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## Managing geochemical data within the U.S. Geological Survey: An overview of policies and approaches from the perspective of the Energy Resources Program

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The mission of the U.S. Geological Survey (USGS) Energy Resources Program (ERP) is to provide unbiased scientific information to stakeholders by conducting and disseminating research into energy-related issues mandated by the Administration or Congress or guided by ERP and USGS leadership. USGS Fundamental Science Practices (FSP) form the foundation for these efforts, representing a set of consistent procedures, ethical requirements, and operational principles that direct how research activities are conducted to ensure the highest standard of scientific integrity and transparency. Policies created to meet the goals of FSP guide how work is performed and how resulting information products are curated through the development, review, and approval processes. Though FSP have been a core part of the USGS mission since its inception, several new policies have been developed and implemented over the last decade related to data generation, management, and distribution to make practices, particularly those involving laboratory-generated geochemical data, more standardized and consistent across the USGS' different scientific mission areas.

The ERP has been at the forefront of implementing these policies, particularly those that relate to laboratory-based science. For example, a new USGS-wide Quality Management System (QMS) was initially rolled out in ERP laboratories. QMS quality assurance requirements for laboratories were developed to ensure generation of data of known and documented quality and to support a culture of continuous improvement. QMS requirements include controls on sample receipt, login, and storage; documentation of data generation methods and standard operating procedures for sample preparation and analysis; and quality control procedures around equipment calibration and maintenance and data acceptance criteria. Many of the requirements are currently being met in the Petroleum Geochemistry Research Laboratory (PGRL) through the use of a laboratory information management system (LIMS) which provides a centralized storage location for data recording, reduction, review, and reporting. Samples processed by PGRL are identified from login to reporting by a unique lab-assigned number. Data are reviewed by the analyst, a secondary reviewer, and the laboratory manager before being accepted or considered qualified to address issues identified during analysis. A similar documentation approach is also applied to new

research methods, experimental work, or modifications of existing processes.

Once reported to a submitter, geochemistry data are then interpreted and incorporated into USGS reports and other outside publications that are tracked using a single information product data system (IPDS). IPDS facilitates management of the internal review and approval processes for USGS information products. For geochemistry studies, data releases containing machine-readable laboratory-generated results along with associated metadata documentation typically accompany publications and have their own review and approval process. Once generated, data releases are given unique digital object identifiers for citation and access persistence, stored in Science Base, a Trusted Digital Repository for USGS products, and are made accessible through the USGS Science Data Catalog (<https://data.usgs.gov>). This collection of systems makes it possible for ERP personnel to collect, manage, and track geochemical data and facilitate the timely delivery of high-quality scientific publications and datasets to the public and support decision makers to manage domestic natural resources.