1	Ordovician to Silurian graptolite specimen images for global
2	correlation and shale gas exploration
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16	Abstract
17	Multi- elemental and -dimensional data are more and more important
18	induring the development of data-driven research, as is the case in modern
19	palaeontology, in which visual examination, by experts or someday the artificial
20	intelligence, to every fossil specimen acts a crucial and fundamental role. We
21	here release an integrated image dataset of 113 Ordovician to Silurian
22	graptolite species or subspecies that are significant in global stratigraphy and
23	shale gas exploration. The dataset contains <u>2 951</u> 1550 high-resolution
24	graptolite specimen images and their related scientific information related to
25	the specimen, e.g., every specimen's taxonomic, geologic, and geographic_
26	information, and related references. We develop a tool, FSIDvis (Fossil
27	Specimen Image Dataset Visualiser), to facilitate the human-interactive
28	exploration of the rich-attribution image dataset. We employ aA nonlinear
29	dimension reduction technique, t-SNE (t-Distributed Stochastic Neighbor
30	Embedding), is employed to project the images into the two-dimensional space
31	to visuali <u>z</u> se and explore the similarities. Our dataset potentially contributes to
32	the analysis of the global bio <u>-</u> stratigraphic correlations and improves the shale
33	gas exploration efficiency by developing an image-based automated
34	classification model. All images are available from
35	https://doi.org/10.5281/zenodo.61949435205216 (Xu, 20221).
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38 **1. Background**

39 Graptolite iswas a marine colonial organic-walled hemichordate and hads over 210 genera/3,000 species worldwide fossil records, extending from the 40 Cambrian to the Carboniferous (c. 510~320 Ma) shale sediments (Maletz, 41 42 2017). Graptolite extensively diversified in the Ordovician and witnessed the second-largest mass extinction in geological life history, i.e., the 43 end-Ordovician mass extinction (Goldman et al., 2020). Graptolite evolved 44 quickly and spread globally in the Paleozoic (Fig. 1); therefore, its species are 45 widely used as significant index fossils for determining rock ages and regional 46 47 bio-stratigraphical correlations. Graptolite Bbio-zones based on graptolite species divided the Ordovician and Silurian sediments and are generally less 48 than one million years in duration; such a short geological moment makes it 49 possible for a better and preciseaccurate understanding of the stratigraphy 50 and ancient life macro-evolution in geological history (Chen et al., 2012; 2018). 51 Up to 102 Ordovician and Silurian graptolite species were selected as global 52 53 bio-zones for dating rocks, biostratigraphy, regional correlation, and understanding the evolutionary patterns of paleobiologyancient life; and 13 54 global stratotype section and point (GSSP) have been defined by the first 55 56 appearance datum (FAD) of graptolite species from in the Lower Paleozoic, i.e., 57 Cambrian, Ordovician, and Silurian systems (Goldman et al., 2020). Two of 58 these GSSPs are situated in southern China, (i.e., the bases of the Darriwilian) Stage of in the Middle Ordovician and the Hirnantian Stage of in the UpperLate 59 Ordovician) (Goldman et al., 2020; Zhang et al., 2020) (Fig. 2). 60 61 Additionally, bio-zones or indication zones based on graptolite species

assist with identifying mining beds for shale gas exploration (Fig. 1). Graptolite

63 shale comprises more than 9% of hydrocarbons rocks and yields the <u>a most</u>

significant volume of shale gas globally (Klemme and Ulmishek, 1991;

65 Podhalańska, 2013). In China, over 61.4% of the natural gas is yielded from

the Ordovician and Silurian graptolite shale of southern China (Zou et al.,

⁶⁷ 2019). Identification of graptolite species helps to locate shale ga<u>s</u>le mining

⁶⁸ beds; especially, 16 graptolite species were chosen as "gold <u>calliperscaliper</u>"

69 to locate favourable exploration beds (FEB) of shale gas fromin China (Zou et

70 al., 2015) (Fig. 2).

71 In this paper, we release a unique graptolite specimen image dataset, 72 which consists of 113 key graptolite species used for dating rocks, global 73 correlation, and "gold caliper" for locating shale gas FEBs fromin China. All images were taken from 1,550 carefully curated graptolite specimens collected 74 from the Ordovician to Silurian sediments of China. We incorporated revision 75 76 suggestions from distinguished palaeontologists to generate the ground-truth 77 labels, providing a taxonomical authority of the dataset. The dataset potentially contributes to a range of scientific activities and provides 1) an easy access to 78 high-resolution images of 1,550 specimens of 113 graptolite species for 79 80 teaching and training in palaeontology and geologic survey; 2) global 81 bio-stratigraphical correlation using graptolites, especially with those bio-zone species; 3) a standard fossil specimen image dataset used in shale gas 82 83 industry to improve exploration efficiency, and 4) athe potential aid of 84 developing image-based automated classification model.

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2. Materials and methods

87 Images of our dataset were taken from 1,550 graptolite specimens, which taxonomically belong to 113 graptolite species or subspecies. These 88 89 specimens are preserved as shale and were collected from 154 representative 90 geological sections of China. All specimens are housed at the Nanjing Institute 91 of Geology and Palaeontology (NIGP), Chinese Academy of Sciences (CAS) 92 the world's largest palaeontological research centre, and one of the top threespecimen collection centres. The NIGP-CAS hosts over 180 palaeontological 93 researchers and laboratory technicians and collecting over 800,000 pieces of 94 95 fossil specimens from all around the world since 1928 (NIGP, 2011).

Every piece of the specimen is tagged with scientific information, including 96 97 scientific names (genus and species names), nominator, nomination year, 98 specimens' serial number, collection -number, locality (province, city, county), 99 geological horizon and section, collector name, collecting time, identifier, 100 identifying time, related references, and published illustrations. Specimens can be indexed and located in their detailed housing drawers and cabinets using 101 102 any of the above information. Their detailed research-related information can also be obtained from the geological section-based database, the 103 104 Geobiodiversity Database (Xu et al., 2020) and forms key elements of fossil specimen metadata (Xu et al., in press). All this related information is collected 105

and recorded in a separate spreadsheet file released with our image dataset. 106 107 We spent over two years to complete photographing every specimen using a single-lens reflex camera Nikon D800E with Nikkor 60 mm macro-lens and 108 Leica M125 and M205C microscopes equipped with Leica cameras (Fig. 3). 109 Every image is well focused and better shows the morphology of graptolite 110 111 bodies. In total, we took 40,597 images, including 20,644 camera photos (each with a resolution of $4,912 \times 7,360$) and 19,953 microscope photos (each with a 112 resolution of 2,720 × 2,048). Photos of low contrast or bad focus were 113 removed from the whole collection. We only kept and selected the photos that 114 show the visual morphology of every specimen and the diagnostic character of 115 116 each graptolite species that the specimens represent (Fig. 4). We selected one or two images for each specimen as the present final dataset, uploaded to, and 117 stored in our cloud server (Fig. 3). Every specimen has at least one original 118 photo, and another image shows specimen with a scale bar. Occasionally in 119 some cases of large image, the scale bar is embedded, just beside the fossil 120 itself. 121

Considering some of the specimens of our collection have a long research history since 1958, and their taxonomical status might change in the new light of graptolite systematic study (Maletz, 2017; Zhang et al., 2020), we invited graptolite palaeontologists to curate every specimen to make sure that its scientific information is updated and widely accepted. The emendation results are showed in the spreadsheet file of our dataset.

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129 **3. Data description**

Our dataset consists of 2,9511,550 high-resolution images and a related 130 131 spreadsheet file. Every image is a high-resolution photo taken from the collection of 1550 graptolite specimens. These specimens were formally 132 published in 1958-2020, and taxonomically belonging to 113 graptolite species 133 or subspecies, of 41 genera and 16 families of the Order Graptoloidea (see the 134 uploaded spreadsheet file, Fig 5). The geological age of these graptolite 135 species ranges from the Middle Ordovician to (467.3 Ma) to the Telychian 136 (433.4 Ma) of the Silurian Pperiod (Fig. 5). 137 These graptolite species have relatively abundant fossil records and are 138

significant in regional and global bio-stratigraphical correlations<u>- and locating</u>
 favourable exploration bed (FEB) of shale gas in China. They are commonly

141 used in geological age determination and shale gas favourable exploration bed 142 (FEB)FEB indication, including 32 graptolite bio_zones from the Darriwilian <u>S</u>stage of the Ordovician <u>Period</u> (467.3 Ma) to the Telychian <u>S</u>stage of the 143 Silurian Period (433.4 Ma) and 16 "gold callipers" of shale gas favourable 144 exploration beds (FEBs) for the cases of 20 m to 80 m thick graptolite shale in 145 146 China (Fig. 6). These species also include two "golden spike" graptolite 147 species for the two GSSPs in southern China (i.e., bases of the Darriwilian Stage in the Middle Ordovician System and the Hirnantian Stage in the Upper-148 149 Late Ordovician System).

The name of the individual image file is initialled by the specimens' unique
number and then its taxonomical species name. The image file is in JPG
format. <u>T</u>, and the single JPG file size ranges from 82240 KB to 7.05510.59 MB.
The whole volume of the dataset is 10.46.41 GB.

In the spreadsheet file, we incorporated revision suggestions of several 154 distinguished palaeontologists for the authority of the graptolite taxonomy. The 155 spreadsheet file shows the detailed scientific information of every graptolite 156 157 specimen. The spreadsheet file includes following fields: species ID, Phylum, Class, Order, Suborder, Infraorder, Family, Subfamily, Genus, Revised species 158 name, tagged species name, total number of specimens, specimens 159 160 number, image file name, microscope photo numbers, SLR photo number, 161 Stage, Age from, Age to, mean age value, Locality, Longitude, Latitude, 162 hHorizon, and specimens firstly published reference.

163 164

4. Data visualization

We have developed an interactive web exploration tool, FSIDvis (Fossil Specimen Image Dataset Visualizer), to assist users to examine better the scientific contents of our data (Fig. 7).

We further explore the distribution of these graptolite images and visualize 168 169 the t-SNE feature embedding of our graptolite dataset (Fig. 8) using different colors to denote different families. In detail, for each annotated image, we first 170 resized it into 448×448 pixels and fed it into the trained CNN model. The output 171 172 1×1×2048 feature map from the last average pooling layer is flattened and projected to a 113 (number of species) dimensional fully connected layer to 173 represent an image embedding. After that, we use t-SNE (t-Distributed 174 175 Stochastic Neighbor Embedding), a nonlinear dimension reduction technique

for high-dimensional data, to project the image embeddings into the two-dimensional space for visualization. Finally, we indicate the image data distribution by a scatter plot, we use 15 colors to represent 15 families of the order Graptoloidea, covering 42 genera and 113 species, so the distribution of the images in this figure is based on species, which shows a "big mixed, small."

the images in this figure is based on species, which shows a "big mixed, small
 settlements" posture.

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5. Conclusions

A graptolite specimen image dataset containing <u>2,951</u>1550 high-resolution images is released. The formation of our dataset includes two steps. 1) 113 Ordovician to Silurian graptolite species or subspecies are selected for their significances in global <u>stratcorrelation</u>igraphy and shale gas exploration; 2) 1550 pieces of fossil specimens that typically represent these 113 species are carefully curated and photographed.

Scientific information related to these graptolite specimens is also included
 and recorded for further study. The structured records include taxonomical,
 geologic, geographic, and related references of every specimen.

Our dataset potentially contributes to global bio-stratigraphical correlation, especially with those <u>bio-zone</u> graptolite-<u>bio-zone</u> species, in the shale gas industry to improve exploration efficiency and develop an image-based automated classification model.

The whole dataset has visualized the tool FSIDvis (Fossil Specimen
Image Data Visualizer). A nonlinear dimension reduction technique, t-SNE
(t-Distributed Stochastic Neighbor Embedding), is used to our data and project
the image embeddings into the two-dimensional space for visualisation.

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Data availability. The dataset is archived and publicly available from
 https://doi.org/10.5281/zenodo.5205216. Visualized version is available at
 https://fossil-ontology.com/FSIDvis/graptolite/.

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Author contributions. H.-H.X. and Z.-B.N. equally designed the project, developed the model, and performed the simulations. H.-H.X. prepared the manuscript with contributions from Z.-B.N. Y.-S.C. gave technician supports. X.M. revised and curated fossil specimens. Others contributed in specimen photography.

- 211
- 212 **Competing interests.** The authors declare that they have no conflict of
- 213 214
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interest.

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264	C) Main shale gas production region
265	Figure 1. Global distribution of graptolite shales and shale gas production
266	region. Most graptolites were yielded from the shale and their distribution is
267	based on graptolite fossil occurrence records in global Ordovician and Silurian
268	sediments. All data are from Peters and McClennen (2016) and Xu et al.
269	(2020). Graptolite shale comprises over 9% of hydrocarbons rocks in the world
270	and yields the largest volume of shale gas in the world. In China, over 61.4%
271	natural gas was yielded from the Ordovician and Silurian graptolite shales of
272	southern China. The map is from ${ m \textcircled{C}}$ OpenStreetMap contributors 2021.
273	Distributed under the Open Data Commons Open Database License (ODbL)
274	v1.0.
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Figure 2. Geological significance and application of graptolites. Our dataset of 278 graptolites is significant to biostratigraphy and the dating of the Ordovician and 279 Silurian sediments. They are widely distributed around the world and useful for 280 regional correlation. These graptolites have also witnessed several 281 macro-evolutional events, including the great Ordovician biodiversity event, 282 Late Ordovician mass extinction, radiation in several graptolite groups, and 283 global stratotype section and point (GSSP), based on graptolite species. To 284 date, 13 GSSPs have been defined by the FAD of graptolites in the early 285 Paleozoic. Two are in South China (i.e., the bases of the Darriwilian in the 286 Middle Ordovician and Hirnantian in the Late Ordovician) (the spike marks in 287 the figure) (data from Goldman et al., 2020). Bio- or indication zones based on 288 289 graptolite species assist with identifying mining beds for shale gas exploration in southern China. 16 graptolite indicator-zones are used in the shale gas 290 exploration in China (Zou et al., 2015). 291



Figure 3. The process of creating the graptolite specimen image dataset.

295 The graptolite specimens were carefully curated and revised to select the

species with biostratigraphy and application significance. Every image was

297 obtained from specimens that were macro-photographed using a single-lens

reflex camera and microscope. After professional revision and cleaning, the

- 299 whole dataset was uploaded to and stored in our cloud server.
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Figure 4. Typical images of our dataset. Every image was taken from a unique graptolite specimen. Photos of low contrast or bad focus were removed. Our dataset only selected the photos that well show visual morphology of every specimen and diagnostic character of each graptolite species that the specimens represent. The scientific species name of every specimen is given on each image.



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Figure 5. Geographic distribution (A) and geologic range (B) of graptolite 311 species of our dataset. Each graptolite specimen locality is represented by a 312 pie chart where each colour is encoded as one graptolite family of the Order 313 Graptoloidea. The sector size is proportional to the specimen number for every 314 315 family. The radius of the pie chart is proportional to the total number of specimens from the same locality. The dashed-lines circle the main areas of 316 shale gas production. The map is from © OpenStreetMap contributors 2021. 317 Distributed under the Open Data Commons Open Database License (ODbL) 318 v1.0. 319 320

System	Series	Stage	Graptolite biozone (22)
	Wenlock	Homerian	Colonograptus deubeli
			Colonograptus praedeubeli
		Sheinwoodian	
	Llandovery	Telychian	Spirograptus turriculatus
Silurian		Aeronian	Lituigraptus convolutus
Silunan			Demirastrites triangulatus
		Rhuddanian	Coronograptus cyphus
			Cystograptus vesiculosus
			Parakidograptus acuminatus
			Akidograptus ascensus
	Upper	Hirnantian	Metabolograptus persculptus
			Metabolograptus extraordinarius
		Katian	Paraorthograptus pacificus
			Dicellograptus complexus
			Dicellograptus ornatus
			Dicellograptus complanatus
Ordovician		Sandbian	Orthograptus calcaratus
	Middle	Darriwilian	Hustedograptus teretiusculus
			Archiclimacograptus riddellensis
			Pterograptus elegans
			Nicholsonograptus fasciculatus
			Levisograptus dentatus
		Dapingian	Levisograptus austrodentatus

Stage	Graptolite indicator zone for shale gas FEB (16)
Telychian	Spirograptus turriculatus (N2)
reiychian	Spirograptus guerichi (N1)
	Stimulograptus sedgwickii (LM8)
Aeronian	Lituigraptus convolutus (LM7)
	Demirastrites triangulatus (LM6)
	Coronograptus cyphus (LM5)
	Cystograptus vesiculosus (LM4)
Rhuddanian	Parakidograptus acuminatus (LM3)
	Akidograptus ascensus (LM2)
	Metabolograptus persculptus (LM1)
Hirnatian	Metabolograptus extraordinarius (WF4)
	Dicellograptus mirus (WF3c)
	Tangyagraptus typicus (WF3b)
Katian	Paraorthograptus pacificus (WF3a)
	Dicellograptus complexus (WF2)
	Dicellograptus complanatus (WF1)

323 **Figure 6.** Graptolite species selected as global biozone (left) and indicator

324 zone (right) for shale gas favourable exploration beds of our dataset. Among

325 our dataset of 113 graptolite species, there are 22 graptolite index species

from global correlation from the Middle Ordovician to (470.0 Ma) to the

327 Wenlock of the Silurian Period (427.4 Ma), and 16 graptolite species as 'gold

328 callipers' to locate favourable exploration beds (FEBs) of shale gas in China.

Note that some graptolite species are duplicate in the two lists.



333	Figure 7. FSIDvis (Fossil Specimen Image Dataset Visualizer) system
334	interface. a) Fossil <u>on geographic distribution</u> -map view <u>, showing fossil</u>
335	specimen location on the map. The lens (a.1), is a tailor-designed specimens'
336	picker that facilitates users to collect interest fossils of a region where the inner
337	ring and outer ring represent the family and genus. When the user chooses a
338	genus, the corresponding detailed species with images will be listed in the
339	fossil list a.2 view (a.2), where the detailed information and further
340	high-resolusion image if the specimens are given. Hit the space bar for locking
341	the selection. b) <u>Geological age scale</u> Time view, providing the <u>geologic</u>
342	agetime selection ability; the top one is the chronostratigraphic agetime scale,
343	and the bottom one is a <u>n agetime</u> slider that facilitates the users to choose a
344	specific agetime slot interactively. The web exploration tool of graptolite is
345	provided at https://fossil-ontology.com/FSIDvis/graptolite/. The map is from ©
346	OpenStreetMap contributors 2021. Distributed under the Open Data
347	Commons Open Database License (ODbL) v1.0.
348	



- 350 **Figure 8.** t-SNE embedding visualization of our <u>graptolite specimen</u> image
- 351 dataset. Individual specimens are denoted by different colors and grouped in
- 352 the visualization. These groups also taxonomically match different graptolite
- 353 <u>families (blocks with several small images).</u>