

# SISALv3: A global speleothem stable isotope and trace element database

Nikita Kaushal<sup>1</sup>, Franziska A. Lechleitner<sup>2</sup>, Micah Wilhelm<sup>3</sup>, Janica C. Bühler<sup>4</sup>, Kerstin Braun<sup>5</sup>,

- 5 Yassine Ait Brahim<sup>6</sup>, Khalil Azennoud<sup>6</sup>, Andy Baker<sup>7</sup>, Yuval Burstyn<sup>8</sup>, Laia Comas-Bru<sup>9</sup>, Yonaton Goldsmith<sup>10</sup>, Sandy P. Harrison<sup>11</sup>, István G. Hatvani<sup>12,13</sup>, Kira Rehfeld<sup>4</sup>, Magdalena Ritzau<sup>4</sup>, Vanessa Skiba<sup>14</sup>, Heather M. Stoll<sup>15</sup>, József G. Szűcs<sup>16</sup>, Pauline C. Treble<sup>7,17</sup>, Vitor Azevedo<sup>18</sup>, Jonathan L. Baker<sup>19</sup>, Sakonvan Chawchai<sup>20</sup>, Andrea Columbu<sup>21</sup>, Laura Endres<sup>15</sup>, Jun Hu<sup>22</sup>, Zoltán Kern<sup>12,13</sup>, Alena Kimbrough<sup>23</sup>, Koray Koç<sup>24,25</sup>, Monika Markowska<sup>26</sup>, Belen Martrat<sup>27</sup>, Syed Masood Ahmad<sup>28</sup>, Carole
- 10 Nehme<sup>29</sup>, Valdir Felipe Novello<sup>4</sup>, Carlos Pérez-Mejías<sup>19</sup>, Jiaoyang Ruan<sup>30,31</sup>, Natasha Sekhon<sup>32,33</sup>, Nitesh Sinha<sup>30,31</sup>, Carol V. Tadros<sup>7,17</sup>, Benjamin H. Tiger<sup>34,35</sup>, Sophie Warken<sup>36,37</sup>, Annabel Wolf<sup>38</sup>, Haiwei Zhang<sup>19</sup> and SISAL Working Group members<sup>+</sup>

<sup>1</sup>Exeter College, University of Oxford, Oxford OX1 3DP, UK

- <sup>2</sup>Department of Chemistry, Biochemistry and Pharmaceutical Sciences, and Oeschger Centre for Climate Change Research, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland <sup>3</sup>Swiss Federal Institute for Forest, Snow and Landscape Research WSL, Zürcherstrasse 111, 8903 Birmensdorf, Switzerland <sup>4</sup>Department of Geoscience and Department of Physics, Geo- und Umweltforschungszentrum (GUZ), Schnarrenbergstr. 94/96, 72076 Tübingen, Germany
- <sup>5</sup>Arizona State University, Institute of Human Origins, PO Box 878404, Tempe, AZ 85287, USA
   <sup>6</sup>International Water Research Institute, Mohammed VI Polytechnic University, Lot 660 Hay Moulay Rachid, 43150, Benguerir, Morocco
   <sup>7</sup>Control Control Contron Control Control Control Control Control Control Control Con

<sup>7</sup> School of Biological, Earth and Environmental Sciences, UNSW Sydney, Sydney, NSW, 2052, Australia

<sup>8</sup>UC Davis Institute for the Environment, UC Davis Earth and Planetary Sciences, University of California Davis, One Shields
 Avenue, Davis, CA 95616, USA

<sup>9</sup>Barcelona, Spain

<sup>10</sup>The Fredy & Nadin Herrman Institute of Earth Sciences, The Hebrew University, The Edmond J. Safra Campus - Givat Ram, Jerusalem 9190401, Israel

<sup>11</sup>Department of Geography and Environmental Science, University of Reading, Reading RG6 6AH, UK

30 <sup>12</sup> Institute for Geological and Geochemical Research, Research Centre for Astronomy and Earth Sciences, Budaörsi út 45, H-1112 Budapest, Hungary

<sup>13</sup>CSFK, MTA Centre of Excellence, Budapest, Konkoly Thege Miklós út 15-17, 1121 Budapest, Hungary

<sup>14</sup> Potsdam Institute for Climate Impact Research (PIK), Potsdam, Germany

<sup>15</sup>Department of Earth Sciences, ETH Zurich, Sonneggstrasse 5, 8092 Zurich, Switzerland

<sup>16</sup>Institute of Geography and Earth Sciences, Department of Geophysics and Space Science, ELTE Eötvös Loránd University, Budapest, 1117, Hungary

<sup>17</sup>ANSTO, New Illawarra Road, Lucas Heights, NSW 2234, Australia

<sup>18</sup>Department of Geology, Trinity College Dublin, Dublin 2, Ireland

<sup>19</sup>Institute of Global Environmental Change, Xi'an Jiaotong University, Xi'an, Shaanxi, China 710049

<sup>20</sup>Department of Geology, Faculty of Science, Chulalongkorn University, Bangkok 10330 Thailand <sup>21</sup>University of Pisa, Department of Earth Sciences. Via Santa Maria 53, 56126 Pisa Italy <sup>22</sup>College of Ocean and Earth Sciences, Xiamen University, Xiamen, Fujian, 361102, China <sup>23</sup>School of Earth, Atmospheric and Life Sciences, University of Wollongong, Northfields Ave Wollongong, NSW 2522, Australia





<sup>24</sup>Department of Geological Engineering, Akdeniz University, 07100, Antalya, Türkiye
 <sup>25</sup>Quaternary Geology, Department of Environmental Sciences, University of Basel, 4056, Switzerland
 <sup>26</sup>Department of Climate Geochemistry, Max Planck Institute for Chemistry, Mainz, Germany
 <sup>27</sup>Department of Environmental Chemistry, Institute of Environmental Assessment and Water Research (IDAEA-CSIC), Jordi Girona, 18; 08034 Barcelona, Spain
 <sup>28</sup>Inter-University Accelerator Centre, New Delhi 110067, India
 <sup>29</sup>UMR IDEES 6266, CNRS, University of Rouen Normandy, 1, Rue Thomas Becket, Mont Saint-Aignan, 76130, France
 <sup>30</sup>Center for Climate Physics, Institute for Basic Science, Busan, 46241, Republic of Korea
 <sup>31</sup>Pusan National University, Busan, 46241, Republic of Korea

- <sup>32</sup>Department of Earth, Environmental and Planetary Science, Brown University, Providence 02908, Rhode Island, USA
   <sup>33</sup>Institute at Brown for Environment and Society, Brown University, Providence 02908, Rhode Island, USA
   <sup>34</sup>Department of Earth, Atmospheric and Planetary Sciences, Massachusetts Institute of Technology, Cambridge, MA, USA
   <sup>35</sup>Department of Geology and Geophysics, Woods Hole Oceanographic Institution, Woods Hole, MA, USA
   <sup>36</sup>Ruprecht Karls University Heidelberg, Institute of Earth Sciences, Im Neuenheimer Feld 234, 69120 Heidelberg
   <sup>37</sup>Ruprecht Karls University Heidelberg, Institute of Environmental Physics, Im Neuenheimer Feld 229, 69120 Heidelberg
- <sup>38</sup>Department of Earth System Science, University of California Irvine, Croul Hall, Irvine, CA 92697-3100, USA
   <sup>+</sup> A full list of authors appears at the end of the paper.

*Correspondence to*: Nikita Kaushal (<u>nikitageologist@gmail.com</u>), Franziska Lechleitner (<u>Franziska.lechleitner@unibe.ch</u>), Micah Wilhelm (<u>micah.wilhelm@wsl.ch</u>)

Abstract. Paleoclimate information on multiple climate variables at different spatiotemporal scales is increasingly important

- 65 to understand environmental and societal responses to climate change. A lack of high-quality reconstructions of past hydroclimate has recently been identified as a critical research gap. Speleothems, with their precise chronologies, widespread distribution, and ability to record changes in local to regional hydroclimate variability, are an ideal source of such information. Here we present a new version of the Speleothem Isotopes Synthesis and AnaLysis database (SISALv3), which has been expanded to include trace element ratios and Sr-isotopes as additional, hydroclimate-sensitive geochemical proxies. The
- 70 oxygen and carbon isotope data included in previous versions of the database have been substantially expanded. SISALv3, contains speleothem data from 364 sites from across the globe, including 94 Mg/Ca, 83 Sr/Ca, 51 Ba/Ca, 25 U/Ca, 29 P/Ca and 14 Sr-isotope records. The database also has increased spatiotemporal coverage for stable oxygen (831) and carbon (588) isotope records compared to SISALv2. Additional meta information has been added to improve machine-readability and filtering of data. Standardized chronologies are included for all new entities together with the originally published
- 75 chronologies. The SISALv3 database thus constitutes a unique resource of speleothem paleoclimate information that allows regional-to-global paleoclimate analyses based on multiple geochemical proxies, allowing more robust interpretations of past hydroclimate and comparisons with isotope-enabled climate models and other earth system and hydrological models.

## **1** Introduction

Speleothems, secondary cave carbonate precipitates, are a rich paleoenvironmental archive of geochemical data (Wong and 80 Breecker, 2015). Due to their widespread distribution (Comas-Bru et al., 2020) and their precise chronologies (Henderson,





2006), they can provide paleoclimate data at seasonal (Baldini et al., 2021) to multi-annual resolution spanning millennial and longer time scales (Cheng et al., 2016; Stoll et al., 2022).

The Speleothem Isotopes Synthesis and AnaLysis working group (SISAL WG) is an international effort to synthesize speleothem data under the umbrella of the Past Global Changes (PAGES) project (Comas-Bru et al., 2017; Comas-Bru and

- 85 Harrison, 2019). The SISAL WG aims to answer critical open questions in paleoclimate science with a focus on regional to global trends and event synchronization. To address these questions, the SISAL WG has been developing standardized and quality checked databases. The first three versions of the database (SISALv1, SISALv1b and SISALv2) provided the paleoclimate community with a growing resource of speleothem geochemical data (Atsawawaranunt et al., 2018; Comas-Bru et al., 2020, 2019), specifically oxygen (δ<sup>18</sup>O) and carbon (δ<sup>13</sup>C) isotope records. The SISAL database versions have been
- 90 exploited (i) to better understand the drivers of speleothem environmental proxies and improve their interpretations (Baker et al., 2019, 2021; Fohlmeister et al., 2020; Treble et al., 2022; Skiba and Fohlmeister, 2023), (ii) to provide a resource on the interpretation of speleothem records at a regional level, identifying key gaps and future work (Kaushal et al., 2018; Lechleitner et al., 2018; Braun et al., 2019; Burstyn et al., 2019; Deininger et al., 2019; Kern et al., 2019; Oster et al., 2019; Zhang et al., 2019; Lorrey et al., 2020), and (iii) to understand the mechanisms of past climate change including through comparison with
- 95 isotope-enabled climate models (Comas-Bru et al., 2019; Parker et al., 2021a; Bühler et al., 2022; Parker and Harrison, 2022; Parker et al., 2021b).

The new SISALv3 database provides an expanded dataset of oxygen and carbon isotope data, interpreted as records of hydroclimate and vegetation dynamics/bioproductivity (Wong and Breecker, 2015), and has been significantly expanded to include data on Sr, Mg, Ba, U, typically tracers for hydrological processes in the karst and cave (Fairchild et al., 2000; Johnson

- 100 et al., 2006; Fairchild and Treble, 2009; Wassenburg et al., 2016), and P, recognized as tracer for surface bioproductivity (Treble et al., 2003; Borsato et al., 2007; McDonough et al., 2022). Also included are data on Sr-isotopes, as these are an important proxy for hydroclimatic processes and may provide information on local hydrology and soil source, production and/or erosion (e.g., Li et al., 2005; Ünal-İmer et al., 2016; Wortham et al., 2017; Weber et al., 2018; Ward et al., 2019; Utida et al., 2020). Ratios of Sr/Ca, Mg/Ca, Ba/Ca and U/Ca, coupled with δ<sup>13</sup>C information, are sensitive to water-rock interactions
- 105 and residence time (Fairchild et al., 2000; Johnson et al., 2006). An important mechanism that drives variability in these multiple proxies in quantifiable ways is the process of prior calcite/carbonate precipitation (PCP), through which carbonate precipitated along flow paths in the karst and on the cave roof will lead to altered element concentration in cave drip waters from which the speleothem ultimately precipitates (Fairchild et al., 2000; Day and Henderson, 2013). An increase in PCP usually occurs in times of drought that facilitate increased water-rock residence times and degassing in the karst (Fairchild et al., 2000; Day and Henderson, 2013).
- 110 al, 2000). The SISALv3 database, augmented with trace element proxies thus provides a multi-proxy dataset that can be used for long-term drought reconstructions in the past, and to better understand the forcings, mechanisms and periodicities of such events. In addition to the new geochemical data, extensive metadata including information on parameters such as vegetation and karst type as well as entity (i.e. speleothem dataset) images are provided to aid robust interpretations.



The SISALv3 database will allow the systematic and global analysis of stable isotope and trace element variability, and 115 elucidate how trace element data can be used to strengthen climatic interpretations from speleothem oxygen ( $\delta^{18}$ O) and carbon ( $\delta^{13}$ C) records.

## 2 Data and Methods

#### 2.1 New data formatting and processing

All trace elements are reported normalized as ratios with respect to Ca (X/Ca) in units of mmol/mol. In the following 120 manuscript, "trace element" refers to the normalized ratio to Ca. A standardized conversion sheet is used to facilitate conversions from gram to mol units (available in the repository). Sr-isotope data is reported as <sup>87</sup>Sr/<sup>86</sup>Sr values. For internal consistency, and to facilitate future intercomparison and synthesis studies, the measurement method and standards used, and measurement precision are also reported for both trace elements and Sr-isotopes.

- Mechanisms relevant to hydroclimate interpretations from speleothems are based on a multi-proxy approach of stable isotopes and one or more trace element ratios. Therefore, the SISALv3 database structure allows for trace element measurements to be added at the depths of the stable isotope measurements on a given entity. However, between 35 and 86% of the records (depending on element) were measured using in-situ techniques, such as laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS), and these datasets are typically generated at a higher resolution (10-100 µm) than the stable isotope records (Jochum et al., 2012). These data have been downsampled to the resolution of the stable isotope data for the
- 130 same speleothem. Downsampling was performed by computing averages (and standard deviations) of the trace element measurements falling into the stable isotope sampling depths. This implicitly assumes that the same or a parallel sampling track were used for trace elements and stable isotopes and that the isotope sampling was continuous. Downsampling allows the trace element data to be represented by the same depth-age model as the stable isotope record. For records submitted by the authors where the originally published dataset was at higher resolution than reported in the SISAL database, standardized \*.txt datafiles are also available in the repository (see Code and Data accessibility). No new chronological information or

separate age models are reported for these datasets.

# 2.2 Additional metadata

New metadata fields are included in the Entity table (see database structure; Figure 1) to allow users to select sites with similar environmental conditions and to take account of factors that might influence the interpretation of individual records. These

include information on vegetation, land use, land cover, and host rock type above the cave. This information is often missing from publications and was not available from data contributors, so information from data products has been added as additional fields to the database for completeness. Vegetation type and land use information were provided by the original investigators. Information on land use and land cover was taken from the Copernicus Global Land Service Land Cover database (LCC v3.0.1 Epoch 2019; (Buchhorn et al., 2021, 2020), extracted with a radius of 250 m around the cave site. Information on the



145 carbonate/evaporite host rock at the cave sites was taken from the WOKAM database (Goldscheider et al., 2020) extracted with a radius of 1000 m.

The database also indicates if the trace element content of the host rock and drip water feeding the speleothem is available (but does not include the actual values). Drip height (i.e., the distance the drip falls from the ceiling of the cave to the speleothem), and the difference between dripwater and carbonate  $\delta^{18}$ O values are given, based on information provided by the original

150 investigators.

The SISAL WG repository now hosts images of the entities (speleothem sections) and maps of cave sites. These allow users to evaluate petrographic features that may influence the trace element and stable isotopic records and to check whether cave morphology could potential influence the climate in the cave (Covington and Perne, 2015). The entity table in the database contains fields indicating whether maps and images are available.

## 155 2.3 Changes to database structure

The structure of the SISALv3 database (Figure 1) has been changed to accommodate additional data and metadata, and to optimise the organisation of information, as described below.

#### 2.3.1 New geochemical data and metadata fields

The elemental ratio for each trace element and the Sr-isotope data are given in individual tables that contain sample identifiers (*sample\_id*), the measurement value and the measurement precision. The *sample\_id* provides the link to the Sample table and thus links these data to the stable isotope data (Figure 1, Table 1).

Metadata for the measurements are stored in the Entity table. For each elemental ratio (Sr/Ca, Mg/Ca, U/Ca, Ba/Ca and P/Ca), the Entity table indicates whether the data are available ("yes/no/other/unknown"), the measurement method, the laboratory standards used and, where applicable, the downsampling methods used. The table also indicates if high-resolution trace

- 165 element data is available. For Sr-isotopes, the Entity table specifies whether this dataset is available, what measurement method was employed and how the measurement was standardized (Figure 1, Table 1). SISALv3 now provides a unique, persistent identifier for each speleothem (*persist\_id*) in the Entity table (Figure 1, Table 1). This was needed because there was an increasing issue with non-unique entity names, and to deal with the fact that different datasets from the same stalagmite had different *entity\_ids* (e.g., for datasets covering different time periods in the same
- 170 speleothem). Thus, the field *entity\_id* provides a unique identifier for a specific dataset, but not necessarily for a specific speleothem, while the *persist\_id* uniquely identifies the speleothem. The *persist\_id* were created by combining the *site\_id* and *entity\_name* (without special characters). There are 837 unique *persist\_id*s and 901 unique *entity\_id*s in the database.

#### 2.3.2 Changes in existing database fields and options

The fields "geology" and "rock age" were moved from the Site table to the Entity table (Figure 1, Table 1). This was done to allow for variability in these parameters within the same cave system, particularly relevant for the interpretation of  $\delta^{13}$ C and





trace element data. The field "trace elements" (yes/no) in the Entity table was removed as it is now redundant. The field "iso\_std" describing the standard used for measurement of  $\delta^{18}$ O and  $\delta^{13}$ C values was moved from the stable isotope tables to the Entity metadata table. A number of options for entries in the metadata fields were changed (Table 2). The majority of these changes were additions to the previously available options in light of the entries made in the 'Notes' section to allow for more "metadata-filterable" database mining. A few options were removed from the metadata fields since they have never been used in previous database versions.





Figure 1: Structure of the SISALv3 database. Fields and tables marked with (\*) refer to new information added in SISALv3;
see table 1 for details. The colors 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 the Supplementary information (Table S1).





Action	Field label	Description	Format	Constraints
Changes m	ade to the SITE table	L		I
Field	geology			
removed				
Field	rock_age			
Terrioved				
Changes m	ade to the ENTITY table			
Field	norsist id	persistent unique identifier for each	Text	
added	persist_id	speleothem	TEX	
Field	geology	Information on geology	Text	Selection from
added				predefined list
Field added	rock_age	Information on bedrock age	Text	Selection from predefined list
Field	wokam	Information on type of carbonate/evaporite	Text	Added by SISAL SC at
added		rock from WOKAM database		database level
Field	vegetation_type	Information on vegetation cover	Text	Selection from
added				predefined list
Field	land_use	Information on land use (publication/data	Text	Selection from
added		contributors)		predefined list
Field	copernicus Icc	Information on land cover from Copernicus	Text	Added by SISAL SC at
added		land cover classification dataset	1 OA	database level
Field	cover_type	Information on land cover (publication/data	Text	Selection from
added		contributors)		predefined list
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Field	host_rock_trace_elements	Indication whether trace element data from	Text	Selection from
auueu		the host fock has been measured		predenned list
Field	drin water trace clamente	Indiantian whether trace element data from	Tout	Coloction from
added	drip_water_trace_elements	the drip water has been measured	Text	predefined list
aaaba				production
Field	drin height	Information on drip beight (in m)	Numeric	Free to fill
added	anp_noight	internation of any height (in m)	Numeno	
Field	iso_std	Information on standard used for oxygen and	Text	Selection from
added		carbon isotope measurements		predefined list



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Field added	d180_dripwater_carbonate_difference	Information on difference between dripwater and carbonate oxygen isotope values	Numeric	neric Free to fill	
Field removed	trace_elements				
Field added	Sr_Ca	Indication whether Sr/Ca data has been measured	Text	Selection predefined list	from
Field added	Sr_Ca_method	Information on measurement method for Sr/Ca	Text	Selection predefined list	from
Field added	Sr_Ca_std	Information on standard used for Sr/Ca measurements	Text	Selection predefined list	from
Field added	Sr_Ca_downsampled	Information on whether Sr/Ca data had to be downsampled	Text	Selection predefined list	from
Field added	Sr_Ca_downsampling_method	Information on downsampling method for Sr/Ca, if applicable	Text	Selection predefined list	from
Field added	Mg_Ca_method	Information on measurement method for Mg/Ca	Text	Selection predefined list	from
Field added	Mg_Ca_std	Information on standard used for Mg/Ca measurements	Text	Selection predefined list	from
Field added	Mg_Ca_downsampled	Information on whether Mg/Ca data had to be downsampled	Text	Selection predefined list	from
Field added	Mg_Ca_downsampling_method	Information on downsampling method for Mg/Ca, if applicable	Text	Selection predefined list	from
Field added	Ba_Ca	Indication whether Ba/Ca data has been measured	Text	Selection predefined list	from
Field added	Ba_Ca_method	Information on measurement method for Ba/Ca	Text	Selection predefined list	from
Field added	Ba_Ca_std	Information on standard used for Ba/Ca measurements	Text	Selection predefined list	from
Field added	Ba_Ca_downsampled	Information on whether Ba/Ca data had to be downsampled	Text	Selection predefined list	from
Field added	Ba_Ca_downsampling_method	Information on downsampling method for Ba/Ca, if applicable	Text	Selection predefined list	from



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Field added	U_Ca	Indication whether U/Ca data has been measured	Text	Selection predefined list	from
Field added	U_Ca_method	Information on measurement method for U/Ca	Text	Selection predefined list	from
Field added	U_Ca_std	Information on standard used for U/Ca measurements	Text	Selection predefined list	from
Field added	U_Ca_downsampled	Information on whether U/Ca data had to be downsampled	Text	Selection predefined list	from
Field added	U_Ca_downsampling_method	Information on downsampling method for U/Ca, if applicable	Text	Selection predefined list	from
Field added	P_Ca	Indication whether P/Ca data has been measured	Text	Selection predefined list	from
Field added	P_Ca_method	Information on measurement method for P/Ca	Text	Selection predefined list	from
Field added	P_Ca_std	Information on standard used for P/Ca measurements	Text	Selection predefined list	from
Field added	P_Ca_downsampled	Information on whether P/Ca data had to be downsampled	Text	Selection predefined list	from
Field added	P_Ca_downsampling_method	Information on downsampling method for P/Ca, if applicable	Text	Selection predefined list	from
Field added	Sr_isotopes	Indication whether Sr isotope data has been measured	Text	Selection predefined list	from
Field added	Sr_isotopes_method	Information on measurement method for Sr isotopes	Text	Selection predefined list	from
Field added	Sr_isotopes_std	Information on standard used for Sr isotope measurements	Text	Selection predefined list	from
Field added	trace_elements_datafile	Information on whether the original trace elements data is available in the repository	Text	Selection predefined list	from
Field added	trace_elements_metadatafile	Information whether original trace element metadata is available in the repository	Text	Selection predefined list	from





Field added	cave_map	Information whether a copy of cave map is available in the repository	Text	Selection predefined list	from
Field	entity_scan	Information whether a scan of the speleothem	Text	Selection	from
added		in the repository		predefined list	
Changes m	ade to the d18O and d13C tables				
Field	iso_std	Information on standard used for d18O and	Text	Selection	from
removed		d13C measurements		predefined list	

Table 1: Changes made to the Site, Entity and stable isotope tables compared to SISALv2.

Table name	Action	Field label	Reason	Format	Constraints
Entity	Added "mixed (see notes)"	speleothem_type	Standardisation of option	Text	Selected from
	option		across fields		pre-defined list
Entity	Added "other (see notes)"	speleothem_type	Standardisation of option	Text	Selected from
	option		across fields		pre-defined list
Entity	Removed "magmatic" option	geology	Not used	Text	Selected from
					pre-defined list
Entity	Removed "granite" option	geology	Not used	Text	Selected from
					pre-defined list
Entity	Added "dolomite limestone"	geology	Machine-readable format	Text	Selected from
	option		option		pre-defined list
Entity	Added "marly limestone" option	geology	Machine-readable format	Text	Selected from
			option		pre-defined list
Entity	Added "calcarenite" option	geology	Machine-readable format	Text	Selected from
			option		pre-defined list
Entity	Added "other (see notes)"	geology	Option to include free	Text	Selected from
	option		text in notes		pre-defined list
Entity	Added "other (see notes)"	rock_age	Option to include free	Text	Selected from
	option		text in notes		pre-defined list



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Entity	Added "mixed (see notes)"	rock_age	Reflect overburden with	Text	Selected from
	option		rocks of different ages		pre-defined list
Entity	Removed "mixture"	drip_type	Replaced with "mixed	Text	Selected from
			(see notes)" option		pre-defined list
Entity	Removed "not applicable"	drip_type	Not used	Text	Selected from
					pre-defined list
Entity	Added "mixed (see notes)"	drip_type	Standardisation of option	Text	Selected from
	option		across fields		pre-defined list
Entity	Added "other (see notes)"	drip_type	Option to include free	Text	Selected from
	option		text in notes		pre-defined list
Entity	Added "other (see notes)"	d180_water_equilibrium	Option to include free	Text	Selected from
	option		text in notes		pre-defined list
Entity	Added "other (see notes)"	organics	Option to include free	Text	Selected from
	option		text in notes		pre-defined list
Entity	Added "other (see notes)"	fluid_inclusions	Option to include free	Text	Selected from
	option		text in notes		pre-defined list
Entity	Added "other (see notes)"	mineralogy_petrology_fabric	Option to include free	Text	Selected from
	option		text in notes		pre-defined list
Entity	Added "other (see notes)"	clumped_isotopes	Option to include free	Text	Selected from
	option		text in notes		pre-defined list
Entity	Added "other (see notes)"	noble_gas_temperatures	Option to include free	Text	Selected from
	option		text in notes		pre-defined list
Entity	Added "other (see notes)"	C14	Option to include free	Text	Selected from
	option		text in notes		pre-defined list
Entity	Added "other (see notes)"	ODL	Option to include free	Text	Selected from
	option		text in notes		pre-defined list
Dating	Added "mixed (see notes)"	material_dated	Align with options in the	Text	Selected from
	option		sample table		pre-defined list
Dating_lamina	Added "Year of chemistry"	modern_reference	Align with options in the	Text	Selected from
	option		dating table		pre-defined list
Sample	Removed "secondary calcite"	mineralogy	Not used	Text	Selected from
	option				pre-defined list



Sample	Removed "vaterite" option	mineralogy	Not used	Text	Selected from pre-defined list
Sample	Added "organic" option	mineralogy	Addition of option	Text	Selected from pre-defined list
Sample	Added "other (see notes)" option	mineralogy	Option to include free text in notes	Text	Selected from pre-defined list
Sample	Removed "combination of methods" option	age_model_type	Standardisation of option across fields	Text	Selected from pre-defined list
Sample	Added "mixed (see notes)" option	age_model_type	Standardisation of option across fields	Text	Selected from pre-defined list
Sample	Added "other (see notes)" option	dep_rate_check	Option to include free text in notes	Text	Selected from pre-defined list

190 Table 2: Changes made to the predefined options for metadata fields compared to SISALv2.

#### **3** Quality control

The SISAL WG has used several levels of quality control (QC) and this practice was continued for SISALv3 (Figure 2). The initial data compilation is performed by SISAL regional coordinators (from datasets archived on public repositories or in publications) and/or in liaison with the data contributors into standardized excel workbooks. The first QC level consists in the

- 195 expert assessment by the SISAL regional coordinators who double-check completeness of entered data and correctness of measurement units where applicable. Standardised unit conversion sheets for common conversions (e.g. degrees-minutesseconds to decimal degrees for site information; atomic ratios to activity ratios for dating information; mg/g to mmol/mol for trace element-to-Ca ratios for trace element information) have been provided to regional coordinators (see repository). The completed workbook(s) are subjected to a series of automated QC (e.g., age model matches discreet dating information,
- 200 hiatuses are placed at the correct depth) by the database managers. If the dataset fails to pass the automated QC, it is sent back to the data contributors and regional coordinators for correction. When the datasets pass automated QC, and no further corrections are necessary, the dataset workbook and auto generated QC figures are sent to the data contributors for final evaluation and approval. The same workflow has been followed for the \*.txt trace element datafiles. The new metadata fields of vegetation\_type and land\_use that have been added to SISALv3 for entities that were included in SISALv2 from
- 205 publications.

Data already included in SISALv2 has been checked, and mistakes / unknowns identified during previous data analysis or during the process of trace element data addition were corrected. A comprehensive summary of the changes made to existing entities between SISALv2 and SISALv3 is shown in Table 3.







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Figure 2: Quality checking workflow adopted for inclusion of datasets in SISALv3. The colors indicate different quality check levels: blue - data contributing sources (original authors or datasets deposited in repositories and publication supplementary information); yellow - SISAL regional coordinator group with regional expertise; orange - SISAL database managers.

Modification	v2 to v3
Site table	
Number of new sites	71
Sites with new entities	37
Entity table	
Number of new entities	210
Entities added to pre-existing sites	71
Entities with updated entity.entity_status	33
Entities with altered entity.corresponding_current	1
Entities with altered geology	106



Entities with altered rock_age	58
Entities with altered entity.cover_thickness	6
Entities with altered distance_entrance	1
Entities with altered d13C	109
Entities with altered d18O	15
Entities with altered organics	9
Entities with altered fluid_inclusions	9
Entities with altered mineralogy_petrology_fabric	14
Entities with altered clumped_isotopes	9
Entities with altered noble_gas_temperatures	12
Entities with altered C14	3
Entities with altered ODL	7
Entities with altered contact	62
Entities with altered data_DOI_url	20
Dating table	
Entities with changes in the dating table	
Addition of "event: hiatus" to an entity	1
Changes in hiatus depths	1
Changes in depths of "Event: start/end of laminations"	1
Alterations in dating.date_type	2
Alterations in dating.depth_dating	5
Alterations in dating.material_dated	2
Alterations in dating.min_weight	6
Alterations in dating.max_weight	6
Alterations in dating.uncorr_age	15
Alterations in dating.uncorr_age_uncert_pos	13
Alterations in dating.uncorr_age_uncert_neg	13
Alterations in dating.date_used	27
Alterations in dating.238U_content	25
Alterations in dating.238U_uncertainty	25
Alterations in dating.232Th_content	91
Alterations in dating.232Th_uncertainty	80
Alterations in dating.230Th_232Th_ratio	201
Alterations in dating.230Th_232Th_ratio_uncertainty	195

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Alterations in dating.230Th_238U_activity	19
Alterations in dating.230Th_238U_activity_uncertainty	19
Alterations in dating.234U_238U_activity	374
Alterations in dating.234U_238U_activity_uncertainty	431
Alterations in dating.ini_230Th_232Th_ratio	519
Alterations in dating.ini_230Th_232Th_ratio_uncertainty	485
Alterations in dating.decay_constant	24
Alterations in dating.corr_age	70
Alterations in dating.corr_age_uncert_pos	26
Alterations in dating.corr_age_uncert_neg	28
Sample table	
Altered sample.depth_sample	1084
Altered sample.mineralogy	294
Altered sample.arag_corr	294
Entities that had d18O time series altered (changes in depth/ duplicate isotope values)	4
Entities that had d13C time series altered (changes in depth/ duplicate isotope values)	4
Original chronology	
Altered original_chronology.interp_age	7440
References	
How many entities had changes in references?	100
How many citations have a different pub_DOI?	100
Notes	
Sites with notes modified	121

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Table 3: Summary of the modifications applied to records in version 2 (Comas-Bru et al., 2020) of the SISAL database. Note that the changes in the dating and sample table were counted by dating\_id and sample\_id, respectively, which leads to a large number of changes.



### 4 Overview of database contents

#### 220 4.1 Trace element and Sr-isotope records

SISALv3 contains 94 Mg/Ca, 83 Sr/Ca, 51 Ba/Ca, 25 U/Ca, 29 P/Ca and 14 Sr-isotope records (Table 4). This corresponds to ~60% of the known published data. There is a clear regional bias in the database with European entities dominating every elemental ratio (Figure 3). The Sr-isotope records are more evenly distributed, with records from every region except Asia and Oceania. Temporal coverage for the combined trace element and Sr-isotope dataset is high during the last 2000 years (~60

- entities per 20 year interval) and the Holocene (~60 entities per 250 year interval), and then drops to 20-40 entities per 10,000 year interval for the last glacial cycle (12-120 ka BP, where ka stands for 1000 years and BP for "before present", defined as 1950, Figure 4). Beyond ~120 ka BP, the number of entities gradually decreases until the U-Th dating limit is reached (~640 ka).
- Where the original measured laser ablation data have been provided by data contributors, these have been made available as
  \*.txt datafiles in the repository (Table 4). 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).

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-	-	$\mathcal{I}$

Geochemical data	Total number in SISAL	Downsampled by original authors	Downsampled by SISAL	Only in repository
Mg/Ca	94	12	15	15
Sr/Ca	83	11	11	17
Ba/Ca	51	11	9	4
U/Ca	21	2	6	5
P/Ca	29	4	12	5

Table 4: Summary of number of trace element records in SISAL and downsampling methods applied.



## 4.2 New stable isotope records

SISALv3 provides a significantly expanded oxygen isotope dataset compared to SISALv2 (Table 5, Figure 5), with 831 δ<sup>18</sup>O
records from 364 sites, compared to 673 records in SISALv2. The most significant increases in δ<sup>18</sup>O records are in Africa (+38%), Europe (+30%), and the Middle-East (+27%; Table 5). SISALv3 contains 338 entities covering the last 2000 years, of which 82 are new (Figure 6). As record density begins to decrease with age (Figure 6), the spatial distribution is reduced as well. For the Last Glacial Maximum (20 – 22 ka BP), SISALv3 contains 96 entities (15 new), while for the Last Interglacial (124 – 126 ka BP), only 67 entities are available (16 new).

245 There has also been a significant increase in the number of  $\delta^{13}$ C records added, with 588 records in SISALv3 compared to 430 in SISALv2 (Table 5, Figure 7). At the regional scale, the biggest increase in  $\delta^{13}$ C records is for Africa (+37%), followed by Asia, the Middle East, and Europe (+31% each, Table 5). The  $\delta^{13}$ C record coverage decreases following the same patterns as the trace elements and  $\delta^{18}$ O records (Figure 8).

Region	$\delta^{18}$ O records in v3	Increase	δ <sup>13</sup> C records in v3	Increase
		compared to v2		compared to v2
		(%)		(%)
Africa	73	38	63	37
Asia	237	21	105	31
Europe	243	30	213	31
Middle East	59	27	42	31
Oceania	100	11	66	17
North and Central	88	10	72	12
America				
South America	97	22	54	24

250 Table 5: Summary of the new  $\delta^{18}O$  and  $\delta^{13}C$  records added to SISALv3 compared to SISALv2.









Figure 3: Trace element ratios and Sr isotope records included in SISALv3 by region. 255







Figure 4: Temporal coverage of the trace element and Sr-isotope records in SISALv3 by region. Entities with multiple trace elements were counted multiple times. Bin sizes: 0-2,000 a (years) BP (top panel) - 20 years; 2,000-21,000 a BP (middle panel) - 250 years; 21,000-750,000 a BP (bottom panel) - 10,000 years.

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Figure 5: Global map of  $\delta^{18}O$  records included in SISAL v2 and v3. The shaded background shows the global karst distribution extracted from the World Karst Aquifer Map (WOKAM, Goldscheider et al., 2020).







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Figure 6: Temporal coverage of the  $\delta^{18}O$  records in SISALv3 by region. Bin sizes: 0-2,000 a BP (top panel) - 20 years; 2,000-21,000 a BP (middle panel) - 250 years; 21,000-750,000 a BP (bottom panel) - 10,000 years.

![](_page_21_Picture_1.jpeg)

![](_page_21_Picture_2.jpeg)

![](_page_21_Figure_3.jpeg)

Figure 7: Map of available  $\delta^{13}C$  records in SISALv3 compared to all records in the database. The shaded background shows the global karst distribution extracted from the World Karst Aquifer Map (WOKAM, Goldscheider et al., 2020).

![](_page_22_Picture_1.jpeg)

![](_page_22_Picture_2.jpeg)

![](_page_22_Figure_3.jpeg)

Figure 8: Temporal coverage of the  $\delta^{13}C$  records in SISALv3 by region. Bin sizes: 0-2,000 a BP (top panel) - 20 years; 2,000-21,000 a BP (middle panel) - 250 years; 21,000-750,000 a BP (bottom panel) - 10,000 years.

![](_page_23_Picture_1.jpeg)

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![](_page_23_Picture_2.jpeg)

## 275 4.4 Vegetation and land cover metadata

Interpretation of the site-to-site variability in speleothem data sensitive to vegetation changes is facilitated by providing information on *vegetation\_type* and *land\_use*. The dropdown list for these fields includes options typically used in speleothem publications. Additional information provided by the authors (e.g. species names) has been added to the Notes table. About 40% of the database entries lack the author-reported information on land cover (Figure 9A). Satellite-derived land cover classifications provides information for many more sites (unknown: 1.7%). Forested sites (evergreen, deciduous, and mixed) comprise ~56.5% (Figure 9B), shrub- and grassland makes up 25.1% and this dataset also denotes sites that are affected by anthropogenic land use (managed vegetation, agriculture, urban), which make up 13%.

![](_page_24_Picture_1.jpeg)

![](_page_24_Picture_2.jpeg)

![](_page_24_Figure_3.jpeg)

Figure 9: A – vegetation description from the original publications or provided by authors and B – land cover categories extracted from the Copernicus LCC database (Buchhorn et al., 2021, 2020) with a radius of 250 m around the cave sites. Background shading in the map shows the global karst distribution extracted from the World Karst Aquifer Map (WOKAM, (Goldscheider et al., 2020). To allow comparison between the two datasets, the Copernicus LCC vegetation data was grouped into broader categories, e.g., "deciduous" includes all closed and open broad-leaf and needle forest marked as deciduous.
The entries in the database are more detailed.

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![](_page_25_Picture_1.jpeg)

## **5** Recommendations for use

The SISALv3 database is a standardized, quality checked dataset that allows regional to global assessments of spatial and temporal trends in multiple environmental proxies from speleothem records. The addition of trace element data at stable isotope equivalent depths to the database together with machine-readable metadata fields allow examination of hydroclimatic controls on speleothem trace element distribution. Metadata fields, including distance from coast (*latitude, longitude, elevation*), lithology (*geology, wokam*), and land cover (*cover\_type, cover\_thickness, vegetation\_type, land\_use, copernicus\_lcc*), allow identification of the primary controls on trace elements. We recommend using all cover fields together since they provide complementary information, with the caveat that anthropogenic and natural changes in the cover parameters over time need to be considered.

Where trace elements are measured on aliquots of the same powder as stable isotopes, the sample-to-sample variability in depth-time space is minimal. Where samples for stable isotopes and trace elements have been drilled at different times or *in situ* methods have been used for trace element measurements, there may be depth-time variability that may impact results. Extensive metadata on sampling and measurement methods, as well as the original high resolution *in-situ* measurements

305 against depth, are provided in the database and linked repository and should be used to check for such impacts. Measurements may also be sensitive to stalagmite petrography; image scans have been provided in the linked repository so the user can evaluate whether this is important for interpretation of the record.

#### 5.3 Code and data availability

- 310 The database is available in CSV and SQL format from https://doi.org/10.5287/ora-mzy8pozvk (Kaushal et al., 2023). This dataset is licensed by the rights holder(s) under a Creative Commons Attribution 4.0 International License: https://creativecommons.org/licenses/by/4.0/. The workbook used to submit data to the SISAL database and the codes for automatic quality checking are available at https://doi.org/10.5287/ora-mzy8pozvk (Kaushal et al., 2023) (scripts licensed by the right holder(s) under a Creative Commons Attribution 4.0 International).
- 315 The codes for standardisation and downsampling of trace element and Sr-isotope records are available at zenodo 10.5281/zenodo.8234066 (Skiba, 2023); licensed by the right holder(s) under Creative Commons Attribution 4.0 International).

The database contains both the original age model for individual entities and a standardized age modelling ensemble. The original age model often takes account of site- and sample-specific conditions; the standardized age model ensemble allows

320 for robust assessment of age uncertainties and sensitivity testing (Comas-Bru et al., 2020). All codes for constructing the age model ensembles using linear interpolation, linear regression, Bchron, Bacon, copRa, and StalAge can be found at https://github.com/paleovar/SISAL.AM (last access: 23 July 2020; codes licensed by the right holder(s) under a GPL-3 license.). These codes are licensed by the right holder(s) under a Creative Commons Attribution 4.0 International. All age

![](_page_26_Picture_1.jpeg)

![](_page_26_Picture_2.jpeg)

model ensembles are available at https://doi.org/10.5281/zenodo.3816804 (Rehfeld et al., 2020). These codes are licensed by 325 the right holder(s) under a Creative Commons Attribution 4.0 International.

The SISALv3 database, like its predecessors, lists the original references, and users are encouraged to consult original authors for interpretative details.

#### 5.4 How to cite the database

330 The SISALv3 database is a community driven effort to synthesize, standardize and make speleothem data to the wider paleoclimate community. In agreement with the FAIR principles for scientific data management and stewardship, the database itself should be cited (available at https://doi.org/10.5287/ora-mzy8pozvk; (Kaushal et al., 2023), together with this publication (and previous version publications). If individual records are extracted from the database, the original publications should also be listed. More details on Terms of Use are provided in the repository (https://doi.org/10.5287/ora-mzy8pozvk; (Kaushal et 335 al., 2023).

#### **Author contributions**

NK, FL and MW designed the new version of the database. KR and JB ran the SISAL standardized age-depth models for new entities. Downsampling of trace element records to stable isotope resolution was performed by VS and MR. Standardization of trace element datafiles was done by YB and NK. Reworking and additions to the metadata fields was done by KB and KA. 340 JGS and NK collected citations, copyright information and license terms for the cave maps and speleothem images. Regional data collection and screening was coordinated by VA, JLB, SC, AC, LE, JH, ZK, AK, KK, MK, BM, SMA, CN, VFN, CPM, JR, NS, NiS, CT, BHT, SW, AW, HZ. Quality control of the submitted datasets was performed by MW, FL, and NK. Figures 1 and 2 were created by FL, figures 3-9 were created by JB. All authors listed as "Data contributors" provided data for this version of the database or helped to complete existing data entries. FL wrote the paper with input from NK, JB, KR, AB, PT,

345 SPH, and all authors contributed to the final version.

## **Team list**

The following SISAL working group members contributed with either data or age-modelling advice to SISALv3: 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,

350 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

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University, Nanjing 210023, China), Dominik Fleitmann (Department of Environmental Sciences, University of Basel, Bernoullistrasse 32 4056 Basel, Switzerland), Dominik Hennhoefer (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, Türkiye), 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,

365 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), Judit Torner (CRG Marine Geosciences, Facultat de Ciències de la Terra, Universitat de Barcelona, Barcelona, 08028, Spain), Kathleen A Wendt (1. College of Earth, Ocean, and

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

- 370 Atmospheric Sciences, Oregon State University, Corvallis, Oregon 97331, USA), 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 (Division of Agrarian History, Department of
- 375 Urban and Rural Development, Swedish University of Agricultural Sciences, Uppsala, 756 51, Sweden), 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, Department 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
- 380 (Institute for Geosciences, Johannes Gutenberg University Mainz, J.-J.-Becher-Weg 21, 55128 Mainz, Germany), Nick Scroxton (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 (Proteomics and Mass Spectrometry Core Facility, Department of Cellular, Computational and Integrative
- 385 Biology (DeCIBIO), 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

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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).

#### **Competing interests**

395 The authors declare that they have no conflict of interest.

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