In Reply Refer To:
Mail Stop 911

October 27, 2015

Memorandum

To: Suzette Kimball, Acting Director, USGS
Dave Applegate, Acting Deputy Director, USGS

From: Alan D. Thornhill, USGS Bureau Scientific Integrity Officer and Director, Office of Science Quality and Integrity

Subject: Concerns regarding the Inorganic Section of the Energy Geochemistry Laboratory Inquiry

Herein, we transmit issues of concern (outside of the scope of the original allegation of loss of scientific integrity (SI)) that were revealed during an SI inquiry focused on allegations of data manipulation within the Inorganic Section of the Energy Geochemistry Laboratory inquiry (ESO-S0000422) that the USGS Office of Science Quality and Integrity (OSQI) conducted with the assistance of a Scientific Integrity Review Panel* (SIRP).

This memorandum is intended to provide a recommendation for the development of a Corrective Action Plan to investigate then promptly and completely address the concerns described below. It does not contain sufficient documentation to substantiate taking any management or personnel action.

In February 2015, the OSQI was contacted by the USGS Energy Resources Program, regarding a recent Energy Geochemistry Laboratory (EGL) Quality Assurance program report, EGLCAPA050, entitled: "Data traceability loss and manipulation of ICP-MS data." Although an internal investigation of this concern was underway by the EGL, we recommended that OSQI conduct an independent preliminary review of this concern. During the preliminary review, OSQI determined that the alleged misconduct was very similar to problems in the same laboratory for the period between 1996 and 2008 where a USGS report summarized that "data adjustment of raw data that exceeded 10% and/or was not constrained by an adequate number of control standards" and reported that this data issue had been resolved. The informal preliminary review completed in April 2015 determined that further inquiry was warranted. The OSQI therefore submitted a formal scientific integrity complaint to the DOI Office of the Secretariat, and for purposes of that complaint, identified the Center Director, Central Energy Resources Science Center, as the complainant. An SIRP was assembled by the OSQI and was charged with investigating the allegations of data traceability loss and manipulation of ICP-MS data.

Inquiry Finding of Loss of Scientific Integrity and Scientific Misconduct

Based on documentation provided by the OSQI and information gathered from the 2-day on-site visit, the SIRP determined that there has been a chronic pattern of loss of scientific integrity and scientific misconduct in the Inorganic Section - EGL, Energy Resources Science Center, Denver, CO. The SIRP concluded that ICP-MS data produced by the Inorganic Section - EGL were:

"...intentionally manipulated by the line-chemist, with conscious acquiescence and inattentiveness of others in the Laboratory and/or the Center's management. Data manipulation involved: 1) assembly of inappropriate (non-standard) determinations to be used as elemental standards during unknown-sample data collection; 2) global adjustments of standard elemental values obtained prior and during analytical sessions; 3) fabrication of elemental concentrations for samples submitted by researchers; and 4) fraudulent and negligent archiving of data in USGS databases. Laboratory procedures adopted in the Inorganic Section – EGL were considered by the SIRP to be abnormal and well outside common practices in other laboratories in the USGS, or as performed in other National laboratories, academic institutions, or in the private sector. The SIRP determined that over the past 7 years or so, the Inorganic Section - EGL's (b) (7)(C) [redacted] and line-chemist have shown a complete disregard for standard protocols practiced in reputable ICP-MS analytical facilities."

Inquiry Findings Beyond the Scope of the Allegation of Loss of Scientific Integrity

Laboratory Management/Personnel Issues

The inquiry revealed that management inattentiveness to preserving healthy working conditions in the Inorganic Section - EGL strongly influenced day-to-day operations of the facility and materially contributed to its sub- standard performance and loss of scientific integrity. Further, the inquiry concluded that the management of the Inorganic Section - EGL is "dysfunctional and broken", and that there is ineffective leadership at all levels within the Inorganic Section - EGL. There was no clear evidence of active oversight on the Inorganic Section - EGL's activities emanating from the current and past Central Energy Science Center Director's office, at least since 2008. The SIRP reported:

> "At a minimum, management has thus failed to provide, enact, and supervise timely and effective QA/QC protocols that were recommended in prior audits and a serious scientific integrity breach identified in 2008. Moreover, the interactions and communications between personnel involved with the Inorganic Section - EGL are plagued with mistrust and disrespect."

The SIRP further noted a complete breakdown in the lines of communication within the Inorganic Section - EGL and among its personnel, and the situation deteriorated even further after EGL's (b) (7)(C) [redacted] internally reported the data manipulation in October 2014.

The SIRP determined that the Inorganic Section - EGL has suffered from "chronic mismanagement and non-productive/dysfunctional inter-personnel relationships" that the SIRP grouped into the following main themes:

1) A pervasive "disconnect" and lack of communication between managers and technical staff;
2) Mistrust and resentment between management and technical staff; and
3) Willful supervisory neglect, along with a pattern of disengagement at higher levels of management.

It is apparent that the inappropriate activities by the line-chemist and (b) (7)(C) started as early as 2008 and have continued since. The pervasive scientific dysfunction in the Inorganic Section - EGL appears to have been widely known to other parts of the Science Center, such as members of other laboratories within the Energy Resources Science Center (e.g., Organic Section - EGL), and to end-users in Reston and Denver, since at least 2008.

The SIRP visited USGS locations in Denver that house the mass spectrometer, ancillary equipment, and sample preparation facilities that are part of the Inorganic Section - EGL. The SIRP reported that sites and equipment used for single-element analyses such as Hg or Se (unrelated to the ICP-MS effort) seemed adequate to perform the work. However, the specific location that houses the mass spectrometer currently used to do the ICP-MS work on coals and water in the Inorganic Section - EGL, is considerably substandard. The SIRP reported:

> "The lab space is reported to experience undesirable and periodic cycles of extreme temperature (up to mid 90° F), and high humidity fluctuations that most certainly induce extreme and significant drift in ICP-MS instrumental performance; consequently, the latter most certainly generate unacceptable analytical results that most likely require "massaging" or data manipulation beyond acceptable practices and protocols. Moreover, the ICP-MS Laboratory space and others in this part of the building are reported to experience periodic water leaks from the ceiling."

Of disturbing importance is when the SIRP asked the EGL manager if he was aware of Laboratory infrastructure deficiencies, he responded that the "lab was not any worse than other labs present at the Denver facility", and "that the poor lab infrastructure should not be used as an excuse to produce inferior quality data". These rather 'hands off' responses led SIRP members to believe that the EGL manager did not possess the necessary skills and expertise to lead a world-class ICP-MS facility. Moreover, sample handling prior to ICP-MS analysis is also deficient and not up to the common standards in the ICP-MS analytical community. Unacceptable open-beaker sample dilutions, handling of standard solutions and manipulation of acids and waters occur in an open, unprotected laboratory setting with exposure to settling dust and other contaminant particulates. Such procedures are unlike those used in most other National, academic, and private sector labs, which often house ICP-MS equipment in cleaner environments (Class 1000 labs or better) and perform sample preparation and dilution procedures in environmentally-protected conditions.

The SIRP found evidence that Laboratory management also failed to correct inappropriate personnel work habits, including attendance issues, verbal and other types of harassment by select Laboratory personnel ((b) (7)(C) and line-chemist), years after having been made aware of these issues. The SIRP concluded that:

> "...management failed to correct the overall toxic work conditions in the Laboratory, particularly as they affected (b) (7)(C) . (b) (7)(C) staff (b) (7)(C) reported inappropriate incidences involving use of offensive language and behavior."

The incidents, as related to the SIRP, did not appear to represent single events, which could be dismissed as anomalies. Rather, these inappropriate activities were described (by (b) (7)(C) numerous times to the EGL manager, but no apparent corrective actions were taken. The SIRP was informed by the EGL manager that the incident(s) were reported to him too late for corrective action to be taken. Also, consultation by the EGL manager with the Employee Relations office was futile because he was told that the Employee Relations office could not get involved. (b) (7)(C) also reported these incidents to the Employee Relations office and was also informed that the Employee Relations office was unwilling to be involved. Several interviewees emphasized that (b) (7)(C) was "flippant, difficult to work with, and prone to inappropriate behavior." The sequence of offensive behavior by several members of the Inorganic Section - EGL (line-chemist, (b) (7)(C) has interfered with the work performance of a staff member and as such constitutes peer-on-peer harassment. The SIRP concluded that management failed to protect the staff from unhealthy peer-on-peer pressure. Consequently, management did not correct and preserve a productive work environment for the Inorganic Section - EGL staff. The OSQI recommends the Deputy Associate Director for Human Capital further examine these allegations.

Quality Assurance/Quality Control (QA/QC) Procedures

The SIRP determined that the QA/QC issues are explicit in the performance expectations for the Inorganic Section - EGL personnel. In FY14, the line-chemist received a minimally successful rating on his employee performance appraisal plan (EPAP). The line-chemist's FY14 EPAP notes multiple instances of data manipulation that violated QA procedures, which led to the minimally successful performance rating and a denial of a within-grade promotion by the EGL manager. Specifically, the line-chemist was warned in May 2014 to stop data manipulation, but the discovery of data manipulation in October 2014 clearly indicated that the practice continued. This begs the question of why the EGL waited until the October 2014 reporting of data manipulation to conduct its internal investigation. The line-chemist disclosed to the SIRP that in March 2015, the line-chemist received a Notice of Proposed Removal (proposed termination from Federal service) from the EGL manager based on data falsification during FY14. EPAP plans for FY13–15 are explicit about the responsibility for QA/QC by the physical scientists/chemists, and in FY15 appear to reflect the concerns of prior reports and performance evaluations. According to their FY13–15 EPAP critical elements, line-chemist was tasked with performing QC analyses and calibrations according to documented methods and practices, and preparing data for input into the Laboratory Information Management System (LIMS). During that multi-year period when data manipulation occurred, (b) (7)(C) in the Inorganic Section- EGL was tasked with reviewing and approving data to ensure that QA measures were satisfied, and was further responsible for confirming the validity of the data entered into the LIMS. Hence, the line-chemist and (b) (7)(C) (b) (7)(C) shared responsibility for the QA/QC process and data validation. During the period of data manipulation, the EGL manager's performance standards included development of a QA plan, periodic reports summarizing Inorganic Section - EGL performance and data quality issues, and reporting of any significant QA issues to the Science Center Director, but the performance standards did not include data verification.

Current Status of the Inorganic Section - EGL

It is my recommendation, and the unanimous counsel of the SIRP's, that the Inorganic Section – EGL be immediately and permanently shut down. The SIRP stated that, under the current conditions, there appears to be no portion of the Inorganic Section – EGL, in its current state that can be salvaged and ordered to resume work. The principal reasons for the SIRP recommendation are:

1). Irreparable Loss of Scientific Integrity/Reputation:

Given the Inorganic Section - EGL's prior serious history of loss of scientific integrity and data falsification during the period 1996-2008, and the claim that this issue had been resolved, combined with the current analogous situation, the SIRP found that serious and irreparable damage has occurred to the Inorganic Section - EGL's scientific credibility and reputation at both national and international levels. Based on the SIRP's interviews and interactions with previous and main end-users of the Inorganic Section - EGL, it is clear that none of them wish to use the facility in the future due to the Inorganic Section - EGL's pervasive history that led to substantial loss of scientific integrity. Moreover, the Organic Section - EGL also has suffered some "collateral damage" to its reputation as a result of the) of the EGL between 1996 and 2014. The Organic Section – EGL is an extremely productive, well-organized, and structured laboratory (under the stewardship of a senior (b) (7)(C) within the Section) that is successfully conducting important scientific research.

2) Outdated and Ineffective Cost Structure:

Previous end users are now using external, reputable, and certified ICP-MS analytical facilities that deliver high quality results at a fraction of the cost and with lower turnaround time (TAT). The SIRP reported that the Inorganic Section - EGL has processed an average of 576 samples a year between the period of 2009 and 2014 with a TAT of 224 days. The extensive TAT is completely unacceptable and much longer relative to those offered by commercial ICP-MS laboratories.

3) Ineffective Management and Irreconcilable Personnel Issues:

Based on the SIRP's interactions and exchanges with all of the personnel directly involved with the Inorganic Section - EGL, including current and previous Center Directors, the EGL manager, the Inorganic Section scientists, the SIRP clearly noted disengagement from standard operating procedures (SOPs) at all levels since at least 2008. The SIRP reported that the current Science Center Director has also been disengaged from the management and oversight of the Inorganic Section - EGL until the most recent report of loss of scientific integrity in October 2014.

The SIRP heard from several members of the Inorganic Section - EGL that the line-chemist lacked adequate expertise and knowledge with routine or rudimentary Microsoft Excel-based mathematical operations (i.e., freshman college-level).

The SIRP also heard of line-chemist's failure to understand the concept of macros within Excel, and how these worked within the new spreadsheet (emplaced in November 2013), which is used to determine elemental abundances from ICP-MS-based raw data. It was incomprehensible to the SIRP that the line-chemist was hired to work within an ICP-MS facility without possessing adequate Excel data processing

skills, which are of elementary importance to an analyst in this position. The SIRP does not endorse the line-chemist's excuse that data manipulation was unintentional and a result of his incomprehension of Excel-based macro operations. (b) (7)(C) claims that he was not aware of line-chemist's data manipulation between the period of 2008 and 2014; however, the SIRP found this claim somewhat disingenuous given the line-chemist and (b) (7)(C) close personal and professional inter-relationship, which dates back many years—to their time as co-workers at the USGS laboratory in Florida, prior to their present employment at the USGS Denver facility.

The SIRP was also informed of unprofessional behavior and conduct by Inorganic Section - EGL members. It is also clear to the SIRP that since the "whistleblowing" regarding the most recent loss of scientific integrity in October 2014, the inter-personnel relationships within the Inorganic Section - EGL have become even more strained, with feelings of mistrust and resentment present at all levels. Therefore, given the past and current issues between the Inorganic Section's personnel and management, it was the SIRP's unanimous opinion that this facility cannot reopen or restart operations with the current personnel in place since they are incapable of working together in an atmosphere of civility and cohesiveness that is required for operation of a world-class ICP-MS facility.

4) Mishandling and Lack of Implementation of Essential QA/QC Procedures:

Despite having undergone several audits and reviews by different panels and organizations (e.g. OIG, internal review)and the previous history of data manipulation within the Inorganic Section - EGL, it was surprising to the SIRP that remedial QA/QC protocols took so long to be drawn-up and implemented. In the opinion of the SIRP members, this should have been the Laboratory's first priority. The SIRP was informed by the Acting Associate Director- Energy Resources, of the new action taken by the Energy Program to put into place a Program-wide Quality Management System, which has been supervised by their analyst over the past couple of years on a part-time basis, and will also involve the hiring of a full-time QA person within the next couple of years. The Acting Associate Director informed the SIRP that this action will address one of the deficiencies listed in an OIG report that resulted from a prior investigation, and it will be the responsibility of the Science Center Director to ensure that implementation of this action is completed.

Although the Acting Associate Director and the EGL manager have attempted to address inadequate QA/QCs issues over the past 5 years and this should be commended, the SIRP unanimously agreed that this and other actions should have been implemented much sooner with more stringent control and oversight by the Laboratory's management (EGL manager and Science Center Directors since 2008). Regrettably, revision of QA/QC protocols and procedures were not accomplished in a timely manner, and now the Inorganic Section - EGL has suffered yet another serious setback to its already tarnished scientific reputation at both the national and international levels.

5) Inadequate ICP-MS Laboratory Infrastructure:

During its Denver on-site visit (August 12th and 13th), the SIRP had the opportunity to visit all of the Inorganic Section - EGL's related facilities. Although sample preparation areas, such as the weighing, crushing, and sieving areas, and sample digestion space were deemed adequate, the ICP-MS Laboratory

conditions are deemed completely inadequate and it lacks the standards expected of reputable ICP-MS laboratories worldwide. Among the most significant deficiencies cited are the following:

a) Complete lack of temperature and humidity controls – this most certainly had a significant effect on instrument drift throughout the course of any individual analytical session, which consequently would have required important normalization factor corrections on the acquired data;

b) Final standard/sample preparation was conducted in the ICP-MS instrument laboratory (neighboring the ICP-MS instruments), in an open atmosphere and not in a HEPA- filtered class 1000 (or lower) environment, which is the minimal norm in accredited and reputable ICP-MS laboratories worldwide. The Inorganic Section - EGL will never receive certification or respectable scientific credibility in its current physical condition;

c) Several of the Inorganic Section - EGL personnel questioned the purchase of the Nexion Instrument (from Perkin Elmer) in 2013 by the EGL manager. In their respective opinions, the Nexion is too sensitive and therefore requires excessive dilutions for trace element analysis of coal samples. SIRP members concur with these opinions, namely because there are other available High Resolution-ICP-MS instruments that have more flexibility relative to acquiring larger ion signals via the use of an added Faraday collector (Element2 XR ICP-MS from Thermo Scientific), or automated ion signal attenuation filter (Attom ICP-MS from Nu Instruments). The purchase of the Nexion ICP-MS instrument by the EGL manager may indicate his lack of appropriate expertise in the field of ICP-MS technology, and confirms statements made by several individuals interviewed during the SIRP's Denver on-site visit.

In addition to the recommended closure of the Inorganic Section - EGL, the SIRP further recommended that the Organic Section - EGL (analytical services) join the Organic Geochemistry Laboratory (research unit), which is currently under separate supervision. Although this separate laboratory is more research-oriented, there is sufficient overlap between both groups in terms of instrumentation and techniques/analytical methods. As a former member of the analytical services Organic Section- EGL, the research lab supervisor understands its structure and operations, and is therefore the ideal research scientist for its oversight. Management will also need to ensure that an effective funding strategy is in place to meet the needs of this newly merged Organic Geochemistry Laboratory.

Impact on Published Research and the Science Community

This most recent breach involving both a loss of scientific integrity and scientific misconduct within the Inorganic Geochemistry Laboratory of the EGL, which was the focus of the SI inquiry, has severely affected and hampered production of scientific publications for end users. Of utmost importance, the science community at-large and end users (and respective collaborators) of the ICP-MS facility within the Inorganic Section - EGL require immediate and effective notification of the fraudulent data produced during 2008 and 2014. Currently, the USGS Energy Resources Program has posted on its website an announcement entitled, "Quality Assurance Update" (http://energy.usgs.gov/GeochemistryGeophysics/GeochemistryLaboratories.aspx#3898252- data),

which describes the nature of the data breach that occurred between 1996 and 2008. Given the current situation described in this memorandum, this announcement is no longer applicable and should be removed. The exact manner in which the data was fraudulently manipulated within the Inorganic Geochemistry Laboratory cannot be reproduced and adequately explained; it is also impossible to determine the exact number of analyses that have been compromised. Therefore, the SIRP recommended that management respond to this current scientific integrity breach in two ways:

1) Contact affected end users and inform them that their 2008-2014 ICP-MS results are suspect, and therefore any published journal articles containing suspect ICP-MS data should carefully be evaluated and possibly retracted, and
2) The Energy Resources Program should immediately place an announcement on their web site indicating that the ICP-MS facility of the EGL is closed for the foreseeable future.

Considerations for Future Reopening of the Inorganic Section – EGL

If the USGS Energy Program decides to re-open the ICP-MS facility in the future, the SIRP's additional recommendations should be considered, to facilitate enabling the Inorganic Section - EGL of the EGL to attain a viable scientific program and peer respectability. These additional SIRP recommendations are as follows:

1) Replacement of all current Inorganic Section - EGL personnel with the possible exception of the analyst scientist. If the Inorganic Geochemistry Laboratory is re-opened, then the new personnel in place should be completely vested into the laboratory's operations and this new personnel would include a [redacted] (b) (7)(C) [redacted] that interacts with the laboratory scientists and chemists on a daily basis and effectively communicates with the Center Director at regular (weekly/monthly) intervals.

2) Current Inorganic Section - EGL infrastructure and conditions are unacceptable. Consider moving the entire Inorganic Section - EGL facility to Reston, VA since this is the location of most of the end users of the ICP-MS facility, and only if credibility can be regained, and only after a comprehensive cost-benefit analysis indicates the Laboratory is viable, and only if appropriate infrastructure and leadership in Reston can be identified.

3) The Inorganic Section - EGL will require complete restructuring so management has a direct stake in the success of the Laboratory. Viability also requires the strict implementation of SOPs and QA/QC protocols and procedures, including the employment of a QA/QC assessor external to the ICP-MS facility. This should include periodic internal (several times per year) analyses of blinds/standards and participation in the external CANSPEX round robin program WITHOUT the prior knowledge of sample/standard background submission information.

4) The Inorganic Section - EGL infrastructure must be upgraded to acceptable standards similar to those used in ICP-MS laboratories worldwide. This includes housing the ICP-MS instrumentation in a temperature and humidity controlled area that is supplied with HEPA- filtered air (minimum class 1000

environment), and under positive pressure to eliminate or render instrument drift negligible, and significantly reduce possible contamination from the ambient atmosphere.

***The SIRP membership included:**

- USGS Senior Research (b) (7)(C), Ph.D.
- USGS Senior Research (b) (7)(C), Ph.D., lead in a major USGS (b) (7)(C) with (b) (7)(C) background.
- USGS Senior Research (b) (7)(C) Ph.D., lead of (b) (7)(C) (editor of major science journal)
- Associate Professor (with tenure), Department of Environmental Engineering and Earth Science at a major US University, Ph.D., research and courses taught include (b) (7)(C), (b) (6)