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A database for igneous rocks of the Newfoundland Appalachians

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Databases are increasingly playing a pivotal role in the field of Earth Sciences. This paper presents a comprehensive database of igneous rocks from the Newfoundland Appalachians. The database comprises a collection of 15,202 datasets with a data analysis platform. Each dataset includes detailed information on geographic location (latitude and longitude), geological background, petrology, geochronology, major and trace elements, isotopes, and references. The data were compiled from published papers, publicly available databases, geological survey reports, and academic dissertations. The database offers several advantages: (1) a systematic and complementary data model aligned with the knowledge systems of igneous rock; (2) a broad range of data collected from diverse sources over a period of more than 50 years; and (3) an efficient platform for searchability and usability. This dataset is helpful to support a wide range of scientific research objectives related to igneous rocks in the Newfoundland Appalachians.

Background & Summary

Data- and model-driven scientific research has become a new paradigm[1–4]. Earth Science is developing towards Earth system science[5,6]. Therefore, collecting and sharing data, particularly establishing mutually sharable dataset, are crucial for accelerating and facilitating innovative geological research[7,8]. The Deep-Time Digital Earth (DDE)[9], a program sponsored by the International Union of Geological Sciences (IUGS), aims to compile deep-time Earth data, share global geoscience knowledge, and facilitate data-driven discovery to enhance our understanding of Earth's evolution.

Igneous rocks are the major constituent of Earth's lithosphere. Geochemical, geochronological, and geospatial data for igneous rocks have been widely used to reconstruct plate tectonic histories[10,11], study continental growth[12–14], investigate material recycling[15–17], and explore metallogenesis[14,18]. The DDE petrology working group, also known as DDE-OnePetrology, is constructing a global igneous rock database with an integrated research platform to support data-driven research of igneous rocks (https://dde.igeodata.org/)[19].

The igneous rock dataset of the Newfoundland Appalachians is integrated into the database that has been established on DDE-OnePetrology[19]. This dataset comprises detailed and updated data for the igneous rocks in Newfoundland. Several global databases have presented some data of the igneous rocks in Newfoundland, including GEOROC[20] (https://georoc.eu and EarthChem[21] (https://www.earthchem.org/). Additionally, the Geoscience Atlas[22–24] (http://geoatlas.gov.nl.ca) has provided a public online portal for accessing geoscience data for Newfoundland and Labrador. These databases have significantly contributed to the research of igneous rocks. However, they primarily present raw data, and many entries lack information on ages, precise locations (coordinates), geological or tectonic background, and the geochemical parameters used to calculate the isotopic values. This limitation restricts the effective use of the data in practical research. Therefore, it is necessary and significant to establish a comprehensive dataset that integrates all these critical pieces of information for the igneous rocks of the Newfoundland Appalachians.

The Newfoundland Appalachians (Newfoundland Island) represents one of the most complete and best exposed cross-sections through the Appalachian mountain belt[25] (Fig. 1a,b). Some researchers[26–29] have divided Newfoundland from west to east into the Humber margin, Dashwoods, Ganderia (i.e., the Penobscot and Popelogan–Victoria [PPV] arcs and Gander margin), and Avalonia (Fig. 1b,c). The five tectonic units are now juxtaposed along the Baie Verte-Bromopton Line (BBL), Beothuk Lake Line (BLL; formerly the Red Indian Line), Dog Bay Line (DBL), and Dover-Hermitage Fault (DHF), respectively (Fig. 1b,c). Progressive accretion of

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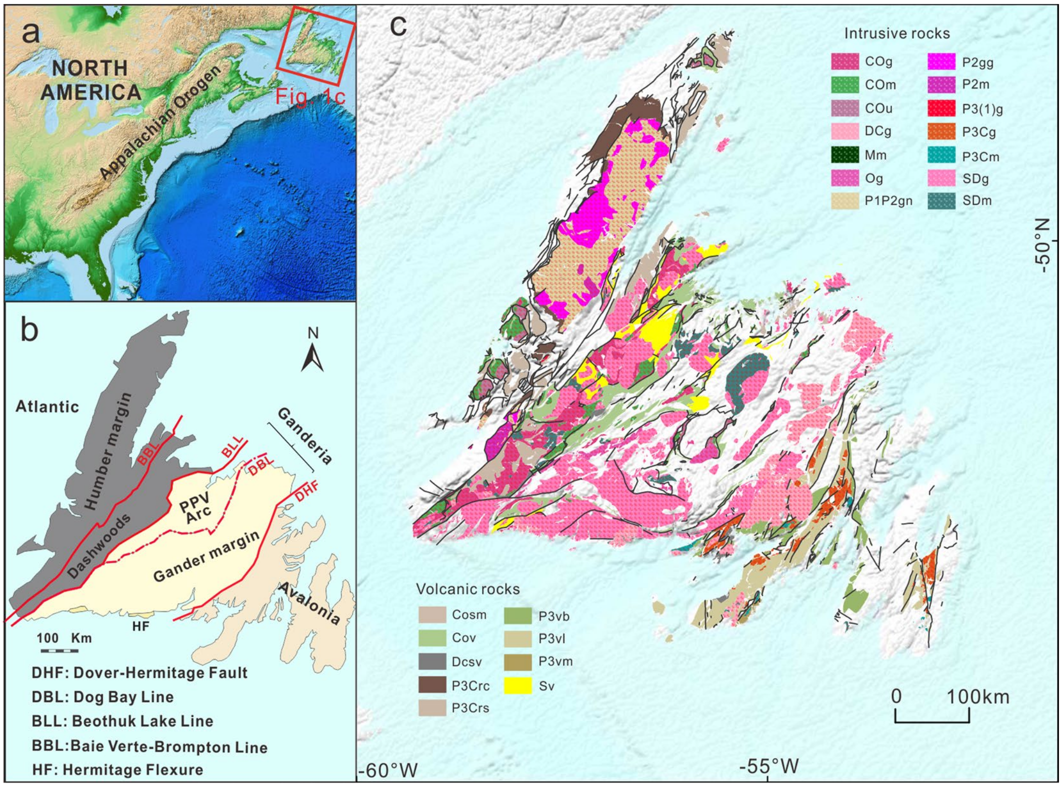

Fig. 1 (**a**) Location map of Newfoundland. (**b**) A simplified tectonic map of the Newfoundland Appalachians[30]. (**c**) A map of igneous rocks in the Newfoundland Appalachians[43].

these peri-Laurentian and exotic peri-Gondwanan elements to Laurentia is thought to have formed a composite Laurentia[30]. The BLL forms the tectonic boundary between the peri-Laurentian and peri-Gondwanan tectonic elements and is considered to represent the main Iapetan suture[29,31–33]. Newfoundland Island is an excellent region to research the progressive orogenesis of the Appalachians, including the early to late Ordovician Taconic (~500–450 Ma), the early to late Silurian Salinic (~450–420 Ma), and the latest Silurian to middle-late Devonian Acadian (~440–370 Ma) orogenic cycles[30]. The Salinic and Acadian orogenic cycles partly overlapped temporally due to coeval convergence in two separate oceanic basins[29]. These orogenic processes record the evolution of the outboard peri-Laurentian and peri-Gondwanan terranes that were progressively accreted to composite Laurentia with the closures of the Iapetus and Rheic Oceans and several associated marginal seaways[29,30,33,34].

The widespread igneous rocks of Newfoundland cover a time range of 1,500 Myr, extending from the Mesoproterozoic basement in the western Grenville Province[35,36] to the Tithonian lamprophyric rocks in the Notre Dame Bay[37,38]. The igneous rocks constitute over 58% of the island's surface, with intrusive rocks covering ~43,000 km^2 and volcanic rocks covering ~20,000 km^2. Numerous studies have been carried out on the age, petrogenesis, tectonic significance, and mineralization (e.g., Cu-Au, Zn, and W-Sn-Mo) of the igneous rocks in Newfoundland[39–48]. Thus, Newfoundland provides an excellent region for the construction of an igneous dataset and upon which igneous rock research can be tested.

This paper introduces a new database with emphasis on the dataset for igneous rocks of the Newfoundland Appalachians. The dataset integrates diverse data of igneous rocks from all available resources. It also provides a simple, queryable platform for plotting lithogeochemistry data of igneous rocks in Newfoundland.

Methods

Igneous rock data encompass a broad range of geological aspects, including geochronology, petrology, geochemistry, and isotopes. Systematically extracting and compiling diverse information remains a significant challenge[49]. Source data were found by searching Google Scholar using keywords as listed in Supplementary Table 1. We collected data manually and also employed digital techniques including the GeoGPT tool (https://geogpt.zero2x.org)[50] to compile data from published papers, publicly available databases, geological survey reports, and academic dissertations. We selected over 40 potential literature or website sources that contain data on igneous rocks in the Newfoundland Appalachian. The compiled data were checked and de-duplicated and then exported to Excel. Finally, the data were integrated into our specialized DDE-OnePetrology platform[19], facilitating easy access for researchers.

Data model construction. Our data model was designed to compile diverse igneous rock data of the Newfoundland Appalachians and to inter-operate with existing igneous rock databases[7,21,51–53]. The model, structured with samples as the core, consists of six modules (144 fields): general information, petrology,

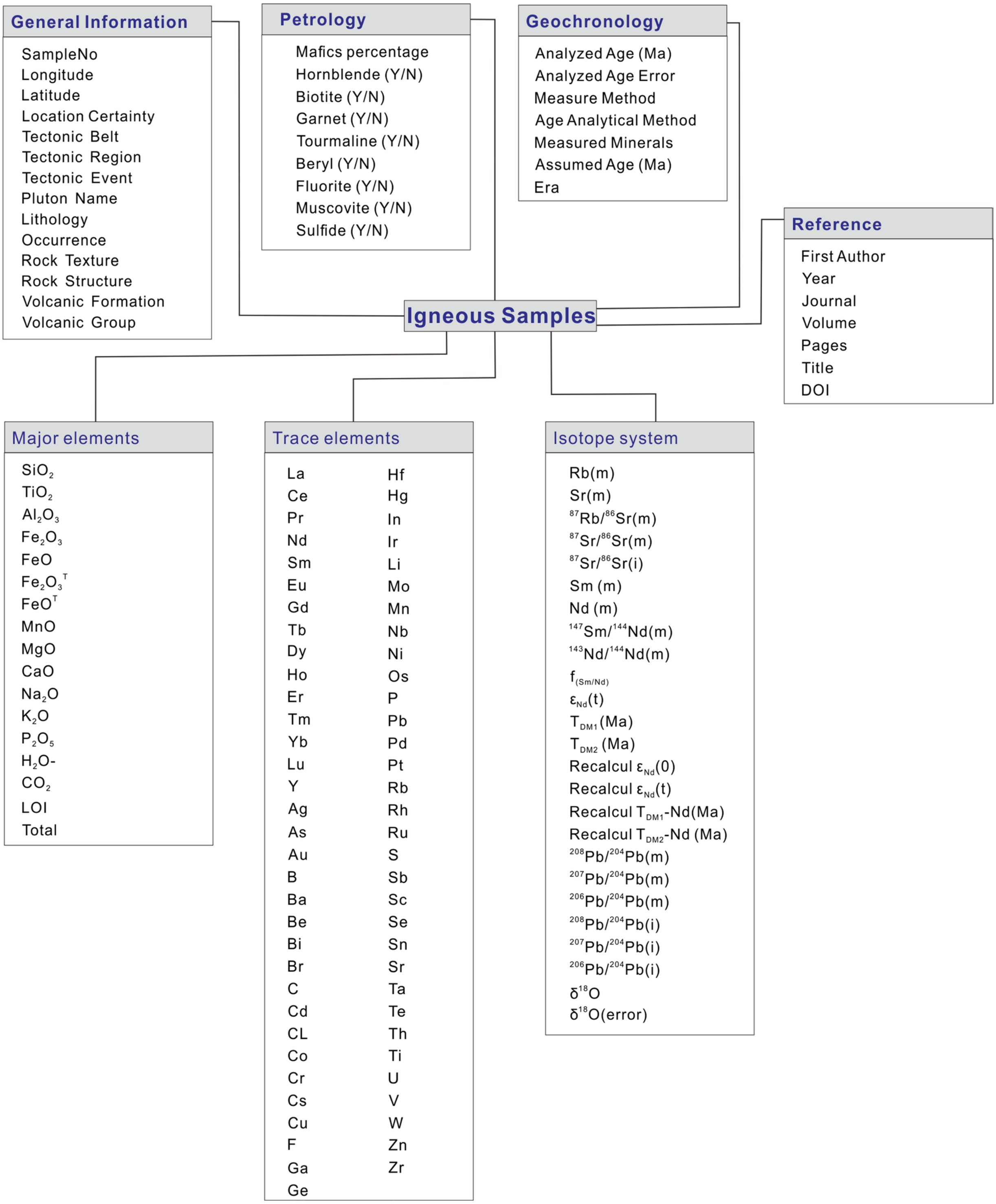

Fig. 2 Data relational model in the dataset. All field names are described in detail in the Supplementary Table 2.

geochronology, major elements, trace elements, isotopes and references (Fig. 2). General information includes geographic details, rock classification, and data sources. Sample locations were expressed using the WGS 84 reference coordinate system and recorded in decimal–degree format. The location is expressed as the "Location Certainty" field. This field has two choices: "Measured" and "Estimated". The former is to be filled with coordinates of data provided in the source. The latter is to be filled with coordinates that were estimated from sample points on geological maps. We also have a tectonic unit classification in the data model. This classification follows the latest tectonic unit classification scheme[26,30] and designates tectonic event classifications to the majority of samples. These samples are considered to comprise rocks of the Appalachian orogen and are categorized into three major tectonic events: Taconic, Salinic and Acadian orogenic cycles. The petrological characteristics of

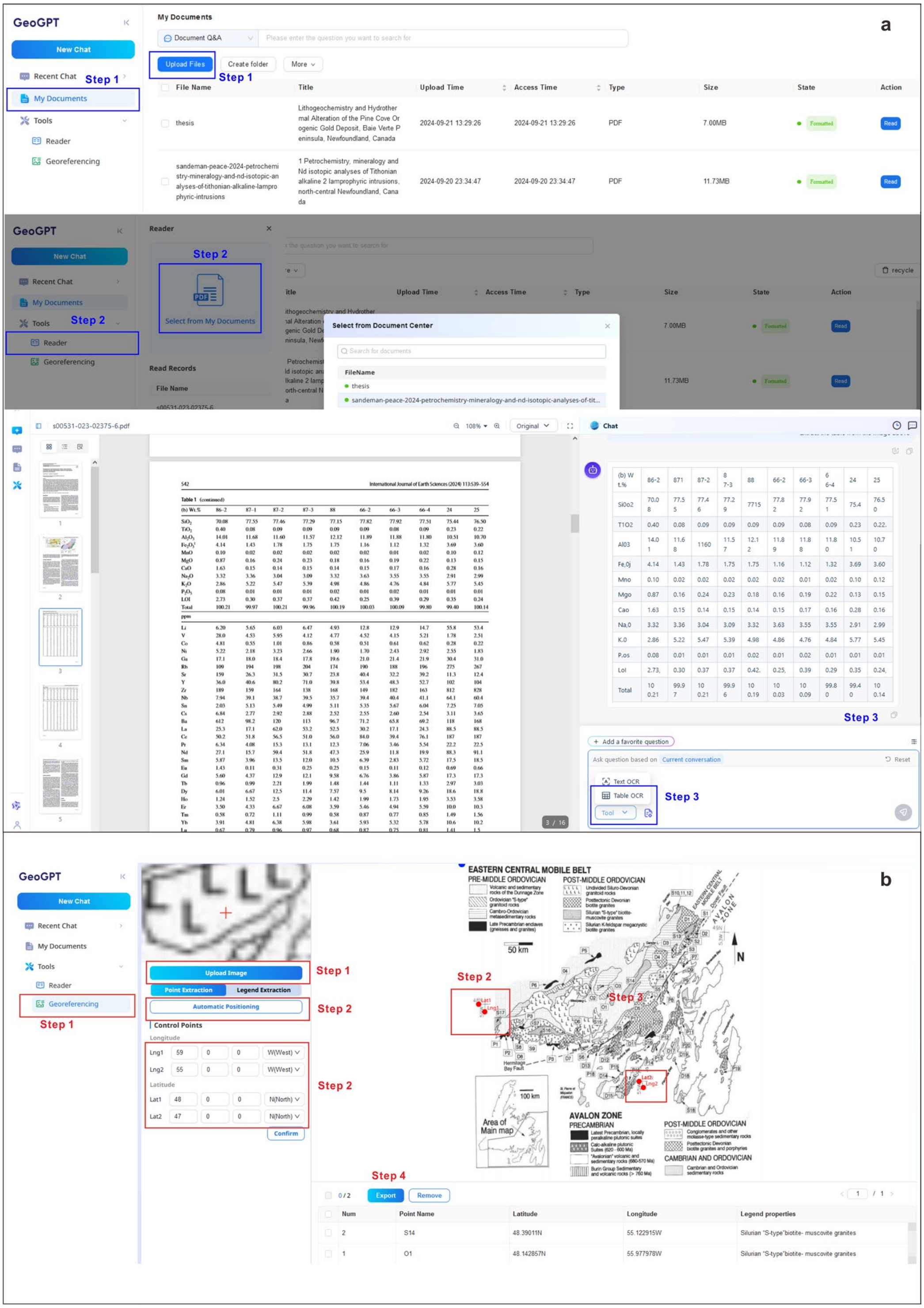

Fig. 3 (**a**) The process of table extraction by GeoGPT. (**b**) The process of coordinate extraction by GeoGPT.

the samples, including the mafic mineral percentage and the occurrence of minerals such as hornblende, garnet, muscovite, and sulfide, are cited from the online Newfoundland and Labrador Geoscience Atlas (https://gis.geosurv.gov.nl.ca/). These minerals play a critical role in the study of igneous rock types, the petrogenesis of igneous rocks, and may have implications for mineralization. Sample ages mostly refer to the zircon crystallization ages (in Ma) of igneous rock samples based on the interpreted age in the data sources. Age errors, which were not consistently reported at the 2σ level, are consistent with the data source. Many samples have only geochemical data, and few have been geochronologically constrained. An accurate and precise age is crucial for a study of the timing and evolution of magmatism. Therefore, we have attempted to add appropriate ages for all these data. Some are measured data cited from sources. Others were estimated from the ages of contemporary igneous rocks

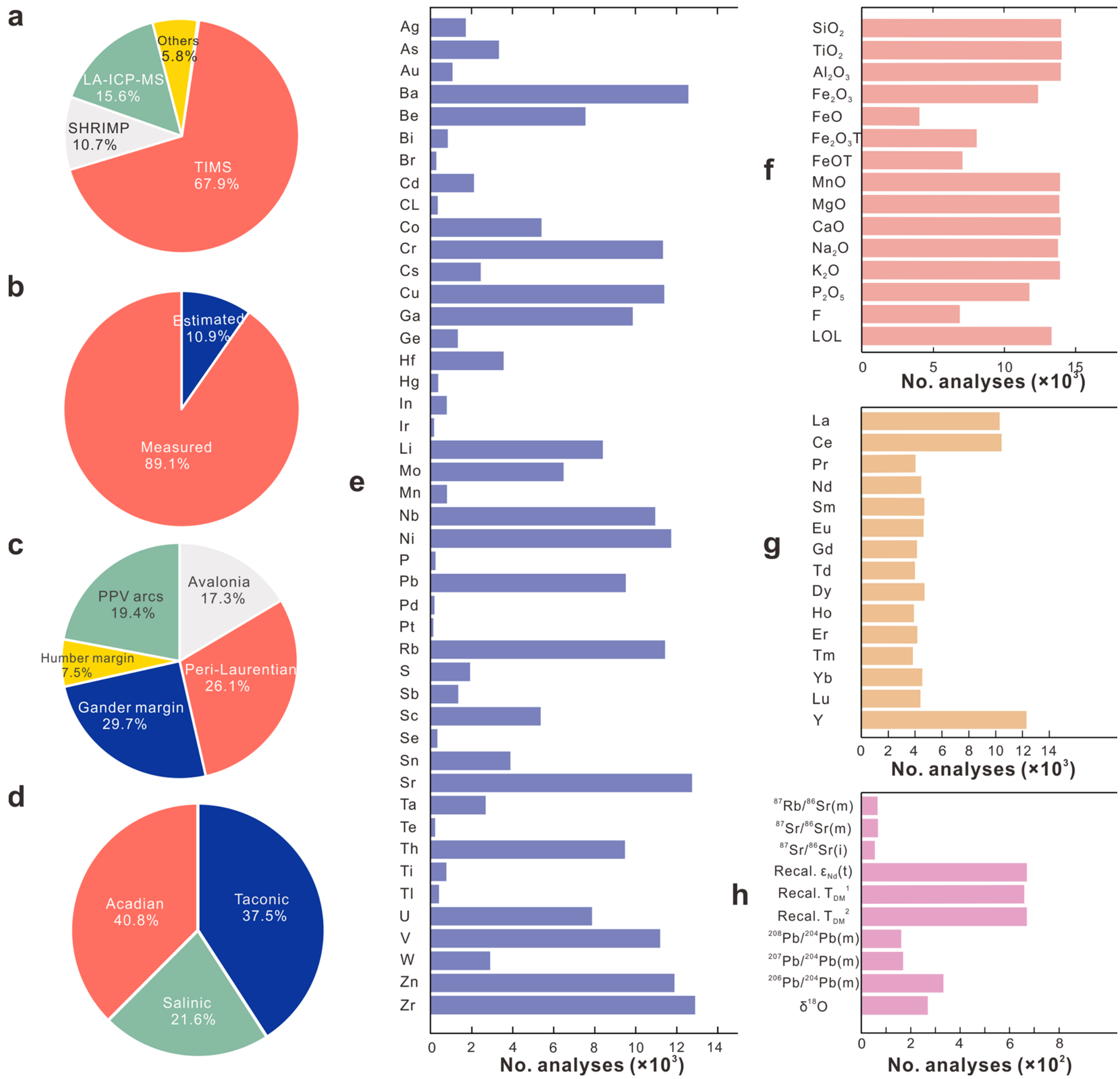

Fig. 4 Pie charts of the core data records: (**a**) Chronological analysis methods, (**b**) Location Certainty, (**c**) Tectonic Belts, and (**d**) Tectonic events. Histogram of analyses: (**e**) Trace elements, (**f**) Major elements, (**g**) REE elements, and (**h**) Isotope ratios and epsilon values.

in the same location. Major elements are reported in weight percent oxides (wt.%) and trace elements in parts per million (ppm = μg/g). Where applicable, trace element normalization values are from McDonough and Sun[54]. For the Sm-Nd isotopes of the samples, we have retained the original data from the literature as much as possible. We used the chondritic values [$(^{143}Nd/^{144}Nd)_{CHUR} = 0.512638$ and $(^{147}Sm/^{144}Nd)_{CHUR} = 0.196753$[55,56]] to recalculate $\varepsilon_{Nd}(t)$ values and depleted mantle Nd model ages (one-stage = T_{DM1}; two-stage = T_{DM2}; Supplementary Table 2). The $\delta^{18}O$ values are reported in per mil (‰) relative to Standard Mean Ocean Water (SMOW). In this study, references follow the APA (American Psychological Association) citation style, with sources obtained from the Google Scholar search engine.

Table and coordinate extraction. The rapid growth in data production has not been matched by advancements in automating the data collection process, particularly in the geosciences. While some scholars have explored the use of machine learning to handle large datasets, balancing efficiency with data quality remains a challenge[43,44]. To address this, we combine automated and semi-automated techniques, including GeoGPT[50], for data extraction and georeferencing. This approach enhances the construction of an igneous rock dataset, enabling more effective data processing. We utilized GeoGPT to streamline the extraction of data tables from the literature, significantly reducing the time and effort typically required for manual data compilation. The process is initiated by selecting and uploading PDF documents for digital parsing. GeoGPT's built-in OCR (Optical Character Recognition) capabilities then enable automated table extraction. To output the data into an Excel-compatible

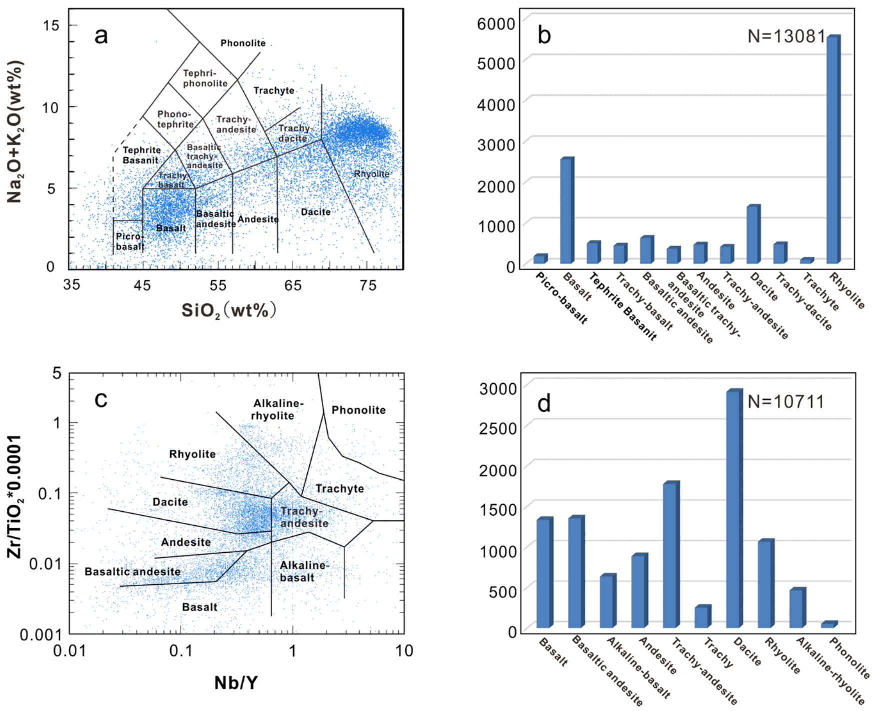

Fig. 5 Rock-type classification information. (**a**) TAS igneous classification[60]. (**b**) Histogram of rock types according to the TAS diagram. (**c**) The Nb/Y-Zr/TiO_2*0.0001 diagram[61]. (**d**) Histogram of rock types according to the Nb/Y-Zr/TiO_2*0.0001 diagram.

format, the user highlights the tables of interest, which are converted into editable data sheets for further analysis (Fig. 3a). This method balances automation with the need for accuracy, ensuring both efficiency and data integrity. Moreover, accurate spatial information is crucial when visualizing and analyzing magmatic rock data, particularly in tectonic studies. Spatial analysis allows researchers to constrain magmatic activity and understand potential migration patterns. For samples lacking precise geographic coordinates in their original sources, GeoGPT's georeferencing function provides a solution. The tool extracts latitude and longitude data from images, geological maps, and other visual sources. This process involves uploading an image, pinpointing relevant locations, and exporting the derived spatial coordinates into the dataset (Fig. 3b). Manual adjustments can be made to ensure accuracy where needed. These automated techniques for data extraction and georeferencing are integral to constructing a high-quality igneous rock dataset. By combining efficient data collection with accurate spatial analysis, our approach ensures that the dataset serves as a reliable tool for ongoing geological research, particularly in the study of the Newfoundland Appalachians.

Data Records

The dataset for igneous rocks of the Newfoundland Appalachians, along with other relevant files, is available as open access via Zenodo Data (https://doi.org/10.5281/zenodo.15043586)[57]. The supplementary materials include three tables: (1) Keywords and references for searching data, (2) Detailed description of the column headers, and (3) The igneous rocks of the Newfoundland Appalachians. This section provides a brief overview of the core data of the dataset, highlighting its value to users.

Geochronology. The geochronological information contains 546 age records. Among them, most age data are obtained from U-Pb dating, with analytical methods including high-precision thermal ionization mass spectrometry (TIMS), laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS), and sensitive high-resolution ion microprobe (SHRIMP), among others (Fig. 4a). The most age samples are associated with the Taconic, Salinic, and Acadian orogenic cycles. These entries represent the most comprehensive collection of geochronological data, providing valuable insights into the different orogenic cycles between the Laurentian and Gondwana continents[29,58,59].

Location information. Although GeoGPT extracted latitude and longitude data for only 10.9% of the samples, most entries already had precise spatial information, ensuring high accuracy in sample location data (Fig. 4b). The distribution of igneous samples across tectonic units is noteworthy. Samples from the Humber margin, Peri-Laurentia (Dashwoods), PPV arcs, Gander margin, and Avalonia account for 7.5%, 26.1%, 19.4%, 29.7%, and 17.3% of the total dataset, respectively (Fig. 4c). These figures reflect the varying intensity of research devoted to different tectonic regions. In addition, igneous rock samples related to the Taconic, Salinic, and Acadian orogenic cycles represent 37.5%, 21.6%, and 40.8% of the dataset (Fig. 4d), which aligns closely with the extent of exposed igneous rocks from each cycle.

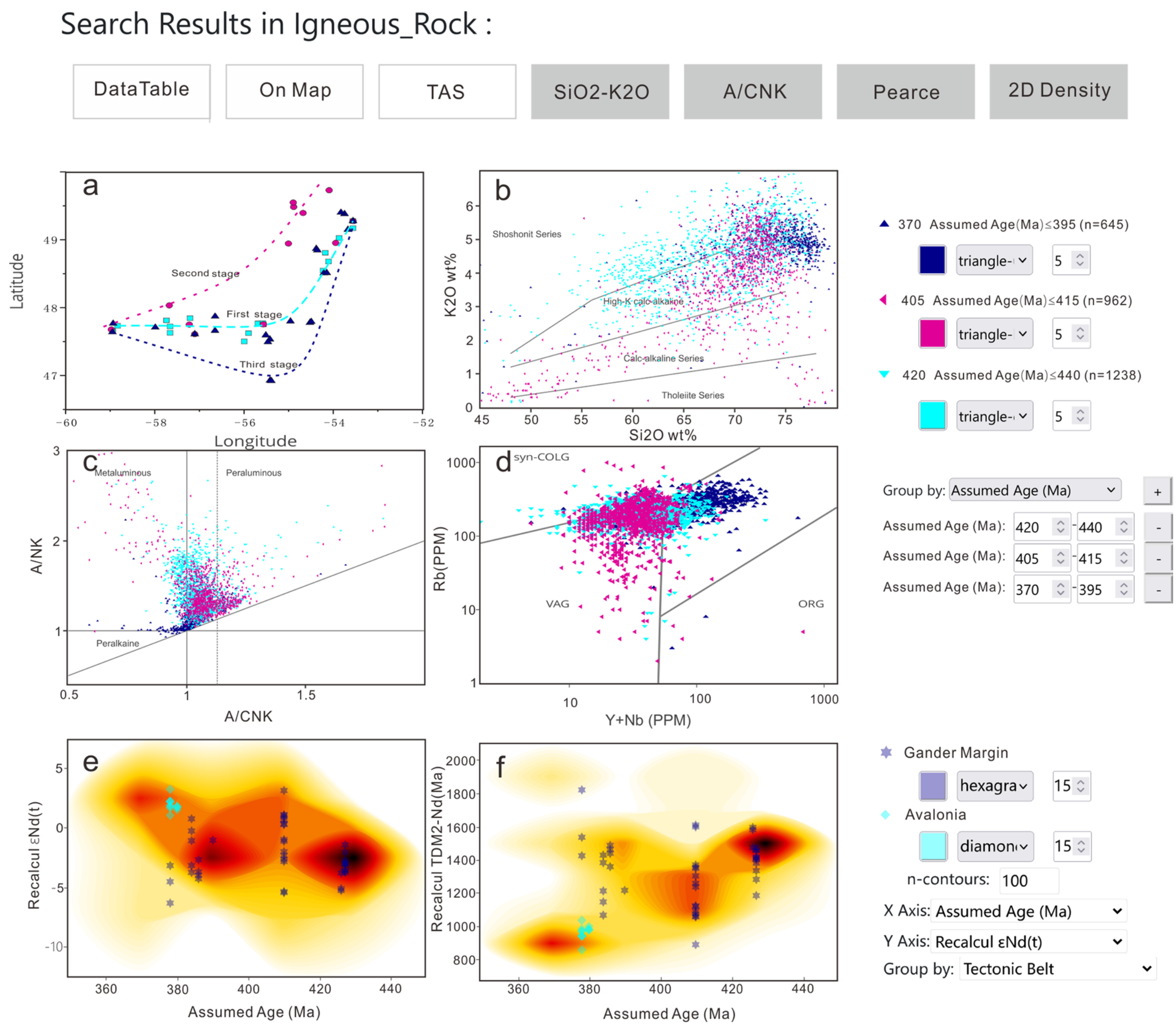

Fig. 6 The examples of using dataset. (**a**) Spatial variation of data. (**b**) SiO_2–K_2O diagram[62]. (**c**) A/NK–A/CNK diagram[63]. (**d**) Pearce diagrams[64]. (**e–f**) 2D density diagrams of age–ε_{Nd}(t) and age–T_{DM2}.

Major, trace, and isotope data. The geochemical diversity within the dataset reveals significant differences in the major, trace, and isotope data recorded across samples. The number of fields for major elements and some trace elements such as La, Ce, Ba, Cr, Cu, Ga, Nb, Ni, Ba, Rb, Sr, V, Y, Zn, and Zr, all exceed 10,000 records (Fig. 4e-g). Isotope data, primarily sourced from recent literature, have been standardized, ensuring consistency. Among the isotope data, over 600 entries of Sm-Nd isotope records are notably more abundant than those for Rb-Sr, Pb, and O isotopes (Fig. 4h), offering a robust representation of available geochemical information.

In conclusion, the dataset provides a comprehensive resource for understanding the magmatic history of the Newfoundland Appalachians. By integrating a wide range of lithologic, geochemical, isotopic, and geochronological data, this dataset supports a variety of scientific research objectives. Its extensive spatial coverage and the inclusion of precise geochronological and isotope data make it a valuable tool for studying orogenic processes and tectonic evolution in the region.

Technical Validation

Data validation is a crucial step in ensuring the accuracy and reliability of the igneous rock dataset for the Newfoundland Appalachian. We verified the consistency of the dataset using the key geochemical fields of SiO_2 (wt%), Na_2O (wt%), and K_2O (wt%) to classify rock types based on the Total Alkali-Silica (TAS) scheme[60] (Fig. 5a). This approach allowed for systematic identification and validation of igneous rock names (assuming volcanic origin), thus ensuring the classification aligns with established geological standards. Following the classification process, we conducted a statistical analysis of 15,202 samples. The results revealed that samples classified as rhyolite are dominant, with over 5,000 samples (Fig. 5b). Additionally, dacite, subalkalic basalt, and alkalic basalt samples each accounted for more than 1,000 entries (Fig. 5b). In additions, the Nb/Y–Zr/TiO_2*0.0001 diagram[61] was also plotted, again using volcanic rock terminology (Fig. 5c). This diagram is generally considered to be effective for assessing the original nature of altered or metamorphosed volcanic rocks[61]. As shown in Fig. 5d, more than 2500 out of 10,711 samples fall mainly within the dacite field, whereas the fields of basalt, basaltic andesite, trachy-andesite and rhyolite have more than 1,000 entries. These distributions reflect the extensive presence of both volcanic and plutonic rocks of rhyolitic and dacitic composition on the island and dataset aligns with known geological characteristics of the Newfoundland Appalachians. These findings underscore the region's complex magmatic history and highlight the importance of felsic magmatism (both volcanic and plutonic) in shaping the island's geological framework. The large volume of basaltic plus andesitic rocks further provides key information for constraining tectonic settings and helps establish the role played by directly mantle-derived magmas[29,34]. The reader is referred to these data sources for much more comprehensive interpretations of the rock types in specific areas of our dataset.

Usage Notes

Our dataset has been integrated into the DDE-OnePetrology platform to enhance its application value (https://dde.igeodata.org/subject/detail.html?id=67). The platform enables multidimensional data retrieval and analytical functions[19]. Through systematic sample classification, our high-quality dataset demonstrates clear distribution patterns on the analytical platform (Fig. 6a-f). This evidence also indicates its strong potential to facilitate research reproducibility via traceable metadata and support novel scientific discoveries.

Code availability

The code developed for this database is available in the GitHub repository (https://github.com/dingyichina/OnePetrology). Additional code that contributed to the development of DDE-OnePetrology is also available in this repository.

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Tao Wang designed the research. Chaoyang Wang and Tao Wang wrote the paper. Chaoyang Wang drew Figures. Yi Ding wrote the code and curated the database. Cees R. van Staal, Zengqian Hou, Ying Tong, and Shoufa Lin contributed to the concept development and refinement of the final presentation.

Competing interests
The authors declare no competing interests.

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