1 2	Ordovician to Silurian graptolite specimen images for global correlation and shale gas exploration
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17	Abstract
18	Multi- elemental and -dimensional data are more and more important in the
19	development of data-driven research, as is the case in modern paleontology, in
20	which visual examination, by experts or someday the artificial intelligence, to
21	every fossil specimen acts a fundamental role. We here release an integrated
22	image dataset of 113 Ordovician to Silurian graptolite species or subspecies
23	that are significant in global stratigraphy and shale gas exploration. The
24	dataset contains 2 951 high-resolution graptolite specimen images and their
25	related scientific information, e.g., every specimen's taxonomic, geologic, and
26	geographic information and related references. We develop a tool, FSIDvis
27	(Fossil Specimen Image Dataset Visualiser), to facilitate the human-interactive
28	exploration of the rich-attribution image dataset. We employ a nonlinear
29	dimension reduction technique, t-SNE (t-Distributed Stochastic Neighbor
30	Embedding), to project the images into the two-dimensional space to visualize
31	and explore the similarities. Our dataset potentially contributes to the analysis
32	of the global bio-stratigraphic correlations and improves the shale gas
33	exploration efficiency by developing an image-based automated classification
34	model. All images are available from <u>https://doi.org/10.5281/zenodo.6194943</u>
35	<u>(Xu, 2022)</u> .

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#### 37 **1. Background**

Graptolite was a marine colonial organic-walled hemichordate and had 38 over 210 genera/3,000 species worldwide fossil records from the Cambrian to 39 the Carboniferous (c. 510~320 Ma) shale sediments (Maletz, 2017). Graptolite 40 41 extensively diversified in the Ordovician and witnessed the second-largest mass extinction in geological life history, i.e., the end-Ordovician mass 42 extinction (Goldman et al., 2020). Graptolite evolved quickly and spread 43 globally in the Paleozoic (Fig. 1); therefore, its species are widely used as 44 significant index fossils for determining rock ages and regional 45 46 bio-stratigraphical correlations. Bio-zones based on graptolite species divide the Ordovician and Silurian sediments and are generally less than one million 47 years in duration; such a short geological moment makes it possible for a 48 49 precise understanding of the life evolution in geological history (Chen et al., 2012; 2018). Up to 102 Ordovician and Silurian graptolite species were 50 selected as global bio-zones for dating rocks, biostratigraphy, regional 51 52 correlation, and understanding the evolutionary pattern of paleobiology; and 13 global stratotype section and point (GSSP) have been defined by the first 53 appearance datum (FAD) of graptolite species from the Cambrian, Ordovician, 54 55 and Silurian systems (Goldman et al., 2020). Two of these GSSPs are situated 56 in southern China, i.e., the bases of the Darriwilian Stage of the Middle 57 Ordovician and the Hirnantian Stage of the Upper Ordovician) (Goldman et al., 2020; Zhang et al., 2020) (Fig. 2). 58

59 Additionally, bio-zones or indication zones based on graptolite species assist with identifying mining beds for shale gas exploration (Fig. 1). Graptolite 60 shale comprises more than 9% hydrocarbons rocks and yields a significant 61 62 volume of shale gas globally (Klemme and Ulmishek, 1991; Podhalańska, 63 2013). In China, over 61.4% natural gas is yielded from the Ordovician and Silurian graptolite shale of southern China (Zou et al., 2019). Identification of 64 graptolite species helps to locate shale gas mining beds; especially, 16 65 graptolite species were chosen as "gold callipers" to locate favourable 66 exploration beds (FEB) of shale gas from China (Zou et al., 2015) (Fig. 2). 67 68 In this paper, we release a unique graptolite specimen image dataset, which consists of 113 key graptolite species used for dating rocks, global 69 correlation, and "gold caliper" for locating shale gas FEBs from China. All 70

71 images were taken from 1,550 carefully curated graptolite specimens collected 72 from the Ordovician to Silurian sediments of China. We incorporated revision suggestions from distinguished paleontologists to generate the ground-truth 73 labels, providing a taxonomical authority of the dataset. The dataset potentially 74 contributes to a range of scientific activities and provides 1) an easy access to 75 76 high-resolution images of 1,550 specimens of 113 graptolite species for teaching and training in paleontology and geologic survey; 2) global 77 78 bio-stratigraphical correlation using graptolites, especially with those bio-zone 79 species; 3) a standard fossil specimen image dataset used in shale gas industry to improve exploration efficiency, and 4) a potential aid of developing 80 81 image-based automated classification model.

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### 2. Materials and methods

Images of our dataset were taken from 1,550 graptolite specimens, which
taxonomically belong to 113 graptolite species or subspecies. These
specimens are preserved as shale and were collected from 154 representative
geological sections of China. All specimens are housed at the Nanjing Institute
of Geology and Palaeontology (NIGP), Chinese Academy of Sciences (CAS).

89 Every piece of specimen is tagged with scientific information, including 90 genus and species names, nominator, nomination year, specimen number, 91 collection number, locality (province, city, county), geological horizon and 92 section, collector name, collecting time, identifier, identifying time, related references, and published illustrations. Specimens can be indexed and located 93 in their detailed housing drawers and cabinets using any of the above 94 95 information. Their detailed research-related information can also be obtained 96 from the geological section-based database, the Geobiodiversity Database 97 (Xu et al., 2020) and forms key elements of fossil specimen metadata (Xu et al., in press). All this related information is collected and recorded in a separate 98 99 spreadsheet file released with our image dataset.

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 Leica M125 and M205C microscopes equipped with Leica cameras (Fig. 3). Every image is well focused and better shows the morphology of graptolite bodies. In total, we took 40,597 images, including 20,644 camera photos (each with a resolution of 4,912 × 7,360) and 19,953 microscope photos (each with a

3 / 16

resolution of 2,720 × 2,048). Photos of low contrast or bad focus were 106 107 removed from the whole collection. We only kept and selected the photos that 108 show the visual morphology of every specimen and the diagnostic character of each graptolite species that the specimens represent (Fig. 4). We selected one 109 or two images for each specimen as the present final dataset, uploaded to, and 110 111 stored in our cloud server (Fig. 3). Every specimen has at least one original photo, and another image shows specimen with a scale bar. Occasionally in 112 113 some cases of large image, the scale bar is embedded, just beside the fossil itself. 114

115 Considering some of the specimens of our collection have a long research 116 history since 1958, and their taxonomical status might change in the new light 117 of graptolite systematic study (Maletz, 2017; Zhang et al., 2020), we invited 118 graptolite palaeontologists to curate every specimen to make sure that its 119 scientific information is updated and widely accepted. The emendation results 120 are showed in the spreadsheet file of our dataset.

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### 3. Data description

Our dataset consists of 2,951 high-resolution images and a related 123 spreadsheet file. Every image is a high-resolution photo taken from the 124 125 collection of 1550 graptolite specimens. These specimens were formally 126 published in 1958-2020, and taxonomically belonging to 113 graptolite species 127 or subspecies, of 41 genera and 16 families of the Order Graptoloidea (see the uploaded spreadsheet file, Fig 5). The geological age of these graptolite 128 species ranges from the Middle Ordovician to (467.3 Ma) to the Telychian 129 (433.4 Ma) of the Silurian Period (Fig. 5). 130

131 These graptolite species have relatively abundant fossil records and are 132 significant in regional and global bio-stratigraphical correlations. They are commonly used in geological age determination and shale gas favourable 133 134 exploration bed (FEB) indication, including 32 graptolite bio-zones from the Darriwilian Stage of the Ordovician Period (467.3 Ma) to the Telychian Stage of 135 the Silurian Period (433.4 Ma) and 16 "gold callipers" of shale gas FEBs for the 136 cases of 20 m to 80 m thick graptolite shale in China (Fig. 6). These species 137 also include two "golden spike" graptolite species for the two GSSPs in 138 southern China (i.e., bases of the Darriwilian Stage in the Middle Ordovician 139 System and the Hirnantian Stage in the Upper Ordovician System). 140

The name of the individual image file is initialled by the specimen' unique number and taxonomical species name. The image file is in JPG format. The single JPG file size ranges from 822 KB to 7.055 MB. The whole volume of the dataset is 10.4 GB.

In the spreadsheet file, we incorporated revision suggestions of several 145 146 distinguished palaeontologists for the authority of the graptolite taxonomy. The spreadsheet file shows the detailed scientific information of every graptolite 147 specimen. The spreadsheet file includes following fields: species ID, Phylum, 148 Class, Order, Suborder, Infraorder, Family, Subfamily, Genus, Revised species 149 name, tagged species name, total number of specimens, specimen serial 150 151 number, image file name, microscope photo number, SLR photo number, 152 Stage, Age from, Age to, mean age value, locality, longitude, latitude, horizon, and specimen firstly published reference. 153

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## 155 **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 159 160 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 161 162 resized it into 448×448 pixels and fed it into the trained CNN model. The output 1×1×2048 feature map from the last average pooling layer is flattened and 163 projected to a 113 (number of species) dimensional fully connected layer to 164 represent an image embedding. After that, we use t-SNE (t-Distributed 165 166 Stochastic Neighbor Embedding), a nonlinear dimension reduction technique for high-dimensional data, to project the image embeddings into the 167 two-dimensional space for visualization. Finally, we indicate the image data 168 169 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 170 the images in this figure is based on species, which shows a "big mixed, small 171 172 settlements" posture.

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## **5.** Conclusions

A graptolite specimen image dataset containing 2,951 high-resolution

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images is released. The formation of our dataset includes two steps. 1) 113 176 Ordovician to Silurian graptolite species or subspecies are selected for their 177 significances in global correlation and shale gas exploration; 2) 1550 pieces of 178 fossil specimens that typically represent these 113 species are carefully 179 curated and photographed. 180 181 Scientific information related to these graptolite specimens is also included and recorded for further study. The structured records include taxonomical, 182 geologic, geographic, and related references of every specimen. 183 Our dataset potentially contributes to global bio-stratigraphical correlation, 184 especially with those bio-zone graptolite species, in the shale gas industry to 185 186 improve exploration efficiency and develop an image-based automated 187 classification model. The whole dataset has visualized the tool FSIDvis (Fossil Specimen Image 188 Data Visualizer). A nonlinear dimension reduction technique, t-SNE 189 (t-Distributed Stochastic Neighbor Embedding), is used to our data and project 190 the image embeddings into the two-dimensional space for visualisation. 191 192 Data availability. The dataset is archived and publicly available from 193 https://doi.org/10.5281/zenodo.5205216. Visualized version is available at 194 https://fossil-ontology.com/FSIDvis/graptolite/. 195 196 197 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 198 manuscript with contributions from Z.-B.N. Y.-S.C. gave technician supports. 199 X.M. revised and curated fossil specimens. Others contributed in specimen 200 201 photography. 202 **Competing interests.** The authors declare that they have no conflict of 203 204 interest. 205 Acknowledgments. We thank Dr. Pan Zhaohui, Institute of Vertebrate 206 207 Paleontology and Paleoanthropology, CAS; Mr. Pan Yaohua and Mr. Wu Jungi, College of Intelligence and Computing, Tianjin University, for constructive 208 suggestions and help. 209 210

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# 216References

- Chen, X., Chen, Q., Zhen, Y., Wang, H., Zhang, L., Zhang, J. and Xiao, Z.:
- 218 Circumjacent distribution pattern of the Lungmachian graptolitic black
- shale (early Silurian) on the Yichang Uplift and its peripheral region.
- 220 Science China Earth Sciences, 61, 1195–1203, 2018.
- 221 Chen, X., Zhang, Y., Li, Y., Fan, J., Tang, P., Chen, Q. and Zhang, Y.:
- Biostratigraphic correlation of the Ordovician black shales in Tarim Basin
- and its peripheral regions. Science China Earth Sciences, 55, 1230–1237,
  2012.
- Goldman, D., Sadler, P.M. and Leslie, S.A.: The Ordovician Period, in Geologic
  Time Scale 2020. Elsevier. p. 631–694, 2020.
- Klemme, H.D. and Ulmishek, G.F.: Effective petroleum source rocks of the
   world: stratigraphic distribution and controlling depositional factors. AAPG
   Bulletin, 75, 1809–1851. 1991.
- Maletz, J.: Part V, Second Revision, Chapter 13: The history of graptolite
   classification. Treatise Online, 88:1–11, 2017.
- Peters, S. E. and McClennen, M.: The Paleobiology Database application
   programming interface. Paleobiology, 42, 1–7, 2016.
- 234 Podhalańska, T.: Graptolites–stratigraphic tool in the exploration of zones
- prospective for the occurrence of unconventional hydrocarbon deposits.
  Przegląd Geologiczny, 61, 621–629, 2013.
- Xu H.H, Nie T., Guo W., Chen Y-S, Yuan W-W.: Palaeontological fossil
   specimen metadata standard. Acta Palaeotologica Sinica, in press.
- Xu, H.-H., Niu, Z.-B. and Chen, Y.-S.: A status report on a section-based
- stratigraphic and palaeontological database–the Geobiodiversity Database.
  Earth System Science Data, 12, 3443–3452, 2020.
- 242 Xu, H.-H.: High-resolution images of 1550 Ordovician to Silurian graptolite
- specimens for global correlation and shale gas exploration.

244 <u>https://doi.org/10.5281/zenodo.6194943</u>. 2022.

Z45 Zhang, Y.D. Zhan, R.B., Wang, Z.H., Yuan, W., Fang., Liang, Y., Yan, Wang, Y.,

- Liang, K. et al.: 2020. Illustrations of index fossils from the Ordovician
- strata in China. Zhejiang University Press 1–575, 2020.
- Zou, C.N., Dong, D., Wang, Y., Li, J., Huang., Wang, S., Guan, Q. et al.: Shale
- gas in China: Characteristics, challenges and prospects (I). Petroleum
- Exploration and Development. 42, 689–701, 2015.
- Zou, C.N., Gong, J., Wang, H.Y. and Shi, Z.: Importance of graptolite evolution
- and biostratigraphic calibration on shale gas exploration. China Petroleum
  Exploration. 24, 1–6, 2019.



255	(_) Main shale gas production region
256	Figure 1. Global distribution of graptolite shales and shale gas production
257	region. Most graptolites were yielded from the shale and their distribution is
258	based on graptolite fossil occurrence records in global Ordovician and Silurian
259	sediments. All data are from Peters and McClennen (2016) and Xu et al.
260	(2020). Graptolite shale comprises over 9% of hydrocarbons rocks in the world
261	and yields the largest volume of shale gas in the world. In China, over 61.4%
262	natural gas was yielded from the Ordovician and Silurian graptolite shales of
263	southern China. The map is from ${ m \bigcirc}$ OpenStreetMap contributors 2021.
264	Distributed under the Open Data Commons Open Database License (ODbL)
265	v1.0.
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Figure 2. Geological significance and application of graptolites. Our dataset of 269 graptolites is significant to biostratigraphy and the dating of the Ordovician and 270 Silurian sediments. They are widely distributed around the world and useful for 271 regional correlation. These graptolites have also witnessed several 272 macro-evolutional events, including the great Ordovician biodiversity event, 273 Late Ordovician mass extinction, radiation in several graptolite groups, and 274 global stratotype section and point (GSSP), based on graptolite species. To 275 date, 13 GSSPs have been defined by the FAD of graptolites in the early 276 Paleozoic. Two are in South China (i.e., the bases of the Darriwilian in the 277 Middle Ordovician and Hirnantian in the Late Ordovician) (the spike marks in 278 the figure) (data from Goldman et al., 2020). Bio- or indication zones based on 279 280 graptolite species assist with identifying mining beds for shale gas exploration in southern China. 16 graptolite indicator-zones are used in the shale gas 281 exploration in China (Zou et al., 2015). 282

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

The graptolite specimens were carefully curated and revised to select the

species with biostratigraphy and application significance. Every image was

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

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

- 290 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.



302 Figure 5. Geographic distribution (A) and geologic range (B) of graptolite species of our dataset. Each graptolite specimen locality is represented by a 303 pie chart where each colour is encoded as one graptolite family of the Order 304 Graptoloidea. The sector size is proportional to the specimen number for every 305 306 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 307 shale gas production. The map is from © OpenStreetMap contributors 2021. 308 Distributed under the Open Data Commons Open Database License (ODbL) 309 v1.0. 310 311

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

Stage	Graptolite indicator zone for shale gas FEB (16)
Tolyobion	Spirograptus turriculatus (N2)
Terychian	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)

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

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

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

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

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

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



Figure 7. FSIDvis (Fossil Specimen Image Dataset Visualizer) system 324 interface. a) Fossil on geographic distribution view, showing fossil specimen 325 location on the map. The lens (a.1) is a tailor-designed specimens' picker that 326 facilitates users to collect interest fossils of a region where the inner ring and 327 328 outer ring represent the family and genus. When the user chooses a genus, the corresponding detailed species with images will be listed in the fossil list 329 view (a.2), where the detailed information and further high-resolusion image if 330 the specimens are given. Hit the space bar for locking the selection. b) 331 Geological age scale view, providing the geologic age selection ability; the top 332 333 one is the chronostratigraphic age scale, and the bottom one is an age slider that facilitates the users to choose a specific age slot interactively. The web 334 exploration tool of graptolite is provided at 335 https://fossil-ontology.com/FSIDvis/graptolite/. The map is from © 336 OpenStreetMap contributors 2021. Distributed under the Open Data 337

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341 Figure 8. t-SNE embedding visualization of our graptolite specimen image

342 dataset. Individual specimens are denoted by different colors and grouped in

343 the visualization. These groups also taxonomically match different graptolite

344 families (blocks with several small images).