1. Project

Title: SISAL (Speleothem Isotopes Synthesis and AnaLysis Working Group) database Version 2.0

Dates: 2017-2020

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2. Dataset

Title: SISAL (Speleothem Isotopes Synthesis and AnaLysis Working Group) database version 2.0

Summary description. 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. 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 second version of the SISAL database contains oxygen and carbon isotope measurements from 673 individual speleothem records, and 18 composites from 293 cave systems worldwide, and metadata describing the cave settings and age models of these records. This version also contains 2,138 alternative age-depth models constructed for 503 SISAL entities. Ensembles of the new sisal-chronologies are available at Rehfeld et al. (2020).

Publication year: 2020

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3. Terms of use

In order to assure traceability, any presentation, report, or publication that uses the SISALv2 database should cite the dataset (https:/doi.org/10.17864/1947.256) 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) and Comas-Bru et al. (2020; https://doi.org/10.5194/essd-2020-39). 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 Contact information of data contributors of unpublished data is also provided, and these should be contacted when unpublished records are used on an individual basis.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 ($\delta^{18}O$, $\delta^{13}C$) 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.

There is a single MySQL database file (sisalv2.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 (sisalv1.zip) comprising 15 CSV files corresponding to the 15 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 1-15. 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 (sisalv1_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:

- An html file (sisal_intro_example.html) which shows example SQL queries on the database
- A python file (sisal_connect2db.py) demonstrating how to connect python to the database once the database has been uploaded into MySQL.
- An R file (sisal_connect2db.R) demonstrating how to connect R to the database once the database has been uploaded into MySQL.
- An R file (sisal_csv_db.R) demonstrating how to load the CSV files into R and query these CSV files without the need to install MySQL.
- An R file (sisal_v2_extract_csv.R) to extract csv files from the sql file loaded in MySQL.
- A Julia file (sisal_connect2db.jl) demonstrating how to load the CSV files into Julia and query these without the need to install MySQL.
- A Matlab file (sisal_connect2db.m) demonstrating how to connect Matlab to the database once the database has been uploaded into MySQL.
- A pdf with Matlab instructions (sisal_csv_db_matlab_instructions.m) to load the CSV files.

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 2 is an updated version of the SISAL database version 1b (Atsawawaranunt et al., 2019; Comas-Bru et al., 2019). New records have been added, and additional data (such as elevation, rock_age and geology which in some cases were unknown) have also been added to records already in previous versions. Moreover, some records have been amended where mistakes were found.

The SISAL working group has created new linear age-depth models for 503 entities. These have been added to a new table (sisal_chronology). Information on which dates were used to produce these new age-depth models can be found in the new columns in the dating table.

For details on what has been added or amended to the SISAL database version 1b to produce version 2, see document named 'sisalv2_updates_since_sisalv1b.pdf' and the dataset paper Comas-Bru et al. (2020).

File structure: The data is stored in a relational database (MySQL), which consists of 15 linked tables. Specifically: Site, entity, sample, dating, dating lamina, gap, hiatus, original chronology, d13C, d18O, 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., Pérez-Mejías, 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, in review.

Rehfeld, K., Roesch, C., Comas-Bru, L., and Amirnezhad-Mozhdehi, S. (2020): Age-depth model ensembles for SISAL v2 speleothem records (Version 1.0) [Data set]. Zenodo. http://doi.org/10.5281/zenodo.3816804

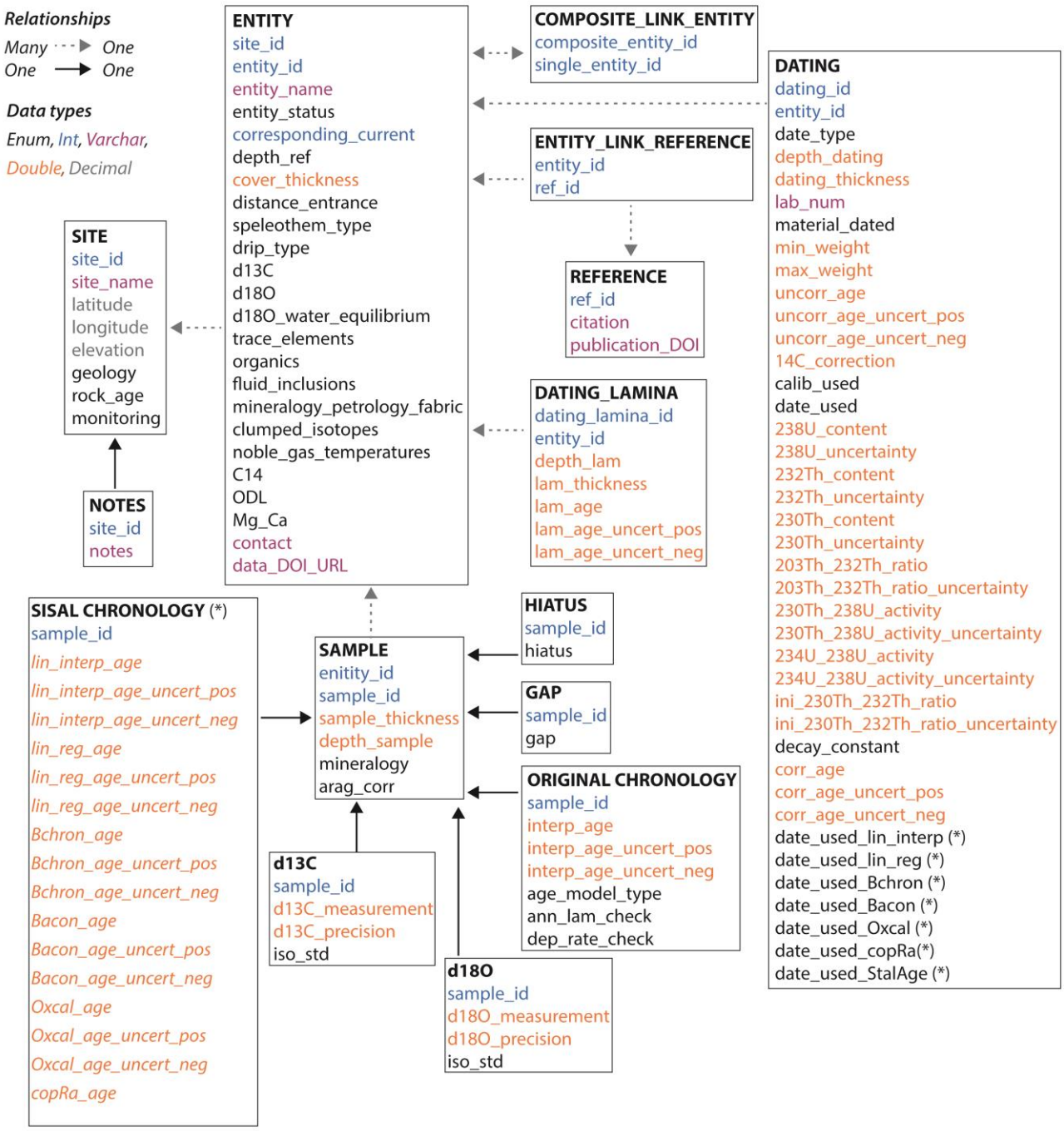

Figure 1: The structure of the SISAL database, showing individual tables (and their contents) and the nature of the relationships between them (where "many to one linkages" indicate that it is possible to have several entries in one table linked to a single entry in another table). Fields and table marked with (*) refer to new information added to SISALv1b (see Comas-Bru et al., 2020 for further details). The colours refer to the format of that field: Enum, Int, Varchar, Double or Decimal. More information on the list of pre-defined menus can be found in Atsawawaranunt et al. (2018). Figure from Comas-Bru et al. (2020).

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 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	Longitude of the cave site, given in decimal degrees, E is positive and W is negative	Numeric	None
elevation	Elevation of the cave, in meters above sea level (where negative values indicate elevations below sea level)	Numeric	None
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
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	Refers to the unique identifier for each site (as given in site table)	Numeric	Positive integer
entity_id	Unique identifier for each entity, where an entity is defined as a speleothem or a speleothem composite	Numeric	Positive integer
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.	Numeric	Positive integer
depth_ref	Indication of whether the reference point is the top or base of the speleothem	Text	selected from pre-defined list
cover_thickness	Thickness of overlying bedrock above the speleothem (m)	Numeric	Positive decimal
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
d13C	Indication of whether $\delta^{13}C$ measurements have been made of the speleothem	Text	selected from pre-defined list
d18O	Indication of whether $\delta^{18}O$ measurements have been measured	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
trace_elements	Indication of whether trace elements have been measured	Text	selected from pre-defined list
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_fabric	Indication of whether 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 ^{14}C 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
Mg_Ca	Indication of whether the Mg/Ca ratio measurements have been made	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 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 entity table)	Numeric	Positive integer
sample_id	Unique identifier for the sample	Numeric	Positive integer
sample_thickness	Thickness of the sample analysed (mm)	Numeric	Positive decimal
depth_sample	Distance in mm from a reference point	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 in aragonite samples	Text	selected from pre-defined list

Table 4: Characteristics of the dating information 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 entity table)	Numeric	Positive integer
date_type	Description of the dating method used	Text	selected from pre-defined list
depth_dating	Distance in mm from a reference point	Numeric	Positive decimal
dating_thickness	Thickness of dated sample in mm	Numeric	Positive decimal
lab_num	The 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 in mg	Numeric	Positive decimal
max_weight	Maximum weight of the dated sample in mg	Numeric	Positive decimal
uncorr_age	Uncorrected age of the dated sample in years	Numeric	None
uncorr_age_uncert_pos	Positive uncertainty of the uncorrected age of the dated sample in years	Numeric	Positive decimal
uncorr_age_uncert_neg	Negative uncertainty of the uncorrected age of the dated sample in 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 is used in the original age model	Text	selected from pre-defined list
238U_content	^{238}U content of the dated sample in ppb	Numeric	None
238U_uncertainty	^{238}U 2-sigma uncertainty of dated sample in ppb	Numeric	None
232Th_content	^{232}Th content of the dated sample in ppt	Numeric	None
232Th_uncertainty	^{232}Th 2-sigma uncertainty of the dated sample in ppt	Numeric	None
230Th_content	^{230}Th content of the dated sample in ppt	Numeric	None
230Th_uncertainty	^{230}Th 2-sigma uncertainty of the dated sample in ppt	Numeric	None
230Th_232Th_ratio	$^{230}Th/^{232}Th$ activity ratio of the dated sample	Numeric	None
230Th_232Th_ratio_uncertainty	$^{230}Th/^{232}Th$ activity ratio 2-sigma uncertainty of the dated sample	Numeric	None
230Th_238U_activity	$^{230}Th/^{238}U$ activity ratio of the dated sample	Numeric	None
230Th_238U_activity_uncertainty	$^{230}Th/^{238}U$ activity ratio 2-sigma uncertainty of the dated sample	Numeric	None
234U_238U_activity	$^{234}U/^{238}U$ activity ratio of the dated sample	Numeric	None
234U_238U_activity_uncertainty	$^{234}U/^{238}U$ activity ratio 2-sigma uncertainty of the dated sample	Numeric	None
ini_230Th_232Th_ratio	Initial $^{230}Th/^{232}Th$ activity ratio for the detrital correction	Numeric	None
ini_230Th_232Th_ratio_uncertainty	Initial $^{230}Th/^{232}Th$ activity ratio uncertainty for the detrital correction	Numeric	None
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 in years	Numeric	None
corr_age_uncert_pos	Positive uncertainty of corrected age of the dated sample in years	Numeric	Positive decimal
corr_age_uncert_neg	Negative uncertainty of corrected age of the dated sample in years	Numeric	Positive decimal

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 entity table)	Numeric	Positive integer
depth_lam	Depth of the midpoint of the lamina in mm from a reference point	Numeric	Positive integer
lam_thickness	Thickness in mm of the sample dated	Numeric	Positive decimal
lam_age	Age in years of individual lamina	Numeric	None
lam_age_uncert_pos	Positive counting uncertainty of individual lamina in years	Numeric	Positive decimal
lam_age_uncert_neg	Negative counting uncertainty of individual lamina in 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 sample table)	Numeric	Positive integer
hiatus	Indication of an 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 the sample (as given in 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 sample table)	Numeric	Positive integer
interp_age	Calendar age of the sample in years	Numeric	Positive decimal
interp_age_uncert_pos	Positive uncertainty on the age of the sample in years	Numeric	Positive decimal
interp_age_uncert_neg	Negative uncertainty on the age of the sample in 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	Indication that verification that laminae are annual, in cases where lamina counting is used to construct the age model	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 data table

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in sample table)	Numeric	Positive integer
d13C_measurement	Original $\delta^{13}C$ measurement	Numeric	None
d13C_precision	Laboratory precision on the $\delta^{13}C$ measurement	Numeric	None
iso_std	Description of isotopic standard used	Text	selected from pre-defined list

Table 10: Characteristics of the oxygen isotope data table

Field	Description	Format	Constraints
sample_id	Refers to the unique identifier for the sample (as given in sample table)	Numeric	Positive integer
d18O_measurement	Original $\delta^{18}O$ measurement	Numeric	None
d18O_precision	Laboratory precision on the $\delta^{18}O$ measurement	Numeric	None
iso_std	Description of isotopic standard used	Text	selected from pre-defined list

Table 11: Characteristics of the publication information table

Field	Description	Type	Constraints
ref_id	Unique identifier for the reference	Numeric	Positive integer
Citation	Full citation for the original publication	Text	None
publication_DOI	Digital Object Identifier (DOI) of publication	Text	None

Table 12: 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 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 13: 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 entity table)	Numeric	Positive integer
single_entity_id	Refers to the unique identifier for each single entity in the composite (as given in entity table)	Numeric	Positive integer

Table 14: Characteristics of the notes table

Field	Description	Format	Constraints
site_id	Refers to the unique identifier for each site (as given in site table)	Numeric	Positive integer
notes	Notes and additional information about the site	Text	None

Table 15: Characteristics of the sisal_chronology table

Field label	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 calculated with linear interpolation between dates	Numeric	None
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 calculated with linear regression	Numeric	None
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 calculated with Bchron	Numeric	None
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 calculated with Bacon	Numeric	None
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 calculated with OxCal	Numeric	None

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 calculated with copRa	Numeric	None
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 calculated with StalAge	Numeric	None
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