APPENDIX B

NJ Drinking Water Quality Institute
Testing Subcommittee

Report on the Development of a Practical Quantitation Level for Perfluorooctanesulfonic Acid (PFOS) in Drinking Water

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Background

The New Jersey Department of Environmental Protection (NJDEP) perfluoroalkyl substances (PFAS) study of 2006 was initiated to determine the occurrence of perfluorooctanoic acid (PFOA) in New Jersey drinking water sources. The method used by the laboratory contracted for the study included the analysis of both PFOA and perfluorooctanesulfonic acid (PFOS). Of the 23 New Jersey drinking water systems monitored in the NJDEP 2006 PFAS study, 27% had quantifiable levels of PFOS in their drinking water sources or finished drinking water. The 2009 PFAS follow-up study determined the occurrence of PFOA, PFOS and eight additional PFASs in drinking water sources of 31 public water systems throughout New Jersey. In contrast to the 2006 PFAS study which was a targeted study for PFOA and included samples from both raw (untreated) and treated water sources, samples for the 2009 study were taken from 20 of the 21 counties and included only *untreated* water samples to determine source water occurrence for these parameters. In the 2009 study, 25% of the 31 public water systems sampled had PFOS levels greater than 5 ng/L in at least one of their drinking water sources.

In 2014, the New Jersey Drinking Water Quality Institute (DWQI) was tasked with recommending a Maximum Contaminant Level (MCL) for PFOS to the Commissioner of the NJDEP. This advisory panel comprised of 15 members from academia, regulated water systems, governmental agencies, and public health experts is responsible for providing MCL recommendations as part of the regulatory process in setting an MCL specific to New Jersey. The DWQI recommendations are a result of the collaboration of three DWQI Subcommittees: the Health Effects Subcommittee, the Treatment Subcommittee and the Testing Subcommittee. The Health Effects Subcommittee is responsible for recommending "health-based MCL[1]" levels for contaminants. The Treatment Subcommittee is responsible for evaluating the best available treatment technologies for removal of the contaminant from drinking water supplies. The Testing Subcommittee is responsible for developing Practical Quantitation Levels (PQL) for contaminants. A PQL is the minimum concentration for which the contaminant under review can be reliably quantitated within acceptable limits of uncertainty.

Developing a PQL involves researching analytical methods that are reliable and have the sensitivity to detect the contaminant at or as close as possible to the health-based MCL developed by the Health Effects Subcommittee. When developing a PQL, the Testing Subcommittee considers available analytical methods and laboratory performance. In 2008, the EPA published Method 537, revision 1.0 a solid-phase extraction and liquid chromatography/ tandem mass spectrometry

[1] Health-based MCLs are goals, not enforceable standards, similar to USEPA Maximum Contaminant Level Goals (MCLG). For carcinogens, health-based MCLS are set at levels that are not expected to result in cancer in more than one in one million persons ingesting the contaminant for a lifetime, and for non-carcinogens, at levels not expected to result in "any adverse physiological effects from ingestion" for a lifetime. The enforceable MCLs consider other factors such as analytical quantitation limits and availability of treatment removal technology and may be set higher than the MCLGs.

(LC/MS/MS) method for perfluorinated alkyl acids. Prior to the availability of EPA 537, laboratories developed proprietary methods such as SOP DEN-LC-0012 Rev. 4, the method developed by Test America Denver used for NJDEP's 2006 PFAS study. More recently, labs have made modifications to EPA 537 to enhance performance.

If the health-based MCL for a contaminant is known at the time of the PQL development, the Testing Subcommittee attempts to establish a PQL at a level less than that health-based MCL. This is not always feasible due to the limitations of analytical sensitivity. It is ultimately the performance data from robust analytical methods and accredited laboratories that determine the PQL if those methods exist or are in development due to the emerging nature of the environmental contaminant of interest the DWQI. In the current process of developing an MCL recommendation for PFOS, the health-based MCL and the PQL were developed simultaneously. As such, the PQL for PFOS recommended by the Testing Subcommittee in this document was derived solely on the performance data obtained from drinking water laboratories that met criteria established by the Testing Subcommittee for this purpose.

Data Sources for PQL Determination

The first step in the PQL development process was to compile data from drinking water laboratories with capable of quantitating PFOS at the concentration less than the 40 ng/L required by EPA for the Unregulated Contaminant Monitoring Rule 3 (UCMR3) UCMR3:

1) Laboratories that performed analysis for the NJDEP PFAS studies of 2006 and 2009 and follow-up monitoring of water systems;
2) Laboratories that are certified for the analysis of PFOS in drinking water by the NJDEP Office of Quality Assurance (NJDEP/OQA) using NJDEP/OQA approved methods called Department Sanctioned Analytical Methods (DSAMs[2]); and
3) National laboratories that had obtained US Environmental Protection Agency (EPA) approval to analyze PFASs (including PFOS) under theUCMR3 program using EPA Method 537 and that had demonstrated that they are capable of reporting PFOS lower than the required UCMR3 minimum reporting level (MRL) of 40 ng/L.

Performance data compiled from these three data sources was used to determine the PQL for PFOS.

1) The NJDEP PFAS Database:

The NJDEP PFAS Database was originally designed to house the results of the NJDEP 2006 and 2009 PFAS studies. At the time that these studies were performed, the laboratories and methods which generated the study data were reviewed and certified by the NJDEP/OQA by both the NJDEP/OQA. , PFAS results from public water systems conducting their own PFAS monitoring were added to this database. Public water system data include follow-up testing results based on recommendations made by the NJDEP because of findings of the 2006 and 2009 studies and data from water systems

[2] DSAMs are methods that laboratories may be certified to perform if they quality under the requirements of the Regulations Governing the Certification of Laboratories and Environmental Measurements (N.J.A.C. 7:18)

that voluntarily initiated PFAS testing. Several New Jersey drinking water purveyors also supplied PFAS treatment efficiency data from their unit operations (Granular Activated Carbon contactors) that were added to the ground water treatment train at water treatment facilities where PFAS contamination was detected.

The NJDEP PFAS database contains approximately 1000 PFOS results, 33% of which were generated by Test America-Denver STL-Denver, 20% by MWH Laboratories, 40% by Eurofins Eaton Analytical and 7% by Underwriters Laboratories. Since this database was established, several laboratories have been acquired or have merged: Severn Trent Laboratory (STL-Denver) became Test America-Denver in 2007; Montgomery Watson Haworth (MWH) Laboratories became Eurofins Eaton Analytical (California) in 2012, and part of the Underwriters Laboratory in South Bend, Indiana became Eurofins Eaton Analytical, Inc. (Indiana) in 2014. Therefore, Test America-Denver (Colorado) analyzed 33% of the test results in the database, Eurofins Eaton Analytical (California) analyzed 60%, and Eurofins Eaton Analytical (Indiana) analyzed 7%.

In 2006, PFASs such as PFOA and PFOS were considered emerging contaminants and few laboratories had developed analytical methods with low levels of sensitivity. In preparing for the 2006 PFAS occurrence study, the BSDW requested that NJDEP/OQA review the available methods and choose an acceptable method for the analysis of the drinking water samples. The NJDEP/OQA reviewed the analytical method developed by Test America (DEN-LC 0012 Rev 4) and approved it as a DSAM. While the focus of the 2006 study was PFOA, the STL-Denver (Test America-Denver) proprietary method could analyze for both PFOA and PFOS where the Reporting Limit (RL) and low calibration standard for both were 10 ng/L and 4 ng/L, respectively.

By 2009 there were additional PFAS drinking water methods available. MWH Labs in Monrovia California developed a proprietary method that was capable of reporting PFOA, PFOS, PFNA, PFBS and 5 other PFASs to 5 ng/L. This proprietary method called MWH PFC Extra was officially MWH SOP-HPLC 12 and was approved by the NJDEP/OQA as a DSAM. MWH Labs was contracted for analysis of the 2009 PFAS drinking water samples using the MWH PFC Extra method.

Based on the results the of the NJDEP 2006 and 2009 PFC studies, the NJDEP recommended that those water systems found to have PFOA and/or PFOS in their drinking water conduct follow-up testing within each quarter of the calendar (or every three months) for a year. Letters from NJDEP to water systems following the 2006 and 2009 PFAS studies included a recommendation to use a method certified by the NJDEP/OQA (DSAM).

Test America-Denver

The NJDEP selected STL-Denver (Test America-Denver) for the 2006 PFAS study. STL-Denver's proprietary method, SOP DEN-LC-0012 Revision 4, used a RL of 10 ng/L for PFOS. The lowest PFOS calibration standard was 4 ng/L.

In February 2009, Revision 7 of the Test America-Denver SOP, DEN-LC-0012, included 14 additional PFAS compounds on the analyte target list. Although Revision 7 of SOP DEN-LC-0012 expanded the capability of Test America-Denver to analyze and report 16 PFASs, in

many cases only PFOA and PFOS results were reported based upon instructions provided to the laboratory by the water system (client).

Test America-Denver analyzed New Jersey water system drinking water samples from 2006 to 2013, during which time several different revisions of the method were used. Revision 4 was used for the 2006 PFAS study; the most recent version used was Revision 12.[3] Table 1 shows that over the course of seven years, Test America-Denver reported PFOS data using different RLs with the most frequently occurring RL in the PFAS database being 10 ng/L. This RL in addition to the lowest calibration standard of 4 ng/L used in the 2006 PFAS study (where the actual laboratory reporting limit was 10 ng/L) are the values selected from the NJDEP database to represent Test America-Denver's performance data in the consideration of a PQL value (see Table 2).

Table 1.
Test America Denver PFOS Data from the NJDEP Historical Database using their Proprietary Method, SOP DEN-LC 0012
June 2006 to August 2013

Reporting Limit (ng/L)	% of Results	Method Detection Limit (ng/L)	% of Results
30	12	13	2
10	77	10	4
4	11	1.6	9
		2	49
		0.5	36

MWH Laboratory

The analytical method used for the 2009 NJDEP PFAS study was a proprietary method developed by MWH Laboratories. This proprietary method, MWH SOP-HPLC 12, is also referred to as MWH PFC Extra. This method was approved by NJDEP/OQA and offered lower reporting limits for the PFASs of concern. The MWH PFC Extra method includes PFOS, PFOA, PFNA and seven other PFASs. The MWH-PFC Extra RL for PFOS was 5 ng/L. Eurofins Eaton Analytical (formally MWH Labs) also offers the method MWH PFC which

[3] The revision number of the method was not noted in the PFA database. However, if needed, this could be determined based on the date of the analysis. The solid phase extraction method used to prepare the water samples for analysis exists as a stand-alone extraction method (DV-OP-0019).

analyzes PFOA, PFOS and PFNA using the same RLs as in MWH PFC Extra. The MWH PFC Extra method was recently renamed EEA LCMS-SOP2434 by Eurofins Eaton Analytical.

Underwriters Laboratory

Several water systems used Underwriters Laboratory for their follow up testing. PFC proprietary method L400 was developed by Underwriters Laboratory and was capable of reporting both PFOS and PFOA to 10 ng/L. (The official name for L400 was UL-SBN-LCMS-013-03 and subsequently, 06-LO-S0442). Underwriters Laboratory was certified by NJDEP/OQA for analysis of PFOS and PFOA by L400 until 2014 when Eurofins purchased the South Bend, Indiana Underwriters Laboratory. Eurofins Eaton Indiana no longer utilizes the Underwriter's L400 method.

Table 2 provides a summary of PFOS laboratory information obtained from the three laboratories in the NJDEP PFAS database that performed most of the PFAS analyses between June 2006 and August 2017. It includes analytical methods, RLs, method detection limits (MDLs), and the number of analyses performed with those RLs/MDLs by three laboratories.

An MDL is defined as the minimum concentration of a substance that can be reported with 99% confidence that the analyte concentration is greater than zero (or present in the drinking water sample). Usually laboratories report analytical results based on the MDL and RL for the analyte. A RL is a concentration used by a laboratory for reporting quantifiable detections of an analyte in a sample. It is a concentration equal to or greater than the lowest calibration standard used in the calibration of the instrument. Any reported concentration that is at or above the reporting limit is considered a valid quantified result for the analyte. If the reported concentration is at or greater than the MDL but less than the reporting limit, the reported concentration will be an estimated value and should be qualified as such on the laboratory report.

Table 2.
Laboratories/Methods with Reporting Limits and MDLs from the NJDEP PFC Database
PFOS Data from the NJDEP Historical Database[4] June 2006 to August 2017

Laboratory	Method	Reporting Limit (ng/L)	MDL (ng/L)	# of Analyses
Test America Denver	SOP DEN-LC-0012	4	NP*	32
		10	0.5, 2	258
		30	1.5, 10	37
Underwriters Laboratories	L400	10	NP	66
MWH Laboratories /Eurofins Eaton Analytical CA	EPA 537 PFAA	2.5	NP	290
	MWH PFC /PFC EXTRA	5	NP	307

*NP =Information not provided in the PFAS database.
* The most frequent reporting limit of Test America Denver in NJDEP PFAS database (see Table 1).

[4] The laboratories presented in this table are those that analyzed samples for the NJDEP PFA occurrence studies and those that analyzed follow up samples for those water systems that had detections of PFAS in the NJDEP occurrence studies. This does not include all laboratories capable of performing PFAS analysis, only those that analyzed New Jersey public water systems samples during June 2006-August 2017.

2) NJDEP/OQA Sanctioned Methods and Laboratories Certified to Report PFOS in Drinking Water

There are currently three drinking water analytical methods that have been approved by NJDEP/OQA as DSAMs for the analysis of PFOS in drinking water: EPA 537 and two proprietary methods, DV-LC-0012 Rev 14 (developed and used by Test America-Denver) and EEA LCMS-SOP2434 used by Eurofins Eaton Analytical. The three DSAMs are similar in that they utilize solid phase extraction, isotope dilution and electrospray ionization with LC/MS/MS.

The method developed by EPA for the analysis of PFAS is EPA 537 "Determination of Selected Perfluorinated Alkyl Acids in Drinking Water by Solid Phase Extraction and Liquid Chromatography/Tandem Mass Spectrometry (LC/MS/MS)" Rev. 1.0. EPA 537 allows laboratories to modify the sample enrichment technique, the separation technique, the LC column, the mobile phase composition, LC conditions, the MS and MS/MS conditions to improve selectivity, resolution, and sensitivity provided that the laboratory documents the modifications and provides method performance information. Other changes, such as use of different extraction volumes, is not allowed and would require the lab to consider the modified EPA 537 a proprietary method. Since 2006, several laboratories have petitioned the NJDEP/OQA and have obtained approval for their proprietary methods to be listed as approved methods for use in New Jersey (DSAMs).

There currently are ten labs that have NJDEP/OQA certification to analyze PFOS in drinking water using EPA 537. These are:

- American Water Central Laboratory (Illinois)
- Eurofins Eaton Analytical Inc. (California)
- Eurofins Lancaster Labs Environmental (Pennsylvania)
- Eurofins Eaton Analytical Inc. (Indiana)
- SGS Accutest Inc. (Orlando, FL)
- Vista Analytical Laboratory
- Pace Analytical Services, LLC (Ormond Beach, FL)
- SGS North America Inc. (North Carolina)
- GEL Laboratories, LLC (South Carolina) and
- Test America (Sacramento, CA)

Table 3 lists these 10 laboratories performing EPA 537 (plus 2 additional methods) with the associated RLs, MDLs and low calibration standards, plus an additional laboratory that only runs a DSAM (Test America-Denver).

In EPA 537, the minimum reporting level (MRL) is a standard for reporting analytical results. EPA 537 describes the MRL as the minimum concentration that can be reported as a quantitated value for a method analyte in a sample following analysis. It is a defined concentration that can be no lower than the concentration of the lowest calibration standard for that analyte and can only be used if acceptable quality control (QC) criteria for this standard are met. The MRL description is like that of a reporting limit, however there are additional quality control requirements associated with the MRL. The accuracy and precision of the reporting limit within most analytical methods is

usually validated with quality control calibration checks and laboratory fortified blanks. The EPA 537 MRL is an RL that requires additional quality control criteria to be met such as a confirmation MRL procedure in Section 9.2.5 of EPA 537. This allows labs to use a different MRL for reporting PFOS results provided that the lab can demonstrate through successfully completing the quality control procedures using that MRL.

In Table 3, the RL of those labs certified for EPA 537, is an MRL. In six out of the ten EPA 537 labs, the lowest calibration standard is lower than their MRL. This indicates that, if necessary, these labs may be able to lower their MRL. If the analytical sensitivity is an issue (e.g., the criteria, if known, is less than the derived PQL), the NJDEP reserves the right to utilize the low calibration data as a PQL because it meets the known quality criteria established for a quantifiable analytical result.

3) UCMR3 EPA-Approved Laboratories for PFAS Analysis

The Unregulated Contaminant Monitoring Rule (UCMR) is a national monitoring program administered every five years by the EPA in which all community water systems serving a population of 10,000 and over, and 800 small water systems selected by the EPA, throughout the country are required to test their drinking water for a specific set of 30 unregulated contaminants. The UCMR analytes are usually chosen from the corresponding EPA Candidate Contaminant List (CCL) as was the case with the selection of most of the analytes for the third round of UCMR sampling (UCMR3). Besides PFOA and PFOS, the UCMR3 includes four additional PFCs - perfluorononanoic acid (PFNA), perfluorohexane sulfonate (PFHxS), perfluoroheptanoic acid (PFHpA), and perfluorobutane sulfonate (PFBS) - in the UCMR3 List 1 Assessment Monitoring.

The Testing Subcommittee identified the UCMR3 participating laboratories as a potential source of information to access for consideration in the PFOS PQL determination. As part of the UCMR3 rule, laboratories performing analyses for any of the UCMR3 contaminants were required to obtain approval from the EPA. NELAP or state certification was not required for the laboratories participating in the UCMR3 but they had to meet several EPA approval requirements such as proficiency testing and on-site audits. EPA required analytical method Version 1.1 of EPA 537 published in 2009 for the analysis of PFOS and the five other PFASs for the UMCR3. UCMR3 results for PFOS were to be reported to an MRL of 40 ng/L.

The EPA derived MRL of 40 ng/L for PFOS is only required for analyses conducted for the UCMR3. Depending on the needs of the client, the method allows a laboratory to use a different MRL provided that the MRL QC is met at that concentration. For example, in addition to the MRL of 40 ng/L for PFOS offered for UCMR3 clients, Eurofins Eaton Analytical-California also offers an MRL of 2.5 ng/L. These client driven reporting limits must be evaluated by the drinking water program when considering the target objective of quantifying parameters at or below the human health criteria developed by the Health Effects Subcommittee to be protective for the citizens of New Jersey but also provide a base of occurrence data that is valid at this lifetime exposure level.

Table 3.
New Jersey Laboratories Certified by NJDEP/OQA
For PFOS in Drinking Water

NJDEP/OQA Certified Lab	Location (State)	DSAM	Reporting Limit (ng/L)	Lowest Calibration Standard (ng/L)	MDL (ng/L)
American Water Central Laboratory	IL	EPA 537	5	5	1.4
Eurofins Eaton Analytical, Inc.	CA	EPA 537	2.5	2.4	0.717
Eurofins Eaton Analytical, Inc.	CA	EEA LCMS-SOP2434	5	4.79	3.664
Eurofins Eaton Analytical, Inc.	IN	EPA 537	2	2	0.5
Eurofins Lancaster Labs Environmental	PA	EPA 537	5	4	2
GEL Laboratories, LLC	SC	EPA 537	2	2	0.66
Pace Analytical Services, LLC Ormond Beach FL	FL	EPA 537	40	4	1.3
SGS Accutest Inc. - Orlando	FL	EPA 537	8	3.2	2
SGS North America Inc.	NC	EPA 537	2	2	0.2
Test America Denver	CO	DV-LC-0012 Rev 14	30	4	1.12
Test America Sacramento	CA	EPA 537	40	4	6.8
Vista Analytical Laboratory	CA	EPA 537	10	1	1.04

NR=Not Required.

The EPA's goal in developing this MRL was to establish a reporting concentration where laboratories across the nation would be able to reliably analyze PFASs for the UCMR3 during the proficiency evaluation. When discussing the MRLs for the six UCMR3 PFASs, the EPA states in the May 2, 2012 Federal Register, "While particular laboratories may be able to meet MRLs lower than those proposed, the selected MRLs reflect those achievable by the national array of laboratories that support the program."

The EPA determination of 40 ng/L as the MRL to use for UCMR3 was statistically determined from three laboratories' Lowest Concentration MRLs (LCMRL) which were generated using the procedure described in the Environmental Science Technology article, *Statistical Procedures for Determination and Verification of MRLs for Drinking Water Methods* (Winslow et. al., 2006). The LCMRL is defined as the lowest spiking concentration at which recovery of between 50 and 150% is expected 99% of the time by a single analyst. The EPA determined the MRL using a Bayesian bootstrap of the LCMRL study data from each of three experienced drinking water laboratories. The Bayesian bootstrap replicates that were generated from each laboratory's data, serve to estimate the distribution of estimated LCMRL values that each laboratory might generate on repeated performance of the LCMRL study. The distribution of pooled Bayesian bootstrap replicates, generated from the LCMRL study data from a sample of experienced drinking water laboratories, approximates the distribution of estimated LCMRL values which might be generated from the *population* of experienced drinking water laboratories. The EPA statistical software, the LCMRL Calculator, performing this process was designed such that the MRL would be an estimate of the LCMRL that is achievable with 95% confidence by a capable analyst/laboratory at least 75% of the time.[5] For PFOS, three laboratory LCMRLs of 13 ng/L, 7.2 ng/L and 48 ng/L were integrated into the EPA statistical software resulting in the MRL of 40 ng/L.

In 2016 the NJDEP, on behalf of the DWQI Testing Subcommittee, conducted a phone inquiry of the EPA laboratories approved for PFAS analysis for the UCMR3 to determine if any of these laboratories were using PFOS reporting limits less than 40 ng/L for purposes other than the UCMR3. Of the 20 UCMR3 participating laboratories solicited for information,

- five stated that they are reporting PFOS lower than 40 ng/L;
- five stated either that they were in the process of lowering the reporting limit or were confident that they could achieve lower reporting limits if requested;
- three laboratories conducted low level calibrations or MRL confirmations proving that they could achieve MRLs for PFOS lower than 40 ng/L in response to our inquiry;
- five stated that they do not report lower than 40 ng/L;
- two labs did not respond.

Listed in Table 4 are those UCMR3 participating laboratories contacted through the phone inquiry capable of reporting PFOS less than 40 ng/L. To report to concentrations less than 40 ng/L several

[5] Technical Basis for the Lowest Concentration Minimum Reporting Level (LCMRL) Calculator (EPA 815-R-11-001). http://water.epa.gov/scitech/drinkingwater/labcert/analyticalmethods_ogwdw.cfm

of these laboratories use a modified EPA 537 method or a proprietary method (as indicated in Table 4) rather than EPA 537. Laboratories using EPA 537 did not always provide an MDL since it is an optional study in EPA 537.

The following data was provided through the phone inquiry conducted in 2016. Since that time, more recent data has been acquired for most of these labs which are reflected in the other tables within the document.

Table 4.

UCMR3 Laboratories using PFAS Analytical Methods with Reporting Limits or Low Calibration Standards Lower than 40 ng/L for PFOS

UCMR3 Participating Laboratory	State	Analytical Method	Reporting Limit (ng/L)	Low Calibration Standard	MDL (ng/L)
Advanced Water Quality Assurance Lab	CA	EPA 537	4	4	NR
American Water Central Laboratory	IL	EPA 537	2	2	0.345
Columbia Analytical Services ALS	WA	Modified EPA 537	2	2	0.60
Eurofins Eaton Analytical	CA	EPA 537	2.5	2.5	0.2
Eurofins Eaton Analytical	CA	MWH-PFC Extra	5	5	0.239
Eurofins Eaton Analytical	IN	EPA 537	4	4	0.493
State Hygienic Laboratory-Coralville	IA	EPA 537	39	15.7	NR
Test America- Sacramento	CA	WS-LC-0025 Rev 1.2	2	2	1.28
Weck Laboratories	CA	Modified EPA 537	5	5	2.33

NR=Not Required.

The variability of the reporting limits that UCMR3 labs are capable of achieving with EPA 537, modifications of EPA 537 and proprietary methods shows that the current reporting limits being used for PFOS are mostly client driven. It is likely that if requested, several of these laboratories would be able to accommodate a PFOS reporting limit lower than the 40 ng/L MRL required with the UCMR3.

PQL Determination

In developing the PQL for PFOS, the DWQI Testing Subcommittee considered the RLs, low calibration standards, and MDLs from laboratories meeting at least one of the criteria below:

1) The laboratories that analyzed water samples for PFOS in the NJDEP 2006 and 2009 studies and follow-up sampling by water systems;

2) Laboratories currently having NJDEP/OQA approval for analysis of PFOS in drinking water for New Jersey using methods have that have been approved as Department Sanctioned Analytical Methods (DSAMS); and
3) Laboratories that are EPA UCMR3 approved using PFAS methods and are capable of reporting PFOS lower than the UCMR3 MRL of 40 mg/L and that have been vetted by the NJDEP/OQA, NELAP or EPA.

Table 5 consolidates the RL, the low calibration standard and MDL data from Tables 2, 3 and 4. The last column in Table 5 indicates the source of the data being considered and which is designated as 1, 2 or 3 based on the criteria described above. Test America-Sacramento and Pace Analytical Services - Florida are included in Table 5 because while their MRL is not lower than 40 ng/L, they are NJDEP/OQA certified labs for which New Jersey public water systems can select for their PFOS analyses. Other than the MRL of 40 ng/L developed by EPA, there are presently no other reporting requirements for PFOS.

Prior to a Lifetime Health Advisory issued by EPA in May 2016 for a combined PFOA and PFOS concentration of 70 ng/L,[6] the EPA had published Provisional Health Advisories for PFOA and PFOS of 0.4 µg/L (400 ng/L) and 0.2 µg/L (200 ng/L) respectively, in January 2009, which did not provide laboratories with an incentive to detect low level concentrations of PFOA and PFOS. However, in the 2006 study and in follow-up monitoring of New Jersey water systems, detection limits of 10 ng/L were commonly reported showing that since 2006, laboratories have been capable of using reporting limits less than 40 ng/L for PFOS.

As seen in Table 5, there is very little difference between the average (mean) and the median of the low calibration standards. However, there is a large difference between the mean and median of the reporting limits. The large statistical spread of the data in indicates that the RL does not represent the capability of the laboratory and supports the fact that the some of the reporting limits are client driven.

[6] https://www.epa.gov/ground-water-and-drinking-water/drinking-water-health-advisories-pfoa-and-pfos

Table 5.
Consolidation of Performance Data from
Laboratories Meeting Established Criteria for Determining the PQL[7]

Laboratory	State	Method	RL (ng/L)	Low Calibration Standard (ng/L)	MDL (ng/L)	Source[8]
Advanced Water Quality Assurance Laboratory	CA	EPA 537	4	4	NR	3
American Water Central Laboratory	IL	EPA 537	5	5	1.4	2
Columbia Analytical Services	WA	Modified EPA 537	2	2	0.60	3
Eurofins Eaton Analytical	CA	EEA LCMS-SOP2434	5	4.8	3.664	2
Eurofins Eaton Analytical	CA	EPA 537	2.5	2.4	0.717	2
Eurofins Eaton Analytical	IN	EPA 537	2	2	0.5	2
Eurofins Lancaster Laboratories Environmental	PA	EPA 537	5	4	2	2
GEL Laboratories, LLC	SC	EPA 537	2	2	0.66	2
Pace Analytical Services Inc. Florida	FL	EPA 537	40	4	1.3	2
SGS Accutest – Orlando	FL	EPA 537	8	3.2	2	2
SGS North America Inc.	NC	EPA 537	2	2	0.2	2
State Hygienic Laboratory- Coralville	IO	EPA 537	39	15.7	NP	3
Test America-Denver	CO	DV-LC-0012 Rev 4	10	4	2	1
Test America-Denver	CO	DV-LC-0012 Rev 14	30	4	1.12	2
Test America-Sacramento	CA	EPA 537	40	4	6.8	2
Test America-Sacramento	CA	Proprietary WS-LC-0025 Rev 1.2	2	2	1.28	3
Underwriters Laboratory	IN	L400	10	0.5	0.35	1
Vista Analytical Laboratory	CA	EPA 537	10	1	1.04	2
Weck Labs	CA	Modified EPA 537	5	5	2.33	3
Mean			**11.8**	**3.8**		
Median			**5**	**4**		

NP= Not Provided; NR=Not Required.

[7] Table 5 is a consolidation of Table 2: PFOS Reporting Limits and MDLs from Laboratory Data in the NJDEP PFC Database, Table 3: Laboratories Certified by NJDEP Office of Quality Assurance for Analysis of PFOS Reporting Limit and MDL Information Acquired by Phone or Email (2016) and Table 4: UCMR3 Laboratories with Reporting Limits Lower than 40 ng/L.

[8] See the paragraph above for a description of the sources of the laboratory performance data.

Determination of the PQL using MDLs

The determination of the PQL using MDLs requires a sample size of at least five MDLs from which to obtain an inter-laboratory MDL value. The individual MDL value from each laboratory for a given method is used to obtain a median MDL value as a representative inter-laboratory MDL. This inter-laboratory MDL is then multiplied by a factor of five. In 1993, a research project was conducted by NJDEP to determine if the MDL multiplied by a certain factor could yield a supportable PQL value. The outcome of this research concluded that a factor of 4, 5 or 6 could be used to derive a PQL (Eaton, et. al., 1993). In 1994, the Testing Subcommittee chose to use a multiplier of five to determine the PQLs generated as part of the DWQI MCL contaminant recommendations. This multiplier approach for determination of a PQL is also consistent with that outlined in the Ground Water Quality Standards (N.J.A.C. 7:9-6).

For PFOS, the Testing Subcommittee derived a PQL from a sample size of 17 MDLs, from 15 laboratories and 7 different methods. Two of the 19 laboratories in Table 6 did not provide MDLs, as this is not required by EPA 537. As seen in Table 6 the median MDL value of these 17 MDLs is 1.3 ng/L. This median value when multiplied by 5 is 6.5 ng/L.

Table 6.
Laboratory Reported MDLs in order of Increasing Values[9]

Laboratory	Analytical Method	MDL (ng/L)
SGS North America Inc.	EPA 537	0.2
Underwriters Laboratory	L400	0.35
Eurofins Eaton Analytical-IN	EPA 537	0.5
Columbia Analytical Services	Modified EPA 537	0.60
GEL Laboratories, LLC	EPA 537	0.66
Eurofins Eaton Analytical-CA	EPA 537	0.717
Vista Analytical Laboratory	EPA 537	1.04
Test America-Denver	DV-LC-0012 Rev 14	1.12
Test America-Sacramento	Proprietary WS-LC-0025 Rev 1.2	**1.28**
Pace Analytical Services, Inc.	EPA 537	1.3
American Water Central Laboratory	EPA 537	1.4
SGS Accutest – Orlando	EPA 537	2
Eurofins Lancaster Laboratories Environmental	EPA 537	2
Test America-Denver	DV-LC-0012 Rev 4	2
Weck Laboratories	Modified EPA 537	2.33
Eurofins Eaton Analytical-CA	EEA LCMS SOP 2434	3.664
Test America-Sacramento	EPA 537	6.8
Median of the MDLs		**1.3**
PQL = Median of MDLs x 5		**6.5**

[9] Two of the 19 laboratories listed in Table 5 did not provide MDLs, as this calculation is not required of labs performing EPA 537. Seventeen MDLs are listed on this table

Determination of PQL Using Minimum Reporting Levels

Analytical reporting standards based on multiples of the standard deviation, such as the MDL, do not account for non-ideal instrumental and analytical occurrences of interference, analyte degradation, matrix enhancement and background contamination which can, particularly at low concentrations, contribute to false positive and false negative results. The MDL is a statistically derived value where the procedure requires that precision criteria be met. EPA 537 does not require the MDL study to be performed but instead requires the completion of the MRL confirmation procedure. While the MDL is optional within the method, the method does indicate that the MDL may be required based on the state regulations. According to EPA 537, "While an MDL determination is not a specific requirement of the method, it may be required by various regulatory bodies associated with compliance monitoring."

The MRL in EPA 537 differs from an MDL in that it accounts for both accuracy and precision as a quantitation level. Laboratories using EPA 537 report results to a MRL which is a concentration equal to or greater than the lowest calibration standard, but must also meet the QC criteria at Section 9.2.5 of EPA 537. This criterion is a verification of laboratory proficiency at the laboratory's designated MRL. EPA 537 does not require laboratories to perform the previously discussed LCMRL procedure, but does require this less rigorous MRL confirmation. Both the LCMRL procedure and the confirmation MRL procedure account for the combined effect accuracy and precision have on these quantitation levels.

As mentioned previously, an MRL can be established either by the laboratory for their own specific purpose or by a regulatory agency such as the required MRL of 40 ng/L for the EPA UCMR3 program. Since EPA 537 describes the MRL as the lowest analyte concentration that meets the Data Quality Objectives developed for the intended use of this method, the MRL is an important factor in determining the PQL for PFOS. It would follow that, in addition to using inter-laboratory MDLs, the PQL should be assessed by considering the MRLs from laboratories that use EPA 537 for the analysis of PFOS in drinking water.

In addition to the laboratory performance data presented in Table 5, the laboratory performance data for labs using EPA 537 is seen in Table 7. The median of the MRLs for the 12 labs using EPA 537 in Table 7 is 5 ng/L. The MRLs used by labs is largely influenced by the needs of the client. The two labs in Table 7 with MRLs of 40 ng/L were analyzing PFASs for the UCMR3 however, they also used a low calibration standard of 4 ng/L. This low calibration standard would indicate that these labs would most likely be capable of lowering their MRL if needed. The median of the low calibration standards from Table 7 is the same (4 ng/L) as the median of the low calibration standards for the list of labs in Table 5 that comprise those using either EPA 537 or proprietary methods. Therefore, the median of the low calibration standard used by these 12 labs using EPA 537, 4 ng/L, was used for consideration of the PQL. The average of the low calibration standards was 4.1 ng/L.

PFAS such as PFOS have not been regulated by the EPA, however six PFAS were included in the UCMR3 and the EPA issued a Lifetime Health Advisory in May 2016 for a combined PFOA and PFOS concentration of 70 ng/L. For this reason the performance data of those labs using EPA 537 were

reviewed separately. EPA 537, as an EPA developed method for PFAS, was required for the UCMR3 and most likely would become an approved method should any of the target PFCs in the method become federally regulated. In this case for New Jersey any proprietary methods that are NJDEP DSAMS would be required to apply to the EPA as an alternate test method and would be unable to be used for compliance purposes until the EPA approval was obtained.

Table 7
Performance Data from Laboratories
Using EPA 537

Laboratory	Method	MRL (ng/L)	Low Calibration Standard (ng/L)	MDL (ng/L)
Advanced Water Quality Assurance Laboratory	EPA 537	4	4	NR
American Water Central Laboratory	EPA 537	5	5	1.4
Eurofins Eaton Analytical California	EPA 537	2.5	2.4	0.717
Eurofins Eaton Analytical Indiana	EPA 537	2	2	0.5
Eurofins Lancaster Laboratories Environmental	EPA 537	5	4	2
SGS North America Inc.	EPA 537	2	2	0.2
Pace Analytical Services Inc. Florida	EPA 537	40	4	1.3
SGS Accutest – Orlando	EPA 537	8	3.2	2
State Hygienic Laboratory-Coralville	EPA 537	39	15.7	NP
GEL Laboratories, LLC	EPA 537	2	2	0.66
Test America-Sacramento	EPA 537	40	4	6.8
Vista Analytical Laboratory	EPA 537	10	1	1.04
Mean		**13.3**	**4.1**	
Median		**5**	**4**	

Determination of PQL Using Reporting Limits or Low Calibration Standards

In most cases proprietary methods such as those sanctioned by the NJDEP/OQA were developed prior to the publication of EPA 537 and do not include the MRL confirmation procedure. Several laboratories not certified by the NJDEP/OQA, however, voluntarily provided details on their proprietary methods. Each of the proprietary methods required confirmation of the reporting limit within the analytical batch analysis. Two different reporting limits were considered for Test America-Denver since the data were generated using different versions of the original method. The median of the reporting limits of the nineteen RLs used by labs in Table 5 is 5 ng/L.

As previously stated, since the RLs are mostly client driven, it is not obvious from the reporting limits alone that greater sensitivity can be achieved. When considering both EPA 537 and proprietary methods, the laboratories' low calibration standard can be considered when it is lower than the reporting limit or MRL in the PQL assessment. The median of the low calibration standards of those labs only using EPA 537 (Table 7) and the median of the low calibration standards of the nineteen labs using either EPA 537 or proprietary methods (Table 5) are both 4 ng/L. The calculated average (mean) of the low calibration standards used by labs only using EPA 537 (Table 7) was determined to be 4.5 ng/L while that of the nineteen labs using EPA 537 or proprietary methods was 3.8 ng/L (Table 5). This indicates that whether the lab is using EPA 537 or a proprietary method, it is very possible that a lower reporting limit can be offered by the lab if offered by a client.

Bootstrap Estimate of a Confidence Interval of a Mean

Basic statistics were used to determine the median of the 17 MDL values in Table 6. The minimum criteria of five laboratories was met for the PQL calculation using the median of the MDLs and the value was determined to be 6.5 ng/L following the convention of multiplying the inter-laboratory MDL value of 1.3 ng/L (rounded to two significant figures) by a factor of five (5).

Another approach that has been used most recently by the EPA for LCMRL range calculation is a statistical technique called "Bootstrap Estimate of a Confidence Interval of the Mean." This technique was applied to generate a normal distribution and associated 95 % upper and lower confidence intervals from the a) inter-laboratory MDL values from Table 6 and b) the RLs or c) the low calibration standards from Table 5. The bootstrap calculations were extended to the results of the laboratories using EPA 537 from d) their MRLs and e) their low calibration standards from Table 7.

a) Bootstrap Analysis using Inter-laboratory MDLs

A bootstrap analysis of the MDL data presented in Table 6 resulted in a distribution where the upper confidence limit for MDL values reported by laboratories was 2.5 ng/L. The results of this data analysis are shown below in Table 8.

Table 8.
Bootstrap Estimate of Inter-laboratory MDLs

Lower Confidence Limit (ng/L)	Mean (ng/L)	Upper Confidence Limit (ng/L)	Confidence Level Range	Number of Randomly Selected Values[10]
1.0	1.6	2.5	95%	2000

Two laboratories reported MDL values above the upper confidence limit of 2.5 ng/L and were not included in a second iteration of the bootstrap analysis. The second iteration bootstrap

[10] The Bootstrap Technique uses a default value of 2000 iterations to calculate the statistics presented.

analysis resulted in a distribution where the upper confidence limit was 1.5 ng/L. These data are presented in Table 9.

Table 9.
Second Iteration: Bootstrap Estimate of Inter-laboratory MDLs
(Excluding two laboratories with MDLs above the UCL of 2.5 ng/L)

Lower Confidence Limit (ng/L)	Mean (ng/L)	Upper Confidence Limit (ng/L)	Confidence Level Range	Number of Randomly Selected Values[11]
0.9	1.2	1.5	95%	2000

Four additional laboratories reported an MDL above the upper confidence limit of 1.5 ng/L value and were not included in a third iteration of the bootstrap analysis. The third iteration bootstrap analysis resulted in a distribution where the upper confidence limit was 1.1 ng/L. These data are presented in Table 10.

Table 10.
Third Iteration: Bootstrap Estimate of Inter-laboratory MDLs
(Excluding six laboratories with an MDL above the UCL of 1.5 ng/L)

Lower Confidence Limit (ng/L)	Mean (ng/L)	Upper Confidence Limit (ng/L)	Confidence Level Range	Number of Randomly Selected Values[11]
0.6	0.8	1.1	95%	2000

Using the 95% upper confidence level from the bootstrap method, a PQL value (5 times the Upper Confidence Limit of the MDL) can be calculated following the regulatory convention that has been used by the NJDEP in the past. This value would be 1.1 ng/L x 5 which would be 5.5 ng/L. This MDL value and the PQL calculated from this value is achievable by 95% of the laboratory community that voluntarily provided the performance data presented in this recommendation.

b) Bootstrap Analysis using MRLs or Reporting Limits

To incorporate more recent techniques of calculating quantification levels, the bootstrap technique can also be applied to evaluate the consistency of the 19 laboratory reporting limits (RLs) found in Table 5. This generated a distribution of 2000 randomly selected values and produced an upper confidence limit of 18.4 ng/L as a reporting limit that 95% of the laboratory community should be able to achieve. The data generated by this bootstrap analysis is in Table 11. Two of these labs use the MRL of 40 ng/L required in the UCMR3 as their RL while their low calibration standard is an order of magnitude lower indicating that, if needed, these labs would

[11] The Bootstrap Technique uses a default value of 2000 iterations to calculate the statistics presented.

be able to demonstrate use of a lower MRL for PFOS. Another lab uses a proprietary method with a RL of 30 ng/L and a low calibration standard of 4 ng/L almost an order or magnitude lower.

Table 11.
Bootstrap Estimate of Reporting Limits

Lower Confidence Limit (ng/L)	Mean (ng/L)	Upper Confidence Limit (ng/L)	Confidence Level Range	Number of Randomly Selected Values
6.1	11.7	18.4	95%	2000

Four laboratories from Table 5 have RL values above the upper confidence level of 18.4 ng/L. Three laboratories reported RL values, which were MRLs equivalent to the requirements of the UCMR3 and two of which use low calibration standards of an order of magnitude lower indicating that if necessary these labs would be able to use a lower MRL for PFOS. Another lab uses a proprietary method with a RL of 30 but a low calibration standard of 4 almost an order or magnitude lower. Therefore, because these four laboratories have RL values outside of the 95% confidence interval, they were not included and the statistical analysis was rerun, producing the following information in Table 12.

Table 12.
Second Iteration: Bootstrap Estimate of Reporting Limits
(Excluding 4 Reporting Limits above the Upper Confidence Level of 18.4 ng/L)

Lower Confidence Limit (ng/L)	Mean (ng/L)	Upper Confidence Limit (ng/L)	Confidence Level Range	Number of Randomly Selected Values
3.5	5.0	6.6	95%	2000

This bootstrap analysis generated an upper confidence limit of 6.6 ng/L. This distribution shows that 95% of the laboratory community can achieve a RL level of 6.6 ng/L.

c) Bootstrap Analysis using Low Calibration Standards

Since it can be seen from the performance data that in four cases, the RL and the low calibration standard are at least an order of magnitude apart, the bootstrap technique was also applied to evaluate the consistency of the 19 laboratory low calibration standards found in Table 5. This generated distribution of 2000 randomly selected values produced an upper confidence limit of 5.6 ng/L as a low calibration standard 95% of the laboratory community should be able to achieve. The data generated by this bootstrap analysis is in Table 13.

Table 13.
Bootstrap Estimate of Low Calibration Standards

Lower Confidence Limit (ng/L)	Mean (ng/L)	Upper Confidence Limit (ng/L)	Confidence Level Range	Number of Randomly Selected Values
2.7	4.0	5.6	95%	2000

One laboratory from Table 5 uses 15.7 ng/L as a low calibration standard value which is above the upper confidence level of 5.6 ng/L. This laboratory is an out of state laboratory that had analyzed PFOS for the UCMR3. Because this laboratory had a low calibration standard value outside of the 95% confidence interval, it was not included and the statistical analysis was rerun, producing the following information in Table 14.

Table 14.
Second Iteration: Bootstrap Estimate of Low Calibration Standards
(Excluding one laboratory using with a low calibration standard above the UCL of 5.6 ng/L)

Lower Confidence Limit (ng/L)	Mean (ng/L)	Upper Confidence Limit (ng/L)	Confidence Level Range	Number of Randomly Selected Values
2.6	3.4	4.2	95%	2000

This bootstrap analysis generated an upper confidence limit of 4.2 ng/L. This distribution shows that 95% of the laboratory community can achieve a low calibration standard of 4.2 ng/L.

d) Bootstrap Analysis of MRLs of Laboratories using EPA 537

As mentioned previously, the RL used for EPA 537 is considered an MRL. The bootstrap technique was applied to evaluate the consistency of the 12 MRLs used with EPA 537 (Table 7) and for comparison to the bootstrap analysis of the combined reporting limits of EPA 537 labs and of labs using the proprietary methods (Table 12). This generated distribution of 2000 randomly selected values produced an upper confidence limit of 22.6 ng/L as an MRL that 95% of the laboratory community should be able to achieve. The data generated by this bootstrap analysis is in Table 15.

Table 15.
Bootstrap Estimate of MRLs used with EPA 537

Lower Confidence Limit (ng/L)	Mean (ng/L)	Upper Confidence Limit (ng/L)	Confidence Level Range	Number of Randomly Selected Values
5.0	13.3	22.6	95%	2000

Three laboratories from Table 7 have MRL values above the upper confidence level of 22.6 ng/L. These three laboratories reported MRL values equivalent to the requirements of the UCMR3; the remaining nine laboratories provided data to demonstrate performance better than that required of the UCMR3. Therefore, because these three laboratories have MRL values outside of the 95% confidence interval, they were not included and the statistical analysis was rerun, producing the following information in Table 16.

Table 16.
Second Iteration: Bootstrap Estimate of MRLs used with EPA 537
(Excluding three laboratories with MRLs above the Upper Confidence Level of 22.6 ng/L)

Lower Confidence Limit (ng/L)	Mean (ng/L)	Upper Confidence Limit (ng/L)	Confidence Level Range	Number of Randomly Selected Values
2.8	4.5	6.3	95%	2000

This bootstrap analysis generated an upper confidence limit of 6.3 ng/L. This distribution shows that 95% of the laboratory community using EPA 537 can achieve an MRL of 6.3 ng/L.

e) Bootstrap Analysis using Low Calibration Standards for EPA 537

The bootstrap technique can be applied to evaluate the consistency of the 12 laboratory low calibration standards for EPA 537 found in Table 7 and for comparison to the bootstrap analysis of the combined low calibration standards of EPA 537 labs and labs using the proprietary methods (Table 14). Four laboratories use MRLs of an order of magnitude higher than their low calibration standard indicating that they could possibly report to a lower MRL. For this reason, the bootstrap analysis was run using the low calibration standards in addition to the MRLs.

This generated distribution of 2000 randomly selected values produced an upper confidence limit of 6.9 ng/L as a low calibration standard 95% of the laboratory community using EPA 537 should be able to achieve. The data generated by this bootstrap analysis is in Table 17.

Table 17.
Bootstrap Estimate of Low Calibration Standards for 537

Lower Confidence Limit (ng/L)	Mean (ng/L)	Upper Confidence Limit (ng/L)	Confidence Level Range	Number of Randomly Selected Values
2.7	4.5	6.9	95%	2000

Two laboratories from Table 7 have low calibration standards above the upper confidence level of 6.9 ng/L. These two laboratories used low calibration standards that met the method criteria for reporting PFOS data for the UCMR3; the remaining nine laboratories provided data to demonstrate performance better than that required of the UCMR3. Therefore, because these two laboratories have low calibration standard values outside of the 95% confidence interval,

they were not included and the statistical analysis was rerun, producing the following information in Table 18.

Table 18.
Second Iteration: Bootstrap Estimate of Low Calibration Standards for 537
(Excluding two laboratories with a low calibration standard above the UCL of 6.9 ng/L)

Lower Confidence Limit (ng/L)	Mean (ng/L)	Upper Confidence Limit (ng/L)	Confidence Level Range	Number of Randomly Selected Values
2.2	3.0	3.8	95%	2000

This bootstrap analysis generated an upper confidence limit of 3.8 ng/L. This distribution shows that 95% of the laboratory community using EPA 537 can achieve a low calibration standard of 3.8 ng/L.

Summary and Recommendations

The Testing Subcommittee of the DWQI evaluated several methods for deriving a drinking water Practical Quantitation Limit (PQL) for PFOS. This PQL is used in conjunction with the information generated by the Health Effects Subcommittee and Treatment Subcommittee to recommend a PFOS MCL to the Commissioner of the NJDEP.

The PQLs derived from several approaches are listed in Tables 19 and 20. Table 19 lists the PQLs derived using non-parametric statistical analyses of the mean and median from actual laboratory data.

Table 19.
Approaches considered in determination of the PFOS PQL using basic statistical analysis of actual laboratory population (non-parametric statistical analysis)

PQL Approach	**Value (ng/L)**
5 x Median of MDLs (Table 6)	6.5
Mean of RLs (Table 5)	11.8
Median of RLs (Table 5)	5
Mean of low calibration standards (Table 5)	3.8
Median of low calibration standards (Table 5)	4
Mean of MRLs used with EPA 537 (Table 7)	13.3
Median of MRLs used with Method 537 (Table 7)	5
Mean of low calibration standards used with Method 537 (Table 7)	4.1
Median of low calibration standards used with Method 537 (Table 7)	4

The traditional use of the median MDL multiplied by a factor of five (mentioned previously) results in a value of 6.5 ng/L as seen in Table 19. The MDL is a statistical determination where accurate quantitation is not expected at that level. Recently developed EPA methods such as EPA 537, as well as EPA 544, EPA 545, EPA 557, EPA 524.4 and EPA 524.3 require an MRL rather than an MDL for reporting data since the QA for the MRL encompasses the additional confidence in the accuracy of that reporting limit besides the precision provided with the MDL. This trend by EPA of using MRLs rather than MDLs for reporting detections of analytes has been included in the Federal regulations for rules such as the EPA UCMR3 and UCMR4 and the EPA Disinfection By-Product (DBP) rule for regulated trihalomethanes, haloacetic acids, chlorite and bromate. Based on direction in which EPA is structuring compliance for drinking water parameters, the proposed PQL will not be based on the MDL.

From Table 5, the mean and the median of the reporting limits are 11.8 ng/L and 5 ng/L respectively indicating a non-normal distribution of the reporting limit data. Normal distribution of data would be such that mean and median are identical. This is also the case with the mean and median of the MRLs (reporting limits for the EPA 537 method) from Table 7 which are 13.3 ng/L and 5 ng/L respectively. In these two instances, the application of the bootstrap technique to the MRLs and reporting limits was used to normalize this data. This is seen in Table 20 below where the UCL of the RLs are 4.2 ng/L and the UCL of the MRLs (reporting limits for EPA 537) are 6.3 ng/L.

Table 20 lists the results of analyzing the data using the bootstrap technique by statistically generate additional data points to produce a more normalized distribution for each of the various categories of data such as MDL, reporting limits, and low calibration standards.

The bootstrap estimate of a confidence interval of a mean is a statistical technique that has been used most recently by the USEPA. It is applied to generate a normal distribution and associated 95% upper and lower confidence intervals from skewed mean values for the inter-laboratory MDLs, RLs, and low calibration standards. Table 20 lists the five parametric statistical approaches in which the bootstrap technique was used to determine a proposed PQL. The technique uses the samples at hand to generate additional statistically derived sample results that provide a normal distribution (also known as a bell curve) of the sample data.

The Testing Subcommittee used laboratory low calibration standard data as the basis of the PQL and applied the bootstrap technique to normalize the data.. The low calibration standard serves as a more appropriate gauge for determining the ability of labs to achieve a lower reporting limit and to approach increased sensitivity of the analysis.

The upper confidence limit for the RL (and MRL) may be higher than that which the laboratory is truly capable of achieving since performance data on emerging contaminants such as PFOS is largely client-driven. Unless requested there would be no incentive for a lab to restrict themselves to more sensitive quality control criteria. There are several cases in Table 5 where the low calibration standards were significantly lower than the reporting limits indicating probability that these labs would be able to use a lower reporting limit if asked. The mean and median of the low calibration standards using actual lab data are closer to each other at 3.8 ng/L and 4 ng/L

respectively indicating a more normal distribution of data than what was observed with the reporting limits and MRLs.

Table 20.

Approaches considered in determination of the PFOS PQL using Bootstrap Estimate of a Confidence Interval of a Mean

PQL Approach	Value (ng/L)
5 x Bootstrap analysis of MDLs (Table 10)	5.5
Bootstrap Upper Confidence Limit of RLs (Table 12)	6.6
Bootstrap Upper Confidence Limit of low calibration standards (Table 14)	4.2
Bootstrap Upper Confidence Limit of MRLs used in EPA 537 (Table 16)	6.3
Bootstrap Upper Confidence Limit of low calibration standards used with Method 537 (Table 18)	3.8

For PFOS, the Testing Subcommittee recommends that a PQL of 4.2 ng/L which was derived using the bootstrap upper confidence limit of the low calibration standards . The Testing Committee's bootstrap analysis of the low calibration standards indicates that 15 of the 16 laboratories reviewed can meet the PQL of 4.2 ng/L 95 % of the time.

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