NIST Data Collection Instruments
NIST DCI 005

Practical Guide for Collecting Feedback from NIST SRM & RM Users

Survey Development Process

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The NIST Data Collection Instruments series includes questionnaires or survey instruments, interview guides, and other structured means of collecting data. Some of these instruments are designed for human subjects research focused on households, social institutions, and businesses. The instruments are approved by both NIST Institutional Review Board (IRB) and OMB/Paperwork Reduction Act.

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Abstract

One way NIST ensures that measurements are accurate and compatible is by certifying and providing over 1 300 Standard Reference Materials® (SRM®) with well-characterized composition, properties, or both. Customers use these materials to calibrate instruments, verify specific measurements, and develop new measurement methods. However, sales data alone is insufficient to determine when to update or restock these materials. Collecting customer data systematically can help in making informed decisions and reducing waste and missed opportunities.

In 2023, NIST SRM 1950, Metabolites in Frozen Human Plasma, had a supply remaining for approximately 4 years. A decision was needed on whether to renew SRM 1950 and/or develop new reference materials in the coming years–a process that typically takes 5 to 7 years. The Information Technology Laboratory (ITL) Information Access Division (IAD) and the Material Measurement Laboratory (MML) Chemical Sciences Division (CSD) collaborated to conduct an online customer and stakeholder survey following an established and rigorous methodology. The survey development process and the artifacts produced can serve as a model for future measurement services projects to gather market research data and inform planning and development in a repeatable and consistent way.

This document provides a practical, step-by-step guide to the survey development process for collecting feedback from users and customers of NIST reference materials. It aims to provide concise guidance, complete with artifacts and templates, using the 2023 NIST SRM 1950 customer feedback survey project to illustrate how to conduct a user feedback survey following an 8-step survey development process. This practical guide outlines a process for developing surveys to incorporate stakeholder feedback into decision-making for new measurement service projects, which can be reused or adapted.

Keywords

Survey instrument; survey development process; Reference Materials (RM); stakeholders; Standard Reference Materials (SRM).

Table of Contents

List of Figures

BACKGROUND

One way that NIST supports accurate and compatible measurements is by certifying and providing over 1 300 Standard Reference Materials® (SRM®) with well-characterized composition, properties, or both. Customers use these materials to perform instrument calibrations as part of overall quality assurance programs, verify the accuracy of specific measurements, and support the development of new measurement methods. NIST currently provides six named types of "reference materials" intended to be used as measurement standards: primary standards (PSs), Standard Reference Materials (SRMs), Research Gas Mixtures (RGMs), NIST Traceable Reference Materials (NTRMs), Reference Materials (RMs), and Research-Grade Test Materials (RGTMs) [1].

While sales information regarding "reference materials" is known (for example, average units sold per year), this information is insufficient to determine when, what, and to what extent updates such as renewals or restocks should occur. A systematic and scientific method of collecting customer data can more precisely inform decision-making and minimize potential material waste and missed opportunities.

SRM 1950 Metabolites in Frozen Human Plasma was first made available in 2011 and sold an average of 285 units/year, within the top 15 SRMs for sales in FY21. The material is value-assigned for 90 components, mainly based on NIST Reference Measurement Procedure measurements and other higher-order method measurements at NIST. SRM 1950 initially required intense staff and instrumental resources to value assign many components and continues to need these resources to maintain the material through stability testing. While the material currently provides SI-traceable values for many components, it is yet to be known whether customers are utilizing these values to establish accuracy or traceability. Many of these measurands are also value assigned in similar serum SRMs. In addition, multiple publications by NIST authors and others outside of NIST have demonstrated that metabolomic/lipidomic communities have used SRM 1950 as a common research material independent of its assigned values.

In 2023, SRM 1950 had an approximate 4-year supply remaining, and a decision needed to be made on whether to renew SRM 1950 and/or develop new reference materials in the coming years–a process that typically takes 5 years to 7 years. A collaborative effort was formed between the Information Technology Laboratory (ITL) Information Access Division (IAD) and the Material Measurement Laboratory (MML) Chemical Sciences Division (CSD) to conduct an online customer and stakeholder survey by engaging the SRM 1950 user community to understand what portions of the ninety value-assigned components have been used (or not used) and to collect customer requirements and needs for updating or developing SRMs. The survey project will be coded as the ***2023 NIST SRM 1950 Customer Feedback Survey*** throughout this document.

Collaboratively, ITL-IAD provided survey development expertise related to survey question development, survey software tools, survey fielding, and data analysis following an established

methodology and process with replicable user-centered designs. MML-CSD provided domain-specific knowledge and expertise in SRM 1950, context of use, and customer outreach. This cross-laboratory collaboration demonstrated the inherently multi-disciplinary techniques necessary to meet the requirements of attaining customer feedback and advance SRMs. By directly engaging the customers, the survey results provided customer-focused data on the current utilization of SRM 1950 and customer-driven requirements on updates and renewal of the SRM.

One direct impact from this well-designed and well-executed customer and stakeholder survey project was applying the survey results to a new FY24 WCF project for the renewal material SRM 1950a Metabolites in Frozen Human Plasma. The survey results also informed the technical specifications of the procured plasma and will further inform value assignment decisions in the following FYs.

In addition, the rigorous and repeatable survey development process and the artifacts produced from each step can be valuable and serve as a model with templates for future measurement services projects to capture market research data and inform planning and development. Documenting the process and sharing artifacts of the survey methodology can facilitate repeatability and consistency in the future when information from stakeholders and users is needed for measurement services projects.

This document offers a practical, step-by-step guide to the survey development process for gathering input from NIST reference materials users and customers. Its objective is to provide concise guidance with exemplary artifacts from the SRM 1950 survey project to illustrate how to conduct a user feedback survey, including the end-to-end process, survey methodology, and templates.

HOW TO USE THIS GUIDE

NOTE: This document is not intended to replace the involvement of crucial personnel, such as researchers or team members trained in survey design and methodology. Instead, it is intended to guide project planning and management and involve relevant personnel at appropriate stages throughout the project.

Throughout the document, the development of the ***2023 NIST SRM 1950 Customer Feedback Survey*** serves as an exemplary process, illustrated via outcomes and artifacts from each step. All relevant artifacts are documented and provided in **Appendices A** to **P.**

The survey development process follows an 8-step structure, as shown in Fig. 1. The bullet list includes a hyperlink for each step to its relevant section, which provides details on how to carry out each step.

1. **Conceptualization**
2. **Initial Design**
3. **Expert Reviews**
4. **Revisions**
5. **Implementation & Pilot Testing**
6. **Sampling & Outreach**
7. **Fielding & Monitoring**
8. **Data Analysis & Reporting**

Fig. 1. Survey Development Process

STEP 1 – CONCEPTUALIZATION

OUTCOMES

- Project scope and relevant background information
- Problem, Purpose, and Questions (PPQs)
- Intended use of the survey results
- Project plan

Before designing a survey, it is critical to define the project scope–what is in scope and what is out of scope; gather background information relevant to the project; define the problem, purpose, and questions (PPQs) that the project is to solve; and the intended use of the survey results. Outcomes and artifacts from those activities should be documented and used to guide the survey design and development.

PPQs provide the focus and structure of the survey development effort:

1. **Problem** – identifying the problem in a broad and high-level sense
   - Why is it a problem?
   - How do you know the problem exists?
   - Why is the problem important?
   - What or who does it impact?
   - What have others already done about the problem?
2. **Purpose** – clarifying the purpose
   - What do you want to do, and why does it matter?
   - From the problem statement in #1 above, narrow down what you want to attend to.
   - How will the project address the problem in #1?
3. **Questions** – developing questions aligned with the problem and purpose
   - What do you want to know?
   - Specifically, what questions will guide your survey and inform the project's problem?
   - Questions need to be written clearly and carefully.

Documenting the intended use of the survey is also important. For example, the intended use of the SRM 1950 Customer Feedback Survey is to inform decisions such as what, and to what extent, the SRM updates should take place. Depending on your project scope, examples of other survey use might be to describe the status quo; to examine relationships or differences; to make predictions; or to inform product, process or training quality or improvements.

Appendix A shows the PPQs and intended use of the ***2023 NIST SRM 1950 Customer Feedback Survey***.

During this phase, a project plan should be developed with tasks, activities, personnel assignments, milestones, and a projected timeline. The project plan needs to be constantly updated to facilitate team communication and progress tracking. A project plan template is

provided in **Appendix B**. The final project plan of the ***2023 NIST SRM 1950 Customer Feedback Survey*** is provided in **Appendix C**.

STEP 2 – INITIAL DESIGN

OUTCOMES

- Initial survey instrument
- Survey alignment matrix

The initial survey instrument design should use the PPQs defined in STEP 1 to direct the development of survey items and the selection of response options. It's important to note that survey design, development, evaluation, and testing is a complex scientific field, and a full description of it is beyond the scope of this document. Here, only a high-level overview of the process is provided, rather than an in-depth description of designing and selecting appropriate survey items and response options. As mentioned earlier, following this guide does not replace the need to involve a trained survey design expert at this step.

Many survey development references exist, e.g.,[2][3][4][5][6][7][8]. To list a few high-level survey design considerations, for example, Dillman et al. [7] provide guidelines on wording and formatting questions properly and deciding on response options (e.g., closed-ended or open-ended). For closed-ended response options, what types are most appropriately aligned with the PPQs? Should they collect data such as nominal, ordinal, interval, or ratio? Do you need to use rating scales? If so, what scales should you use? Common rating scales include Adjective checklist, Comparative, Forced rank order, Frequency scale, Likert-type scale, Multiple Rating Matrix, Paired comparison, Pick some, Semantic differential, Semantic distance, and Visual analog/slider. The visual design and presentation layout of the survey questions also need to be considered. Ordering and grouping of questions can affect how respondents take the survey. Quality survey items should be relevant, focused, clear, and lack bias. Note that the considerations described here only cover a very limited portion of a rigorously planned and executed survey design, development, evaluation, and testing. Readers are encouraged to consult with survey design experts and read the references provided. The initial draft of the ***2023 NIST SRM 1950 Customer Feedback Survey*** is provided in **Appendix D**.

One useful process is to create an alignment matrix to ensure the survey is aligned with the project's PPQs. For tracking purposes, the first page of the alignment matrix should list the survey title and its PPQs, as well as the intended use of the survey results. The second page should show alignment between the survey items and the project questions to ensure all questions are covered by the survey items.

A template of the Alignment Matrix is provided in **Appendix E,** and an example of the ***2023 NIST SRM 1950 Customer Feedback Survey*** Alignment Matrix is provided in **Appendix F**.

STEP 3 – EXPERT REVIEWS

OUTCOMES

- Expert review comments and revision suggestions (linked to STEP 4)

There are various methods to understand and evaluate the quality of survey instruments in order to catch and correct any problems identified prior to fielding the surveys, e.g., [4][8][10]. One such approach is conducting expert reviews. The initial design from STEP 2 should go through a rigorous, iterative review (in STEP 3) and revision (in STEP 4) cycle by asking a team of experts to review the survey instrument. This review and revision cycle is essential in helping identify question problems; judge the alignment between project objectives and question selection, format, and wording; and suggest revisions. A typical outcome of an expert review is improved question wording, response formats, instructions, and survey flow. The focus of expert reviews includes not only the content but also the ease and efficiency of survey completion, avoidance of errors, and presentation of the content (e.g., overall appearance, organization, and layout of the instrument).

Who should be included and invited to be the experts to help evaluate the quality of the survey instruments? Readers are encouraged to consult with references provided to identify the types and numbers of experts that best suit their project goals. The ***2023 NIST SRM 1950 Customer Feedback Survey*** underwent four types of reviews, including the following.

- **Content expert**: three subject-matter experts (SMEs) who are familiar with SRM 1950 and possess knowledge in clinical chemistry, metabolomics, and lipidomics.
- **Survey expert**: one expert with expertise in survey development, measurement, and evaluation.
- **Statistics expert**: one expert who has expertise in statistical methodology and analysis of survey data.
- **Pseudo participant:** two participants who are representative of the survey's target audience– one was an existing SRM 1950 user, and the other was a potential customer interested in purchasing SRM 1950 for their research.

There are various ways to conduct expert reviews, such as evaluation forms, card sorting tasks, individual interviews, and cognitive interviews.

The ***2023 NIST SRM 1950 Customer Feedback Survey*** used a mixture of methods to conduct the expert reviews. For content, survey, and statistics experts, electronic copies of the initial survey draft in Microsoft Word format were emailed to them, and the experts provided comments and suggested revisions directly on the Word documents. It should be noted that the PPQs and alignment matrix should be accompanied when sending the survey draft for experts to review. Providing the PPQs and alignment matrix helps the experts better provide feedback relevant to your project objectives. **Appendix G** provides a template of evaluation questions for requesting experts to offer their feedback.

After collecting feedback from the content, survey, and statistic experts, the initial survey draft was revised based on the experts' comments and suggestions (see STEP 4 for details). Then, to gather pseudo-participant reviews, individual cognitive interviews were conducted using a concurrent-think-aloud protocol (e.g., [5][9][10][11][12][13]). Concurrent-think-aloud interviewing requested participants actively verbalize their thoughts as they attempt to answer the survey questions and select response options. The role of the interviewer is mainly to support the activity by asking the participant to "keep talking" and to document the verbal record for later analysis. To minimize interviewer interference during the participant's think-aloud process, each interview session was audio and video recorded to collect verbatim data. All interview sessions were conducted in 2023 virtually using Zoom. A template for conducting cognitive concurrent-think-aloud interviews with pseudo-participants for the ***2023 NIST SRM 1950 Customer Feedback Survey*** is included in **Appendix H**.

STEP 4 – REVISIONS

OUTCOMES

- Iterative Survey Instrument Revisions (linked to STEP 3)

All reviews collected in STEP 3 should be discussed with team members to resolve. The comments and resolutions (including justifications if suggested revisions were not addressed) should be well documented with an adequate audit trail. It is an iterative cycle to revise the survey instrument based on the reviews and resolutions.

Appendix I includes a template for documenting expert review comments and resolutions. **Appendix J** provides an exemplary survey item whose original wording induced critical confusion from the pseudo-participants and resulted in a major revision of the survey item language. The revised survey draft for the ***2023 NIST SRM 1950 Customer Feedback Survey*** is included in **Appendix K** as an example.

STEP 5 – IMPLEMENTATION and PILOT TESTING

OUTCOMES

- Survey Programming Specifications
- Data Dictionary
- Finalized and implemented survey instrument
- Study Protocol reviewed/approved by the NIST Research Protections Office (RPO)
- Survey Instrument reviewed/cleared by the Office of Management and Budget (OMB) regarding the Paperwork Reduction Act (PRA)

Before the survey can be launched and data collection can start, the instrument must be implemented and piloted with representative participants to check for survey usability and to estimate the response timing. Usually, there could be minor adjustments based on the pilot testing results. Another important consideration for pilot testing is creating a data dictionary and checking for data validity.

The project team decided to conduct the ***2023 NIST SRM 1950 Customer Feedback Survey*** online. Thus, the survey was implemented within an online survey platform called Qualtrics, making it ready for performing the pilot testing. It is a best practice to document the implementation process specifications detailing survey items and response options, variables, and data types, as well as any logic for branching and skipping. The programming document helped guide implementation and debugging. **Appendix L** provides examples from the programming specifications documentation and the data dictionary for the ***2023 NIST SRM 1950 Customer Feedback Survey***.

For survey projects involving data collection from human subjects, the NIST Research Protections Office (RPO) needs to review and approve the study protocols and recruitment text. For guidance, refer to the RPO's page: https://inet.nist.gov/rpo/human-subjects-research.

If the target audience includes non-federal participants, the survey instrument needs to be reviewed/cleared by the Office of Management and Budget (OMB) regarding the Paperwork Reduction Act (PRA). The PRA submission should go through the NIST Management and Organization Office (M&O) which liaises with the project team, DOC, and OMB to make sure all aspects of conformance with the PRA law are met. For guidance, refer to the M&O's PRA page: https://inet.nist.gov/mando/paperwork-reduction-act.

For the ***2023 NIST SRM 1950 Customer Feedback Survey***, the process of procuring the RPO study approval and OMB PRA approval took about six weeks. Note that the OMB PRA approval process required screenshots of the implemented survey instrument. Exemplar screenshots of the implemented ***2023 NIST SRM 1950 Customer Feedback Survey*** are shown in **Appendix M**.

STEP 6 – SAMPLING and OUTREACH

OUTCOMES

- Sampling and outreach plan
- Recruitment text

Before fielding the survey, the project team must determine how to sample and reach the target audience to collect responses. A sampling and outreach plan should be developed and documented to determine the survey fielding timeframe, recruitment, and dissemination strategies. NOTE that although this step is listed in Fig. 1 as a sequential step after the previous five steps, the team can (and is encouraged to) start discussing the sampling and outreach plan any time after *Step 1. Conceptualization*. Resources related to survey sampling methods are provided, e.g., [7][14][15][16].

Follow the guiding questions below to develop and document the sampling plan.

- **Target population** – a collection of elements that we draw an inference about using a sample
- **Sampling frame(s)** – a list of units in the population that the sample is drawn from; a sample is a collection of sampling units drawn from a frame(s)
- **Context characteristics** –attributes of the sampling that are important to consider in the sampling plan with respect to PPQs identified in STEP 1
- **Sampling types and techniques** – which sampling types and techniques meet the project objectives? Consider:
    - Probabilistic sampling: for example, Simple random sampling, Stratified random sampling, Proportional random sampling, cluster sampling
    - Non-probabilistic sampling: for example, Convenience sampling, Homogeneous sampling, Snowball or chain sampling. Convenience sampling selects participants because of availability and accessibility.
- **Recruitment and dissemination strategies** – consider:
    - Identify the source(s) of information about your populations, for example:
        - Directories
        - Public records
        - Member lists
        - Existing databases
    - How would you contact members in the sampling frame(s)
- **Fielding timeframe and duration**
    - What are the best time windows for data collection? For example, if the sampling frame(s) includes academic researchers, do you need to consider time?
    - How much time, i.e., duration, do you want the survey to be open for collecting responses?
- **Protocol for responding to inquiries**

- Establish a protocol for addressing any inquiries from the respondents, including a point of contact (POC) and mechanism (e.g., email, phone, or online form).

Appendix N includes the sampling and recruitment plan for the ***2023 NIST SRM 1950 Customer Feedback Survey*** as an example.

STEP 7 – FIELDING and MONITORING

OUTCOMES

- Survey fielding and monitoring documentation

Survey fielding should follow the sampling and recruitment plan prepared in Step 6. The project team should monitor data collection closely to address and document any unanticipated incidents or respondent inquiries. Sometimes, it is necessary to adjust or extend the timeframe and duration of data collection.

It is helpful to keep an up-to-date tally of completed survey responses with some basic demographic information to determine whether the responses show adequate coverage of the intended sampling frames. This can be done weekly or more/less frequently, depending on the project objectives.

The ***2023 NIST SRM 1950 Customer Feedback Survey*** was fielded on April 12, 2023, based on the sampling and recruitment plan described in Step 6. We reached out to potential respondents in the sampling frames through multiple channels. These channels included using the NIST Office of Reference Materials (ORM) MarketingCloud to reach both current and past customers of SRM 1950. We also reached out to three professional organizations seeking assistance for survey dissemination to their members: the Metabolomics Association of North America, the Metabolomics Society, and the Metabolomics Quality Assurance and Quality Control Consortium (mQACC). Project team members also reached out to personal contacts and used word-of-mouth strategies at conferences. The Metabolomics Society utilized their monthly newsletter, MetaboNews, to help announce the survey opportunity. To align with the timing of MetaboNews newsletter announcement, the survey duration was extended to July 15, 2023 from the initially planned date of June 30, 2023. **Appendix O** shows examples of how survey fielding and data collection monitoring were carried out for the ***2023 NIST SRM 1950 Customer Feedback Survey***.

STEP 8 – DATA ANALYSIS and REPORTING

OUTCOMES

- Survey data file(s) of completed responses
- Data analysis and report

When data collection is concluded, the survey data needs to be processed before data analysis can be performed. Data processing can include:

- Judge survey completeness by creating agreed-upon standards to determine:
  - How complete does it need to be to include in the final sample?
  - Is information missing on critical items? How should missing data be handled?
- Data cleaning, if necessary:
  - Separate/redact personally identifiable information (PII). For example, the last section in the ***2023 NIST SRM 1950 Customer Feedback Survey*** asked for respondents' contact information (name, email, organization) if they were willing to be contacted by NIST for further information regarding SRM 1950. The raw survey data file was separated into two data files.
    (1) One file contains only survey responses to questions related to experiences/needs of SRM 1950. Within this file, each participant will be assigned a unique participant number.
    (2) The other file contains only contact information for those who indicate their willingness to be contacted for further information.

    Once this cleaning process was completed, the original raw survey data was permanently purged making it impossible to link between those two separate data files.
  - Processing data by scale type. For example, for nominal data, it's common to assign labels or shorter names to help with data analysis. For ordinal data, it's common to assign numerical values for analysis.
  - Recoding data. Depending on the data, sometimes it helps to understand survey results by recoding data such as recoding into meaning categories, recoding for fewer values – starting with more narrow categories, then further collapsing as to preserve logically as much meaning as possible. For example, for 5-point Likert-type scales (Strongly Disagree, Disagree, Neither Disagree Nor Agree, Agree, Strongly Agree), it can be recoded into three categories of: Disagree, Neutral, Agree.

After data processing, the project team needs to discuss and plan the appropriate data analysis methods and techniques that best meet the project objectives. It is encouraged to consult with ITL's Statistical Engineering Division (SED) for further guidance on inferential statistical analysis methodology.

The objectives of the ***2023 NIST SRM 1950 Customer Feedback Survey*** focused on collecting customer feedback on their experiences and needs of NIST SRM 1950 and other potential reference materials. The intent is not to draw statistical inferences on people's opinions, perceptions, or attitudes toward topics of interest. So, descriptive statistics were used and reported on the quantitative data. Results were intended to guide future SRM development activities. The survey results of the ***2023 NIST SRM 1950 Customer Feedback Survey*** are included in **Appendix P**. Results from the survey provided user feedback to help MML-CSD chemists plan the procurement package for the renewal material SRM 1950a and helped inform the specifications of the renewal material in FY24. In the following FYs, the survey feedback will further help inform which analytes will be value assigned in the material.

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Appendix A. Example – PPQs and Intended Use of NIST SRM 1950 Customer Feedback Survey

Problem

SRM 1950 Metabolites in Frozen Human Plasma was first made available in 2011 and has approximate 4-year supply remaining. The material is value assigned for 90 components. However, it is not known which values are utilized by customers. In addition, multiple publications by NIST authors and others outside of NIST have demonstrated that SRM 1950 has been used by metabolomic/lipidomic communities as a common research material independent of its assigned values, for example as a long-term QC (quality control) material. There is not sufficient information to determine when, what, and to what extent the SRM updates should take place or whether a different new SRM is needed for the target customer communities.

Purpose

This project aims to engage the user community through an online customer and stakeholder survey to determine whether customers require a renewal material with many values (certified and/or non-certified) similar to SRM 1950 or if current or new materials more similar to recently introduced metabolomics RMs would fulfill customer needs for a common harmonization material.

Questions

Q1. What is the feedback on existing classes of analytes and their values?

Q1a. Which ones are/will be used and to what extent (e.g., importance to their research)?

Q1b. How do/will analytes support their needs? And to what extent? (e.g., calibration, validation, benchmarking)

Q2. Are there additional requirements for SRM 1950 renewal?

Q2a. Are additional components/analytes needed?

Q2b. Do users prefer:

i. same or a different amount per vial?
ii. same or different anticoagulant (current: lithium heparin)?
iii. similar or different sample pool demographic?

Q3. What do users prefer (RMs and/or SRMs) for new materials for metabolomics?

Intended Use

The intended use of the SRM 1950 Customer Feedback Survey is to inform decisions such as what, and to what extent, the SRM updates should take place.

Appendix B. Template–Project Plan

The project plan template below shows each survey stage, tasks within the stage, and activities within each task. It's recommended to keep the project plan updated by color-coding activities planned (orange) and completed (green), as well as grey for non-applicable activities.

Survey Stage	Task	Activity	Assigned to	OCT-20xx	NOV-20xx	(add as needed)
1. CONCEPTUALIZATION	T1. Scoping & Project Goals	*Define scope and gather background info*	[name][name]			
		Develop the problems, purpose, and questions (PPQs)	[name][name]			
2. INITIAL DESIGN	T2. Survey Design	*Design of Survey Items and Responses*	[name][name]			
		Create alignment matrix to ensure coverage	[name][name]			
3. EXPERT REVIEWS	T3. Survey Reviews	*Content expert reviews*	[name][name]			
		Survey expert reviews	[name][name]			
		Statistics expert reviews	[name][name]			
		Pseudo participant reviews	[name][name]			
4. REVISIONS	T4. Iterative Survey Revisions	*Revise survey instrument based on reviews*	[name][name]			
5. IMPLEMENTATION & PILOT TESTING	T5.a. Implementation & Pilot Testing	*Implement online survey (e.g., Qualtrics)*	[name][name]			
		Define data dictionary (variable names, data types, and values)	[name][name]			
		Pilot testing to estimate survey timing and ensure valid data collection	[name][name]			
	T5.b. Final Survey	*Finalize survey instrument*	[name][name]			
		Develop initial data analysis plan	[name][name]			
	T5.c. PRA & RPO Approvals	*PRA - prepare and submit PRA packages for approval*	[name][name]			
		RPO - prepare and submit study in iMedRis for approval	[name][name]			
6. SAMPLING & OUTREACH	T6. Sampling plan	*Define Sampling frame (e.g., current/past customers) & Develop sampling plan*	[name][name]			
		Develop recruitment/dissemination plan (initial invite; reminders, follow-ups, etc.)	[name][name]			
		Determine fielding timeframe and duration	[name][name]			
		Establish Protocol for Responding to Inquiries	[name][name]			
7. FIELDING & MONITORING	T7. Survey fielding & Data collection	*Launch survey online*	[name][name]			
		Monitor data collection	[name][name]			
8. DATA ANALYSIS & REPORTING	T8.a. Data cleaning & Data analysis	*Identify completes, incompletes, missing data, etc.*	[name][name]			
		Perform data cleaning (if needed): e.g., recoding, rebinning, collapsing, etc.	[name][name]			
		Refine data analysis plan on cleaned dataset	[name][name]			
		Perform data analysis	[name][name]			
	T8.b. Reporting	*Develop descriptive and toplines of the data*	[name][name]			
		Report findings, results, and recommendations	[name][name]			

Color Legend:

Planned
Completed
N/A

Appendix C. Example–Final Project Plan of the 2023 NIST SRM 1950 Customer Feedback Survey

Task	Activity	Names	Nov 2022	Dec 2022	Jan 2023	Feb 2023	Mar 2023	Apr 2023	May 2023	Jun 2023	Jul 2023	Aug 2023	Sep 2023
1. Scoping & Background Info	*Scoping and background info gathering*	Yee-Yin, Johanna, Tracey, Clay											
	Defining Sampling frame & Developing sampling plan (e.g., current/past custom	Yee-Yin, Johanna, Tracey, Clay											
2. Survey Design	*Design of Survey Items and Responses*	Yee-Yin											
3. Survey Reviews & Revisions	*Content expert reviews*	Yee-Yin, Johanna, Tracey, Clay											
	Survey expert reviews	Yee-Yin											
	Statistics expert reviews	Yee-Yin											
	Pseudo participant reviews	Yee-Yin, Johanna, Tracey, Clay											
	Revisions based on reviews	Yee-Yin											
4. Implementation & Pilot Testing	*Implement online survey (e.g., Qualtrics)*	Yee-Yin											
	Define data dictionary (variable names, data types, and values)	Yee-Yin											
	Pilot testing: survey timing; test against data dictionary to ensure valid data coll	Yee-Yin, Johanna, Tracey, Clay											
5. Final Survey	*Finalize survey instrument*	Yee-Yin											
	Develop initial data analysis plan	Yee-Yin											
6. Survey fielding plan	*Recruitment/Dissemination plan (initial invite; reminders, follow-ups, etc.)*	Yee-Yin, Johanna, Tracey, Clay											
	Fielding timeframe and duration	Yee-Yin, Johanna, Tracey, Clay											
	Establish Protocol for Responding to Inquiries	Yee-Yin, Johanna, Tracey, Clay											
7. PRA & RPO Approvals	*PRA - prepare and submit PRA packages for approval*	Yee-Yin, Johanna, Tracey, Clay				Submitted 2023FEB2	Approved 2023MAR2						
	RPO - prepare and submit study in iMedRis for approval	Yee-Yin, Johanna, Tracey, Clay				Approved 2023FEB1		Amendment2023APR17					
8. Survey fielding & Data collection	*Launch survey online*	Yee-Yin, Johanna, Tracey, Clay						2023APR12					
	Monitor data collection	Yee-Yin, Johanna, Tracey, Clay						2023APR12			2023JUL15		
9. Data cleaning & Data analysis	*Identify completes, incompletes, missing data, etc.*	Yee-Yin											
	Recoding, rebinning, collapsing, etc.	Yee-Yin											
	Refine data analysis plan on cleaned dataset	Yee-Yin											
	Perform data analysis	Yee-Yin											
10. Reporting	*Develop descriptive and toplines of the data*	Yee-Yin											
	Report findings, results, and recommendations	Yee-Yin										2023AUG22	

Appendix D. Example–Initial Survey Draft of the *2023 NIST SRM 1950 Customer Feedback Survey*

We anticipated target respondents from existing NIST SRM 1950 customers and prospective users who might be interested in purchasing and using the SRM. There could also be resellers/distributors who were not users but could help forward the survey to their customers. Thus, the survey instrument included conditional branching to provide tailored text and survey items depending on the customer types. The initial survey draft is divided into parts as below:

1. **Landing Page:** the first page was displayed when a respondent followed the survey link. This page is the same for all customer types. The details of this part are shown in sec. D.1 below.
2. **Version A – Existing Customers:** this version was shown when a respondent indicated they were an SRM 1950 customer (either current or past). The details of this part are shown in sec. D.2 below.
3. **Version B – Prospective Customers:** this version was shown when a respondent indicated they were not an SRM 1950 customer, but were interested in purchasing the SRM. This version had some tailored texts, but shared mostly the same structure and survey items as Version A. The detail of this part is shown in sec. D.3 below.
4. **Version C – Reseller/Distributor:** this version was shown when a respondent indicated they were a reseller or distributor of SRM 1950. They were only asked to provide minimal information and to help forward the survey to their customers. The details of this part are shown in sec. D.4 below.
5. **Matrix Questions for Analytes:** this part is shared for both Version A and Version B. The details of this part are shown in sec. D.5 below.

D.1 Landing Page

[LANDING PAGE] [1]

NIST SRM 1950 Metabolites in Frozen Human Plasma was first made available in 2011. It has been used by researchers and scientists in the metabolomic and lipidomic communities. NIST will be renewing SRM 1950 and/or developing new reference materials in the coming years. We are conducting a survey with existing and prospect users to gather feedback on their experiences and needs of SRM 1950. The survey results will help NIST devise future reference materials formulation to better fulfill user needs and support the metabolomic and lipidomic communities.

It is important to have your individual and collective voices heard from the metabolomic and lipidomic communities. We hope you will encourage other researchers and scientists to take the survey. Please share the link widely with others as well. We appreciate your assistance and your time.

This survey takes approximately [xx] minutes.

If you are a reseller/distributor of NIST SRM 1950, please help forward this survey to your customers.

[OMB control #xxxx-xxxx]

[NEXT]

[1] **NOTE**: Blue text in brackets, such as [LANDING PAGE], is not part of the survey. It indicates survey flow, conditional jumps/skips, or content to be provided later.

[BRANCHING]

Has your organization used NIST SRM 1950?

- ○ Yes – current customer of SRM 1950
- ○ Yes – used SRM 1950 before, but not currently
- ○ No, but my organization is interested in SRM 1950
- ○ No, my organization is a reseller/distributor of SRM 1950

[NEXT]

CONDITIONS:

- IF [Yes, current/past customers] JUMPTO **[Version A – Existing Customers]**
- IF [No, but interested] JUMPTO **[Version B – Prospective Customers]**
- IF [No, reseller/distributor] JUMPTO **[Version C – Reseller/Distributor]**

D.2 Version A – Existing Customers

About You and Your Organization

1. Where are you located?
   - ○ United States (US)
   - ○ Non-US (please specify your country): _____

2. What of the following best describe(s) your organization? (check all that apply)
   - ☐ Academic laboratory
   - ☐ Federal Government laboratory
   - ☐ Local Government laboratory
   - ☐ Pharmaceutical laboratory
   - ☐ Third-party testing laboratory
   - ☐ Research and development
   - ☐ Contractor
   - ☐ Other (please specify): _____

3. What of the following best describe(s) your role? (check all that apply)
   - ☐ Researcher/Scientist
   - ☐ Management
   - ☐ Technician
   - ☐ Tester
   - ☐ Other (please specify): _____

4. What of the following best describe(s) your research area or interest? (check all that apply)
   - ☐ Lipidomics
   - ☐ Metabolomics
   - ☐ Other (please specify): _____

[NEXT]

Use of NIST SRM 1950 Metabolites in Frozen Human Plasma

5. For what purpose(s) has your laboratory used SRM 1950? (check all that apply)
   - ☐ Calibration
   - ☐ Benchmarking
   - ☐ In-house calibrants, control materials
   - ☐ Method development/optimization
   - ☐ Method validation
   - ☐ Precision: Intra-study (within study)
   - ☐ Comparability: Inter-study (across studies)
   - ☐ Comparability: Inter-laboratory (across laboratories)
   - ☐ Process stability assessment
   - ☐ Quantitation
   - ☐ Normalization
   - ☐ Identification
   - ☐ Quality Assurance/Quality Control
   - ☐ Other (please specify): _____

6. Which class(es) of analytes has your laboratory used SRM 1950? (check all that apply)
   - ☐ Cholesterol and Total Glycerides
   - ☐ Fatty acids
   - ☐ Amino acids
   - ☐ Fat-soluble vitamins and Carotenoids
   - ☐ Water-soluble vitamins
   - ☐ Organic clinical markers
   - ☐ Electrolytes
   - ☐ Hormones
   - ☐ Trace Elements
   - ☐ Proteins
   - ☐ Perfluorinated Compounds (PFCs)
   - ☐ Other (please specify): _____

[NEXT]

[FOR each class selected above in Q6, SHOW the matrix questions below.]

a. [class name from Q6]

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	**1**	**2**	**3** (essential)
Individual analyte (e.g. Cholesterol if the 1st checkbox is checked)	○	○	○	○
[repeated for all analytes in a class]	○	○	○	○

[Repeated for each class selected in Q.6]

[NEXT]

Future SRM 1950 Renewals or Development of New Materials

7. A unit of SRM 1950 consists of five vials, each containing approximately 1.0 mL of plasma.
   a. Typically, how much plasma do you use per analysis? _____ (mL)
   b. Would you prefer a **similar** volume of plasma per vial for future renewals of SRM 1950?
      - ○ Yes
      - ○ No, please specify how much would you prefer per vial: _____ (mL)

8. The current SRM 1950 contains lithium heparin as the anticoagulant. Would you prefer a **similar** anticoagulant for future renewals of SRM 1950?
   - ○ Yes
   - ○ No, please specify: _____

9. The source for current SRM 1950 was plasma obtained from 100 individuals with an equal number of men and women in age range of 40-50 years (detail of the sample pool demographic can be found in the SRM Certificate of Analysis). Would you prefer a **similar** sample pool demographic for future renewals of SRM 1950?
   - ○ Yes
   - ○ No, please specify: _____

10. NIST currently provides various types of materials intended to be used as measurement standards. We want to get your feedback on two types below:
    - NIST Reference Materials (RM): [need definition and links]
    - NIST Standard Reference Materials (SRM): [need definition and links]

    a. Based on the above definitions and your research needs, if NIST develops new materials, what would you prefer them to be?
       - ○ Reference Materials (RMs)
       - ○ Standard Reference Materials (SRMs)
       - ○ It doesn't matter to my research
       - ○ I don't know the difference between RMs and SRMs

    [SHOW 10b if RMs or SRMs is selected]

    b. Please explain why you chose [RMs/SRMs]: _____

11. What characteristics are important to you when selecting future reference materials for your research? (check all that apply)
    - ☐ Availability
    - ☐ Composition
    - ☐ Cost
    - ☐ Homogeneity
    - ☐ Matrix
    - ☐ Purity
    - ☐ Stability
    - ☐ Traceability to SI unit
    - ☐ Uncertainty
    - ☐ Other (please specify): _____

[NEXT]

12. Please share any additional thoughts.

13. May NIST contact you for further discussion on your experience with SRM 1950 or other reference materials?
    - ☐ Yes, please provide contact information:
      Name: _____ (First/Last)
      Email: _____
      Laboratory/Affiliation: _____

14. The Metabolomics Quality Assurance and Quality Control Consortium (mQACC), an international working group, not affiliated with NIST, is interested in compiling SRM 1950 data from metabolomics researchers in order to fully characterize the compositional components in benefit to the community. Are you willing to share your SRM 1950 data with mQACC?
    - ○ Yes
    - ○ No

Thank You!

[SUBMIT/FINISH]

D.3 Version B – Prospective Customers

About You and Your Organization

1. Where are you located?
   - ○ United States (US)
   - ○ Non-US (please specify your country): _____

2. What of the following best describe(s) your laboratory? (check all that apply)
   - ☐ [same list as in Version A]

3. What of the following best describe(s) your role? (check all that apply)
   - ☐ [same list as in Version A]

4. What of the following best describe(s) your research area or interest? (check all that apply)
   - ☐ [same list as in Version A]

5. What are the reasons that your laboratory does not use SRM 1950? (check all that apply)
   - ☐ Availability due to location
   - ☐ Cost
   - ☐ Lack of analyte-specific certified values
   - ☐ Time required for analysis
   - ☐ I use other reference materials in my work.
   - ☐ I am not aware of this reference material.
   - ☐ Other (please specify): _____

[NEXT]

Use of NIST SRM 1950 Metabolites in Frozen Human Plasma

6. If your laboratory would purchase SRM 1950, for what purpose(s) will your laboratory use it? (check all that apply)
   ☐ [same list as in Version A]

7. If your laboratory would purchase SRM 1950, for which class(es) of analytes will your laboratory use it? (check all that apply)
   ☐ [same list as in Version A]

[NEXT]

[FOR each class selected above in Q7, SHOW the matrix questions below.]

a. [class name from Q7]

For the value assigned for each analyte listed, how important will it be to your research? (0=not used; 3=essential)

[same Matrix Q as in Version A]

[Repeated for each class selected in Q7]

[NEXT]

Future SRM 1950 Renewals or Development of New Reference Materials

8. A unit of current SRM 1950 consists of five vials, each containing approximately 1.0 mL of plasma intended for one-time use.
   a. Will the **same** volume of 1.0 mL plasma per vial meet your needs?
      - ○ Yes
      - ○ No, please specify how much would you prefer per vial: _____ (mL)

9. The current SRM 1950 contains lithium heparin as the anticoagulant. Will the **same** anticoagulant meet your needs?
   - ○ Yes
   - ○ No, please specify: _____

10. The source for current SRM 1950 was plasma obtained from 100 individuals with an equal number of men and women in age range of 40-50 years (detail of the sample pool demographic can be found in the SRM Certificate of Analysis). If SRM 1950 will be renewed, will a **similar** sample pool demographic meet your needs?
    - ○ Yes
    - ○ No, please specify: _____

11. NIST currently provides various types of materials intended to be used as measurement standards. We want to get your feedback on two types below:?
    - NIST Reference Materials (RM): [same as Ver. A for existing users]
    - NIST Standard Reference Materials (SRM): [same as Ver. A for existing users]

    a. Based on the above definitions and your research needs, if NIST develops new materials, what would you prefer them to be?
       - ○ Reference Materials (RMs)
       - ○ Standard Reference Materials (SRMs)
       - ○ It doesn't matter to my research
       - ○ I don't know the difference between RMs and SRMs

    [SHOW 1qb if RMs or SRMs is selected]

    b. Please explain why you chose [RMs/SRMs]: _____

12. What characteristics are important to you when selecting future reference materials for your research? (check all that apply)
    - ☐ [same list as in Version A]

[NEXT]

13. May NIST contact you for further discussion on your interest in SRM 1950 or other reference materials?
    - ☐ Yes, please provide contact information:
      Name: _____ (First/Last)
      Email: _____
      Laboratory/Affiliation: _____

14. Please share any additional thoughts.

Thank You!

[SUBMIT/FINISH]

D.4 Version C – Reseller/Distributor

1. Where are you located?
   - ○ United States (US)
   - ○ Non-US (please specify your country): _____

2. About how many NIST SRM 1950 customers do you have? _____

We sincerely appreciate your help in forwarding this survey [survey link] to your customers.

Thank You!

[SUBMIT/FINISH]

D.5 Matrix Questions for Analytes (shared by Version A and Version B)

[BRANCHING from Q6 in Version A OR Q7 in Version B]

[IF Cholesterol and Total Glycerides is checked, SHOW the matrix questions below.]

a. Cholesterol and Total Glycerides

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	1	2	3 (essential)
Cholesterol	○	○	○	○
Total Glycerides (as triolein)	○	○	○	○

[NEXT]

[IF Fatty acids is checked, SHOW the matrix questions below.]

b. **Fatty Acids**

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	1	2	3 (essential)
C12:0 Dodecanoic Acid (Lauric Acid)	○	○	○	○
C16:0 Hexadecanoic Acid (Palmitic Acid)	○	○	○	○
C16:1 n-7 (Z)-9-Hexadecenoic Acid (Palmitoleic Acid)	○	○	○	○
C18:0 Octadecanoic Acid (Stearic Acid)	○	○	○	○
C18:3 n-3 (Z,Z,Z)-9,12,15-Octadecatrienoic Acid (α-Linolenic Acid)	○	○	○	○
C18:1 n-9 (Z)-9-Octadecenoic Acid (Oleic Acid)	○	○	○	○
C18:2 n-6 (Z,Z)-9,12-Octadecadienoic Acid (Linoleic Acid)	○	○	○	○
C22:0 Docosanoic Acid (Behenic Acid)	○	○	○	○
C14:0 Tetradecanoic Acid (Myristic Acid)	○	○	○	○
C14:1 (Z)-9-Tetradecenoic Acid (Myristoleic Acid)	○	○	○	○
C15:0 Pentadecanoic Acid	○	○	○	○
C17:0 Heptadecanoic Acid (Margaric Acid)	○	○	○	○
C18:3 n-6 (Z,Z,Z)-6,9,12-Octadecatrienoic Acid (γ-Linolenic Acid)	○	○	○	○
C18:1 n-7 (Z)-11-Octadecenoic Acid (Vaccenic Acid)	○	○	○	○
C20:0 Eicosanoic Acid (Arachidic Acid)(c,d)	○	○	○	○
C20:1 (Z)-11-Eicosenoic Acid (Gondolic Acid)	○	○	○	○
C20:2 (Z,Z)-1,14-Eicosadienoic Acid(c,d)	○	○	○	○
C20:3 n-6 (Z,Z,Z)-8,11,14-Eicosatrienoic Acid (Dihomo-γ-Linolenic Acid)	○	○	○	○
C20:4 n-6 (Z,Z,Z,Z)-5,8,11,14-Eicosatetraenoic Acid (Arachidonic Acid)	○	○	○	○
C20:5 n-3 (Z,Z,Z,Z,Z) -5,8,11,14,17-Eicosapentaenoic Acid (EPA)	○	○	○	○
C22:1 (Z)-13-Docosenoic Acid (Erucic Acid)	○	○	○	○

C22:4 n-6 (Z,Z,Z,Z)-7,10,13,16-Docosatetraenoic Acid	○	○	○	○
C22:5 n-3 (Z,Z,Z,Z,Z)-7,10,13,16,19-Docosapentaenoic Acid (DPA)	○	○	○	○
C22:5 n-6 (Z,Z,Z,Z,Z)-4,7,10,13,16-Docosapentaenoic Acid	○	○	○	○
C22:6 n-3 (Z,Z,Z,Z,Z,Z)-4,7,10,13,16,19-Docosahexaenoic Acid (DHA)	○	○	○	○
C24:0 Tetracosanoic Acid (Lignoceric Acid)	○	○	○	○
C24:1 (Z)-15-Tetracosenoic Acid (Nervonic Acid)	○	○	○	○

[NEXT]

[IF Amino acids is checked, SHOW the matrix questions below.]

c. **Amino acids**

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	**1**	**2**	**3** (essential)
Arginine	○	○	○	○
Alanine	○	○	○	○
Cysteine	○	○	○	○
Cystine	○	○	○	○
Glycine	○	○	○	○
Histidine	○	○	○	○
Isoleucine	○	○	○	○
Leucine	○	○	○	○
Lysine	○	○	○	○
Methionine	○	○	○	○
Phenylalanine	○	○	○	○
Proline	○	○	○	○
Serine	○	○	○	○
Threonine	○	○	○	○
Tyrosine	○	○	○	○
Valine	○	○	○	○

[NEXT]

[IF Fat-soluble vitamins and Carotenoids is checked, SHOW the matrix questions below.]

d. Fat-soluble vitamins and Carotenoids

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	**1**	**2**	**3** (essential)
Retinol	○	○	○	○
α-Tocopherol	○	○	○	○
γ- + β-Tocopherol	○	○	○	○
Lutein	○	○	○	○
Zeaxanthin	○	○	○	○

β-Cryptoxanthin	○	○	○	○
Total α-Carotene	○	○	○	○
Total β-Carotene	○	○	○	○
25-Hydroxyvitamin D_3	○	○	○	○
5-Methyltetrahydrofolate	○	○	○	○
Pyridoxal 5'-phosphate	○	○	○	○

[NEXT]

[IF Water-soluble vitamins is checked, SHOW the matrix questions below.]

e. **Water-soluble vitamins**

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	**1**	**2**	**3** (essential)
Trans-Lycopene	○	○	○	○
Total Lycopene	○	○	○	○
Trans-β-Carotene	○	○	○	○
Cis-β-Carotene	○	○	○	○
25-Hydroxyvitamin D_2	○	○	○	○
Folic acid	○	○	○	○
Total folate	○	○	○	○
4-Pyridoxic acid	○	○	○	○

[NEXT]

[IF Organic clinical markers is checked, SHOW the matrix questions below.]

f. **Organic clinical markers**

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	**1**	**2**	**3** (essential)
Creatinine	○	○	○	○
Glucose	○	○	○	○
Urea	○	○	○	○
Uric Acid	○	○	○	○

[NEXT]

[IF Electrolytes is checked, SHOW the matrix questions below.]

g. **Electrolytes**

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	**1**	**2**	**3** (essential)
Calcium	○	○	○	○
Magnesium	○	○	○	○

Potassium	○	○	○	○
Sodium	○	○	○	○

[NEXT]

[IF Hormones is checked, SHOW the matrix questions below.]

h. **Hormones**

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	**1**	**2**	**3** (essential)
Homocysteine	○	○	○	○
Cortisol	○	○	○	○
Progesterone	○	○	○	○
Testosterone	○	○	○	○

[NEXT]

[IF Trace Elements is checked, SHOW the matrix questions below.]

i. **Trace Elements**

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	**1**	**2**	**3** (essential)
Copper	○	○	○	○
Selenium	○	○	○	○
Glutathione Peroxidase	○	○	○	○
Seleno-Albumin	○	○	○	○
Bilirubin (mg/dL)	○	○	○	○

[NEXT]

[IF Proteins is checked, SHOW the matrix questions below.]

j. **Proteins**

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	**1**	**2**	**3** (essential)
Selenoprotein P	○	○	○	○
Total Protein (g/L)	○	○	○	○
Vitamin D-Binding Protein (mg/L)	○	○	○	○

[NEXT]

[IF Perfluorinated Compounds (PFCs) is checked, SHOW the matrix questions below.]

k. **Perfluorinated Compounds (PFCs)**

For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)

	0 (not used)	**1**	**2**	**3** (essential)
Perfluorooctanoic Acid (PFOA)	○	○	○	○
Perfluorononanoic Acid (PFNA)	○	○	○	○
Perfluorodecanoic Acid (PFDA)	○	○	○	○
Perfluoroundecanoic Acid (PFUnA)	○	○	○	○
Perfluorohexansulfonate (PFHxS)	○	○	○	○
Perfluorooctanesulfonic Acid (PFOS)	○	○	○	○

[NEXT – return to Q7 in Version A or Q8 in Version B]

Appendix E. Template Alignment Matrix Template and Examples

For tracking purposes, the first page of the alignment matrix should list the survey title and its PPQs, as well as the intended use of the survey results. The 2nd page should show alignment between the survey items and the project questions to ensure all questions are covered by survey items.

[Insert survey title] – Alignment Matrix

Problems:

- [Insert why it is a problem]

Purpose:

- [Insert what you want to do and why it matters]

Questions:

- [Insert what you want to know]

Intended Use:

- [Insert the intended use of the survey results]

Survey Alignment Matrix

Suggest use: Duplicate the following table for each survey item and map to its relevant research question(s) as identified in the PPQs, as demonstrated in Appendix F on the next page.

RQs [list research questions covered by the survey items]		
Survey Items	**Response Options**	**Plan for Reporting**
Q.		[Insert plan for report, e.g. Descriptive stat, Qualitative, linkage]

Demographic Questions		
Demographic Questions	**Response Options**	**Plan for Reporting**
D.		[Insert plan for report, e.g. Descriptive stat, Qualitative, linkage]

Appendix F. Example–Alignment Matrix for 2023 NIST SRM 1950 Customer Feedback Survey

Survey Alignment Matrix

RQ1 What is the feedback on existing classes of analytes and their values? Q1a. Which ones are/will be used and to what extent (e.g., importance to their research)? ***RQ2*** Are there additional requirements for SRM 1950 renewal? Q2a. Are additional components/analytes needed?			
Version	**Survey Items**	**Response Options**	**Plan for Reporting**
A	Which class(es) of analytes has your laboratory used SRM 1950? (check all that apply)	☐ Cholesterol and Total Glycerides ☐ Fatty acids ☐ Amino acids ☐ Fat-soluble vitamins and Carotenoids ☐ Water-soluble vitamins ☐ Organic clinical markers ☐ Electrolytes ☐ Hormones ☐ Trace Elements ☐ Proteins ☐ Perfluorinated Compounds (PFCs) ☐ Other (please specify): _____	Descriptive
A	For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential) [Repeat this survey item for all analytes in each selected class from the survey item above]	○ 0 (not used) ○ 1 ○ 2 ○ 3 (essential	Descriptive
B	If your laboratory would purchase SRM 1950, for which class(es) of analytes will your laboratory use it? (check all that apply)	☐ Cholesterol and Total Glycerides ☐ Fatty acids ☐ Amino acids ☐ Fat-soluble vitamins and Carotenoids	Descriptive

		☐ Water-soluble vitamins ☐ Organic clinical markers ☐ Electrolytes ☐ Hormones ☐ Trace Elements ☐ Proteins ☐ Perfluorinated Compounds (PFCs) ☐ Other (please specify): _____	
B	For the value assigned for each analyte listed, how important will it be to your research? (0=not used; 3=essential) [Repeat this survey item for all analytes in each selected class from the survey item above]	○ 0 (not used) ○ 1 ○ 2 ○ 3 (essential	Descriptive

RQ1 What is the feedback on existing classes of analytes and their values? Q1b. How do/will analytes support their needs? And, to what extent? (e.g., calibration, validation, benchmarking)			
Version	**Survey Items**	**Response Options**	**Plan for Reporting**
A	For what purpose(s) has your laboratory used SRM 1950? (check all that apply)	☐ Calibration ☐ Benchmarking ☐ In-house calibrants, control materials ☐ Method development/optimization ☐ Method validation ☐ Precision: Intra-study (within study) ☐ Comparability: Inter-study (across studies) ☐ Comparability: Inter-laboratory (across laboratories) ☐ Process stability assessment ☐ Quantitation ☐ Normalization ☐ Identification ☐ Quality Assurance/Quality Control	Descriptive

		☐ Other (please specify): _____	
B	If your laboratory would purchase SRM 1950, for what purpose(s) will your laboratory use it? (check all that apply)	☐ Calibration ☐ Benchmarking ☐ In-house calibrants, control materials ☐ Method development/optimization ☐ Method validation ☐ Precision: Intra-study (within study) ☐ Comparability: Inter-study (across studies) ☐ Comparability: Inter-laboratory (across laboratories) ☐ Process stability assessment ☐ Quantitation ☐ Normalization ☐ Identification ☐ Quality Assurance/Quality Control ☐ Other (please specify): _____	Descriptive

RQ2 Are there additional requirements for SRM 1950 renewal?
Q2b. Do users prefer:
i. Same or different amount per vial?
ii. Same or different anticoagulant (current: lithium heparin)?
iii. Similar or different sample pool demographic

Version	Survey Items	Response Options	Plan for Reporting
A	A unit of SRM 1950 consists of five vials, each containing approximately 1.0 mL of plasma. a. Typically, how much plasma do you use per analysis?	_____ (mL)	Descriptive
A	A unit of SRM 1950 consists of five vials, each containing approximately 1.0 mL of plasma. b. Would you prefer a **similar** volume of plasma per vial for future renewals of SRM 1950?	○ Yes ○ No, please specify how much would you prefer per vial: _____ (mL)	Descriptive

A	The current SRM 1950 contains lithium heparin as the anticoagulant. Would you prefer a **similar** anticoagulant for future renewals of SRM 1950?	○ Yes ○ No, please specify: _____	Descriptive
A	The source for current SRM 1950 was plasma obtained from 100 individuals with an equal number of men and women in age range of 40-50 years (detail of the sample pool demographic can be found in the SRM Certificate of Analysis). Would you prefer a **similar** sample pool demographic for future renewals of SRM 1950?	○ Yes ○ No, please specify: _____	Descriptive
B	A unit of SRM 1950 consists of five vials, each containing approximately 1.0 mL of plasma. a. Will the **same** volume of 1.0 mL plasma per vial meet your needs?	○ Yes ○ No, please specify how much would you prefer per vial: _____ (mL)	Descriptive
B	The current SRM 1950 contains lithium heparin as the anticoagulant. Will the **same** anticoagulant meet your needs?	○ Yes ○ No, please specify: _____	Descriptive
B	The source for current SRM 1950 was plasma obtained from 100 individuals with an equal number of men and women in age range of 40-50 years (detail of the sample pool demographic can be found in the SRM Certificate of Analysis). If SRM 1950 will be renewed, will a **similar** sample pool demographic meet your needs?	○ Yes ○ No, please specify: _____	Descriptive

RQ3 What do users prefer (RMs and/or SRMs) for new materials for metabolomics?			
Version	**Survey Items**	**Response Options**	**Plan for Reporting**
A, B	NIST currently provides various types of materials intended to be used as measurement standards. We want to get your feedback on two types below: • NIST Reference Materials (RM): [need definition and links] • NIST Standard Reference Materials (SRM): [need definition and links] c. Based on the above definitions and your research needs, if NIST develops new materials, what would you prefer them to be?	○ Reference Materials (RMs) ○ Standard Reference Materials (SRMs) ○ It doesn't matter to my research ○ I don't know the difference between RMs and SRMs	Descriptive

A, B	[SHOW b if RMs or SRMs is selected in the survey item above] d. Please explain why you chose [RMs/SRMs]	_____	Descriptive
A, B	What characteristics are important to you when selecting future reference materials for your research? (check all that apply)	☐ Availability ☐ Composition ☐ Cost ☐ Homogeneity ☐ Matrix ☐ Purity ☐ Stability ☐ Traceability to SI unit ☐ Uncertainty ☐ Other (please specify): _____	Descriptive

Additional information to be collected			
Version	**Survey Items**	**Response Options**	**Plan for Reporting**
A, B	Please share any additional thoughts.	_____	Descriptive
A, B	May NIST contact you for further discussion on your experience with SRM 1950 or other reference materials?	☐ Yes, please provide contact information: Name: _____ (First/Last) Email: _____ Laboratory/Affiliation: _____	Descriptive
A, B	The Metabolomics Quality Assurance and Quality Control Consortium (mQACC), an international working group, not affiliated with NIST, is interested in compiling SRM 1950 data from metabolomics researchers in order to fully characterize the compositional components in benefit to the community. Are you willing to share your SRM 1950 data with mQACC?	○ Yes ○ No	Descriptive

Demographic Questions			
Version	**Demographic Questions**	**Response Options**	**Plan for Reporting**
A, B, C	Where are you located?	○ United States (US) ○ Non-US (please specify your country): _____	Descriptive
A, B	What of the following best describe(s) your organization? (check all that apply)	☐ Academic laboratory ☐ Federal Government laboratory ☐ Local Government laboratory ☐ Pharmaceutical laboratory ☐ Third-party testing laboratory ☐ Research and development ☐ Contractor ☐ Other (please specify): _____	Descriptive
A, B	What of the following best describe(s) your role? (check all that apply)	☐ Researcher/Scientist ☐ Management ☐ Technician ☐ Tester ☐ Other (please specify): _____	Descriptive
A, B	What of the following best describe(s) your research area or interest? (check all that apply)	☐ Lipidomics ☐ Metabolomics ☐ Other (please specify): _____	Descriptive
B	What are the reasons that your laboratory does not use SRM 1950? (check all that apply)	☐ Availability due to location ☐ Cost ☐ Lack of analyte-specific certified values ☐ Time required for analysis ☐ I use other reference materials in my work. ☐ I am not aware of this reference material. ☐ Other (please specify): _____	Descriptive
C	About how many NIST SRM 1950 customers do you have?	_____	Descriptive

Appendix G. Template– Evaluation Questions for Requesting Expert Reviews

As described in STEP 3, when requesting feedback from experts, it's a best practice to include the project's PPQs and/or alignment matrix providing experts with relevant contextual information.

In the copy of the survey, for each survey item, add the table below for experts to review and provide feedback.

Evaluation questions	Yes or No	Please explain your answer and provide comments on recommended refinements
Does the item align with the research questions?		
Are the directions clear?		
Is the item wording clear?		
Are the rating scales appropriate?		
Are the response options appropriate?		
Are there any missing elements?		

[Repeat the table for each survey item]

Then, at the end of the survey, add the table below to get the overall comments for the entire survey.

Evaluation questions for the overall survey	Yes or No	Please explain your answer and provide comments on recommended refinements
Do the items align with the research questions?		
Are there any missing elements?		
Is the survey layout appropriate?		
Do you have other comments?		

Appendix H. Template–Pseudo Participant Cognitive Interview

This template shows survey Version A as an example. The cognitive interview process is the same for other versions.

----------[TEMPLATE] ----------

Interviewer's Script and Notes for Pseudo-Participant Cognitive Think-Aloud Protocol

Pseudo-Participant ID: _____**Interviewer**: _____ **Date/Time**: _____

Project Title: 2023 NIST SRM 1950 Customer Feedback Survey – Version A

Materials needed
Cognitive interview script; Survey Instrument; Recording platform/device (e.g., Zoom)

Observation Notes (preferably, have another team member help take notes)
Throughout the interview, note problematic items/words:

- When a participant completely misinterprets an item
- Non-verbal behavior that you think is important (such as the participant seems distracted, fatigued, anxious, nervous, or slow to respond, puzzled or confused, irritated)

Interviewer's Script (what the interviewer will say is in blue text)
Review interview purpose, say:

> Thank you for agreeing to help review the survey we are developing. Today's focus is on getting your feedback. Your feedback is extremely valuable. Your perspective will help ensure our questions and response options are clear and complete.

Review study purpose, say:

> This survey aims to gather feedback directly from existing and prospective users of NIST SRM 1950. The results will help NIST devise future reference material formulations to fulfill user needs and continue to support the metabolomic and lipidomic communities.

> We will be going through each survey question one by one. For each question, I'd ask you to "think aloud." Have you ever done think-aloud? [If not] so for a think-aloud, all I want you to do is explain what you're thinking when you hear a question asked.
>
> - Read the question out loud.
> - Tell me what this question is asking you.
> - Tell me if you could answer the question – if not, why not?

There are no right or wrong answers to these questions, only what you think is right for you. Please answer as if you were taking the questionnaire.

You can skip any questions that you do not feel comfortable answering and stop at any time.

Review the per-question feedback process, say:

To recap, for each question, I will ask you to read the question out loud, tell me what it is asking, and tell me if you could answer the question—if not, why not?

I know it's tempting to read the question and then choose your answer immediately. But please wait for my prompt so that I can ensure that your feedback is recorded properly.

- I will let you know when we can move on to the next question.
- We'll go question by question, and then I'll ask for your overall impressions at the end.

Do you have any questions before we start? One last thing before we get started: Would you mind if we recorded this session? Recording helps ensure that we catch everything you're saying.

Are you ready to start?

[If in-person, hand the participant a copy of the survey. If virtually, show participants the survey instrument on the screen; for example, share the screen using a PowerPoint presentation with one question on each slide.]

Example question

First, let's start with an example question so you are comfortable with "thinking aloud" and step through the feedback process.

EX1. How would you classify the weather today?

- ○ Cloudy
- ○ Sunny
- ○ Hot
- ○ Rainy
- ○ Unsure
- ○ Other (please specify) _____

Cognitive Interview Script	Notes
1. First, please read the example question aloud.	
2. What is the question asking you? [follow-up–if participate doesn't understand the question] How would you ask the question in your own words?	
3. Could you answer the question using the response options? [If not] Why not?	
[just for the example question] 4. Do you have any questions on the feedback process?	
5. Let's move on to the next question.	

NIST SRM 1950 Customer Feedback Survey

The National Institute of Standards and Technology (NIST) SRM 1950 Metabolites in Frozen Human Plasma was first made available in 2011 and has been widely used by researchers and scientists in the metabolomic and lipidomic communities and beyond. NIST will be renewing SRM 1950 and/or developing new reference materials in the coming years, a process that typically takes 5-7 years. We are conducting an information gathering survey with existing and prospective users to collect feedback on their experiences with SRM 1950. The survey results will help NIST devise future reference material formulations to fulfill user needs and continue to support the metabolomic and lipidomic communities.

Voices from SRM 1950 customers and the metabolomic and lipidomic communities are important to this endeavor. We hope you will play a part in SRM 1950's succession and encourage colleagues and other scientists to participate as well. Please share the [survey link] widely. We appreciate your assistance and your time.

This survey takes approximately 10 minutes.

If you are a purchasing official or reseller/distributor of NIST SRM 1950, please help forward this survey [survey link] to your group members or customers.

The NIST SRM 1950 survey team would like to express our gratitude to the Metabolomics Quality Assurance and Quality Control Consortium (mQACC) Best Practices QA/QC task group for their inspiration on some of the survey questions.

[NEXT]

Cognitive Interview Script	Notes
1. First, please read the text aloud.	
2. What is the text asking you? [follow-up–if participate doesn't understand the question] How would you say it in your own words?	

[BRANCHING]
Has your organization used NIST SRM 1950 ?

- ○ Yes – current customer of SRM 1950
- ○ Yes – used SRM 1950 before, but not currently
- ○ No, but my laboratory is interested in SRM 1950
- ○ No, my laboratory is not interested in SRM 1950
- ○ No, my organization is a reseller/distributor of SRM 1950

Cognitive Interview Script	Notes
1. First, please read the question aloud.	
2. What is the question asking you? [follow-up–if participate doesn't understand the question] How would you ask the question in your own words?	
3. Could you answer the question using the response options? [If not] Why not?	
[just for the example question] 4. Do you have any questions on the feedback process?	
5. Let's move on to the next question.	

-------[Repeat this process, one question at a time, for all questions and response options] --------

Appendix I. Template–Expert Review Comments and Resolutions

It's suggested that a spreadsheet be used to record experts' review comments and decisions on the resolutions.

Experts	Survey Items					
	Item1	**Item 2**	**Item 3**	**…**	**…**	**Item n**
Survey Expert 1						
Survey Expert 2						
…						
SME 1						
SME 2						
…						
Pseudo Participant 1						
Pseudo Participant 2						
…						
Resolution Decisions	[state what will be done addressing experts' feedback; or include justifications if suggested revisions were not addressed.]					

Appendix J. Example–Pseudo-Participants Comments and Resolutions

Many comments were collected during the cognitive Interviews with pseudo-participants for the ***2023 NIST SRM 1950 Customer Feedback Survey***. For illustration purposes, only one exemplary survey item is shown here, in which the original wording induced significant confusion from the pseudo-participants and resulted in a major revision of the survey item language.

	Survey Items
Experts	6. Which class(es) of analytes has your laboratory used SRM 1950? (check all that apply) ☐ Cholesterol and Total Glycerides ☐ Fatty acids ☐ Amino acids ☐ Fat-soluble vitamins and Carotenoids ☐ Water-soluble vitamins ☐ Organic clinical markers ☐ Electrolytes ☐ Hormones ☐ Trace Elements ☐ Proteins ☐ Perfluorinated Compounds (PFCs) ☐ Other (please specify): _____
Pseudo Participant 1	your top question asks on this page "for each class… has your laboratory used SRM 1950" but then the list doesn't cover all the categories of metabolites, you are only focusing on the ones which you have certified values in SRM 1950. You have a huge set of values that may not be certified. But, I can use SRM 1950 for many other things. It will be very tricky on the categories and how people are going to interpret them. The list will be bigger than you have. People will have different names/categories. The "Other" category can get very messy.
Pseudo Participant 2	Most people would buy SRM 1950 and add things to it in order to create the sample and use it for their own purpose. Different people might group things differently, some classes are missing from the list; The moment you open the door to Perfluorinated Compounds, you open the door to non-natural; but there are many other things that are not natural (not listed)
Resolution Decisions	After discussing with the project team, we realized the problem is not so much about those classes (or how they are grouped), but actually stemmed from how the question is worded. The original wording sounded like asking what classes people use SRM 1950 for - which both PP1 & PP2 indicated that people could use SRM 1950 for many other things. So, we need to make it clear that we are only asking about the classes provided/available in current SRM 1950 certificate. • Reworded survey item to: 6. SRM 1950 currently provides values of 90 analytes in the following 10 classes. Which class(es) of these analytes has your laboratory used SRM 1950? (check all that apply) Subsequently, for analytes under each class, we will ask their importance to your work. • Revised response options to: ☐ Cholesterol and Total Glycerides ☐ Fatty acids ☐ Amino acids ☐ Fat-soluble vitamins and Carotenoids ☐ Water-soluble vitamins ☐ Organic clinical markers

	☐ *Inorganic clinical markers* ☐ Electrolytes ☐ Hormones *(e.g., steroid hormones)* ☐ Trace Elements ☐ Proteins ☐ Perfluorinated Compounds (PFCs) ☐ *None of the above. I do not use assigned values provided in SRM 1950 Certificate of Analysis.* • Added an open-ended question: Are there other classes (not provided in current SRM 1950) that you use for your work? Please specify: [ ]

Appendix K. Example–Revised Survey Draft of the 2023 NIST SRM 1950 Customer Feedback Survey

This example illustrates revisions made to the initial draft after iterative rounds of expert reviews, team members' discussions, and resolution decisions.

The revised survey draft has the same part divisions as in the initial draft in Appendix D. For illustration purposes, only the revised Landing Page, Version A (including the Matrix Questions for Analytes) are shown in this Appendix.

Notations:

- Revisions: red, underlined text
- *Additions*: green, italicized text
- ~~Deletions~~: strike-out text
- Blue text in brackets, such as [LANDING PAGE], is not part of the survey. It indicates survey flow, conditional jumps/skips, or content to be provided later.

[LANDING PAGE]

*The National Institute of Standards and Technology (*NIST*)* SRM 1950 Metabolites in Frozen Human Plasma was first made available in 2011~~. It~~ *and* has been *widely* used by researchers and scientists in the metabolomic and lipidomic communities *and beyond*. NIST will be renewing SRM 1950 and/or developing new reference materials in the coming years*, a process that typically takes 5-7 years*. We are conducting *an information gathering* ~~a~~ survey with existing and prospect*ive* users to collect feedback on their experiences ~~and needs of~~ *with* SRM 1950. The survey results will help NIST devise future reference material~~s~~ formulation*s* to ~~better~~ fulfill user needs and *continue to* support the *clinical chemistry,* metabolomic and lipidomic communities.

~~It is important to have your individual and collective voices heard from the~~ *Feedback from SRM 1950 customers and the clinical chemistry,* metabolomic and lipidomic communities *are important to this endeavor*. We hope you will *play a part in SRM 1950's succession and* encourage *colleagues and* other ~~researchers and~~ scientists to *participate as well* ~~take the survey~~. Please *copy and* share the link widely~~ with others as well~~. We appreciate your assistance and your time.

This survey takes approximately [xx] minutes.

If you are a *purchasing official or* reseller/distributor of NIST SRM 1950, please help forward the survey to your *group members or* customers.

The NIST SRM 1950 survey team would like to express our gratitude to the Metabolomics Quality Assurance and Quality Control Consortium (mQACC) Best Practices QA/QC task group for their inspiration on some of the survey questions.

[OMB control #xxxx-xxxx]

[NEXT]

[BRANCHING]

Has your organization used NIST SRM 1950?

- ○ Yes – current user of SRM 1950
- ○ Yes – used SRM 1950 before, but not currently
- ○ No, but my laboratory is interested in SRM 1950
- ○ *No, my laboratory is **not** interested in SRM 1950*
- ○ No, my organization is a reseller/distributor of SRM 1950

[NEXT]

CONDITIONS:

- IF [Yes, current/past customers] JUMPTO **[Version A – Existing Customers]**
- IF [No, but interested] JUMPTO **[Version B – Prospective Customers]**
- IF [No, but interested] JUMPTO **[Version B – Prospective Customers, only show the "About You and Your Organization" part of the survey]**
- IF [No, reseller/distributor] JUMPTO **[Version C – Reseller/Distributor]**

[Version A – Existing Users]

About You and Your Organization

1. Where is your laboratory located?
   - ○ United States (US)
   - ○ Non-US, ~~(~~please specify your country~~)~~: _____

2. Which of the following best describe(s) your laboratory? (check all that apply)
   - ☐ Academic laboratory*: Metabolomics Service Core Facility*
   - ☐ *Academic laboratory:* Research and development
   - ☐ *Clinical research institute*
   - ☐ Federal Government laboratory
   - ☐ Local Government laboratory
   - ☐ *In Vitro Diagnostic Manufacturer laboratory*
   - ☐ *Industry: Biotechnology*
   - ☐ *Industry: Food/Nutrition laboratory*
   - ☐ *Industry: Instrument vendor*
   - ☐ *Industry: Metabolomics Service Company*
   - ☐ *Industry:* Pharmaceutical laboratory
   - ☐ Reference testing laboratory
   - ~~☐ Contractor~~
   - ☐ Other (please specify): _____

3. Which of the following best describe(s) your role? (check all that apply)
   - ☐ Management
   - ☐ *Principal Investigator*
   - ☐ *Project Lead*
   - ☐ Researcher/Scientist
   - ☐ Technician
   - ☐ *Trainee: graduate student, postdoctoral fellow*
   - ~~☐ Tester~~
   - ☐ Other (please specify): _____

4. Which of the following best describe(s) your research area or interest? (check all that apply)
   - ☐ *Bioanalysis*
   - ☐ *Clinical analysis*
   - ☐ Lipidomics
   - ☐ Metabolomics
   - ☐ *Proteomics*
   - ☐ Other (please specify): _____

[NEXT]

Use of NIST SRM 1950 Metabolites in Frozen Human Plasma

5. For what purpose(s) has your laboratory used SRM 1950? (check all that apply)
   - ☐ Calibration
   - ~~☐ Benchmarking~~
   - ☐ Comparability: Inter-study (across studies)
   - ☐ Comparability: Inter-laboratory (across laboratories)
   - ☐ Identification
   - ☐ *Instrument benchmarking/System suitability test*
   - ~~☐ In-house calibrants, control materials~~
   - ☐ Method development/optimization
   - ☐ Method validation
   - ☐ Normalization
   - ☐ Precision: Intra-study (within study)
   - ~~☐ Process stability assessment~~
   - ☐ Quantitation
   - ~~☐ Quality Assurance/Quality Control~~
   - ☐ Other (please specify): _____

6. *SRM 1950 currently provides values of 90 analytes in the following 10 classes.* Which class(es) of *these* analytes has your laboratory used ~~SRM 1950~~? (check all that apply)
   Subsequently, for analytes under each class, we will ask their importance to your work.

   - ☐ Cholesterol and ~~Total~~ Glycerides
   - ☐ Fatty acids
   - ☐ Amino acids
   - ☐ Fat-soluble vitamins and Carotenoids
   - ☐ Water-soluble vitamins
   - ☐ Organic clinical markers
   - ☐ *Inorganic clinical markers*
   - ~~☐ Electrolytes~~
   - ☐ Hormones *(e.g., steroid hormones)*
   - ~~☐ Trace Elements~~
   - ☐ Proteins
   - ☐ Perfluorinated Compounds (PFCs)
   - ☐ *None of the above. I do not use assigned values provided in SRM 1950 Certificate of Analysis.*
   - ~~☐ Other (please specify): _____~~

Are there other classes (not provided in current SRM 1950) that you use for your work? Please specify:

[NEXT]

[**HIDE** IF no item or "None of the above" was selected in Q6 above; **SHOW** IF otherwise]

[IF Cholesterol and Total Glycerides was checked, SHOW the matrix questions below.]

a. Cholesterol and ~~Total~~ Glycerides

For the value *currently* assigned *in SRM 1950* for each analyte~~-listed~~, how **important** is it to your work? ~~(0=not used; 3=essential)~~

	0 Do not use	1 *Somewhat Important*	2 *Very Important*	3 Essential
Cholesterol	○	○	○	○
Total Glycerides (as triolein)	○	○	○	○

Are there other analytes in this class that will be important to your work? Please specify:

[IF Fatty acids is checked, SHOW the matrix questions below.]

b. **Fatty Acids**

For the value *currently* assigned *in SRM 1950* for each analyte~~-listed~~, how **important** is it to your work? ~~(0=not used; 3=essential)~~

	0 Do not use	1 *Somewhat Important*	2 *Very Important*	3 Essential
C12:0 Dodecanoic Acid (Lauric Acid)	○	○	○	○
C16:0 Hexadecanoic Acid (Palmitic Acid)	○	○	○	○
C16:1 n-7 (Z)-9-Hexadecenoic Acid (Palmitoleic Acid)	○	○	○	○
C18:0 Octadecanoic Acid (Stearic Acid)	○	○	○	○
C18:3 n-3 (Z,Z,Z)-9,12,15-Octadecatrienoic Acid (α-Linolenic Acid)	○	○	○	○
C18:1 n-9 (Z)-9-Octadecenoic Acid (Oleic Acid)	○	○	○	○
C18:2 n-6 (Z,Z)-9,12-Octadecadienoic Acid (Linoleic Acid)	○	○	○	○
C22:0 Docosanoic Acid (Behenic Acid)	○	○	○	○
C14:0 Tetradecanoic Acid (Myristic Acid)	○	○	○	○
C14:1 (Z)-9-Tetradecenoic Acid (Myristoleic Acid)	○	○	○	○
C15:0 Pentadecanoic Acid	○	○	○	○
C17:0 Heptadecanoic Acid (Margaric Acid)	○	○	○	○
C18:3 n-6 (Z,Z,Z)-6,9,12-Octadecatrienoic Acid (γ-Linolenic Acid)	○	○	○	○
C18:1 n-7 (Z)-11-Octadecenoic Acid (Vaccenic Acid)	○	○	○	○
C20:0 Eicosanoic Acid (Arachidic Acid)(c,d)	○	○	○	○
C20:1 (Z)-11-Eicosenoic Acid (Gondolic Acid)	○	○	○	○
C20:2 (Z,Z)-1,14-Eicosadienoic Acid(c,d)	○	○	○	○
C20:3 n-6 (Z,Z,Z)-8,11,14-Eicosatrienoic Acid (Dihomo-γ-Linolenic Acid)	○	○	○	○

C20:4 n-6 (Z,Z,Z,Z)-5,8,11,14-Eicosatetraenoic Acid (Arachidonic Acid)	○	○	○	○
C20:5 n-3 (Z,Z,Z,Z,Z) -5,8,11,14,17-Eicosapentaenoic Acid (EPA)	○	○	○	○
C22:1 (Z)-13-Docosenoic Acid (Erucic Acid)	○	○	○	○
C22:4 n-6 (Z,Z,Z,Z)-7,10,13,16-Docosatetraenoic Acid	○	○	○	○
C22:5 n-3 (Z,Z,Z,Z,Z)-7,10,13,16,19-Docosapentaenoic Acid (DPA)	○	○	○	○
C22:5 n-6 (Z,Z,Z,Z,Z)-4,7,10,13,16-Docosapentaenoic Acid	○	○	○	○
C22:6 n-3 (Z,Z,Z,Z,Z,Z)-4,7,10,13,16,19-Docosahexaenoic Acid (DHA)	○	○	○	○
C24:0 Tetracosanoic Acid (Lignoceric Acid)	○	○	○	○
C24:1 (Z)-15-Tetracosenoic Acid (Nervonic Acid)	○	○	○	○

Are there other analytes in this class that will be important to your work? Please specify:

[IF Amino acids is checked, SHOW the matrix questions below.]

c. **Amino acids**

For the value *currently* assigned *in SRM 1950* for each analyte ~~listed~~, how **important** is it to your work? ~~(0=not used; 3=essential)~~

	0 Do not use	**1** *Somewhat Important*	**2** *Very Important*	**3** Essential
Arginine	○	○	○	○
Alanine	○	○	○	○
Cysteine	○	○	○	○
Cystine	○	○	○	○
Glycine	○	○	○	○
Histidine	○	○	○	○
Isoleucine	○	○	○	○
Leucine	○	○	○	○
Lysine	○	○	○	○
Methionine	○	○	○	○
Phenylalanine	○	○	○	○
Proline	○	○	○	○
Serine	○	○	○	○
Threonine	○	○	○	○
Tyrosine	○	○	○	○
Valine	○	○	○	○

Are there other analytes in this class that will be important to your work? Please specify:

[IF Fat-soluble vitamins and Carotenoids is checked, SHOW the matrix questions below.]

d. Fat-soluble vitamins and Carotenoids

For the value *currently* assigned *in SRM 1950* for each analyte ~~listed~~, how **important** is it to your work? ~~(0=not used; 3=essential)~~

	0 Do not use	1 *Somewhat Important*	2 *Very Important*	3 Essential
Retinol	○	○	○	○
α-Tocopherol	○	○	○	○
γ- + β-Tocopherol	○	○	○	○
Lutein	○	○	○	○
Zeaxanthin	○	○	○	○
β-Cryptoxanthin	○	○	○	○
Total α-Carotene	○	○	○	○
Total β-Carotene	○	○	○	○
25-Hydroxyvitamin D_2	○	○	○	○
25-Hydroxyvitamin D_3	○	○	○	○
~~5-Methyltetrahydrofolate~~	○	○	○	○
~~Pyridoxal 5'-phosphate~~	○	○	○	○
Trans-Lycopene	○	○	○	○
Total Lycopene	○	○	○	○
Trans-β-Carotene	○	○	○	○
Cis-β-Carotene	○	○	○	○

Are there other analytes in this class that will be important to your work? Please specify:

[IF Water-soluble vitamins is checked, SHOW the matrix questions below.]

e. **Water-soluble vitamins**

For the value *currently* assigned *in SRM 1950* for each analyte ~~listed~~, how **important** is it to your work? ~~(0=not used; 3=essential)~~

	0 Do not use	1 *Somewhat Important*	2 *Very Important*	3 Essential
~~*Trans*-Lycopene~~	○	○	○	○
~~Total Lycopene~~	○	○	○	○
~~*Trans*-β-Carotene~~	○	○	○	○
~~*Cis*-β-Carotene~~	○	○	○	○
~~25-Hydroxyvitamin D_2~~	○	○	○	○

Folic acid	○	○	○	○
Total folate	○	○	○	○
4-Pyridoxic acid	○	○	○	○
5-Methyltetrahydrofolate	○	○	○	○
Pyridoxal 5'-phosphate	○	○	○	○

Are there other analytes in this class that will be important to your work? Please specify:

[IF Organic clinical markers is checked, SHOW the matrix questions below.]

f. **Organic clinical markers**

For the value *currently* assigned *in SRM 1950* for each analyte ~~listed~~, how **important** is it to your work? ~~(0=not used; 3=essential)~~

	0 Do not use	**1** *Somewhat Important*	**2** *Very Important*	**3** Essential
Bilirubin	○	○	○	○
Creatinine	○	○	○	○
Homocysteine	○	○	○	○
Glucose	○	○	○	○
Urea	○	○	○	○
Uric Acid	○	○	○	○

Are there other analytes in this class that will be important to your work? Please specify:

[IF Electrolytes is checked, SHOW the matrix questions below.]

g. ***Inorganic Clinical Markers*** ~~**Electrolytes**~~

For the value *currently* assigned *in SRM 1950* for each analyte ~~listed~~, how **important** is it to your work? ~~(0=not used; 3=essential)~~

	0 Do not use	**1** *Somewhat Important*	**2** *Very Important*	**3** Essential
Calcium	○	○	○	○
Magnesium	○	○	○	○
Potassium	○	○	○	○
Sodium	○	○	○	○
Copper	○	○	○	○
Selenium	○	○	○	○

Are there other analytes in this class that will be important to your work? Please specify:

[IF Hormones is checked, SHOW the matrix questions below.]

h. **Hormones**

For the value *currently* assigned *in SRM 1950* for each analyte ~~listed~~, how **important** is it to your work? ~~(0=not used; 3=essential)~~

	0 Do not use	**1** *Somewhat Important*	**2** *Very Important*	**3** Essential
~~Homocysteine~~	○	○	○	○
Cortisol	○	○	○	○
Progesterone	○	○	○	○
Testosterone	○	○	○	○

Are there other analytes in this class that will be important to your work? Please specify:

[IF Trace Elements is checked, SHOW the matrix questions below.]

~~**i.Trace Elements**~~

~~For the value assigned for each analyte listed, to what extent is it needed for your research? (0=not used; 3=essential)~~

	0 ~~(not use)~~	**1**	**2**	**3** ~~(essential)~~
~~Copper~~	○	○	○	○
~~Selenium~~	○	○	○	○
~~Glutathione Peroxidase~~	○	○	○	○
~~Seleno-Albumin~~	○	○	○	○
~~Bilirubin (mg/dL)~~	○	○	○	○

[IF Proteins is checked, SHOW the matrix questions below.]

i. **Proteins**

For the value *currently* assigned *in SRM 1950* for each analyte ~~listed~~, how **important** is it to your work? ~~(0=not used; 3=essential)~~

	0	**1**	**2**	**3**

	Do not use	*Somewhat Important*	*Very Important*	Essential
Selenoprotein P	○	○	○	○
Glutathione Peroxidase	○	○	○	○
Seleno-Albumin	○	○	○	○
Total Protein ~~(g/L)~~	○	○	○	○
Vitamin D-Binding Protein ~~(mg/L)~~	○	○	○	○

Are there other analytes in this class that will be important to your work? Please specify:

[IF Perfluorinated Compounds (PFCs) is checked, SHOW the matrix questions below.]

j. **Perfluorinated Compounds (PFCs)**
For the value *currently* assigned *in SRM 1950* for each analyte ~~listed~~, how **important** is it to your work? ~~(0=not used; 3=essential)~~

	0 Do not use	**1** *Somewhat Important*	**2** *Very Important*	**3** Essential
Perfluorooctanoic Acid (PFOA)	○	○	○	○
Perfluorononanoic Acid (PFNA)	○	○	○	○
Perfluorodecanoic Acid (PFDA)	○	○	○	○
Perfluoroundecanoic Acid (PFUnA)	○	○	○	○
Perfluorohexansulfonate (PFHxS)	○	○	○	○
Perfluorooctanesulfonic Acid (PFOS)	○	○	○	○

Are there other analytes in this class that will be important to your work? Please specify:

[NEXT]

Future SRM 1950 Renewals or Development of New Reference Materials

7. A unit of *current* SRM 1950 consists of five vials, each containing approximately 1.0 mL of plasma *intended for one-time use. Would you prefer the **same** volume of **1.0 mL** plasma per vial for future renewals of SRM 1950?*
   a. ~~Typically, how much plasma do you use per analysis? _____ (mL)~~
   b. ~~Would you prefer a **similar** volume of plasma per vial for future renewals of SRM 1950?~~
      - Yes
      - No, please specify preferred amount per vial in mL~~per vial~~:_____ ~~(mL)~~

8. The current SRM 1950 contains lithium heparin as the anticoagulant. Would you prefer the **same** anticoagulant for future renewals of SRM 1950?
   - Yes
   - No, please specify *preferred anticoagulant*: _____

9. The source for current SRM 1950 was plasma obtained from 100 individuals with an equal number of men and women in age range of 40-50 years (details of the sample pool demographics can be found in the SRM Certificate of Analysis). Would you prefer a **similar** sample pool demographic for future renewals of SRM 1950?
   - Yes
   - No, please specify *other demographics you would prefer*: _____

10. NIST currently provides various types of materials intended to be used as measurement standards. We want to get your feedback on two types below (*as defined in NISTSP 260-136*):
    - NIST Reference Materials (RM): *RMs only possess non-certified values and are accompanied by a NIST Reference Material Information Sheet. RMs are materials that are sufficiently homogeneous and stable with respect to one or more specified properties established by NIST in a measurement process.*
    - NIST Standard Reference Materials (SRM): *SRM 1950 is a NIST Standard Reference Material. SRMs are accompanied by a NIST Certificate or Certificate of Analysis. SRMs are materials that are characterized by a metrologically valid and traceable procedure for one or more specified properties. The certificate provides the value of the specified property, its associated uncertainty, and a statement of metrological traceability*

    e. Based on the above definitions and your research needs, if NIST develops new materials *for metabolomics*, what would you prefer them to be?
       - Reference Materials (RMs)
       - Standard Reference Materials (SRMs)
       - *Both RMs and SRMs*
       - It doesn't matter to my work
       - I don't know the difference between RMs and SRMs

    [SHOW 10b if RMs or SRMs *or BOTH* is selected]
    f. Please explain why you chose [RMs/SRMs]: _____

11. What characteristics are important to you when selecting future reference materials for your research? (check all that apply)
    - ☐ Availability
    - ☐ Composition *of assigned values*
    - ☐ Cost
    - ☐ Homogeneity
    - ☐ Matrix *(e.g., plasma, serum)*
    - ☐ *Measurement* Uncertainty
    - ☐ Purity
    - ☐ Stability
    - ☐ Traceability to SI unit *for purpose of quantitation*
    - ☐ Other (please specify): _____

[NEXT]

12. May NIST contact you for further discussion on your experience with SRM 1950 or other reference materials?
    If "Yes," please provide contact information. We will not share your contact information outside of the NIST research team.

    ☐ ~~Yes, please provide contact information:~~
    Name: _____ (First/Last)
    Email: _____
    Laboratory/Affiliation: _____

13. Please share any additional thoughts.

14. ~~The Metabolomics Quality Assurance and Quality Control Consortium (mQACC), an international working group, not affiliated with NIST, is interested in compiling SRM 1950 data from metabolomics researchers in order to fully characterize the compositional components in benefit to the community. Are you willing to share your SRM 1950 data with mQACC?~~
    ~~○ Yes~~
    ~~○ No~~

Thank You!

[SUBMIT/FINISH]

Appendix L. Example–Survey Programming Specifications and Data Dictionary

J.1 Survey Programming Specifications for the 2023 NIST SRM 1950 Customer Feedback Survey

Base Survey

[BLOCK1] LANDING PAGE

NIST SRM 1950 Customer Feedback Survey

The National Institute of Standards and Technology (NIST) SRM 1950 Metabolites in Frozen Human Plasma was first made available in 2011 and has been widely used by researchers and scientists in the metabolomic and lipidomic communities and beyond. NIST will be renewing SRM 1950 and/or developing new reference materials in the coming years, a process that typically takes 5-7 years. We are conducting an information gathering survey with existing and prospective users to collect feedback on their experiences with SRM 1950. The survey results will help NIST devise future reference material formulations to fulfill user needs and continue to support the clinical chemistry, metabolomic and lipidomic communities.

Feedback from SRM 1950 customers and the clinical chemistry, metabolomic and lipidomic communities are important to this endeavor. We hope you will play a part in SRM 1950's succession and encourage colleagues and other scientists to participate as well. Please copy and share the [survey link] widely. We appreciate your assistance and your time.

This survey takes approximately 10 minutes.

If you are a purchasing official or reseller/distributor of NIST SRM 1950, please help forward the survey [survey link] to your group members or customers.

The NIST SRM 1950 survey team would like to express our gratitude to the Metabolomics Quality Assurance and Quality Control Consortium (mQACC) Best Practices QA/QC task group for their inspiration on some of the survey questions.

Click for additional information about this study.

[OMB control #xxxx-xxxx]

[NEXT-NEW PAGE]

[BLOCK2] CUSTOMER STATUS

Question Number: **D0**
Question Label: D0_STATUS
Question Text: Has your organization used NIST SRM 1950?
Question Type: Radio buttons
Logic:
- IF D0_STATUS=NOW OR D0_STATUS=PAST OR D0_STATUS=MAYBE, continue to [BLOCK3] DEMOGRPHICS
- IF D0_STATUS=NO, JUMPTO [BLOCK8] NOT-INTERESTED
- IF D0_STATUS=RESELL, JUMPTO [BLOCK9] RESELLER

#	Answer Choice Text	Variable Name
1	Yes – current user of SRM 1950	NOW
2	Yes – used SRM 1950 before, but not currently	PAST
3	No, but my laboratory is **interested** in SRM 1950	MAYBE
4	No, my laboratory is **not** interested in SRM 1950	NO
5	No, my organization is a reseller/distributor of SRM 1950	RESELL

[NEXT-NEW PAGE]

[BLOCK3] DEMOGRAPHICS

Question Number: **D1**
Question Label: D1_LOC
Question Text: Where is your laboratory located?
Question Type: Radio buttons
Logic: SHOW D1 IF D0_STATUS = NOW OR D0_STATUS = PAST OR D0_STATUS = MAYBE

#	Answer Choice Text	Variable Name
1	United States (US)	US
2	Non-US, please specify your country:	NONUS

Question Number: D1_2
Question Label: D1_2_TEXT
Question Text: please specify your country:
Question Type: Single line text
Logic: NA

NO CHARACTER LIMIT

Question Number: **D2**
Question Label: D2_LAB

Question Text: Which of the following best describe(s) your laboratory? (check all that apply)
Question Type: Check boxes
Logic: SHOW D2 IF D0_STATUS = NOW OR D0_STATUS = PAST OR D0_STATUS = MAYBE

#	Answer Choice Text	Variable Name
1	Academic laboratory: Metabolomics service core facility	ACA_CORE
2	Academic laboratory: Research and Development	ACA_R&D
3	Clinical research institute	CLINICAL
4	Federal Government laboratory	FED_GOV
5	Local Government laboratory	LOC_GOV
6	In Vitro Diagnostic Manufacturer laboratory	INVITRO
7	Industry: Biotechnology	IND_BIO
8	Industry: Food/Nutrition laboratory	IND_FOOD
9	Industry: Instrument vendor	IND_INST
10	Industry: Metabolomics Service Company	IND_METAB
11	Industry: Pharmaceutical laboratory	IND_PHARM
12	Reference testing laboratory	REF_TEST
13	Other, please specify:	OTH

Question Number: D2_13
Question Label: D2_13_TEXT
Question Text: please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

Question Number: **D3**
Question Label: D3_ROLE
Question Text: Which of the following best describe(s) your role? (check all that apply)
Question Type: Check boxes
Logic: SHOW D3 IF D0_STATUS = NOW OR D0_STATUS = PAST OR D0_STATUS = MAYBE

#	Answer Choice Text	Variable Name
1	Management	MGR
2	Principal Investigator	PI
3	Project Lead	PL
4	Researcher/Scientist	RS
5	Technician	TECH
6	Trainee: graduate student, postdoctoral fellow	TRAINEE

7	Other, please specify:	OTH

Question Number: D3_7
Question Label: D3_7_TEXT
Question Text: please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

Question Number: D4
Question Label: D4_RSRCH
Question Text: Which of the following best describe(s) your research area or interest? (check all that apply)
Question Type: Check boxes
Logic: SHOW D4 IF D0_STATUS = NOW OR D0_STATUS = PAST OR D0_STATUS = MAYBE

#	Answer Choice Text	Variable Name
1	Bioanalysis	BIO
2	Clinical analysis	CLN
3	Lipidomics	LIP
4	Metabolomics	META
5	Proteomics	PRO
6	Other, please specify:	OTH

Question Number: D4_6
Question Label: D4_6_TEXT
Question Text: please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

Question Number: D5
Question Label: D5_NONCUS_REASON
Question Text: What are the reasons that your laboratory does not use SRM 1950? (check all that apply)
Question Type: Check boxes
Logic: SHOW D5 IF D0_STATUS= MAYBE

#	Answer Choice Text	Variable Name
1	Difficult to access/purchase	HARDACCESS
2	Not knowing how to purchase	HOWBUY
3	Cost	COST
4	Lack of desired analyte-specific certified values	LACK
5	Time required for analysis	TIME
6	I use other reference materials in my work.	DIFFRM
7	I am not aware of this reference material.	NOTAWARE
8	Other, please specify:	OTH

Question Number: D5_8
Question Label: D5_8_TEXT
Question Text: please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

[BLOCK4] SRM 1950 USAGE

Question Number: **Q1**
Question Label: Q1_PURP
Question Text: [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] (check all that apply)
Question Type: Check boxes
Logic:
- SHOW Q1 IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="For what purpose(s) has your laboratory used SRM 1950?"
  - IF D0=MAYBE, then DYNAMIC TEXT="If your laboratory would purchase SRM 1950, for what purpose(s) will your laboratory use it?"

#	Answer Choice Text	Variable Name
1	Calibration	CALI
2	Comparability: Inter-study (across studies)	COMP_STUDY
3	Comparability: Inter-laboratory (across laboratories)	COMP_LAB
4	Identification	IDENT
5	Instrument benchmarking/System suitability test	BENCHMARK
6	Method development/optimization	MTHD_DEV
7	Method validation	MTHD_VALID
8	Normalization	NORM

9	Precision: Intra-study (within study)	PRCISE
10	Quantitation	QUANT
11	Other, please specify:	OTH

Question Number: Q1_11
Question Label: Q1_11_TEXT
Question Text: please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

Question Number: **Q2**
Question Label: Q2_CLASS
Question Text: SRM 1950 currently provides values of 90 analytes in the following 10 classes. [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] (check all that apply)
Subsequently, for analytes under each class, we will ask their importance to your work.
Question Type: Check boxes
Logic:
- SHOW Q2 IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="Which class(es) of these analytes has your laboratory used?"
  - IF D0=MAYBE, then DYNAMIC TEXT="If your laboratory would purchase SRM 1950, which class(es) of these analytes will your laboratory use?"

#	Answer Choice Text	Variable Name
1	Cholesterol and Glycerides	CHOL
2	Fatty acids	FATTY
3	Amino acids	AMINO
4	Fat-soluble vitamins and Carotenoids	V_FATSOL
5	Water-soluble vitamins	V_WATER
6	Organic clinical markers	ORG
7	Inorganic clinical markers	INORG
8	Hormones (e.g., steroid hormones)	HRMN
9	Proteins	PROTN
10	Perfluorinated Compounds (PFCs)	PFCS
11	None of the above. I do not use assigned values provided in SRM 1950 Certificate of Analysis.	NONE

Question Number: Q2_OTH
Question Label: Q2_CLASS_OTH
Question Text: Are there other classes (not provided in current SRM 1950) that you [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] use for your work? Please specify:
Question Type: Multi line text
Logic:
- SHOW Q2_OTH IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT=""
  - IF D0=MAYBE, then DYNAMIC TEXT="will"

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

[BLOCK5] ANALYTES

Question Number: **Q2a**
Question Label: Q2_CHOL
Question Text: **Cholesterol and Glycerides**
For the value currently assigned in SRM 1950 for each analyte, [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] to your work?
Question Type: Matrix
Logic:
- SHOW Q2_a IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="how **important** is it"
  - IF D0=MAYBE, then DYNAMIC TEXT="how **important** will it be"

ROW TABLE

#	Row Text	Alias
1	Cholesterol	Q2_a_CHOL
2	Total Glycerides (as triolein)	Q2_a_GLYC

COLUMN TABLE

#	Column Text	Alias	VALUE
1	0 Do not use	NOT_USE	0
2	1 Somewhat Important	SOMEWHAT	1
3	2 Very Important	VERY	2
4	3 Essential	ESSENTIAL	3

Question Number: Q2a_OTH

Question Label: Q2a_CHOL_OTH
Question Text: Are there other analytes in this class that will be important to your work? Please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

Question Number: **Q2b**
Question Label: Q2_FATTY
Question Text: **Fatty Acids**
For the value currently assigned in SRM 1950 for each analyte, [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] to your work?
Question Type: Matrix
Logic:
- SHOW Q2_b IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="how **important** is it"
  - IF D0=MAYBE, then DYNAMIC TEXT="how **important** will it be"

ROW TABLE

#	Row Text	Alias
1	**C12:0** Dodecanoic Acid (Lauric Acid)	Q2_b_C12-0
2	**C14:0** Tetradecanoic Acid (Myristic Acid)	Q2_b_C14-0
3	**C14:1** (Z)-9-Tetradecenoic Acid (Myristoleic Acid)	Q2_b_C14-1
4	**C15:0** Pentadecanoic Acid	Q2_b_C15-0
5	**C16:0** Hexadecanoic Acid (Palmitic Acid)	Q2_b_C16-0
6	**C16:1 n-7** (Z)-9-Hexadecenoic Acid (Palmitoleic Acid)	Q2_b_C16-1
7	**C17:0** Heptadecanoic Acid (Margaric Acid)	Q2_b_C17-0
8	**C18:0** Octadecanoic Acid (Stearic Acid)	Q2_b_C18-0
9	**C18:1 n-7** (Z)-11-Octadecenoic Acid (Vaccenic Acid)	Q2_b_C18-1-n7
10	**C18:1 n-9** (Z)-9-Octadecenoic Acid (Oleic Acid)	Q2_b_C18-1-n9
11	**C18:2 n-6** (Z,Z)-9,12-Octadecadienoic Acid (Linoleic Acid)	Q2_b_C18-2
12	**C18:3 n-3** (Z,Z,Z)-9,12,15-Octadecatrienoic Acid (α-Linolenic Acid)	Q2_b_C18-3-n3
13	**C18:3 n-6** (Z,Z,Z)-6,9,12-Octadecatrienoic Acid (γ-Linolenic Acid)	Q2_b_C18-3-n6
14	**C20:0** Eicosanoic Acid (Arachidic Acid)	Q2_b_C20-0
15	**C20:1** (Z)-11-Eicosenoic Acid (Gondolic Acid)	Q2_b_C20-1
16	**C20:2** (Z,Z)-1,14-Eicosadienoic Acid	Q2_b_C20-2
17	**C20:3 n-6** (Z,Z,Z)-8,11,14-Eicosatrienoic Acid (Dihomo-γ-Linolenic Acid)	Q2_b_C20-3
18	**C20:4 n-6** (Z,Z,Z,Z)-5,8,11,14-Eicosatetraenoic Acid (Arachidonic Acid)	Q2_b_C20-4
19	**C20:5 n-3** (Z,Z,Z,Z,Z) -5,8,11,14,17-Eicosapentaenoic Acid (EPA)	Q2_b_C20-5

20	**C22:0** Docosanoic Acid (Behenic Acid)	Q2_b_C22-0
21	**C22:1** (Z)-13-Docosenoic Acid (Erucic Acid)	Q2_b_C22-1
22	**C22:4 n-6** (Z,Z,Z,Z)-7,10,13,16-Docosatetraenoic Acid	Q2_b_C22-4
23	**C22:5 n-3** (Z,Z,Z,Z,Z)-7,10,13,16,19-Docosapentaenoic Acid (DPA)	Q2_b_C22-5-n3
24	**C22:5 n-6** (Z,Z,Z,Z,Z)-4,7,10,13,16-Docosapentaenoic Acid	Q2_b_C22-5-n6
25	**C22:6 n-3** (Z,Z,Z,Z,Z,Z)-4,7,10,13,16,19-Docosahexaenoic Acid (DHA)	Q2_b_C22-6
26	**C24:0** Tetracosanoic Acid (Lignoceric Acid)	Q2_b_C24-0
27	**C24:1** (Z)-15-Tetracosenoic Acid (Nervonic Acid)	Q2_b_C24-1

COLUMN TABLE

#	Column Text	Alias	VALUE
1	0 Do not use	NOT_USE	0
2	1 Somewhat Important	SOMEWHAT	1
3	2 Very Important	VERY	2
4	3 Essential	ESSENTIAL	3

Question Number: Q2b_OTH
Question Label: Q2b_FATTY_OTH
Question Text: Are there other analytes in this class that will be important to your work? Please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

Question Number: **Q2c**
Question Label: Q2_AMINO
Question Text: **Amino Acids**
For the value currently assigned in SRM 1950 for each analyte, [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] to your work?
Question Type: Matrix
Logic:
- SHOW Q2_c IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="how **important** is it"
  - IF D0=MAYBE, then DYNAMIC TEXT="how **important** will it be"

ROW TABLE

#	Row Text	Alias

1	Arginine	Q2_c_ARG
2	Alanine	Q2_c_ALA
3	Cysteine	Q2_c_CYSTEINE
4	Cystine	Q2_c_CYSTINE
5	Glycine	Q2_c_GLY
6	Histidine	Q2_c_HIS
7	Isoleucine	Q2_c_ISO
8	Leucine	Q2_c_LEU
9	Lysine	Q2_c_LYS
10	Methionine	Q2_c_MET
11	Phenylalanine	Q2_c_PHE
12	Proline	Q2_c_PRO
13	Serine	Q2_c_SER
14	Threonine	Q2_c_THR
15	Tyrosine	Q2_c_TYR
16	Valine	Q2_c_VAL

COLUMN TABLE

#	Column Text	Alias	VALUE
1	0 Do not use	NOT_USE	0
2	1 Somewhat Important	SOMEWHAT	1
3	2 Very Important	VERY	2
4	3 Essential	ESSENTIAL	3

Question Number: Q2c_OTH
Question Label: Q2c_AMINO_OTH
Question Text: Are there other analytes in this class that will be important to your work?
Please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

Question Number: **Q2d**
Question Label: Q2_V_FATSOL
Question Text: **Fat-soluble Vitamins and Carotenoids**
For the value currently assigned in SRM 1950 for each analyte, [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] to your work?
Question Type: Matrix

Logic:

- SHOW Q2_d IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="how **important** is it"
  - IF D0=MAYBE, then DYNAMIC TEXT="how **important** will it be"

ROW TABLE

#	Row Text	Alias
1	Retinol	Q2_d_RET
2	α-Tocopherol	Q2_d_A-TOC
3	γ- + β-Tocopherol	Q2_d_TOCO
4	Lutein	Q2_d_LUT
5	Zeaxanthin	Q2_d_ZEA
6	β-Cryptoxanthin	Q2_d_CRY
7	Total α-Carotene	Q2_d_A-CAR
8	Total β-Carotene	Q2_d_B-CAR
9	25-Hydroxyvitamin D_2	Q2_d_25-HD2
10	25-Hydroxyvitamin D_3	Q2_d_25-HD3
11	*Trans*-Lycopene	Q2_d_TRANS-L
12	Total Lycopene	Q2_d_TOTAL-L
13	*Trans*-β-Carotene	Q2_d_TRANS-B
14	*Cis*-β-Carotene	Q2_d_CIS-B

COLUMN TABLE

#	Column Text	Alias	VALUE
1	0 Do not use	NOT_USE	0
2	1 Somewhat Important	SOMEWHAT	1
3	2 Very Important	VERY	2
4	3 Essential	ESSENTIAL	3

Question Number: Q2d_OTH
Question Label: Q2d_V_FATSOL_OTH
Question Text: Are there other analytes in this class that will be important to your work? Please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

Question Number: **Q2e**

Question Label: Q2_V_WATER
Question Text: **Water-soluble Vitamins**
For the value currently assigned in SRM 1950 for each analyte, [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] to your work?
Question Type: Matrix
Logic:
- SHOW Q2_e IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="how **important** is it"
  - IF D0=MAYBE, then DYNAMIC TEXT="how **important** will it be"

ROW TABLE

#	Row Text	Alias
1	Folic acid	Q2_e_FOLIC
2	Total folate	Q2_e_TOTAL-F
3	4-Pyridoxic acid	Q2_e_4-PYR
4	5-Methyltetrahydrofolate	Q2_e_5-METH
5	Pyridoxal 5'-phosphate	Q2_e_PYR

COLUMN TABLE

#	Column Text	Alias	VALUE
1	0 Do not use	NOT_USE	0
2	1 Somewhat Important	SOMEWHAT	1
3	2 Very Important	VERY	2
4	3 Essential	ESSENTIAL	3

Question Number: Q2e_OTH
Question Label: Q2e_V_WATER_OTH
Question Text: Are there other analytes in this class that will be important to your work?
Please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

Question Number: **Q2f**
Question Label: Q2_ORG
Question Text: **Organic Clinical Markers**
For the value currently assigned in SRM 1950 for each analyte, [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] to your work?

Question Type: Matrix
Logic:
- SHOW Q2_f IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="how **important** is it"
  - IF D0=MAYBE, then DYNAMIC TEXT="how **important** will it be"

ROW TABLE

#	Row Text	Alias
1	Bilirubin	Q2_f_BIL
2	Creatinine	Q2_f_CRE
3	Homocysteine	Q2_f_HOM
4	Glucose	Q2_f_GLU
5	Urea	Q2_f_UREA
6	Uric Acid	Q2_f_URIC

COLUMN TABLE

#	Column Text	Alias	VALUE
1	0 Do not use	NOT_USE	0
2	1 Somewhat Important	SOMEWHAT	1
3	2 Very Important	VERY	2
4	3 Essential	ESSENTIAL	3

Question Number: Q2f_OTH
Question Label: Q2f_ORG_OTH
Question Text: Are there other analytes in this class that will be important to your work?
Please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

Question Number: **Q2g**
Question Label: Q2_INORG
Question Text: **Inorganic Clinical Markers**
For the value currently assigned in SRM 1950 for each analyte, [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] to your work?
Question Type: Matrix
Logic:
- SHOW Q2_g IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT

- IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="how **important** is it"
- IF D0=MAYBE, then DYNAMIC TEXT="how **important** will it be"

ROW TABLE

#	Row Text	Alias
1	Calcium	Q2_g_CAL
2	Magnesium	Q2_g_MAG
3	Potassium	Q2_g_POT
4	Sodium	Q2_g_SOD
5	Copper	Q2_g_COP
6	Selenium	Q2_g_SEL

COLUMN TABLE

#	Column Text	Alias	VALUE
1	0 Do not use	NOT_USE	0
2	1 Somewhat Important	SOMEWHAT	1
3	2 Very Important	VERY	2
4	3 Essential	ESSENTIAL	3

Question Number: Q2g_OTH
Question Label: Q2g_INORG_OTH
Question Text: Are there other analytes in this class that will be important to your work? Please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

Question Number: **Q2h**
Question Label: Q2_HRMN
Question Text: **Hormones** (e.g., steroid hormones)
For the value currently assigned in SRM 1950 for each analyte, [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] to your work?
Question Type: Matrix
Logic:

- SHOW Q2_h IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="how **important** is it"
  - IF D0=MAYBE, then DYNAMIC TEXT="how **important** will it be"

ROW TABLE

#	Row Text	Alias
1	Cortisol	Q2_h_COR
2	Progesterone	Q2_h_PRO
3	Testosterone	Q2_h_TES

COLUMN TABLE

#	Column Text	Alias	VALUE
1	0 Do not use	NOT_USE	0
2	1 Somewhat Important	SOMEWHAT	1
3	2 Very Important	VERY	2
4	3 Essential	ESSENTIAL	3

Question Number: Q2h_OTH
Question Label: Q2h_HRMN_OTH
Question Text: Are there other analytes in this class that will be important to your work?
Please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

Question Number: **Q2i**
Question Label: Q2_PROTN
Question Text: **Proteins**
For the value currently assigned in SRM 1950 for each analyte, [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] to your work?
Question Type: Matrix
Logic:
- SHOW Q2_i IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="how **important** is it"
  - IF D0=MAYBE, then DYNAMIC TEXT="how **important** will it be"

ROW TABLE

#	Row Text	Alias
1	Seleno-Albumin	Q2_i_SEL-A
2	Glutathione Peroxidase	Q2_i_GLU
3	Selenoprotein P	Q2_i_SEL-P
4	Total Protein	Q2_i_PROT

5	Vitamin D-Binding Protein	Q2_i_VITA-D

COLUMN TABLE

#	Column Text	Alias	VALUE
1	0 Do not use	NOT_USE	0
2	1 Somewhat Important	SOMEWHAT	1
3	2 Very Important	VERY	2
4	3 Essential	ESSENTIAL	3

Question Number: Q2i_OTH
Question Label: Q2i_PROTN_OTH
Question Text: Are there other analytes in this class that will be important to your work? Please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

Question Number: **Q2j**
Question Label: Q2_PFCS
Question Text: **Perfluorinated Compounds (PFCs)**
For the value currently assigned in SRM 1950 for each analyte, [DYNAMIC TEXT using EMBEDDED DATA in Qualtrics] to your work?
Question Type: Matrix
Logic:
- SHOW Q2_j IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="how **important** is it"
  - IF D0=MAYBE, then DYNAMIC TEXT="how **important** will it be"

ROW TABLE

#	Row Text	Alias
1	Perfluorooctanoic Acid (PFOA)	Q2_j_PFOA
2	Perfluorononanoic Acid (PFNA)	Q2_j_PFNA
3	Perfluorodecanoic Acid (PFDA)	Q2_j_PFDA
4	Perfluoroundecanoic Acid (PFUnA)	Q2_j_PFUnA
5	Perfluorohexansulfonate (PFHxS)	Q2_j_PFHxS
6	Perfluorooctanesulfonic Acid (PFOS)	Q2_j_PFOS

COLUMN TABLE

#	Column Text	Alias	VALUE
1	0 Do not use	NOT_USE	0
2	1 Somewhat Important	SOMEWHAT	1
3	2 Very Important	VERY	2
4	3 Essential	ESSENTIAL	3

Question Number: Q2j_OTH
Question Label: Q2j_PFCS_OTH
Question Text: Are there other analytes in this class that will be important to your work? Please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

[BLOCK6] FUTURE SRMs & RMs

Question Number: **Q3**
Question Label: Q3_VIAL
Question Text: A unit of current SRM 1950 consists of five vials, each containing approximately 1.0 mL of plasma intended for one-time use.
[DYNAMIC TEXT using EMBEDDED DATA in Qualtrics]
Question Type: Radio
Logic:
- SHOW Q3 IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="Would you prefer the **same** volume of **1.0 mL** plasma per vial for future renewals of SRM 1950?"
  - IF D0=MAYBE, then DYNAMIC TEXT="If SRM 1950 will be renewed, will the **same** volume of **1.0 mL** plasma per vial meet your needs?"

#	Answer Choice Text	Variable Name
1	Yes	Y
2	No, please specify preferred amount per vial in mL	N

Question Number: Q3_2
Question Label: Q3_2_TEXT
Question Text: please specify preferred amount per vial in mL

Question Type: Single line text
Logic: Validate numbers (real)

NO CHARACTER LIMIT

Question Number: **Q4**
Question Label: Q4_ANTICO
Question Text: The current SRM 1950 contains **lithium heparin** as the anticoagulant.
[DYNAMIC TEXT using EMBEDDED DATA in Qualtrics]
Question Type: Radio
Logic:
- SHOW Q4 IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="Would you prefer the **same** anticoagulant for future renewals of SRM 1950?"
  - IF D0=MAYBE, then DYNAMIC TEXT="If SRM 1950 will be renewed, will the **same** anticoagulant meet your needs?"

#	Answer Choice Text	Variable Name
1	Yes	Y
2	No, please specify anticoagulant	N

Question Number: Q4_2
Question Label: Q4_2_TEXT
Question Text: please specify preferred anticoagulant
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

Question Number: **Q5**
Question Label: Q5_SOURCE
Question Text: The source for current SRM 1950 was plasma obtained from 100 individuals with an equal number of men and women in age range of 40-50 years (detail of the sample pool demographic can be found in the SRM 1950 Certificate of Analysis).
[DYNAMIC TEXT using EMBEDDED DATA in Qualtrics]
Question Type: Radio
Logic:
- SHOW Q5 IF D0 ≠ NO OR D0 ≠ RESELL
- DYNAMIC TEXT
  - IF D0=NOW OR D0=PAST, then DYNAMIC TEXT="Would you prefer a **similar** sample pool demographic for future renewals of SRM 1950?"

- IF D0=MAYBE, then DYNAMIC TEXT="If SRM 1950 will be renewed, will a **similar** sample pool demographic meet your needs"

#	Answer Choice Text	Variable Name
1	Yes	Y
2	No, please specify other demographics you would prefer	N

Question Number: Q5_2
Question Label: Q5_2_TEXT
Question Text: please specify other demographics you would prefer
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

Question Number: **Q6_a**
Question Label: Q6_RM-SRM
Question Text: NIST currently provides various types of materials intended to be used as measurement standards. We want to get your feedback on two types below (as defined in NISTSP 260-136):

- **NIST Reference Materials (RM)**: RMs only possess non-certified values and are accompanied by a NIST Reference Material Information Sheet. RMs are materials that are sufficiently homogeneous and stable with respect to one or more specified properties established by NIST in a measurement process.
- **NIST Standard Reference Materials (SRM)**: SRM 1950 is a NIST Standard Reference Material. SRMs are accompanied by a NIST Certificate or Certificate of Analysis. SRMs are materials that are characterized by a metrologically valid and traceable procedure for one or more specified properties. The certificate provides the value of the specified property, its associated uncertainty, and a statement of metrological traceability.

a. Based on the above definitions and your research needs, if NIST develops new materials for metabolomics, what would you prefer them to be?

Question Type: Radio
Logic:

- SHOW Q6_a IF D0 ≠ NO OR D0 ≠ RESELL

#	Answer Choice Text	Variable Name
1	Reference Materials (RMs)	RM
2	Standard Reference Materials (SRMs)	SRM
3	Both RMs and SRMs	BOTH
4	It doesn't matter to my work	NODIFF

5	I don't know the difference between RMs and SRMs	DNK

Question Number: Q6_b
Question Label: Q6_ OPEN
Question Text: Please explain why you chose [RMs/SRMs/Both]:
Question Type: Multi line text
Logic: SHOW Q6_b IF Q6_a=RM OR Q6_a=SRM OR Q6_a=BOTH

NO CHARACTER LIMIT

Question Number: **Q7**
Question Label: Q7_DECISION
Question Text: What **characteristics** are important to you when selecting future reference materials for your research? (check all that apply)
Question Type: Check boxes
Logic: NA

#	Answer Choice Text	Variable Name
1	Assigned values for specific analytes (provided in Certificate of Analysis for SRMs, or Information Sheet for RMs)	VALUES
2	Availability	AVAIL
3	Cost	COST
4	Homogeneity	HOM
5	Matrix (e.g., plasma, serum)	MATRX
6	Measurement Uncertainty	MEAS
7	Stability	STAB
8	Traceability to SI unit for purpose of quantitation	TRACE
9	Other, please specify:	OTH

Question Number: Q7_10
Question Label: Q7_10_TEXT
Question Text: please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[NEXT-NEW PAGE]

[BLOCK] CATCHALL

Question Number: **Q8**
Question Label: Q8_CONTACT
Question Text: May NIST contact you for further discussion on your experience with SRM 1950 or other reference materials?
If "Yes," please provide contact information. We will not share your contact information outside of the NIST research team.
Question Type: Form Fields (3 fields)
Logic:
- SHOW Q8 IF D0 ≠ NO OR D0 ≠ RESELL

#	Answer Choice Text	Variable Name
1	Name (First/Last):	NAME
2	Email:	EMAIL
3	Laboratory/Affiliation:	LAB

Question Number: **Q9**
Question Label: Q9_FINAL
Question Text: Please share any additional thoughts. Thank you!
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[FINISH/SUBMIT]

[BLOCK8] NOT-INTERESTED

Question Number: **N1**
Question Label: N1_LOC
Question Text: Where is your laboratory located?
Question Type: Radio buttons
Logic: SHOW N1 IF D0_STATUS = NO

#	Answer Choice Text	Variable Name
1	United States (US)	US
2	Non-US, please specify your country:	NONUS

Question Number: N1_2
Question Label: N1_NONUS_OPEN
Question Text: please specify your country:
Question Type: Single line text

Logic: NA

NO CHARACTER LIMIT

Question Number: **N2**
Question Label: N2_LAB
Question Text: What of the following best describe(s) your laboratory? (check all that apply)
Question Type: Check boxes
Logic: SHOW N2 IF D0_STATUS = NO

#	Answer Choice Text	Variable Name
1	Academic laboratory: Metabolomics service core facility	ACA_CORE
2	Academic laboratory: Research and Development	ACA_R&D
3	Clinical research institute	CLINICAL
4	Federal Government laboratory	FED_GOV
5	Local Government laboratory	LOC_GOV
6	In Vitro Diagnostic Manufacturer laboratory	INVITRO
7	Industry: Biotechnology	IND_BIO
8	Industry: Food/Nutrition laboratory	IND_FOOD
9	Industry: Instrument vendor	IND_INST
10	Industry: Metabolomics Service Company	IND_METAB
11	Industry: Pharmaceutical laboratory	IND_PHARM
12	Reference testing laboratory	REF_TEST
13	Other, please specify:	OTH

Question Number: N2_13
Question Label: N2_OTH_OPEN
Question Text: please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

Question Number: **N3**
Question Label: N3_ROLE
Question Text: Which of the following best describe(s) your role? (check all that apply)
Question Type: Check boxes
Logic: SHOW N3 IF D0_STATUS = NO

#	Answer Choice Text	Variable Name
1	Management	MGR

2	Principal Investigator	PI
3	Project Lead	PL
4	Researcher/Scientist	RS
5	Technician	TECH
6	Trainee: graduate student, postdoctoral fellow	TRAINEE
7	Other, please specify:	OTH

Question Number: N3_7
Question Label: N3_OTH_OPEN
Question Text: please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

Question Number: N4
Question Label: N4_RSRCH
Question Text: Which of the following best describe(s) your research area or interest? (check all that apply)
Question Type: Check boxes
Logic: SHOW N1 IF D0_STATUS = NO

#	Answer Choice Text	Variable Name
1	Bioanalysis	BIO
2	Clinical analysis	CLN
3	Lipidomics	LIP
4	Metabolomics	META
5	Proteomics	PRO
6	Other, please specify:	OTH

Question Number: N4_6
Question Label: N4_OTH_OPEN
Question Text: please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

Question Number: N5
Question Label: N5_NONCUS_REASON

Question Text: What are the reasons that your laboratory does not use SRM 1950? (check all that apply)
Question Type: Check boxes
Logic: SHOW N1 IF D0_STATUS = NO

#	Answer Choice Text	Variable Name
1	Difficult to access/purchase	HARDACCESS
2	Not knowing how to purchase	HOWBUY
3	Cost	COST
4	Lack of desired analyte-specific certified values	LACK
5	Time required for analysis	TIME
6	I use other reference materials in my work.	DIFFRM
7	I am not aware of this reference material.	NOTAWARE
8	Other, please specify:	OTH

Question Number: N5_8
Question Label: N5_OTH_OPEN
Question Text: please specify:
Question Type: Multi line text
Logic: NA

NO CHARACTER LIMIT

[FINISH/SUBMIT]

[BLOCK9] RESELLER

Question Number: **R1**
Question Label: R1_LOC
Question Text: Where are you located?
Question Type: Radio buttons
Logic: NA

#	Answer Choice Text	Variable Name
1	United States (US)	US
2	Non-US (please specify your country):	NONUS

Question Number: **R2**
Question Label: R2_CUSNUM
Question Text: About how many NIST SRM 1950 customers do you have?
Question Type: Single line text
Logic: Validate whole number

whole number/digits

Question Number:	**R_FINAL**
Question Label:	NULL
Question Text:	We sincerely appreciate your help in forwarding this survey [survey link] to your customers. ***Thank You!***
Question Type:	Static text
Logic:	NA

[FINISH/SUBMIT]

[END OF SURVEY]

Thank you for taking this survey.

If you have any questions about this study, please contact Yee-Yin Choong at yee-yin.choong@nist.gov. If you have any questions about your rights as a research participant, please contact the NIST Research Protections Office and/or Institutional Review Board at 301-975-5445 or email rpoffice@nist.gov.

J.1 Data Dictionary Example of the 2023 NIST SRM 1950 Customer Feedback Survey

For illustration purposes, only partial portions of the data dictionary of the ***2023 NIST SRM 1950 Customer Feedback Survey*** are shown below. The data dictionary typically is in a spreadsheet format such as Microsoft Excel.

QID	Data Variables	Survey Question	Type	Measure	Value	Value Label
ResponseId	Response ID	Qualtrics Generated	String	Nominal		
[BLOCK2] CUSTOMER STATUS						
D0	D0_STATUS	Has your organization used NIST SRM 1950?				
			String	Nominal	NOW	Yes – current user of SRM 1950
			String	Nominal	PAST	Yes – used SRM 1950 before, but not currently
			String	Nominal	MAYBE	No, but my laboratory is **interested** in SRM 1950
			String	Nominal	NO	No, my laboratory is **not** interested in SRM 1950
			String	Nominal	RESELL	No, my organization is a reseller/distributor of SRM 1950
[BLOCK3] DEMOGRAPHICS						
D1	D1_LOC	Where is your laboratory located?				
			String	Nominal	US	United States (US)
			String	Nominal	NONUS	Non-US, please specify your country:
D1_2	D1_2_TEXT	please specify your country:	String	Nominal	OPEN	
			Numeric	Nominal	-99	(non-response)
D2	D2_LAB	Which of the following best describe(s) your laboratory? (check all that apply)				
			String	Nominal	ACA_CORE	Academic laboratory: Metabolomics service core facility
			String	Nominal	ACA_R&D	Academic laboratory: Research and Development
			String	Nominal	CLINICAL	Clinical research institute
			String	Nominal	FED_GOV	Federal Government laboratory
			String	Nominal	LOC_GOV	Local Government laboratory
			String	Nominal	INVITRO	In Vitro Diagnostic Manufacturer laboratory
			String	Nominal	IND_BIO	Industry: Biotechnology
			String	Nominal	IND_FOOD	Industry: Food/Nutrition laboratory
			String	Nominal	IND_INST	Industry: Instrument vendor
			String	Nominal	IND_METAB	Industry: Metabolomics Service Company
			String	Nominal	IND_PHARM	Industry: Pharmaceutical laboratory
			String	Nominal	REF_TEST	Reference testing laboratory
D2_13	D2_13_TEXT	Other, please specify:	String	Nominal	OTH	Other, please specify:

			Numeric	Nominal	-99	(non-response)
			Numeric	Nominal	-100	(valid skip)
D3	D3_ROLE	Which of the following best describe(s) your role? (check all that apply)				
			String	Nominal	MGR	Management
			String	Nominal	PI	Principal Investigator
			String	Nominal	PL	Project Lead
			String	Nominal	RS	Researcher/Scientist
			String	Nominal	TECH	Technician
			String	Nominal	TRAINEE	Trainee: graduate student, postdoctoral fellow
D3_7	D3_7_TEXT	Other, please specify:	String	Nominal	OTH	Other, please specify:
			Numeric	Nominal	-99	(non-response)
			Numeric	Nominal	SKIP	(valid skip)
D4	D4_RSRCH	Which of the following best describe(s) your research area or interest? (check all that apply)				
			String	Nominal	BIO	Bioanalysis
			String	Nominal	CLN	Clinical analysis
			String	Nominal	LIP	Lipidomics
			String	Nominal	META	Metabolomics
			String	Nominal	PRO	Proteomics
D4_6	D4_6_TEXT	Other, please specify:	String	Nominal	OTH	Other, please specify:
			Numeric	Nominal	-99	(non-response)
			Numeric	Nominal	-100	(valid skip)
D5	D5_NONCUS_REASON	What are the reasons that your laboratory does not use SRM 1950? (check all that apply)				
			String	Nominal	HARDACCESS	Difficult to access/purchase
			String	Nominal	HOWBUY	Not knowing how to purchase
			String	Nominal	COST	Cost
			String	Nominal	LACK	Lack of desired analyte-specific certified values
			String	Nominal	TIME	Time required for analysis
			String	Nominal	DIFFRM	I use other reference materials in my work.
			String	Nominal	NOTAWARE	I am not aware of this reference material.
D5_8	D5_8_TEXT	Other, please specify:	String	Nominal	OTH	Other, please specify:
			Numeric	Nominal	-99	(non-response)
			Numeric	Nominal	-100	(valid skip)
[BLOCK4] SRM 1950 USAGE						
Q1	Q1_PURP	[NOW or PAST] For what purpose(s) has your laboratory used SRM 1950? [MAYBE] If your laboratory would purchase SRM 1950, for what purpose(s) will your laboratory use it?				
			String	Nominal	CALI	Calibration

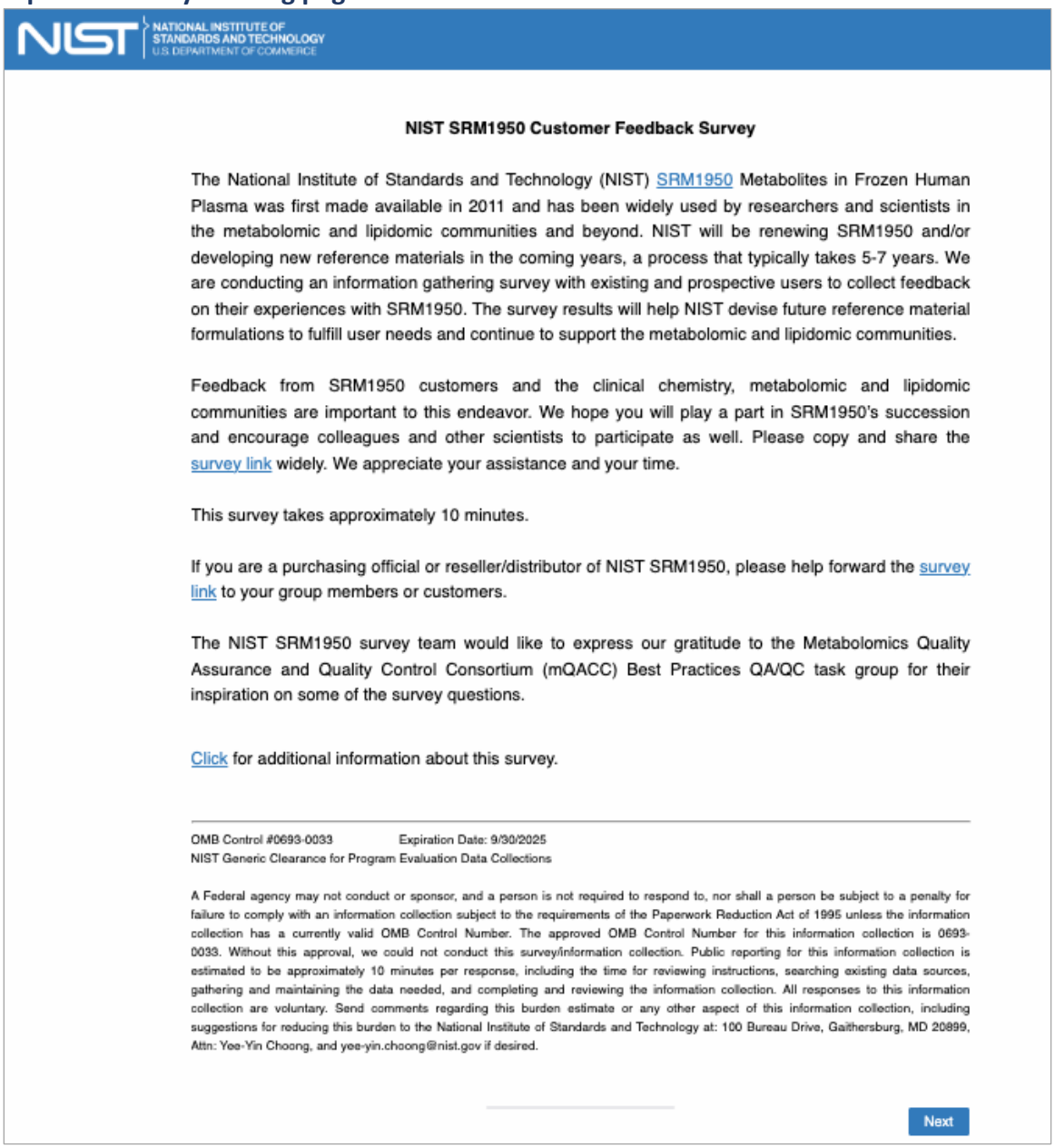
			String	Nominal	COMP_STUDY	Comparability: Inter-study (across studies)
			String	Nominal	COMP_LAB	Comparability: Inter-laboratory (across laboratories)
			String	Nominal	IDENT	Identification
			String	Nominal	BENCHMARK	Instrument benchmarking/System suitability test
			String	Nominal	MTHD_DEV	Method development/optimization
			String	Nominal	MTHD_VALID	Method validation
			String	Nominal	NORM	Normalization
			String	Nominal	PRCISE	Precision: Intra-study (within study)
			String	Nominal	QUANT	Quantitation
Q1_11	Q1_11_TEXT	Other, please specify:	String	Nominal	OTH	Other, please specify:
			Numeric	Nominal	-99	(non-response)
			Numeric	Nominal	-100	(valid skip)
Q2	Q2_CLASS	SRM 1950 currently provides values of 90 analytes in the following 10 classes. [EXISTING] Which class(es) of these analytes has your laboratory used? [PROSPECTIVE] If your laboratory would purchase SRM 1950, which class(es) of these analytes will your laboratory use?				
			String	Nominal	CHOL	Cholesterol and Glycerides
			String	Nominal	FATTY	Fatty acids
			String	Nominal	AMINO	Amino acids
			String	Nominal	V_FATSOL	Fat-soluble vitamins and Carotenoids
			String	Nominal	V_WATER	Water-soluble vitamins
			String	Nominal	ORG	Organic clinical markers
			String	Nominal	INORG	Inorganic clinical markers
			String	Nominal	HRMN	Hormones (e.g., steroid hormones)
			String	Nominal	PROTN	Proteins
			String	Nominal	PFCS	Perfluorinated Compounds (PFCs)
			String	Nominal	NONE	None of the above. I do not use assigned values provided in SRM 1950 Certificate of Analysis.
			Numeric	Nominal	-99	(non-response)
			Numeric	Nominal	-100	(valid skip)
Q2_OTH	Q2_CLASS_OTH	Are there other classes (not provided in current SRM 1950) that you [Field-Q2_CLASS_OTH_PIPE]use for your work? Please specify:	String	Nominal	OTH	
			Numeric	Nominal	-99	(non-response)
			Numeric	Nominal	-100	(valid skip)

Q2a		For the value currently assigned in SRM 1950 for each analyte, how important is it/will it be to your work?				
Q2_a_CHOL	Q2_a_CHOL	Cholesterol	String	Ordinal	0	Do Not Use
Q2_a_GLYC	Q2_a_GLYC	Total Glycerides (as triolein)	String	Ordinal	1	Somewhat Important
			String	Ordinal	2	Very Important
			String	Ordinal	3	Essential
			Numeric	Nominal	-99	(non-response)
			Numeric	Nominal	-100	(valid skip)
Q2a_OTH	Q2a_CHOL_OTH	Are there other analytes in this class that will be important to your work? Please specify:			OPEN	
			Numeric	Nominal	-99	(non-response)
			Numeric	Nominal	-100	(valid skip)
[similar for other variables]						

Appendix M. Example–Screenshots of the Implemented 2023 NIST SRM 1950 Customer Feedback Survey

Below are exemplary screenshots from the implemented 2023 NIST SRM 1950 Customer Feedback Survey for illustration purposes.

Example 1 – Survey Landing page:



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NIST SRM1950 Customer Feedback Survey

The National Institute of Standards and Technology (NIST) SRM1950 Metabolites in Frozen Human Plasma was first made available in 2011 and has been widely used by researchers and scientists in the metabolomic and lipidomic communities and beyond. NIST will be renewing SRM1950 and/or developing new reference materials in the coming years, a process that typically takes 5-7 years. We are conducting an information gathering survey with existing and prospective users to collect feedback on their experiences with SRM1950. The survey results will help NIST devise future reference material formulations to fulfill user needs and continue to support the metabolomic and lipidomic communities.

Feedback from SRM1950 customers and the clinical chemistry, metabolomic and lipidomic communities are important to this endeavor. We hope you will play a part in SRM1950's succession and encourage colleagues and other scientists to participate as well. Please copy and share the survey link widely. We appreciate your assistance and your time.

This survey takes approximately 10 minutes.

If you are a purchasing official or reseller/distributor of NIST SRM1950, please help forward the survey link to your group members or customers.

The NIST SRM1950 survey team would like to express our gratitude to the Metabolomics Quality Assurance and Quality Control Consortium (mQACC) Best Practices QA/QC task group for their inspiration on some of the survey questions.

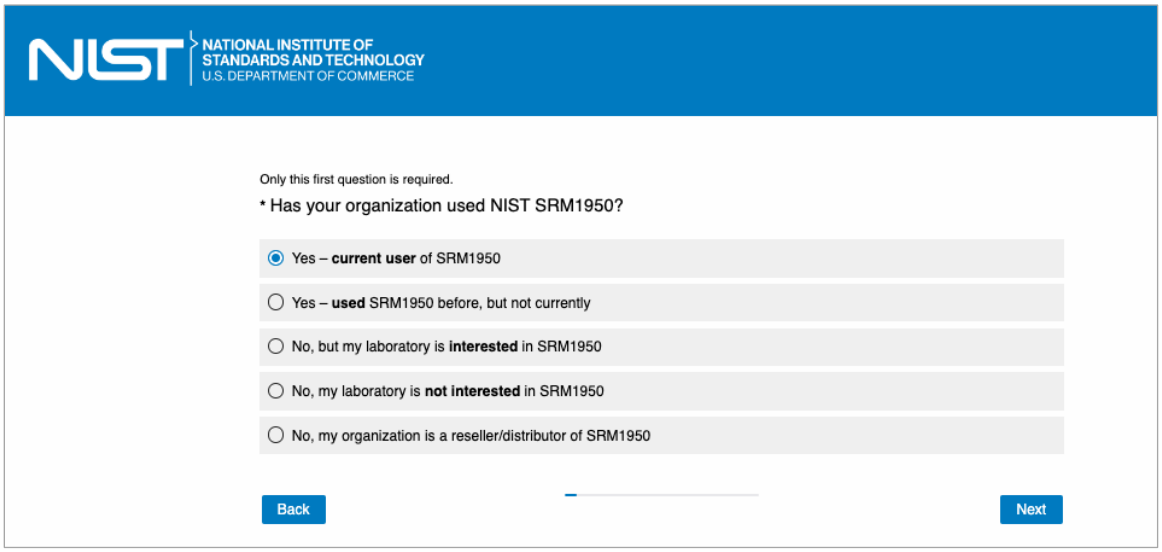
Click for additional information about this survey.

OMB Control #0693-0033 Expiration Date: 9/30/2025
NIST Generic Clearance for Program Evaluation Data Collections

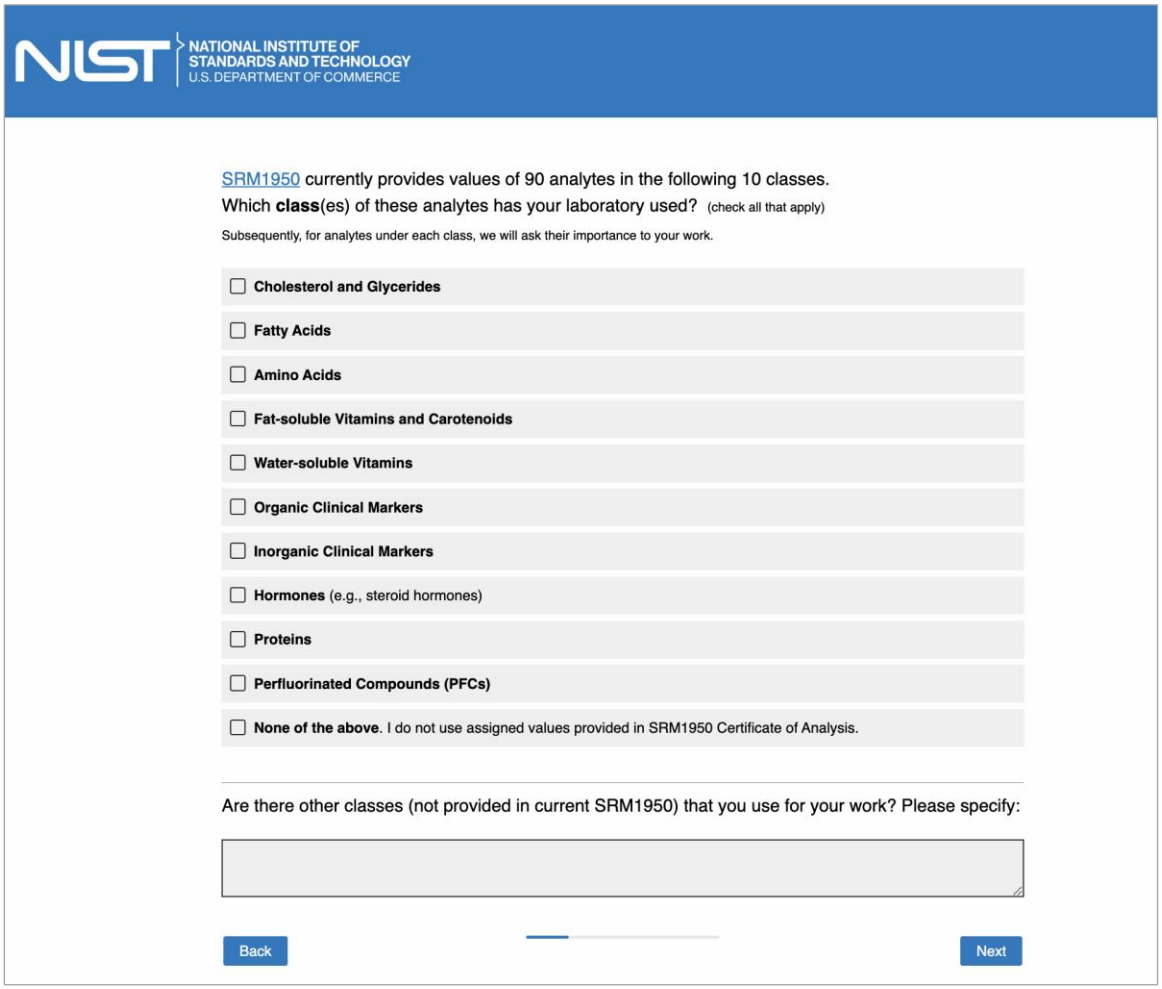
A Federal agency may not conduct or sponsor, and a person is not required to respond to, nor shall a person be subject to a penalty for failure to comply with an information collection subject to the requirements of the Paperwork Reduction Act of 1995 unless the information collection has a currently valid OMB Control Number. The approved OMB Control Number for this information collection is 0693-0033. Without this approval, we could not conduct this survey/information collection. Public reporting for this information collection is estimated to be approximately 10 minutes per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the information collection. All responses to this information collection are voluntary. Send comments regarding this burden estimate or any other aspect of this information collection, including suggestions for reducing this burden to the National Institute of Standards and Technology at: 100 Bureau Drive, Gaithersburg, MD 20899, Attn: Yee-Yin Choong, and yee-yin.choong@nist.gov if desired.

Next

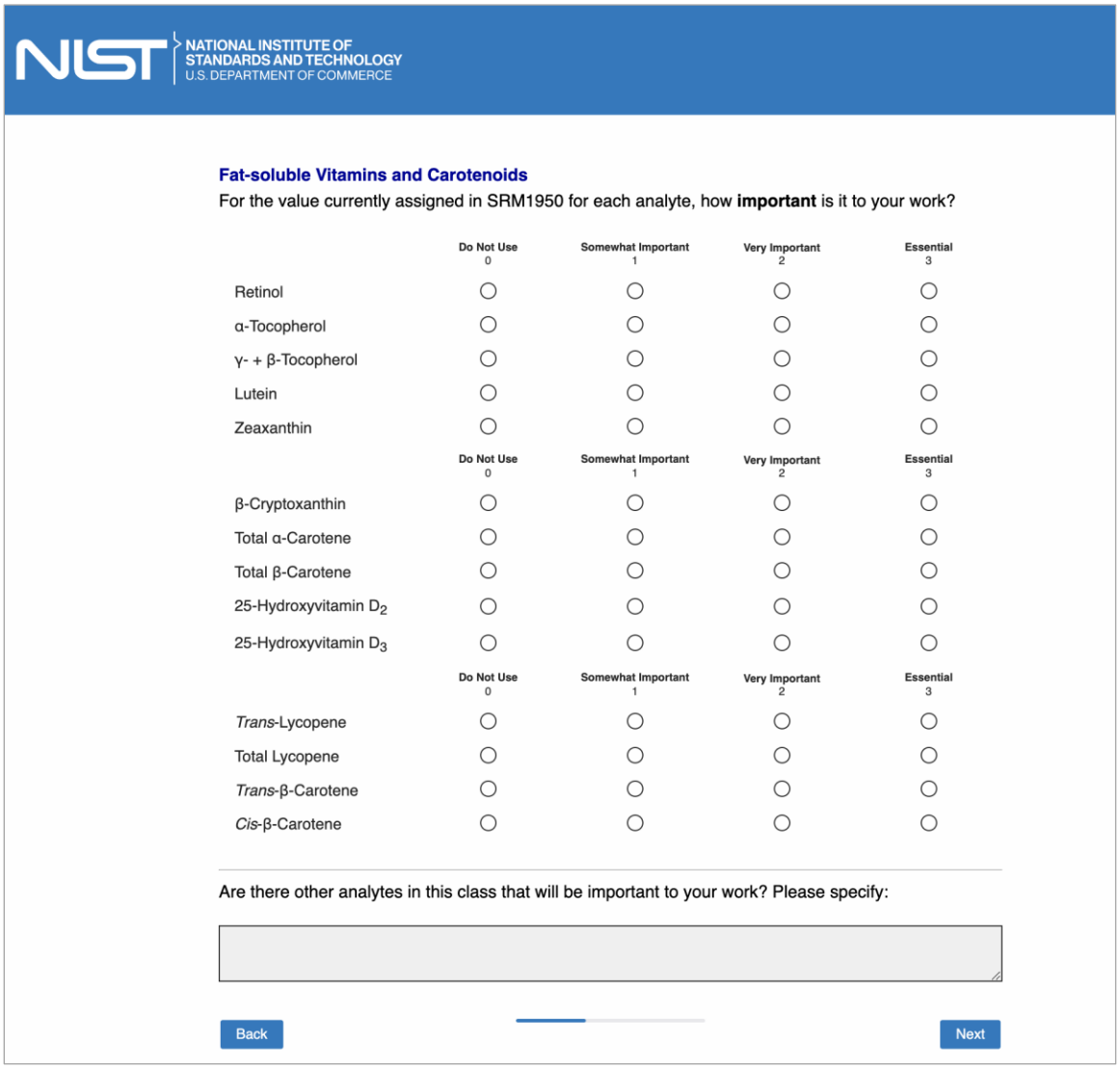
Example 2 – Customer status page:



Example 3 – SRM 1950 Class Usage page:



Example 4 – SRM 1950 Usage page (if "Fat-soluble vitamins and Carotenoids" was checked):



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U.S. DEPARTMENT OF COMMERCE

Fat-soluble Vitamins and Carotenoids

For the value currently assigned in SRM1950 for each analyte, how **important** is it to your work?

	Do Not Use 0	Somewhat Important 1	Very Important 2	Essential 3
Retinol	○	○	○	○
α-Tocopherol	○	○	○	○
γ- + β-Tocopherol	○	○	○	○
Lutein	○	○	○	○
Zeaxanthin	○	○	○	○

	Do Not Use 0	Somewhat Important 1	Very Important 2	Essential 3
β-Cryptoxanthin	○	○	○	○
Total α-Carotene	○	○	○	○
Total β-Carotene	○	○	○	○
25-Hydroxyvitamin D_2	○	○	○	○
25-Hydroxyvitamin D_3	○	○	○	○

	Do Not Use 0	Somewhat Important 1	Very Important 2	Essential 3
Trans-Lycopene	○	○	○	○
Total Lycopene	○	○	○	○
Trans-β-Carotene	○	○	○	○
Cis-β-Carotene	○	○	○	○

Are there other analytes in this class that will be important to your work? Please specify:

Back Next

Appendix N. Example–Sampling and Recruitment Plan for 2023 NIST SRM 1950 Customer Feedback Survey

	2023 NIST SRM 1950 Customer Feedback Survey
Target population	Existing SRM 1950 customers and prospective customers in the clinical chemistry, metabolomic and lipidomic communities
Sampling frame(s)	• ***Existing SRM 1950 customers***: Existing SRM 1950 customers (current and past) • ***Prospective customers***: members in professional organizations of the clinical chemistry, metabolomic and lipidomic communities
Sampling types and techniques	Non-probabilistic, convenience sampling

Recruitment and dissemination strategies	• ***Sources:***
	  ○ NIST Office of Reference Materials (ORM) database of existing SRM 1950 customers (current and past)
	  ○ The Metabolomics Association of North America (MANA)
	  ○ The Metabolomics Society
	  ○ The Metabolomics Quality Assurance and Quality Control Consortium (mQACC)
	• ***Recruitment***: recruitment text and template (see below)
	• ***Dissemination strategies***:
	  ○ ORM sends invitation to existing SRM 1950 customers (current and past) via MarketingCloud
	  ○ NIST PAO assists with posting survey invite on social media, i.e., Twitter (X)
	  ○ Reach out to three professional organizations listed seeking assistance for survey dissemination to their members: MANA, the Metabolomics Society, and mQACC
	  ○ Project team members reach out to personal contacts and use word-of-mouth strategies at conferences

Fielding timeframe and duration	Initial planned timeframe: • ***Fielding***: launch survey mid-April, 2023 • ***Duration***: open survey for 10 weeks, concluding in end of June, 2023
Protocol for responding to inquiries	Single point of contact using email

[1st email invitation template – change highlighted date based on dissemination path, 4 weeks from the sent date**]**

Email Invitation Template – NIST SRM 1950 Customer Feedback Survey

To line: <ORM SRM 1950 mailing list of existing customers><members from metabolomic and lipidomic communities for prospective users>
Subject line: NIST SRM 1950 Customer Feedback Survey

Dear Colleagues,

The National Institute of Standards and Technology (NIST) is conducting a survey about SRM 1950 to gather feedback directly from existing and potential users on their experiences and needs to better design SRM products in the future.

SRM 1950 Metabolites in Frozen Human Plasma was first made available in 2011 and has been widely used by researchers and scientists in the metabolomic and lipidomic communities and beyond. NIST will be renewing SRM 1950 and/or developing new reference materials in the coming years, a process that typically takes 5-7 years. The survey results will help NIST devise future reference material formulations to fulfill your needs and continue to support the clinical chemistry, metabolomic and lipidomic communities. Feedback from SRM 1950 customers and the clinical chemistry, metabolomic and lipidomic communities are important to this endeavor.

We hope you will play a part in SRM 1950's succession and encourage colleagues and other scientists to participate as well. We appreciate your assistance and your time. Please take the survey and share the survey widely. This survey takes approximately 10 minutes.

If you are a purchasing official or reseller/distributor of NIST SRM 1950, please help forward this survey to your group members or customers.

The survey will be open until [month date], 2023, and can be accessed by using the direct link below (or copy-and-paste the link in a web browser):

LINK to survey: [insert survey url]

If you have any questions regarding the survey, please don't hesitate to email the survey point of contact, Yee-Yin Choong (yee-yin.choong@nist.gov).

Best regards,

The NIST SRM 1950 Survey Team:
Yee-Yin Choong, Human Factors Scientist, Information Technology Laboratory
Johanna Camara, Research Chemist, Material Measurement Laboratory
Tracey Schock, Research Chemist, Material Measurement Laboratory
Clay Davis, Research Chemist, Material Measurement Laboratory
National Institute of Standards and Technology

[2nd email reminder template – sent 2 weeks after the 1st invitation email**]**

Email Reminder Template – NIST SRM 1950 Customer Feedback Survey

To line: <ORM SRM 1950 mailing list of existing customers><members from metabolomic and lipidomic communities for prospective users>
Subject line: REMINDER – NIST SRM 1950 Customer Feedback Survey

Dear Colleagues,

This is a friendly reminder. Please provide your invaluable feedback on SRM 1950 by taking the survey, if you have not already done so. The survey will be open until [month date], 2023

The National Institute of Standards and Technology (NIST) is conducting a survey about SRM 1950 to gather feedback directly from existing and potential users on their experiences and needs to better design SRM products in the future.

SRM 1950 Metabolites in Frozen Human Plasma was first made available in 2011 and has been widely used by researchers and scientists in the metabolomic and lipidomic communities and beyond. NIST will be renewing SRM 1950 and/or developing new reference materials in the coming years, a process that typically takes 5-7 years. The survey results will help NIST devise future reference material formulations to fulfill your needs and continue to support the clinical chemistry, metabolomic and lipidomic communities. Feedback from SRM 1950 customers and the clinical chemistry, metabolomic and lipidomic communities are important to this endeavor.

We hope you will play a part in SRM 1950's succession and encourage colleagues and other scientists to participate as well. We appreciate your assistance and your time. Please take the survey and share the survey widely. This survey takes approximately 10 minutes.

If you are a purchasing official or reseller/distributor of NIST SRM 1950, please help forward this survey to your group members or customers.

The survey can be accessed by using the direct link below (or copy-and-paste the link in a web browser):

LINK to survey: [insert survey url]

If you have any questions regarding the survey, please don't hesitate to email the survey point of contact, Yee-Yin Choong (yee-yin.choong@nist.gov).

Best regards,

The NIST SRM 1950 Survey Team:
Yee-Yin Choong, Human Factors Scientist, Information Technology Laboratory
Johanna Camara, Research Chemist, Material Measurement Laboratory
Tracey Schock, Research Chemist, Material Measurement Laboratory
Clay Davis, Research Chemist, Material Measurement Laboratory
National Institute of Standards and Technology

Appendix O. Example–Fielding and Data Collection Monitoring for 2023 NIST SRM 1950 Customer Feedback Survey

M1. Survey Fielding Logs

Recruitment/ Dissemination	Sampling Frame	Timeframe	Assigned to
ORM marketing cloud	Existing/Past customers	Initial: 2023-04-12 Reminder: 2023-04-26	Johanna NIST ORM
The Metabolomics Society	Prospective customers	Tweet: 2023-04-13	Tracey/Clay
Metabolomics journal	Prospective customers	Tweet: 2023-04-13	Tracey
The Metabolomics Quality Assurance and Quality Control Consortium (mQACC)	Prospective customers	Tweet: 2023-04-13	Tracey/Clay
The Metabolomics Association of North America (MANA)	Prospective customers	Initial: 2023-04-17 Reminder: 2023-04-xx	Tracey
MetaboNews	Prospective customers	Posted in newsletter: 2023-07-1	Tracey
Personal contacts/conferences	Prospective customers	No specific timeframe, just send them the survey link	Johanna/Tracey/Clay

M2. Weekly tally of completed survey responses

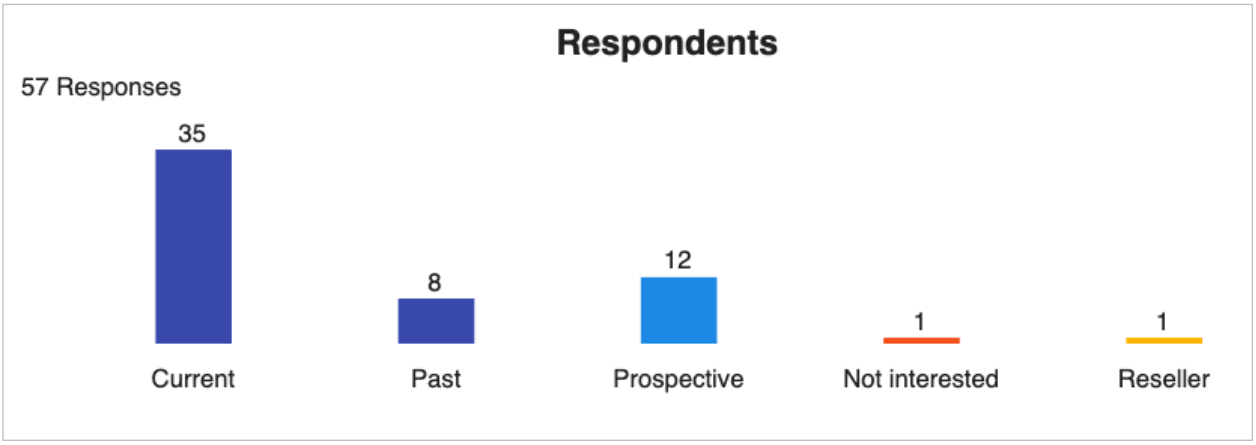
Time Recorded	Response Count	Cumulative Count	Customer Type			Location		
			Current	Past	Prospective	US	Non-US	Not specified
4/12/23 to 4/15/23	8	8	6	1	1	2	6	
4/16/23 to 4/22/23	19	27	11	1	7	14	5	
4/23/23 to 4/29/23	7	34	5	2		2	5	
4/30/23 to 5/06/23	5	39	3	2			5	
5/07/23 to 5/13/23	7	46	6	1		6	1	
5/14/23 to 5/20/23	1	47			1		1	
5/21/23 to 5/27/23								
5/28/23 to 6/03/23								
6/04/23 to 6/10/23								
6/11/23 to 6/17/23								
6/18/23 to 6/24/23	1	48	1				1	
6/25/23 to 7/01/23	3	51	1	1	1	2	1	
7/02/23 to 7/15/23	4	55	2		2	1	2	1
Subtotal	55	55	35	8	12	27	27	1

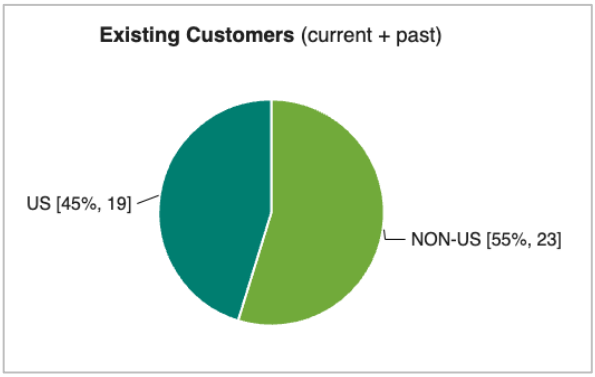
In addition, one respondent indicated they were not interested in SRM 1950, and another indicated that they were an SRM 1950 reseller rather than a user.

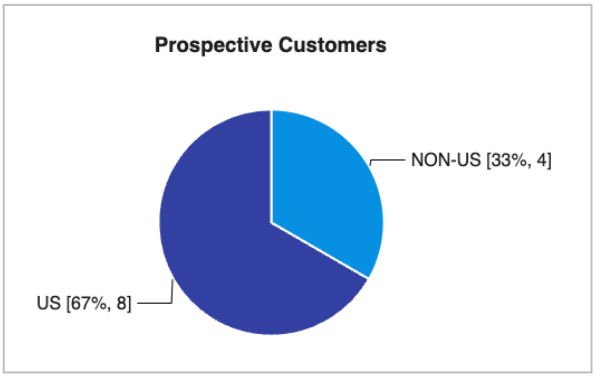
Appendix P. Example–Survey Results of the 2023 NIST SRM 1950 Customer Feedback Survey

A total of 55 completed responses were collected from existing and prospective users of SRM 1950 – 35 were current users, 8 were past users, and 12 were prospective users.

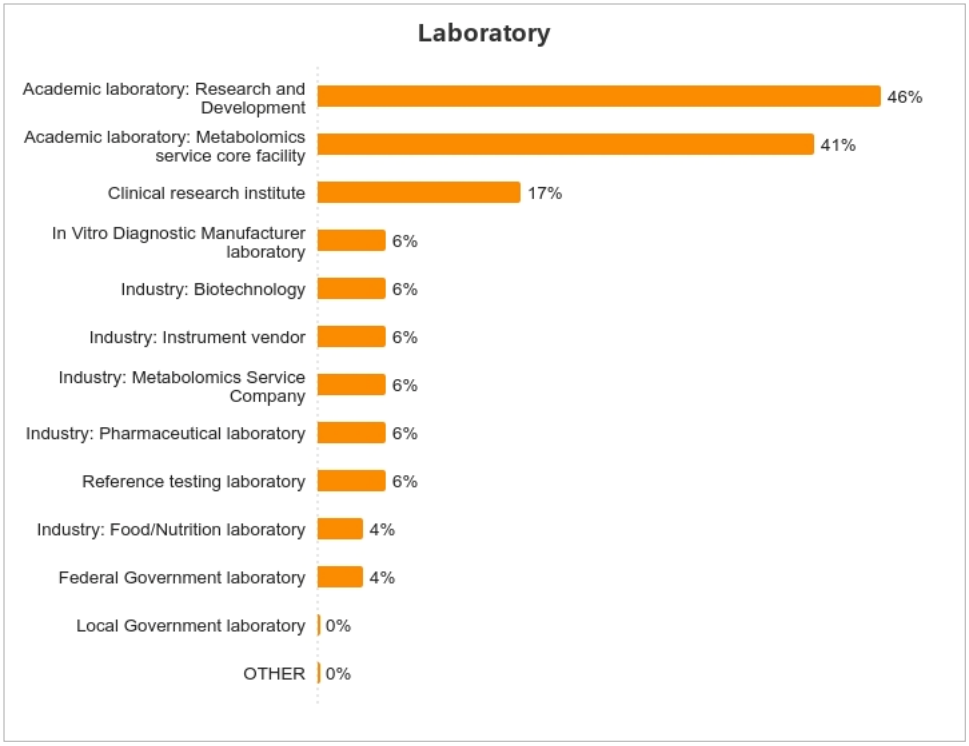
N.1. Respondent Characteristics

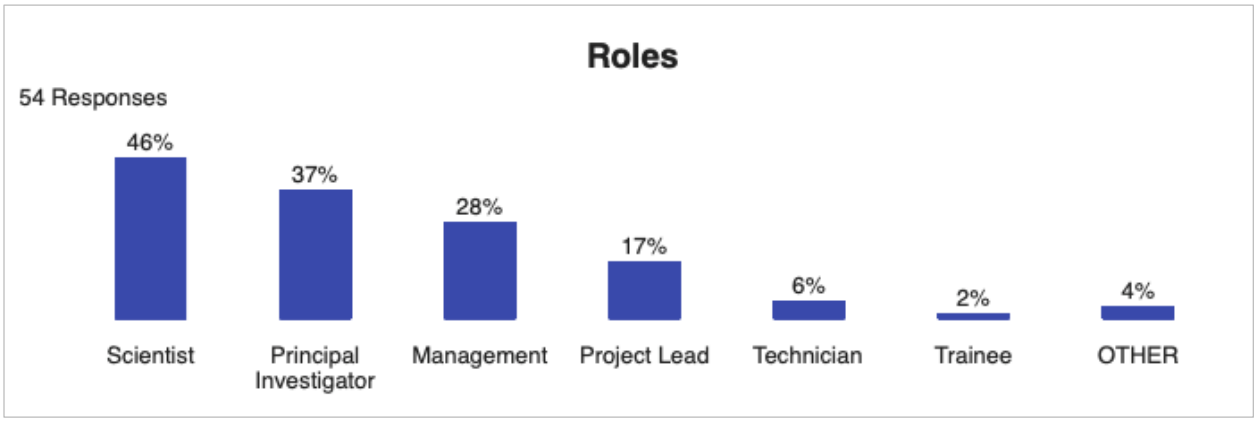




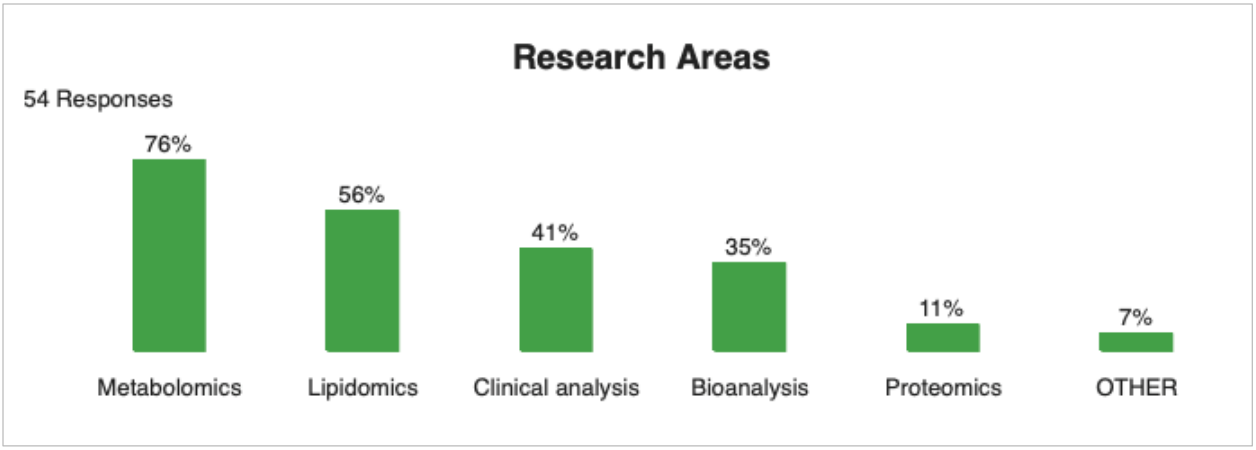


[Non-US countries entered] Australia (2); Belgium (1); Canada (6); Czech Republic (1); Finland (1); India (1); Italy (1); Japan (1); Norway (1); Singapore (1); South Korea (1); Switzerland (3); Taiwan (1); UK (3); Unspecified (3).



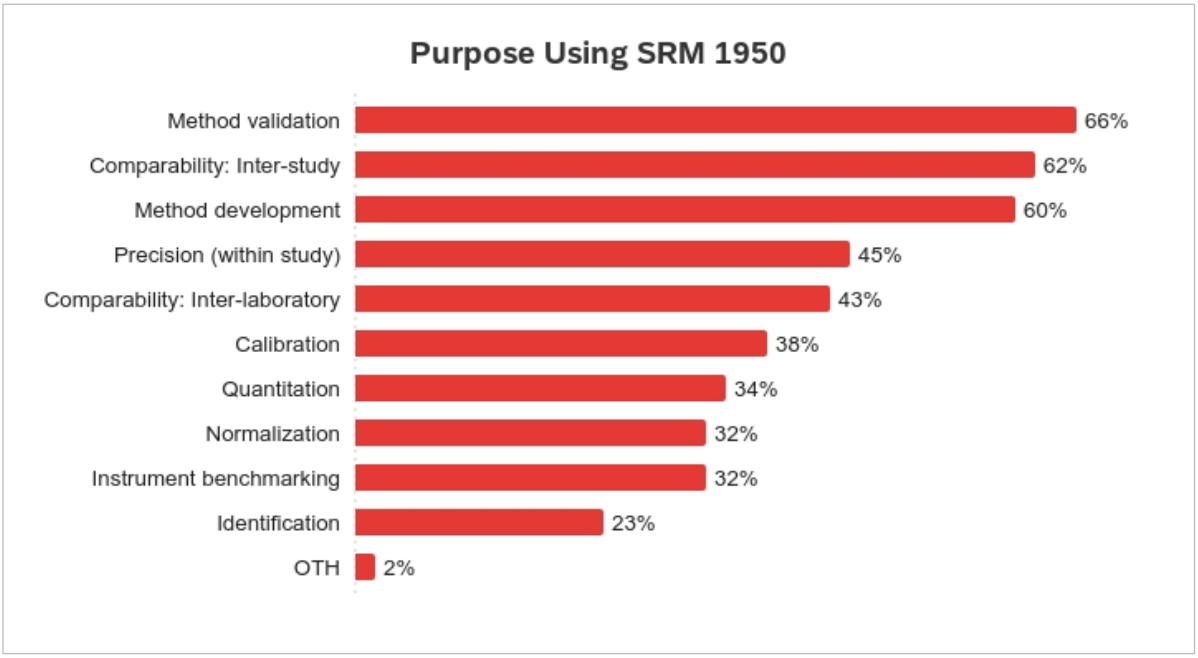


[Other roles entered] Citizen Science Initiative--Participant and Designate, Mass spectrometry research coordinator, Research Associate

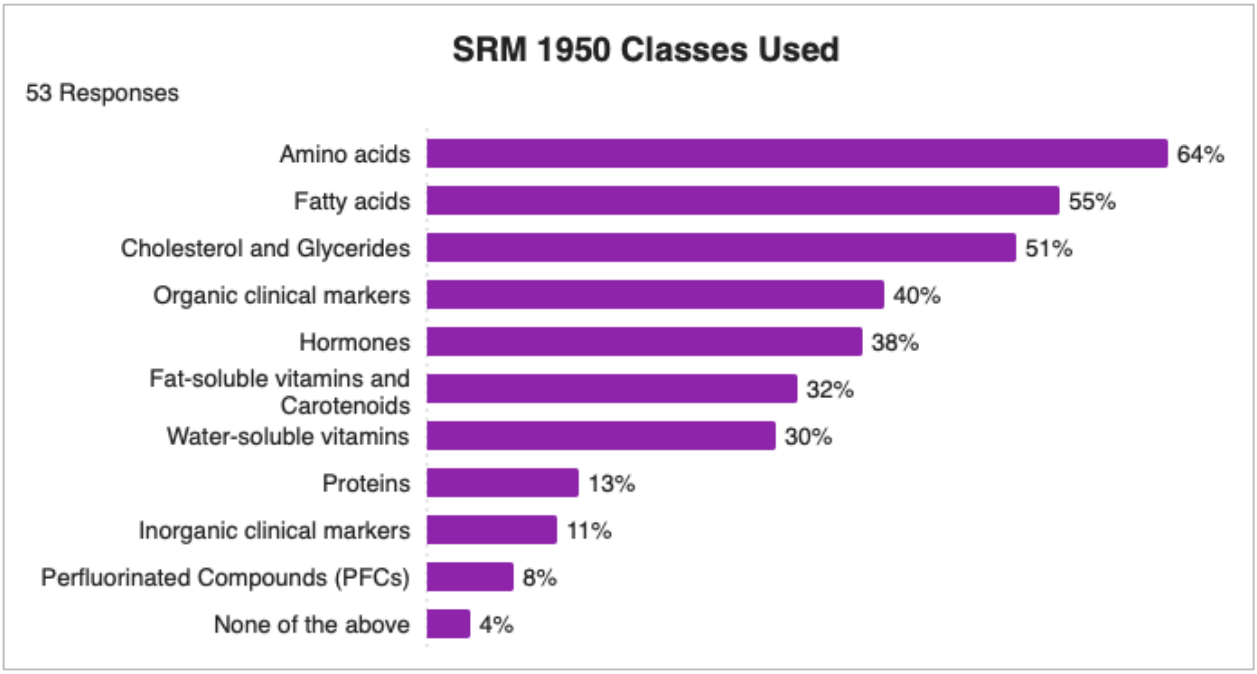


[Other research areas entered] isotope metallomics, Chemical exposure agent analysis, Exposomics, Food and Nutritional Sciences

N.2. SRM 1950 Usage – General



[Other purpose entered] Traceability



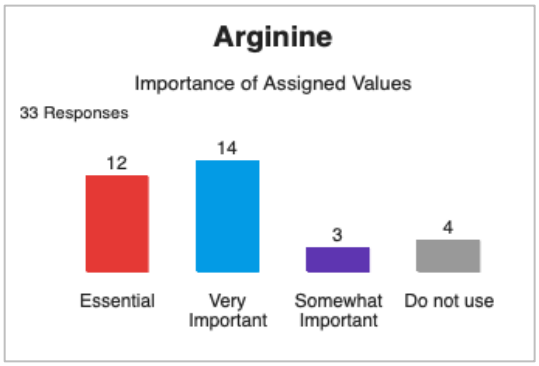
[Other classes used for their work, verbatim as entered by respondents]

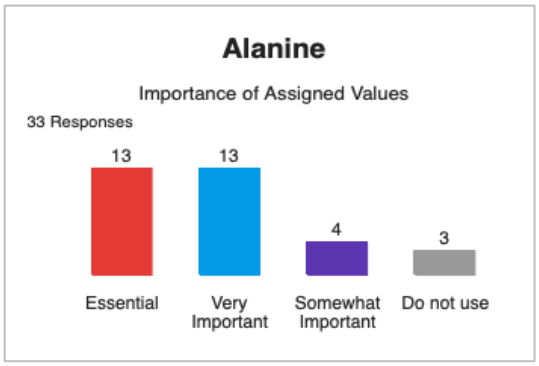
- Acyl carnitines, short chain organic acids
- Apolipoproteins
- Bile acids
- Biogenic amines in general
- Cholesterol biosynthesis intermediates
- comparison of the distributions of unbound free fatty acids in adults versus infants
- endocannabinoids, oxylipins
- Homocysteine
- isotope signatures of the inorganic clinical markers are of primary interest
- Metal isotope ratios
- Organic acids
- Phenols, Phthalates, Pesticides, Pharmaceuticals, Flame retardants, Plastic Additives
- Phospholipids, sphingolipids, acyl-carnitines, eicosanoids, water soluble metabolites (e.g. dicarboxylic acids, polyamines, sugars)
- polar metabolites
- primary and secondary bile acids; metabolites derived from microbiome (e.g. indoxyl sulfate, p-cresyl sulfate), common prescription and OTC drugs (e.g. NSAIDs and their metabolites, metformin, statins), metabolites (e.g. kyurenine pathway), common food constituents (e.g. caffeine and metabolites)
- Secondary metabolites related to the environment
- Various phospholipids and other lipid sub-classes (the lipidomics harmonization study was helpful). Also, vitamin K related metabolites (e.g., K1, MK-4, MK-7, coenzyme Q10), TMAO related metabolites (e.g., carnitine, choline, betaine), and dietary/exposure biomarkers of interest (e.g., proline betaine, 3-methylhistidine, omega-3 index)

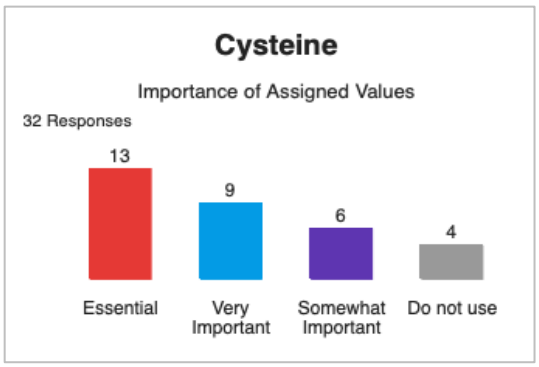
N.3. **SRM 1950 Usage –** the importance of assigned values

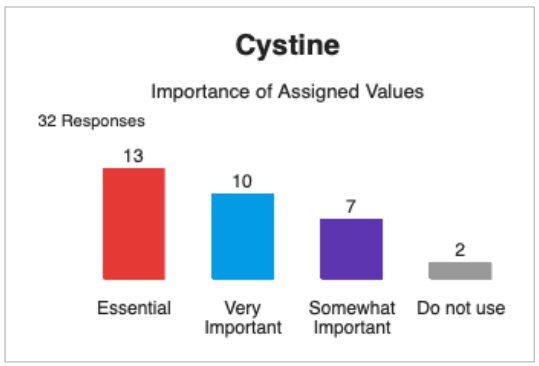
The sub-sections below list classes in the order of the number of responses as shown in Section N.2 above, from the largest number of responses (i.e., Amino Acids) to the smallest number of responses (i.e., Perfluorinated Compounds). Each sub-section shows results regarding the importance of assigned values for analytes to users' work.

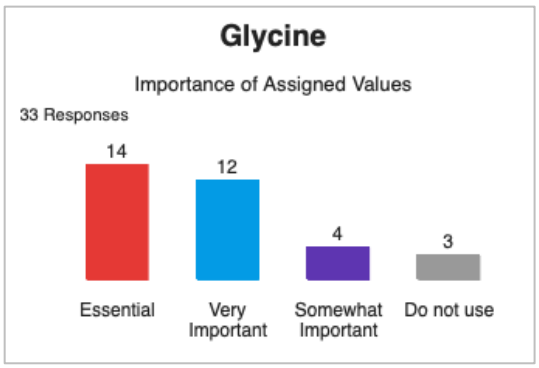
N.3.1. Amino Acids

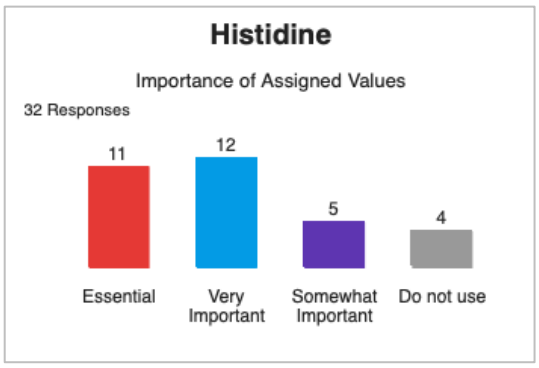


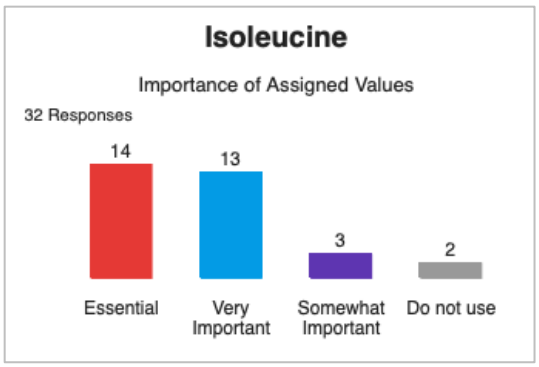


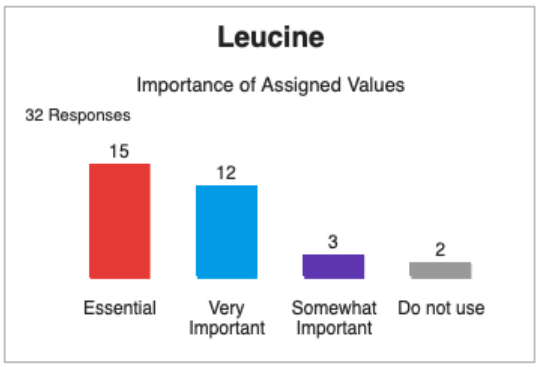


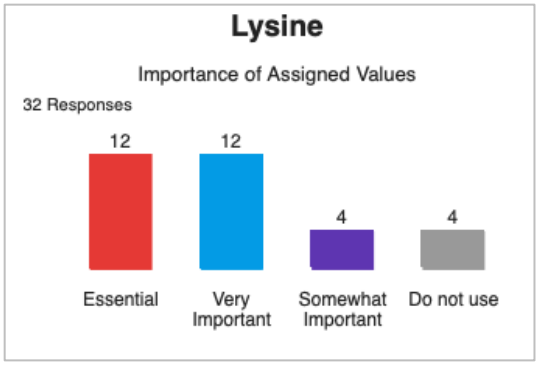


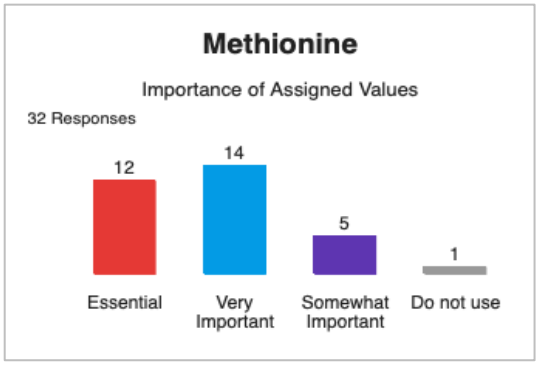


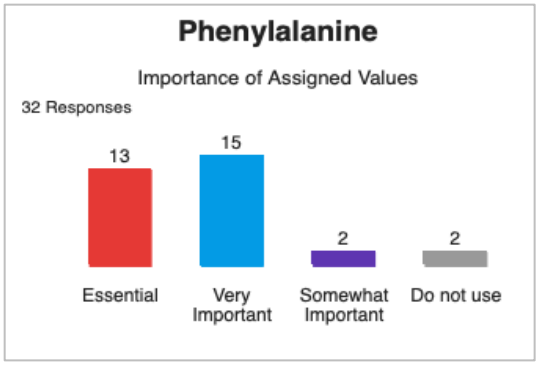


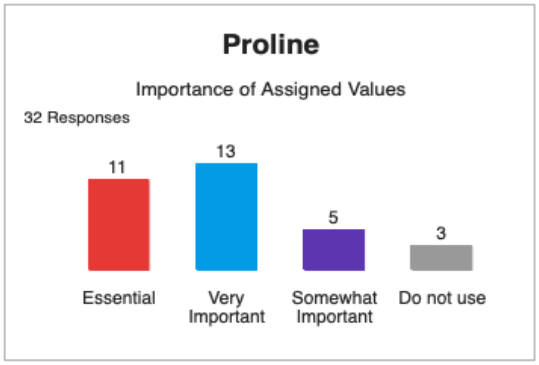

Isoleucine
Importance of Assigned Values
32 Responses
14
13
3
2
Essential
Very Important
Somewhat Important
Do not use

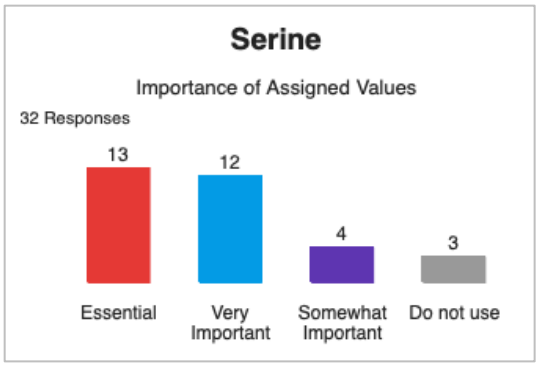

Leucine
Importance of Assigned Values
32 Responses
15
12
3
2
Essential
Very Important
Somewhat Important
Do not use

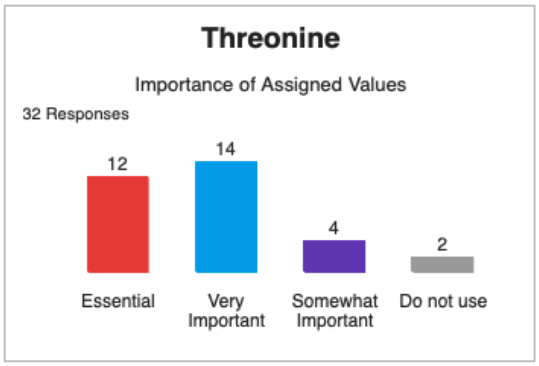

Lysine
Importance of Assigned Values
32 Responses
12
12
4
4
Essential
Very Important
Somewhat Important
Do not use

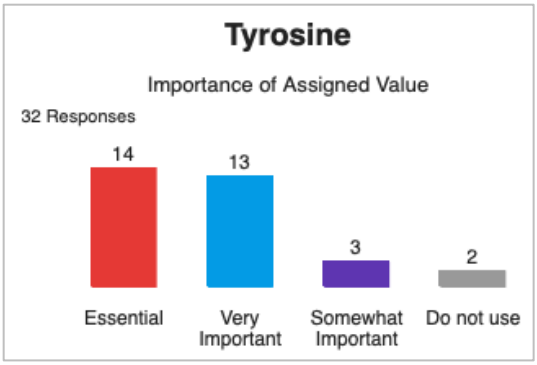

Methionine
Importance of Assigned Values
32 Responses
12
14
5
1
Essential
Very Important
Somewhat Important
Do not use

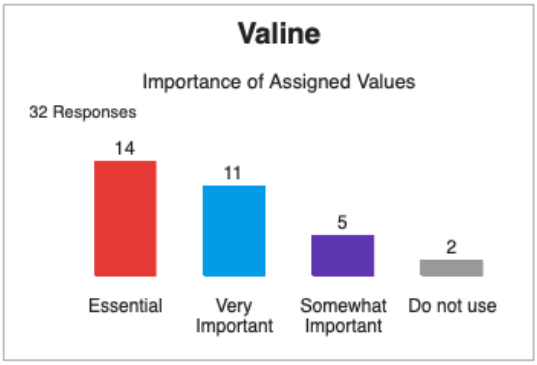

Phenylalanine
Importance of Assigned Values
32 Responses
13
15
2
2
Essential
Very Important
Somewhat Important
Do not use


Proline
Importance of Assigned Values
32 Responses
11
13
5
3
Essential
Very Important
Somewhat Important
Do not use


Serine
Importance of Assigned Values
32 Responses
13
12
4
3
Essential
Very Important
Somewhat Important
Do not use


Threonine
Importance of Assigned Values
32 Responses
12
14
4
2
Essential
Very Important
Somewhat Important
Do not use

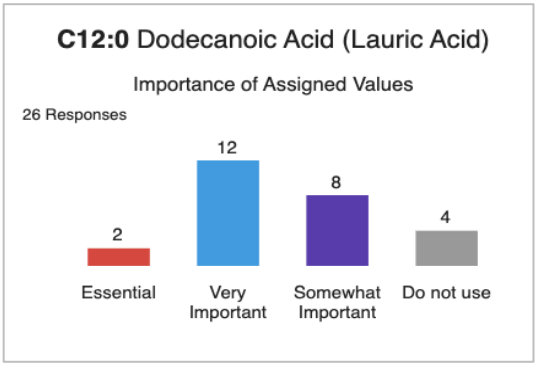


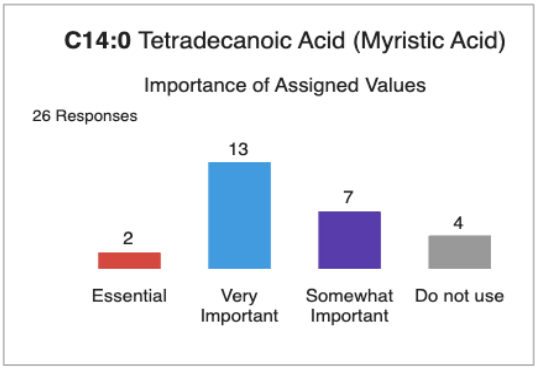


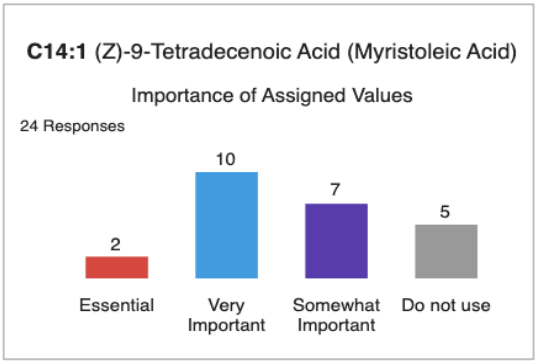
[Other analytes needed, verbatim as entered by respondents]

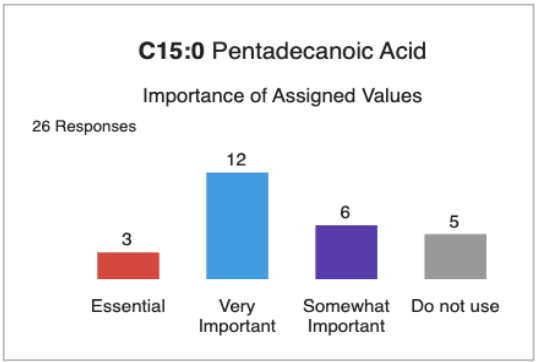
- maybe methylated amino acids
- Aspartic Acid, Asparagine, Glutamate, Citrulline, Ornithine, N-acetyl-ornithine
- Tryptophan, 3-Nitro Tyrosine and Methionine Sulfoxide can be interesting as well information about Allo-Isoleucine and anaytical method capability regarding the quantitation of IsoLeucine and Allo-Isoleucine. An other important topic is the analtical method used for Cystein determination, a sample preparation maintaining a low temperature durin all the process is not well fitted against the commonly used sample preparation using reducting agent as DTT, DTE etc...
- Aspartic acid We hope that the 20 amino acids will be covered at a minimum.
- Homocysteine
- Please expand to include all major amino acids (e.g., Asp, Glu, Trp) and related catabolites (e.g., hydroxyproline, S-methylcysteine, 3-methylhistidine, N-acetyllysine), and potentially D-amino acids (D-Ser, D-Glu, D-Ala etc)
- biogenic amines
- Methylhistidine, various betaine derivatives of amino acids, oxidized forms of methionine

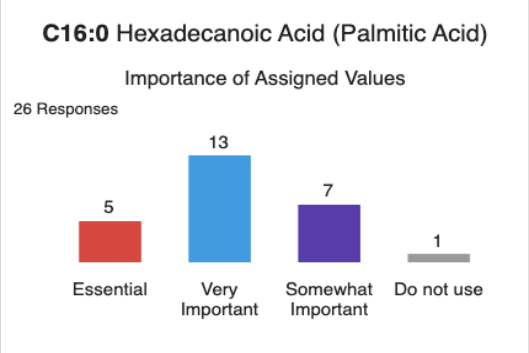
N.3.2. Fatty Acids

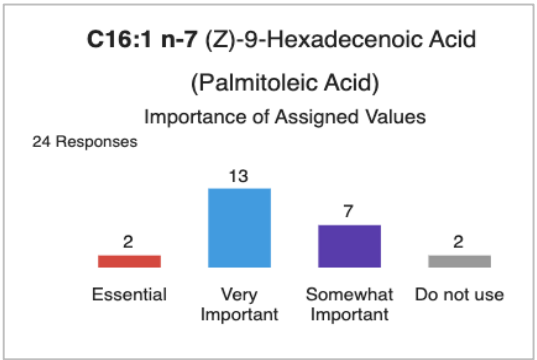


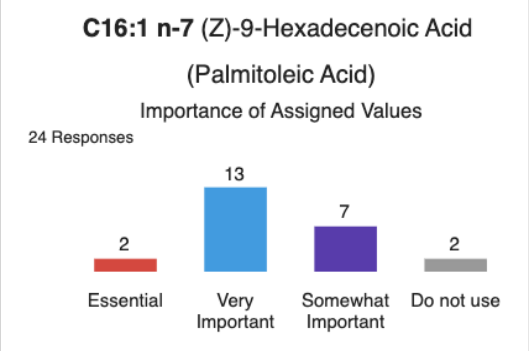


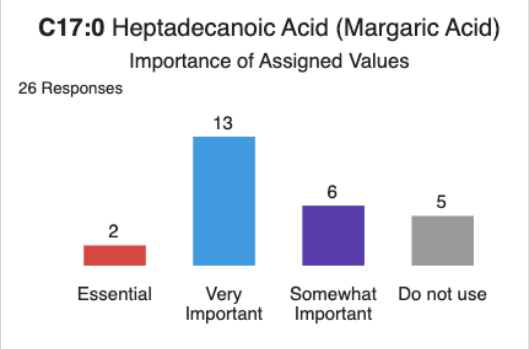

C14:1 (Z)-9-Tetradecenoic Acid (Myristoleic Acid)
Importance of Assigned Values
24 Responses
2
10
7
5
Essential
Very Important
Somewhat Important
Do not use

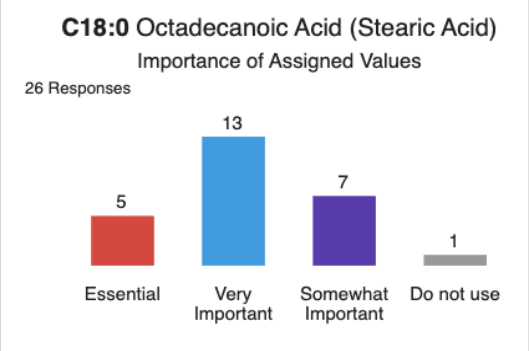

C15:0 Pentadecanoic Acid
Importance of Assigned Values
26 Responses
3
12
6
5
Essential
Very Important
Somewhat Important
Do not use

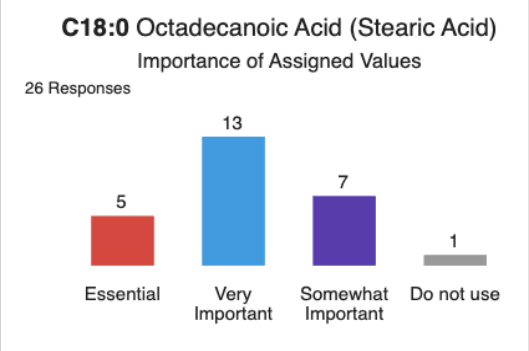

C16:0 Hexadecanoic Acid (Palmitic Acid)
Importance of Assigned Values
26 Responses
5
13
7
1
Essential
Very Important
Somewhat Important
Do not use

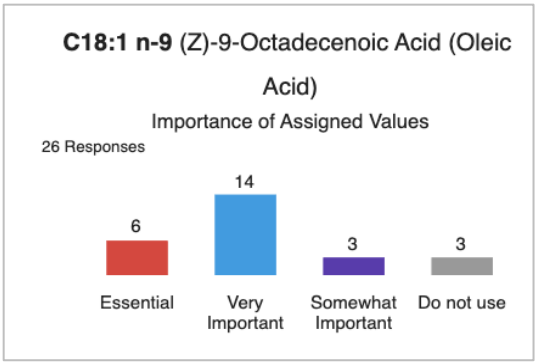

C16:1 n-7 (Z)-9-Hexadecenoic Acid
(Palmitoleic Acid)
Importance of Assigned Values
24 Responses
2
13
7
2
Essential
Very Important
Somewhat Important
Do not use

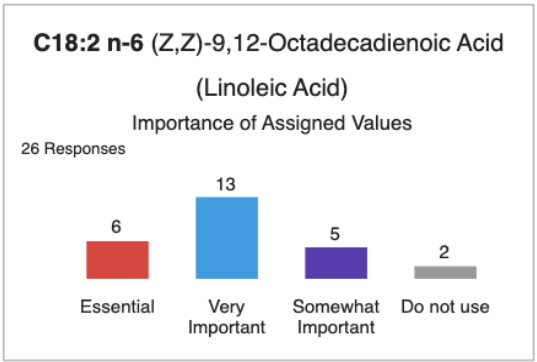

C16:1 n-7 (Z)-9-Hexadecenoic Acid
(Palmitoleic Acid)
Importance of Assigned Values
24 Responses
2
13
7
2
Essential
Very Important
Somewhat Important
Do not use

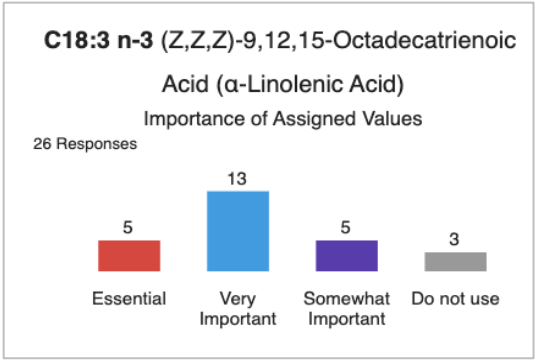

C17:0 Heptadecanoic Acid (Margaric Acid)
Importance of Assigned Values
26 Responses
2
13
6
5
Essential
Very Important
Somewhat Important
Do not use

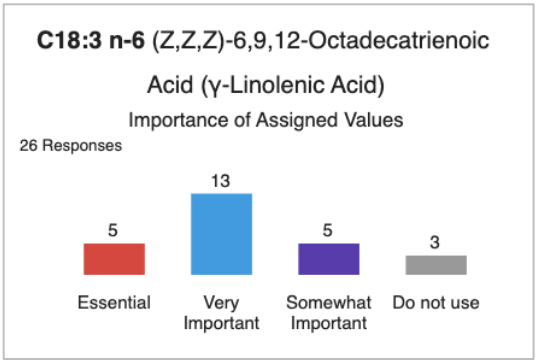

C18:0 Octadecanoic Acid (Stearic Acid)
Importance of Assigned Values
26 Responses
5
13
7
1
Essential
Very Important
Somewhat Important
Do not use

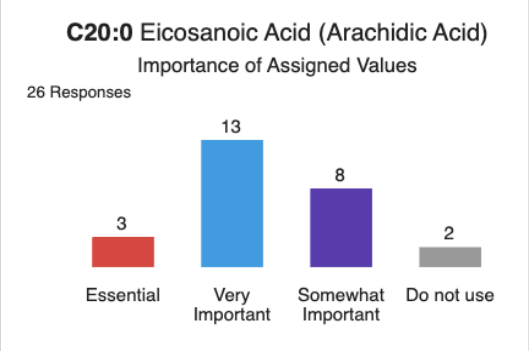

C18:0 Octadecanoic Acid (Stearic Acid)
Importance of Assigned Values
26 Responses
5
13
7
1
Essential
Very Important
Somewhat Important
Do not use

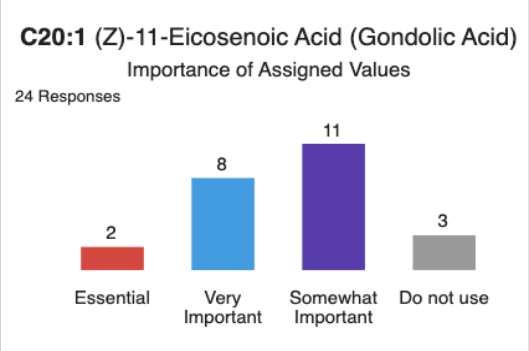

C18:1 n-9 (Z)-9-Octadecenoic Acid (Oleic Acid)
Importance of Assigned Values
26 Responses
6
14
3
3
Essential
Very Important
Somewhat Important
Do not use

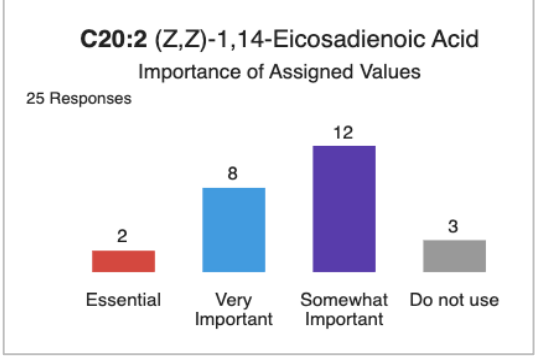

C18:2 n-6 (Z,Z)-9,12-Octadecadienoic Acid (Linoleic Acid)
Importance of Assigned Values
26 Responses
6
13
5
2
Essential
Very Important
Somewhat Important
Do not use

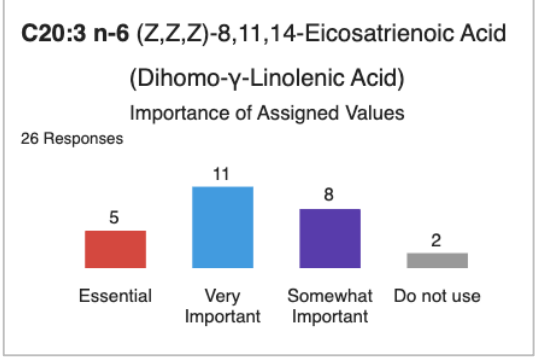

C18:3 n-3 (Z,Z,Z)-9,12,15-Octadecatrienoic Acid (α-Linolenic Acid)
Importance of Assigned Values
26 Responses
5
13
5
3
Essential
Very Important
Somewhat Important
Do not use

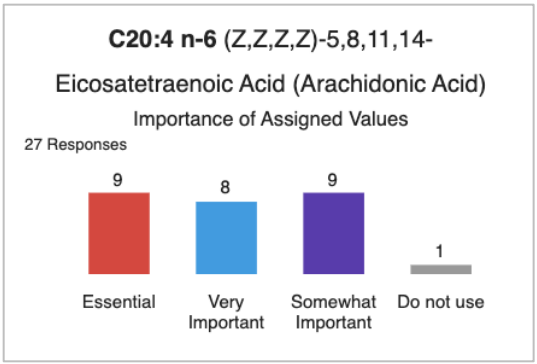

C18:3 n-6 (Z,Z,Z)-6,9,12-Octadecatrienoic Acid (γ-Linolenic Acid)
Importance of Assigned Values
26 Responses
5
13
5
3
Essential
Very Important
Somewhat Important
Do not use

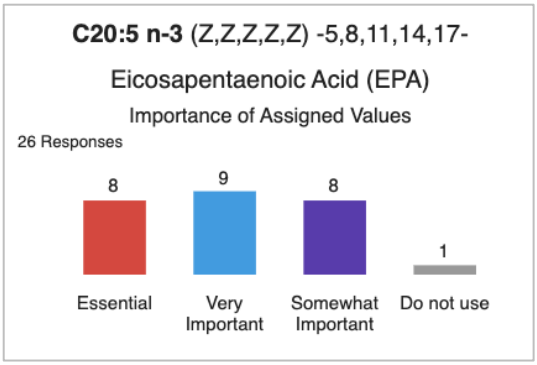

C20:0 Eicosanoic Acid (Arachidic Acid)
Importance of Assigned Values
26 Responses
3
13
8
2
Essential
Very Important
Somewhat Important
Do not use

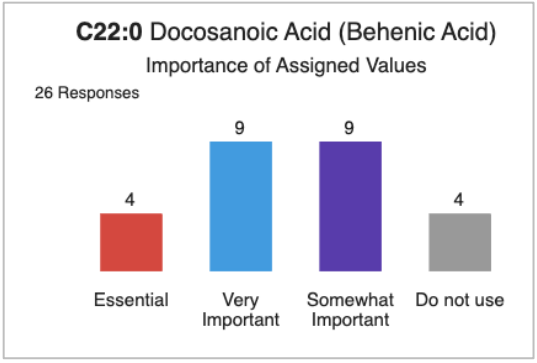

C20:1 (Z)-11-Eicosenoic Acid (Gondolic Acid)
Importance of Assigned Values
24 Responses
2
8
11
3
Essential
Very Important
Somewhat Important
Do not use

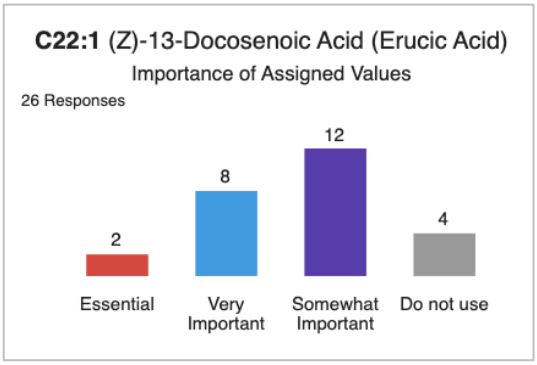

C20:2 (Z,Z)-1,14-Eicosadienoic Acid
Importance of Assigned Values
25 Responses
2
8
12
3
Essential
Very Important
Somewhat Important
Do not use

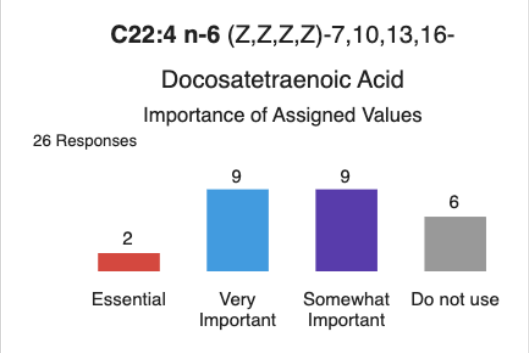

C20:3 n-6 (Z,Z,Z)-8,11,14-Eicosatrienoic Acid (Dihomo-γ-Linolenic Acid)
Importance of Assigned Values
26 Responses
5
11
8
2
Essential
Very Important
Somewhat Important
Do not use

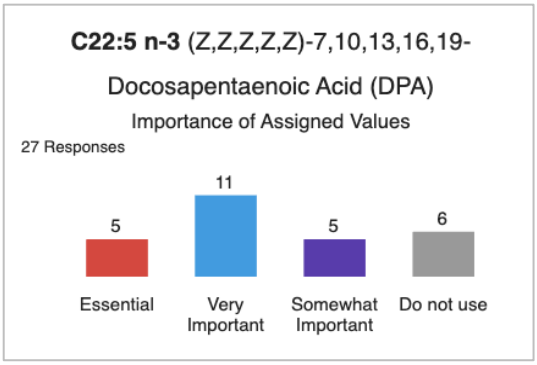

C20:4 n-6 (Z,Z,Z,Z)-5,8,11,14-
Eicosatetraenoic Acid (Arachidonic Acid)
Importance of Assigned Values
27 Responses
9
8
9
1
Essential
Very Important
Somewhat Important
Do not use

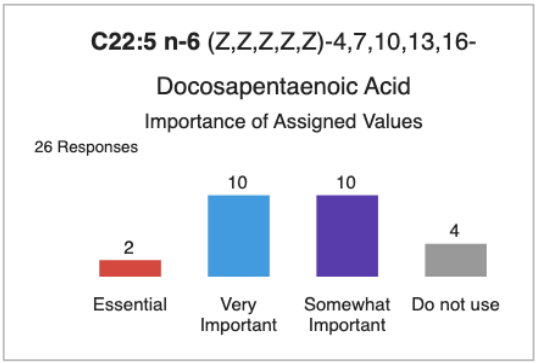

C20:5 n-3 (Z,Z,Z,Z,Z) -5,8,11,14,17-
Eicosapentaenoic Acid (EPA)
Importance of Assigned Values
26 Responses
8
9
8
1
Essential
Very Important
Somewhat Important
Do not use

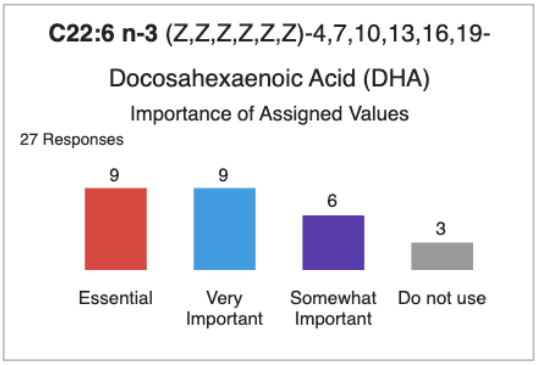

C22:0 Docosanoic Acid (Behenic Acid)
Importance of Assigned Values
26 Responses
4
9
9
4
Essential
Very Important
Somewhat Important
Do not use

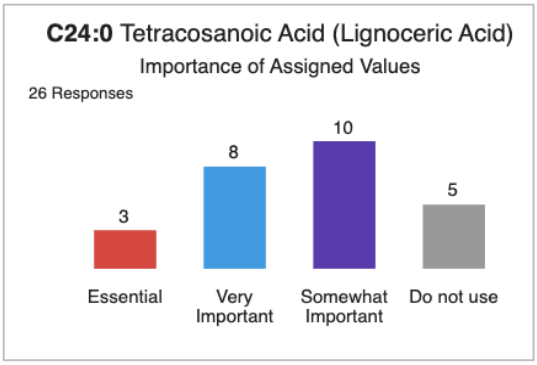

C22:1 (Z)-13-Docosenoic Acid (Erucic Acid)
Importance of Assigned Values
26 Responses
2
8
12
4
Essential
Very Important
Somewhat Important
Do not use

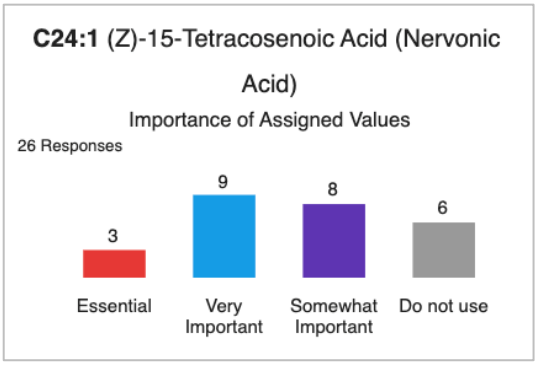

C22:4 n-6 (Z,Z,Z,Z)-7,10,13,16-
Docosatetraenoic Acid
Importance of Assigned Values
26 Responses
2
9
9
6
Essential
Very Important
Somewhat Important
Do not use


C22:5 n-3 (Z,Z,Z,Z,Z)-7,10,13,16,19-
Docosapentaenoic Acid (DPA)
Importance of Assigned Values
27 Responses
5
11
5
6
Essential
Very Important
Somewhat Important
Do not use


C22:5 n-6 (Z,Z,Z,Z,Z)-4,7,10,13,16-
Docosapentaenoic Acid
Importance of Assigned Values
26 Responses
2
10
10
4
Essential
Very Important
Somewhat Important
Do not use


C22:6 n-3 (Z,Z,Z,Z,Z,Z)-4,7,10,13,16,19-
Docosahexaenoic Acid (DHA)
Importance of Assigned Values
27 Responses
9
9
6
3
Essential
Very Important
Somewhat Important
Do not use

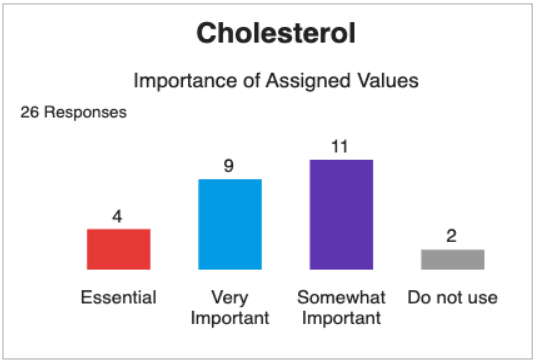


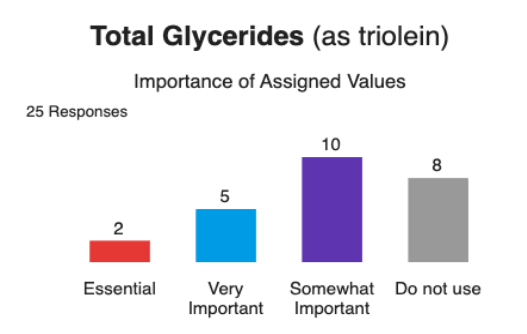


[Other analytes needed, verbatim as entered by respondents]

- Total concentration of fatty acids.
- C24:5 n-3
- Short chain fatty acids as Acetate, Butyrate, Propionate etc...
- Note: We investigate the fraction of the water soluble FFA i.e. UNBOUND FFAu
- Branched-chain fatty acids. Fatty acid measurements as their NEFAs as well as hydrosylates.
- branched odd-carbon number fatty acids

N.3.3. Cholesterol and Glycerides (response count=26)

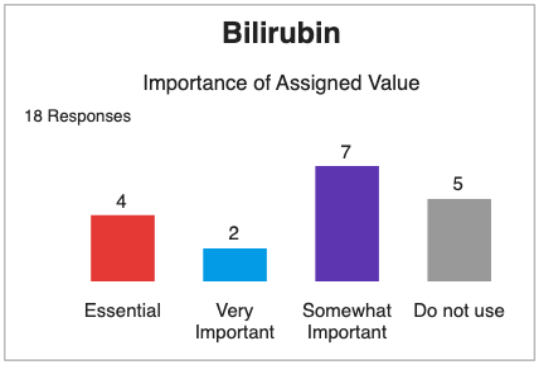


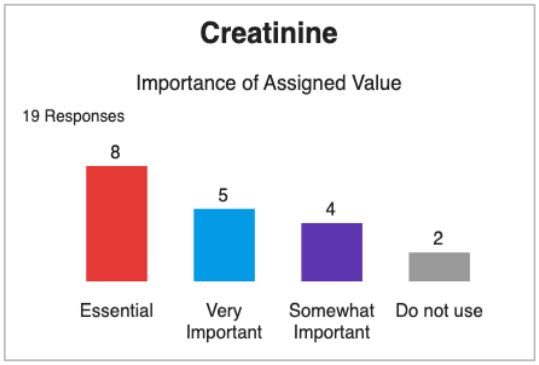


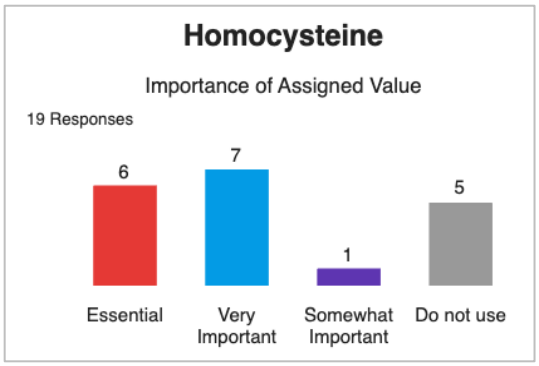
[Other analytes needed, verbatim as entered by respondents]

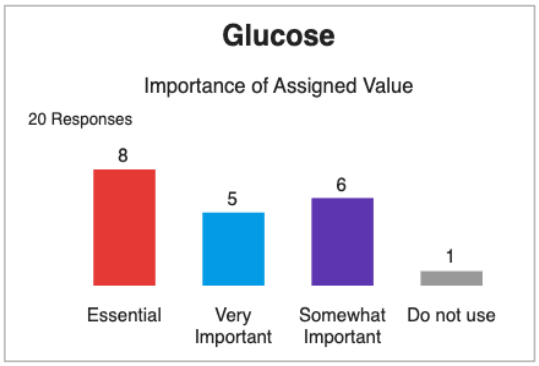
- Generally, more compound-resolved analytical results would be great
- LDL Cholesterol, HDL Cholesterol, VLDL Cholesterol
- Cholesterol biosynthesis intermediates
- amino acids, biogenic amines, phospholipids

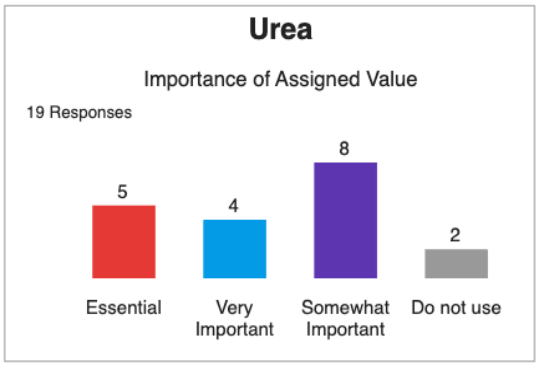
N.3.4. Organic Clinical Markers

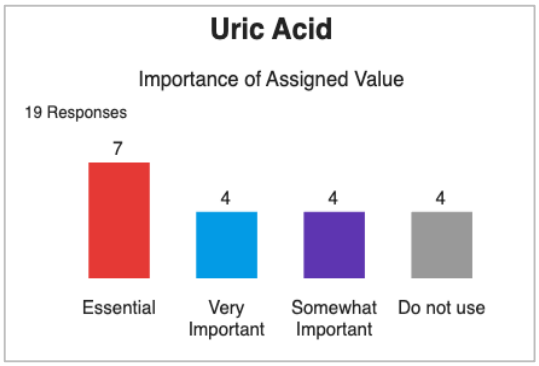








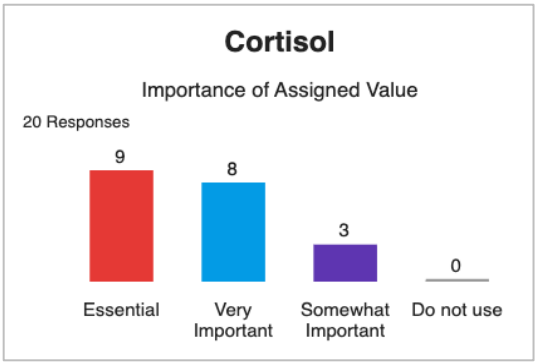


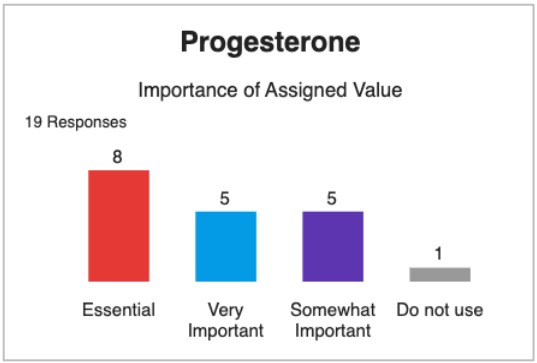


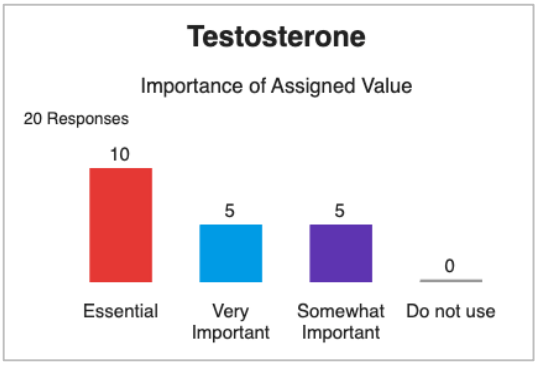
[Other analytes needed, verbatim as entered by respondents]

- Also include creatine, TMAO, asymmetric dimethylarginine (ADMA), symmetric dimethylarginine (SDMA), and uremic toxins (cresol sulfate, indoxyl sulfate, hippuric acid etc.)
- bilirubin photo isomers
- Bilirubin/biliverdin degradation products

N.3.5. Hormones



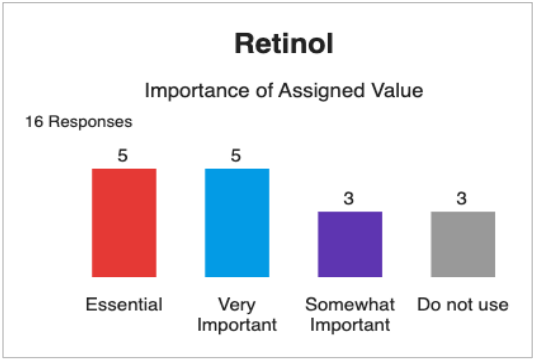


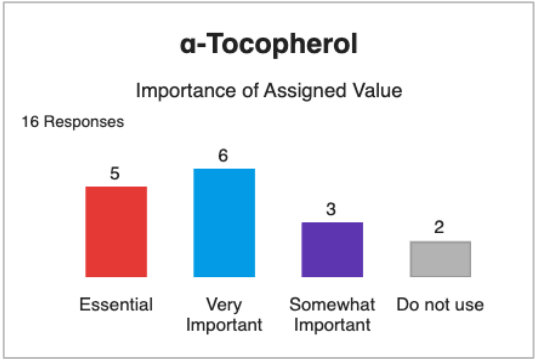


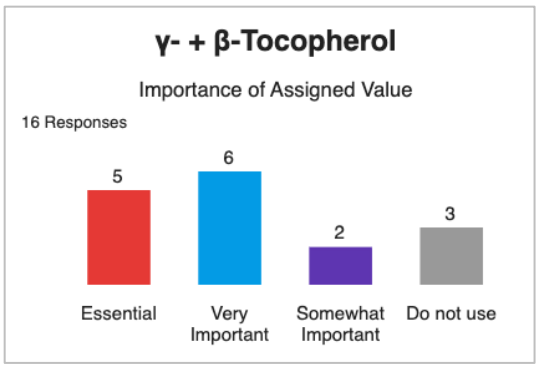
[Other analytes needed, verbatim as entered by respondents]

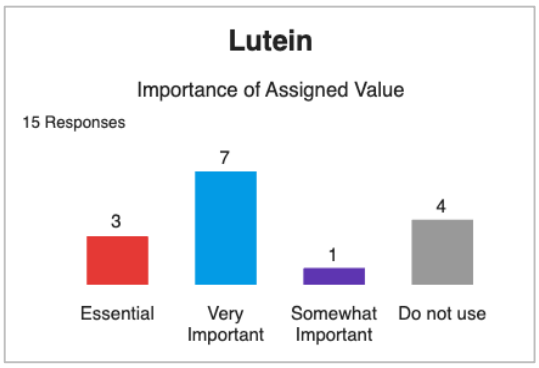
- 17B-estradiol
- 17-hydroxyprogesterone, estradiol, estriol, aldosterone, androstenedione, dihydrotestosterone
- glucuronide and sulfate conjugated forms

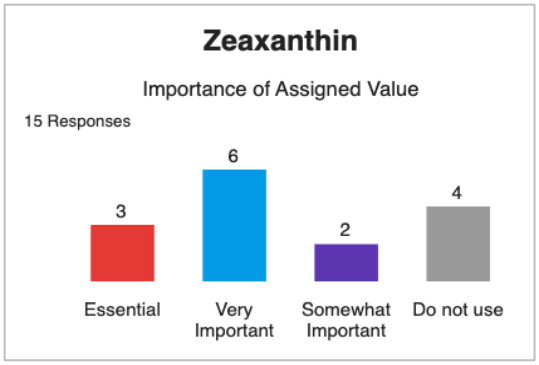
N.3.6. Fat-soluble Vitamins and Carotenoids

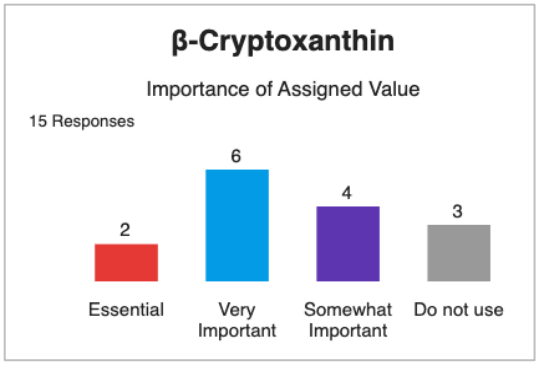


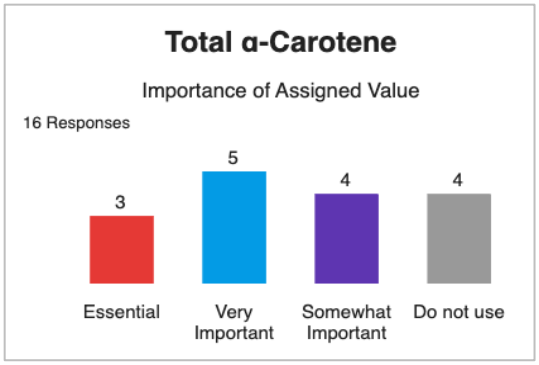


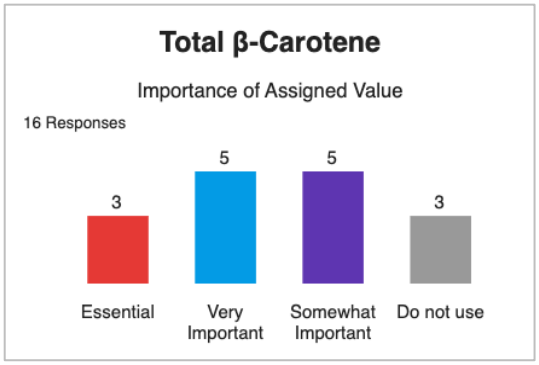

γ- + β-Tocopherol
Importance of Assigned Value
16 Responses
5
6
2
3
Essential
Very Important
Somewhat Important
Do not use

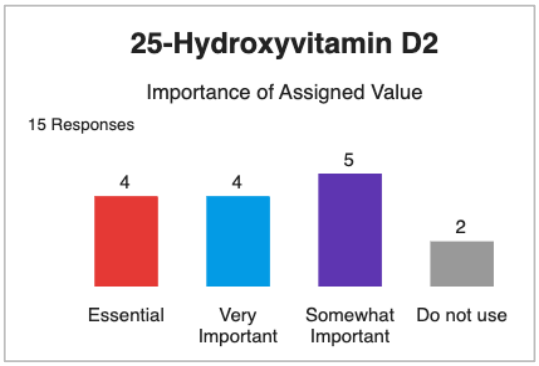

Lutein
Importance of Assigned Value
15 Responses
3
7
1
4
Essential
Very Important
Somewhat Important
Do not use

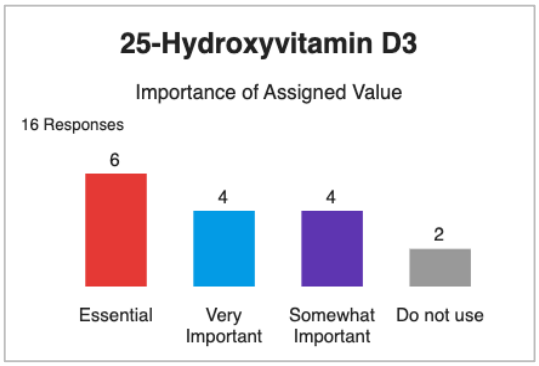

Zeaxanthin
Importance of Assigned Value
15 Responses
3
6
2
4
Essential
Very Important
Somewhat Important
Do not use

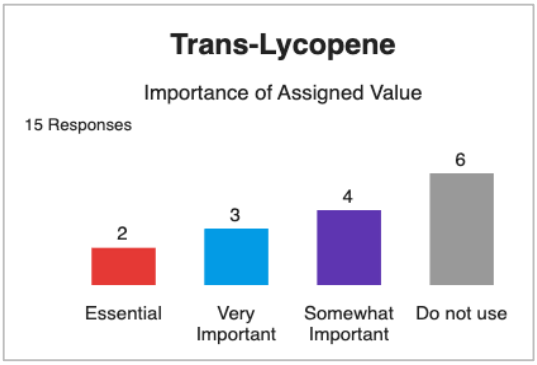

β-Cryptoxanthin
Importance of Assigned Value
15 Responses
2
6
4
3
Essential
Very Important
Somewhat Important
Do not use

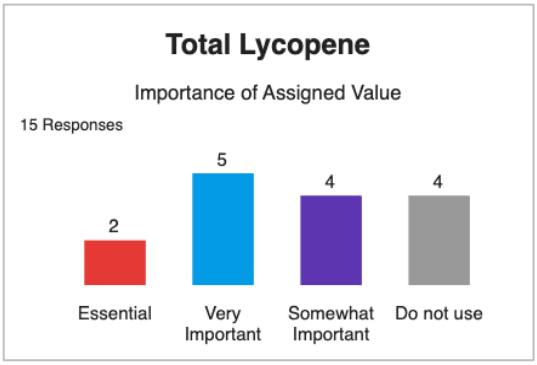

Total α-Carotene
Importance of Assigned Value
16 Responses
3
5
4
4
Essential
Very Important
Somewhat Important
Do not use

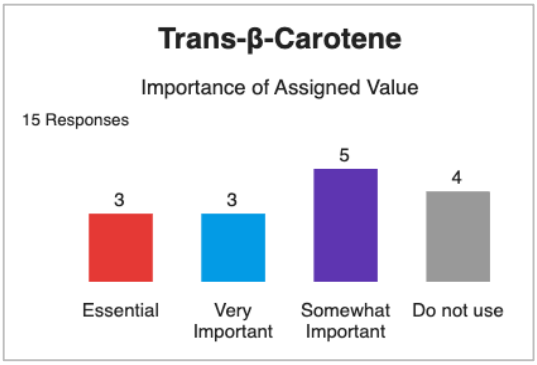

Total β-Carotene
Importance of Assigned Value
16 Responses
3
5
5
3
Essential
Very Important
Somewhat Important
Do not use

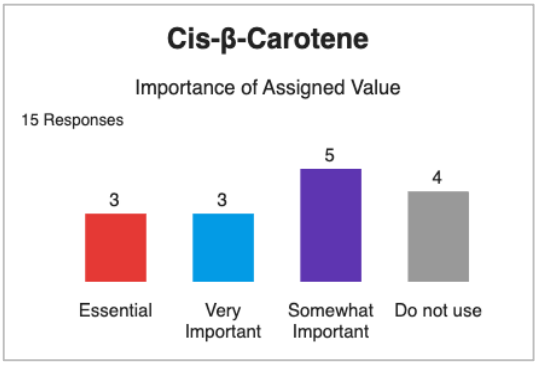

25-Hydroxyvitamin D2
Importance of Assigned Value
15 Responses
4
4
5
2
Essential
Very Important
Somewhat Important
Do not use


25-Hydroxyvitamin D3
Importance of Assigned Value
16 Responses
6
4
4
2
Essential
Very Important
Somewhat Important
Do not use





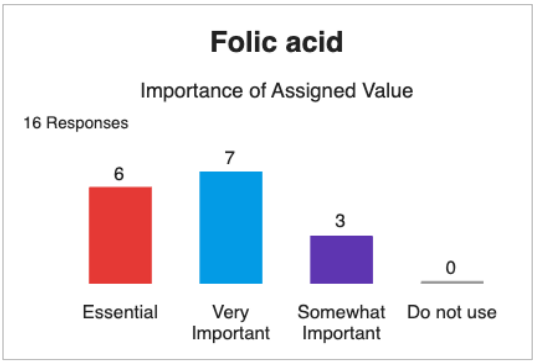


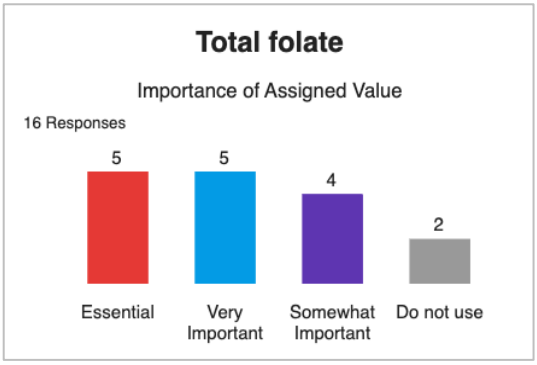


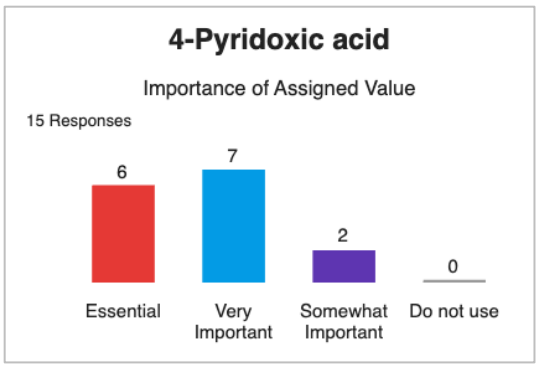
[Other analytes needed, verbatim as entered by respondents]

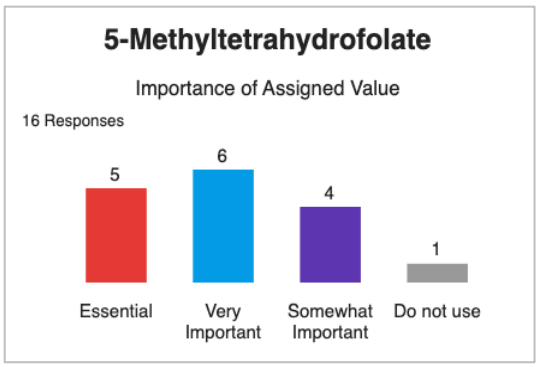
- Tocotrienol forms and Vitamin K1 (and K2 as MK-4 and MK-7)
- Other vitamin D metabolites (3-epi-25-OH D3, 24,25-(OH)2D3 etc) as well as vitamin K species (K1, MK-4, MK-7, coenzyme Q10)
- 20-S-hydroxy vitamin D3, 24,25-dihydroxy vitamin D3

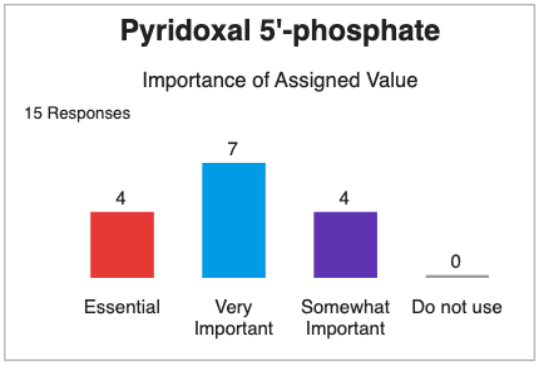
N.3.7. Water-soluble Vitamins







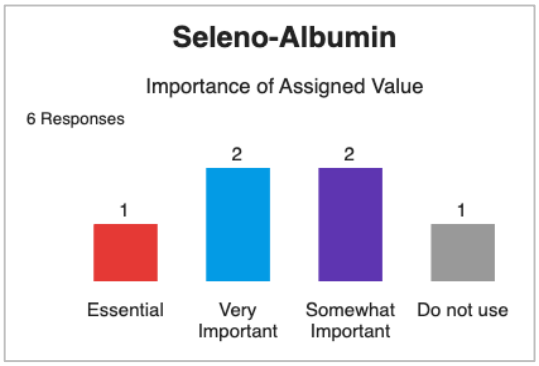


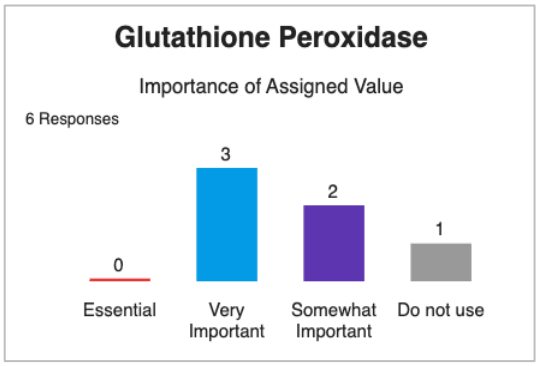


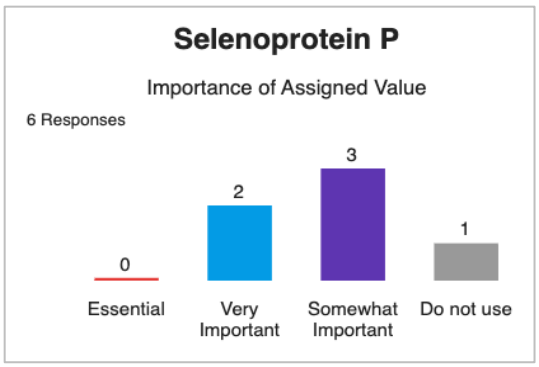
[Other analytes needed, verbatim as entered by respondents]

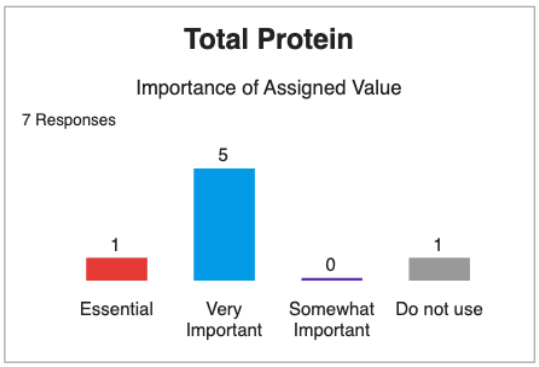
- No, but we would really appreciate higher concentrations in a folate reference standard
- Thiamine, Riboflavin, Nicotinamide, Nicotinic Acid, Nicotinuric Acid, Pyridoxal, Pyridoxine, Pyridoxamine.

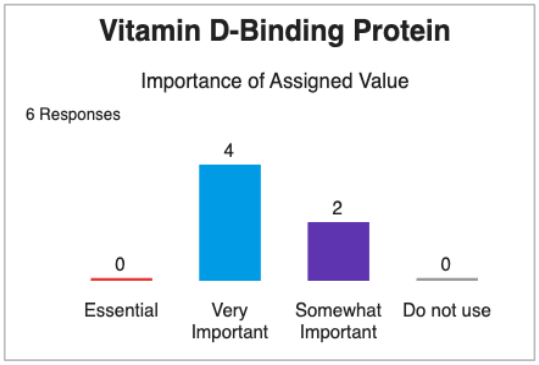
N.3.8. Proteins







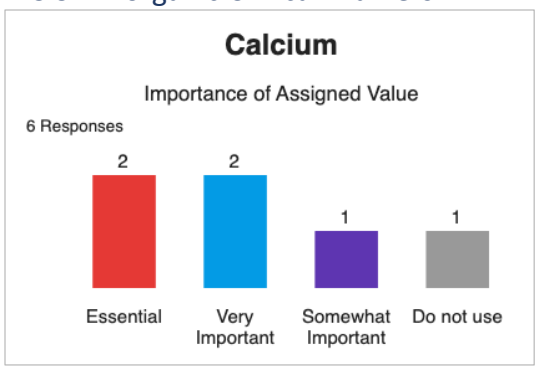


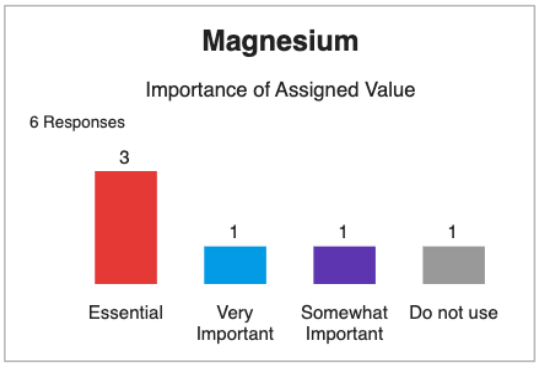


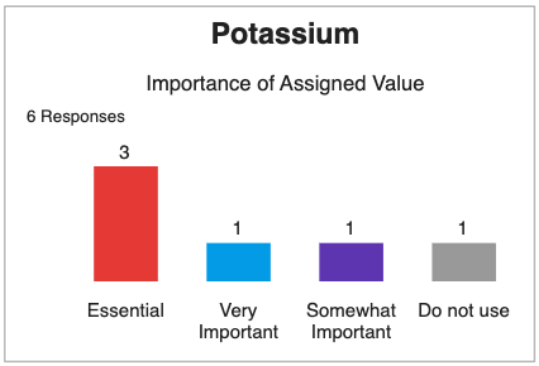
[Other analytes needed, verbatim as entered by respondents]

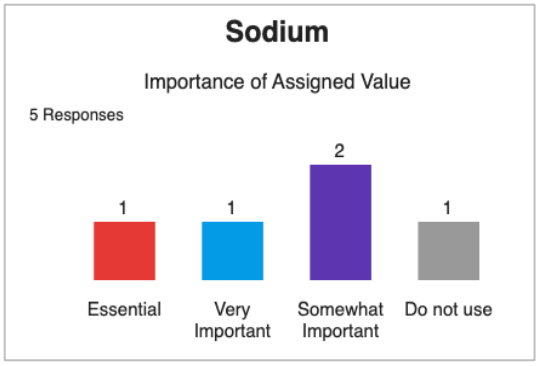
- (no resonses)

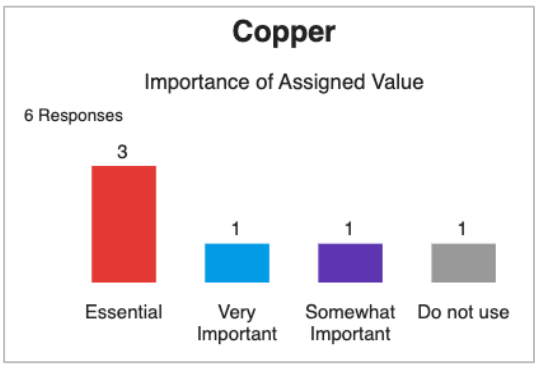
N.3.9. Inorganic Clinical Markers

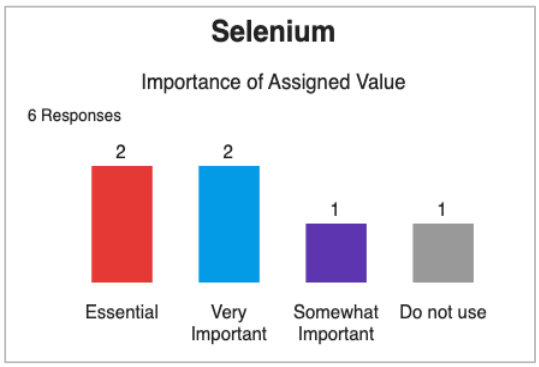








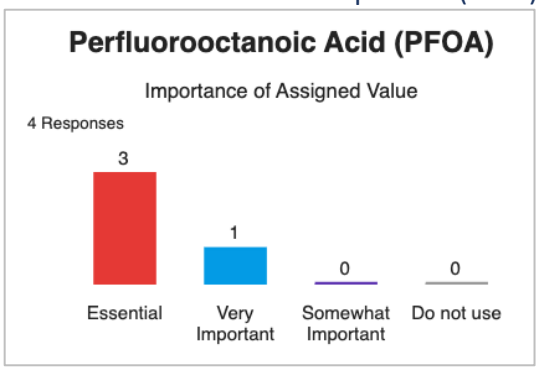


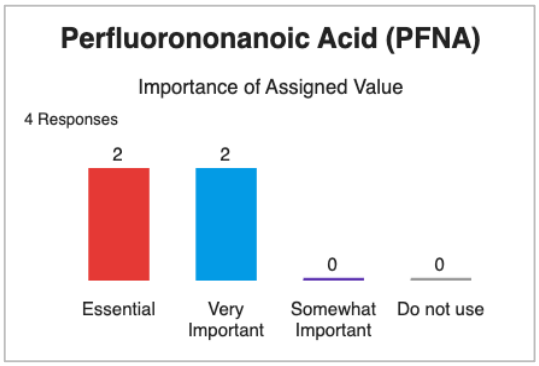


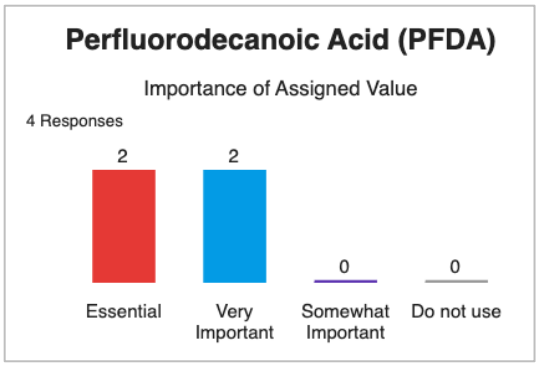
[Other analytes needed, verbatim as entered by respondents]

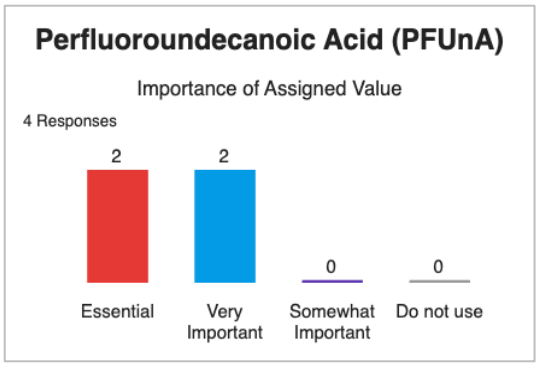
- Iron

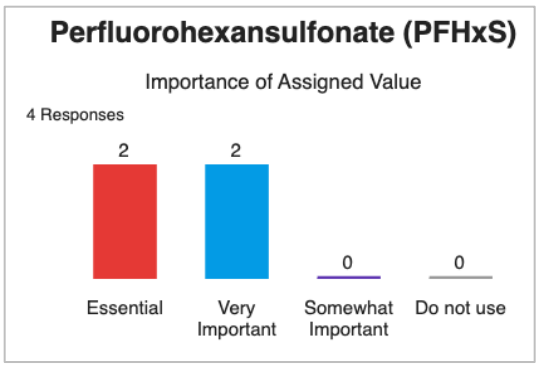
N.3.10. Perfluorinated Compounds (PFCs)

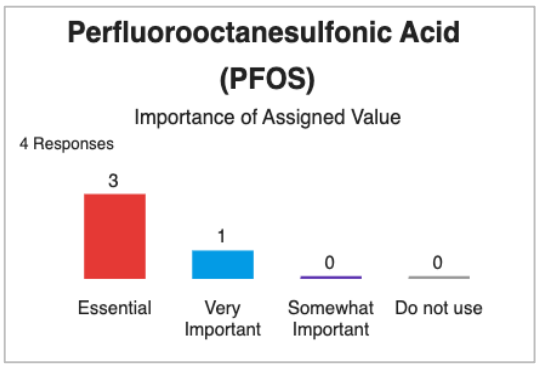










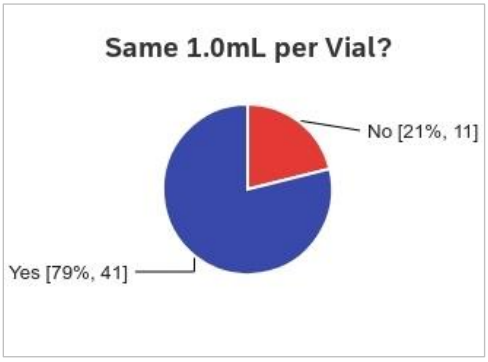


[Other analytesneeded, verbatim as entered by respondents]

- Would prefer information about all of the PFAS analytes detected using EPA Draft Method 1633 (~ 40 compounds).

N.4. Future SRM 1950

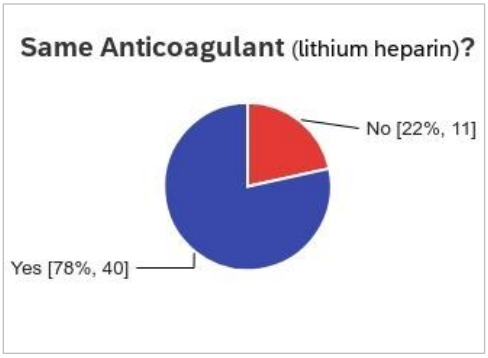
N.4.1. Preferred volume per vial



If "No," different volume per vial preferred (mL)	# of responses
0.01	1
0.1	1
0.2	3
0.25	1
2	1
5	1
10	1
250	1

N.4.2. Preferred anticoagulant

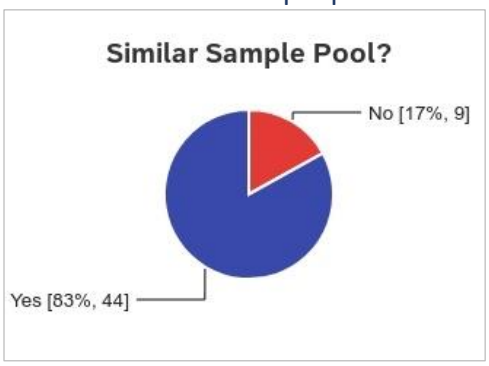
If "No," different anticoagulant preferred
Serum without an anticoagulant. If that is not possible, then lithium heparin.
K3 – EDTA
K2EDTA
EDTA
EDTA
EDTA
An EDTA-K2 K3 based must be more usefull.
EDTA・2Na or EDTA・2K
In addition to this anticoagulant, it would be nice to also have an EDTA option.
Serum separator tubes, SST™ II advance, BD Vacutainer®



[If "No," different anticoagulant preferred]

- Serum without an anticoagulant. If that is not possible, then lithium heparin.
- K3 – EDTA
- K2EDTA
- EDTA
- EDTA
- EDTA
- An EDTA-K2 K3 based must be more usefull.
- EDTA・2Na or EDTA・2K
- In addition to this anticoagulant, it would be nice to also have an EDTA option.
- Serum separator tubes, SST™ II advance, BD Vacutainer®

N.4.3. Preferred sample pool

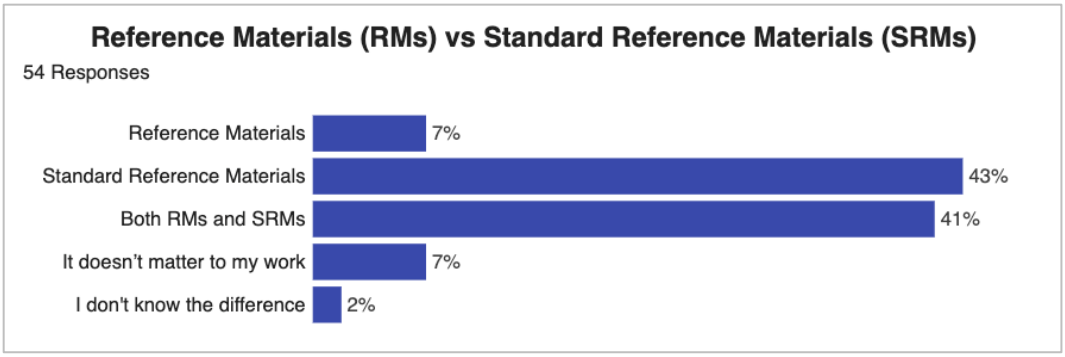


[If "No," different sample pool preferred]

- Larger participant pool from more ethically diverse populations across US would be preferred.
- Instead of one pool, provide two or more pools with, e.g., low/high total cholesterol (correlated with fatty acids too), or fasting/non-fasting (correlated with, e.g., amino acid concentrations).
- females and males separate
- 1. Wider age range from 10-80 years 2. Range of BMI 3. Fed and fasted
- Male & female cohorts separated

- Pediatric population(s)
- would prefer to include individuals of child-bearing age
- Age specific - 40-50 is perimenopausal. Premenopausal women. Postmenopausal (55+)
- prefer men and women separated but this should also work for a bulk material.

N.5. Preferred RMs or SRMs for new materials for metabolomics



N.5.1. SRMs Preferred – Reasons

- We need material that is as stable and reproducible as possible for a wide range of analytes
- Use of certified values are important
- Fields like machine learning progress quickly when there are established benchmarks many labs can compare methods against. We expect NIST standards to serve a similar role of highly accurate benchmarks to compare methods that progress research in mass spectrometry
- We are a national metrology institute
- I can generate RMs in house but it is difficult and time consuming to prepare biologically relevant SRMs.
- GXP/GLP studies
- Better validation
- in our folate work, method is important so we appreciate the values given for different methods
- Need quantitative value to test the precision and reproducibility of our analysis
- In order to provide accurate clinical diagnosis data
- Traceability to SI unit
- We clearly use your SRM to understand statues of our own methods in clinical and non-clinical project and your metrology expertise has a great value and help a lot.
- Because we intend to use it for validation of our measurement methods.
- To check our calbirator's traceability
- The accurate absolute concentration of SRM would be helpful for quantitative studies of metabolomics.
- We need it to ensure assay calibration traceability for FDA approved IVD devices
- Because it is traceable to a gold standard.

- As a reference for our human plasma metabolomics analysis
- Prefer a NIST level of certification
- Higher standards for reporting
- Higher reliability of reference values

N.5.2. BOTH RMs & SRMs Preferred – Reasons

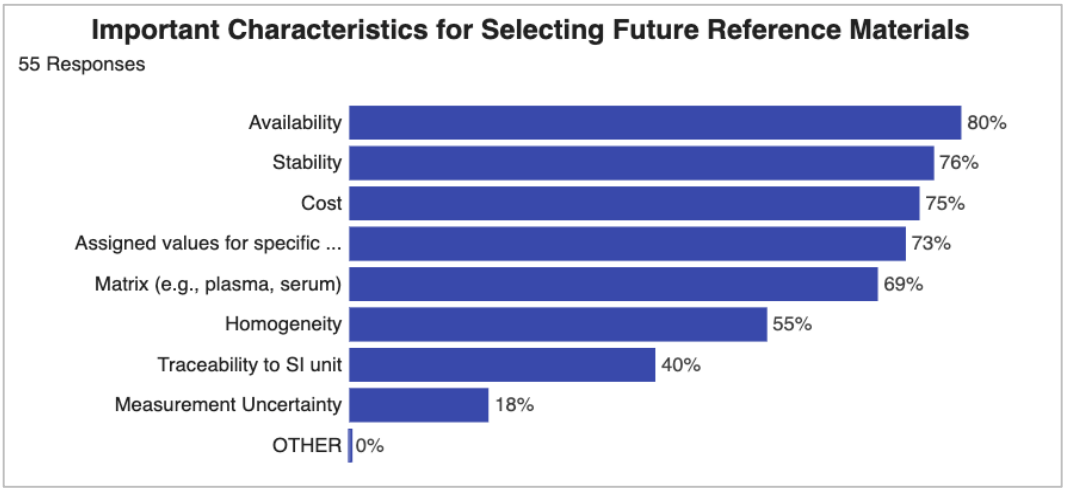
- We use the SRM's to check for accuracy to current reference methods and as QC material where no other commercial material or EQA scheme exists but we could use RM rather than SRM for the latter.
- I am not sure I fully understood the difference between RM and SRMs. We use SRMs now in my lab for inter-laboratory comparison and external validation of our methods. I am not sure clients or collaborators would be fine with an RM as external control. We are however not a clinically certified lab, so from a practical point of view, RMs sound fine to me. Again, depending on the actual difference and related possible impact on level of validation we can do with RM vs. SRM, we may need to purchase both.
- SRM is not needed for all application, and thus (potentially) cheaper RM would be enough. For traceability purposes, however, SRM is needed.
- Study-dependence sometimes requires SRM, but in instances where it doesn't RM is still needed.
- SRMs are used as yardstick and to normalize across studies RMs are mainly used within studies, but not between studies
- It's nice to have the gold standard value for some references materials. But would prefer a higher diversity of reference materials than having everything be an SRM
- Not all projects require strict certification that can be potentially used for quantitation
- We would use RMs where there are large numbers of sample batches (e.g. many thousands of samples), and compare RM results occasionally to SRMs.
- Can show instrument quantitation is in line with NIST standards and thus instrument sensitivity by serial dilution
- because I am working on method development and validation.
- For validation work, SRM is needed to establish diagnostic assays.
- RMs for non quantitative purposes, SRMs for quantitative purposes
- I think for most studies RMs would be sufficient as long as there is a huge pool that the whole community can access. We typically look at much more metabolites than the certified ones anyway. However, I have in the past enjoyed the SRM aspect in that you can really use it for validation of quantitative methods. (Unfortunately) most larger metabolomics studies can usually not be performed quantitatively.
- Comparison and validation
- Presumably RMs are cheaper so that is a consideration, but it's also good to have the SRMs available as they provide better accuracy on the reported metabolite levels.

N.5.3. RMs Preferred – Reasons

- I do not need to go to the lengths of traceability / certification, and am assuming RMs would be cheaper to produce/purchase than SRM.

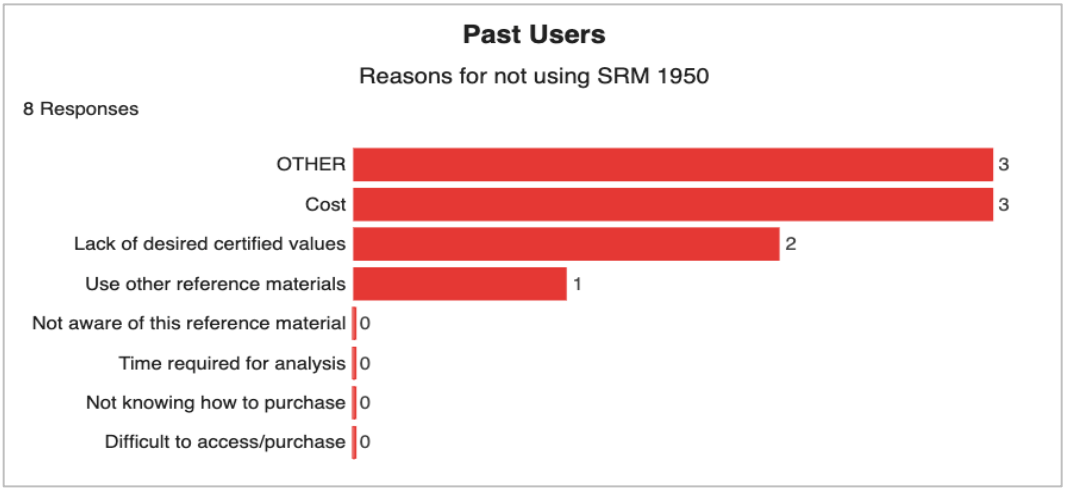
- We need the same RMs for calibration of our studies
- It is sufficient for comparability, validation and system suitability
- It is sufficient for our needs.

N.6. Important Characteristics for Selecting Future Reference Materials



N.7. Reasons for not using SRM 1950 currently

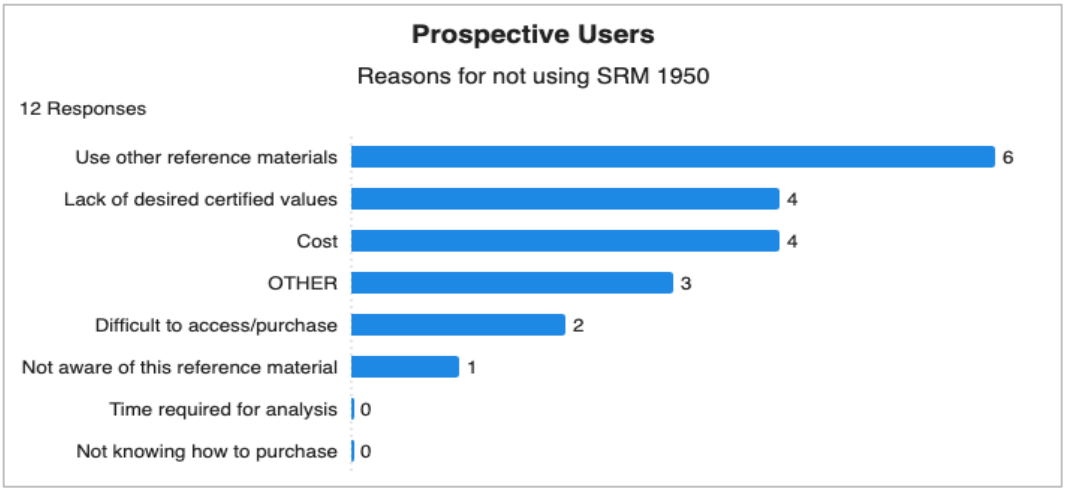
N.7.1. Past SRM 1950 Users



[Other reasons entered]

- Project status not needing it at this time.
- It was not available for some time then after we didn't need it anymore.
- Used for troubleshooting. Not routine use.

N.7.2. Prospective SRM 1950 Users



[Other reasons entered]

- Preparing to purchase
- Would like to have isotope-delta values assigned for the Mg, Cu, Se, and K.

N.8. Final Comments

N.8.1. Current SRM 1950 Users

- What I really need is untargeted metabolomics proficiency tests to document if I can detect up- and downregulation of key metabolites in biological samples
- NIST SRM 1950 has been invaluable to the community. Would like to see some sort of cellular extract next.
- thank you!
- Please don't hesitate to connect to our lab if feedback needed. Nestlé is promoting usage of NIST reference and strongly trust your expertise.
- We used it for validation purposes, and 1 mL was sufficient. We would like you to consider selling the product in units of 1 mL instead of 1 mLx5 to keep the price low and make it available to more researchers.
- Please make NIST 1955 again if possible.
- Thank you for working on providing a continued supply of this important product
- Love what you guys are doing, so essential for science, keep up the good work!

N.8.2. Prospective SRM 1950 Users

- For the parameters we are interested in, freeze-dried material would be preferable.
- Appreciate you reaching out to the communities that use this material and the one's they may potential use this material!
- I have been using ChromSystems Steroid Serum Controls (MassCheck) which has made huge difference to that method development process.
- If you want us to be part of inter-lab studies, we are happy to participate if you can send us a sample.