

1. Project

Title - SISALv3: Speleothem Isotopes Synthesis and AnaLysis database version 3.0

Dates – 2020 to 2024

Funding organizations - Past Global Changes (PAGES) programme which receives financial support from the Swiss Academy of Sciences and the Chinese Academy of Sciences.

2. Dataset

Title - SISALv3: Speleothem Isotopes Synthesis and AnaLysis database version 3.0

Summary description - Stable isotope and trace elements records from speleothems provide information on past climate changes, most particularly information that can be used to reconstruct past changes in precipitation and atmospheric circulation. SISAL (Speleothem Isotope Synthesis and Analysis) is an international working group of the Past Global Changes (PAGES) project. The working group aims to provide a comprehensive compilation of speleothem isotope and trace elements records for climate reconstruction and model evaluation. SISALv3 database contains 892 oxygen isotope, 620 carbon isotope, 95 Mg/Ca, 85 Sr/Ca, 52 Ba/Ca, 25 U/Ca, 29 P/Ca and 14 Sr isotope records from 838 speleothems from 365 cave sites worldwide, and metadata describing the cave settings and age models of these records. This version also contains standardized age-depth models.

Publication year – 2023

Creators - Kaushal, Nikita, Lechleitner, Franziska, Wilhelm, Micah and SISAL working group members

Right holders - University of Oxford

The following SISAL Working Group members contributed with running the standardised SISAL age-depth models for the new entities that were added to SISALv3 version of the database: Kira Rehfeld (Geo- and Umweltforschungszentrum, Tübingen, Germany) and Janica Buehler (Institute of Environmental Physics and Interdisciplinary Center for Scientific Computing, Heidelberg University, Germany).

The following SISAL Working Group members contributed with down sampling the trace element records to stable isotope equivalent depths: Vanessa Skiba (Potsdam Institute for Climate Impact Research, Potsdam, Germany) and Magdalena Ritzau (Geo- and Umweltforschungszentrum, Tübingen, Germany).

The following SISAL Working Group members contributed with adding metadata information, where available in publications, to the newly added metadata fields in SISALv3 version of the database: Khalil Azennoud (Sidi Mohamed Ben Abdellah University, Morocco) and Kerstin Braun (Arizona State University, United States of America).

The following SISAL Working Group members contributed with standardising the submitted trace element datafiles: Yuval Burstyn (UC Davis, United States of America) and Nikita Kaushal (University of Oxford, United Kingdom).

The following SISAL Working Group members contributed with gathering the citation, copyright statement and licence terms for the cave map and speleothem section image files in the database: Jozsef G. Szucs (Eotvos Lorand University, Hungary) and Nikita Kaushal (University of Oxford, United Kingdom).

The following SISAL Working Group members coordinated the regional data collection and/or assisted in the quality control procedure of the SISALv3 database: Vitor Azevedo (Department of Geology, Trinity College Dublin, Dublin 2, Ireland), Jonathan Lloyd Baker (Institute of Global Environmental Change, Xi'an Jiaotong University, Xi'an, 710049, China), Sakonvan Chawchai (Department of Geology, The Faculty of Science, Chulalongkorn University, Bangkok, 10330, Thailand), Andrea Columbu (University of Pisa, Department of Earth Sciences, Via Santa Maria 53, 56126 Pisa Italy), Laura Endres (ETH Zurich, Switzerland), Jens Fohlmeister (Federal Office for Radiation Protection, Koepenicker Allee 120, 10318 Berlin Germany), Jun Hu (College of Ocean and Earth Sciences, Xiamen University, Xiamen, Fujian, 361102, China), Zoltan Kern ((Institute for Geological and Geochemical Research, Research Centre for Astronomy and Earth Sciences, H-1112, Budaörsi út 45, Budapest, Hungary), Alena Kimbrough (Research School of Earth Sciences, The Australian National University, Acton, ACT, 2601, Australia), Koray Koc (Department of Geological Engineering, Akdeniz University, 07058, Antalya, Türkiye and Department of Environmental Sciences, Quaternary Geology, University of Basel, 4056 Basel, Switzerland), Monika Markowska (Max Planck Institute for Chemistry, Mainz, Germany), Belen Martrat (Department of Environmental Chemistry, Spanish Council for Scientific Research (CSIC), Institute of Environmental Assessment and Water Research (IDAEA), Barcelona, Spain), Syed Masood Ahmad (Department of Geography, Faculty of Natural Sciences, Jamia Millia Islamia, New Delhi, India), Carole Nehme (UMR IDEES 6266, CNRS, University of Rouen Normandy, 1, Rue Thomas Becket, Mont Saint-Aignan, 76130, France), Valdir Felipe Novello (Department of Geosciences, University of Tübingen, Tübingen, 72076, Germany), Carlos Pérez-Mejías (Institute of Global Environmental Change, Xi'an Jiaotong University, 710049 Xi'an, China), Jiaoyang Ruan (Center for Climate Physics, Institute for Basic Science, Busan, Republic of Korea and Pusan National University, Busan, Republic of Korea), Natasha Sekhon (Department of Earth, Environmental and Planetary Science, Brown University, Providence 02908, Rhode Island, USA 2 and Institute at Brown for Environment and Society, Brown University, Providence 02908, Rhode Island, USA), Nitesh Sinha (Center for Climate Physics, Institute for Basic Science, Busan, Republic of Korea. Pusan National University, Busan, Republic of Korea), Carol Tadros (ANSTO, New Illawarra Road, Lucas Heights, NSW 2234, Australia and School of Biological, Earth and Environmental Sciences, UNSW Sydney, Sydney, NSW, 2052, Australia), Benjamin H. Tiger (MIT, Cambridge, Massachusetts, United States of America), Sophie Warken (Institute of Earth Sciences, Ruprecht Karls University Heidelberg, Im Neuenheimer Feld 234, 69120 Heidelberg, Germany and Institute of Environmental Physics, Ruprecht Karls University Heidelberg, Im Neuenheimer Feld 229, 69120 Heidelberg, Germany), Annabel Wolf (Northumbria University, Department of Geography and Environmental Sciences, Newcastle upon Tyne NE1 8ST, United Kingdom), Haiwei Zhang (Institute of Global Environmental Change, Xi'an Jiaotong University, Xi'an, 710049, China).

The following SISAL group members contributed data to SISALv3 database: Asfawossen Asrat (Department of Mining and Geological Engineering, Botswana International University of Science and Technology, Private Bag 16, Palapye, Botswana), Charlotte Honiat (Institute of Geology, University of Innsbruck, Innrain 52, Innsbruck, Austria), Dana Felicitas Christine Riechelmann (Institute for Geosciences, Johannes Gutenberg University Mainz, Johann-Joachim-Becher-Weg 21, 55128 Mainz, Germany), Denis Scholz (Institute for Geosciences, Johannes Gutenberg University Mainz, Johann-Joachim-Becher-Weg 21, 55128 Mainz, Germany), Dianbing Liu (School of Geography, Nanjing Normal University, Nanjing 210023, China), Dominik Fleitmann (Department of Environmental Sciences, University of Basel, Bernoullistrasse 32 4056 Basel, Switzerland), Dominik Hennhofer (Department of Earth Sciences, Khalifa University (SAN Campus), Abu Dhabi, 127788, United Arab Emirates), Ezgi Ünal İmer (Geological Engineering Department, Middle East Technical University, 06800 Çankaya, Ankara, Turkey), Gina E. Moseley (Institute of Geology, University of Innsbruck, Innrain 52, 6020 Innsbruck, Austria), Giselle Utida (Institute of Geosciences, University of São Paulo, 05508-080, Brazil), Hai Cheng (Institute of Global Environmental Change, Xi'an Jiaotong University, China), Helen Green (The University of Melbourne, Parkville VIC 3010, Australia), Hsun-Ming Hu (High-Precision Mass Spectrometry and Environment Change Laboratory (HISPEC), Department of Geosciences, National Taiwan University, Taipei 10617 Taiwan), James Apaéstegui (Instituto Geofísico del Perú, Lima, 15012, Peru), Jan Esper (Department of Geography, Johannes Gutenberg University, Becherweg 21, 55099 Mainz, Germany), Jasper A. Wassenburg (1. Center for Climate Physics, Institute for Basic Science, 10,11th Fl. M-building, 2 Busandaehak-ro 63beon-gil, Geumjeong-gu, Busan 46241, Republic of Korea 2. Pusan National University, 2 Busandaehak-ro 63beon-gil, Geumjeong-gu, Busan, Republic of Korea), Jeronimo Aviles Olguin (Museo del Desierto. Blvd. Carlos Abedrop Dávila 3745, Nuevo Centro Metropolitano de Saltillo, 25022 Saltillo, Coah. Mexico), Jessica Leigh Oster (Department of Earth and Environmental Sciences, Vanderbilt University, Nashville, TN 37240, USA), Jesús M. Pajón Morejón (National Museum of Natural History of Cuba, Department of Paleogeography and Paleobiology, Obispo 61, Plaza de Armas, Habana Vieja, CP 10 100, La Habana, Cuba), Jonathan Lloyd Baker (Institute of Global Environmental Change, Xi'an Jiaotong University, Xi'an, 710049, China), Judit Torner (CRG Marine Geosciences, Facultat de Ciències de la Terra, Universitat de Barcelona, Barcelona, 08028, Spain), Kathleen A Wendt (1. Oregon State University, Corvallis, Oregon 97331, USA 2. Institute of Geology, University of Innsbruck, Innrain 52, 6020 Innsbruck, Austria), Liangcheng Tan (State Key Laboratory of Loess and Quaternary Geology, Institute of Earth Environment, Chinese Academy of Sciences, Xi'an 710061, China), Lijuan Sha (Institute of Global Environmental Change, Xi'an Jiaotong University, Xi'an 710049, China), Liza Kathleen McDonough (ANSTO, New Illawarra Road, Lucas Heights, NSW 2234, Australia), Maša Surić (Department of Geography, University of Zadar, Ul. dr. F. Tuđmana 24 i, Zadar 23000, Croatia), Matthew J. Jacobson (Department of Archaeology, School of Humanities, Molema Building, Lilybank Gardens, University of Glasgow, Glasgow, G12 8QQ, UK), Mercè Cisneros (1. GRC Geociències Marines, Departament de Dinàmica de la Terra i de l'Oceà, Facultat de Ciències de la Terra, Universitat de Barcelona. c/ Martí i Franqués s/n, 08028 Barcelona, Spain 2. Centre en Canvi Climàtic, Departament de Geografia, Facultat de Turisme i Geografia, Universitat Rovira i Virgili, c/ Joanot Martorell 15, 43480, Vila-seca, Tarragona, Spain), Michael L. Griffiths (Department of Environmental Science, William Paterson University, Wayne NJ, 07739, USA), Michael Weber (Institute for Geosciences, Johannes Gutenberg University Mainz, J.-J.-Becher-Weg 21, 55128 Mainz, Germany), Nick Scropton (Irish Climate and Analysis Research UnitS (ICARUS), Department of Geography, Maynooth University, Maynooth, Co. Kildare, Ireland), Paul S. Wilcox (Institute of Geology, University of Innsbruck, Innrain 52, 6020 Innsbruck, Austria), R. Lawrence Edwards (Department of

Earth and Environmental Sciences, University of Minnesota, Minneapolis, MN 55455, USA), Romina Belli (1. Proteomics and Mass Spectrometry Core Facility, Department of Chemistry, The University of Georgia, Athens, GA 30602, USA 2. Department of Cellular, Computational and Integrative Biology (DeCBIO), University of Trento, Via Sommarive 9, 38123 Trento, Italy), Sebastian F.M. Breitenbach (Department of Geography and Environmental Sciences, Northumbria, Newcastle upon Tyne NE1 8ST, UK), Shraddha T Band (National Taiwan University, Address: Institute of Oceanography, National Taiwan University No.1, Sec. 4, Roosevelt Road, Taipei 106, Taiwan), Simon Dominik Steidle (Institute of Geology, University of Innsbruck, Innrain 52, 6020 Innsbruck, Austria), Stacy Anne Carolin (Department of Earth Sciences, University of Cambridge, Downing Street, Cambridge, CB23 8AD, UK), Vanessa E. Johnston (Karst Research Institute ZRC SAZU, Titov trg 2, 6230 Postojna, Slovenia), Wuhui Duan (1. Key Laboratory of Cenozoic Geology and Environment, Institute of Geology and Geophysics, Chinese Academy of Sciences, Beijing, 100029, China 2. CAS Center for Excellence in Life and Paleoenvironment, Beijing, 100044 China).

3. Terms of use

This dataset is licensed by the rights-holder(s) under a Creative Commons Attribution 4.0 International Licence: <https://creativecommons.org/licenses/by/4.0/>. In order to assure traceability, any presentation, report, or publication that uses the SISALv3 database should cite the datasets (<https://doi.org/10.5287/ora-2nanwp4rk>) along with the following publications: Atsawawaranunt et al. (2018; <https://doi.org/10.5194/essd-10-1687-2018>), Comas-Bru et al. (2019; <https://doi.org/10.5194/cp-15-1557-2019>), Comas-Bru et al. (2020; <https://doi.org/10.5194/essd-2020-39>) and Kaushal et al. (2023; DOI***). If using individual sites, the literature citations for published work provided in the database should also be cited. Contact information of data contributors of unpublished data is also provided, and these should be contacted when unpublished records are used on an individual basis.

4. Contents

Abstract: Stable isotope records from speleothems provide information on past climate changes, most particularly information that can be used to reconstruct past changes in precipitation and atmospheric circulation. These records are increasingly being used to provide “out-of-sample” evaluations of isotope-enabled climate models. SISAL (Speleothem Isotope Synthesis and Analysis) is an international working group of the Past Global Changes (PAGES) project. The working group aims to provide a comprehensive compilation of speleothem isotope records for climate reconstruction and model evaluation. The SISAL database contains data for individual speleothems, grouped by cave system. Stable isotopes of oxygen and carbon ($\delta^{18}\text{O}$, $\delta^{13}\text{C}$) and trace element (Mg/Ca, Sr/Ca, Ba/Ca, U/Ca and Sr isotope) measurements are referenced by distance from the top or youngest part of the speleothem. Additional tables provide information on dating, including information on the dates used to construct the original age model and sufficient information to assess the quality of each data set and to create a standardized chronology across different speleothems. The metadata table provides location information, information about the full range of measurements carried out on each speleothem and information about the cave system that is relevant to the interpretation of the records, as well as citations for both publications and archived data. Cave site and entity (speleothem) scan images are provided in the SISAL folder in the repository along with datafiles that include trace element data that could not be entered into the database (see Kaushal et al., 2023 for details). Associated citation, copyright and license information are provided in an excel file. Indication of whether these data are

available in the repository is provided in the database. The repository also includes the latest SISAL workbook version and standardized conversion files.

There is a single MySQL database file (sisalv3.sql). Please check <https://dev.mysql.com/downloads/> to download and install MySQL. Once MySQL Community Server and MySQL Workbench are installed, the database can be imported and visualised. A schema must be created upon import. To import the SQL file, you follow:

1. Open MySQL Workbench
2. Connect to the connection you would like to store your database in. A connection is usually created during the installation process (usually root@localhost with the password defined during the installation process)
3. Server>Data Import>Import from Self-contained file
4. Browse to the SQL file you have downloaded
5. Press New... next to the Default Target Schema to create a new schema (name this as appropriate, such as sisalv2)
6. Press Import

Please note that once the database is imported, there are packages and modules in several programming languages which will allow you to connect to the database such as RMySQL in R, and MySQLdb in python. There is a single compressed archive file (sisalv3.zip) comprising 21 CSV files corresponding to the 21 individual tables in the MySQL database. The CSV file names correspond to the table names. As these are flat CSV files, no relationships are defined here but the tables can be joined in different programming languages (R, Python, etc.) based on the foreign keys (shared column names between tables such as site_id in the site and entity tables). The relationships are described in figure 1 and the characteristics of each table are described in tables 1-20. Please note that CSV files are in UTF-8 characters, and special characters (such as Greek characters, and letters with accents which may appear in site names and in citations) may not be reproduced correctly when open as default in Excel.

Therefore, due to the multilingual nature of the site/entity names, you will need to follow these steps to open the csv data files with Excel in Windows computers (otherwise the UTF-8 encoding is not recognised):

1. Open Excel
2. Import the data using Data -> Import External Data--> Import Data
3. Select the file type of "csv" and browse to your file
4. In the import wizard change the File_Origin to "65001 UTF-8"
5. Change the Delimiter to comma
6. Select where to import to and Finish

There is a single compressed archive file (sisalv3_codes.zip) comprising examples of codes and queries that can be used with the MySQL database, but also with the CSV files. Within this compressed archive file, there is:

- A pdf file (sisalv3_mysql_intro.pdf) which shows extraction of data from the sisalv3.sql file and gives example SQL queries on the database
- Python files (sisal_connect2db_v3.py) demonstrating how to connect python to the database once the database has been uploaded into MySQL and (sisal3_extractCSVdata.py) demonstrating how to load the CSV files into Python and query these CSV files without the need to install MySQL.

- A Julia file (read_sisalv3.jl) demonstrating how to load the CSV files into Julia and query these without the need to install MySQL.

Note: Repository folders of the previous versions of the SISAL database contain codes for extraction using programs such as R and MATLAB which can be tweaked to enable sisalv3. They are available here:

SISALv1:

<https://doi.org/10.17864/1947.139>

SISALv2:

<https://doi.org/10.17864/1947.256>

Please note that there may be some authentication issues when using MySQL 8.0, especially when trying to connect from R/Python. This could be due to the change in the default authentication plugin from `mysql_native_password` to `caching_sha2_password`. One way around this is to run the following MySQL query in MySQL Workbench:

```
ALTER USER 'username'@'host' IDENTIFIED WITH mysql_native_password BY 'password';
```

where 'username' refers to the user's username ('root' if MySQL is run locally), 'host' refers to the host name ('localhost' if MySQL is run locally) and 'password' refers to the password (if MySQL is run locally, this is usually the password set up when installing MySQL).

SISAL database version 3 is an updated version of the SISAL database version 2 (Atsawawaranunt et al., 2019; Comas-Bru et al., 2019; Comas-Bru et al., 2020). New proxies and records (entities) have been added, and additional metadata fields and metadata have also been added to records already in previous versions. Some records have been amended where mistakes were found. The SISAL working group has created linear age-depth models for new entities added to SISALv3 version of the database. These have been added to the table (`sisal_chronology`). Information on which dates were used to produce these new age-depth models can be found in the dating table. For details on what has been added or amended to the SISAL database version 3 see the dataset paper Kaushal et al. (2023).

The 'sisal_data_entry_workbook_standardised_sheets' folder provides the standardized excel/GoogleSheet conversion sheets for

- Atomic to activity ratios calculator for uranium-thorium data.
- Grams to moles conversion file for trace element data.
- Latitude-longitude decimalization sheet.
- SISAL entity scan wish list with 'best practices' information to be submitted with a speleothem scan for the database and any speleothem-publications..
- SISAL trace elements metadata wish list with 'best practices' information to be submitted with speleothem trace element measurements for the database and any speleothem-publications.
- SISAL_workbook_v14 which was used for primary data entry.

The 'sisalv3_cave_map_entity_images' folder provides

- Speleothem section images as provided by data contributors or permitted by journals. The database 'entity' table – 'entity_scan' field indicates if these images are available

in the repository. The images in the repository are labelled with 'site_id entity_id persist_id site_name entity_scan'.

- Cave map images where provided by data contributors or permitted by journals. The database 'entity' table – 'cave_map' field indicates if these images are available in the repository. The images in the repository are labelled with 'site_id cave_name cave_map'
- The 'sisalv3_cave_site_entity_images_citation_copyright_license_information.xlsx' file provides information linked to the entity_scan and cave_map image files. Users must adhere to the 'reuse permission information' given in this document when using the images for their research work. The file contains the following information:
 - o Image publication DOI
 - o Parent journal
 - o Copyright statement
 - o License terms
 - o Reuse permission information
 - o Reference

The 'sisalv3_standardised_trace_elements_datafiles' folder provides data that could not be entered directly into the database due to sampling resolution or units of measurement. Where the original measured laser ablation data have been provided by data contributors, these have been made available as *.txt datafiles in the repository. Forty-six trace element records (Mg/Ca: 15, Sr/Ca: 17, Ba/Ca: 4, U/Ca: 5, P/Ca: 5, Sr-isotopes: 2) are only provided in the original format (*.txt files), either because they could not be converted to mmol/mol or because the trace element data were not measured at stable isotope equivalent depths and were at an insufficiently high resolution for accurate resampling. Additional elements that are not included in the database, but have been submitted by data contributors, are also provided as *.txt files (e.g., Mn, Fe, Zn, Th, Pb, K, Na). This folder contains sub-folders labelled by the site_name. Each sub-folder contains the following files for each entity from that site:

- 'trace_elements_datafile_site_name_entity_id' which is the original file submitted by the data contributor.
- 'trace_elements_datafile_site_name_entity_id_standardised.xlsx' which contains the original data submitted by the data contributor standardized by the database managers in .xlsx format.
- 'trace_elements_datafile_site_name_entity_id_standardised.txt' which contains the original data submitted by the data contributor standardized by the database managers in .txt format.
- 'trace_elements_datafile_site_name_entity_id_standardised.pdf' which contains the figures of the data contained in the standardized files.

File structure: The data is stored in a relational database (MySQL), which consists of 21 linked tables. Specifically: Site, entity, sample, dating, dating lamina, gap, hiatus, original chronology, d13C, d18O, Sr/Ca, Mg/Ca, Ba/Ca, U/Ca, P/Ca, Sr isotopes, entity link reference, references, composite link entity and sisal_chronology. Figure 1 shows the relationships between these tables. The structure and contents of each table is described below.

5. References:

Atsawawaranunt, K., Harrison, S. and Comas Bru, L. (2018): SISAL (Speleothem Isotopes Synthesis and AnaLysis Working Group) database Version 1.0. University of Reading. Dataset. <https://doi.org/10.17864/1947.147>

Atsawawaranunt, K., Comas-Bru, L., Amirnezhad Mozhdehi, S., Deininger, M., Harrison, S. P., Baker, A., Boyd, M., Kaushal, N., Ahmad, S. M., Ait Brahim, Y., Arienzo, M., Bajo, P., Braun, K., Burstyn, Y., Chawchai, S., Duan, W., Hatvani, I. G., Hu, J., Kern, Z., Labuhn, I., Lachniet, M., Lechleitner, F. A., Lorrey, A., PérezMejías, C., Pickering, R., Scroxton, N., and SISAL Working Group Members (2018): The SISAL database: a global resource to document oxygen and carbon isotope records from speleothems, *Earth Syst. Sci. Data*, 10, 1687–1713, <https://doi.org/10.5194/essd-10-1687-2018>

Atsawawaranunt, K., Harrison, S. and Comas-Bru, L. (2019): SISAL (Speleothem Isotopes Synthesis and AnaLysis Working Group) database version 1b. University of Reading. Dataset. <https://doi.org/10.17864/1947.189> Comas-Bru, L., Harrison, S. P., Werner, M., Rehfeld, K., Scroxton, N., Veiga-Pires, C., and SISAL working group members (2019): Evaluating model outputs using integrated global speleothem records of climate change since the last glacial, *Clim. Past*, 15, 1557–1579, <https://doi.org/10.5194/cp-15-1557-2019>

Comas-Bru, L., Atsawawaranunt, K., Harrison, S. and SISAL working group members (2020): SISAL (Speleothem Isotopes Synthesis and AnaLysis Working Group) database version 2.0. University of Reading. Dataset. <https://doi.org/10.17864/1947.256>

Comas-Bru, L., Rehfeld, K., Roesch, C., Amirnezhad-Mozhdehi, S., Harrison, S. P., Atsawawaranunt, K., Ahmad, S. M., Ait Brahim, Y., Baker, A., Bosomworth, M., Breitenbach, S. F. M., Burstyn, Y., Columbu, A., Deininger, M., Demény, A., Dixon, B., Fohlmeister, J., Hatvani, I. G., Hu, J., Kaushal, N., Kern, Z., Labuhn, I., Lechleitner, F. A., Lorrey, A., Martrat, B., Novello, V. F., Oster, J., Pérez-Mejías, C., Scholz, D., Scroxton, N., Sinha, N., Ward, B. M., Warken, S., Zhang, H., and the SISAL members (2020): SISALv2: A comprehensive speleothem isotope database with multiple age-depth models, *Earth Syst. Sci. Data Discuss.*, <https://doi.org/10.5194/essd-2020-39>

Kaushal, K., Lechleitner, F., Wilhelm, M., and SISAL Working Group members (2023): SISALv3: Speleothem Isotopes Synthesis and AnaLysis database version 3.0. University of Oxford. Dataset., <https://doi.org/10.5287/ora-2nanwp4rk>

Kaushal, K., Lechleitner, F., Wilhelm, M., Buehler, J., Braun, K., Ait Brahim, Y., Azennoud, K., Baker, A., Burstyn, Y., Comas-Bru, L., Goldsmith, Y., Harrison, S., Hatvani, I.G., Rehfeld, K., Ritzau, M., Skiba, V., Stoll, H.M., Szucs, J.G., Treble, P.C., and SISAL Working Group members (2023): SISALv3: A global speleothem stable isotope and trace element database, *Earth Syst. Sci. Data Discuss.*, DOI:***

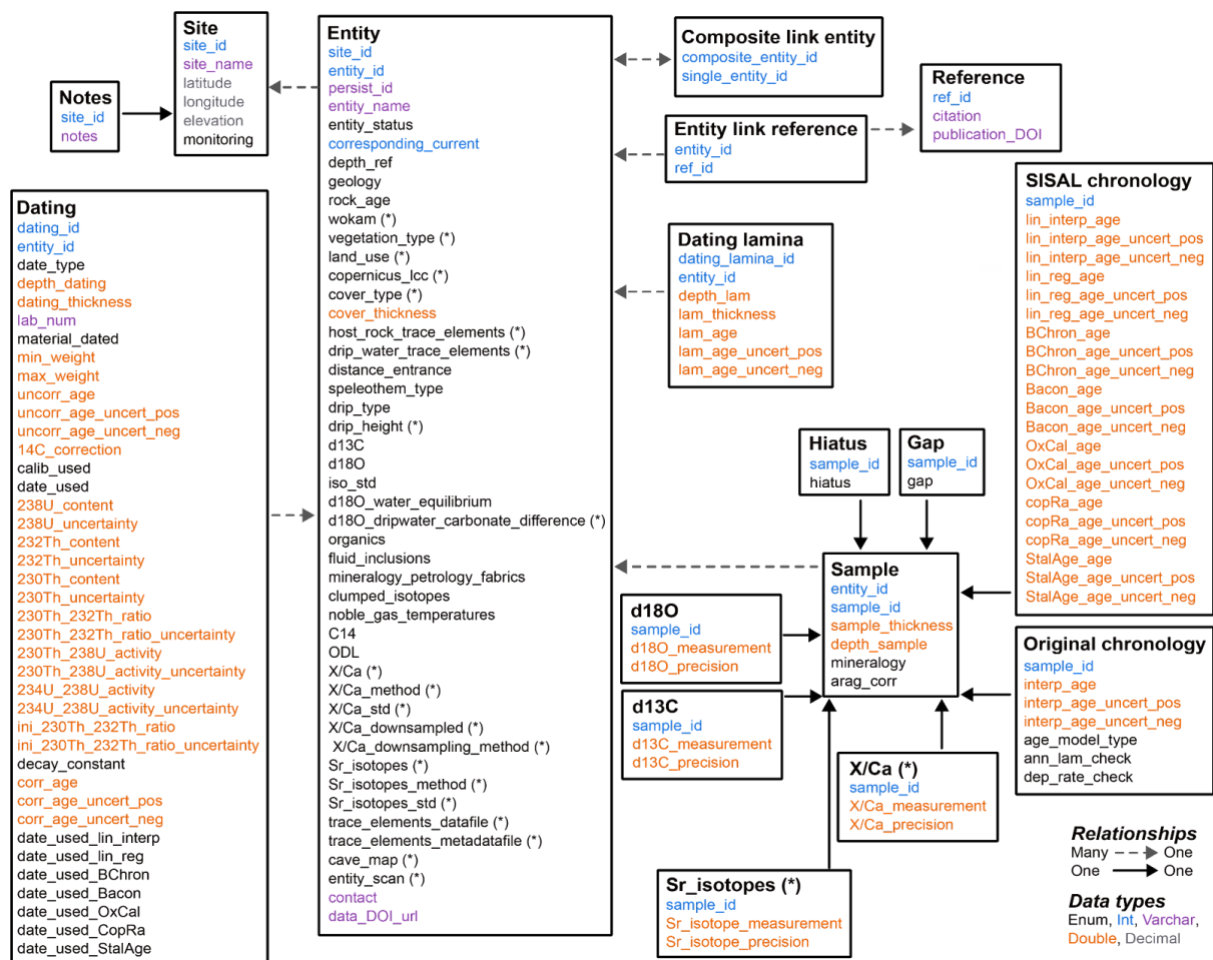


Figure 1: The structure of the SISAL database, showing individual tables (and their contents) and the nature of the relationships between them (where “many to one linkages” indicate that it is possible to have several entries in one table linked to a single entry in another table). Fields and table marked with (*) refer to new fields / tables added to SISALv3. The colours refer to the format of that field: Enum, Int, Varchar, Double or Decimal. Figure from Kaushal et al. (2023).

Table 1: Characteristics of the site table.

Field label	Definition	Format	Constraints
site_id	Unique identifier for each site, where a site is defined as a cave or cave system	Numeric	Positive integer
site_name	Site name as given by original authors / data contributors or as defined by us where there was no unique name given to the site	Text	None
latitude	Latitude of the cave site, given in decimal degrees, where N is positive and S is negative	Numeric	None
longitude	Latitude of the cave site, given in decimal degrees, where E is positive and W is negative	Numeric	None
elevation	Elevation of the cave, in meters above sea level (where negative values indicate elevation below sea level)	Numeric	None

monitoring	Indication of whether long-term monitoring of cave conditions have been carried out	Text	Selected from pre-defined list
------------	---	------	--------------------------------

Table 2: Characteristics of the entity table.

Field	Definition	Format	Constraints
site_id	Unique identifier for each site, where a site is defined as a cave or cave system	Numeric	Positive integer
entity_id	Unique identifier for each entity, where an entity is defined as a speleothem dataset or a speleothem composite dataset	Numeric	Positive integer
persist_id	Unique identifier for each speleothem, where an entity is defined as a speleothem or a speleothem composite	Alpha-numeric	Formulaically generated combination of site and entity name
entity_name	Entity (speleothem) name as given by the author	Text	None
entity_status	Status of the entity record, specifically whether it is current, is current but includes modifications or additional information, or it has been superseded by another record	Text	Selected from pre-defined list
corresponding_current	This refers to the entity_id of the record which replaces a superceded record or to the entity_id of other current records that are linked to a current but partially modified record	Text	Selected from pre-defined list
depth_ref	Indication of whether the reference point is the top or base of the speleothem	Numeric	Selected from pre-defined list
geology	Description of the rock type	Text	Selected from pre-defined list
rock_age	Description of age of the rock	Text	Selected from pre-defined list
wokam (*)	Information on type of carbonate/evaporite rock from WOKAM database	Text	Added by SISAL SC at database level
vegetation_type (*)	Information on vegetation cover (publication/data contributors)	Text	Selected from pre-defined list

land_use (*)	Information on land use (publication/data contributors)	Text	Selected from pre-defined list
copernicus_lcc (*)	Information on land cover from Copernicus land cover classification dataset	Text	Added by SISAL SC at database level
cover_type (*)	Information on land cover (publication/data contributors)	Text	Selected from pre-defined list
cover_thickness	Thickness of overlying bedrock above the speleothem (m)	Text	Positive decimal
host_rock_ trace_elements (*)	Indication whether trace element data from the host rock has been measured	Text	Selected from pre-defined list
drip_water_ trace_elements (*)	Indication whether trace element data from the drip water has been measured	Text	Selected from pre-defined list
distance_entrance	Distance of the speleothem from the cave entrance (m)	Numeric	Positive decimal
speleothem_type	Description of the speleothem type	Text	Selected from pre-defined list
drip_type	Description of the drip type	Text	Selected from pre-defined list
drip_height (*)	Information on drip height (in m)	Numeric	Positive decimal
d13C	Indication of whether $\delta^{13}\text{C}$ has been measured	Text	Selected from pre-defined list
d18O	Indication of whether $\delta^{18}\text{O}$ has been measured	Text	Selected from pre-defined list
iso_std	Information on standard used for oxygen and carbon isotope measurements	Text	Selected from pre-defined list
d18O_water equilibrium	Indication of whether studies assessing if the speleothem is precipitating in equilibrium with dripwaters have been done	Text	Selected from pre-defined list
d18O_dripwater_ carbonate_difference(*)	Information on difference between dripwater and carbonate oxygen isotope values	Numeric	Positive decimal
organics	Indication of whether organics have been measured	Text	Selected from pre-defined list

fluid_inclusions	Indication of whether fluid inclusions have been measured	Text	Selected from pre-defined list
mineralogy_petrology_fabrics	Indication of whether mineralogy and/or petrology and/or fabric measurements have been made	Text	Selected from pre-defined list
clumped_isotopes	Indication of whether clumped isotopes have been measured	Text	Selected from pre-defined list
noble_gas_temperatures	Indication of whether noble gases have been measured	Text	Selected from pre-defined list
C14	Indication of whether 14C measurements have been made	Text	Selected from pre-defined list
ODL	Indication of whether the optical density of luminosity measurements have been made	Text	Selected from pre-defined list
Sr_Ca (*)	Indication whether Sr/Ca data has been measured	Text	Selected from pre-defined list
Sr_Ca_method (*)	Information on measurement method for Sr/Ca	Text	Selected from pre-defined list
Sr_Ca_std (*)	Information on standard used for Sr/Ca measurements	Text	Selected from pre-defined list
Sr_Ca_downsampled (*)	Information on whether Sr/Ca data had to be downsampled	Text	Selected from pre-defined list
Sr_Ca_downsampling_method (*)	Information on downsampling method for Sr/Ca	Text	Selected from pre-defined list
Mg_Ca (*)	Indication whether Mg/Ca data has been measured	Text	Selected from pre-defined list
Mg_Ca_method (*)	Information on measurement method for Mg/Ca	Text	Selected from pre-defined list
Mg_Ca_std (*)	Information on standard used for Mg/Ca measurements	Text	Selected from pre-defined list
Mg_Ca_downsampled (*)	Information on whether Mg/Ca data had to be downsampled	Text	Selected from pre-defined list
Mg_Ca_downsampling_method (*)	Information on downsampling method for Mg/Ca	Text	Selected from pre-defined list

Ba_Ca (*)	Indication whether Ba/Ca data has been measured	Text	Selected from pre-defined list
Ba_Ca_method (*)	Information on measurement method for Ba/Ca	Text	Selected from pre-defined list
Ba_Ca_std (*)	Information on standard used for Ba/Ca measurements	Text	Selected from pre-defined list
Ba_Ca_downsampled (*)	Information on whether Ba/Ca data had to be downsampled	Text	Selected from pre-defined list
Ba_Ca_downsampling_method (*)	Information on downsampling method for Ba/Ca	Text	Selected from pre-defined list
U_Ca (*)	Indication whether U/Ca data has been measured	Text	Selected from pre-defined list
U_Ca_method (*)	Information on measurement method for U/Ca	Text	Selected from pre-defined list
U_Ca_std (*)	Information on standard used for U/Ca measurements	Text	Selected from pre-defined list
U_Ca_downsampled (*)	Information on whether U/Ca data had to be downsampled	Text	Selected from pre-defined list
U_Ca_downsampling_method (*)	Information on downsampling method for U/Ca	Text	Selected from pre-defined list
P_Ca (*)	Indication whether P/Ca data has been measured	Text	Selected from pre-defined list
P_Ca_method (*)	Information on measurement method for P/Ca	Text	Selected from pre-defined list
P_Ca_std (*)	Information on standard used for P/Ca measurements	Text	Selected from pre-defined list
P_Ca_downsampled (*)	Information on whether P/Ca data had to be downsampled	Text	Selected from pre-defined list
P_Ca_downsampling_method (*)	Information on downsampling method for P/Ca	Text	Selected from pre-defined list
Sr_isotopes (*)	Indication whether Sr isotopes data has been measured	Text	Selected from pre-defined list

Sr_isotopes_method (*)	Information on measurement method for Sr isotopes	Text	Selected from pre-defined list
Sr_isotopes_std (*)	Information on standard used for Sr isotopes measurements	Text	Selected from pre-defined list
trace_elements_datafile (*)	Information on whether the original trace elements data is available in the repository	Text	Selected from pre-defined list
trace_elements_metadatafile (*)	Information on whether trace elements metadata is available in the repository	Text	Selected from pre-defined list
cave_map (*)	Information on whether the cave map is available in the repository	Text	Selected from pre-defined list
entity_scan (*)	Information on whether the entity scan is available in the repository	Text	Selected from pre-defined list
contact	Name of the person who entered the data into the workbook	Text	None
data_DOI_url	Digital Object Identifier (DOI) of the data or URL of the webpage from which the data was / can be obtained.	Text	None

Table 3: Characteristics of the sample table.

Field	Description	Format	Constraints
entity_id	Refers to the unique identifier for each entity (as given in the entity table)	Numeric	Positive integer
sample_id	Unique identifier for the sample	Numeric	Positive integer
sample_thickness	Thickness of the sample analyzed (mm)	Numeric	Positive decimal
depth_sample	Distance from a reference point (mm)	Numeric	Positive decimal
mineralogy	Description of the mineralogy of the sample	Text	Selected from pre-defined list
arag_corr	Indication of whether the isotope measurements have been corrected for aragonite samples to calcite-equivalent values	Text	Selected from pre-defined list

Table 4: Characteristics of the dating table.

Field	Description	Format	Constraints
dating_id	Unique identifier for each date	Numeric	Positive integer
entity_id	Refers to the unique identifier for each entity (as given in the entity table)	Numeric	Positive integer
date_type	Description of the dating method used	Text	Selected from pre-defined list
depth_dating	Distance from a reference point (mm)	Numeric	Positive decimal
dating_thickness	Thickness of dated sample (mm)	Numeric	Positive decimal
lab_num	Laboratory number of the dated sample	Text	None
material_dated	Mineralogy of the dated sample	Text	Selected from pre-defined list
min_weight	Minimum weight of the dated sample (mg)	Numeric	Positive decimal
max_weight	Maximum weight of the dated sample (mg)	Numeric	Positive decimal
uncorr_age	Uncorrected age of the dated sample (years BP)	Numeric	Positive decimal
uncorr_age_uncert_pos	Positive uncertainty of the uncorrected age (years)	Numeric	Positive decimal
uncorr_age_uncert_neg	Negative uncertainty of the uncorrected age (years)	Numeric	Positive decimal
14C_correction	Percentage dead carbon present in dated sample	Numeric	Positive decimal
calib_used	Calibration method used to convert C ¹⁴ dates to calendar years	Text	Selected from pre-defined list
date_used	Indication of whether the date was used in the author-generated original age model	Text	Selected from pre-defined list
238U_content	²³⁸ U content of the dated sample (ppb)	Numeric	Positive decimal
238U_uncertainty	²³⁸ U 2-sigma uncertainty of dated sample (ppb)	Numeric	Positive decimal
232Th_content	²³² Th content of the dated sample (ppt)	Numeric	Positive decimal
232Th_uncertainty	²³² Th 2-sigma uncertainty of dated sample (ppb)	Numeric	Positive decimal
230Th_content	²³⁰ Th content of the dated sample (ppb)	Numeric	Positive decimal
230Th_uncertainty	²³⁰ Th 2-sigma uncertainty of dated sample (ppb)	Numeric	Positive decimal

230Th_232Th_ratio	$^{230}\text{Th}/^{232}\text{Th}$ activity ratio of the dated sample	Numeric	Positive decimal
230Th_232Th_ratio_uncertainty	$^{230}\text{Th}/^{232}\text{Th}$ activity ratio 2-sigma uncertainty of the dated sample	Numeric	Positive decimal
230Th_238U_activity	$^{230}\text{Th}/^{238}\text{U}$ activity ratio of the dated sample	Numeric	Positive decimal
230Th_238U_activity_uncertainty	$^{230}\text{Th}/^{238}\text{U}$ activity ratio 2-sigma uncertainty of the dated sample	Numeric	Positive decimal
234U_238U_activity	$^{234}\text{U}/^{238}\text{U}$ activity ratio of the dated sample	Numeric	Positive decimal
234U_238U_activity_uncertainty	$^{234}\text{U}/^{238}\text{U}$ activity ratio 2-sigma uncertainty of the dated sample	Numeric	Positive decimal
ini_230Th_232Th_ratio	Initial $^{230}\text{Th}/^{232}\text{Th}$ activity ratio for the detrital correction	Numeric	Positive decimal
ini_230Th_232Th_ratio_uncertainty	Initial $^{230}\text{Th}/^{232}\text{Th}$ activity ratio uncertainty for the detrital correction	Numeric	Positive decimal
decay_constant	Description of the half-life used for ^{230}Th and ^{234}U for U/Th samples	Text	Selected from pre-defined list
corr_age	Corrected age of the dated sample (years BP)	Numeric	Positive decimal
corr_age_uncert_pos	Positive uncertainty of corrected age of the dated sample (years)	Numeric	Positive decimal
corr_age_uncert_neg	Negative uncertainty of corrected age of the dated sample (years)	Numeric	Positive decimal
date_used_lin_interp	Indication of whether the date has been used to run the linear interpolation SISAL chronology.	Text	Pre-defined text added at database level
date_used_lin_reg	Indication of whether the date has been used to run the linear regression SISAL chronology.	Text	Pre-defined text added at database level
date_used_Bchron	Indication of whether the date has been used to run the Bchron SISAL chronology.	Text	Pre-defined text added at database level
date_used_Bacon	Indication of whether the date has been used to run the Bacon SISAL chronology.	Text	Pre-defined text added at database level
date_used_OxCal	Indication of whether the date has been used to run the OxCal SISAL chronology.	Text	Pre-defined text added at database level
date_used_copRa	Indication of whether the date has been used to run the copRa SISAL chronology.	Text	Pre-defined text added at database level

date_used_StalAge	Indication of whether the date has been used to run the StalAge SISAL chronology.	Text	Pre-defined text added at database level
-------------------	---	------	--

Table 5: Characteristics of the lamina dating table.

Field	Description	Format	Constraints
dating_lamina_id	Unique identifier for each lamina	Numeric	Positive integer
entity_id	Refers to the unique identifier for each entity (as given in the entity table)	Numeric	Positive integer
depth_lam	Depth of the midpoint of the lamina from a reference point (mm)	Numeric	Positive decimal
lam_thickness	Thickness of the sample dates (mm)	Numeric	Positive decimal
lam_age	Age of individual lamina (years BP)	Numeric	Positive decimal
lam_age_uncert_pos	Positive counting uncertainty of individual lamina (years)	Numeric	Positive decimal
lam_age_uncert_neg	Negative counting uncertainty of individual lamina (years)	Numeric	Positive decimal

Table 6: Characteristics of the hiatus place mark information table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for each sample (as given in the sample table)	Numeric	Positive integer
hiatus	Indication of a hiatus	Text	Selected from pre-defined list

Table 7: Characteristics of the gap place mark information table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for each sample (as given in the sample table)	Numeric	Positive integer
gap	Indication of a gap	Text	Selected from pre-defined list

Table 8: Characteristics of the original chronology information table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in the sample table)	Numeric	Positive integer
interp_age	Calendar age of the sample (years BP)	Numeric	Positive decimal
interp_age_uncert_pos	Positive uncertainty on the age of the sample (years)	Numeric	Positive decimal
interp_age_uncert_neg	Negative uncertainty on the age of the sample (years)	Numeric	Positive decimal
age_model_type	Description of the age model used in the original publication	Text	Selected from pre-defined list

ann_lam_check	This is an indication that it has been verified that laminae are annual	Text	Selected from pre-defined list
dep_rate_check	Indication that verification of the deposition rate has been made	Text	Selected from pre-defined list

Table 9: Characteristics of the carbon isotope table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in the sample table)	Numeric	Positive integer
d13C_measurement	Original $\delta^{13}\text{C}$ measurement (‰)	Numeric	Positive decimal
d13C_precision	Laboratory precision on the $\delta^{13}\text{C}$ measurement (‰)	Numeric	Positive decimal

Table 10: Characteristics of the oxygen isotope table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in the sample table)	Numeric	Positive integer
d18O_measurement	Original $\delta^{18}\text{O}$ measurement (‰)	Numeric	Positive decimal
d18O_precision	Laboratory precision on the $\delta^{18}\text{O}$ measurement (‰)	Numeric	Positive decimal

Table 11: Characteristics of the Sr_Ca table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in the sample table)	Numeric	Positive integer
Sr_Ca_measurement	Original Sr/Ca measurement mmol/mol	Numeric	Positive decimal
Sr_Ca_precision	Laboratory precision on the Sr/Ca measurement mmol/mol	Numeric	Positive decimal

Table 12: Characteristics of the Mg_Ca table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in the sample table)	Numeric	Positive integer
Mg_Ca_measurement	Original Mg/Ca measurement mmol/mol	Numeric	Positive decimal
Mg_Ca_precision	Laboratory precision on the Mg/Ca measurement mmol/mol	Numeric	Positive decimal

Table 13: Characteristics of the Ba_Ca table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in the sample table)	Numeric	Positive integer
Ba_Ca_measurement	Original Ba/Ca measurement mmol/mol	Numeric	Positive decimal
Ba_Ca_precision	Laboratory precision on the Ba/Ca measurement mmol/mol	Numeric	Positive decimal

Table 14: Characteristics of the U_Ca table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in the sample table)	Numeric	Positive integer
U_Ca_measurement	Original U/Ca measurement mmol/mol	Numeric	Positive decimal
U_Ca_precision	Laboratory precision on the U/Ca measurement mmol/mol	Numeric	Positive decimal

Table 15: Characteristics of the P_Ca table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in the sample table)	Numeric	Positive integer
P_Ca_measurement	Original P/Ca measurement mmol/mol	Numeric	Positive decimal
P_Ca_precision	Laboratory precision on the P/Ca measurement mmol/mol	Numeric	Positive decimal

Table 16: Characteristics of the Sr_isotopes table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in the sample table)	Numeric	Positive integer
Sr_isotopes_measurement	Original Sr isotopes ($^{87}\text{Sr}/^{86}\text{Sr}$) measurement	Numeric	Positive decimal
Sr_isotopes_precision	Laboratory precision on the Sr isotopes ($^{87}\text{Sr}/^{86}\text{Sr}$) measurement	Numeric	Positive decimal

Table 17: Characteristics of the publication information table.

Field	Description	Format	Constraints
ref_id	Unique identifier for the reference	Numeric	Positive integer
citation	Full citation for the original publication / data contribution	Text	None
publication_doi	Digital Object Identifier (DOI) of publication	Text	None

Table 18: Characteristics of the link entity and publication information table.

Field	Description	Format	Constraints
entity_id	Refers to the unique identifier for the entity (as given in the entity table)	Numeric	Positive integer

ref_id	Refers to the unique identifier for the publication (as given in the publication information table)	Numeric	Positive integer
--------	---	---------	------------------

Table 19: Characteristics of the link composite and entity table.

Field	Description	Format	Constraints
composite_entity_id	Refers to the unique identifier for a composite entity (as given in the entity table)	Numeric	Positive integer
single_entity_id	Refers to the unique identifier for each single entity that makes the composite (as given in the entity table)	Numeric	Positive integer

Table 20: Characteristics of the notes table.

Field	Description	Format	Constraints
site_id	Refers to the unique identifier for each site (as given in the site table)	Numeric	Positive integer
notes	Additional information on the site or entity	Text	None

Table 21: Characteristics of the SISAL chronology table.

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in the sample table)	Numeric	Positive integer
lin_interp_age	Age of the sample in years BP calculated with linear interpolation between dates	Numeric	Positive decimal
lin_interp_age_uncert_pos	Positive 2-sigma uncertainty of the age of the sample in years calculated with linear interpolation between dates	Numeric	Positive decimal
lin_interp_age_uncert_neg	Negative 2-sigma uncertainty of the age of the sample in years calculated with linear interpolation between dates	Numeric	Positive decimal
lin_reg_age	Age of the sample in years BP calculated with linear regression	Numeric	Positive decimal
lin_reg_age_uncert_pos	Positive 2-sigma uncertainty of the age of the sample in years calculated with linear regression	Numeric	Positive decimal
lin_reg_age_uncert_neg	Negative 2-sigma uncertainty of the age of the sample in years calculated with linear regression	Numeric	Positive decimal
Bchron_age	Age of the sample in years BP calculated with Bchron	Numeric	Positive decimal

Bchron_age_uncert_pos	Positive 2-sigma uncertainty of the age of the sample in years calculated with Bchron	Numeric	Positive decimal
Bchron_age_uncert_neg	Negative 2-sigma uncertainty of the age of the sample in years calculated with Bchron	Numeric	Positive decimal
Bacon_age	Age of the sample in years BP calculated with Bacon	Numeric	Positive decimal
Bacon_age_uncert_pos	Positive 2-sigma uncertainty of the age of the sample in years calculated with Bacon	Numeric	Positive decimal
Bacon_age_uncert_neg	Negative 2-sigma uncertainty of the age of the sample in years calculated with Bacon	Numeric	Positive decimal
OxCal_age	Age of the sample in years BP calculated with OxCal	Numeric	Positive decimal
OxCal_age_uncert_pos	Positive 2-sigma uncertainty of the age of the sample in years calculated with OxCal	Numeric	Positive decimal
OxCal_age_uncert_neg	Negative 2-sigma uncertainty of the age of the sample in years calculated with OxCal	Numeric	Positive decimal
copRa_age	Age of the sample in years BP calculated with copRa	Numeric	Positive decimal
copRa_age_uncert_pos	Positive 2-sigma uncertainty of the age of the sample in years calculated with copRa	Numeric	Positive decimal
copRa_age_uncert_neg	Negative 2-sigma uncertainty of the age of the sample in years calculated with copRa	Numeric	Positive decimal
Stalage_age	Age of the sample in years BP calculated with StalAge	Numeric	Positive decimal
Stalage_age_uncert_pos	Positive 2-sigma uncertainty of the age of the sample in years calculated with StalAge	Numeric	Positive decimal
Stalage_age_uncert_neg	Negative 2-sigma uncertainty of the age of the sample in years calculated with StalAge	Numeric	Positive decimal