Chapter 7. Reporting Requirements

Specifications for the Conduct of Chemistry Activities for Toxicology Research Performed by the Division of Translational Toxicology at the National Institute of Environmental Health Sciences

7. Reporting Requirements

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7.1. General

All final deliverables[1] in electronic format must be Section 508 compliant. Currently, Section 508 compliance for PDF files is defined as passing the full compliance check found in Adobe Acrobat X or above with no reported errors and meeting the requirements found in the accessibility conformance checklist.[2]

Deliverables include, but are not limited to:

- Functional Activity reports – reports of work done for specific assignments, e.g., CCA report
- Periodic Status reports – reports of contract activities, e.g., Monthly Progress Report, Annual Report, etc.
- Contract Management Reports – quality management plan, health and safety plan, etc.
- Final QA'd data – typically Excel spreadsheets of data generated under a specific assignment (e.g., BSA functional activity) that has undergone QA review
- Interim data – spreadsheets, figures, supporting literature accumulated during execution of an assignment
- Study protocol (e.g., TKS protocol)
- Assignment-Specific plans – validation plan, characterization plan, etc.
- Hard copy of study files for a given assignment
- Electronic copy (e.g., pdf format) of study files for a given assignment

7.2. Required Reports

Required reports (see below) for all contract activities shall comply with the requirements described below with respect to submission milestones, report formats and content, and reporting timeframes.

[1]Refer to Glossary of Terms.
[2]https://www.hhs.gov/web/section-508/accessibility-checklists/index.html

7.2.1. Contract Management

Contract management reports consist of the quality management plan (QMP), health and safety plan (HASP), information technology (IT) system security plan (SSP), standard operating procedures (SOPs), chemical inventory, and annual water report.

7.2.2. Periodic Status

Periodic status reports, including a **monthly status report (MSR)** that describes all test articles or samples shipped or received; all reports issued and their status (draft or final); health and safety, quality assurance (QA), information and data management, and IT security activities during the month; the status of all active assignments; and current costs for active assignments, cumulative costs for the contract, including direct and administrative costs; an **annual report** consisting of a compilation of all reports completed during the just-ended contract year; and a final report consisting of the annual report for the last year of the contract.

7.2.3. Functional Activity (Chemistry)

Chemistry reports consist of the following report types.

Interim reports consisting of preliminary results of an assignment in electronic format, usually as a data table. Interim reports are considered drafts and do not need to be Section 508 compliant. The format for interim data reports can be found in Appendix A.2. Data Submission Requirements.

Formal reports of all work performed for each assignment for each functional activity. These reports consist of a draft final report, submitted for review and approval of the contracting officer's representative (COR), and a final report, which is the COR-approved version of the report.

Letter reports, which may be issued in lieu of a formal report at the direction of the COR. Letter reports are typically issued for special studies assignments, or canceled assignments for which work was performed and are formatted as a letter to the COR describing the work performed.

7.2.4. Data Sheets

Data sheets consist of a one- or two-page summary report that contains a short narrative summary and lists in tabular form, the results of all analyses performed on a given chemical, test article, formulation, or sample, along with representative instrument output, as directed by the COR (e.g., MIPS report).

7.2.5. Other Deliverables

- A PDF of the study file for a given chemistry functional activity including a copy of the final report, data sheets, and all raw data supporting the information presented in the report. The PDF document is not currently required to be Section 508 compliant.
- Spreadsheets, consisting of the final QA results. Typically issued for biological sample analysis (BSA) and special chemical analysis assignments involving biosample analysis. Labeling, formatting, and data inclusion requirements for data spreadsheets can be found in Appendix A.2. Data Submission Requirements.

- Any incident or unforeseeable occurrences not listed in this document, or any physical modifications to the laboratory facilities, as well as any change in personnel that might have an effect on the conduct and results of studies, shall be reported immediately to the Division of Translational Toxicology (DTT).
- Monthly cost report supporting monthly invoices. See Section 7.10. Monthly Invoices and Cost Reporting.

7.3. General Reporting Requirements

The contractor shall ensure that the relevant chemistry functional activity reporting timeframes given below are met.

All reports submitted under this contract shall reference the contract number, the title and type of report, any applicable DTT numbers (e.g., DTTID), and the represented period on the first page of the report.

Chemistry Functional Activity reports shall include a header, an Executive Summary, a signed statement from the quality assurance unit (QAU), a Good Laboratory Practices (GLP) compliance statement (where applicable), and copies of representative instrumental output to support the data presented.

- Reports shall be signed and dated by the principal investigator (PI) and the responsible key personnel or task leader.
- Reports shall include the name of the relevant functional activity in the report header. See Appendix A.1.2. Report Header and Cover Page Formats for more detailed information.
- Section 7.6. Chemistry Functional Activity Reports provide requirements regarding report format, content, and submission deadlines.

The PI and the person who prepared the report shall sign the financial reports and status reports.

7.3.1. Electronic Reports

Electronic copies of all approved final chemistry reports and data sheets shall be submitted to the DTT Program Management System (PMS) at a URL specified by the COR.

Electronic copies of contract management and status reports shall be submitted to the DTT PMS. The COR will designate a forum for these reports.

Electronic reports of chemistry functional activity study files shall be submitted to a location designated by the COR.

Electronic copies of financial reports shall be emailed to the contracting officer (CO). The CO will provide the email address to the contractor.

7.3.2. Report Mailing Addresses

When required, hard copies of fiscal, status, or functional activity reports required shall be delivered to the COR at the following address and within the time periods specified below.

Contracting Officer's Representative
National Institute of Environmental Health Sciences
111 T.W. Alexander Drive
P.O. Box 12233
Research Triangle Park, NC 27709-2233

When required, hard copies of reports required for the CO shall be addressed and delivered to the CO at the address provided by the CO.

7.3.3. Study File Mailing Address

Hard copies of the study files for chemistry functional activities completed during the contract year and all associated raw data shall be mailed to the following address, as directed by the COR, at the end of each contract year:

Experimental Pathology Lab, Inc.
615 Davis Drive, Suite 400
Morrisville, North Carolina 27560

7.3.4. Reporting Subcontracted Work

When reporting subcontracted work, the contractor shall summarize the work in a report to DTT and attach as an appendix the original report submitted to the contractor by the subcontractor.

7.4. Contract Management Reports

7.4.1. Quality Management Plan

The contractor shall submit a QMP that addresses the quality requirements found in Chapter 5. Project Management. The QMP shall be submitted to the COR within 60 calendar days of the start of the contract.

The contractor shall update the QMP on a biannual basis and resubmit the updated QMP to the COR.

7.4.2. Health and Safety Plan

The contractor shall submit a copy of their HASP to the COR within 60 days of the award of the contract.

7.4.3. Information Technology Security Plan

The contractor shall submit a copy of their IT SSP to the COR within 60 days of the award of the contract.

7.4.4. Standard Operating Procedures

Within 6 months of the start of the contract, the contractor shall post electronic copies of the general SOPs applicable to all functional activities covered by Chapter 6. Functional Areas into the DTT PMS.

Subsequently, the contractor shall submit copies of these SOPs whenever they are changed.

It is not necessary for the contractor to submit copies of chemical-specific SOPs within 6 months of the start of the contract, as those SOPs will be submitted to the DTT PMS as needed for individual assignments.

7.4.5. Bulk Chemical Inventory

On the 15th day of each month of this contract, beginning with the second month after award, the contractor shall provide an electronic version of the inventory of test articles stored at their facility under this contract.

At the direction of the COR, the contractor shall provide an inventory of the analytical and reference standards stored at their facility under this contract in an electronic format.

Report Contents

An electronic file listing the chemicals stored at the contractor's facility, including the Chemical Abstracts Service registry number® (CASRN), DTXSID, and lot number of each chemical, and the amount on hand. Tabs in the file shall include, but are not limited to, test articles (bulk chemicals) and component standards.

The electronic file format shall be tab-delimited or.xlsx (Excel).

Delivery Requirements

The contractor shall post a copy of the electronic file to the DTT PMS. The COR shall designate a forum to receive the electronic chemical inventory.

7.4.6. Toxicity Screening Inventory

The contractor shall maintain an electronic inventory of all chemicals stored in the toxicity screening chemical library. In addition to the chemical name, the inventory shall include the Chemical List Identification number (CLID), Chemical Abstracts Service registry number® (CASRN), DTXSID, and lot number of each chemical, and the amount on hand, chemical class and use information, and other information designated by the COR.

The electronic file format shall be tab-delimited or.xlsx (Excel) and shall be uploaded in DTT PMS on the 15th day of each month.

7.4.7. Annual Water Analysis Report

The contractor shall post an electronic copy of their annual water analysis (AWA) report to the DTT PMS when animal studies are actively occurring under the contract.

Report Contents

Report the results of the analysis, including at minimum, values for each parameter required by the AWA functional activity (see Section 6.6.2. Annual Water Analysis (AWA)).

Include a reference to the entity performing the analysis, or to the relevant lab notebooks if performed by the contractor.

7.5. Periodic Status Reports

7.5.1. Monthly Status Report

On the 15th day of the second month after the start of the contract, and each month thereafter, the contractor shall provide an MSR of the activities on the contract during the previous calendar month. The format of this status report shall conform to that given in Appendix A.1. Report Formatting Requirements and shall include the following information:

- A cover page listing the report date, report title "Monthly Status Report" followed by the contractor's contract number, and date of the report. The middle of the page shall contain the phrase "Status Report –" followed by a number that indicates in sequential order for each month, the number of the current report; followed below by the reporting period; the contract title; the National Institutes of Health (NIH) contract number; and "Approved By" sign-off areas. At the bottom of the page, the contractor shall include the phrase "Submitted To:" followed below by the COR mailing address given in Section 7.3. General Reporting Requirements, above.
- The report shall have page headers indicating the report title, number, date, and page number.
- MSR Section 1, Introduction, shall state the period of the report and include definitions of the status flags used by the contractor in the report. For example, if the status flag "STARTED" is used in the report it could be defined as: "Work initiated during the reporting period but not completed." In addition, MSR Section 1 shall include tables that serve as keys to the program and funding codes (Table 1.1) and assignment acronyms (Table 1.2) used in the report. Refer to Section 7.9, Special Data Tables for Selected Reports, for a list of program and funding codes as well as functional activity acronyms.
- MSR Section 2, Reports Issued, shall consist of tables for the base and option years and for each exercised option listing all reports issued during the reporting period sorted by funding source and subsequently by program supported (Tables 2.1 and 2.2). The table shall include the functional activity, chemical name, a concise description of the work, the species/strain of any biosamples analyzed or toxicokinetic studies (TKS) performed, the report status code (final or interim), the contractor's internal tracking number, and the DTT organizational resource and business information tool (ORBIT) Project Task ID.
- MSR Section 3, Materials Handling, shall consist of tables for the base and option years and for each exercised optional activity listing all materials handling activities that have occurred during the reporting period sorted by funding source and then by program supported (Tables 3.1.1–3.3.2). MSR Section 3 is to be divided into subsections by activity i.e., sample receipt, sample processing, and shipment. The table is specific to the subsection being reported, but in general should include the following: sample or aliquot type, species/strain (for biosamples), a brief sample description, lab-assigned sample codes, lab-assigned work assignment number or code, and the associated DTT ORBIT Project Task ID.

- MSR Section 4, Safety Program, describes all accidents and/or injuries, industrial hygiene, and training activities involving contract staff during the reporting period.
  - Accidents/Injuries
  - Industrial Hygiene
  - Hazardous Chemicals/Waste
  - Training
  - Incident Response
  - Other Items
- MSR Section 5, Quality Assurance, is a summary of the activities of the QAU along with a table that summarizes the work performed on individual assignments for the base contract and all exercised options during the reporting period. MSR Section 5 includes a discussion of any project-related QA problem areas that arose during the reporting period.
- MSR Section 6, Information Management, describes activities relating to computer facilities, software, and equipment used under the contract, including work performed on the contractors' information management system and databases. Activities include routine maintenance, software and hardware upgrades, and software development projects related to the contract. MSR Section 6 also reports project-related electronic data collection, processing, and transmission problem areas that arose during the reporting period.
- MSR Section 7, Status Summary, consists of two subsections, sorted by funding source and program. The first subsection consists of a table that reports the status of all the work started, continued, reported, or completed during the reporting period. The table shall include columns for the following: DTT ORBIT Project Task ID, contractor-assigned work number, chemical name, functional activity, species/strain or matrix for biosample analysis or TKS, or vehicle for formulation work; a status code, due date, and date completed.
- MSR Section 8, Fiscal Data, reports monthly and cumulative summaries of total expenditures, direct costs, and labor incurred on the contract during the reporting period. MSR Section 8 consists of five subsections.
  - MSR Sections 8.1 and 8.2 report monthly and cumulative direct, administrative, and total costs for the base and option years, and each active option, respectively.
    - Direct costs are defined as labor and materials costs applied directly to the completion of assignments.
    - Administrative costs are defined as labor and materials costs applied to management of the workload (e.g., quality control [QC], QA).
    - Total cost is defined as invoiced cost.
  - MSR Section 8.3, Active Assignment Costs, reports the costs of all the work started, continued, reported, or completed during the reporting period for the base and each exercised option in tabular form (Table 8.3.1) meeting the following criteria:

        - Columns: DTT ORBIT Project Task ID, contractor-assigned work number, chemical name, CAS number, functional activity, estimated cost for the assignment, costs incurred for the assignment during the reporting period, and cumulative cost for the assignment since its inception.
        - Subtables: The table is split into subtables sorted by funding source and then by program.
        - Cost Data:
      - Data in cost columns may be footnoted to clarify issues related to the cost of a particular assignment.
      - Any assignment whose cumulative cost exceeds 150% of its estimated cost shall be flagged and footnoted.
      - Any assignment with a cumulative cost that is 80% of its estimated cost shall be flagged using a flag different from the "cost exceeded" flag.
      - Total costs for each program shall be reported after each subtable. Total costs for each funding source shall be reported after the last subtable for each funding source.
      - Footnotes shall describe the reason(s) for any cost overrun.
  - MSR Section 8.4, Cost Summary, presents invoiced monthly costs for the current contract year for the base contract and each exercised option (Table 8.4.1) and for each program and funding code (Table 8.4.2). Relevant program and funding codes are specified in Section 7.9. Special Data Tables for Selected Reports, below.
        - Table 8.4.1. shall include a line listing the cumulative total for the base and each exercised option along with a line listing the annual awarded amount for the base and each exercised option.
        - Table 8.4.2. Shall include three columns for each program and funding code: Direct Costs, Administrative Costs, and Total Costs. The cost summary shall be divided by contract year and each row in the table shall correspond to 1 month. The last row in each annual table shall contain the cumulative totals for each column.
  - MSR Section 8.5, Graphs, shall present plots showing dollars and person-hours expended for a running year, which are cumulative for the contract. The plots shall be furnished for the base, all active options, and the total contract.
- MSR Section 9, IT Security.
  - MSR Section 9 shall report on all activities specified in the contractor's submitted SSP. This information would typically include, though not be limited by, the following information for the reporting period:
        - Staff training performed.
        - Results of routine system scans.
        - Software updates/rollouts related to DTT work.

        - Reports of any IT incursions or suspicious activities.
        - Documentation of backups of DTT data performed.
- The MSR may include other information deemed pertinent as directed by the COR.
- Delivery Requirements.
    - One copy posted to the DTT PMS.
    - Reporting timeframe.
        - The MSR shall be submitted during each month of the contract, beginning during the second month after award. The report is due within 15 calendar days following the end of each reporting period.

7.5.2. Annual Report

Within 60 calendar days of the end of each year of this contract, the contractor shall submit an annual report, except for the final contract year. This report shall include the following information:

- A list of all reports completed during the just-ended contract year in PDF and Excel format.
- Reports may include other information as directed by the COR.

Delivery Requirements

- One electronic copy to the COR and one electronic copy to the CO or contract specialist.
- A copy of the annual report shall be posted to the DTT PMS in a location specified by the COR.

Reporting Timeframe

- Once a year for the base contract and option years.
- The first annual report shall cover the period comprising the first full 12 calendar months following the effective start date of this contract in addition to any fractional part of the initial month.
- The annual report must be received within 60 calendar days following each reporting period.

7.5.3. Final Report

The contractor shall submit a final report, which shall consist of the annual report for the last year of the contract.

Delivery Requirements

- One electronic copy of the final report shall be sent to the COR and one electronic copy to the CO or contract specialist.
- A copy of the final report shall be posted to the DTT PMS in a location specified by the COR.

Reporting Timeframe

- The contract's final report is due on or before the expiration date of the contract.

7.6. Chemistry Functional Activity Reports

7.6.1. General Requirements

For all assignments, the contractor shall post all reports in the DTT PMS under the respective project task. The COR may request copies of some documents to also be posted elsewhere.

For all assignments performed under the contract that generate data, the contractor shall issue interim reports consisting of the preliminary results of an assignment in electronic format.

- Interim reports are considered drafts and do not need to be Section 508 compliant.
- Interim data and/or reports provided by the contractor do not have to be formally quality-checked by the QAU but must be reviewed by the laboratory staff and PI prior to release.
- Interim data and/or reports shall be posted as soon as available. The COR will direct the contractor to the exact location for interim data (e.g., task timeline).

For all assignments performed, the contractor shall issue a draft final report upon completion of an assignment that describes the work performed for the assignment and details the results obtained, as required herein, and in the specific report requirements for each functional activity.

- The draft final report shall include all the information required in Section 7.6.2, Content Requirements and following.
- Draft final reports (both Word and PDF files) shall be posted as review documents.
- Draft final reports do not need to be Section 508 compliant.
- If a review of the draft final report by the COR results in changes to the report, the contractor shall submit a revised version of the draft final report to the COR that reflects the required changes, prior to submission of the final report.

After the COR approves the draft final report, the contractor shall issue a final report consisting of the approved final report, with a signed QA statement, uploaded as a Section 508-compliant electronic document in PDF.

7.6.2. Content Requirements

Reports shall contain a header with information about the analyzed sample(s). All report headers shall contain the contract number, OTBIT task and project ID, sample name or descriptor, lot/batch numbers, all assigned sample codes, the sample source, and the date the sample was obtained or received. Other information that may be included in the report header depends on the reported assignment and may include any or all of the following:

- Chemical name
- CASRN
- DTXSID

- CLID (for MHTS assignments)
- Analysis date(s)
- Shipping date
- Archival date
- Archival mass
- Number of samples collected
- Person(s) responsible for sample collection
- See Appendix A.1.2. Report Header and Cover Page Formats for additional information

The report shall include an Executive Summary that summarizes the work performed and the results obtained.

The report shall include all contractor-assigned codes, presented so that they are traceable to the original source material.

When analysis results for samples are reported, and whenever the contractor reports test article(s), chemical(s), or samples shipped or received, the report shall include a table identifying all the samples shipped, received and/or analyzed. The table shall list all sample identification codes, including animal numbers, color codes, dose group codes, contractor-assigned log numbers, and/or sample source-assigned codes; and other identifying information (e.g., nominal concentrations, species/strain information, lot numbers, and/or dose route).

The contractor shall report all procedures developed or used, including (for method development activities) the process leading up to the final method(s) and references to all applicable development report(s), substance-specific analysis protocol(s), dose analysis, and/or characterization reports.

Analysis reports shall include a description summarizing all methods used for sampling (when applicable) and analysis, the results of the assignment, normally in tabular form, a discussion of the results of each analysis performed, including the measurement limits of the method, the mean, and an estimate of sample variability (e.g., % relative standard deviation [RSD]) for all replicate analyses, including replicate QC standards. Additionally, analysis reports shall include a tentative identification (when the method used allows for such) for each substance measured, a written results summary, data tables, and relevant figures.

Reports shall include references to other relevant reports (e.g., the BSA report shall include a reference to the corresponding BMD report).

Special Content Requirements for Selected Reports

Absorption, Distribution, Metabolism, and Excretion Studies (ADMES)

The results of absorption, distribution, metabolism, and excretion (ADME) studies by phase. Each phase shall include discussion of the data, including a comparison between species, sexes, doses, and dose routes, as applicable.

Report contents:

- Cover
- Header
- Executive Summary
- GLP Compliance (if applicable)
- QA Statement (if applicable)
- Table of Contents
- Introduction
- Study Design
- Methods
  - Test article
  - Animals
  - Animal study conduct
  - Sample analysis
- Results
  - Chemical purity results
  - Formulation analysis results (when applicable)
  - Sample analysis data and/or tables
- Discussion/Conclusion
- Acknowledgments/References
- Appendices (as required)

BSA = Biological Sample Analysis; GLP = Good Laboratory Practices; QA = quality assurance.

Biological Sample Analysis (BSA)

The following also applies to other functional activities for which biosample analysis was performed. In addition to the formal report, the contractor shall submit a spreadsheet to the DTT PMS, which meets the following requirements.

The spreadsheet must be in Microsoft Excel or an Excel-compatible file format. The spreadsheet data shall be a true and accurate copy of the data in the final report and shall have been reviewed by the contractor's QAU.

One spreadsheet with tabs for one matrix, sex, and species shall be issued per a BSA assignment (e.g., plasma, male rat, plasma in one tab).

Each tab shall contain header information describing the study from which the samples to be analyzed came. At minimum, the header shall specify:

- The animal species, strain, and sex of sample results reported
- The name of the study from which the samples came (e.g., TKS, 2-year bioassay)
- The date(s) the samples were received

- The date(s) the samples were analyzed

All individual sample data reported in any spreadsheet shall be clearly identifiable and traceable to the animal from which the sample data came, and the dose group shall be clearly labeled. A dose is defined as a specific administered formulation concentration, with the animal's sex and life stage (e.g., 25 mg/kg bwt, adult, nonpregnant female).

BSA reports shall include a reference to the study and/or source from which the samples analyzed came.

Report contents:

- Cover
- Header
- Executive Summary
- GLP Compliance
- QA Statement (as applicable)
- Table of Contents
- Introduction/Objectives
- Study Samples
- Methods
- Results
- Conclusion
- References
- Appendices (as required)

Biosample Method Development (BMD)

A report of the method development activities conducted including a presentation of the validation and stability results, a conclusion regarding the acceptability of the method, and a discussion of the sample storage requirements.

Report contents:

- Cover
- Header
- Executive Summary, including method validation and stability summary table(s)
- GLP Compliance
- QA Statement
- Table of Contents
- Introduction/Objectives
- Method Development Notes
- Experimental Design

- Definitions
- Method Validation
  - Validation data
  - Analysis period stability
  - Method verification (if needed to extend the standard curve range)
  - Specificity testing (if needed)
- Storage Stability
- Acknowledgment/References
- Appendices (as required)

GLP = Good Laboratory Practices; QA = quality assurance.

Chemical Reanalysis (CRA)

Chemical reanalysis (CRA) reports shall include a plot of the results for all previous analyses of the same lot, formatted as percent relative purity versus time, with 95% confidence intervals indicated, when applicable.

Formulation Development (FD)

The effective range of the method must be specified in the report along with method qualification or validation data.

Report contents:

- Cover
- Header
- Executive Summary
- GLP Compliance (not required for FD reports)
- QA Statement (as applicable)
- Table of Contents
- Methods
- Introduction
- Method Development Notes
- Description of Method
- Method Validation (as applicable)
- Homogeneity and Stability Results
- Summary and Conclusion
- Acknowledgments/References
- Appendices (as required)

FD = formulation development; GLP = Good Laboratory Practices; QA = quality assurance.

Formulation Preparation, Analysis, and Shipment (FA and FPAS)

The results of analysis for feed formulations shall be reported as milligram test article per gram vehicle. All other formulations shall be reported as milligram test article per milliliter vehicle.

Table 7–1. Formulation Analysis Results Format

Sample	Target Concentration (mg/mL)	Determined Concentration (mg/mL)	Mean Determined Concentration ± SD (%RSD)	Mean % Target	Mean %RE
0–1	0	ND			
0–2	0	ND	NA	NA	NA
0–3	0	ND			
75–1	75	75.83			
75–2	75	75.60	75.82 ± 0.22 (0.3%)	101.1	1.1
75–3	75	75.03			
150–1	150	151.3			
150–2	150	151.4	152.0 ± 1.1 (0.7%)	101.3	1.3
150–3	150	153.2			
300–1	300	301.8			
300–2	300	302.7	303.5 ± 2.2 (0.7%)	101.2	1.2
300–3	300	305.9			
450–1	450	454.5			
450–2	450	449.9	456.0 ± 7.0 (1.5%)	101.3	1.3
450–3	450	463.6			

NA = not available; ND = not detected; RE = relative error; RSD = relative standard deviation; SD = standard deviation.

In vitro Assays

Report contents:

- Cover
- Header
- Executive Summary
- GLP Compliance (if applicable)
- QA Statement (if applicable)
- Table of Contents
- Introduction
- Study Design
- Methods
  - Model system
  - Analytical method development (if applicable)

  - Study conduct
  - Sample analysis
  - Data analysis
- Results
  - Analytical method development data (if applicable)
  - Sample analysis data
  - Data analysis/modeling
- Discussion
- Conclusion
- Acknowledgments
- References
- Appendices (as required)

GLP = Good Laboratory Practices; QA = quality assurance.

Multiple Chemical Handling (MCH)

- Cover
- Header/Chemical Information
- Executive Summary
- Quality Statement
- Table of Contents
- Introduction/Objectives
- List of Equipment/Solvents/Reagents Used
- Table 1: Chemicals Prepared and Concentrations[3]
  - Column 1: DTT Chemical Name
  - Column 2: CASRN
  - Column 3: DTXSID
  - Column 4: Supplier
  - Column 5: Lot Number
  - Column 6: COA Purity
  - Column 7: DMSO Concentration
  - Column 8: Plate Address (plate number, row, and column ID)[4]
- Table 2: Chemicals Not Prepared (if necessary)
  - Column 1: DTT Chemical Name

[3]If multiple researchers are receiving the same chemicals, one table is appropriate, if chemicals to be prepared are different, a separate table for each researcher is required.
[4]When micro-plates (96- or 384-well) are prepared.

  - Column 2: CASRN
  - Column 3: DTXSID
  - Column 4: Reason for Not Preparing (e.g., insoluble in DMSO, physical change upon dissolving, gas generation upon dissolving)
- Conclusion
- Table 3: Summary Table (include CLID in table title)
  - Column 1: Type
  - Column 2: Number
  - Row 1: "Type," "Number"
  - Row 2: "Chemicals Prepared," ##[5]
  - Row 3: "Chemicals Not Prepared," ##
  - Row 4 (Sub R3): "Insoluble," ##
  - Row 5 (Sub R3): "Solution Change," ##
  - Row 6: (Sub R3): "Gas Generation," ##
  - Rows 7-nn (Sub R3): {*Additional Conditions*}, ##
  - Final Row: "Total," ## (total of Rows 1 and 2)

CASRN = Chemical Abstracts Service Registry Number; COA = Certificate of Analysis; DMSO = dimethyl sulfoxide; DTT = Division of Translational Toxicology.

Multiple Chemical Identity and Purity Screening (MIPS)

- Cover
- Header/Chemical Information
  - Citation of Tables
- Executive Summary
- Quality Statement
- Table of Contents
- Introduction/Objectives
- List of Equipment/Chemicals/Solvents/Reagents Used
- Method Development Notes
- Experimental Design
  - Include all analysis methods
  - Table 1: Summary Table Outlining Chemical Types

Type	Number
Mixture	
Flame Retardant	
Ionic liquid	

[5]## is the number of chemicals that fall into the specific category (e.g., the number of chemicals prepared).

Type	Number
Etc.	
Total	1408

  - Table 2: Chemical Analysis Results (include CLID in table title)
    - Column 1: Tox21_ID
    - Column 2: DTT Chemical Name
    - Column 3: CASRN
    - Column 4: DTXSID
    - Column 5: Supplier
    - Column 6: Lot
    - Column 7: COA Purity
    - Column 8: MIPS Purity
    - Column 9: Purity Method (GC/MS, LC/MS, NMR, etc.)
- Acknowledgments/References
- Appendices (as needed)
- Appendix 1: Definitions of Terms Used in Tables (e.g., Tox21_ID, STRUCTURE_Formula)

CASRN = Chemical Abstracts Service Registry Number; CID = Chemical Identifier; COA = Certificate of Analysis; DMSO = dimethyl sulfoxide; DTT = Division of Translational Toxicology; DTT_Set# = Reference Tox21 Plate Set #; GS-MS = Gas Chromatography-Mass Spectrometry; HIPS = High-Throughput Identity and Purity Screen; HTS = high-throughput screening; InChI = International Chemical Identifier; IUPAC = International Union of Pure and Applied Chemistry; LC-MS = Liquid Chromatography-Mass Spectrometry; NMR = Nuclear Magnetic Resonance; RID = reference identifier; SID = substance identifier; SMILES = Simplified Molecular Input Line Entry System.

Multiple Chemical Procurement (MCP)

- Cover
- Header/Chemical Information
- Introduction/Objectives
- Quality Statement
- List of all suppliers with addresses, contact phone numbers, and web addresses
- Table 1: Supplier Order Information (landscape)
  - Column 1: DTT Chemical Name
  - Column 2: CASRN
  - Column 3: DTXSID
  - Column 4: Supplier Name
  - Column 5: Supplier Lot No.
  - Column 6: Supplier Unit Size (e.g., 100 mg, 5 g, 1 kg)
  - Column 7: Amount Ordered
  - Column 8: Supplier COA Purity
  - Column 9: Method of COA Analysis

- Table 2: Chemicals Not Ordered
  - Column 1: DTT Chemical Name
  - Column 2: CASRN
  - Column 3: DTXSID
  - Column 4: Reason for Not Ordering (e.g., rare, not available, insoluble in dimethyl sulfoxide (DMSO), gas at 25°C, explosive, degrades, expensive)
- Conclusion
- Table 3: Summary Table (include CLID in table title)
  - Column 1: Type
  - Column 2: Number
  - Row 1: "Type," "Number"
  - Row 2: "Chemicals Ordered," ##[6]
  - Row 3: "Chemicals Not Ordered," ##
    - Row 4 (Sub Row 3): "Insoluble," ##
    - Row 5 (Sub Row 3): "Gas @25ºC," ##
    - Row 6 (Sub Row 3): "Explosive," ##
    - Row 7-nn (Sub Row 3): {*Additional Conditions*}, ##
  - Final Row: "Total," ## (total of Rows 1 and 2)
- Acknowledgments/References
- Appendices (as needed)
  - Appendix 1: Supplier information for chemicals whose supplier information differs from DTT information (e.g., different name or CASRN).
    - Table A-1: Supplier Information Differs from DTT
      - Column 1: DTT Chemical Name
      - Column 2: DTT CASRN
      - Column 3: Supplier
      - Column 4: Supplier Chemical Name
      - Column 5: Supplier CASRN

BSA = biological sample analysis; CASRN = Chemical Abstracts Service Registry Number; COA = Certificate of Analysis; DMSO = dimethyl sulfoxide; DTT = Division of Translational Toxicology; GLP = Good Laboratory Practices.

OMICS

Report contents:

- Cover
- Header

[6]## is the number of chemicals that fall into the specific category (e.g., the number of chemicals prepared).

- Executive Summary
- GLP Compliance (if applicable)
- QA Statement (if applicable)
- Table of Contents
- Introduction/scope
- Study Design (if applicable)
- Methods
  - Analytical method development (if applicable)
  - Sample preparation and analysis
  - Data analysis
- Results
  - Analytical method development data (if applicable)
  - Sample analysis data
  - Data analysis/modeling
- Discussion
- Conclusion
- Acknowledgments
- References
- Appendices (as required)

GLP = Good Laboratory Practices; QA = quality assurance.

Palatability Studies (PALS)

The results of the palatability study including a presentation of the food and/or water consumption and body weight gains at each dose and a discussion of the implications of the data for the palatability of the dose.

Report contents:

- Cover
- Header
- Executive Summary
- GLP Compliance
- QA Statement
- Table of Contents
- Introduction/Objectives
  - Description of study
- Methods

  - Test article
  - Animals
  - Experimental design
- Discussion/Conclusion
- Acknowledgments/References
- Appendices (as required)

GLP = Good Laboratory Practices; QA = quality assurance.

Preliminary Formulation Studies (PFS)

The contractor shall report the maximum concentration (mg/mL) at which the test article was soluble in the vehicles tested and the Merck Index or other reference solubility when available.

The contractor shall report the results of storing the maximum concentration solution in the refrigerator for 24 hours.

For each vehicle tested, the contractor shall report the maximum concentration (mg/mL) of test article solution, which was shown to be syringeable through an 18-, 20-, or 22-gauge gavage needle.

When a solution is syringeable with an 18-gauge gavage needle, the contractor shall report whether it is also syringeable with a 22-gauge needle.

The contractor shall report the observed stability of the suspension/emulsion with respect to homogeneity and test article settling rate.

The contractor shall report the results electronically in tabular form.

Protocols Development (PD)

Protocols development (PD) reports shall include references to the formulation and/or characterization reports that are the source of the method described in the protocol.

Typical analytical output of the method performed shall be included in the PD report.

Shipment of Multiple Chemicals

In addition to the report header (see Section 7.9.2. Required Report Formats) information, shipping reports for multiple chemicals shall contain a table (Table 1) with the following information:

- Column 1: Code (if required)
- Column 2: DTT-CID No. (for HTS chemicals)
- Column 3: Chemical Name
- Column 4: CASRN
- Column 5: DTXSID
- Column 6: Supplier
- Column 7: Lot No.

- Column 8: COA Purity (%)
- Column 9: Determined Purity (%) (CIPS, CCA, HIPS, etc.)
- Column 10: Storage Conditions (abbreviate: RT, RF, FR, PFL, IG, etc.)
- Column 11: Amount Shipped (e.g., Aliquot Weight)

CASRN = Chemical Abstracts Service Registry Number; CCA = Comprehensive Chemical Analysis; CID = Chemical Identifier; CIPS = Chemical Identity and Purity Screen; COA = Certificate of Analysis; DTT = Division of Translational Toxicology; FR = freeze; HIPS = High-Throughput Identity and Purity Screen; HTS = high-throughput screening; IG = inert gas; PFL = protect from light; RF = refrigerate; RT = room temperature.

Special Studies

Report titles for special studies reports shall include a reference to the functional activity(ies) from which the report was derived when applicable (e.g., the title of a special dose FD report would be "Special Chemical Activity: Dose Formulation Development," followed by a short subtitle describing the work).

Toxicokinetic Studies (TKS)

The report shall cover the following:

- Formulation preparation and analysis and biosample analysis and data. Documentation detailing formulation preparation and analysis and biosample analysis and data shall be included as appendices to the TKS report.
- Results of TKS, including the resulting toxicokinetic modeling parameters and a discussion of the data, including a comparison between species, sexes, doses, and dose routes, as applicable.
- The spreadsheets for biosample analysis data (refer to BSA) and final toxicokinetic parameter tables in Microsoft Word format.

Report contents:

- Cover
- Header
- Executive Summary
- GLP Compliance
- QA Statement
- Table of Contents
- Introduction/Objectives
  - Description of study
- Study Design
- Methods
  - Test article
  - Animals
  - Animal study conduct

    - Toxicokinetic evaluation
- Results
    - Summary of formulation analysis
    - Summary of biosample analysis
    - Animal information (e.g., observations, animal body weights)
    - Summary of toxicokinetic evaluation
- Discussion/Conclusion
- Acknowledgments/References
- Appendices (e.g., formulation analysis and data, biosample analysis data)

BSA = Biological Sample Analysis; GLP = Good Laboratory Practices; QA = quality assurance.

Required Chemistry Report Appendices

Appendices may vary depending on the task. When appropriate, reports may include appendices containing, for example, a substance-specific analysis protocol, a method summary, a study protocol, a mixing protocol, raw data tables, computer modeling and/or simulation outputs, or other chemistry reports that support the work being reported.

TKS and ADMES reports shall include the following appendices as applicable:

- Study protocol (with all amendments and deviations)
- All associated analysis data (formulation preparation and analysis and biosample analysis data; animal body weights tables; water and food and water consumption; compound consumption; toxicokinetic evaluation supporting documentation [e.g., output from modeling programs])

7.6.3. Reporting Results

Results should be presented in tabular form whenever practical.

Discussions of the results of any analyses shall reference accepted literature values when applicable.

Results of all analyses of samples, standard curves, and QC standards shall be reported. These results may be presented as summary information in the body of the report, but in that case, the raw data must be included in an appendix.

- Chromatographic purity assays shall report all peaks with integrated areas ≥0.1% of the total area and include the contractor's best information (from literature, synthesis routes, manufacturer, etc.) on what these peaks represent.
- Formulation analysis reports shall flag any result that is outside the specified acceptability criteria, typically ± 10% of nominal.
- Vehicle analysis reports shall flag any result that exceeds the specified limit value for that vehicle.

- Raw data includes but is not limited to standard concentrations (nominal or prepared), responses and found concentrations, sample responses and found concentrations, and modeling program outputs.

Plots of analytical results shall be reported when appropriate (e.g., standard curves, dose-response curves, time-course data, QC plots).

Reports shall include a representative instrument or other analytical output, which supports the reported analysis results. These data include chromatograms, spectra, plots, or other output, which may be presented as figures, photos, tables, principal component analysis plots, and/or heat maps. All reported instrument output figures, including photographs and photomicrographs, spectra, chromatograms, etc., supplied as supporting documentation in any report, shall be clear, in focus and unambiguously labeled to allow trace-back to the source bulk chemical, test article, dose formulation, or sample from which they were produced.

When system suitability is performed for any analysis, the report shall include a table of the results.

7.6.4. Letter Reports

Reports of incomplete or canceled assignments for which work was performed may be reported as letter reports, at the direction of the COR.

- The contractor shall describe the work performed, including (when applicable), samples received, sample and standards preparation, analytical method parameters, including instrument settings, and any calculations performed.
- Letter reports shall be formatted as a letter to the COR describing the work performed.
    - The contractor shall present the results obtained from the work (if any), including summary tables, graphs, and/or figures as appropriate to illustrate the results.
    - Letter reports are not required to have a cover page, report header, GLP compliance page, QA statement, Executive Summary, or table of contents unless specifically requested by the COR.
    - Letter reports must be dated with their date of issuance, include the chemical name or study for which they were created, the CASRN, and the ORBIT Project Task ID for which the work was performed.
    - The contractor's PI must sign letter reports.
- Letter reports shall be considered draft final reports until they are approved by the COR and follow the same reporting process as the formal draft final reports.

7.6.5. Draft Final Reports

The contractor shall provide a draft final report a specified number of calendar days after all laboratory work is completed depending on the report category (see below).

Draft final reports shall be considered final by the contractor but shall not be signed.

The contractor shall post electronic copies of draft final reports to the DTT PMS for review by the COR. If the COR requests revisions to a draft final report, the contractor shall submit a new version of the draft final report to the DTT PMS reflecting the requested changes, prior to the submission of a final report.

7.6.6. Final Reports

Once the COR approves the draft final report, a certified electronic copy of the final report shall be uploaded to the DTT PMS at a location specified by the COR.

Final reports must be posted to the DTT PMS specified folder within 1 week from the date of COR approval.

7.6.7. Amending Reports

When an error is found in an approved final report, the report shall be amended to correct the error at the direction of the COR. An appendix shall be included in the amended report, indicating all of the changes made in the report by page number.

The revised final report shall be submitted to the COR for review and approval.

Once the revisions are approved by the COR, the report shall be reissued as an amended final report. The report date of the amended report shall reflect the date of COR approval for the revisions and the title page shall reflect its amended status. The report title shall clearly indicate that the report has been amended.

Amended final reports shall be uploaded to the DTT PMS as certified electronic copies within 1 week from the date of COR approval.

7.6.8. Reporting Deadlines

Chemistry report deadlines for each assignment category are given below. Deadline exceptions may be granted on a case-by-case basis with the approval of the COR.

- Logistics and Handling: 4 weeks after all laboratory work is completed.
- Characterization: 8 weeks after all laboratory work is completed.
- Formulation: 8 weeks after all laboratory work is completed.
- Biosample Analysis: 8 weeks after all laboratory work is completed.
- Animal Studies: 12 weeks after all laboratory work is completed.
- Special Studies: 8 weeks after all laboratory work is completed.
- OMICS: 8 weeks after all laboratory work is completed.
- In Vitro Assays: 8 weeks after all laboratory work is completed.

7.7. Data Sheet Reports

A data sheet report consists of a one- or two-page report listed in tabular form and presents the results of all analyses performed on a given bulk chemical, test article, formulation, or sample.

The data sheet shall include an abbreviated report header that shall minimally include the chemical or sample name, CAS number, lot number and/or source- and contractor-supplied sample codes, sample source, and sample receipt or mixing date. See Appendix A.1.2. Report Header and Cover Page Formats, for more information.

The reported results shall include:

- A table listing the instrument and instrument parameters used to measure the sample.
- For characterization activities, a table listing all substances found in the sample at an apparent concentration of ≥0.1%.
    - For chromatographic-mass spectrometric data, the table shall include a peak identification number, the determined molecular mass, the retention time (in minutes), and the percent total area value for that peak.
    - For non-chromatographic data, the table shall include identification numbers, determined values (e.g., chemical shifts), and a percentage of sample estimate, for each substance reported.
- Figures of instrument output for the sample and reference (library or reference standard).
    - For chromatographic non-mass spectrometric data, the figures shall include the chromatogram of the sample and the reference standard run with the samples, along with any applicable standard curves.
    - For chromatographic-mass spectrometric data, the figures shall include the total ion chromatogram, and the sample, standard reference (if applicable) and library reference mass spectra, along with any applicable standard curves.
    - For NMR data, the figures shall include the sample spectrum and library reference, along with any 2-D NMR data plots produced.
- A brief summary of the sample and standards (when applicable) preparation procedure.

Data sheets will be issued as an additional deliverable for the following functional activities:

- Multiple Chemical Identity and Purity (MIPS) Studies

Data sheets may be submitted in lieu of a formal chemistry report for the CIPS functional activity and as stand-alone reports accompanying MIPS functional activity reports.

Stand-alone data sheets for MIPS tasks shall be submitted as draft final reports and shall be subject to the same reporting requirements as chemistry reports (Sections 7.6.5–7.6.8, above).

7.8. Additional Reporting Requirements

7.8.1. Electronic Data Submission

Copies of all approved chemistry reports, including the supporting raw data and all supporting instrument outputs shall be submitted to the DTT PMS forum library associated with the DTT PMS task entry for that work, or as specified by the COR, in accordance with the requirements described below. The PDF document is not required to be Section 508 compliant unless otherwise specified by the COR.

The contractor shall verify and certify that the data submitted represent a clear complete copy of the original data and final approved report.

The uploaded data shall be labeled with the contract number, and lab-assigned work number, DTT-assigned ORBIT Project Task ID, for which the work was done, the species/strain and study codes associated with the work (if applicable), the functional activity(ies) for which the report was generated, and the date of the report.

Additional information may be included at the discretion of the contractor.

Data included on the upload must be readable on all commercially available operating systems at the time of issuance. The COR shall approve file types for specific categories of data.

Copies of approved reports and supporting raw data shall be uploaded once the report has been approved, but not less than semi-annually.

7.8.2. Good Laboratory Practice Compliance Statements in Reports

At the time of task assignment, the COR will designate a task needing GLP compliance.

GLP compliance statements are required to be present in reports of all work conducted in compliance with Food and Drug Administration GLP regulations.

The GLP compliance statement shall precede the QA statement in all reports for which it appears.

Typically, reports for the following functional activities will require a GLP compliance statement:

- Protocols Development (PD)
- Comprehensive Chemical Analysis (CCA)
- Chemical Reanalysis (CRA)
- Formulation Development (FD)
- Formulation Analysis (FA) including referee analysis
- Formulation Preparation, Analysis, and Shipment (FPAS)
- Biosample Method Development (BMD)
- Biological Sample Analysis (BSA)

- Toxicokinetic Studies (TKS)
- Absorption, Distribution, Metabolism, and Excretion Studies (ADMES)

7.9. Special Data Tables for Selected Reports

7.9.1. Program and Funding Codes

Codes are used to track contract expenditures by funding source and program supported. Each assignment will be assigned funding and program codes prior to commencement of work. Status reports issued by the contractor shall reference the funding and program codes when tabulating expenses.

Funding Codes shall be as listed in Table 7–2. Additional funding codes may be added during the course of the contract at the discretion of the COR.

Table 7–2. Funding Codes

Funding Source	Funding Code
NIH AIDS	AIDS
National Institute of Environmental Health Sciences (NIEHS, not DTT)	DIR
Superfund	SPR
Other Government Agency	OGA

Program Codes shall be as listed in Table 7–3. Program Codes may be changed or added during the course of the contract at the discretion of the COR. A current list is provided below.

Table 7–3. Program Codes

Program/Initiative	Program Code
	HTS
Toxicity Testing	TOX
NIEHS (in-house, not DTT)	DIR
AIDS	AIDS
Per and Polyfluoroalkyl substances	PFAS
Other Program	OTH

7.9.2. Required Report Formats

See Appendix A.1. Report Formatting Requirements for more information regarding the formatting and content requirements for the MSR and chemistry report headers and cover pages.

7.10. Monthly Invoices and Cost Reporting

7.10.1. Invoices (Monthly)

Title/Cover page - Standard Form 1034, Revised January 1980. Department of the Treasury, I TFRM 4-2000, 1034-118.

Summary page containing:

- Invoice Number and Date
- Bill To and Remit To information
- Customer information, including contract number, project number, project name, project period of performance, terms, and due date
- A table listing Direct Other Direct and indirect costs, Fee and Invoice Costs with columns for the monthly performance period and the Cumulative Amount (Contract Year to Date).

Project Labor Summary Report

- Actual Hours and Costs presented in tabular format for the current performance period and year to date for each person working on the contract
- Data should be presented by labor category and by assignment

Non-Labor Summary (Supplies and Materials)

- Actual costs presented by category, e.g., Purchased Services, Word Processing, Lab Supplies, Chemicals and Gases, Books and Subscriptions, Postage and Shipping

7.10.2. Cost Reports

Monthly Hours and Cost by Assignment (Monthly)

- Excel Spreadsheet submitted monthly summarizing hours and costs for staff by assignment
  - Hours for each person by assignment for the reporting period
  - Costs for the reporting period for each assignment
  - Admin hours for each person not charging to a specific assignment
  - Total admin cost
- Example:

Administrative $25,540
– Bill Smollet 4.0 h
– Susan Miller 20.0 h

SCA 123456 $Total reporting period cost
– Jane Doe. 2.5 h
– John Smith 42.3 h
CCA 234567 $Total reporting period cost

Quarterly Cost Summary (Quarterly)

- Excel spreadsheet submitted quarterly summarizing costs per task per month sorted by DTT cost category (e.g., AIDS, PFAS, Flame Retardants, etc.)
- Provide summary costs for each cost category within the spreadsheet