

NISTIR 8146

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Comparison Study of Fatty Acid
Concentrations in Human Serum-
Results for Exercise 03:
QA16FASER03**

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NIST
National Institute of
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QA16FASER03**

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U.S. Department of Commerce
Penny Pritzker, Secretary

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Willie May, Under Secretary of Commerce for Standards and Technology and Director

ABSTRACT

The National Institute of Standards and Technology (NIST), at the request of the National Institute of Health's (NIH's) Office of Dietary Supplements (ODS) and in conjunction with the Centers for Disease Control and Prevention (CDC), initiated a third interlaboratory analytical comparison study of fatty acid concentrations in human serum in 2016. Three unknown serum samples were distributed along with Standard Reference Material (SRM) 1950 Metabolites in Frozen Human Plasma as the control sample. This is a performance-based program so participating laboratories were requested to use the analytical procedures that they typically use in their laboratories for these analyses and report data for those fatty acids that they typically quantify. The results from the third exercise are reported along with a summary of the analytical methods used by each laboratory.

Background

The National Institute of Standards and Technology (NIST) currently offers three quality assurance programs (QAPs) for the determination of micronutrients, vitamin D metabolites, and fatty acids in serum and plasma matrices, the Micronutrients Measurement QAP (MMQAP), the Vitamin D QAP (VitDQAP), and the Fatty Acid QAP (FAQAP), respectively. Given the similarity in the operations of these programs, NIST has consolidated the three programs into one larger program, the NIST Clinical Quality Assurance Program, or ClinQAP (<http://www.nist.gov/mml/csd/clinqap.cfm>). The primary goals of the ClinQAP are to support the comparability of clinical measurements through the MMQAP, VitDQAP, and the FAQAP and to monitor and support the emerging measurement needs of the clinical community.

The first exercise of the FAQAP was conducted in 2012 with 11 laboratories returning data for the content of individual fatty acids in Standard Reference Material (SRM) 2378 Fatty Acids in Frozen Human Serum (a candidate material at that time) along with SRM 1950 Metabolites in Frozen Human Plasma which was distributed as the control sample. Candidate SRM 2378 consists of three serum materials collected from: donors who have not taken fish or flaxseed oil supplements for one month prior to collection; donors who have taken flaxseed oil supplements for a minimum of one month prior to collection; and donors who have taken fish oil supplements for a minimum of one month prior to collection. SRM 1950 is designed to represent “normal” human plasma. Plasma was obtained from 100 individuals (equal number of men and women in a narrow age range (40 to 50 years) who had undergone an overnight fast prior to blood draw. The results from the first exercise were published in NIST Internal Report (NISTIR) 7953. [1]

The second exercise of the FAQAP was conducted in 2015 with 14 laboratories returning data for the content of individual fatty acids in three serum samples, that had been originally collected for use in the MMQAP, and in each of the three levels of SRM 2378 (as control samples). The results from the second exercise were published in NISTIR 8086 [2].

Overview of Exercise 03: QA16FASER03

For the third FAQAP exercise, the intercomparison materials were three serum samples previously used in the VitDQAP studies. [3] The samples used were:

SRM 972a Level 2 relabeled as	FAQAP Unk 004 (black label)
VitDQAP Sample I relabeled as	FAQAP Unk 005 (red label)
VitDQAP Sample II relabeled as	FAQAP Unk 006 (green label)

In addition, participants were requested to run SRM 1950 as the control material. The laboratories were provided with three vials of each unknown material, each vial contained approximately 1 mL of serum, and were requested to do triplicate measurements of each unknown sample using their laboratory's and/or program's analytical protocols for the concentrations of the fatty acids currently being determined in their laboratory. In addition, they

were requested to analyze one subsample of the control material, SRM 1950. A target list of fatty acids was provided; however, participants did not need to quantify all of these compounds and could add additional compounds when reporting data. They were requested to report results, using three significant figures, in units of either $\mu\text{g/g}$ or $\mu\text{mol/L}$ (μM) and to provide brief descriptions of their cleanup and analytical procedures.

Reported Results

Thirteen laboratories returned data and were assigned numerical identification codes in order of receipt of data with the exception of the NIST laboratory, which is Lab 1 in this exercise. The fatty acids included in the study are listed in Table 1 with the suggested list of fatty acids at the top of the table and the additional fatty acids reported listed below. For the total (esterified and free) fatty acids, the laboratory mean values, standard deviations, and relative standard deviations are shown in Tables 2, 4, and 6 in $\mu\text{g/g}$ for unknowns 004, 005, and 006, respectively, and in Tables 3, 5, and 7 in μM for unknowns 004, 005, and 006, respectively. The laboratory values reported for the control sample, SRM 1950, are summarized in Tables 8 and 9 in $\mu\text{g/g}$ and in μM , respectively. The summary statistics (median, number of laboratories reporting, and lowest and highest value reported) are given in Table 10 for the total fatty acids.

This is the first study in which the laboratories were also given the option of reporting data for the free fatty acids in the serum samples. Only one laboratory (Lab 12) did so, however. Their data for the free fatty acids are shown in Table 11, and the % of free to total fatty acid based only on that laboratory's data are shown in Table 12.

Summaries of the methods used and notes submitted by each laboratory are in Appendix A, and charts of the mean numerical results reported by each laboratory for each analyte in the exercise materials are in Appendix B.

Discussion

NIST contacted over 40 laboratories in early 2016 regarding participation in the third interlaboratory analytical comparison study of fatty acid concentrations in human serum. Of the laboratories contacted, 15, including NIST, replied with interest in participating in this study. As stated above, laboratories were also given the option of reporting free fatty acids along with total fatty acids for the samples received. Of the 15 laboratories requesting samples, four (4) said that they were interested in quantifying the free fatty acids in addition to the total fatty acids and two (2) were interested in quantifying the free fatty acids. Only one of those laboratories, designated as Lab 12 in this study, reported data for the free fatty acids.

Samples were sent on dry ice between March 14 and 21, 2016. The deadline for submission of data to NIST was June 1, 2016. All but two laboratories returned data by June 30, 2016. One of the remaining laboratories reported that they would not be sending in data because they had

problems with the hydrolysis step resulting in low results on the control material. The last laboratory did not respond to requests for a status report on their analyses.

After submitting data, one of the laboratories (designated as Lab 11 in this study) asked that their data be removed from the data summary. Their results were 5 to 10 times higher than expected based on the SRM 1950 values. They stated that their method is semi-quantitative, reported as normalized area percents. They have had success with the method for foods but speculate that the residue mass from the serum and plasma samples is composed of more than fatty acids thus overestimating the concentrations of each fatty acid.

Another laboratory (designated as Lab 13 in this study) provided a recalculated set of data on July 12. The recalculated data set has been incorporated into this report. The laboratory did not report what the recalculation involved.

An alphabetical list of laboratories that returned data is given in Appendix C. Note that the numerical codes in the following tables and figures are based on the receipt of the data and therefore do not follow the order in Appendix C.

Laboratories were requested to submit data for the fatty acids that they typically monitor in similar samples (Table 1) for three subsamples of each unknown sample received and one subsample of SRM 1950 in units of either $\mu\text{g/g}$ or μM along with the density of each sample. Summaries of the results submitted by each laboratory are presented in Tables 2 through 7 as the means, standard deviations, and relative standard deviations for the three values submitted for each unknown sample in both $\mu\text{g/g}$ and μM . Three (3) laboratories reported the data in $\mu\text{g/g}$, and nine (9) laboratories reported the data in μM . The conversions between the units reported and the alternate units were calculated using the densities provided by each laboratory except for labs 1, 2, 5, 7, and 13. These laboratories did not report a density so the density was assumed to be 1 g/mL for the conversion. The densities reported by the remaining laboratories are shown in the tables and range from 0.954 g/mL to 1.09 g/mL. Summaries of the results from each participant for the analysis of one subsample of SRM 1950 are presented in tables 8 and 9 in $\mu\text{g/g}$ and μM , respectively, along with the certified and reference values for the fatty acids.

As shown in Tables 2 through 7, the relative standard deviations (RSDs) for each participating laboratory for the analyses of three subsamples for each unknown serum sample are generally < 10 %. Lab 13 had a few analytes, particularly in unknown 004, with higher RSDs as well as high RSDs (> 90 %) for C22:1n9 in unknown 005 and unknown 006. The higher RSDs for C22:1n9 came from reporting one or more 0 values for the subsamples.

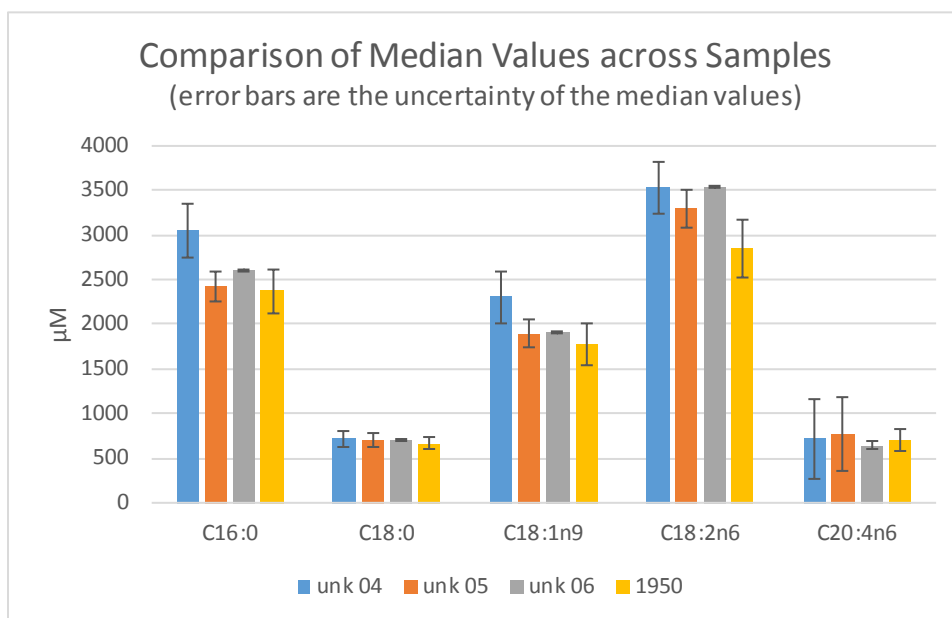
Several laboratories reported data for additional fatty acids. These fatty acids are included at the bottom of Table 1 and summarized at the bottom of Tables 2 through 9.

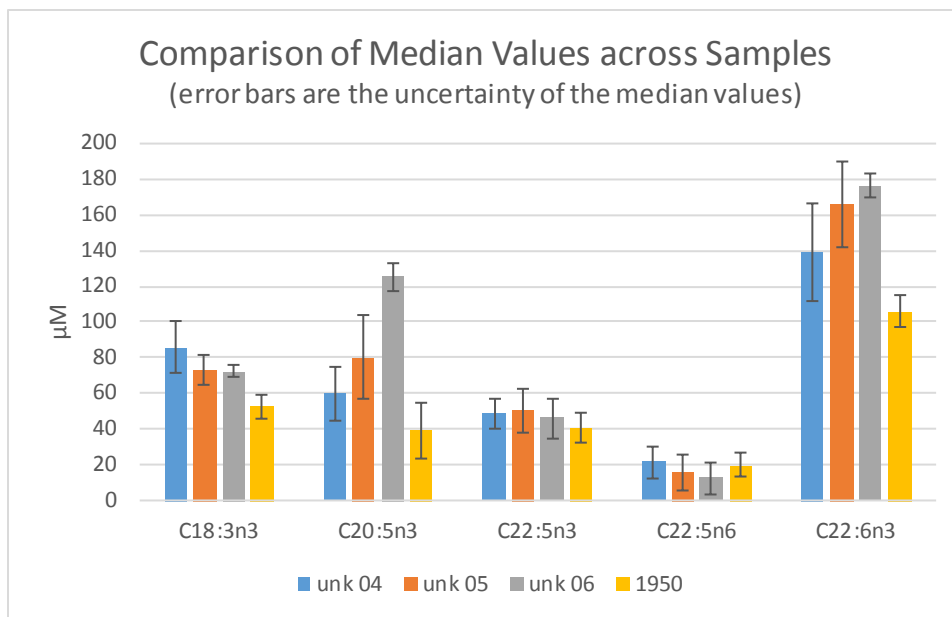
The data in terms of μM are plotted by analyte in each material in Appendix B. Each data point is the mean and associated standard deviation of the data reported by the laboratory of the indicated analyte in the indicated sample. The medians calculated from the data received for the fatty acid in each unknown sample are summarized in Table 10 and included on each chart for

the unknown samples. The charts for SRM 1950 include the certified or reference values for comparison purposes.

The relative expanded uncertainty for the medians ranged from 9 % to 66 % for unknown 004, from 7 % to > 300 % for unknown 005, and < 1 % to > 200 % for unknown 006. The high relative uncertainties for C22:1n9 in unknown 005 and 006 are due to a limited number of laboratories reporting data (n=4), and one of those laboratories (Lab 13) appearing to be an outlier. As mentioned above, this is also the compound for which Lab 13 reported several 0 values resulting in high RSDs for their data. In general, the agreement among the laboratories was best in all of the samples for those fatty acids at highest concentrations, particularly C16:0, C18:0, C18:1n9, and C18:2n6.

Examples of the comparison of the median values and associated uncertainties are shown below for 10 of the fatty acids quantified in this study.





The concentrations of the individual fatty acids in the four (4) samples quantified in this study were similar with the uncertainty of the median values overlapping for most of the fatty acids with the exception of C20:5n3 being highest in unknown 006. It is interesting to note that the agreement among the laboratories was best for the majority of the fatty acids in unknown 006.

In the past exercises [1,2], there were some trends across all fatty acids in the samples with a particular laboratory reporting high data or low data. In this exercise, that does not appear to be the case. The laboratories reporting the highest or lowest data tend to vary from fatty acid to fatty acid within the samples, however, tend to be consistent across samples. Using C20:4n6 as an example, Lab 2 reported the lowest values for unknown 004, unknown 005, and SRM 1950 and the second lowest value for unknown 006; whereas Lab 7 reported the highest value for all of the samples. These results could be obtained by incomplete extraction (low), coelution with other fatty acids or matrix components on the analytical column used (high), misidentification of the chromatographic peaks (low or high), or from some other method variations such as inaccurate calibration.

The methods used by each laboratory are summarized in Appendix A with the procedures for the total fatty acids in Table A-1, Lab 12's procedures for the free fatty acids in Table A-2, the calibration information in Table A-3, and notes submitted by laboratories in Table A-4. For the laboratories reporting an hydrolysis method, they used both acid and base, and the extraction methods were typically liquid-liquid. Most laboratories used gas chromatography (GC) with either flame ionization detection (FID) or mass spectrometry (MS) following a derivatization. The derivatizing reagents used by each laboratory are summarized in Appendix A. The exception being lab 7, which used a liquid chromatography (LC)/MS/MS method. They, however, reported data for only three fatty acids, C20:4n6, C20:5n3, and C22:6n3.

For the GC analyses, the columns used ranged in polarity from relatively non-polar (5% phenyl methylpolysiloxane phase) to relatively polar (cyanopropyl phase). For the calibration information (Table A-3), labs 1, 2, 7, 8, 9, 10 used a linear regression, labs 3, 4, and 12 used a quadratic regression, and lab 6 used a mix of linear and quadratic regression tailored by analyte. Lab 5 only reported the limits of their calibration range, and labs 11 and 13 did not report calibration information. Combining the method information with the trends in the data reported does not lead to obvious explanations of the variations noted in the data submitted by individual laboratories.

Lab 12 reported data for the free fatty acids (Table 11) in addition to the total fatty acids. Using only lab 12's data, the relative amount of free to total for each fatty acid in the four samples has been calculated and is summarized in Table 12. The free fatty acids are from < 1% to 34 % of the total fatty acids with most in the 2 % to 10 % range. Hopefully, more laboratories will report data for free fatty acids in future intercomparison exercises.

The data from this exercise can be used to assess the comparability across a limited number of laboratories (see Appendix C). The data do not indicate specific method biases but do indicate the need for such intercomparisons and for the use of control materials to increase the comparability of data across laboratories.

Acknowledgments

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The time and effort of the analysts and management of the participating laboratories are gratefully acknowledged.

Disclaimer

Certain commercial equipment, instruments, or materials are identified in this report to specify adequately the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are the best available for the purpose.

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Table 1. Fatty Acids Included in Study		
Code	Common Name	mol wt (g/mol)
C14:0	Myristic acid	228.38
C14:1n5	Myristoleic acid	226.38
C16:0	Palmitic acid	256.43
C16:1n7	Palmitoleic acid	254.43
C18:0	Stearic acid	284.48
C18:1n7	cis-Vaccenic acid	282.48
C18:1n9	Oleic acid	282.48
C18:2n6	Linoleic acid	280.48
C18:3n3	alpha-Linolenic acid	278.48
C18:3n6	gamma-Linolenic acid	278.48
C20:0	Arachidic acid	312.54
C20:1n9	11-Eicosenoic acid	310.54
C20:2n6	11,14-Eicosadienoic acid	308.53
C20:3n6	homo-gamma-Linolenic acid	306.53
C20:4n6	Arachidonic acid	304.52
C20:5n3	Eicosapentaenoic acid	302.52
C22:0	Docosanoic acid	340.59
C22:1n9	Docosenoic acid	338.59
C22:4n6	Docosatetraenoic acid	332.57
C22:5n3	Docosapentaenoic acid	330.57
C22:5n6	Docosapentaenoic acid	330.57
C22:6n3	Docosahexaenoic acid	328.57
C24:0	Lignoceric acid	368.64
C24:1n9	Nervonic acid	366.63
List any additional information such as known coelutions or results for additional fatty acids below:		
C8:0	Caprylic acid	144.26
C10:0	Decanoic acid	172.3
C10:1n1	9-Decenoic acid	170.3
C12:0	Lauric acid	200.34
C12:1n1	11-Dodecenoic acid	198.34
C12:1n7	cis-5-dodecenoic	198.34
C14:2		224.38
C15:0	Pentadecanoic acid	242.42
C16:1n7t	Palmitelaidic acid	254.43
C16:1n9		254.43
C16:2		252.43
C17:0	Margaric acid	270.46
C17:1n9	10-Heptadecenoic acid	268.46
9c,11t-C18:2n6	Rumenic acid	280.48
C18:4n3	Stearidonic acid	276.48
C19:0	Nonadecanoic acid	298.54
C20:3n3	11,14,17-Eicosatrienoic acid	306.53
C20:3n9	5,8,11-Eicosatrienoic acid (Mead acid)	306.53
C20:4n3	Arachidonic acid (Omega 3)	304.53
C21:0	Heneicosanoic acid	326.58
C22:2n6	Docosadienoic acid	336.59
C23:0	Tricosanoic acid	354.62
C26:0	Hexacosanoic acid	396.68
C26:1		394.68
PhA	Phytanic acid	312.54
PrA	Pristanic acid	298.5

Table 2. Interlaboratory data received for total fatty acids in Unknown 004 (µg/g)												
Code	Lab 1			Lab 2 ^a			Lab 3			Lab 4 ^a		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	35.3	1.5	4.17%	44.4	1.9	4.19%	34.9	0.5	1.52%	33.1	0.7	2.15%
C14:1n5	<10			4.75	0.23	4.76%	Not analyzed			3.18	0.06	1.75%
C16:0	828	63	7.61%	777	30	3.84%	740	43	5.79%	771	21	2.77%
C16:1n7	73.1	5.2	7.05%	74.3	4.2	5.72%	72.3	2.5	3.40%	84.9	1.4	1.69%
C18:0	178	16	8.83%	261	12	4.68%	207	1	0.28%	208	7	3.26%
C18:1n7	51.2	4.8	9.45%	83.0	4.5	5.47%	45.5	0.3	0.55%	70.4	1.4	1.99%
C18:1n9	672	40	5.89%	622	33	5.27%	639	10	1.59%	666	14	2.06%
C18:2n6	1024	79	7.72%	817	32	3.97%	973	21	2.11%	991	27	2.73%
C18:3n3	27.8	1.3	4.62%	23.0	0.6	2.79%	24.6	0.4	1.65%	24.1	0.3	1.05%
C18:3n6	15.5	0.8	5.00%	15.3	0.7	4.81%	15.1	0.6	4.14%	14.8	0.3	2.27%
C20:0	<10			10.2	0.5	4.68%	Not analyzed			7.16	0.13	1.79%
C20:1n9	<10			Not analyzed			Not analyzed			Not analyzed		
C20:2n6	Not analyzed			Not analyzed			Not analyzed			Not analyzed		
C20:3n6	Not analyzed			39.2	2.5	6.25%	50.2	0.5	0.98%	58.6	0.4	0.63%
C20:4n6	240	6	2.44%	173	7	4.02%	210	2	0.99%	224	5	2.22%
C20:5n3	20.3	0.6	3.18%	16.7	0.9	5.52%	17.5	0.3	1.75%	17.9	0.8	4.26%
C22:0	<10			24.0	1.0	4.33%	15.9	0.3	1.66%	19.9	0.6	3.17%
C22:1n9	<10			3.61	0.20	5.41%	NA			3.38	0.11	3.29%
C22:4n6	Not analyzed			9.31	0.58	6.19%	7.18	0.14	1.98%	10.43	0.36	3.49%
C22:5n3	16.1	1.2	7.15%	15.0	0.7	4.59%	14.1	0.4	2.68%	14.6	0.6	3.76%
C22:5n6	Not analyzed			8.26	0.66	8.00%	Not analyzed			5.67	0.19	3.41%
C22:6n3	53.0	3.0	5.65%	45.3	4.1	9.05%	44.2	0.5	1.14%	46.6	2.2	4.79%
C24:0	<20			21.4	1.0	4.56%	13.9	0.4	2.91%	20.7	0.8	3.93%
C24:1n9	<20			31.5	1.5	4.65%	20.0	0.4	1.80%	26.2	1.1	4.27%
List any additional information such as known coelutions or results for additional fatty acids below:												
C8:0										1.12	0.04	3.18%
C10:0										1.07	0.02	2.31%
C10:1n1										1.07	0.06	5.62%
C12:0										4.23	0.09	2.13%
C12:1n1										1.02	0.06	5.49%
C12:1n7										0.920	0.054	5.85%
C14:2										0.317	0.020	6.23%
C15:0										5.41	0.15	2.80%
C16:1n-7t												
C16:1n9										12.9	0.4	2.81%
C16:2										1.67	0.02	1.36%
C17:0										6.79	0.19	2.74%
C17:1n9												
9c,11t-CLA												
C18:4n-3												
C19:0										0.691	0.055	7.90%
C 20:3n-3												
C20:3n9										4.91	0.09	1.82%
C20:4n3												
C21:0										0.605	0.030	4.94%
C 22:2n-6												
C23:0										13.8	1.1	8.21%
C26:0										0.204	0.008	3.92%
C26:1										0.171	0.004	2.33%
PhA										0.363	0.005	1.32%
PrA										0.064	0.002	2.71%
density (g/mL)	Not analyzed			Not analyzed			1.06	0.01	0.55%	0.992	0.001	0.10%

^a Reported as µM

Code	Lab 5 ^a			Lab 6 ^a			Lab 7 ^a			Lab 8		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	38.7	1.1	2.91%	38.6	1.0	2.54%	Not analyzed			46.2	3.9	8.33%
C14:1n5				2.52	0.04	1.67%	Not analyzed			Not analyzed		
C16:0	780	17	2.15%	845	19	2.23%	Not analyzed			1050	73	6.93%
C16:1n7	62.6	1.9	3.11%	78.6	2.7	3.50%	Not analyzed			97.5	7.0	7.14%
C18:0	206	5	2.65%	183	2	1.14%	Not analyzed			277	20	7.23%
C18:1n7				44.2	2.3	5.29%	Not analyzed			Not analyzed		
C18:1n9	625	13	2.02%	677	28	4.10%	Not analyzed			861	59	6.85%
C18:2n6	977	19	1.94%	1029	39	3.78%	Not analyzed			1084	78	7.21%
C18:3n3	23.2	0.5	1.98%	28.8	1.2	4.09%	Not analyzed			35.9	3.0	8.31%
C18:3n6				16.3	0.8	4.98%	Not analyzed			Not analyzed		
C20:0				6.60	0.18	2.79%	Not analyzed			Not analyzed		
C20:1n9				5.57	0.35	6.27%	Not analyzed			9.41	0.94	9.99%
C20:2n6	5.96	0.89	14.89%	7.77	0.36	4.59%	Not analyzed			Not analyzed		
C20:3n6				52.4	1.7	3.32%	Not analyzed			68.4	4.9	7.22%
C20:4n6	205	5	2.40%	239	6	2.65%	858	41	4.83%	317	16	5.18%
C20:5n3	15.4	0.5	3.07%	19.4	0.1	0.36%	27.4	1.7	6.07%	28.7	3.6	12.44%
C22:0				22.6	0.1	0.37%	Not analyzed			Not analyzed		
C22:1n9							Not analyzed			Not analyzed		
C22:4n6				8.93	0.21	2.36%	Not analyzed			11.2	1.2	10.43%
C22:5n3	18.5	1.2	6.28%	16.8	0.8	4.81%	Not analyzed			18.5	1.2	6.61%
C22:5n6				7.32	0.08	1.05%	Not analyzed			Not analyzed		
C22:6n3	37.6	1.8	4.84%	53.4	2.7	5.10%	70.2	0.8	1.18%	18.5	1.2	6.61%
C24:0				20.3	0.5	2.51%	Not analyzed			Not analyzed		
C24:1n9				31.4	0.8	2.50%	Not analyzed			Not analyzed		

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0												
C10:1n1												
C12:0												
C12:1n1												
C12:1n7												
C14:2												
C15:0				5.99	0.22	3.70%						
C16:1n-7t												
C16:1n9												
C16:2												
C17:0				8.22	0.16	1.89%						
C17:1n9												
9c,11t-CLA												
C18:4n-3				1.10	0.05	4.30%						
C19:0												
C 20:3n-3												
C20:3n9				2.34	0.09	4.02%						
C20:4n3												
C21:0												
C 22:2n-6												
C23:0				10.3	0.2	1.89%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	Not analyzed			0.963	0.003	0.32%	Not analyzed			1.03	0.01	1.12%

^a Reported as µM

Code	Lab 9 ^a			Lab 10 ^a			Lab 12 ^a			Lab 13 ^a		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	35.4	0.3	0.96%	32.5	0.6	1.78%	62.2	1.8	2.89%	24.2	2.1	8.54%
C14:1n5	3.41	0.02	0.65%	1.81	0.04	2.41%	3.93	0.06	1.52%	1.77	0.19	10.87%
C16:0	794	0.3	0.04%	670	2	0.37%	767	36	4.68%	719	15	2.13%
C16:1n7	74.2	0.3	0.37%	67.1	0.3	0.44%	65.5	2.8	4.31%	105.1	4.7	4.51%
C18:0	193	3	1.64%	196	2	0.78%	193	11	5.76%	185	3	1.80%
C18:1n7	47.8	0.3	0.59%	48.1	0.7	1.47%	45.4	2.2	4.75%	78.7	3.1	3.97%
C18:1n9	636	2	0.33%	600	8	1.38%	685	32	4.61%	407	10	2.50%
C18:2n6	1006	3	0.33%	877	2	0.26%	1106	55	4.93%	776	6	0.75%
C18:3n3	23.3	0.2	0.72%	21.6	0.2	0.73%	18.1	0.6	3.58%	15.9	1.9	12.21%
C18:3n6	15.1	0.2	1.08%	13.2	0.1	0.98%	18.6	0.6	3.45%	Not analyzed		
C20:0	6.98	0.12	1.74%	4.81	0.20	4.24%	4.49	0.19	4.27%	4.02	0.85	21.07%
C20:1n9	Not analyzed			5.04	0.21	4.13%	10.29	0.63	6.15%	3.18	0.95	29.90%
C20:2n6	7.35	0.14	1.91%	7.28	0.12	1.71%	7.57	0.11	1.48%	6.41	1.49	23.29%
C20:3n6	51.2	0.6	1.17%	45.8	0.4	0.97%	31.5	2.3	7.28%	47.8	5.0	10.51%
C20:4n6	213	0	0.21%	193	1	0.39%	170	13	7.47%	205	12	6.07%
C20:5n3	17.1	0.1	0.61%	15.7	0.1	0.58%	10.81	0.19	1.76%	33.3	4.0	11.90%
C22:0	20.9	0.2	1.11%	12.79	0.42	3.24%	3.23	0.21	6.58%	9.97	1.26	12.68%
C22:1n9	Not analyzed			3.02	0.23	7.65%	Not analyzed			4.81	8.33	173.21%
C22:4n6	7.29	0.12	1.64%	6.77	0.23	3.33%	7.00	0.51	7.26%	11.69	2.00	17.12%
C22:5n3	14.33	0.26	1.84%	6.05	0.20	3.37%	17.5	0.9	4.87%	18.0	3.4	19.03%
C22:5n6	6.01	0.06	1.04%	13.23	0.13	0.99%	7.20	0.24	3.37%	4.08	0.56	13.73%
C22:6n3	46.2	0.6	1.24%	40.6	0.7	1.78%	30.5	2.8	9.19%	40.8	7.4	18.15%
C24:0	18.8	0.2	0.82%	11.31	0.47	4.14%	1.75	0.04	2.16%	8.22	2.35	28.57%
C24:1n9	25.7	0.1	0.53%	16.1	0.4	2.66%	4.52	0.56	12.28%	15.19	3.75	24.70%

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0				1.19	0.16	13.48%						
C10:1n1												
C12:0				3.53	0.55	15.64%	97.1	2.5	2.58%			
C12:1n1				0.601	0.126	20.91%						
C12:1n7												
C14:2												
C15:0							6.89	0.13	1.95%	7.67	0.26	3.45%
C16:1n-7t							21.9	0.5	2.20%			
C16:1n9												
C16:2												
C17:0				7.45	0.09	1.14%	7.39	0.16	2.10%	16.0	1.2	7.32%
C17:1n9							6.18	0.41	6.72%			
9c,11t-CLA							6.14	0.16	2.68%			
C18:4n-3							1.03	0.15	14.90%			
C19:0							3.82	0.31	8.15%			
C 20:3n-3				0.750	0.121	16.09%	3.53	0.27	7.64%			
C20:3n9				2.93	0.15	5.06%						
C20:4n3							1.82	0.06	3.45%			
C21:0							2.07	0.19	9.00%			
C 22:2n-6				0.635	0.195	30.75%	4.05	0.17	4.31%			
C23:0				5.79	0.17	2.90%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	1.02	0.01	1.13%	1.04	0.01	0.58%	1.03	0.00	0.00%	Not analyzed		

^a Reported as µM

Table 3. Interlaboratory data received for total fatty acids in Unknown 004 (μM)												
Code	Lab 1 ^a			Lab 2			Lab 3 ^a			Lab 4		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	155	6	4.17%	194	8	4.19%	161	2	1.52%	144	3	2.15%
C14:1n5				21.0	1.0	4.76%	Not analyzed			13.9	0.2	1.75%
C16:0	3228	246	7.61%	3031	116	3.84%	3048	177	5.79%	2983	83	2.77%
C16:1n7	287	20	7.05%	292	17	5.72%	300	10	3.40%	331	6	1.69%
C18:0	626	55	8.83%	916	43	4.68%	768	2	0.28%	725	24	3.26%
C18:1n7	181	17	9.45%	294	16	5.47%	170	1	0.55%	247	5	1.99%
C18:1n9	2378	140	5.89%	2202	116	5.27%	2390	38	1.59%	2339	48	2.06%
C18:2n6	3652	282	7.72%	2914	116	3.97%	3664	77	2.11%	3504	96	2.73%
C18:3n3	100	5	4.62%	82.7	2.3	2.79%	93	2	1.65%	86.0	0.9	1.05%
C18:3n6	55.7	2.8	5.00%	55.0	2.6	4.81%	57.3	2.4	4.14%	52.8	1.2	2.27%
C20:0				32.7	1.5	4.68%	Not analyzed			22.7	0.4	1.79%
C20:1n9				Not analyzed			Not analyzed			Not analyzed		
C20:2n6	Not analyzed			Not analyzed			Not analyzed			Not analyzed		
C20:3n6	Not analyzed			128	8	6.25%	173	2	0.98%	190	1	0.63%
C20:4n6	789	19	2.44%	567	23	4.02%	728	7	0.99%	730	16	2.22%
C20:5n3	67.1	2.1	3.18%	55.3	3.1	5.52%	61.0	1.1	1.75%	58.6	2.5	4.26%
C22:0				70.6	3.1	4.33%	49.3	0.8	1.66%	58.0	1.8	3.17%
C22:1n9				10.7	0.6	5.41%	Not analyzed			9.89	0.33	3.29%
C22:4n6	Not analyzed			28.0	1.7	6.19%	22.8	0.5	1.98%	31.1	1.1	3.49%
C22:5n3	48.7	3.5	7.15%	45.3	2.1	4.59%	45.2	1.2	2.68%	43.9	1.7	3.76%
C22:5n6	Not analyzed			25.0	2.0	8.00%	Not analyzed			17.0	0.6	3.41%
C22:6n3	161	9	5.65%	138	12	9.05%	142	2	1.14%	141	7	4.79%
C24:0				58.0	2.6	4.56%	39.8	1.2	2.91%	55.7	2.2	3.93%
C24:1n9				86.0	4.0	4.65%	57.6	1.0	1.80%	71.0	3.0	4.27%
List any additional information such as known coelutions or results for additional fatty acids below:												
C8:0										7.72	0.25	3.18%
C10:0										6.15	0.14	2.31%
C10:1n1										6.26	0.35	5.62%
C12:0										20.9	0.4	2.13%
C12:1n1										5.11	0.28	5.49%
C12:1n7										4.60	0.27	5.85%
C14:2										1.40	0.09	6.23%
C15:0										22.1	0.6	2.80%
C16:1n-7t												
C16:1n9										50.2	1.4	2.81%
C16:2										6.57	0.09	1.36%
C17:0										24.9	0.7	2.74%
C17:1n9												
9c,11t-CLA												
C18:4n-3												
C19:0										2.30	0.18	7.90%
C 20:3n-3												
C20:3n9										15.9	0.3	1.82%
C20:4n3												
C21:0										1.84	0.09	4.94%
C 22:2n-6												
C23:0										38.6	3.2	8.21%
C26:0										0.510	0.020	3.92%
C26:1										0.430	0.010	2.33%
PhA										1.15	0.02	1.32%
PrA										0.213	0.006	2.71%
density (g/mL)	Not analyzed			Not analyzed			1.06	0.01	0.55%	0.992	0.001	0.10%

^a Reported as $\mu\text{g/g}$

Table 3 (cont). Interlaboratory data received for total fatty acids in Unknown 004 (μM)

Code	Lab 5			Lab 6			Lab 7			Lab 8 ^a		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	169	5	2.91%	163	4	2.54%	Not analyzed			208	17	8.33%
C14:1n5				10.7	0.2	1.67%	Not analyzed			Not analyzed		
C16:0	3042	65	2.15%	3171	71	2.23%	Not analyzed			4202	291	6.93%
C16:1n7	246	8	3.11%	297	10	3.50%	Not analyzed			393	28	7.14%
C18:0	723	19	2.65%	620	7	1.14%	Not analyzed			998	72	7.23%
C18:1n7				151	8	5.29%	Not analyzed			Not analyzed		
C18:1n9	2212	45	2.02%	2306	95	4.10%	Not analyzed			3128	214	6.85%
C18:2n6	3484	68	1.94%	3531	134	3.78%	Not analyzed			3969	286	7.21%
C18:3n3	83.3	1.6	1.98%	99.5	4.1	4.09%	Not analyzed			132	11	8.31%
C18:3n6				56.5	2.8	4.98%	Not analyzed			Not analyzed		
C20:0				20.3	0.6	2.79%	Not analyzed			Not analyzed		
C20:1n9				17.3	1.1	6.27%	Not analyzed			31.1	3.1	9.99%
C20:2n6	19.1	2.8	14.89%	24.2	1.1	4.59%	Not analyzed			Not analyzed		
C20:3n6				164	5	3.32%	Not analyzed			229	17	7.22%
C20:4n6	675	16	2.40%	756	20	2.65%	2818	136	4.83%	1070	55	5.18%
C20:5n3	51.0	1.6	3.07%	61.7	0.2	0.36%	90.6	5.5	6.07%	97	12	12.44%
C22:0				63.9	0.2	0.37%	Not analyzed			Not analyzed		
C22:1n9							Not analyzed			Not analyzed		
C22:4n6				25.8	0.6	2.36%	Not analyzed			34.5	3.6	10.43%
C22:5n3	55.9	3.5	6.28%	48.8	2.3	4.81%	Not analyzed			57.5	3.8	6.61%
C22:5n6				21.3	0.2	1.05%	Not analyzed			Not analyzed		
C22:6n3	115	6	4.84%	156	8	5.10%	214	3	1.18%	57.9	3.8	6.61%
C24:0				53.1	1.3	2.51%	Not analyzed			Not analyzed		
C24:1n9				82.4	2.1	2.50%	Not analyzed			Not analyzed		

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0												
C10:1n1												
C12:0												
C12:1n1												
C12:1n7												
C14:2												
C15:0				23.8	0.9	3.70%						
C16:1n-7t												
C16:1n9												
C16:2												
C17:0				29.2	0.6	1.89%						
C17:1n9												
9c,11t-CLA												
C18:4n-3				3.82	0.16	4.30%						
C19:0												
C 20:3n-3												
C20:3n9				7.36	0.30	4.02%						
C20:4n3												
C21:0												
C 22:2n-6												
C23:0				28.0	0.5	1.89%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	Not analyzed			0.963	0.003	0.32%	Not analyzed			1.03	0.01	1.12%

^a Reported as $\mu\text{g/g}$

Table 3 (cont). Interlaboratory data received for total fatty acids in Unknown 004 (μM)

Code	Lab 9			Lab 10			Lab 12			Lab 13		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	159	2	1.31%	148	3	1.78%	279	8	2.89%	106	9	8.54%
C14:1n5	15.4	0.2	1.30%	8.31	0.20	2.41%	17.8	0.3	1.52%	7.80	0.85	10.87%
C16:0	3170	35	1.09%	2715	10	0.37%	3065	144	4.68%	2802	60	2.13%
C16:1n7	298	3	1.02%	274	1	0.44%	264	11	4.31%	413	19	4.51%
C18:0	694	12	1.72%	716	6	0.78%	694	40	5.76%	650	12	1.80%
C18:1n7	173	2	1.16%	177	3	1.47%	165	8	4.75%	279	11	3.97%
C18:1n9	2303	21	0.90%	2205	30	1.38%	2486	115	4.61%	1440	36	2.50%
C18:2n6	3670	36	0.98%	3247	8	0.26%	4040	199	4.93%	2766	21	0.75%
C18:3n3	85.6	1.4	1.66%	80.6	0.6	0.73%	66.7	2.4	3.58%	57.2	7.0	12.21%
C18:3n6	55.6	0.7	1.20%	49.1	0.5	0.98%	68.5	2.4	3.45%	Not analyzed		
C20:0	22.9	0.5	2.02%	16.0	0.7	4.24%	14.7	0.6	4.27%	12.88	2.71	21.07%
C20:1n9	Not analyzed			16.9	0.7	4.13%	34.0	2.1	6.15%	10.19	3.05	29.90%
C20:2n6	24.4	0.5	1.94%	24.5	0.4	1.71%	25.1	0.4	1.48%	20.51	4.78	23.29%
C20:3n6	171	3	1.55%	155	1	0.97%	105	8	7.28%	156	16	10.51%
C20:4n6	717	9	1.30%	660	3	0.39%	571	43	7.47%	672	41	6.07%
C20:5n3	57.7	0.6	0.95%	54.1	0.3	0.58%	36.6	0.6	1.76%	110.1	13.1	11.90%
C22:0	62.9	1.0	1.63%	39.0	1.3	3.24%	9.73	0.64	6.58%	29.3	3.7	12.68%
C22:1n9	Not analyzed			9.26	0.71	7.65%	Not analyzed			14.20	24.60	173.21%
C22:4n6	22.4	0.5	2.29%	21.1	0.7	3.33%	21.6	1.6	7.26%	35.1	6.0	17.12%
C22:5n3	44.4	1.2	2.61%	19.0	0.6	3.37%	54.2	2.6	4.87%	54.4	10.3	19.03%
C22:5n6	18.6	0.2	0.93%	41.6	0.4	0.99%	22.3	0.8	3.37%	12.35	1.70	13.73%
C22:6n3	144	3	2.08%	128	2	1.78%	95.2	8.7	9.19%	124.0	22.5	18.15%
C24:0	52.2	1.0	1.94%	31.9	1.3	4.14%	4.87	0.10	2.16%	22.3	6.4	28.57%
C24:1n9	71.7	1.0	1.42%	45.6	1.2	2.66%	12.6	1.6	12.28%	41.4	10.2	24.70%

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0				7.19	0.97	13.48%						
C10:1n1												
C12:0				18.3	2.9	15.64%	497	13	2.58%			
C12:1n1				3.15	0.66	20.91%						
C12:1n7												
C14:2												
C15:0							29.1	0.6	1.95%	31.6	1.1	3.45%
C16:1n-7t							88.1	1.9	2.20%			
C16:1n9												
C16:2												
C17:0				28.6	0.3	1.14%	28.0	0.6	2.10%	59.1	4.3	7.32%
C17:1n9							23.6	1.6	6.72%			
9c,11t-CLA							22.4	0.6	2.68%			
C18:4n-3							3.81	0.57	14.90%			
C19:0							13.1	1.1	8.15%			
C 20:3n-3				2.54	0.41	16.09%	11.8	0.9	7.64%			
C20:3n9				9.94	0.50	5.06%						
C20:4n3							6.10	0.21	3.45%			
C21:0							6.51	0.59	9.00%			
C 22:2n-6				1.96	0.60	30.75%	12.3	0.5	4.31%			
C23:0				17.0	0.5	2.90%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	1.02	0.01	1.13%	1.04	0.01	0.58%	1.03	0.00	0.00%	Not analyzed		

^a Reported as $\mu\text{g/g}$

Code	Lab 1			Lab 2 ^a			Lab 3			Lab 4 ^a		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	25.0	1.1	4.25%	29.5	0.8	2.80%	23.1	0.2	0.90%	22.4	0.9	4.12%
C14:1n5	<10			2.57	0.13	5.09%	Not analyzed			1.79	0.05	2.83%
C16:0	621	22	3.58%	620	16	2.58%	608	6	0.99%	625	40	6.47%
C16:1n7	47.5	2.9	6.02%	43.2	1.7	3.92%	46.0	0.7	1.52%	53.7	2.3	4.28%
C18:0	167	7	3.99%	243	6	2.48%	199	3	1.53%	207	14	6.76%
C18:1n7	29.3	2.6	8.89%	56.4	1.8	3.26%	34.5	0.7	1.90%	41.7	1.6	3.72%
C18:1n9	582	44	7.55%	505	9	1.70%	519	5	1.02%	549	32	5.75%
C18:2n6	905	3	0.36%	726	7	0.97%	903	8	0.88%	935	56	5.96%
C18:3n3	23.9	1.3	5.25%	18.6	0.7	3.77%	21.6	0.3	1.49%	21.4	1.3	6.24%
C18:3n6	13.9	0.6	4.35%	14.5	0.7	5.09%	13.4	0.1	0.86%	15.7	1.0	6.14%
C20:0	<10			9.90	0.18	1.82%	Not analyzed			7.54	0.29	3.85%
C20:1n9	<10			Not analyzed			Not analyzed			Not analyzed		
C20:2n6	Not analyzed			Not analyzed			Not analyzed			Not analyzed		
C20:3n6	Not analyzed			37.4	0.9	2.46%	47.5	1.4	2.97%	55.1	3.5	6.37%
C20:4n6	247	4	1.53%	168	8	4.49%	223	4	1.86%	240	13	5.47%
C20:5n3	26.0	1.1	4.24%	20.4	0.9	4.54%	23.1	0.2	1.00%	24.7	1.8	7.28%
C22:0	<10			24.3	0.5	2.25%	16.9	0.8	4.47%	21.2	0.6	2.78%
C22:1n9	<10			1.69	0.00	0.00%	Not analyzed			2.72	0.04	1.32%
C22:4n6	Not analyzed			7.32	0.33	4.55%	6.16	0.12	1.90%	9.09	0.61	6.74%
C22:5n3	16.6	0.4	2.65%	14.5	0.6	3.94%	14.9	0.1	0.67%	15.7	1.1	7.06%
C22:5n6	Not analyzed			5.73	0.38	6.66%	Not analyzed			4.24	0.23	5.38%
C22:6n3	61.5	3.7	6.05%	48.3	3.1	6.49%	51.9	0.4	0.80%	54.9	5.3	9.60%
C24:0	<20			23.2	0.6	2.75%	16.1	0.6	3.98%	24.1	1.6	6.71%
C24:1n9	<20			28.4	0.2	0.75%	18.9	1.3	6.88%	25.6	1.7	6.58%
List any additional information such as known coelutions or results for additional fatty acids below:												
C8:0										0.968	0.061	6.33%
C10:0										1.00	0.02	1.81%
C10:1n1										1.01	0.01	1.25%
C12:0										2.48	0.05	2.01%
C12:1n1										0.843	0.035	4.19%
C12:1n7										0.737	0.029	3.91%
C14:2										0.305	0.021	6.92%
C15:0										5.45	0.29	5.30%
C16:1n-7t												
C16:1n9										11.8	0.5	3.90%
C16:2										1.09	0.07	6.52%
C17:0										6.66	0.40	6.01%
C17:1n9												
9c,11t-CLA												
C18:4n-3												
C19:0										0.750	0.050	6.70%
C 20:3n-3												
C20:3n9										5.74	0.56	9.83%
C20:4n3												
C21:0										0.597	0.064	10.67%
C 22:2n-6												
C23:0										14.5	1.1	7.62%
C26:0										0.227	0.016	7.13%
C26:1										0.190	0.014	7.37%
PhA										0.439	0.022	5.04%
PrA										0.063	0.003	4.76%
density (g/mL)	Not analyzed			Not analyzed			1.05	0.01	1.10%	0.989	0.004	0.38%

^a Reported as μM

Code	Lab 5 ^a			Lab 6 ^a			Lab 7 ^a			Lab 8		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	25.4	0.3	1.01%	25.3	0.4	1.45%	Not analyzed			24.6	0.3	1.28%
C14:1n5				1.38	0.04	3.25%	Not analyzed			Not analyzed		
C16:0	615	2	0.32%	679	7	1.07%	Not analyzed			768	10	1.31%
C16:1n7	33.8	0.6	1.78%	50.3	0.4	0.77%	Not analyzed			52.5	0.8	1.48%
C18:0	199	1	0.56%	179	3	1.41%	Not analyzed			248	2	0.73%
C18:1n7				34.6	0.4	1.28%	Not analyzed			Not analyzed		
C18:1n9	509	2	0.34%	572	0	0.08%	Not analyzed			586	4	0.70%
C18:2n6	912	2	0.25%	992	6	0.61%	Not analyzed			918	16	1.71%
C18:3n3	20.2	0.1	0.54%	25.2	0.1	0.41%	Not analyzed			26.8	0.3	1.21%
C18:3n6				14.69	0.23	1.59%	Not analyzed			Not analyzed		
C20:0				6.52	0.18	2.74%	Not analyzed			Not analyzed		
C20:1n9				4.91	0.05	0.98%	Not analyzed			7.30	0.08	1.15%
C20:2n6	6.10	0.19	3.12%	6.93	0.10	1.48%	Not analyzed			Not analyzed		
C20:3n6				48.5	0.6	1.30%	Not analyzed			60.4	0.4	0.65%
C20:4n6	220	1	0.52%	256	2	0.59%	831	42	5.10%	307	5	1.71%
C20:5n3	21.6	0.2	0.86%	26.09	0.36	1.40%	25.0	0.9	3.58%	32.3	0.5	1.54%
C22:0				23.9	0.2	0.87%	Not analyzed			Not analyzed		
C22:1n9							Not analyzed			Not analyzed		
C22:4n6				7.26	0.26	3.64%	Not analyzed			8.68	0.20	2.28%
C22:5n3	18.2	0.4	2.42%	17.40	0.70	4.02%	Not analyzed			18.1	0.5	2.74%
C22:5n6				5.41	0.12	2.19%	Not analyzed			Not analyzed		
C22:6n3	46.1	1.1	2.37%	66.2	2.9	4.43%	72.9	2.0	2.70%	62.6	1.7	2.64%
C24:0				22.6	0.9	4.08%	Not analyzed			Not analyzed		
C24:1n9				28.9	0.3	0.99%	Not analyzed			Not analyzed		

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0												
C10:1n1												
C12:0												
C12:1n1												
C12:1n7												
C14:2												
C15:0				6.11	0.10	1.56%						
C16:1n-7t												
C16:1n9												
C16:2												
C17:0				8.19	0.21	2.62%						
C17:1n9												
9c,11t-CLA												
C18:4n-3				0.963	0.047	4.86%						
C19:0												
C 20:3n-3												
C20:3n9				2.49	0.11	4.28%						
C20:4n3												
C21:0												
C 22:2n-6												
C23:0				10.9	0.2	1.46%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	Not analyzed			0.967	0.002	0.18%	Not analyzed			1.04	0.01	0.56%

^a Reported as μM

Code	Lab 9 ^a			Lab 10 ^a			Lab 12 ^a			Lab 13 ^a		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	23.2	0.5	2.01%	21.4	0.1	0.40%	51.4	2.8	5.46%	19.8	1.0	4.99%
C14:1n5	1.78	0.09	4.95%	0.875	0.108	12.37%	2.96	0.09	2.95%	1.22	0.21	17.15%
C16:0	621	3	0.52%	532	3	0.54%	594	31	5.30%	650	13	2.00%
C16:1n7	45.8	0.4	0.81%	41.7	0.3	0.64%	37.6	1.3	3.44%	79.5	1.3	1.57%
C18:0	188	1	0.34%	183	1	0.61%	182	6	3.28%	201	2	1.22%
C18:1n7	36.0	0.2	0.66%	35.7	0.4	1.11%	34.0	1.9	5.48%	62.3	1.1	1.75%
C18:1n9	509	4	0.78%	477	4	0.76%	523	30	5.70%	367	4	1.20%
C18:2n6	917	7	0.79%	805	5	0.62%	979	55	5.63%	789	1	0.12%
C18:3n3	19.9	0.3	1.71%	18.3	0.3	1.65%	15.3	0.5	3.14%	20.1	0.9	4.63%
C18:3n6	13.1	0.2	1.08%	11.5	0.1	1.27%	16.3	0.7	4.19%	Not analyzed		
C20:0	6.99	0.02	0.31%	4.79	0.04	0.75%	4.30	0.09	2.08%	4.70	0.69	14.70%
C20:1n9	Not analyzed			4.30	0.06	1.51%	9.95	0.06	0.57%	3.39	0.40	11.82%
C20:2n6	6.55	0.09	1.45%	6.55	0.07	1.08%	7.13	0.20	2.82%	7.62	0.74	9.66%
C20:3n6	48.0	0.2	0.46%	43.1	0.4	0.84%	29.2	6.8	23.33%	64.4	4.5	7.04%
C20:4n6	222	2	0.84%	202	2	0.86%	165	5	2.73%	255	7	2.80%
C20:5n3	22.4	0.2	0.89%	20.4	0.4	1.84%	13.9	0.3	1.90%	53.6	4.8	8.97%
C22:0	22.1	0.1	0.43%	13.67	0.55	4.01%	3.17	0.04	1.11%	14.07	0.84	5.98%
C22:1n9	Not analyzed			1.45	0.17	11.49%	Not analyzed			14.72	14.65	99.57%
C22:4n6	6.22	0.08	1.35%	5.26	0.24	4.55%	6.48	0.15	2.35%	13.53	1.98	14.61%
C22:5n3	14.9	0.0	0.17%	4.17	0.49	11.70%	18.7	1.8	9.56%	28.5	2.6	9.22%
C22:5n6	4.37	0.09	2.10%	13.16	0.02	0.13%	5.97	0.12	1.94%	4.44	0.42	9.56%
C22:6n3	52.7	0.1	0.21%	46.6	0.1	0.31%	30.3	2.3	7.61%	61.4	6.0	9.77%
C24:0	21.8	0.6	2.89%	13.30	0.58	4.33%	1.74	0.09	5.06%	11.50	0.47	4.12%
C24:1n9	24.4	0.6	2.62%	15.77	1.00	6.31%	4.52	0.31	6.94%	17.94	1.11	6.18%

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0				1.49	0.38	25.70%						
C10:1n1												
C12:0				1.51	0.37	24.69%	96.5	10.3	10.67%			
C12:1n1				0.575	0.145	25.23%						
C12:1n7												
C14:2												
C15:0							6.83	0.26	3.77%	9.13	0.55	6.08%
C16:1n-7t							18.4	1.0	5.41%			
C16:1n9												
C16:2												
C17:0				7.11	0.08	1.17%	6.91	0.18	2.63%	18.7	0.5	2.79%
C17:1n9							4.90	0.19	3.95%			
9c,11t-CLA							5.56	0.03	0.53%			
C18:4n-3							0.614	0.217	35.37%			
C19:0							3.81	0.04	1.12%			
C 20:3n-3				0.502	0.121	24.17%	3.44	0.26	7.53%			
C20:3n9				3.06	0.15	4.76%						
C20:4n3							1.81	0.14	7.67%			
C21:0							2.07	0.01	0.54%			
C 22:2n-6				0.600	0.201	33.43%	4.06	0.28	6.81%			
C23:0				6.05	0.21	3.55%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	1.03	0.01	0.56%	1.09	0.01	0.68%	1.03	0.00	0.00%	Not analyzed		

^a Reported as µM

Table 5. Interlaboratory data received for total fatty acids in Unknown 005 (μM)

Code	Lab 1 ^a			Lab 2			Lab 3 ^a			Lab 4		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	109	5	4.25%	129	4	2.80%	106	1	0.86%	97.2	4.0	4.17%
C14:1n5				11.3	0.6	5.09%	Not analyzed			7.80	0.22	2.83%
C16:0	2423	87	3.58%	2419	62	2.58%	2495	25	0.99%	2411	156	6.47%
C16:1n7	187	11	6.02%	170	7	3.92%	190	3	1.52%	209	9	4.28%
C18:0	586	23	3.99%	855	21	2.48%	737	11	1.53%	721	49	6.76%
C18:1n7	104	9	8.89%	200	7	3.26%	128	2	1.90%	146	5	3.72%
C18:1n9	2059	155	7.55%	1789	30	1.70%	1932	20	1.02%	1924	111	5.75%
C18:2n6	3228	11	0.36%	2587	25	0.97%	3386	30	0.88%	3297	197	5.96%
C18:3n3	85.9	4.5	5.25%	66.7	2.5	3.77%	81.7	1.2	1.49%	76.1	4.7	6.24%
C18:3n6	50.0	2.2	4.35%	52.0	2.6	5.09%	50.7	0.4	0.86%	55.7	3.4	6.14%
C20:0				31.7	0.6	1.82%	Not analyzed			23.9	0.9	3.85%
C20:1n9				Not analyzed			Not analyzed			Not analyzed		
C20:2n6	Not analyzed			Not analyzed			Not analyzed			Not analyzed		
C20:3n6	Not analyzed			122	3	2.46%	163	5	2.97%	178	11	6.37%
C20:4n6	812	12	1.53%	553	25	4.49%	771	14	1.86%	779	43	5.47%
C20:5n3	86.1	3.6	4.24%	67.3	3.1	4.54%	80	1	1.00%	80.6	5.9	7.28%
C22:0				71.3	1.6	2.25%	52.2	2.3	4.47%	61.5	1.7	2.78%
C22:1n9				5.00	0.00	0.00%	Not analyzed			7.96	0.11	1.32%
C22:4n6	Not analyzed			22.0	1.0	4.55%	19.5	0.4	1.90%	27.0	1.8	6.74%
C22:5n3	50.3	1.3	2.65%	44.0	1.7	3.94%	47.4	0.3	0.67%	47.0	3.3	7.06%
C22:5n6	Not analyzed			17.3	1.2	6.66%	Not analyzed			12.7	0.7	5.38%
C22:6n3	187	11	6.05%	147	10	6.49%	166	1	0.80%	165	16	9.60%
C24:0				63.0	1.7	2.75%	46.0	1.8	3.98%	64.8	4.3	6.71%
C24:1n9				77.3	0.6	0.75%	54.2	3.7	6.88%	69.0	4.5	6.58%

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0										6.64	0.42	6.33%
C10:0										5.76	0.10	1.81%
C10:1n1										5.88	0.07	1.25%
C12:0										12.3	0.2	2.01%
C12:1n1										4.20	0.18	4.19%
C12:1n7										3.68	0.14	3.91%
C14:2										1.34	0.09	6.92%
C15:0										22.3	1.2	5.30%
C16:1n-7t												
C16:1n9										46.0	1.8	3.90%
C16:2										4.27	0.28	6.52%
C17:0										24.4	1.5	6.01%
C17:1n9												
9c,11t-CLA												
C18:4n-3												
C19:0										2.49	0.17	6.70%
C 20:3n-3												
C20:3n9										18.5	1.8	9.83%
C20:4n3												
C21:0										1.81	0.19	10.67%
C 22:2n-6												
C23:0										40.6	3.1	7.62%
C26:0										0.567	0.040	7.13%
C26:1										0.477	0.035	7.37%
PhA										1.39	0.07	5.04%
PrA										0.210	0.010	4.76%
density (g/mL)	Not analyzed			Not analyzed			1.05	0.01	1.10%	0.989	0.004	0.38%

^a Reported as $\mu\text{g/g}$

Code	Lab 5			Lab 6			Lab 7			Lab 8 ^a		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	111	1	1.01%	107	2	1.50%	Not analyzed			112	1	1.24%
C14:1n5				5.89	0.19	3.25%	Not analyzed			Not analyzed		
C16:0	2399	8	0.32%	2558	27	1.07%	Not analyzed			3104	41	1.31%
C16:1n7	133	2	1.78%	191	1	0.77%	Not analyzed			214	3	1.48%
C18:0	700	4	0.56%	608	9	1.41%	Not analyzed			905	7	0.73%
C18:1n7				118	2	1.28%	Not analyzed			Not analyzed		
C18:1n9	1803	6	0.34%	1958	2	0.08%	Not analyzed			2149	15	0.70%
C18:2n6	3253	8	0.25%	3419	21	0.61%	Not analyzed			3394	58	1.71%
C18:3n3	72.5	0.4	0.54%	87.3	0.4	0.41%	Not analyzed			100	1	1.21%
C18:3n6				51.0	0.8	1.59%	Not analyzed			Not analyzed		
C20:0				20.2	0.6	2.74%	Not analyzed			Not analyzed		
C20:1n9				15.3	0.1	0.98%	Not analyzed			24.4	0.3	1.15%
C20:2n6	19.5	0.6	3.12%	21.7	0.3	1.48%	Not analyzed			Not analyzed		
C20:3n6				153	2	1.30%	Not analyzed			204	1	0.65%
C20:4n6	723	4	0.52%	814	5	0.59%	2727	139	5.10%	1046	18	1.71%
C20:5n3	71.4	0.6	0.86%	83.4	1.2	1.40%	82.6	3.0	3.58%	111	2	1.54%
C22:0				67.8	0.6	0.87%	Not analyzed			Not analyzed		
C22:1n9							Not analyzed			Not analyzed		
C22:4n6				21.1	0.8	3.64%	Not analyzed			27.1	0.6	2.28%
C22:5n3	55.0	1.3	2.42%	50.9	2.0	4.02%	Not analyzed			56.7	1.6	2.74%
C22:5n6				15.8	0.3	2.19%	Not analyzed			Not analyzed		
C22:6n3	140	3	2.37%	195	9	4.43%	222	6	2.70%	198	5	2.64%
C24:0				59.3	2.4	4.08%	Not analyzed			Not analyzed		
C24:1n9				76.1	0.8	0.99%	Not analyzed			Not analyzed		

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0												
C10:1n1												
C12:0												
C12:1n1												
C12:1n7												
C14:2												
C15:0				24.4	0.4	1.56%						
C16:1n-7t												
C16:1n9												
C16:2												
C17:0				29.3	0.8	2.62%						
C17:1n9												
9c,11t-CLA												
C18:4n-3				3.37	0.16	4.86%						
C19:0												
C 20:3n-3												
C20:3n9				7.86	0.34	4.28%						
C20:4n3												
C21:0												
C 22:2n-6												
C23:0				29.6	0.4	1.46%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	Not analyzed			0.967	0.002	0.18%	Not analyzed			1.04	0.01	0.56%

^a Reported as $\mu\text{g/g}$

Code	Lab 9			Lab 10			Lab 12			Lab 13		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	104	2	1.46%	103	0	0.37%	231	12	5.33%	86.9	4.3	4.99%
C14:1n5	8.09	0.36	4.39%	4.22	0.52	12.37%	13.4	0.4	2.95%	5.39	0.92	17.15%
C16:0	2487	12	0.46%	2264	12	0.54%	2375	126	5.30%	2535	51	2.00%
C16:1n7	185	2	0.94%	179	1	0.64%	151	5	3.44%	312	5	1.57%
C18:0	678	6	0.90%	701	4	0.61%	657	22	3.28%	707	9	1.22%
C18:1n7	131	2	1.17%	138	2	1.11%	123	7	5.48%	220	4	1.75%
C18:1n9	1850	10	0.54%	1843	14	0.76%	1896	108	5.70%	1297	16	1.20%
C18:2n6	3357	15	0.46%	3132	19	0.62%	3577	201	5.63%	2813	3	0.12%
C18:3n3	73.3	1.2	1.57%	71.8	1.2	1.65%	56.3	1.8	3.14%	72.0	3.3	4.63%
C18:3n6	48.4	0.9	1.84%	45.0	0.6	1.27%	59.9	2.5	4.19%	Not analyzed		
C20:0	23.0	0.1	0.25%	16.7	0.1	0.75%	14.1	0.3	2.08%	15.0	2.2	14.70%
C20:1n9	Not analyzed			15.1	0.2	1.51%	32.9	0.2	0.57%	10.9	1.3	11.82%
C20:2n6	21.8	0.4	2.00%	23.2	0.3	1.08%	23.7	0.7	2.82%	24.4	2.4	9.66%
C20:3n6	161	2	0.95%	154	1	0.84%	97.5	22.8	23.33%	210	15	7.04%
C20:4n6	750	3	0.35%	724	6	0.86%	555	15	2.73%	838	23	2.80%
C20:5n3	76.1	1.0	1.26%	73.7	1.4	1.84%	47.2	0.9	1.90%	177	16	8.97%
C22:0	66.5	0.3	0.40%	43.8	1.8	4.01%	9.54	0.11	1.11%	41.3	2.5	5.98%
C22:1n9	Not analyzed			4.67	0.54	11.49%	Not analyzed			43.5	43.3	99.57%
C22:4n6	19.2	0.4	1.88%	17.3	0.8	4.55%	20.0	0.5	2.35%	40.7	5.9	14.61%
C22:5n3	46.1	0.2	0.45%	13.8	1.6	11.70%	57.9	5.5	9.56%	86.2	8.0	9.22%
C22:5n6	13.6	0.4	2.59%	43.5	0.1	0.13%	18.5	0.4	1.94%	13.4	1.3	9.56%
C22:6n3	165	1	0.35%	155	0	0.31%	94.7	7.2	7.61%	187	18	9.77%
C24:0	60.7	2.1	3.44%	39.4	1.7	4.33%	4.84	0.24	5.06%	31.2	1.3	4.12%
C24:1n9	68.3	2.2	3.17%	47.0	3.0	6.31%	12.6	0.9	6.94%	48.9	3.0	6.18%

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0				9.43	2.42	25.70%						
C10:1n1												
C12:0				8.21	2.03	24.69%	494	53	10.67%			
C12:1n1				3.17	0.80	25.23%						
C12:1n7												
C14:2												
C15:0							28.9	1.1	3.77%	37.7	2.3	6.08%
C16:1n-7t							73.9	4.0	5.41%			
C16:1n9												
C16:2												
C17:0				28.7	0.3	1.17%	26.2	0.7	2.63%	69.3	1.9	2.79%
C17:1n9							18.7	0.7	3.95%			
9c,11t-CLA							20.3	0.1	0.53%			
C18:4n-3							2.28	0.81	35.37%			
C19:0							13.1	0.1	1.12%			
C 20:3n-3				1.79	0.43	24.17%	11.5	0.9	7.53%			
C20:3n9				10.9	0.5	4.76%						
C20:4n3							6.10	0.47	7.67%			
C21:0							6.48	0.03	0.54%			
C 22:2n-6				1.95	0.65	33.43%	12.4	0.8	6.81%			
C23:0				18.6	0.7	3.55%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	1.03	0.01	0.56%	1.09	0.01	0.68%	1.03	0.00	0.00%	Not analyzed		

^aReported as $\mu\text{g/g}$

Code	Lab 1			Lab 2 ^a			Lab 3			Lab 4 ^a		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	31.7	1.5	4.69%	36.8	1.0	2.85%	29.0	0.3	0.87%	27.6	0.4	1.57%
C14:1n5	<10			3.47	0.13	3.77%	NA			2.23	0.10	4.38%
C16:0	709	13	1.88%	666	27	4.10%	637	13	2.00%	646	8	1.16%
C16:1n7	51.2	4.7	9.09%	48.9	1.6	3.25%	50.3	1.0	2.03%	57.6	0.7	1.23%
C18:0	182	16	8.88%	259	8	3.05%	212	3	1.42%	207	3	1.40%
C18:1n7	37.0	1.6	4.29%	57.4	1.7	2.96%	35.6	0.6	1.55%	42.3	2.3	5.48%
C18:1n9	537	42	7.80%	513	11	2.22%	534	3	0.60%	548	7	1.34%
C18:2n6	993	28	2.80%	781	18	2.28%	989	8	0.77%	973	13	1.36%
C18:3n3	24.2	1.0	4.24%	20.0	1.4	6.88%	21.1	0.3	1.45%	20.4	0.2	1.01%
C18:3n6	13.2	0.6	4.42%	14.0	0.4	3.03%	13.5	0.6	4.12%	13.2	0.2	1.71%
C20:0	<10			11.0	0.4	3.27%	Not analyzed			8.29	0.08	1.01%
C20:1n9	<10			Not analyzed			Not analyzed			Not analyzed		
C20:2n6	Not analyzed			Not analyzed			Not analyzed			Not analyzed		
C20:3n6	Not analyzed			34.1	1.7	5.11%	40.5	0.6	1.36%	45.5	0.7	1.49%
C20:4n6	205	17	8.35%	151	2	1.53%	194	7	3.38%	198	3	1.51%
C20:5n3	40.6	2.9	7.25%	34.2	0.6	1.77%	37.9	0.6	1.69%	37.2	0.4	1.10%
C22:0	<10			25.0	1.0	4.09%	17.1	0.7	3.99%	21.4	0.4	2.08%
C22:1n9	<10			1.81	0.20	10.83%	NA			2.91	0.07	2.51%
C22:4n6	Not analyzed			6.54	0.38	5.87%	5.38	0.28	5.16%	7.09	0.08	1.19%
C22:5n3	15.2	1.3	8.40%	14.2	1.1	8.06%	14.4	0.4	2.43%	13.87	0.15	1.11%
C22:5n6	ND			5.07	0.19	3.77%	NA			3.33	0.06	1.79%
C22:6n3	68.2	5.7	8.29%	54.1	0.9	1.75%	56.1	0.4	0.64%	53.8	0.8	1.43%
C24:0	<20			23.1	0.9	3.69%	15.5	0.4	2.58%	22.9	0.3	1.21%
C24:1n9	<20			34.7	1.5	4.27%	24.7	1.6	6.28%	32.1	0.6	1.81%
List any additional information such as known coelutions or results for additional fatty acids below:												
C8:0										1.05	0.05	4.34%
C10:0										1.15	0.02	1.46%
C10:1n1										1.02	0.02	2.37%
C12:0										3.67	0.06	1.65%
C12:1n1										0.906	0.020	2.26%
C12:1n7										0.816	0.013	1.55%
C14:2										0.298	0.022	7.42%
C15:0										4.23	0.06	1.46%
C16:1n-7t												
C16:1n9										10.4	0.2	1.55%
C16:2										1.21	0.03	2.14%
C17:0										6.00	0.06	1.01%
C17:0												
C17:1n9												
9c,11t-CLA												
C18:4n-3										0.684	0.010	1.43%
C19:0												
C 20:3n-3										4.19	0.14	3.26%
C20:3n9												
C20:4n3										0.531	0.013	2.37%
C21:0												
C 22:2n-6												
C23:0										14.7	0.1	0.95%
C26:0										0.225	0.002	1.04%
C26:1										0.243	0.006	2.53%
PhA										0.433	0.007	1.53%
PrA										0.108	0.002	1.63%
density (g/mL)	Not analyzed			Not analyzed			1.03	0.01	1.01%	0.979	0.002	0.21%

^a Reported as μM

Code	Lab 5 ^a			Lab 6 ^a			Lab 7 ^a			Lab 8		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	32.8	0.2	0.54%	32.1	0.6	1.76%	Not analyzed			32.7	0.5	1.47%
C14:1n5				1.84	0.03	1.53%	Not analyzed			NA		
C16:0	671	8	1.19%	719	13	1.84%	Not analyzed			806	11	1.36%
C16:1n7	40.0	1.1	2.80%	55.3	1.7	3.08%	Not analyzed			58.3	0.7	1.17%
C18:0	214	3	1.26%	190	1	0.42%	Not analyzed			258	4	1.62%
C18:1n7				35.8	1.6	4.55%	Not analyzed			NA		
C18:1n9	529	5	0.89%	575	20	3.44%	Not analyzed			577	6	1.09%
C18:2n6	1013	8	0.82%	1062	44	4.14%	Not analyzed			945	8	0.88%
C18:3n3	20.1	0.2	1.09%	24.7	0.7	2.98%	Not analyzed			26.2	0.3	1.11%
C18:3n6				14.4	0.6	3.91%	Not analyzed			NA		
C20:0				7.28	0.15	2.08%	Not analyzed			NA		
C20:1n9				3.98	0.16	3.92%	Not analyzed			6.54	0.06	0.86%
C20:2n6	5.63	0.17	2.94%	5.97	0.07	1.24%	Not analyzed			NA		
C20:3n6				43.1	1.1	2.50%	Not analyzed			51.4	0.8	1.47%
C20:4n6	194	1	0.66%	217	6	2.66%	585	21	3.60%	250	4	1.68%
C20:5n3	35.5	0.2	0.65%	41.3	1.6	3.83%	39.9	2.4	6.01%	49.1	0.8	1.62%
C22:0				24.1	0.3	1.12%	Not analyzed			NA		
C22:1n9							Not analyzed			NA		
C22:4n6				6.07	0.30	4.99%	Not analyzed			7.31	0.78	10.73%
C22:5n3	18.7	0.3	1.50%	16.2	0.4	2.68%	Not analyzed			17.3	0.4	2.27%
C22:5n6				4.30	0.12	2.80%	Not analyzed			NA		
C22:6n3	51.1	0.9	1.78%	69.5	1.7	2.39%	80.5	5.2	6.41%	66.7	1.1	1.60%
C24:0				22.1	0.5	2.46%	Not analyzed			NA		
C24:1n9				35.9	0.6	1.73%	Not analyzed			NA		

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0												
C10:1n1												
C12:0												
C12:1n1												
C12:1n7												
C14:2												
C15:0				4.69	0.12	2.54%						
C16:1n-7t												
C16:1n9												
C16:2												
C17:0				7.46	0.17	2.28%						
C17:0												
C17:1n9												
9c,11t-CLA				1.18	0.04	3.44%						
C18:4n-3												
C19:0												
C 20:3n-3				1.90	0.02	0.98%						
C20:3n9												
C20:4n3												
C21:0												
C 22:2n-6												
C23:0				11.2	0.2	1.36%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	Not analyzed			0.954	0.001	0.13%	Not analyzed			1.03	0	0.00%

^a Reported as μM

Code	Lab 9 ^a			Lab 10 ^a			Lab 12 ^a			Lab 13 ^a		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	29.2	0.1	0.40%	26.7	0.2	0.65%	58.7	4.5	7.69%	24.4	1.1	4.57%
C14:1n5	2.38	0.05	1.90%	1.35	0.14	10.13%	3.65	0.62	17.02%	1.71	0.21	12.52%
C16:0	661	4	0.57%	561	2	0.29%	652	48	7.37%	665	28	4.17%
C16:1n7	50.6	0.1	0.28%	44.9	0.2	0.36%	44.3	3.7	8.40%	85.0	2.4	2.85%
C18:0	196	3	1.35%	193	1	0.63%	191	15	7.98%	202	4	2.17%
C18:1n7	37.1	0.1	0.14%	35.6	0.1	0.30%	38.4	2.1	5.43%	63.8	0.8	1.20%
C18:1n9	518	3	0.49%	485	1	0.20%	548	37	6.80%	356	7	1.87%
C18:2n6	995	5	0.49%	872	1	0.08%	1113	87	7.83%	821	8	1.03%
C18:3n3	20.2	0.3	1.65%	18.1	0.1	0.59%	16.2	1.3	8.26%	16.7	0.6	3.56%
C18:3n6	13.2	0.2	1.58%	11.3	0.1	0.72%	17.8	1.1	6.05%	Not analyzed		
C20:0	7.84	0.10	1.30%	5.23	0.35	6.65%	4.70	0.48	10.11%	4.83	1.22	25.24%
C20:1n9	Not analyzed			3.84	0.14	3.74%	9.96	1.03	10.31%	3.18	0.43	13.37%
C20:2n6	5.85	0.03	0.58%	5.92	0.15	2.61%	6.66	0.55	8.19%	7.17	0.73	10.14%
C20:3n6	40.8	0.3	0.79%	37.1	0.1	0.37%	23.6	2.3	9.92%	59.1	3.0	5.09%
C20:4n6	189	1	0.66%	173	0	0.10%	127.1	9.6	7.52%	215	15	7.03%
C20:5n3	36.3	0.2	0.43%	33.2	0.1	0.32%	23.7	2.6	11.10%	65.3	1.0	1.58%
C22:0	22.1	0.3	1.21%	13.6	0.6	4.11%	3.69	0.37	10.03%	12.9	2.2	16.85%
C22:1n9	Not analyzed			1.71	0.16	9.54%	Not analyzed			11.2	10.2	90.29%
C22:4n6	5.19	0.09	1.72%	4.50	0.20	4.47%	6.00	1.11	18.51%	11.6	0.8	6.74%
C22:5n3	14.04	0.17	1.19%	3.69	0.31	8.32%	19.9	1.9	9.55%	24.5	2.1	8.40%
C22:5n6	3.69	0.08	2.17%	12.6	0.3	2.42%	6.23	0.49	7.92%	3.42	0.16	4.57%
C22:6n3	57.1	0.4	0.61%	50.0	0.1	0.18%	35.6	7.3	20.42%	59.2	2.8	4.64%
C24:0	20.8	0.3	1.51%	12.2	0.6	5.32%	2.15	0.19	8.63%	10.5	2.3	22.35%
C24:1n9	30.9	0.6	1.85%	19.1	0.9	4.97%	5.26	0.97	18.47%	21.1	5.9	28.10%

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0				1.65	0.40	24.08%						
C10:1n1												
C12:0				2.48	0.41	16.58%	103	7	7.09%			
C12:1n1				0.875	0.256	29.25%						
C12:1n7												
C14:2												
C15:0							6.16	0.24	3.86%	6.97	0.31	4.48%
C16:1n-7t							18.6	0.9	5.10%			
C16:1n9												
C16:2												
C17:0				6.58	0.05	0.79%	6.93	0.52	7.46%	15.7	1.1	6.74%
C17:0							5.27	0.44	8.29%			
C17:1n9												
9c,11t-CLA							1.42	0.20	13.98%			
C18:4n-3							4.11	0.47	11.38%			
C19:0				0.550	0.066	12.03%	3.61	0.47	12.94%			
C 20:3n-3				2.48	0.10	4.04%						
C20:3n9							1.46	0.33	22.50%			
C20:4n3							2.10	0.22	10.26%			
C21:0				0.464	0.194	41.93%	4.60	0.52	11.23%			
C 22:2n-6				0.478	0.200	41.93%	4.74	0.53	11.23%			
C23:0				5.70	0.39	6.89%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	1.02	0.01	0.57%	1.09	0.00	0.40%	1.03	0.00	0.00%	Not analyzed		

^a Reported as µM

Code	Lab 1 ^a			Lab 2			Lab 3 ^a			Lab 4		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	139	7	4.69%	161	5	2.85%	130	1	0.87%	118	2	1.57%
C14:1n5				15.3	0.6	3.77%	Not analyzed			9.63	0.42	4.38%
C16:0	2766	52	1.88%	2599	107	4.10%	2553	51	2.00%	2466	29	1.16%
C16:1n7	201	18	9.09%	192	6	3.25%	203	4	2.03%	222	3	1.23%
C18:0	641	57	8.88%	911	28	3.05%	766	11	1.42%	713	10	1.40%
C18:1n7	131	6	4.29%	203	6	2.96%	130	2	1.55%	147	8	5.48%
C18:1n9	1902	148	7.80%	1817	40	2.22%	1945	12	0.60%	1901	25	1.34%
C18:2n6	3539	99	2.80%	2783	64	2.28%	3627	28	0.77%	3397	46	1.36%
C18:3n3	86.8	3.7	4.24%	71.7	4.9	6.88%	78.0	1.1	1.45%	71.7	0.7	1.01%
C18:3n6	47.5	2.1	4.42%	50.3	1.5	3.03%	49.9	2.1	4.12%	46.6	0.8	1.71%
C20:0				35.3	1.2	3.27%	Not analyzed			26.0	0.3	1.01%
C20:1n9				Not analyzed			Not analyzed			Not analyzed		
C20:2n6	Not analyzed			Not analyzed			Not analyzed			Not analyzed		
C20:3n6	Not analyzed			111	6	5.11%	136	2	1.36%	145	2	1.49%
C20:4n6	672	56	8.35%	494	8	1.53%	655	22	3.38%	637	10	1.51%
C20:5n3	134	10	7.25%	113	2	1.77%	129	2	1.69%	121	1	1.10%
C22:0				73.5	3.0	4.09%	51.5	2.1	3.99%	61.6	1.3	2.08%
C22:1n9				5.33	0.58	10.83%	Not analyzed			8.41	0.21	2.51%
C22:4n6	Not analyzed			19.7	1.2	5.87%	16.6	0.9	5.16%	20.9	0.2	1.19%
C22:5n3	46.0	3.9	8.40%	43.0	3.5	8.06%	44.9	1.1	2.43%	41.1	0.5	1.11%
C22:5n6	Not analyzed			15.3	0.6	3.77%	Not analyzed			9.86	0.18	1.79%
C22:6n3	207	17	8.29%	165	3	1.75%	176	1	0.64%	160	2	1.43%
C24:0				62.7	2.3	3.69%	43.2	1.1	2.58%	60.8	0.7	1.21%
C24:1n9				94.7	4.0	4.27%	69	4	6.28%	85.9	1.6	1.81%
List any additional information such as known coelutions or results for additional fatty acids below:												
C8:0										7.16	0.31	4.34%
C10:0										6.55	0.10	1.46%
C10:1n1										5.87	0.14	2.37%
C12:0										17.9	0.3	1.65%
C12:1n1										4.47	0.10	2.26%
C12:1n7										4.03	0.06	1.55%
C14:2										1.30	0.10	7.42%
C15:0										17.1	0.3	1.46%
C16:1n-7t												
C16:1n9										40.2	0.6	1.55%
C16:2										4.68	0.10	2.14%
C17:0										21.7	0.2	1.01%
C17:1n9												
9c,11t-CLA												
C18:4n-3												
C19:0										2.24	0.03	1.43%
C 20:3n-3												
C20:3n9										13.4	0.4	3.26%
C20:4n3												
C21:0										1.71	0.04	2.37%
C 22:2n-6												
C23:0										40.6	0.4	0.95%
C26:0										0.557	0.006	1.04%
C26:1										0.603	0.015	2.53%
PhA										1.36	0.02	1.53%
PrA										0.353	0.006	1.63%
density (g/mL)	Not analyzed			Not analyzed			1.03	0.01	1.01%	0.979	0.002	0.21%

^a Reported as $\mu\text{g/g}$

Table 7 (cont). Interlaboratory data received for total fatty acids in Unknown 006 (μM)

Code	Lab 5			Lab 6			Lab 7			Lab 8 ^a		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	143	1	0.54%	134	2	1.76%	Not analyzed			147	2	1.47%
C14:1n5				7.74	0.12	1.53%	Not analyzed			Not analyzed		
C16:0	2616	31	1.19%	2675	49	1.84%	Not analyzed			3237	44	1.36%
C16:1n7	157	4	2.80%	207	6	3.08%	Not analyzed			236	3	1.17%
C18:0	752	9	1.26%	638	3	0.42%	Not analyzed			933	15	1.62%
C18:1n7				121	5	4.55%	Not analyzed			Not analyzed		
C18:1n9	1872	17	0.89%	1944	67	3.44%	Not analyzed			2103	23	1.09%
C18:2n6	3610	29	0.82%	3615	150	4.14%	Not analyzed			3472	31	0.88%
C18:3n3	72.3	0.8	1.09%	84.8	2.5	2.98%	Not analyzed			97	1	1.11%
C18:3n6				49.3	1.9	3.91%	Not analyzed			Not analyzed		
C20:0				22.2	0.5	2.08%	Not analyzed			Not analyzed		
C20:1n9				12.2	0.5	3.92%	Not analyzed			21.7	0.2	0.86%
C20:2n6	18.0	0.5	2.94%	18.5	0.2	1.24%	Not analyzed			Not analyzed		
C20:3n6				134	3	2.50%	Not analyzed			173	3	1.47%
C20:4n6	636	4	0.66%	679	18	2.66%	1920	69	3.60%	846	14	1.68%
C20:5n3	117	1	0.65%	130	5	3.83%	132	8	6.01%	167	3	1.62%
C22:0				67.6	0.8	1.12%	Not analyzed			Not analyzed		
C22:1n9							Not analyzed			Not analyzed		
C22:4n6				17.4	0.9	4.99%	Not analyzed			22.7	2.4	10.73%
C22:5n3	56.7	0.9	1.50%	46.8	1.3	2.68%	Not analyzed			53.9	1.2	2.27%
C22:5n6				12.4	0.3	2.80%	Not analyzed			Not analyzed		
C22:6n3	156	3	1.78%	202	5	2.39%	245	16	6.41%	209	3	1.60%
C24:0				57.2	1.4	2.46%	Not analyzed			Not analyzed		
C24:1n9				93.5	1.6	1.73%	Not analyzed			Not analyzed		

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0												
C10:1n1												
C12:0												
C12:1n1												
C12:1n7												
C14:2												
C15:0				18.5	0.5	2.54%						
C16:1n-7t												
C16:1n9												
C16:2												
C17:0				26.3	0.6	2.28%						
C17:1n9												
9c,11t-CLA												
C18:4n-3				4.06	0.14	3.44%						
C19:0												
C 20:3n-3												
C20:3n9				5.92	0.06	0.98%						
C20:4n3												
C21:0												
C 22:2n-6												
C23:0				30.1	0.4	1.36%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	Not analyzed			0.954	0.001	0.13%	Not analyzed			1.03	0.00	0.00%

^a Reported as $\mu\text{g/g}$

Code	Lab 9			Lab 10			Lab 12			Lab 13		
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd
C14:0	130	1	0.77%	127	1	0.65%	264	20	7.69%	107	5	4.57%
C14:1n5	10.7	0.2	1.43%	6.50	0.66	10.13%	16.5	2.8	17.02%	7.57	0.95	12.52%
C16:0	2620	0	0.00%	2382	7	0.29%	2608	192	7.37%	2593	108	4.17%
C16:1n7	202	1	0.50%	192	1	0.36%	179	15	8.40%	334	10	2.85%
C18:0	702	9	1.21%	741	5	0.63%	689	55	7.98%	711	15	2.17%
C18:1n7	134	1	0.43%	137	0	0.30%	139	8	5.43%	226	3	1.20%
C18:1n9	1863	6	0.31%	1870	4	0.20%	1989	135	6.80%	1260	24	1.87%
C18:2n6	3607	12	0.32%	3389	3	0.08%	4066	318	7.83%	2926	30	1.03%
C18:3n3	73.7	1.0	1.34%	70.9	0.4	0.59%	59.7	4.9	8.26%	59.9	2.1	3.56%
C18:3n6	48.3	0.5	1.04%	44.4	0.3	0.72%	65.4	4.0	6.05%	Not analyzed		
C20:0	25.5	0.3	1.18%	18.2	1.2	6.65%	15.4	1.6	10.11%	15.44	3.90	25.24%
C20:1n9	Not analyzed			13.5	0.5	3.74%	32.9	3.4	10.31%	10.24	1.37	13.37%
C20:2n6	19.3	0.1	0.60%	20.9	0.5	2.61%	22.1	1.8	8.19%	23.2	2.4	10.14%
C20:3n6	135	2	1.13%	132	0	0.37%	78.8	7.8	9.92%	193	10	5.09%
C20:4n6	630	3	0.40%	619	1	0.10%	428	32	7.52%	707	50	7.03%
C20:5n3	122	1	0.82%	120	0	0.32%	80.2	8.9	11.10%	216	3	1.58%
C22:0	66.1	0.8	1.14%	43.4	1.8	4.11%	11.1	1.1	10.03%	37.7	6.4	16.85%
C22:1n9	Not analyzed			5.49	0.52	9.54%	Not analyzed			33.2	30.0	90.29%
C22:4n6	15.9	0.4	2.21%	14.8	0.7	4.47%	18.5	3.4	18.51%	34.9	2.4	6.74%
C22:5n3	43.2	0.7	1.54%	12.2	1.0	8.32%	61.6	5.9	9.55%	74.2	6.2	8.40%
C22:5n6	11.3	0.3	2.70%	41.5	1.0	2.42%	19.3	1.5	7.92%	10.33	0.47	4.57%
C22:6n3	177	1	0.65%	166	0	0.18%	111	23	20.42%	180	8	4.64%
C24:0	57.5	0.9	1.50%	36.1	1.9	5.32%	5.97	0.52	8.63%	28.5	6.4	22.35%
C24:1n9	85.7	1.6	1.82%	56.7	2.8	4.97%	14.7	2.7	18.47%	57.5	16.2	28.10%

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0												
C10:0				10.5	2.5	24.08%						
C10:1n1												
C12:0				13.5	2.2	16.58%	524	37	7.09%			
C12:1n1				4.81	1.41	29.25%						
C12:1n7												
C14:2												
C15:0							26.1	1.0	3.86%	28.7	1.3	4.48%
C16:1n-7t							75.0	3.8	5.10%			
C16:1n9												
C16:2												
C17:0				26.5	0.2	0.79%	26.3	2.0	7.46%	58.1	3.9	6.74%
C17:1n9							20.1	1.7	8.29%			
9c,11t-CLA							21.0	2.0	9.44%			
C18:4n-3							5.27	0.74	13.98%			
C19:0							14.1	1.6	11.38%			
C 20:3n-3				1.96	0.24	12.03%	12.1	1.6	12.94%			
C20:3n9				8.83	0.36	4.04%						
C20:4n3							4.90	1.10	22.50%			
C21:0							7.06	0.72	10.26%			
C 22:2n-6				1.55	0.65	41.93%	14.4	1.6	11.23%			
C23:0				17.5	1.2	6.89%						
C26:0												
C26:1												
PhA												
PrA												
density (g/mL)	1.02	0.01	0.57%	1.09	0.00	0.40%	1.03	0.00	0.00%	Not analyzed		

^a Reported as µg/g

Table 8. Interlaboratory data received for total fatty acids in SRM 1950 ($\mu\text{g/g}$)

Code	COA ^a	Lab 1	Lab 2 ^b	Lab 3	Lab 4 ^b	Lab 5 ^b	Lab 6 ^b	Lab 7 ^b	Lab 8	Lab 9 ^b	Lab 10 ^b	Lab 12 ^b	Lab 13 ^b
C14:0	17.9 ± 3.8	20.9	28.8	22.2	23.1	26.1	25.1	NA	27.0	22.5	20.1	62.2	21.8
C14:1n5	1.57 ± 0.03	<10	3.17	NA	2.34		1.82	NA	NA	2.21	1.29	3.93	1.57
C16:0	594 ± 19	595	595	581	639	623	643	NA	786	594	504	767	683
C16:1n7	53.5 ± 6.4	57.4	58.8	62.1	81.9	55.8	70.5	NA	75.9	63.7	59.0	65.5	133
C18:0	179 ± 12	185	218	179	201	191	163	NA	235	167	166	193	199
C18:1n7	37.7 ± 0.9	47.3	70.6	37.6	85.5		36.2	NA	NA	39.7	45.1	45.4	99.0
C18:1n9	447 ± 43	468	480	485	550	511	528	NA	601	470	456	685	365
C18:2n6	780 ± 39	742	646	769	862	822	851	NA	836	780	690	1106	751
C18:3n3	14.9 ± 1.0	14.6	12.8	13.7	15.2	14.7	16.4	NA	18.6	13.0	12.3	18.1	19.6
C18:3n6	10.9 ± 2.3	11.1	13.1	14.2	15.2		15.1	NA	NA	13.8	12.09	18.6	NA
C20:0	5.5 ± 0.2	<10	8.13	NA	6.07		5.14	NA	NA	5.57	3.80	4.49	3.86
C20:1n9	3.5 ± 0.1	<10	NA	NA	NA		3.30	NA	6.12	NA	3.02	10.29	NA
C20:2n6	5.7 ± 0.2	NA	NA	NA	NA	5.15	5.64	NA	NA	5.32	5.34	7.57	NA
C20:3n6	41.8 ± 1.1	NA	32.5	39.4	50.2		41.1	NA	53.2	40.1	36.6	31.5	40.6
C20:4n6	293 ± 54	295	150	200	229	214	228	336	255	198	182	170	232
C20:5n3	11.4 ± 0.1	11.6	10.6	12.3	13.7	12.1	13.5	11.6	17.0	11.56	10.63	10.81	34.0
C22:0	15.9 ± 1.5	<10	19.2	13.6	17.6		18.3	NA	NA	17.1	10.65	3.23	11.79
C22:1n9	1.1 ± 0.4	<10	2.03	NA	2.43		0.0	NA	NA	NA	0.058	NA	26.7
C22:4n6	8.3 ± 0.2	NA	8.98	7.92	12.50		9.17	NA	10.2	7.80	6.95	7.00	15.30
C22:5n3	12.5 ± 0.2	12.2	11.6	12.6	14.25	15.2	14.32	NA	15.5	12.34	5.22	17.5	19.4
C22:5n6	6.3 ± 0.1	NA	7.60	NA	6.06		6.94	NA	NA	5.73	10.90	7.20	4.65
C22:6n3	37.9 ± 6.8	37.8	28.9	30.9	36.8	29.5	39.4	39.1	39.2	32.3	27.9	30.5	38.4
C24:0	16.8 ± 0.9	<20	17.3	11.9	19.0		16.7	NA	NA	15.62	9.09	1.75	7.83
C24:1n9	25.6 ± 1.2	<20	26.0	18.2	26.2		26.5	NA	NA	22.1	13.87	4.52	14.81

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0					0.772								
C10:0					0.729						1.03		
C10:1n1					0.974								
C12:0	1.86 ± 0.11				2.47						1.69	103	
C12:1n1					0.903						0.492		
C12:1n7					0.804								
C14:2					0.271								
C15:0	1.08 ± 0.01				3.71		3.78					5.33	6.39
C16:1n-7t												18.2	
C16:1n9					10.2								
C16:2					1.41								
C17:0	4.7 ± 0.2				5.84		6.60				5.55	5.95	13.9
C17:1n9												5.46	
9c,11t-CLA												5.79	
C18:4n-3							0.860					0.674	
C19:0					0.676							3.59	
C 20:3n-3											0.455	3.47	
C20:3n9					5.64		2.56				3.07		
C20:4n3												1.49	
C21:0					0.492							1.94	
C 22:2n-6					0.000						0.501	4.07	
C23:0					11.952		7.45				3.77		
C26:0					0.182								
C26:1					0.209								
PhA					0.231								
PrA					0.042								
density (g/mL)	NA ^c	NA ^c	NA ^c	1.04	1.00	NA ^c	0.948	NA ^c	1.03	1.01	1.07	1.03	NA ^c

^a Certified (bold) and reference values from the Certificate of Analysis (COA) for SRM 1950

^b Reported as μM

^c NA = not analyzed

Table 9. Interlaboratory data received for total fatty acids in SRM 1950 (μM)

Code	COA ^a	Lab 1 ^b	Lab 2	Lab 3 ^b	Lab 4	Lab 5	Lab 6	Lab 7	Lab 8 ^b	Lab 9	Lab 10	Lab 12	Lab 13
C14:0	80.1 ± 17.0	91.4	126	101	101	114	104	NA	122	99.3	94.5	279	95.3
C14:1n5	7.1 ± 0.1		14.0	NA	10.4		7.62	NA	NA	9.84	6.13	17.8	6.93
C16:0	2364 ± 77	2320	2319	2356	2498	2428	2377	NA	3158	2340	2110	3065	2664
C16:1n7	215 ± 26	225	231	254	323	219	263	NA	307	253	249	264	523
C18:0	644 ± 41	650	768	654	709	671	544	NA	850	592	625	694	701
C18:1n7	136 ± 3	167	250	138	303		122	NA	NA	142	171	165	351
C18:1n9	1614 ± 154	1657	1699	1786	1950	1810	1771	NA	2192	1680	1732	2486	1291
C18:2n6	2838 ± 143	2645	2302	2851	3078	2931	2877	NA	3072	2810	2639	4040	2678
C18:3n3	54.6 ± 3.6	52.4	46.0	51.2	54.8	52.8	55.9	NA	68.9	47.3	47.5	66.7	70.4
C18:3n6	39.9 ± 8.5	39.9	47.0	53.0	54.6		51.5	NA	NA	49.9	46.6	68.5	NA
C20:0	18.0 ± 0.5		26.0	NA	19.5		15.6	NA	NA	18.0	13.1	14.7	12.33
C20:1n9	11.5 ± 0.5			NA	NA		10.1	NA	20.3	NA	10.4	34.0	5.24
C20:2n6	18.8 ± 0.6	NA		NA	NA	16.7	17.3	NA	NA	17.4	18.6	25.1	13.61
C20:3n6	139 ± 4	NA	106	134	164		127	NA	179	132	128	105	132.3
C20:4n6	984 ± 180	969	493	683	754	703	709	1103	864	657	640	571	762
C20:5n3	38.6 ± 0.5	38.3	35.0	42.3	45.4	40.1	42.2	38.3	57.8	38.6	37.7	36.6	112.5
C22:0	47.8 ± 4.6		56.5	41.5	51.8		51.0	NA	NA	50.8	33.6	9.73	34.6
C22:1n9	3.4 ± 1.3		6.00	NA	7.20			NA	NA	NA	0.183	NA	78.9
C22:4n6	25.5 ± 0.6	NA	27.0	24.8	37.7		26.1	NA	31.6	23.7	22.4	21.6	46.0
C22:5n3	38.5 ± 0.7	37.0	35.0	39.6	43.2	45.9	41.1	NA	48.4	37.7	16.9	54.2	58.8
C22:5n6	19.5 ± 0.4	NA	23.0	NA	18.4		19.9	NA	NA	17.5	35.4	22.3	14.05
C22:6n3	118 ± 21	115	88.0	98	112	89.8	114	119	123	99.4	91.1	95.2	117.0
C24:0	46.6 ± 2.6		47.0	33.6	51.6		42.8	NA	NA	42.8	26.5	4.87	21.2
C24:1n9	71.3 ± 3.2		71.0	51.6	71.5		68.6	NA	NA	60.8	40.6	12.6	40.4

List any additional information such as known coelutions or results for additional fatty acids below:

C8:0					5.36								
C10:0					4.24						6.42		
C10:1n1					5.73								
C12:0	9.47 ± 0.57				12.4					9.06		527	
C12:1n1					4.56					2.66			
C12:1n7					4.06								
C14:2					1.21								
C15:0	4.56 ± 0.04				15.4		14.8					22.5	25.7
C16:1n-7t												73.1	
C16:1n9					40.2								
C16:2					5.6								
C17:0	17.6 ± 0.7				21.6		23.1				22.0	22.6	37.6
C17:1n9												20.8	
9c,11t-CLA												21.3	
C18:4n-3							2.95					2.50	
C19:0					2.27							12.3	
C 20:3n-3											1.59	11.6	
C20:3n9					18.4		7.92				10.7		
C20:4n3												4.98	
C21:0					1.51							6.09	
C 22:2n-6											1.60	12.4	
C23:0					33.8		19.9				11.4		
C26:0					0.460								
C26:1					0.530								
PhA					0.740								
PrA					0.140								
density (g/mL)	NA ^c	NA ^c	NA ^c	1.04	1.00	NA ^c	0.948	NA ^c	1.03	1.01	1.07	1.03	NA ^c

^a Certified (bold) and reference values from the Certificate of Analysis (COA) for SRM 1950

^b Reported as $\mu\text{g/g}$

^c NA = not analyzed

Table 10. Summary statistics for total fatty acids (μM)

Unknown 004								
Code	median	unc	rel unc	n ^a	lowest value		highest value	
C14:0	161	33	20.7%	11	106	Lab 13	279	Lab 12
C14:1n5	13.9	4.7	33.4%	7	7.80	Lab 13	21.0	Lab 2
C16:0	3048	291	9.6%	11	2715	Lab 10	4202	Lab 8
C16:1n7	297	39	13.1%	11	246	Lab 5	413	Lab 13
C18:0	716	89	12.4%	11	620	Lab 6	998	Lab 8
C18:1n7	177	45	25.4%	9	151	Lab 6	294	Lab 2
C18:1n9	2306	292	12.7%	11	1440	Lab 13	3128	Lab 8
C18:2n6	3531	296	8.4%	11	2766	Lab 13	4040	Lab 12
C18:3n3	85.6	14.6	17.1%	11	57.2	Lab 13	132	Lab 8
C18:3n6	55.7	4.9	8.8%	8	49.1	Lab 10	68.5	Lab 12
C20:0	20.3	6.3	31.2%	7	12.9	Lab 13	32.7	Lab 2
C20:1n9	17.3	11.4	65.9%	5	10.2	Lab 13	34.0	Lab 12
C20:2n6	24.3	2.6	10.6%	6	19.1	Lab 5	25.1	Lab 12
C20:3n6	164	29	17.8%	9	105	Lab 12	229	Lab 8
C20:4n6	722	447	61.8%	12	567	Lab 2	2818	Lab 7
C20:5n3	59.8	15.4	25.8%	12	36.6	Lab 12	110	Lab 13
C22:0	53.7	18.2	34.0%	8	9.73	Lab 12	70.6	Lab 2
C22:1n9	10.3	2.8	26.9%	4	9.26	Lab 10	14.2	Lab 13
C22:4n6	25.8	4.6	17.8%	9	21.1	Lab 10	35.1	Lab 13
C22:5n3	48.7	7.9	16.3%	11	19.0	Lab 10	57.5	Lab 8
C22:5n6	21.3	8.8	41.3%	7	12.3	Lab 13	41.6	Lab 10
C22:6n3	139	27	19.5%	12	57.9	Lab 8	214	Lab 7
C24:0	46.0	16.7	36.4%	8	4.87	Lab 12	58.0	Lab 2
C24:1n9	64.3	21.7	33.7%	8	12.6	Lab 12	86.0	Lab 2

List any additional information such as known coelutions or results for additional fatty acids below:

C15:0	26.5	5.6	21.1%	4	22.1	Lab 4	31.6	Lab 13
C17:0	28.6	15.8	55.2%	5	24.9	Lab 4	59.1	Lab 13
density (g/mL)	1.03	0.03	2.9%	7	0.963	Lab 6	1.06	Lab 3

^a n is number of laboratories reporting a value.

Table 10 (cont). Summary statistics for total fatty acids (μM)

Unknown 005								
Code	median	unc	rel unc	n ^a	lowest value		highest value	
C14:0	107	29	27.3%	11	86.9	Lab 13	231	Lab 12
C14:1n5	7.80	3.14	40.2%	7	4.22	Lab 10	13.4	Lab 12
C16:0	2423	164	6.8%	11	2264	Lab 10	3104	Lab 8
C16:1n7	187	35	18.6%	11	133	Lab 5	312	Lab 13
C18:0	701	71	10.2%	11	586	Lab 1	905	Lab 8
C18:1n7	131	32	24.8%	9	104	Lab 1	220	Lab 13
C18:1n9	1896	163	8.6%	11	1297	Lab 13	2149	Lab 8
C18:2n6	3297	216	6.6%	11	2587	Lab 2	3577	Lab 12
C18:3n3	73.3	8.8	12.0%	11	56.2	Lab 12	100	Lab 8
C18:3n6	50.9	4.0	7.9%	8	45.0	Lab 10	60.0	Lab 12
C20:0	20.2	5.8	28.8%	7	14.1	Lab 12	31.7	Lab 2
C20:1n9	15.3	9.9	64.7%	5	10.9	Lab 13	32.9	Lab 12
C20:2n6	22.5	1.8	7.9%	6	19.5	Lab 5	24.4	Lab 13
C20:3n6	161	30	18.6%	9	97.5	Lab 12	210	Lab 13
C20:4n6	775	420	54.2%	12	553	Lab 2	2727	Lab 7
C20:5n3	80.4	23.1	28.8%	12	47.2	Lab 12	177	Lab 13
C22:0	56.9	18.0	31.7%	8	9.54	Lab 12	71.3	Lab 2
C22:1n9	6.48	23.6	363.8%	4	4.67	Lab 10	43.5	Lab 13
C22:4n6	21.1	6.0	28.4%	9	17.3	Lab 10	40.7	Lab 13
C22:5n3	50.3	12.7	25.2%	11	13.8	Lab 10	86.2	Lab 13
C22:5n6	15.8	10.3	65.1%	7	12.7	Lab 4	43.5	Lab 10
C22:6n3	166	24	14.4%	12	94.7	Lab 12	222	Lab 7
C24:0	52.7	18.3	34.7%	8	4.84	Lab 12	64.8	Lab 4
C24:1n9	61.3	18.9	30.8%	8	12.6	Lab 12	77.3	Lab 2
List any additional information such as known coelutions or results for additional fatty acids below:								
C15:0	26.6	8.5	32.1%	4	22.3	Lab 4	37.7	Lab 13
C17:0	28.7	21.2	73.9%	5	24.4	Lab 4	69.3	Lab 13
density (g/mL)	1.03	0.04	3.9%	7	0.967	Lab 6	1.09	Lab 10

^a n is number of laboratories reporting a value.

Table 10 (cont). Summary statistics for total fatty acids (μM)								
Unknown 006								
Code	median	unc	rel unc	n ^a	lowest value		highest value	
C14:0	134	10	7.3%	11	107	Lab 13	264	Lab 12
C14:1n5	9.63	3.8	40.0%	7	6.50	Lab 10	16.5	Lab 12
C16:0	2608	11	0.4%	11	2382	Lab 10	3237	Lab 8
C16:1n7	202	9	4.5%	11	157	Lab 5	334	Lab 13
C18:0	713	10	1.3%	11	638	Lab 6	933	Lab 8
C18:1n7	137	8	6.1%	9	121	Lab 6	226	Lab 13
C18:1n9	1901	13	0.7%	11	1260	Lab 13	2103	Lab 8
C18:2n6	3539	17	0.5%	11	2783	Lab 2	4066	Lab 12
C18:3n3	72.3	3.3	4.6%	11	59.7	Lab 12	97.0	Lab 8
C18:3n6	48.8	2.4	5.0%	8	44.4	Lab 10	65.4	Lab 12
C20:0	22.2	4.2	18.7%	7	15.4	Lab 12 & 13	35.3	Lab 2
C20:1n9	13.5	6.7	49.5%	5	10.2	Lab 13	32.9	Lab 12
C20:2n6	20.1	1.2	6.2%	6	12.0	Lab 5	23.2	Lab 13
C20:3n6	135	8	5.7%	9	78.8	Lab 12	193	Lab 13
C20:4n6	646	43	6.7%	12	428	Lab 12	1920	Lab 7
C20:5n3	125	8	6.2%	12	80.2	Lab 12	216	Lab 13
C22:0	56.5	7.8	13.8%	8	11.1	Lab 12	73.5	Lab 2
C22:1n9	6.95	14.6	209.9%	4	5.33	Lab 2	33.2	Lab 13
C22:4n6	18.5	4.0	21.4%	9	14.8	Lab 10	34.9	Lab 13
C22:5n3	46.0	11.0	24.0%	11	12.2	Lab 10	74.2	Lab 13
C22:5n6	12.4	8.9	72.1%	7	9.86	Lab 4	41.5	Lab 10
C22:6n3	176	7	3.8%	12	111	Lab 12	245	Lab 7
C24:0	50.2	8.2	16.4%	8	5.97	Lab 12	62.7	Lab 2
C24:1n9	77.5	8.9	11.5%	8	14.7	Lab 12	94.7	Lab 2
List any additional information such as known coelutions or results for additional fatty acids below:								
C15:0	22.3	3.4	15.5%	4	17.1	Lab 4	28.7	Lab 13
C17:0	26.3	8.0	30.3%	5	21.7	Lab 4	58.1	Lab 13
density (g/mL)	1.03	0.11	10.7%	7	0.954	Lab 6	1.09	Lab 10

^a n is number of laboratories reporting a value.

Table 10 (cont). Summary statistics for total fatty acids (μM)

SRM 1950								
Code	median	unc	rel unc	n ^a	lowest value		highest value	
C14:0	101	41	39.9%	11	91.4	Lab 1	279	Lab 12
C14:1n5	9.84	4.0	40.4%	7	6.13	Lab 10	17.8	Lab 12
C16:0	2377	245	10.3%	11	2110	Lab 10	3158	Lab 8
C16:1n7	254	65	25.4%	11	219	Lab 5	523	Lab 13
C18:0	671	63	9.3%	11	544	Lab 6	850	Lab 8
C18:1n7	167	67	40.2%	9	122	Lab 6	351	Lab 13
C18:1n9	1771	232	13.1%	11	1291	Lab 13	2486	Lab 12
C18:2n6	2851	330	11.6%	11	2302	Lab 2	4040	Lab 12
C18:3n3	52.8	6.7	12.7%	11	46.0	Lab 2	70.4	Lab 13
C18:3n6	50.7	7.3	14.5%	8	46.4	Lab 10	68.5	Lab 12
C20:0	15.6	4.4	28.5%	7	12.3	Lab 13	26.0	Lab 2
C20:1n9	10.4	12.8	122.6%	5	5.24	Lab 13	34.0	Lab 12
C20:2n6	17.4	3.9	22.5%	6	13.6	Lab 13	25.1	Lab 12
C20:3n6	132	20	15.2%	9	105	Lab 12	179	Lab 8
C20:4n6	706	122	17.2%	12	493	Lab 2	1103	Lab 7
C20:5n3	39.4	15.5	39.3%	12	35.0	Lab 2	113	Lab 13
C22:0	46.2	13.5	29.2%	8	9.73	Lab 12	56.5	Lab 2
C22:1n9	6.60	46.7	707.0%	4	0.182	Lab 10	78.9	Lab 13
C22:4n6	26.1	6.8	25.9%	9	21.9	Lab 12	46.0	Lab 13
C22:5n3	41.1	8.3	20.2%	11	16.9	Lab 10	58.8	Lab 13
C22:5n6	19.9	6.4	32.4%	7	14.1	Lab 13	35.4	Lab 10
C22:6n3	106	9	8.7%	12	88.0	Lab 2	123	Lab 8
C24:0	38.2	13.8	36.1%	8	4.87	Lab 12	51.6	Lab 4
C24:1n9	56.2	18.0	32.0%	8	12.6	Lab 12	71.5	Lab 4
List any additional information such as known coelutions or results for additional fatty acids below:								
C15:0	18.9	6.7	35.5%	4	14.8	Lab 6	25.7	Lab 13
C17:0	22.6	7.6	33.8%	5	21.6	Lab 4	37.6	Lab 13
density (g/mL)	1.03	0.04	3.9%	7	0.948	Lab 6	1.07	Lab 10

^a n is number of laboratories reporting a value.

Table 11. Laboratory 12's data for free fatty acids (μM)										
	Unknown 004 (n=3)			Unknown 005 (n=3)			Unknown 006 (n=3)			SRM 1950 (n=1)
	mean	stdev	rsd	mean	stdev	rsd	mean	stdev	rsd	
C14:0	12.84	0.95	7.41%	9.17	0.70	7.64%	9.83	0.62	6.29%	7.96
C14:1n5	2.38	0.21	8.74%	1.83	0.20	11.15%	1.74	0.18	10.21%	1.60
C16:0	125.35	12.41	9.90%	86.98	8.53	9.81%	88.71	4.61	5.20%	80.42
C16:1n7	15.02	1.65	10.98%	7.60	0.66	8.65%	8.18	0.26	3.22%	10.38
C18:0	42.22	2.44	5.78%	37.43	3.61	9.65%	37.67	1.53	4.05%	30.65
C18:1n7	7.68	0.62	8.03%	4.79	0.32	6.59%	5.00	0.21	4.23%	5.55
C18:1n9	138.26	11.83	8.56%	100.25	7.25	7.23%	95.47	1.63	1.71%	86.75
C18:2n6	77.85	6.43	8.26%	54.97	4.41	8.02%	57.81	2.45	4.23%	47.89
C18:3n3	6.81	0.51	7.50%	5.17	0.46	8.85%	4.75	0.21	4.34%	4.19
C18:3n6	1.00	0.03	2.59%	7.83	12.38	158.25%	0.73	0.04	5.00%	0.70
C20:0	1.25	0.02	1.85%	1.21	0.12	9.75%	1.28	0.06	4.31%	1.46
C20:1n9	2.04	0.04	1.89%	1.76	0.02	0.89%	1.73	0.04	2.42%	1.91
C20:2n6	1.51	0.05	3.45%	1.36	0.08	5.98%	1.28	0.13	9.86%	1.34
C20:3n6	15.41	0.85	5.50%	13.48	2.07	15.33%	16.46	1.37	8.33%	10.61
C20:4n6	14.65	0.80	5.44%	15.50	2.52	16.25%	13.23	1.21	9.15%	10.71
C20:5n3	0.37	0.01	3.37%	0.34	0.01	2.95%	0.35	0.02	4.91%	0.31
C22:0	0.62	0.01	1.53%	0.57	0.03	5.22%	0.60	0.01	2.44%	0.53
C22:1n9	Not analyzed (NA)			NA			NA			NA
C22:4n6	1.06	0.08	7.14%	0.91	0.04	4.76%	0.99	0.11	11.52%	1.11
C22:5n3	1.19	0.07	6.00%	1.19	0.04	2.95%	1.20	0.08	6.58%	0.97
C22:5n6	1.03	0.06	5.90%	0.91	0.10	10.61%	0.89	0.04	4.56%	0.93
C22:6n3	1.51	0.06	4.21%	1.79	0.57	31.68%	2.78	0.26	9.20%	0.81
C24:0	0.48	0.03	6.71%	0.42	0.03	6.10%	0.61	0.08	13.70%	0.43
C24:1n9	0.92	0.12	13.20%	0.76	0.07	8.69%	0.98	0.22	22.79%	0.85
List any additional information such as known coelutions or results for additional fatty acids below:										
C12:0	5.80	0.14	2.41%	4.23	0.26	6.18%	4.90	0.64	13.08%	3.79
C15:0	2.19	0.14	6.63%	1.96	0.19	9.63%	2.08	0.10	4.77%	1.54
C16:1n7t	3.00	0.31	10.49%	2.27	0.18	8.04%	3.77	2.08	55.20%	2.10
C17:0	2.12	0.12	5.72%	1.89	0.12	6.36%	1.84	0.05	2.59%	1.60
C17:1n9	1.43	0.07	4.54%	1.18	0.09	7.67%	1.08	0.04	3.33%	1.21
9c,11t-CLA	2.06	0.07	3.23%	1.79	0.06	3.11%	1.77	0.06	3.38%	2.01
C18:4n3	0.24	0.16	64.90%	0.25	0.15	60.06%	0.31	0.05	15.88%	0.09
C19:0	0.75	0.03	3.69%	0.65	0.02	2.70%	0.69	0.02	2.56%	0.63
C20:3n3	0.77	0.05	6.54%	0.66	0.01	1.96%	0.73	0.08	10.87%	0.64
C20:4n3	0.98	0.01	1.46%	0.96	0.09	9.66%	1.67	0.16	9.89%	0.66
C21:0	0.41	0.07	17.98%	0.36	0.03	9.35%	0.47	0.15	31.37%	0.36
C22:2n6	0.76	0.05	6.76%	0.70	0.01	1.54%	0.69	0.01	1.28%	0.81
C22:1n9 (Docosenoic acid) was used as a surrogate.										

Table 12. % of free to total fatty acids based on Laboratory 12's data				
	Unknown 004	Unknown 005	Unknown 006	SRM 1950
C14:0	4.60%	3.98%	3.73%	2.85%
C14:1n5	13.34%	13.66%	10.55%	8.99%
C16:0	4.09%	3.66%	3.40%	2.62%
C16:1n7	5.69%	5.02%	4.58%	3.93%
C18:0	6.09%	5.70%	5.47%	4.42%
C18:1n7	4.66%	3.88%	3.59%	3.36%
C18:1n9	5.56%	5.29%	4.80%	3.49%
C18:2n6	1.93%	1.54%	1.42%	1.19%
C18:3n3	10.22%	9.18%	7.97%	6.28%
C18:3n6	1.47%	13.06%	1.12%	1.02%
C20:0	8.51%	8.57%	8.33%	9.88%
C20:1n9	5.99%	5.34%	5.26%	5.61%
C20:2n6	6.01%	5.73%	5.81%	5.33%
C20:3n6	14.64%	13.82%	20.88%	10.08%
C20:4n6	2.57%	2.79%	3.09%	1.87%
C20:5n3	1.02%	0.71%	0.43%	0.85%
C22:0	6.35%	5.93%	5.44%	5.41%
C22:1n9	Not analyzed			
C22:4n6	4.90%	4.58%	5.35%	5.15%
C22:5n3	2.19%	2.05%	1.94%	1.78%
C22:5n6	4.61%	4.90%	4.61%	4.17%
C22:6n3	1.59%	1.89%	2.51%	0.85%
C24:0	9.85%	8.58%	10.14%	8.85%
C24:1n9	7.29%	5.99%	6.64%	6.69%
List any additional information such as known coelutions or results for additional fatty acids below:				
C12:0	1.17%	0.86%	0.93%	0.72%
C15:0	7.50%	6.77%	8.00%	6.82%
C16:1n7t	3.40%	3.06%	5.02%	2.88%
C17:0	7.56%	7.21%	7.00%	7.09%
C17:1n9	6.08%	6.33%	5.37%	5.83%
9c,11t-CLA	9.18%	8.81%	8.41%	9.44%
C18:4n3	6.27%	11.12%	5.92%	3.53%
C19:0	5.70%	4.99%	4.90%	5.15%
C20:3n3	6.56%	5.69%	6.07%	5.47%
C20:4n3	16.04%	15.76%	34.01%	13.29%
C21:0	6.31%	5.59%	6.68%	5.84%
C22:2n6	6.18%	5.64%	4.75%	6.51%

Appendix A.

Methods reported by the participating laboratories

Table A-1. Procedures used

Table A-2. Calibration information

Table A-3. Additional notes provided by laboratories

Table A-1 Procedures used for total fatty acids					
Lab #	1	2	3	4	5
Reporting date	5/9/2016	5/18/2016	5/23/2016	5/25/2016	5/31/2016
Volume of sample extracted (mL):	0.50	0.05	0.20	0.10	0.02
Mass of samples extracted (g) (average of 3):					
FAQAP unk004	0.49	not recorded	0.211	0.10	
FAQAP unk005	0.52	not recorded	0.210	0.10	
FAQAP unk006	0.48	not recorded	0.206	0.10	
Mass of samples extracted (g) :					
SRM 1950	0.51	not recorded	0.208	0.10	
Analytical method reference, if available	Sánchez-Ávila N, Mata-Granados JM, Ruiz-Jiménez J, Luque de Castro MD. J Chromatog A 1216 (2009) 6864-6872	Lagerstedt SA, Hinrichs DR, Batt SM, Magera MJ, Rinaldo P, McConnell JP. (2001) Quantitative determination of plasma C8-C26 total fatty acids for the biochemical diagnosis of nutritional and metabolic disorders. Mol Genet Metab.,73:38-45.		Lagerstedt SA, Hinrichs DR, Batt SM, Magera MJ, Rinaldo P, McConnell JP. Quantitative determination of plasma C8-C26 total fatty acids for the biochemical diagnosis of nutritional and metabolic disorders. Mol Genet Metab 2001;73:38-45	Bagga D, Capone S, Wang HJ, Heber D, Lill M, Chap L, Glasphy JA. J Nat Cancer Ins 1997; 89:1123-1131.
Analytical method used:					
Hydrolysis method	0.4 M KOH methanol followed by 1 M H ₂ SO ₄ methanol	Acid and Base Hydrolysis	Acetic acid with Methanol	Acid hydrolysis followed by basic hydrolysis and re-acidification	Add sample to 1ml methanol:benzene (4:1). Add 100 ul acetyl chloride. Heat for 60 minutes at 100 C.
Extraction method	Liquid-liquid	Liquid Liquid Extraction (LLE)	Liquid/Liquid Extraction	liquid-liquid	
Extraction solvent	hexane with 40 mg/g BHT	Hexane	Hexane	Hexane	
Extraction time	vortex 30 s each time	2 min	14 per batch; each batch about 8 hours for extraction	20 min on rotary mixer	
Extraction - other details	Hexane extraction performed 2x following base addition and 2x following acid addition			Extraction solvent evaporated, samples derivatized then reconstituted in hexane + 0.5N HCl	Cool sample to room T and add 4 ml of potassium carbonate (6%). Centerifuge and inject supernatant into GC.
Sample extract cleanup method	none	Hexane LLE from derivatizing reagent	None	Centrifugation of samples and removal of supernatant for injection	
Derivatization reagent	acidic methanol	pentafluorobenzylbromide	Methyl ester is formed from the methanol	2,3,4,5,6-Pentafluorobenzyl bromide (10% solution in acetonitrile)	
Analytical instrument	GC-FID	6890N/5973N Gas Chromatograph/Mass Spectrometer	Agilent MSD 5973N, Agilent GC 6890N	Agilent 6890 GC/5975C CI MSD in negative ion mode	Agilent Technologies 5890A gas chromatograph
Column phase	crossbonded polyethylene glycol (FAMEWAX, Restek)	5% phenyl-95% methylpolysiloxane	DB-23	DB-5MS	SP2380 stabilized phase fused silica capillary column (Sigma-Aldrich)
Column length, m	30	20	60	30m + 10m guard	30
Column i.d., mm	0.32	0.18	0.25	0.25	0.32
Column film thickness, µm	0.25	0.18	0.15	0.25	0.20
Injection method (split, splitless, etc)	split	split and splitless	Split	Split and splitless injections for different fatty acids	split injection
Method of quantitation:					
ES = external standards (Y/N)		N	N	Y	Y
Number of ES used		0		37 compounds at 6 levels each	12
IS = internal standards (Y/N)	yes	Y	Y	Y	
Number of IS used	2	13	4	13 in one solution	
IS added PRIOR to extraction of sample	yes	Y	Y	Y	

Table A-1 Continued					
Lab #	6	7	8	9	10
Reporting date	5/31/2016	06/01/2016	6/1/2016	6/1/2016	6/1/2016
Volume of sample extracted (mL):	0.10	0.0031	0.10	0.10	0.05
Mass of samples extracted (g) (average of 3):					
FAQAP unk004	0.096		0.103	0.10	0.052
FAQAP unk005	0.097		0.104	0.10	0.055
FAQAP unk006	0.095		0.103	0.10	0.054
Mass of samples extracted (g) :					
SRM 1950	0.095		0.103	0.10	0.054
Analytical method reference, if available	Lagertedt S, Hinrichs D, Batt S, Magera M, Rinaldo P, McConnell J. Quantitative Determination of Plasma C8-C26 Total Fatty Acids for the Biochemical Diagnosis of Nutritional and Metabolic Disorders. Mol Genet & Metab 2001; 73: 38-45.				
Analytical method used:				Acidic and alkaline hydrolysis using 10% 6N HCl in acetonitrile and 10% 10N NaOH in MeOH	
Hydrolysis method	Acid/Base				
Extraction method	Liquid-liquid	Liquid extraction	Liquid-liquid Extraction	Liquid-liquid extraction	Modified Folch
Extraction solvent	hexane	0.001% BHT in Methanol	Chloroform-Methanol (2:1)	Hexanes	3mL 2:1 chloroform:methanol
Extraction time	20-30 minutes per extraction	At 300 rpm for 15 Minutes	3 min	15 minutes	24 hours in 2:1 chloroform:methanol
Extraction - other details	triple extraction via automated liquid handler	Follow by 90% Acetonitrile		samples extracted 3x	Addition of 500uL sodium phosphate buffer, vortex, centrifuge, double extraction of organic phase
Sample extract cleanup method	Speedvac			Solvent evaporated and samples derivatized	Hexane/water
Derivatization reagent	PFBBR - pentafluorobenzyl bromide		METH-PREP II, Grace Davision Discovery Sciences	pentafluorobenzyl-bromide	14% boron trifluoride in methanol
Analytical instrument	GC/MS	LC-MS/MS	Agilent 7890A GC, 5975C MSD	Agilent 7890/5975B GC-MS	Varian 3900 GC-FID
Column phase	90% biscyanopropyl/10% phenylcyanopropyl polysiloxane	C18	Non bonded, Poly (80% biscyanopropyl/20% cyanopropyl phenyl siloxane) phase	Select-FAME	DB-FFAP
Column length, m	60	0.005	30	200	15
Column i.d., mm	0.25	2.1	0.25	0.25	0.10
Column film thickness, µm	0.2	3	0.20	0.25	0.10
Injection method (split, splitless, etc)	split		splitless	split 20:1	50:1 split ratio
Method of quantitation:					
ES = external standards (Y/N)	N	Y	N	N	Y
Number of ES used		3			28
IS = internal standards (Y/N)	Y	Y	Y	Y	Y
Number of IS used	17	1	2	16	1
IS added PRIOR to extraction of sample	Y	Y	Y	Y	Y

Table A-1 Continued			
Lab #	11	12	13
Reporting date	6/8/2016	6/23/2016	6/29/2016
Volume of sample extracted (mL):	0.15	0.05	0.20
Mass of samples extracted (g) (average of 3):			
FAQAP unk004	0.152		0.21
FAQAP unk005	0.153		0.21
FAQAP unk006	0.148		0.21
Mass of samples extracted (g) :			
SRM 1950	0.152		0.21
Analytical method reference, if available:			Liu et al 2010
Analytical method used:			
Hydrolysis method	Acid-catalyzed transesterification	0.5M dry methanolic sodium methoxide (as part of derivatization)	
Extraction method	Organic Phase with Vortexing	Based on F. Smèdes, Analyst, 1999,124, 1711-1718	Solvent extraction
Extraction solvent	3:2 Hexane-Isopropanol	0.41mL 2-propanol, 0.52mL cyclohexane, 0.57mL 0.1M ammonium acetate	Hexane:2-propanol (3:2, v/v)
Extraction time	10 minutes	6 minutes	
Extraction - other details		Transfer cyclohexane fraction and re-extract with added 0.57mL cyclohexane	
Sample extract cleanup method	One wash in Hexane/dd-water and wash in dd-water	Evaporate to dryness and reconstitute in 1:1 methanol/toluene	
Derivatization reagent	4% Sulfuric Acid in Methanol	0.5M dry methanolic sodium methoxide, 60°C 60 min, +0.1mL 3N Methanolic HCl, 60°C 30 min, neutralize, extract with 0.4mL hexanes	
Analytical instrument	Hewlett-Packard Model (now Agilent) GC 6890 FID gas chromatograph with 7673 Autosampler injector	Agilent 6890 Plus+ GC, 5973N MSD, 7683 Injector, DB-225ms column	Thermo Trace GC-DSQ system
Column phase	fused silica capillary cis/trans column SP2560	(50%-Cyanopropylphenyl)-dimethylpolysiloxane	Rxi-5MS-coated 5% diphenyl/95% dimethyl polysiloxane capillary column
Column length, m	100	30	30.00
Column i.d., mm	0.25	0.25	0.25
Column film thickness, µm	0.20	0.25	0.25
Injection method (split, splitless, etc)	splitless	splitless	splitless
Method of quantitation:			
ES = external standards (Y/N)	Y (NOTE: Used for identification not quantification)	N	N
Number of ES used	43	0	
IS = internal standards (Y/N)	N	Y	Y
Number of IS used	N/A	1	Methyl tridecanoate
IS added PRIOR to extraction of sample (Y/N)		Y	Y

Table A-2 Procedures used for free fatty acids	
Lab #	12
Reporting date	6/23/2016
Volume of sample extracted (mL):	0.05
Mass of samples extracted (g) (average of 3):	
FAQAP unk004	
FAQAP unk005	
FAQAP unk006	
Mass of samples extracted (g) :	
SRM 1950	
Analytical method reference, if available:	
Analytical method used:	
Extraction method	Based on F. Smedes, Analyst, 1999,124, 1711-1718
Extraction solvent	0.41mL 2-propanol, 0.52mL cyclohexane, 0.57mL 0.1M ammonium acetate
Extraction time	6 minutes
Extraction - other details	Transfer cyclohexane fraction and re-extract with added 0.57mL cyclohexane
Sample extract cleanup method	Evaporate to dryness and reconstitute in 1:1 methanol/toluene
Derivatization reagent	2M Tri(methylsilyl)diazomethane (in hexanes)
Analytical instrument	Agilent 6890 Plus+ GC, 5973N MSD, 7683 Injector, DB-225ms column
Column phase	(50%-Cyanopropylphenyl)-dimethylpolysiloxane
Column length, m	30
Column i.d., mm	0.25
Column film thickness, μ m	0.25
Injection method (split, splitless, etc)	splitless
Method of quantitation:	
ES = external standards (Y/N)	N
Number of ES used	0
IS = internal standards (Y/N)	Y
Number of IS used	1
IS added PRIOR to extraction of sample	Y

Table A-3 Calibration information										
Lab	Fatty Acid Code	Fatty Acid Name	Lowest std (µmol/L)	Highest std (µmol/L)	LOD (µmol/L)	LOQ (µmol/L)	Curve Type	Weighting	IS used for quantitation	
1	C14:0	Myristic acid	used response factors based on three independently prepared calibration solutions							Myristic-d ₂₇
	C14:1n5	Myristoleic acid	used response factors based on three independently prepared calibration solutions							Myristic-d ₂₇
	C16:0	Palmitic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C16:1n7	Palmitoleic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C18:0	Stearic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C18:1n7	<i>cis</i> -Vaccenic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C18:1n9	Oleic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C18:2n6	Linoleic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C18:3n3	<i>alpha</i> -Linolenic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C18:3n6	<i>gamma</i> -Linolenic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C20:0	Arachidic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C20:1n9	11-Eicosenoic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C20:4n6	Arachidonic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C20:5n3	Eicosapentaenoic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C22:0	Docosanoic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C22:1n9	Docosenoic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C22:5n3	Docosapentaenoic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C22:6n3	Docosahexaenoic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C24:0	Lignoceric acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	C24:1n9	Nervonic acid	used response factors based on three independently prepared calibration solutions							Palmitic-d ₃₁
	2	C14:0	Myristic acid	12.5	150	0.3	3000	Linear	None	Myristic acid-d ₃
		C14:1n5	Myristoleic acid	1.25	15	0.013	300	Linear	None	Pentadecanoic acid-d ₄
		C16:0	Palmitic acid	25	300	2.81	6000	Linear	None	Palmitic-d ₃
		C16:1n7	Palmitoleic acid	12.5	150	0.045	3000	Linear	None	Myristic acid-d ₃
C18:0		Stearic acid	25	300	3.719	6000	Linear	None	Stearic acid-d ₃	
C18:1n7		<i>cis</i> -Vaccenic acid	25	300	0.089	6000	Linear	None	Stearic acid-d ₄	
C18:1n9		Oleic acid	25	300	0.21	6000	Linear	None	Stearic acid-d ₅	
C18:2n6		Linoleic acid	25	300	0.15	6000	Linear	None	Stearic acid-d ₆	
C18:3n3		<i>alpha</i> -Linolenic acid	12.5	150	0.009	3000	Linear	None	Arachidic acid-d ₃	
C18:3n6		<i>gamma</i> -Linolenic acid	12.5	150	0.009	3000	Linear	None	Arachidic acid-d ₃	
C20:0		Arachidic acid	12.5	150	0.25	3000	Linear	None	Arachidic acid-d ₃	
C20:3n6		homo- <i>gamma</i> -Linolenic acid	0.625	7.5	0.004	150	Linear	None	Docosanoic acid-d ₄	
C20:4n6		Arachidonic acid	12.5	150	0.021	3000	Linear	None	Arachidic acid-d ₃	
C20:5n3		Eicosapentaenoic acid	12.5	150	0.019	3000	Linear	None	Arachidic acid-d ₃	
C22:0		Docosanoic acid	0.625	7.5	0.036	150	Linear	None	Docosanoic acid-d ₄	
C22:4n6		Docosatetraenoic acid	0.625	7.5	0.002	150	Linear	None	Docosanoic acid-d ₄	
C22:5n3		Docosapentaenoic acid	0.625	7.5	0.021	150	Linear	None	Docosanoic acid-d ₄	
C22:5n6		Docosapentaenoic acid	0.625	7.5	0.021	150	Linear	None	Docosanoic acid-d ₄	
C22:6n3		Docosahexaenoic acid	12.5	150	0.03	3000	Linear	None	Arachidic acid-d ₃	
C24:0		Lignoceric acid	0.625	7.5	0.029	150	Linear	None	Tetracosanoic acid-d ₄	
C24:1n9		Nervonic acid	0.625	7.5	0.004	150	Linear	None	Tetracosanoic acid-d ₄	
3		C14:0	myristic	12.7	845	0.963	13.1	quadratic	1/x	Methyl Tridecenoate
		C16:0	palmitic	111	7430	29	234	quadratic	1/x	Methyl trans-Heptadecenoate
		C16:1	palmitoleic	11.4	757	3.69	23.6	quadratic	1/x	Methyl Tridecenoate
	C18:0	stearic	100	6700	6.22	105	quadratic	1/x	Methyl trans-Heptadecenoate	
	C18:1n7	vaccenic	10.2	682	2.8	21.2	quadratic	1/x	Methyl Heneicosanoate	
	C18:1n9	oleic	102	6790	36.3	212	quadratic	1/x	Methyl trans-Heptadecenoate	
	C18:2n6	linoleic	103	6840	26	214	quadratic	1/x	Methyl trans-Heptadecenoate	
	C18:3n3	<i>alpha</i> -linolenic	10.4	691	0.718	10.8	quadratic	1/x	Methyl Heneicosanoate	
	C18:3n6	<i>gamma</i> -linolenic	10.4	690	0.682	10.8	quadratic	1/x	Methyl Heneicosanoate	
	C20:3n6	homo- <i>gamma</i> -linolenic	9.41	628	2.19	19.6	quadratic	1/x	Methyl Heneicosanoate	
	C20:4n6	arachidonic	93.5	6230	5.12	98.5	quadratic	1/x	Methyl trans-Heptadecenoate	
	C20:5n3	eicosapentaenoic	9.53	635	0.794	9.92	quadratic	1/x	Methyl Tricosenoate	
	C22:0	docosanoic	8.5	566	0.382	8.81	quadratic	1/x	Methyl Tricosenoate	
	C22:4n6	docosatetraenoic	8.67	578	0.481	9.02	quadratic	1/x	Methyl Tricosenoate	
	C22:5n3	docosapentaenoic	8.72	581	0.424	9.08	quadratic	1/x	Methyl Tricosenoate	
	C22:6n3	docosahexaenoic	8.79	586	1.46	18.3	quadratic	1/x	Methyl Tricosenoate	
	C24:0	lignoceric	7.83	522	0.353	8.14	quadratic	1/x	Methyl Tricosenoate	
	C24:1n9	nervonic	7.87	525	0.409	8.18	quadratic	1/x	Methyl Tricosenoate	

Lab	Fatty Acid Code	Fatty Acid Name	Lowest std (µmol/L)	Highest std (µmol/L)	LOD (µmol/L)	LOQ (µmol/L)	Curve Type	Weighting	IS used for quantitation	
4	C8:0	Octanoic acid	14	120			quadratic	equal	C8:0 D3	
	C10:0	Decanoic acid	13	110			quadratic	equal	C10:0 D3	
	C10:1	9-Decenoic acid	16	120			quadratic	equal	C10:0 D3	
	C12:0	Lauric acid	12	101			quadratic	equal	C12:0 D3	
	C12:1w1	11-Dodecenoic acid	13	108			quadratic	equal	C12:0 D3	
	C12:1w7	cis-5-Dodecenoic acid	14	115			quadratic	equal	C12:0 D3	
	C14:0	Myristic acid	44	365			quadratic	equal	C14:0 D3	
	C14:1	Myristoleic acid	14	115			quadratic	equal	C15:0 D3	
	C15:0	Pentadecanoic acid	23	190			quadratic	equal	C15:0 D3	
	C16:0	Palmitic acid	468	3900			quadratic	equal	C16:0 D3	
	C16:1w7	Palmitoleic acid	127	1058			quadratic	equal	C14:0 D3	
	C17:0	Heptadecanoic acid	22	180			quadratic	equal	C15:0 D3	
	C18:0	Stearic acid	89	745			quadratic	equal	C18:0 D3	
	C18:1w7	Vaccenic acid	241	2010			quadratic	equal	C18:0 D3	
	C18:1w9	Oleic acid	600	5000			quadratic	equal	C18:0 D3	
	C18:2w6	Linoleic acid	474	3950			quadratic	equal	C18:0 D3	
	C18:3w3	<i>n</i> -linolenic acid	55	460			quadratic	equal	C18:0 D3	
	C18:3w6	<i>g</i> -linolenic acid	60	500			quadratic	equal	C18:0 D3	
	C19:0	Nonadecanoic acid	5	43			quadratic	equal	C22:0 D3	
	C20:0	Arachidic acid	115	960			quadratic	equal	C20:0 D3	
	C20:3w6	Eicosatrienoic acid (w6) (Homo- <i>g</i> -linolenic acid)	13	112			quadratic	equal	C22:0 D3	
	C20:3w9	5,8,11-Eicosatrienoic acid (MEAD)	7	55			quadratic	equal	C22:0 D3	
	C20:4w6	Arachidonic acid	121	1000			quadratic	equal	C20:0 D3	
	C20:5w3	Eicosapentaenoic acid (w3)	78	650			quadratic	equal	C20:0 D3	
	C21:0	Heneicosanoic acid	11	95			quadratic	equal	C22:0 D3	
	C22:0	Docosanoic acid (Behenic acid)	14	115			quadratic	equal	C22:0 D3	
	C22:1w9	Erucic acid (w9)	9	72			quadratic	equal	C22:0 D3	
	C22:4w6	Docosatetraenoic acid (w6)	6	46			quadratic	equal	C22:0 D3	
	C22:5w3	Docosapentaenoic acid (w3)	25	210			quadratic	equal	C22:0 D3	
	C22:5w6	Docosapentaenoic acid	6	50			quadratic	equal	C22:0 D3	
	C22:6w3	Docosahexaenoic acid (w3)	13	108			quadratic	equal	C22:0 D3	
	C23:0	Tricosanoic acid	12	97			quadratic	equal	C24:0 D4	
	C24:0	Tetracosanoic acid	6	51			quadratic	equal	C24:0 D4	
	C24:1w9	Nervonic acid (w9)	23	195			quadratic	equal	C24:0 D4	
	C26:0	Hexacosanoic acid	1.4	11.3			quadratic	equal	C26:0 D4	
	PhA	Phytanic acid	2.6	21.7			quadratic	equal	PhA D3	
	PrA	Pristanic acid	0.25	2.05			quadratic	equal	PrA D3	
	5	C14:0	<i>Myristic acid</i>	56.8	909.9					
		C14:1n5	<i>Myristoleic acid</i>	NA	NA					
		C16:0	<i>Palmitic acid</i>	151.7	2428.3					
		C16:1n7	<i>Palmitoleic acid</i>	51.9	832.4					
		C18:0	<i>Stearic acid</i>	91.7	1467.9					
		C18:1n7	<i>cis</i> -Vaccenic acid	NA	NA					
		C18:1n9	<i>Oleic acid</i>	92.4	1479					
C18:2n6		<i>Linoleic acid</i>	46.7	749.1						
C18:3n3		<i>alpha</i> -Linolenic acid	47	750.5						
C18:3n6		<i>gamma</i> -Linolenic acid	NA	NA						
C20:0		<i>Arachidic acid</i>	NA	NA						
C20:1n9		11-Eicosenoic acid	NA	NA						
C20:2n6		11,14-Eicosadienoic acid	21.1	337.4						
C20:3n6		homo- <i>gamma</i> -Linolenic acid	NA	NA						
C20:4n6		<i>Arachidonic acid</i>	39.7	654.1						
C20:5n3		<i>Eicosapentaenoic acid</i>	36.2	580.70						
C22:0		<i>Docosanoic acid</i>	NA	NA						
C22:1n9		<i>Docosenoic acid</i>	NA	NA						
C22:4n6		<i>Docosatetraenoic acid</i>	NA	NA						
C22:5n3		<i>Docosapentaenoic acid</i>	39.9	636.7						
C22:5n6		<i>Docosapentaenoic acid</i>	NA	NA						
C22:6n3		<i>Docosahexaenoic acid</i>	39.6	632.8						
C24:0		<i>Lignoceric acid</i>	NA	NA						
C24:1n9		<i>Nervonic acid</i>	NA	NA						

Table A-3 (cont) Calibration information									
Lab	Fatty Acid Code	Fatty Acid Name	Lowest std (µmol/L)	Highest std (µmol/L)	LOD (µmol/L)	LOQ (µmol/L)	Curve Type	Weighting	IS used for quantitation
6	C18:3n3	<i>alpha</i> -Linolenic acid	6.53	653	1.54	not available	linear	1/x ²	<i>alpha</i> -Linolenic-d14
	C20:0	Arachidic acid	0.90	89.5	0.82	not available	linear	1/x ²	Arachidic-d39
	C20:4n6	Arachidonic acid	23.4	2337	7.34	not available	linear	1/x ²	Arachidonic-d8
	C10:0	Capric acid	0.44	43.9	1.59	not available	quadratic	1/x ²	Capric-d3
	C22:0	Docosanoic acid	1.83	183	0.68	not available	linear	1/x ²	Docosanoic-d4
	C22:6n3	Docosahexaenoic acid	7.88	788	1.84	not available	linear	1/x ²	Docosahexaenoic-d5
	C22:5n3	Docosapentaenoic n-3 acid	2.49	249	0.55	not available	linear	1/x ²	Docosahexaenoic-d5
	C22:5n6	Docosapentaenoic n-6 acid	1.59	159	0.24	not available	linear	1/x ²	Docosahexaenoic-d5
	C22:4n6	Docosatetraenoic acid	1.48	148	0.31	not available	quadratic	1/x ²	Docosahexaenoic-d5
	C20:2n6	11,14-Eicosadienoic acid	0.98	97.7	0.31	not available	quadratic	1/x ²	Arachidic-d39
	C20:1n9	11-Eicosenoic acid	1.00	100	0.87	not available	quadratic	1/x ²	Arachidic-d39
	C20:5n3	Eicosapentaenoic acid	7.15	715	0.79	not available	quadratic	1/x ²	Eicosapentaenoic-d5
	C20:3n9	5Z, 8Z, 11Z-Eicosatrienoic acid	0.64	64.3	0.39	not available	quadratic	1/x ²	Arachidic-d39
	C18:3n6	<i>gamma</i> -Linolenic acid	2.93	293	0.42	not available	linear	1/x ²	<i>alpha</i> -Linolenic-d14
	C20:3n6	<i>homo-gamma</i> -Linolenic acid	4.62	462	1.14	not available	quadratic	1/x ²	<i>alpha</i> -Linolenic-d14
	C12:0	Lauric acid	2.33	233	2.33	not available	quadratic	1/x ²	Lauric-d3
	C24:0	Lignoceric acid	1.47	147	1.09	not available	linear	1/x ²	Tetracosanoic-d4
	C18:2n6	Linoleic acid	82.7	8274	22.6	not available	linear	1/x ²	13C-Linoleic
	C14:1n5	Myristoleic acid	1.42	142	0.29	not available	quadratic	1/x ²	Myristic-d27
	C14:0	Myristic acid	10.1	1012	4.90	not available	quadratic	1/x ²	Myristic-d27
	C17:0	Margaric acid	1.50	150	3.36	not available	quadratic	1/x	Margaric-d3
	C24:1n9	Nervonic acid	1.95	195	0.69	not available	quadratic	1/x ²	Tetracosanoic-d4
	C18:1n9	Oleic acid	85.0	8496	17.7	not available	linear	1/x ²	13C-Oleic
	C15:0	Pentadecanoic acid	0.95	95.0	0.75	not available	linear	1/x ²	Pentadecanoic-d3
	C16:1n7	Palmitoleic acid	25.1	2514	6.56	not available	quadratic	1/x ²	Palmitoleic-d14
	C16:0	Palmitic acid	87.4	8742	78.1	not available	quadratic	1/x ²	Palmitic-d31
	C18:4n3	Stearidonic acid	0.47	46.9	0.24	not available	quadratic	1/x	Arachidic-d39
	C18:0	Stearic acid	25.0	2505	39.1	not available	quadratic	1/x ²	Stearic-d35
	C23:0	Tricosanoic acid	0.98	97.6	0.90	not available	linear	1/x ²	Docosanoic-d4
	C18:1n7	<i>cis</i> -Vaccenic acid	7.42	742	2.31	not available	quadratic	1/x ²	13C-Oleic
7	C20:4n6	Arachidonic acid	317	2952			Linear	1/x	Docosahexaenoic-d5
	C20:5n3	Eicosapentaenoic acid	12.50	116			Linear	1/x	Docosahexaenoic-d5
	C22:6n3	Docosahexaenoic acid	38.1	354			Linear	1/x	Docosahexaenoic-d5
8	C14:0	Myristic	54.70	1094.7			Linear	Equal	Margaric
	C16:0	Palmitic	195	3899.7			Linear	Equal	Margaric
	C16:1n7	Palmitoleic	49.1	982.6			Linear	Equal	Margaric
	C18:0	Stearic	87.90	1757.6			Linear	Equal	Margaric
	C18:1n9	Oleic	177	3540.1			Linear	Equal	Margaric
	C18:2n6	Linoleic	178.3	3565.3			Linear	Equal	Margaric
	C18:3n3	<i>alpha</i> -Linolenic	22.40	448.9			Linear	Equal	Margaric
	C20:1n9	11-Eicosenoic	20.10	402.5			Linear	Equal	Margaric
	C20:3n6	<i>homo-gamma</i> -Linolenic	20.4	407.8			Linear	Equal	Margaric
	C20:4n6	Arachidonic	82.1	1641.9			Linear	Equal	Arachidonic-d8
	C20:5n3	Eicosapentaenoic	82.6	1652.8			Linear	Equal	Arachidonic-d8
	C22:4n6	Docosatetraenoic	18.80	375.9			Linear	Equal	Arachidonic-d8
	C22:5n3	Docosapentaenoic	18.9	378.1			Linear	Equal	Arachidonic-d8
	C22:6n3	Docosahexaenoic	38.0	760.9			Linear	Equal	Arachidonic-d8

Table A-3 (cont) Calibration information									
Lab	Fatty Acid Code	Fatty Acid Name	Lowest std (µmol/L)	Highest std (µmol/L)	LOD (µmol/L)	LOQ (µmol/L)	Curve Type	Weighting	IS used for quantitation
9	C14:0	Myristic acid	24.3	608	0.33		Linear	none	Myristic-d27
	C14:1n5	Myristoleic acid	4.11	103	0.29		Linear	none	Myristic-d27
	C16:0	Palmitic acid	315	7896	17		Linear	none	Palmitic-13C16
	C16:1n7	Palmitoleic acid	47.9	1198	0.76		Linear	none	Palmitoleic-13C16
	C18:0	Stearic acid	80	2000	4.02		Linear	none	Stearic-d35
	C18:1n7	cis-Vaccenic acid	31.6	790	1.06		Linear	none	cis-Vaccenic-13C5
	C18:1n9	Oleic acid	240	5994	14.3		Linear	none	Oleic-13C18
	C18:2n6	Linoleic acid	320	8007	4.9		Linear	none	Linoleic-13C18
	C18:3n3	alpha-Linolenic acid	15.9	398	0.82		Linear	none	alpha-Linolenic-d14
	C18:3n6	gamma-Linolenic acid	8.18	204	0.43		Linear	none	alpha-Linolenic-d14
	C20:0	Arachidic acid	8.05	201	0.47		Linear	none	Arachidic-d39
	C20:1n9	11-Eicosenoic acid	NA	NA	NA	NA	NA	NA	NA
	C20:2n6	11,14-Eicosadienoic acid	2.07	51.7	0.16		Linear	none	Arachidic-d39
	C20:3n6	homo-gamma-Linolenic acid	9.96	249	1		Linear	none	Arachidonic-d8
	C20:4n6	Arachidonic acid	79.3	1983	0.36		Linear	none	Arachidonic-d8
	C20:5n3	Eicosapentaenoic acid	31.4	786	1.29		Linear	none	Eicosapentaenoic-d5
	C22:0	Docosanoic acid	8.02	200	1.77		Linear	none	Docosanoic-d43
	C22:1n9	Docosenoic acid	NA	NA	NA	NA	NA	NA	NA
	C22:4n6	Docosatetraenoic acid	4.15	104	0.34		Linear	none	Docosahexaenoic-d5
	C22:5n3	Docosapentaenoic acid	8.15	204	0.51		Linear	none	Docosahexaenoic-d5
	C22:5n6	Docosapentaenoic acid	4.23	106	0.33		Linear	none	Docosahexaenoic-d5
	C22:6n3	Docosahexaenoic acid	40	999	1.96		Linear	none	Docosahexaenoic-d5
	C24:0	Lignoceric acid	8.05	201	1.59		Linear	none	Lignoceric-d47
	C24:1n9	Nervonic acid	8.03	201	1.38		Linear	none	Lignoceric-d47
10	C 10:0	Capric acid	0.0839	4028.7492	2.6858	26.8583	Linear	Equal weight%	Methyl-nonadecanoate
	C 12:0	Lauric acid	0.0729	3501.5101	2.3343	23.3434	Linear	Equal weight%	Methyl-nonadecanoate
	C 14:0	Myristic acid	0.0645	3096.2999	2.0642	20.6420	Linear	Equal weight%	Methyl-nonadecanoate
	C 16:0	Palmitic acid	0.0578	2775.1476	1.8501	18.5010	Linear	Equal weight%	Methyl-nonadecanoate
	C 18:0	Stearic Acid	0.0524	2514.3553	1.6762	16.7624	Linear	Equal weight%	Methyl-nonadecanoate
	C 20:0	Arachidic acid	0.0479	2298.3680	1.5322	15.3225	Linear	Equal weight%	Methyl-nonadecanoate
	C 22:0	Docosanoic acid	0.0441	2116.5526	1.4110	14.1104	Linear	Equal weight%	Methyl-nonadecanoate
	C 24:0	Lignoceric acid	0.0409	1961.3940	1.3076	13.0760	Linear	Equal weight%	Methyl-nonadecanoate
	C 12:1	Dodecenoic acid	0.0736	3534.7746	2.3565	23.5652	Linear	Equal weight%	Methyl-nonadecanoate
	C 14:1	Myristoleic acid	0.0650	3122.2823	2.0815	20.8152	Linear	Equal weight%	Methyl-nonadecanoate
	C 16:1	Palmitoleic acid	0.0583	2796.0015	1.8640	18.6400	Linear	Equal weight%	Methyl-nonadecanoate
	C 18:1n-7	cis-Vaccenic acid	0.0527	2531.4619	1.6876	16.8764	Linear	Equal weight%	Methyl-nonadecanoate
	C 18:1n-9	Oleic acid	0.0527	2531.4619	1.6876	16.8764	Linear	Equal weight%	Methyl-nonadecanoate
	C 20:1n-9	11-Eicosenoic acid	0.0482	2312.6535	1.5418	15.4177	Linear	Equal weight%	Methyl-nonadecanoate
	C 22:1n-9	Docosenoic acid	0.0443	2128.6614	1.4191	14.1911	Linear	Equal weight%	Methyl-nonadecanoate
	C 24:1n-9	Nervonic acid	0.0411	1971.7882	1.3145	13.1453	Linear	Equal weight%	Methyl-nonadecanoate
	C 18:2n-6	Linoleic acid	0.0531	2548.8019	1.6992	16.9920	Linear	Equal weight%	Methyl-nonadecanoate
	C 18:3n-6	gamma-Linolenic acid	0.0535	2566.3820	1.7109	17.1092	Linear	Equal weight%	Methyl-nonadecanoate
	C 20:2n-6	11,14-Eicosadienoic acid	0.0485	2327.1169	1.5514	15.5141	Linear	Equal weight%	Methyl-nonadecanoate
	C 20:3n-6	homo-gamma-Linolenic acid	0.0488	2341.7632	1.5612	15.6118	Linear	Equal weight%	Methyl-nonadecanoate
	C 20:4n-6	Arachidonic acid	0.0491	2356.5942	1.5711	15.7106	Linear	Equal weight%	Methyl-nonadecanoate
	C 22:2n-6	Docosadienoic acid	0.0446	2140.9089	1.4273	14.2727	Linear	Equal weight%	Methyl-nonadecanoate
	C 22:4n-6	Docosatetraenoic acid	0.0451	2165.8323	1.4439	14.4389	Linear	Equal weight%	Methyl-nonadecanoate
	C 18:3n-3	alpha-Linolenic acid	0.0535	2566.3820	1.7109	17.1092	Linear	Equal weight%	Methyl-nonadecanoate
C 20:3n-3	Eicosatrienoic acid	0.0488	2341.7632	1.5612	15.6118	Linear	Equal weight%	Methyl-nonadecanoate	
C 20:5n-3	Eicosapentaenoic acid	0.0494	2371.6150	1.5811	15.8108	Linear	Equal weight%	Methyl-nonadecanoate	
C 22:5n-3	Docosapentaenoic acid, n3	0.0454	2178.5132	1.4523	14.5234	Linear	Equal weight%	Methyl-nonadecanoate	
C 22:6n-3	Docosahexaenoic acid	0.0457	2191.3428	1.4609	14.6090	Linear	Equal weight%	Methyl-nonadecanoate	

Table A-3 (cont) Calibration information									
Lab	Fatty Acid Code	Fatty Acid Name	Lowest std (µmol/L)	Highest std (µmol/L)	LOD (µmol/L)	LOQ (µmol/L)	Curve Type	Weighting	IS used for quantitation
11	No information								
12	C14:0	Myristic Acid	0.0495	165			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C14:1n5	Myristoleic Acid	0.0083	27.7			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C16:0	Palmitic Acid	0.0592	197			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C16:1n7	Palmitoleic Acid	0.0075	24.8			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C18:0	Stearic Acid	0.0402	134			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C18:1n7	<i>Vaccenic Acid</i>	0.0030	9.8			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C18:1n9	Oleic Acid	0.0270	89.9			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C18:2n6	Linoleic Acid	0.0204	67.9			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C18:3n3	<i>Alpha Linolenic Acid</i>	0.0109	36.2			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C18:3n6	<i>Gamma Linolenic Acid</i>	0.0040	13.4			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C20:0	Arachidic Acid	0.0061	20.4			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C20:1n9	11-Eicosenoic Acid	0.0123	41.1			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C20:2n6	11-14-Eicosadienoic Acid	0.0070	23.4			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C20:3n6	<i>Homogamma Linolenic Acid</i>	0.0036	12.0			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C20:4n6	Arachidonic Acid	0.0344	114.8			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C20:5n3	Eicosapentaenoic Acid	0.0051	17.0			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C22:0	Behenic Acid	0.0056	18.8			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C22:1n9	Erucic Acid	0.0075	25.1			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C22:4n6	Docosic Acidtraenoic Acid	0.0081	27.0			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C22:5n3	Docosapentaenoic Acid	0.0068	22.7			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C22:5n6	Docosapentaenoic Acid N6	0.0078	26.0			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C22:6n3	Docosahexaenoic Acid (DHA)	0.0188	62.7			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C24:0	Ignoceric Acid	0.0052	17.4			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C24:1n9	Nervonic Acid	0.0084	27.9			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C12:0	Lauric Acid	0.0373	124.4			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C15:0	Pentadecanoic Acid	0.0078	26.0			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C16:1n7t	9t-Palmitelaidic Acid (Omega 7)	0.0084	27.9			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C17:0	Heptadecanoic Acid	0.0070	23.4			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C17:1n9	10-Heptadecenoic Acid	0.0071	23.6			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	9c,11t-CLA	9c,11t-Conjugated Linoleic Acid	0.0073	24.5			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C18:4n3	Stearidonic Acid	0.0012	4.1			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C19:0	Nonadecanoic Acid	0.0064	21.3			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C20:3n3	11-14-17 Eicosatrienoic Acid	0.0055	18.3			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C20:4n3	Arachidonic Acid (Omega 3)	0.0030	10.0			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C21:0	Heneicosanoic Acid	0.0031	10.3			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
	C22:2n6	13-16-Docosadienoic Acid	0.0070	23.3			quadratic	1/x	Glyceryl Tri(hexadecanoate-d31)
13	No information								

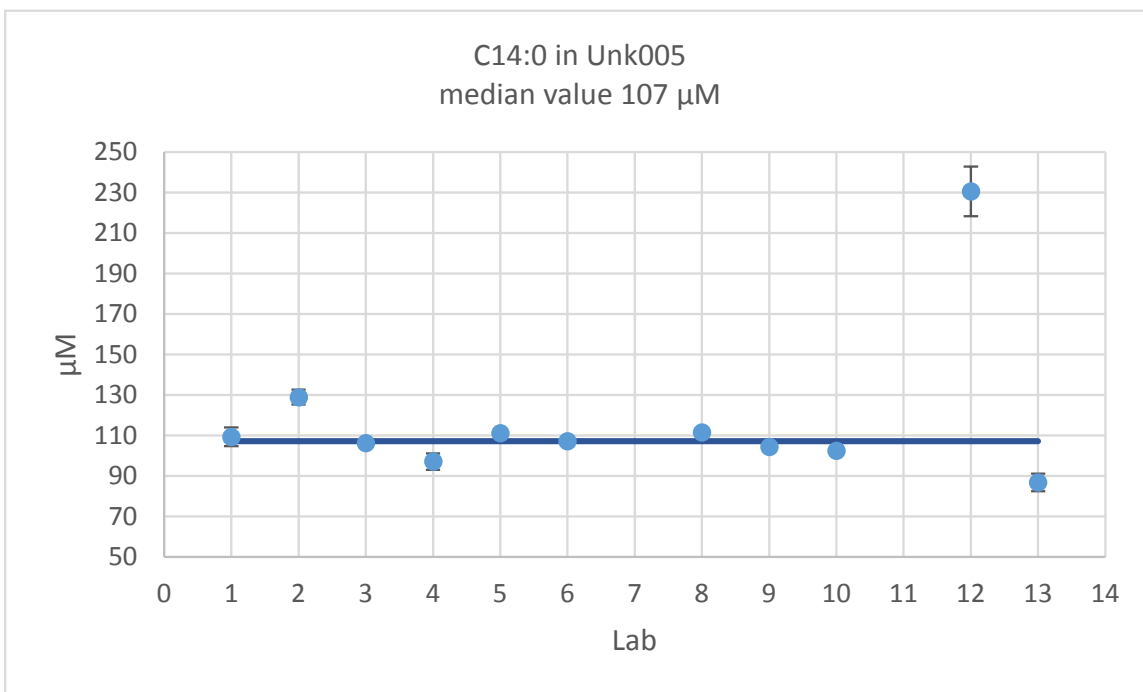
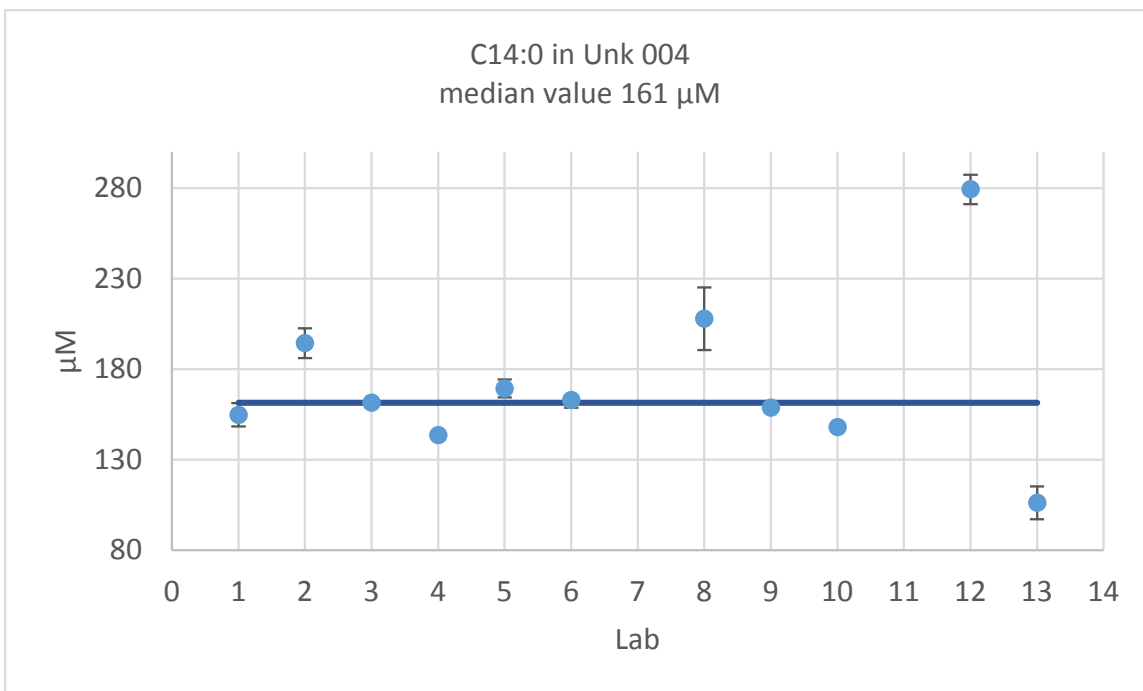
Table A-4 Additional notes provided by laboratories	
Lab #	Note:
1	^a trans-vaccenic acid coelutes with cis-vaccenic acid ND = not determined
2	C20:1n9 and C20:2n6 were not quantitated
11	Method was not quantitative so data were withdrawn.
12 (total fatty acid data)	C22:1n9 (Docosenoic acid) was used as a surrogate.
12 (free fatty acid data)	C22:1n9 (Docosenoic acid) was used as a surrogate.

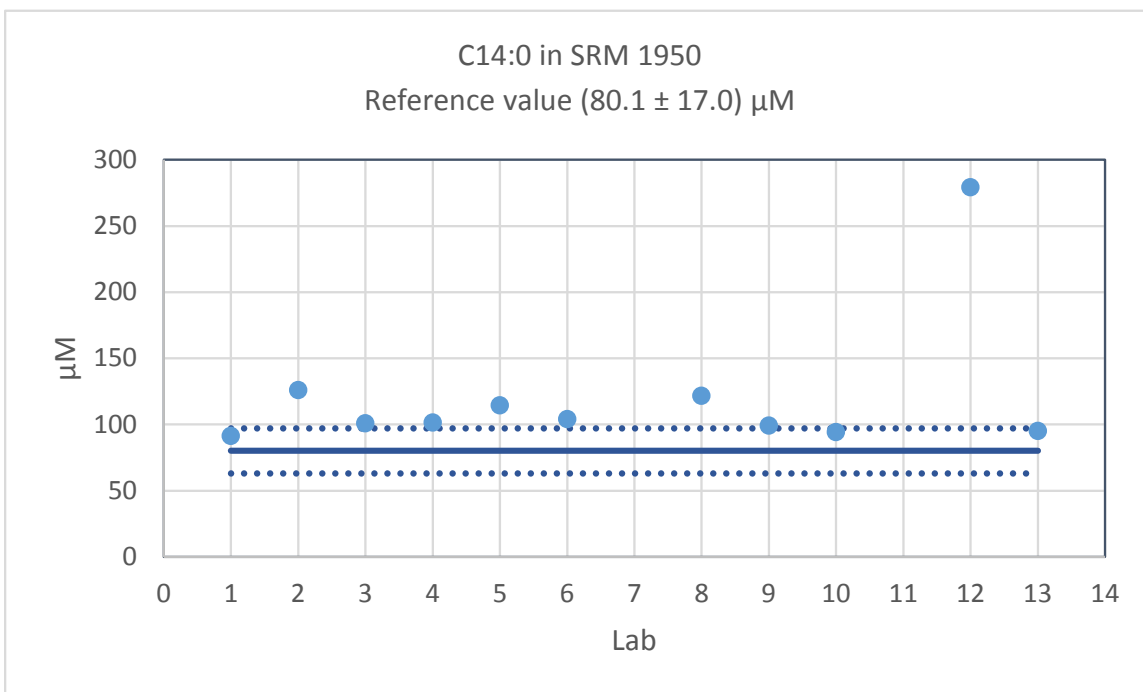
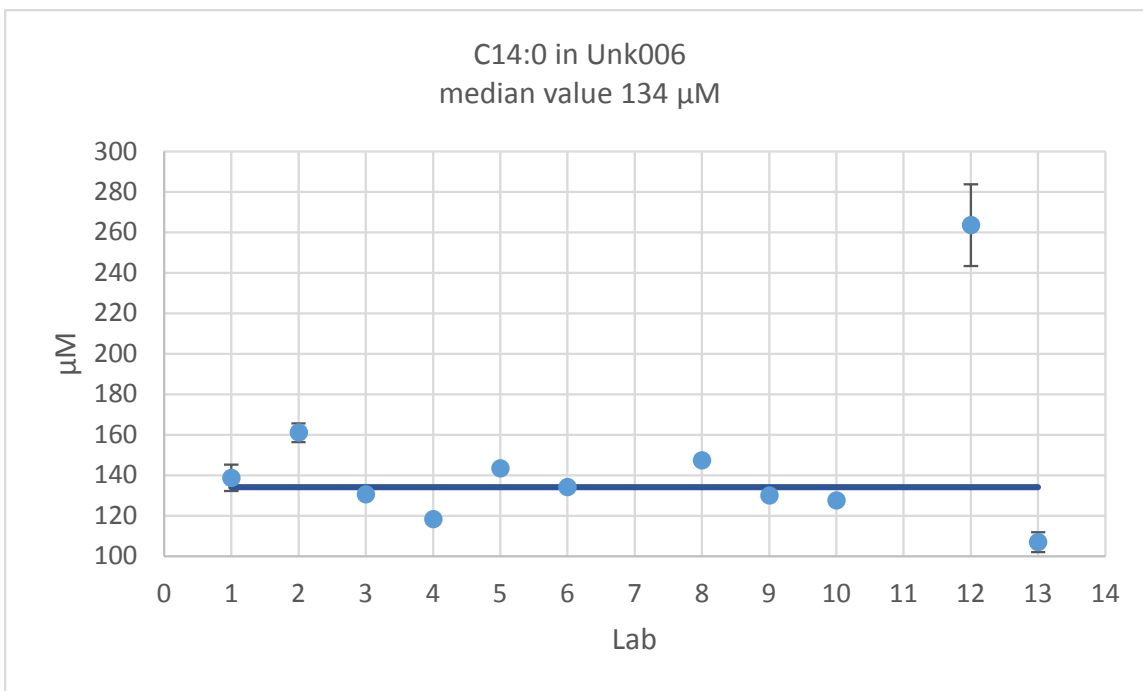
Appendix B.

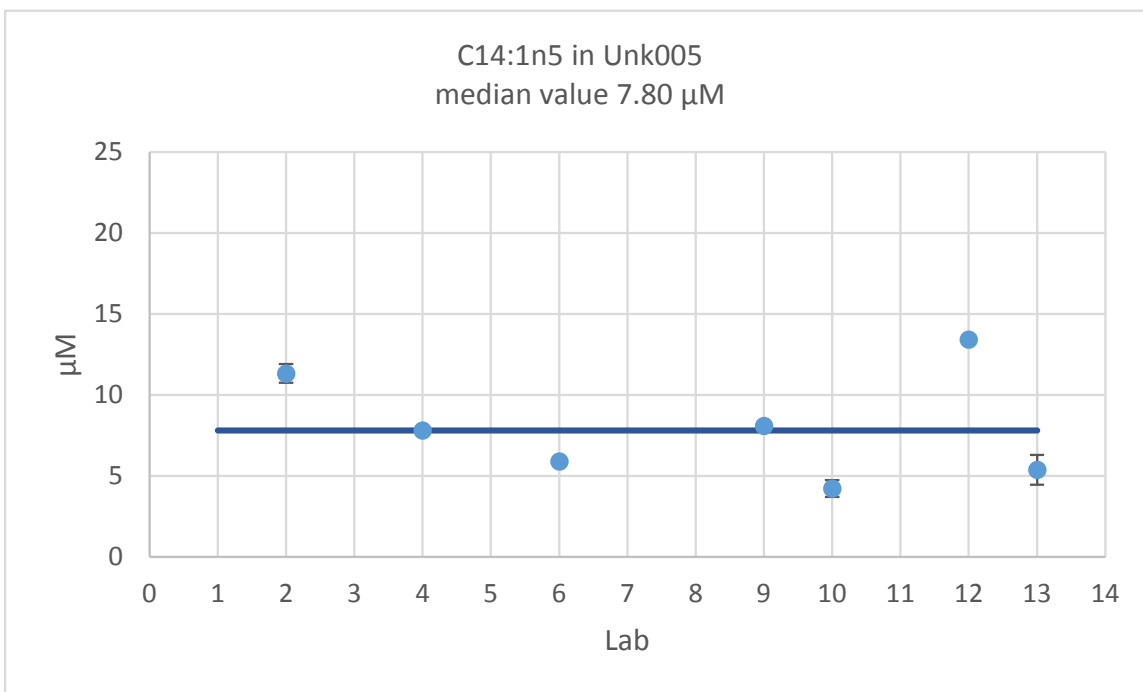
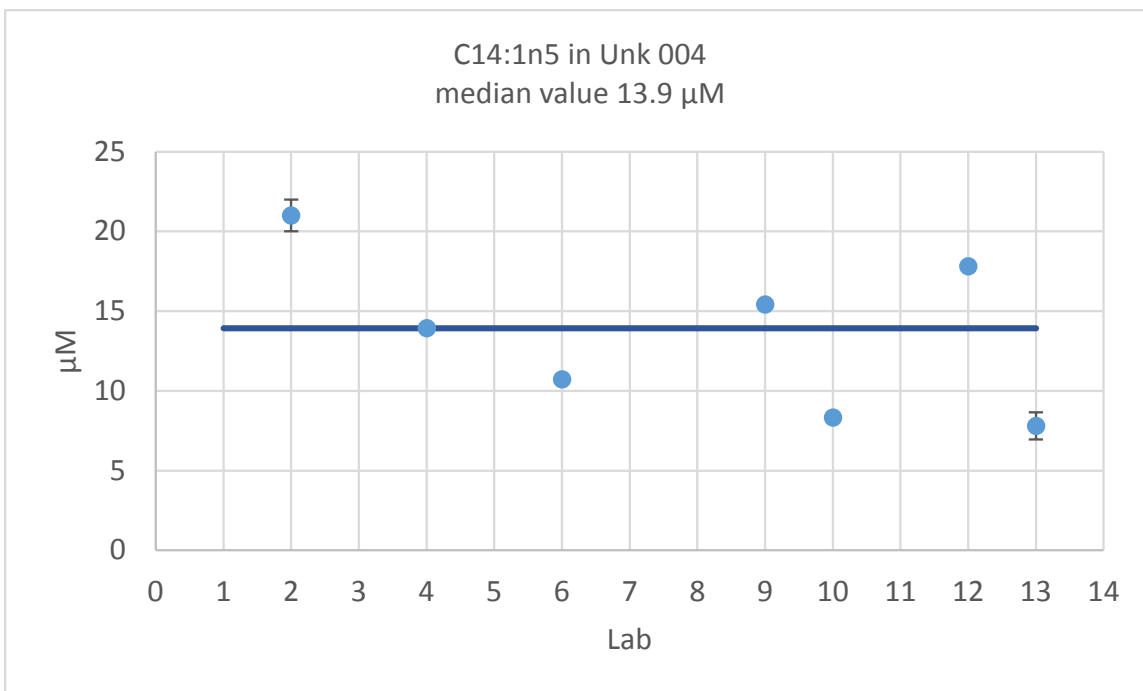
Charts of interlaboratory data received for the individual fatty acids in each material (in terms of μM) with the median identified for the three unknown samples and the certified or reference value with associated confidence interval identified for SRM 1950.

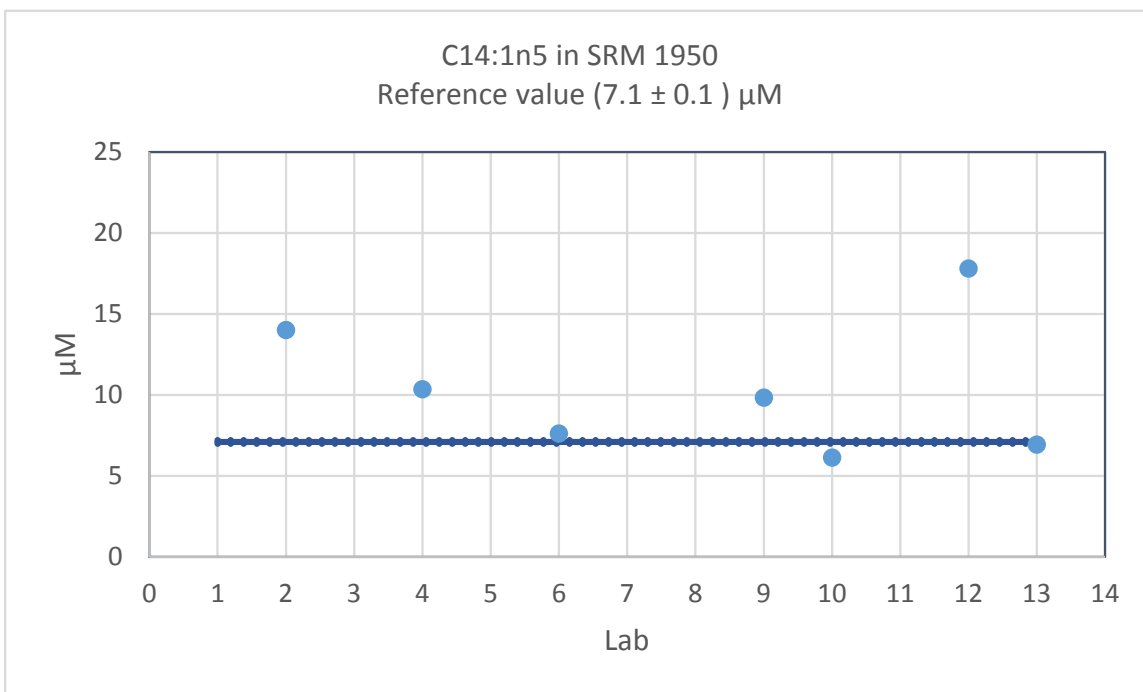
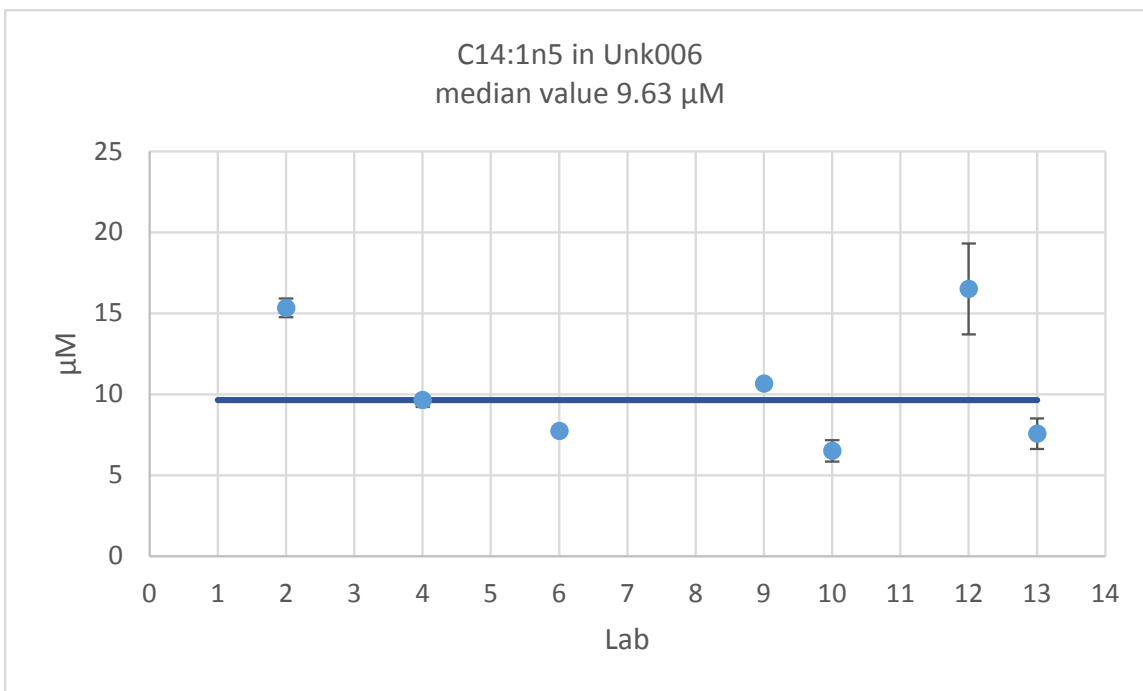
The charts are presented in the order of an individual fatty acid in each of the four materials (unknown 004, unknown 005, unknown 006, and SRM 1950) with the fatty acids in the order presented in Table 1. If fewer than four laboratories reported numerical data for a fatty acid, no chart is presented.

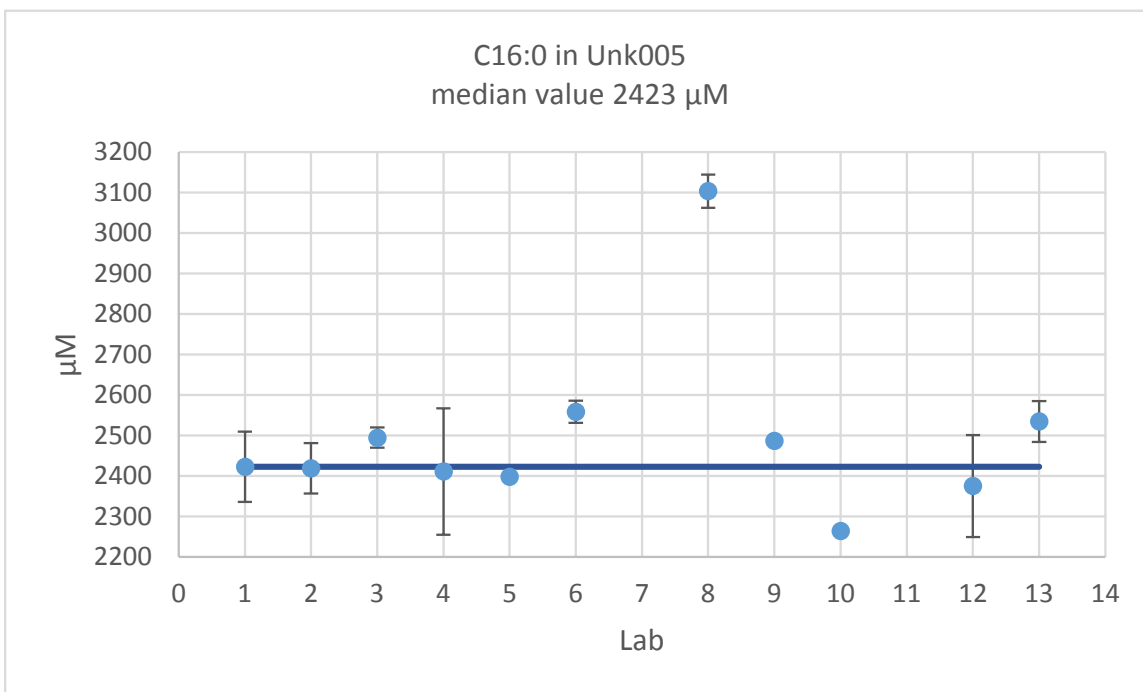
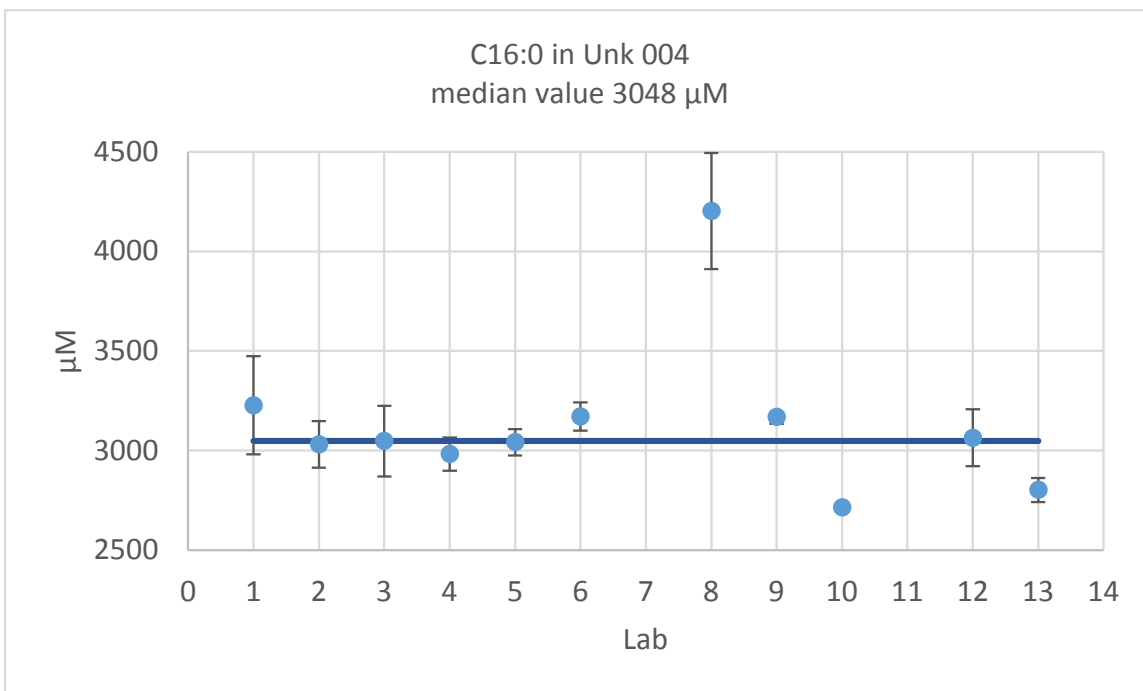
The error bars for each data point represent the laboratory's standard deviation from their analysis of three subsamples.

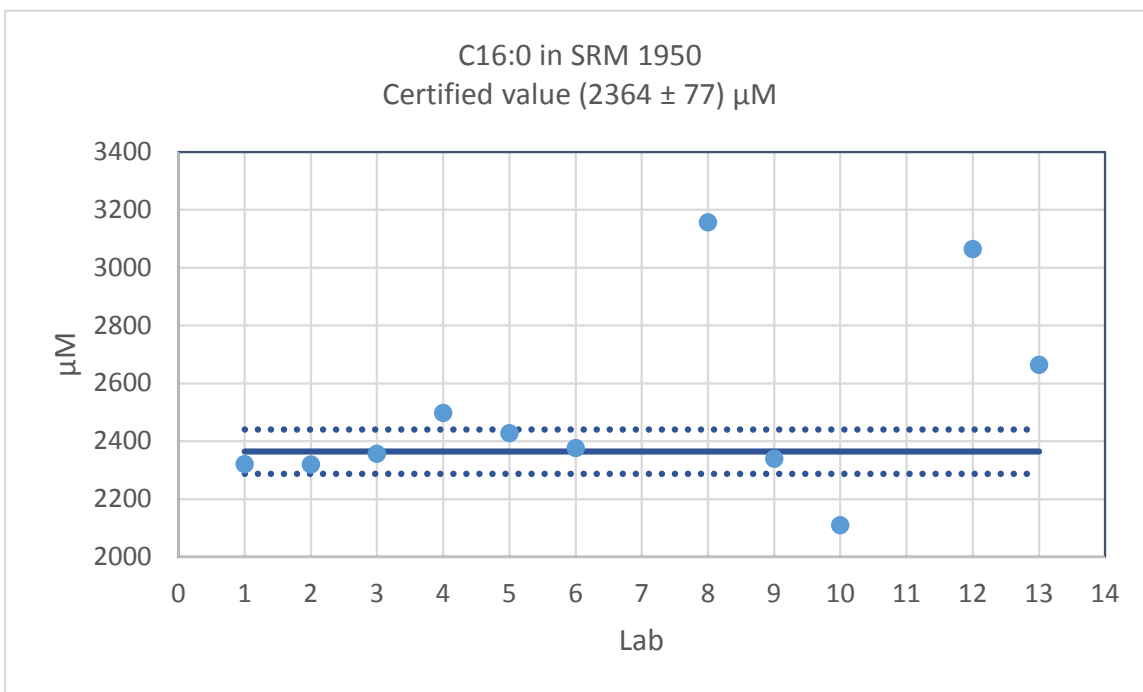
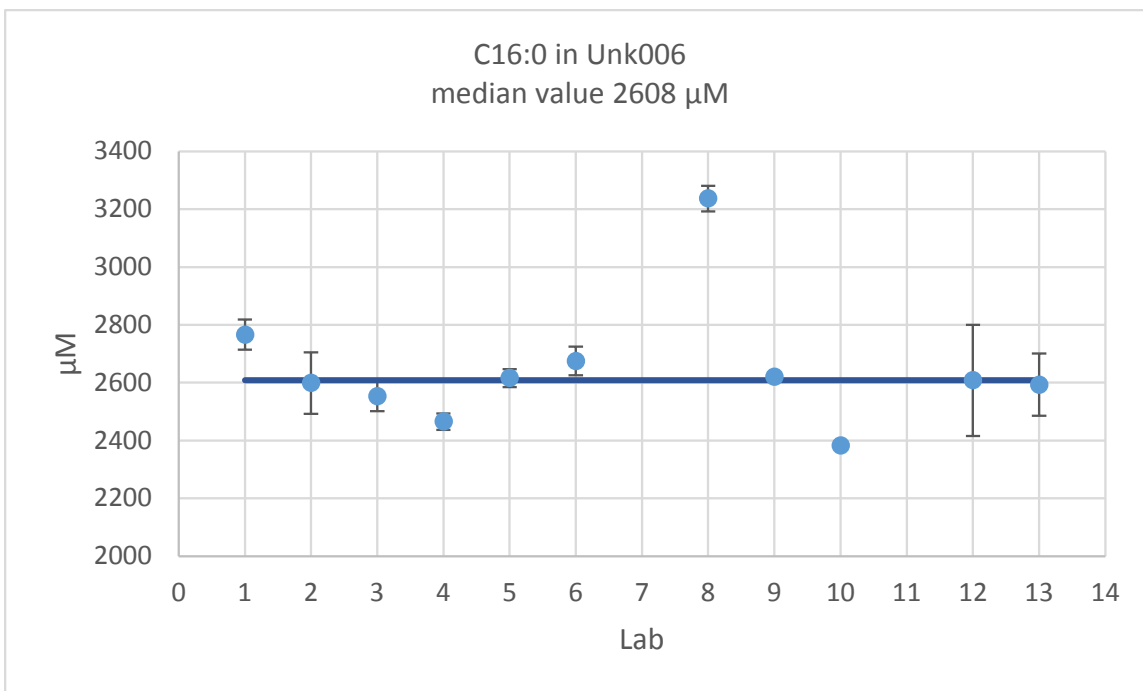


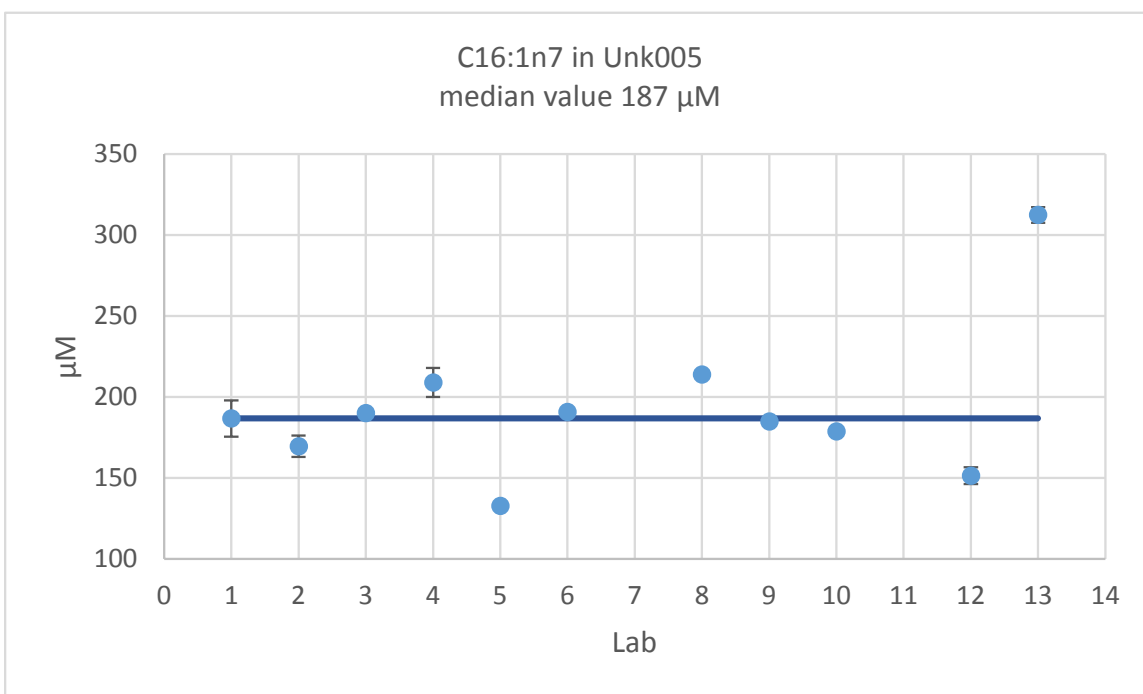
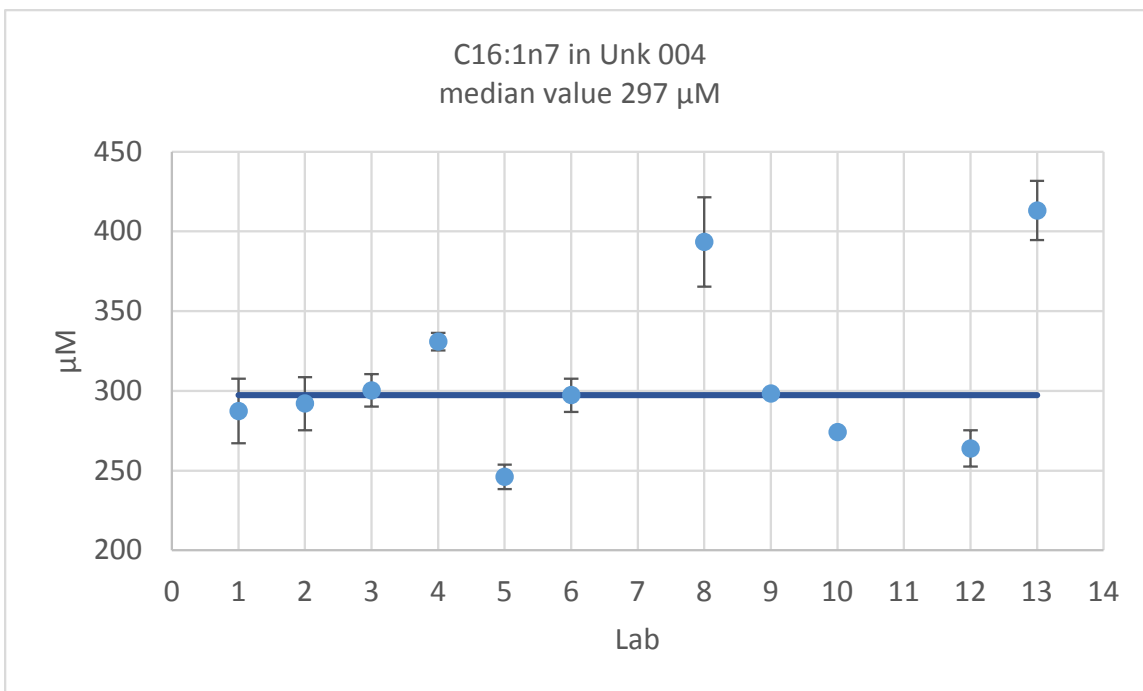


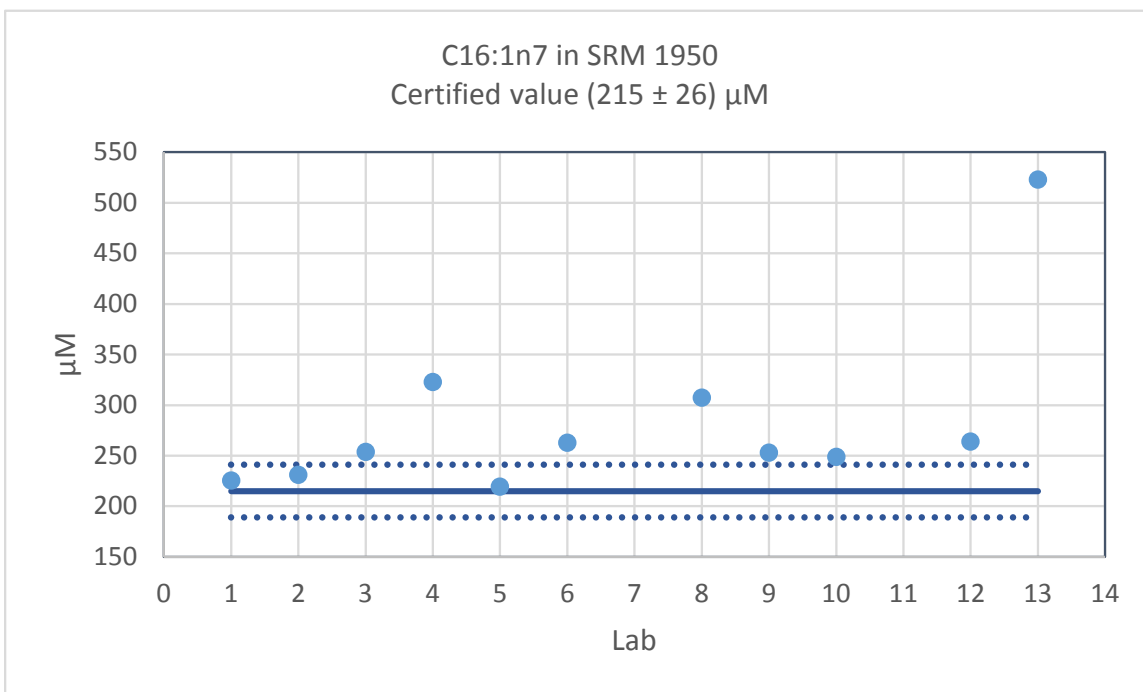
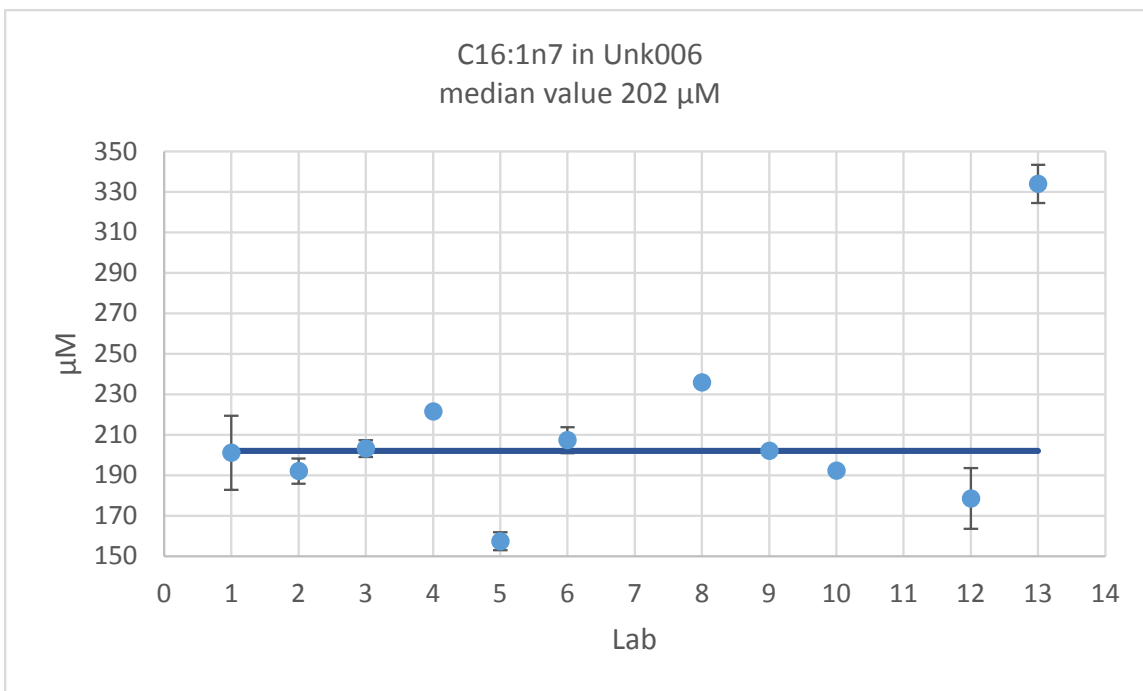


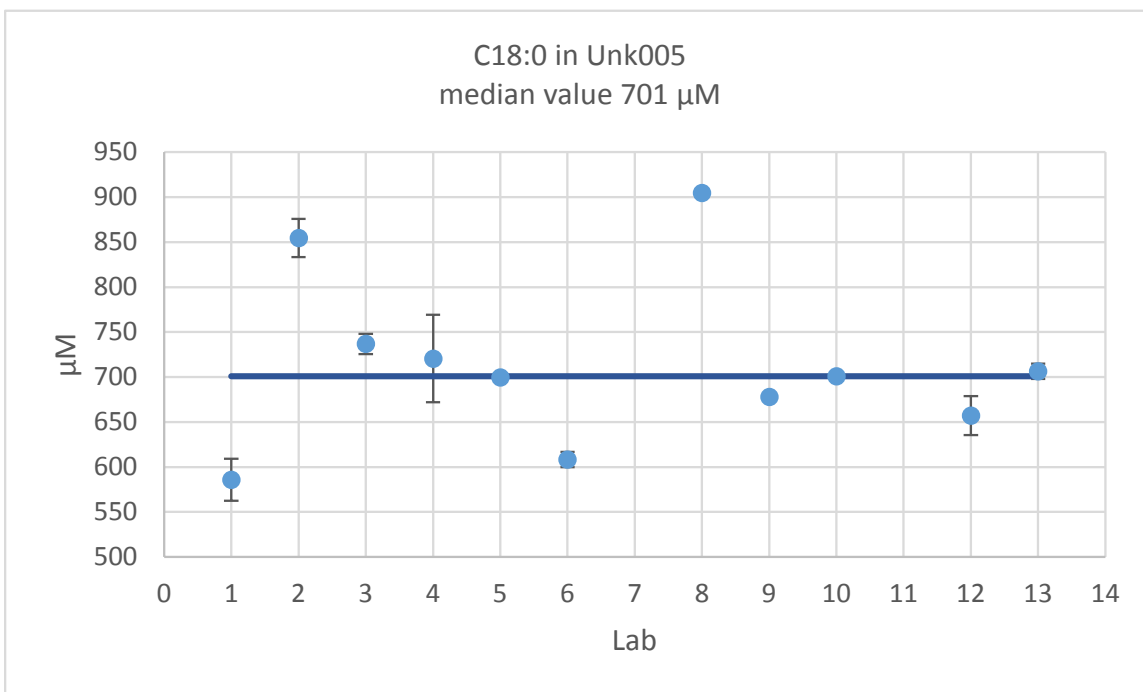
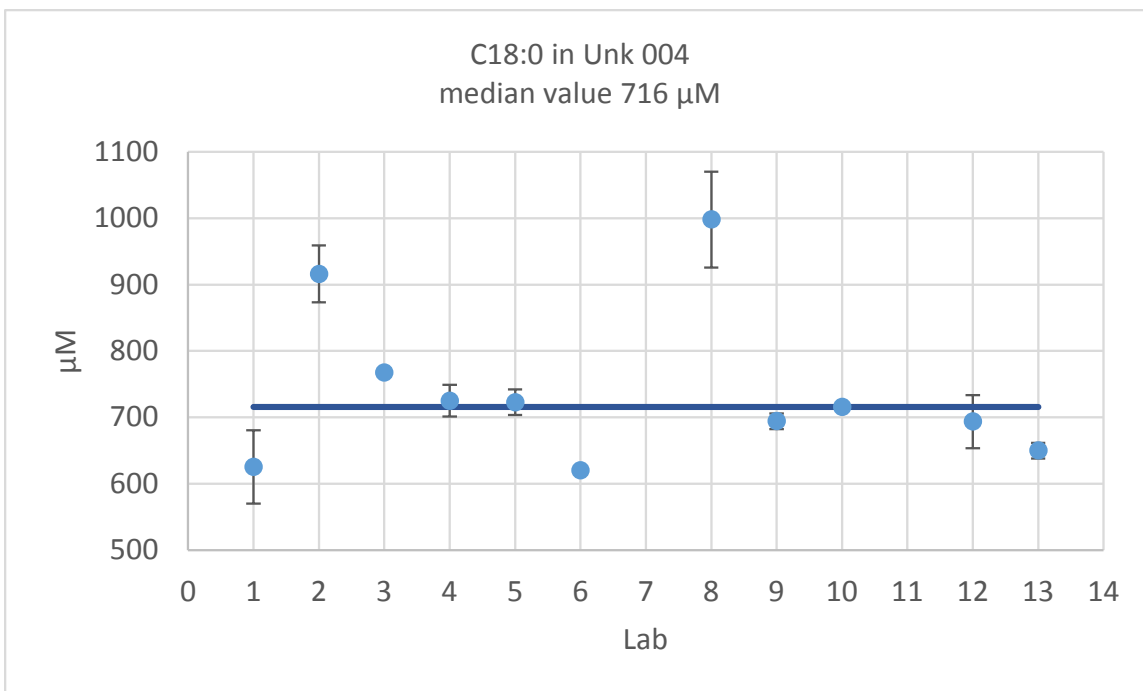


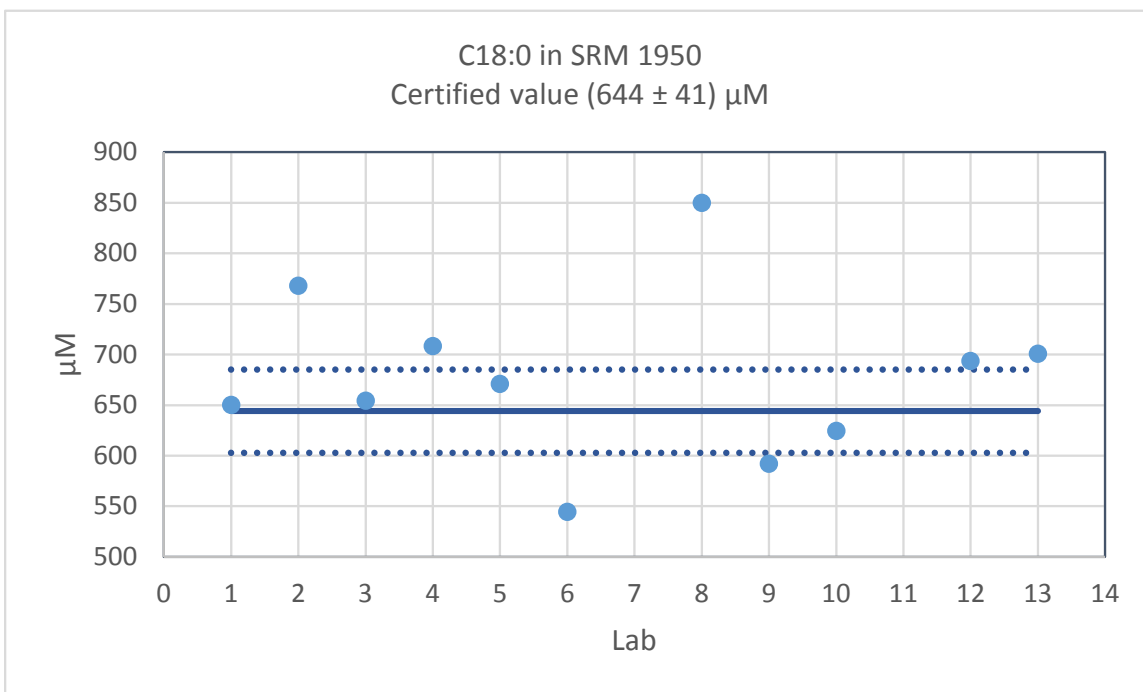
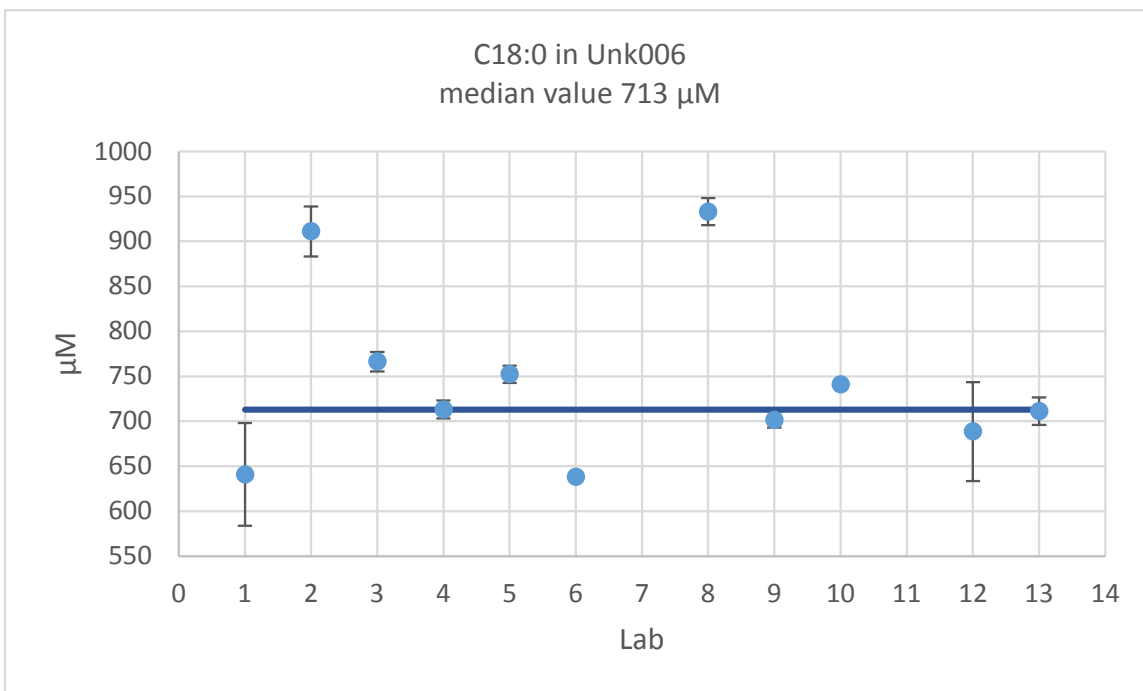


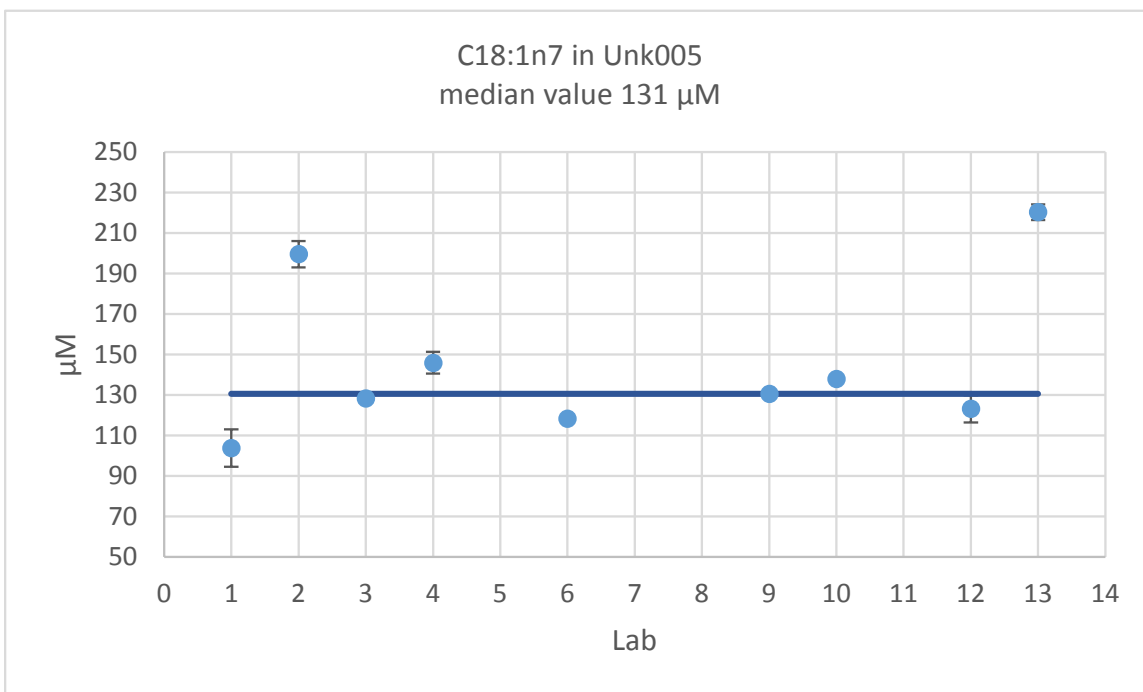
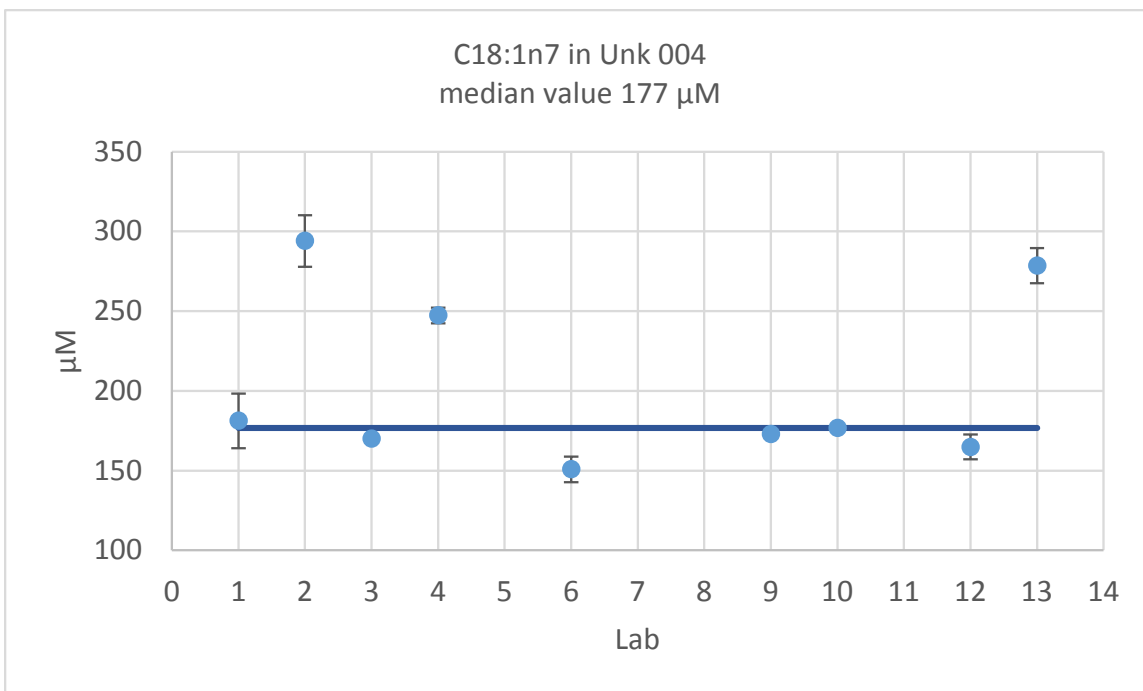


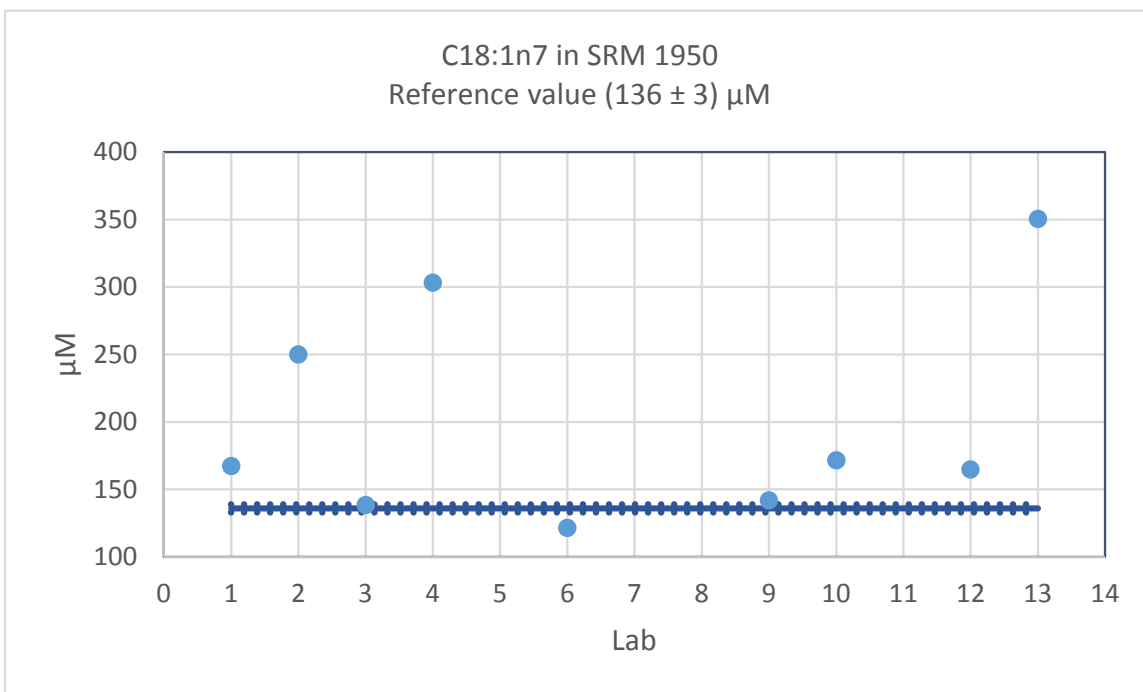
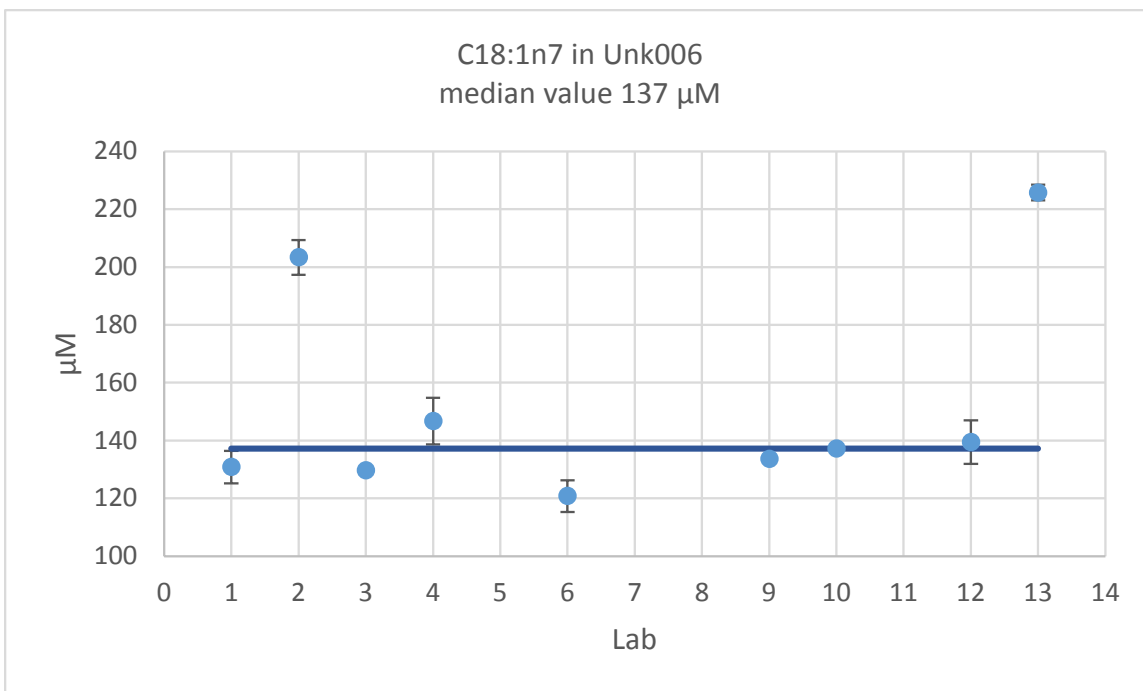


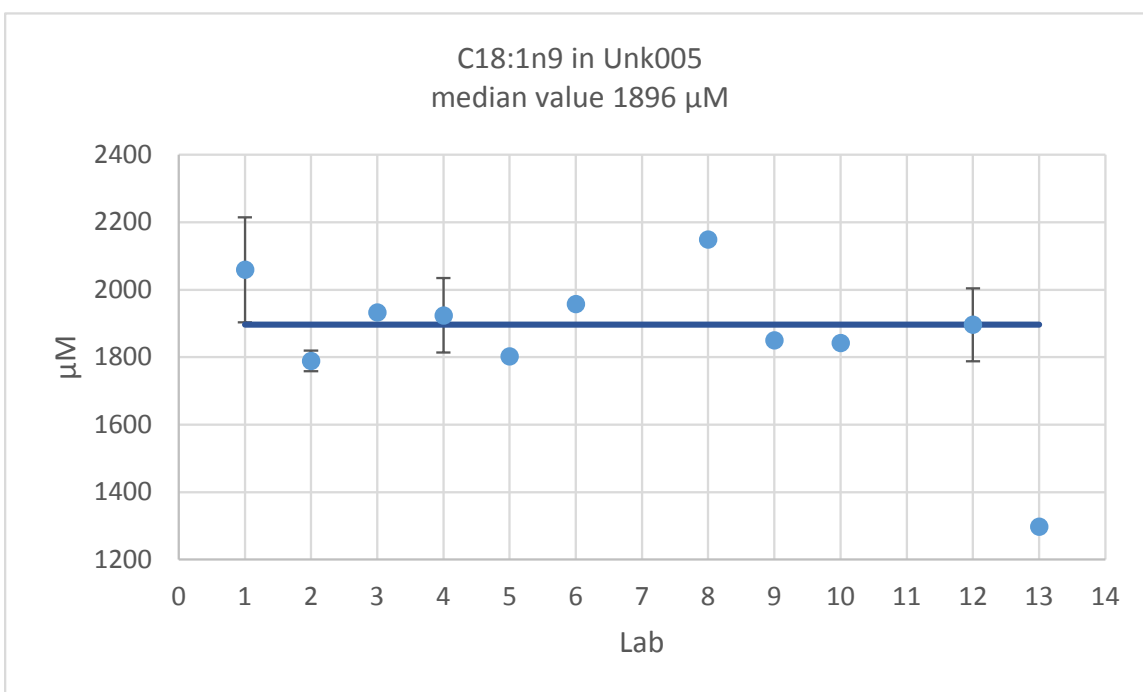
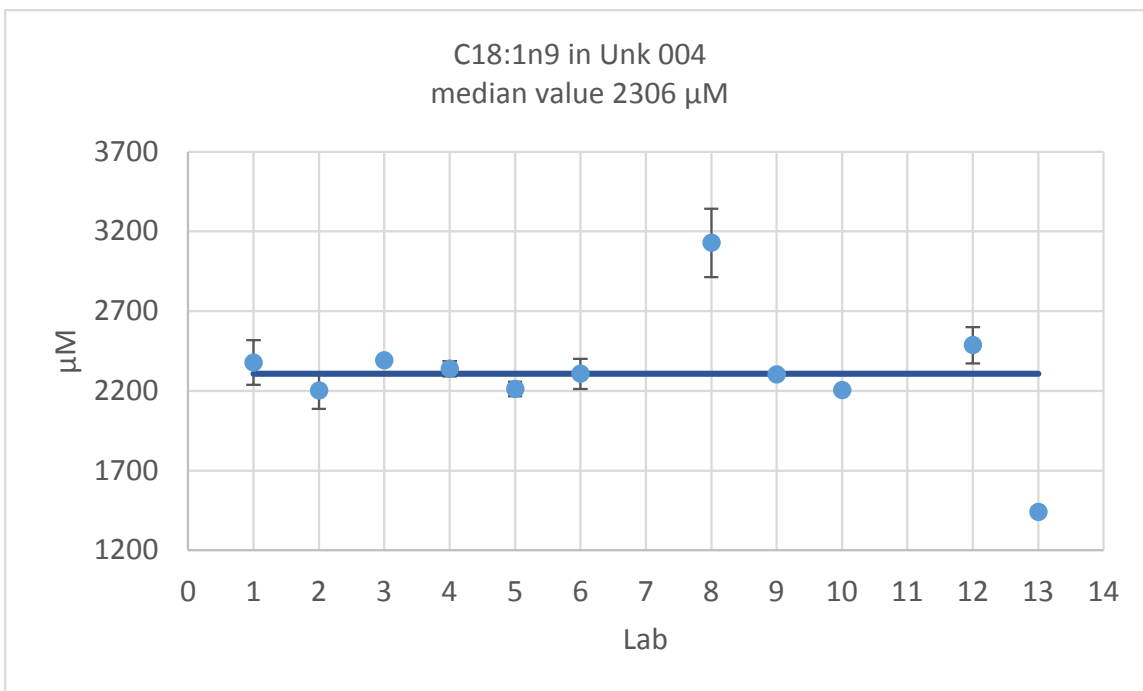


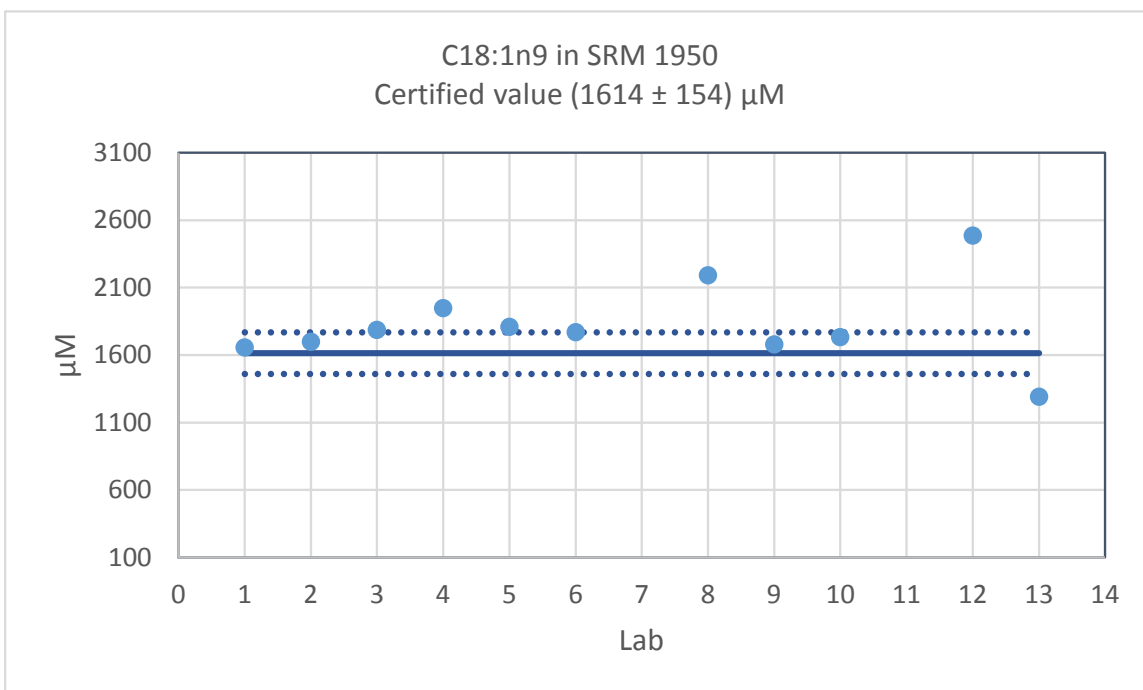
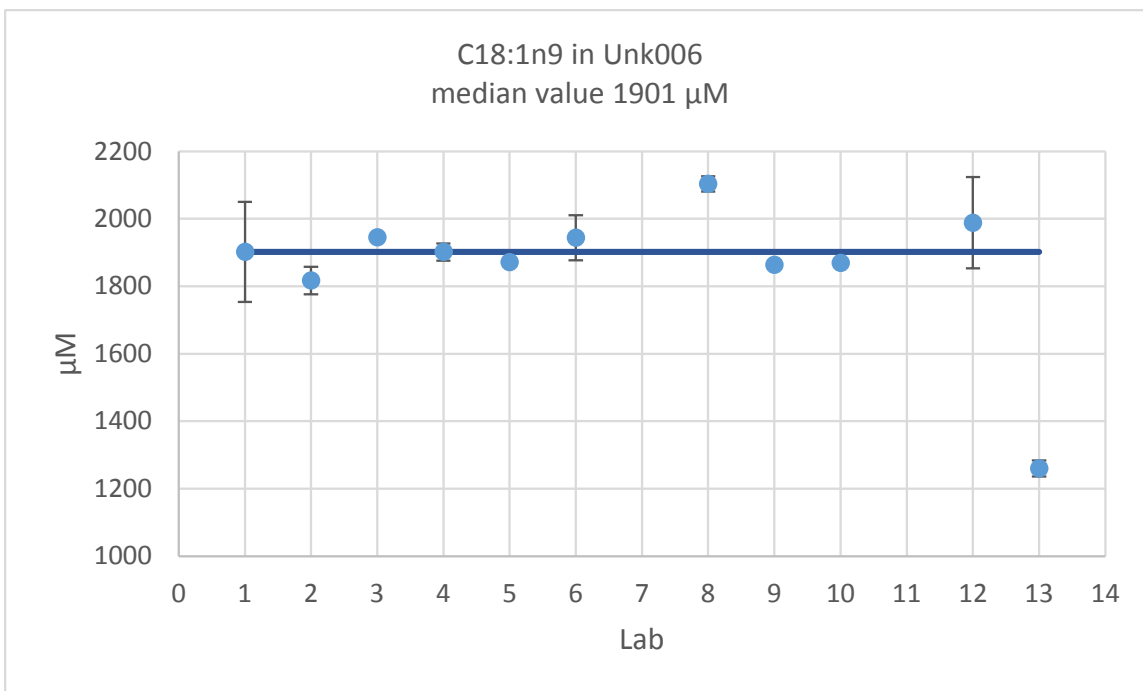


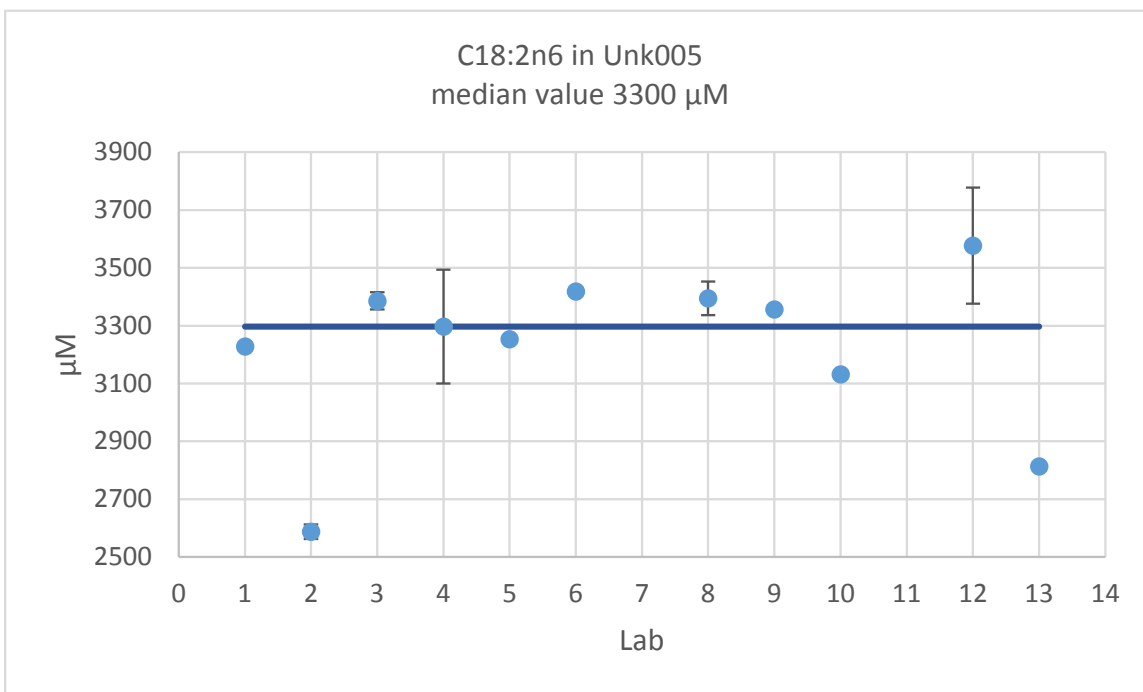
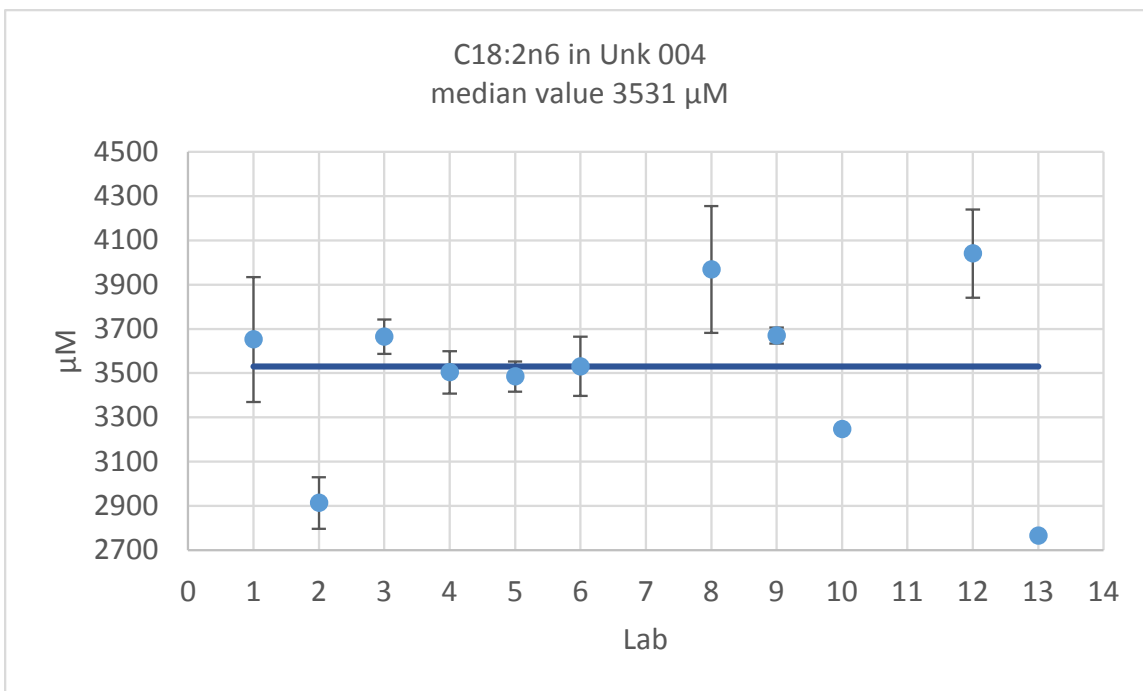


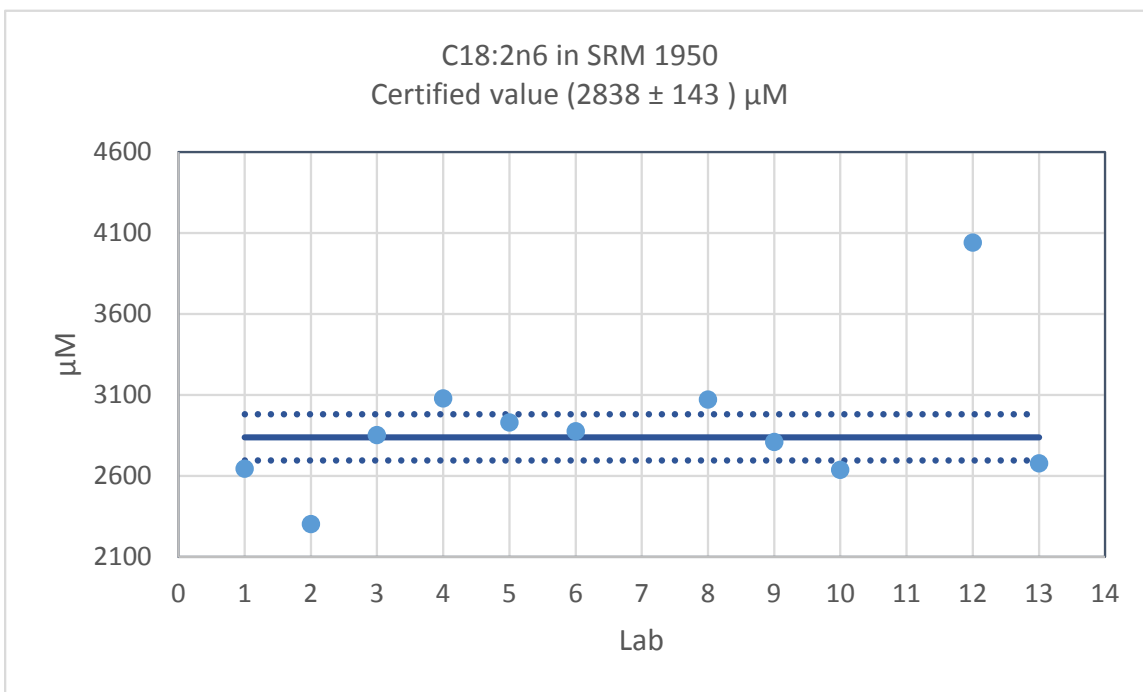
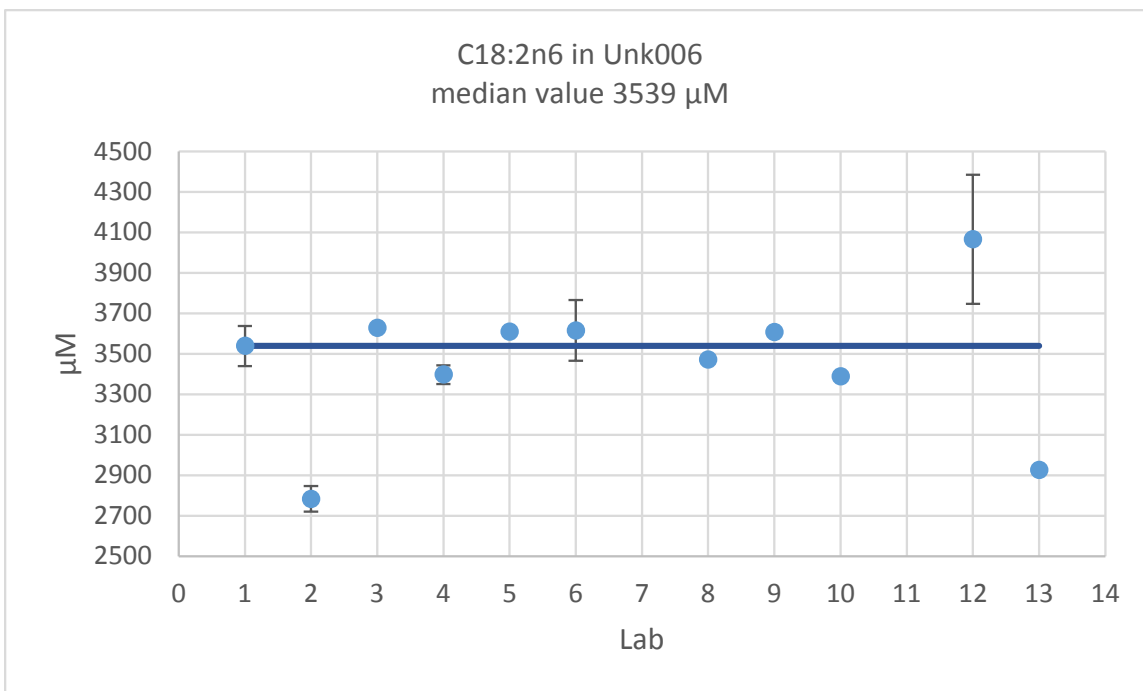


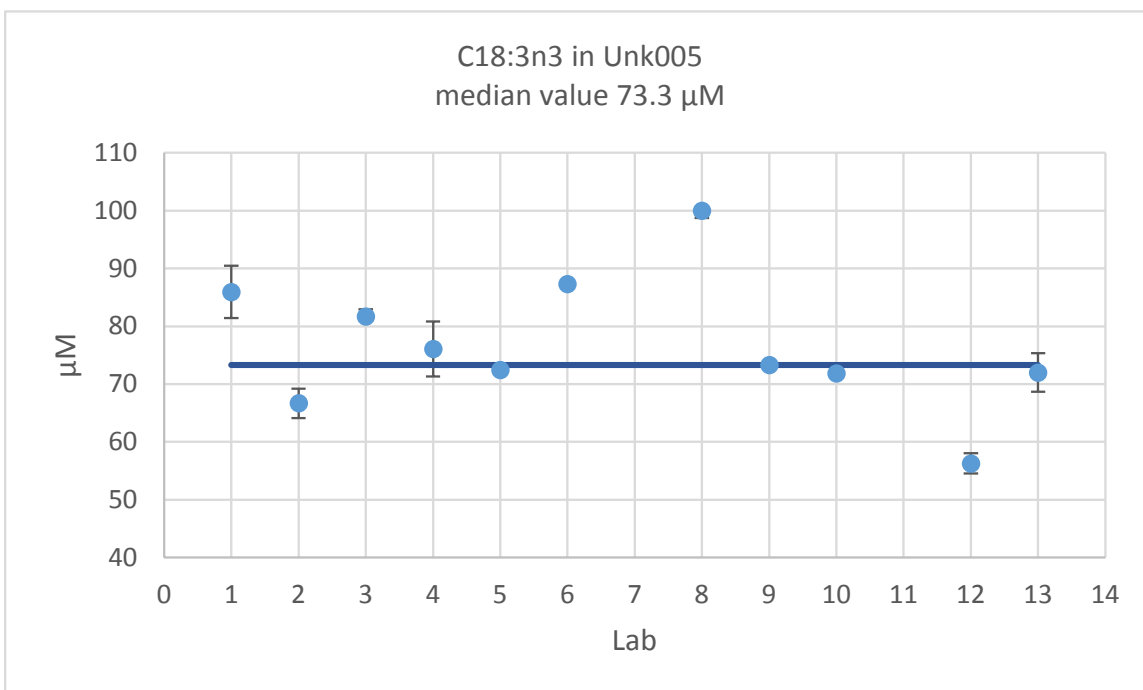
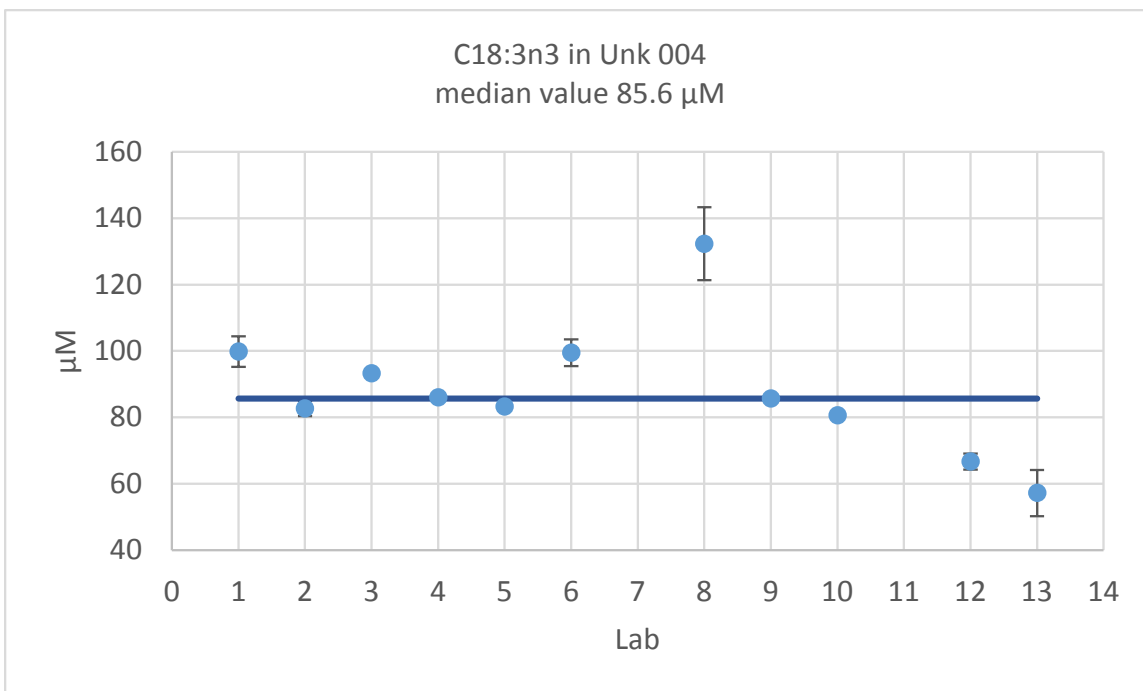


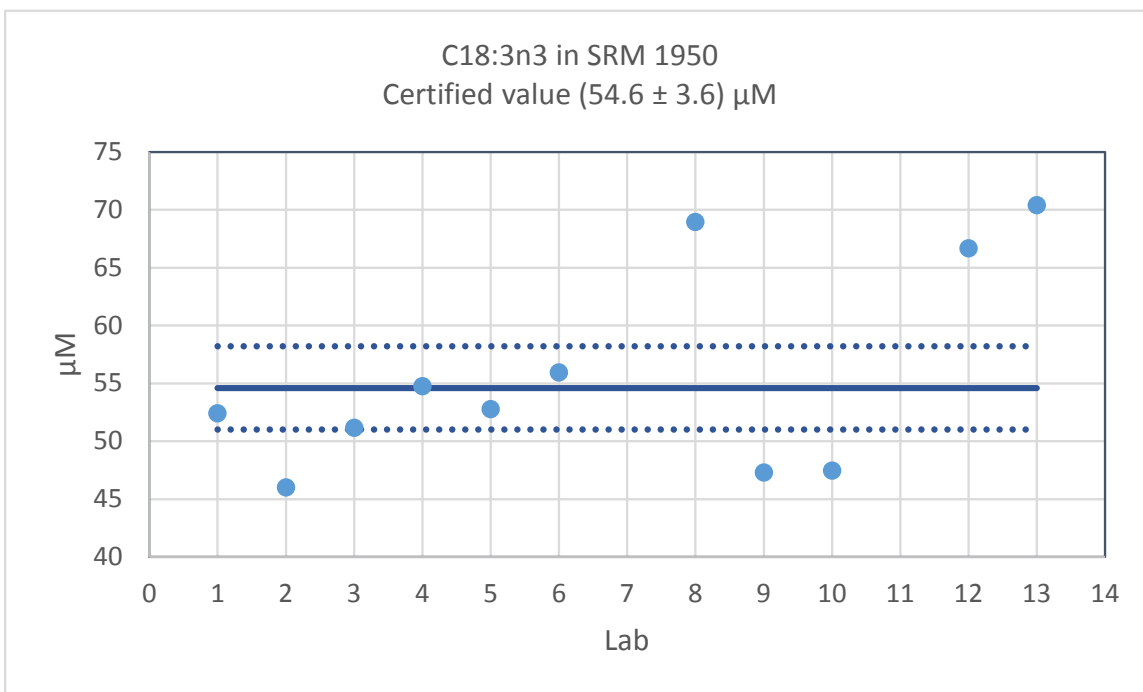
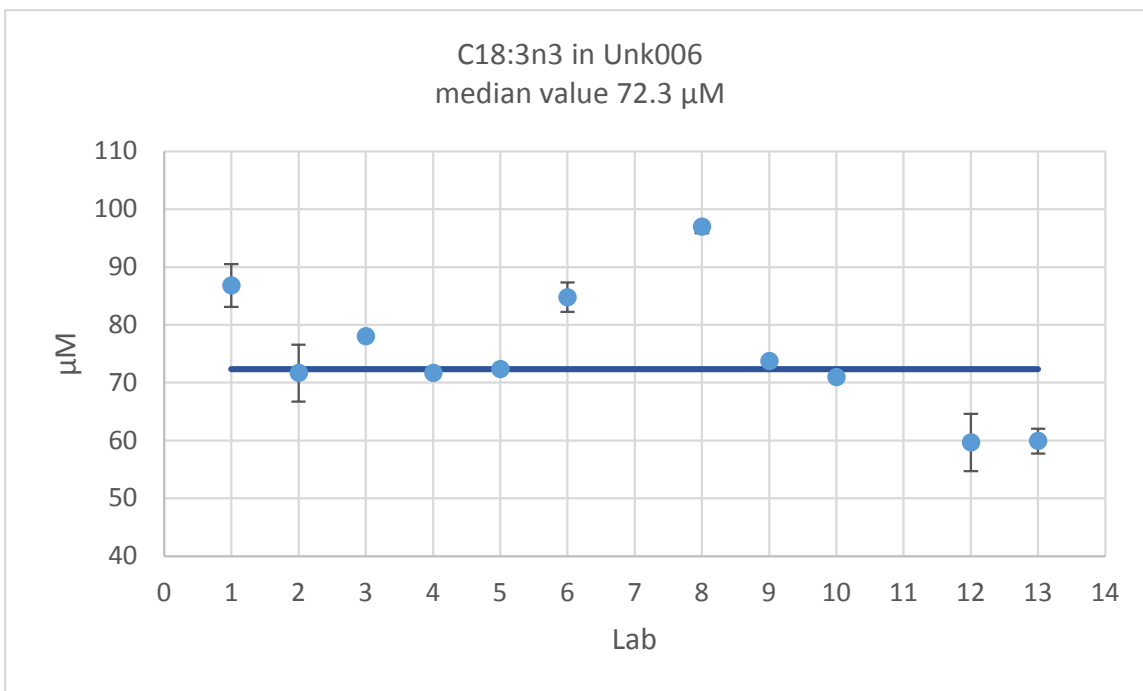


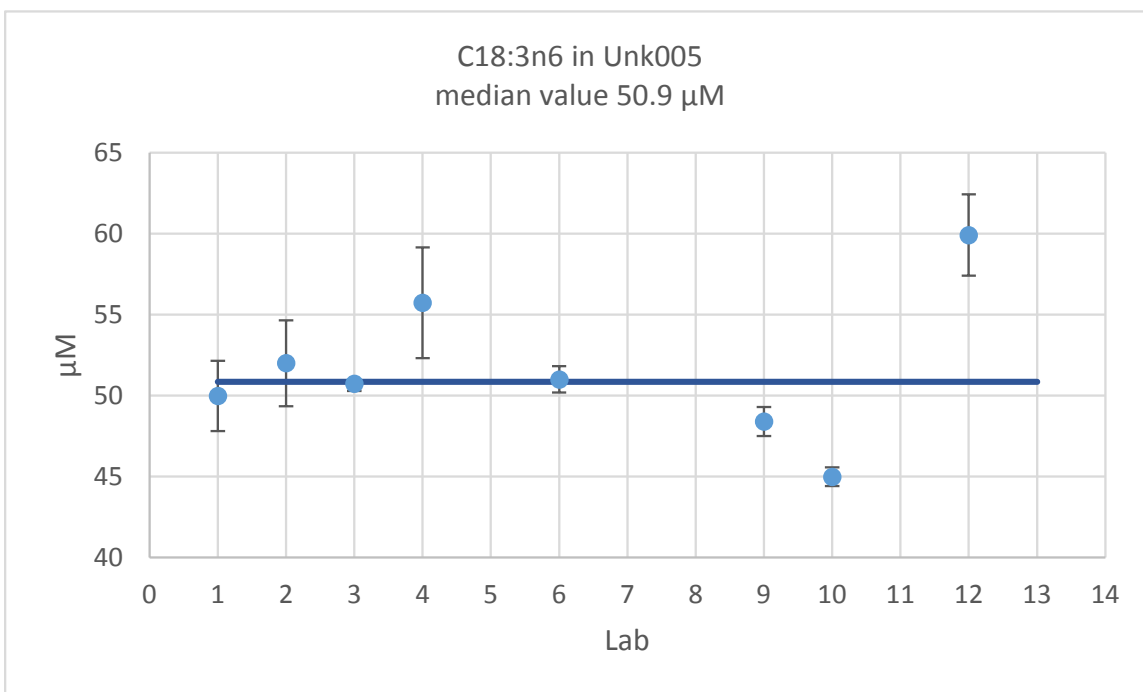
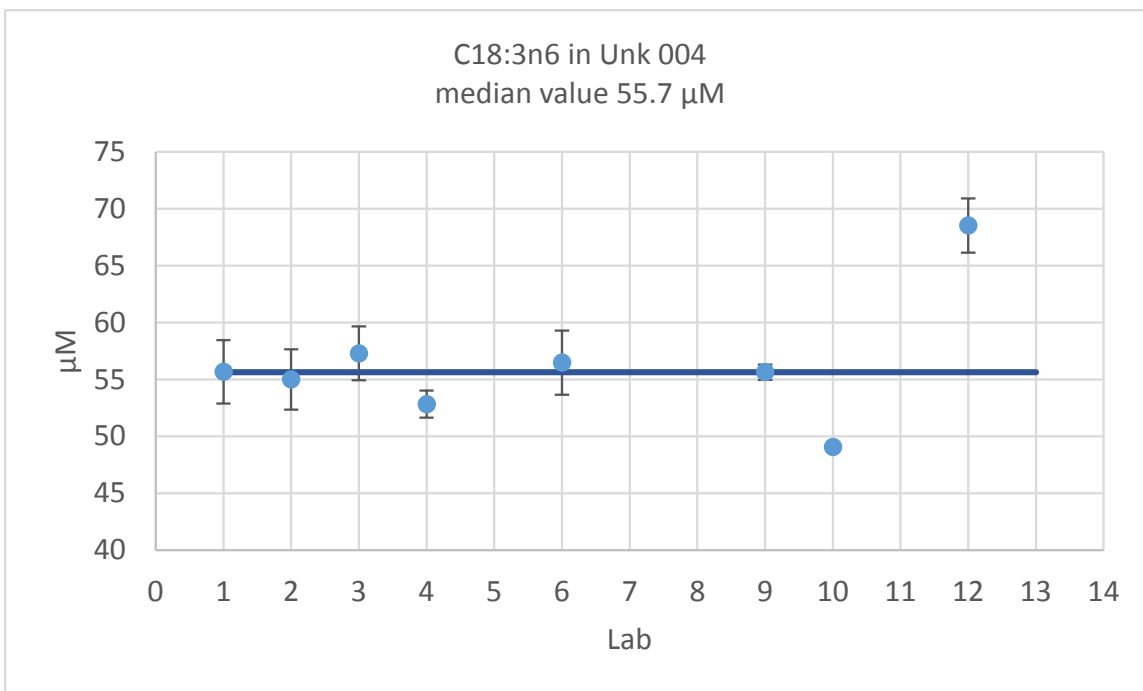


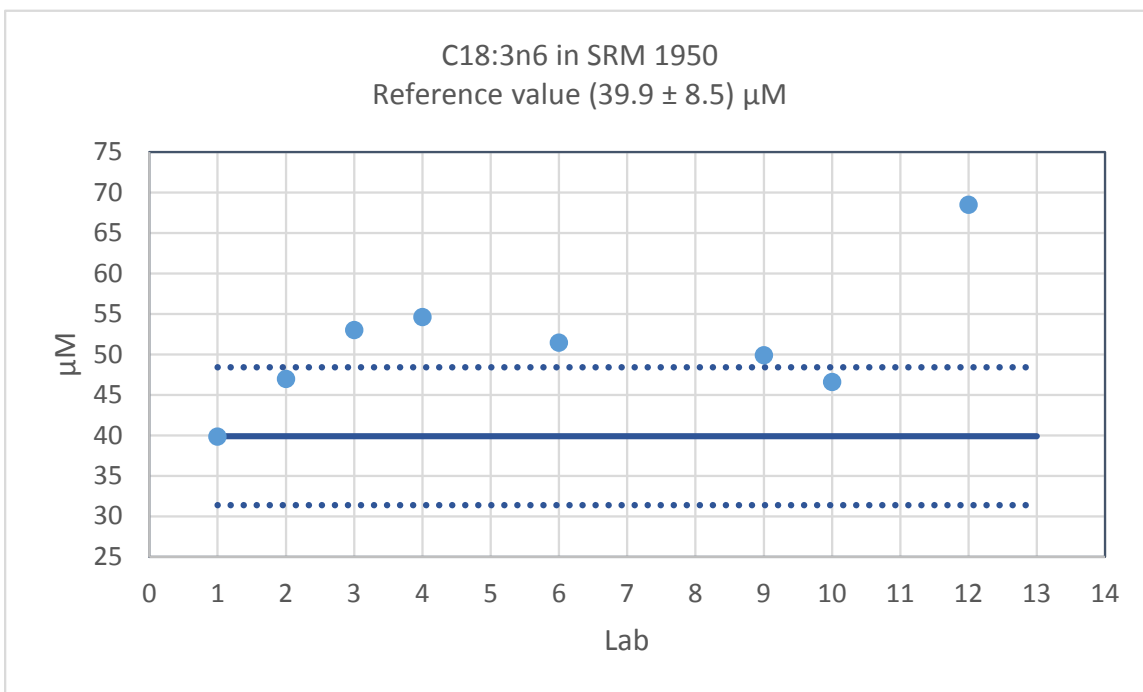
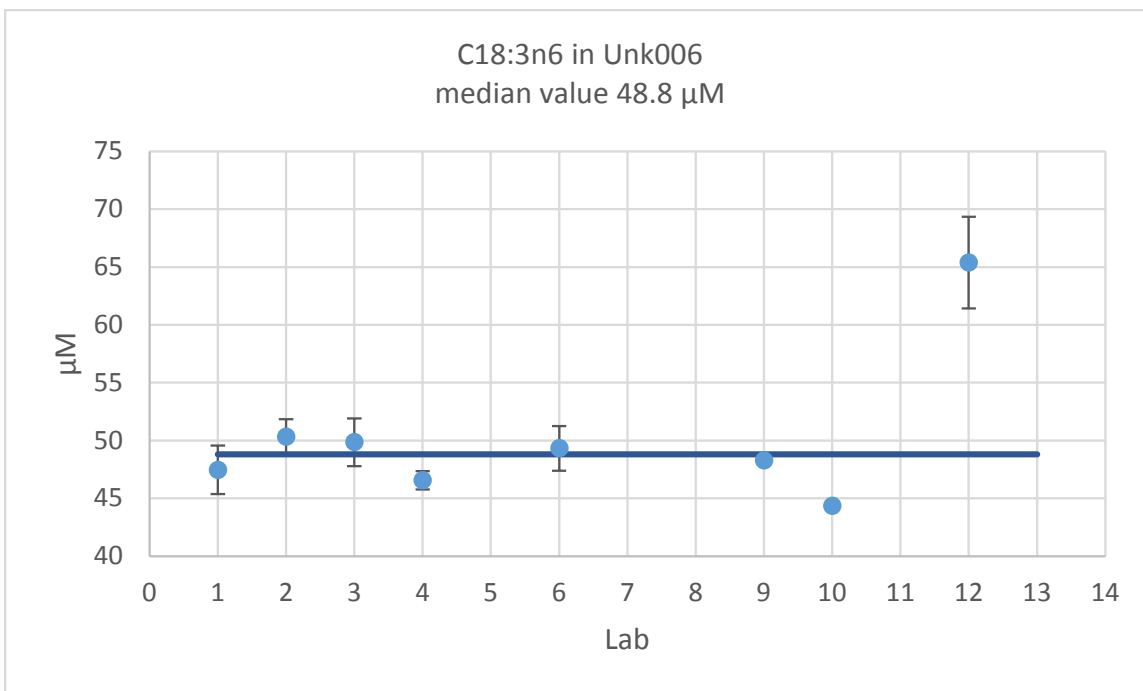


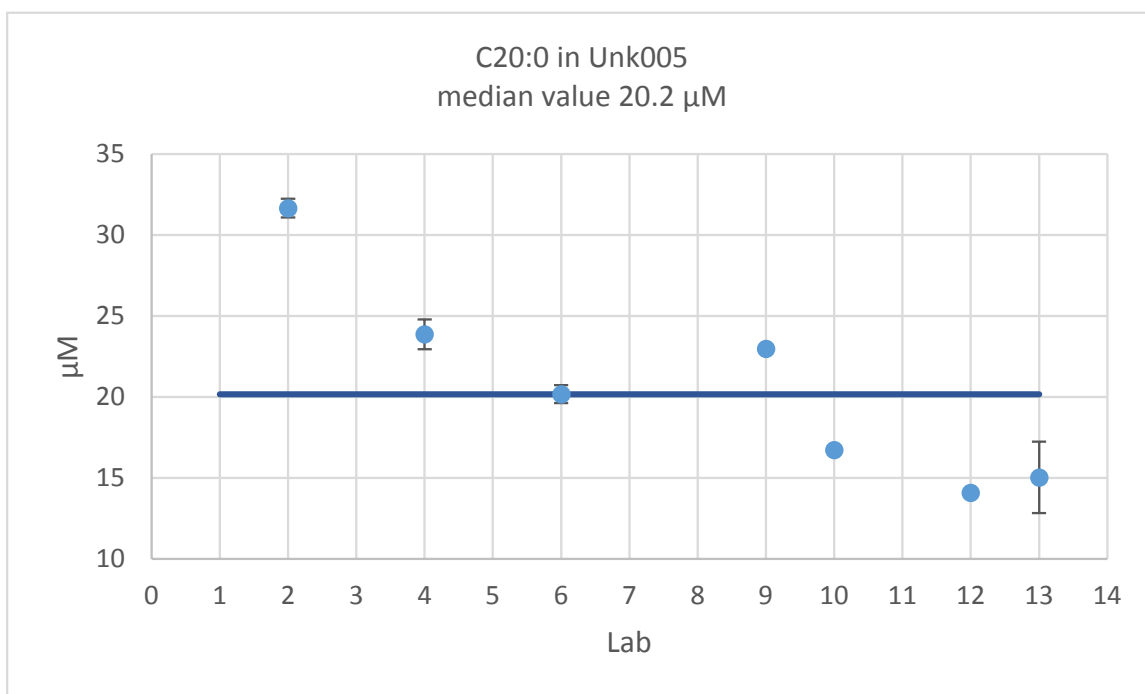
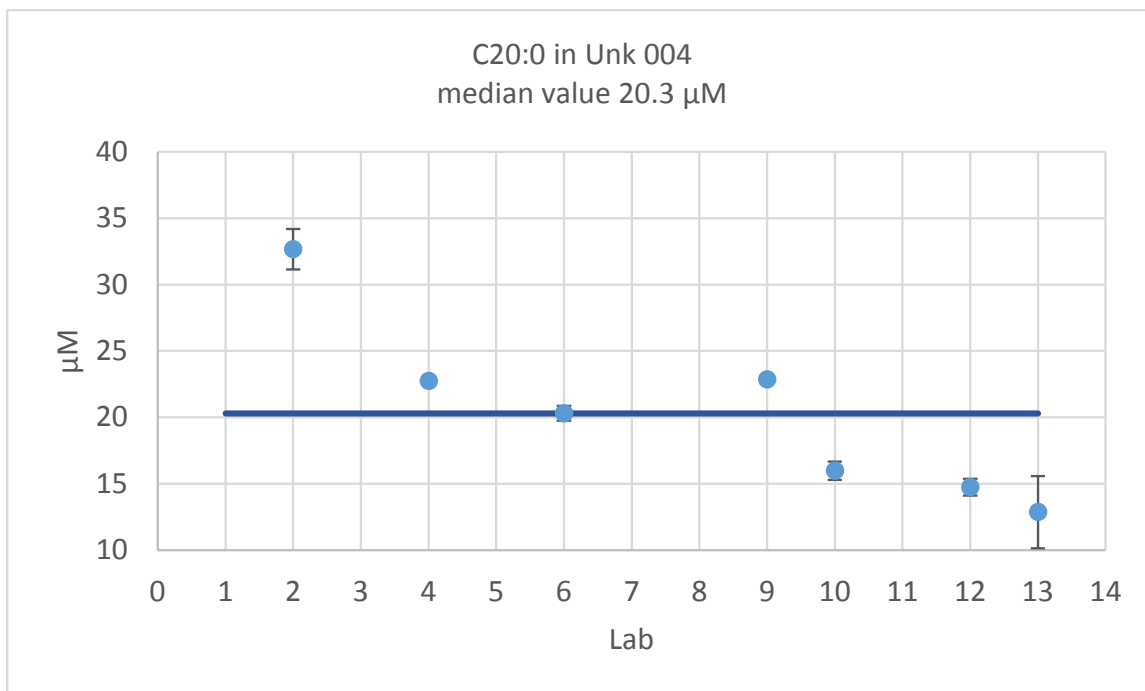


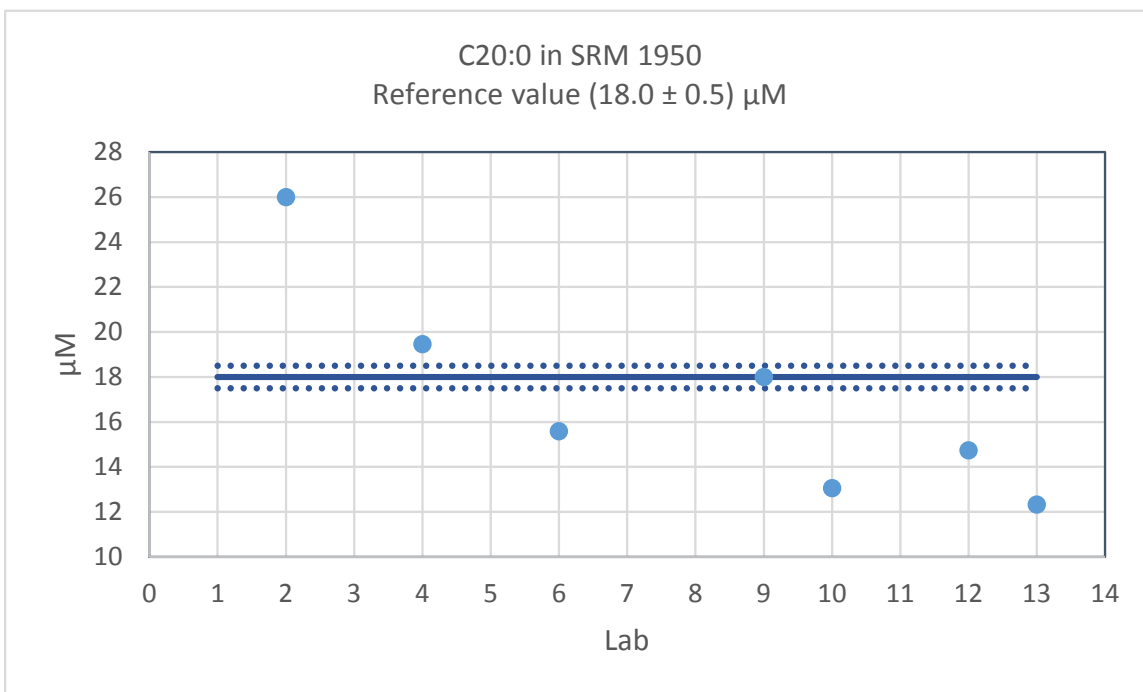
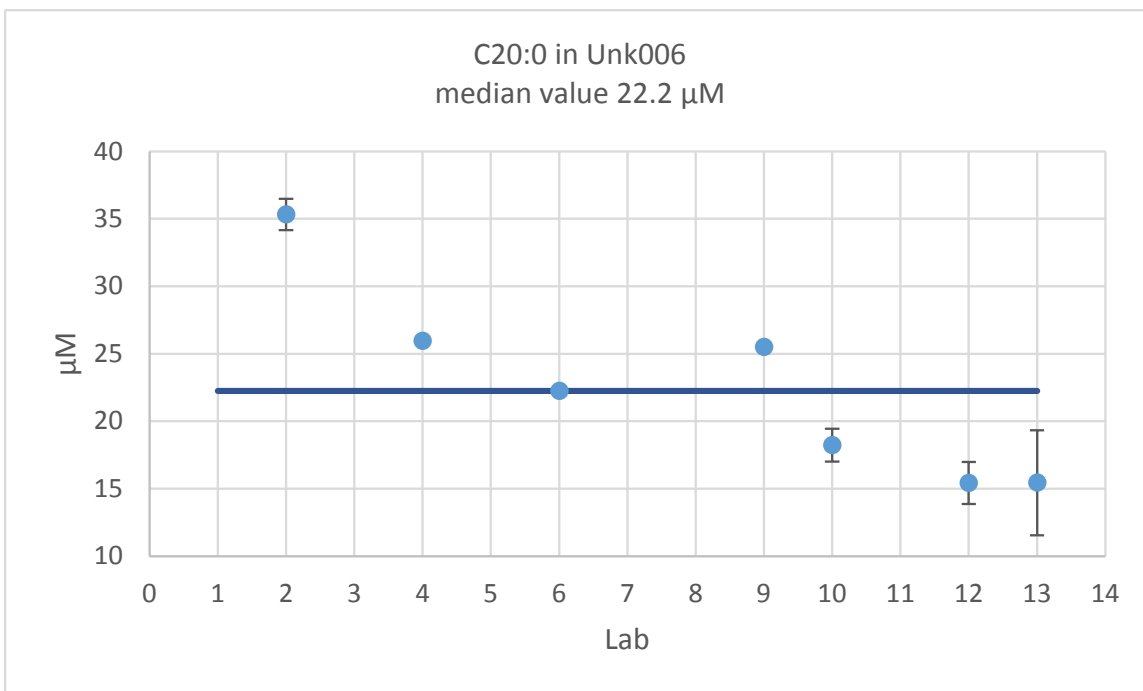




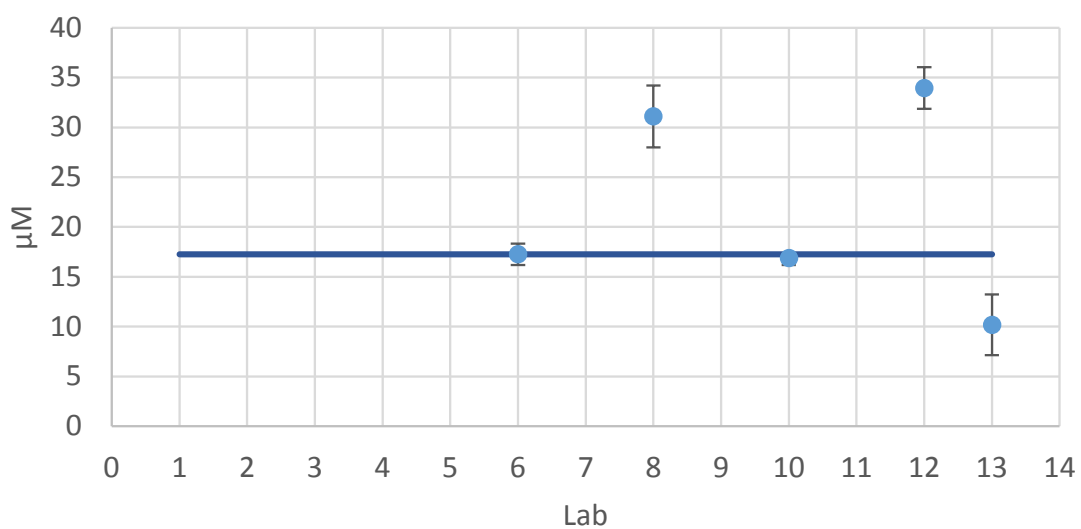




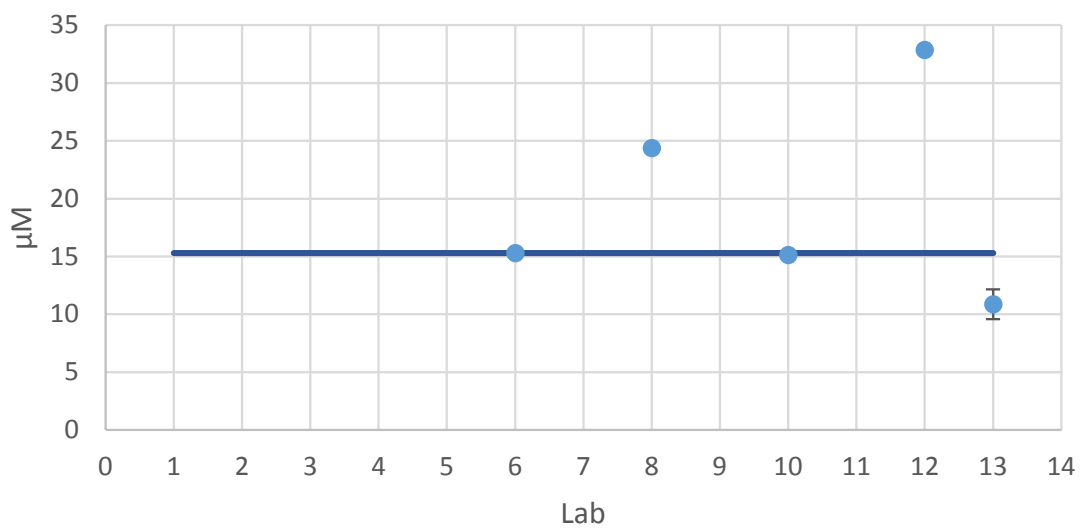


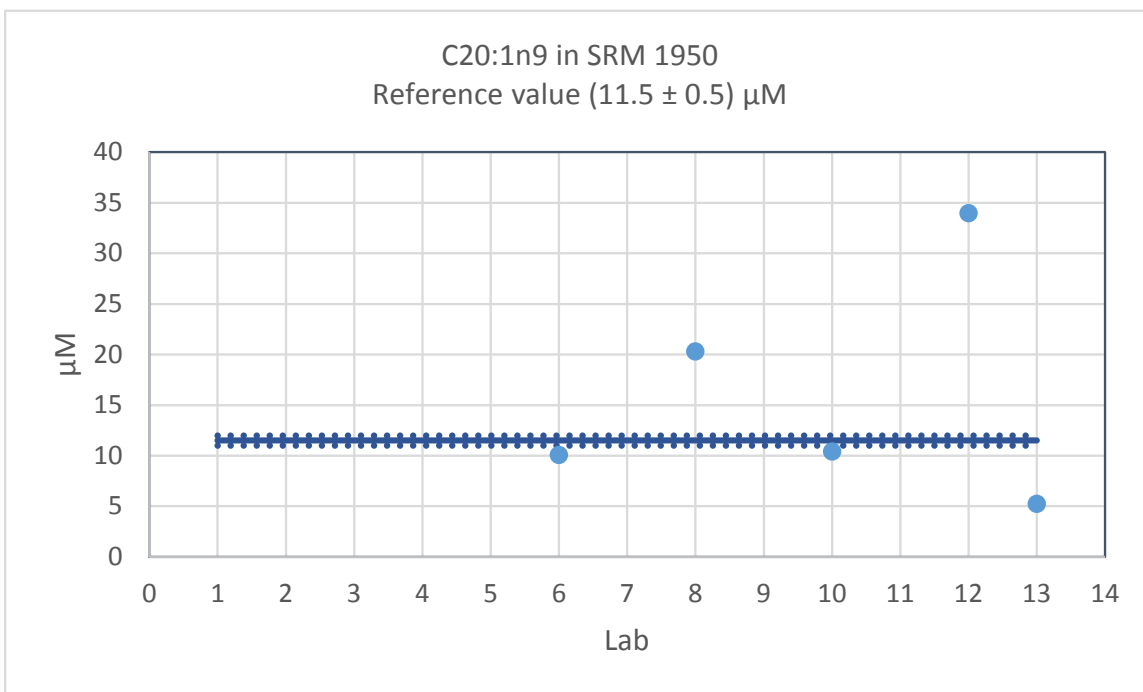
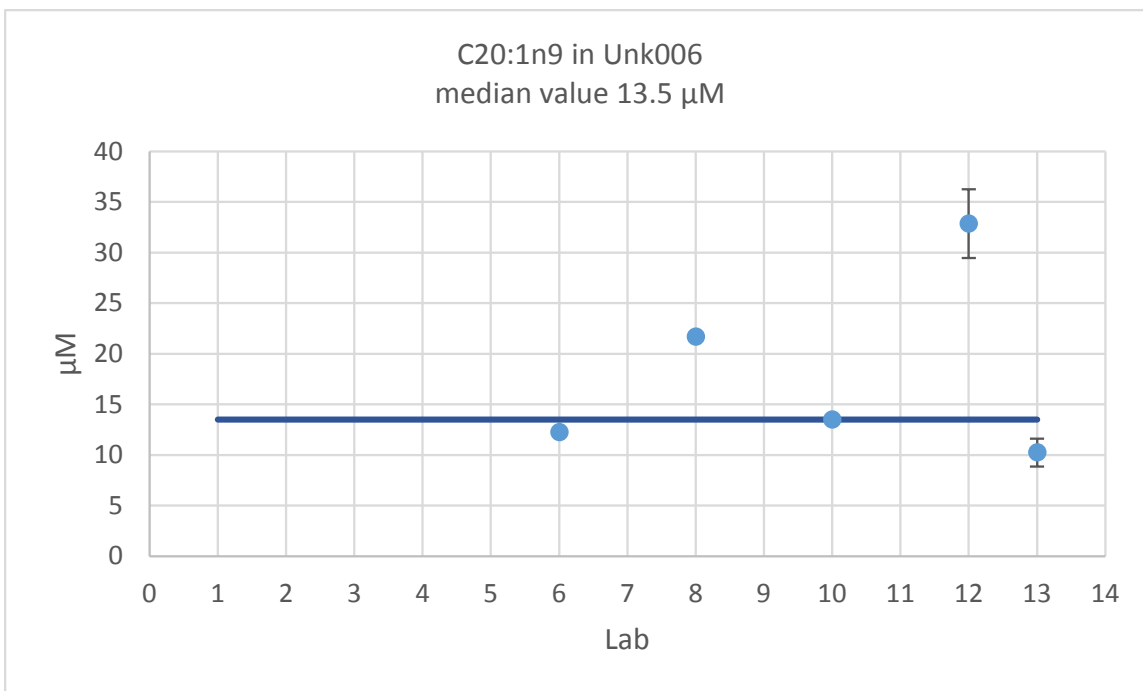


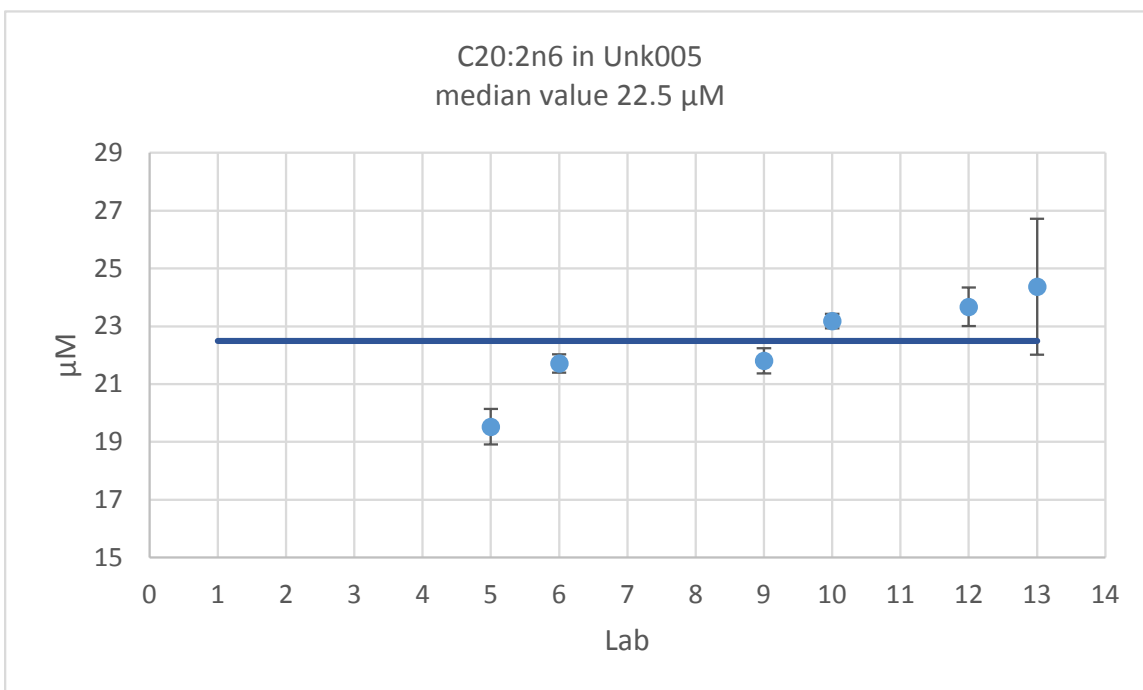
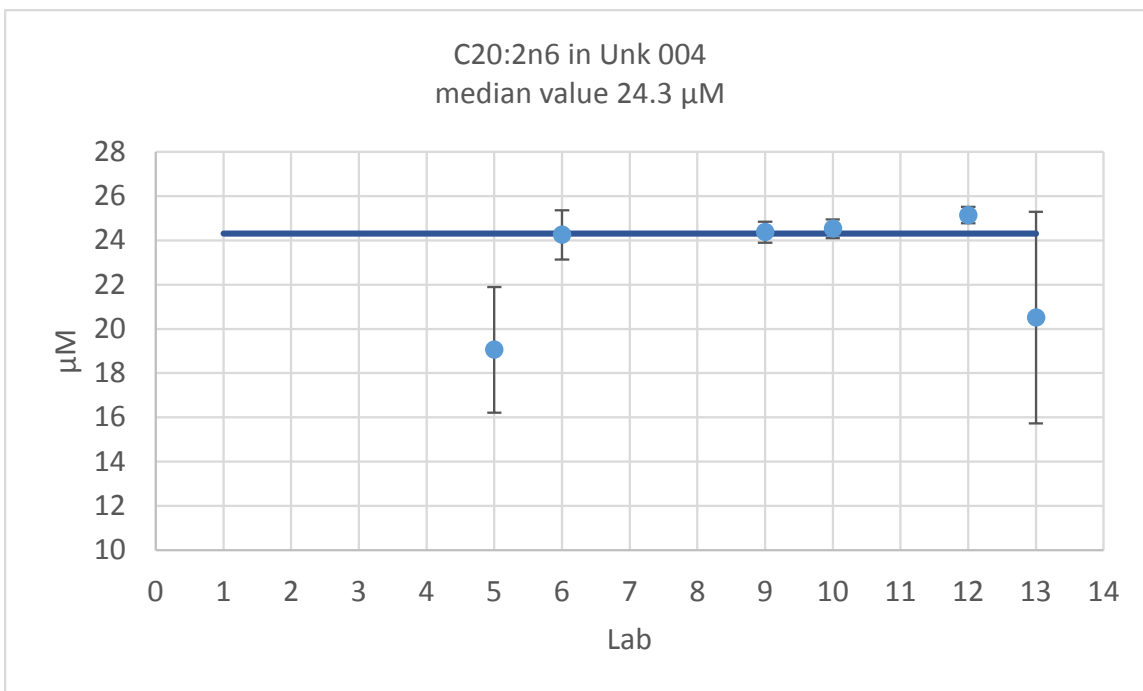
C20:1n9 in Unk 004
median value 17.3 μM

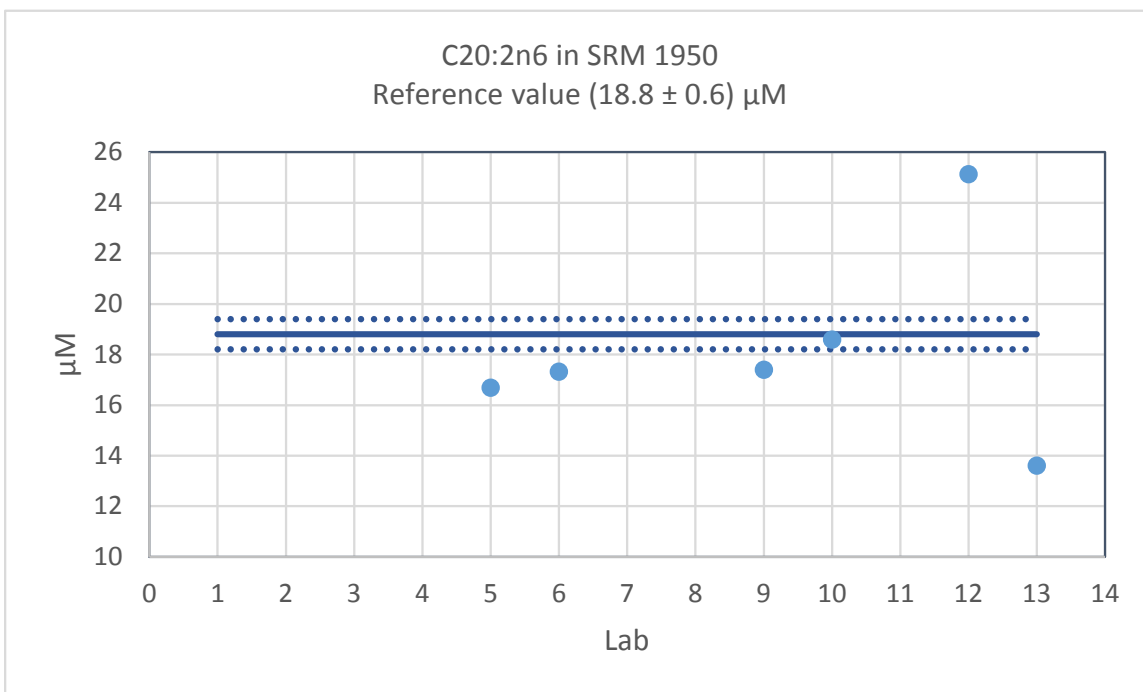
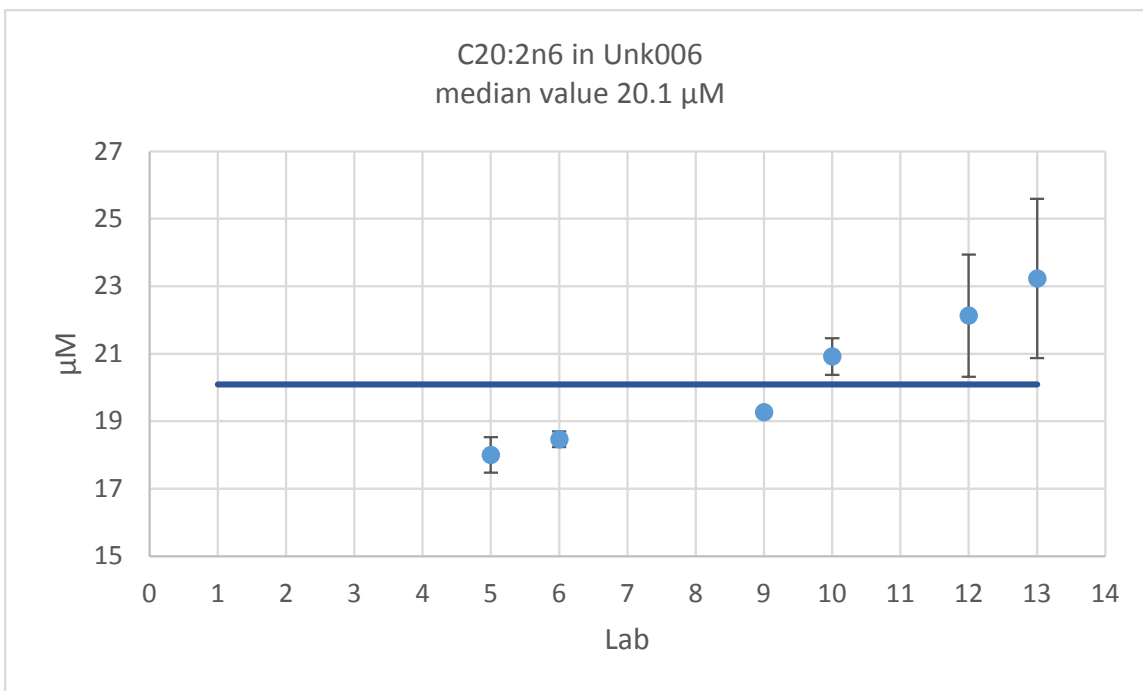


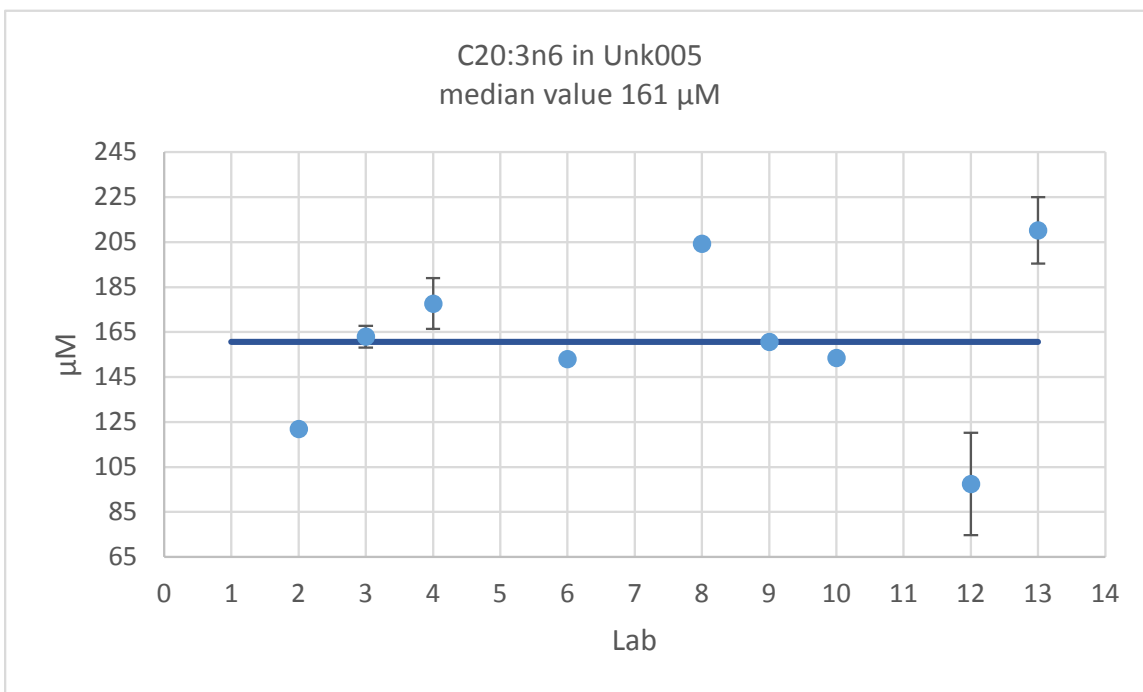
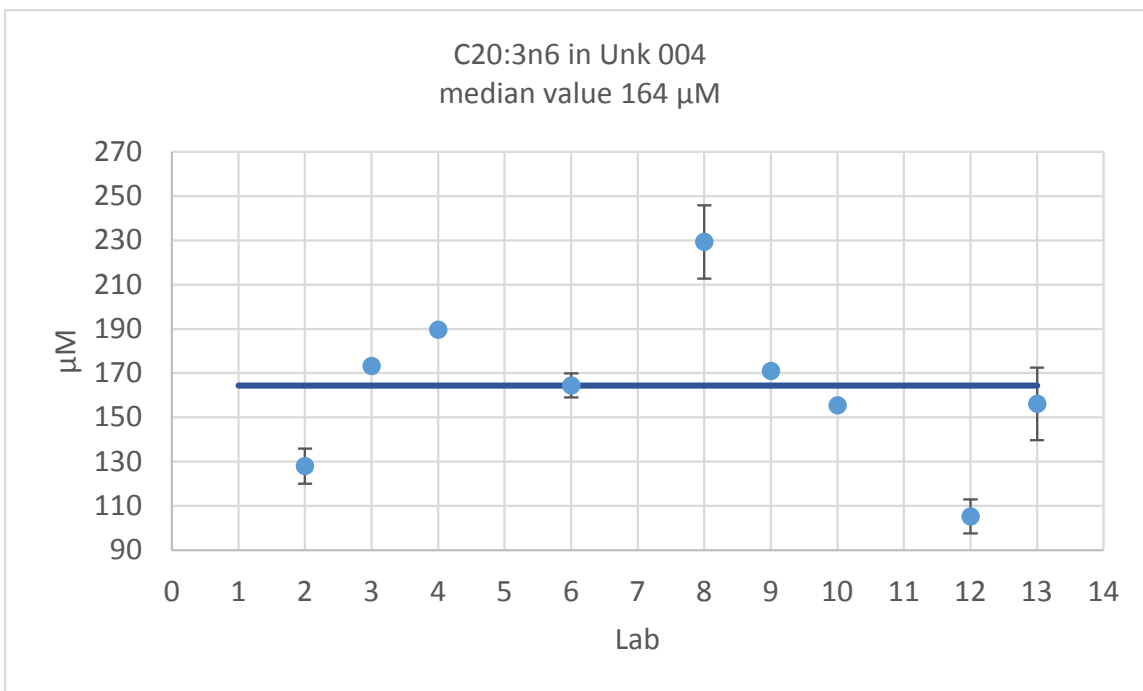
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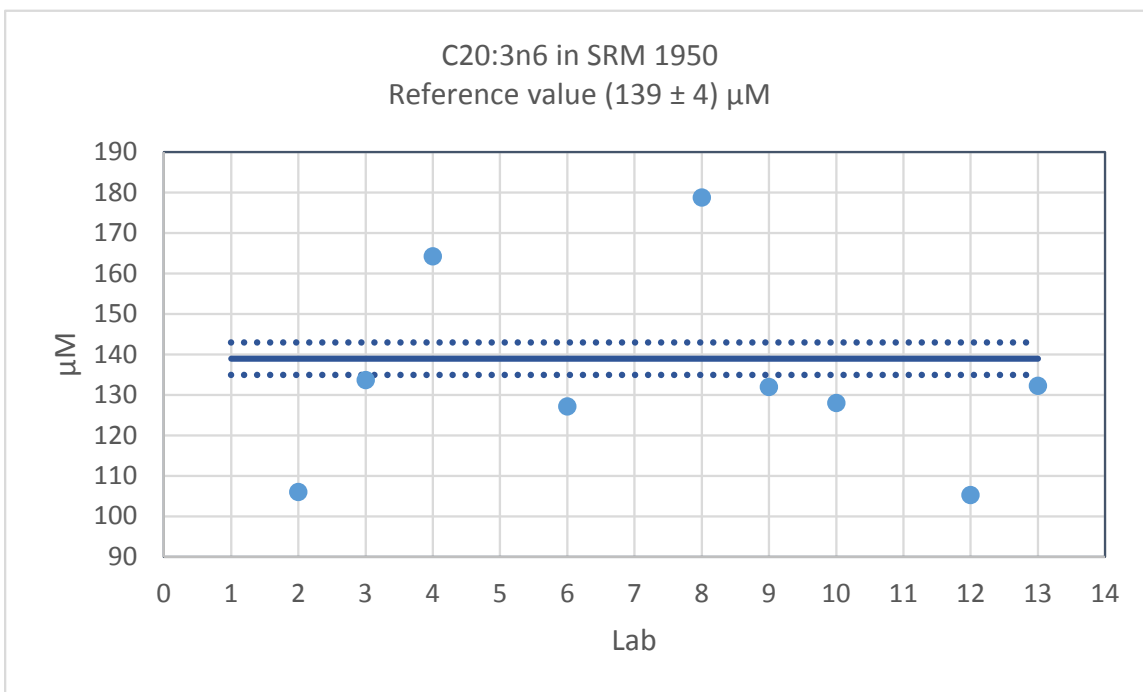
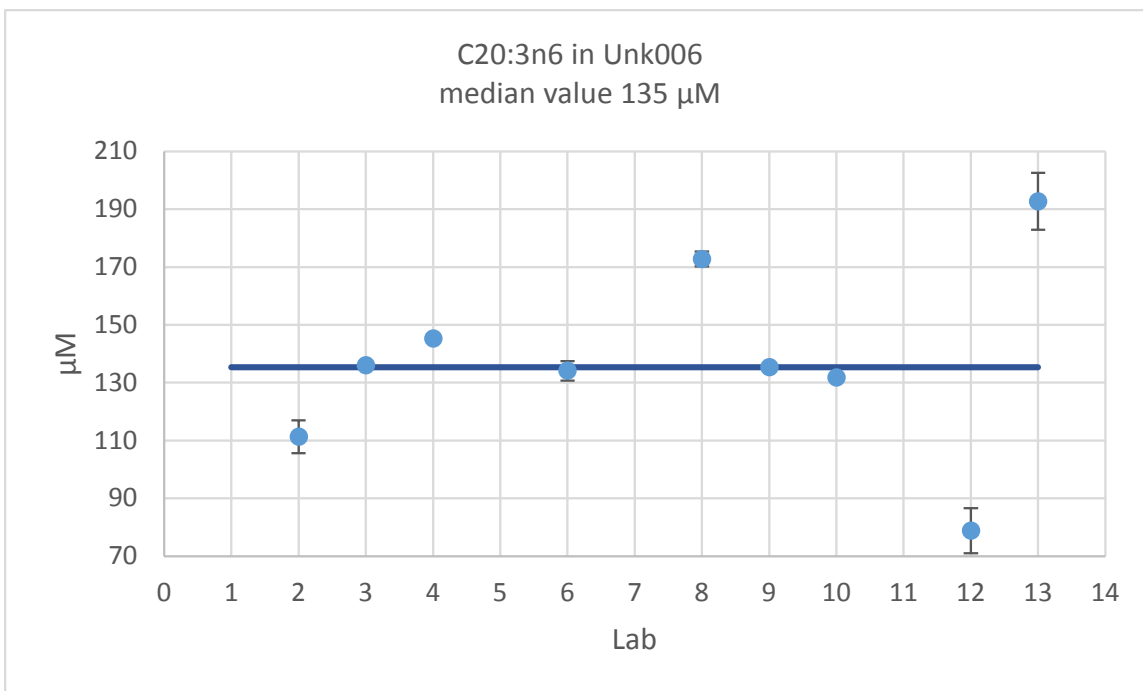


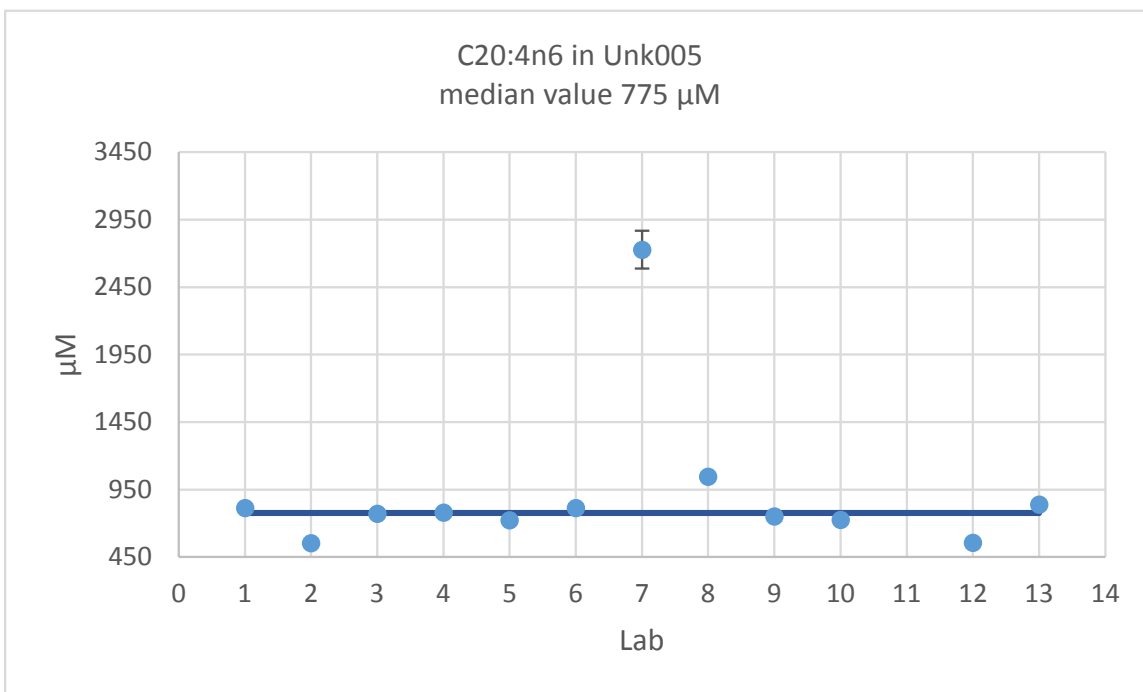
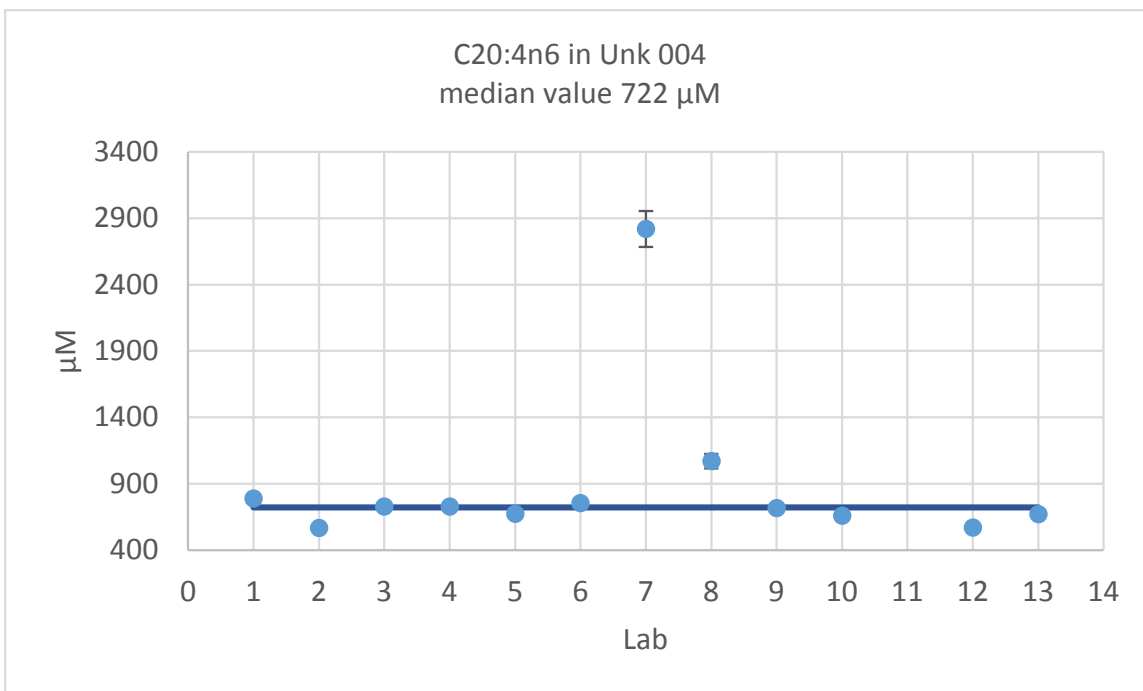


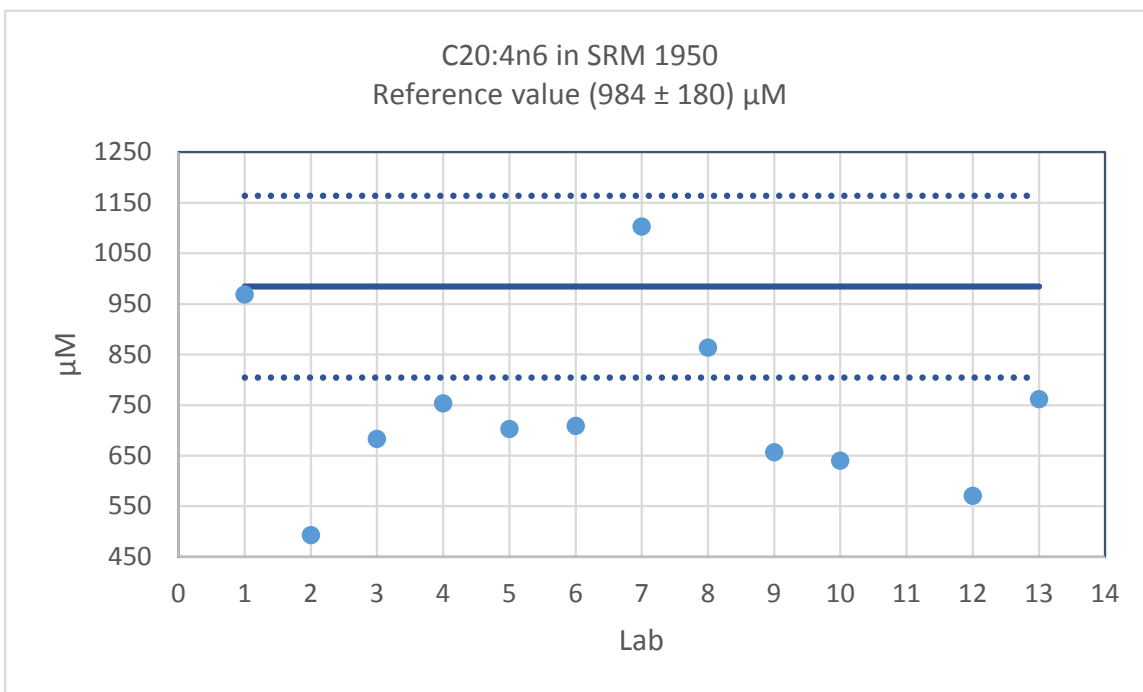
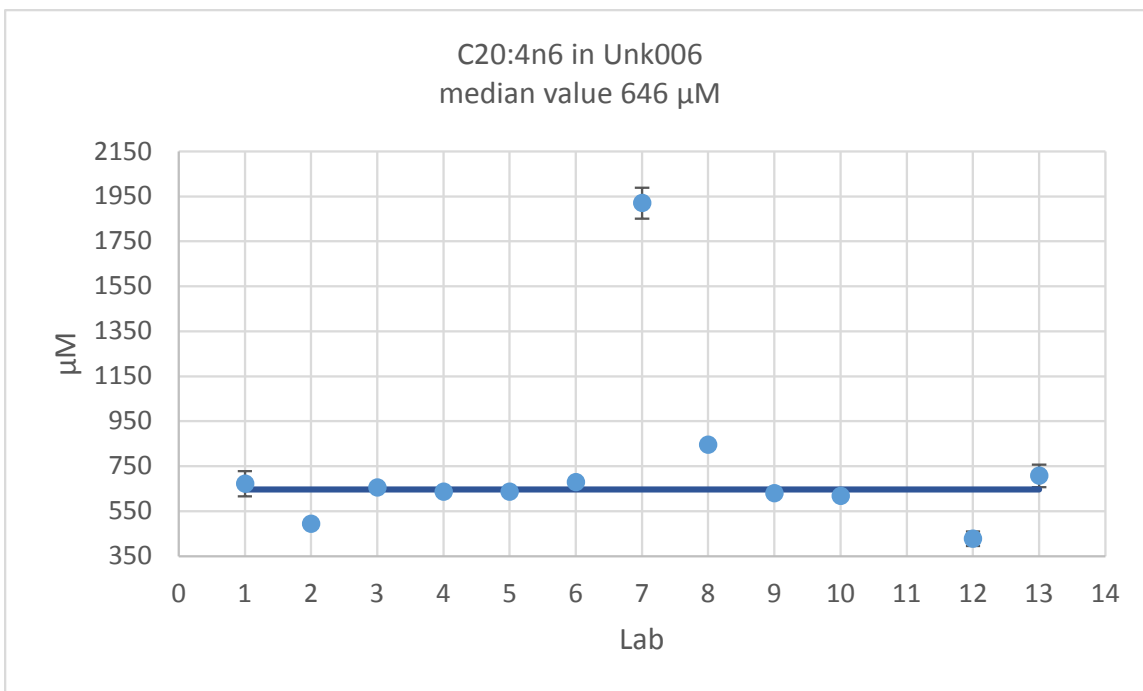


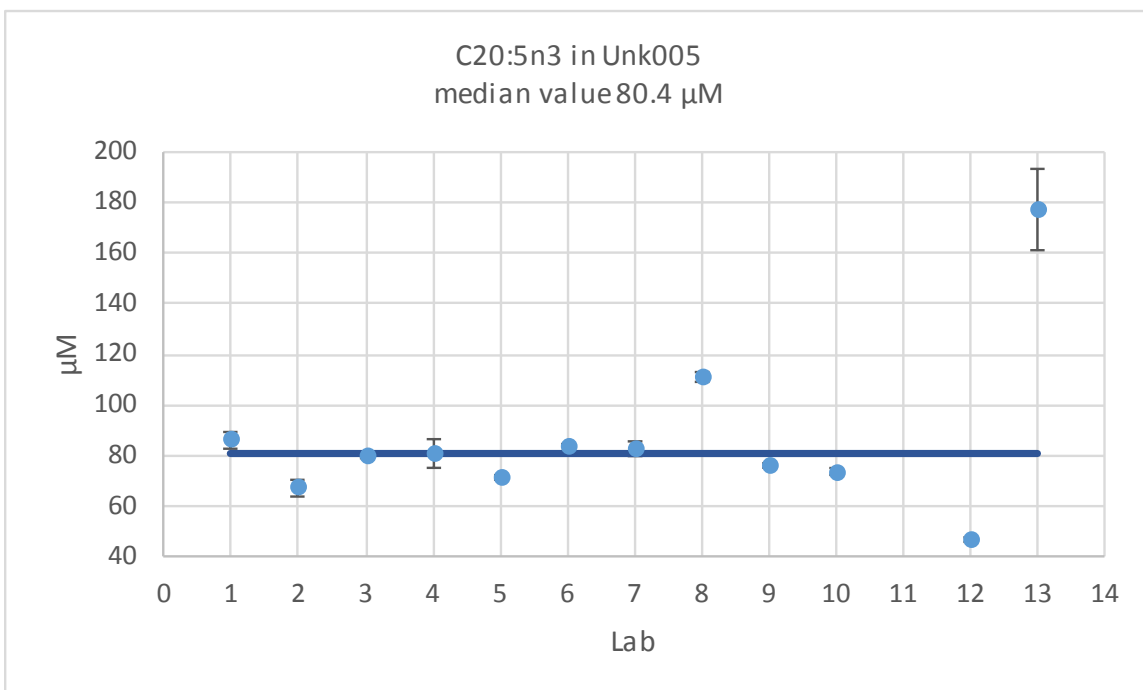
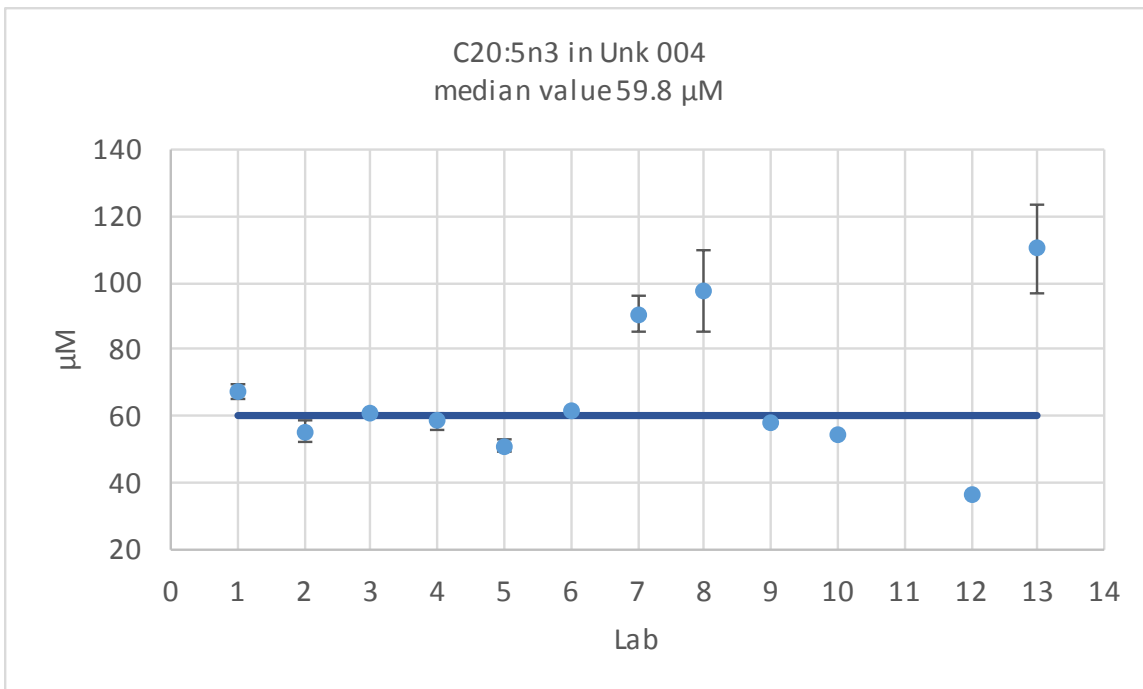


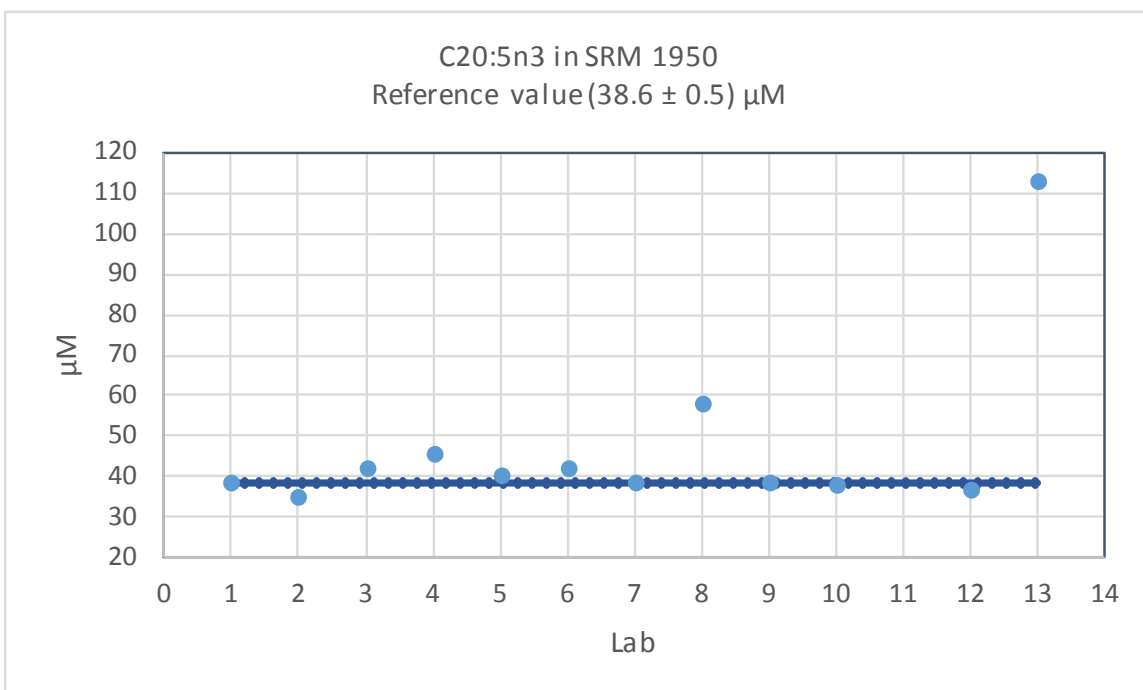
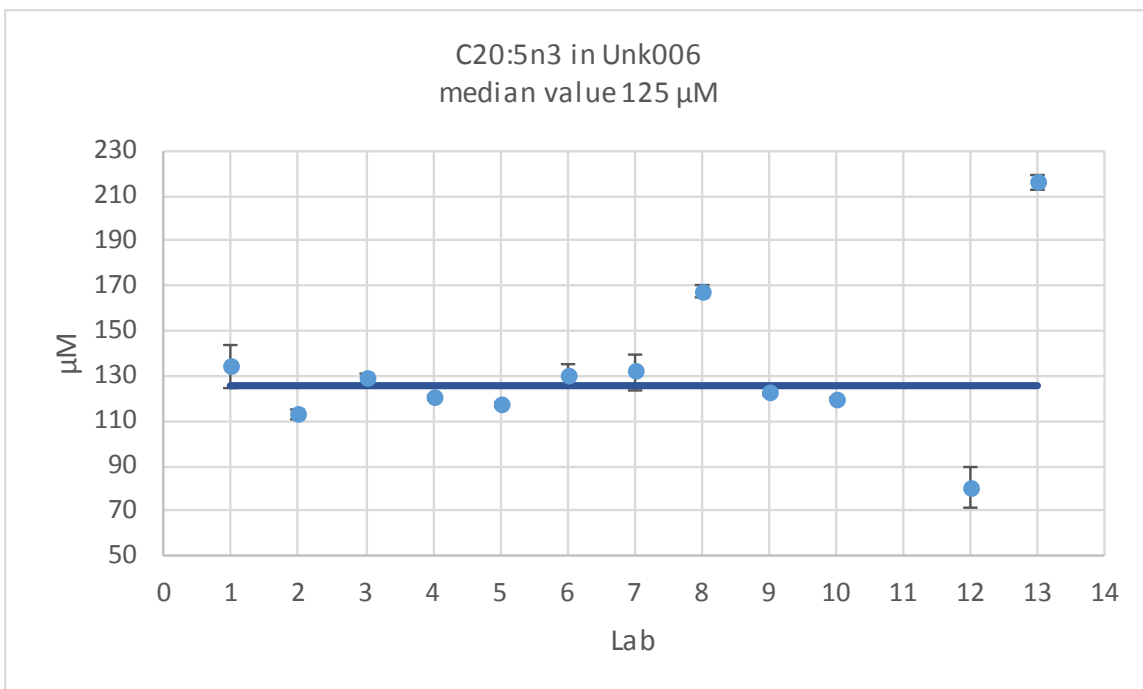


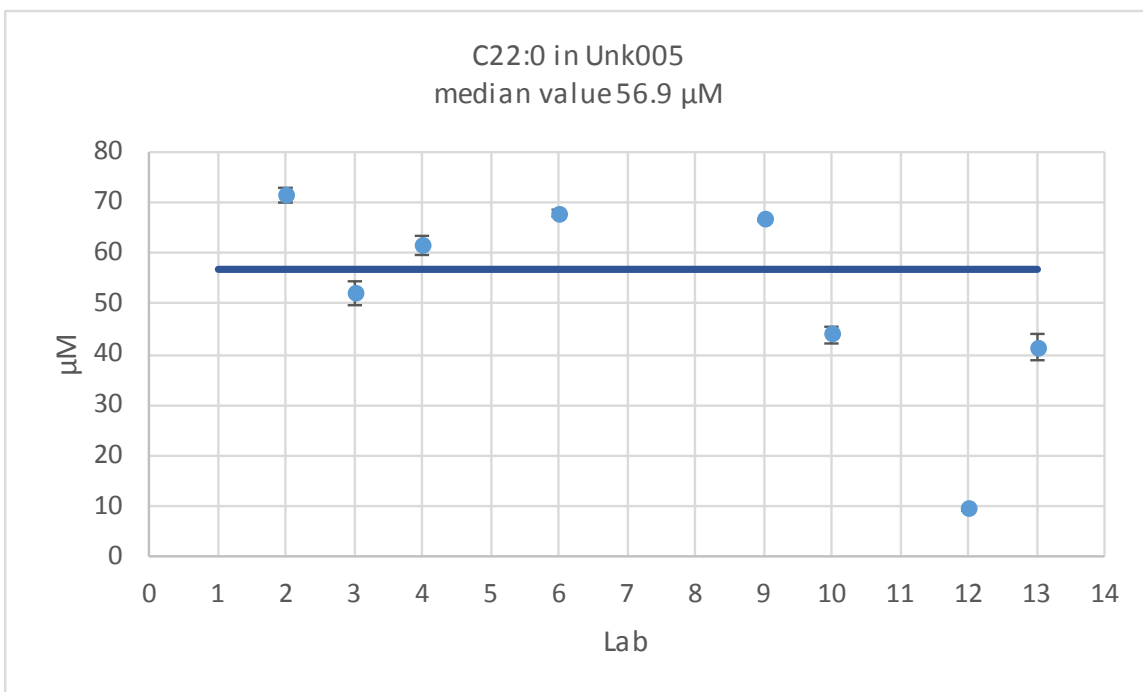
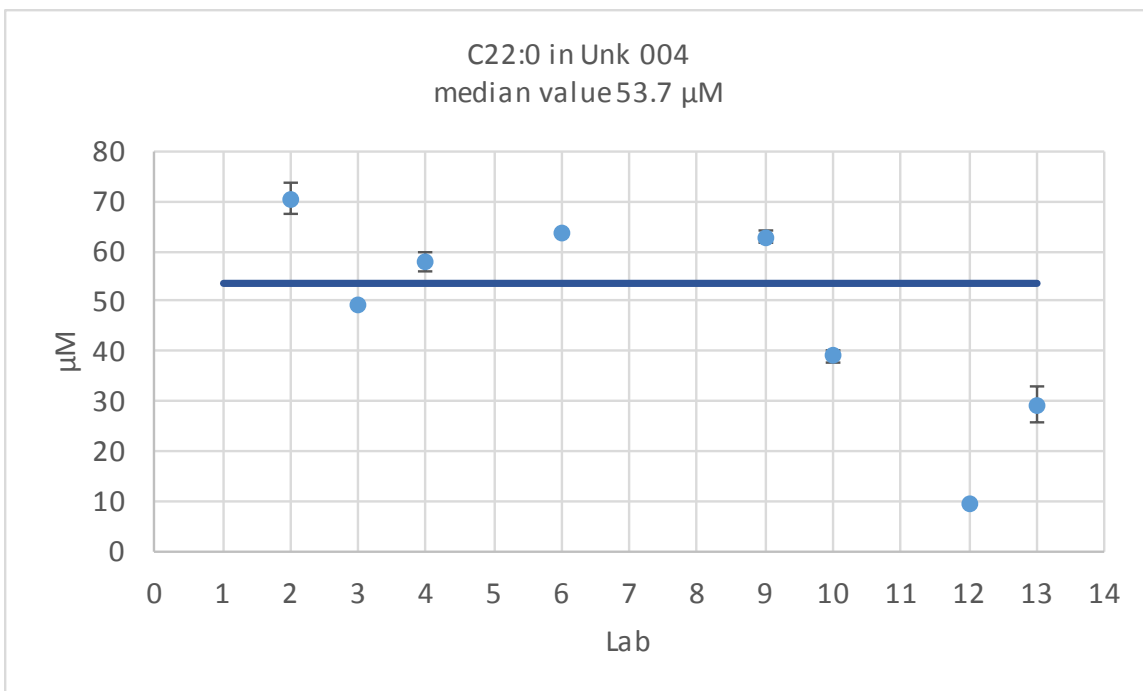


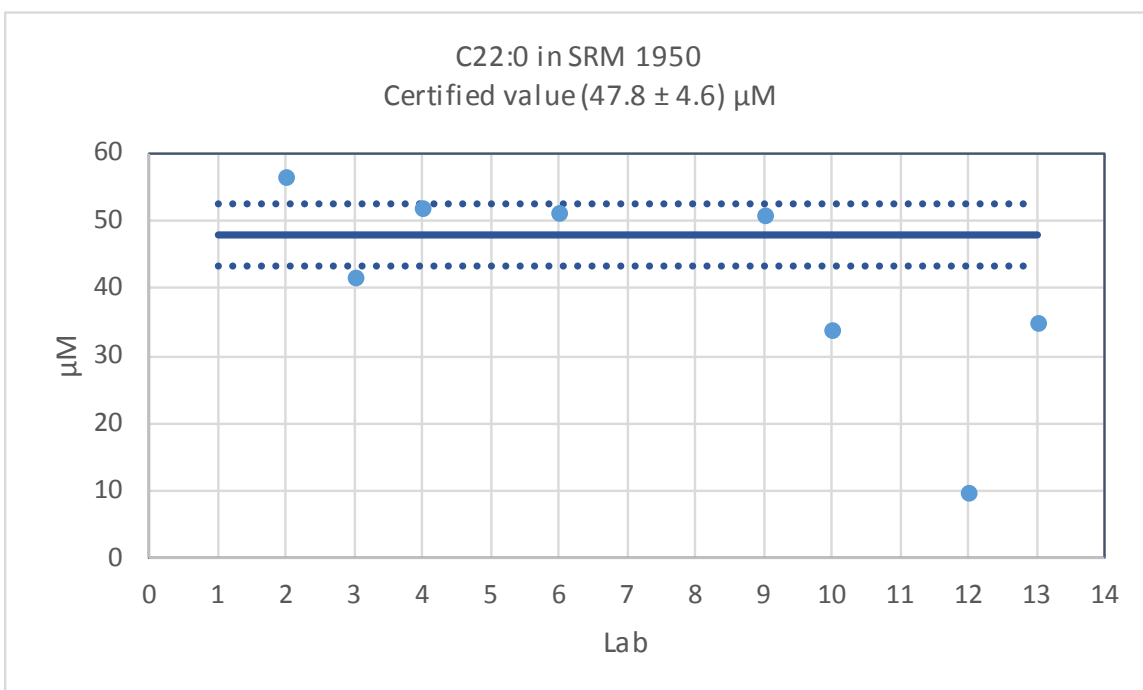
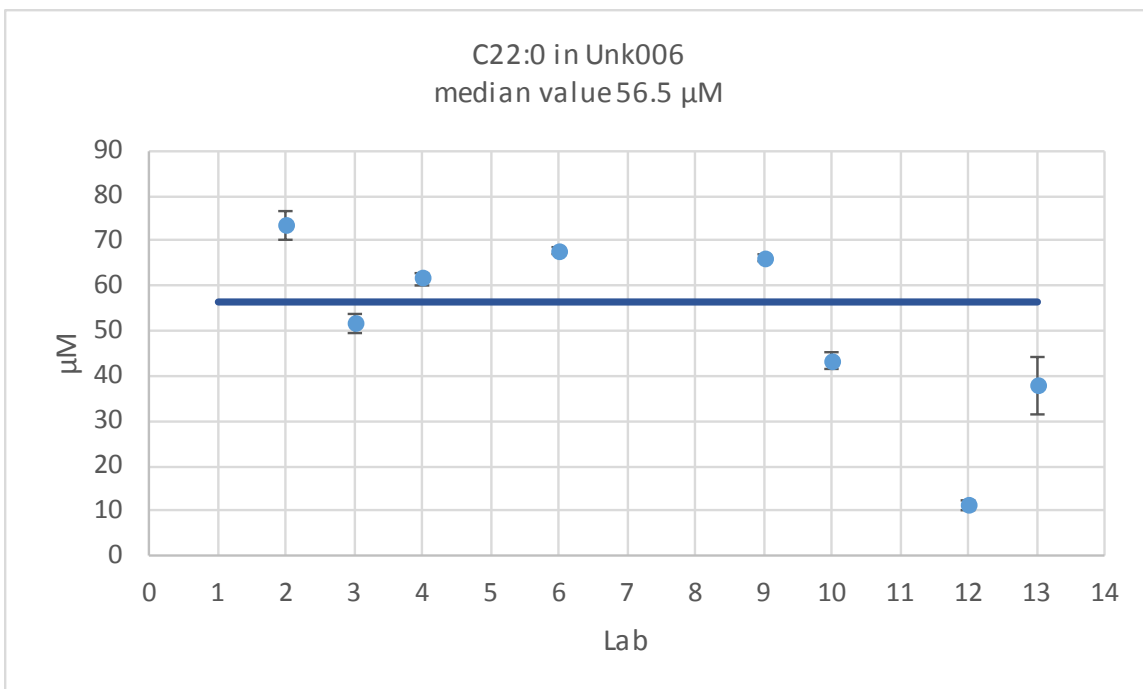


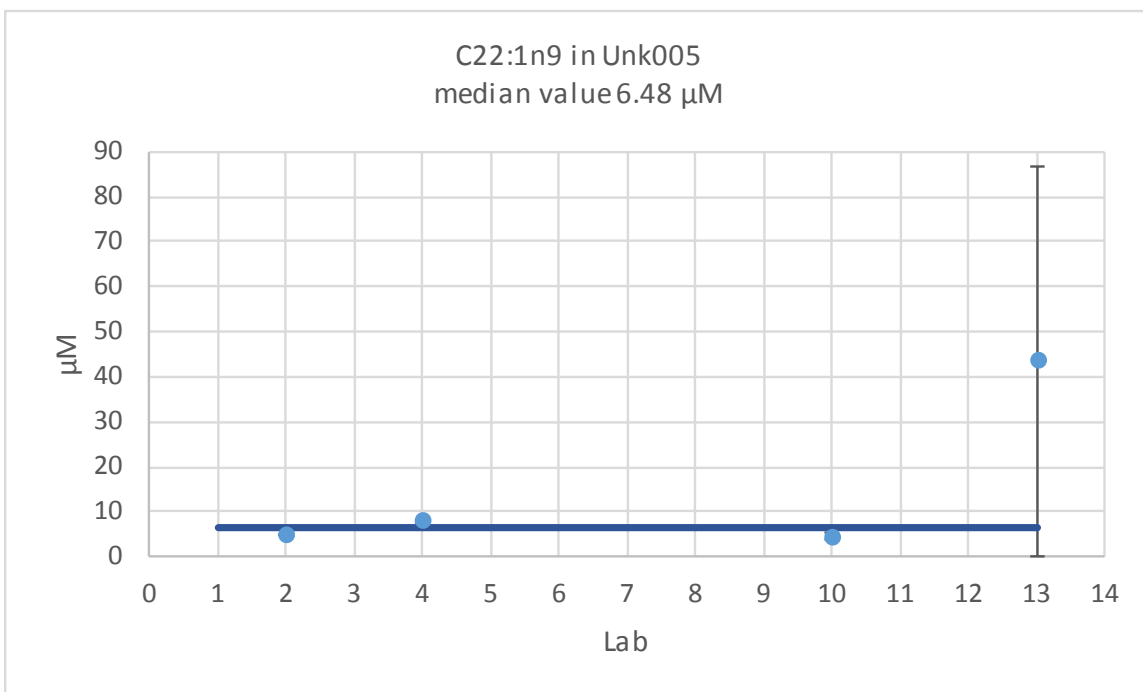
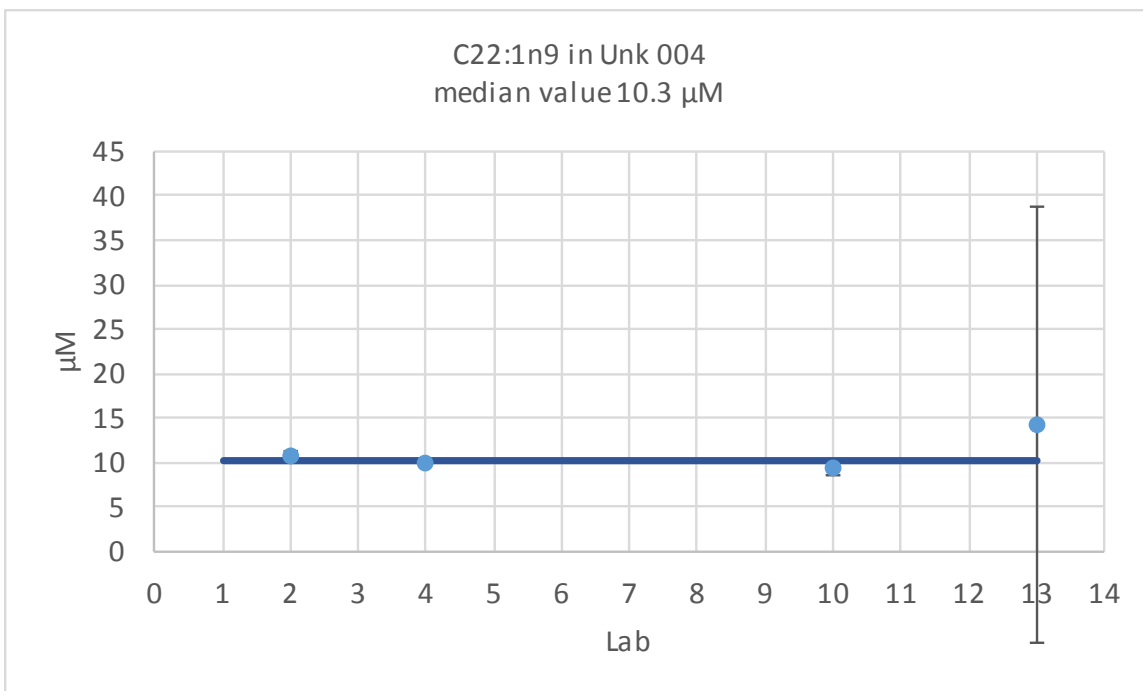


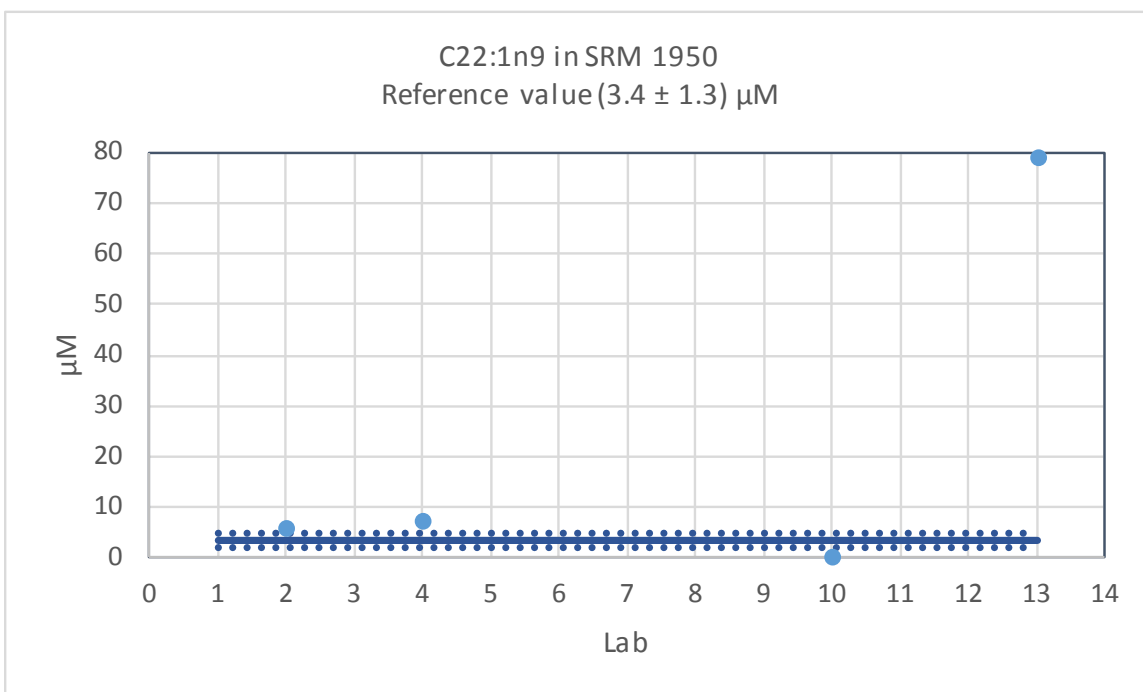
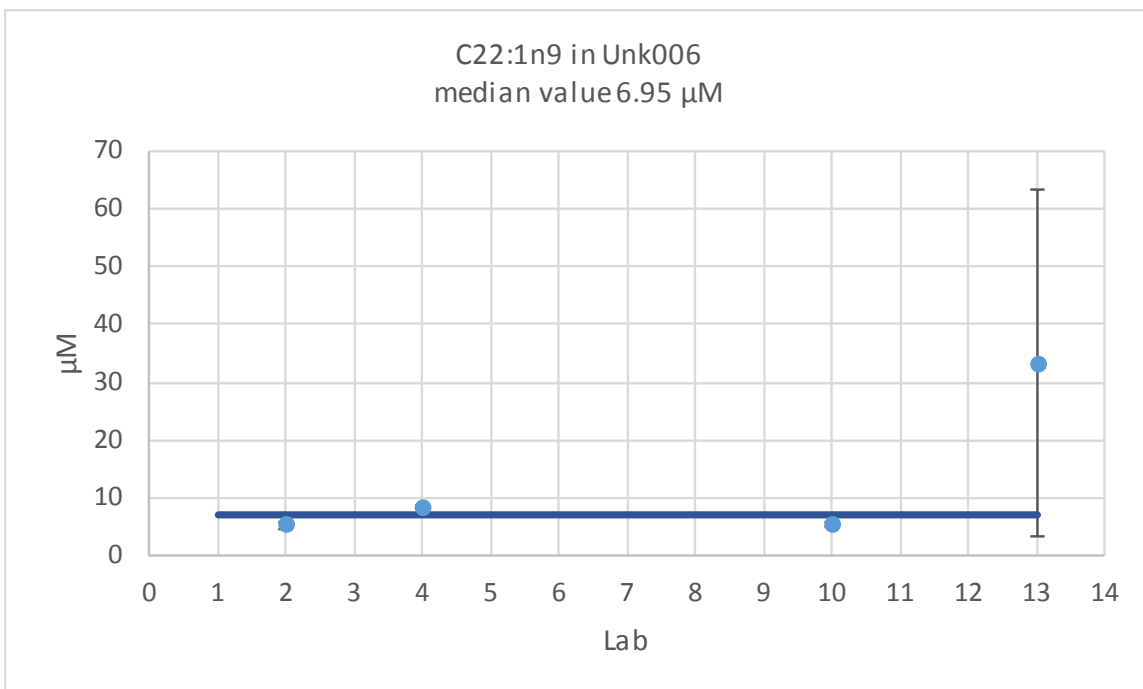


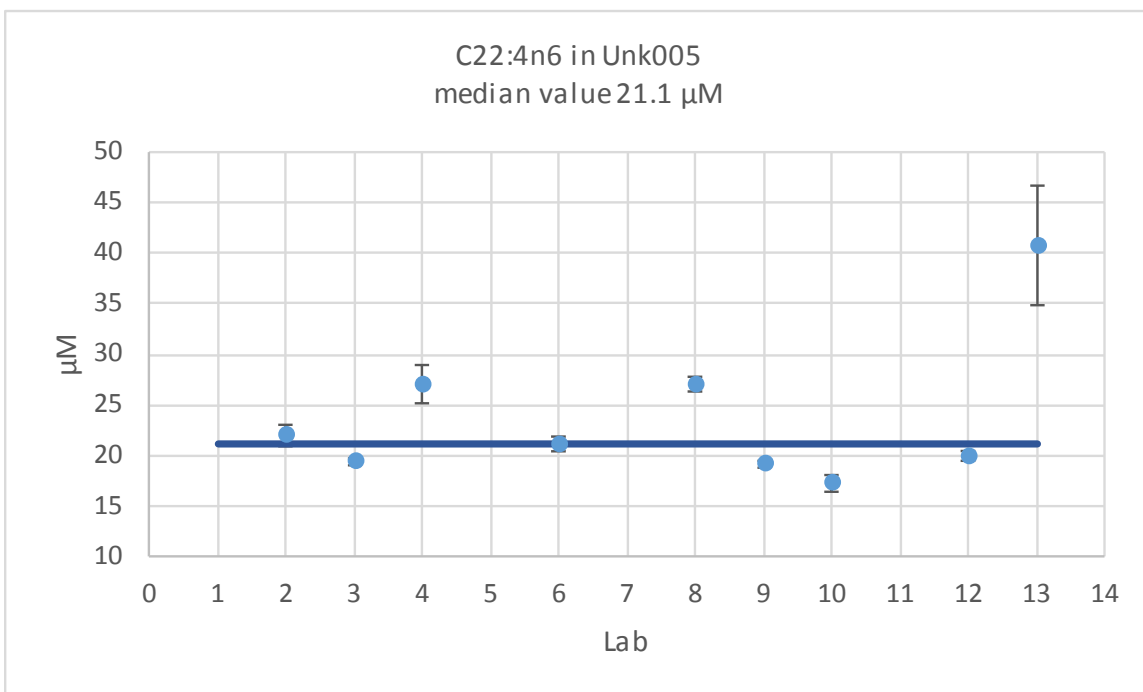
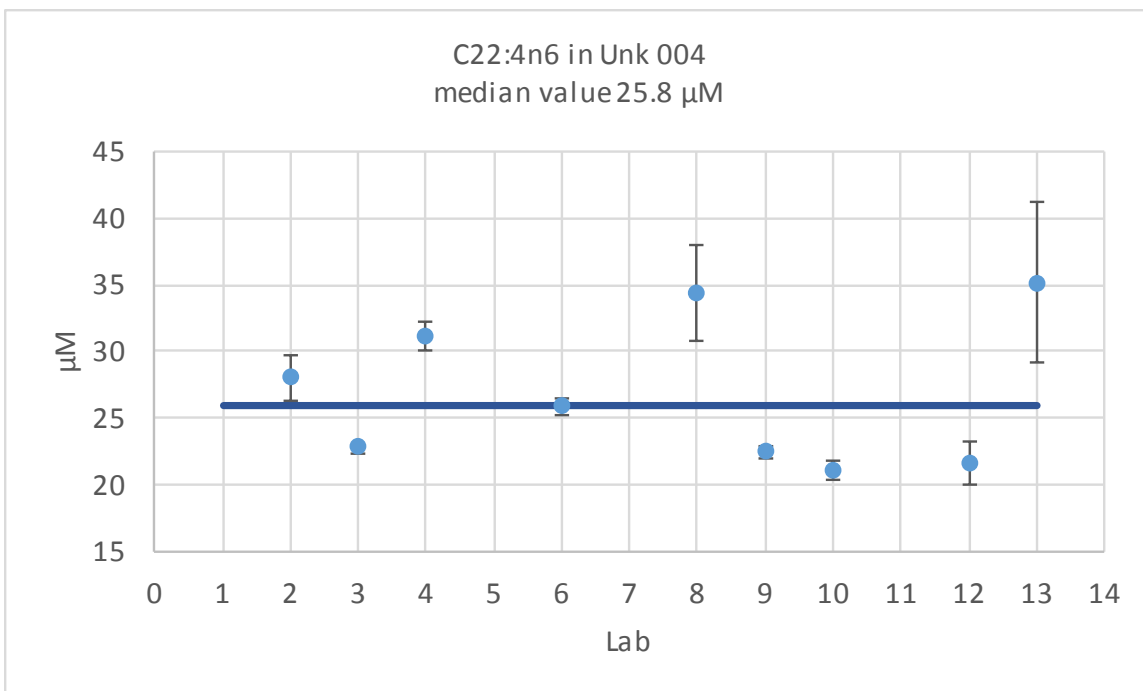


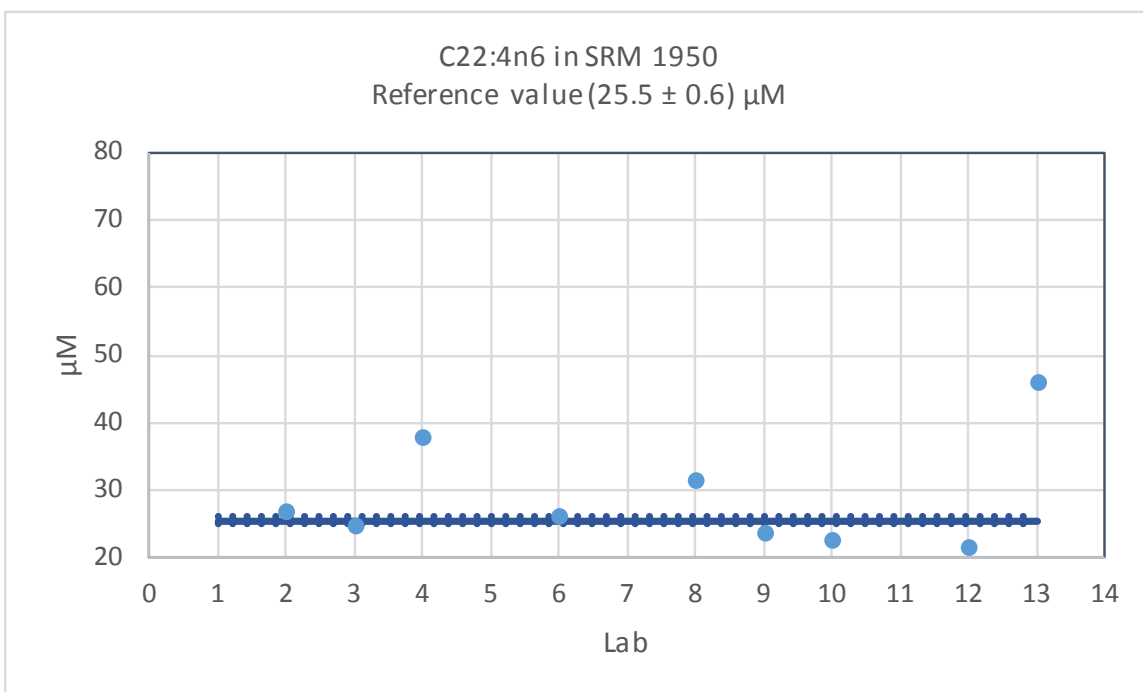
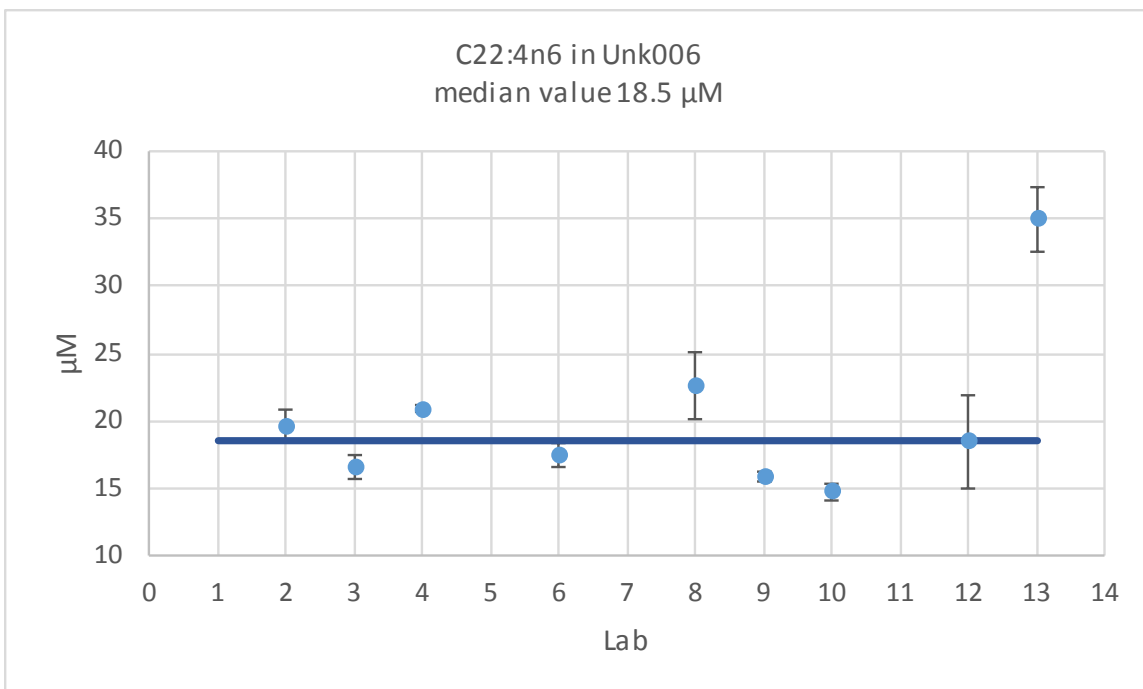


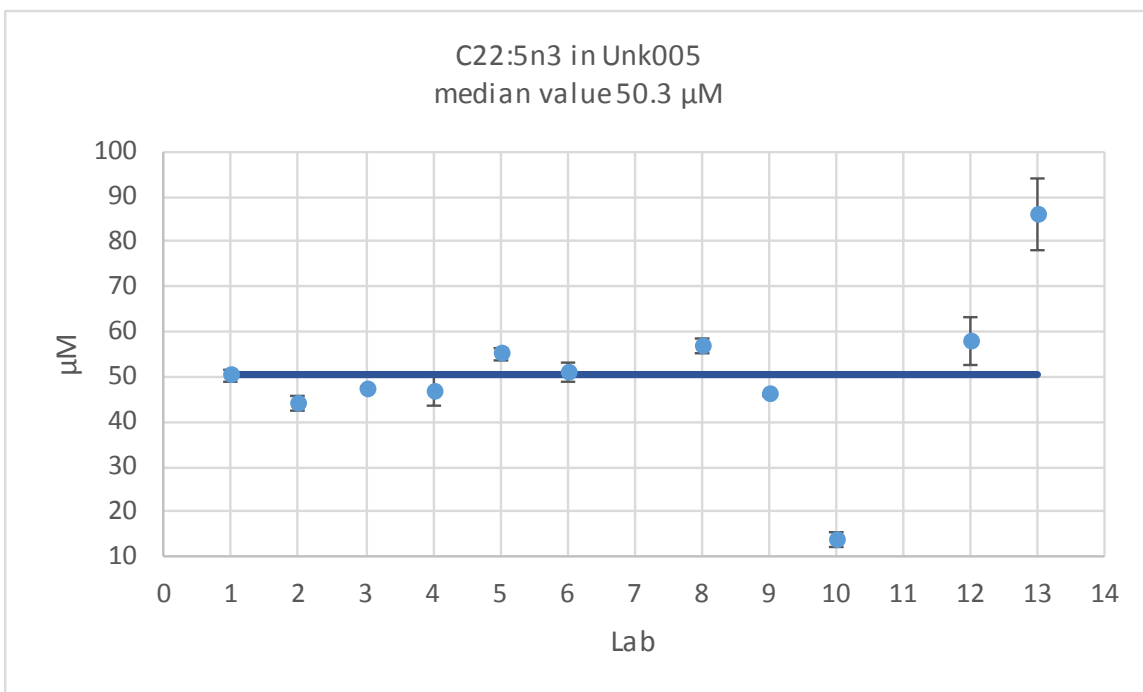
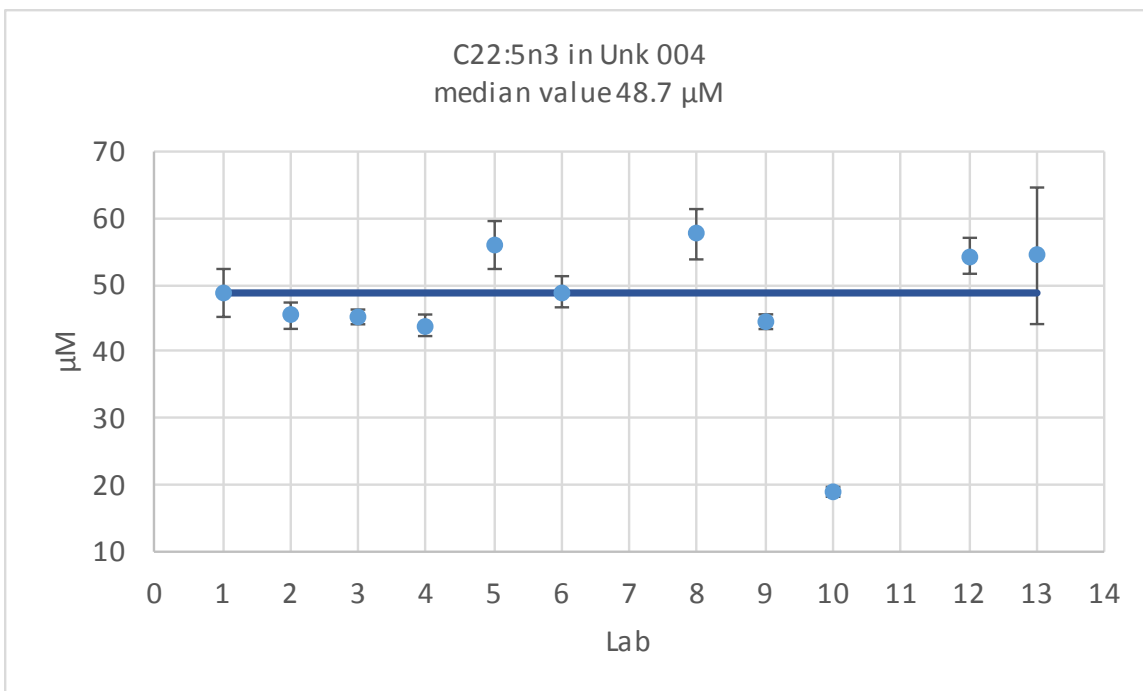


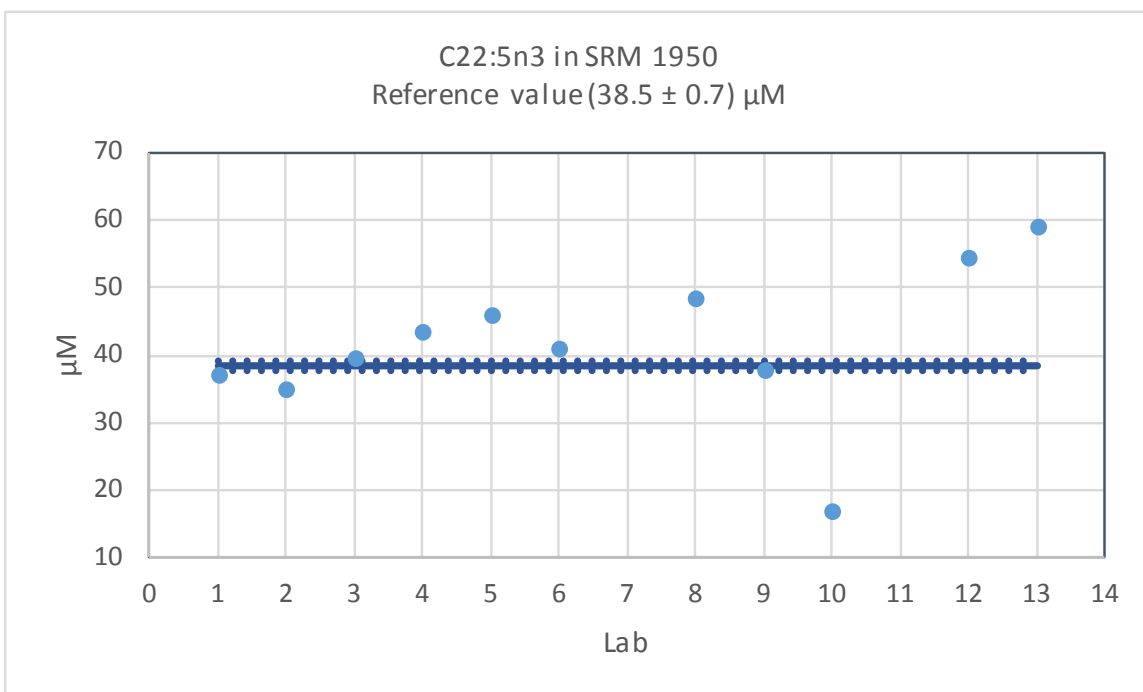
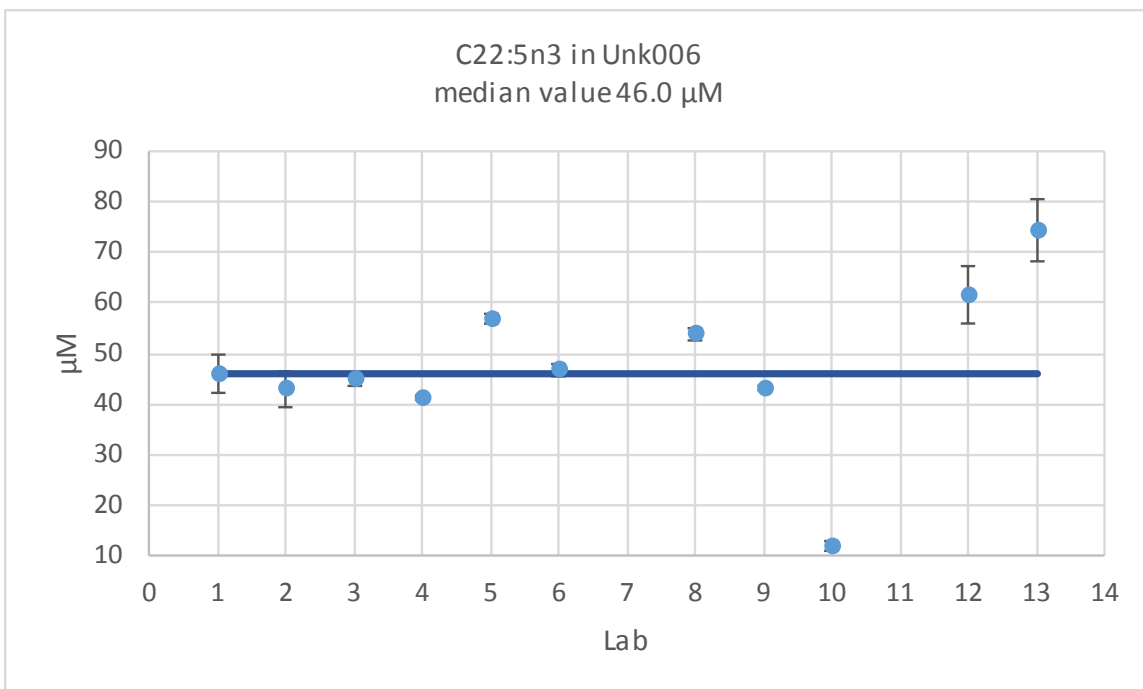


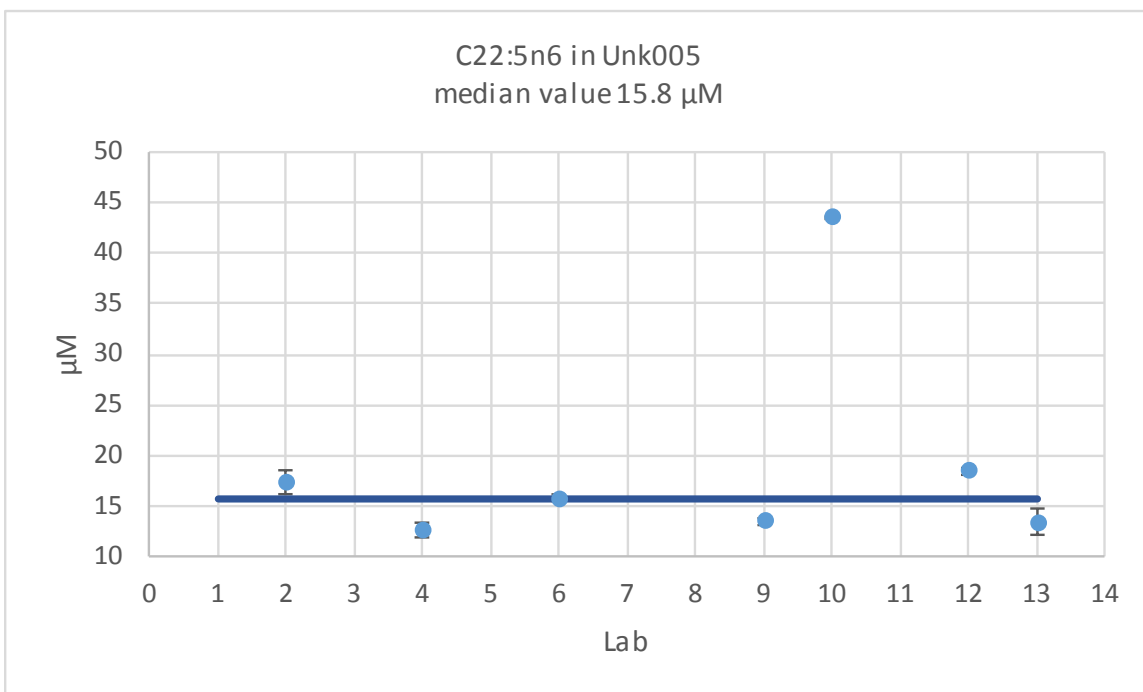
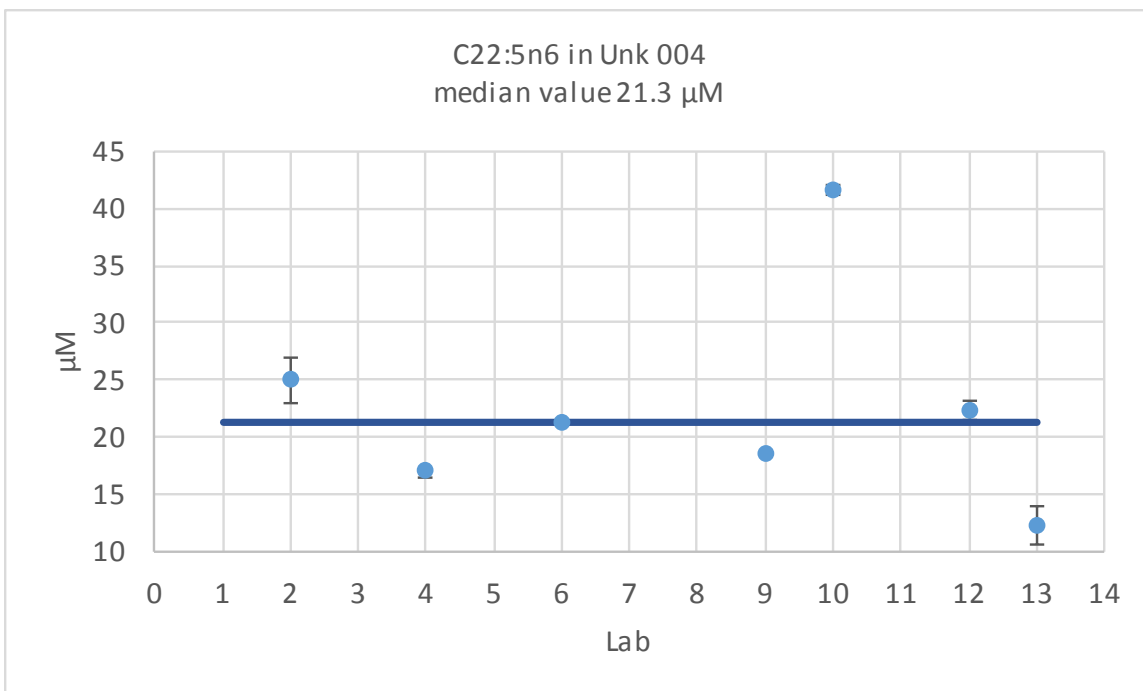


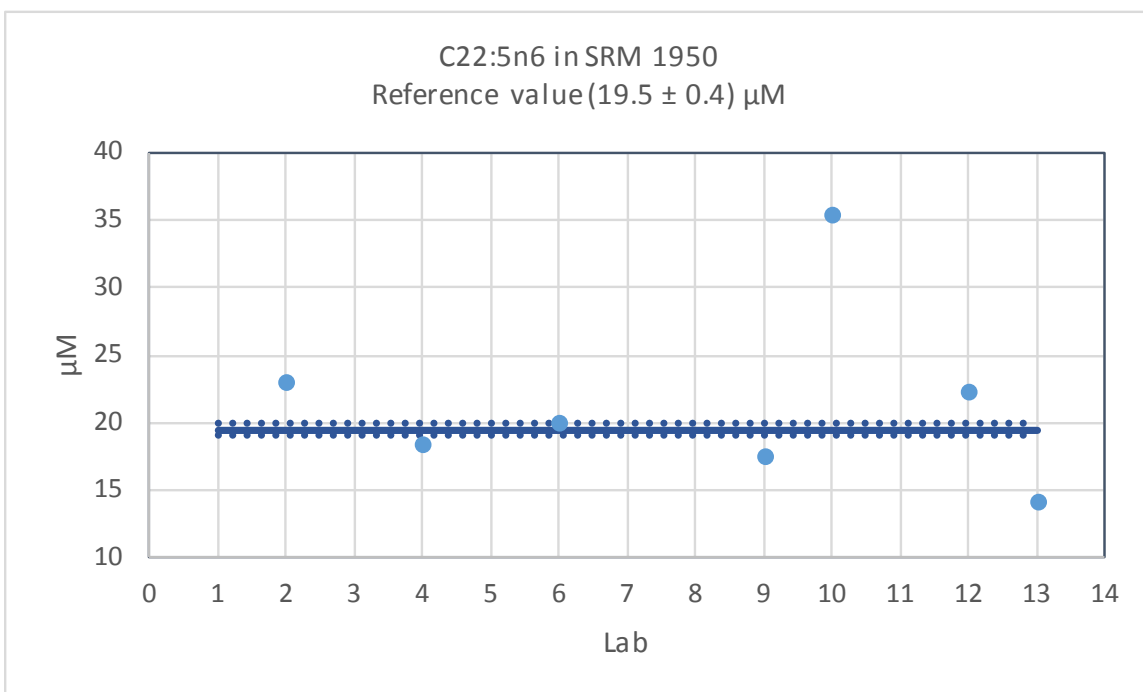
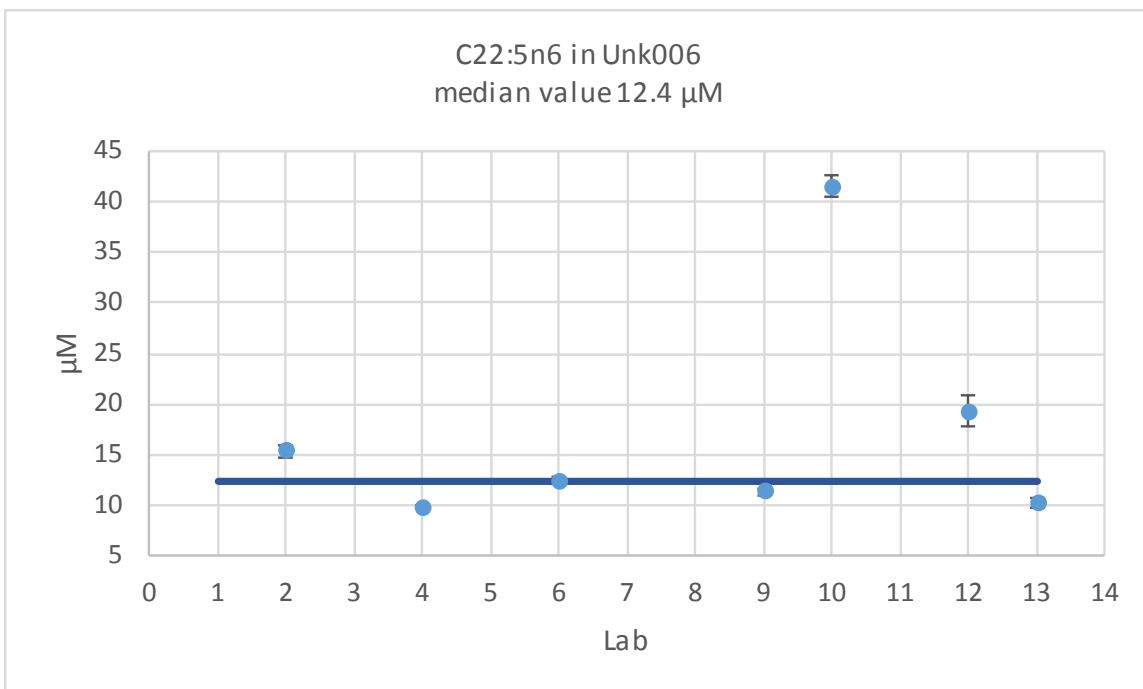


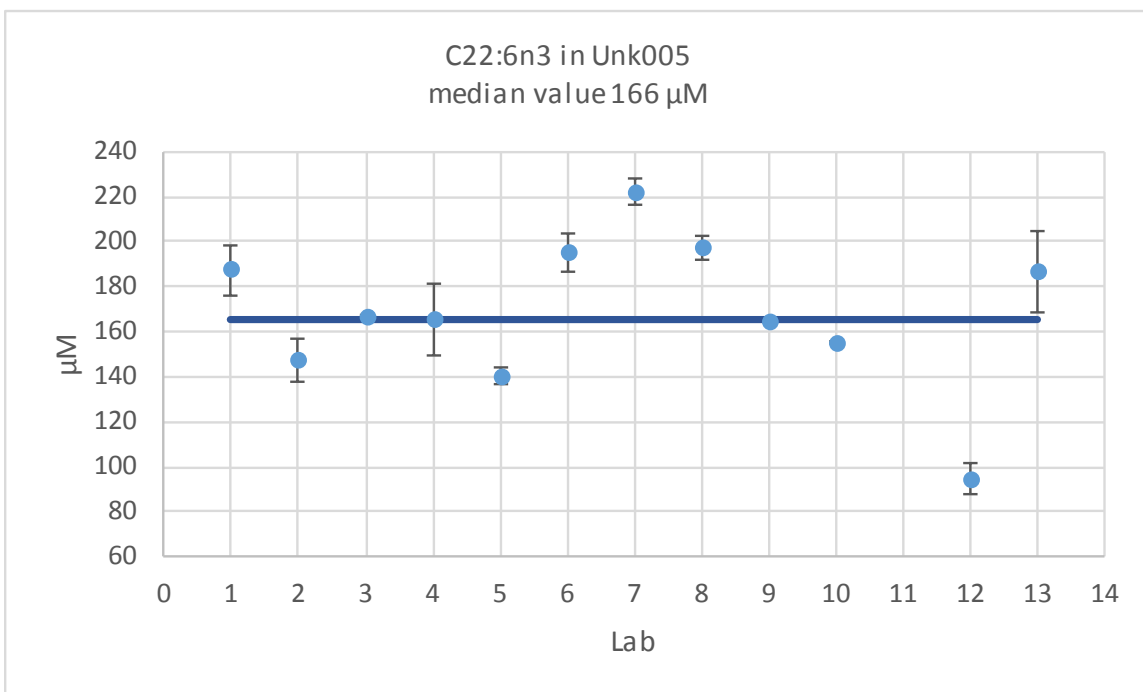
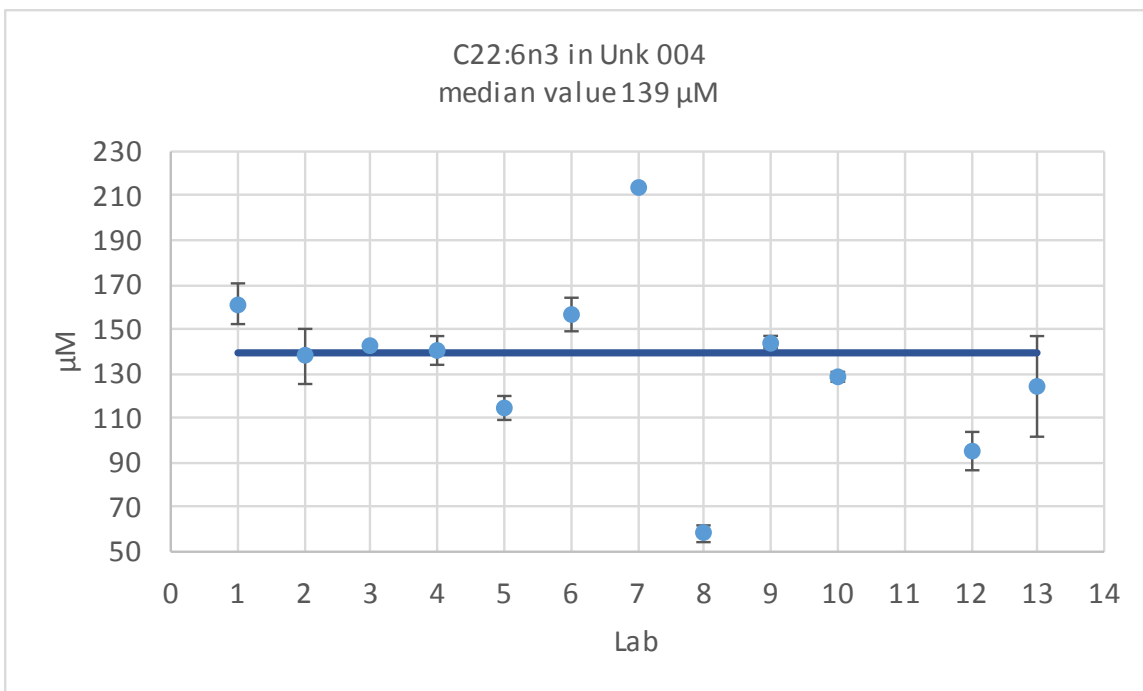


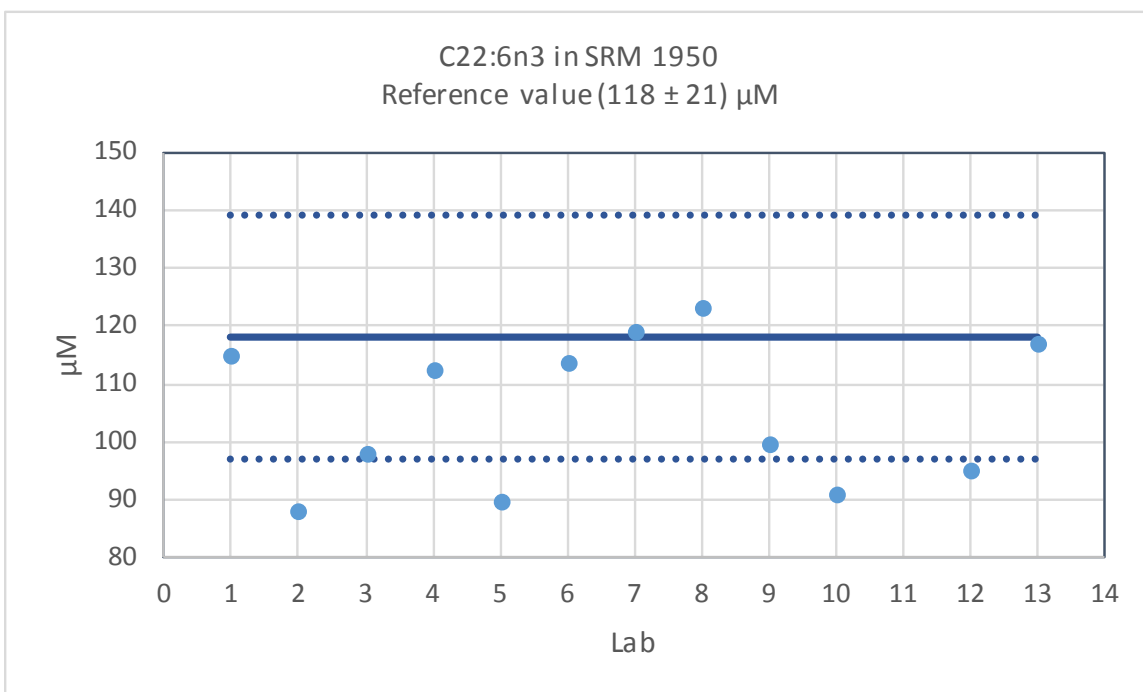
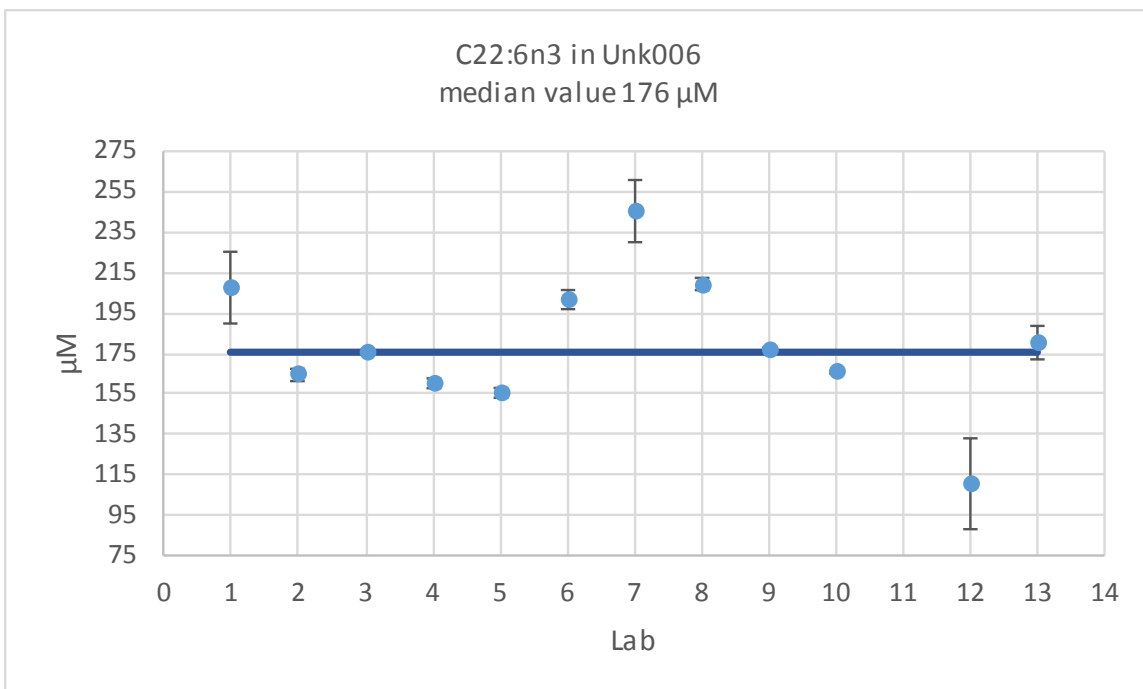


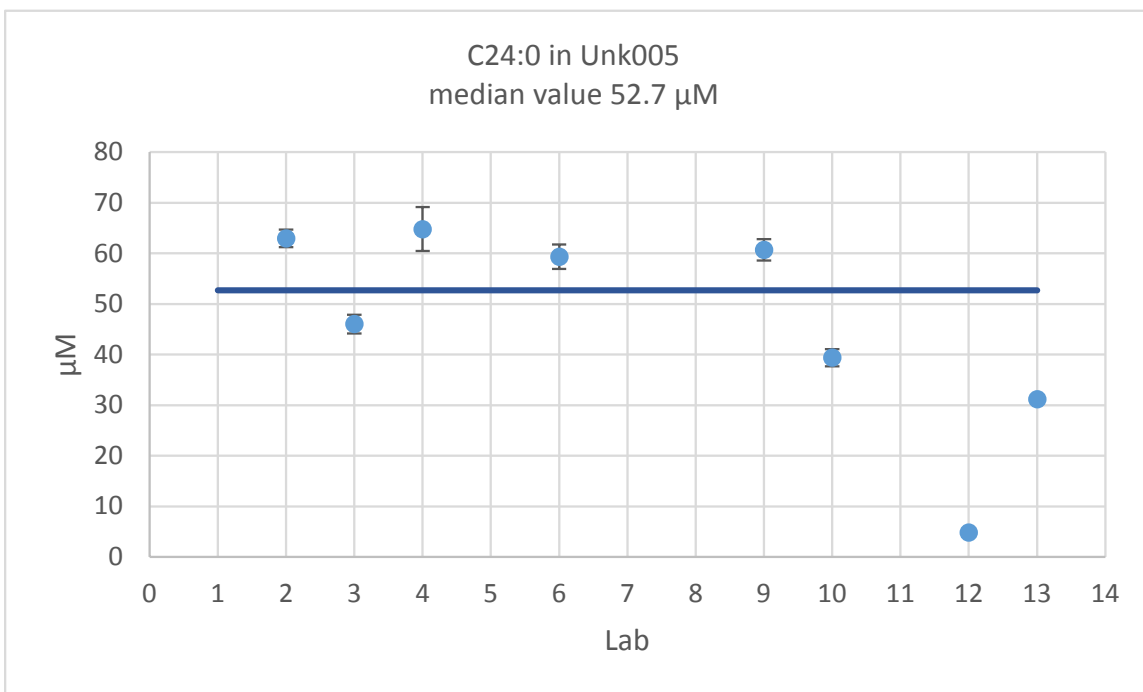
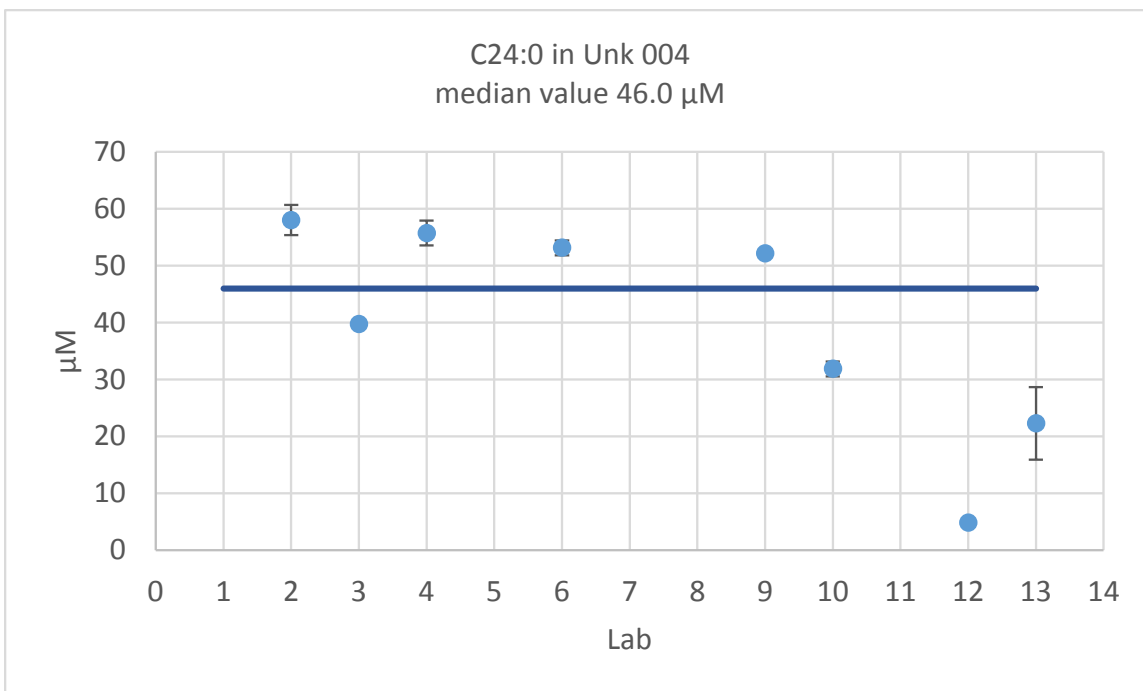


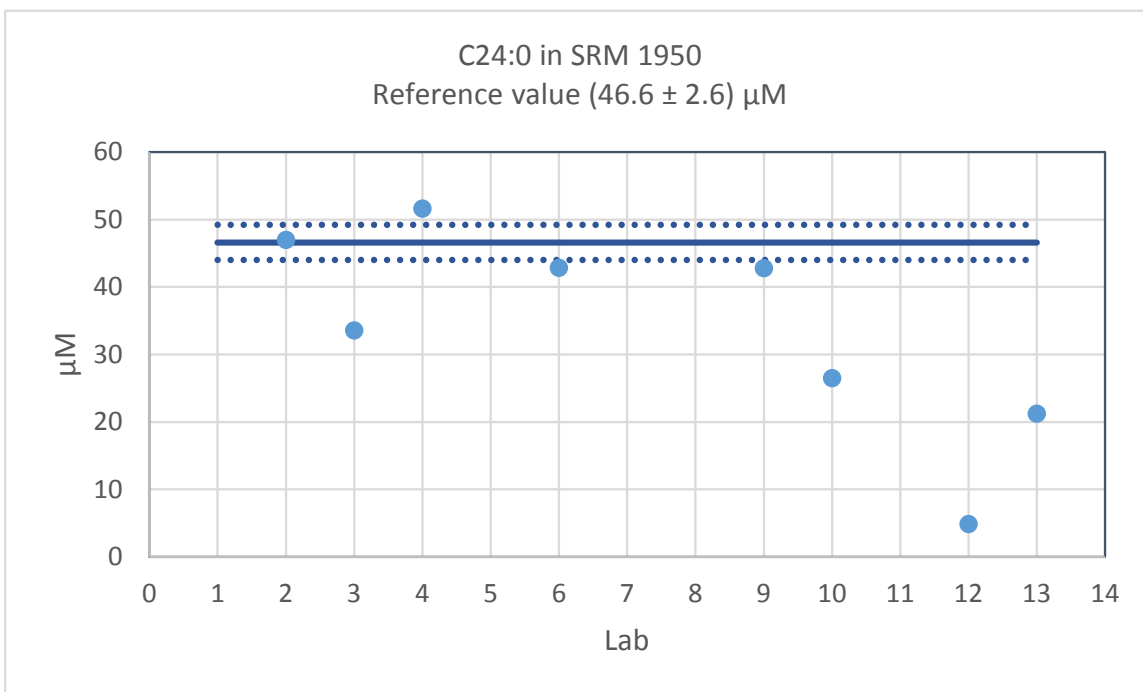
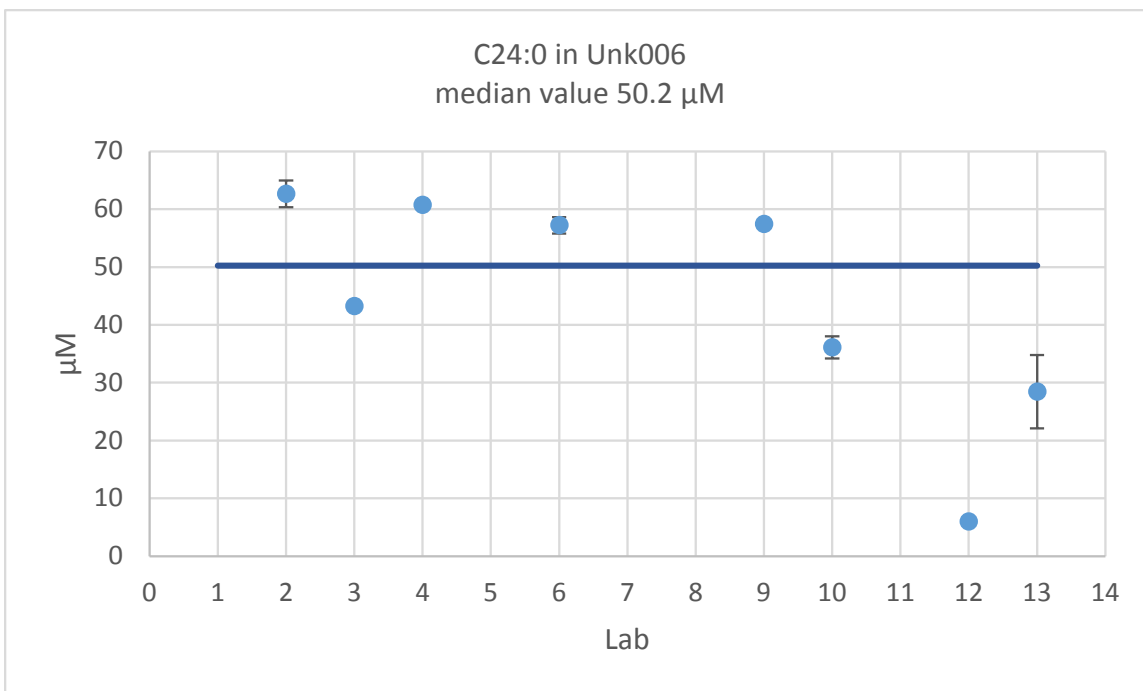


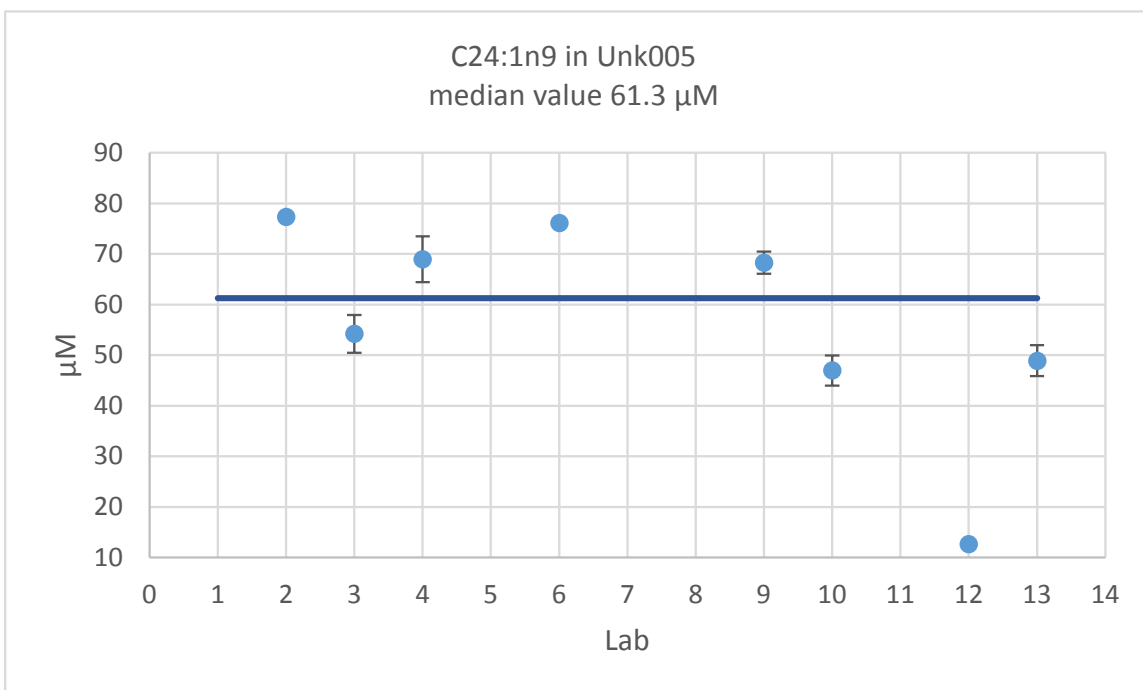
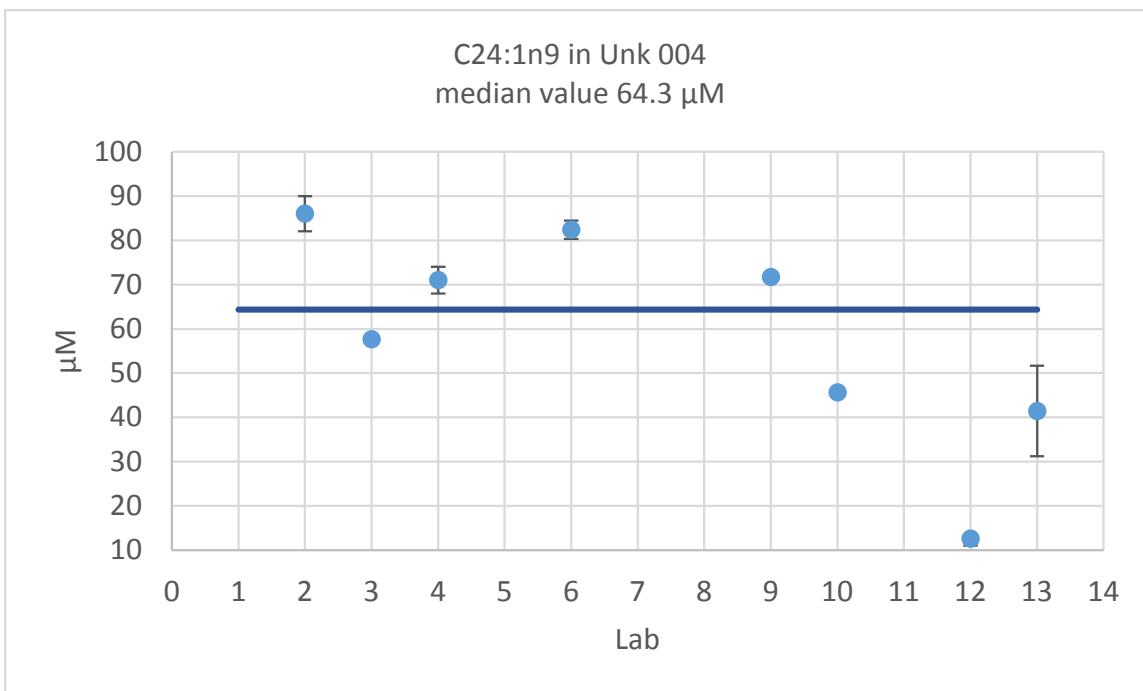


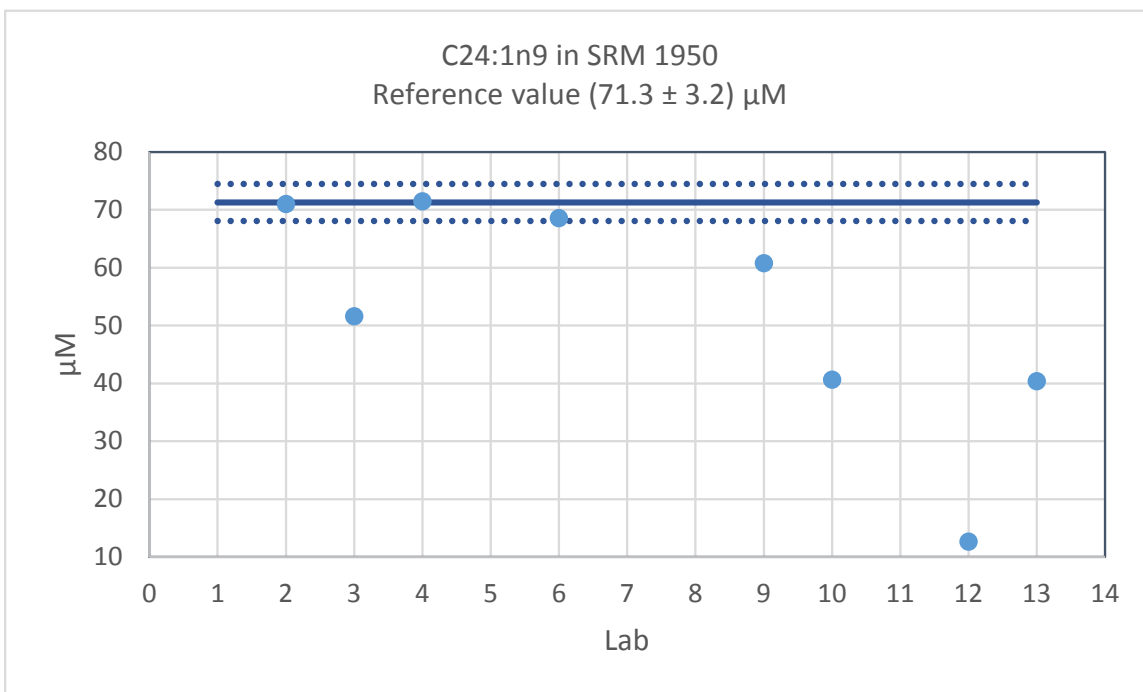
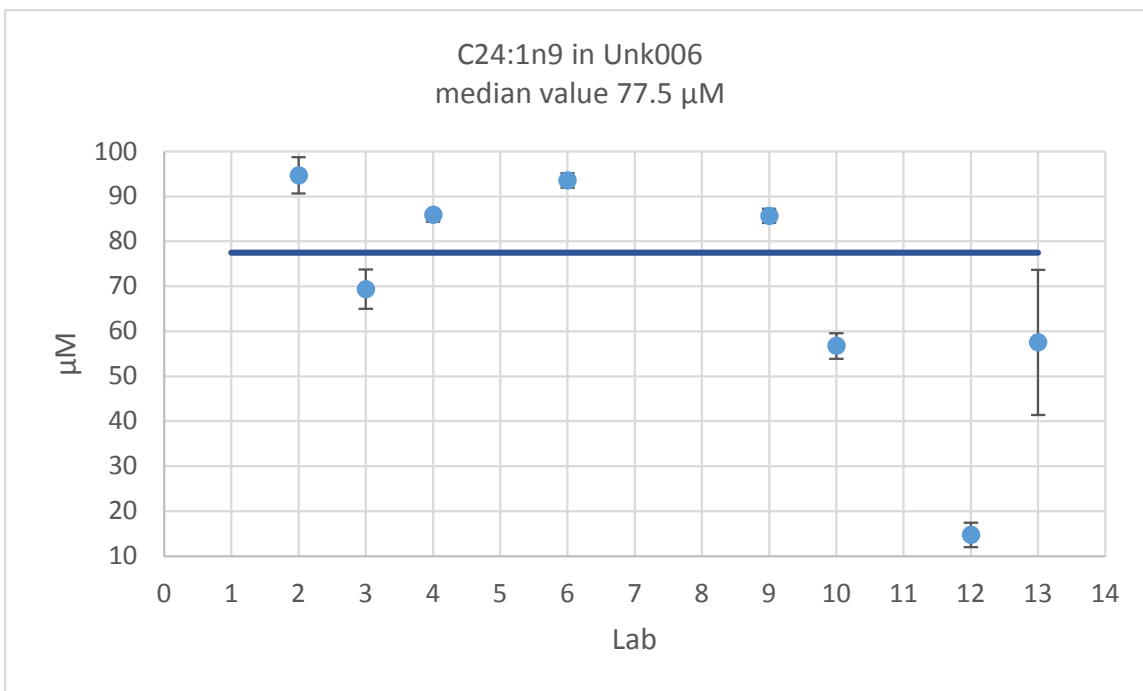


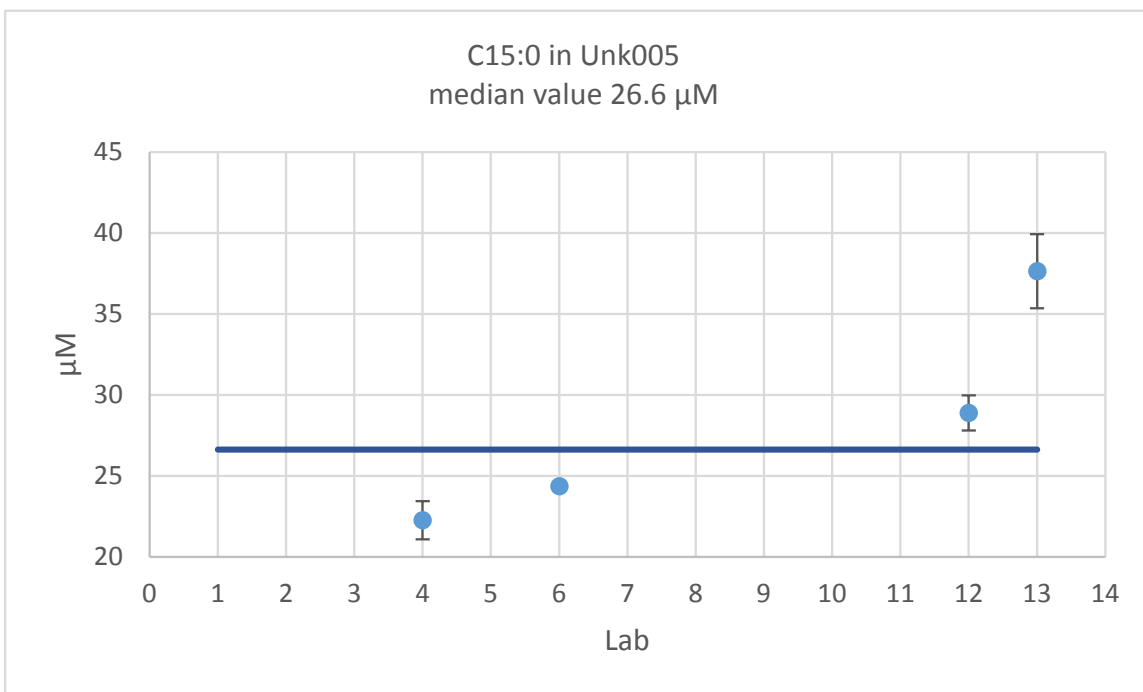
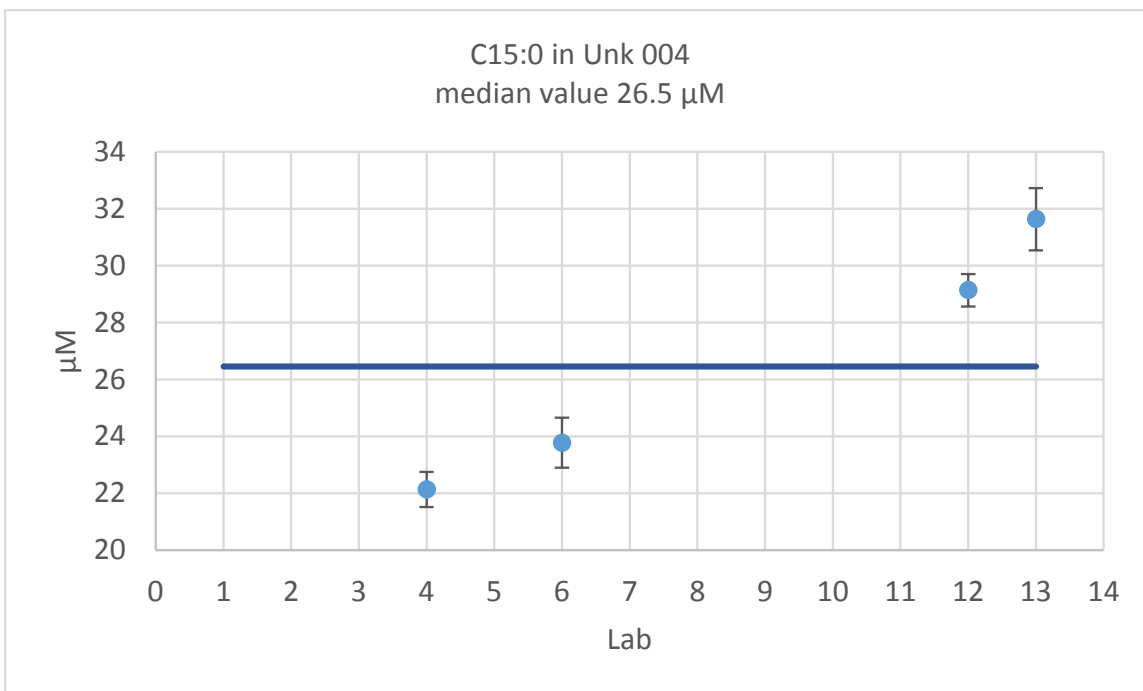


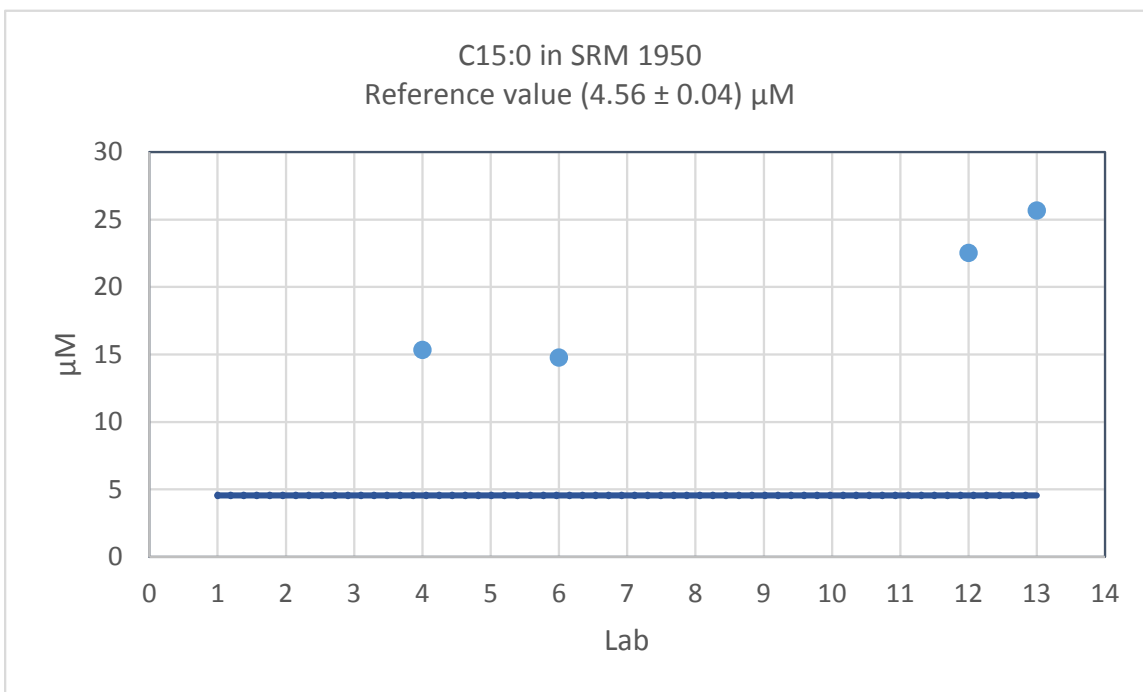
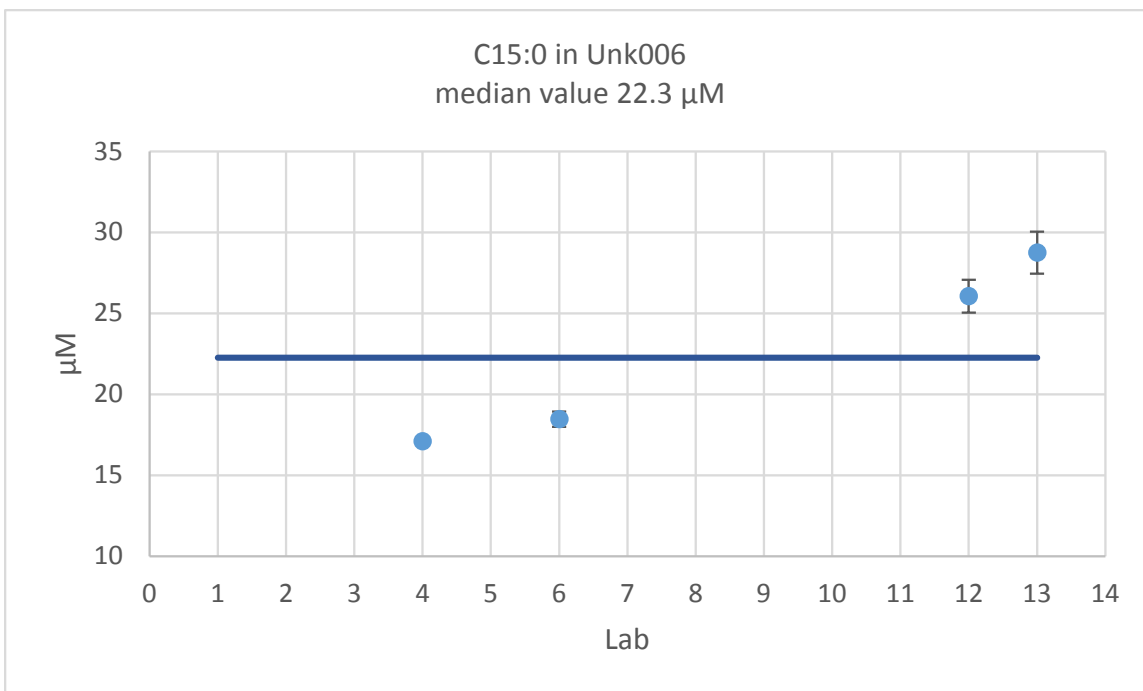


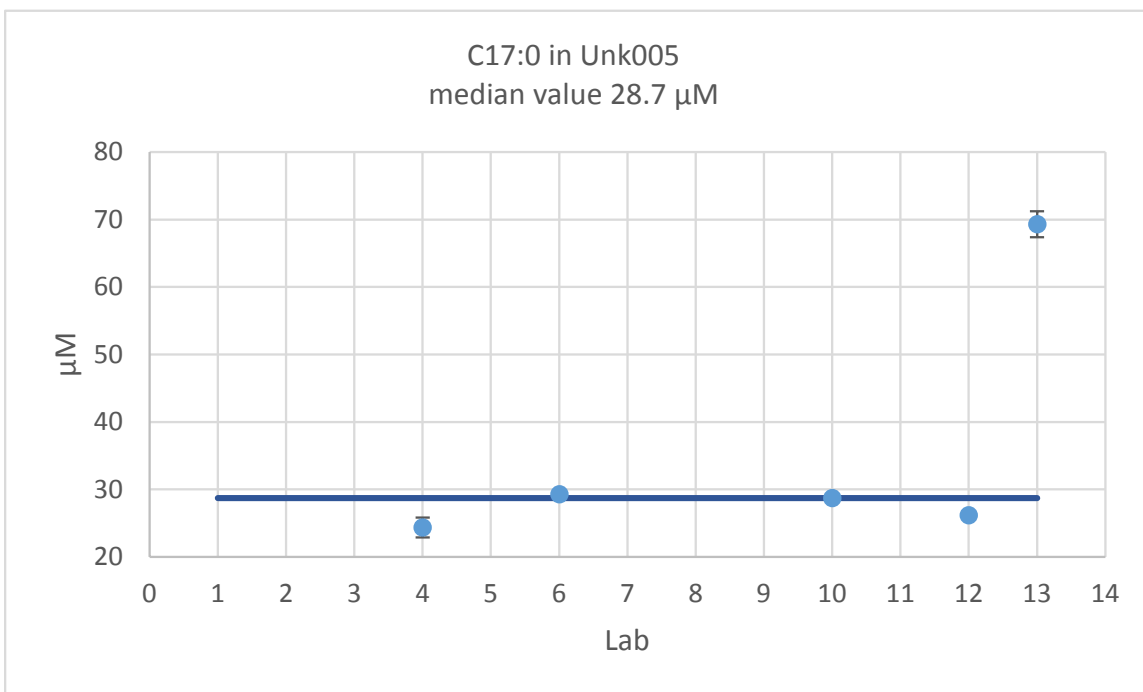
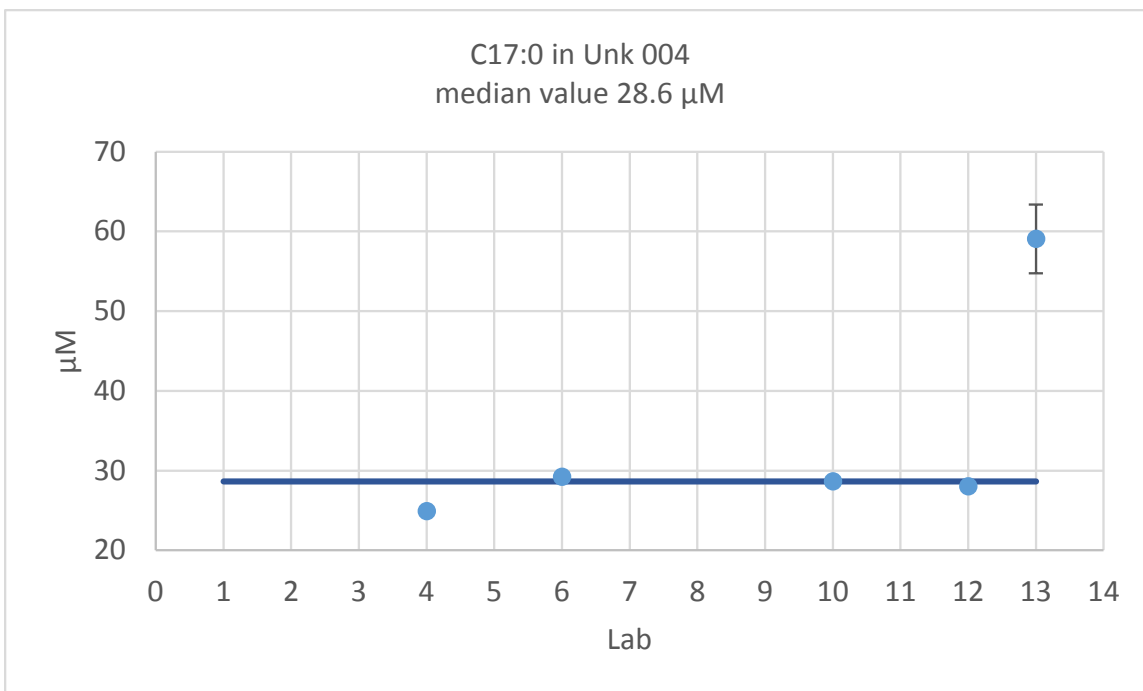


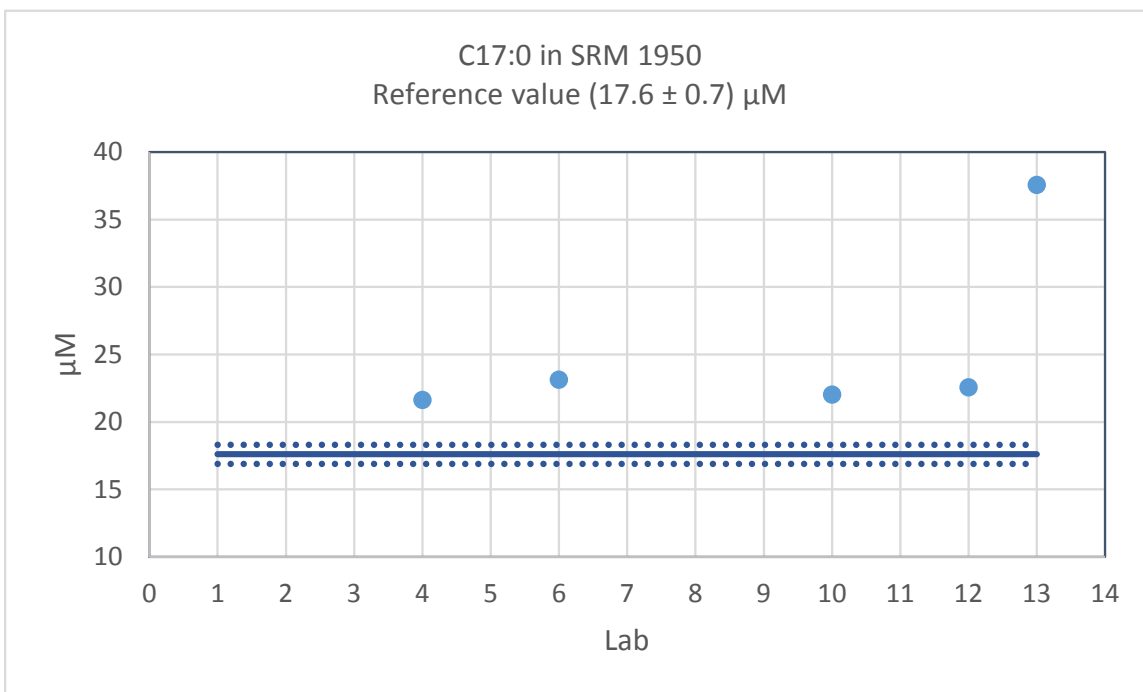
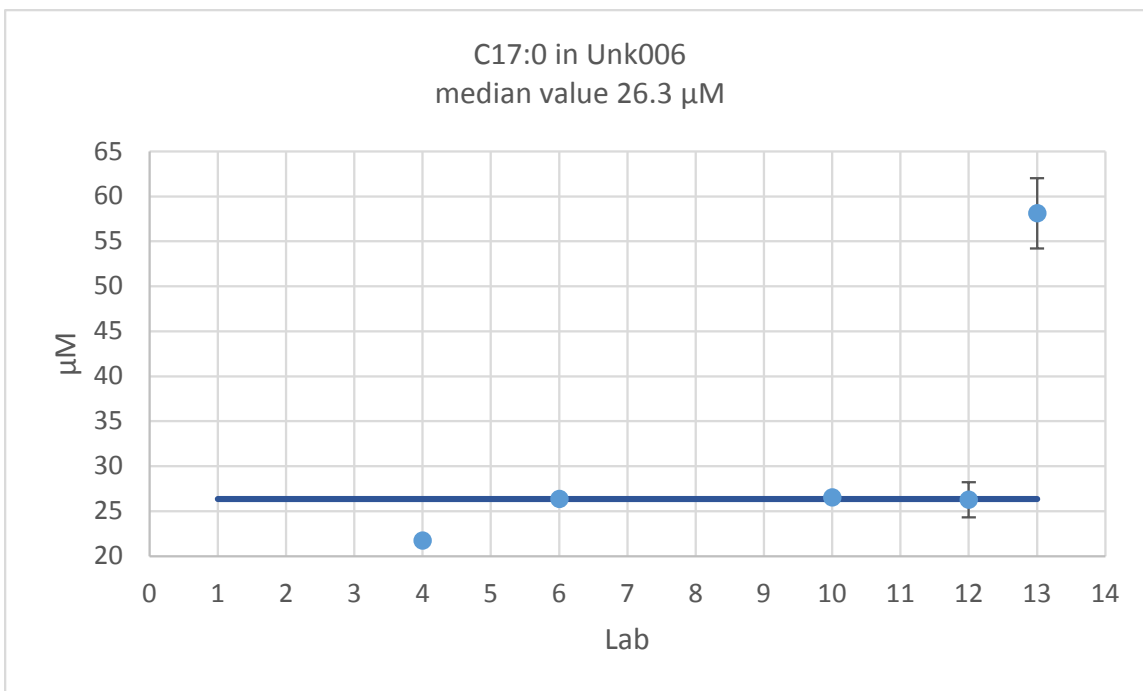












Appendix C.

Participants in the third interlaboratory analytical comparison study of total fatty acid concentrations in human serum (alphabetical order unrelated to the laboratory numbering in this report)

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