Standard Operating Procedures

RTI SOP# Ion3

RTI QT9 QMS # MAP-IONS-SOP-086

Filter Extraction via SimPrep Autodilution System

Analytical Sciences
Laboratory Sciences & Engineering
RTI International*
Research Triangle Park, NC

Prepared by: Adam Conway Date: 12/19/2025

Reviewed by: Andrea McWilliams Date: 12/19/2025

Approved by: Tracy Dombek Date: 12/19/2025

EFFECTIVE DATE: 12/19/2025

Table of Contents

Page

1.0 PURPOSE

This Standard Operating Procedure (SOP) describes the process for delivering deionized (DI) water via the SimPrep Autodilution System to sample tubes containing filters that will be extracted.

2.0 SCOPE

This SOP applies to particulate matter with an aerodynamic diameter of less than or equal to 2.5 micrometers ($PM_{2.5}$) on 47-millimeter (mm) nylon filters from the Chemical Speciation Network (CSN) and 37-mm nylon filters from the National Park Service (NPS). The procedures may also be applied for filters received for special projects; however, the volume should be adjusted accordingly.

3.0 RESPONSIBILITY

Management (Center Directors, Principal Investigators, Study Directors, or equivalent) is responsible for ensuring that the procedures outlined in this SOP are performed by trained laboratory staff supporting the project.

4.0 PROCEDURE

This section of the SOP outlines how to initialize the instrument (**Section 4.1**), set up the sequence (**Section 4.2**), and begin the sequence (**Section 4.3**).

4.1 Initializing the SimPrep Autodilution System

Note: When the SimPrep Autodilution System has been used to extract filters, analysts will leave it drained at the end of each day; therefore, the instrument must be restarted and initialized before use.

The following procedures will be used to initialize the SimPrep Autodilution System:

1. Select the “SimPrep” shortcut

2. Check the following parameters for use:

Location	Parameter	Amount
Settings -> Station -> Misc.	Purge Volume	10,000 microliters
Settings -> Station -> Misc.	Loop Volume	50,000 microliters
Settings -> Station -> Syringes	Syringe Size (S1)	50,000 microliters
Settings -> Station -> Syringes	Syringe Size (S2)	1,000 microliters
Settings -> Station -> Diluents	Diluent	DI water

3. Purge the autodilution system by selecting the purge icon at the top of the screen. Repeat selection five times to fully prime the valve.
4. Set each rack to 3 rows and 7 positions.
5. Set up two bottles filled with DI water for each SimPrep autodilution system. Use a rinse bottle for the probe station and another bottle for providing the volume of DI water to be dispensed into the sample tubes.
6. Empty and rinse the DI water reservoir for the dispenser and probe rinse before every use.

4.2 Setting up the Sequence

The sequence may be added manually or selected from the saved files directory.

The following procedure is used to create a manual sequence:

1. Verify status is set to the green triangle, which indicates that the sample needs to have DI water added.
2. Set Name column to “Dispense”.
3. Set Position to rack number and position number. An example for the first position in rack one would be R1-01.
4. Autodilutor performance is assessed quarterly in accordance with the procedures outlined in the Demonstration Autodilutor Performance worksheet (see **Figure 1** for example of the worksheet). This assessment evaluates and documents both the precision and accuracy of each autodilutor. The final determined volumes are recorded on the performance worksheets and in each autodilutor’s logbook. All logbooks and performance check records are maintained in Johnson 187 alongside the autodilutors. Analysts must refer to each autodilutor logbook to verify the correct volume setting before entering the extraction volume in the

autodilutor software. The required setting depends on the type of extractions being performed:

- NPS extractions 20,000
- CSN extractions 25,000

If you plan to extract non routine samples, you may conduct a check of the system to assess the appropriate volume setting required to meet the targeted accuracy following the procedure used in the "Demonstration of Autodilutor Performance" worksheet.

5. Set up the sequence for the exact number of samples that are to be extracted.

The following procedure is used to load a sequence from the saved files:

1. Select "Open Saved File".
2. Select the file specific for either NPS or CSN sample extraction.

4.3 Beginning the Sequence

The following procedure is used at the beginning of a sequence:

1. Verify that the volume to be added is correct for the samples to be extracted.
2. Select the start button located at the top of the screen.
3. Verify that the probe is aligned correctly, and that water is being dispensed in the correct vial. The sequence will stop when all vials have been filled.
4. When the sequence has ended, replace the caps on extracted samples.

5.0 MAINTENANCE

Verify the accuracy and precision of the instrument quarterly and document results using the *Demonstration of Autodilutor Performance* worksheet.

AUTODILUTOR PROFICIENCY WORKSHEET	RESEARCH TRIANGLE INSTITUTE POST OFFICE BOX 12194 RESEARCH TRIANGLE PARK, NC 27709-2194	DATE: _____ ANALYST: _____

TITLE: Demonstration of Autodilutor Performance

System ID #:_____

General Instructions

This worksheet applies to use of the SimPrep AutoDilution system. The purpose of this worksheet is to demonstrate proficiency for chemists and technicians. If the relative standard deviation is not greater than 5 %, the chemist or technician is deemed qualified to utilize the autodilutor. The review can be completed by any technician or chemist who has previously demonstrated proficiency using the autodilution system. Initial and date each task as soon as it is completed; sign the bottom of the page when all entries have been completed and have reviewer sign bottom of page. Data entries should be performed using indelible blue or black-ink ballpoint pens. Be sure to record scientific observations and deviations from this procedure on this document.

Reagents	Supplier	Date Prepared	Exp. Date
Deionized (DI) Water	Milli-Q IQ7000	Resistivity reading_____	Drawn daily

Equipment	Manufacturer/Model	Serial Number or ID# / Location
Deionized (DI) Water System	Millipore / Milli-Q IQ7000	F2SB29069 / Johnson, Lab 187, Bay 6
SimPrep AutoDilution System	SimPrep	0122138A560/ Johnson, Lab 187, Bay 6
SimPrep AutoDilution System	SimPrep	0122139A560/ Johnson, Lab 187, Bay 6
50 mL Plastic Digestion Tubes	Mold Pro/ MP-108PW	n/a
Analytical Balance (RTI Bal 291)	Mettler Toledo/ XP205	1128372296/ Johnson, Lab 268
Calibration Weight Set	Fisher Scientifics	A-263/ Johnson, Lab 268

Procedure: *RECORD WHICH SYSTEM IS BEING USED:*_____

- ☐ Rinse gloved hands with DI water and dry with KimWipe.
- ☐ Gather 22 empty 50 mL plastic digestion tubes and number each tube and corresponding cap.
- ☐ Calibrate the analytical balance using calibration weight set in accordance with SOP 100-EQP-004.5, "Calibration, Use and Maintenance of Balances"[1]. Take the mass of each empty tube, including cap, and record in table 1, 2, and 3 in "Mass of Tube" column.
- ☐ Fill the 2-liter plastic bottle used with the SimPrep auto dilution system with DI water directly from the Milli-Q system. Resistivity reading **must be 18.2 MΩ.**
- ☐ Purge the SimPrep autodilution system at least 5 times using the system software.
  - ○ **1 2 3 4 5**
- ☐ Program the autodilutor to dispense the current corrected volume for 20,000 microliters of DI water into tubes 1 and 2 and the current corrected volume for 25,000 microliters into tubes 3 and 4. Program in accordance with RTI SOP#IONS3 SOP "Filter Extraction via SimPrep Autodilution System"[2].
- ☐ Uncap tubes 1 to 4 and arrange in order in autosampler racks.
- ☐ Deliver the programed amounts of DI water into tubes 1 through 4 using the SimPrep by hitting start in the program.
- ☐ Cap tubes 1-4 with corresponding caps and use analytical balance to obtain the mass of the filled tubes. Record in Table 1 in "Mass of Tube and Water" column.

1

Analyst Signature: _____ Date: _____ Reviewer Signature: _____ Date: _____

Filename Demonstration of SIMPREP Performance Worksheet. V5_031125

Figure 1. Example of Demonstration of Autodilutor performance (page 1 of 4).

AUTODILUTOR PROFICIENCY WORKSHEET	RESEARCH TRIANGLE INSTITUTE POST OFFICE BOX 12194 RESEARCH TRIANGLE PARK, NC 27709-2194	DATE: _____ ANALYST: _____

- ☐ Calculate the "Volume of Water (D)" using the following equation and record value in Table 1:
  - "Volume of Water in µL (D)" = "[Mass of Tube and Water (C)" – "Mass of Tube (B)]*1000"
- ☐ Calculate the Volume Difference using the following equation and record values in Table 1:
  - "Volume Difference (E)" = "Simprep Volume Setting (D)" – 20000 µL (Target Volume of for tubes 1 and 2); = "simprep Volume Setting (D)" - 25000 µL (Target Volume of water for tubes 3 and 4).

TABLE 1: Determination of Accurate Simprep Settings – SYSTEM 1

	A	B	C	D	E	F
Tube Number	Current Corrected Simprep Volume Setting (uL)	Mass of Empty Tube (g)	Mass of Tube and Water (g)	Volume of Water (mL)	Volume Difference (uL)	Corrected Simprep Volume Setting (uL)
1						
2						
3						
4						

- ☐ Determine new SimPrep volume settings for 20,000 uL and 25,000 uL using the following equation:
  - "Corrected Simprep Volume Setting (F)" = "Simprep Volume Setting (A)" + "Volume Difference (E)"
- ☐ The final Corrected Simprep Volume Setting will be determined by the average of column F for the two tubes of each volume setting :
  - For 20,000 uL: $(F_1 + F_2)/2$
  - For 25,000 uL: $(F_3 + F_4)/2$

Record the results below:

SYSTEM 1:
Corrected Simprep Volume Setting for 20,000 uL:_____
Corrected Simprep Volume Setting for 25,000 uL:_____

- ☐ Program the autodilutor to dispense the "Corrected Simprep Volume Setting for 20,000 ul" of DI water into tubes 5-13 and the "Corrected Simprep Volume Setting for 25,000 uL" into tubes 14-22.
- ☐ Uncap tubes 5-22 and arrange in order in autosampler racks.
- ☐ Deliver the programed amounts of DI water into tubes 5 through 22 using the SimPrep by hitting start in the program.
- ☐ Cap tubes 5-22 with corresponding caps and use analytical balance to obtain the mass of the filled tubes. Record in Table 2 and 3 in "Mass of Tube and Water" column.
- ☐ Calculate the average and standard deviation for the volume of DI water dispensed at both the "Corrected 20,000 uL" setting and the "Corrected 25,000 uL" setting. Calculate the relative standard deviation (RSD) = standard deviation divided by the mean multiplied x 100. The RSD should not be greater than 5%. Record calculated results in appropriate spots below Table 2 and 3.

COMMENTS:

2

Analyst Signature: _____ Date: _____ Reviewer Signature: _____ Date: _____

Filename Demonstration of SIMPREP Performance Worksheet. V5_031125

Figure 2. Copy of Demonstration of Autodilutor performance page 2 of 4).

AUTODILUTOR PROFICIENCY WORKSHEET

RESEARCH TRIANGLE INSTITUTE
POST OFFICE BOX 12194
RESEARCH TRIANGLE PARK, NC 27709-2194

DATE: _____

ANALYST: _____

TABLE 2: Simprep System Check Corrected 20,000 Setting Volume Setting:_____uL

Tube Number	Mass of tube (g)	Mass of tube with water (g)	Volume of water (mL)
5			
6			
7			
8			
9			
10			
11			
12			
13			

Average: _____

Standard Deviation: _____

RSD:_____

TABLE 3: Simprep System Check Corrected 25,000 Setting Volume Setting:_____uL

Tube Number	Mass of tube (g)	Mass of tube with water (g)	Volume of water (mL)
14			
15			
16			
17			
18			
19			
20			
21			
22			

Average: _____

3

Analyst Signature: _____ Date: _____ Reviewer Signature: _____ Date: _____

Filename Demonstration of SIMPREP Performance Worksheet. V5_031125

Figure 3. Copy of Demonstration of Autodilutor Performance (page 3 of 4)

AUTODILUTOR PROFICIENCY WORKSHEET	RESEARCH TRIANGLE INSTITUTE POST OFFICE BOX 12194 RESEARCH TRIANGLE PARK, NC 27709-2194	DATE: _____ ANALYST: _____

Standard Deviation: _____

RSD:_____

COMMENTS:

References:

1. SOP 100-EQP-004, *Calibration, Use and Maintenance of Balances*, v6
2. SOP Ions #3, *Filter Extraction via SimPrep Autodilution System*, v3

4

Analyst Signature: _____ Date: _____ Reviewer Signature: _____ Date: _____

Filename Demonstration of SIMPREP Performance Worksheet. V5_031125

Figure 4. Demonstration of Autodilutor performance (page 4 of 4).

REVIEW AND REVISION HISTORY

Version	Describe Major Changes or Indicate "Reviewed with No Revisions"	Effective Date/ Review Date	New Review Date
1	Create new SOP for new Systems Installed 6/1/2022	6/1/2022	6/1/2023
2	Updated Worksheet for performance demonstration for autodilutor and assign SOP a number and performed general edits with formatting	6/7/2023	6/7/2024
3	Updated location of autodilutor, checks and provided clarity as needed and updated autodilutor performance worksheet example in appendix	12/19/2025	12/19/2026