



1	Ordovician to Silurian graptolite specimen images for global		
2	correlation and shale gas exploration		
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17	Abstract		
18	Multi- elemental and -dimensional data are more and more important		
19	during the development of data-driven research, as is the case in modern		
20	palaeontology, in which visual examination, by experts or someday the		
21	artificial intelligence, to every fossil specimen acts a crucial and fundamental		
22	role. We here release an integrated image dataset of 113 Ordovician to		
23	Silurian graptolite species or subspecies that are significant in global		
24	stratigraphy and shale gas exploration. The dataset contains 1550 high-		
25	resolution graptolite specimen images and scientific information related to the		
26	specimen, e.g., every specimen's taxonomic, geologic, geographic, and		
27	related references. We develop a tool, FSIDvis (Fossil Specimen Image		
28	Dataset Visualiser), to facilitate the human-interactive exploration of the rich-		
29	attribution image dataset. A nonlinear dimension reduction technique, t-SNE		
30	(t-Distributed Stochastic Neighbor Embedding), is employed to project the		
31	images into the two-dimensional space to visualise and explore the		
32	similarities. Our dataset potentially contributes to the analysis of the global		
33	biostratigraphic correlations and improves the shale gas exploration efficiency		
34	by developing an image-based automated classification model. All images are		
35	available from <u>https://doi.org/10.5281/zenodo.5205216 (Xu, 2021)</u> .		





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38	1. Background
39	Graptolite is marine colonial organic-walled hemichordate and has over
40	210 genera/3,000 species worldwide fossil records, extending from the
41	Cambrian to the Carboniferous (c. 510~320 Ma) shale sediments (Maletz,
42	2017). Graptolite extensively diversified in the Ordovician and witnessed the
43	second-largest mass extinction in geological life history, i.e., the end-
44	Ordovician mass extinction (Goldman et al., 2020). Graptolite evolved quickly
45	and spread globally in the Paleozoic (Fig. 1); therefore, its species are widely
46	used as significant index fossils for determining rock ages and regional bio-
47	stratigraphical correlations. Graptolite bio-zones divided the Ordovician and
48	Silurian sediments are generally less than one million years in duration; such
49	a short geological moment makes it possible for a better and accurate
50	understanding of the stratigraphy and ancient life macro-evolution (Chen et
51	al., 2012; 2018). Up to 102 Ordovician and Silurian graptolite species were
52	selected as global bio-zones for dating rocks, biostratigraphy, regional
53	correlation, and understanding the evolutionary patterns of ancient life; and 13
54	global stratotype section and point (GSSP) have been defined by the first
55	appearance datum (FAD) of graptolite species in the Lower Paleozoic, i.e.,
56	Cambrian, Ordovician, and Silurian (Goldman et al., 2020). Two of these
57	GSSPs are situated in southern China (i.e., the bases of the Darriwilian in the
58	Middle Ordovician and Hirnantian in the Late Ordovician) (Goldman et al.,
59	2020; Zhang et al., 2020) (Fig. 2).
60	Additionally, bio-zones or indication zones based on graptolite species
61	assist with identifying mining beds for shale gas exploration (Fig. 1). Graptolite
62	shale comprises more than 9% of hydrocarbons rocks and yields the most
63	significant volume of shale gas globally (Klemme and Ulmishek, 1991;
64	Podhalańska, 2013). In China, over 61.4% of the natural gas is yielded from
65	the Ordovician and Silurian graptolite shale of southern China (Zou et al.,
66	2019). Identification of graptolite species helps to locate shale gale mining
67	beds; especially, 16 graptolite species were chosen as "gold caliper" to locate
68	favourable exploration beds (FEB) of shale gas in China (Zou et al., 2015)
69	(Fig. 2).
70	In this paper, we release a unique graptolite image dataset, which
71	consists of 113 key graptolite species used for dating rocks, global correlation,

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⁷² and "gold caliper" for locating shale gas FEBs in China. All images were taken

- ⁷³ from 1,550 carefully curated graptolite specimens collected from the
- 74 Ordovician to Silurian sediments of China. We incorporated revision
- ⁷⁵ suggestions from distinguished palaeontologists to generate the ground-truth
- 76 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 high-resolution images of 1,550 specimens of 113 graptolite
- r9 species for teaching and training in palaeontology and geologic survey; 2)
- 80 global bio-stratigraphical correlation using graptolites, especially with those
- 81 bio-zone species; 3) a standard fossil specimen image dataset used in shale
- gas industry to improve exploration efficiency, and 4) the potential aid of

83 developing image-based automated classification model.

84 85

2. Materials and methods

Images of our dataset were taken from 1,550 graptolite specimens, which 86 87 taxonomically belong to 113 graptolite species or subspecies. These specimens are preserved as shale and were collected from 154 88 representative geological sections of China. All specimens are housed at the 89 Nanjing Institute of Geology and Palaeontology (NIGP), Chinese Academy of 90 91 Sciences (CAS), the world's largest palaeontological research centre, and one 92 of the top three specimen collection centres. The NIGP-CAS hosts over 180 93 palaeontological researchers and laboratory technicians and collecting over 800,000 pieces of fossil specimens from all around the world since 1928 94 (NIGP, 2011). 95

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

106 We spent over two years to complete photographing every specimen





using a single-lens reflex camera Nikon D800E with Nikkor 60 mm macro-lens 107 and Leica M125 and M205C microscopes equipped with Leica cameras (Fig. 108 3). Every image is well focused and better shows the morphology of graptolite 109 bodies. In total, we took 40,597 images, including 20,644 camera photos 110 (each with a resolution of 4,912 x 7,360) and 19,953 microscope photos (each 111 with a resolution of 2,720 x 2,048). Photos of low contrast or bad focus were 112 removed from the whole collection. We only kept and selected the photos that 113 show the visual morphology of every specimen and the diagnostic character 114 of each graptolite species that the specimens represent (Fig. 4). We selected 115 one image for each specimen as the present final dataset, uploaded to, and 116 stored in our cloud server (Fig. 3). 117 Considering some of the specimens of our collection have a long research 118 history since 1958, and their taxonomical status might change in the new light 119 of graptolite systematic study (Maletz, 2017; Zhang et al., 2020), we invited 120 graptolite palaeontologists to curate every specimen to make sure that its 121 122 scientific information is updated and widely accepted. 123 3. Data description 124 Our dataset consists of 1,550 high-resolution images and a related 125 spreadsheet file. Every image is a high-resolution photo taken from the 126 127 collection of 1550 graptolite specimens. These specimens were formally published in 1958-2020, and taxonomically belonging to 113 graptolite 128 species or subspecies, of 41 genera and 16 families of the Order 129 Graptoloidea (see the uploaded spreadsheet file, Fig 5). The geological age of 130 these graptolite species ranges from the Middle Ordovician to (467.3 Ma) to 131 the Telychian (433.4 Ma) of the Silurian period (Fig. 5). 132 These graptolite species have relatively abundant fossil records and are 133 significant in regional and global bio-stratigraphical correlations and locating 134 favourable exploration bed (FEB) of shale gas in China. They are commonly 135 used in geological age determination and shale gas FEB indication, including 136 137 32 graptolite biozones from the Darriwilian stage of the Ordovician (467.3 Ma) to the Telychian stage of the Silurian (433.4 Ma) and 16 "gold callipers" of 138 shale gas favourable exploration beds (FEBs) for cases of 20 to 80 m thick 139 graptolite shale in China (Fig. 6). These species also include two "golden 140 spike" graptolite species for the two GSSPs in southern China (i.e., bases of 141

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- 142 the Darriwilian in the Middle Ordovician and Hirnantian in the Late
- 143 Ordovician).

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, and the single JPG file size ranges from 840 KB to 10.59 MB. The whole volume of the dataset is 6.41 GB.

In the spreadsheet file, we incorporated revision suggestions of several 148 distinguished palaeontologists for the authority of the graptolite taxonomy. The 149 spreadsheet file shows the detailed scientific information of every graptolite 150 specimen. The spreadsheet file includes following fields: species ID, Phylum, 151 Class, Order, Suborder, Infraorder, Family, Subfamily, Genus, Revised 152 species name, tagged species name, total number of specimens, specimens 153 serial number, image file name, microscope photo numbers, SLR photo 154 number, Stage, Age from, Age to, mean age value, Locality, Longitude, 155

Latitude, Horizon, and specimens firstly published reference.

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4. Data visualization

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

162 We further explore the distribution of these graptolite images and visualize the t-SNE feature embedding of our graptolite dataset (Fig. 8) using 163 different colors to denote different families. In detail, for each annotated 164 image, we first resized it into 448×448 pixels and fed it into the trained CNN 165 model. The output 1×1×2048 feature map from the last average pooling layer 166 is flattened and projected to a 113 (number of species) dimensional fully 167 connected layer to represent an image embedding. After that, we use t-SNE 168 (t-Distributed Stochastic Neighbor Embedding), a nonlinear dimension 169 reduction technique for high-dimensional data, to project the image 170 embeddings into the two-dimensional space for visualization. Finally, we 171 172 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 113 173 species, so the distribution of the images in this figure is based on species, 174 which shows a "big mixed, small settlements" posture. 175





177 **5. Conclusions**

178	A graptolite specimen image dataset containing 1550 high-resolution
179	images is released. The formation of our dataset includes two steps. 1) 113
180	Ordovician to Silurian graptolite species or subspecies are selected for their
181	significances in global stratigraphy and shale gas exploration; 2) 1550 pieces
182	of fossil specimens that typically represent these 113 species are carefully
183	curated and photographed.
184	Scientific information related to these graptolite specimens is also
185	included and recorded for further study. The structured records include
186	taxonomical, geologic, geographic, and related references of every specimen.
187	Our dataset potentially contributes to global bio-stratigraphical correlation,
188	especially with those graptolite bio-zone species, in the shale gas industry to
189	improve exploration efficiency and develop an image-based automated
190	classification model.
191	The whole dataset has visualised the tool FSIDvis (Fossil Specimen
192	Image Data Visualizer). A nonlinear dimension reduction technique, t-SNE (t-
193	Distributed Stochastic Neighbor Embedding), is used to our data and project
194	the image embeddings into the two-dimensional space for visualisation.
195	
196	Data availability. The dataset is archived and publicly available from
197	https://doi.org/10.5281/zenodo.5205216. Visualized version is available at
198	https://fossil-ontology.com/FSIDvis/graptolite/.
199	
200	Author contributions. HH.X. and ZB.N. equally designed the project,
201	developed the model, and performed the simulations. HH.X. prepared the
202	manuscript with contributions from ZB.N. YS.C. gave technician supports.
203	X.M. revised and examined fossil specimens. Others contributed in specimen
204	photography.
205	
206	Competing interests. The authors declare that they have no conflict of
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208	
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Figure 1. Global distribution of graptolite shales and shale gas production 262 region. Most graptolites were yielded from the shale and their distribution is 263 264 based on graptolite fossil occurrence records in global Ordovician and Silurian 265 sediments. All data are from Peters and McClennen (2016) and Xu et al. (2020). Graptolite shale comprises over 9% of hydrocarbons rocks in the 266 world and yields the largest volume of shale gas in the world. In China, over 267 61.4% natural gas was yielded from the Ordovician and Silurian graptolite 268 shales of southern China. The map is from © OpenStreetMap contributors 269 2021. Distributed under the Open Data Commons Open Database License 270 271 (ODbL) v1.0. 272







Figure 2. Geological significance and application of graptolites. Our dataset of 275 graptolites is significant to biostratigraphy and the dating of the Ordovician 276 and Silurian sediments. They are widely distributed around the world and 277 useful for regional correlation. These graptolites have also witnessed several 278 macro-evolutional events, including the great Ordovician biodiversity event, 279 Late Ordovician mass extinction, radiation in several graptolite groups, and 280 global stratotype section and point (GSSP), based on graptolite species. To 281 date, 13 GSSPs have been defined by the FAD of graptolites in the early 282 Paleozoic. Two are in South China (i.e., the bases of the Darriwilian in the 283 284 Middle Ordovician and Hirnantian in the Late Ordovician) (the spike marks in the figure) (data from Goldman et al., 2020). Bio- or indication zones based on 285 graptolite species assist with identifying mining beds for shale gas exploration 286 in southern China. 16 graptolite indicator-zones are used in the shale gas 287 exploration in China (Zou et al., 2015). 288 289







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

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

293 species with biostratigraphy and application significance. Every image was

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

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

whole dataset was uploaded to and stored in our cloud server.







298

299 Figure 4. Typical images of our dataset. Every image was taken from a

- 300 unique graptolite specimen. Photos of low contrast or bad focus were
- removed. Our dataset only selected the photos that well show visual
- 302 morphology of every specimen and diagnostic character of each graptolite
- 303 species that the specimens represent. The scientific species name of every
- 304 specimen is given on each image.
- 305





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Figure 5. Geographic distribution (A) and geologic range (B) of graptolite 308 species of our dataset. Each graptolite specimen locality is represented by a 309 pie chart where each colour is encoded as one graptolite family of the order 310 Graptoloidea. The sector size is proportional to the specimen number for 311 312 every 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 313 shale gas production. The map is from © OpenStreetMap contributors 2021. 314 Distributed under the Open Data Commons Open Database License (ODbL) 315 v1.0. 316 317





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System	Series	Stage	Graptolite biozone (22)	Stage	Graptolite indicator zone for shale gas FEB (
		Homerian	Colonograptus deubeli	Telychian	Spirograptus turriculatus (N2)	
	Wenlock		Colonograptus praedeubeli		Spirograptus guerichi (N1)	
		Sheinwoodian			Stimulograptus sedgwickii (LM8)	
		Telychian	Spirograptus turriculatus	Aeronian	Lituigraptus convolutus (LM7)	
Silurian		Aeronian	Lituigraptus convolutus		Demirastrites triangulatus (LM6)	
Siluriari		Aeronian	Demirastrites triangulatus		Coronograptus cyphus (LM5)	
	Llandovery	Rhuddanian	Coronograptus cyphus		Cystograptus vesiculosus (LM4)	
			Cystograptus vesiculosus	Rhuddanian	Parakidograptus acuminatus (LM3)	
			Parakidograptus acuminatus		Akidograptus ascensus (LM2)	
			Akidograptus ascensus		Metabolograptus persculptus (LM1)	
	Upper	Hirnantian	Metabolograptus persculptus	Hirnatian	Metabolograptus extraordinarius (WF4)	
			Metabolograptus extraordinarius		Dicellograptus mirus (WF3c)	
		Katian	Paraorthograptus pacificus		Tangyagraptus typicus (WF3b)	
			Dicellograptus complexus	Katian	Paraorthograptus pacificus (WF3a)	
			Dicellograptus ornatus		Dicellograptus complexus (WF2)	
			Dicellograptus complanatus		Dicellograptus complanatus (WF1)	
Ordovician		Sandbian	Orthograptus calcaratus			
				Hustedograptus teretiusculus		
		e Darriwilian	Archiclimacograptus riddellensis			
	Middle		Pterograptus elegans			
	Middle		Nicholsonograptus fasciculatus			
			Levisograptus dentatus			
		Dapingian	Levisograptus austrodentatus			

319

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

321 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

324 Wenlock of Silurian period (427.4 Ma), and 16 graptolite species as 'gold

325 calliper' to locate favourable exploration beds (FEB) of shale gas in China.

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





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329	bóna 400na 475ma 475ma 405ma 465ma 466ma 455na 450na 446ma 446ma 445ma 435ma 435ma 425ma 425ma 420m
330	Figure 7. FSIDvis (Fossil Specimen Image Dataset Visualiser) system
331	interface. a) Fossil map view. a.1, is a tailor-designed specimens' picker that
332	facilitates users to collect interest fossils of a region where the inner ring and
333	outer ring represent the family and genus. When the user chooses a genus,
334	the corresponding detailed species with images will be listed in the a.2 view.
335	b) Time view, providing the time selection ability; the top one is the
336	chronostratigraphic time scale, and the bottom one is a time slider that
337	facilitates the users to choose a specific time slot interactively. The web
338	exploration tool of graptolite is provided at https://fossil-
339	ontology.com/FSIDvis/graptolite/. The map is from © OpenStreetMap
340	contributors 2021. Distributed under the Open Data Commons Open
341	Database License (ODbL) v1.0.







344 Figure 8. t-SNE embedding visualization of our image dataset.