A multi-dimensional dataset of Ordovician to Silurian graptolite specimens ~~images~~ for virtual examination, global correlation, and shale gas exploration

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Abstract

Multi- elemental and -dimensional data are more and more important in the development of data-driven research, as is the case in modern paleontology, in which ~~visual~~ examination, by experts or someday the artificial intelligence, to every fossil specimen acts a fundamental role. We here release an integrated ~~image~~ dataset of 1,550 graptolite specimens representing 113 Ordovician to Silurian graptolite species or subspecies that are significant in global stratigraphic~~y~~ correlation and shale gas exploration. The dataset contains 2,951 high-resolution ~~graptolite specimen~~ images and a structured data table of specimens'~~their related~~ scientific information, e.g., every specimen's taxonomic, geologic, and geographic information, comment, and ~~related~~ references. Specimens data of our dataset provide virtual eaxaminations for specialists or laymen worldwide, are visualized, by the tool w~~W~~e developed~~ a tool~~, FSIDvis (Fossil Specimen Image Dataset Visualiz~~s~~er), to facilitate the human-interactive exploration of the rich-attribution image dataset, and also are analysed with~~. We employ~~ a nonlinear dimension reduction technique, t-SNE (t-Distributed Stochastic Neighbor Embedding), to project ~~the~~ images~~s~~ data into the two-dimensional space to visualize and explore the similarities. Our dataset potentially contributes to virtual examination to specimens (VES), ~~the analysis of the~~ global bio-stratigraphic correlation~~s~~ and improvement of ~~s~~ the shale gas exploration efficiency.~~ by developing an image-based automated classification model~~ A fossil specimen database need to fulfil the purpose and the requirement of VES. All data, images and the spreadsheet file, are available from https://doi.org/10.5281/zenodo.6688671 (Xu, 2022).

1. ~~Background~~Introduction

Fossils show the direct evidence of prehistoric life and are probably the most important research object of palaeontology and stratigraphy, during which fossils are collected, sampled, illustrated, described, curated, and deposited as permanent specimens in museum or institution for any further investigation (Shute and Foster, 1999). Examinations of fossil specimens is a key and indispensable part in descriptional study of palaeontology. Such can be potentially achieved in a convenient and low-cost way, with aid of multi-dimensional fossil specimen dataset as in this study.

Graptolite is an extinct group of~~was a~~ marine colonial organic-walled hemichordates and has~~d~~ over 210 genera/3,000 species worldwide fossil records from the Cambrian to~~ the~~ Carboniferous (c. 510~320 Ma) shale sediments (Maletz, 2017). Graptolite extensively diversified in the Ordovician Period and witnessed the second-largest mass extinction in geological life history, i.e., the end-Ordovician mass extinction (Goldman et al., 2020). Graptolite evolved quickly and spread globally in the Paleozoic (Fig. 1); and~~therefore,~~ its species are widely used as significant index fossils for determining rock ages and regional bio-stratigraphical correlations. Bio-zones based on graptolite species dividing~~e~~ the Ordovician and Silurian sediments ~~and~~ are generally less than one million years in duration; such a short geological moment makes it possible for a precise understanding of ~~the~~ life evolution in geological history (Chen et al., 2012; 2018). Up to 102 Ordovician and Silurian graptolite species were selected as global bio-zones for dating sediments~~rocks~~, bio-stratigraphic ~~y, regional~~ correlation, and understanding the evolutionary pattern of paleobiology; and 13 global stratotype sections and points (GSSPs) are ~~have been~~ defined by the first appearance datum (FAD) of graptolite species from the Cambrian, Ordovician, and Silurian systems (Goldman et al., 2020)~~. Two of these GSSPs are situated in southern China, i.e., the bases of the Darriwilian Stage of the Middle Ordovician and the Hirnantian Stage of the Upper Ordovician) (Goldman et al., 2020; Zhang et al., 2020)~~ (Fig. 2).

Additionally, bio-zones or indication zones based on graptolite species assist with identifying mining beds for shale gas exploration (Fig. 1). Graptolite shale yields a significant volume of shale gas and comprises more than 9% global hydrocarbons rocks~~ and yields a significant volume of shale gas globally~~ (Klemme and Ulmishek, 1991; Podhalańska, 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 graptolite species helps to locate shale gas mining beds; especially, 16 graptolite species were chosen as “gold callipers” to locate favourable exploration beds (FEBs) of shale gas from

China (Zou et al., 2015) (Fig. 2).

In this paper, we describe a multi-dimensional and integrated dataset of release a unique graptolite specimens image dataset, which consists of 113 key graptolite species used for dating rocks, global correlation, and "gold caliper" for locating shale gas FEBs from China. All images were taken from 1,550 carefully curated graptolite specimens collected from the Ordovician to Silurian sediments of China. We incorporated revision suggestions from distinguished paleontologists to generate the ground-truth labels, providing a taxonomical authority of the dataset. The dataset potentially contributes to a range of scientific activities and provides 1) an easy access and the virtual examination to high-resolution images of 1,550fossil specimens through high-resolution images and detailed scientific information of 113 graptolite species for teaching and training in paleontology and geologic survey, and researching in; 2) global bio-stratigraphical correlation using graptolites, especially with those bio-zone species; 23) a standard fossil specimen image dataset used in shale gas industry to improve exploration efficiency, and 34) a potential aid of developing image-based automated classification model.

2. Materials and methods

All iImages of our dataset were taken from 1,550 graptolite specimens that, 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. These All specimens are housed at the Nanjing Institute of Geology and Palaeontology (NIGP), Chinese Academy of Sciences (CAS), with serial numbers and prefix NIGP.

Every piece of specimen is tagged with scientific information, including genus and species names, nominator, nomination year, specimen number, collection number, locality (province, city, county), geological horizon and section, collector name, collecting time, identifier, identifying time, related references, and published illustrations. Specimens can be indexed and located in their detailed housing drawers and cabinets using any of the above information. Their detailed research-related information can also be obtained from the geological section-based database, the Geobiodiversity Database (Xu et al., 2020) and forms key elements of fossil specimen metadata (Xu et al., 2022). All this related information is collected and recorded in a separate

~~spreadsheet file released with our image dataset.~~

We spent over two years to ~~complete~~ photograph~~ing~~ 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 resolution of 2,720 × 2,048). Photos of low contrast or bad focus were removed from the whole collection. We only kept and selected the photos that show the ~~visual~~ morphology of every specimen and the diagnostic character of each graptolite species that the specimen~~s~~ represents (Fig. 4). We selected one or two images for each specimen as the present final dataset, uploaded to, and 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 some cases of large image, the scale bar is embedded, just beside the fossil itself.

~~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.~~

3. Data description

Our dataset consists of 2,951 high-resolution images and a related spreadsheet file. Every image is a high-resolution photo taken from a~~the~~ collection of 1,550 graptolite specimens. These specimens were formally published in 1958-2020, and taxonomically belonging to 113 graptolite species 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 species ranges from the Middle Ordovician to (467.3 Ma) to the Telychian (433.4 Ma) of the Silurian Period (Fig. 5).

These graptolite species have relatively abundant fossil records and are significant in regional and global bio-stratigraphical correlations. They are commonly used in geological age determination and shale gas favourable 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 the Silurian Period (433.4 Ma) and 16 "gold callipers" of shale gas FEBs for the cases of 20 m to 80 m thick graptolite shale in China (Fig. 6). These species also include two "golden spike" graptolite 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 Ordovician System).

The name of the individual image file is initialled by the specimen' unique number and taxonomical species name. Every specimen has two photos, one is original, another shows specimen with a scale bar. Occasionally in some large image the scale bar is embedded and beside the fossil specimen. For example, in the file name: '9721Cardiograptus_amplus_S.jpg', genus name and species epithet are connected by the underline symbol, avoiding the space symbol. '9721' is the specimen number, 'Cardiograptus_amplus' means species name is *Cardiograptus amplus*, '_S' means it is a photo with scale bar. In all scale bar, the minimum unit is millimetre.

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. The quality of specimen images in our dataset is much better than that in any previous version for that most specimens were firstly studied many years ago and their illustrations were in black and white, in low-resolution and/or printed on paper publications only. Most of these specimens were illustrated only once, or never clearly photographed. The image collection of our dataset provides necessary complement for these specimens and furthermore, once again unfolds their scientific value to experts or anyone who is interested with fossils.

Every piece of specimen is tagged with scientific information, including genus and species names, nominator, nomination year, specimen number, collection number, locality (province, city, county), geological horizon and section, collector name, collecting time, identifier, identifying time, related references, and published illustrations. Specimens can be indexed and located in their detailed housing drawers and cabinets using any of the above information. Their detailed research-related information can also be obtained from the geological section-based database, the Geobiodiversity Database (Xu et al., 2020) and forms key elements of fossil specimen metadata (Xu et al., 2022). All this related information is collected and recorded in a separate spreadsheet file released with our image dataset.

Additionally, considering some 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 comments, as emendation results, are also showed in the spreadsheet file of our dataset.

All specimen images are in 49 folders, every of which is zipped to one file that is about tens of MB to 740 MB in size. Folders are named after the tagged genus names of individual graptolite specimens. One spreadsheet file is given in the whole dataset showing the metadata and the arrangement of the species names.

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

Our dataset, with the image collection and comprehensive information of a large batch of fossil specimens, provides virtual examinations to specimens in a convenient and low-cost way. Experts or laymen can look through, examine, study, and even measure fossil specimens without need for regional/international travel and formalities. Such greatly benefits palaeontology in research, teaching, and science communication (Rahman et al., 2012).

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 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 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 projected to a 113 (number of species) dimensional fully connected layer to represent an image embedding. After that, we use t-SNE (t-Distributed 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 settlements" posture.

5. Conclusions

A multi-dimensional, integrated dataset based on 1,550 pieces of graptolite specimens is released. It contains ~~image dataset containing~~ 2,951 high-resolution images and a spreadsheet file showing structured records of every specimen's scientific information ~~is released~~. ~~The formation of our dataset includes two steps.~~ During the preparation of the dataset,~~1)~~ 113 Ordovician to Silurian graptolite species or subspecies were~~are~~ selected for their significances in stratigraphic ~~global~~ correlation and shale gas exploration, and~~; 2) 1550 pieces of fossil~~ these specimens ~~that typically represent these 113 species are~~ were carefully ~~curated and~~ photographed and taxonomically curated.

~~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 provide experts or laymen virtual examination to a batch of fossil specimens in a convenient and low-cost way. It potentially contributes to global bio-stratigraphical correlation, especially with those bio-zone graptolite species, and in the shale gas industry to improvement of exploration efficiency. A fossil specimen database need to fulfil the purpose and the requirement of virtual examination to specimens, such great benefits palaeontology research and science communication. ~~and develop an image-based automated classification model.~~

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

Data availability. The dataset is archived and publicly available from https://doi.org/10.5281/zenodo.6688671. Visualized version is available at https://fossil-ontology.com/FSIDvis/graptolite/.

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

Competing interests. The authors declare that they have no conflict of interest.

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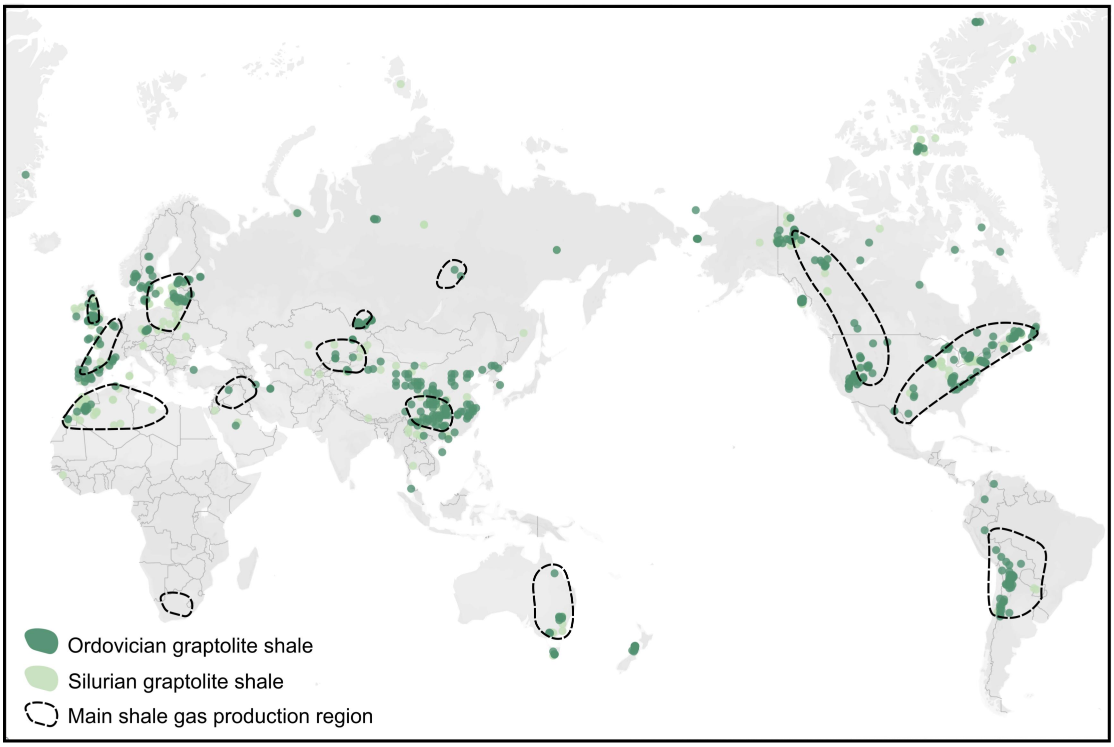

Figure 1. Global distribution of graptolite shales and shale gas production region. Most graptolite fossils were yielded from these shale sediments and their distribution is based on their graptolite fossil occurrence records in global Ordovician and Silurian sediments. All data are from Peters and McClennen (2016) and Xu et al. (2020). Graptolite shale comprises over 9% of hydrocarbons rocks in the world and yields the largest volume of shale gas in the world. In China, over 61.4% natural gas was yielded from the Ordovician and Silurian graptolite shales of southern China. The map is from © OpenStreetMap contributors 2021. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

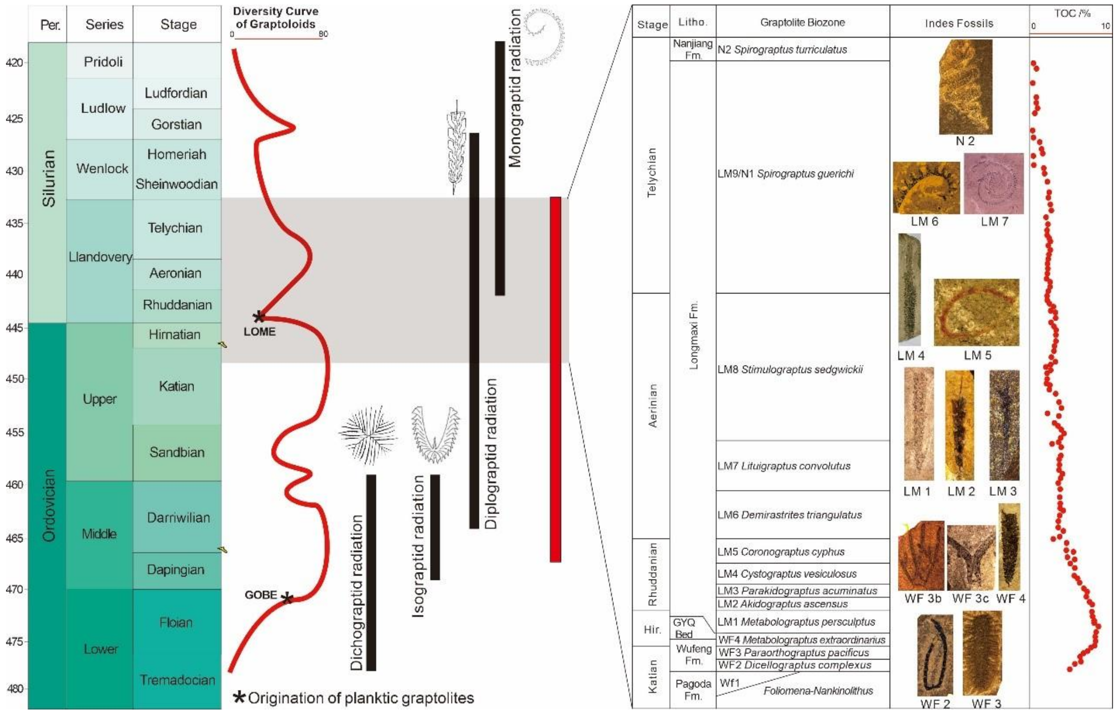

Figure 2. ~~Geological significance and application of graptolites. Our dataset of graptolites is~~Graptolite species of our dataset are significant to biostratigraphy and ~~the~~ dating of ~~the~~ Ordovician and Silurian sediments. ~~They are widely distributed around the world and useful for regional correlation.~~ These graptolites ~~have~~ also witnessed several macro-evolution~~al~~ events, including the great Ordovician biodiversity event (GOBE), Late Ordovician mass extinction (LOME). R~~, r~~adiation of ~~in~~ several graptolite groups (bold vertical lines) occurs in this geological time. Two~~, and~~ global stratotype sections and points (GSSPs), based on graptolite species record,~~. To date, 13 GSSPs have been defined by the FAD of graptolites in the early Paleozoic. Two~~ are in s~~S~~outhern China (i.e., the bases of the Darriwilian in the Middle Ordovician and Hirnantian in the Late Ordovician) (the spike marks in left~~the figure~~) (data from Goldman et al., 2020). Bio- or indication zones based on graptolite species assist with identifying mining beds for shale gas exploration in southern China. 16 graptolite indicator-zones are used in the shale gas exploration in China (Zou et al., 2015) (right part in the figure).

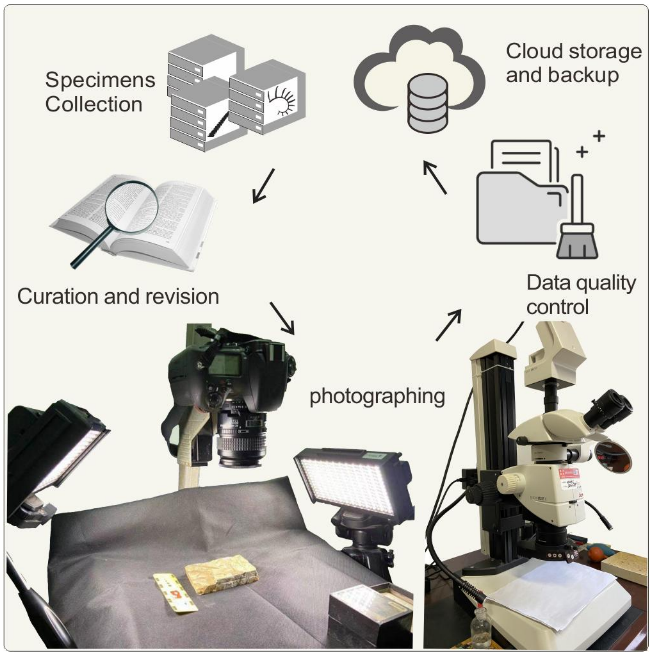

Figure 3. The process of creating the graptolite specimen image dataset. The graptolite specimens were carefully curated and revised to select the species with biostratigraphy and application significances. Every image was obtained from specimens that were macro-photographed using a single-lens reflex camera and microscope. After professional revision and cleaning, the whole dataset was uploaded to and stored in our cloud server.

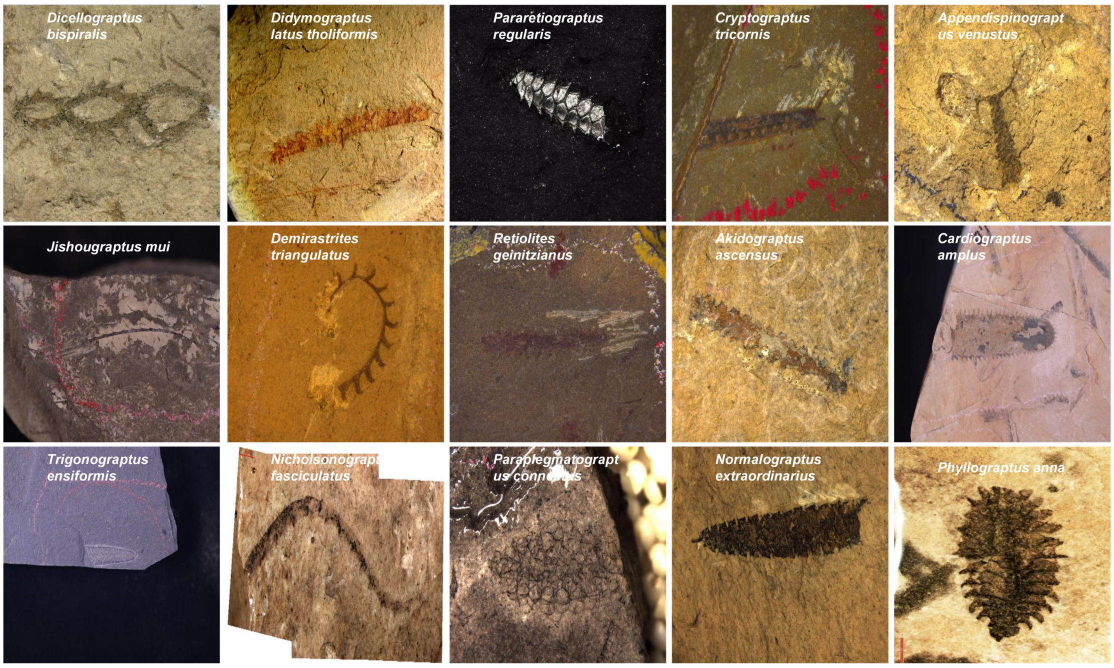

Figure 4. Typical images of graptolite specimens in our dataset. Every image was taken from a unique graptolite specimen. ~~Photos of low contrast or bad focus were removed.~~ Our dataset only selected the photos that well show ~~visual~~ morphology of every specimen and diagnostic character of each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

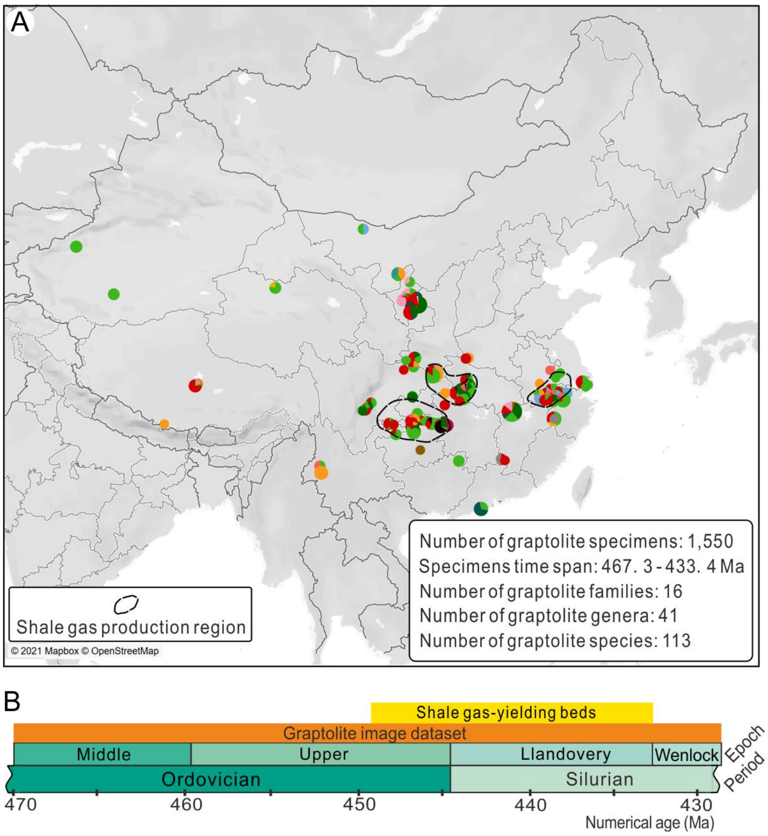

Figure 5. Geographic distribution (A) and geologic range (B) of graptolite species of our dataset. Each graptolite specimen locality is represented by a pie chart where each colour is encoded as one graptolite family of the Order Graptoloidea. The sector size is proportional to the specimen number for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

System	Series	Stage	Graptolite biozone (22)
Silurian	Wenlock	Homerian	*Colonograptus deubeli*
			Colonograptus praedeubeli
		Sheinwoodian	
	Llandovery	Telychian	*Spirograptus turriculatus*
		Aeronian	*Lituigraptus convolutus*
			Demirastrites triangulatus
		Rhuddanian	*Coronograptus cyphus*
			Cystograptus vesiculosus
			Parakidograptus acuminatus
			Akidograptus ascensus
Ordovician	Upper	Hirnantian	*Metabolograptus persculptus*
			Metabolograptus extraordinarius
		Katian	*Paraorthograptus pacificus*
			Dicellograptus complexus
			Dicellograptus ornatus
			Dicellograptus complanatus
		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)
	Spirograptus guerichi (N1)
Aeronian	*Stimulograptus sedgwickii* (LM8)
	Lituigraptus convolutus (LM7)
	Demirastrites triangulatus (LM6)
Rhuddanian	*Coronograptus cyphus* (LM5)
	Cystograptus vesiculosus (LM4)
	Parakidograptus acuminatus (LM3)
	Akidograptus ascensus (LM2)
	Metabolograptus persculptus (LM1)
Hirnatian	*Metabolograptus extraordinarius* (WF4)
Katian	*Dicellograptus mirus* (WF3c)
	Tangyagraptus typicus (WF3b)
	Paraorthograptus pacificus (WF3a)
	Dicellograptus complexus (WF2)
	Dicellograptus complanatus (WF1)

Figure 6. Graptolite species selected as global bio-zone (left) and indicator zone (right) for shale gas favourable exploration beds (FEBs) 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 Wenlock of the Silurian Period (427.4 Ma), and 16 graptolite species as ‘gold callipers’ to locate ~~favourable exploration beds (~~FEBs~~)~~ of shale gas in China. Note that some graptolite species are duplicate in the two lists.

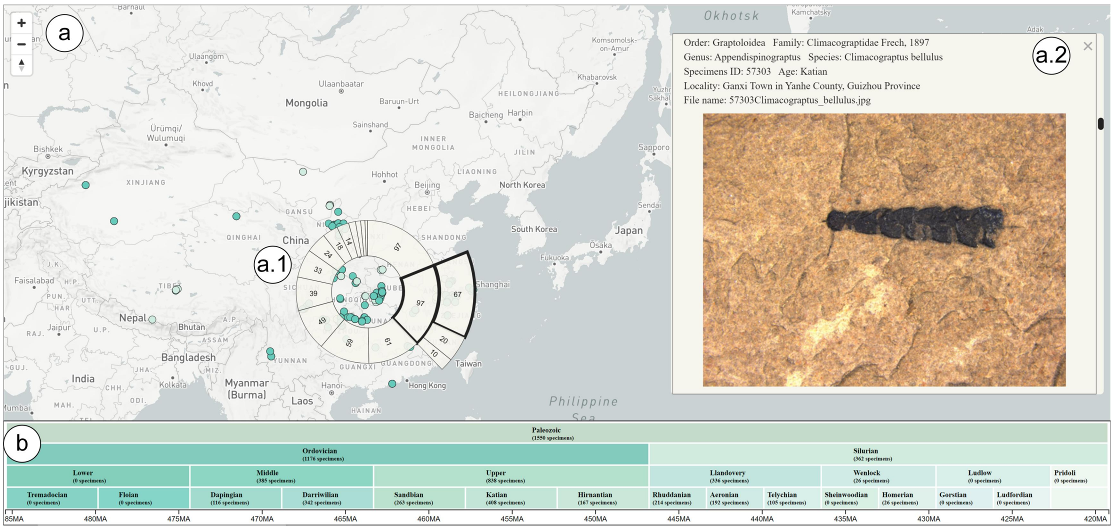

Figure 7. FSIDvis (Fossil Specimen Image Dataset Visualizer) system interface. a) Fossil on geographic distribution view, showing fossil specimen location on the map. The lens (a.1) is a tailor-designed specimens' picker that facilitates users to collect interest fossils of a region where the inner ring and 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 view (a.2), where the detailed information and further high-resolution image if the specimens are given. Hit the space bar for locking the selection. b) Geological age scale view, providing the geologic age selection ability; the top 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 exploration tool of graptolite is provided at https://fossil-ontology.com/FSIDvis/graptolite/. The map is from © OpenStreetMap contributors 2021. Distributed under the Open Data Commons Open Database License (ODbL) v1.0.

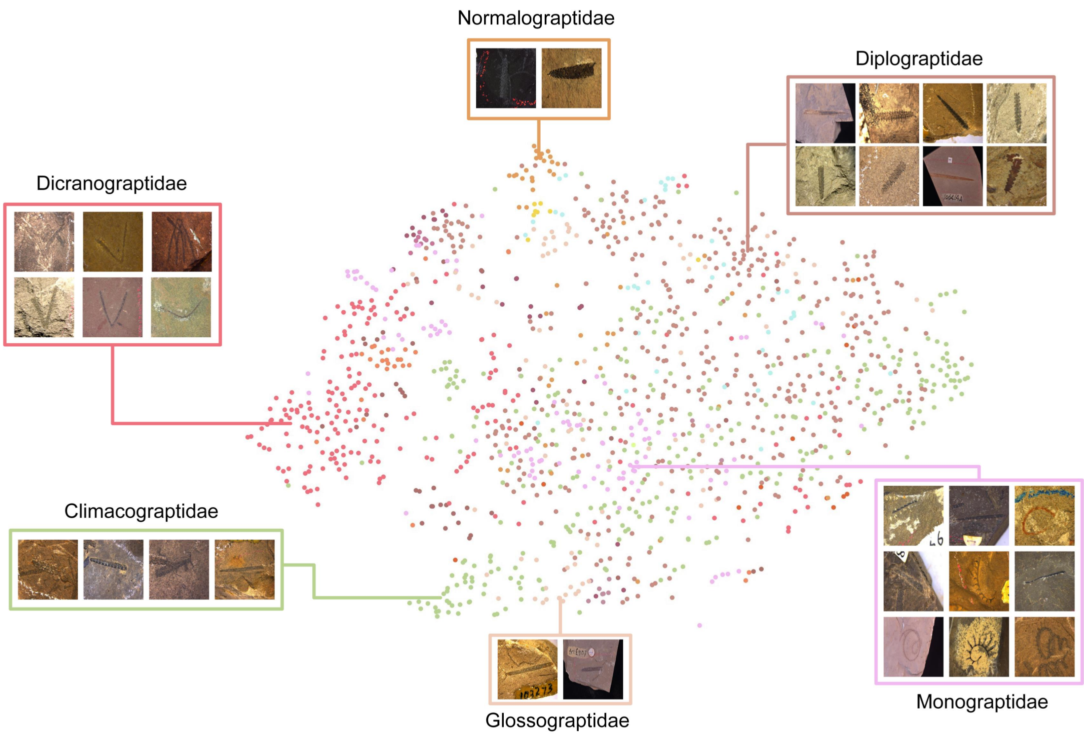

Figure 8. t-SNE embedding visualization of our graptolite specimen images~~-dataset~~. Individual specimens are denoted by different colors and grouped in the visualization. These groups also taxonomically match different graptolite families (blocks with several small images).