1	Deep-Time Marine Sedimentary Element Database
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18	Abstract. Geochemical data from ancient marine sediments are crucial forto studying
19	palaeoenvironments, palaeoclimates, and elementals' cycles. With increased accessibility to
20	geochemical data, many databases have emerged. However, there remains a need for a more
21	comprehensive database that focuses on deep-time marine sediment records. Here, we introduce the
22	"Deep-Time Marine Sedimentary Element Database" (DM-SED). The DM-SED has been built upon the
23	"Sedimentary Geochemistry and Paleoenvironments Project" (SGP) database with the new compilation
24	of 34,93834,874 data entries from 433 studies, totalling 63,69163,627 entries. The DM-SED contains
25	2,412,0852,522,255 discrete marine sedimentary data points, including major and trace elements and
26	some stable isotopes. It includes 9,2719,207 entries from the Precambrian and 54,420 entries from the
27	Phanerozoic, thus providing significant references for reconstructing deep-time Earth system evolution.
28	The data files described in this paper are available at
29	https://doi.org/10.5281/zenodo.13898366https://doi.org/10.5281/zenodo.14771859 (Lai et al., 2024Lai

32 1 Introduction

33 Geochemical data from deep-time marine sediments are fundamental for reconstructing the evolution of 34 the Earth system. By analysing the conetentrations of chemical elements in sediments and their isotopic 35 compositions, we can reconstruct the past cycling of elements in the Earth's surface systems and reveal 36 the evolution of Earth's surface systems through time Earth's evolution through time (Large et al., 2015; 37 Reinhard et al., 2017; Farrell et al., 2021; Planavsky et al., 2023). For instance, total organic carbon 38 (TOC), phosphorus (P), biogenic barium (Babio), copper (Cu), zinc (Zn), nickel (Ni), etc., enable 39 reconstructing marine primary productivity and carbon cycle perturbationschanges, thereby revealing 40 mechanisms driving past climate fluctuationspast climate change mechanisms (Scott et al., 2013; 41 Schoepfer et al., 2015; Shen et al., 2015; Schoepfer et al., 2016; Xiang et al., 2018; Jin et al., 2020; 42 Tribovillard, 2021; Wang et al., 2022; Zhang et al., 2022; Li et al., 2023; Sweere et al., 2023; Zhao et al., 43 2023). Elements such as uranium (U), vanadium (V), and molybdenum (Mo) can reveal how marine 44 redox conditions changed during critical periods in animal evolution, including mass extinctions and 45 evolutionary radiations (Algeo and Liu, 2020; Schobben et al., 2020; Stockey et al., 2024). Oxygen 46 isotopes (δ^{18} O) from fossilized marine organismsin the remains of marine fossil animals can reveal 47 oceanic palaeo-temperature changes (Veizer and Prokoph, 2015; Song et al., 2019; Grossman and 48 Joachimski, 2020; Scotese et al., 2021; Judd et al., 2022). However, many geochemical studies have 49 focused on high-resolution research of limited time intervals and/or regions, and there is little 50 comprehensive exploration across large-scale geological time and globally.

Fortunately, with more journals and institutions adopting strict data archiving rules and promoting adherence to FAIR (Findability, Accessibility, Interoperability, and Reusability) principles (Wilkinson et al., 2016; "FAIR Play in Geoscience Data," 2019), a large amount of geochemical data has become accessible, and sample meta-data records are more detailed. Several geochemical databases of varying scales and foci have emerged, such as the following:

EarthChem, which covers igneous, sedimentary, and metamorphic rocks and comprises numerous
 joint databases (https://www.earthchem.org/, last accessed: 16 July 2024).

Petrological Database of the Ocean Floor (PetDB), which includes elemental chemical, isotopic, and
 mineralogical data of global ocean floor igneous rocks, metamorphic rocks, minerals, and inclusions
 (https://www.earthchem.org/petdb, last accessed: 16 July 2024).

- Geochemistry of Rocks of the Oceans and Continents (GEOROC), a comprehensive compilation of chemical, isotopic, and other data on igneous rock samples, including whole rock, glass, mineral, and inclusion analyses and metadata (http://georoc.mpch-mainz.gwdg.de, last access: 16 July 2024).
 Data Publisher for Earth & Environmental Science (PANGAEA), which is used for archiving, publishing, and disseminating georeferenced data from earth, environmental, and biodiversity sciences and includes a large number of sediment core data (https://www.pangaea.de, last accessed:
- 67 16 July 2024).

Stable Isotope Database for Earth System Research (StabisoDB) containing δ¹⁸O and δ¹³C data for
 more than 67,000 macrofossil and microfossil samples, including benthic and planktonic
 foraminifera, benthic and nektonic mollusks, brachiopods, fish teeth, and conodonts
 (https://cnidaria.nat.uni-erlangen.de/stabisodb/, last accessed: 16 July 2024).

- Sedimentary Geochemistry and Paleoenvironments Project (SGP), which collects multi-proxy
 sedimentary geochemical data with an emphasis on Neoproterozoic-Palaeozoic shale data in its first
 data release (https://sgp-search.io/, last accessed: 12 June 2024).
- NOAA and MMS Marine Minerals Geochemical Database, which contains geochemical analyses
 and auxiliary information on present-day marine deposits of primarily ferromanganese nodules and
- 77 crusts, as well as some data for heavy minerals and phosphorites
- 78 (https://www.ncei.noaa.gov/access/metadata/landing-
- 79 page/bin/iso?id=gov.noaa.ngdc.mgg.geology:G01323, last accessed: 7 January 2025).
- An International Study of the Marine Biogeochemical Cycles of Trace Elements and Isotopes
 (GEOTRACES), which provides hydrographical and marine geochemical data acquired over the
 past decade (https://www.geotraces.org/, last accessed: 7 January 2025).
- 83 Many other government initiatives also host databases:
- The United States Geological Survey (USGS) National Geochemical Database, an archive of
 geochemical information and related metadata from USGS research (https://www.usgs.gov/energy and-minerals/mineral-resources-program/science/national-geochemical-database, last accessed: 16
- 87 July 2024).

- The British Geological Survey (BGS), which provides data and information on UK geology,
 boreholes, geomagnetism, groundwater, rocks, etc. (http://www.bgs.ac.uk/, last accessed: 16 July
 2024).
- The Australian National Whole Rock Geochemistry Database (OZCHEM), including chemical
 compositions of rock, soil, and sediment samples (https://ecat.ga.gov.au/geonetwork/srv/, last
 accessed: 16 July 2024).
- 94 <u>NOAA and MMS Marine Minerals Geochemical Database, which contains geochemical analyses</u>
 95 <u>and auxiliary information on present day marine deposits of primarily ferromanganese nodules and</u>
 96 <u>crusts, as well as some data for heavy minerals and phosphorites</u>
 97 (https://www.ncei.noaa.gov/access/metadata/landing-
- 98 page/bin/iso?id=gov.noaa.ngdc.mgg.geology:G01323, last accessed: 7 January 2025).
- 99 <u>An International Study of the Marine Biogeochemical Cycles of Trace Elements and Isotopes</u>
 100 (<u>GEOTRACES</u>), which provides hydrographical and marine geochemical data acquired over the
 101 <u>past decade (https://www.geotraces.org/, last accessed: 7 January 2025).</u>
- 102 Although some of these databases (Table 1) include data on ancient marine sediments, they have 103 shortcomings such as limited spatial coverage, the lack of age data and coarse age resolution, the absence 104 of recent publications, and missing information from original publicationsdata on ancient marine 105 sediments, they are often limited to specific countries or regions and have certain shortcomings, such as 106 the lack of age data, the absence of many recent publications, missing information from original 107 individual publications, and relatively coarse age resolutions. Thus, we propose have established the 108 Deep-Time Marine Sedimentary Element Database (DM-SED), which focuses on the elemental content 109 changes in marine sediments across geological history. The current version of the DM-SED database 110 contains 63,69163,627 entries, enabling research on a series of scientific issues related to 111 palaeoenvironmental, palaeoclimatic, and elemental cycles in deep-time Earth history.
- 112 DM-SED version 0.0.1 is presented in table (.csv) format. Dynamic versions of the most recent 113 release can be found on Zenodo (https://doi.org/10.5281/zenodo.14771859, last accessed: 30 January 114 2025) (Lai et al., 2025), and a static copy of Version 0.0.1 is archived in the Geobiology database 115 (http://202.114.198.132/dmgeo-geobiology-portal/, last accessed: 25 September 2024). In the following 116 sections, we provide a brief overview of the database, information on the data sources and selection 117 criteria, and a review of the definitions and decisions behind the metadata fields associated with each

118	proxy measurement. We explore the spatial and temporal distribution trends of the compiled data and
119	discuss future uses and limitations of the database.
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133 Table 1. Overview of different databases (Note: not all databases have a clear number of records).

Database name	Content	Website information	Number of records	Data regions
EarthChem	Igneous, sedimentary, and metamorphic rocks; various joint databases	https://www.earthchem.org/, last accessed: 16 July 2024	Over 2,596 digital content files in EarthChem Library	Global
PetDB	Elemental chemical, isotopic, and mineralogical data of global ocean floor rocks	https://www.earthchem.org/ petdb, last accessed: 16 July 2024	<mark>⊖O</mark> ver 6,000,000 samples	Global
GEOROC	Chemical, isotopic, and other data on igneous rock samples	http://georoc.mpch- mainz.gwdg.de, last access: 16 July 2024	672,990 samples	Global
PANGAEA	Georeferenced data from earth, environmental, and biodiversity sciences	https://www.pangaea.de, last accessed: 16 July 2024	Extensive dataset	Global
StabisoDB	$\delta^{18}O$ and $\delta^{13}C$ data for macrofossil and microfossil samples	https://cnidaria.nat.uni- erlangen.de/stabisodb/, last accessed: 16 July 2024	Over 67,000 samples	Global

SGP	Multi-proxy sedimentary geochemical data from the Palaeozoic and Neoproterozoic	https://sgp-search.io/, last accessed: 12 June 2024	82,578 samples	Global
NOAA and MMS Marine Minerals Geochemical Database	Geochemical analyses on ferromanganese nodules and crusts, as well as some heavy minerals and phosphorites	https://www.ncei.noaa.gov/a ccess/metadata/landing- page/bin/iso?id=gov.noaa.n gdc.mgg.geology:G01323, last accessed: 7 January 2025	Over 140,000 element/oxide analyses	Global
GEOTRACES	Hydrographical and marine geochemical data	https://www.geotraces.org/, last accessed: 7 January 2025	Data from-77 cruises and more than 800 hydrographic and geochemical parameters	Global
USGS	Geochemical information and related metadata from USGS research	https://www.usgs.gov/energ y-and-minerals/mineral- resources- program/science/national- geochemical-database, last accessed: 16 July 2024	Extensive dataset	United States
BGS	Data on UK geology, boreholes, geomagnetism, groundwater, rocks, etc.	http://www.bgs.ac.uk/, last accessed: 16 July 2024	Extensive dataset	United Kingdom
OZCHEM	Chemical compositions of rock, soil, and sediment samples	https://ecat.ga.gov.au/geonet work/srv/, last accessed: 16 July 2024	Extensive dataset	Australia
NOAA and MMS Marine Minerals Geochemical Database	Geochemical analyses on	https://www.ncei.noaa.gov/a ccess/metadata/landing- page/bin/iso?id=gov.noaa.n gdc.mgg.geology:G01323, last accessed: 7 January 2025	<u>Over 140,000</u> element/oxide analyses	<u>Global</u>
GEOTRACES	Hydrographical and marine geochemical data	https://www.geotraces.org/, last accessed: 7 January 2025	Data from 77 cruises and more than 800 hydrographic and geochemical parameters	<u>Global</u>

DM SED version 0.0.1 is presented in table (.csv) format. Dynamic versions of the most recent
 release can be found on Zenodo (https://doi.org/10.5281/zenodo.13898366, last accessed: 7 October
 2024) (Lai et al., 2024), and a static copy of Version 0.0.1 is archived in the Geobiology <u>database</u>data

(http://202.114.198.132/dmgeo geobiology portal/, last accessed: 25 September 2024). In the following
sections, we provide a brief overview of the database, information on the data sources and selection
criteria, and a review of the definitions and decisions behind the metadata fields associated with each
proxy measurement. We explore the spatial and temporal distribution trends of the compiled data and
discuss future uses and limitations of the database.

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144 2 Dataset overview

145 The DM-SED aims at collecting geochemical data from deep-time marine sediments. The database is 146 primarily sourced from based on the SGP database, supplemented with additional by 34,874 newly 147 compiled entries. The SGP contains a total of 82,578 entries, from which we selected 28,753 entries 148 specifically related to marine sedimentary geochemical data, and is comprised of three parts: two parts 149 from the U.S. Geological Survey (USGS), i.e. the National Geochemical Database (USGS NGDB, 150 https://mrdata.usgs.gov/ngdb/rock, last accessed: 9 September 2024) and the Global Geochemical 151 Database for Critical Metals in Black Shales project (USGS CMIBS, Granitto et al., 2017), with samples 152 mainly from North America and Phanerozoic shales from various continents, respectively (Farrell et al., 153 2021). The third part comprises direct inputs by SGP members. The direct inputs in the Phase 1 SGP 154 data release primarily focused on Neoproterozoic-Palaeozoic shales, although there are other lithologies 155 and other time periods represented (Farrell et al., 2021). Our DM-SED database, built upon the SGP, 156 includes a new compilation of 34,93834,874 entries from 433 studies, spanning approximately 3800 Ma 157 and including entries entries from 433 literatures, covering a time range from approximately 3800 Ma to 158 the present, and including entries from North America, Europe, Asia, Africa, South America, Oceania, 159 Pacific and Atlantic, thus This supplementings the temporal and spatial distribution gaps in the SGP 160 database, and thereby creating a more comprehensive sedimentary marine geochemical database. The 161 new compiled literatures span the time range from 1965 to 2023, with the number of papers per decade 162 gradually increasing (Fig. 1). It should be noted that the top of the DM-SED version 0.0.1 data is the new 163 compilation, and the bottom contains data imported from SGP.

164 <u>Table 2. Summary of data entries and points in the DM-SED.</u>

Entries Data points





168 Figure 1. The distribution of publication years for newly compiled literature (the dashed line denotes the

169 predicted literature from 2023 to 2030).

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171 Table 2. Summary of data entries and points in the DM-SED.

	Entries	Data points
New compilation	<u>34,938<u>34,874</u></u>	1,345,589<u>1,454,400</u>
SGP	28,753	1,066,496<u>1,067,855</u>
DM-SED	<u>63,691<u>63,627</u></u>	2,412,085 <u>2,522,255</u>

The DM-SED database comprises 63,69163,627 entries with 2,412,0852,522,255 discrete data
points (Table 2), each including location (SampleID, SampleName, SiteName, Region, Elevation,
SampleDepth, ModLat, ModLon, PalaeoLat, PalaeoLon), age (Age, Period, Stage, Biozone),
stratigraphic information (LithName, LithType, Formation, Facies), carbon element (total carbon (Total
C), inorganic carbon (C_{inorg}), TOC, fin wt%), isotopic values (δ¹⁸O_{carb}, δ¹³C_{Ker}, δ¹³C_{TOC}, δ¹³C_{carb}, δ³⁴S_{CAS},

- 177 $\delta^{34}S_{pyr}, \delta^{15}N_{total}, \delta^{15}N_{org}, in \infty)$, major element (P, Al, Si, Ti, Fe, Ca, Mg, Na, K, S, N, in wt%), trace
- 178 element (Ag, Ar, As, B, Ba, Be, Bi, Br, Cd, Ce, Co, Cr, Cs, Cu, Dy, Er, Eu, Ga, Gd, Ge, Hf, Hg, Ho, In,
- 179 La, Li, Lu, Mn, Mo, Nb, Nd, Ni, Pb, Pr, Rb, Re, Sb, Sc, Se, Sm, Sn, Sr, Ta, Tb, Te, Th, Tl, Tm, U, V,
- 180 W, Y, Yb, Zn, Zr, in ppm), methodology (TOC methods, Major elements methods, Trace elements
- 181 <u>methods</u>), and data sources (Reference, Project). The specific names and descriptions of each field in the
- database are shown in Table 3. The standards and descriptions of isotope ratios in the database are shownin Table 4.
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187 Table 3. Field names and descriptions.

Field name	Description of field (units)	
Location fields		
SampleID	Unique sample identification code	
SampleName	Author denoted title for the sample (often non-unique)	
SiteName	Name of the drill core site or section	
Region	Country or ocean of the data collection site	
Elevation	Distance between sampling location and sea level (m)	
SampleDepth	Stratigraphic height or depth (m)	
ModLat	Modern latitude of collection site rounded to two decimals; negative values indicate the Southern Hemisphere (decimal degrees)	
ModLon	Modern longitude of the collection site rounded to two decimals; negative values indicate the Western Hemisphere (decimal degrees)	
PalaeoLat	Palaeolatitude of collection site rounded to two decimals; negative values indicate the Southern Hemisphere (decimal degrees)	
PalaeoLon	Palaeolongitude of the collection site rounded to two decimals; negative values indicate the Western Hemisphere (decimal degrees)	
Age fields		
Age	Absolute Age, in reference to GTS2020 (Ma)	
Period	The geologic period	
Stage	The geologic stage (i.e. geochronologic age)	
Biozone	Conodont, graptolite, ammonite biozone, etc	
Stratigraphy		
LithName	Lithological name of the sample, as originally published	
LithType	Lithology type of sample (e.g. carbonate, siliciclastic)	
Formation	Geologic formation name	
Facies	Depositional environment (e.g. mid-shelf, ramp)	
Proxy fields		

Carbon	The content of carbon, including Total C, C _{inorg} , TOC, rounded to two decimals (wt%)
Isotopes	The isotope value, rounded to two decimals (‰)
Major elements	The content of major elements such as P, Al, and Si, rounded to two decimals (wt%)
Trace elements	The content of trace elements such as Ag, Ar, As, B, and Ba, rounded to two decimals (ppm)
<u>Methodology</u>	
TOC content methods	A brief description of the testing methods for TOC
Major elements methods	A brief description of the testing methods for major elements
Trace elements methods	A brief description of the testing methods for trace elements
Data sources	
Reference	Data sources, including published literature or other databases
Project	Two parts: new compilation and SGP

191 Table 4. Standards and descriptions of isotope ratios in the DM-SED.

Symbol	Standard	Description
$\delta^{18}O_{carb}$	Vienna Pee Dee Belemnite (VPDB)	Oxygen isotope ratio of carbonate minerals, used in palaeoclimate studies.
$\delta^{13}C_{Ker}$	VPDB	Carbon isotope ratio of kerogen, used to study the source and depositional environment of organic matter.
$\delta^{13}C_{TOC}$	VPDB	Carbon isotope ratio of total organic carbon, used to analyse the source of organic matter and biogeochemical cycles in sediments.
$\delta^{13}C_{carb}$	VPDB	Carbon isotope ratio of carbonate minerals, used in palaeoclimate and carbon cycle research.
$\delta^{34}S_{CAS}$	Vienna Canyon Diablo Troilite (VCDT)	Sulfur isotope ratio of carbonate-associated sulfate, used to study the sulfur cycle and redox conditions.
$\delta^{34} S_{pyr}$	VCDT	Sulfur isotope ratio of pyrite, typically used to investigate the sulfur cycle and redox conditions in ancient oceans.
$\delta^{15} N_{total}$	Atmospheric Nitrogen (air N ₂)	Nitrogen isotope ratio of total nitrogen, used to study the nitrogen cycle and nutrient sources.
$\delta^{15}N_{org}$	air N ₂	Nitrogen isotope ratio of organic nitrogen, often used to analyse the source of organic matter and the nitrogen cycle.

193 **3 Dataset screening and processing**

- 194 This section details the screening and processing criteria for sample location, age, lithology and facies,
- specific geochemical values, and data source information (Fig. 2).



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Figure 2. The data filtering and processing criteria for DM-SED.

198 For sample location, the datasetbase includes SampleID, SampleName, SiteName, Region, 199 Elevation, SampleDepth, ModLat, ModLon, PalaeoLat, and PalaeoLon. A unique SampleID is assigned 200 to each sample in the DM-SED. The SampleName corresponds to the identifier given in each referenced 201 publication, facilitating cross-referencing with the original data. The SiteName includes well name or 202 outcrop information, representing the smallest unit of location information. The Region indicates the 203 country or ocean area where the sample has been collected and represents a broader geographical range. 204 The Elevation data are mainly related to samples from the Deep Sea Drilling Project (DSDP) and the 205 Ocean Drilling Program (ODP) collected from post-Cretaceous sediments and indicate whether the 206 samples originate from deep or shallow marine environments. SampleDepth refers to the relative position 207 (in metres) of the sample within the well or outcrop, which is crucial for calculating sample age. In some publications, specific heights are not provided directly but are given as relative heights through figures. 208 209 We manually extracted these heights using WebPlotDigitizer, rounding to two decimal places (Drevon 210 et al., 2017). For publications in which heights are expressed in feet or centimetres, we converted the 211 units to metres. Modern latitude and longitude (ModLat and ModLon) information are the most precise location data. Although some publications provide exact coordinates, many offer only section names (i.e. 212 213 SiteName) and regions or merely a map marking the location of the section. For publications providing

214 section names, we determined accurate coordinates by consulting other studies carried out in the same 215 section. For those providing only a map marking the location of the section, we used Google Maps to 216 estimate relative coordinates. To ensure consistency, we recorded sample coordinates in decimal degrees, 217 rounded to two decimal places, with positive values indicating north latitude and east longitude and 218 negative values indicating south latitude and west longitude. And-Tthe coordinate reference system is 219 WGS 84 (World Geodetic System 1984). For palaeo-coordinates, we reconstructed palaeo-latitude and 220 palaeo-longitude (PalaeoLat, and PalaeoLon) using the sample age and modern coordinates, employing 221 the PointTracker v7 rotation files from the PALEOMAP project, which are based on current geographic 222 reference data and global tectonic history models (Scotese, 2008). It is important to note that we only 223 generated palaeogeographic locations for samples from the Phanerozoic, as the geological records from 224 this time are more complete and abundant compared to those from the Precambrian, making the 225 reconstruction of geographic features (such as ancient oceans, mountains, plains, etc.) relatively more 226 reliable and accurate (Scotese and Wright 2018). We plotted the sample points on palaeogeographic maps 227 based on Scotese's data using QGIS 3.16 (Scotese and Wright 2018).

228 To assign specific ages to each sample in the database, we assumed a constant sedimentation 229 rate within the same formation or group of section. If the original studies provided numerical ages for 230 two or more samples, we calculated the precise age for each sample based on the sedimentation rate and 231 assigned it accordingly. If absolute ages were not provided in the original literature, we assigned 232 approximate ages based on corresponding fossil zones or the general age of the same lithostratigraphic 233 unit in the same region (Farrell et al., 2021; Judd et al., 2022). For samples with completely missing 234 height information in the original text, we assigned the same age to all samples within the section based 235 on lithostratigraphic information. However, the primary age constraints for these samples (mainly from 236 USGS NGDB and USGS CMIBS) remain derived from SGP age calls.For samples with completely 237 missing height information in the original text, we assigned the same age to all samples within the section 238 based on lithostratigraphic information (mainly samples from USGS NGDB and USGS CMIBS). Once 239 each sample had a specific age, we assigned it to a specific Period and Stage according to its age. We 240 attempted to incorporate the most recent age models; however, due to the extensive size of the data 241 compilation, it was not feasible to update all of them. All ages were based on the timescale provided by 242 the Geologic Time Scale 2020 (Gradstein et al., 2020). Although GTS 2020 is accurate, readers are 243 advised to consult the incremental updates of the International Chronostratigraphic Chart (ICS) for the

most accurate stratigraphic intervals

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246 For lithology and facies, the lithologies include shale, mudstone, sandstone, limestone, 247 dolostonedolomite, and others. We classified these into two-major types of rocks: siliciclastic 248 sedimentary rocks (88.7%) and carbonate rocks (11.3%). For outcrop sections, the lithostratigraphic unit 249 was generally available; however, for data from marine drilling sitesfor marine drilling data, there was 250 oftenwere no corresponding lithostratigraphic unit informationgroup names. Regarding facies 251 classification, before the Cretaceous, the primary depositional environment was marine settings on 252 continental crust, including specific facies such as tidal flats, inner shelves, outer shelves, and basinal. 253 However, after the Cretaceous, with most samples coming from DSDP and ODP, deep ocean 254 depositional environments emerged. However, after the Cretaceous, with most samples coming from the 255 DSDP and ODP, shallow marine depositional environments still existed and were sampled, but deep-sea pelagic settings began to be sampled as well-emerge. 256

- For specific geochemical values in the DM-SED database, we standardized the units, converting oxides to elements (e.g. P (ppm) to P (wt%), P_2O_5 (wt%) to P (wt%)). If a sample was analysed multiple times, we averaged the value. For literature before 2000, some data were preserved as images, requiring manual extraction of values, and some images were slightly blurry, potentially leading to minor human error. We excluded data that were beyond detection limits (e.g. the trace element content is too low and the value provided in the text represents the minimum detection limit) or unreasonable (e.g. negative values for major and trace elements).
- 264 For the testing methods of the datageochemical methodology, we briefly documented them based
 265 on the descriptions in the original text, focusing primarily on the testing methods and instrument models
 266 used for TOC, major elements, and trace elements. Methods for stable iI sotopes were not documented,
 267 as the testing methods vary for different isotopes, and due to the limited amount of isotope data, recording
 268 them holds little significance.

Regarding data sources, we ensured that each corresponding reference was collected and listed in full citation format, including authors, title, publication date, journal, page numbers, and DOI. Most data in the SGP database came directly from USGS NGDB and USGS CMIBS, without corresponding literature sources, so we marked them individually. The entire database for this Project was divided into two parts: new compilation and SGPAnd the project includes two parts: new compilation and SGP. We used keyword searches in Google Scholar to identify missing references and made efforts to target
literature for data-scarce regions (e.g. South America) and time intervals (e.g. Silurian, Jurassic).

276 4 Data distribution

277 The elemental data content distribution for the entire database is shown in Fig. 3. Overall, major elements 278 have the highest data quantity, followed by trace elements and carbon elements, with isotope data having 279 the lowest quantity. Among the major elements, N has the fewest entries, with 3,164 records, whereas 280 the other major elements all have more than 10,000 entries. All has the highest quantity, with 501,568906281 records. Among trace elements, Mn has the largest record (412,058499 records), followed by Ba 282 (401,1634701 records). Ar and Br have the fewest records, with 9 and 16276 records, respectively. Other 283 elements such as Ag, B, Bi, Ge, Hg, Ho, In, Pr, Re, Sb, Se, Sn, Ta, Te, Tl, Tm, and W have data quantities 284 ranging from 1,000 to 10,000. Elements such as As, Be, Cd, Ce, Co, Cr, Cs, Cu, Dy, Er, Eu, Ga, Gd, Hf, 285 Ho, La, Li, Lu, Mo, Nb, Nd, Ni, Pb, Pr, Rb, Sb, Sc, Sm, Sr, Ta, Tb, Th, U, V, Y, Yb, Zn, and Zr all have 286 more than 10,000 records each. For carbon elements, TOC has the largest record (32,9046 entries), 287 followed by Total C (9,386 entries), while C_{inorg} has the lowest record (7,215 entries) For carbon elements, 288 TOC has the most records, with 33,216 entries, followed by Total C with 9,201 entries. Cinorg has the 289 fewest records, with 7,194 entries. Isotope data are overall less abundant, with none exceeding 10,000 290 entries; the most abundant is $\delta^{13}C_{TOC}$, with 8,166 records, and the least abundant is $\delta^{13}C_{Ker}$, with only 291 <u>112</u>29 records.

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Figure 3. Histogram distribution of different subsets. (a) Trace elements. (b) Major elements. (ea) Carbon
elements. (d) Isotopes. (c) Major elements. (d) Trace elements.

The temporal trend of data density in the entire database, shown in Fig. 4a, indicates that the data are primarily distributed in the Phanerozoic Eon, which accounts for 85% of the entire database. Within the Phanerozoic From this, the Cenozoic Era accounts for 19% of the database, the Mesozoic Era accounts for 21%, and the Palaeozoic Era accounts for 45%. Precambrian data account for only 15% of the entire database. The SGP data are most concentrated in the Palaeozoic Era, in which they make up 27% of the total database, with the new compiled data contributing only 18%. In other eras, the new compiled data outnumber the SGP data: 4% versus 15% in the Cenozoic, 7% versus 14% in the Mesozoic, and 7%

versus 8% in the Precambrian. This is mainly the case because the SGP data in the first phase wereprimarily from the Neoproterozoic and Palaeozoic eras (Farrell et al., 2021).

(a) Number of entries (by period) New compilation SGP Ors Stt СІ Ec Stn Tn Cry Ed Age (Ma) (b) Number of entries (by stage) S Ν 300 250 Age (Ma)



Figure 4. The age distribution of samples in the database. (a) Age distribution of samples (excluding a small number of samples with ages >2500 Ma from the figure, a total of 12958 samples). (b) Age distribution of
Phanerozoic samples at the stage level. Sd, Siderian; R, Rhyacian; Sd, Siderian; Ors, Orosirian; Stt,
Statherian; Cl, Calymmian; Ec, Ectasian; Stn, Stenian; Tn, Tonian; Cry, Cryogenian; Ed, Ediacaran; Cm,
Cambrian; O, Ordovician; S, Silurian; D, Devonian; C, Carboniferous; P, Permian; T, Triassic; J, Jurassic;
K, Cretaceous; Pg, Paleogene; N, Neogene; O, Quaternary.

317 For the distribution of sample ages within the Phanerozoic, we divided the samples by stage, as 318 shown in Fig. 4b. For the Quaternary Period, due to its short duration, data were not subdivided by Stage, 319 but only into Holocene and Pleistocene.the data were not subdivided by Stage but were instead divided 320 into the Holocene and Pleistocene Series. Data distribution is not uniform, with the highest concentration 321 in the Quaternary Period. These data mainly come from DSDP and ODP, which are characterised by a 322 high number of core samples and high resolution. There are fewer data for the Upper Permian, Lower 323 Triassic, and Lower to Middle Jurassic, possibly because of the existence of Pangaea at that time, which 324 reduced the area of continental margins and inhibited marine transgressions, resulting in fewer preserved 325 marine environments in comparison to those of other geological periods (Mackenzie and Pigott, 1981; 326 Walker et al., 2002). The distribution of sample quantities in other periods fluctuates, often corresponding 327 to periods of significant research interest, such as the end-Ordovician, end-Devonian, end-Permian, Early 328 Jurassic Toarcian and Early Cretaceous Albian, which had peaks in sample numbers due to their 329 association with major mass extinction events and oceanic anoxic events (Fan et al., 2020).





331 Figure 5. Bubble chart of modern geographical distribution and sample quantities in the database.

In terms of spatial trends, the spatial distribution of sampling points in the DM-SED database is inherently uneven, both in modern and palaeogeographic locations. Modern locations are primarily concentrated in North America, Europe, South Africa, and China (Fig. 5). When modern coordinates are converted to palaeogeographic coordinates and projected onto palaeogeographic maps, Cambrian to Jurassic data come predominantly from continental margin environments, as oceanic crust plates subductingsubduction of oceanic crust before the Cretaceous resulted inled to preservation of very few deep-sea environments (Fig. 6). Cambrian and Ordovician data are distributed mainly on the Laurentia, Baltica, and South China plates, with a few along the Gondwana margin. Silurian data occur mainly on
Laurentia, South China, and <u>eastern Gondwanaright side of Gondwana</u>. Devonian and Carboniferous
data are primarily on the Laurussia plate, with sparse distribution in South China and Gondwana. Permian
and Triassic data are mainly on the Laurussia and South China plates, with sparse distribution in
Gondwana. Jurassic data are primarily on the North American, European-shelf, with sparse distribution
on other plates. From the Cretaceous to the Quaternary, sample locations, dominated by data from the
DSDP, ODP, and USGS NGDB projects, are mainly <u>located</u> in the deep oceans and North America.



346

347 Figure 6. The palaeogeographic distribution of sample sites in the DM-SED.

When averaging all Phanerozoic data by stage and spatially averaging them into 15° palaeolatitude bins (Fig. 7), Palaeozoic data records are mainly biased toward tropical regions. Cambrian data are concentrated between 15° S and 30° N, Ordovician to Carboniferous data are concentrated between 45° S and 15° N, and Permian data are concentrated between 0° N and 30° N, with data mainly fluctuating around the equator. As continents migrated northward through the Mesozoic and into the Cenozoic, records began to show bias toward mid-latitudes in the Northern Hemisphere. From the Triassic to the Cretaceous, data are mainly concentrated between 0° N and 60° N. <u>And-Paleogene to Quaternary data</u>

are concentrated between 45° S and 45° N.



Figure 7. The spatiotemporal distributions of sample quantities (categorized temporally by stage and spatially
by palaeolatitude intervals of 15°).

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360 5 Usage instructions

The ultimate goal of the DM-SED database is to provide the geoscience community with a valuable resource of knowledge and geographic information. By deriving meaningful conclusions from a large marine sediment geochemistry datasetbase, we aim to enhance our understanding of Earth's environmental changes over time and space. All entries in DM-SED contain the source of original proxy values, ensuring traceability between DM-SED and the original datasets from which the data were extracted.

However, our database has some limitations. The criteria for age determination, relying variously
on fossil zones and lithostratigraphic unit information, are not entirely uniform. Some age determinations
are still coarse, with samples from a single section <u>allwere</u> assigned the same age. Additionally, the data
quantity for some elements is still low. The testing methods for elements are not annotated, and there
may be significant differences in methodological precision between older and newer literature. Currently,

these issues remain largely unresolved. Despite our best efforts to identify data from the literature and process quality control for each entry, the sheer volume of data in DM-SED means that some errors or omissions are inevitable. Prompt corrections and continuous updates are expected to ensure the credibility of this datasetbase.

Finally, it is important to recognize that DM-SED merely compiles these various datasets and cannot impose any requirements on their generation. When using the data (and where practicable), we recommend citing both DM-SED and the original data sources to ensure proper attribution.

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380 6 Data availability

381 Version controlled releases of the DM-SED can be found on Zenodo 382 (https://doi.org/10.5281/zenodo.13898366https://doi.org/10.5281/zenodo.14771859, last accessed: 30 383 January 2025last accessed: 7-October 2024) (Lai et al., 2024Lai et al., 2025). A static copy of DM-SED 384 version 0.0.1 is archived in the Geobiology databasedata (http://202.114.198.132/dmgeo-geobiology-385 portal/, last accessed: 25 September 2024). We plan to supplement and improve the datasetbase 386 continuously and hope to collaborate with existing compilation authors to assist in adding new content. 387

388 7 Code availability

The software tools used in this study are available at the following links: WebPlotDigitizer can be downloaded from https://github.com/automeris-io/WebPlotDigitizer/releases (last accessed: 20 July 2024); the PointTracker v7 tool can be found at http://www.paleogis.com (last accessed: 20 July 2024); QGIS 3.16 can be downloaded from the https://qgis.org/project/overview/ (last accessed: 20 July 2024).

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