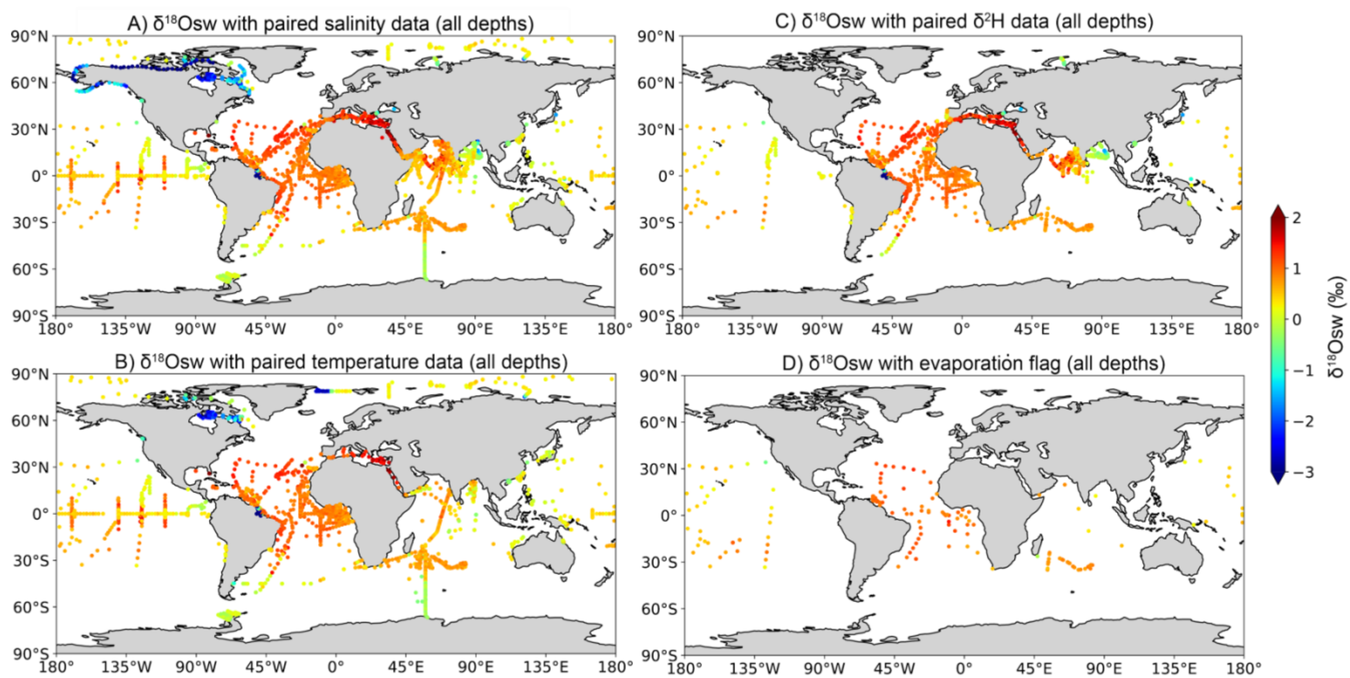

Figure 3: Locations and seawater $\delta^{18}O$ values of the data in the database with (A) paired salinity measurements, (B) paired temperature measurements, (C) paired δ^2H measurements, and (D) an evaporation flag.

Compared to the seawater $\delta^{18}O$ database presented in LeGrande and Schmidt (2006), data coverage in the surface ocean (upper 5 m) is substantially improved in the tropics and subtropics, particularly in the northern Indian Ocean, the eastern Atlantic Ocean, the northeast coast of South America, the Mediterranean Sea, and the equatorial Pacific Ocean. However, poor data coverage still exists in the western Pacific Ocean and Maritime Continent region, the southeastern Indian Ocean, and the subtropical Pacific Ocean regions in both hemispheres. Below 5 m depth, the data coverage is even more limited (Fig. 1B). At all depths, regions with reasonable spatial coverage of $\delta^{18}O_{sw}$ data contain limited temporal coverage (Fig. 4A). Typically, only a few years of regular measurements are available from the most highly sampled regions. For example, only 21% of locations contain at least 12 measurements spanning two years within a 2º latitude x 2º longitude grid box and only 8% of the grid boxes contain data that cover at least 50% of the annual cycle (i.e., 6/12 months of the calendar year; Fig. 4B). While the coverage of seawater isotope data has been growing over the last decade, these measurements are still sparse in space and time, thus highlighting the need for globally coordinated sampling campaigns and archiving efforts.

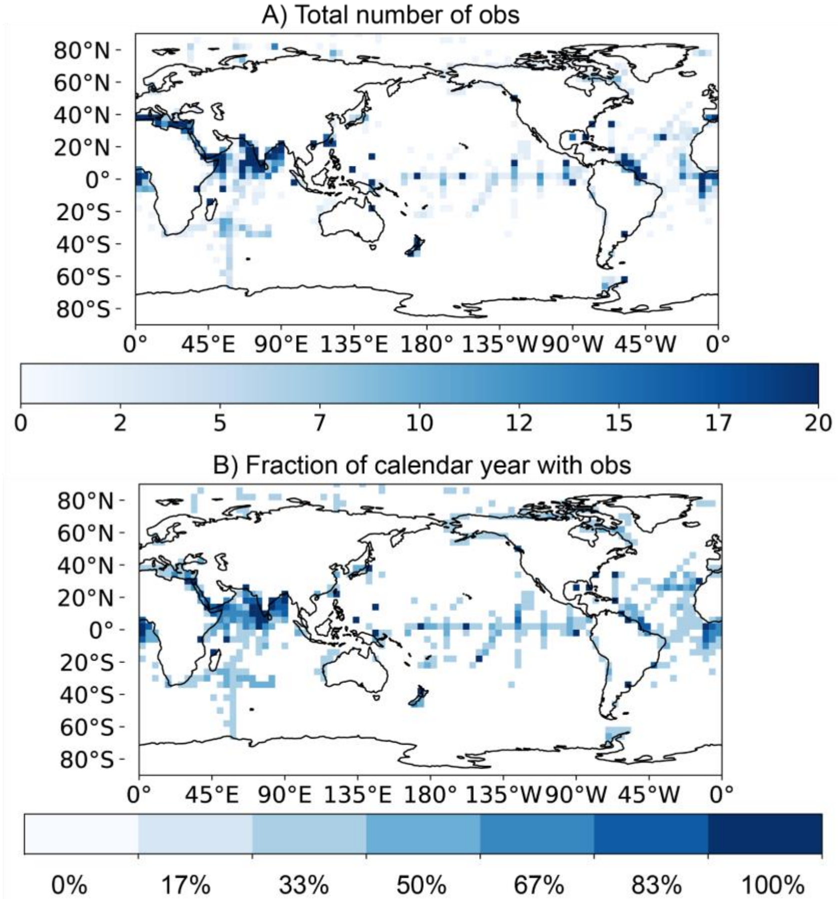

Figure 4: Temporal distribution of near-surface (upper 5m) $\delta^{18}O_{sw}$ measurements in the database, aggregated in 2°x2° (latitude x longitude) grid boxes. (A) Total number of $\delta^{18}O_{sw}$ measurements in each grid box. (B) Fraction of calendar year with $\delta^{18}O_{sw}$ measurements.

Outside of the tropics and subtropics, the coverage of $\delta^{18}O$ data in the CoralHydro2k Seawater $\delta^{18}O$ Database is sparser, since only hidden datasets were collected from all latitudes and all depths across the global ocean, while datasets from public repositories were only incorporated into the database if the measurements were made in the upper 50 m between 35°N and 35°S. Future database development efforts will include incorporating additional hidden and public datasets.

3.2 Data-model comparisons of the seawater $\delta^{18}O$ data

To assess how the $\delta^{18}O_{sw}$ data in the database compares with isotope-enabled climate model simulations and other products, we compare the climatological annual cycle in $\delta^{18}O_{sw}$ at different island sites using four data products: two simulations of isotope-enabled General Circulation Models [the National Center for Atmospheric Research Community Earth System Model Last Millennium Ensemble (1000 years; Brady et al., 2019) and the NASA Goddard Institute for Space Studies E2-R last millennium simulation (ensemble member E4rhLMgTck; 255 years; Colose et al., 2016)], a regional ocean model of the Pacific called isoROMS (44 years; Stevenson et al., 2018), and a gridded dataset of global monthly mean $\delta^{18}O_{sw}$ based on data assimilation with the MITgcm (Breitkreuz et al., 2018). The Breitkreuz dataset is based on a 400-year quasi-equilibrated simulation of a water isotope-enabled global ocean general circulation model constrained by global monthly $\delta^{18}O_{sw}$ data collected from 1950 to 2011 and climatological salinity and temperature data collected from 1951 to 1980.

The characteristics of $\delta^{18}O_{sw}$ variability at the four selected sites in the tropical Pacific and Atlantic Oceans vary widely across the different data products and the $\delta^{18}O_{sw}$ observations from the CoralHydro2k Seawater $\delta^{18}O$ Database, with large differences in both the amplitude and phase of the annual cycle of $\delta^{18}O_{sw}$ (Fig. 5). These differences could be due to deficiencies in the models (associated with subgrid-scale parameterizations, treatment of atmospheric exchange and ocean mixing processes, and/or the limited spatial resolution of the models not capturing the local influence of evaporation, precipitation, runoff, and upwelling at the sampling sites), and/or uncertainties in the observational data given the low temporal resolution of the $\delta^{18}O_{sw}$ measurements. Clearly, more observational data is needed to determine the source of the discrepancies, pointing to the need for more coordinated and sustained seawater isotope sampling programs. Seawater isotope sampling at multinational observing systems that are already in place, such as the Tropical Pacific Observing System (TPOS), Bermuda Atlantic Time-series Study (BATS), GO-SHIP, and GEOTRACES, could expand and complement existing observational programs. For example, incorporating new sampling devices such as long-term osmotically pumped fluid samplers (Jannasch et al., 2004; Khare et al., 2021) could provide a relatively straightforward way to add $\delta^{18}O_{sw}$ measurements to existing programs. The development of sustained seawater isotope measurements at a network of observational hotspots around the global ocean would provide powerful new constraints on hydrologic changes in the modern ocean, generating data that could be used to test theoretical predictions, assess climate model performance and skill, and calibrate paleoclimate proxies for improved paleoclimate reconstruction.

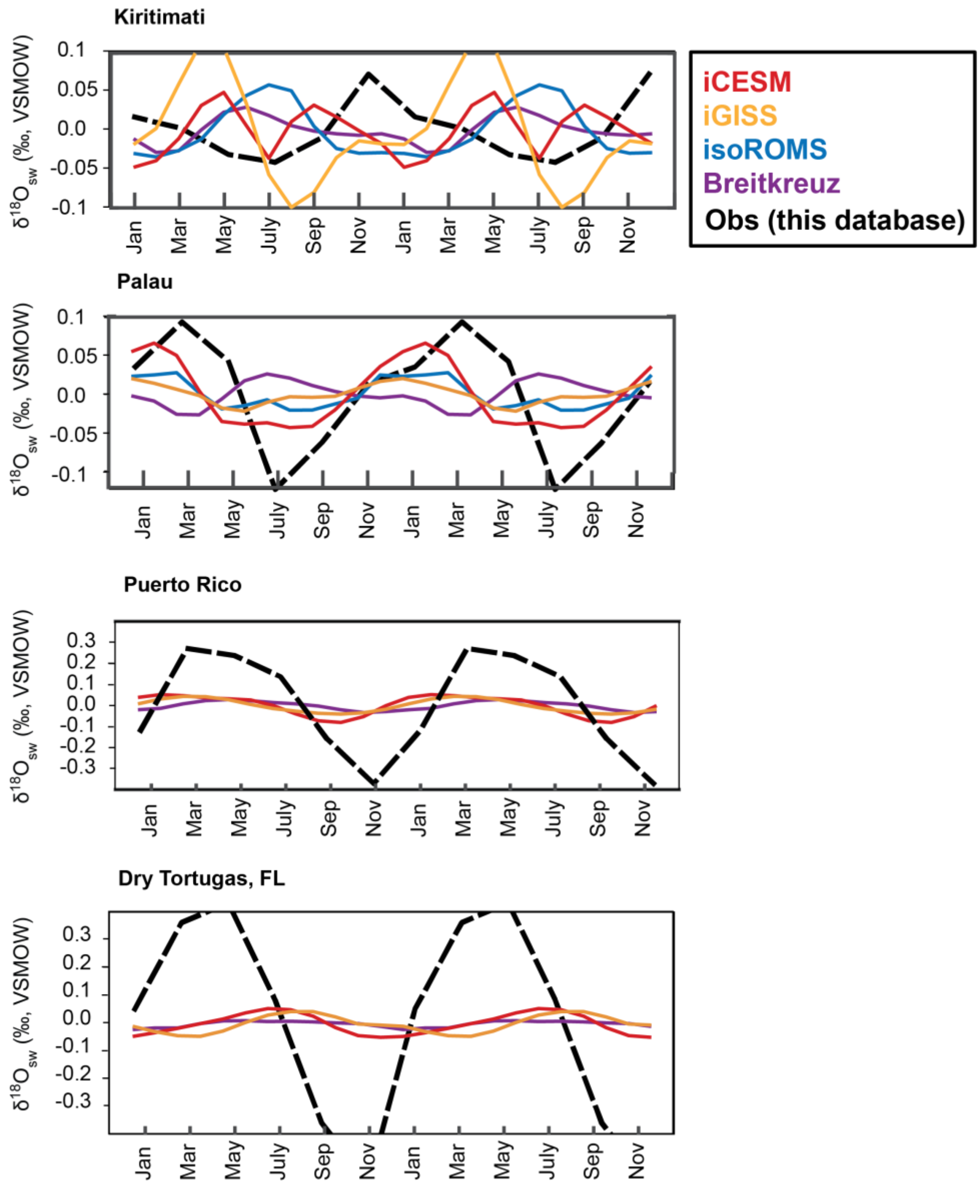

Figure 5: Monthly climatology of $\delta^{18}O_{sw}$ at four island locations: Kiritimati Atoll in the Central Pacific Ocean, Palau in the western Pacific Ocean, Puerto Rico in the Caribbean Sea, and Dry Tortugas in the Gulf of Mexico. Five data sources are shown: observed $\delta^{18}O_{sw}$ (from this database; black dashed line), simulated $\delta^{18}O_{sw}$ from iCESM, iGISS, and isoROMS, and $\delta^{18}O_{sw}$ from the reanalysis product of Breitkreuz et al., 2018 (purple; monthly climatology constrained by observed monthly $\delta^{18}O_{sw}$ data collected from 1950 to 2011 and climatological salinity and temperature data collected from 1951 to 1980). The three Earth system models are the National Center for Atmospheric Research Community Earth System Model Last Millennium Ensemble (1,000 years; red) (Brady et al., 2019), the NASA Goddard Institute for Space Studies E2-R last millennium simulation (ensemble member E4rhLMgTck; 255 years; yellow) (Colose et al., 2016), and the isoROMs Pacific Ocean simulation (44 years; blue) (Stevenson et al., 2018).

4 Applications of the database

While the primary motivation of the CoralHydro2k Seawater $\delta^{18}O$ Database was for coral paleoclimate research, this database was designed to be useful to researchers from a wide range of disciplines, including paleoceanography and paleoclimatology, oceanography, marine biology, Earth science, and climatology. Of relevance to paleoclimate applications, the pairing of seawater oxygen isotope data with salinity data can provide transfer equations for reconstructing past salinity variations (e.g., Gagan et al., 1998; Kilbourne et al., 2004; McCulloch et al., 1994; Ren et al., 2003). For example: coral Sr/Ca, a temperature proxy, paired with coral $\delta^{18}O$, a proxy for both temperature and $\delta^{18}O_{sw}$, can be used to remove the temperature component from the coral $\delta^{18}O$ signal. The derived $\delta^{18}O_{sw}$ can then be converted to salinity using the local $\delta^{18}O_{sw}$ to salinity transfer equation (e.g., Kilbourne et al., 2004). The same method can be applied to foraminifera Mg/Ca and $\delta^{18}O$ records to reconstruct salinity variations and can also potentially be applied to bivalves, coralline algae, ostracods, and otoliths (e.g., Light et al., 2018; Schmidt and Lynch-Stieglitz, 2011; Stott et al., 2004; Trofimova et al., 2020; Warner et al., 2022). Many studies have used this paired approach to reconstruct $\delta^{18}O_{sw}$ variations for a wide range of time scales (e.g., Brocas et al., 2019; Felis et al., 2009; Giry et al., 2013; Gorman et al., 2012; Hereid et al., 2013; Knebel et al., 2024; Wu et al., 2013); however, few studies have been able to validate their reconstructions with observed $\delta^{18}O_{sw}$ records that span more than one year (Conroy et al., 2017; O'Connor et al., 2021). Instead, most studies use reanalysis products such as Simple Ocean Data Assimilation (SODA) (Carton et al., 2000, 2018), or satellite-derived sea surface salinity (SSS) products (e.g., NASA Aquarius, NASA SMOS) (Boutin et al., 2021) for validating the reconstructions (e.g., Cahyarini et al., 2008; Harbott et al., 2023; Hetzinger et al., 2006). Typically, these applications assume that the salinity versus $\delta^{18}O_{sw}$ relationship is stable in time; however, this assumption has been shown to break down in many instances: e.g., with temporal variations observed between monsoon and non-monsoon seasons (Ghosh et al., 2013; McConnell et al., 2009), in regions affected by sea ice formation and melting (Strain and Tan, 1993), and under variations in ocean advection, upwelling, and ocean-atmosphere interactions (Conroy et al., 2017; Rohling and Bigg, 1998).

The CoralHydro2k Seawater $\delta^{18}O$ database can be leveraged to explore the relationship between these two parameters by combining the seawater $\delta^{18}O$ data with the paired salinity data in the database (e.g., Conroy et al., 2017; Durack et al., 2012; LeGrande and Schmidt, 2006; Wagner and Slowey, 2011). In this way, the Seawater $\delta^{18}O$ Database also has important applications to modern oceanography. By allowing these relationships to be more comprehensively assessed across space and time, this database (alongside future improvements in data coverage) will have important applications to resolving past and present oceanographic variations and change.

Additionally, the CoralHydro2k Seawater $\delta^{18}O$ Database can be used in proxy-system model development, paleo-data assimilation, and comparison studies between proxy reconstructions and climate model output (Dee et al., 2023; Evans et al., 2013; Reed et al., 2022; Sanchez et al., 2021; Smerdon, 2012; Stevenson et al., 2018; Thompson et al., 2011). Proxy-derived

$\delta^{18}O_{sw}$ data can be directly compared with simulations from isotope-enabled models as part of the validation process and to understand oxygen isotope fractionation processes within the hydrological cycle (Dee et al., 2015; Stevenson et al., 2015, 2023). Furthermore, the proxy-derived salinity reconstructions can be compared with reanalysis and other salinity data products, such as SODA, as a separate validation step (e.g., Cahyarini et al., 2008). Finally, the Seawater $\delta^{18}O$ Database offers the opportunity for improved proxy system models with rigorous uncertainty quantification of proxy-derived estimates of salinity. With such estimates, long reconstructions of salinity would provide valuable insights into the low frequency variability of the hydrological cycle over the data sparse tropical oceans. This Seawater $\delta^{18}O$ Database is the most comprehensive to date and will be updated as new datasets are published to support ongoing research (see Section 6).

5 Code/Data availability

5.1 Accessing the database

The CoralHydro2k Seawater $\delta^{18}O$ Database follows the FAIR data principles (Wilkinson et al., 2016) that strive to make scholarly data findable, accessible, interoperable, and reusable. The CoralHydro2k Seawater $\delta^{18}O$ Database uses the Comma Separated Values (*.CSV) file format, a machine-readable format for archiving and describing seawater isotope data. Access to the database has been granted for reviewers and editors during the review phase. The data are also available upon request for members of the public that wish to participate in the review process by emailing the corresponding author. Once the review period is complete, the database will be available on the NOAA NCEI World Data Service for Paleoclimatology (study page: https://www.ncei.noaa.gov/access/paleo-search/study/34575) and issued a permanent DOI. A mirror copy of the database will also be hosted at Waterisotopes.org.

5.2 Code availability

Example Jupyter notebooks and MATLAB scripts are available on the CoralHydro2k Seawater Database GitHub page (https://github.com/CoralHydro2k/ch2kSeawater_Database) to help users search, filter, and visualize the database. We encourage users of the database to share their scripts on GitHub as well for improved access.

5.3 Underlying data sources

The CoralHydro2k Seawater $\delta^{18}O$ Database includes records (0–50 mbsl, 35ºN to 35ºS) from ten international databases, including GEOTRACES, NASA GISS, PANGAEA, CISE LOCEAN, GLODAPv2, WIDB, NOAA NCEI, and BODC (Table 3). Literature searches were also conducted to find hidden seawater $\delta^{18}O$ data (from all depths and latitudes) published only in tables and supplemental data files of published papers, theses, and dissertations. Data was also sourced from author contributions sent directly to this project or the EarthChem community (earthchem.org/communities/seawater-oxygen-isotopes). Users of this database should adhere to the data use policies for the underlying data sources (see Table 3 and Appendices A1–A4).

Table 3. Databases included

Database	URL (https://)	Notes	References
British Oceanographic Data Centre	https://www.bodc.ac.uk/	See A1 for data usage policies	Acknowledge the source of the information by including an attribution statement, see A1.
CISE LOCEAN Seawater Isotope (SEANOE)	www.seanoe.org/data/00600/71186/)	Public domain, see URL for data usage details.	(waterisotopes-CISE-LOCEAN 2024); Reverdin et al. 2022)
GEOTRACES	geotraces.webodv.awi.de/	See A2 for data usage policies	(GEOTRACES Intermediate Data Product Group, 2023)
Global Ocean Data Analysis Project (GLODAPv2.2022)	www.ncei.noaa.gov/access/metadata/landing-page/bin/iso?id=gov.noaa.nodc:0257247	See A3 for data usage policies	(Key et al., 2023; Olsen et al., 2016)
NASA GISS Global Seawater Oxygen-18 (GISS)	data.giss.nasa.gov/o18data/	Public domain	(Bigg and Rohling, 2000; Schmidt, 1999; Schmidt et al., 1999)
NOAA National Centers for Environmental Information (NCEI)	www.ncei.noaa.gov/	Public domain	Cite original publication, online resource, dataset and publication DOIs (where available), and date accessed
NOAA NCEI Paleoclimatology	www.ncei.noaa.gov/products/paleoclimatology	Public domain	Cite original publication, online resource, dataset and publication DOIs (where available), and date accessed
NOAA NCEI World Ocean	www.ncei.noaa.gov/products/world-ocean-database	Public domain	(Boyer et al., 2018)
PANGAEA	www.pangaea.de/	Terms of use https://www.pangaea.de/about/terms.php	(Felden et al. 2023)
Waterisotopes.org (WIDB)	https://wateriso.utah.edu/waterisotopes/	See A4 for data usage policies	http://waterisotopes.org

6 Database submission of new datasets and versioning scheme

The CoralHydro2k Seawater $\delta^{18}O$ project will accept data submissions for updates to the database. All seawater $\delta^{18}O$ observations are welcomed regardless of location or water depth. To facilitate this process, a Seawater Oxygen Isotopes Community was developed within the EarthChem Library, an open-access repository for geochemical datasets (earthchem.org/communities/seawater-oxygen-isotopes), where researchers can submit their seawater isotope data and obtain a dataset DOI. The Seawater Oxygen Isotopes Community contains a template that can be downloaded to help researchers submit their data. This template is aligned with the CoralHydro2k Seawater $\delta^{18}O$ Database to facilitate future updates to the database. The template has a README tab in the Microsoft Excel file with details on the template and an example. We hope that the creation of this site helps researchers publish their seawater isotope datasets, thus minimizing the number of "hidden" datasets.

The initial release of the CoralHydro2k Seawater $\delta^{18}O$ Database will be Version 1.0.0 for this publication. With new submissions, the database will grow as new datasets are added. Database users who find errors in the database can use the "Report an issue" option in the GitHub site. Datasets submitted to the Seawater Oxygen Isotopes Community within the EarthChem Library (earthchem.org/communities/seawater-oxygen-isotopes) can be updated through that site.

As the CoralHydro2k Seawater $\delta^{18}O$ Database is updated, it will be versioned following the scheme used by other PAGES data collection projects (Ahmed et al., 2013; Emile-Geay et al., 2017; Kaufman et al., 2020; McKay and Kaufman, 2014; Walter et al., 2023). The version number has three counters in the following form: $C_1.C_2.C_3$, where C_1, C_2, and C_3 are incrementing integers. When C_1 increases, C_2 and C_3 reset to zero. When C_2 increases, C_3 resets to zero. C_1 represents the number of publications describing the database. C_2 increments each time the set of records in the database changes (addition or removal of a dataset). C_3 increments when the data or metadata within the dataset changes, but the set of records remains the same. Upon updates, extensions, or corrections to the database, rather than issuing errata to this publication, changes will be included in subsequent versions of the database and updated and described through the online data repository.

7 Citation

This CoralHydro2k Seawater $\delta^{18}O$ Database descriptor publication should be cited when the database is used in whole or in part, including its metadata fields, for subsequent studies. We encourage end users of this database to also cite the original publications and/or data sources of the underlying primary data (Table 3). To facilitate this process, citation information for every data point is included in the metadata, including a full citation and DOI of the original publication, as well as a dataset citation and DOI for the original public archive of the data. Researchers should also adhere to the data use policies for the underlying data sources (see Appendices A1–A4).

8 Conclusions and anticipated applications of the Seawater $\delta^{18}O$ Database

Observational seawater $\delta^{18}O$ and $\delta^{2}H$ data can place powerful constraints on the global water cycle, providing valuable information on the exchange of water between the ocean, atmosphere, and cryosphere, as well as on ocean-mixing processes. As such, these data provide an additional set of constraints for understanding the complex hydrologic system, beyond what standard oceanographic variables like temperature and salinity can offer. They also provide a "common currency" that links paleoclimate reconstructions, modern climate observations, and isotope-enabled model simulations, allowing hydrologic processes to be evaluated on a wide range of time and spatial scales. Given the broad value of this data, and the growing number of seawater $\delta^{18}O$ and $\delta^{2}H$ datasets that have been generated since 2011, the CoralHydro2k Seawater $\delta^{18}O$ Database was developed to improve the accessibility of seawater isotope data for the Earth Science research community. This new, machine-readable, and metadata-rich database contains over 18,600 observational seawater $\delta^{18}O$ data points, paired with seawater $\delta^{2}H$ and salinity data and extensive metadata that makes the database suitable for a myriad of research applications. The metadata template also provides a set of best practices for reporting seawater isotope data in future studies.

The CoralHydro2k Seawater $\delta^{18}O$ Database and its extensive metadata can provide insight into the multiple processes that impact seawater $\delta^{18}O$ and $\delta^{2}H$. Furthermore, the database can be used to better constrain the relationship between $\delta^{18}O_{sw}$ and salinity in the global ocean, and (in conjunction with future improvements in data coverage) provide insight into how this relationship varies in space and time. The database also provides updated seawater $\delta^{18}O$ and $\delta^{2}H$ data critical for the calibration and validation of paleoclimate reconstructions using $\delta^{18}O$ and $\delta^{2}H$ to reconstruct past ocean temperature and salinity variations. For example, recent paleoclimate data assimilation efforts would greatly benefit from a spatial network of observational $\delta^{18}O_{sw}$ data for training the proxy system models that underlie those efforts. This database could also be used to construct a new gridded dataset of $\delta^{18}O_{sw}$ to update that of (LeGrande and Schmidt (2006), which has been widely used for providing climate model boundary conditions and to assess model performance and skill in resolving key features of the hydrologic cycle. In this way, the PAGES CoralHydro2k Seawater $\delta^{18}O$ Database can be used in a wide variety of applications to bolster our understanding of the modern climate system, while also providing new insights into past and future climate variability and change.

9 Author contribution

AA, KD, AM, TF, SL, SS, and ED designed the database, AA, AM, RP, SL, KD, JH, CM, SS, and AV entered data and/or metadata into the database, AA, AM, SL, RP, JH, CM, and ED performed quality control on the database, AA and KD prepared the manuscript, with contributions from all co-authors, RP developed the example Python code, and JH developed the Github site for the database.

10 Competing interests

The authors declare that they have no conflict of interest.

11 Acknowledgements

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We thank the PAGES CoralHydro2k team for their encouragement and effort in building this database, especially the helpful comments and suggestions from Amy Wagner and Hali Kilbourne. We also thank Gilles Reverdin for useful discussions about the database. Many thanks to Erika Ornouski for her work in finding hidden $\delta^{18}O_{sw}$ data files in the early stages of the project. We are grateful to Kerstin Lehnert and the EarthChem team at Lamont Doherty Earth Observatory and Carrie Morrill and Edward Gille and Bruce Bauer at NOAA/WDS Paleoclimatology for providing opportunities to host the new database. We also recognize the efforts of Gavin Schmidt, Eelco Rohling, Grant Bigg, and Allegra LeGrande in building and maintaining the first seawater $\delta^{18}O$ database (https://data.giss.nasa.gov/o18data/), as well as Gabriel Bowen at the University of Utah (waterisotopes.org) and Gilles Reverdin at LOCEAN-IPSL (https://www.locean.ipsl.fr/?lang=fr) for their data collection and compiling efforts in continuing to make such data publicly available.

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