NISTIR 8185

Lipid Concentrations in Standard Reference Material (SRM) 1950: Results from an Interlaboratory Comparison Exercise for Lipidomics

John A. Bowden
Alan Heckert
Candice Z. Ulmer
Christina M. Jones

This publication is available free of charge from:
https://doi.org/10.6028/NIST.IR.8185

National Institute of Standards and Technology
U.S. Department of Commerce

NISTIR 8185

Lipid Concentrations in Standard Reference Material (SRM) 1950: Results from an Interlaboratory Comparison Exercise for Lipidomics

John A. Bowden
Candice Z. Ulmer
Christina M. Jones
Chemical Sciences Division
Material Measurement Laboratory

Alan Heckert
Statistical Engineering Division
Information Technology Laboratory

This publication is available free of charge from:
https://doi.org/10.6028/NIST.IR.8185

August 2017

U.S. Department of Commerce
Wilbur L. Ross, Jr., Secretary

National Institute of Standards and Technology
Kent Rochford, Acting NIST Director and Under Secretary of Commerce for Standards and Technology

OVERVIEW OF EXERCISE

The continued growth of the lipidomics research community, combined with a concomitant increase in the number of lipidomic applications, has culminated in an emerging need for the harmonization and standardization of lipidomics measurement. Harmonization and standardization of lipidomic measurement is a considerable undertaking, owing to the vast structural diversity and complexity of lipids, which also subsequently coincides with the use of a broad range of qualitative and quantitative measurement strategies employed by the lipidomics community. The lipidomics community needs to address the variability present in current lipidomics measurement before harmonization and standardization can begin to occur. Accordingly, this work encompasses the first community-supported harmonization effort via an interlaboratory comparison exercise, focused on ascertaining sources of lipidomic measurement variability and/or agreement, while also highlighting measurement challenges in regards to lipid quantitation.

The main objectives of the interlaboratory comparison exercise were to 1) generate consensus estimates in nmol/mL for those lipids routinely measured by participants, 2) determine the extent of agreement present within the community using current quantitation lipidomics workflows, 3) and identify those lipids or lipid classes that require more attention. The basic framework of the National Institute of Standards and Technology (NIST) interlaboratory comparison for lipidomics was to distribute one vial of Standard Reference Material (SRM) 1950 – Metabolites in Frozen Human Plasma to each participating laboratory, and to encourage each participant to employ the analytical methodologies that they typically use to quantify lipids in their laboratory. SRM 1950 was chosen as the vehicle for the comparison exercise as it has been previously recognized and promoted as an appropriate reference material for metabolomics (1-5). In addition, SRM 1950 was constructed to approximate “normal” blood plasma indicative of the United States population (see http://srm1950.nist.gov/). Invitations were sent to a cohort of laboratories that were representative of the diverse cross-section of lipid measurement methodologies present within the lipidomics community. Consensus estimates (at sum composition level), with corresponding uncertainties, were generated for those lipids measured by at least five laboratories. Additional analyses were performed to further assess the collective submitted data, including coefficient of dispersion (COD) for each consensus estimate and zeta-scores (ζ-scores). COD values were used to evaluate the quality or "usefulness" of the consensus estimates. ζ-scores were used to determine the relative measurement agreement amongst the consensus estimates by lipid species and lipid class.

The final consensus estimates and associated uncertainties generated from this exercise hold considerable potential for the lipidomics community, both to serve as inter- and intra-laboratory benchmarks but also to initiate follow-up efforts to continue measurement harmonization within the lipidomics community.

MATERIALS AND METHODS

Guidelines for Laboratory Participation

Upon receipt of SRM 1950, each laboratory was instructed to identify and quantify those lipids that they routinely measure in their laboratories. We required that the lipids be quantitatively measured in triplicate and the final lipid concentration reported for each replicate in nmol/mL plasma. To aid in the data submission process, an Excel template was provided (Appendix A) that included comment boxes to record method information (e.g., laboratory profile, sample preparation/extraction, sample introduction and chromatography, mass spectrometric analysis, and data handling/processing) and tabs for each potential target lipid class present in SRM 1950. Possible lipid classes included ceramides (CER), cholesteryl esters (CE), diacylglycerols (DAG), free fatty acids (FFA), lysophosphatidylcholines (LPC), lysophosphatidylethanolamines (LPE), phosphatidic acids (PA), phosphatidylcholines (PC), phosphatidylethanolamines (PE), phosphatidylglycerols (PG), phosphatidylinositols (PI), phosphatidylserines (PS), sphingomyelins (SM), and triacylglycerols (TAG). The target list for each lipid class consisted of potential individual lipid species. In addition, an "other" tab was included, which allowed for the submission of bile acids (BA) and eicosanoids. We also encouraged laboratories to provide values for lipids not included in the target lists. In total, 320 lipid species (designated by the sum composition annotation, lipid class and total carbons (C) and degrees of unsaturation in the fatty acyl chains, DB) were listed as potential targets in the submission template (i.e., lipid species with a high probability to be present in SRM 1950 based on the previous LIPID MAPS consortium report (6)). The 320 target lipid species are listed in Appendix A.

Handling of Submitted Lipidomic Data

Lipid identifications and quantitative measurements of lipid species in triplicate for each participating laboratory were submitted to NIST via the provided data template. Each laboratory was given a random laboratory identification number. Therefore, the laboratory identification number is not correlated with the order of the participants listed in this document. For each laboratory submission, mean and standard deviation calculations were performed for each lipid species submitted with three replicate concentrations above zero. Only the lipid species with mean and standard deviation calculated were included in the final consensus estimation (unless otherwise indicated). Data was validated, with respect to proper annotation, *m/z* value, and adduct measured using LipidPioneer (7). Any corrections to the original laboratory submission were sent to each laboratory for approval. We received data from a diverse collection of participating laboratories, encompassing a wide range of lipidomic methodologies (see Table 1), thus we obtained lipid data annotated at the sum compositional level and/or the fatty acyl level. To allow for comparison amongst all laboratory submissions, all lipid data were converted to sum composition level. Thus, the final lipid concentration for each lipid was calculated by summing all the isomers for each replicate, then calculating the average and standard deviation of the summed triplicate concentrations. A lipid isomer was included in the summation if it was reported by at least two laboratories.

Calculation of Final Consensus Locations and Uncertainties

Lipid consensus estimates and associated uncertainties were determined using three methods, the Vangel-Rukhin (VR), the DerSimonian-Laird (DSL), and the median of means (MEDM). The VR method (8, 9) is a weighted mean based on maximum likelihood. The derivation and mathematical details of the VR mean and its associated standard uncertainty are given in a previous publication (8, 9). This method incorporates both inter-laboratory and intra-laboratory variances in determining the weights. Maximum likelihood approaches have excellent statistical properties; however, the VR method is not robust against extreme outliers. In these cases, the VR weighting method gives the outlying laboratory value greater influence and results in unrepresentative estimates (i.e., the resulting value reflects neither the non-outlying values or the outlying value). Thus, to obtain a reasonable mean using this approach, the extreme outlying lipid values would need to be omitted from the estimation. The VR means were calculated with no outliers omitted.

The DSL method (10) is a weighted mean based on the method of moments. The associated standard uncertainties for the DSL mean were determined using several approaches, including the original method (10), a parametric bootstrap (11), and the Horn–Horn Duncan (HHD) (12). As with VR, DSL incorporates both inter- and intra-laboratory variances in determining the weights. However, the DSL weighting scheme is more dependent on the intra-laboratory variances than the VR method. Thus, the DSL method is more robust against extreme outliers in the laboratory means if the associated variance of the outlying laboratory is large relative to the variances of the non-outlying laboratories. When the variance of the extreme outlier is not significantly greater than the variances of the non-outlying laboratories, this robustness breaks down. In these cases, as with VR, these extreme outlier laboratories would need to be omitted to obtain a reasonable mean estimate. Another consequence of the greater emphasis on intra-laboratory variances is that when the smallest or largest laboratory means, excluding the extreme outliers, had significantly smaller variances than the other laboratories, the resulting DSL mean may be over-weighted to these most extreme (but non-outlier) laboratory means. The DSL means were calculated with no outliers omitted.

The median of the means (MEDM) method (13) uses the median of the laboratory means as the estimate of the location. The associated uncertainty, u, is $\sqrt{(\pi/2m)}\times 1.483\times \mathrm{MAD}$, where m and MAD denote the number of laboratories and the median absolute deviation of the laboratory means, respectively. The MEDM method is robust to outliers in the laboratory means regardless of the nature of the intra-laboratory variances. This method will give a "reasonable" location (i.e., half the laboratory values fall above the location and half fall below the location) without omitting any laboratories. In addition, the MEDM location estimate is less likely than VR or DSL to be distorted. The trade-off is that the MEDM method makes no use of the intra-laboratory variance (i.e., all laboratories have equal weight).

Since we aimed to include all laboratory submissions in the lipid concentration estimation, the MEDM method was chosen as it consistently generates a reasonable location value. The final locations (in nmol/mL) were reported using the MEDM method for those lipids measured by at least five laboratories. The consensus estimates determined using all three estimation approaches, with number of laboratories reporting and the standard uncertainty, are shown in Tables 2 to 6. The five lipid categories reported in this study are organized as the following: fatty acyl lipids (FA), glycerolipids (GL), glycerophospholipids (GP), sphingolipids (SL), and sterol lipids (ST),

respectively. Sample coefficient of dispersion (COD) values (14), expressed as a percentage (listed in Tables 2 to 6), were calculated for each lipid with $n \geq 5$ laboratories reporting using the equation: 100*u/MEDM. The COD values were used to assess the quality or "usefulness" of each final MEDM location. We designated lipids with a COD < 40 % as acceptable for use with quality control activities.

Final MEDM Location Plots

MEDM location plots were generated for all lipids (n = 339) that were reported by at least five laboratories. On each plot, the calculated mean and standard deviation of the mean (nmol/mL), from the triplicate measurement made by each laboratory, is shown, as well as the calculated DSL, VR, and MEDM consensus estimates with standard uncertainties. For enhanced visualization, the location plots were often truncated on the y-axis to remove outlying lipid concentrations from laboratories. The final selected MEDM location and associated uncertainty for each lipid is also provided on the plot.

Calculation of Zeta-Scores

Zeta(ζ)-scores were calculated for each lipid ($n \geq 5$ laboratories reporting) using the final calculated MEDM location, standard uncertainty, and the calculated means from the submitted lipid concentration replicates reported by each laboratory. Zeta-scores were obtained using the following equation (15):

$$Zeta(i) = \frac{X(i) - X_{pt}}{\sqrt{u_{x(i)}^2 + u_{pt}^2}}$$

where X_{pt} is the MEDM location, $X(i)$ is the laboratory's submitted average concentration value, u_x is the laboratory's standard uncertainty, and u_{pt} is the standard uncertainty of the MEDM location. ζ-scores were used to evaluate the following: 1) collective laboratory values relative to the MEDM location on a per lipid basis and 2) individual laboratory values relative to the MEDM location for lipids of a single lipid class.

RESULTS AND DISCUSSION

Summary of Laboratories and Lipids Reported in SRM 1950

To initiate the interlaboratory comparison exercise, 100 invitations were sent to a comprehensive and diverse collection of laboratories, with the mindset that this methodological diversity would lead to the creation of robust consensus mean estimates. Upon the data submission closing date, 31 laboratories submitted data for the exercise (one laboratory submitted lipidomic data using two different MS platforms, for a total number of 32 laboratory submissions). Examination of the participating laboratories revealed that 45 % were international (outside of the United States), 52 % were from laboratories that employ global lipidomic methodologies (reported lipids from three or more lipid categories), and 78 % of the laboratories self-identified as academic. These self-reported classifications, along with some additional information (extraction type and instrument platforms used) are found in Table 1. The collective data from all participating laboratories resulted in the identification of 1527 unique lipid species at the sum compositional level ($n \geq 1$ laboratories reporting). Further dissection of the 1527 lipids revealed that five lipid

categories were represented (Appendix B) as follows: FA (n = 177), GL (n = 317), GP (n = 679), SP (n = 236), and ST (n = 118). In Appendix B, all unique lipid species are provided, including a summary table that breaks down the lipid categories into lipid classes and sub-classes.

Consensus estimates were calculated for lipid species reported by at least five laboratories, using the VR, DSL, and MEDM methods. In total, final consensus locations and associated uncertainties were determined using the MEDM method for 339 lipids at the sum composition level ($n \geq 5$ laboratories reporting). The 339 lipids were represented in lipid categories as follows: FA (n = 14), GL (n = 83), GP (n = 150), SP (n = 58), and ST (n = 34). Upon further examination of the MEDM locations (n = 339), several location estimates had large uncertainties, thus limiting their application as a useful quality control benchmark. Thus, to classify the usefulness of the MEDM locations, we calculated COD values for each MEDM location. To be considered acceptable for use with quality control activities, among other validation purposes, we set a requirement that the corresponding COD value must be ≤ 40 %, with smaller COD values indicating that the lipid was measured with increased robustness and was minimally impacted by the methodology employed. In total, there were 254 lipids that fit this criterion and the lipid breakdown was BA (n = 14), CE (n = 15), CER (n = 8), free cholesterol, DAG (n = 5), eicosanoids (n = 3), FFA (n = 5), HexCer (n = 4), LPC (n = 25), LPE (n = 6), PC (n = 53), PE (n = 29), PI (n = 13), PG (n = 1), SM (n = 30), and TAG (n = 42), representing all the major lipid classes, and are shown in Tables 2 to 6.

For those lipids (n = 85) with COD values > 40 % (i.e. the lipids not measured consistently within the exercise), the lipid class breakdown (number of lipid species) was as follows: CE (n = 4), CER (n = 7), DAG (n = 19), FFA (n = 6), HexCer (n = 1), LPE (n = 2), PC (n = 10), PE (n = 6), PG (n = 2), PI (n = 2), PS (n = 1), SM (n = 8), and TAG (n = 17). Furthermore, four lipid classes had ≥ 25 % of the lipid species present with COD > 40 %, including (number of species with COD > 40 % / total number of species with $n \geq 5$ laboratories reporting): TAG (17/59 = 29 %), CER (8/15 = 53 %), FFA (6/11 = 55 %), and DAG (19/24 = 79 %). These finding indicate that measurement of these lipid classes were the most frequently inconsistent. We strongly suggest that the lipids with COD > 40 % not be used for validation purposes, rather we note that the measurement of these lipids is problematic and future improvements should be made.

MEDM location plots for each lipid ($n \geq 5$ laboratories reporting) are shown in Appendix C, see link for each class: BA, CER, CE, cholesterol, DAG, eicosanoids, FFA, HexCer, LPC, LPE, PC, PE, PG, PI, PS, SM, and TAG. On each plot, submitted lipid data from each laboratory (calculated mean and standard deviation of the mean shown in nmol/mL from the triplicate measurement) are shown to the right of the plot (right of the dashed line). On the left of the plot, consensus estimates calculated using the DSL, VR, and MEDM methods are shown with standard uncertainties. Extreme values were truncated from the plot but were not removed from the estimation. The final MEDM location is provided at the bottom of each figure.

Evaluation of all MEDM location COD values, in relation to number of laboratories reporting, showed a generally decreasing COD as the number of laboratories reporting a lipid increased as expected (Figure 1). In addition, it is expected that the impact of outlier laboratories decreases as the total number of laboratories reporting for a lipid increases. To further dissect trends in the final MEDM locations (n = 339), we examined the top-50 and bottom-50 lipids by

concentration (nmol/mL) (Appendix D). The top-50 comprised CE (*n* = 11), FFA (*n* = 4), LPC (*n* = 4), PC (*n* = 11), SM (*n* = 7), and TAG (*n* = 13). The average number of laboratories reporting for the top-50 consensus lipids was (15 ± 4) laboratories with an average COD of (26 ± 11)%. The bottom-50 lipids comprised BA (*n* = 10), CER (*n* = 9), DAG (*n* = 2), eicosanoids (*n* = 3), HexCer (*n* = 1), LPC (*n* = 9), LPE (*n* = 1), PC (*n* = 8), PE (*n* = 2), SM (*n* = 4), and TAG (*n* = 1). The average number of laboratories reporting for the bottom-50 consensus lipids was (7 ± 2) laboratories with an average COD of (35 ± 19)%. This comparison suggests that laboratories measure more concentrated lipid species more precisely and with better harmonization within the community. This is further supported by the top-50 lipids having only three lipid species with COD > 40 % (three fatty acids), while the bottom-50 had 18 lipid species with COD > 40 %.

To increase the coverage of the lipidome examined in this exercise, we extended the analysis to lipids measured by only three or four laboratories. We investigated the utility of these lipids (i.e., lipids could potentially be useful if measured uniformly within the community despite having < 5 laboratories reporting). The MEDM method was not used to determine these estimates, as the associated uncertainty calculations for the MEDM procedure may understate the uncertainty when there are fewer than five laboratories (13). In addition, it is recommended that there be at least six laboratories for the maximum likelihood asymptotics of the VR method to be valid (16). Thus, for the estimation of these lipids (*n* = 192, Table 7 and Table 8), with only three to four laboratories reporting, the DSL estimation method was employed as its uncertainty estimation remains valid for a small number of laboratories (10). To examine the usefulness of these additional DSL means, we set the criteria to be COD ≤ 40 % and a percent difference between the DSL mean and the MEDM location ≤ 20 %, which ensures both a generally reliable consensus estimate and avoids lipids with extreme outliers. For the 192 lipid species, there were 62 lipids which fit the criteria for acceptance as “tentative” consensus means for validation purposes. For the 62 lipid species, the following lipid classes were represented: BA (*n* = 2), CE (*n* = 3), CER (*n* = 4), DAG (*n* = 1), dihydroceramides (DHC, *n* = 4), dhSph-1P (*n* = 1), eicosanoids (*n* = 20), FFA (*n* = 3), HexCer (*n* = 1), LPC (*n* = 4), PC (*n* = 4), PE (*n* = 2), PG (*n* = 2), PS (*n* = 2), SM (*n* = 2), Sph-1P, TAG (*n* = 7), and total cholesterol.

ζ-Score Analysis

To determine the relative agreement of each participating laboratory, in relation to the community-derived MEDM location, ζ-scores were calculated for each submitted lipid concentration. While z-scores are often employed, which subtract the consensus estimate from the laboratory submitted value and divide by the standard uncertainty of the consensus estimate, we employed the zeta(ζ)-score, a variant of the z-score, which takes into account laboratory variances (15).

Upon closer inspection of the collective calculated ζ-scores, several community-wide trends were observed based on lipid species measured (for lipids with n ≥ 5 laboratories reporting). ζ-scores were implemented to normalize the submitted data from all laboratories and to compare values relative to the MEDM location by lipid species (Appendix E) or by laboratory (Appendix F). Untruncated ζ-score averages are included in all plots to help identify those lipids with a higher frequency of atypical measurement in relation to the collective data submitted. For each ζ-score plot, each dot represents the number of combined standard uncertainties a single laboratory-

reported lipid value is from the MEDM location. With normally distributed data, approximately 95 % of the data should fall within ± 2 standard deviations (two solid lines on plots). This normality guideline assumes that the participating laboratories are approximately equal in ability, and thus the differences observed reflect random measurement error. For those lipids by which a majority of the dots reside outside the guidelines (± 2), the ζ-scores indicate that the capability of measuring those lipids is poor for the majority of the laboratories reporting and is not just random measurement error. According to the ζ-scores on a per lipid species basis (all the laboratories scores on the same plot for a lipid species, Appendix E), the ten most variably measured lipids in relation to the MEDM location by untruncated ζ-scores (in parentheses) were SM d34:0 (6.47), CE 22:4 (6.51), CE 22:5 (7.37), SM d41:1 (7.38), PC O-40:6/P-40:5/39:6 (8.71), PC 38:7 (8.76), PE O-40:5/P-40:4/39:5 (8.8), SM d38:0 (9.31), CER d38:1 (9.61), and DAG 38:0 (10.48). The untruncated ζ-score averages indicate that, on average, the lipids were measured more than six times (and greater) the standard uncertainty away from the MEDM location.

The second manner in which ζ-scores were organized was by laboratory on a per lipid class basis. In these plots (Appendix F), the ζ-scores were used to identify which laboratories consistently measured lipid species, organized by lipid class, at different concentrations relative to the MEDM location. The untruncated average ζ-scores reveal how well each laboratory performed relative to the MEDM location. Further examination of the ζ-scores by laboratory, on a per lipid class basis, revealed that five lipid classes had ≥ 3 laboratories with untruncated ζ-score averages above five (i.e., a ζ-score value of 5 for a lipid class indicates, that on average, the laboratory ζ-scores were four times the combined standard uncertainties away from the MEDM location). The five lipid classes were (with number of laboratories with ζ-score averages above five): DAG (3), LPE (3), PE (3), SM (4), and LPC (5).

SUMMARY

To date, there is no community-wide accepted workflow for performing and analyzing lipidomics experiments. Furthermore, there are no lipid benchmark concentrations in complex mixtures that can be used to assess current lipidomic workflows and methods. This interlaboratory study is the first step towards providing a means to increase harmonization and initiating a conversation regarding potential efforts required to improve standardization in lipid measurement within the lipidomics community.

DISCLAIMER

Certain commercial equipment, instruments, or materials are identified in this paper to specify adequately the experimental procedures. 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 necessarily the best for the purpose.

ACKNOWLEDGEMENTS

In addition to acknowledging the contributions (and funding sources) for each participating laboratory (Appendix G), the authors of this report would also like to acknowledge the contributions of Rebecca Pugh, Debra Ellisor, Amanda Moors, David Duewer, Katrice Lippa, John

Kucklick, Stephen Somerville, Theresa Cantu, Jackie Bangma, and Jeremy Koelmel, which helped make this interlaboratory exercise successful.

REFERENCES

1. Beger, R. D., W. Dunn, M. A. Schmidt, S. S. Gross, J. A. Kirwan, M. Cascante, L. Brennan, D. S. Wishart, M. Oresic, and T. Hankemeier. 2016. Metabolomics enables precision medicine: "a white paper, community perspective". Metabolomics **12**: 149.

2. Phinney, K. W., G. Ballihaut, M. Bedner, B. S. Benford, J. E. Camara, S. J. Christopher, W. C. Davis, N. G. Dodder, G. Eppe, and B. E. Lang. 2013. Development of a Standard Reference Material for metabolomics research. *Anal. Chem*. **85**: 11732-11738.

3. Simon-Manso, Y., M. S. Lowenthal, L. E. Kilpatrick, M. L. Sampson, K. H. Telu, P. A. Rudnick, W. G. Mallard, D. W. Bearden, T. B. Schock, and D. V. Tchekhovskoi. 2013. Metabolite profiling of a NIST Standard Reference Material for human plasma (SRM 1950): GC-MS, LC-MS, NMR, and clinical laboratory analyses, libraries, and web-based resources. *Anal. Chem.* **85**: 11725-11731.

4. Telu, K. H., X. Yan, W. E. Wallace, S. E. Stein, and Y. Simón-Manso. 2016. Analysis of human plasma metabolites across different liquid chromatography/mass spectrometry platforms: Cross-platform transferable chemical signatures. *Rapid Comm. Mass Spectrom.* **30**: 581-593.

5. Koal, T., and H.-P. Deigner. 2010. Challenges in mass spectrometry based targeted metabolomics. *Curr. Mol. Med*. **10**: 216-226.

6. Quehenberger, O., A. M. Armando, A. H. Brown, S. B. Milne, D. S. Myers, A. H. Merrill, S. Bandyopadhyay, K. N. Jones, S. Kelly, and R. L. Shaner. 2010. Lipidomics reveals a remarkable diversity of lipids in human plasma. *J. Lipid Res*. **51**: 3299-3305.

7. Ulmer, C. Z., J. P. Koelmel, J. M. Ragland, T. J. Garrett, and J. A. Bowden. 2017. LipidPioneer: A Comprehensive User-Generated Exact Mass Template for Lipidomics. *J. Am. Soc. Mass Spectrom*. **28**: 562-565.

8. Rukhin, A. L., and M. G. Vangel. 1998. Estimation of a common mean and weighted means statistics. *J. Am. Stat. Assoc*. **93**: 303-308.

9. Vangel, M. G., and A. L. Rukhin. 1999. Maximum Likelihood Analysis for Heteroscedastic One-Way Random Effects ANOVA in Interlaboratory Studies. *Biometrics* **55**: 129-136.

10. DerSimonian, R., and N. Laird. 1986. Meta-analysis in clinical trials. *Control. Clin. Trials* **7**: 177-188.

11. Efron, B., and R. J. Tibshirani. 1993. An introduction to the bootstrap. Number 57 in Monographs on statistics and applied probability. Chapman & Hall, New York.

12. Horn, S. D., R. A. Horn, and D. B. Duncan. 1975. Estimating heteroscedastic variances in linear models. Journal of the American Statistical Association **70**: 380-385.

13. CCQM. 2013. CCQM Guidance note: Estimation of a consensus KCRV and associated degrees of equivalence: Version 10 http://www.bipm.org/cc/CCQM/Allowed/19/CCQM13-22_Consensus_KCRV_v10.pdf.

14. Bonett, D. G., Seier, E. 2006. Confidence Interval for a Coefficient of Dispersion in Nonnormal Distributions. *Biometrics* **48**: 144-148.

15. ISO 13528. 2015. Statistical methods for use in proficiency testing by interlaboratory comparison. 2nd Edition. 1-89.

16. Vangel, M. G. personal communication.

Table 1. Participating laboratory and methodological information

Lab #	International/ National*	Lab Type*	Target/ Global	Extraction Type			Instrument #1		Instrument #2		Instrument #3	
							Sample Introduction	MS Used	Sample Introduction	MS Used	Sample Introduction	MS Used
1	International	Academia	Global	Bligh-Dyer			HPLC	HRMS/MS				
2	International	Industry	Global	Matyash			DI	HRMS/MS				
3	International	Academia	Global	Matyash			UHPLC	HRMS/MS				
4†							UHPLC	MS/MS	GC	MS		
5†	International	Industry	Global	Folch			UHPLC	MS/MS				
6	National	Academia	Global	Bligh-Dyer			DI	MS/MS	GC	MS		
7	International	Academia	Global	Modified Bligh-Dyer			DI	MS/MS				
8	National	Academia	Targeted	SPE	Modified Bligh-Dyer		HPLC	MS/MS	GC	MS		
9	National	Academia	Global	Matyash			UHPLC	HRMS/MS				
10	International	Academia	Global	Butanol/Methanol	Methanol Precipitation		UHPLC	MS/MS				
11	International	Industry	Global	SPE	Methanol Precipitation	Folch	DI	MS/MS	GC	MS/MS	UHPLC	MS/MS
12	National	Academia	Global	Matyash			UHPLC	HRMS				
13	National	Academia	Global	SPE			DI	MS/MS	HPLC	MS/MS		
14	National	Academia	Targeted	Isopropanol/Ethyl acetate	Chloroform/water/1N NaCl		HPLC	MS/MS				
15	National	Academia	Global	Matyash			HPLC	HRMS/MS				
16	National	Government	Global	Modified Bligh-Dyer			DI	MS/MS				
17	National	Academia	Targeted	Folch			HPLC	MS/MS				
18	International	Industry	Global	Modified Folch			UHPLC	HRMS				
19	National	Industry	Global	Folch			UHPLC	HRMS/MS				
20	International	Academia	Targeted	SPE	Modified Bligh-Dyer		UHPLC	MS/MS				
21	National	Academia	Targeted	SPE			UHPLC	MS/MS				
22	International	Academia	Targeted	SPE			UHPLC	MS/MS				
23	International	Academia	Global	Matyash			DI	HRMS				
24	National	Academia	Targeted	Acetonitrile Precipitation			UHPLC	MS				
25	National	Academia	Targeted	Acetonitrile Precipitation			UHPLC	MS/MS				
26	National	Academia	Targeted	Methanol Precipitation			DI	MS/MS				
27	International	Academia	Targeted	Bligh-Dyer			DI	MS/MS	GC	MS	HPLC	MS/MS
28	International	Academia	Targeted	Isopropanol			HPLC	HRMS/MS				
30	National	Academia	Targeted	SPE			UHPLC	MS/MS				
31	National	Academia	Targeted	Methanol Precipitation			UHPLC	MS/MS				
32	International	Industry	Targeted	Ethyl Acetate			HPLC	MS/MS				
34	National	Academia	Targeted	Acetonitrile Precipitation			UPLC	MS/MS				

* Self-reported by participating laboratory. † Submissions for laboratory ID 4 and 5 are from the same laboratory, the two submissions were performed on two different mass spectrometric platforms. N/A indicates that the information was not provided. Global = reported ≥ 3 lipid categories, Targeted = reported < 3 lipid categories. HRMS – high resolution-mass spectrometry, MS - low resolution-mass spectrometry, MS/MS – tandem mass spectrometry

Table 2. Consensus estimates and associated uncertainties for fatty acyl lipids (FA) measured by at least five laboratories in SRM 1950

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
FFA 16:0	5	nmol/mL	19	20	75	39	**43**	**13**	31
FFA 16:1	6	nmol/mL	8.4	3.0	8.5	2.7	**6.1**	**2.9**	48
FFA 18:0	5	nmol/mL	34	15	34	13	**15**	**9.0**	62
FFA 18:1	6	nmol/mL	37	12	100	30	**110**	**53**	48
FFA 18:2	6	nmol/mL	64	25	64	23	**44**	**22**	49
FFA 18:3	6	nmol/mL	3.6	0.64	3.6	0.57	**2.9**	**0.62**	21
FFA 20:3	5	nmol/mL	2.7	1.9	3.0	1.8	**1.3**	**0.62**	47
FFA 20:4	7	nmol/mL	8.7	4.8	16	11	**4.7**	**1.5**	31
FFA 20:5	7	nmol/mL	0.42	0.059	0.82	0.44	**0.42**	**0.056**	13
FFA 22:5	5	nmol/mL	1.4	0.67	1.4	0.61	**1.1**	**0.56**	52
FFA 22:6	8	nmol/mL	2.8	1.2	2.9	1.3	**1.5**	**0.17**	11
12-HETE	5	pmol/mL	11	2.9	11	2.6	**6.8**	**1.5**	23
15-HETE	5	pmol/mL	1.8	0.19	2.0	0.21	**2.4**	**0.64**	27
5-HETE	5	pmol/mL	10	1.3	11	1.6	**10**	**1.3**	13

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. The abbreviations identify free fatty acids (FFA) and hydroxyeicosatetraenoic acids (HETE).

Table 3. Consensus estimates and associated uncertainties for glycerolipids measured by at least five laboratories in SRM 1950

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
DAG 30:0	7	nmol/mL	0.55	0.15	0.65	0.13	**0.83**	**0.17**	20
DAG 32:0	11	nmol/mL	0.56	0.35	5.3	2.0	**2.6**	**1.2**	44
DAG 32:1	10	nmol/mL	0.71	0.24	1.00	0.29	**1.2**	**0.62**	51
DAG 32:2	11	nmol/mL	0.29	0.088	0.62	0.20	**0.62**	**0.29**	48
DAG 34:0	10	nmol/mL	5.9	3.7	11	3.6	**6.5**	**3.6**	56
DAG 34:1	16	nmol/mL	4.1	1.2	22	9.6	**6.1**	**2.4**	40
DAG 34:2	14	nmol/mL	2.7	0.71	5.2	1.4	**4.4**	**1.9**	43
DAG 34:3	7	nmol/mL	0.16	0.070	8.7	4.5	**0.31**	**0.20**	63
DAG 36:0	9	nmol/mL	3.7	1.9	13	7.3	**1.6**	**0.98**	60
DAG 36:1	12	nmol/mL	5.2	2.2	6.1	2.8	**2.6**	**1.1**	43
DAG 36:2	16	nmol/mL	2.4	0.89	25	12	**6.2**	**2.2**	36
DAG 36:3	15	nmol/mL	4.2	1.6	6.8	1.6	**8.4**	**3.3**	39
DAG 36:4	12	nmol/mL	0.68	0.29	2.6	0.60	**2.8**	**1.0**	38
DAG 36:5	6	nmol/mL	0.61	0.28	2.9	2.0	**0.89**	**0.54**	61
DAG 38:0	7	nmol/mL	1.8	1.2	1.9	1.1	**0.24**	**0.13**	55
DAG 38:1	5	nmol/mL	0.39	0.35	0.65	0.28	**0.51**	**0.39**	77
DAG 38:2	5	nmol/mL	0.69	0.54	2.2	0.98	**1.5**	**1.2**	81
DAG 38:3	5	nmol/mL	0.45	0.32	2.8	1.4	**1.3**	**1.0**	80
DAG 38:4	11	nmol/mL	0.57	0.19	2.0	0.99	**0.95**	**0.38**	40
DAG 38:5	11	nmol/mL	1.2	0.48	1.6	0.42	**1.8**	**0.82**	47
DAG 38:6	9	nmol/mL	1.6	0.79	2.0	1.1	**0.77**	**0.37**	47
DAG 40:5	5	nmol/mL	0.046	0.021	0.043	0.017	**0.084**	**0.053**	63
DAG 40:6	6	nmol/mL	0.18	0.072	0.18	0.064	**0.28**	**0.17**	60
DAG 40:7	5	nmol/mL	0.060	0.039	0.49	0.22	**0.89**	**0.68**	77
TAG 42:0	5	nmol/mL	0.48	0.20	0.73	0.30	**0.38**	**0.19**	50
TAG 42:1	5	nmol/mL	0.29	0.057	0.29	0.048	**0.37**	**0.17**	45
TAG 42:2	6	nmol/mL	0.12	0.031	0.12	0.026	**0.16**	**0.064**	41
TAG 44:0	5	nmol/mL	1.8	0.82	2.1	0.78	**1.2**	**0.73**	62
TAG 44:1	7	nmol/mL	1.1	0.32	9.3	6.9	**1.7**	**0.84**	50
TAG 44:2	6	nmol/mL	1.1	0.41	3.9	2.7	**0.90**	**0.40**	45

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. The abbreviations identify diacylglycerols (DAG) and triacylglycerols (TAG).

Table 3. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
TAG 46:0	6	nmol/mL	2.0	0.66	3.5	1.2	**2.8**	**1.6**	56
TAG 46:1	8	nmol/mL	6.0	2.1	17	11	**5.7**	**2.6**	46
TAG 46:2	8	nmol/mL	2.4	0.63	2.8	0.63	**3.6**	**1.3**	37
TAG 46:3	5	nmol/mL	0.71	0.21	0.70	0.18	**0.76**	**0.34**	45
TAG 48:0	10	nmol/mL	5.3	1.3	5.3	1.2	**4.5**	**1.2**	26
TAG 48:1	16	nmol/mL	24	11	28	14	**13**	**3.2**	24
TAG 48:2	15	nmol/mL	21	6.9	14	2.0	**16**	**2.8**	18
TAG 48:3	11	nmol/mL	5.1	1.5	7.3	3.0	**3.3**	**1.3**	41
TAG 48:4	5	nmol/mL	1.2	0.13	1.8	0.47	**1.3**	**0.23**	18
TAG 49:1	9	nmol/mL	1.9	0.32	2.4	0.48	**2.0**	**0.42**	21
TAG 49:2	6	nmol/mL	1.5	0.41	1.6	0.37	**1.8**	**0.56**	31
TAG 50:0	11	nmol/mL	4.6	1.2	4.9	0.97	**3.8**	**0.83**	22
TAG 50:1	14	nmol/mL	17	6.9	33	5.6	**38**	**10.0**	26
TAG 50:2	15	nmol/mL	18	5.4	48	7.4	**47**	**12**	26
TAG 50:3	16	nmol/mL	27	4.3	27	4.1	**23**	**6.6**	29
TAG 50:4	15	nmol/mL	8.5	1.7	8.3	1.6	**8.7**	**2.9**	34
TAG 50:5	7	nmol/mL	1.7	0.37	1.8	0.35	**1.6**	**0.64**	40
TAG 51:1	7	nmol/mL	1.2	0.46	1.5	0.33	**1.8**	**0.48**	27
TAG 51:2	8	nmol/mL	4.0	0.48	4.9	0.62	**4.8**	**1.1**	22
TAG 51:3	5	nmol/mL	3.6	0.79	3.6	0.68	**4.8**	**1.9**	39
TAG 51:4	6	nmol/mL	0.96	0.31	1.2	0.32	**1.4**	**0.62**	43
TAG 52:0	8	nmol/mL	2.3	0.76	5.8	2.1	**3.4**	**1.8**	54
TAG 52:1	11	nmol/mL	20	4.5	17	3.5	**14**	**2.9**	20
TAG 52:2	16	nmol/mL	49	23	71	14	**44**	**14**	33
TAG 52:3	16	nmol/mL	22	5.4	170	66	**100**	**29**	28
TAG 52:4	15	nmol/mL	41	26	60	11	**48**	**17**	35
TAG 52:5	13	nmol/mL	17	3.5	17	3.3	**15**	**5.7**	39
TAG 52:6	8	nmol/mL	3.0	0.78	3.1	0.72	**4.0**	**1.4**	35
TAG 52:7	5	nmol/mL	0.37	0.064	0.37	0.055	**0.39**	**0.13**	33

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. The abbreviations identify diacylglycerols (DAG) and triacylglycerols (TAG).

Table 3. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
TAG 53:2	9	nmol/mL	1.9	0.20	2.0	0.20	**1.9**	**0.41**	21
TAG 53:3	6	nmol/mL	3.1	0.72	15	11	**3.7**	**1.1**	29
TAG 53:4	6	nmol/mL	1.6	0.40	4.4	2.3	**2.4**	**0.76**	32
TAG 53:5	6	nmol/mL	0.67	0.21	0.91	0.28	**0.84**	**0.37**	44
TAG 54:0	9	nmol/mL	1.3	0.59	4.2	1.5	**2.4**	**1.3**	51
TAG 54:1	10	nmol/mL	3.0	0.61	20	17	**3.2**	**0.91**	29
TAG 54:2	13	nmol/mL	23	12	47	34	**8.2**	**2.6**	31
TAG 54:3	15	nmol/mL	33	6.2	35	7.3	**26**	**9.8**	37
TAG 54:4	15	nmol/mL	12	5.9	37	6.5	**36**	**13**	35
TAG 54:5	15	nmol/mL	5.7	2.4	30	5.6	**27**	**11**	38
TAG 54:6	16	nmol/mL	2.3	2.3	15	2.9	**14**	**5.1**	37
TAG 54:7	7	nmol/mL	4.5	1.3	4.5	1.2	**5.6**	**1.5**	26
TAG 56:2	5	nmol/mL	0.67	0.14	0.67	0.13	**0.69**	**0.23**	33
TAG 56:3	6	nmol/mL	1.1	0.27	1.1	0.23	**1.4**	**0.14**	10
TAG 56:4	10	nmol/mL	2.4	0.81	5.8	3.7	**2.0**	**0.56**	28
TAG 56:5	12	nmol/mL	3.9	0.86	4.9	1.0	**4.1**	**1.4**	33
TAG 56:6	15	nmol/mL	8.0	1.7	8.1	1.7	**6.4**	**2.7**	42
TAG 56:7	8	nmol/mL	22	13	23	13	**13**	**2.7**	20
TAG 56:8	11	nmol/mL	3.1	0.78	3.1	0.74	**3.3**	**1.3**	40
TAG 56:9	5	nmol/mL	0.75	0.23	0.74	0.20	**0.71**	**0.27**	38
TAG 58:6	5	nmol/mL	1.5	0.39	1.5	0.36	**1.6**	**0.68**	42
TAG 58:7	5	nmol/mL	3.2	1.7	11	8.2	**2.0**	**0.64**	32
TAG 58:8	9	nmol/mL	0.97	0.28	0.96	0.25	**0.68**	**0.21**	31
TAG 58:9	6	nmol/mL	1.5	0.72	1.9	0.90	**1.2**	**0.27**	22

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. The abbreviations identify diacylglycerols (DAG) and triacylglycerols (TAG).

Table 4. Consensus estimates and associated uncertainties for glycerophospholipids measured by at least five laboratories in SRM 1950

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
LPC 14:0	16	nmol/mL	0.99	0.19	1.1	0.19	**1.0**	**0.20**	19
LPC 15:0	9	nmol/mL	0.85	0.27	0.86	0.26	**0.52**	**0.11**	22
LPC 16:0	20	nmol/mL	85	44	79	12	**73**	**11**	15
LPC O-16:0	10	nmol/mL	0.49	0.11	0.50	0.10	**0.55**	**0.16**	29
LPC P-16:0	8	nmol/mL	0.35	0.088	310	290	**0.46**	**0.13**	27
LPC 16:1	19	nmol/mL	1.00	0.21	2.7	0.51	**2.4**	**0.35**	15
LPC 17:0	6	nmol/mL	1.3	0.045	680	620	**1.4**	**0.24**	18
LPC 17:1	6	nmol/mL	0.31	0.12	54	50	**0.25**	**0.071**	29
LPC 18:0	20	nmol/mL	16	5.0	30	4.9	**27**	**3.3**	12
LPC O-18:0	6	nmol/mL	0.49	0.39	0.61	0.44	**0.16**	**0.058**	36
LPC 18:1	19	nmol/mL	22	5.2	20	2.9	**18**	**2.3**	13
LPC 18:2	19	nmol/mL	25	11	25	3.8	**22**	**2.9**	13
LPC 18:3	18	nmol/mL	1.4	0.80	1.8	1.2	**0.44**	**0.13**	30
LPC 20:0	7	nmol/mL	0.18	0.057	65	60	**0.10**	**0.034**	34
LPC 20:1	13	nmol/mL	0.19	0.030	0.29	0.084	**0.19**	**0.024**	12
LPC 20:2	9	nmol/mL	0.43	0.19	0.44	0.18	**0.23**	**0.044**	19
LPC 20:3	18	nmol/mL	1.4	0.34	2.4	0.50	**1.8**	**0.26**	15
LPC 20:4	20	nmol/mL	2.8	0.62	6.4	1.0	**6.0**	**0.60**	10
LPC 20:5	15	nmol/mL	0.47	0.11	0.48	0.11	**0.33**	**0.092**	28
LPC 22:0	5	nmol/mL	0.023	0.0032	15	13	**0.025**	**0.0017**	7
LPC 22:1	5	nmol/mL	0.015	0.0053	12	11	**0.013**	**0.0046**	36
LPC 22:4	8	nmol/mL	0.17	0.077	0.18	0.071	**0.12**	**0.041**	33
LPC 22:5	12	nmol/mL	0.46	0.12	0.56	0.13	**0.43**	**0.13**	30
LPC 22:6	17	nmol/mL	1.3	0.45	1.3	0.41	**0.77**	**0.14**	18
LPC 24:0	5	nmol/mL	0.055	0.017	27	24	**0.046**	**0.015**	33
LPE 16:0	14	nmol/mL	0.69	0.17	0.80	0.14	**0.91**	**0.27**	29
LPE 18:0	15	nmol/mL	2.8	1.1	3.6	1.5	**1.6**	**0.55**	34
LPE 18:1	14	nmol/mL	2.0	0.61	1.8	0.53	**1.4**	**0.47**	35

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. For PC and PE lipid classes, the isobaric species (ether-linked) were summed and the possibilities observed by the participants are separated by a "/". The abbreviations identify lysophosphatidylcholines (LPC) and lysophosphatidylethanolamines (LPE).

Table 4. (cont….)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
LPE 18:2	16	nmol/mL	2.9	0.89	3.5	1.2	**1.9**	**0.56**	30
LPE 20:3	5	nmol/mL	0.47	0.25	0.71	0.37	**0.52**	**0.38**	72
LPE 20:4	14	nmol/mL	1.5	0.60	2.3	0.98	**1.1**	**0.41**	37
LPE 22:1	5	nmol/mL	0.017	0.019	0.090	0.062	**0.036**	**0.030**	82
LPE 22:6	12	nmol/mL	0.57	0.11	0.62	0.12	**0.52**	**0.18**	34
PC 30:0	11	nmol/mL	1.8	0.32	2.0	0.34	**1.6**	**0.32**	20
PC 30:1	5	nmol/mL	0.76	0.54	0.84	0.41	**0.76**	**0.43**	57
PC O-30:0/29:0	7	nmol/mL	0.083	0.028	0.41	0.30	**0.072**	**0.026**	36
PC O-30:1/P-30:0	7	nmol/mL	0.071	0.022	0.13	0.068	**0.047**	**0.0096**	20
PC 32:0	18	nmol/mL	7.0	0.53	8.4	0.77	**7.2**	**1.0**	14
PC O-32:0/31:0	11	nmol/mL	1.4	0.25	1.4	0.24	**1.5**	**0.41**	28
PC 32:1	18	nmol/mL	9.2	1.0	13	1.3	**13**	**1.9**	15
PC O-32:1/P-32:0/31:1	11	nmol/mL	1.7	0.22	1.7	0.20	**1.6**	**0.24**	14
PC O-32:2/P-32:1/31:2	8	nmol/mL	0.29	0.062	18	16	**0.34**	**0.093**	28
PC 32:3	8	nmol/mL	0.27	0.089	6.7	6.0	**0.42**	**0.14**	34
PC P-33:1/32:2	16	nmol/mL	2.1	0.18	3.2	0.45	**2.6**	**0.37**	14
PC 34:0	12	nmol/mL	3.3	1.4	3.6	1.5	**2.1**	**0.37**	18
PC O-34:0/33:0	10	nmol/mL	0.70	0.10	0.70	0.099	**0.76**	**0.17**	22
PC 34:1	19	nmol/mL	33	33	1,500	1,300	**120**	**21**	17
PC O-34:1/P-34:0/33:1	17	nmol/mL	3.1	0.77	5.0	0.69	**4.9**	**0.86**	17
PC O-34:2/P-34:1/33:2	17	nmol/mL	4.7	0.52	6.5	0.86	**5.2**	**1.3**	25
PC O-34:3/P-34:2/33:3	12	nmol/mL	4.5	0.67	250	230	**4.7**	**0.88**	19
PC O-34:4/P-34:3	6	nmol/mL	0.084	0.037	0.11	0.044	**0.12**	**0.079**	66
PC P-35:1/34:2	18	nmol/mL	140	11	2,400	2,100	**240**	**47**	19
PC P-35:2/34:3	18	nmol/mL	9.1	0.90	11	1.1	**12**	**1.7**	14
PC O-35:4/34:4	9	nmol/mL	0.97	0.15	0.98	0.14	**1.0**	**0.25**	24
PC 34:5	5	nmol/mL	0.047	0.016	0.048	0.014	**0.034**	**0.0045**	13
PC 36:1	17	nmol/mL	26	1.6	29	3.6	**26**	**4.6**	17
PC O-36:0/35:0	5	nmol/mL	0.72	0.36	0.69	0.31	**0.72**	**0.53**	74

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. For PC and PE lipid classes, the isobaric species (ether-linked) were summed and the possibilities observed by the participants are separated by a "/". Abbreviations identify lysophosphatidylethanolamines (LPE) and phosphatidylcholines (PC).

Table 4. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
PC O-36:1/P-36:0/35:1	16	nmol/mL	2.7	0.55	3.3	0.64	**3.5**	**0.99**	28
PC 36:2	18	nmol/mL	100	4.9	160	18	**140**	**25**	17
PC O-36:2/P-36:1/35:2	17	nmol/mL	3.2	1.7	7.7	1.2	**7.4**	**1.7**	22
PC 36:3	17	nmol/mL	82	7.1	1,600	1,400	**100**	**14**	14
PC O-36:3/P-36:2/35:3	12	nmol/mL	4.0	0.73	4.4	0.77	**3.7**	**0.82**	22
PC 36:4	19	nmol/mL	48	27	130	18	**150**	**28**	19
PC O-36:4/P-36:3/35:4	17	nmol/mL	12	1.2	440	410	**12**	**1.4**	12
PC 36:5	16	nmol/mL	9.2	0.55	12	1.5	**11**	**1.8**	17
PC O-36:5/P-36:4/35:5	11	nmol/mL	7.9	1.6	290	270	**6.9**	**1.6**	23
PC P-36:5/35:6	5	nmol/mL	0.25	0.056	0.25	0.049	**0.30**	**0.094**	31
PC 36:6	8	nmol/mL	0.32	0.065	70	66	**0.28**	**0.088**	32
PC 38:0	6	nmol/mL	1.9	0.50	2.0	0.47	**2.0**	**0.85**	42
PC 38:1	6	nmol/mL	0.34	0.089	0.36	0.086	**0.37**	**0.17**	47
PC 38:2	15	nmol/mL	2.9	0.49	3.3	0.71	**2.3**	**0.20**	9
PC O-38:2/37:2	6	nmol/mL	0.91	0.21	0.90	0.18	**0.98**	**0.32**	32
PC 38:3	14	nmol/mL	26	0.83	26	3.3	**26**	**5.2**	20
PC O-38:3/P-38:2/37:3	14	nmol/mL	1.5	0.38	1.8	0.39	**1.5**	**0.51**	34
PC 38:4	18	nmol/mL	59	4.5	80	8.4	**84**	**14**	17
PC O-38:4/P-38:3/37:4	12	nmol/mL	5.6	1.6	8.5	1.3	**7.4**	**2.0**	27
PC 38:5	18	nmol/mL	32	4.2	410	360	**42**	**7.9**	19
PC O-38:5/P-38:4/37:5	16	nmol/mL	8.2	0.79	12	1.5	**11**	**1.6**	14
PC 38:6	18	nmol/mL	39	2.2	40	4.4	**41**	**4.4**	11
PC O-38:6/P-38:5/37:6	12	nmol/mL	3.6	0.60	120	120	**3.6**	**1.0**	29
PC P-38:6/36:0	10	nmol/mL	1.1	0.28	1.1	0.26	**1.2**	**0.39**	33
PC 38:7	8	nmol/mL	2.5	1.8	73	66	**0.79**	**0.35**	44
PC 40:2	8	nmol/mL	0.19	0.054	0.21	0.064	**0.23**	**0.10**	44
PC 40:3	7	nmol/mL	0.21	0.084	0.26	0.081	**0.27**	**0.14**	51
PC 40:4	18	nmol/mL	2.8	0.16	3.2	0.39	**2.9**	**0.37**	13
PC O-40:2/P-40:1	5	nmol/mL	0.15	0.10	14	12	**0.069**	**0.021**	30

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. For PC and PE lipid classes, the isobaric species (ether-linked) were summed and the possibilities observed by the participants are separated by a "/". Abbreviations identify phosphatidylcholines (PC).

Table 4. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
PC O-40:4/P-40:3/39:4	8	nmol/mL	1.1	0.31	1.1	0.28	**0.95**	**0.38**	40
PC 40:5	18	nmol/mL	4.3	0.50	6.9	0.82	**6.7**	**1.1**	16
PC O-40:5/P-40:4/39:5	12	nmol/mL	2.0	0.43	2.0	0.41	**1.7**	**0.45**	27
PC 40:6	17	nmol/mL	13	1.6	15	1.8	**14**	**2.6**	19
PC O-40:6/P-40:5/39:6	11	nmol/mL	4.0	2.1	81	75	**1.8**	**0.74**	42
PC 40:7	16	nmol/mL	2.8	0.59	3.8	0.55	**3.5**	**0.76**	21
PC O-40:7/P-40:6/39:7	9	nmol/mL	1.5	0.34	41	37	**1.1**	**0.23**	20
PC 40:8	14	nmol/mL	1.1	0.33	1.1	0.31	**0.73**	**0.20**	28
PC O-42:5/P-42:4	7	nmol/mL	1.1	0.23	1.1	0.21	**0.79**	**0.12**	15
PC 42:6	5	nmol/mL	0.090	0.041	0.12	0.061	**0.079**	**0.041**	52
PE 32:1	6	nmol/mL	0.33	0.092	0.33	0.085	**0.34**	**0.12**	36
PE 34:0	5	nmol/mL	1.4	0.53	1.4	0.47	**1.6**	**1.1**	65
PE 34:1	14	nmol/mL	1.2	0.17	1.1	0.13	**1.2**	**0.17**	14
PE O-34:1/P-34:0	6	nmol/mL	0.62	0.36	1.0	0.55	**0.46**	**0.22**	48
PE 34:2	16	nmol/mL	2.9	0.58	3.1	0.60	**2.2**	**0.26**	12
PE O-34:2/P-34:1	11	nmol/mL	0.72	0.15	0.72	0.13	**0.78**	**0.17**	22
PE O-34:3/P-34:2	11	nmol/mL	2.0	0.42	1.9	0.39	**1.5**	**0.41**	27
PE 36:0	11	nmol/mL	0.63	0.29	9.3	8.1	**0.28**	**0.10**	36
PE 36:1	14	nmol/mL	2.7	1.4	4.1	2.0	**1.3**	**0.26**	20
PE 36:2	16	nmol/mL	6.9	1.0	6.7	0.92	**6.7**	**0.79**	12
PE O-36:2/P-36:1/35:2	12	nmol/mL	1.1	0.25	16	14	**0.93**	**0.22**	23
PE 36:3	16	nmol/mL	2.9	0.65	2.9	0.63	**2.4**	**0.38**	16
PE O-36:3/P-36:2/35:3	15	nmol/mL	2.9	0.51	2.9	0.49	**3.2**	**0.76**	24
PE 36:4	16	nmol/mL	3.0	0.43	2.9	0.38	**3.1**	**0.39**	13
PE O-36:4/P-36:3	14	nmol/mL	2.1	0.47	2.1	0.45	**1.6**	**0.29**	18
PE 36:5	11	nmol/mL	0.27	0.071	0.27	0.067	**0.26**	**0.13**	48
PE O-36:5/P-36:4	15	nmol/mL	4.6	1.2	120	110	**4.9**	**1.9**	38
PE O-36:6/P-36:5	7	nmol/mL	0.47	0.27	0.56	0.24	**0.70**	**0.49**	70

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. For PC and PE lipid classes, the isobaric species (ether-linked) were summed and the possibilities observed by the participants are separated by a "/". The abbreviations identify phosphatidylcholines (PC) and phosphatidylethanolamines (PE).

Table 4. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
PE 38:1	7	nmol/mL	6.2	3.9	6.5	3.4	**2.6**	**1.7**	67
PE 38:2	7	nmol/mL	3.1	1.5	5.7	3.2	**1.9**	**1.2**	64
PE 38:3	14	nmol/mL	1.0	0.16	0.84	0.098	**0.95**	**0.20**	21
PE 38:4	16	nmol/mL	6.9	2.8	7.8	0.87	**8.1**	**1.2**	15
PE O-38:4/P-38:3/37:4	9	nmol/mL	1.1	0.20	1.1	0.18	**0.94**	**0.18**	19
PE 38:5	12	nmol/mL	2.5	0.34	2.4	0.32	**2.7**	**0.47**	17
PE O-38:5/P-38:4	17	nmol/mL	2.8	1.1	6.7	1.4	**5.8**	**1.9**	33
PE 38:6	15	nmol/mL	2.9	0.53	11	6.8	**3.2**	**0.59**	19
PE O-38:6/P-38:5	16	nmol/mL	2.2	0.52	5.3	1.1	**4.9**	**1.2**	25
PE O-38:7/P-38:6	8	nmol/mL	3.6	0.62	49	43	**3.5**	**0.98**	28
PE 40:4	10	nmol/mL	0.23	0.047	0.22	0.041	**0.26**	**0.082**	31
PE 40:5	12	nmol/mL	0.67	0.13	0.67	0.12	**0.73**	**0.23**	31
PE O-40:5/P-40:4/39:5	12	nmol/mL	2.4	1.2	2.4	1.1	**0.73**	**0.13**	17
PE 40:6	14	nmol/mL	1.8	0.29	1.8	0.27	**1.8**	**0.36**	20
PE O-40:6/P-40:5/39:6	14	nmol/mL	1.7	0.45	1.8	0.47	**1.3**	**0.31**	23
PE 40:7	11	nmol/mL	0.91	0.21	1.1	0.22	**0.77**	**0.26**	33
PE O-40:7/P-40:6/39:7	14	nmol/mL	2.3	0.41	2.3	0.40	**2.5**	**0.72**	29
PI 32:1	10	nmol/mL	0.45	0.041	0.45	0.037	**0.56**	**0.11**	19
PI 34:1	14	nmol/mL	2.7	0.39	2.9	0.44	**2.4**	**0.42**	17
PI 34:2	14	nmol/mL	2.7	0.14	2.7	0.17	**2.8**	**0.38**	14
PI 36:1	13	nmol/mL	2.0	0.30	2.0	0.29	**2.1**	**0.59**	28
PI 36:2	15	nmol/mL	9.3	1.3	8.5	0.90	**7.7**	**0.93**	12
PI 36:3	14	nmol/mL	2.0	0.21	1.9	0.19	**2.2**	**0.29**	14
PI 36:4	14	nmol/mL	2.6	0.25	2.6	0.24	**3.0**	**0.48**	16
PI 38:2	8	nmol/mL	0.22	0.073	0.32	0.089	**0.34**	**0.16**	47
PI 38:3	14	nmol/mL	3.0	0.36	3.0	0.34	**3.4**	**0.54**	16

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. For PC and PE lipid classes, the isobaric species (ether-linked) were summed and the possibilities observed by the participants are separated by a "/". The abbreviations identify phosphatidylethanolamines (PE) and phosphatidylinositols (PI).

Table 4. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
PI 38:4	17	nmol/mL	19	2.6	19	2.4	**19**	**2.2**	11
PI 38:5	15	nmol/mL	2.5	0.27	2.3	0.22	**2.5**	**0.44**	18
PI 38:6	10	nmol/mL	0.28	0.019	0.29	0.018	**0.32**	**0.031**	10
PI 40:4	7	nmol/mL	0.34	0.10	0.34	0.091	**0.30**	**0.042**	14
PI 40:5	8	nmol/mL	0.51	0.13	0.58	0.13	**0.63**	**0.26**	40
PI 40:6	12	nmol/mL	0.80	0.094	0.80	0.089	**0.84**	**0.16**	19
PG 34:1	5	nmol/mL	0.82	0.60	1.2	0.38	**1.3**	**0.60**	45
PG 36:1	5	nmol/mL	0.45	0.31	0.50	0.24	**0.83**	**0.61**	73
PG 36:2	6	nmol/mL	0.54	0.20	6.0	5.1	**0.67**	**0.24**	36
PS 38:4	6	nmol/mL	0.26	0.21	2.3	0.96	**2.2**	**1.6**	74

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. For PC and PE lipid classes, the isobaric species (ether-linked) were summed and the possibilities observed by the participants are separated by a "/". The abbreviations identify phosphatidylglycerols (PG), phosphatidylinositols (PI), and phosphatidylserines (PS).

Table 5. Consensus estimates and associated uncertainties for sphingolipids measured by at least five laboratories in SRM 1950

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
HexCer d34:1	6	nmol/mL	0.69	0.18	0.81	0.12	**0.86**	**0.21**	25
HexCer d36:1	5	nmol/mL	0.13	0.033	0.14	0.032	**0.13**	**0.043**	34
HexCer d40:1	5	nmol/mL	2.1	0.48	2.1	0.43	**2.4**	**0.68**	28
HexCer d42:1	6	nmol/mL	2.3	0.56	2.4	0.51	**2.7**	**0.73**	27
HexCer d42:2	6	nmol/mL	1.4	0.43	1.4	0.39	**1.1**	**0.59**	51
CER d32:1	8	nmol/mL	0.034	0.0092	0.034	0.0084	**0.051**	**0.021**	42
CER d34:0	5	nmol/mL	0.025	0.013	0.022	0.0098	**0.045**	**0.031**	70
CER d34:1	17	nmol/mL	0.38	0.11	0.40	0.11	**0.28**	**0.044**	16
CER d36:1	14	nmol/mL	0.12	0.017	0.11	0.014	**0.12**	**0.021**	17
CER d36:2	7	nmol/mL	0.012	0.0047	0.015	0.0047	**0.026**	**0.014**	56
CER d38:1	16	nmol/mL	0.42	0.27	9.4	7.5	**0.11**	**0.021**	20
CER d40:1	18	nmol/mL	0.80	0.13	0.81	0.12	**0.65**	**0.12**	18
CER d40:2	6	nmol/mL	0.13	0.029	4.7	4.2	**0.15**	**0.021**	14
CER d41:1	7	nmol/mL	0.90	0.27	1.0	0.28	**0.67**	**0.27**	40
CER d42:0	6	nmol/mL	0.32	0.19	0.56	0.36	**0.28**	**0.18**	63
CER d42:1	19	nmol/mL	3.0	0.57	2.9	0.54	**1.9**	**0.47**	24
CER d42:2	19	nmol/mL	1.0	0.19	1.0	0.17	**0.82**	**0.10**	12
CER d42:3	5	nmol/mL	0.21	0.094	4.5	3.9	**0.23**	**0.14**	62
CER d44:1	7	nmol/mL	0.069	0.020	0.071	0.018	**0.063**	**0.031**	49
CER d44:2	7	nmol/mL	0.048	0.018	0.033	0.0089	**0.044**	**0.022**	49
SM d31:1	5	nmol/mL	0.14	0.036	50	45	**0.19**	**0.049**	25
SM d32:0	9	nmol/mL	0.93	0.51	8.5	6.7	**0.47**	**0.22**	47
SM d32:1	14	nmol/mL	4.8	1.2	12	3.1	**8.4**	**1.4**	17
SM d32:2	10	nmol/mL	1.0	0.39	1.2	0.40	**0.66**	**0.24**	36
SM d33:1	14	nmol/mL	6.2	1.5	6.6	1.6	**4.7**	**0.64**	14
SM d34:0	14	nmol/mL	11	5.1	43	33	**5.8**	**1.3**	22
SM d34:1	21	nmol/mL	81	9.0	110	13	**100**	**15**	15
SM d34:2	17	nmol/mL	9.2	1.4	22	4.4	**16**	**2.2**	14
SM d35:1	9	nmol/mL	2.2	0.42	2.2	0.35	**2.5**	**0.58**	23

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. The abbreviations identify hexosylceramides (HexCer), ceramides (CER), and sphingomyelins (SM).

Table 5. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
SM d35:2	6	nmol/mL	0.34	0.090	0.44	0.099	**0.52**	**0.21**	39
SM d36:0	11	nmol/mL	1.9	0.62	2.0	0.58	**2.0**	**0.49**	24
SM d36:1	22	nmol/mL	11	1.9	19	2.4	**20**	**3.7**	18
SM d36:2	22	nmol/mL	9.3	1.2	8.8	1.0	**9.6**	**1.5**	16
SM d36:3	13	nmol/mL	1.5	0.30	1.7	0.37	**1.3**	**0.41**	31
SM d37:1	11	nmol/mL	0.99	0.20	24	22	**1.0**	**0.23**	23
SM d37:2	5	nmol/mL	0.22	0.086	0.26	0.091	**0.21**	**0.10**	50
SM d38:0	8	nmol/mL	2.3	1.3	28	17	**0.92**	**0.51**	55
SM d38:1	17	nmol/mL	6.0	0.84	14	2.4	**11**	**3.1**	27
SM d38:2	17	nmol/mL	2.0	1.4	4.2	0.63	**5.2**	**1.3**	25
SM d38:3	8	nmol/mL	0.56	0.16	0.47	0.12	**0.61**	**0.24**	39
SM d39:1	14	nmol/mL	5.2	1.2	110	100	**3.6**	**1.0**	29
SM d39:2	9	nmol/mL	0.66	0.16	1.3	0.63	**0.61**	**0.16**	26
SM d40:0	10	nmol/mL	1.4	0.59	33	26	**1.5**	**0.65**	43
SM d40:1	17	nmol/mL	7.8	6.2	34	9.0	**20**	**5.1**	25
SM d40:2	15	nmol/mL	5.0	2.5	16	3.2	**12**	**2.8**	24
SM d40:3	8	nmol/mL	1.7	0.37	1.6	0.29	**2.2**	**0.79**	37
SM d41:1	14	nmol/mL	15	4.3	300	270	**7.7**	**2.1**	27
SM d41:2	14	nmol/mL	3.8	0.95	8.0	1.6	**5.8**	**1.4**	24
SM d41:3	7	nmol/mL	0.79	0.22	66	60	**0.77**	**0.30**	39
SM d42:1	21	nmol/mL	7.3	0.94	27	5.4	**20**	**5.4**	28
SM d42:2	18	nmol/mL	29	3.9	70	13	**44**	**11**	25
SM d42:3	12	nmol/mL	11	4.0	22	4.2	**17**	**4.7**	27
SM d42:4	8	nmol/mL	1.9	0.48	3.1	0.62	**4.2**	**1.8**	42
SM d43:1	9	nmol/mL	0.66	0.22	0.68	0.23	**0.62**	**0.28**	45
SM d43:2	10	nmol/mL	1.3	0.39	1.4	0.39	**1.0**	**0.29**	29
SM d44:1	9	nmol/mL	0.15	0.064	0.42	0.20	**0.25**	**0.12**	49
SM d44:2	9	nmol/mL	0.41	0.096	11	9.7	**0.40**	**0.13**	32
SM d44:3	5	nmol/mL	0.62	0.40	4.3	3.5	**0.27**	**0.19**	71

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. The abbreviations identify hexosylceramides (HexCer), ceramides (CER), and sphingomyelins (SM).

Table 6. Consensus estimates and associated uncertainties for sterol lipids measured by at least five laboratories in SRM 1950

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
CE 14:0	7	nmol/mL	16	3.7	13	2.0	**16**	**6.0**	37
CE 15:0	6	nmol/mL	5.5	1.2	5.1	0.95	**5.3**	**1.8**	34
CE 16:0	13	nmol/mL	49	16	170	31	**210**	**58**	28
CE 16:1	11	nmol/mL	20	8.6	92	19	**100**	**27**	27
CE 16:2	5	nmol/mL	1.8	0.32	1.8	0.28	**1.9**	**0.46**	25
CE 17:0	6	nmol/mL	2.7	0.57	8.9	4.2	**6.0**	**2.5**	42
CE 17:1	9	nmol/mL	6.2	0.23	6.8	0.51	**8.2**	**1.0**	13
CE 18:0	7	nmol/mL	15	1.9	15	2.0	**15**	**3.7**	25
CE 18:1	14	nmol/mL	180	81	520	120	**450**	**110**	25
CE 18:2	14	nmol/mL	110	63	2,900	1,100	**1,700**	**430**	26
CE 18:3	13	nmol/mL	14	10	230	93	**84**	**24**	28
CE 20:1	6	nmol/mL	0.51	0.11	0.77	0.20	**1.3**	**0.66**	51
CE 20:2	9	nmol/mL	4.9	2.3	5.0	2.1	**5.8**	**3.1**	53
CE 20:3	13	nmol/mL	12	2.0	100	47	**35**	**12**	35
CE 20:4	14	nmol/mL	210	130	960	400	**350**	**58**	17
CE 20:5	12	nmol/mL	23	1.4	99	35	**38**	**8.6**	23
CE 22:4	7	nmol/mL	6.9	5.9	8.0	4.1	**1.2**	**0.70**	59
CE 22:5	6	nmol/mL	25	19	26	17	**4.1**	**1.6**	39
CE 22:6	11	nmol/mL	32	8.7	140	74	**37**	**9.5**	26
Free Cholesterol	8	nmol/mL	710	160	780	70	**770**	**110**	14
CDCA	7	nmol/mL	0.58	0.26	0.67	0.31	**0.30**	**0.11**	38
CA	9	nmol/mL	0.16	0.036	0.24	0.093	**0.12**	**0.034**	28

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. The abbreviations identify chenodeoxycholic acid (CDCA), cholic acid (CA), and cholesteryl ester (CE).

Table 6. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	VR Mean	VR Standard Uncertainty	**MEDM Location**	**MEDM Standard Uncertainty**	COD (%)
DCA	9	nmol/mL	0.51	0.11	3.3	2.7	**0.35**	**0.083**	24
GCDCA	8	nmol/mL	1.0	0.15	1.0	0.14	**1.1**	**0.18**	17
GDCA	7	nmol/mL	0.38	0.064	0.37	0.056	**0.43**	**0.069**	16
GLCA	6	nmol/mL	0.025	0.0053	0.025	0.0045	**0.025**	**0.0018**	7
GUDCA	6	nmol/mL	0.15	0.016	0.15	0.015	**0.15**	**0.024**	16
GCA	6	nmol/mL	0.28	0.064	0.28	0.060	**0.24**	**0.069**	29
LCA	8	nmol/mL	0.015	0.0029	0.69	0.64	**0.014**	**0.0036**	26
TCDCA	9	nmol/mL	0.085	0.0071	0.10	0.024	**0.084**	**0.0050**	6
TCA	9	nmol/mL	0.042	0.016	0.047	0.019	**0.026**	**0.0056**	22
TDCA	8	nmol/mL	0.048	0.0089	0.048	0.0090	**0.040**	**0.0064**	16
TLCA	5	nmol/mL	0.0023	0.00041	0.0026	0.00044	**0.0027**	**0.00069**	26
UDCA	8	nmol/mL	0.15	0.043	0.38	0.19	**0.11**	**0.024**	22

The DSL uncertainty is the Horn-Horn Duncan. The COD (%) was calculated using the MEDM location and standard uncertainty. Final MEDM locations are in bold. The abbreviations identify deoxycholic acid (DCA), glycochenodeoxycholic acid (GCDCA), glycodeoxycholic acid (GDCA), glycolithocholic acid (GLCA), glycoursodeoxycholic acid (GUDCA), glyocholic acid (GCA), lithocholic acid (LCA), taurochenodeoxycholic acid (TCDCA), taurocholic acid (TCA), taurodeoxycholic acid (TDCA), taurolithocholic acid (TLCA), ursodeoxycholic acid (UDCA).

Table 7. Consensus estimates and corresponding uncertainties for those lipids measured by three to four laboratories in SRM 1950.

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	MEDM Location	DSL COD (%)	Percent Difference (%)
Chenodeoxycholic acid-3-Sulfate	3	nmol/mL	0.013	0.051	0.14	389	165
Hyodeoxycholic acid	4	nmol/mL	0.023	0.019	0.035	84	42
Taurolithocholic acid sulfate	3	nmol/mL	0.088	0.018	0.10	21	15
α-Muricholic acid	4	nmol/mL	0.0048	0.0048	0.012	101	85
β-Muricholic acid	4	nmol/mL	0.0018	0.00082	0.0033	46	60
ω-Muricholic acid	3	nmol/mL	0.0056	0.00013	0.0057	2	1
CE 14:1	4	nmol/mL	0.93	0.26	1.2	28	22
CE 20:0	4	nmol/mL	1.4	0.21	3.1	15	79
CE 22:0	4	nmol/mL	0.35	0.034	0.36	10	2
CE 22:1	4	nmol/mL	0.41	0.21	0.52	52	23
CE 24:0	3	nmol/mL	0.28	0.052	0.31	18	7
CE 24:1	3	nmol/mL	0.15	0.014	0.15	9	1
Total Cholesterol	3	nmol/mL	4,000	24	4,000	1	0
LacCer d34:1	3	nmol/mL	2.7	0.72	2.1	26	28
HexCer d38:1	3	nmol/mL	0.20	0.00015	0.20	0	0
LacCer d42:1	3	nmol/mL	0.30	0.079	0.28	26	9
CerG3(d18:1/16:0)	3	nmol/mL	0.27	0.33	0.98	119	113
CerG3(d18:1/24:0)	3	nmol/mL	0.065	0.13	0.37	195	141
CER d16:0	3	nmol/mL	0.052	0.0075	0.056	14	9
CER d18:0	3	nmol/mL	0.031	0.012	0.042	41	31
CER d20:0	3	nmol/mL	0.028	0.0076	0.030	28	8
CER d22:0	3	nmol/mL	0.084	0.029	0.11	35	30
CER d24:0	3	nmol/mL	0.090	0.033	0.084	37	6

The final mean was calculated using the DSL estimation method (grey). The uncertainty associated with MEDM was not provided as it does not hold up when less than five laboratories are reporting. COD (%) is calculated using the DSL mean and standard uncertainty. The percent difference (%) was calculated comparing the DSL mean and MEDM location values. Abbreviations: cholesteryl ester (CE), ceramide (CER), hexosylceramide (HexCer), and lactosylceramide (LacCer).

Table 7. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	MEDM Location	DSL COD (%)	Percent Difference (%)
CER d24:1	3	nmol/mL	0.11	0.095	0.21	88	63
CER d34:2	3	nmol/mL	0.12	0.13	0.033	107	116
CER d38:2	3	nmol/mL	0.013	0.0052	0.019	39	33
CER d38:5	3	nmol/mL	0.0013	0.027	0.37	2015	199
CER d39:1	4	nmol/mL	0.093	0.016	0.11	18	15
CER d40:0	4	nmol/mL	0.12	0.062	0.17	51	34
CER d41:2	3	nmol/mL	0.099	0.042	0.14	43	35
CER d43:1	3	nmol/mL	0.12	0.048	0.16	40	30
CER d44:3	3	nmol/mL	0.32	0.27	0.22	84	38
DHC d16:0	3	nmol/mL	5.3	0.67	5.5	13	4
DHC d22:0	3	nmol/mL	0.26	0.046	0.29	18	12
DHC d24:0	3	nmol/mL	0.40	0.050	0.33	12	20
DHC d24:1	3	nmol/mL	0.97	0.14	1.1	15	13
DAG 30:1	3	nmol/mL	0.41	0.26	0.51	64	22
DAG 32:3	4	nmol/mL	0.24	0.38	0.73	154	101
DAG 34:4	4	nmol/mL	0.44	0.38	0.71	86	46
DAG 40:0	3	nmol/mL	0.53	0.32	0.56	60	5
DAG 40:1	3	nmol/mL	0.017	0.0053	0.021	32	22
DAG 40:4	4	nmol/mL	0.91	0.34	0.83	38	10
FFA 14:0	3	nmol/mL	2.1	3.4	5.1	167	85
FFA 17:0	3	nmol/mL	1.7	0.23	1.7	14	1
FFA 17:1	3	nmol/mL	0.86	0.15	0.86	18	0
FFA 20:1	3	nmol/mL	1.8	0.17	1.6	9	9
FFA 20:2	4	nmol/mL	1.00	0.34	1.3	34	23

The final mean was calculated using the DSL estimation method (grey). The uncertainty associated with MEDM was not provided as it does not hold up when less than five laboratories are reporting. COD (%) is calculated using the DSL mean and standard uncertainty. The percent difference (%) was calculated comparing the DSL mean and MEDM location values. Abbreviations: ceramide (CER), dihydroceramide (DHC), diacylglycerol (DAG), and free fatty acid (FFA).

Table 7. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	MEDM Location	DSL COD (%)	Percent Difference (%)
FFA 22:4	4	nmol/mL	1.0	0.32	1.3	32	22
FFA 24:1	3	nmol/mL	0.66	0.61	1.0	93	45
LPC 14:1	4	nmol/mL	0.0013	0.0012	0.12	92	196
LPC P-18:0	4	nmol/mL	0.37	0.14	0.68	39	60
LPC O-18:1	3	nmol/mL	0.41	0.13	0.35	31	16
LPC 19:0	4	nmol/mL	0.94	0.94	1.6	99	54
LPC 19:1	3	nmol/mL	0.023	0.014	0.037	60	46
LPC O-20:0	4	nmol/mL	0.023	0.0049	0.025	22	9
LPC O-20:1	3	nmol/mL	0.072	0.075	0.024	104	100
LPC O-22:0	3	nmol/mL	1.2	1.4	0.029	112	191
LPC 24:1	3	nmol/mL	0.022	0.0071	0.023	33	4
LPC 26:0	3	nmol/mL	0.015	0.0031	0.016	21	3
LPE 16:1	3	nmol/mL	0.15	0.21	0.77	137	133
LPE P-18:1	3	nmol/mL	0.23	0.17	0.40	73	54
LPE 18:3	3	nmol/mL	0.00034	0.0011	0.45	307	200
LPE 20:1	4	nmol/mL	0.00046	0.0089	1.4	1947	200
LPE 20:2	3	nmol/mL	2.4	2.1	4.4	87	59
LPE 20:5	3	nmol/mL	0.0084	0.080	0.54	942	194
LPE 22:0	3	nmol/mL	0.51	0.76	1.0	147	66
LPE 22:4	3	nmol/mL	2.5	1.8	1.0	73	84
LPE 22:5	3	nmol/mL	0.45	0.71	1.7	158	115
PC 26:0	3	nmol/mL	0.23	0.21	0.44	94	64
PC 28:0	4	nmol/mL	0.16	0.025	0.15	15	5
PC 40:1	3	nmol/mL	0.30	0.25	0.29	82	4

The final mean was calculated using the DSL estimation method (grey). The uncertainty associated with MEDM was not provided as it does not hold up when less than five laboratories are reporting. COD (%) is calculated using the DSL mean and standard uncertainty. The percent difference (%) was calculated comparing the DSL mean and MEDM location values. Abbreviations: free fatty acid (FFA), lysophosphatidylcholine (LPC), lysophosphatidylethanolamine (LPE), and phosphatidylcholine (PC).

Table 7. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	MEDM Location	DSL COD (%)	Percent Difference (%)
PC O-40:8/P-40:7	4	nmol/mL	0.083	0.033	0.11	40	24
PC 42:2	3	nmol/mL	0.097	0.065	0.17	66	56
PC 42:4	3	nmol/mL	0.067	0.053	0.14	79	68
PC O-42:4/P-42:3	4	nmol/mL	0.47	0.14	0.58	31	22
PC 42:5	4	nmol/mL	0.14	0.061	0.19	42	26
PC O-42:6/P-42:5	4	nmol/mL	0.46	0.14	0.55	29	18
PC O-42:7	3	nmol/mL	0.067	0.0011	0.078	2	15
PC O-44:5/P-44:4	3	nmol/mL	1.3	0.30	1.4	24	6
PC O-44:6e/P-44:5	4	nmol/mL	0.69	0.32	0.97	46	34
PE 34:3	4	nmol/mL	0.14	0.020	0.15	14	8
PE 35:1	4	nmol/mL	0.15	0.045	0.14	30	5
PE P-38:2/37:3	3	nmol/mL	0.91	0.40	1.3	44	34
PE O-40:8/P-40:7	4	nmol/mL	11	9.5	2.6	86	124
PE P-42:5	3	nmol/mL	0.30	0.13	0.55	44	60
PE P-42:6	3	nmol/mL	0.86	0.69	0.66	80	26
PG 34:2	4	nmol/mL	0.55	0.22	0.45	40	19
PG 36:3	4	nmol/mL	0.50	0.11	0.43	22	15
PG 38:4	3	nmol/mL	0.040	0.020	0.065	51	47
PG 40:6	3	nmol/mL	0.025	0.023	0.048	94	63
LPI 18:0	4	nmol/mL	0.14	0.078	0.22	56	44
LPI 18:1	3	nmol/mL	0.15	0.12	0.27	77	56
LPI 18:2	4	nmol/mL	0.17	0.083	0.28	48	45
LPI 20:4	4	nmol/mL	0.21	0.082	0.26	40	23
PI 32:0	3	nmol/mL	0.24	0.072	0.30	30	21

The final mean was calculated using the DSL estimation method (grey). The uncertainty associated with MEDM was not provided as it does not hold up when less than five laboratories are reporting. COD (%) is calculated using the DSL mean and standard uncertainty. The percent difference (%) was calculated comparing the DSL mean and MEDM location values. Abbreviations: phosphatidylcholine (PC), phosphatidylethanolamine (PE), phosphatidylglycerol (PG), lysophosphatidylinositol (LPI), and phosphatidylinositol (PI).

Table 7. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	MEDM Location	DSL COD (%)	Percent Difference (%)
PI 34:0	3	nmol/mL	0.056	0.0078	0.086	14	43
PI 36:5	4	nmol/mL	0.13	0.12	1.7	91	172
PS 36:1	4	nmol/mL	0.16	0.066	0.18	43	11
PS 36:2	4	nmol/mL	0.090	0.20	0.73	224	156
PS 36:4	3	nmol/mL	0.19	0.19	0.36	104	63
PS 38:1	3	nmol/mL	0.23	0.046	0.25	20	9
PS 38:2	3	nmol/mL	0.24	0.040	0.27	16	11
PS 40:4	3	nmol/mL	0.39	0.81	2.0	206	134
PS 40:5	3	nmol/mL	0.37	0.93	7.4	253	181
SM d30:1	4	nmol/mL	0.71	0.47	0.70	67	2
SM d33:0	4	nmol/mL	13	14	0.026	108	199
SM d33:2	3	nmol/mL	0.037	0.021	0.056	55	41
SM d34:3	3	nmol/mL	0.14	0.041	0.18	30	27
SM d35:0	3	nmol/mL	0.044	0.0072	0.050	16	13
SM d36:4	3	nmol/mL	0.60	0.43	1.0	71	51
SM d38:4	3	nmol/mL	0.16	0.11	0.25	68	44
SM d40:4	4	nmol/mL	0.15	0.068	0.26	44	53
SM d42:5	3	nmol/mL	0.36	0.021	0.37	6	4
SM d43:3	4	nmol/mL	0.18	0.010	1.4	6	153
dhSph-1P	3	nmol/mL	0.10	0.035	0.10	35	4
Sph-1P	3	nmol/mL	0.42	0.0076	0.41	2	2
TAG 38:0	3	nmol/mL	0.25	0.20	0.14	81	53
TAG 40:0	4	nmol/mL	0.33	0.11	0.44	33	31
TAG 40:1	3	nmol/mL	0.15	0.12	0.83	75	137

The final mean was calculated using the DSL estimation method (grey). The uncertainty associated with MEDM was not provided as it does not hold up when less than five laboratories are reporting. COD (%) is calculated using the DSL mean and standard uncertainty. The percent difference (%) was calculated comparing the DSL mean and MEDM location values. Abbreviations: phosphatidylinositol (PI), phosphatidylserine (PS), sphingomyelin (SM), and triacylglycerol (TAG).

Table 7. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	MEDM Location	DSL COD (%)	Percent Difference (%)
TAG 40:2	3	nmol/mL	0.058	0.025	0.085	43	39
TAG 44:3	4	nmol/mL	0.18	0.0094	0.18	5	1
TAG 45:0	3	nmol/mL	1.6	1.5	0.54	91	99
TAG 46:4	3	nmol/mL	0.27	0.20	0.50	73	61
TAG 46:5	3	nmol/mL	0.044	0.098	1.1	222	184
TAG 47:0	3	nmol/mL	0.43	0.10	0.53	23	22
TAG 47:1	4	nmol/mL	0.47	0.17	0.59	36	24
TAG 47:2	3	nmol/mL	0.21	0.027	0.22	13	7
TAG 47:3	3	nmol/mL	0.078	0.035	0.10	44	29
TAG 48:5	3	nmol/mL	1.1	0.92	2.1	85	64
TAG 48:6	3	nmol/mL	0.029	0.056	1.3	193	191
TAG 48:7	3	nmol/mL	0.018	0.093	0.53	510	187
TAG 49:0	3	nmol/mL	0.31	0.055	0.29	18	5
TAG 49:3	4	nmol/mL	0.43	0.20	0.36	45	18
TAG 50:6	4	nmol/mL	0.24	0.059	0.30	24	22
TAG 50:7	3	nmol/mL	0.077	0.088	0.51	115	148
TAG 51:0	4	nmol/mL	0.42	0.19	0.35	45	18
TAG 51:5	3	nmol/mL	0.55	0.28	0.52	51	5
TAG 53:0	3	nmol/mL	0.053	0.039	0.39	74	152
TAG 53:1	3	nmol/mL	0.73	0.49	0.44	67	50
TAG 54:8	4	nmol/mL	0.92	0.30	0.90	32	2
TAG 55:3	3	nmol/mL	0.43	0.15	0.35	34	20
TAG 55:4	3	nmol/mL	0.32	0.029	0.42	9	28
TAG 55:6	3	nmol/mL	0.17	0.073	0.39	44	78

The final mean was calculated using the DSL estimation method (grey). The uncertainty associated with MEDM was not provided as it does not hold up when less than five laboratories are reporting. COD (%) is calculated using the DSL mean and standard uncertainty. The percent difference (%) was calculated comparing the DSL mean and MEDM location values. Abbreviations: triacylglycerol (TAG).

Table 7. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	MEDM Location	DSL COD (%)	Percent Difference (%)
TAG 56:1	4	nmol/mL	0.68	0.28	0.83	42	20
TAG 57:6	3	nmol/mL	0.034	0.023	0.056	66	48
TAG 57:7	3	nmol/mL	0.049	0.026	0.069	54	35
TAG 58:10	4	nmol/mL	0.92	0.56	0.55	61	51
TAG 58:11	3	nmol/mL	0.11	0.018	0.13	16	13
TAG 58:2	3	nmol/mL	0.53	0.21	0.66	39	22
TAG 58:3	3	nmol/mL	0.19	0.019	0.21	10	8
TAG 60:10	3	nmol/mL	0.26	0.088	0.20	34	24
TAG 60:11	4	nmol/mL	0.42	0.37	0.13	89	107
TAG 60:12	3	nmol/mL	0.34	0.37	0.082	109	123

The final mean was calculated using the DSL estimation method (grey). The uncertainty associated with MEDM was not provided as it does not hold up when less than five laboratories are reporting. COD (%) is calculated using the DSL mean and standard uncertainty. The percent difference (%) was calculated comparing the DSL mean and MEDM location values. Abbreviations: triacylglycerols (TAG).

Table 8. Consensus estimates and associated uncertainties for eicosanoids measured by three to four laboratories in SRM 1950

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	MEDM Location	DSL COD (%)	Percent Difference (%)
11,12-DiHETrE	3	pmol/mL	0.82	0.28	1.0	34	20
11-HDoHE	3	pmol/mL	0.63	0.092	0.61	15	3
11-HEPE	3	pmol/mL	0.22	0.14	0.38	63	54
11-HETE	4	pmol/mL	2.1	1.0	1.5	49	32
12,13-DiHOME	3	pmol/mL	5.1	0.38	5.0	7	3
12,13-EpOME	3	pmol/mL	6.9	2.0	7.8	28	12
12-HEPE	4	pmol/mL	2.1	1.2	0.98	59	71
12-HHTrE	3	pmol/mL	0.23	0.053	0.27	23	18
13-HODE	3	pmol/mL	21	9.5	13	46	47
13-HOTrE	3	pmol/mL	0.54	0.056	0.56	10	4
14,15-DiHETrE	3	pmol/mL	1.6	0.75	1.1	47	37
14-HDoHE	4	pmol/mL	1.3	0.11	1.3	8	2
15-HEPE	4	pmol/mL	0.28	0.16	0.42	57	39
17-HDoHE	3	pmol/mL	0.82	0.036	0.84	4	2
18-HEPE	3	pmol/mL	0.28	0.069	0.25	25	10
19,20-DiHDoPE (19,20-DiHDPA)	3	pmol/mL	0.96	0.15	1.6	16	50
20-HETE	3	pmol/mL	2.1	0.53	2.0	25	7
4-HDoHE	4	pmol/mL	2.5	0.40	3.9	16	43
5,15-DiHETE	4	pmol/mL	0.16	0.045	0.25	28	43
5,6-DiHETrE	3	pmol/mL	1.2	0.34	1.5	30	26
5,6-EET	3	pmol/mL	0.82	0.28	1.0	34	20
5-HEPE	4	pmol/mL	0.85	0.016	0.86	2	2
5-HETrE	3	pmol/mL	0.99	0.27	1.2	27	21

The final mean was calculated using the DSL estimation method (grey). The uncertainty associated with MEDM was not provided as it does not hold up when less than five laboratories are reporting. COD (%) is calculated using the DSL mean and standard uncertainty. The percent difference (%) was calculated comparing the DSL mean and MEDM location values. For nomenclature of eicosanoids, see the LIPID MAPS Structure Database Fatty Acyls [FA] (W) --> Eicosanoids [FA03] (http://www.lipidmaps.org/data/structure/LMSDSearch.php).

Table 8. (cont…)

Lipid	# of Labs	Units	DSL Mean	DSL Standard Uncertainty	MEDM Location	DSL COD (%)	Percent Difference (%)
5-oxoETE (5-KETE)	3	pmol/mL	0.37	0.13	0.48	34	25
8,9-DiHETrE	3	pmol/mL	0.51	0.22	0.65	43	25
8-HDoHE	3	pmol/mL	4.3	3.7	1.0	87	124
8-HEPE	4	pmol/mL	0.30	0.24	0.89	80	100
8-HETE	4	pmol/mL	0.98	0.22	1.1	22	15
8-HETrE	3	pmol/mL	0.38	0.093	0.46	24	19
9,10-EpOME	3	pmol/mL	7.5	3.3	4.2	45	56
9,10-DiHOME	3	pmol/mL	6.7	0.44	7.0	7	5
9-HEPE	4	pmol/mL	0.43	0.087	0.50	20	15
9-HETE	4	pmol/mL	0.85	0.082	0.85	10	0
9-HODE	3	pmol/mL	10	2.6	9.7	25	5
9-HOTrE	3	pmol/mL	0.62	0.18	0.80	28	25
9-OxoODE (9-KODE)	3	pmol/mL	7.3	1.3	6.8	18	7
LTB4	3	pmol/mL	0.019	0.0069	0.030	37	47
PGD2	4	pmol/mL	0.082	0.048	0.17	58	71
PGE2	4	pmol/mL	0.035	0.014	0.040	40	14

The final mean was calculated using the DSL estimation method (grey). The uncertainty associated with MEDM was not provided as it does not hold up when less than five laboratories are reporting. COD (%) is calculated using the DSL mean and standard uncertainty. The percent difference %) was calculated comparing the DSL mean and MEDM location values. For nomenclature of eicosanoids, see the LIPID MAPS Structure Database Fatty Acyls [FA] (W) --> Eicosanoids [FA03] (http://www.lipidmaps.org/data/structure/LMSDSearch.php).

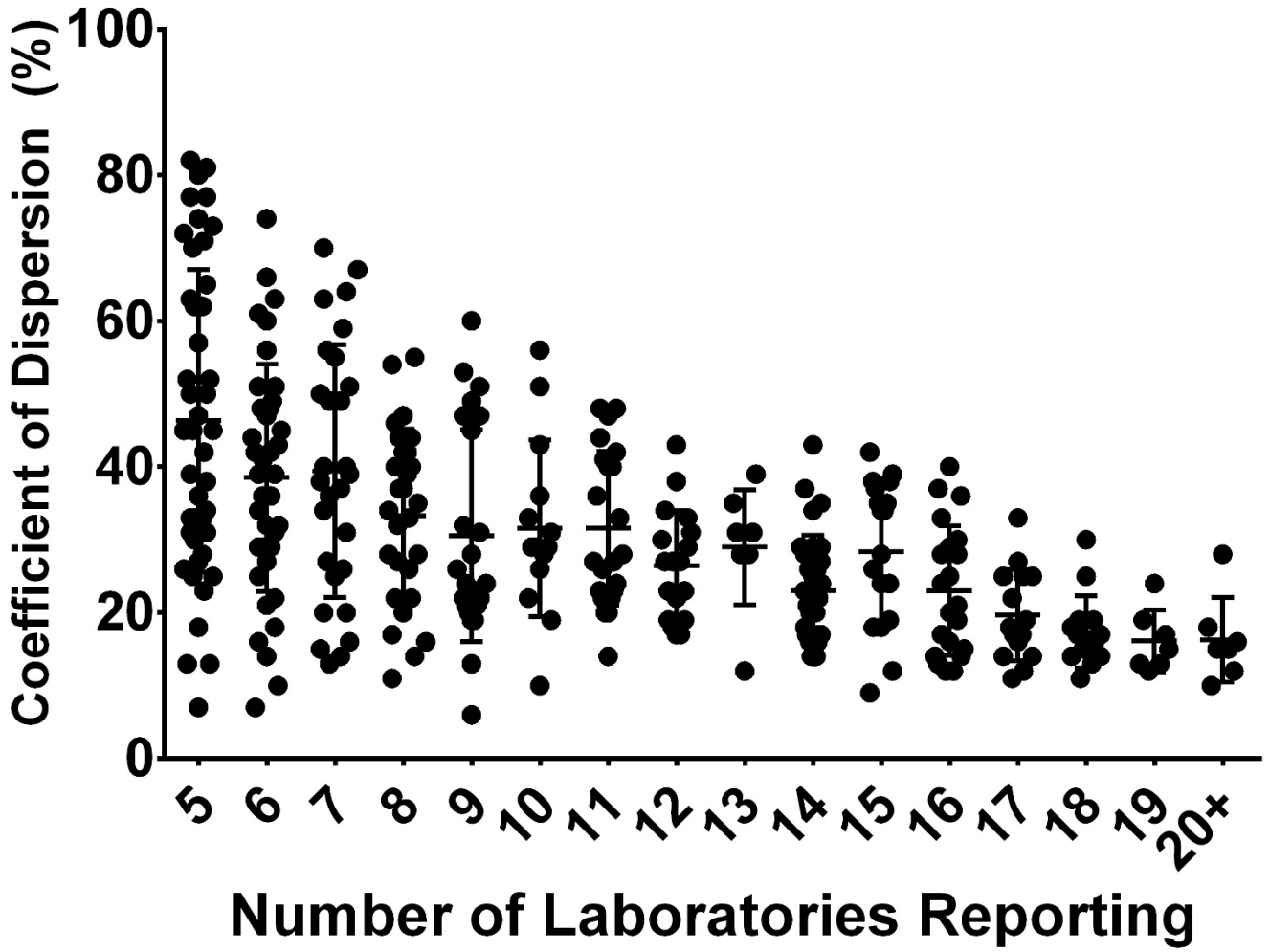


Figure 1. Coefficient of dispersion (COD, %) values plotted against the number of laboratories reporting for each lipid (n = 339, $n \geq 5$ laboratories reporting) measured in SRM 1950. The COD for each lipid was calculated using the MEDM location and standard uncertainty.

Appendix A

Upon agreement to participate in the interlaboratory comparison exercise, this Excel template was provided to each participating laboratory for data submission. The template included tabs for laboratories to provide details on the laboratory and methodological information including sample preparation, sample introduction and/or chromatography, mass spectrometric methods, and data processing software. Additional tabs were provided containing potential target lipid species (see Table S7 for all 320 target lipids). An example is shown for cholesteryl esters (CE, Table S6). On these target lipid tabs, we required the exact mass of lipid identified and the corresponding adduct used for scanning.

Table S1. Data submission template for basic laboratory information

Please fill out what you can	
Date(s) of Analyses	
Main Principal Investigator (PI):	
PI Affiliation:	
Type of affiliation (academia, industry, core lab, etc.):	
Interest in publication? (y/n)	
If yes, who would be listed as a co-author?	provide names as you want them to appear
If yes, who would be listed as an acknowledgement?	provide names as you want them to appear
Do you use quality controls materials for your lipidomics measurements? (y/n)	
Do you think Standard Reference Materials (SRMs) are needed for lipidomics? (y/n)	
If so, what matrices would you find most valuable?	
Would you be interested in participating in a follow-up interlab exercise? (y/n)	

Table S2. Data submission template for sample preparation

Please fill out what you can		
How much material did you use for extraction?		
What type of extraction did you perform (BD, Folch, MTBE, etc.)?		
Extraction protocol:		
What did you reconstitute extract in?		
How long from sample thaw to the samples run on instrument?		
How do you prepare internal standard solutions? (gravimetrically)?		Amt Spiked in?
What internal standards did you employ (for each class)?		
* Fatty acids (FFA)		
* Triacylglycerols (TAG)		
* Diacylglycerols (DAG)		
* Cholesterol (CHOL)		
* Cholesteryl esters (CE)		
* Phosphatidylcholines (PC)		
* Lysophosphatidylcholines (LPC)		
* Phosphatidylethanolamines (PE)		
* Lysophosphatidylethanolamines (LPE)		
* Phosphatidylserines (PS)		
* Phosphatidylinositols (PI)		
* Phosphatidic acids (PA)		
* Sphingomyelins (SM)		
* Ceramides (CER)		
* Other		

Table S3. Data submission template for sample introduction/chromatography

Please fill out what you can	
If shotgun	
Type of instrument:	
Manual, Flow-Injection, Nanomate, etc.	
Shotgun settings:	
Injection amount:	
Which lipids monitored with approach:	
If LC	
Type of LC system:	
Column information:	
Solvent composition/gradient:	
Other LC settings:	
Injection amount:	
Which lipids monitored with approach:	
If GC….	

Table S4. Data submission template for mass spectrometric parameters

Please fill out what you can					
Mass spec instrument:					
	MS or MS/MS	Type of Scan	Scan Fragment	# of Scans	MS or MS/MS Parameters… such as CE, CAD, IS, Temp, etc.
* Fatty acids (FFA)					
* Triacylglycerols (TAG)					
* Diacylglycerols (DAG)					
* Cholesterol (CHOL)					
* Cholesteryl esters (CE)					
* Phosphatidylcholines (PC)					
* Lysophosphatidylcholines (LPC)					
* Phosphatidylethanolamines (PE)					
* Lysophosphatidylethanolamines (LPE)					
* Phosphatidylserines (PS)					
* Phosphatidylinositols (PI)					
* Phosphatidic acids (PA)					
* Sphingomyelins (SM)					
* Ceramides (CER)					
* Other					

Table S5. Data submission template for data processing information

Please fill out what you can	
Software employed:	
Correction factors employed:	
Response factors employed:	
Other processing details:	

Table S6. Example of a data submission tab for cholesteryl esters (CE), which includes potential targets species, *m/z* value used for identification, lipid adduct employed, and triplicate concentrations reported in nmol/mL

Type of adduct: $[M+H]^+$, $[M+Na]^+$, $[M+NH_4]^+$, $[M+Li]^+$, $[M-H]^-$, etc…:				
		in nmol/1 mL plasma		
		Rep 1	Rep 2	Rep 3
Lipid Species	*m/z* value	SRM 1950	SRM 1950	SRM 1950
14:1				
14:0				
15:1				
15:0				
16:1				
16:0				
17:1				
17:0				
18:3				
18:2				
18:1				
18:0				
20:5				
20:4				
20:3				
20:2				
20:1				
20:0				
22:6				
22:4				
22:2				
22:1				
22:0				

Cholesteryl esters are listed in total carbons of fatty acyl chains by total number of double bonds in fatty acyl chains (C:DB).

Table S7. Target lipid species (by class, *n* = 320) provided in the data submission template

CE	FFA	TAG	DAG	PC	PC	LPC	PE	PE	LPE	PS	PA	PG	PI	CER	SM	SM
14:1	12:0	48:2	30:2	30:1	38:1	14:1	32:1	O-40:6	16:0	32:1	32:1	34:2	32:1	14:0	31:0	41:3
14:0	14:1	48:1	30:1	32:2	38:0	14:0	P-34:2	40:6	18:2	34:2	32:0	34:1	34:2	16:0	32:2	41:2
15:1	14:0	50:4	30:0	32:1	40:8	16:1	34:2	O-40:5	18:1	34:1	34:2	36:5	34:1	17:0	32:1	41:1
15:0	15:0	50:3	32:3	32:0	40:7	P-16:0	P-34:1	40:5	18:0	34:0	34:1	36:4	34:0	18:1	32:0	42:4
16:1	16:1	50:2	32:2	34:3	40:6	O-16:0	34:1	40:4	20:4	36:4	34:0	36:3	36:5	18:0	33:1	42:3
16:0	16:0	50:1	32:1	O-34:2	40:5	16:0	34:0	40:1	22:1	36:3	36:4	36:2	36:4	20:0	33:0	42:2
17:1	17:1	50:0	32:0	34:2	40:4	18:3	O-36:5/P-36:4	42:7	22:6	36:2	36:3	36:1	36:3	22:0	34:2	42:1
17:0	17:0	52:5	34:4	O-34:1	40:3	18:2	36:5	P-42:6		36:1	36:2	38:6	36:2	24:1	34:1	43:3
18:3	18:3	52:4	34:3	34:1	40:2	18:1	O-36:4/P-36:3	42:6		36:0	36:1	38:5	36:1	24:0	34:0	43:2
18:2	18:2	52:3	34:2	34:0		O-18:0	36:4	P-42:5		38:6	36:0	38:4	36:0	26:2	35:1	43:1
18:1	18:1	52:2	34:1	36:5		18:0	O-36:3/P-36:2	42:5		38:5	38:6	40:9	38:6	26:1	35:0	44:3
18:0	18:0	52:1	34:0	O-36:4/P-36:3		20:5	36:3	42:1		38:4	38:5	40:8	38:5	26:0	36:3	44:2
20:5	20:5	52:0	36:5	36:4		20:4	O-36:2/P-36:1			38:3	38:4	40:7	38:4		36:2	44:1
20:4	20:4	54:6	36:4	36:3		20:3	36:2			38:2	38:3	40:6	38:3		36:1	
20:3	20:3	54:5	36:3	O-36:2/P-36:1		20:1	36:1			38:1	38:2	40:5	38:2		36:0	
20:2	20:2	54:4	36:2	36:2		22:6	36:0			40:7		40:4	40:6		37:1	
20:1	20:1	54:3	36:1	O-36:1/P-36:0		22:5	O-38:6/P-38:5			40:6			40:5		38:3	
20:0	20:0	54:2	36:0	36:1		22:4	38:6			40:5			40:4		38:2	
22:6	22:6	54:1	38:5	36:0			O-38:5/P-38:4			40:4			40:2		38:1	
22:4	22:5	54:0	38:4	38:6			38:5			40:3					38:0	
22:2	22:4	56:6	38:3	O-38:5/P-38:4			38:4								39:2	
22:1	22:3	56:5	38:2	38:5			38:3								39:1	
22:0	22:1	56:4	38:1	38:4			38:2								40:3	
	22:0		38:0	O-38:3/P-38:2			38:1								40:2	
CHOL	24:1		40:7	38:2			O-40:7								40:1	
	24:0		40:6				40:7								40:0	
	26:0		40:5													
			40:4													

The list was partially derived from the lipids detected in the LIPID MAPS consortium analysis of SRM 1950 (6).

Appendix B: Lipid Breakdown

The total number of lipids reported in SRM 1950 (n = 1527) measured by at least one laboratory at the sum composition level. The 1527 lipids were measured across five lipid categories, as shown in Table S8. Lipid class abbreviations are also provided. Individual lipids reported for each lipid category are shown in Tables S9 to S13, for lipid categories FA, GL, GP, SP, and ST, respectively.

Table S8: Total number of lipids detected in SRM 1950 organized by lipid category and class

Lipid Group	Lipid Class	Abbreviation	# of Lipid Species (Sum Composition)
Fatty acyls (FA)	free fatty acids	FFA	27
	eicosanoids		141
	(o-acyl)-1-hydroxy fatty acid	OAHFA	9
Glycerolipids (GL)	monoacylglycerol	MAG	27
	diacylglycerol	DAG	75
	triacylglycerol	TAG	214
	monogalactosyldiacylglycerol	MGDG	1
Glycerophospholipids (GP)	bis(monoacylglycero)phosphate	BMP	1
	cardiolipin	CL	2
	lysophosphatidic acid	LPA	6
	phosphatidic acid	PA	17
	lysophosphatidylcholine	LPC	84
	phosphatidylcholine	PC	219
	lysophosphatidylethanolamine	LPE	35
	phosphatidylethanolamine	PE	99
	lysophosphatidylglycerol	LPG	5
	phosphatidylglycerol	PG	19
	lysophosphatidylinositol	LPI	11
	phosphatidylinositol	PI	43
	phosphatidylinositol monophosphate	PIP	1
	lysophosphatidylserine	LPS	2
	phosphatidylserine	PS	22
	dimethylphosphatidylethanolamine	dMePE	75
	lysodimethylphosphatidylethanolamine	LdMePE	19
	cyclic phosphatidic acid	cPA	3
	phosphatidylethanol	Pet	14
	phosphatidylmethanol	PMe	2
Sphingolipids (SP)	ceramide	Cer	57
	ceramide-1-phosphate	CerP	1
	dihydroceramide	CerOH	10
	glucosylceramide	GlcCer	1
	hexosylceramide	HexCer	13
	dihexosylceramide	Hex2Cer	6
	trihexosylceramide	Hex3Cer	6
	lactosylceramide	LacCer	13
	GM1 ganglioside	GM1Cer	6
	GM2 ganglioside	GM2Cer	4
	GM3 ganglioside	GM3Cer	6
	acylceramide	1-O-Cer/2-O-Cer	8
	sphingomyelin	SM	91
	sphingosine/sphinganine	SPH/dhSPH	2
	lysosphingomyelin	LSM	1
	sphingosine-1-phosphate	S1P	3
	sphinganine-1-phosphate	dhS1P	1
	phytosphingosine	phSM	5
	psychosine	HexSph	1
	lactosyl sphingosine	LacSph	1
Sterol lipids (ST)	cholesteryl ester	CE	38
	free cholesterol/cholesterol derivatives	FC/CHOL	3
	zymosteryl	ZyE	4
	bile acids and derivatives	BA	73

Table S9. Individual fatty acyl lipid species measured by at least one laboratory in SRM 1950

FA 12:0	15d-D12,14-PGJ3	9,10-DiHOME
FA 14:0	15-HEDE	9,12,13-TriHOME
FA 14:1	15-HEPE	9-HEPE
FA 15:0	15-HETE	9-HETE
FA 16:0	15-HETrE	9-HODE
FA 16:1	15-keto PGE2	9-HOTrE
FA 17:0	15-OxoEDE (15-KEDE)	9-OxoOTrE (9-KOTrE)
FA 17:1	15-OxoETE (15-KETE)	9-OxoODE (9-KODE)
FA 18:0	16,17-EpDPE	Bicyclo PGE2
FA 18:1	16-HDoHE	D12-PGJ2
FA 18:2	16-HETE	D17-PGE1
FA 18:3	17,18-DiHETE	Dihomo PGF2a
FA 18:4	17,18-EpETE	EKODE
FA 20:0	17-HDoHE	iPF2a-IV
FA 20:1	17-HETE	LTB4
FA 20:2	18-HEPE	LTC4
FA 20:3	18-HETE	LTD4
FA 20:4	19,20-EpDPE	LTE4
FA 20:5	19(R)-hydroxy PGE1	LXA4
FA 22:0	19(R)-OH PGF2a	LXA5
FA 22:1	19,20-DiHDoPE (19,20-DiHDPA)	LXB4
FA 22:2	19-HETE	PD1
FA 22:4	2,3 dinor 11b PGF2a	PGA2
FA 22:5	20-COOH AA	PGB2
FA 22:6	20-COOH LTB4	PGD2
FA 24:0	20-HDoHE	PGD3
FA 24:1	20-HETE	PGE1
10-HDoHE	20-OH LTB4	PGE2
10S,17S-DiHDoHE	4,17-DiHDoHE	PGE3
11-HEDE	4-HDoHE	PGF1a
11,12-DiHET (DHET)	4S,14S-diHDHA	PGF2a
11,12-DiHETrE	5,15-DiHETE	PGJ2
11,12-EET	5,6 DiHET (DHET)	RvD1
11,12-EpETrE	5,6-DiHETE	RvD5
11b PGE2	5,6-DiHETE(EPA)	RvD6
11-HDoHE	5,6-DiHETrE	RvE2
11-HEPE	5,6-EET	RvE3
11-HETE	5,6-EpETrE	tetranor 12-HETE
12,13-DiHOME	5-HEPE	tetranor-PGEM
12,13-EpODE	5-HETE	TXB1
12,13-EpOME	5-HETrE	TXB2
12epi LTB4	5-iso PGF2a VI	TXB3
12-HEPE	5-oxoETE (5-KETE)	OAHFA 34:0
12-HETE	5S,12S-diHETE	OAHFA 36:0

12-HHTrE	6-keto-PGF1a	OAHFA 38:2
12-OxoETE (12-KETE)	6-trans-12-epi-LTB4	OAHFA 38:4
12-OxoLTB4	7,8-EpDPE	OAHFA 38:6
13,14-EpDPE	7(S)-Maresin1	OAHFA 41:6
13,14dh-15k-PGD2	7-HDoHE	OAHFA 42:10
13,14dh-15k-PGE2	8,15-DiHETE	OAHFA 42:8
13,14dh-15k-PGF2α	8,9 DiHET (DHET)	OAHFA 43:7
13-HDoHE	8,9-DiHETrE	
13-HODE	8,9-EET	
13-HOTrE	8,9-EpETE	
13-HOTrE(gamma)	8,9-EpETrE	
13-OxoODE (13-KODE)	8-HDoHE	
14,15-EET	8-HEPE	
14,15-DiHET (DHET)	8-HETE	
14,15-DiHETE	8-HETrE	
14,15-DiHETrE	8-iso-PGF2a (8-iso PGF2a III)	
14,15-EpETrE	8-isoPGE2	
14-HDoHE	9,10-EpOME	
15d-D12,14-PGJ2	9,10,13-TriHOME	

Table S10. Individual glycerolipid species measured by at least one laboratory in SRM 1950

MAG 12:0	TAG 33:2	TAG 52:5
MAG 14:0	TAG 33:3	TAG 52:6
MAG 16:1	TAG 34:0	TAG 52:7
MAG 16:0	TAG 34:1	TAG 52:8
MAG 18:4	TAG 35:0	TAG 53:0
MAG 18:3	TAG 35:3	TAG 53:1
MAG 18:2	TAG 35:4	TAG 53:2
MAG 18:1	TAG 36:0	TAG 53:3
MAG 18:0	TAG 36:2	TAG 53:4
MAG 20:5	TAG 36:3	TAG 53:5
MAG 20:4	TAG 37:0	TAG 53:6
MAG 20:3	TAG 37:1	TAG 53:7
MAG 20:2	TAG 38:0	TAG 53:8
MAG 20:1	TAG 38:1	TAG 54:0
MAG 20:0	TAG 38:2	TAG 54:1
MAG 21:2	TAG 38:3	TAG 54:2
MAG 22:6	TAG 39:0	TAG 54:3
MAG 22:5	TAG 39:1	TAG 54:4
MAG 22:4	TAG 39:2	TAG 54:5
MAG 22:3	TAG 40:0	TAG 54:6
MAG 22:2	TAG 40:1	TAG 54:7
MAG 22:1	TAG 40:2	TAG 54:8
MAG 22:0	TAG 40:3	TAG 54:9
MAG 24:1	TAG 40:4	TAG 55:0
MAG 24:0	TAG 41:0	TAG 55:1
MAG 26:0	TAG 41:1	TAG 55:2
MAG 27:4	TAG 41:2	TAG 55:3
DAG 20:0	TAG 41:3	TAG 55:4
DAG 22:0	TAG 42:0	TAG 55:5
DAG 23:0	TAG 42:1	TAG 55:6
DAG 24:1	TAG 42:2	TAG 55:7
DAG 25:1	TAG 42:3	TAG 55:8
DAG 26:2	TAG 42:4	TAG 55:9
DAG 28:0	TAG 42:5	TAG 56:0
DAG 29:1	TAG 42:6	TAG 56:1
DAG 29:2	TAG 43:0	TAG 56:10
DAG 29:3	TAG 43:1	TAG 56:11
DAG 29:5	TAG 43:2	TAG 56:2
DAG 30:0	TAG 43:3	TAG 56:3
DAG 30:1	TAG 43:4	TAG 56:4
DAG 30:2	TAG 44:0	TAG 56:5
DAG 30:5	TAG 44:1	TAG 56:6
DAG 30:6	TAG 44:2	TAG 56:7
DAG 31:0	TAG 44:3	TAG 56:8

DAG 31:1
DAG 31:2
DAG 32:0
DAG 32:1
DAG 32:2
DAG 32:3
DAG 33:0
DAG 33:1
DAG 33:2
DAG 33:3
DAG 33:4
DAG 33:5
DAG 34:0
DAG 34:1
DAG 34:2
DAG 34:3
DAG 34:4
DAG 35:0
DAG 35:1
DAG 35:2
DAG 35:3
DAG 36:0
DAG 36:1
DAG 36:2
DAG 36:3
DAG 36:4
DAG 36:5
DAG 37:0
DAG 37:2
DAG 38:0
DAG 38:1
DAG 38:2
DAG 38:3
DAG 38:4
DAG 38:5
DAG 38:6
DAG 38:7
DAG 39:0
DAG 40:0
DAG 40:1
DAG 40:2
DAG 40:3
DAG 40:4
DAG 40:5
DAG 40:6

TAG 44:4
TAG 44:5
TAG 44:6
TAG 45:0
TAG 45:1
TAG 45:2
TAG 45:3
TAG 45:4
TAG 45:5
TAG 45:6
TAG 46:0
TAG 46:1
TAG 46:2
TAG 46:3
TAG 46:4
TAG 46:5
TAG 46:6
TAG 47:0
TAG 47:1
TAG 47:2
TAG 47:3
TAG 47:4
TAG 47:5
TAG 47:6
TAG 48:0
TAG 48:1
TAG 48:2
TAG 48:3
TAG 48:4
TAG 48:5
TAG 48:6
TAG 48:7
TAG 49:0
TAG 49:1
TAG 49:2
TAG 49:3
TAG 49:4
TAG 49:5
TAG 49:6
TAG 49:7
TAG 50:0
TAG 50:1
TAG 50:2
TAG 50:3
TAG 50:4

TAG 56:9
TAG 57:1
TAG 57:2
TAG 57:3
TAG 57:4
TAG 57:5
TAG 57:6
TAG 57:7
TAG 57:8
TAG 57:9
TAG 58:0
TAG 58:1
TAG 58:10
TAG 58:11
TAG 58:12
TAG 58:13
TAG 58:2
TAG 58:3
TAG 58:4
TAG 58:5
TAG 58:6
TAG 58:7
TAG 58:8
TAG 58:9
TAG 59:1
TAG 59:2
TAG 59:5
TAG 59:9
TAG 60:0
TAG 60:1
TAG 60:10
TAG 60:11
TAG 60:12
TAG 60:13
TAG 60:14
TAG 60:15
TAG 60:2
TAG 60:3
TAG 60:4
TAG 60:5
TAG 60:7
TAG 60:8
TAG 60:9
TAG 62:1
TAG 62:12

DAG 40:7	TAG 50:5	TAG 62:13
DAG 40:8	TAG 50:6	TAG 62:14
DAG 41:0	TAG 50:7	TAG 62:16
DAG 42:0	TAG 50:8	TAG 62:2
DAG 42:1	TAG 51:0	TAG 62:3
DAG 42:2	TAG 51:1	TAG 62:5
DAG 42:5	TAG 51:2	TAG 62:9
DAG 42:6	TAG 51:3	TAG O-48:0
DAG 42:7	TAG 51:4	TAG O-50:0
DAG 48:6	TAG 51:5	TAG O-50:1
DAG 54:6	TAG 51:6	TAG O-50:2
DAG 56:6	TAG 51:7	TAG O-52:1
DAG 56:7	TAG 52:0	TAG O-52:2
TAG 24:0	TAG 52:1	TAG P-52:1
TAG 28:0	TAG 52:2	TAG P-52:2
TAG 32:2	TAG 52:3	MGDG 36:4
TAG 33:1	TAG 52:4	

Table S11. Individual glycerophospholipid species measured by at least one laboratory in SRM 1950

LPC 12:0	PC O-42:0	PG 36:5
LPC 13:0	PC O-42:1	PG 37:0
LPC 14:0	PC O-16:0	PG 37:2
LPC 14:1	PC O-21:1	PG 38:4
LPC 15:0	PC O-23:0	PG 38:5
LPC 15:1	PC O-31:0	PG 38:6
LPC 15:2	PC O-32:4	PG 40:4
LPC 16:0	PC O-33:0	PG 40:6
LPC 16:1	PC O-34:5	PG 40:7
LPC 16:2	PC O-34:6	PG 43:7
LPC 17:0	PC O-36:6	PG 46:0
LPC 17:1	PC O-38:0	PG 50:10
LPC 17:2	PC O-38:1	LPI 16:0
LPC 17:3	PC O-38:7	LPI 16:1
LPC 17:4	PC O-39:4	LPI 18:0
LPC 18:0	PC O-39:5	LPI 18:1
LPC 18:1	PC O-39:6	LPI 18:2
LPC 18:2	PC O-40:1	LPI 20:3
LPC 18:3	PC O-40:3	LPI 20:4
LPC 18:4	PC O-41:1	LPI 20:5
LPC 19:0	PC O-41:6	LPI 22:4
LPC 19:1	PC O-42:2	LPI 22:5
LPC 19:2	PC O-42:3	LPI 22:6
LPC 19:3	PC O-42:7	PI 32:0
LPC 19:4	PC O-43:4	PI 32:1
LPC 19:5	PC O-43:6	PI 32:2
LPC 20:0	PC O-44:4	PI 33:1
LPC 20:1	PC O-44:7	PI 33:2
LPC 20:2	PC 18:0	PI 34:0
LPC 20:3	PC 23:0	PI 34:1
LPC 20:4	PC 27:1	PI 34:2
LPC 20:5	PC 29:1	PI 34:3
LPC 21:3	PC O-30:1/P-30:0	PI 35:1
LPC 21:5	PC O-30:2/P-30:1	PI 35:2
LPC 22:0	PC P-30:3	PI 36:0
LPC 22:1	PC P-31:0	PI 36:1
LPC 22:2	PC P-31:3	PI 36:2
LPC 22:3	PC P-32:2	PI 36:3
LPC 22:4	PC P-32:4	PI 36:4
LPC 22:5	PC P-33:0	PI 36:5
LPC 22:6	PC P-33:2	PI 37:1
LPC 23:0	PC O-34:4/P-34:3	PI 37:2
LPC 23:1	PC P-34:4	PI 37:4
LPC 24:0	PC P-35:6	PI 38:1

LPC 24:1
LPC 24:2
LPC 24:3
LPC 24:4
LPC 24:5
LPC 24:6
LPC 26:0
LPC 26:1
LPC 26:2
LPC 26:4
LPC 28:0
LPC 33:5
LPC 35:4
LPC 35:5
LPC 36:2
LPC 37:4
LPC 37:5
LPC 37:6
LPC 38:4
LPC 38:5
LPC O-14:0
LPC O-16:0
LPC O-16:1
LPC O-18:0
LPC O-18:1
LPC O-18:2
LPC O-20:0
LPC O-20:1
LPC O-22:0
LPC O-22:1
LPC O-24:0
LPC O-24:1
LPC O-24:2
LPC P-16:0
LPC P-16:1
LPC P-18:0
LPC P-18:1
LPC P-18:2
LPC P-20:0
LPC P-20:1
PC 16:0
PC 17:0
PC 18:0
PC 18:1
PC 20:0
PC P-36:6
PC P-36:7
PC P-37:2
PC P-37:4
PC P-37:6
PC P-38:7
PC P-39:2
PC P-39:6
PC O-40:2/P-40:1
PC P-40:2
PC O-40:8/P-40:7
PC P-42:2
PC O-42:4/P-42:3
PC O-42:5/P-42:4
PC O-42:6/P-42:5
PC P-42:6
PC P-42:7
PC P-42:9
PC P-44:2
PC P-44:3
PC O-44:5/P-44:4
PC O-44:6/P-44:5
PC P-44:7
LPA 16:0
LPA 18:0
LPA 18:1
LPA 18:2
LPA 20:4
LPA 22:6
PA 32:1
PA 32:0
PA 34:0
PA 34:1
PA 34:2
PA 36:0
PA 36:1
PA 36:2
PA 36:3
PA 36:4
PA 38:2
PA 38:3
PA 38:4
PA 38:5
PA 38:6
PA P-40:4
PI 38:2
PI 38:3
PI 38:4
PI 38:5
PI 38:6
PI 39:4
PI 40:3
PI 40:4
PI 40:5
PI 40:6
PI 40:7
PI 40:8
PI 42:10
PI 42:11
PI 42:9
PI O-36:2
PI O-36:4
PI O-38:4
PI O-38:5
PI O-38:6
PI P-38:4
PI P-40:6
LPS 18:0
LPS 18:1
PS 32:1
PS 34:0
PS 34:1
PS 34:2
PS 36:0
PS 36:1
PS 36:2
PS 36:3
PS 36:4
PS 38:1
PS 38:2
PS 38:3
PS 38:4
PS 38:5
PS 38:6
PS 40:3
PS 40:4
PS 40:5
PS 40:6
PS 40:7
PS P-36:3

PC 20:2
PC 22:0
PC 22:2
PC 22:3
PC 23:0
PC 24:0
PC 26:0
PC 26:1
PC 26:3
PC 27:0
PC 28:0
PC 28:1
PC 28:2
PC 28:3
PC 29:1
PC 30:0
PC O-30:0/29:0
PC 30:1
PC 30:2
PC 30:3
PC 30:4
PC 32:0
PC O-32:0/31:0
PC 32:1
PC O-32:1/P-32:0/31:1
PC O-32:2/P-32:1/31:2
PC 32:3
PC 32:4
PC 32:5
PC P-33:1/32:2
PC 33:4
PC 34:0
PC O-34:0/33:0
PC 34:1
PC O-34:1/P-34:0/33:1
PC O-34:2/P-34:1/33:2
PC O-34:3/P-34:2/33:3
PC 34:5
PC 34:6
PC P-35:1/34:2
PC P-35:2/34:3
PC O-35:4/34:4
PC 35:7
PC O-36:0/35:0
PC 36:1

PA 48:7
LPE 12:0
LPE 14:0
LPE 16:0
LPE 16:1
LPE 17:0
LPE 18:0
LPE 18:1
LPE 18:2
LPE 18:3
LPE 19:0
LPE 19:1
LPE 20:0
LPE 20:1
LPE 20:2
LPE 20:3
LPE 20:4
LPE 20:5
LPE 22:0
LPE 22:1
LPE 22:2
LPE 22:3
LPE 22:4
LPE 22:5
LPE 22:6
LPE 24:0
LPE 34:1
LPE O-16:0
LPE O-16:1
LPE O-20:1
LPE P-16:0
LPE P-16:1
LPE P-18:0
LPE P-18:1
LPE P-20:0
LPE P-20:1
PE 19:2
PE 21:2
PE 32:0
PE 32:1
PE 34:0
PE 34:1
PE 34:2
PE 34:3
PE 35:1

PS P-38:4
BMP 18:1/18:1
PIP O-34:4
CL 66:3
CL 72:8
dMePE 24:0
dMePE 30:0
dMePE 32:1
dMePE 32:2
dMePE 33:2
dMePE 34:0
dMePE 34:1
dMePE 34:2
dMePE 34:3
dMePE 34:5
dMePE 35:1
dMePE 35:2
dMePE 35:3
dMePE 36:1
dMePE 36:2
dMePE 36:3
dMePE 36:4
dMePE 36:5
dMePE 36:6
dMePE 37:5
dMePE 37:6
dMePE 37:7
dMePE 38:3
dMePE 38:4
dMePE 38:5
dMePE 38:6
dMePE 38:7
dMePE 38:8
dMePE 40:4
dMePE 43:6
dMePE 44:11
dMePE 48:1
dMePE 48:2
dMePE 48:3
dMePE 50:2
dMePE 50:3
dMePE 50:4
dMePE 50:5
dMePE 50:6
dMePE 51:5

PC O-36:1/P-36:0/35:1
PC 36:2
PC O-36:2/P-36:1/35:2
PC 36:3
PC O-36:3/P-36:2/35:3
PC 36:4
PC O-36:4/P-36:3/35:4
PC 36:5
PC O-36:5/P-36:4/35:5
PC P-36:5/35:6
PC 36:6
PC 36:7
PC 37:1
PC 37:7
PC 37:8
PC 37:9
PC 38:0
PC 38:1
PC 38:2
PC O-38:2/37:2
PC 38:3
PC O-38:3/P-38:2/37:3
PC 38:4
PC O-38:4/P-38:3/37:4
PC 38:5
PC O-38:5/P-38:4/37:5
PC 38:6
PC O-38:6/P-38:5/37:6
PC P-38:6/36:0
PC 38:7
PC 38:8
PC 38:9
PC 39:10
PC 39:2
PC 39:3
PC 40:0
PC 40:1
PC 40:10
PC 40:2
PC 40:3
PC 40:4
PC O-40:4/P-40:3/39:4
PC 40:5
PC O-40:5/P-40:4/39:5
PC 40:6

PE 36:0
PE 36:1
PE 36:2
PE O-36:2/P-36:1/35:2
PE 36:3
PE O-36:3/P-36:2/35:3
PE 36:4
PE 36:5
PE 37:1
PE 37:2
PE 37:5
PE 37:6
PE 38:1
PE 38:2
PE P-38:2/37:3
PE 38:3
PE 38:4
PE O-38:4/P-38:3/37:4
PE 38:5
PE 38:6
PE 38:7
PE 39:1
PE 39:3
PE 39:4
PE 40:1
PE 40:2
PE 40:3
PE 40:4
PE 40:5
PE O-40:5/P-40:4/39:5
PE 40:6
PE O-40:6/P-40:5/39:6
PE 40:7
PE O-40:7/P-40:6/39:7
PE 40:8
PE 41:4
PE 42:1
PE 42:5
PE 42:6
PE 42:7
PE 43:5
PE 43:6
PE 44:5
PE 45:8
PE 46:13

dMePE 52:2
dMePE 52:3
dMePE 52:4
dMePE 52:5
dMePE 52:6
dMePE 52:7
dMePE 52:8
dMePE 53:5
dMePE 53:6
dMePE 54:3
dMePE 54:5
dMePE 54:6
dMePE 54:7
dMePE 54:8
dMePE 54:9
dMePE 56:10
dMePE 56:11
dMePE 56:5
dMePE 56:6
dMePE 56:7
dMePE 56:8
dMePE 56:9
dMePE 58:10
dMePE 58:6
dMePE 58:9
dMePE O-32:0
dMePE O-36:4
dMePE P-34:0
dMePE P-34:2
dMePE P-38:1
dMePE P-38:2
dMePE P-38:4
dMePE P-40:4
dMePE P-40:5
dMePE P-40:8
LdMePE 14:0
LdMePE 15:0
LdMePE 16:0
LdMePE 16:1
LdMePE 17:0
LdMePE 17:1
LdMePE 18:0
LdMePE 18:1
LdMePE 18:2
LdMePE 18:3

PC O-40:6/P-40:5/39:6
PC 40:7
PC O-40:7/P-40:6/39:7
PC 40:8
PC 40:9
PC 41:4
PC 41:5
PC 41:6
PC 41:7
PC 41:8
PC 41:9
PC 42:0
PC 42:1
PC 42:10
PC 42:11
PC 42:12
PC 42:2
PC 42:3
PC 42:4
PC 42:5
PC 42:6
PC 42:7
PC 42:8
PC 42:9
PC 43:10
PC 43:4
PC 43:9
PC 44:1
PC 44:11
PC 44:12
PC 44:2
PC 44:4
PC 44:5
PC 44:6
PC 45:11
PC 45:13
PC 46:4
PC 46:5
PC 46:6
PC 46:7
PC 49:3
PC 49:4
PC 51:3
PC 52:8
PC 53:13

PE 47:12
PE 47:9
PE 54:2
PE O-16:0
PE O-17:0
PE O-18:0
PE O-20:0
PE O-22:0
PE O-34:0
PE O-36:1
PE O-38:1
PE P-16:0
PE P-18:0
PE P-20:0
PE P-32:0
PE P-32:1
PE O-34:1/P-34:0
PE O-34:2/P-34:1
PE O-34:3/P-34:2
PE P-34:3
PE P-34:4
PE P-35:1
PE P-35:2
PE P-36:0
PE O-36:4/P-36:3
PE O-36:5/P-36:4
PE O-36:6/P-36:5
PE P-37:1
PE P-37:2
PE P-37:4
PE P-38:1
PE O-38:5/P-38:4
PE O-38:6/P-38:5
PE O-38:7/P-38:6
PE P-39:3
PE O-40:2/P-40:1
PE P-40:2
PE O-40:4/P-40:3
PE P-40:7
PE O-40:8
PE P-40:8
PE P-42:4
PE P-42:5
PE P-42:6
PE P-42:7

LdMePE 20:0
LdMePE 20:1
LdMePE 20:2
LdMePE 20:3
LdMePE 20:4
LdMePE 20:5
LdMePE 22:4
LdMePE 22:5
LdMePE 22:6
cPA 16:0
cPA 18:0
cPA 18:1
PEt 33:0
PEt 37:0
PEt 37:2
PEt 41:6
PEt 43:5
PEt 43:6
PEt 43:8
PEt 44:4
PEt 44:6
PEt 45:7
PEt 46:8
PEt 52:9
PEt O-34:6
PEt P-40:4
PMe 38:0
PMe 47:7

PC 53:5	LPG 16:0
PC 53:7	LPG 18:0
PC 54:12	LPG 18:1
PC 54:4	LPG 18:2
PC 55:6	LPG 20:0
PC 55:8	PG 33:0
PC 56:5	PG 34:1
PC 60:8	PG 34:2
PC 61:9	PG 36:1
PC 62:10	PG 36:2
PC 62:8	PG 36:3
PC 62:9	PG 36:4

For PC and PE lipid classes, the isobaric species (ether-linked) were summed and the possibilities observed by the participants are separated by a “/”.

Table S12. Individual sphingolipid species measured by at least one laboratory in SRM 1950

Cer d14:0	HexCer d40:2	SM d36:1
Cer d16:0	HexCer d42:1	SM d36:2
Cer d18:0	HexCer d42:2	SM d36:3
Cer d18:1	HexCer d44:1	SM d36:4
Cer d20:0	HexCer d44:2	SM d36:5
Cer d20:1	Hex2Cer d34:1	SM d36:6
Cer d22:0	Hex2Cer d36:1	SM d37:1
Cer d22:1	Hex2Cer d38:1	SM d37:2
Cer d24:0	Hex2Cer d40:1	SM d37:4
Cer d24:1	Hex2Cer d42:1	SM d37:5
Cer d26:0	Hex2Cer d42:2	SM d38:0
Cer d26:1	LacCer d30:1	SM d38:1
Cer d28:1	LacCer d32:1	SM d38:2
Cer d30:1	LacCer d34:1	SM d38:3
Cer d32:1	LacCer d36:1	SM d38:4
Cer d32:2	LacCer d36:2	SM d38:5
Cer d33:0	LacCer d38:1	SM d38:7
Cer d33:1	LacCer d38:2	SM d39:0
Cer d34:0	LacCer d40:1	SM d39:1
Cer d34:1	LacCer d40:2	SM d39:2
Cer d34:2	LacCer d42:1	SM d39:3
Cer d35:0	LacCer d42:2	SM d40:0
Cer d35:1	LacCer d44:1	SM d40:1
Cer d35:2	LacCer d44:2	SM d40:2
Cer d36:0	Hex3Cer d34:1	SM d40:3
Cer d36:1	Hex3Cer d36:1	SM d40:4
Cer d36:2	Hex3Cer d38:1	SM d40:5
Cer d36:3	Hex3Cer d40:1	SM d40:7
Cer d36:7	Hex3Cer d42:1	SM d41:1
Cer d37:1	Hex3Cer d42:2	SM d41:2
Cer d38:0	GM1-Cer d41:1	SM d41:3
Cer d38:1	GM1-Cer d34:1	SM d41:4
Cer d38:2	GM1-Cer d40:1	SM d42:0
Cer d38:4	GM1-Cer d42:1	SM d42:1
Cer d38:5	GM1-Cer d42:2	SM d42:2
Cer d39:0	GM1-Cer d42:2	SM d42:3
Cer d39:1	GM2-Cer d34:1	SM d42:4
Cer d40:0	GM2-Cer d42:1	SM d42:5
Cer d40:1	GM2-Cer d42:2	SM d42:6
Cer d40:2	GM2-Cer d34:2	SM d42:7
Cer d40:4	GM3-Cer d34:1	SM d43:1
Cer d41:0	GM3-Cerd 36:1	SM d43:2
Cer d41:1	GM3-Cer d38:1	SM d43:3
Cer d41:2	GM3-Cer d40:1	SM d43:4

Cer d42:0	GM3-Cer d42:1	SM d43:5
Cer d42:1	GM3-Cer d42:2	SM d44:0
Cer d42:2	HexSph (Psychosine)	SM d44:1
Cer d42:3	LacSph	SM d44:2
Cer d42:4	SM d26:1	SM d44:3
Cer d43:1	SM d27:1	SM d44:4
Cer d43:2	SM d28:0	SM d44:5
Cer d44:0	SM d28:1	SM d44:6
Cer d44:1	SM d28:2	SM d45:1
Cer d44:2	SM d29:1	SM d45:4
Cer d44:3	SM d30:0	phSM d20:1
Cer d44:4	SM d30:1	phSM d36:1
Cer d44:5	SM d30:2	phSM d36:4
CerP d34:1	SM d30:4	phSM d36:5
Cer 1-O-d32:1	SM d31:0	phSM d43:0
Cer 1-O-d34:2	SM d31:1	lysoSM d18:1
Cer 1-O-d34:1	SM d31:2	dhSph
Cer 2-O-d34:0	SM d32:0	dhS1P
Cer 1-O-d40:0	SM d32:1	Sph
Cer 1-O-d42:0	SM d32:2	S1P
Cer 2-O-d42:0	SM d32:3	S1P d16:1
Cer 1-O-d44:0	SM d32:4	S1P d18:2
Cer d34:0-OH	SM d32:5	
Cer d36:0-OH	SM d33:0	
Cer d36:1-OH	SM d33:1	
Cer d38:0-OH	SM d33:2	
Cer d38:1-OH	SM d33:3	
Cer d40:0-OH	SM d33:4	
Cer d40:1-OH	SM d34:0	
Cer d42:0-OH	SM d34:1	
Cer d42:1-OH	SM d34:2	
Cer d44:0-OH	SM d34:3	
GlcCer d44:1	SM d34:4	
HexCer d30:1	SM d34:5	
HexCer d32:1	SM d35:0	
HexCer d34:1	SM d35:1	
HexCer d36:1	SM d35:2	
HexCer d36:2	SM d35:3	
HexCer d38:1	SM d35:4	
HexCer d38:2	SM d35:5	
HexCer d40:1	SM d36:0	

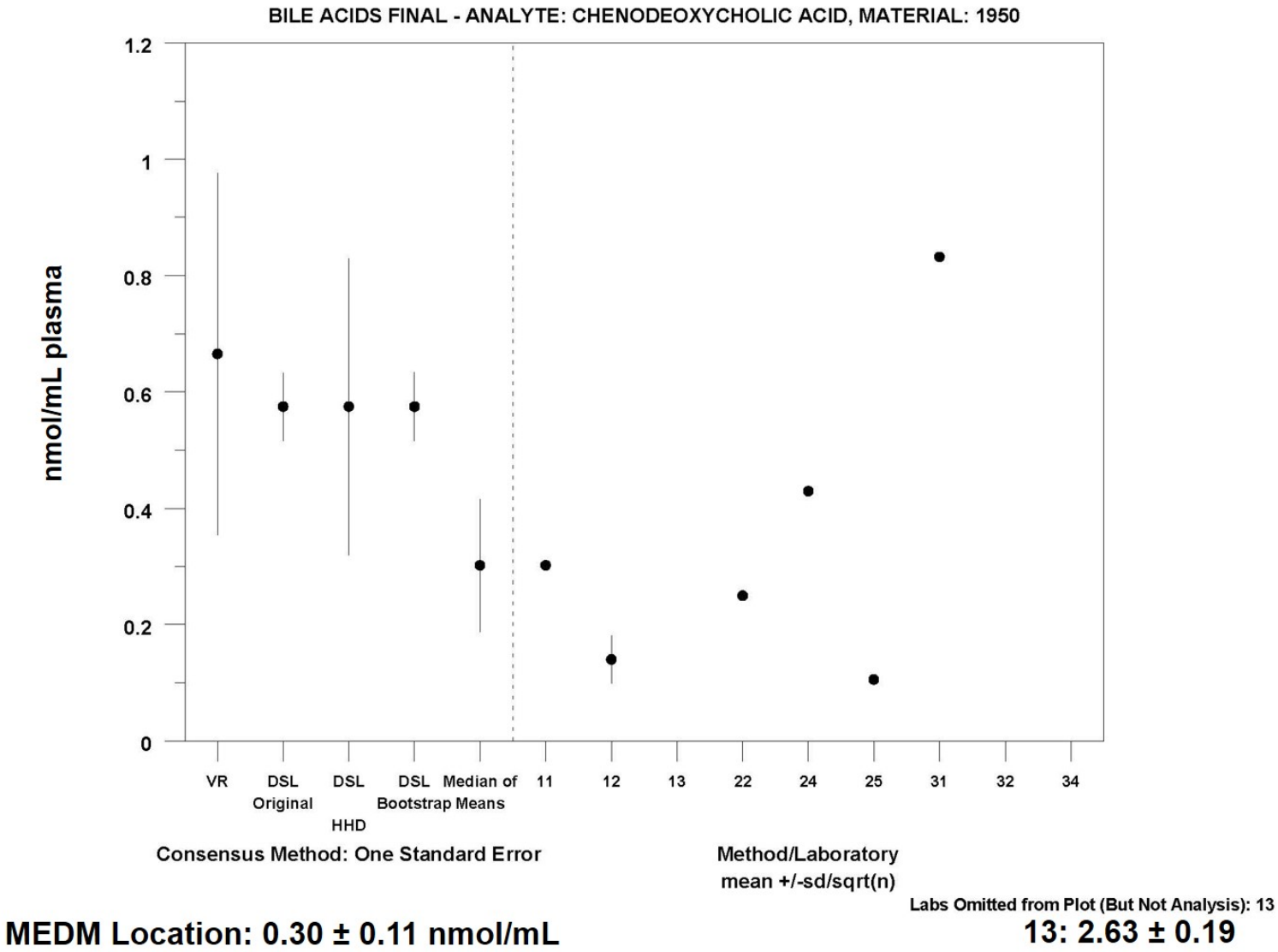
Table S13. Individual sterol lipid species measured by at least one laboratory in SRM 1950

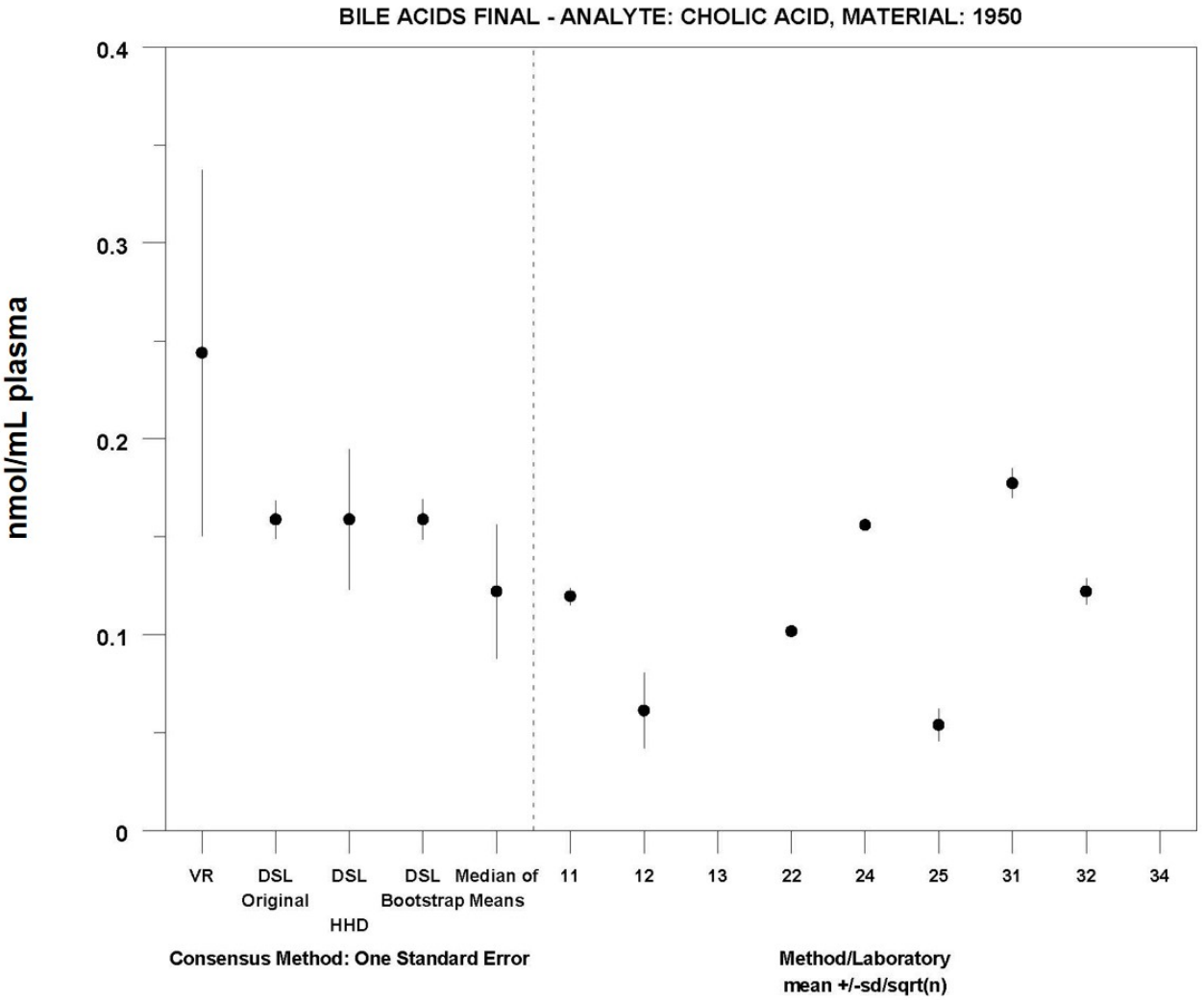
CE 14:0	Thyroxine	Hyocholic acid
CE 14:1	12-Ketochenodeoxycholic acid	Hyodeoxycholic acid
CE 15:0	12-Ketolithocholic acid	isoDeoxycholic acid
CE 15:1	3-Oxocholic acid	isoLithocholic acid
CE 16:0	3α,6α,7α,12α-Tetetrahydroxyl bile acid	Lithocholic acid
CE 16:1	3α,6β,7α,12α-Tetrahydroxyl bile acid	Lithocholic acid-Sulfate (3)
CE 16:2	6,7-Diketolithocholic acid	Murideoxycholic acid
CE 17:0	7-Ketodeoxycholic acid	Murocholic acid
CE 17:1	7-Ketolithocholic acid	Norcholic acid
CE 17:2	7-oxo-Lithocholic acid	Nordeoxycholic acid
CE 17:3	Allocholic acid	Tauro-3α,6α,7α,12α-tetrahydroxyl bile acid
CE 18:0	Alloisolithocholic acid	Tauroallocholic acid
CE 18:1	Chenodeoxycholic acid	Taurochenodeoxycholic acid
CE 18:2	Chenodeoxycholic acid-3-Sulfate	Taurochenodeoxycholic acid-Sulfate
CE 18:3	Cholic acid	Taurocholic acid
CE 19:1	Cholic acid-3-Sulfate	Taurodeoxycholic acid
CE 19:2	Dehydrocholic acid	Taurodeoxycholic acid-Sulfate
CE 19:3	Dehydrolithocholic acid	Taurohyodeoxyocholic acid
CE 20:0	Deoxycholic acid	Taurolithocholic acid
CE 20:1	Deoxycholic acid-3-Sulfate	Taurolithocholic acid sulfate
CE 20:2	Dioxolithocholic acid	Tauromuricholic acid (a+b)
CE 20:3	Glycoallocholic acid	Tauroursodeoxycholic acid
CE 20:4	Glycochenodeoxycholic acid-Sulfate	Tauroursodeoxycholic acid-3-sulfate
CE 20:5	Glycochenodeoxycholic acid	Tauro-α-muricholic acid
CE 21:5	Glycocholic acid	Tauro-β-muricholic acid
CE 22:0	Glycocholic acid-3-sulfate	Tauro-ω-muricholic acid
CE 22:1	Glycodeoxycholic acid	Total of Tauroursodexycholic acid/Taurohyocholic acid
CE 22:2	Glycodeoxycholic acid-Sulfate	Ursocholic acid
CE 22:3	Glycohyocholic acid	Ursodeoxycholic acid
CE 22:4	Glycohyodeoxycholic acid	Ursodeoxycholic acid-3-Sulfate
CE 22:5	Glycolithocholic acid	α-Muricholic acid
CE 22:6	Glycolithocholic acid sulfate	β-Muricholic acid
CE 24:0	Glycomuricholic acid	λ-muricholic acid
CE 24:1	Glycoursocholic acid	ω-Muricholic acid
CE 24:4	Glycoursodeoxycholic acid	ZyE 18:2
CE 24:5	Glycoursodeoxycholic acid-Sulfate	ZyE 18:3
CE 24:6	Glyco-α-muriholic acid	ZyE 20:4
CE 26:0	Glyco-β-muricholic acid	ZyE 23:0
cholesterol	Glyco-ω-muricholic acid	
total cholesterol	Glyocholic acid	

Appendix C: MEDM Location Plots

Plots were created for all lipids measured by at least five laboratories (n = 339). On each plot, every laboratory submission for each lipid species is displayed (calculated mean and standard deviation of the mean in nmol/mL from a triplicate measurement). To enhance visual inspection, the plots were truncated at the y-axis in the presence of extreme outliers (outlying values and laboratory reported on bottom right of the plot). On the left of each plot, calculated consensus estimates using the DSL, VR, or MEDM methods are shown with standard uncertainties. For a few lipids, the VR mean was truncated to improve visualization. The uncertainty values for laboratory 8 are not standard deviation, rather standard error of the mean. If no point is present on the plot for a listed laboratory ID number, this indicates that the laboratory did not report a concentration for that lipid.

The final determined MEDM location is provided at the bottom left of each figure with standard uncertainty. A star (★) on a plot indicates that the uncertainty of this data point is not shown. For plasmanyl lipid species, lipids are identified in the plots using "e" (same as "O-"), while plasmenyl lipids are identified in the plots using a lowercase "p" (same as "P-").

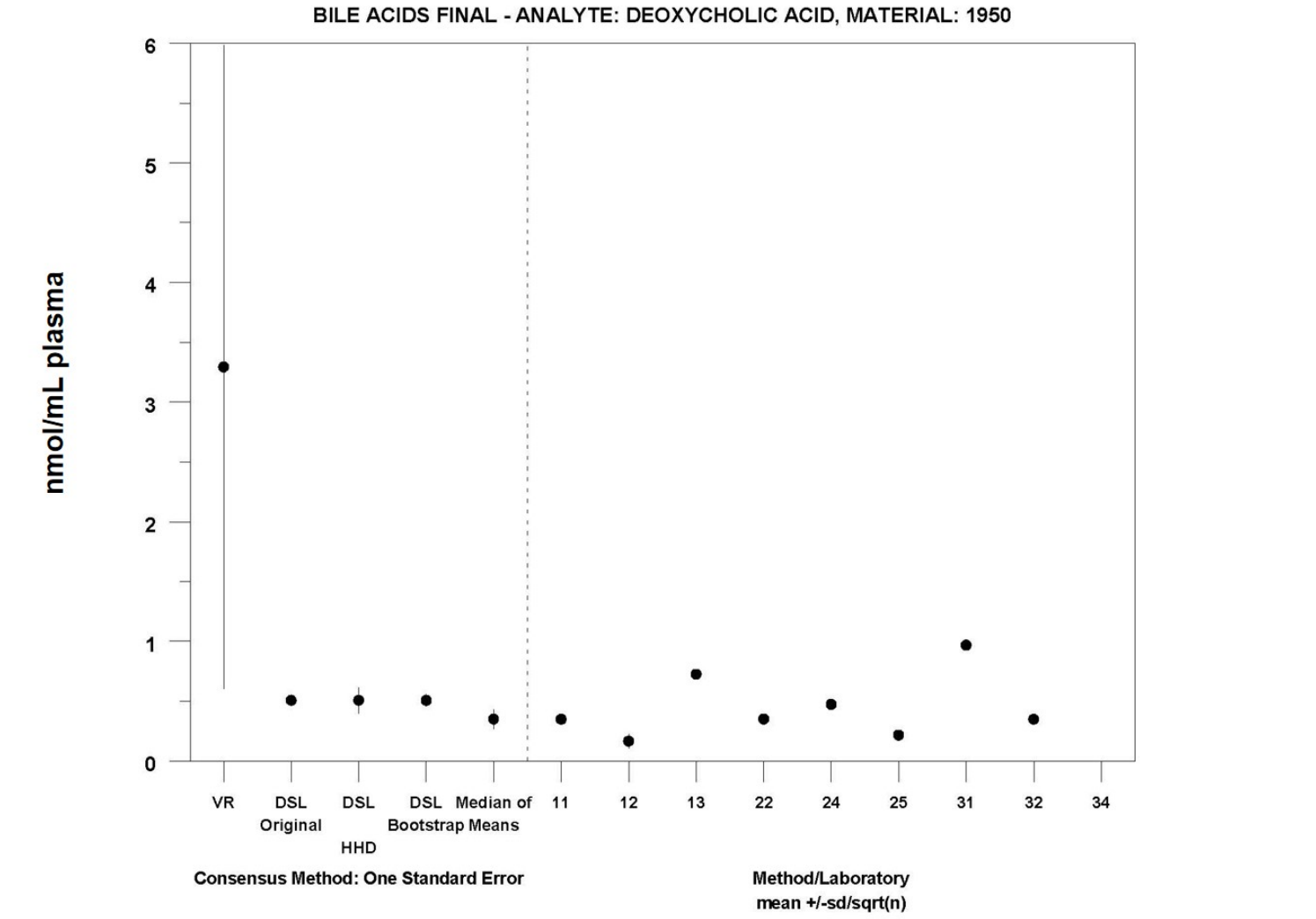




Labs Omitted from Plot (But Not Analysis): 13 34

MEDM Location: 0.12 ± 0.034 nmol/mL

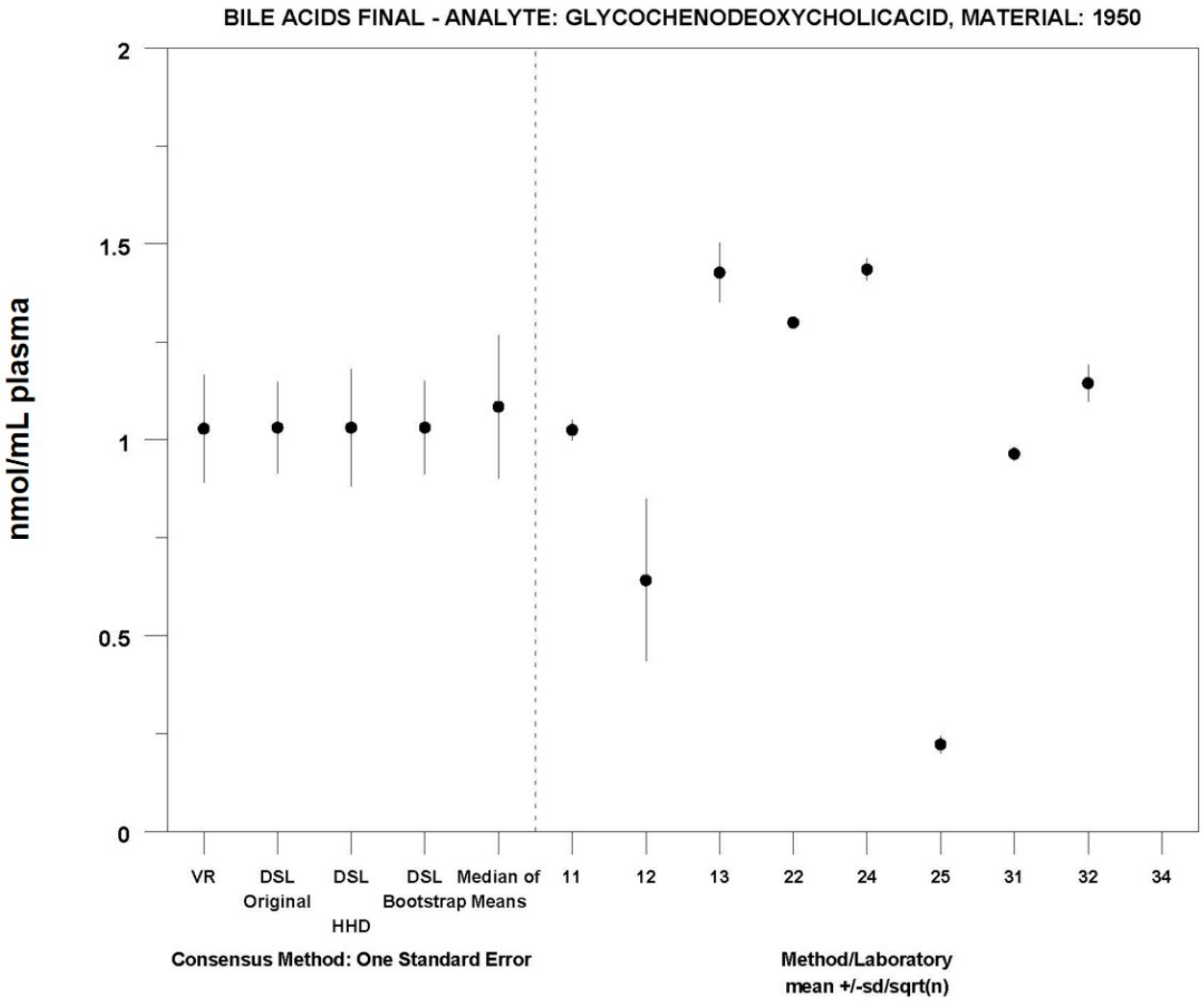
13: 0.44 ± 0.03; 34: 1.04 ± 0.13



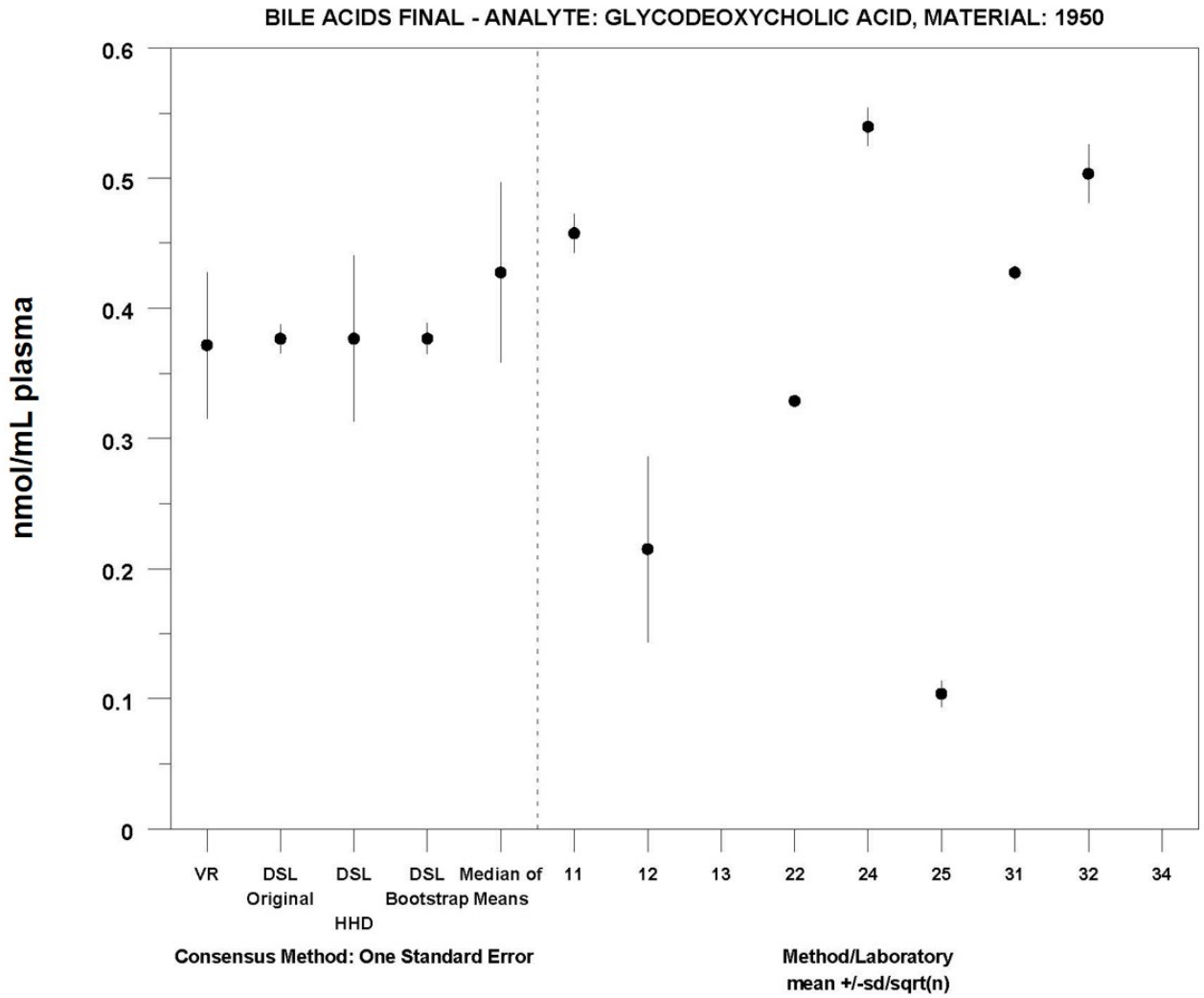
MEDM Location: 0.35 ± 0.083 nmol/mL

Labs Omitted from Plot (But Not Analysis): 34

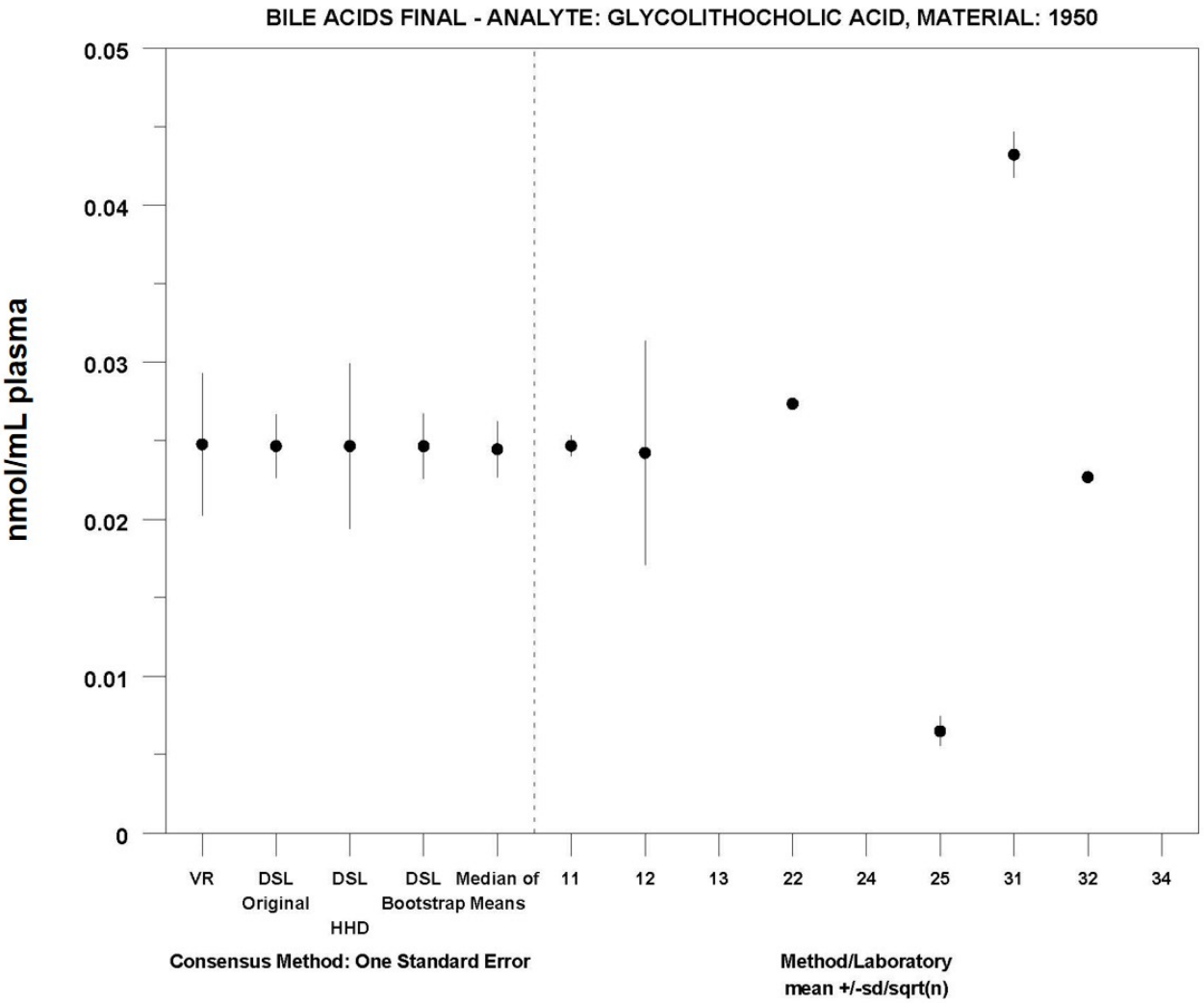
34: 26 ± 2



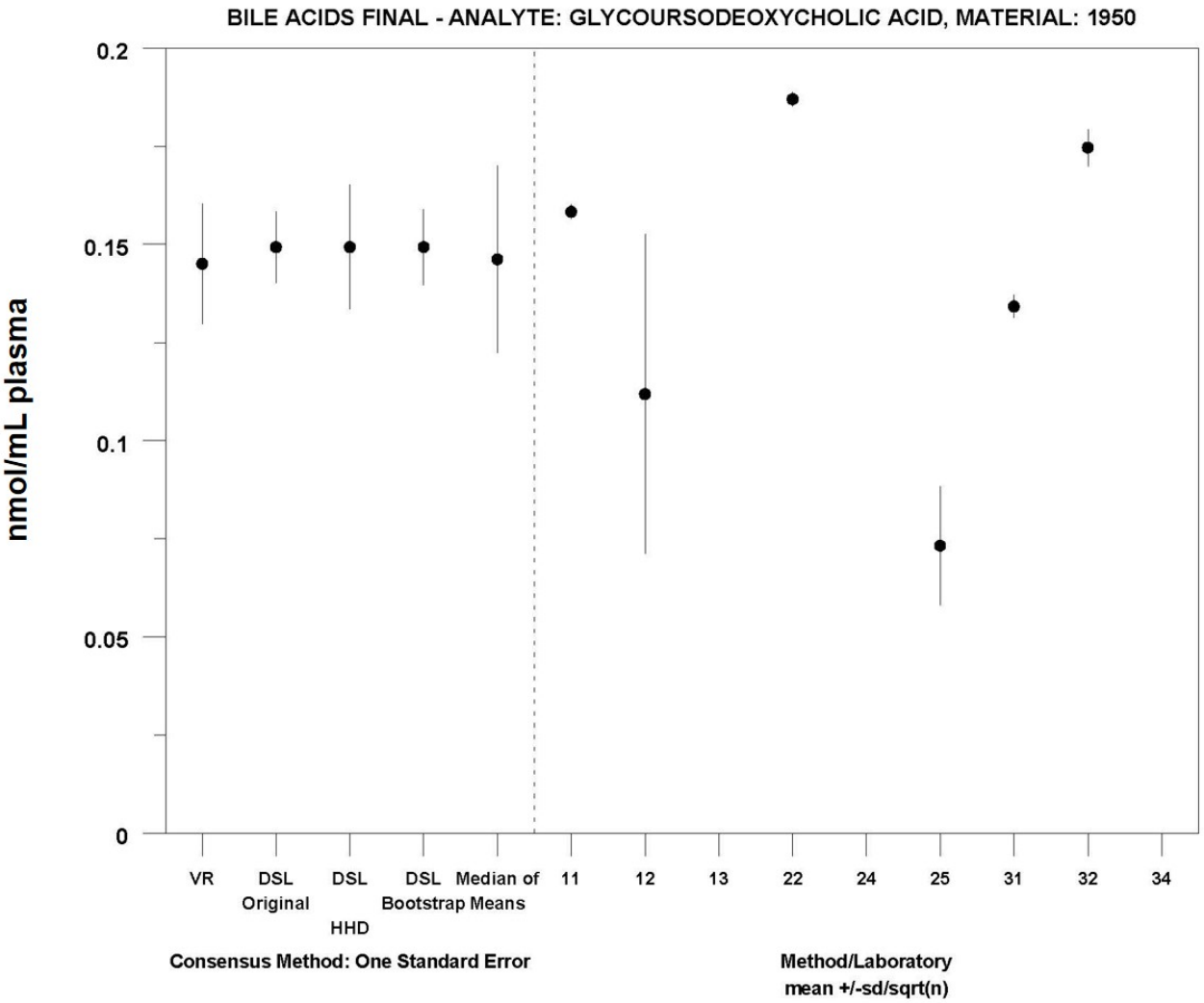
MEDM Location: 1.1 ± 0.18 nmol/mL



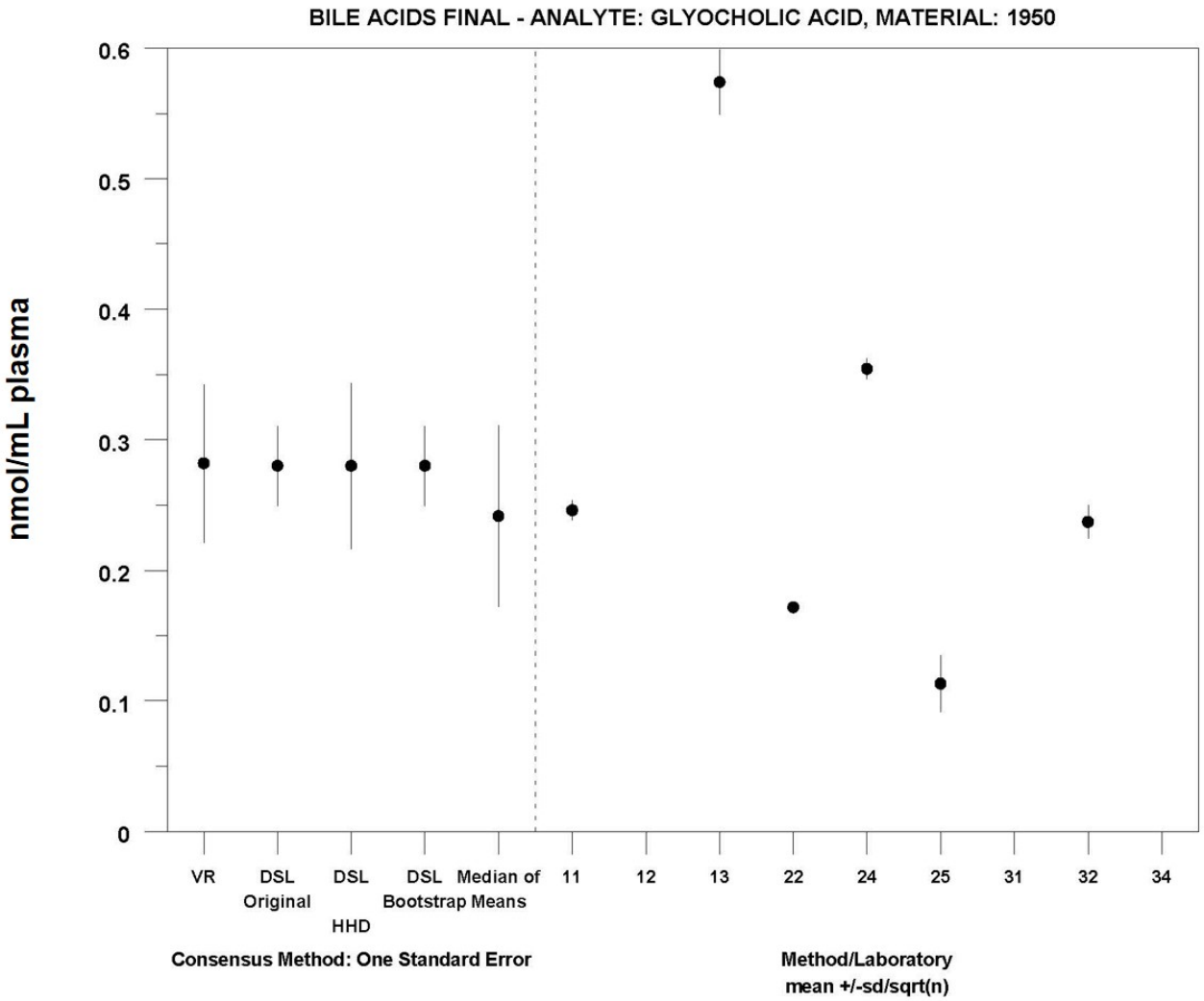
MEDM Location: 0.43 ± 0.069 nmol/mL



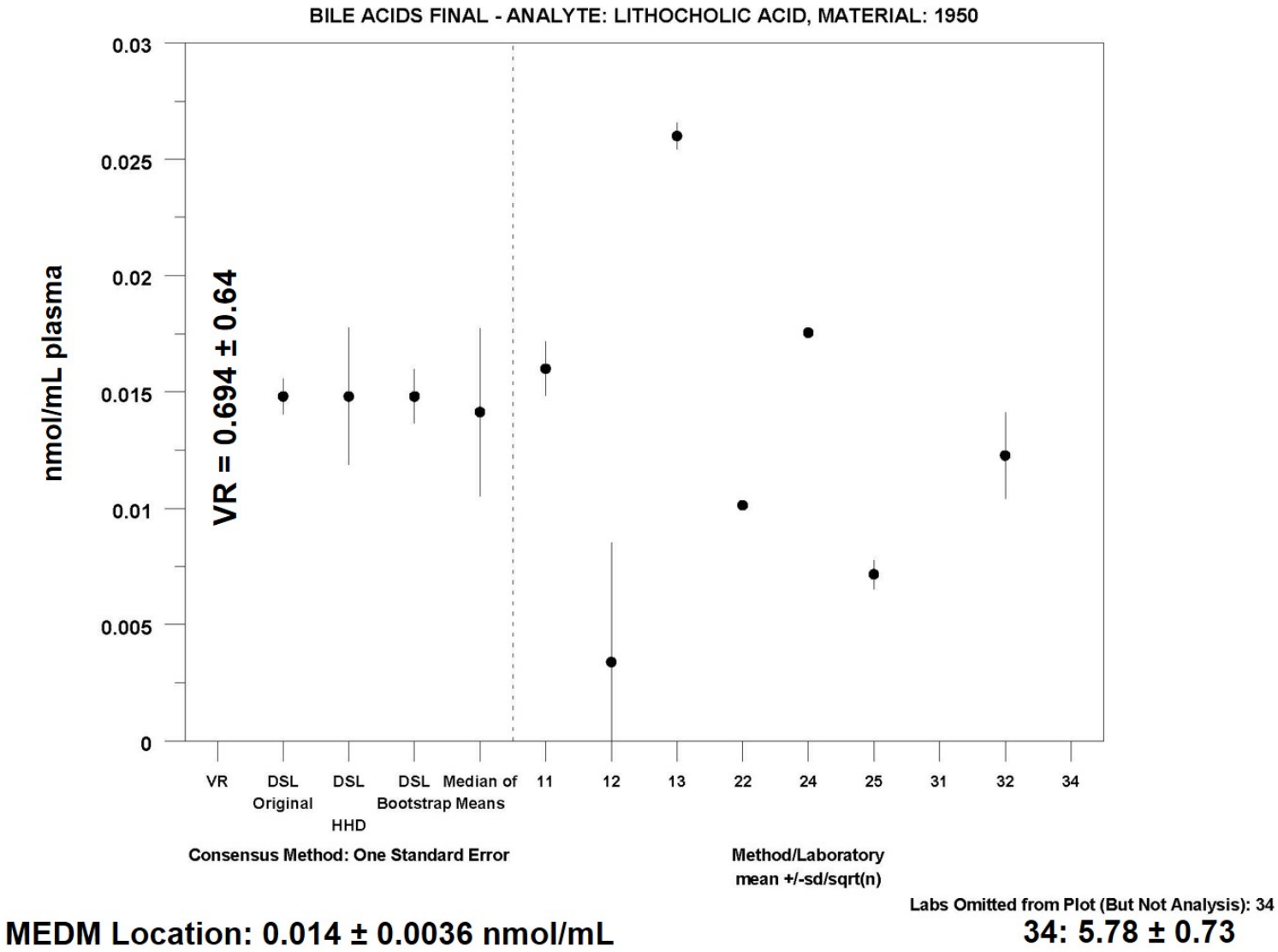
MEDM Location: 0.025 ± 0.0018 nmol/mL

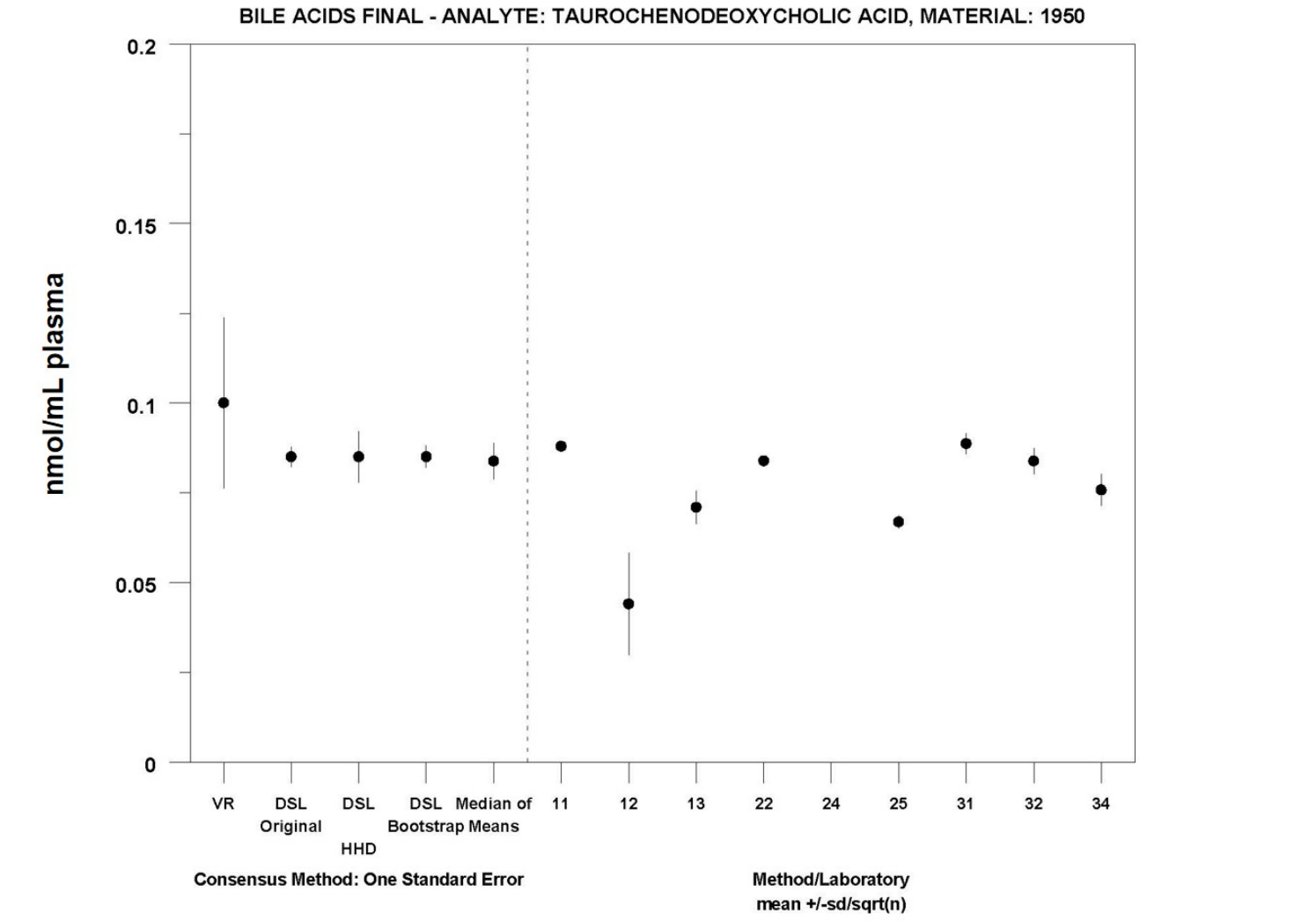


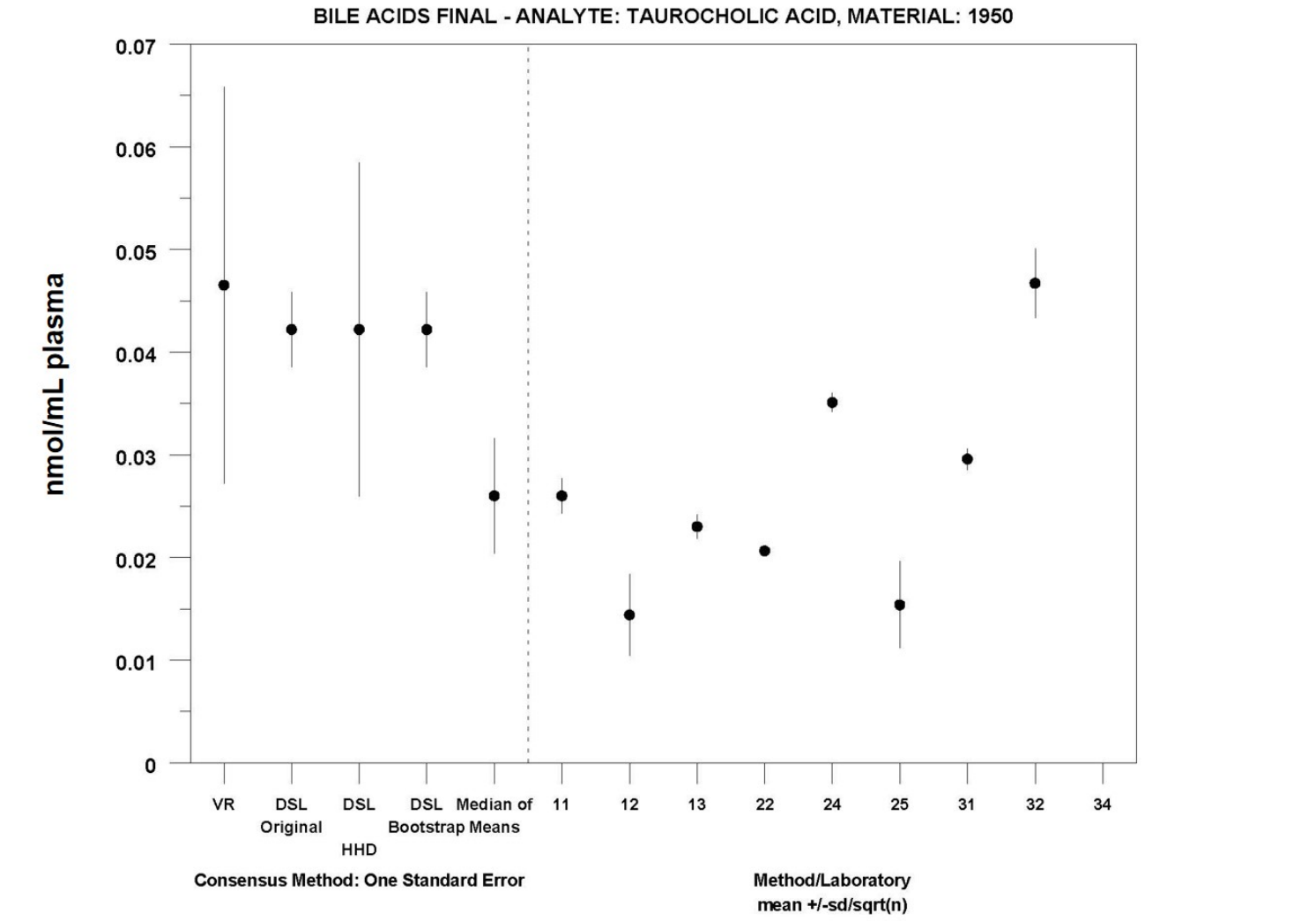
MEDM Location: 0.15 ± 0.024 nmol/mL

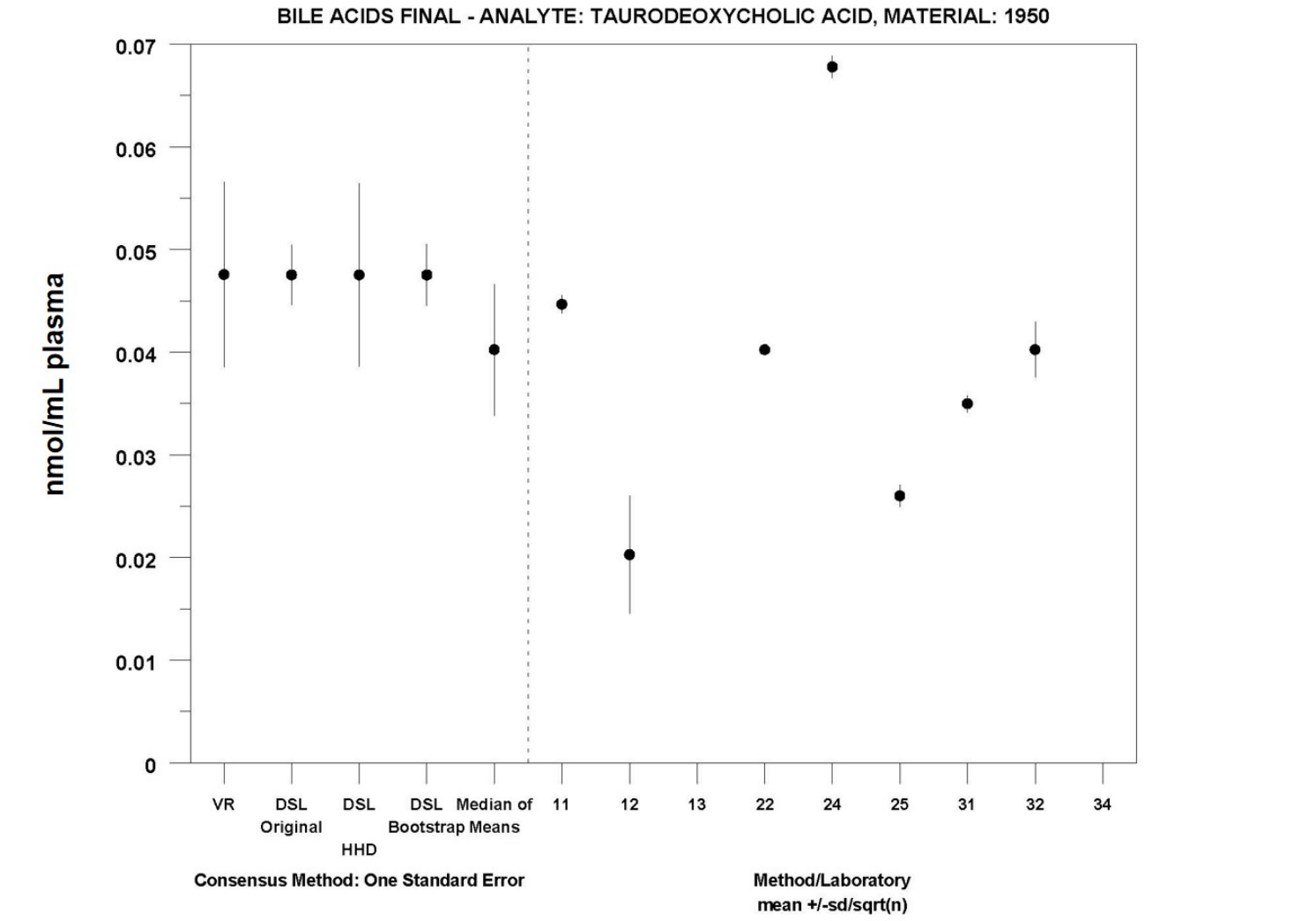


MEDM Location: 0.24 ± 0.069 nmol/mL





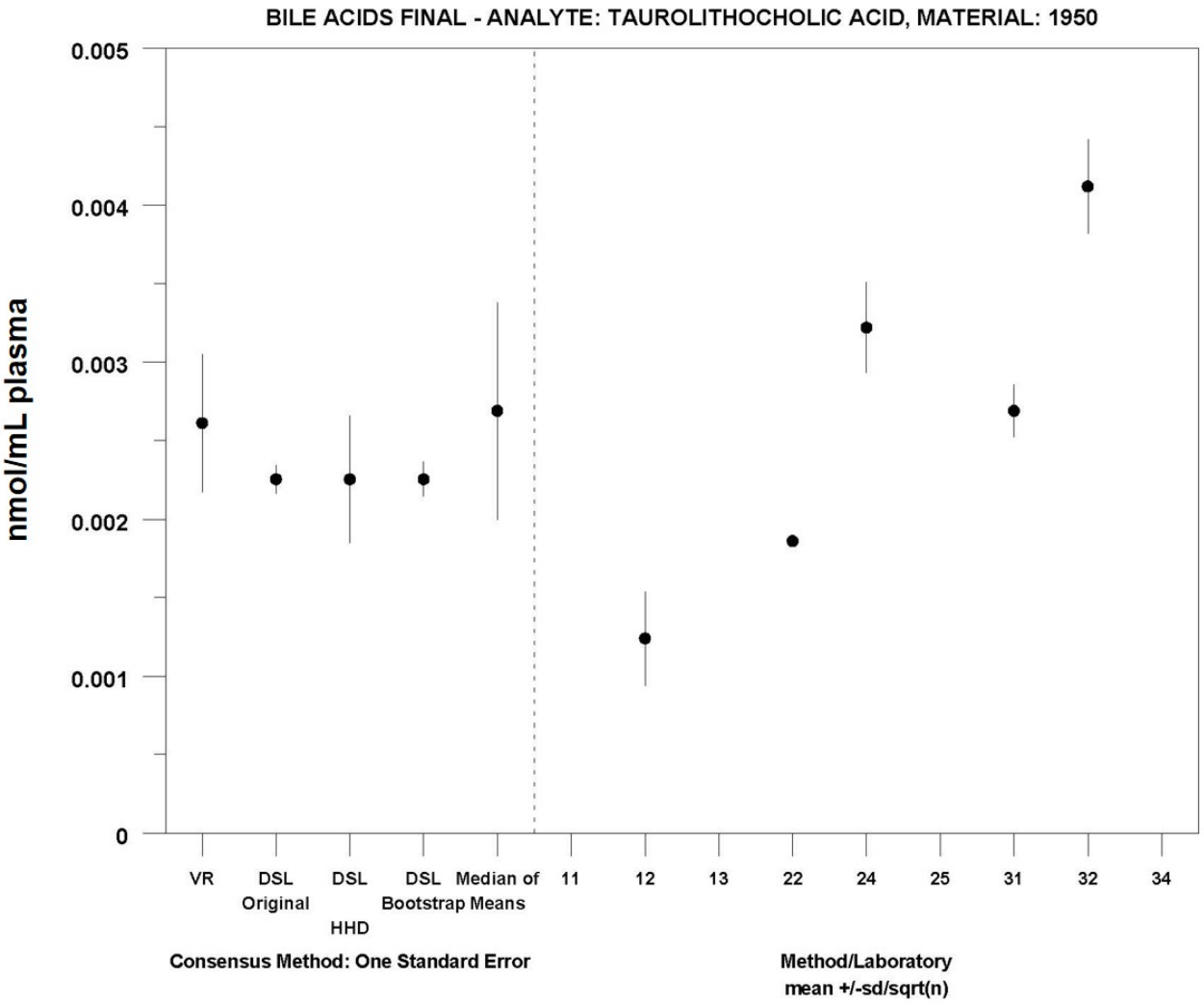




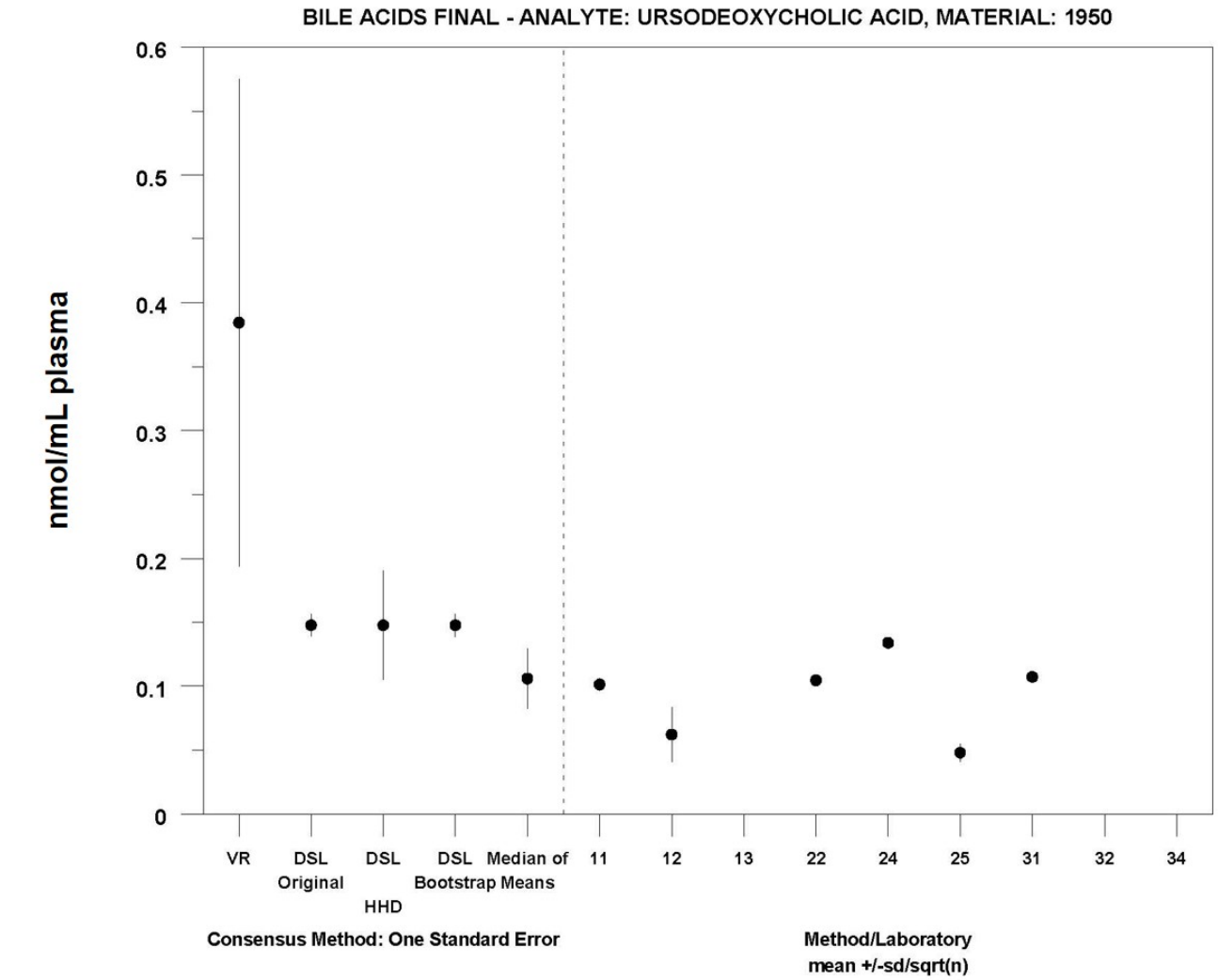
MEDM Location: 0.040 ± 0.0064 nmol/mL

Labs Omitted from Plot (But Not Analysis): 34

34: 0.11 ± 0.01



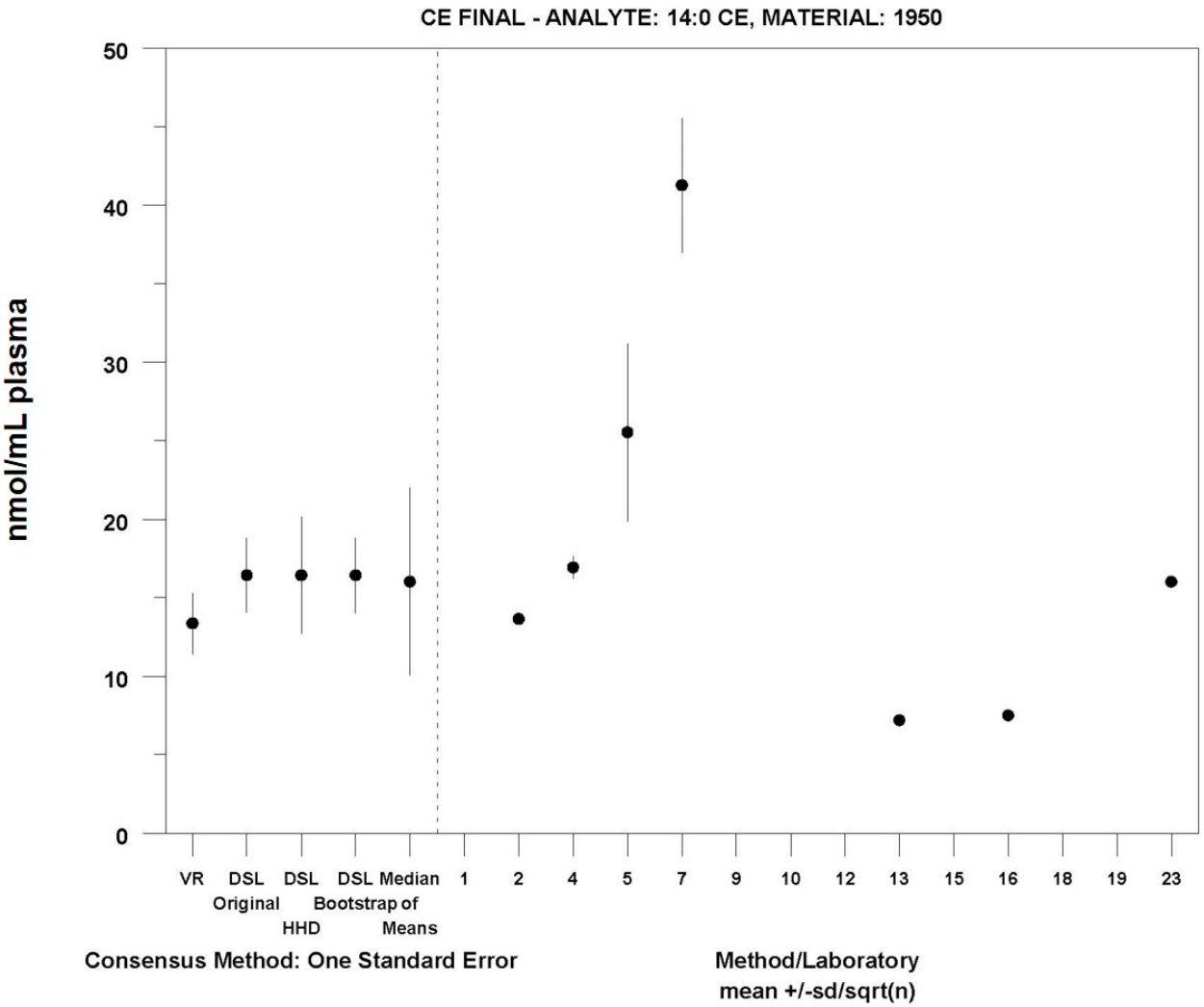
MEDM Location: 0.0027 ± 0.00069 nmol/mL



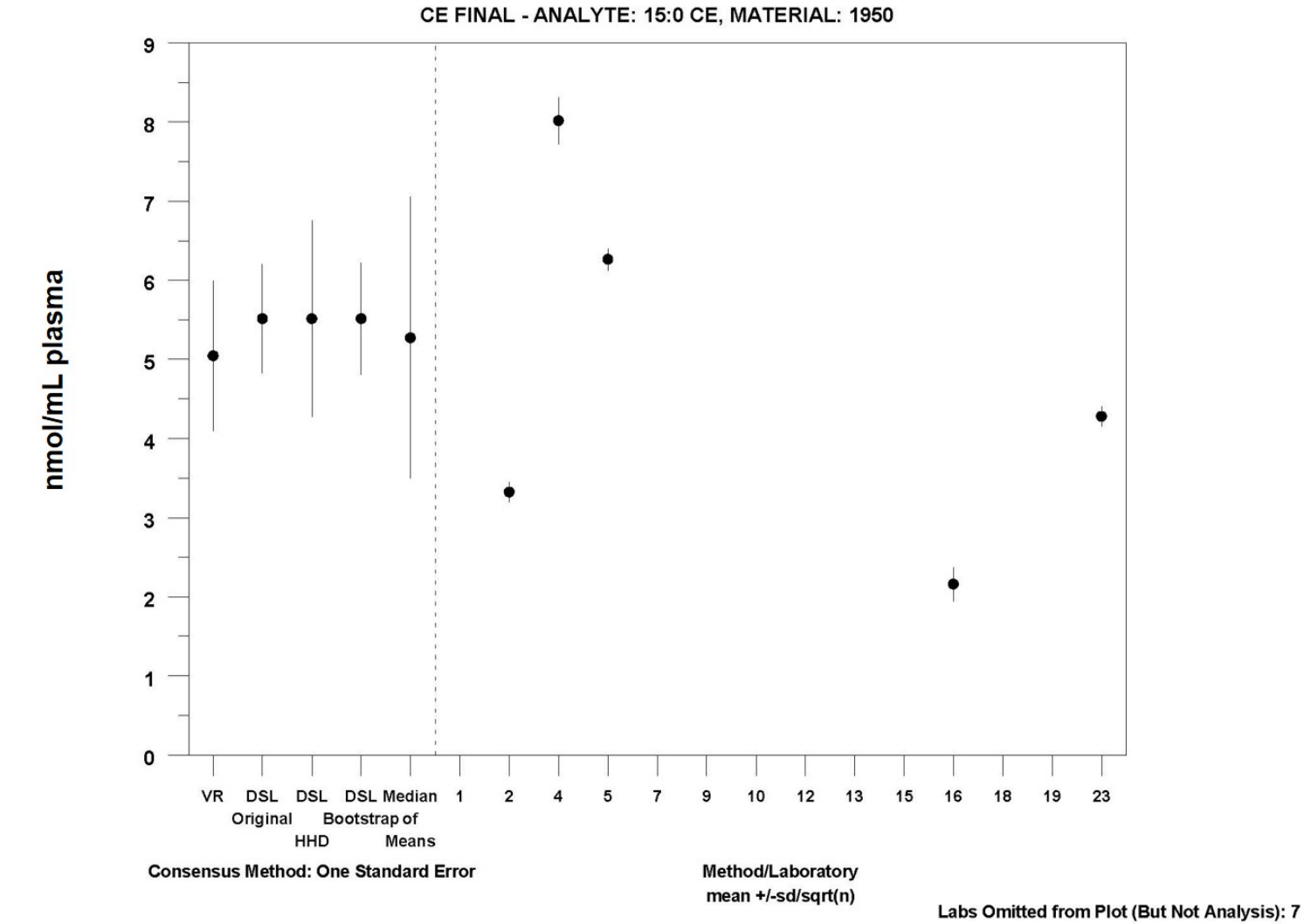
Labs Omitted from Plot (But Not Analysis): 13 34

MEDM Location: 0.11 ± 0.024 nmol/mL

13: 0.89 ± 0.08; 34: 1.64 ± 0.10



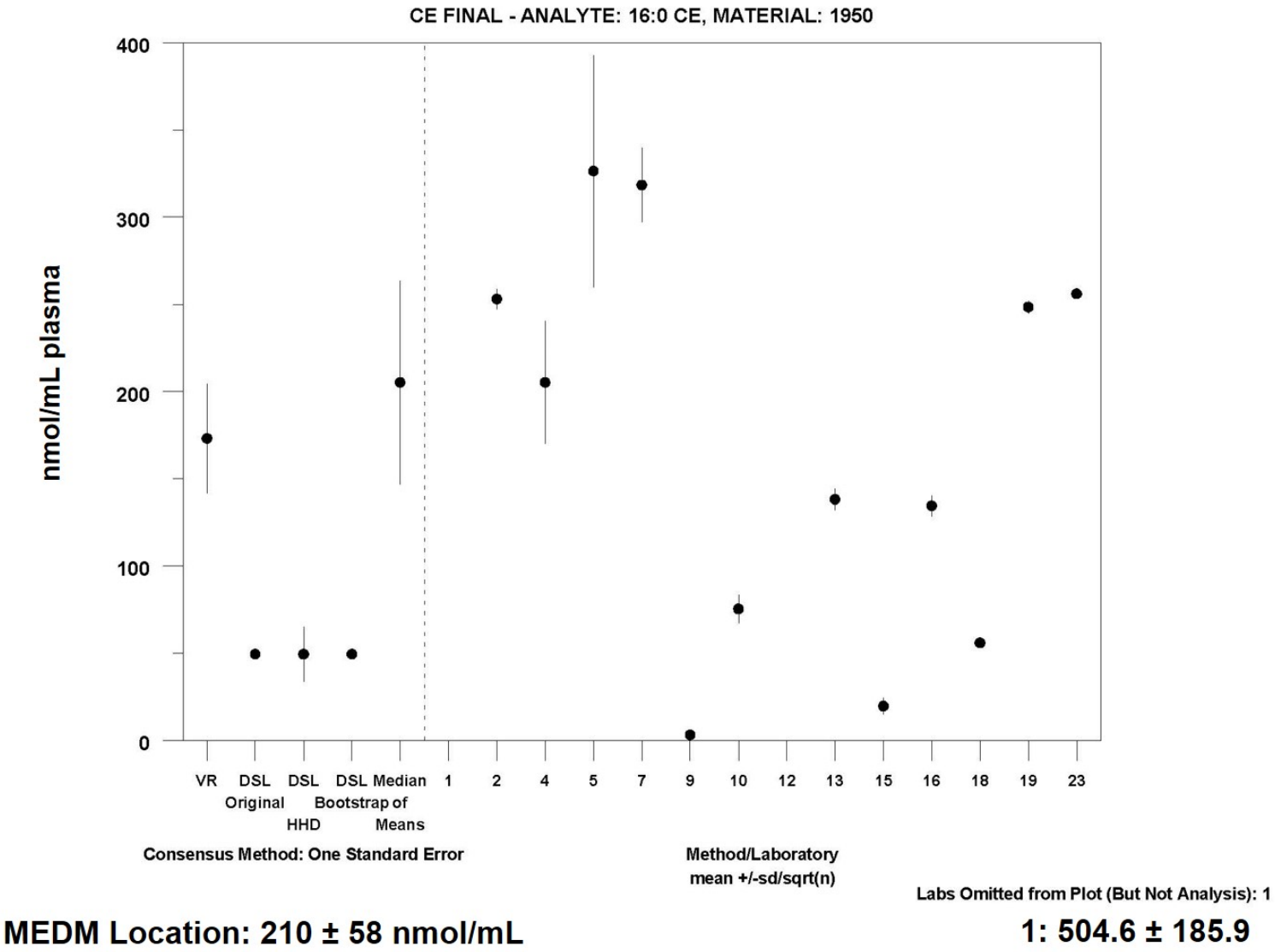
MEDM Location: 16.0 ± 6.0 nmol/mL

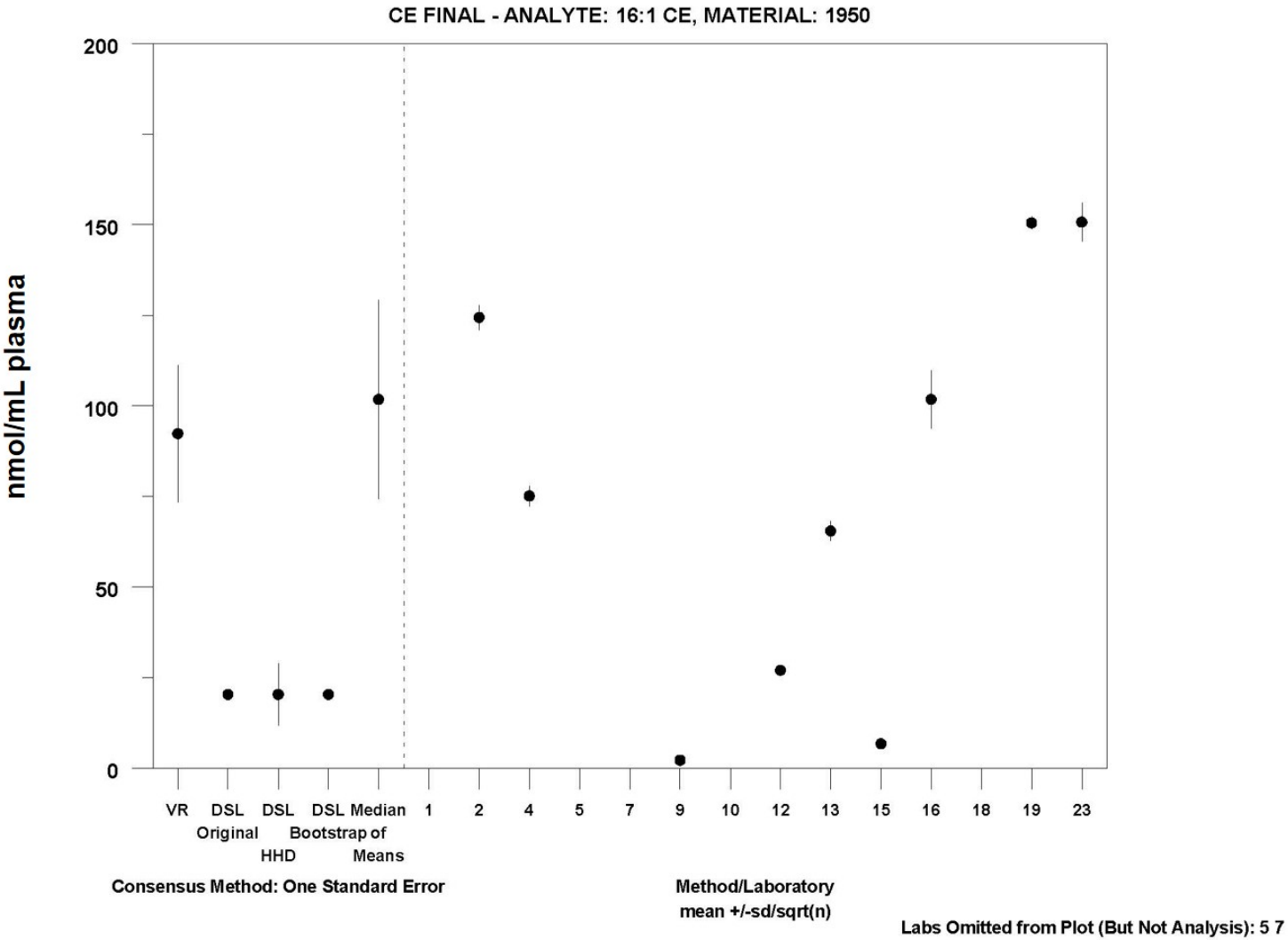


MEDM Location: 5.3 ± 1.8 nmol/mL

Labs Omitted from Plot (But Not Analysis): 7

7: 16.17 ± 3.90

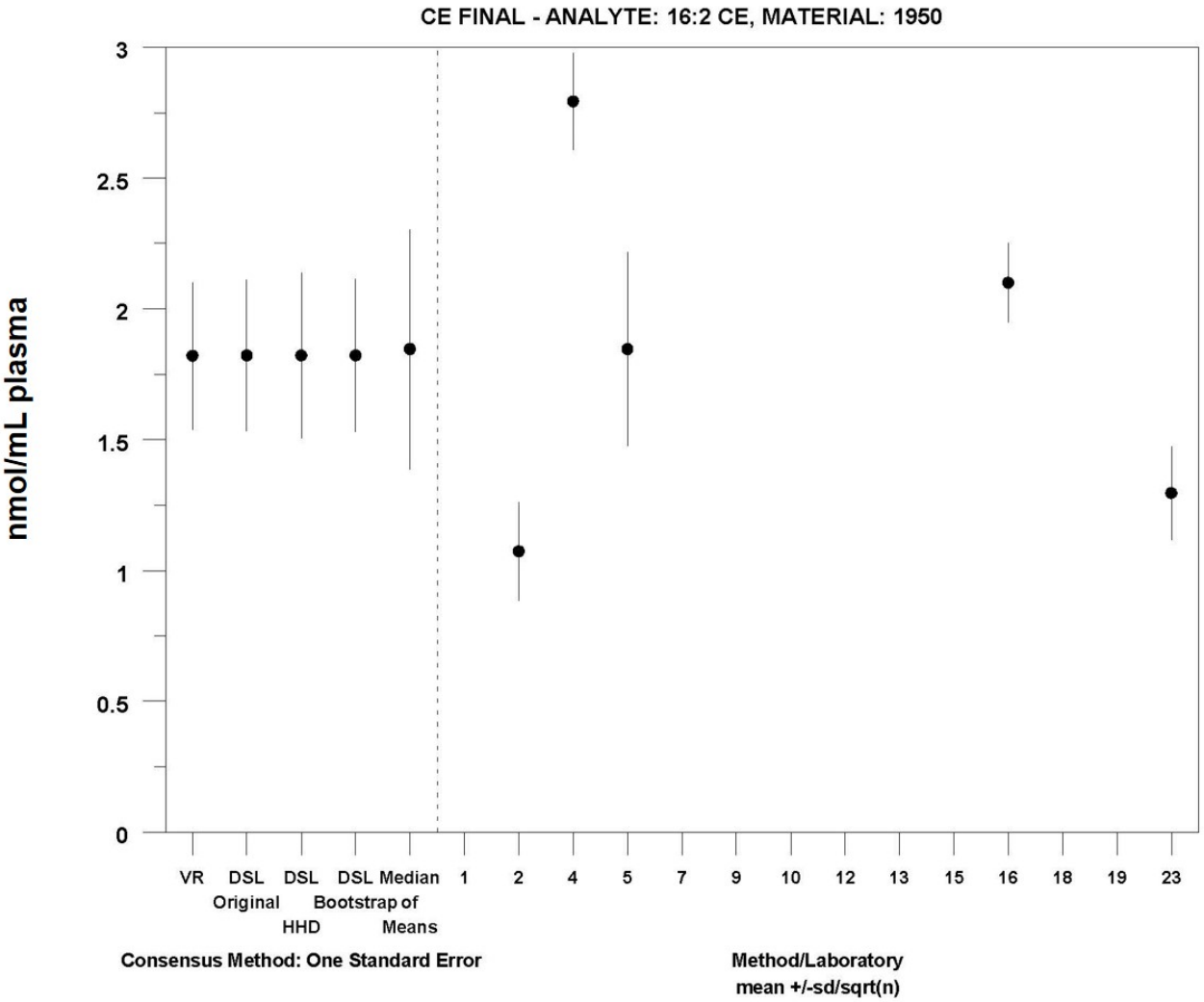




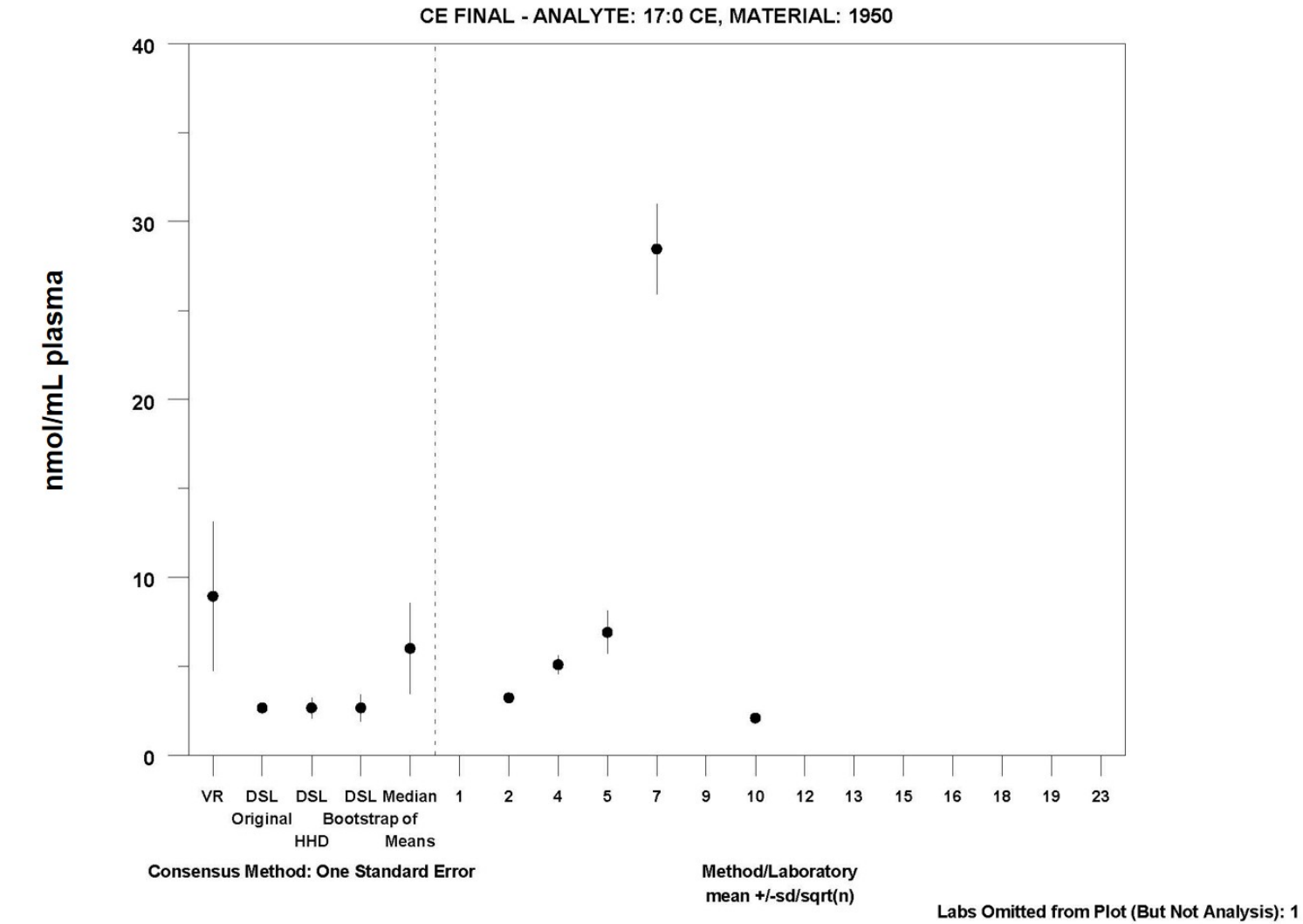
Labs Omitted from Plot (But Not Analysis): 5 7

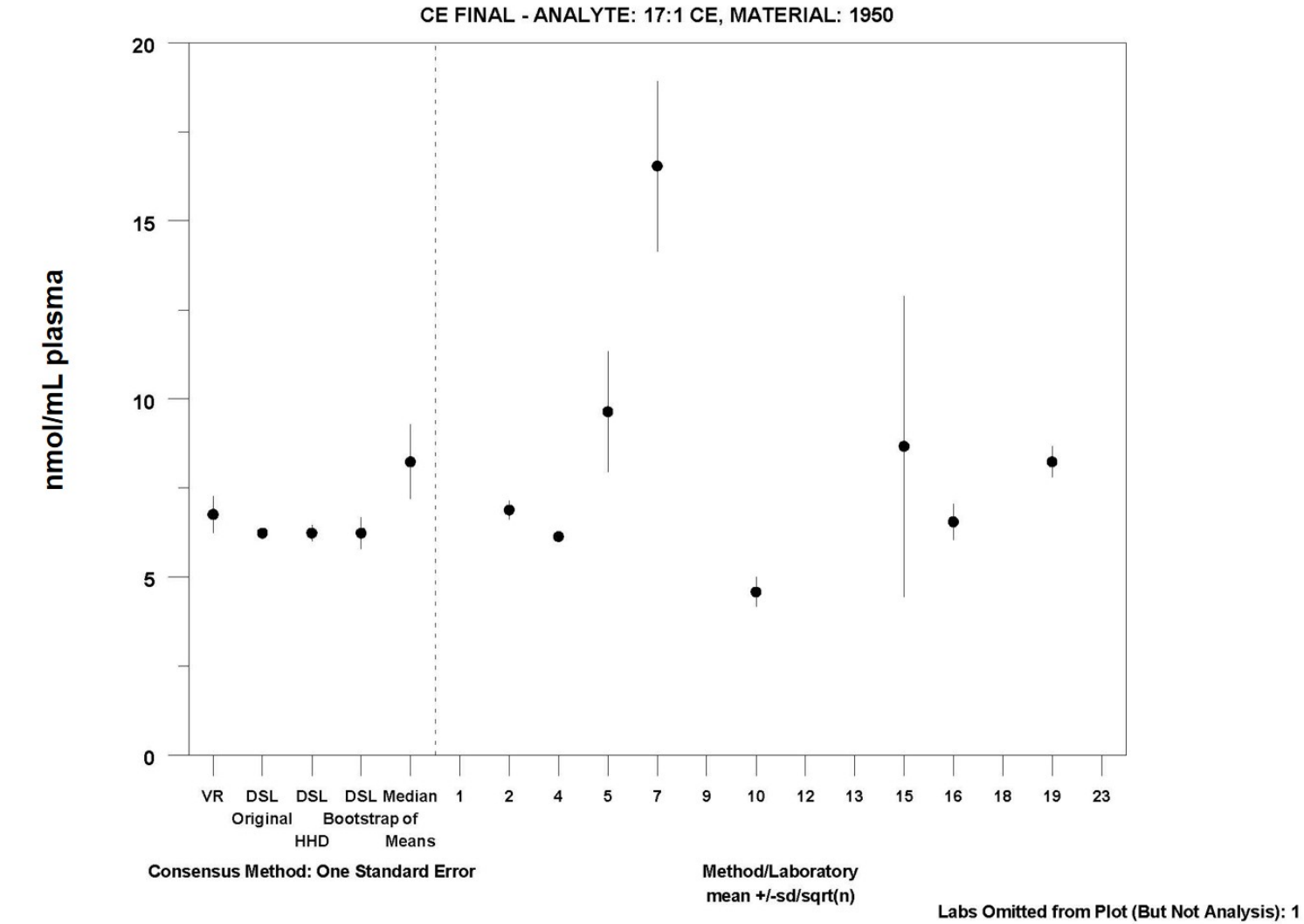
MEDM Location: 100 ± 27 nmol/mL

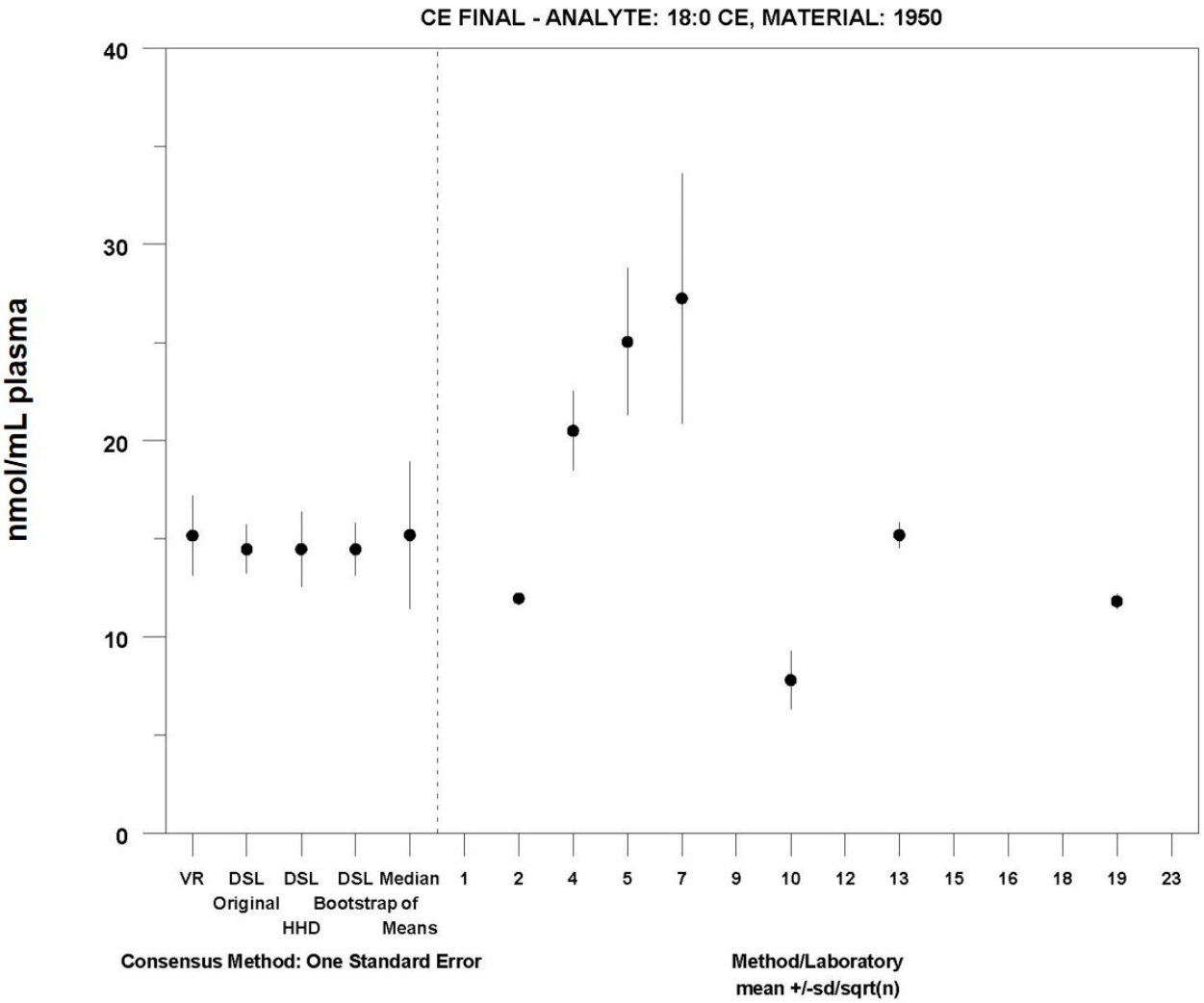
5: 160 ± 41; 7: 287 ± 49



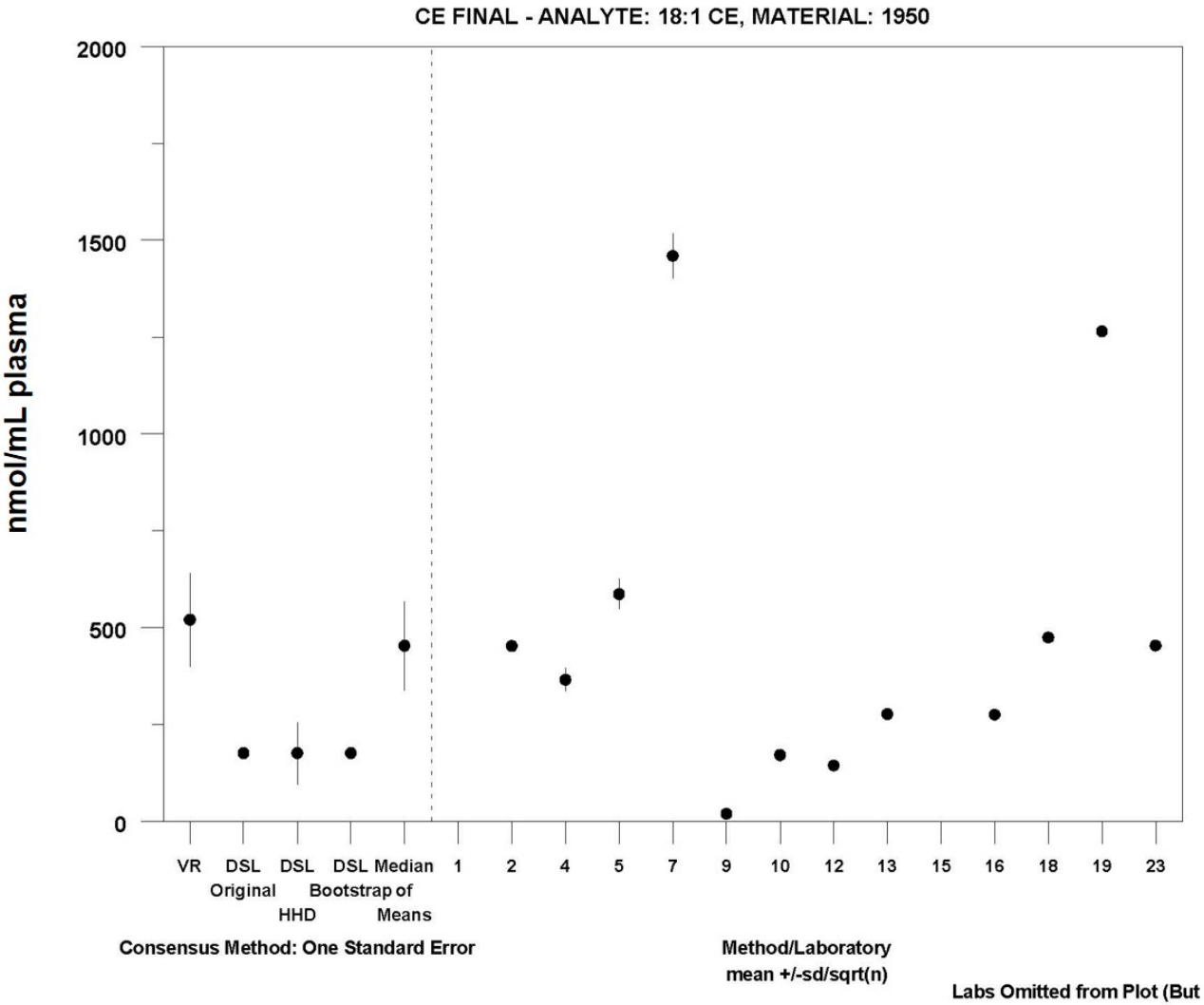
MEDM Location: 1.9 ± 0.46 nmol/mL







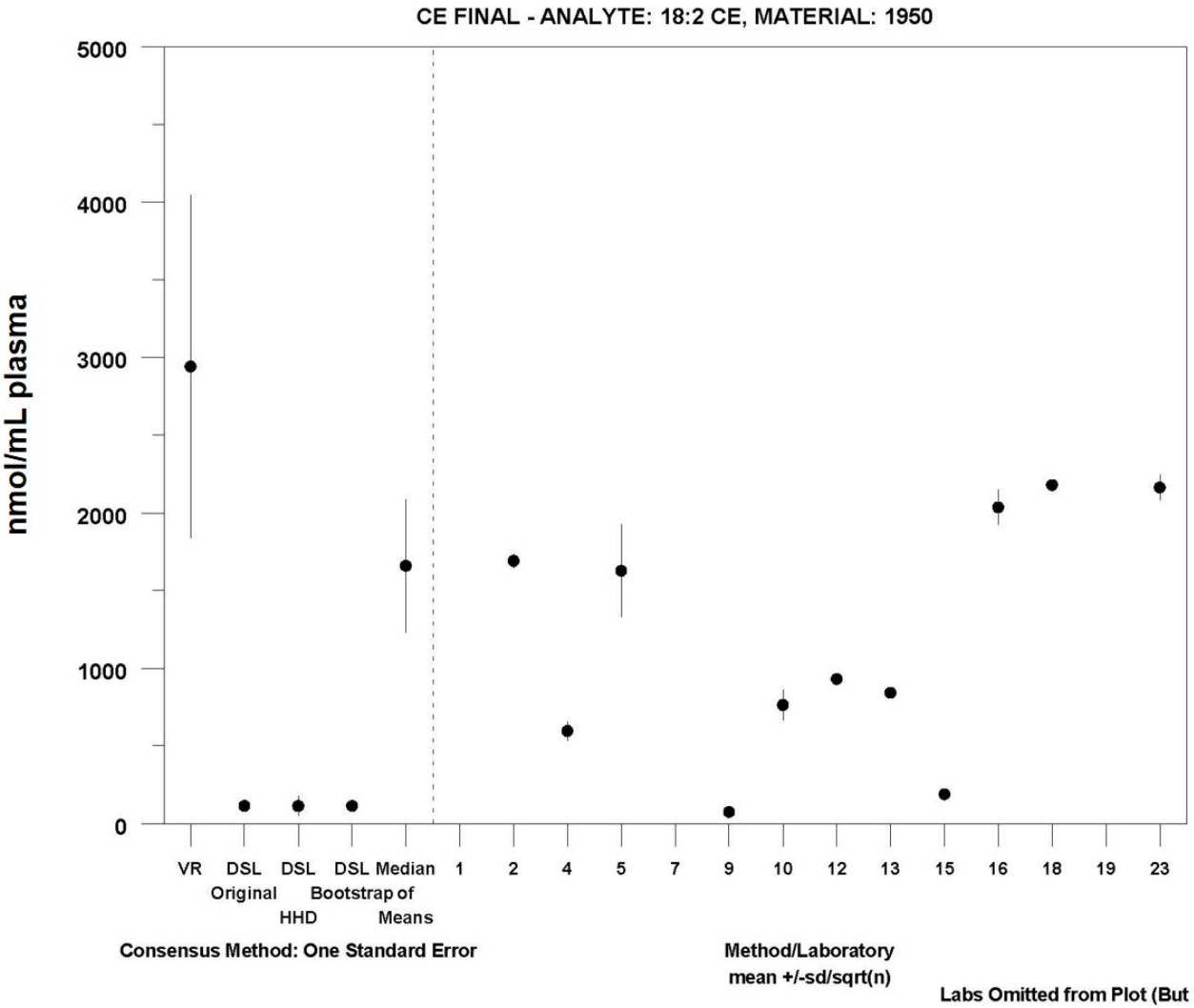
MEDM Location: 15 ± 3.7 nmol/mL



Labs Omitted from Plot (But Not Analysis): 1 15

MEDM Location: 450 ± 110 nmol/mL

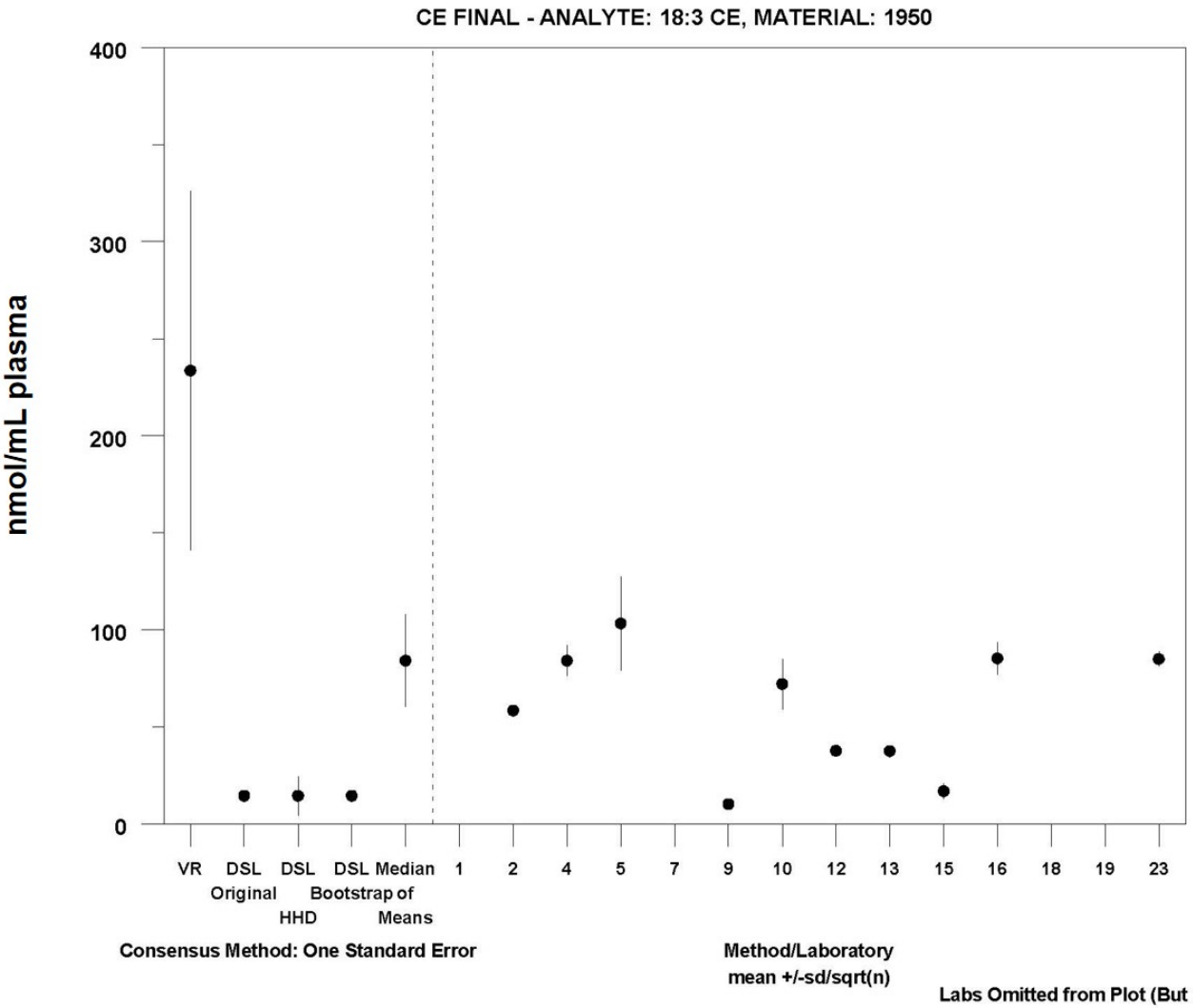
1: 5922 ± 2082; 15: 2116 ± 1315



MEDM Location: 1700 ± 430 nmol/mL

Labs Omitted from Plot (But Not Analysis): 1 7 19

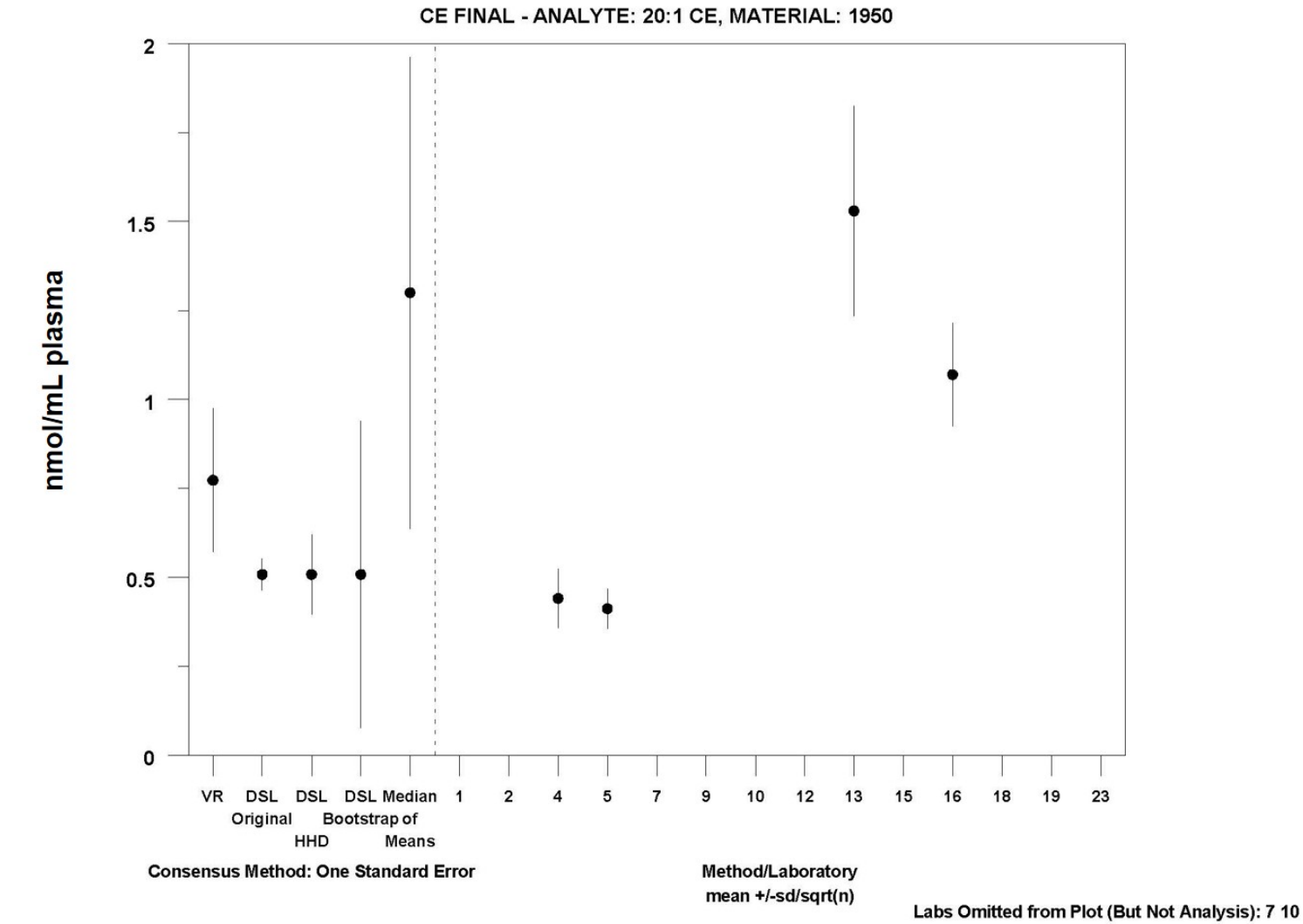
1: 31954 ± 10787; 7: 13910 ± 1084; 19: 9996 ± 294

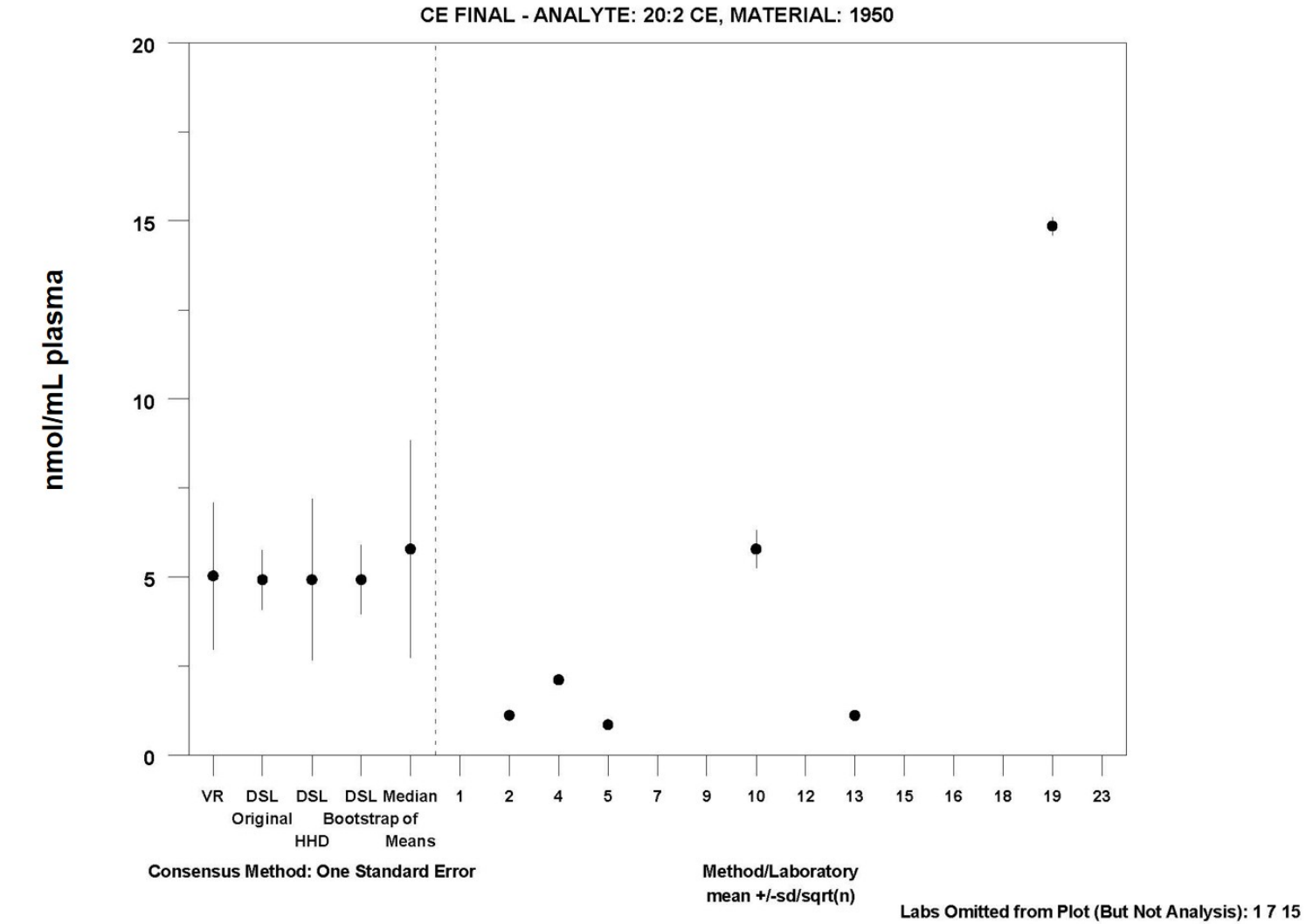


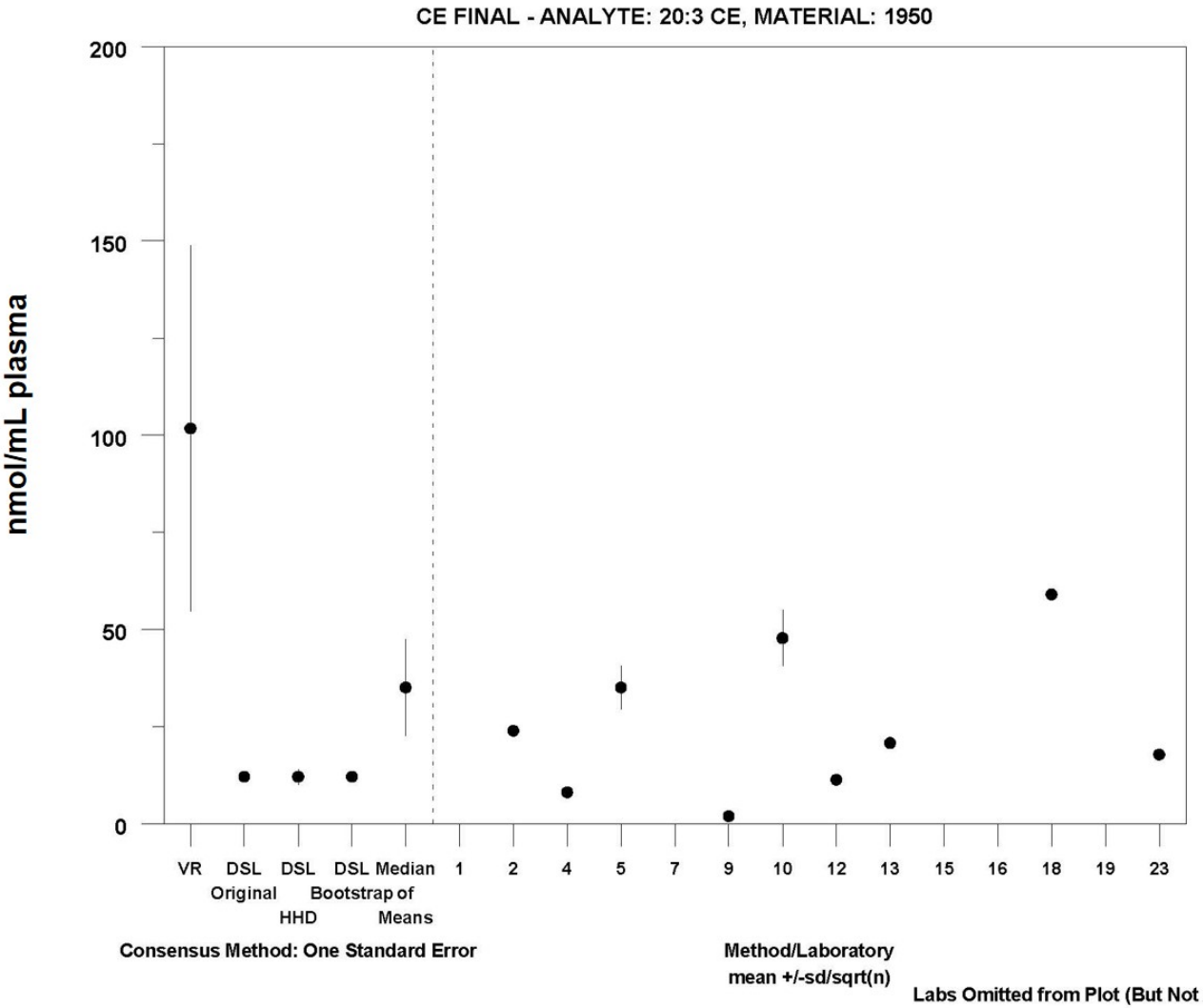
MEDM Location: 84 ± 24 nmol/mL

Labs Omitted from Plot (But Not Analysis): 1 7 19

1: 882 ± 310; 7: 754 ± 93; 19: 1008 ± 32



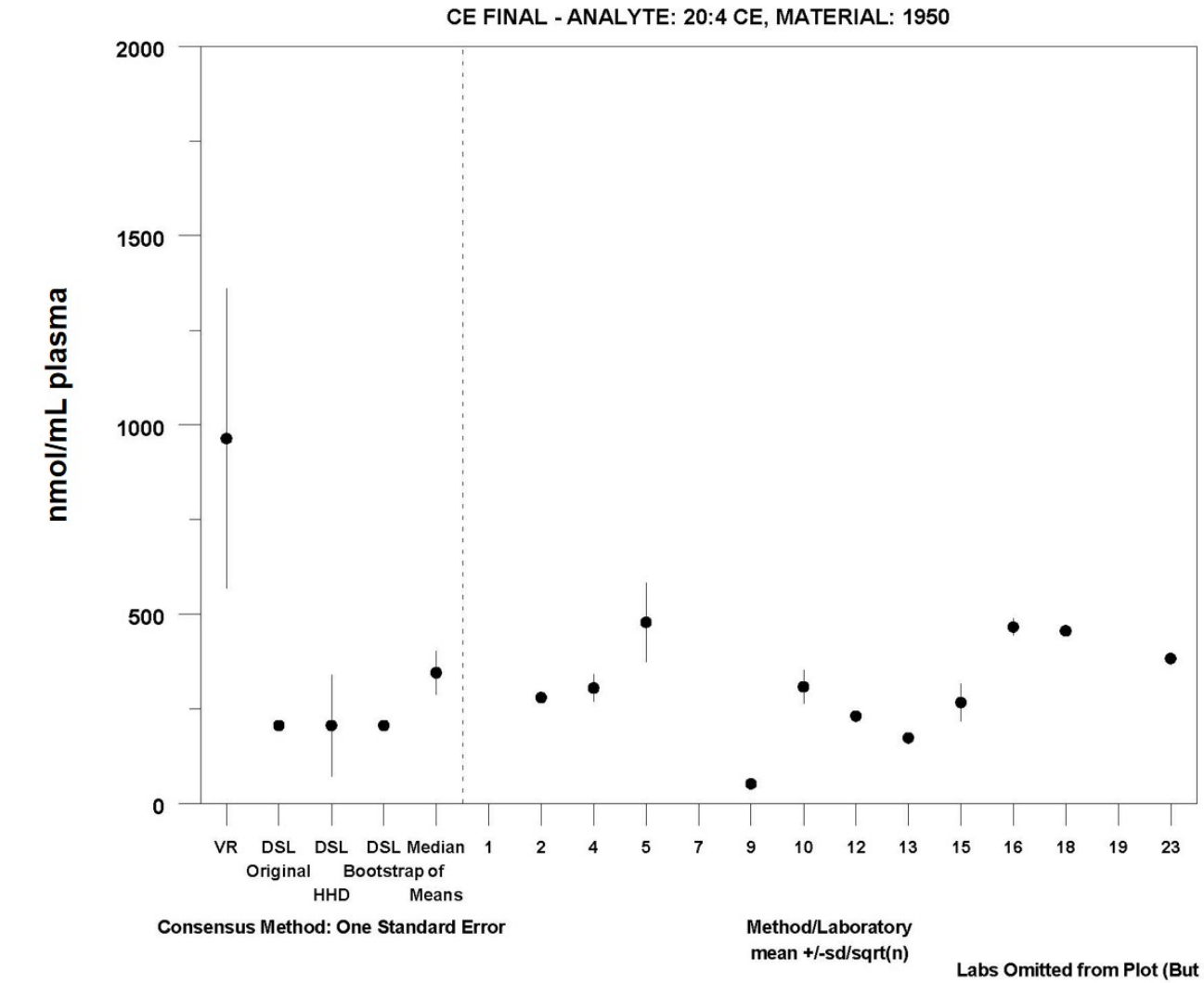




Labs Omitted from Plot (But Not Analysis): 1 7 15 19

MEDM Location: 35 ± 12 nmol/mL

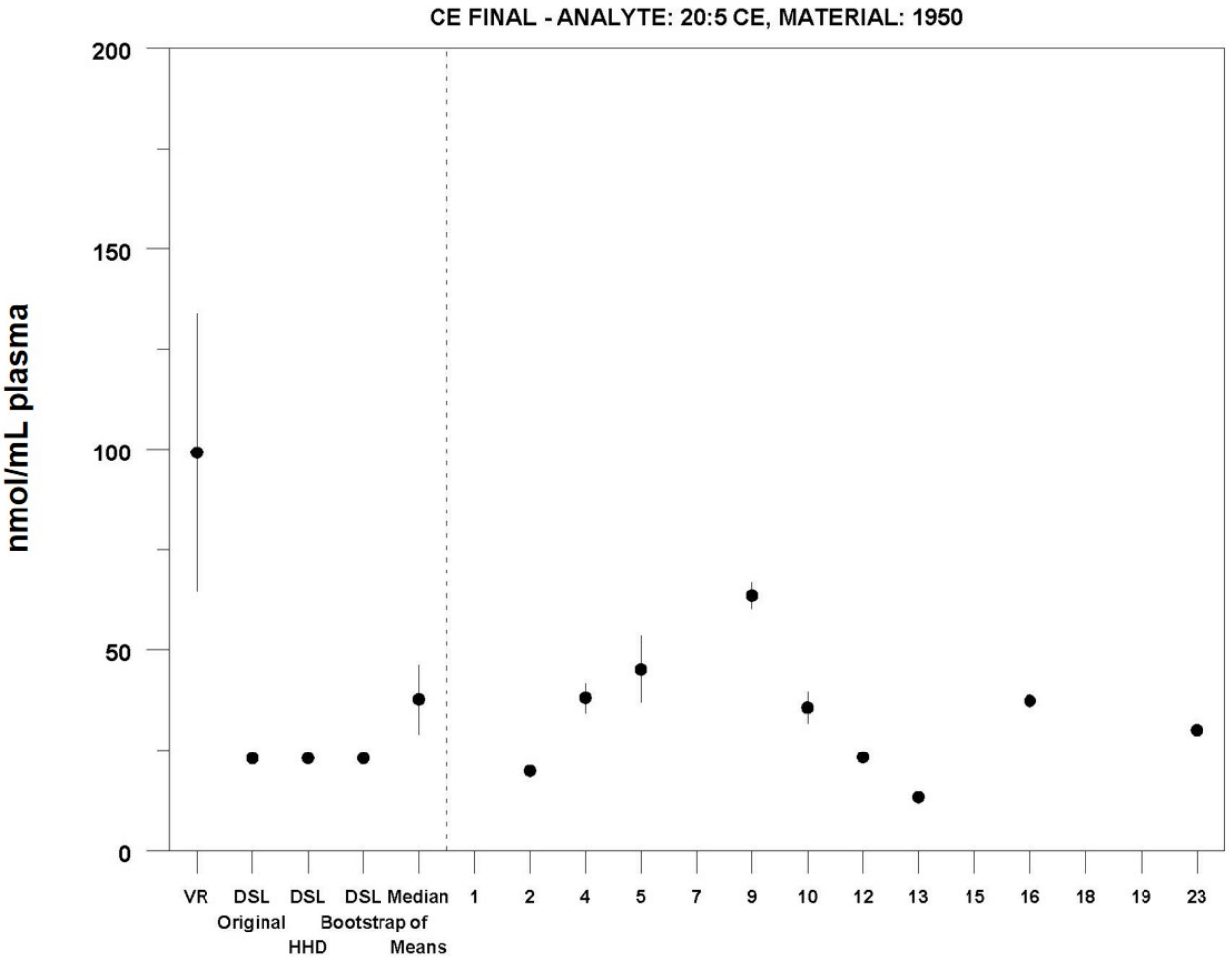
1: 1931 ± 741; 7: 267 ± 55; 15: 1252 ± 149; 19: 531 ± 8



MEDM Location: 350 ± 58 nmol/mL

Labs Omitted from Plot (But Not Analysis): 1 7 19

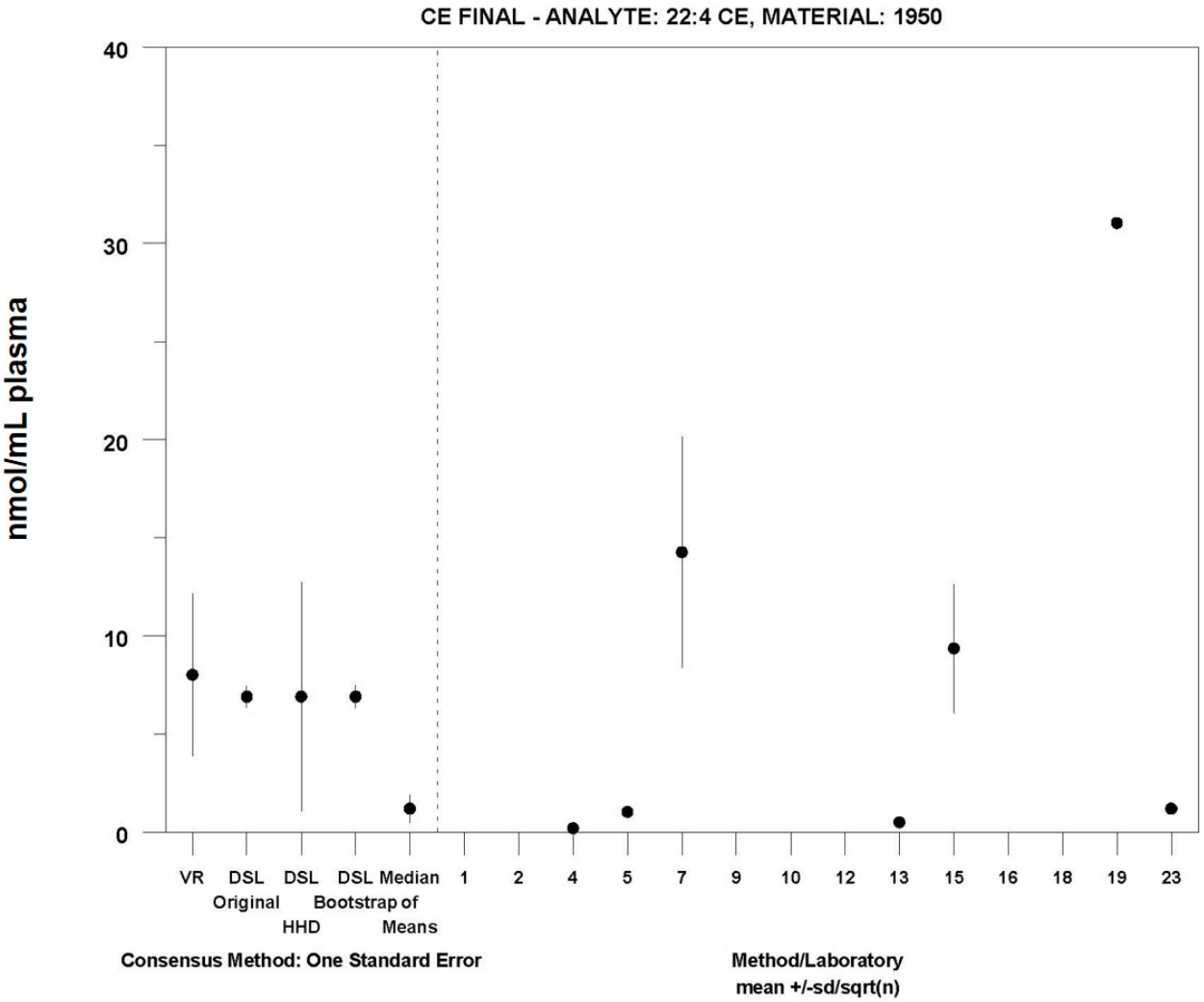
1: 5871 ± 2053; 7: 2653 ± 366; 19: 5250 ± 201



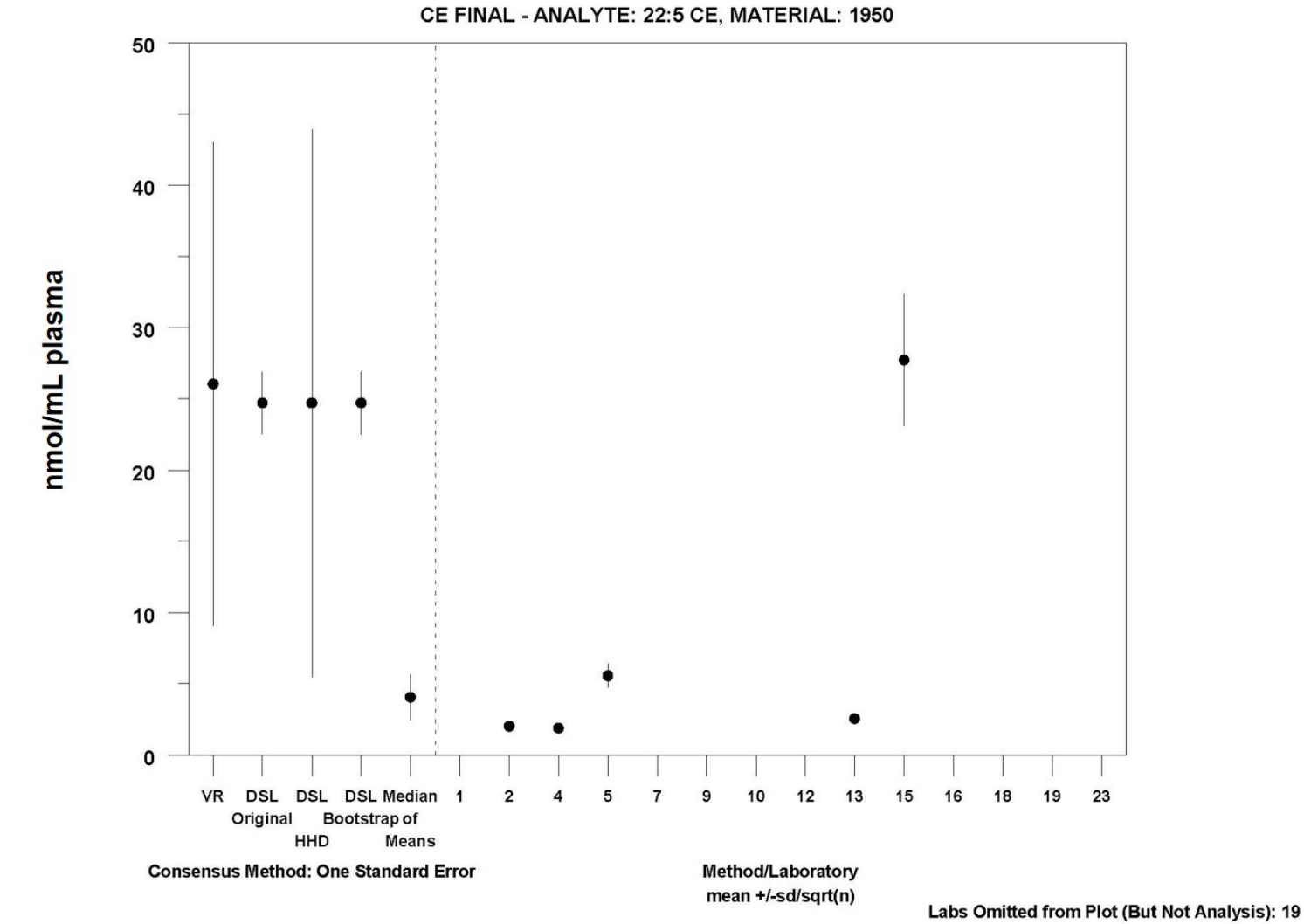
Labs Omitted from Plot (But Not Analysis): 7 15 19

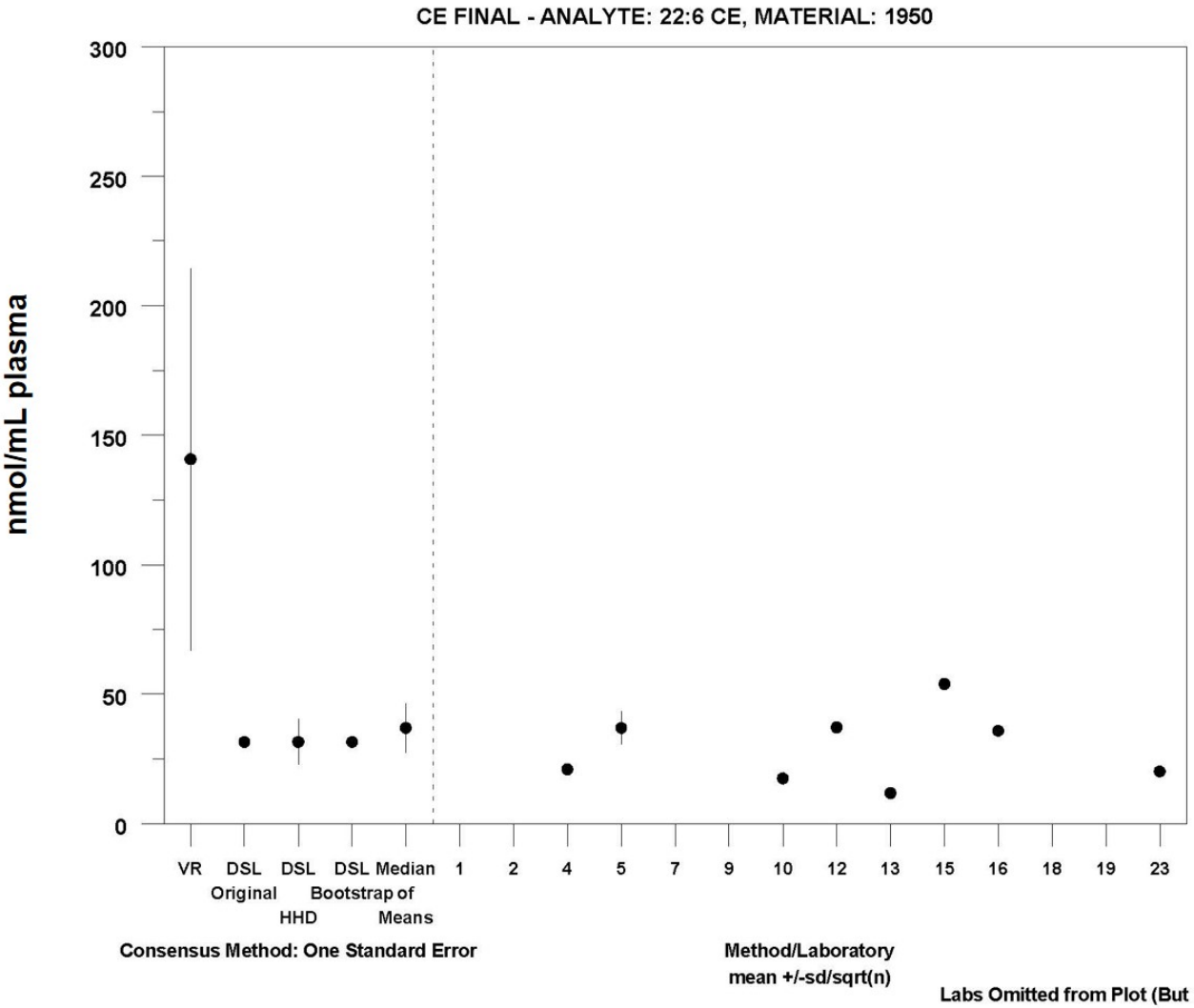
MEDM Location: 38 ± 8.6 nmol/mL

7: 368 ± 32; 15: 365 ± 119; 19: 255 ± 7



MEDM Location: 1.2 ± 0.70 nmol/mL

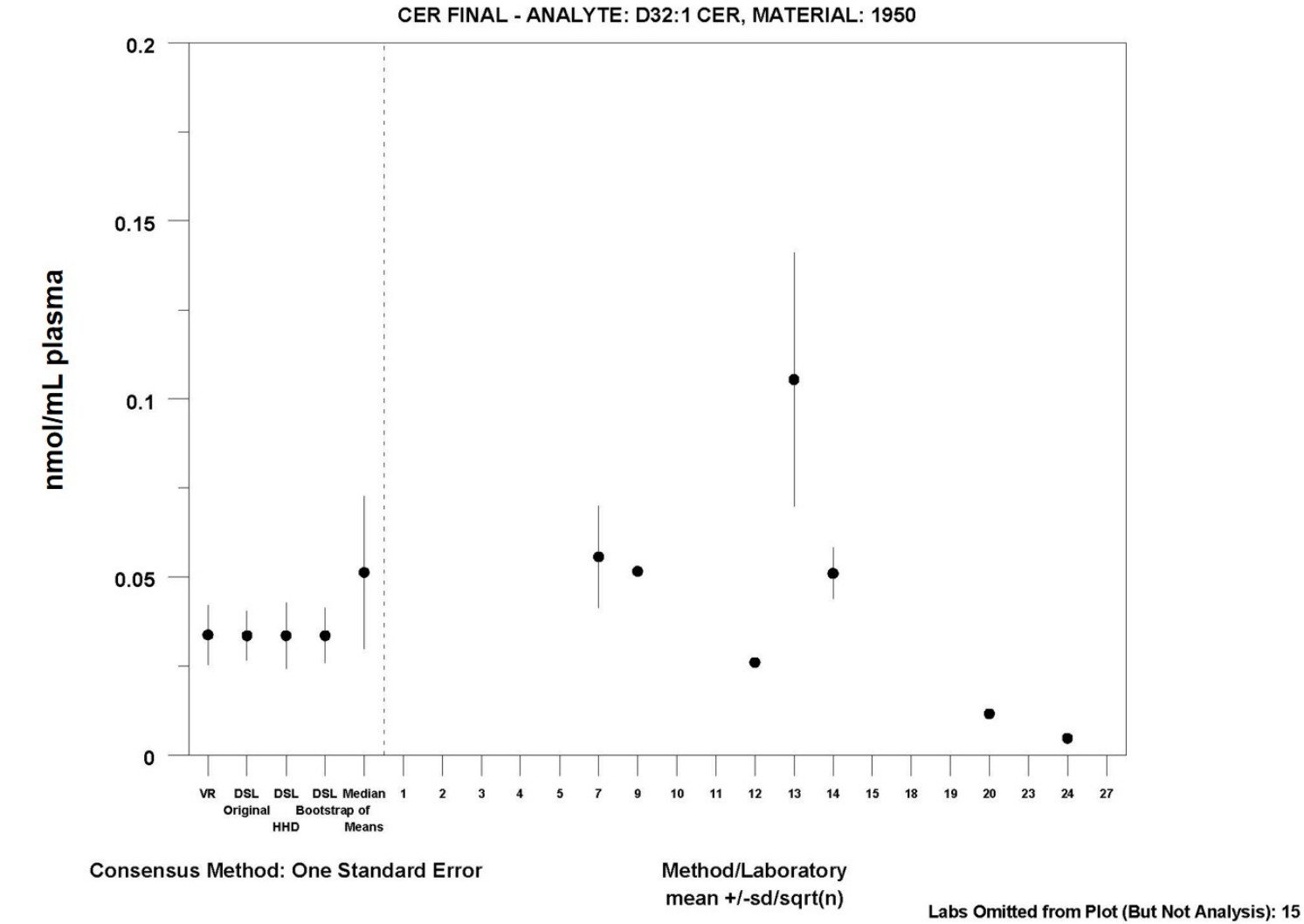


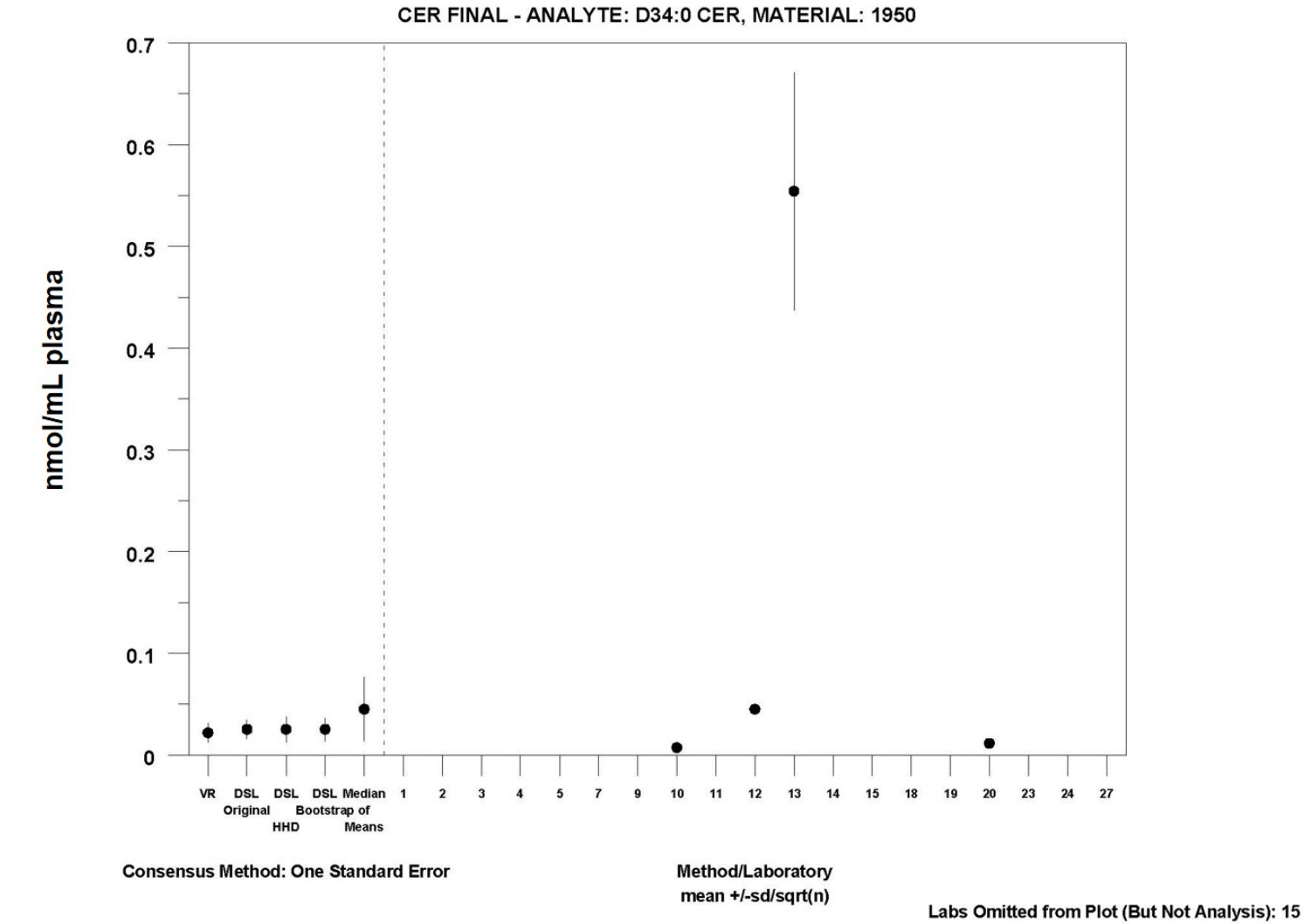


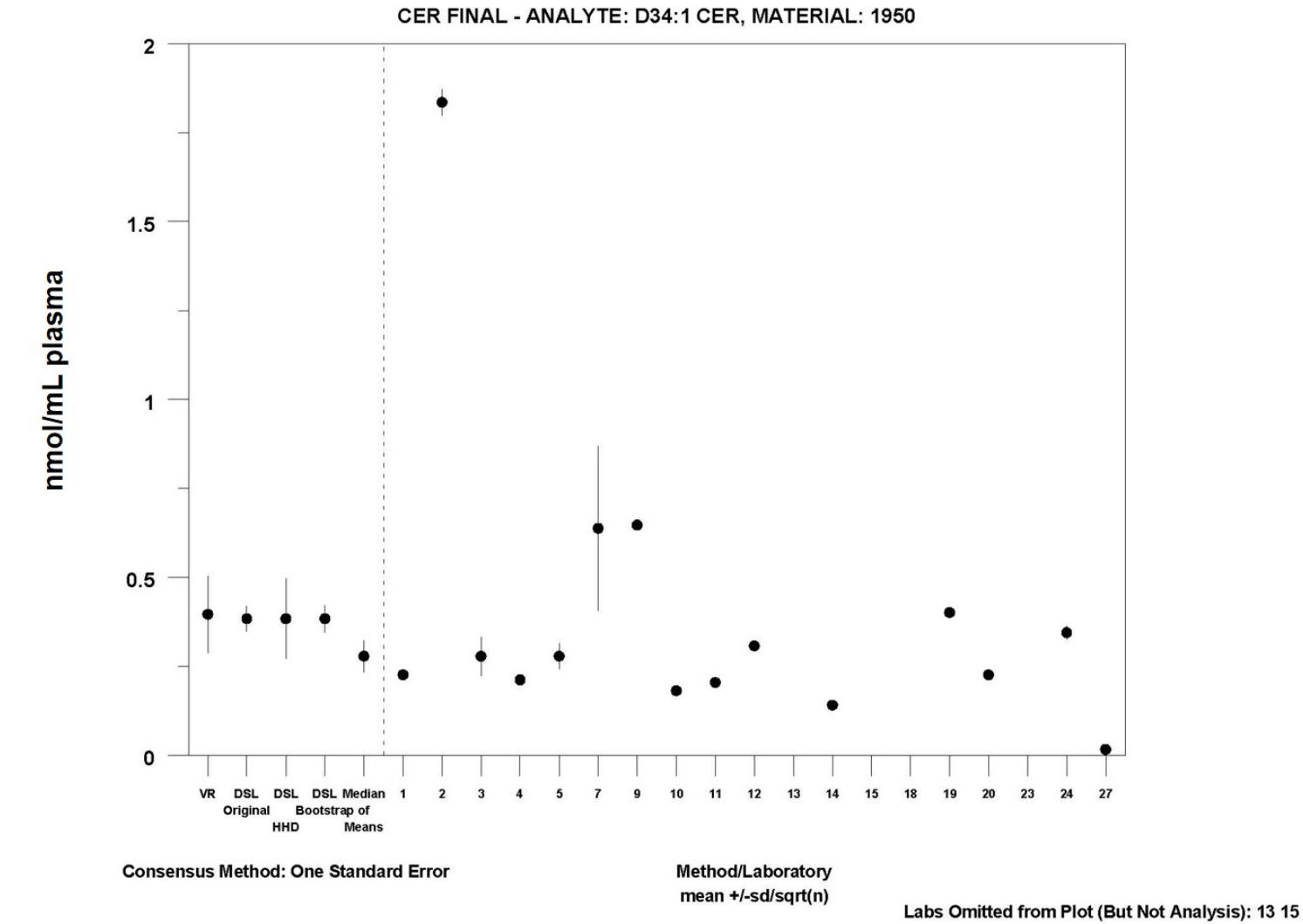
Labs Omitted from Plot (But Not Analysis): 1 7 19

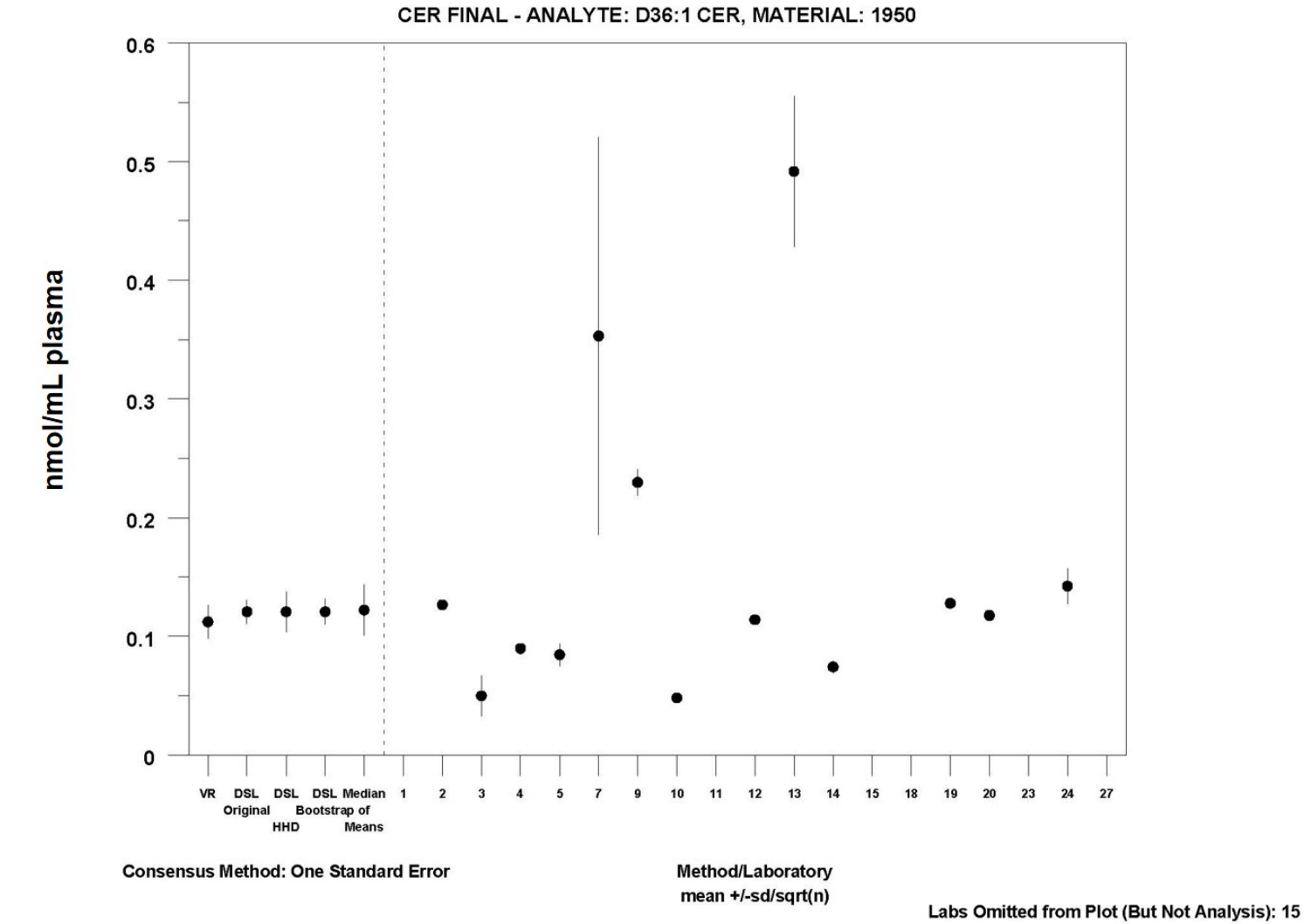
MEDM Location: 37 ± 9.5 nmol/mL

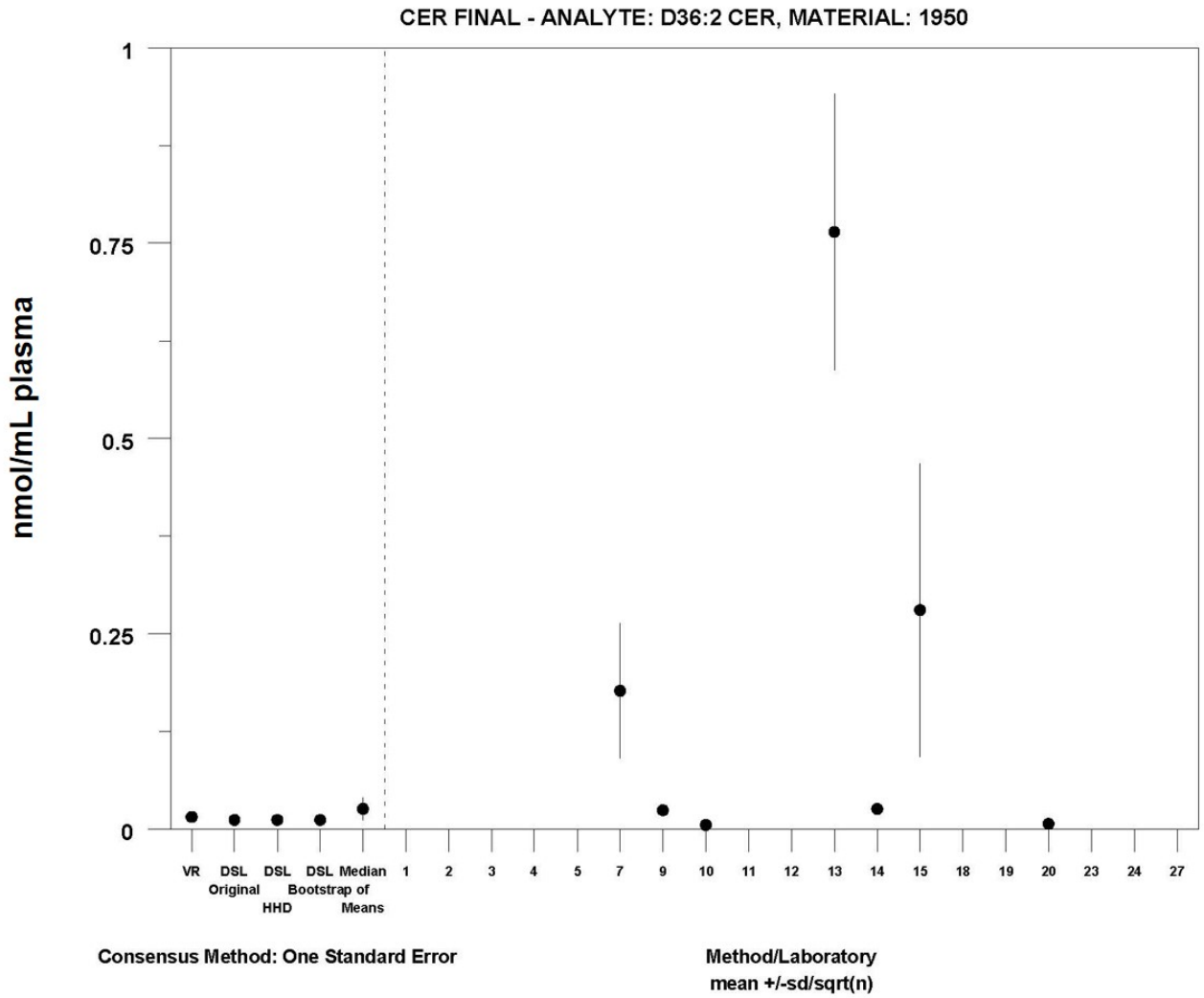
1: 1521 ± 538; 7: 272 ± 40; 19: 792 ± 25



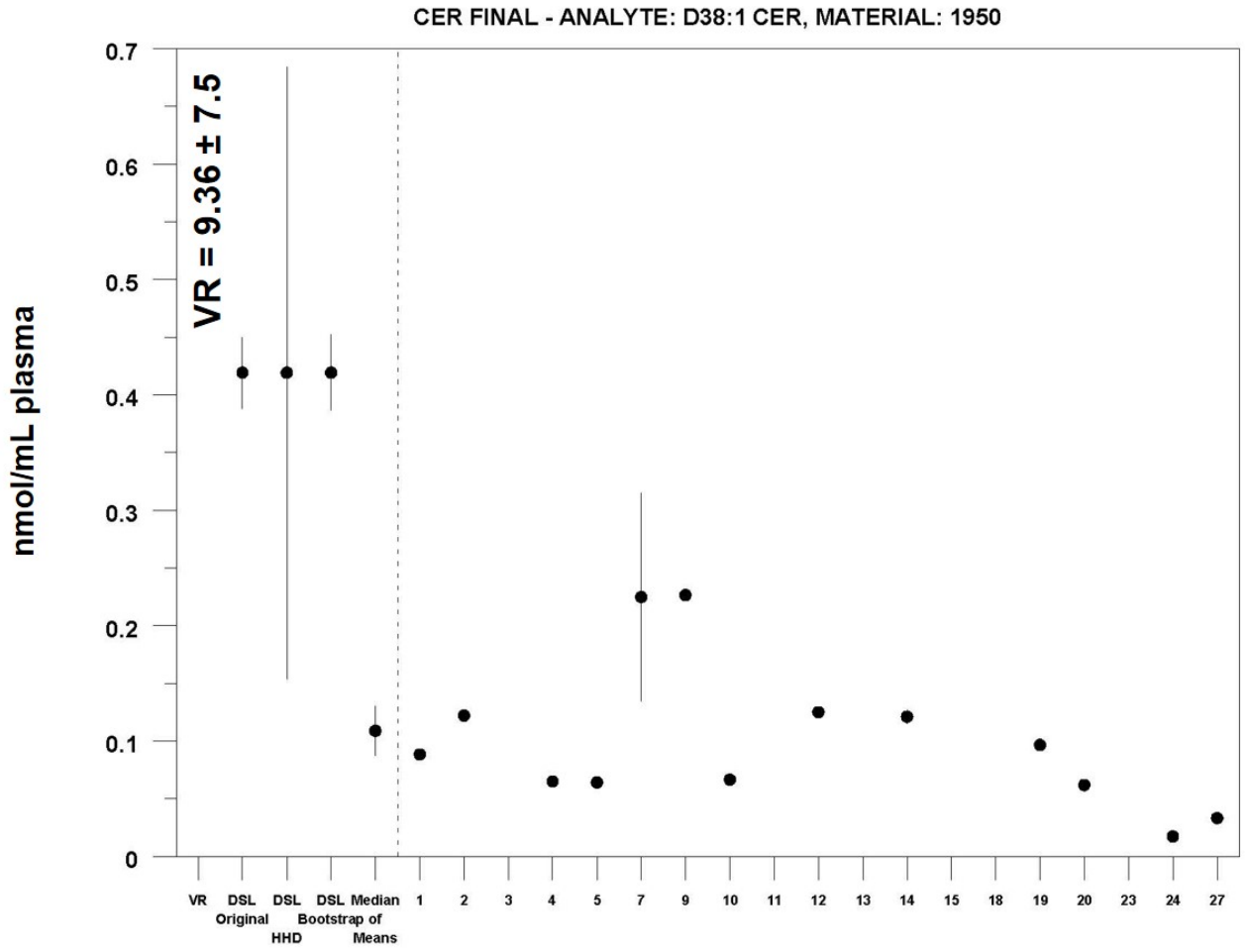








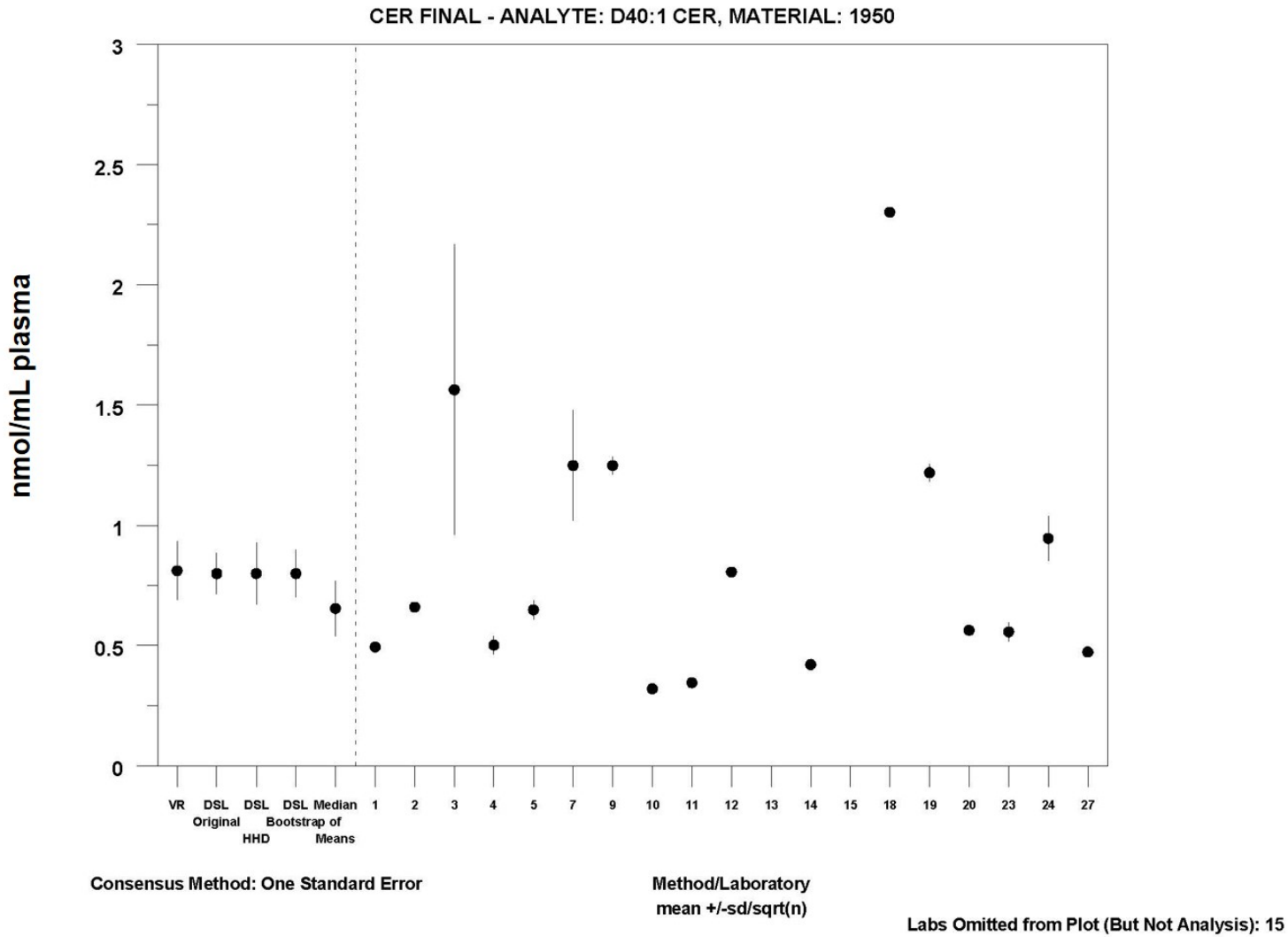
MEDM Location: 0.026 ± 0.014 nmol/mL

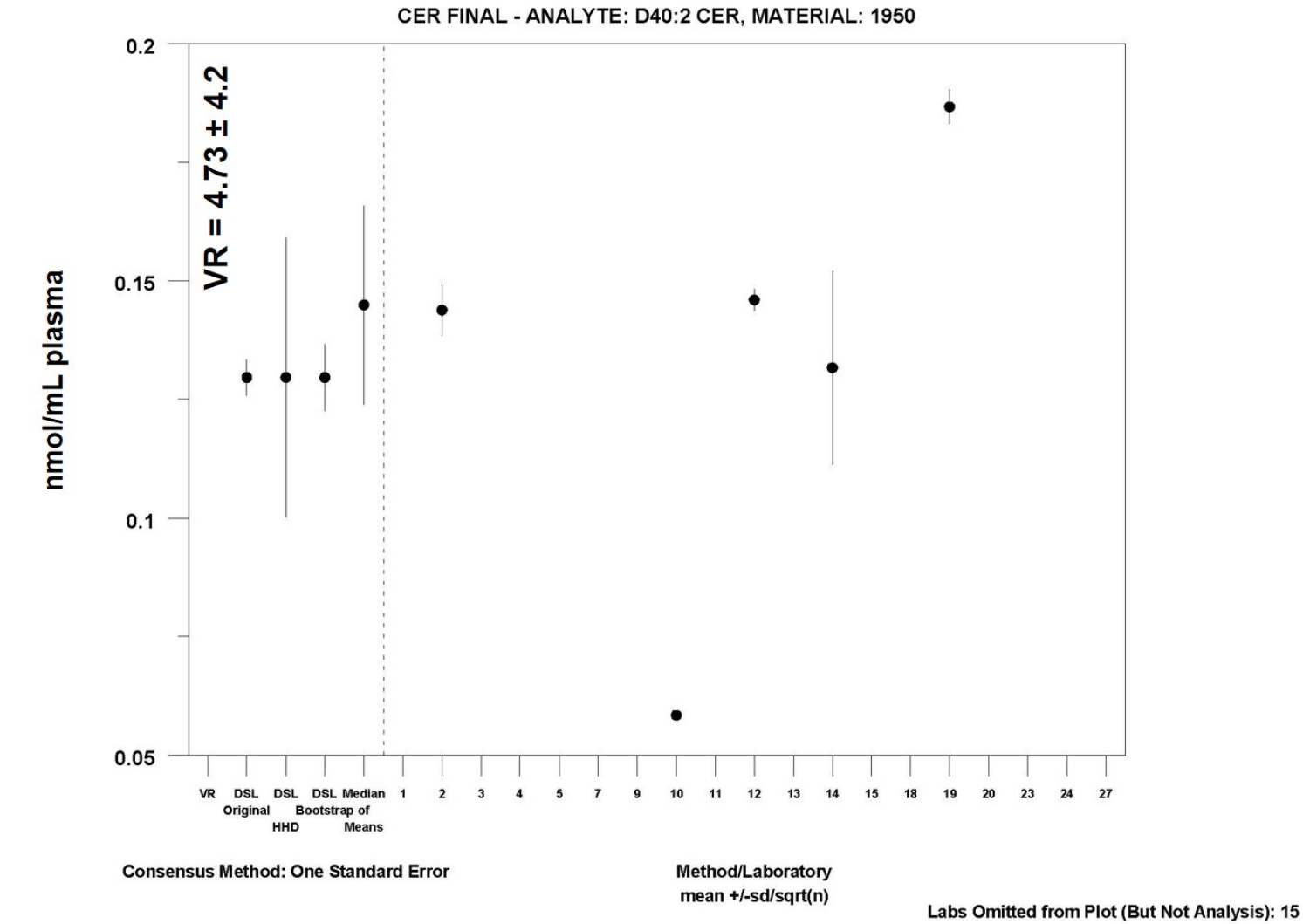


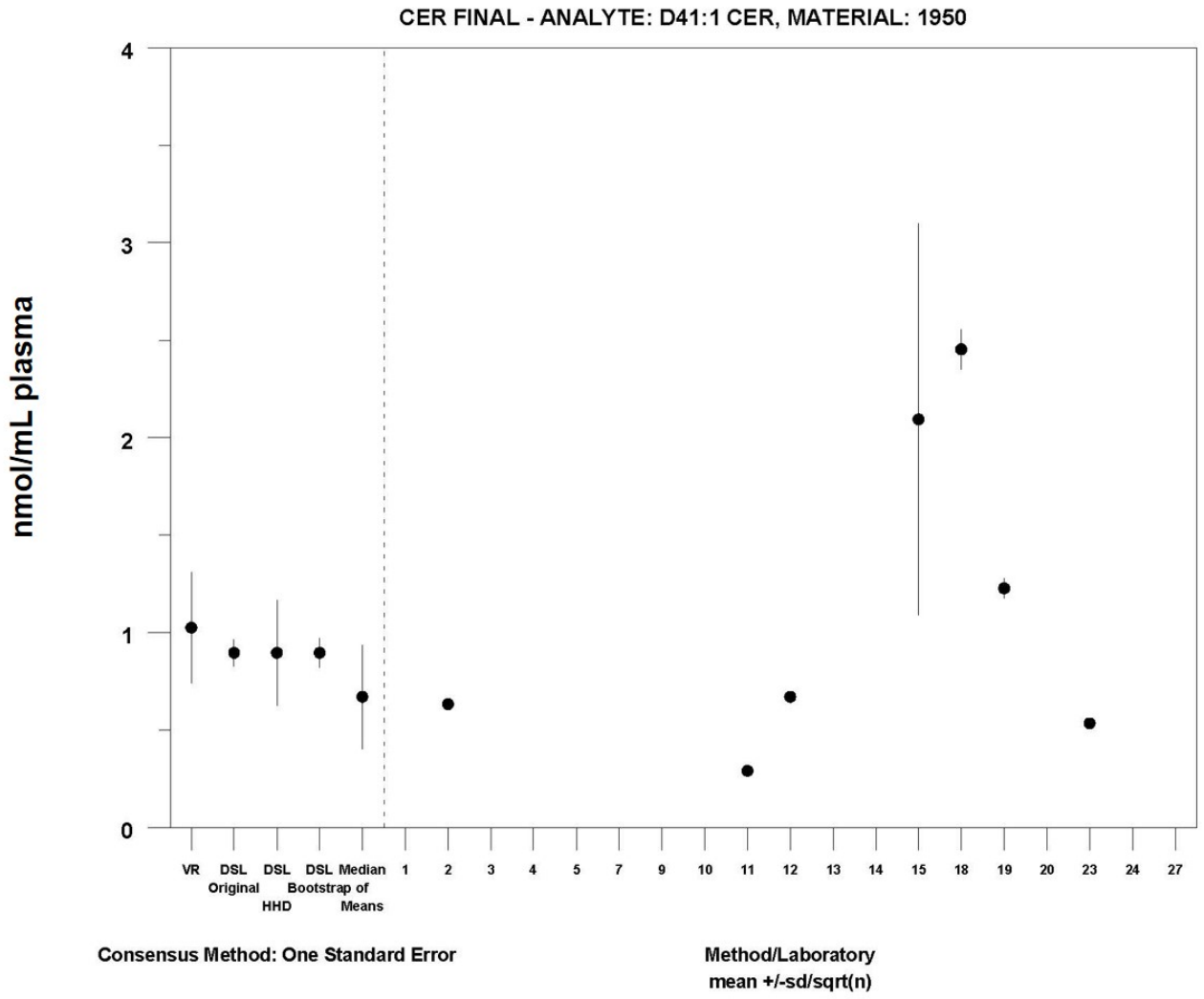
MEDM Location: 0.11 ± 0.021 nmol/mL

Labs Omitted from Plot (But Not Analysis): 13 15 18

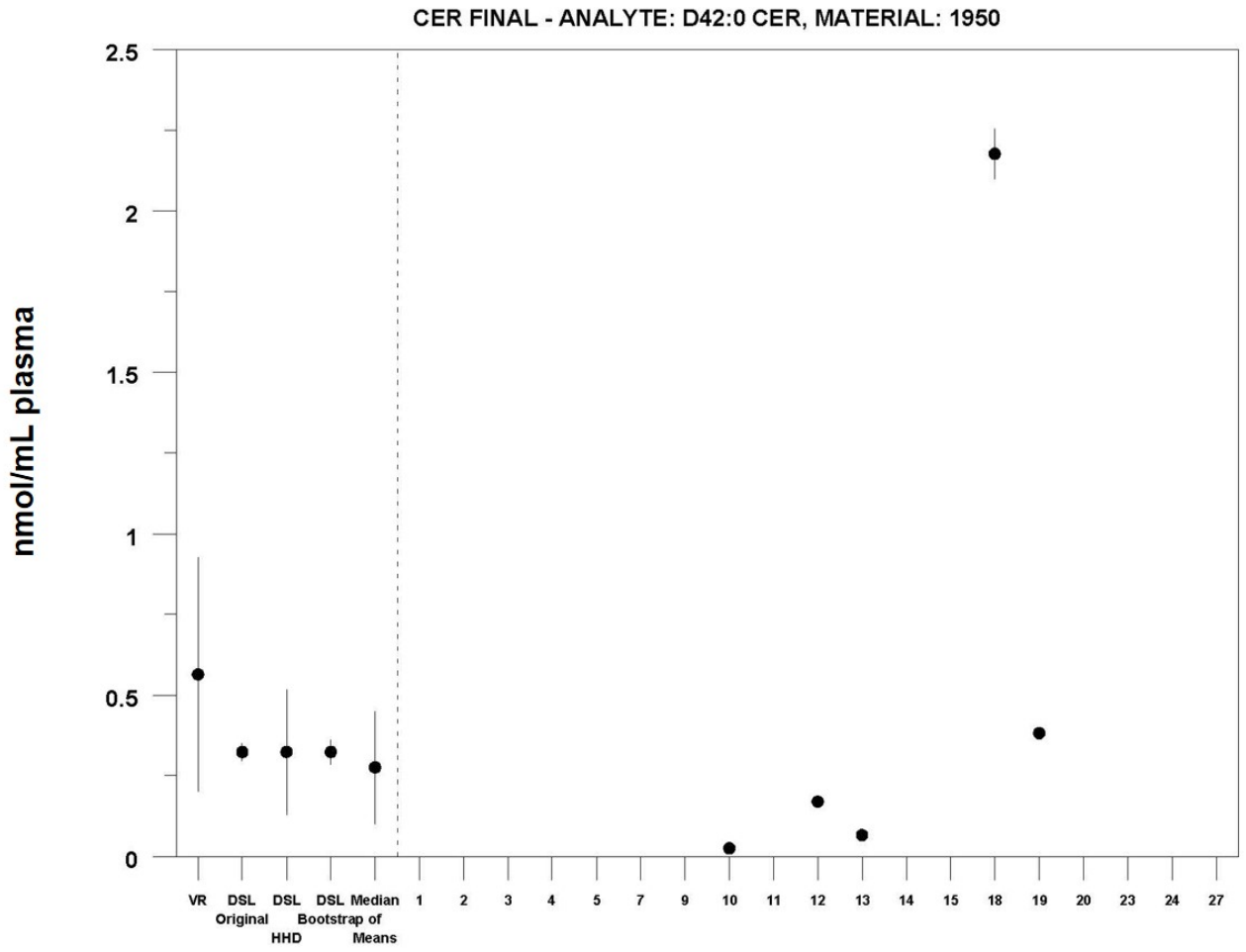
13: 1.25 ± 0.25; 15: 24 ± 1; 18: 123 ± 1







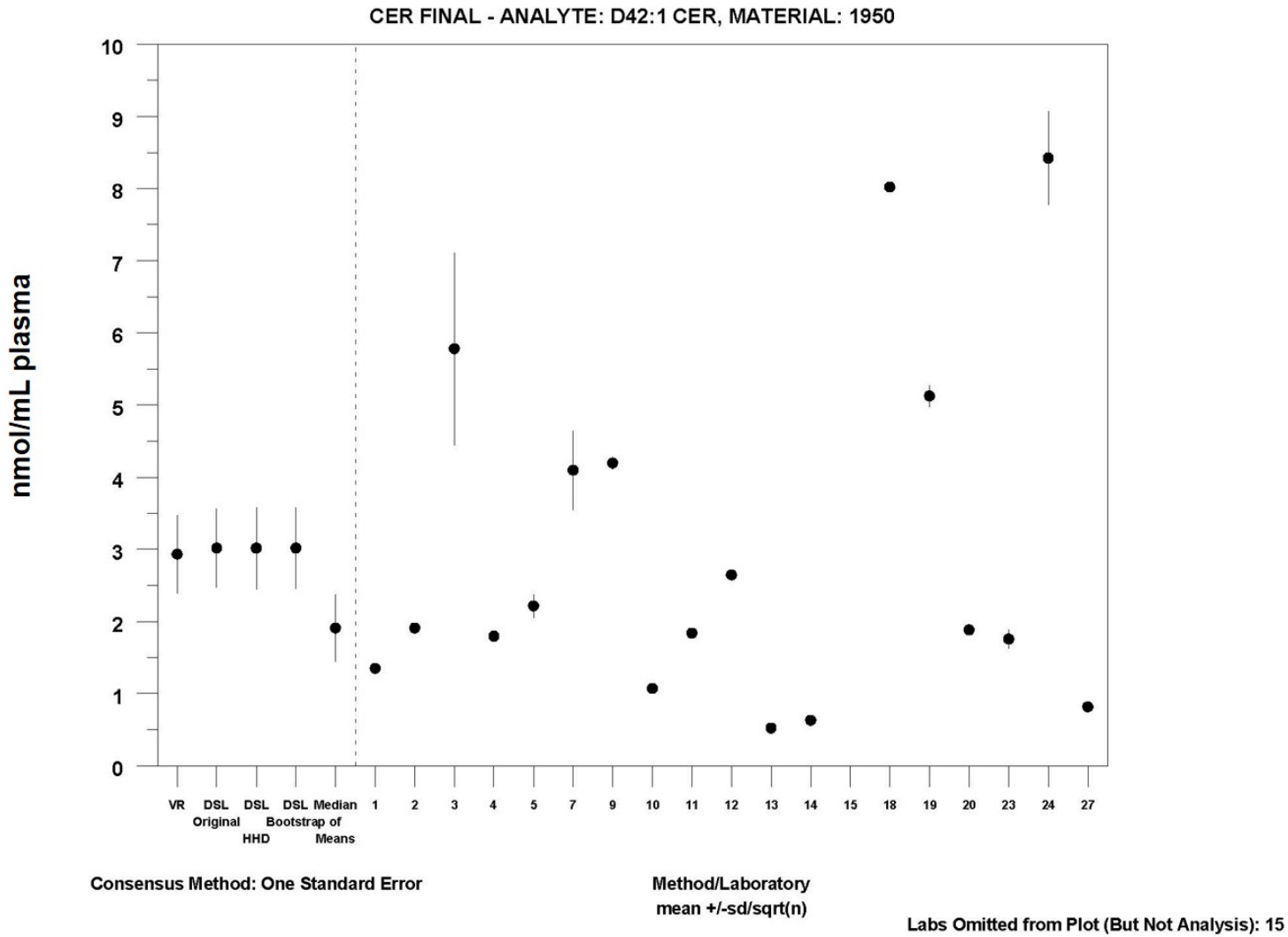
MEDM Location: 0.67 ± 0.27 nmol/mL

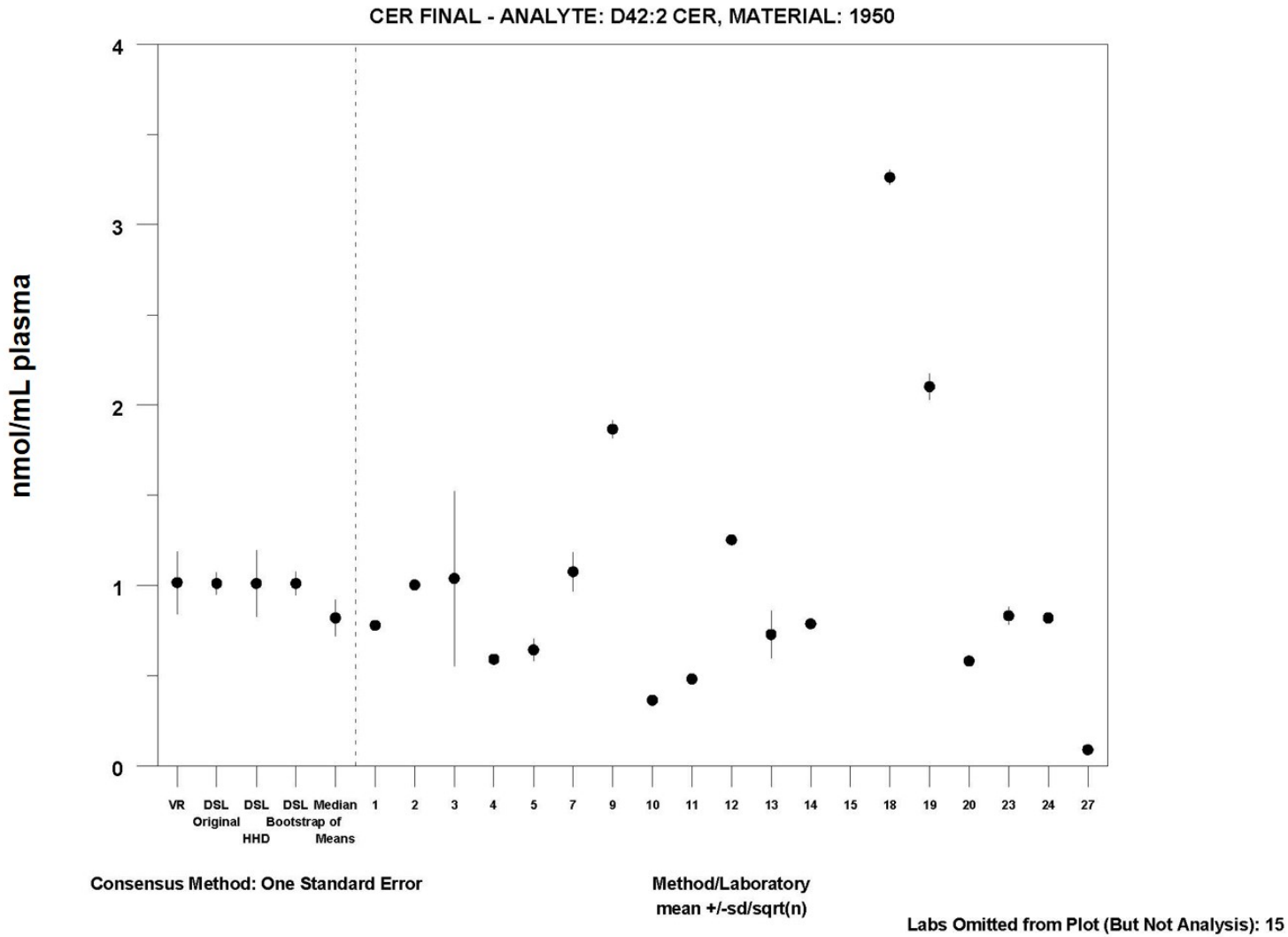


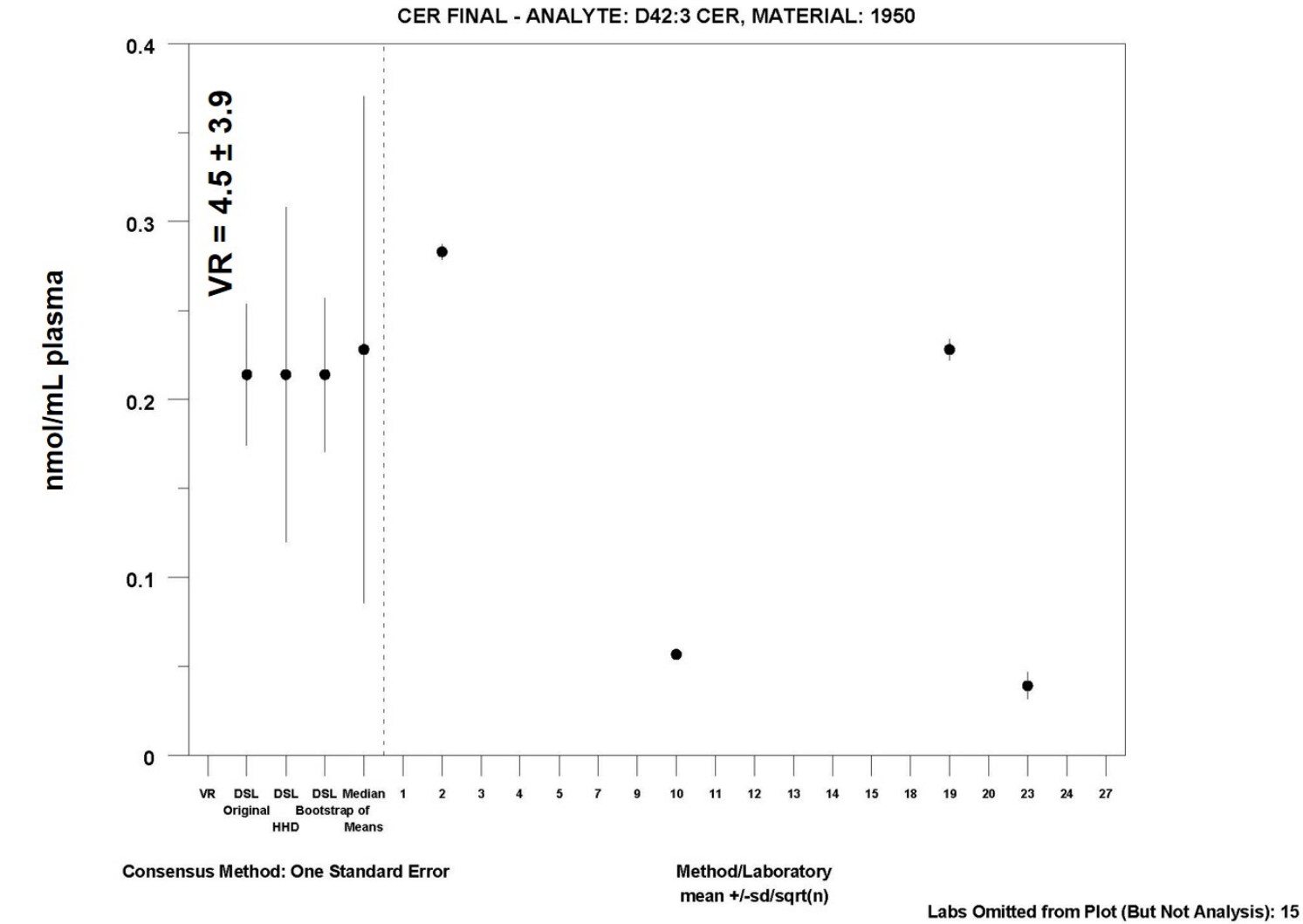
Labs Omitted from Plot (But Not Analysis): 15

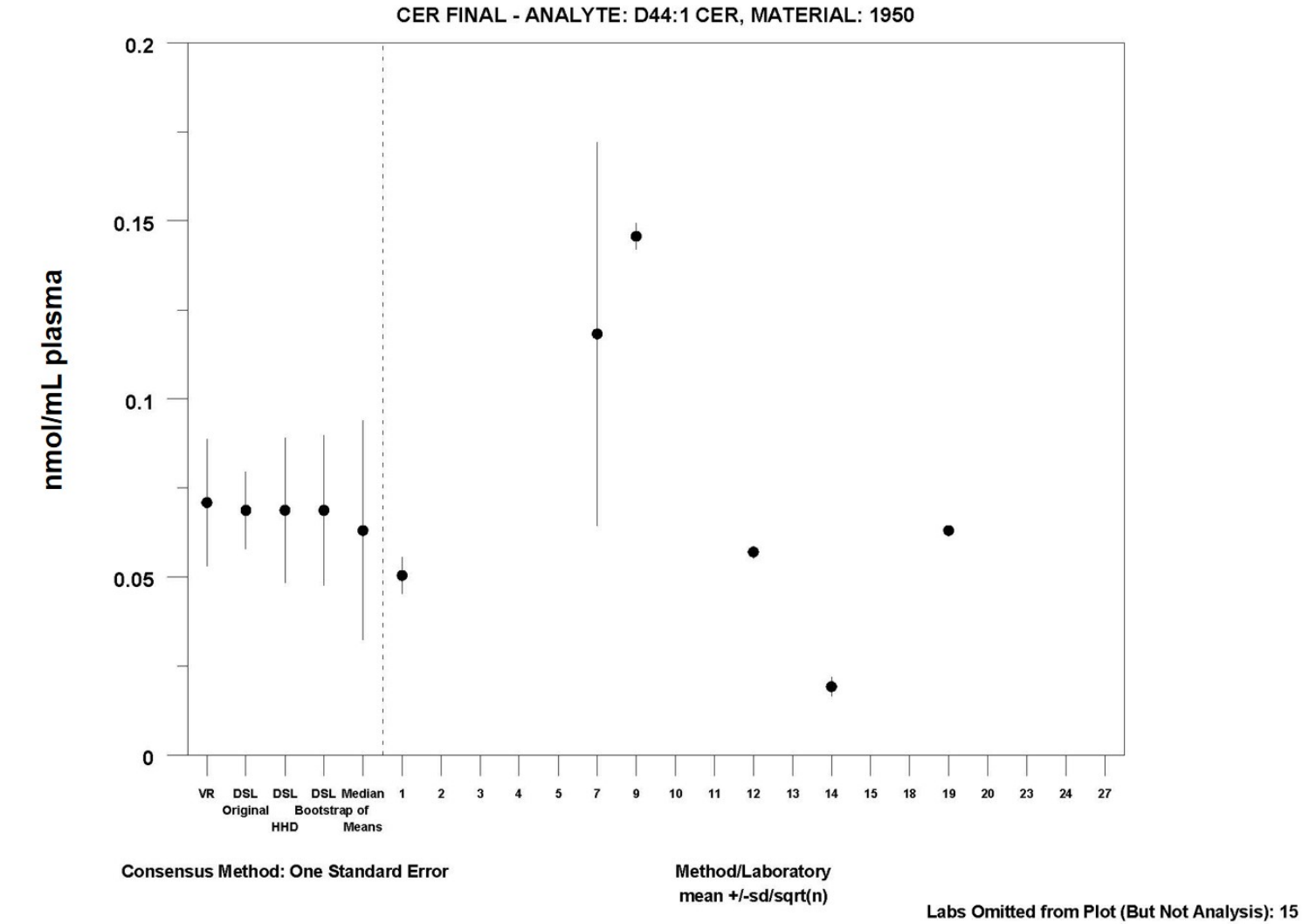
MEDM Location: 0.28 ± 0.18 nmol/mL

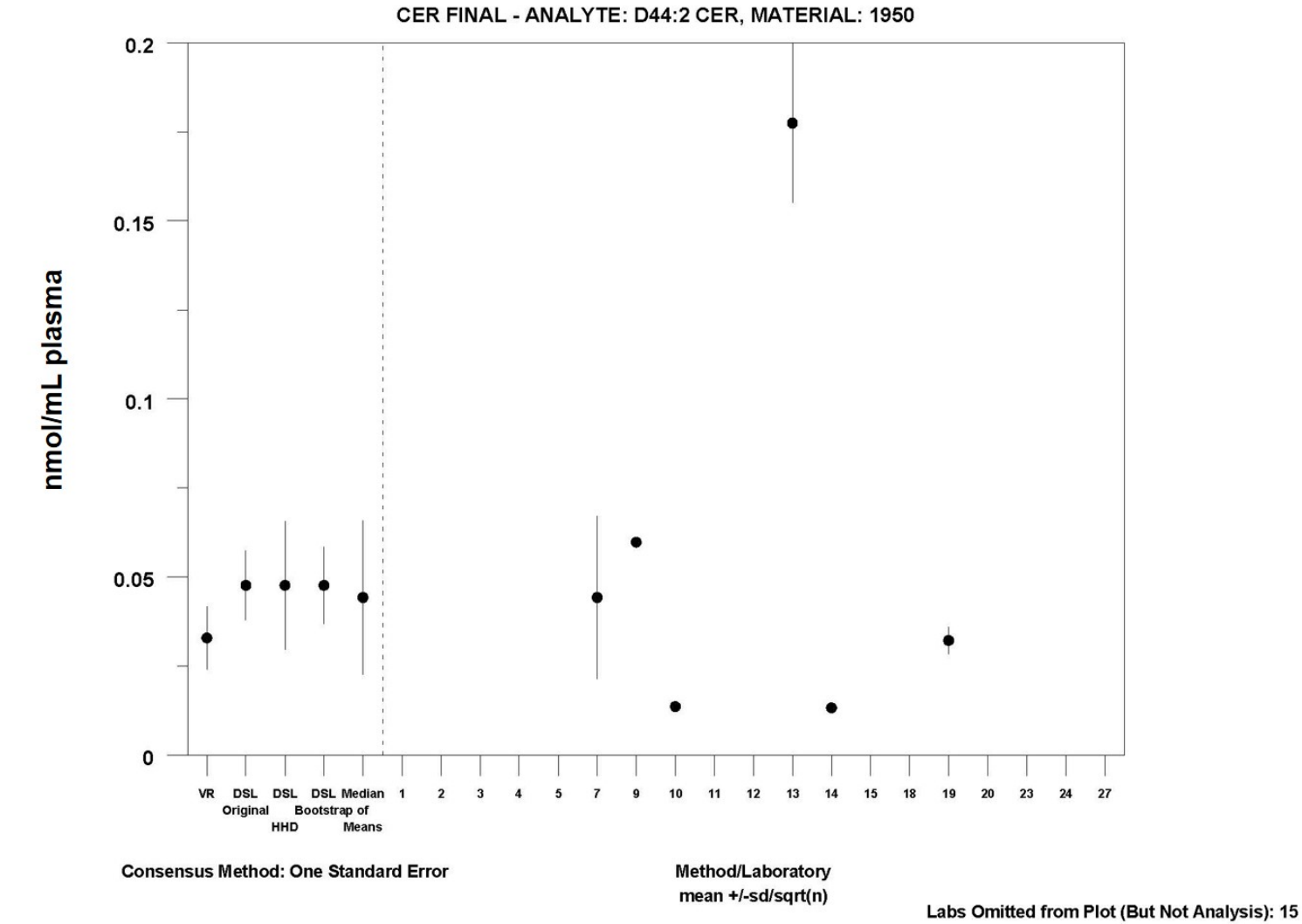
15: 129 ± 40

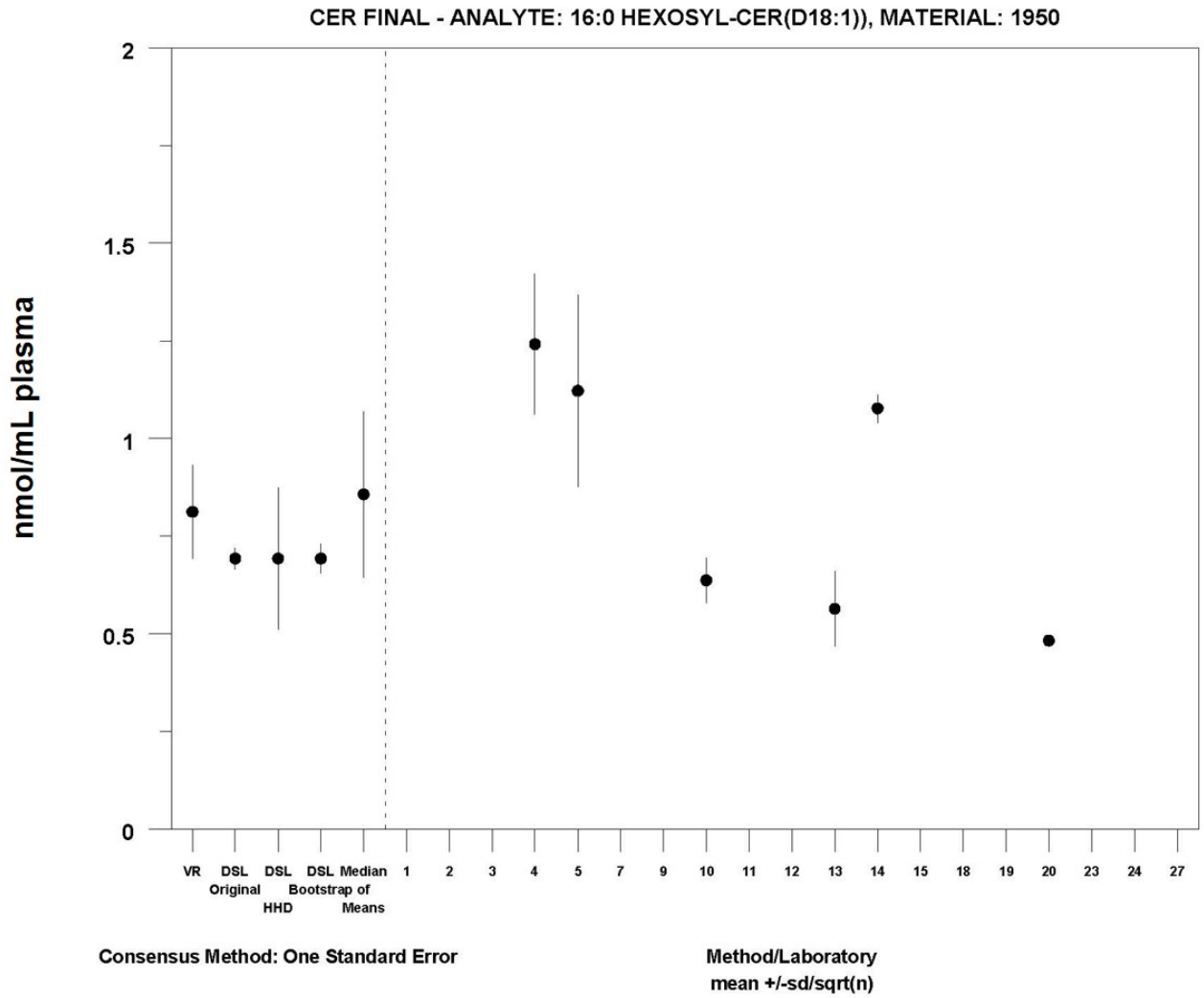




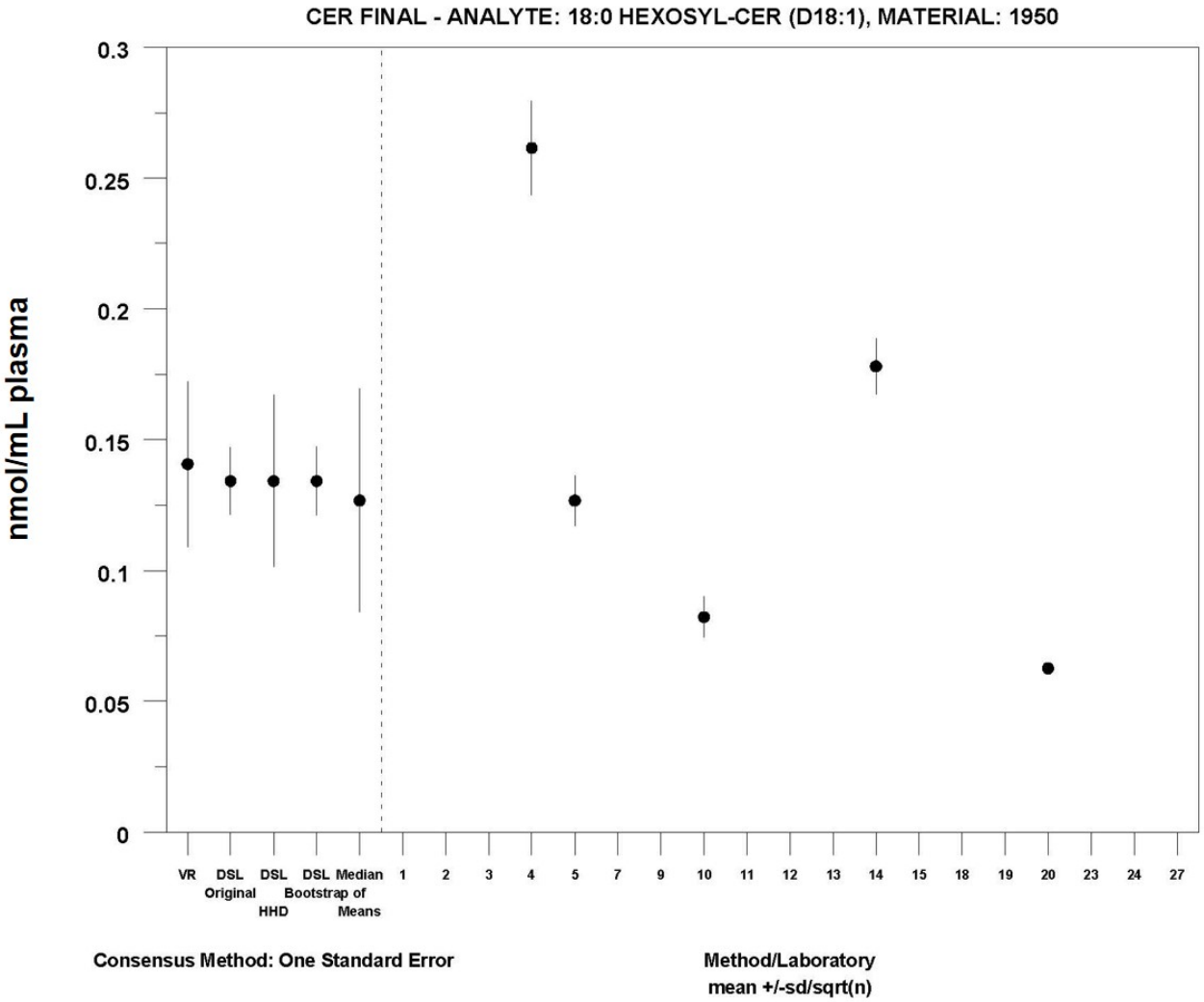




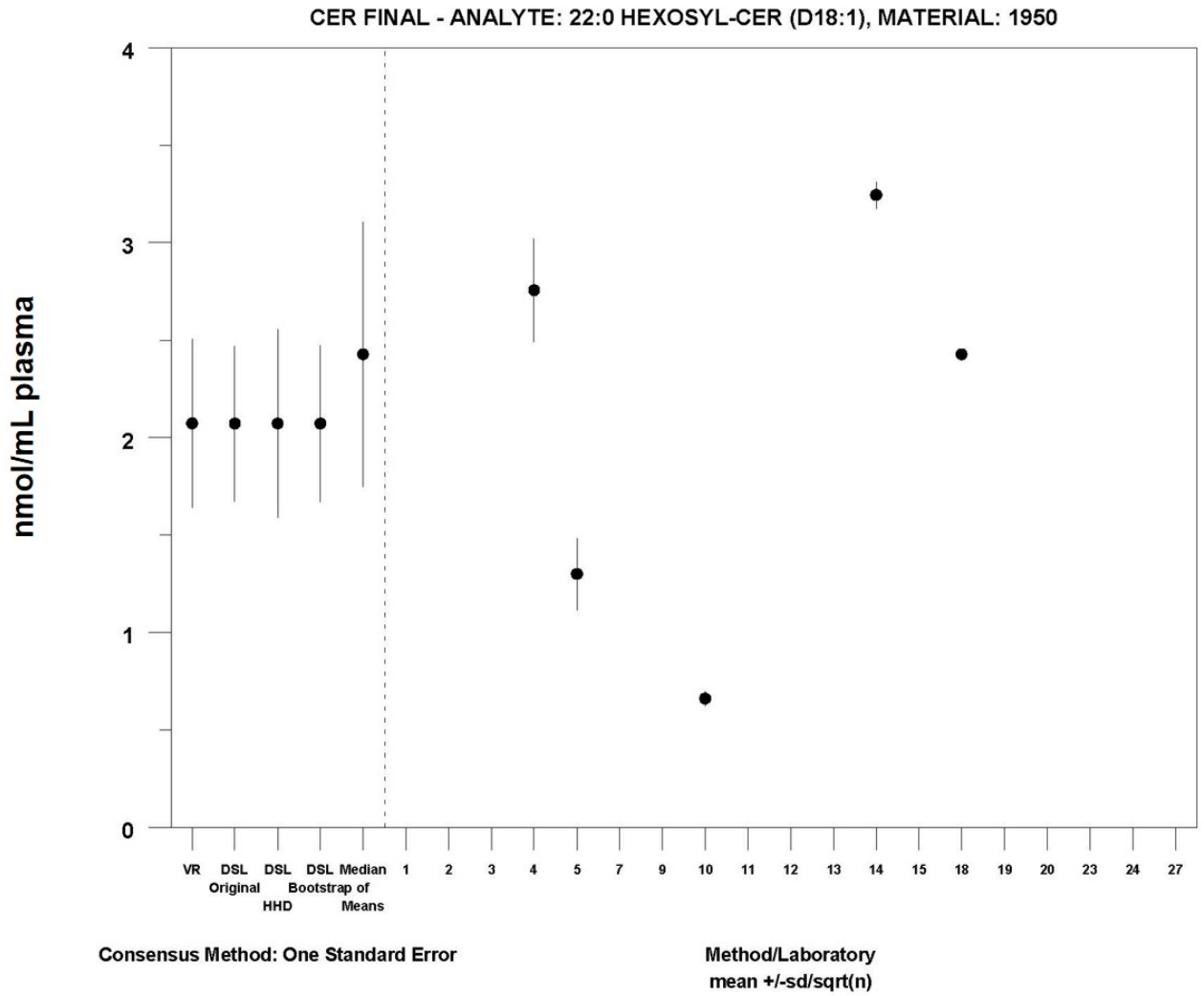




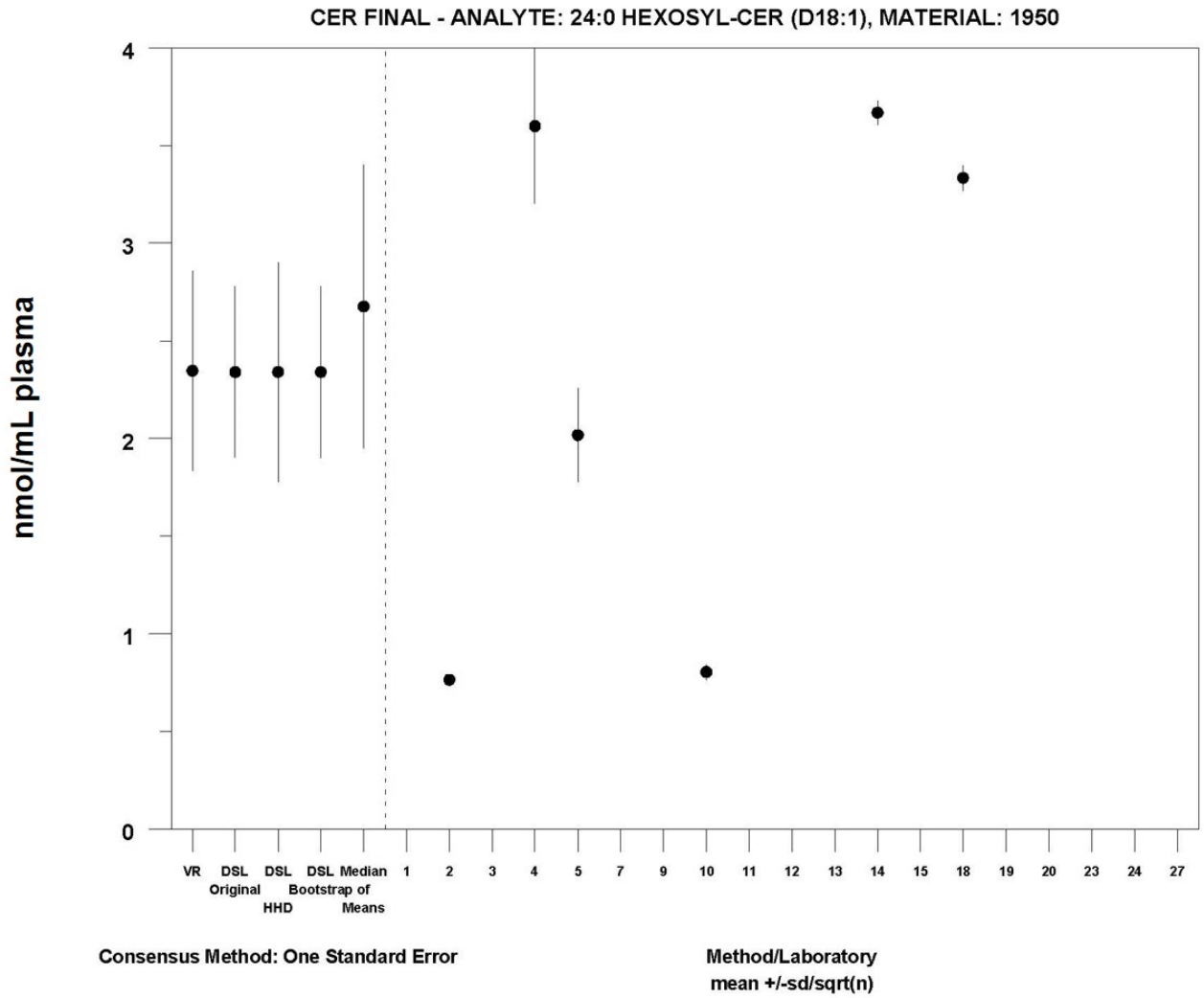
MEDM Location: 0.86 ± 0.21 nmol/mL



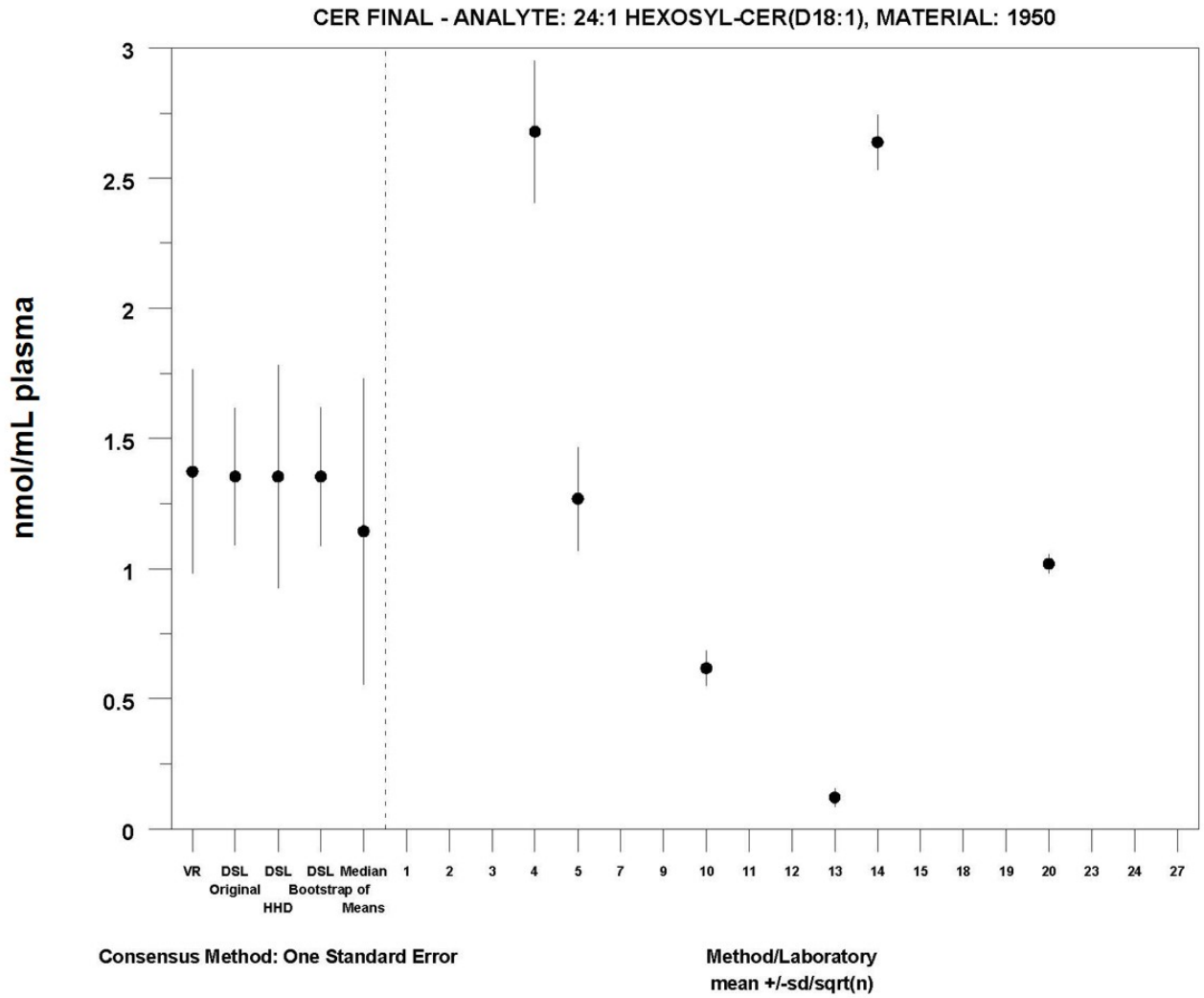
MEDM Location: 0.13 ± 0.043 nmol/mL



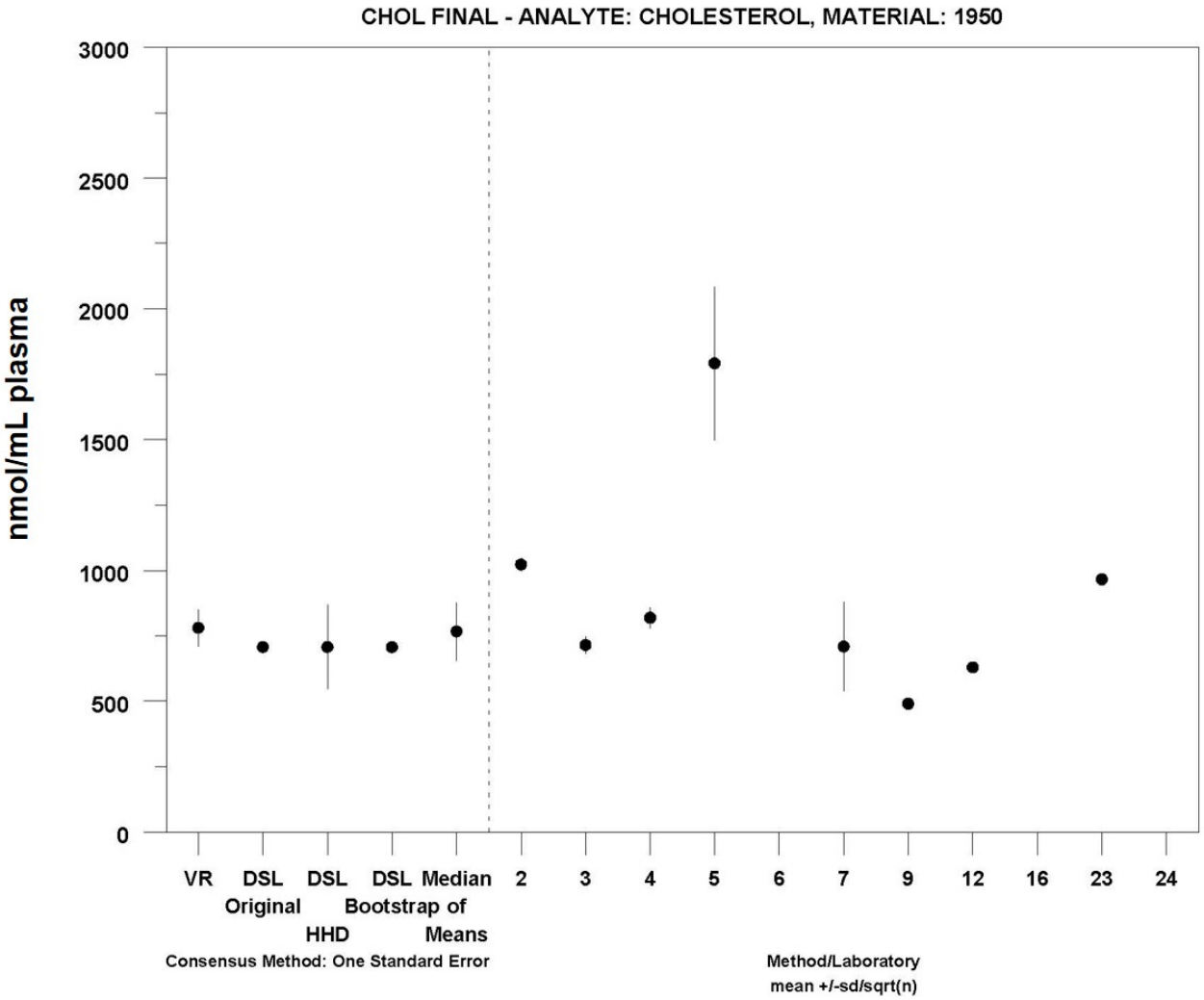
MEDM Location: 2.4 ± 0.68 nmol/mL



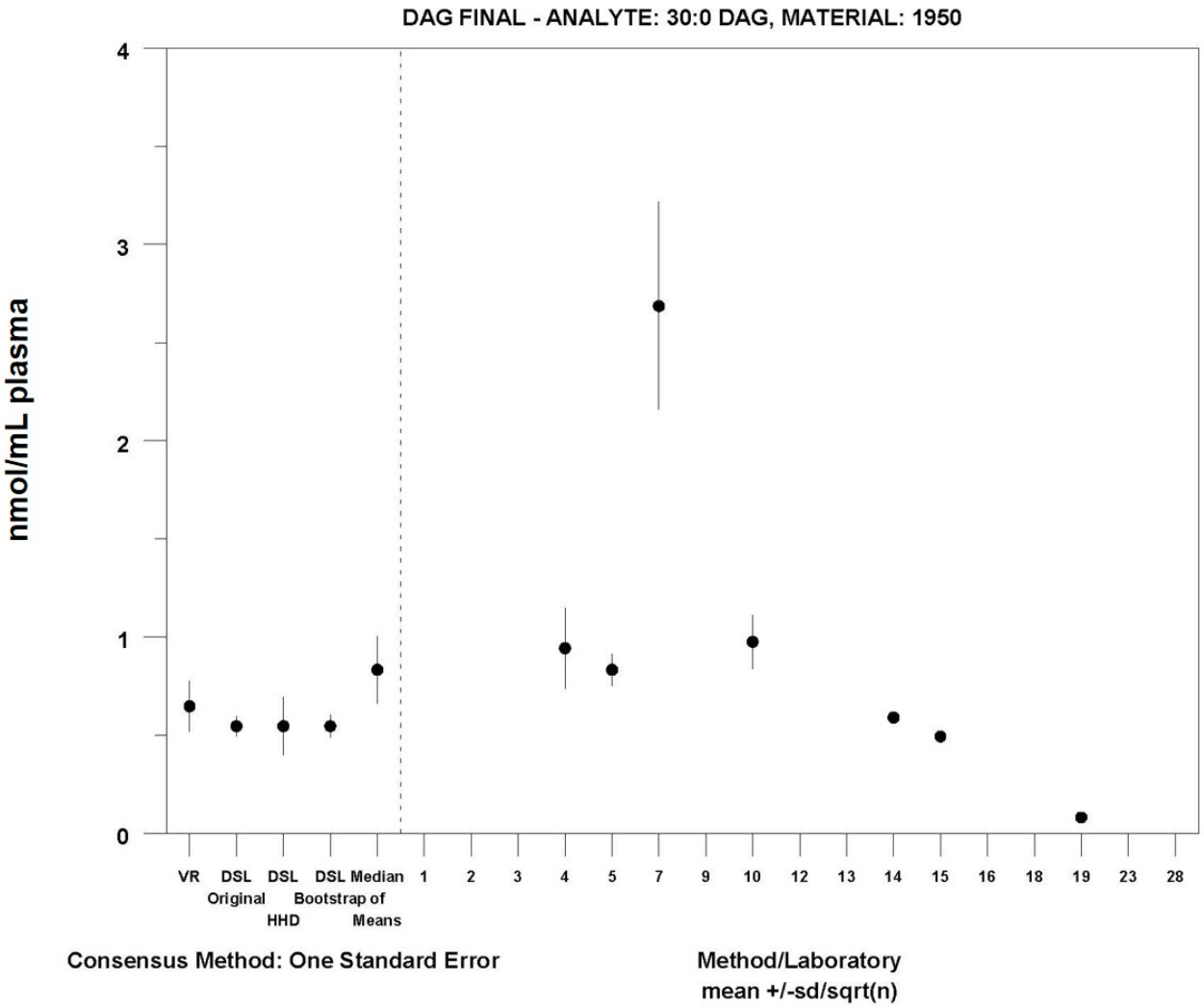
MEDM Location: 2.7 ± 0.73 nmol/mL



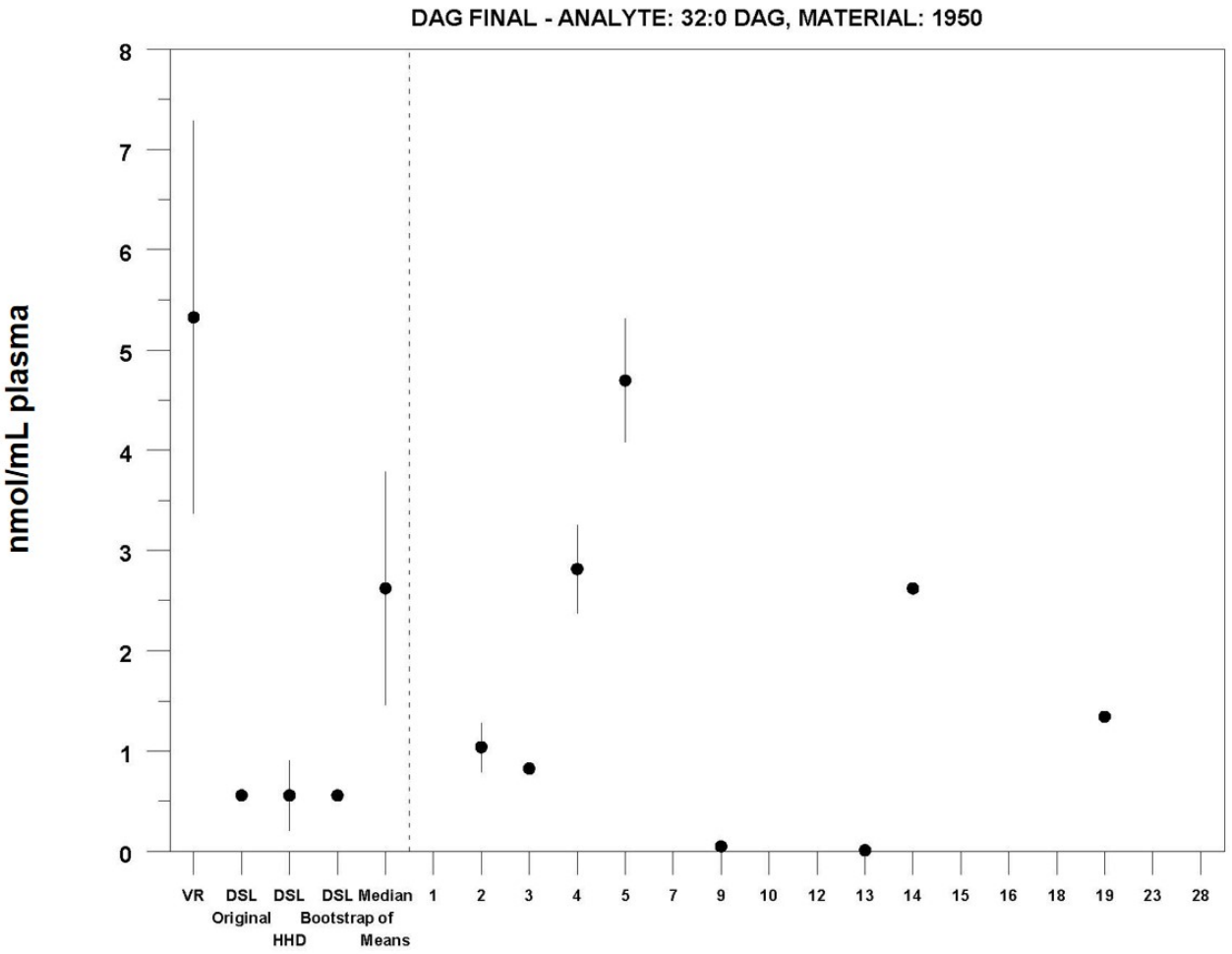
MEDM Location: 1.14 ± 1.17 nmol/mL



MEDM Location: 770 ± 110 nmol/mL



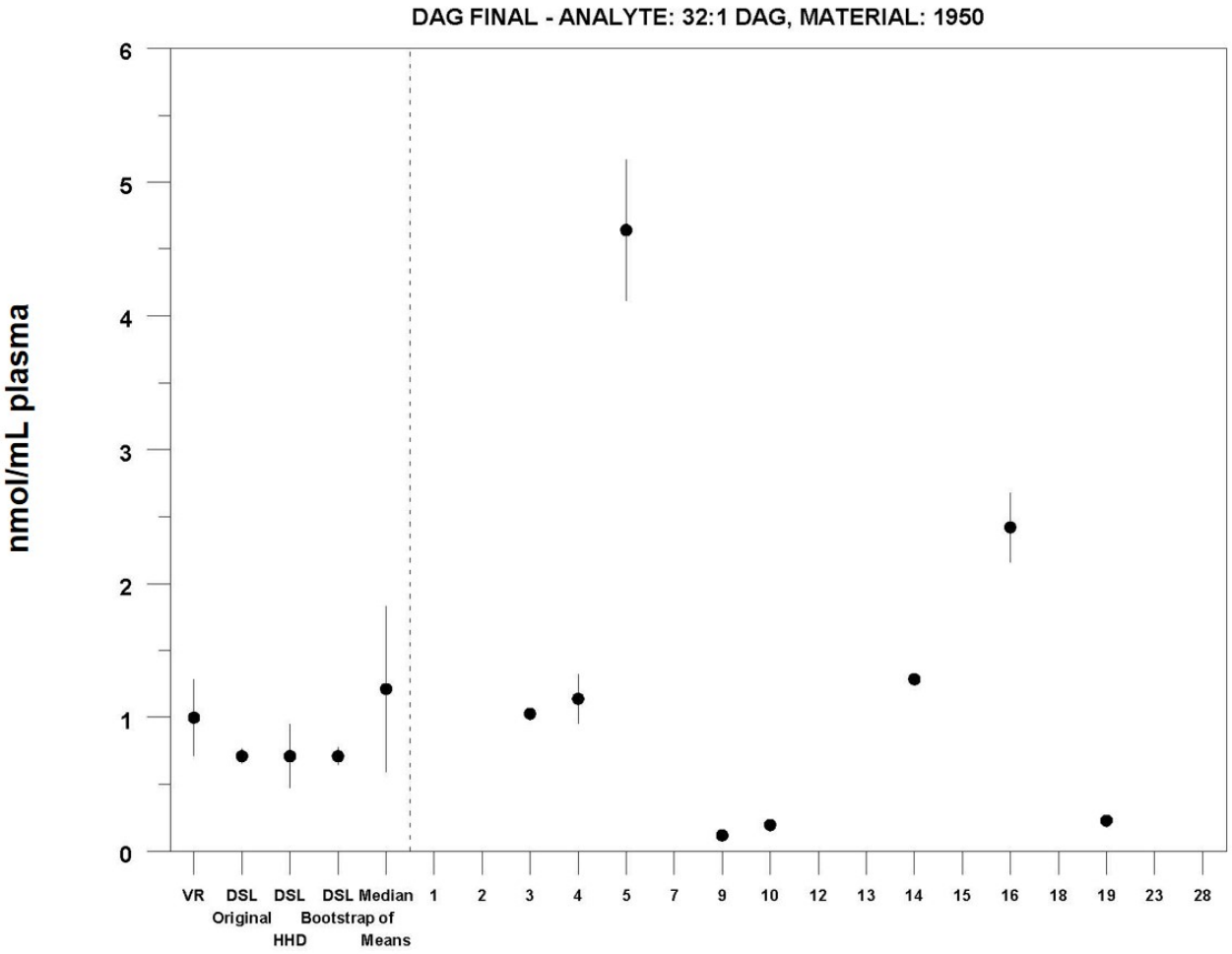
MEDM Location: 0.83 ± 0.17 nmol/mL



MEDM Location: 2.6 ± 1.2 nmol/mL

Labs Omitted from Plot (But Not Analysis): 7 10 15

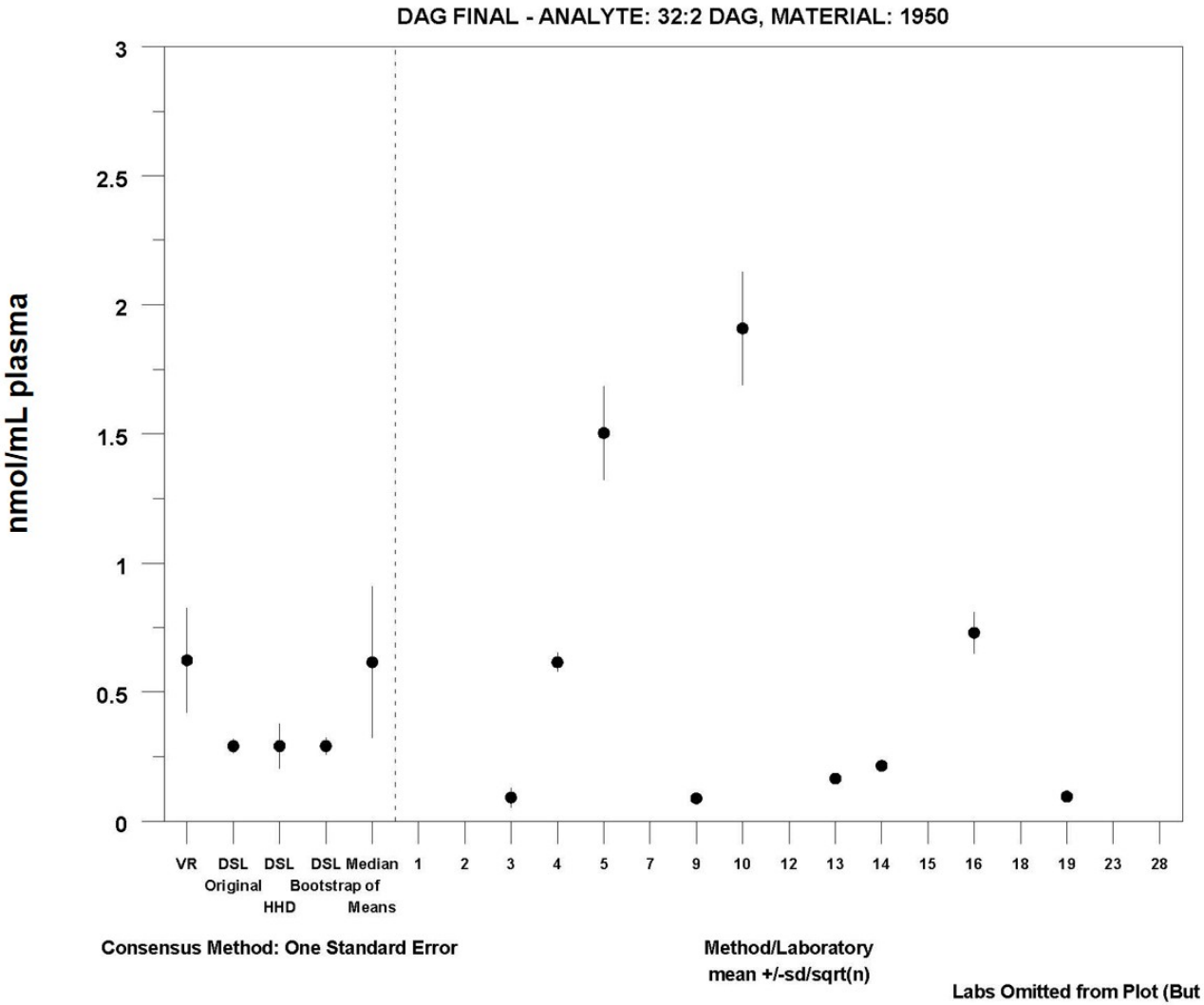
7: 10.37 ± 0.81; 10: 20.87 ± 2.58; 15: 15.34 ± 2.53



Labs Omitted from Plot (But Not Analysis): 7 15

MEDM Location: 1.2 ± 0.62 nmol/mL

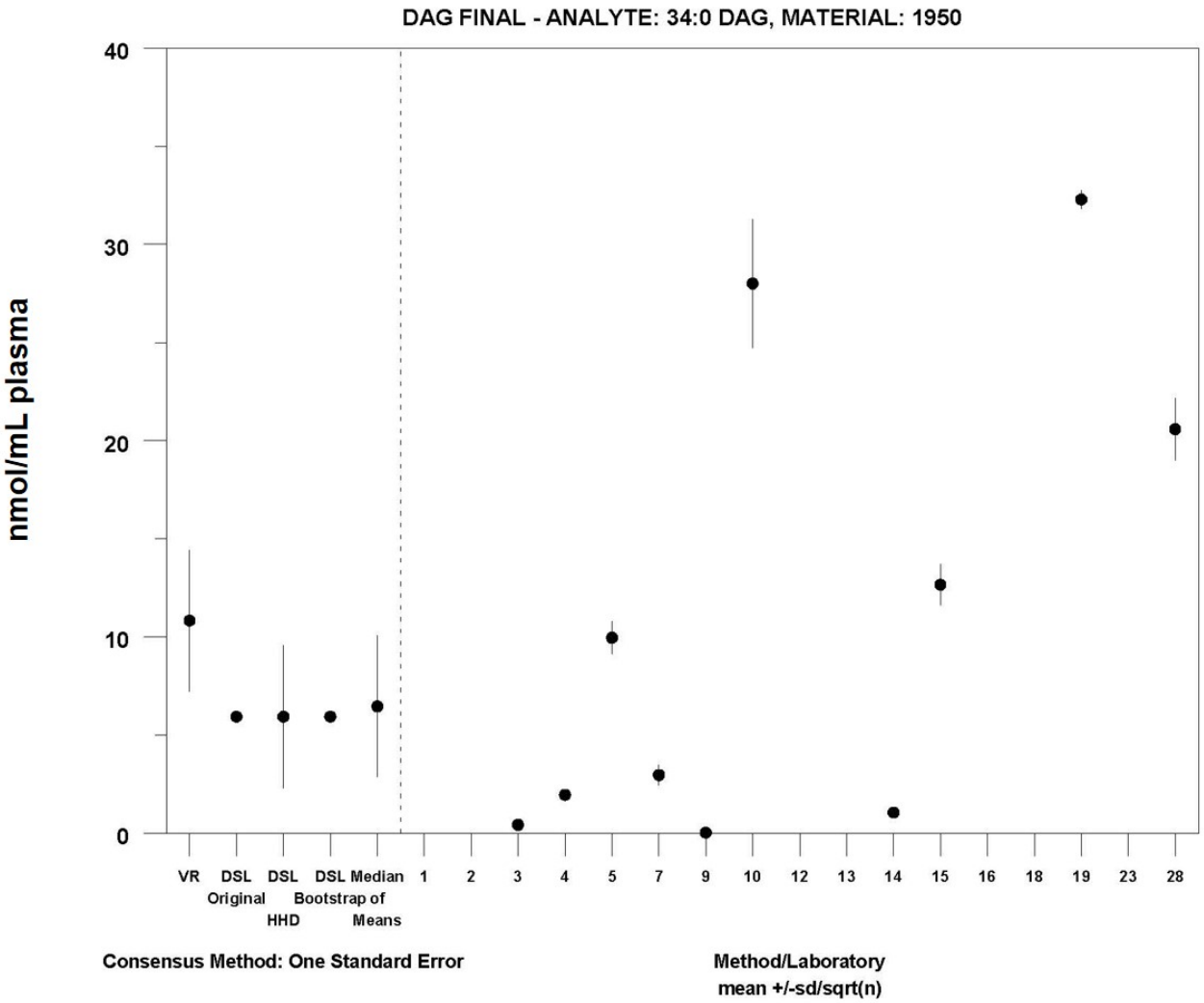
7: 9.71 ± 2.85; 15: 21.97 ± 5.40



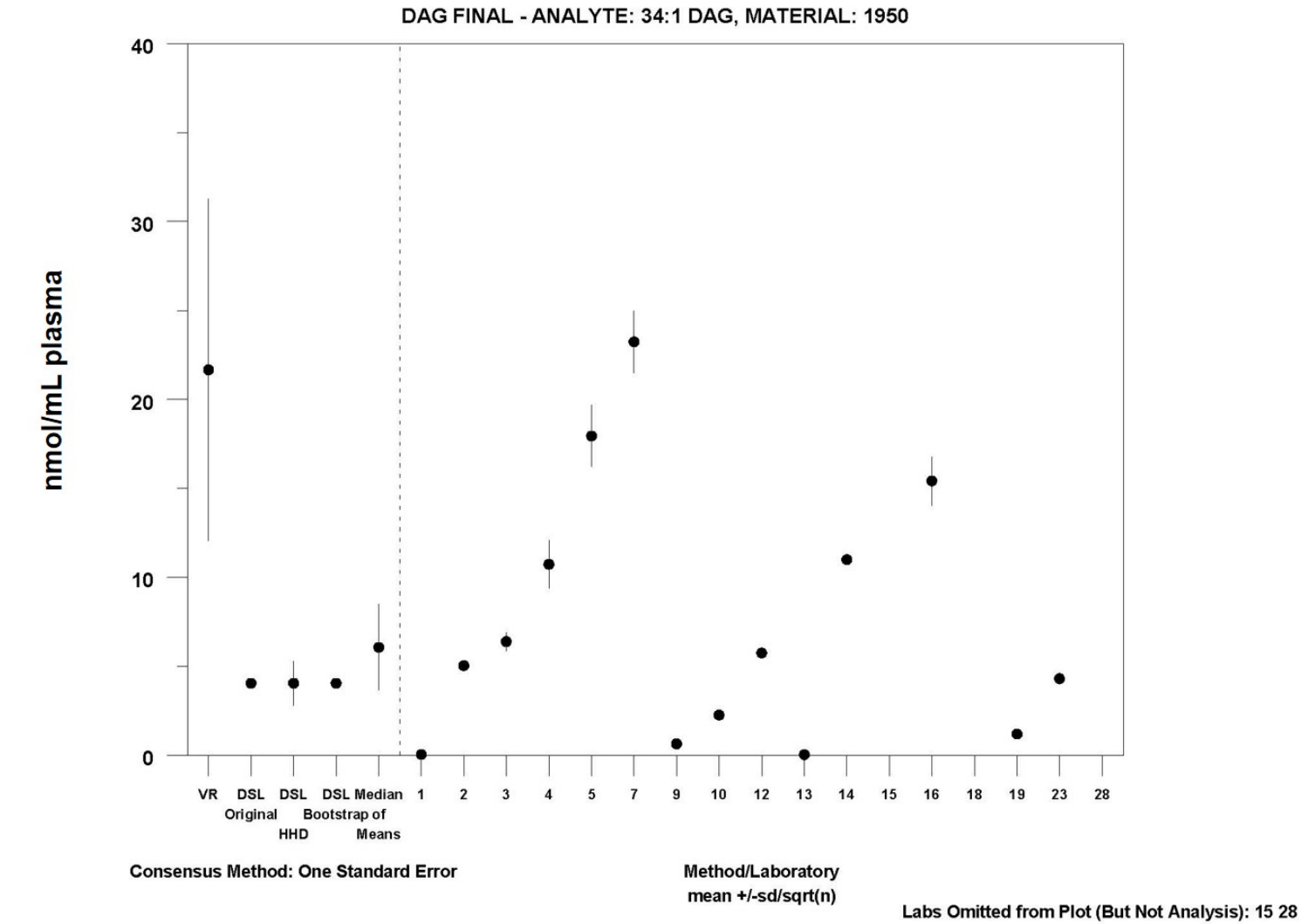
MEDM Location: 0.62 ± 0.29 nmol/mL

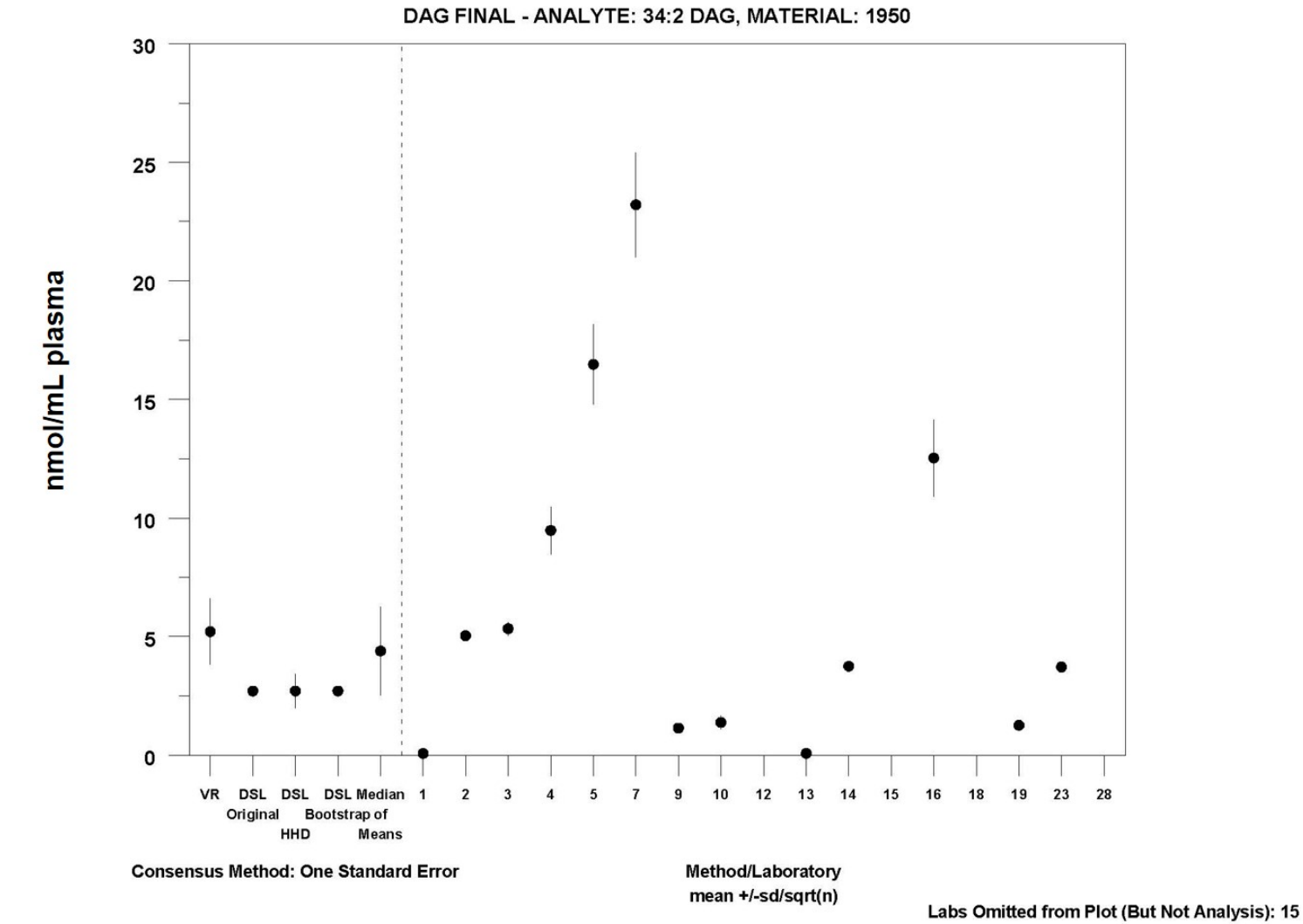
Labs Omitted from Plot (But Not Analysis): 7 15

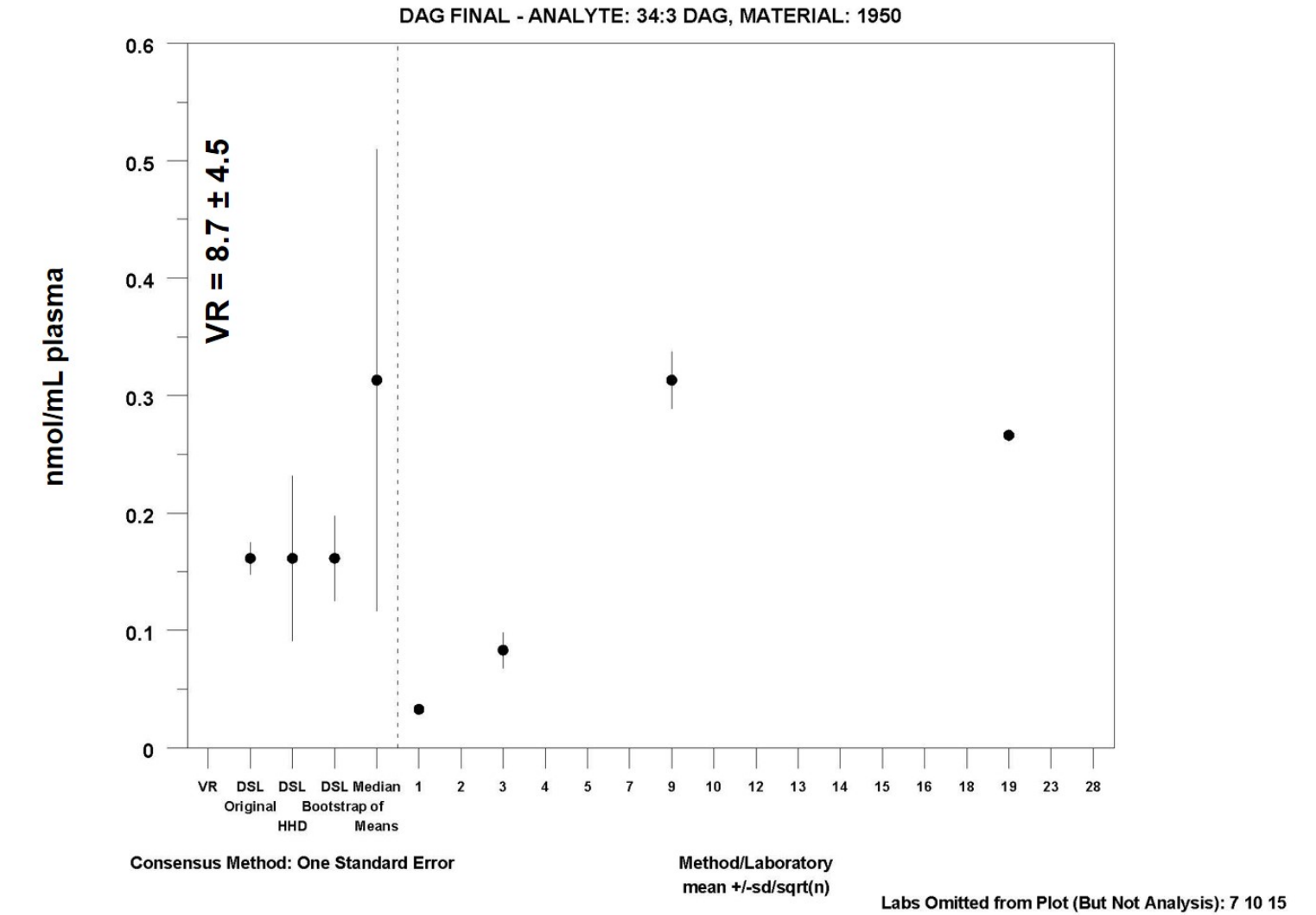
7: 6.55 ± 1.57; 15: 4.30 ± 1.48

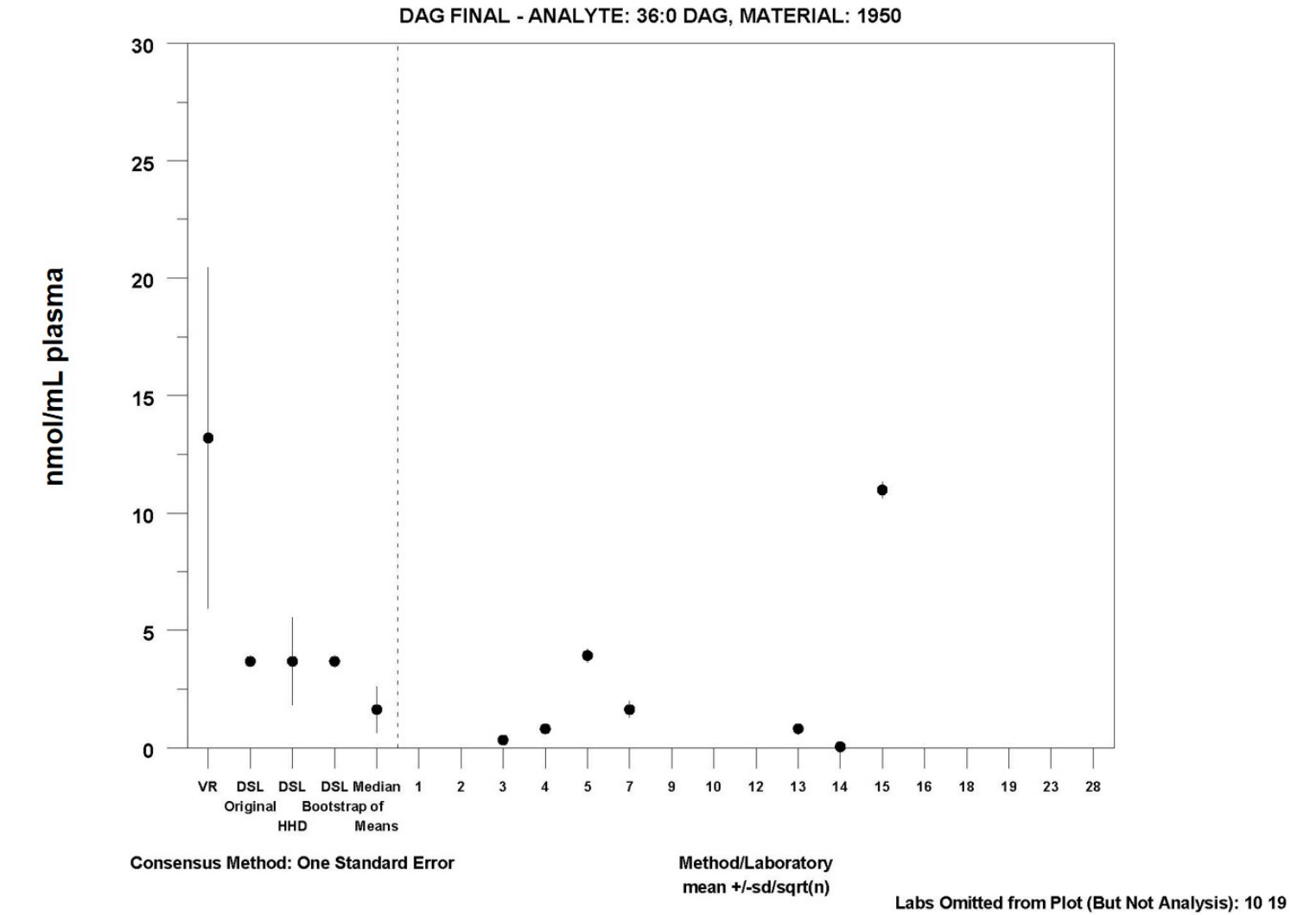


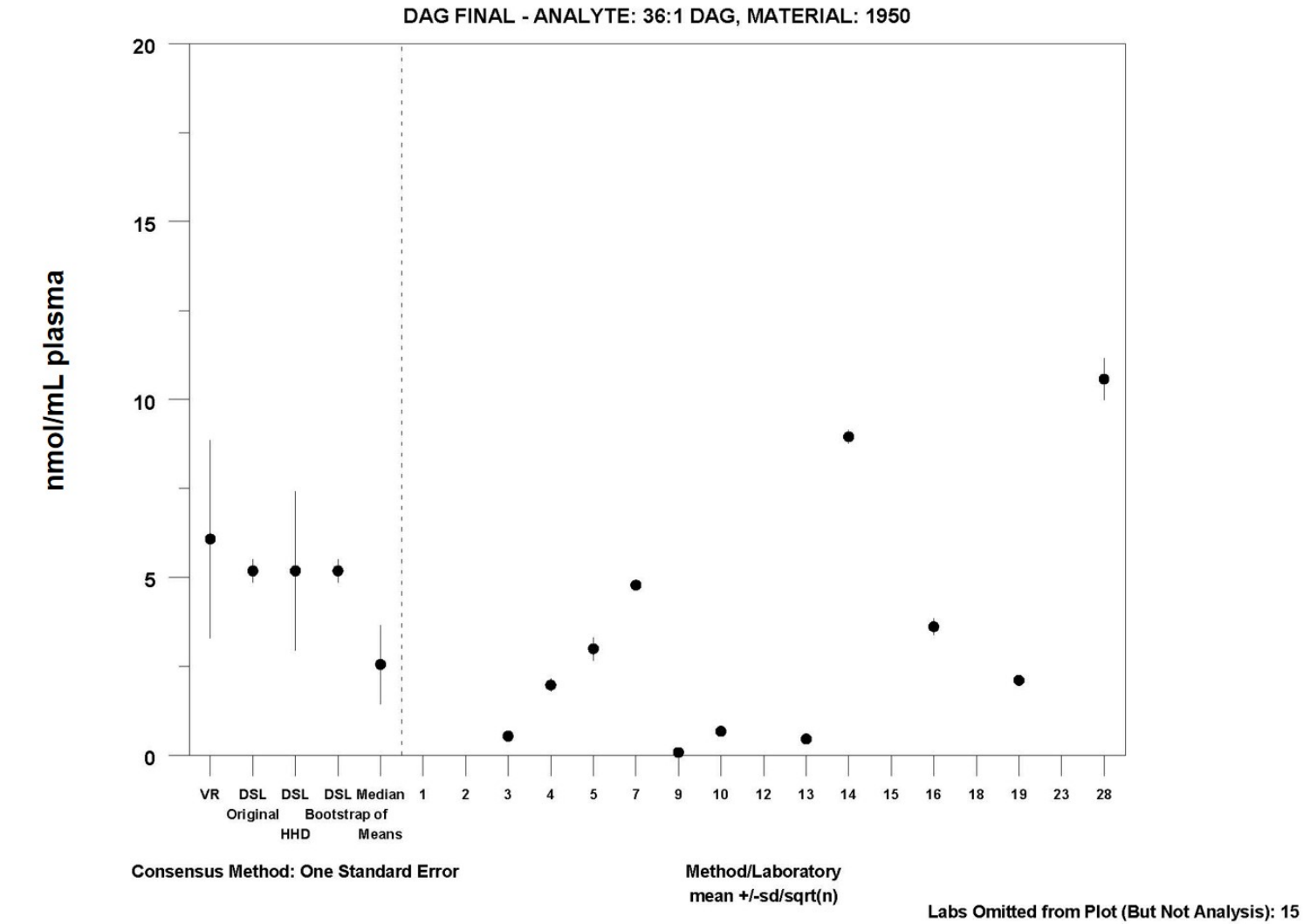
MEDM Location: 6.5 ± 3.6 nmol/mL

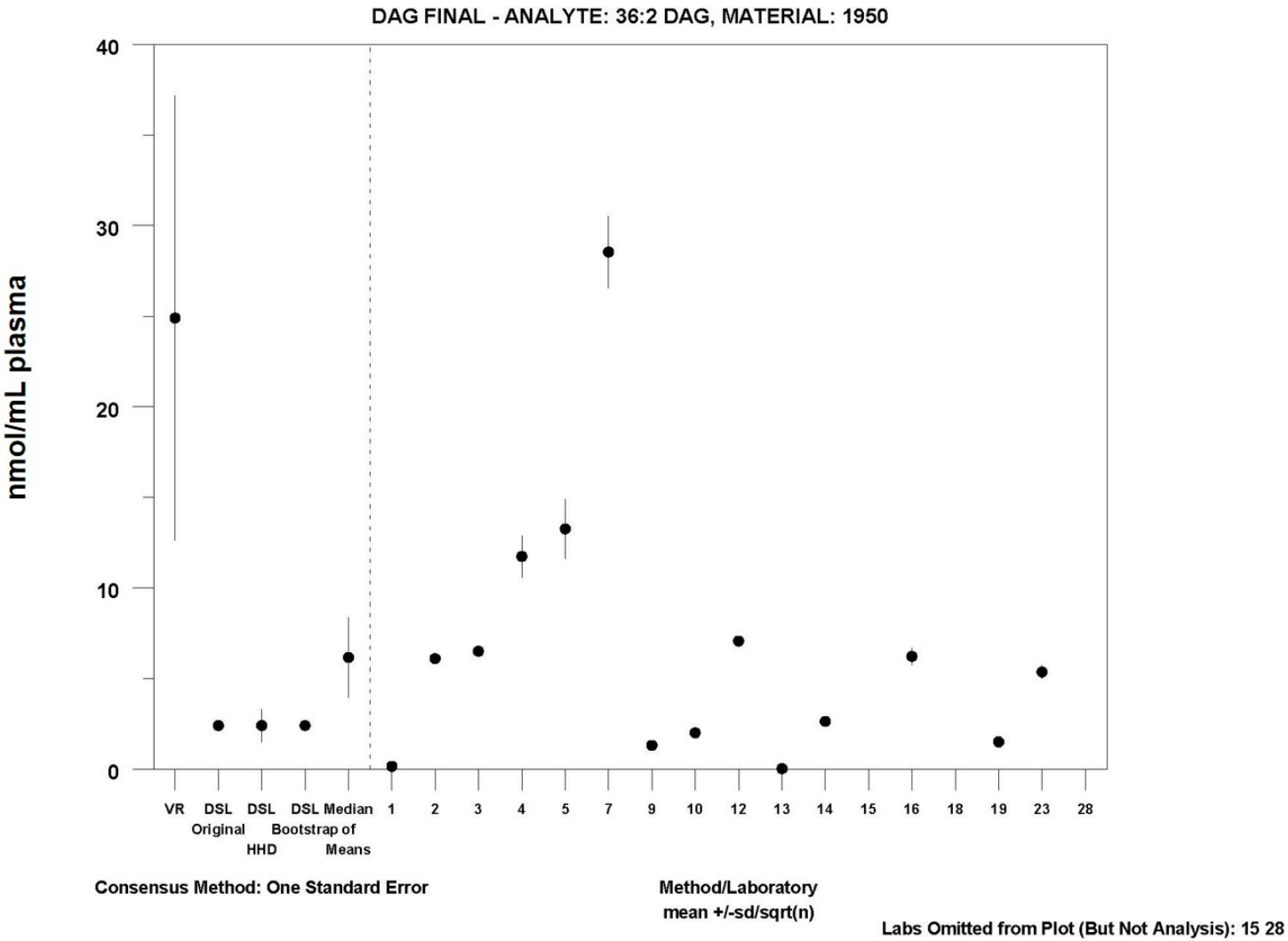


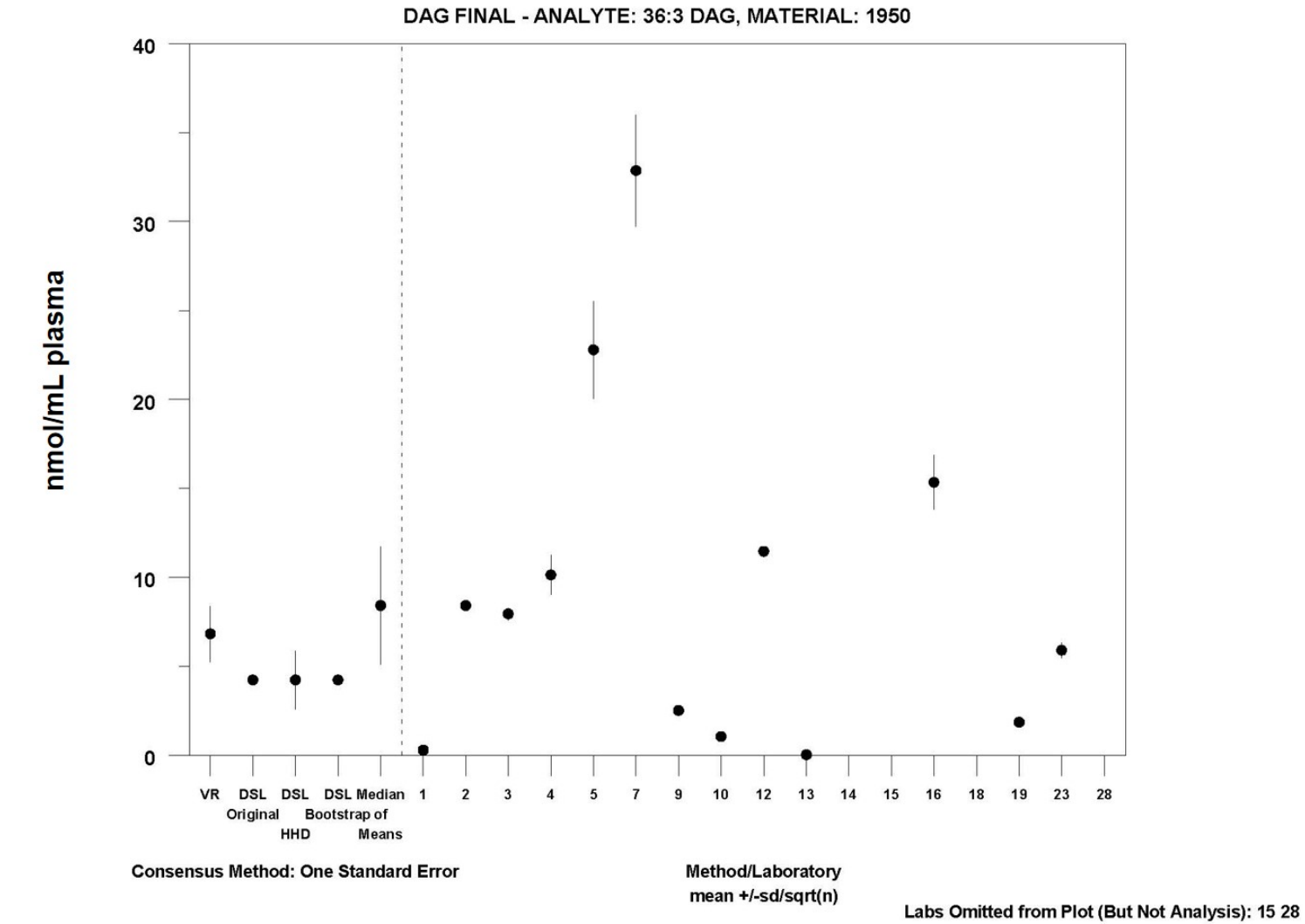


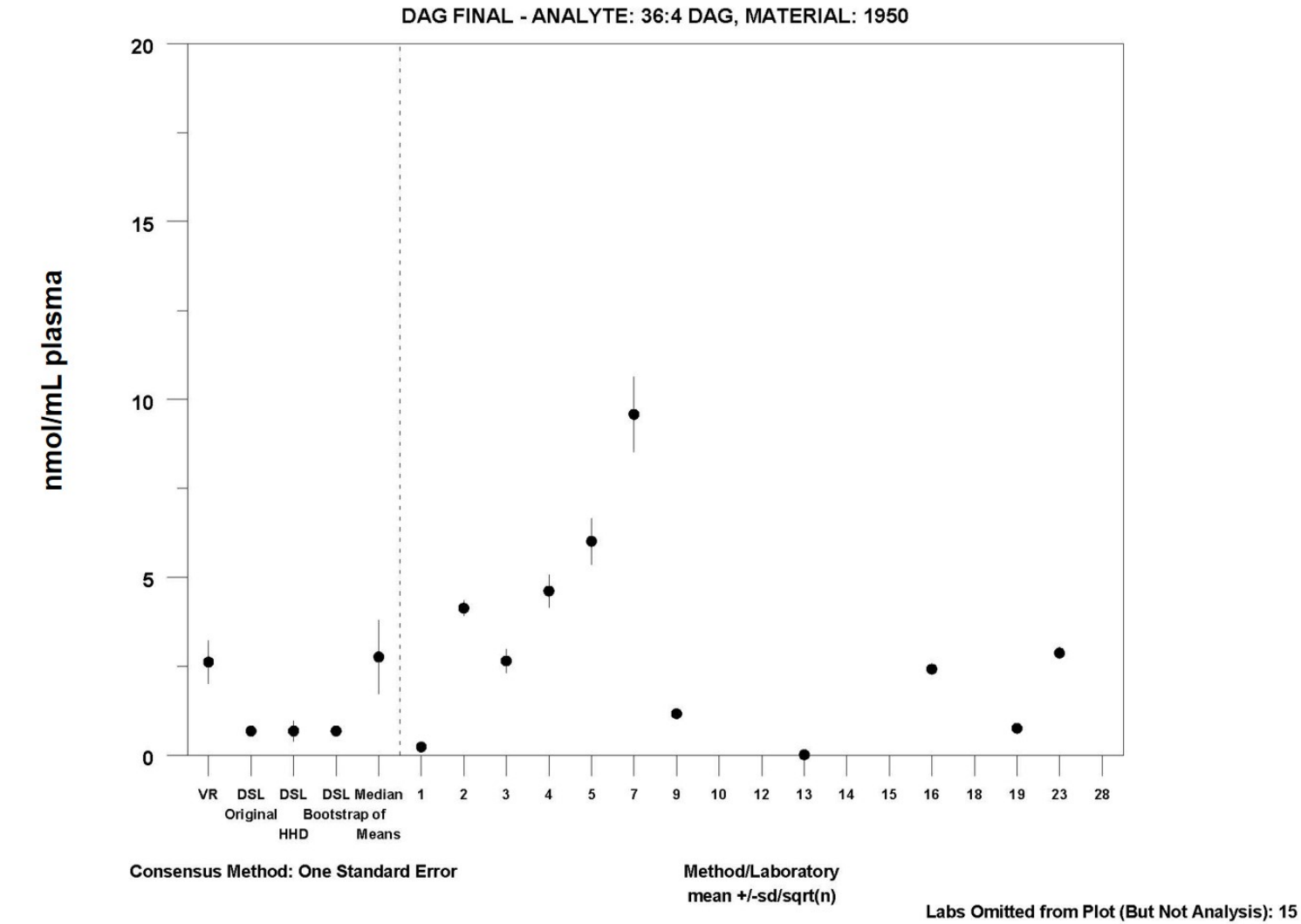


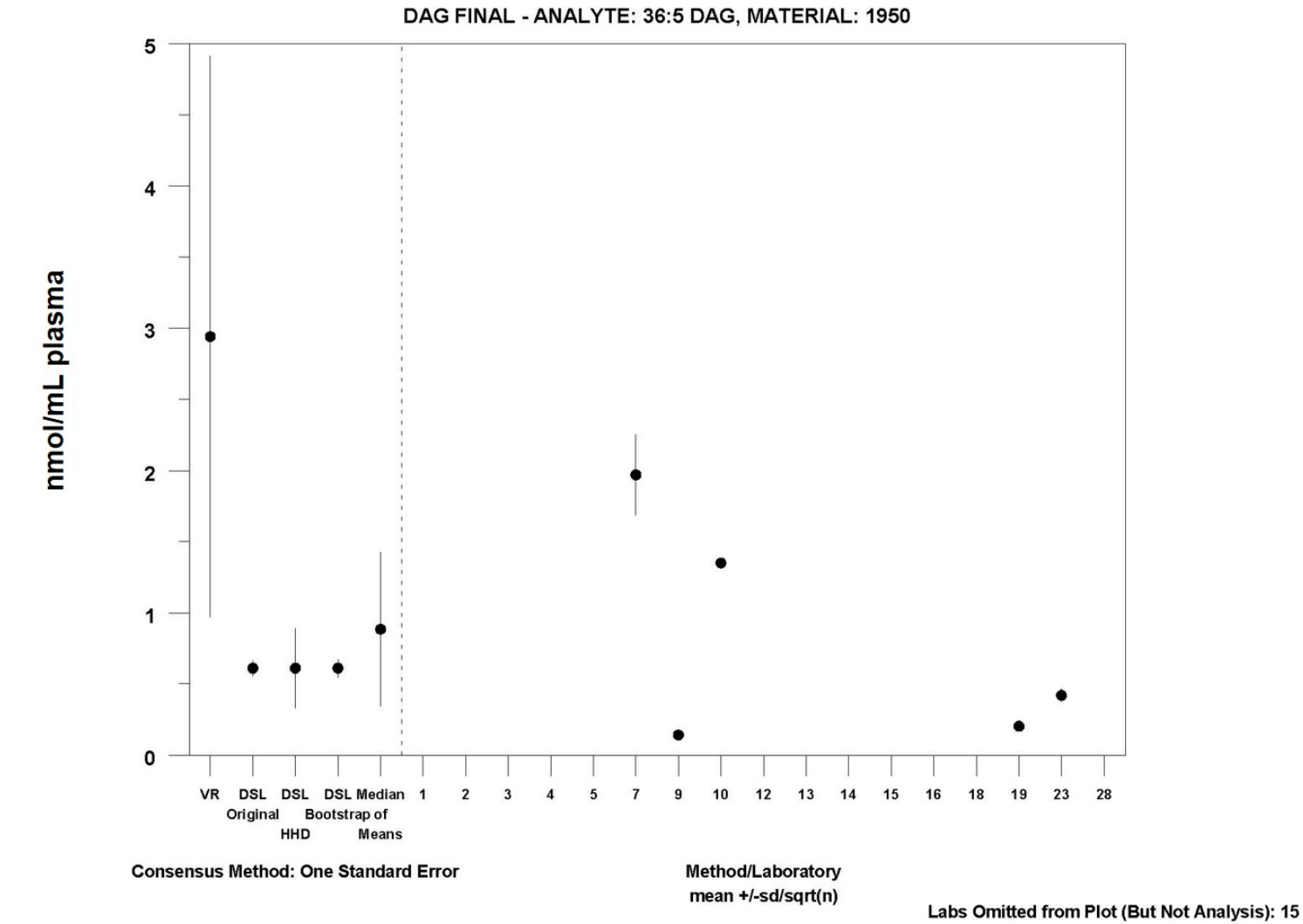


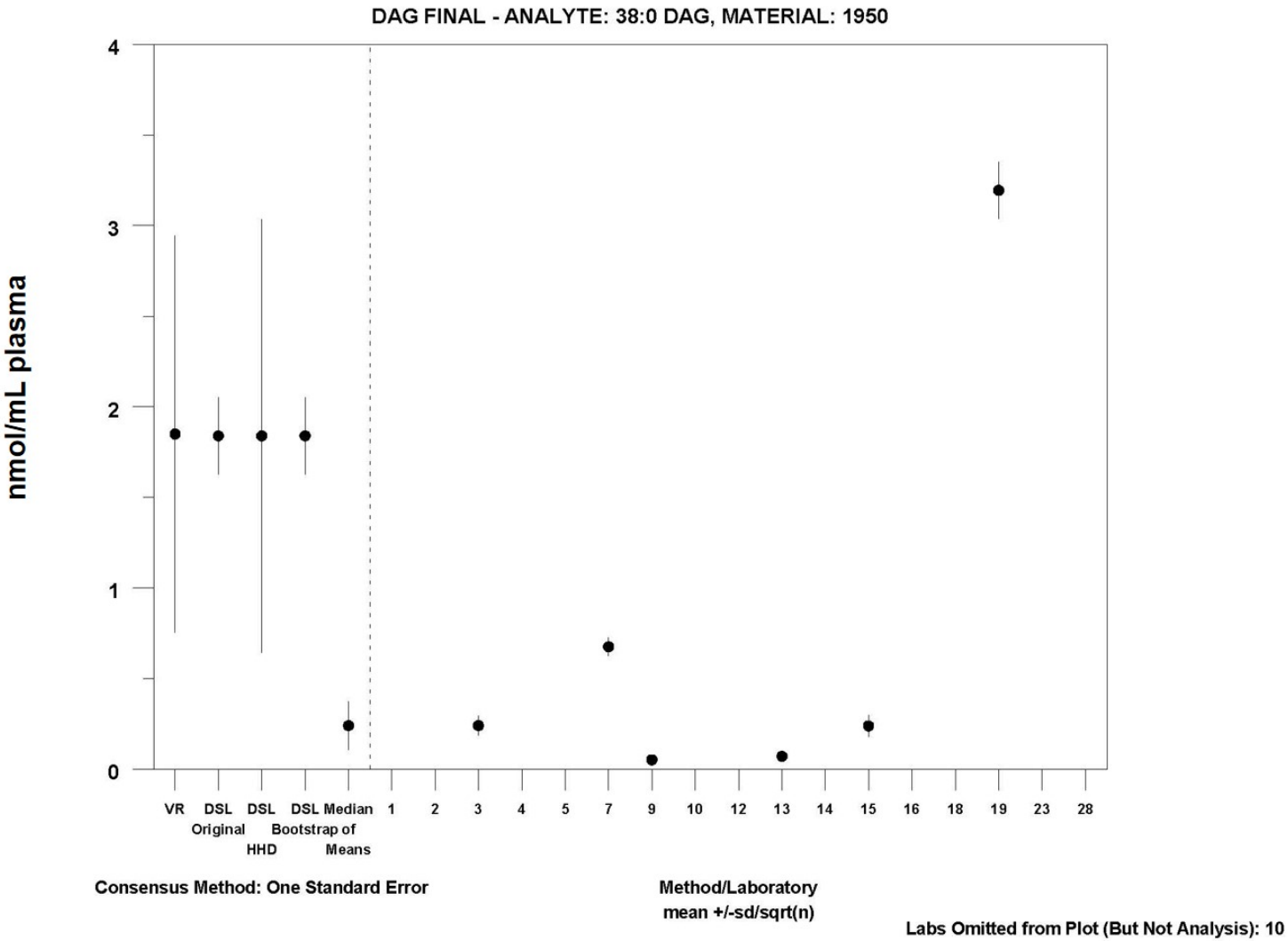


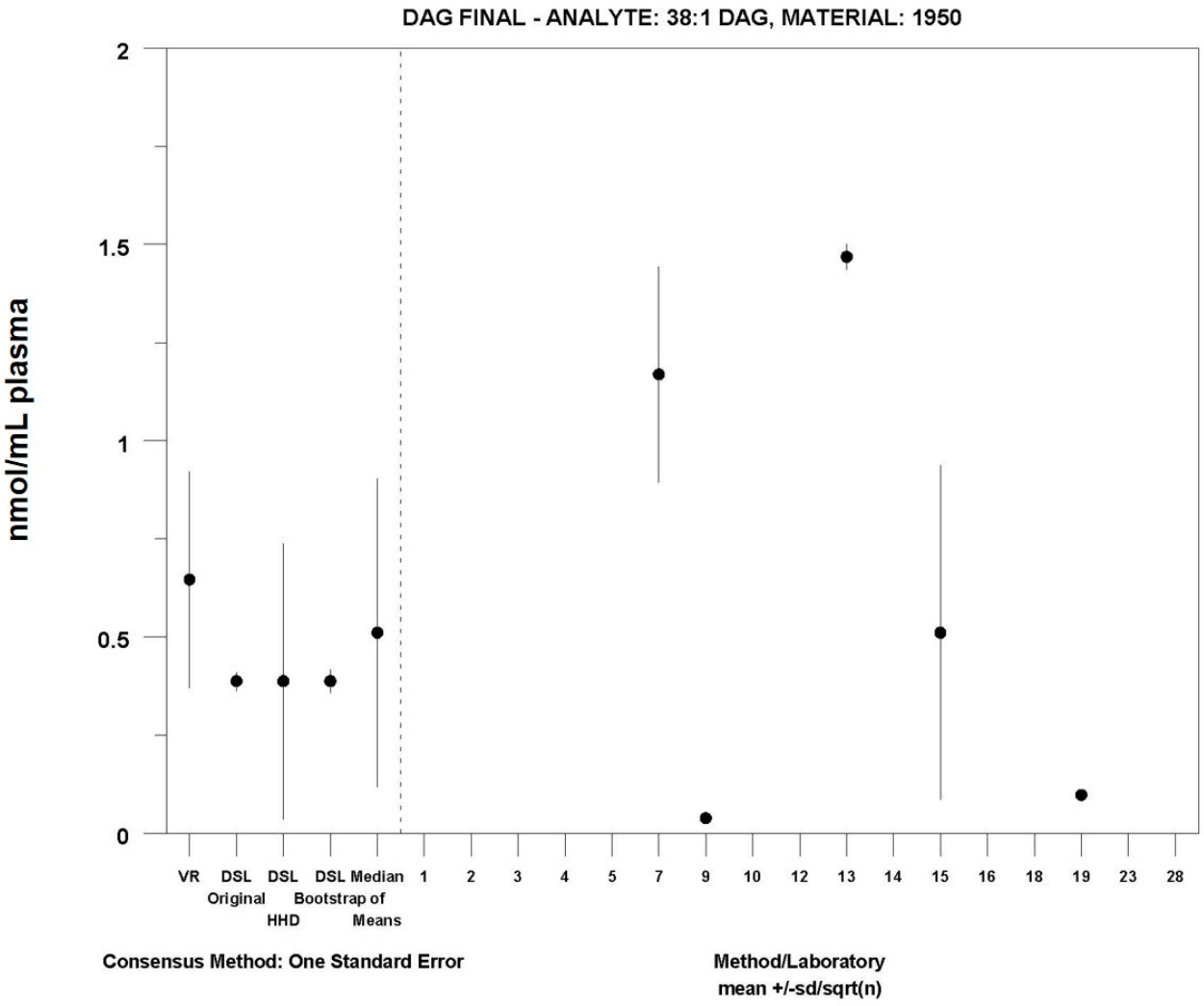




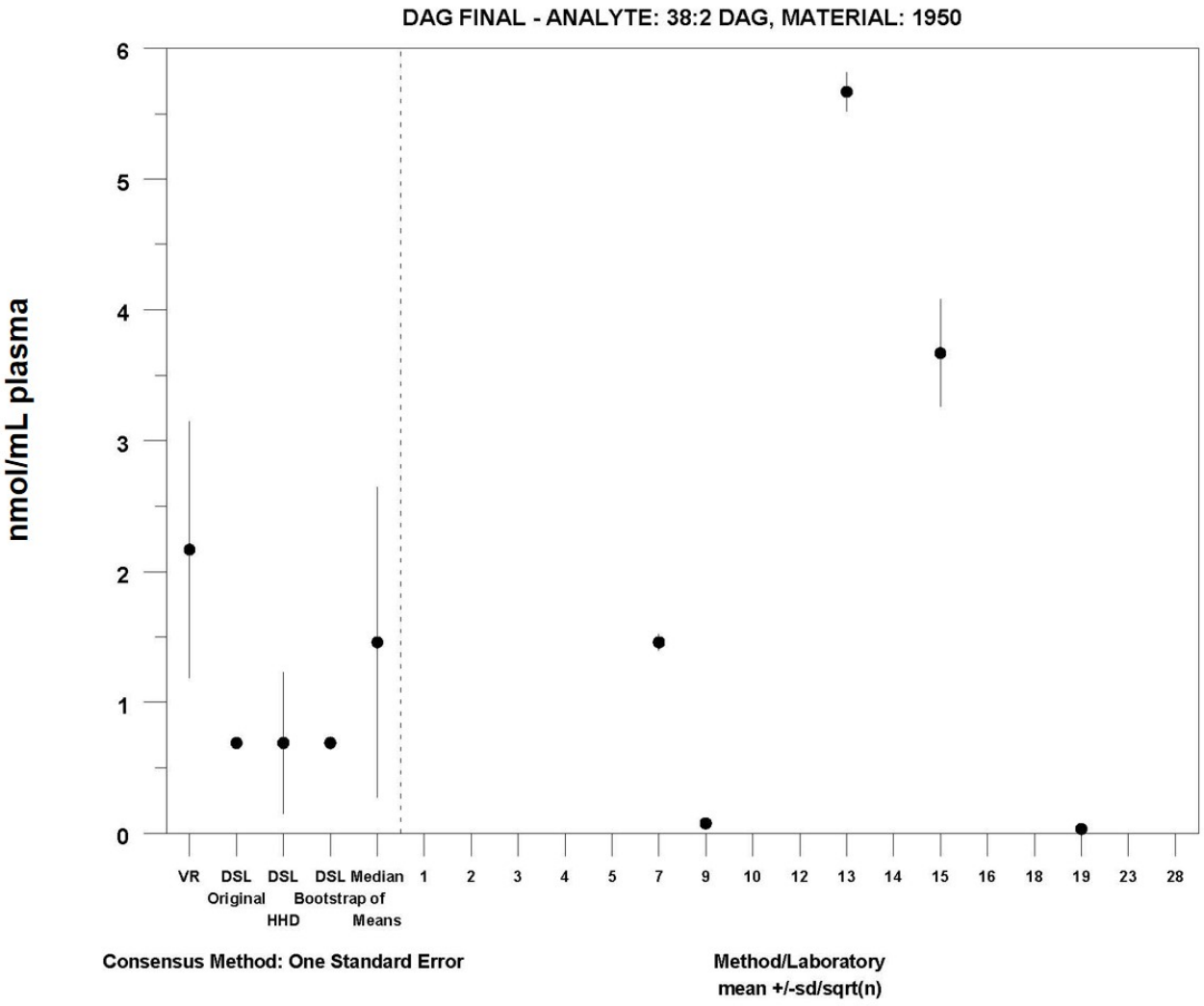




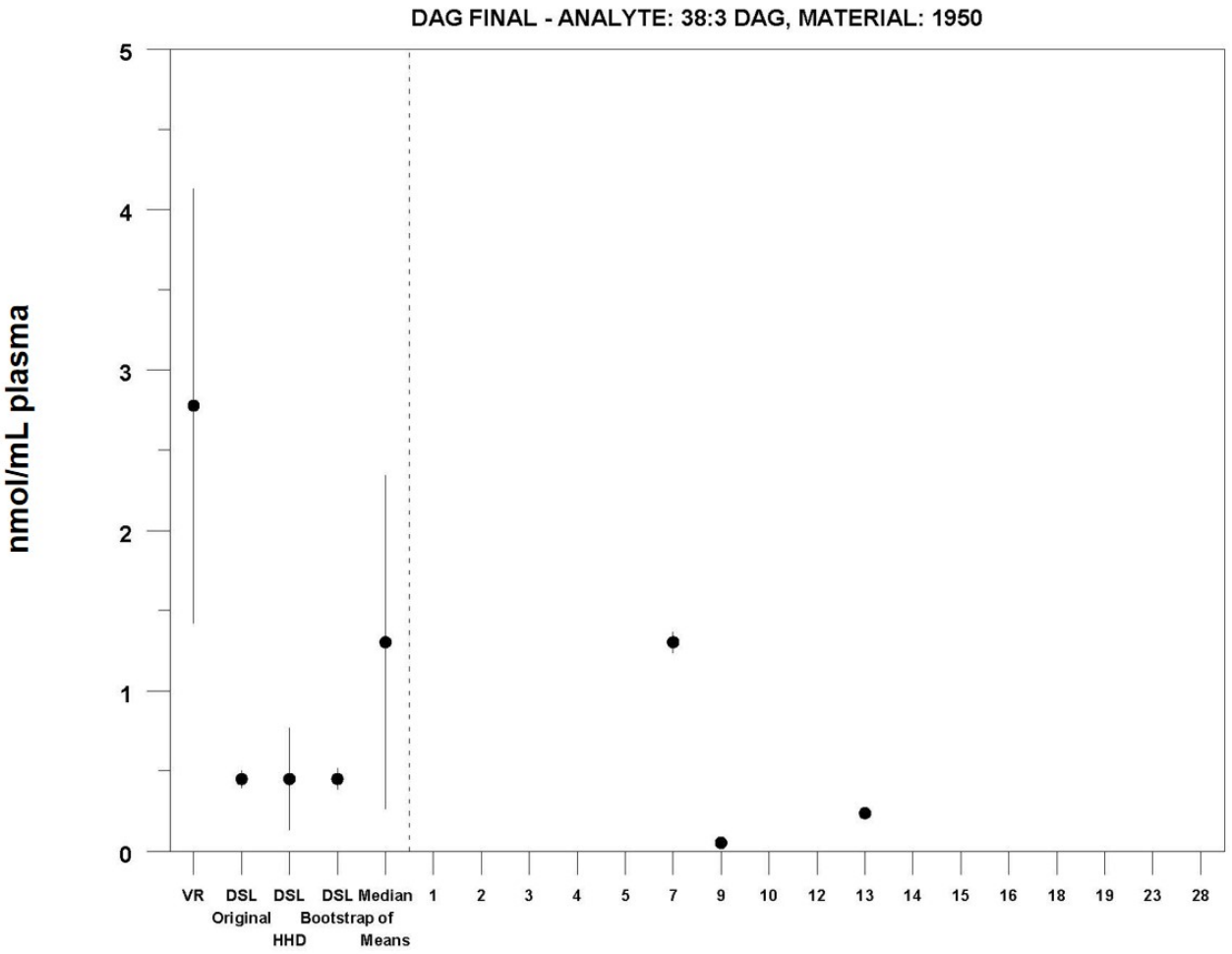




MEDM Location: 0.51 ± 0.39 nmol/mL



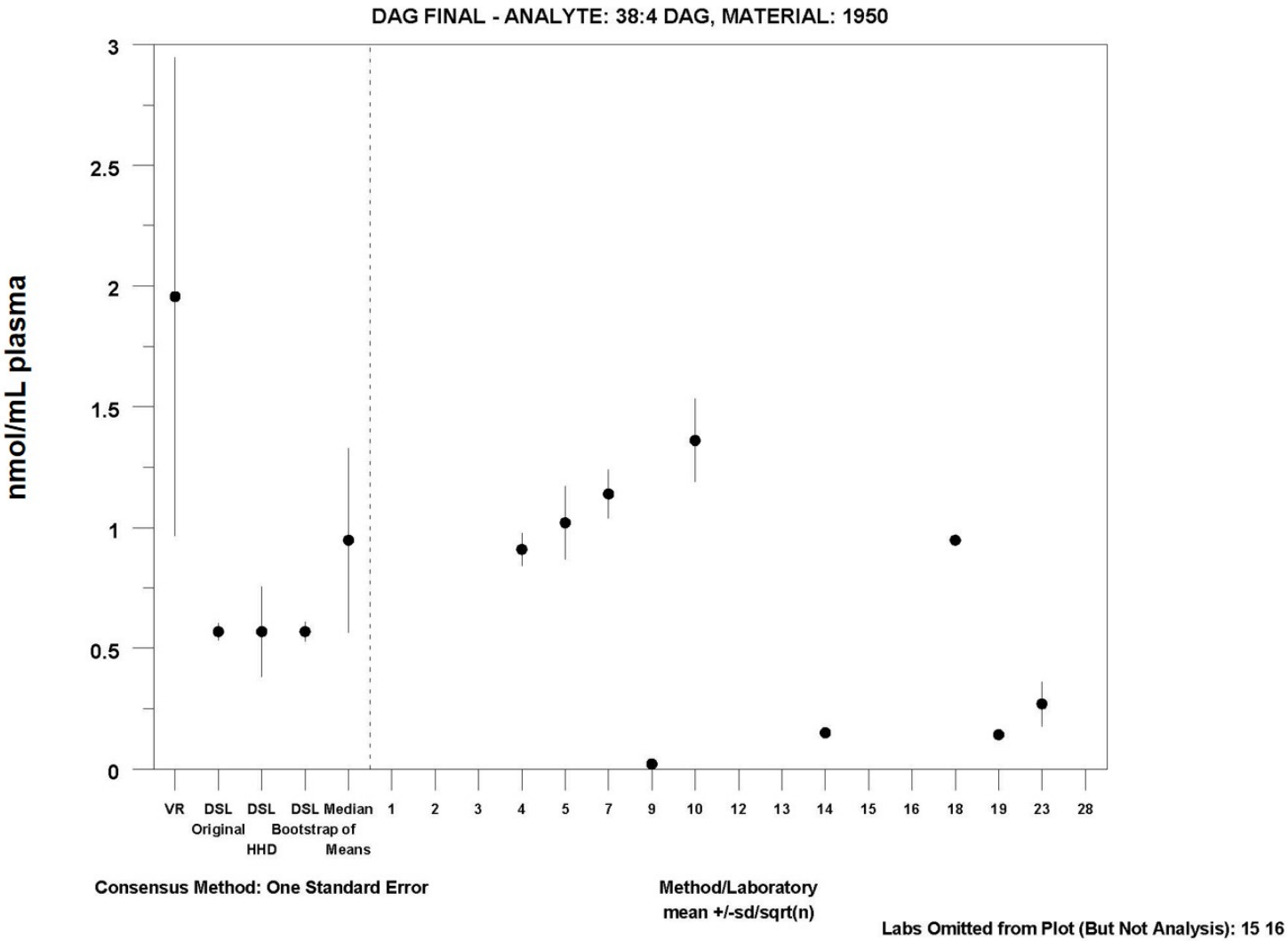
MEDM Location: 1.5 ± 1.2 nmol/mL

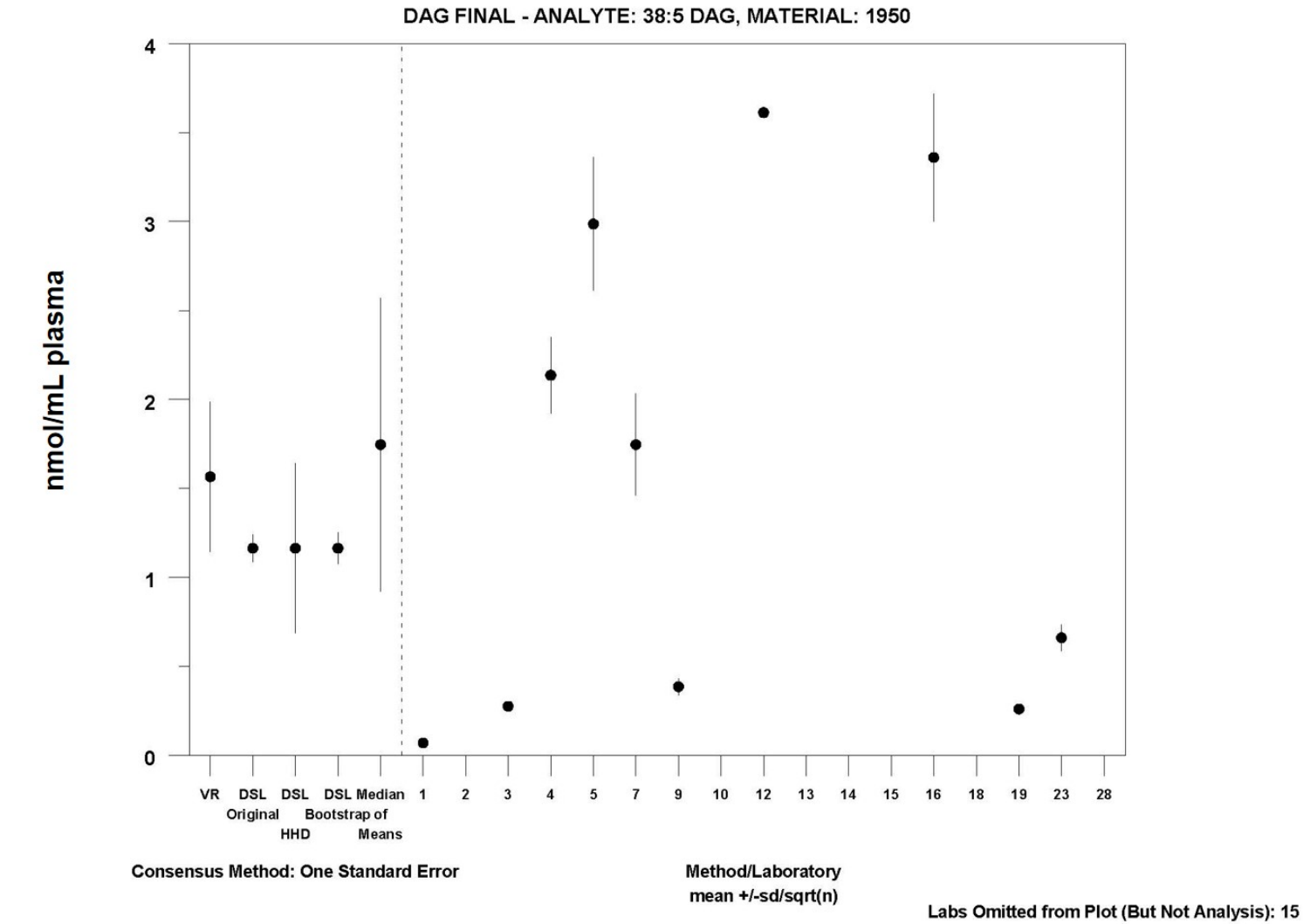


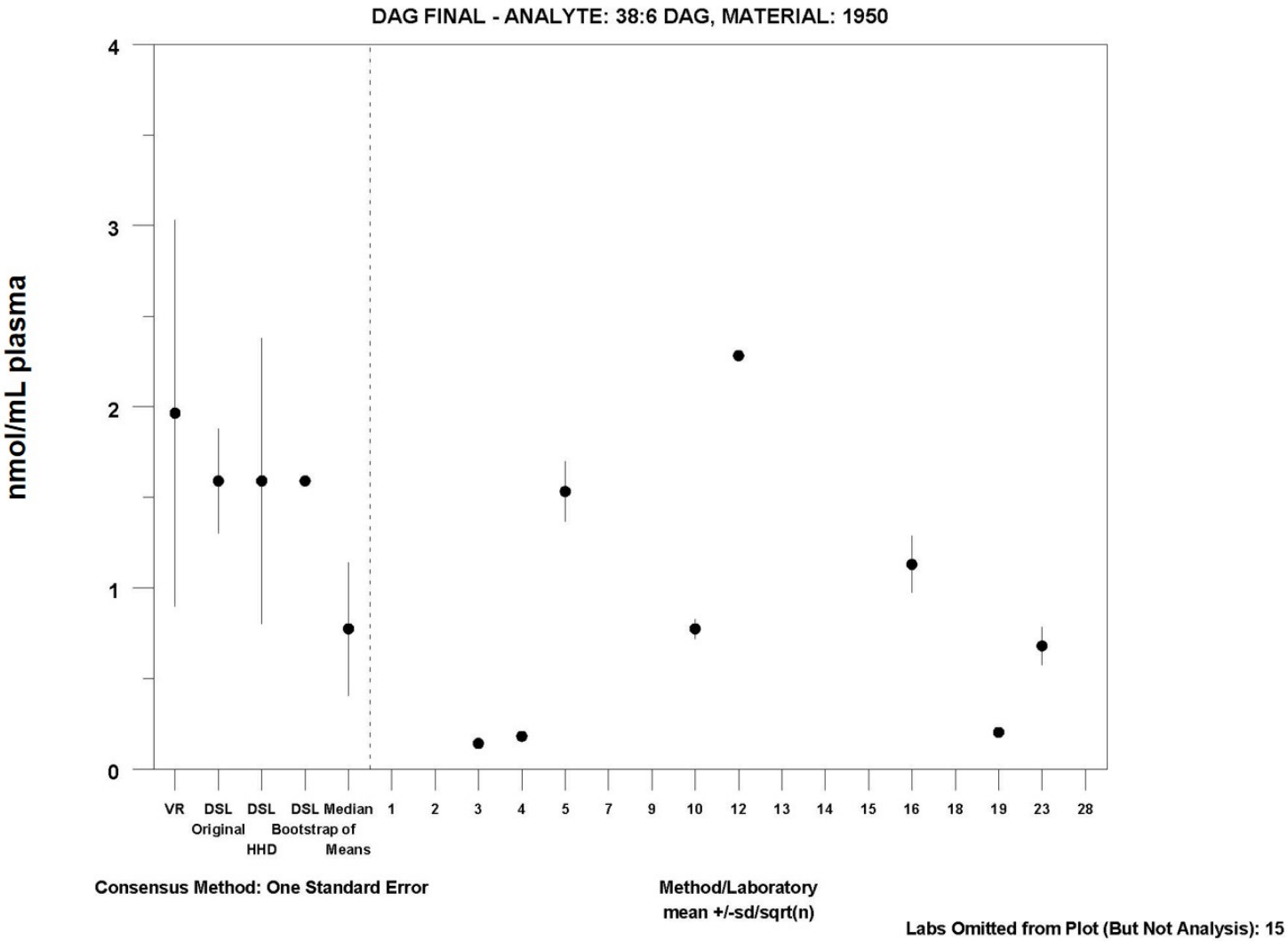
Labs Omitted from Plot (But Not Analysis): 10 15

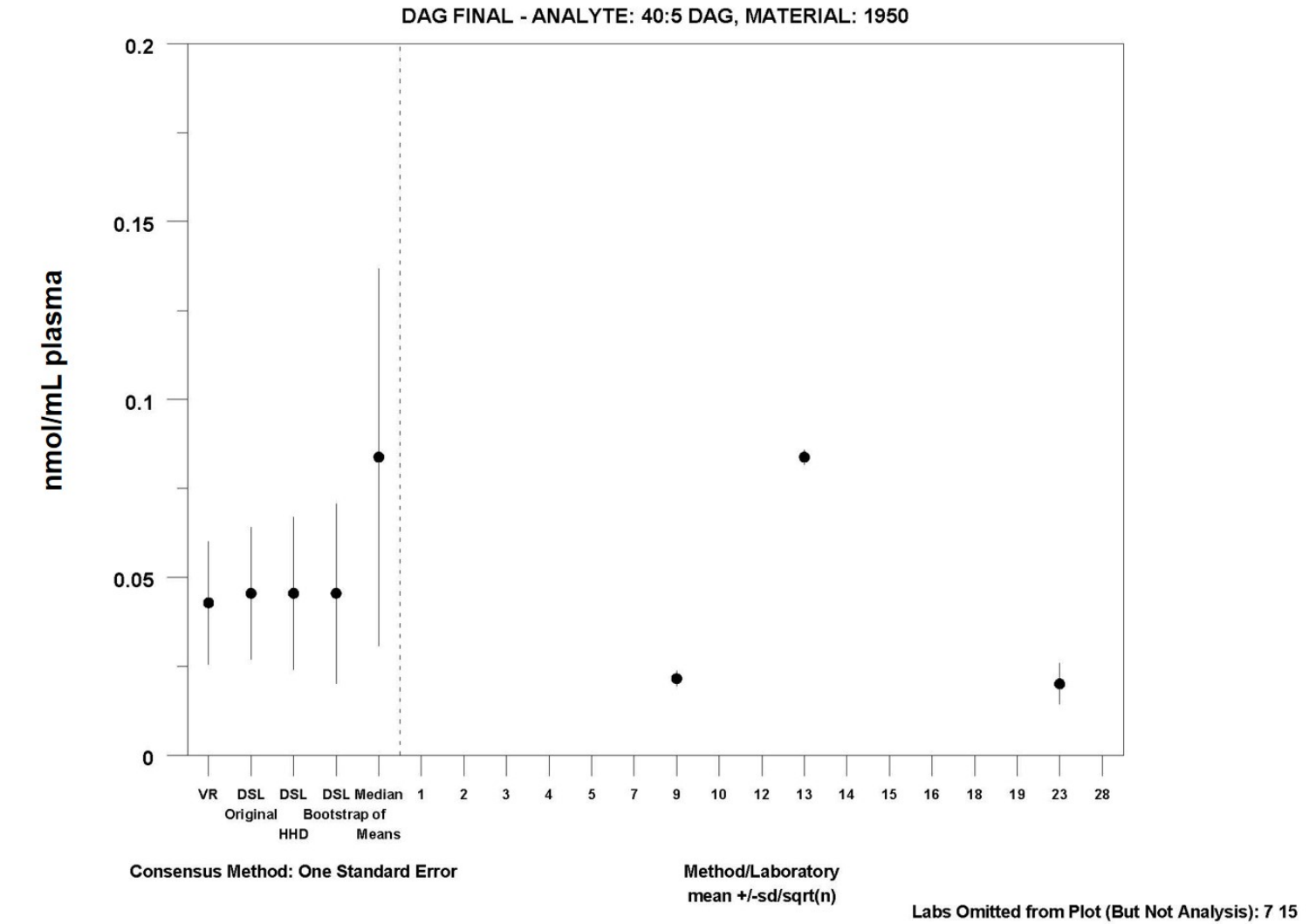
MEDM Location: 1.3 ± 1.0 nmol/mL

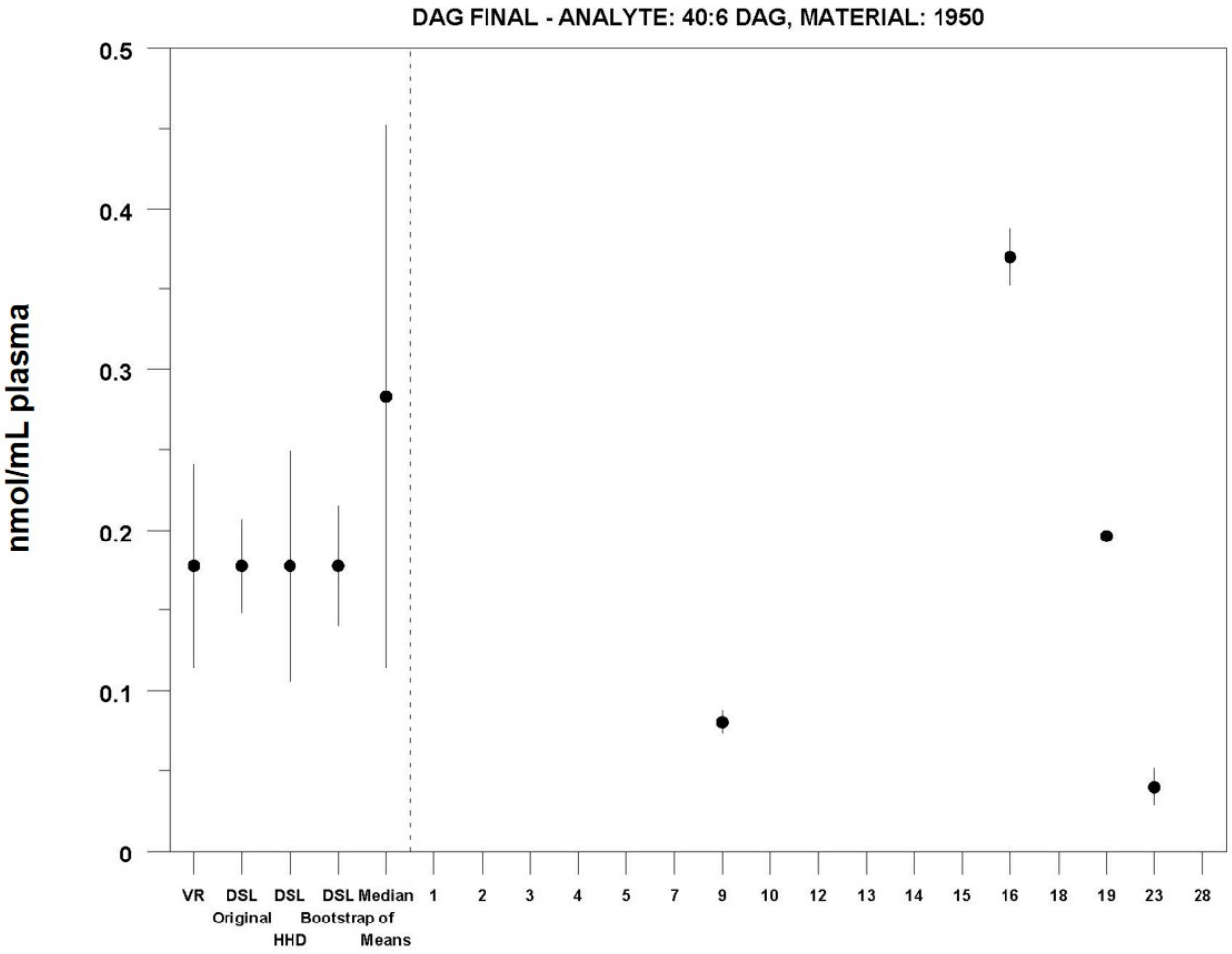
10: 8.30 ± 2.41; 15: 5.40 ± 1.49







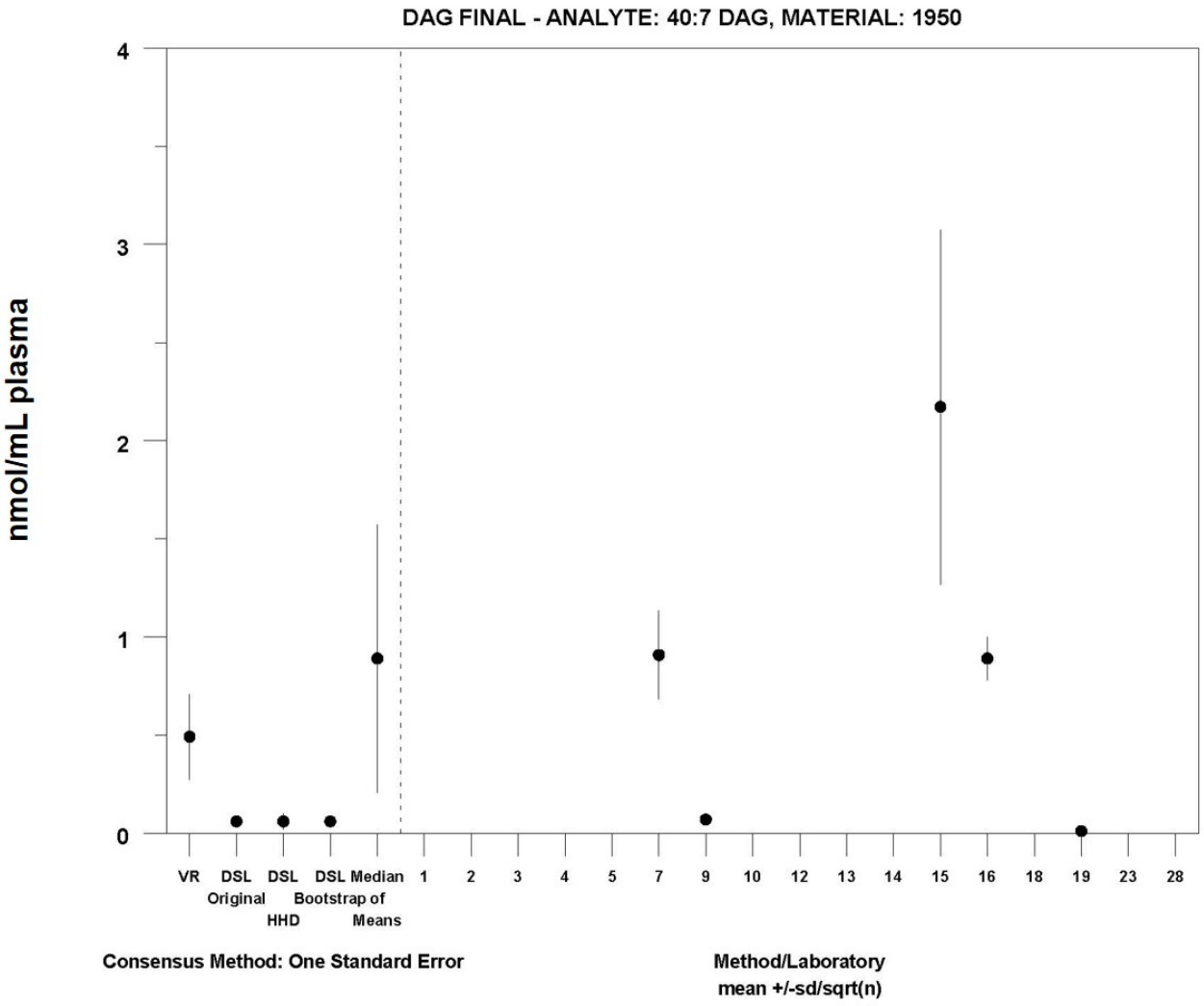




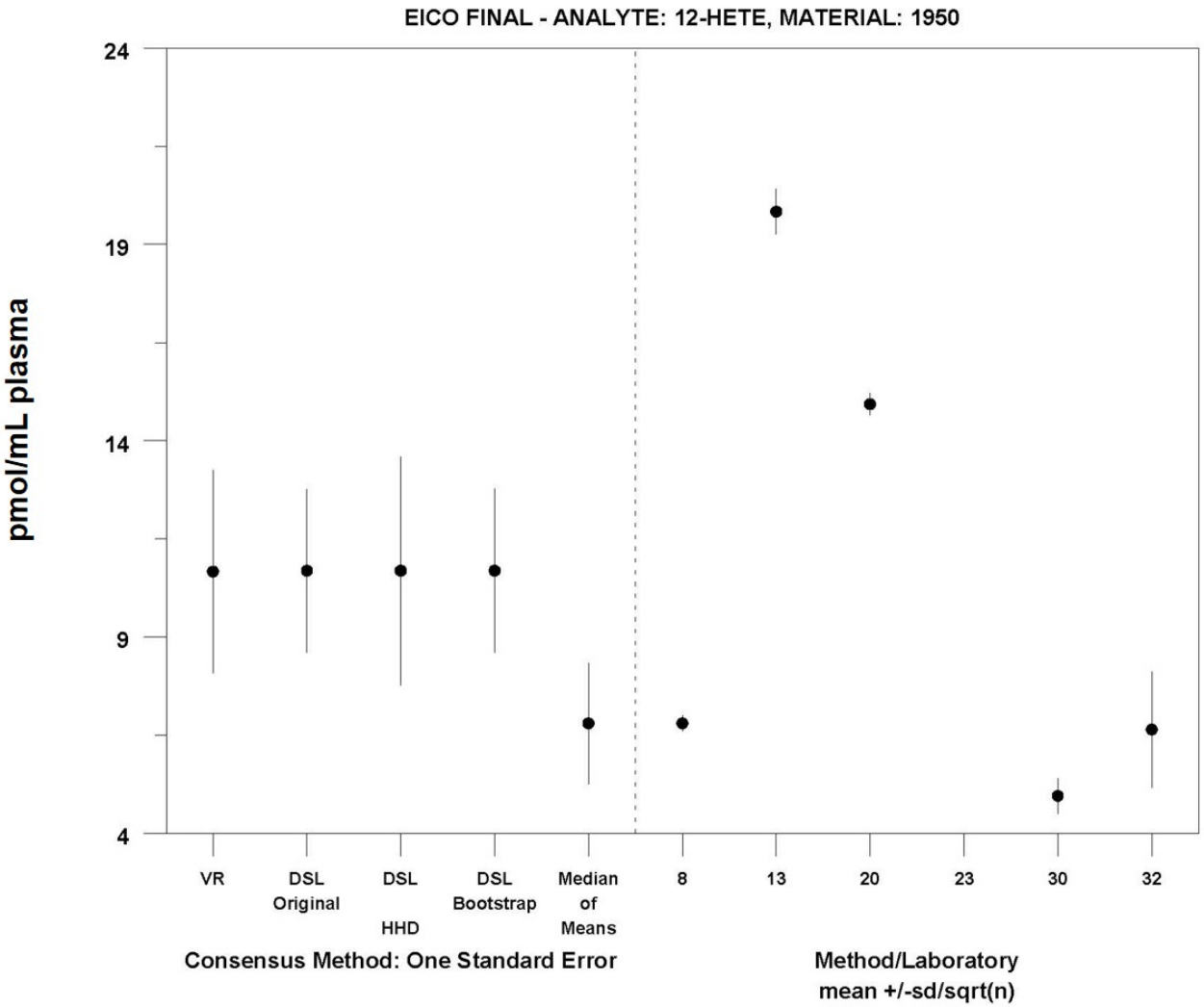
MEDM Location: 0.28 ± 0.17 nmol/mL

Labs Omitted from Plot (But Not Analysis): 7 15

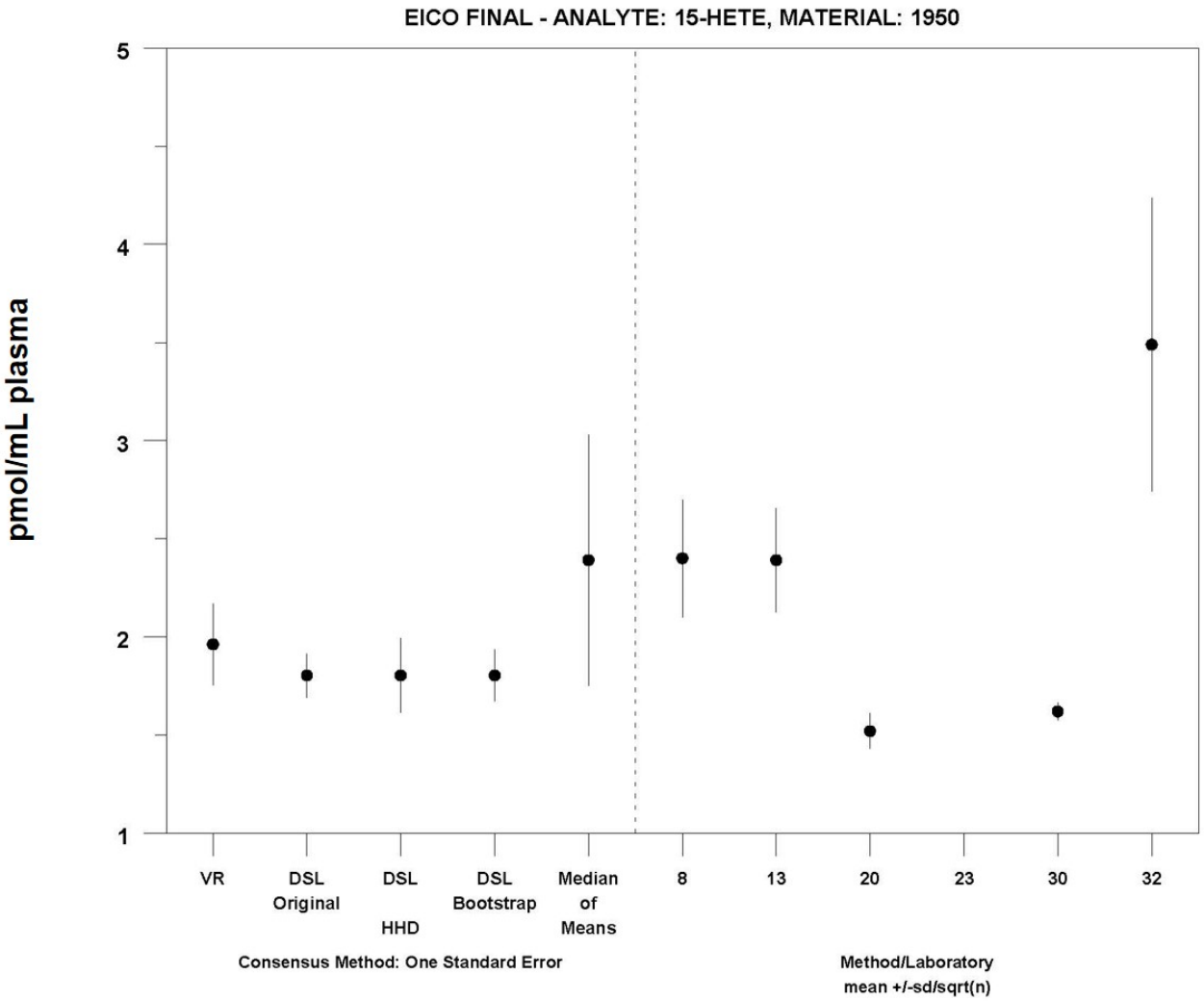
7: 1.61 ± 1.45; 15: 8.00 ± 1.69



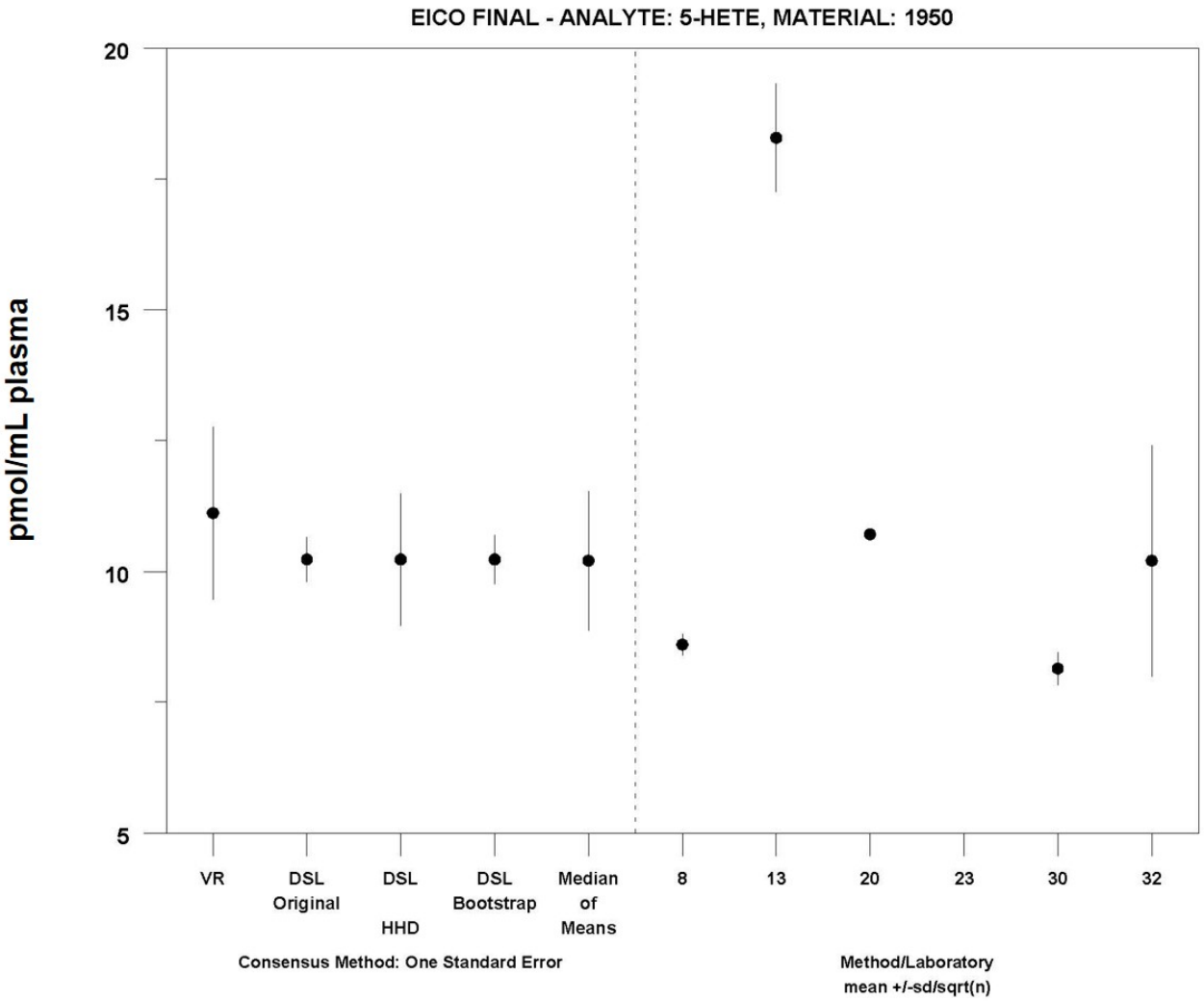
MEDM Location: 0.89 ± 0.68 nmol/mL



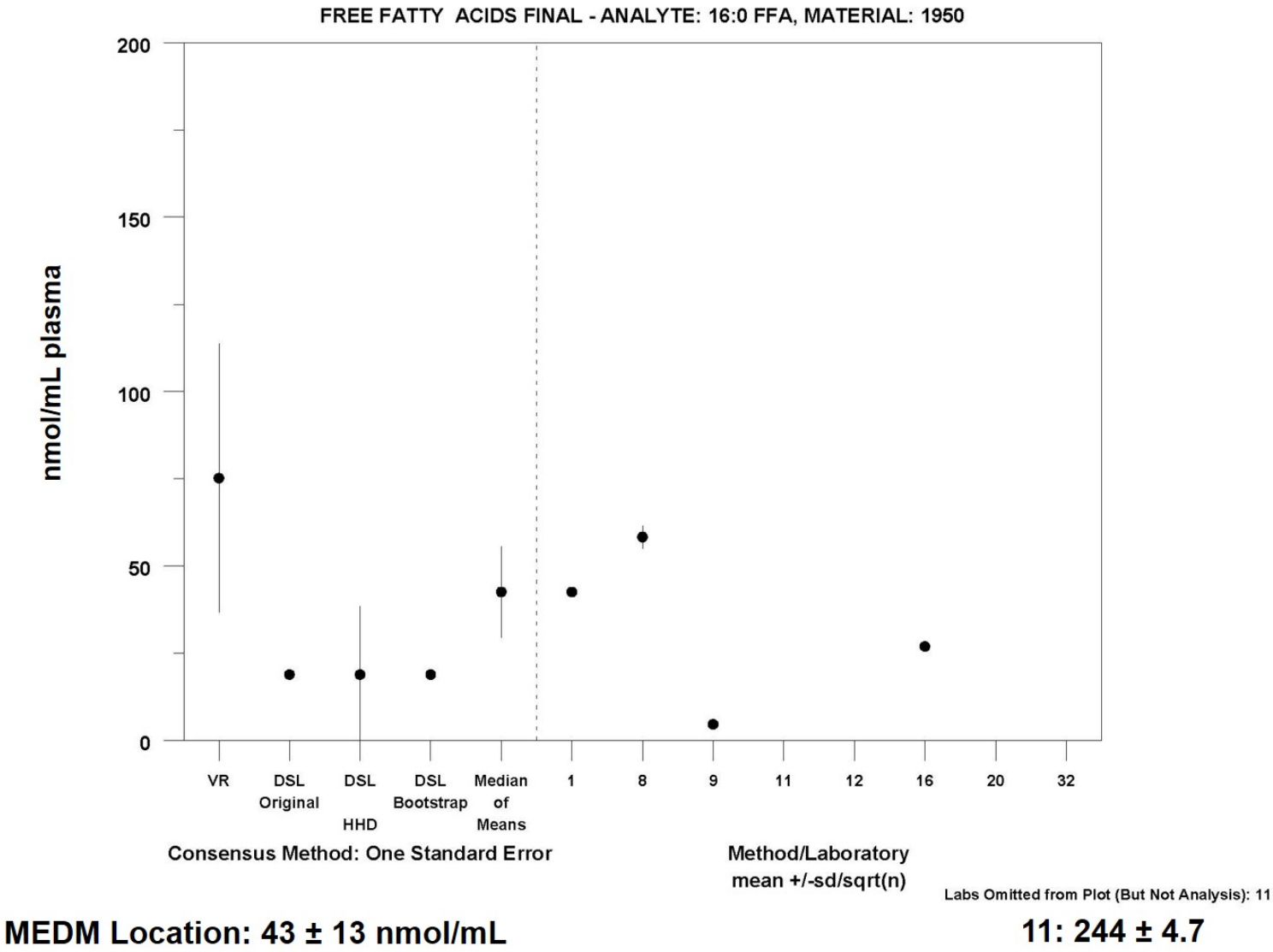
MEDM Location: 6.8 ± 1.5 pmol/mL

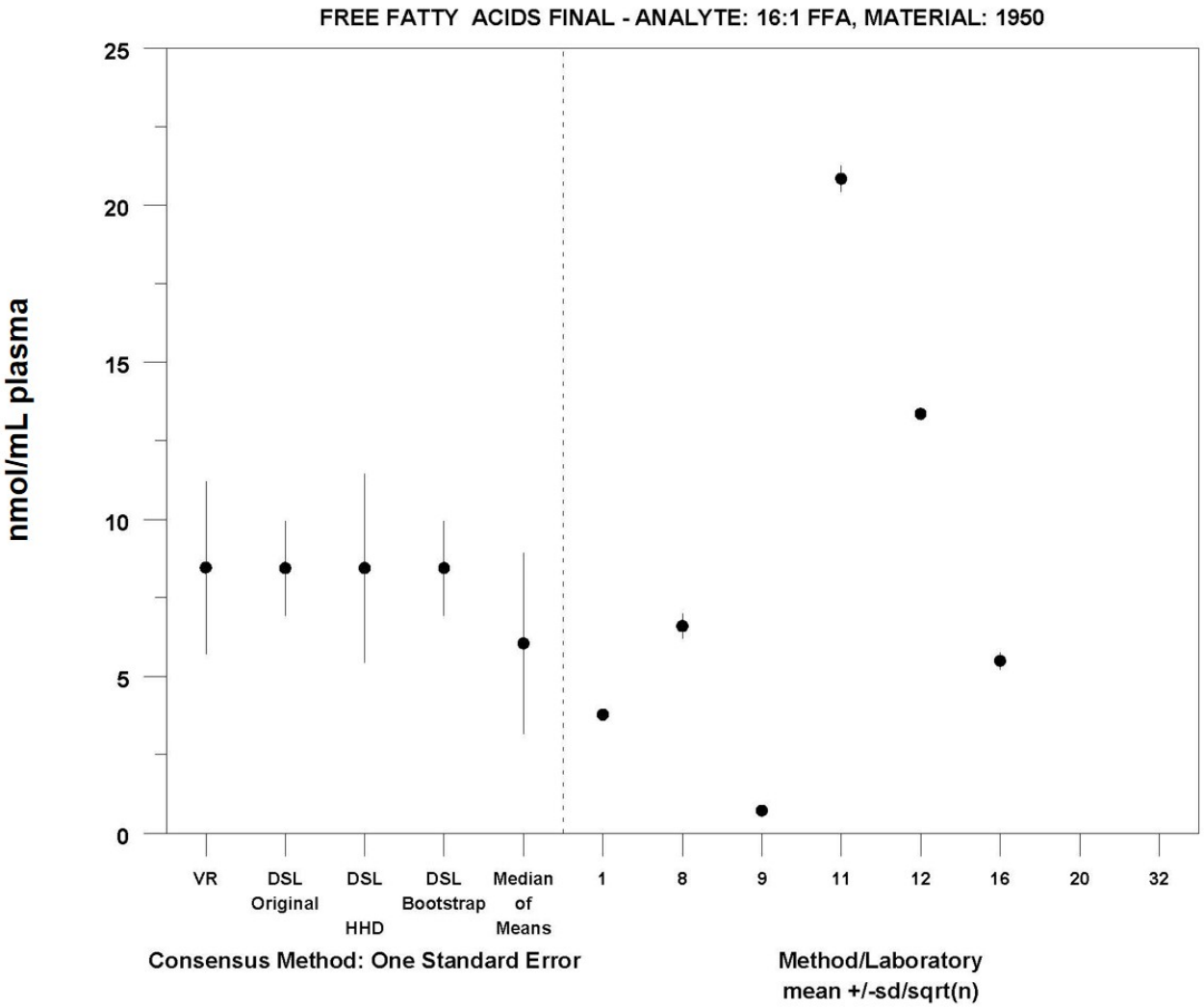


MEDM Location: 2.4 ± 0.64 pmol/mL

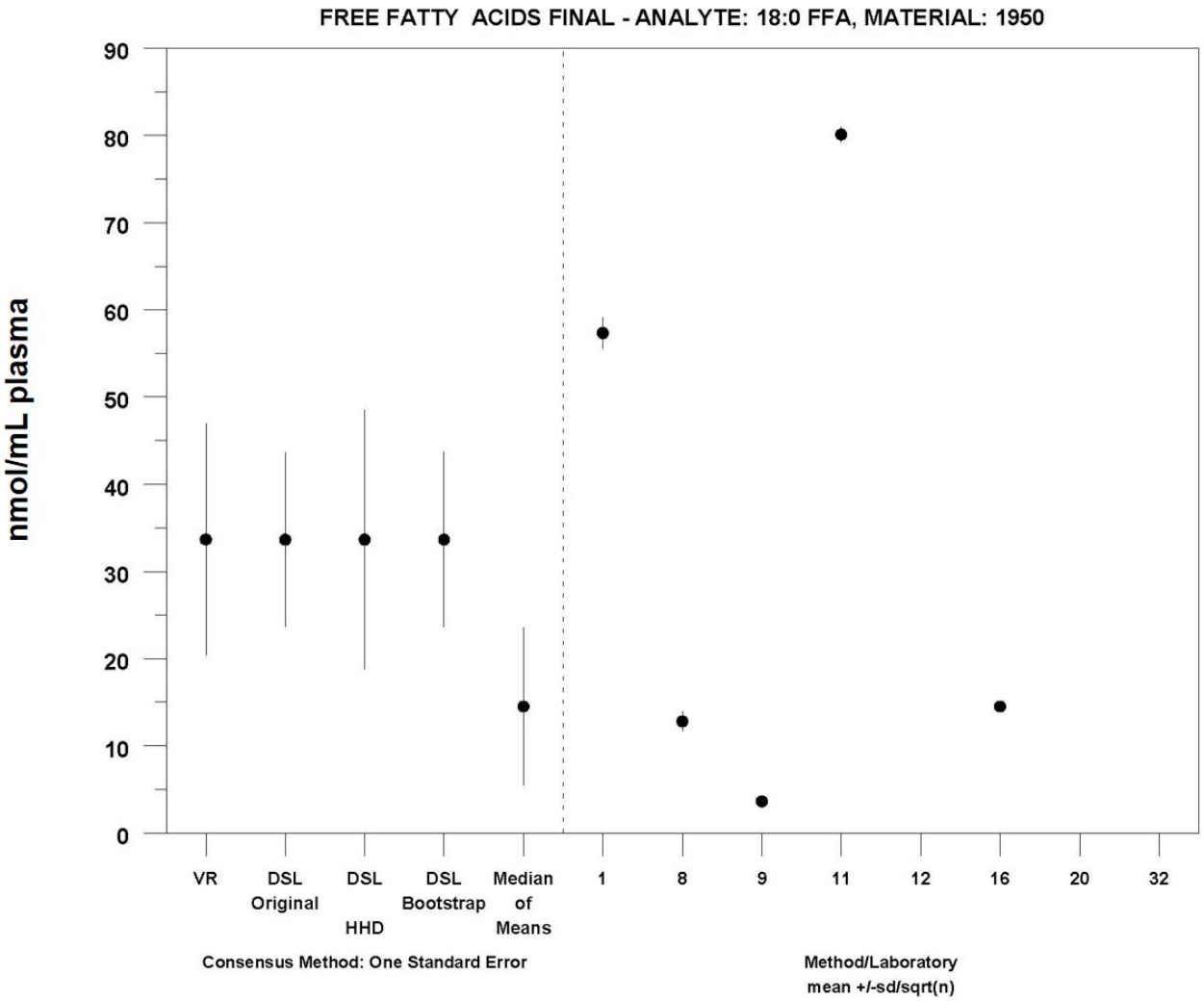


MEDM Location: 10 ± 1.3 pmol/mL

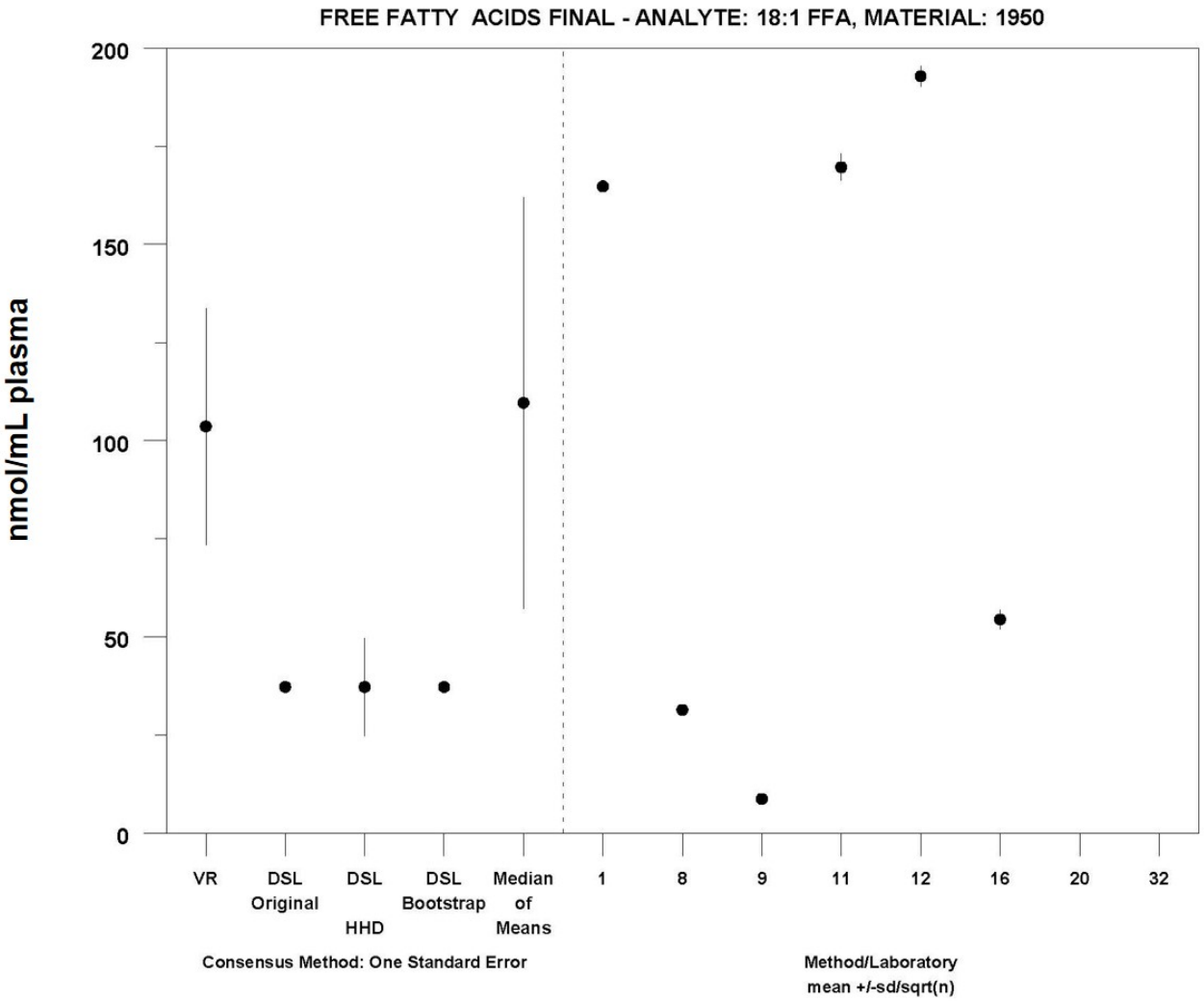




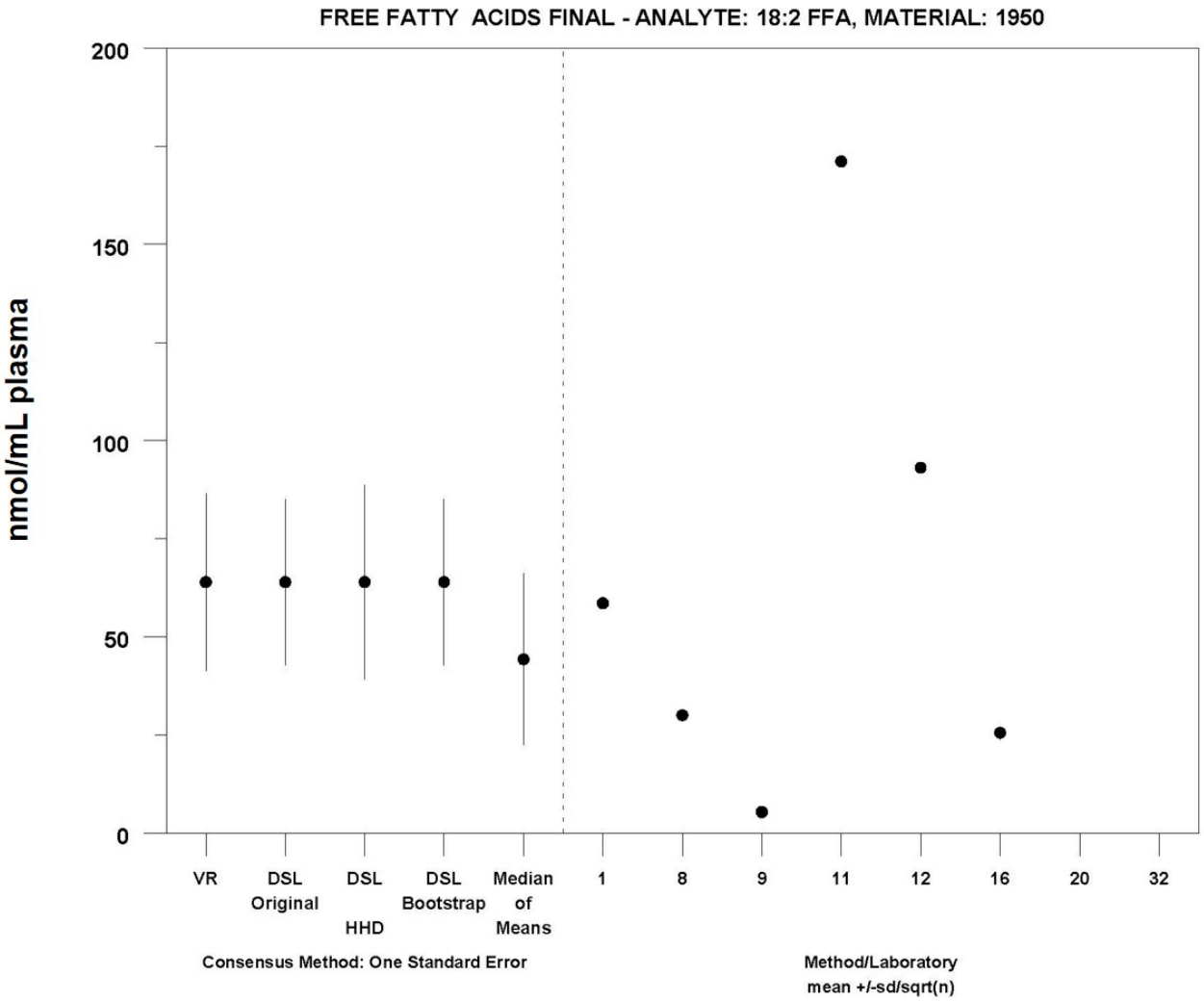
MEDM Location: 6.1 ± 2.9 nmol/mL



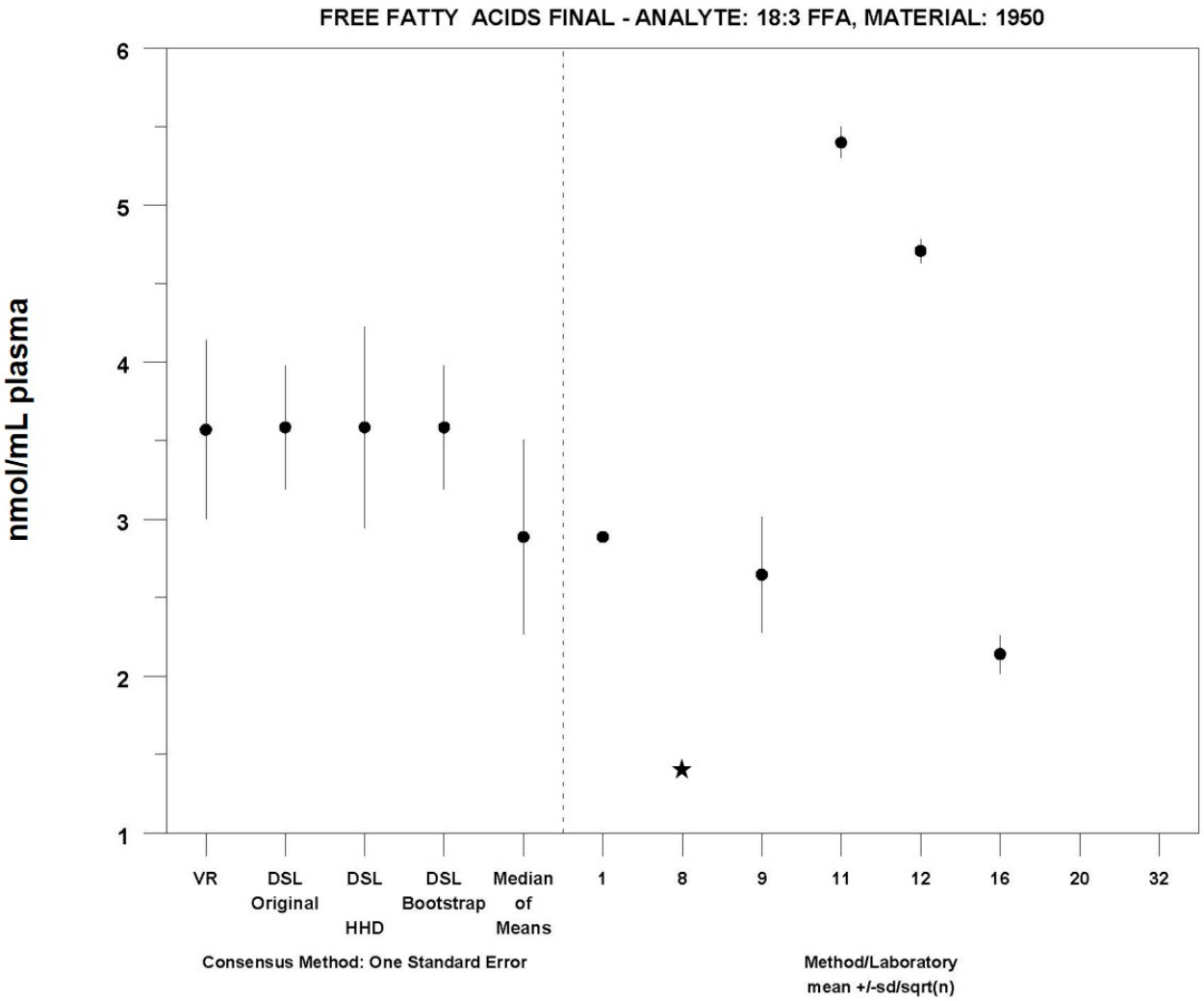
MEDM Location: 15 ± 9.0 nmol/mL



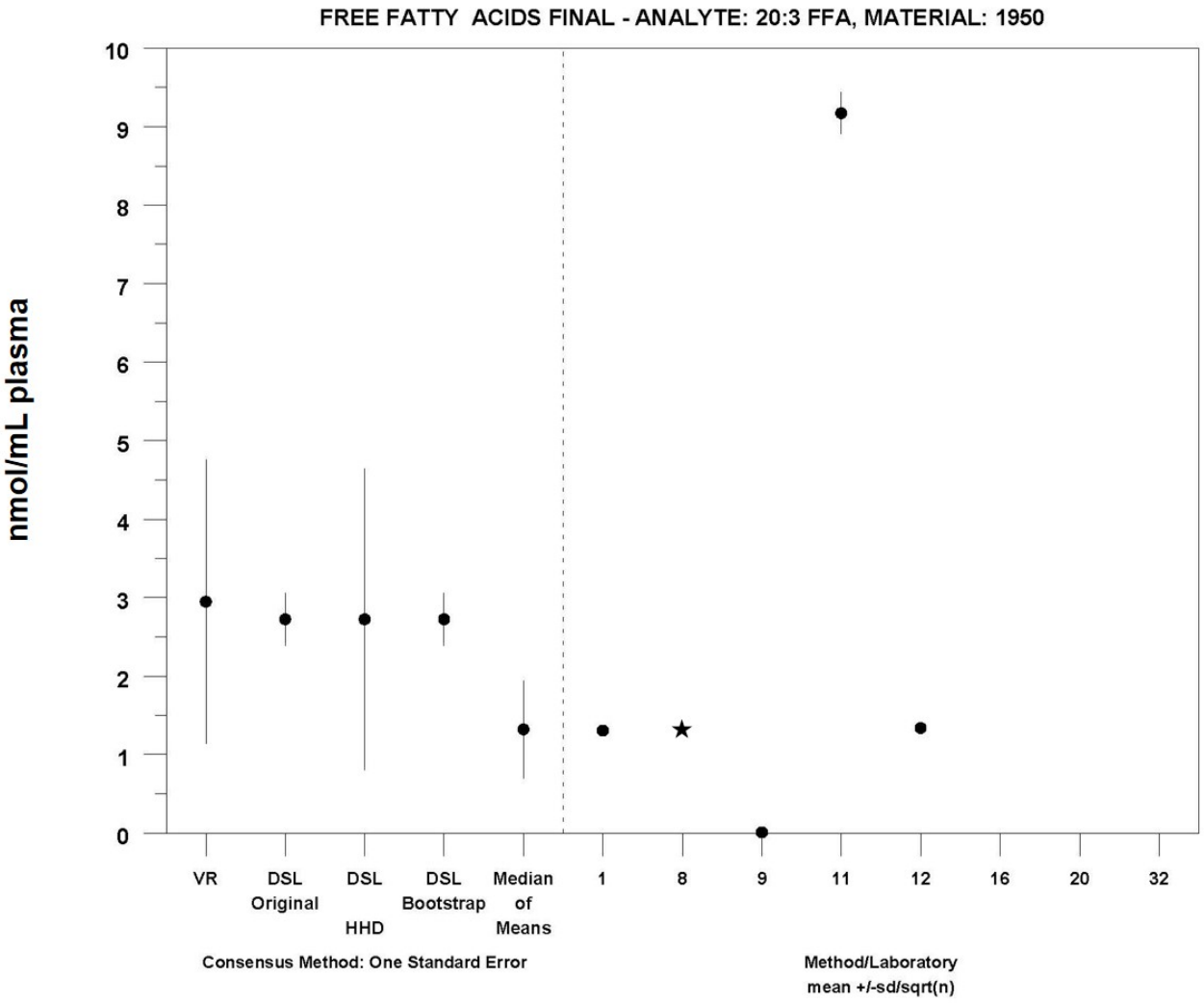
MEDM Location: 110 ± 105 nmol/mL



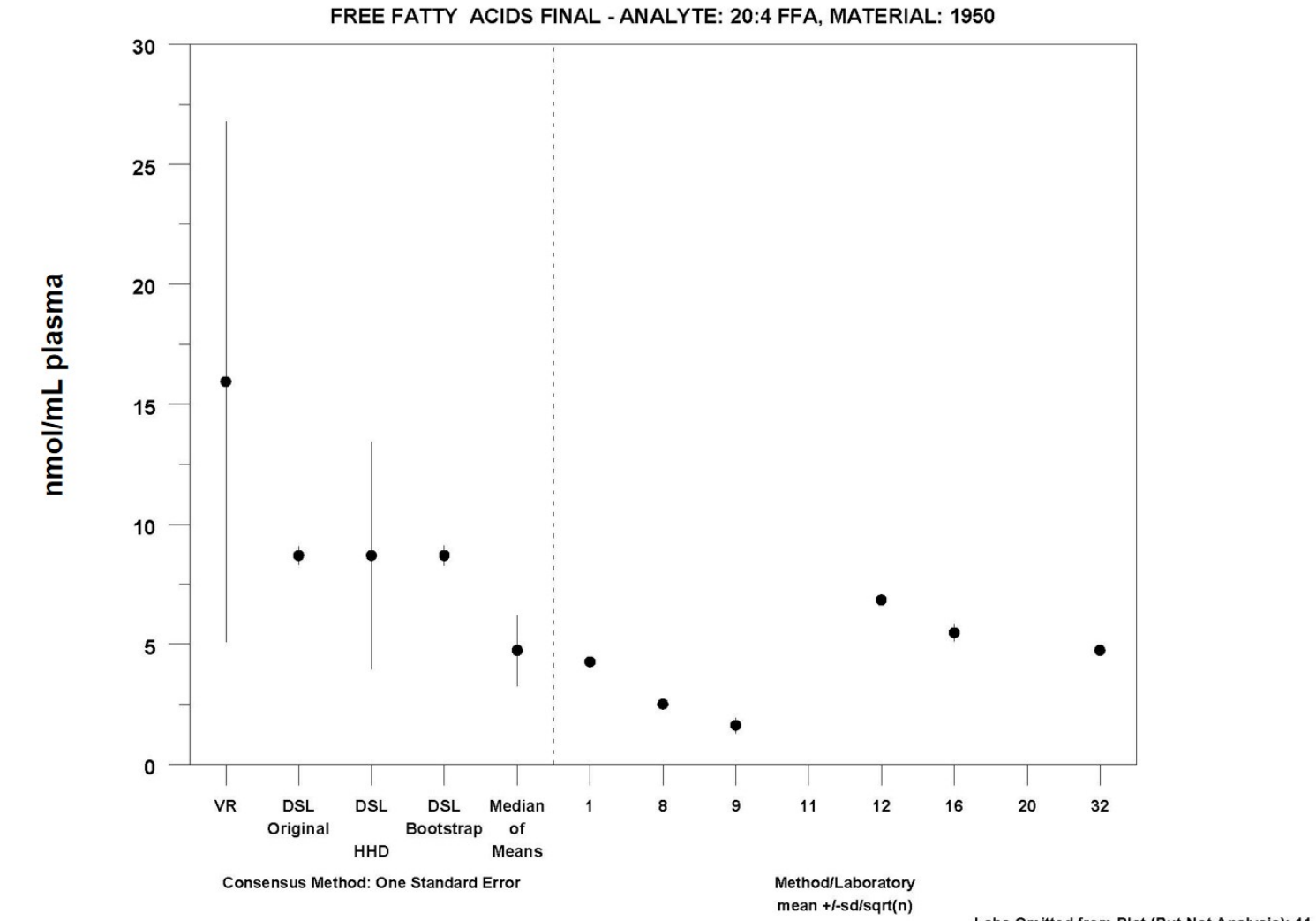
MEDM Location: 44 ± 22 nmol/mL

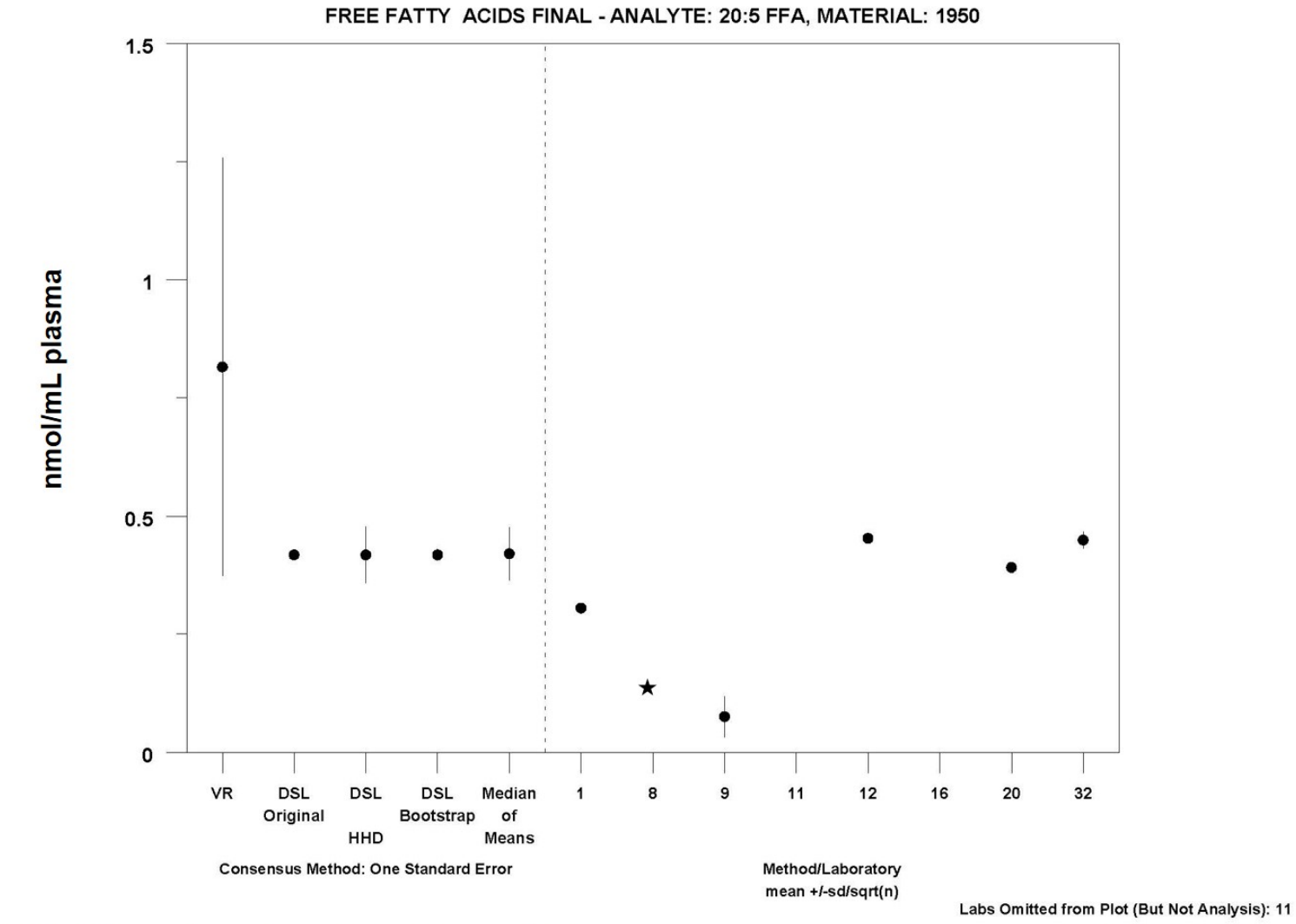


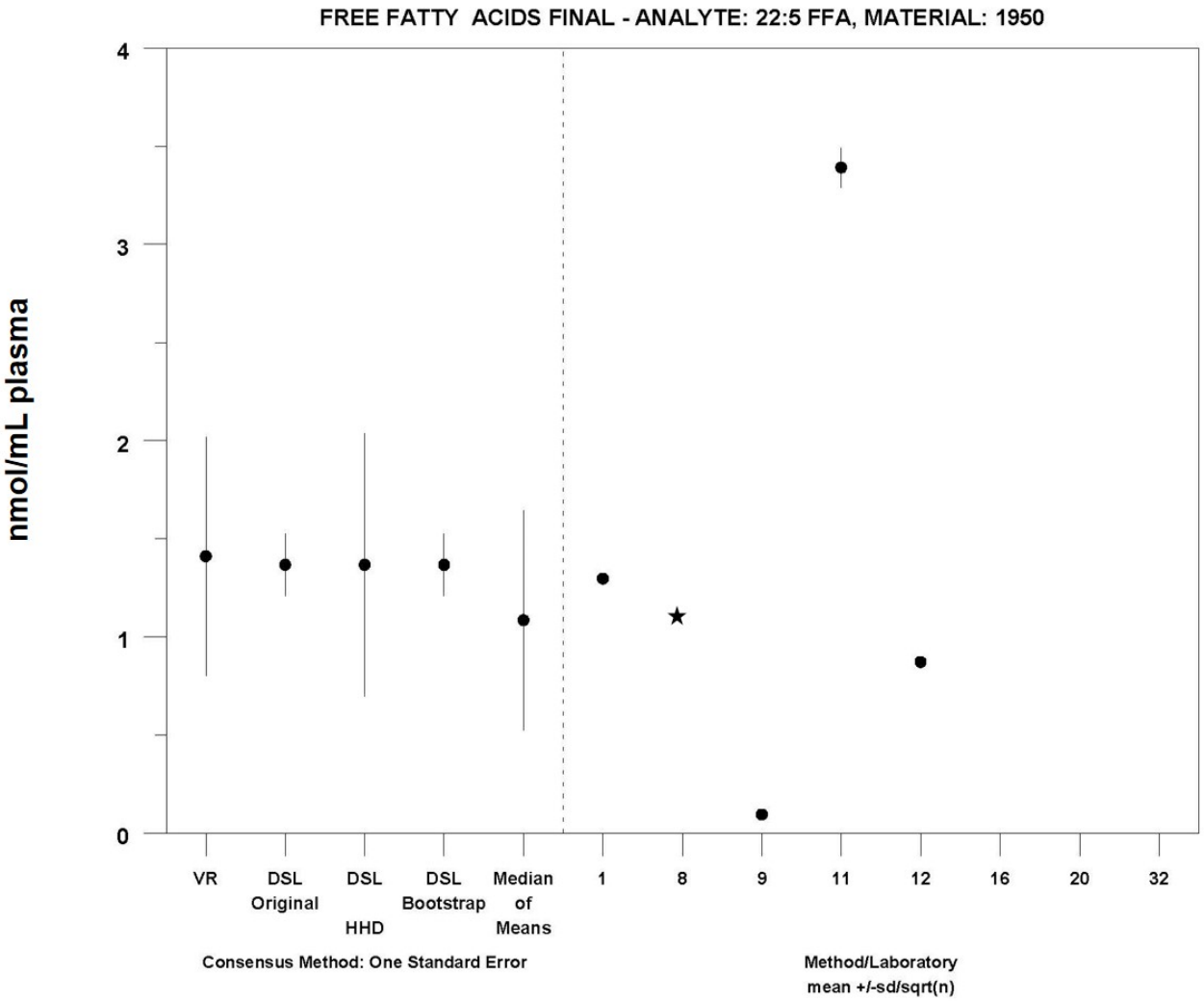
MEDM Location: 2.9 ± 0.62 nmol/mL



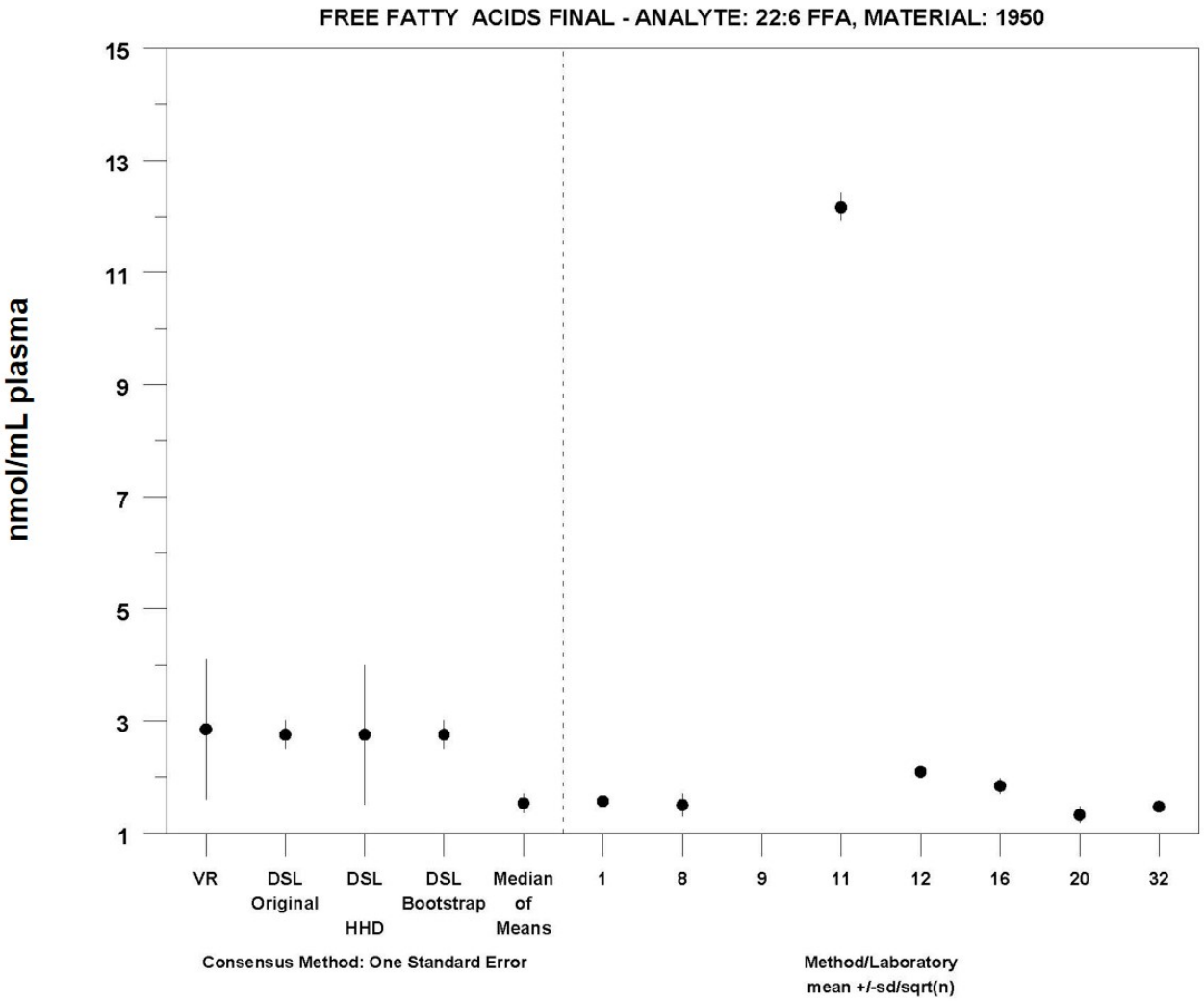
MEDM Location: 1.3 ± 0.62 nmol/mL



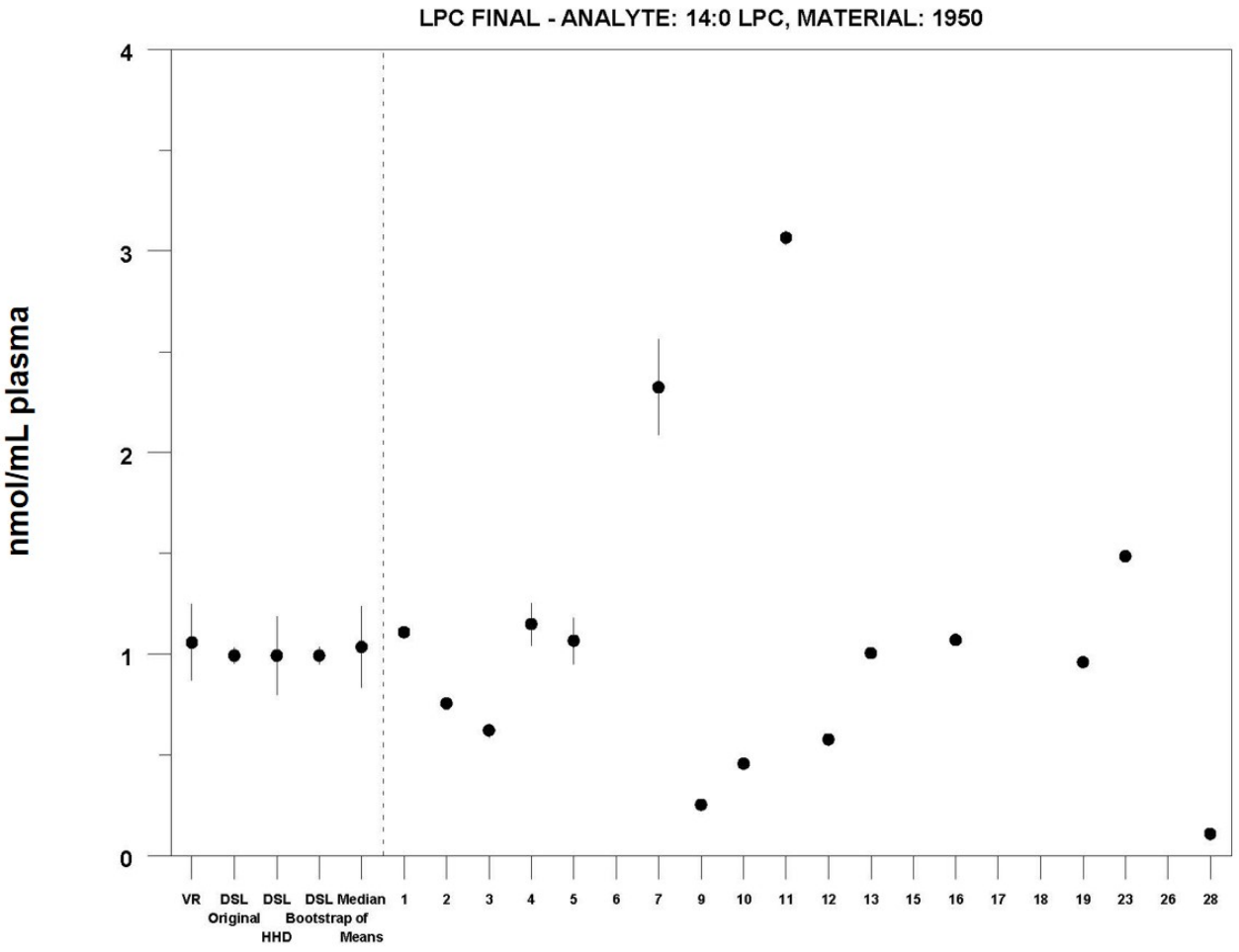


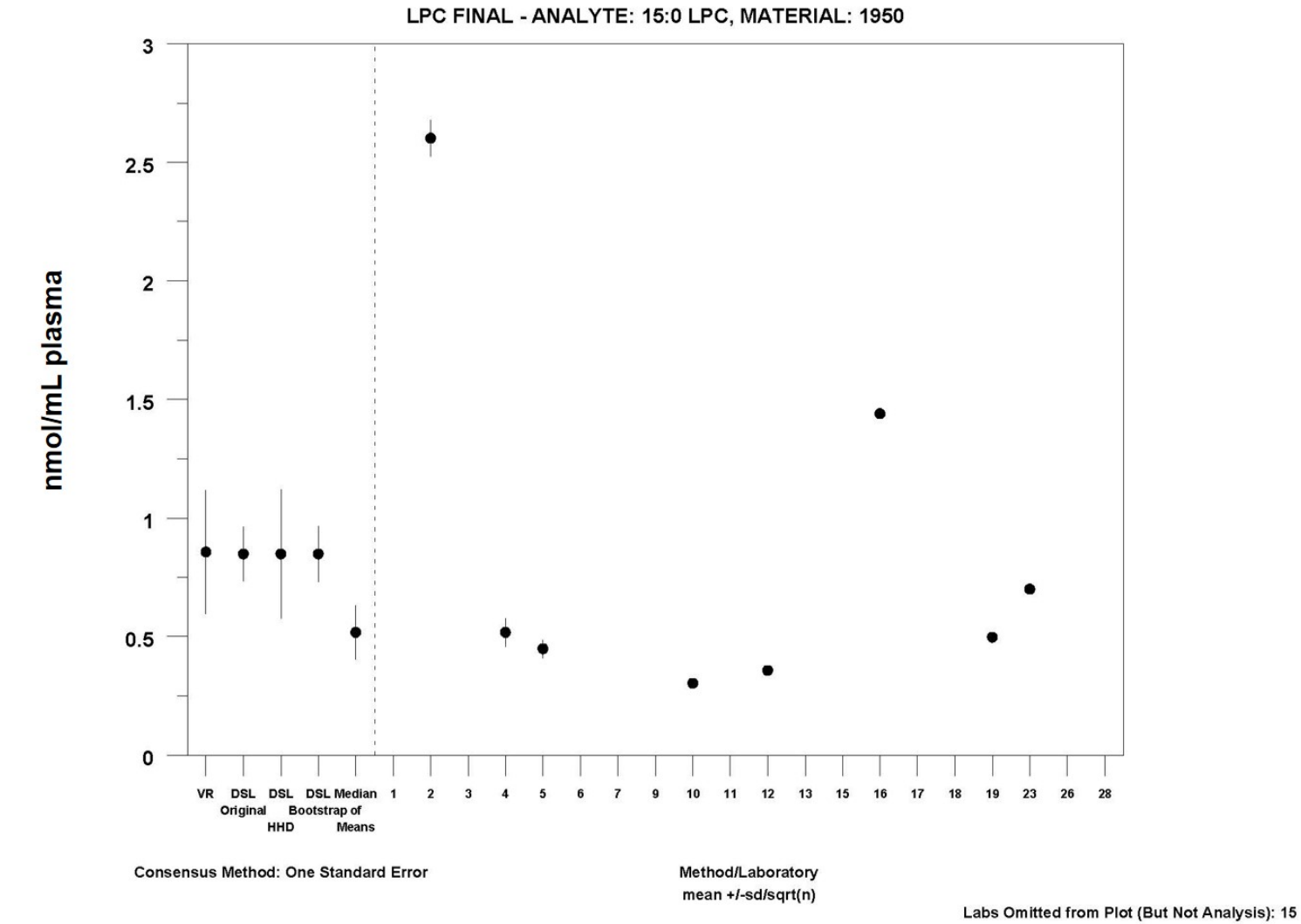


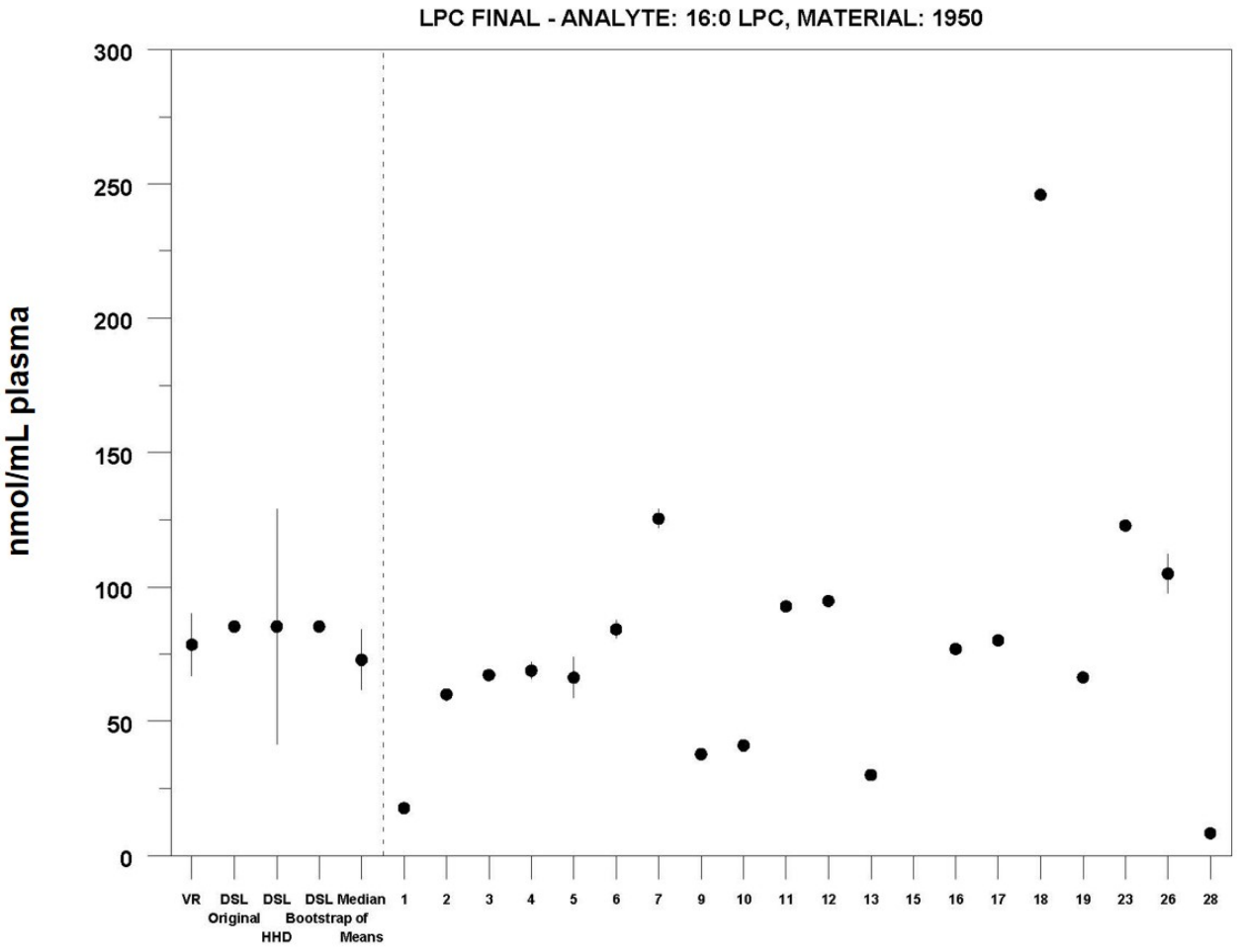
MEDM Location: 1.1 ± 0.56 nmol/mL



MEDM Location: 1.5 ± 0.17 nmol/mL



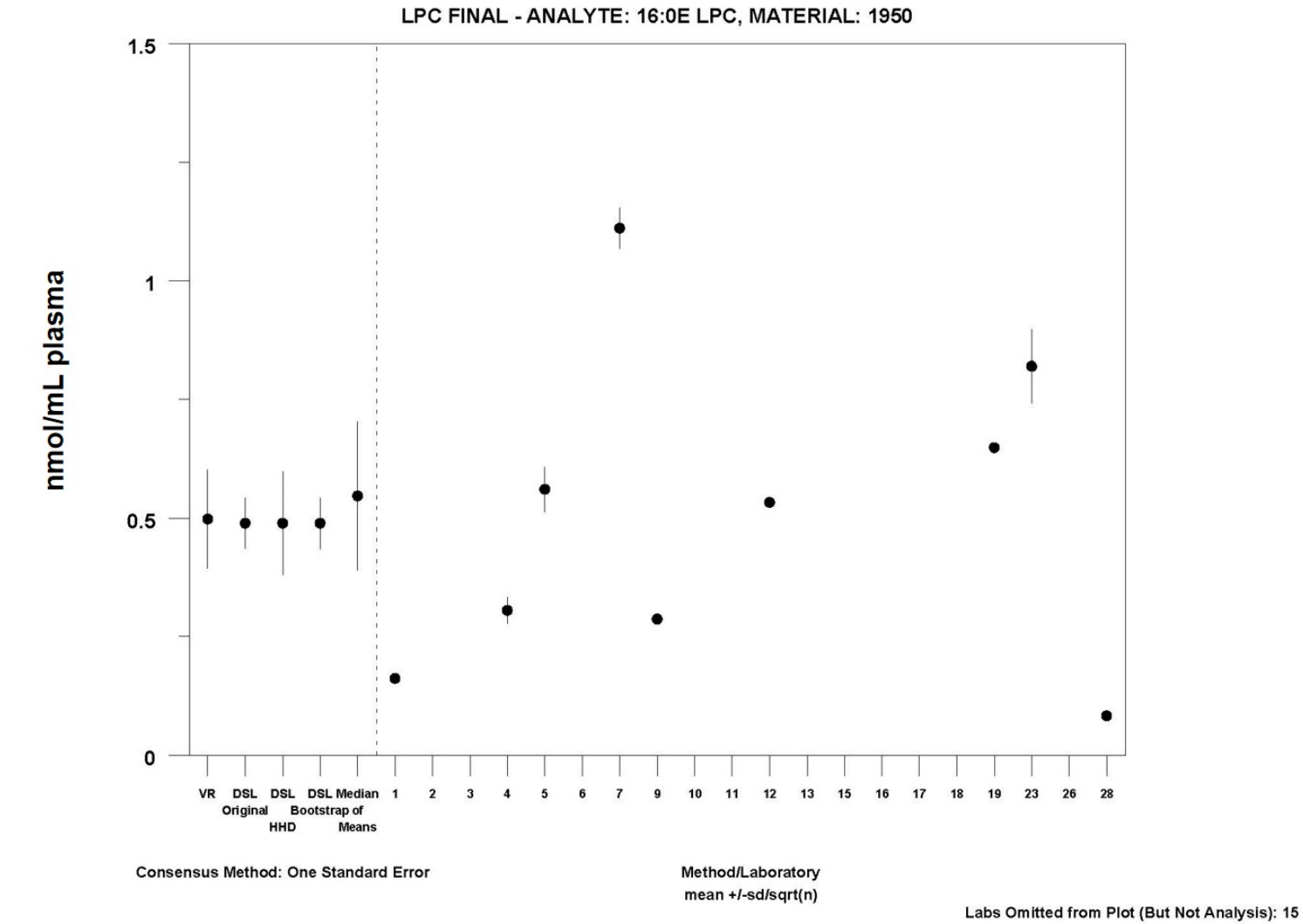


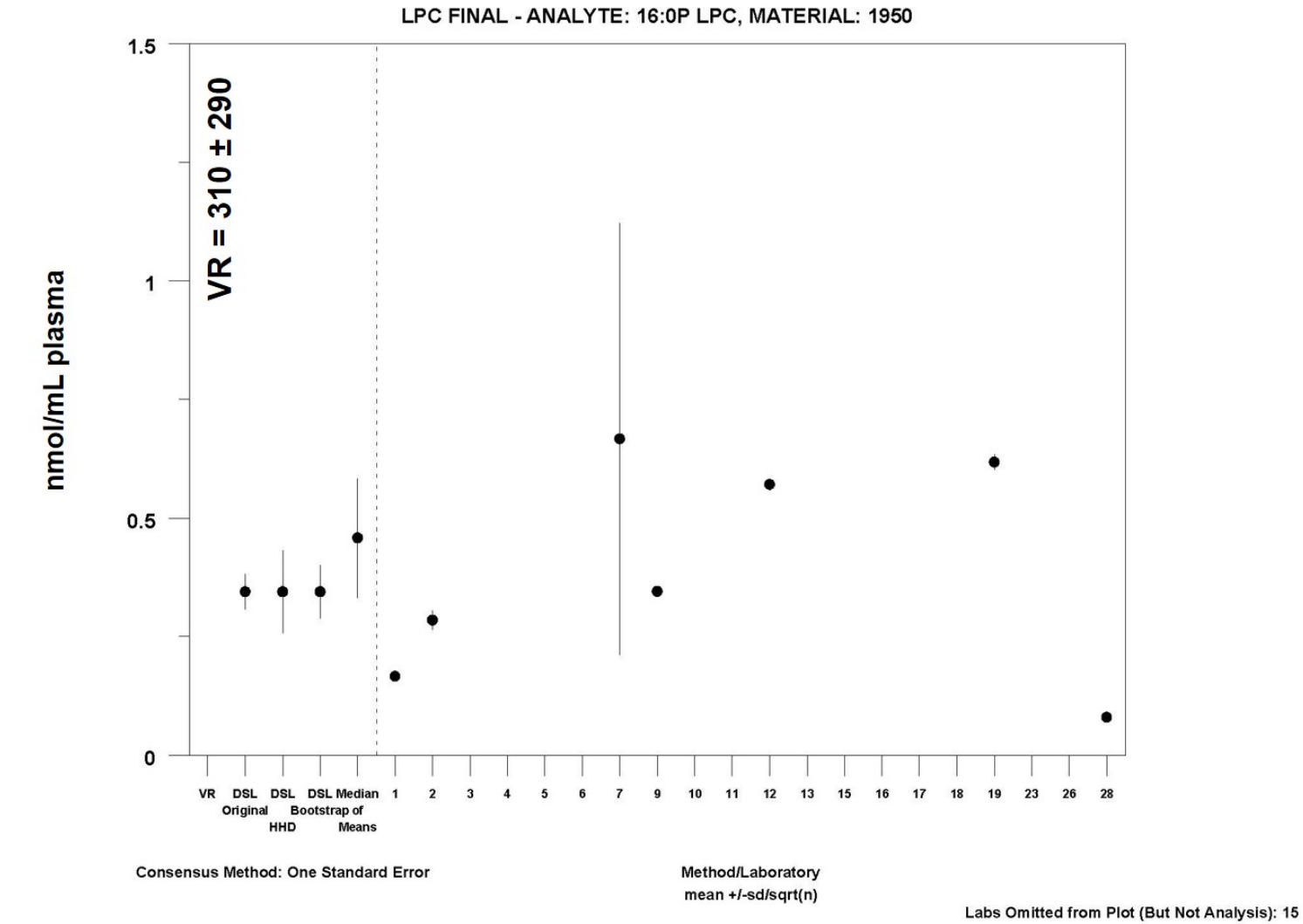


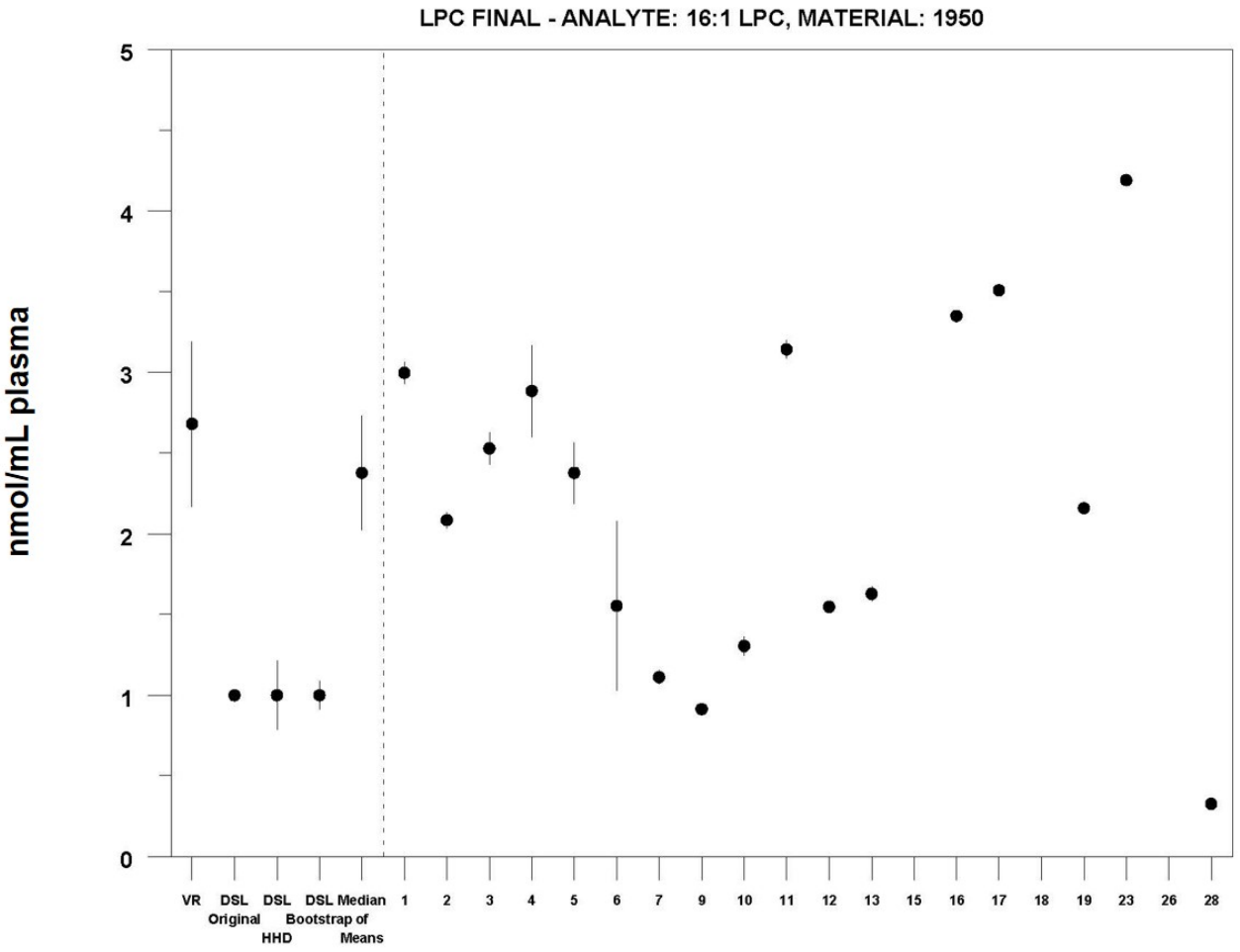
Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 73 ± 11 nmol/mL

15: 91164 ± 17489



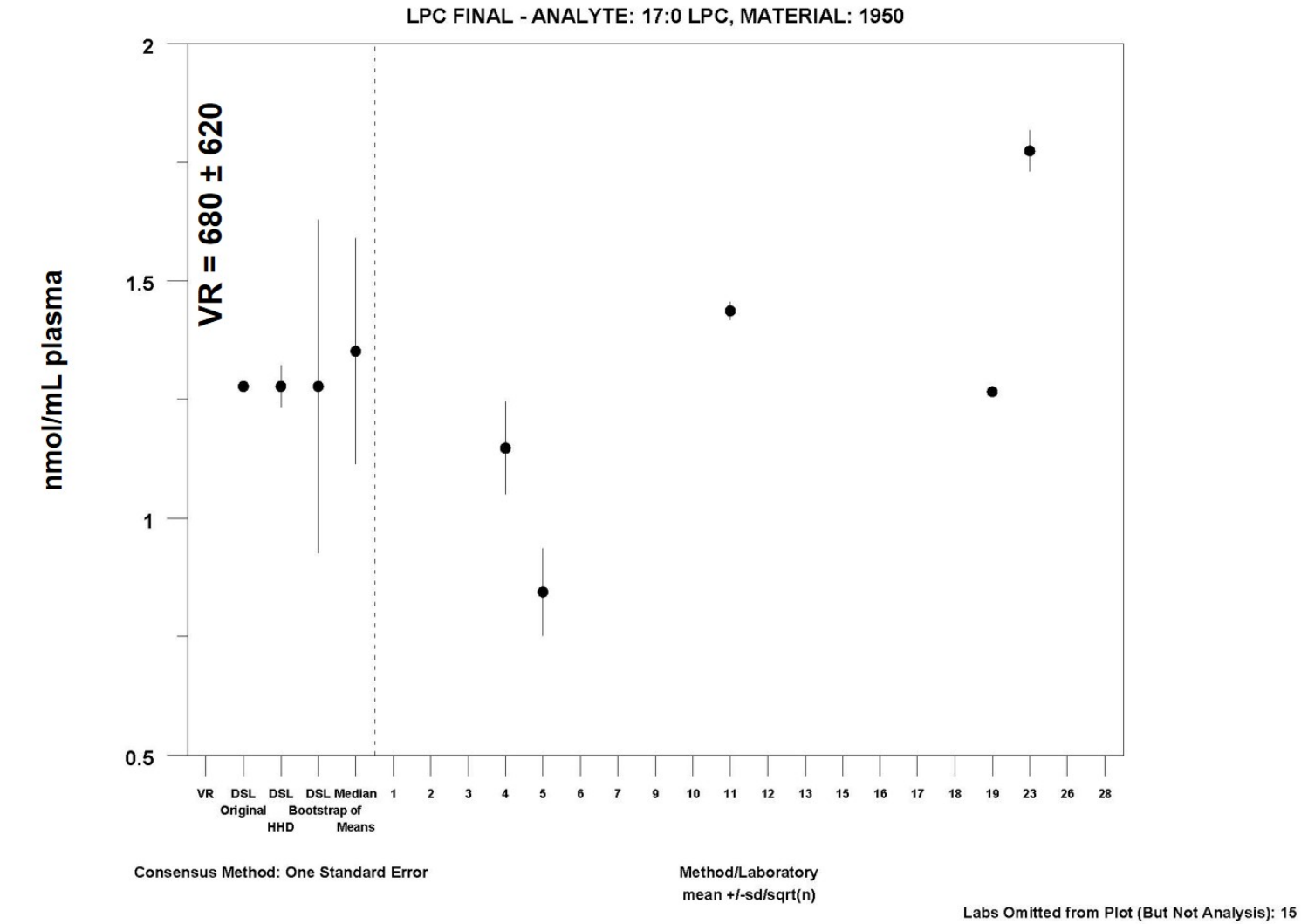


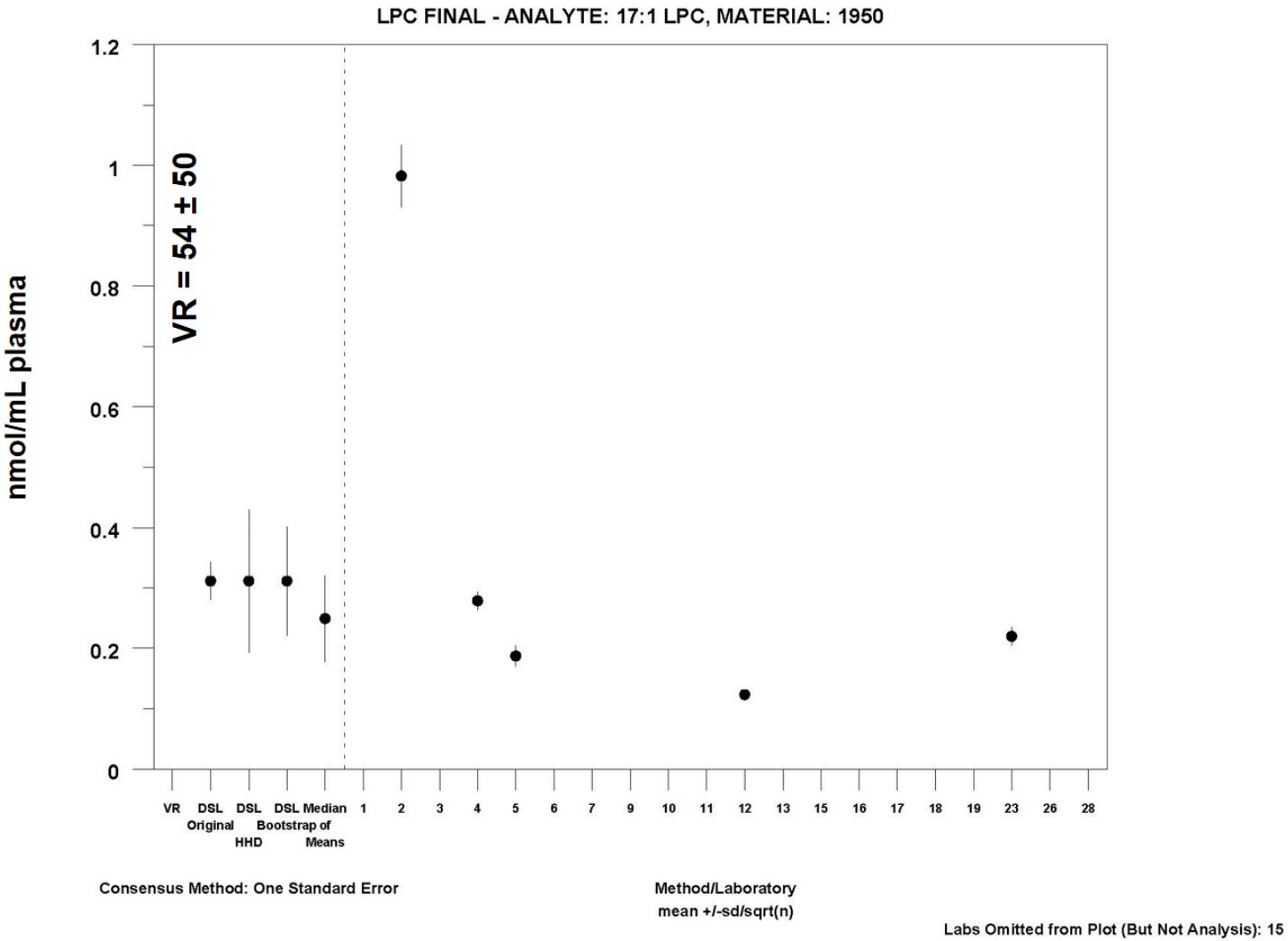


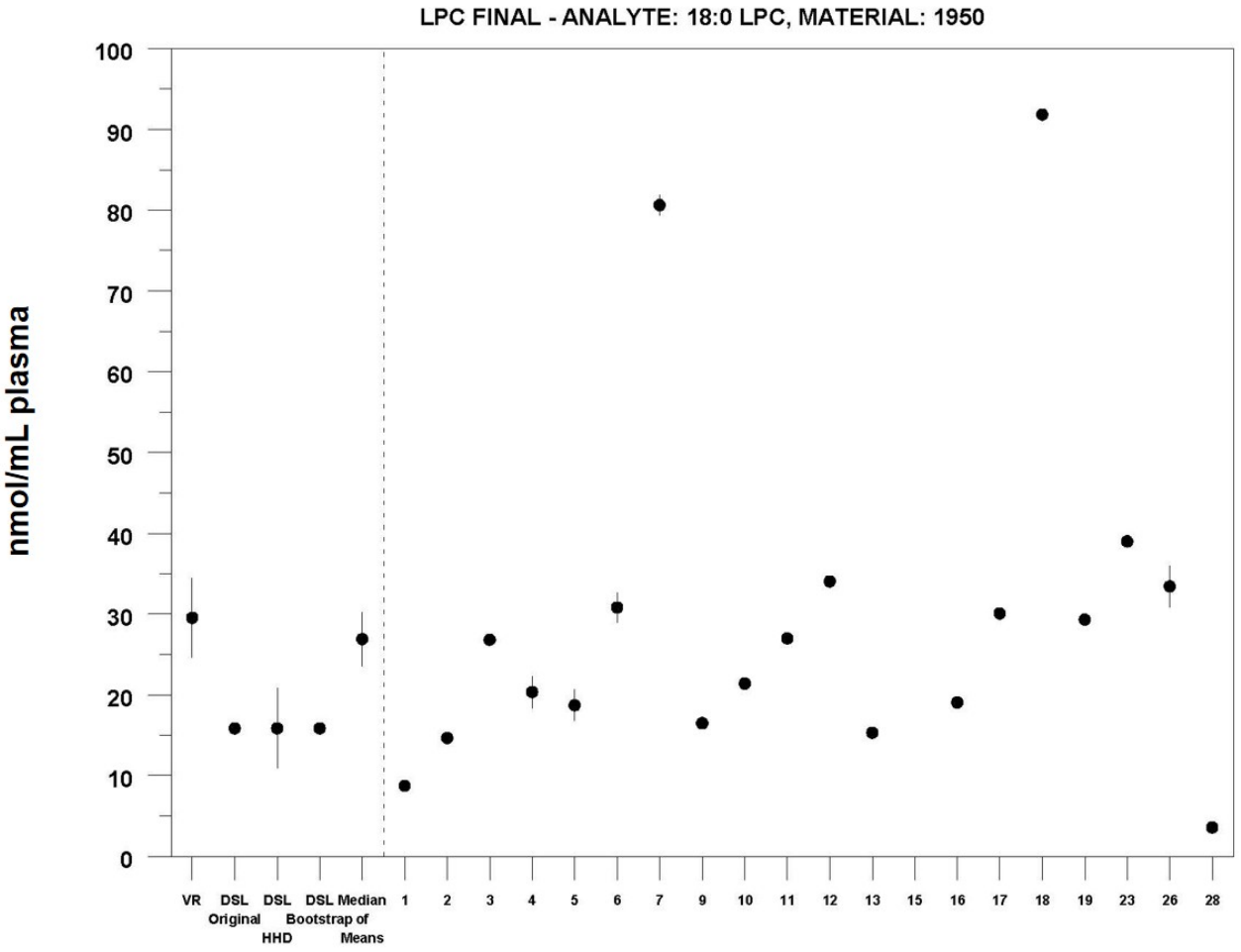
Labs Omitted from Plot (But Not Analysis): 15 18

MEDM Location: 2.4 ± 0.35 nmol/mL

15: 4574 ± 609; 18: 10.6 ± 0.08



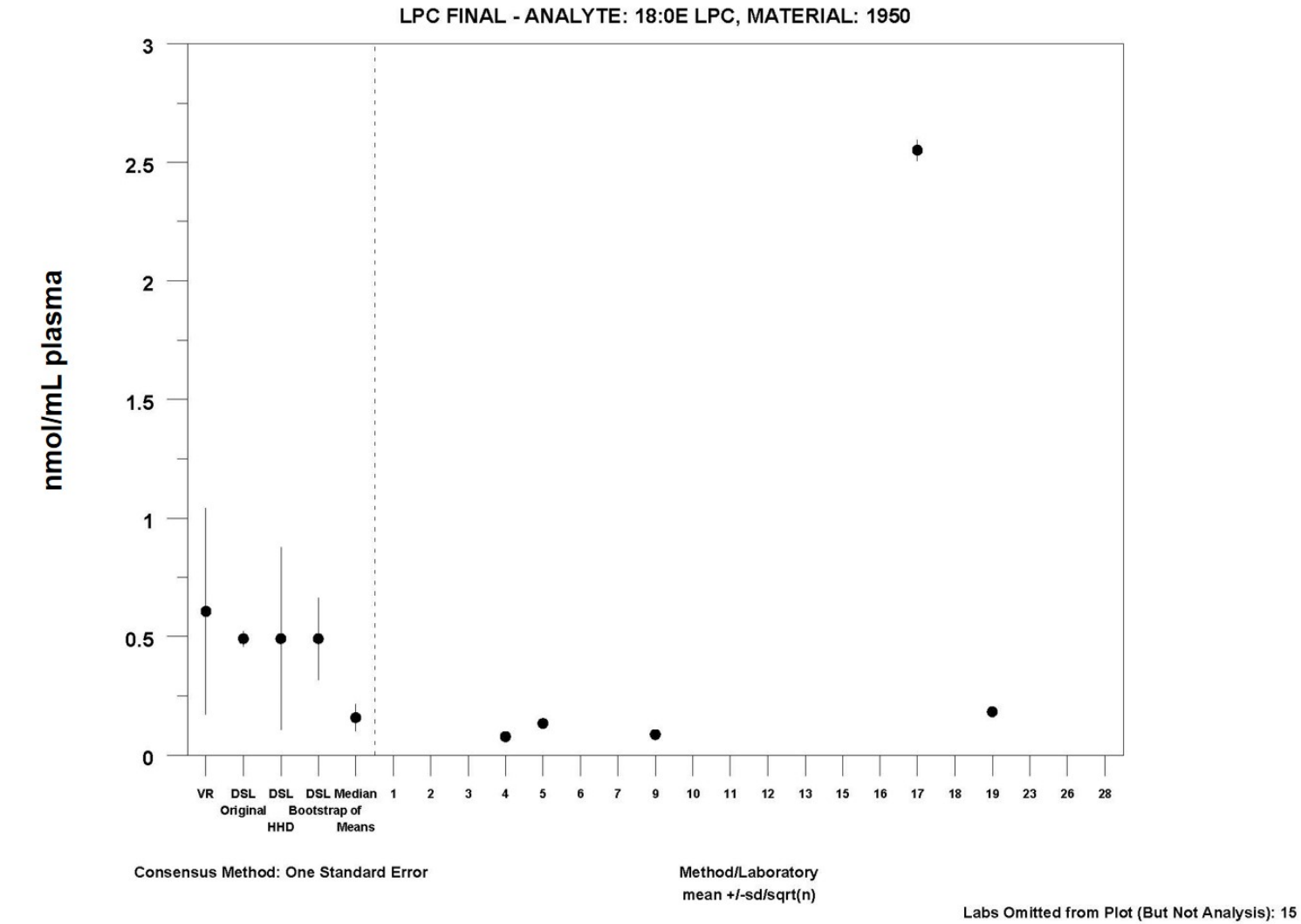


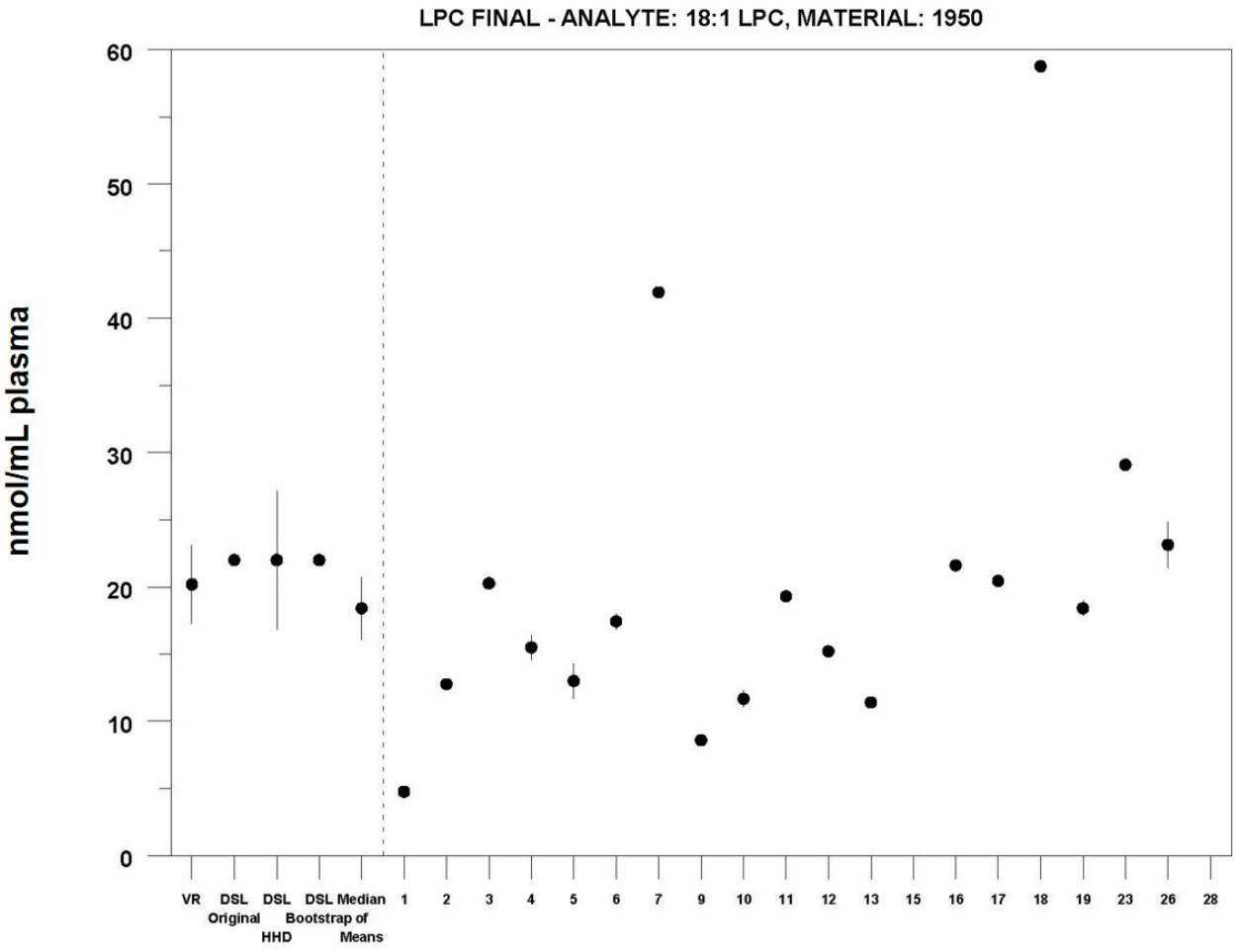


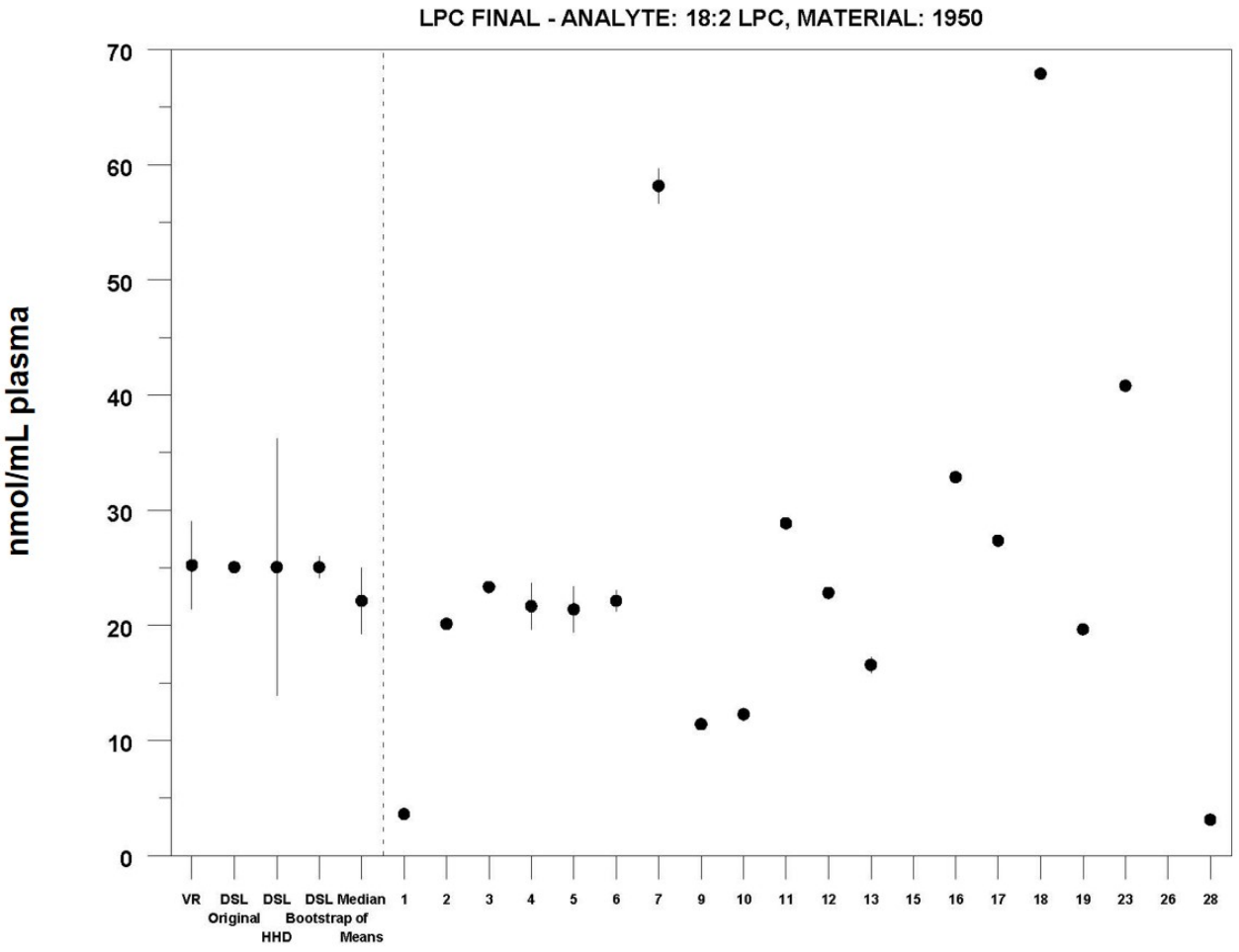
Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 27 ± 3.3 nmol/mL

15: 62272 ± 16163



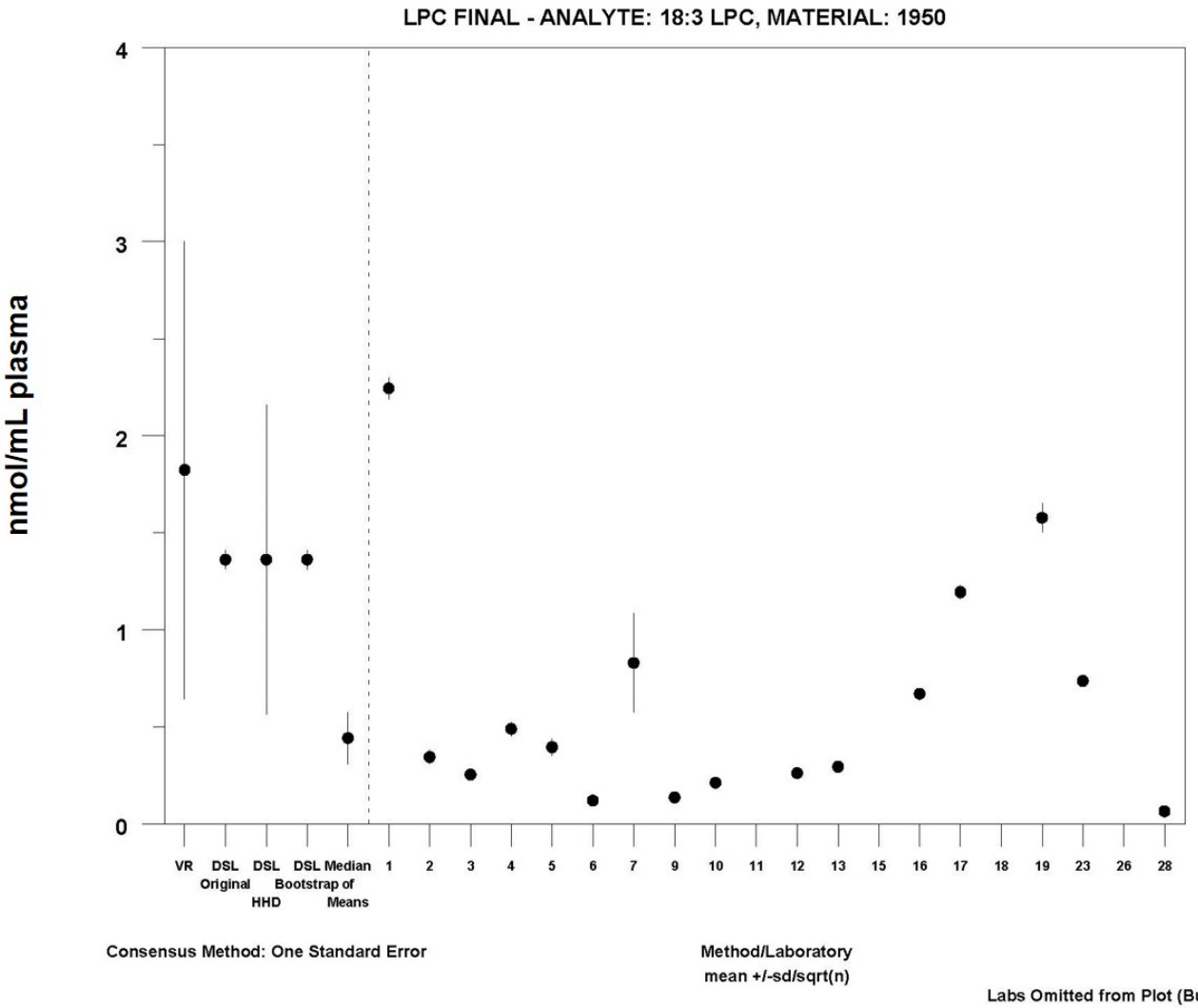


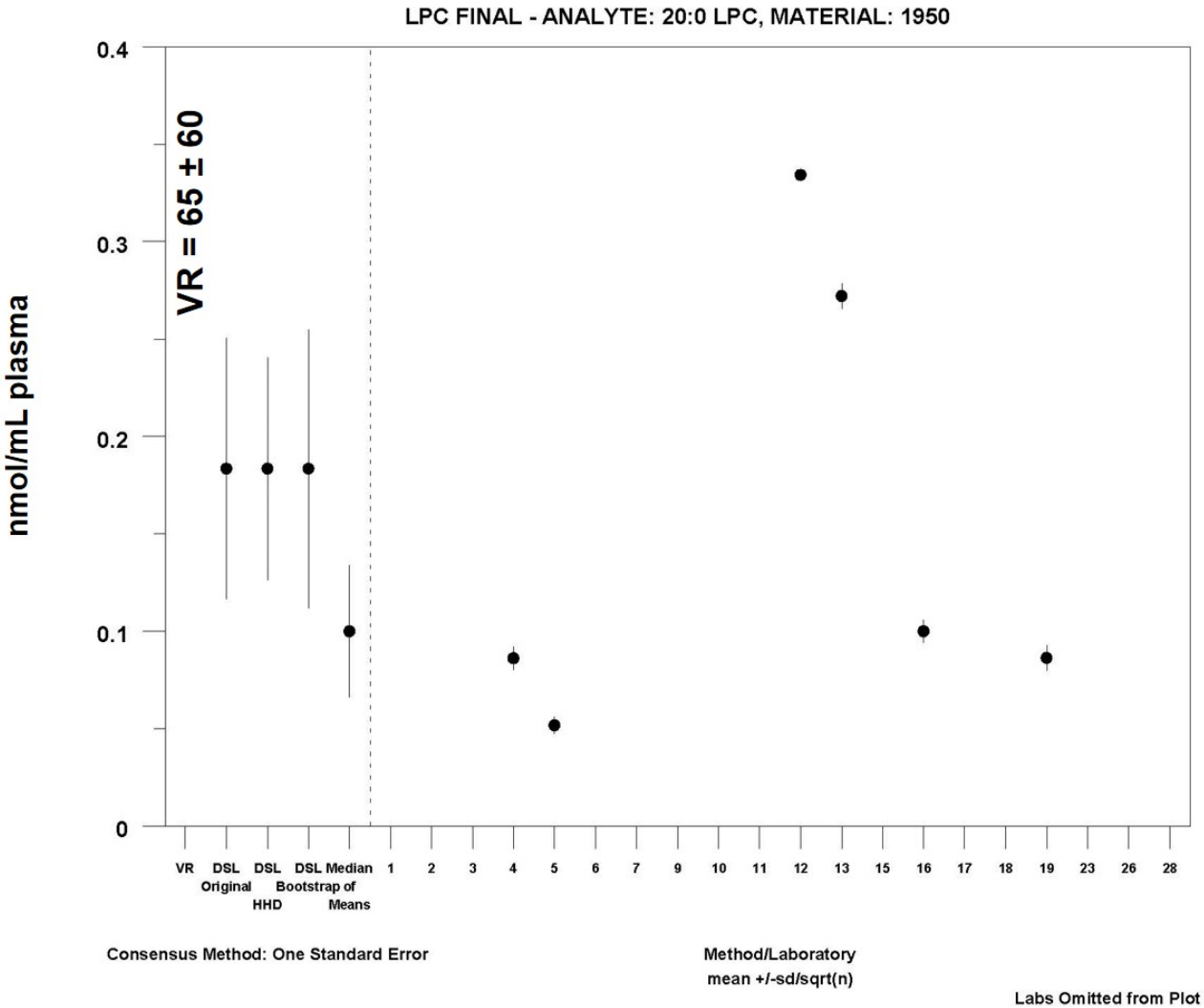


Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 22 ± 2.9 nmol/mL

15: 73529 ± 17862

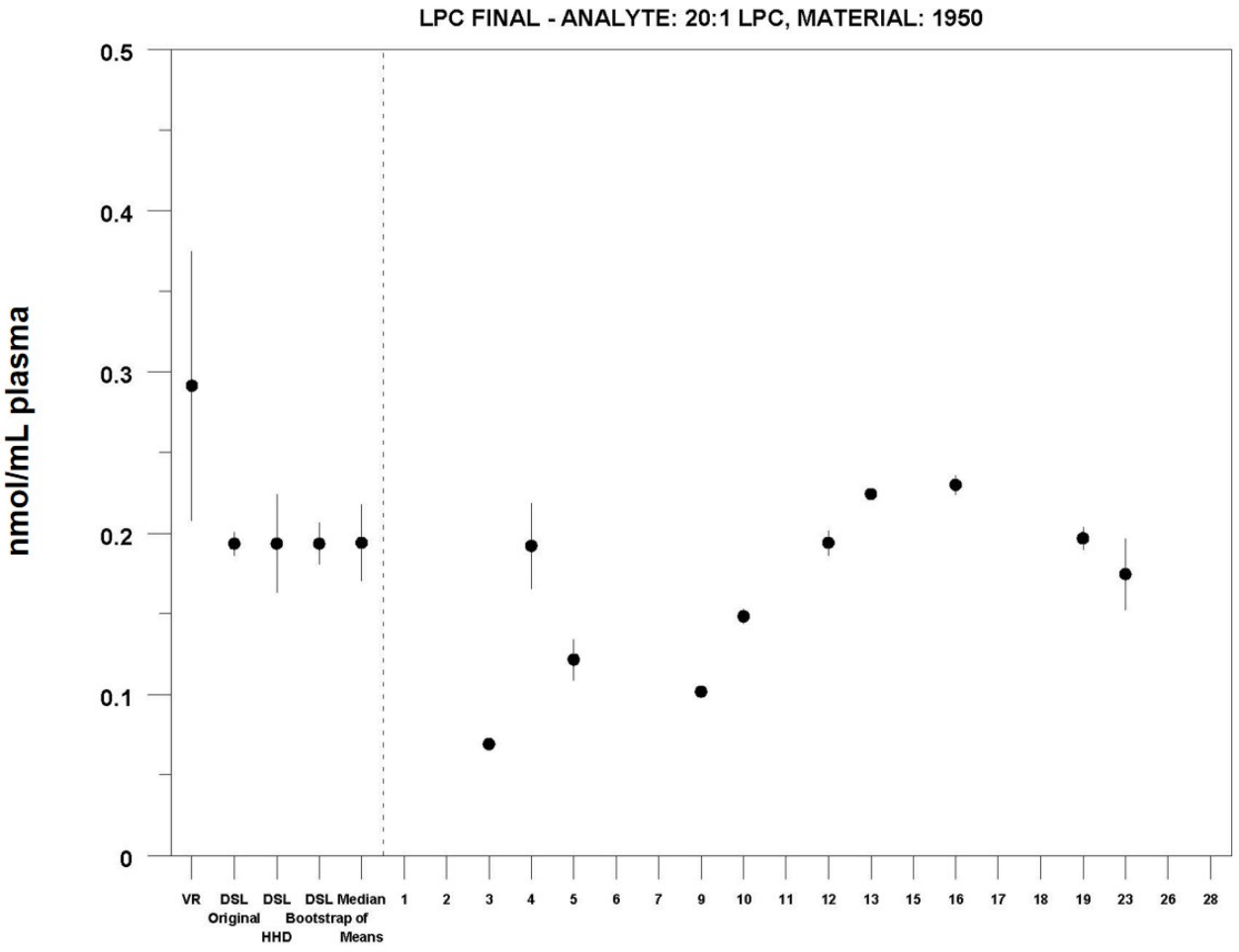




Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 0.10 ± 0.034 nmol/mL

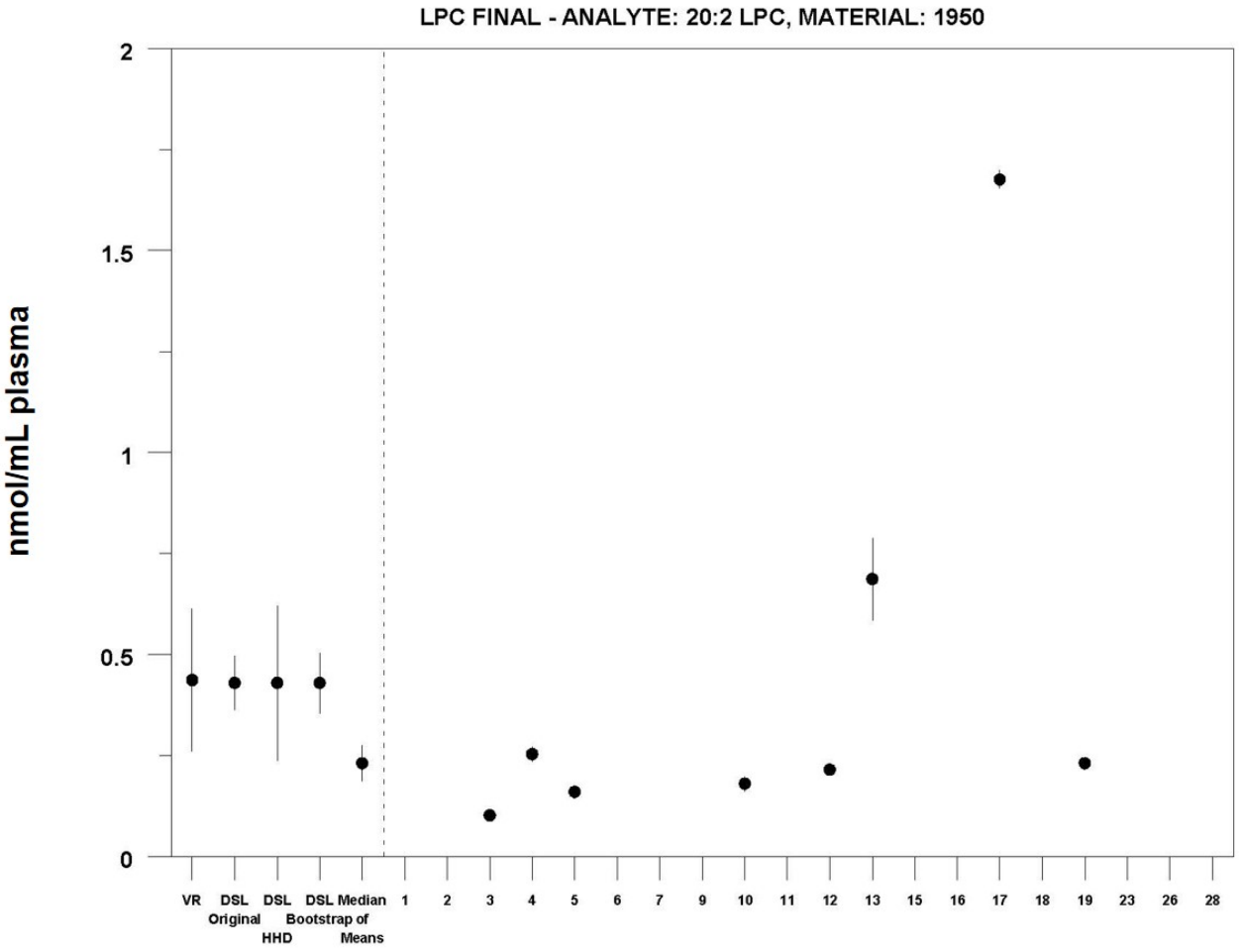
15: 457 ± 15



MEDM Location: 0.19 ± 0.024 nmol/mL

Labs Omitted from Plot (But Not Analysis): 7 15 17

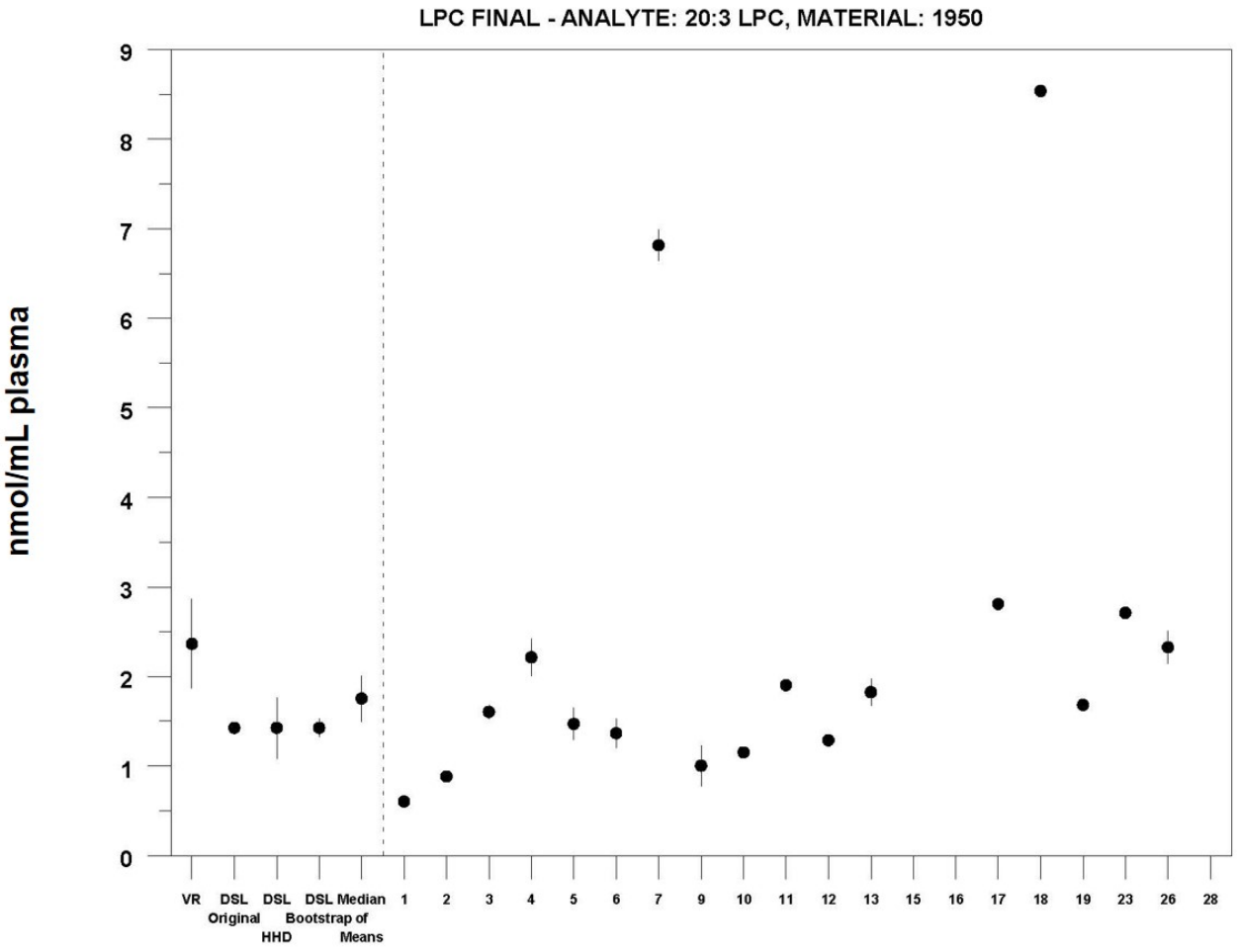
7: 0.86 ± 0.09; 15: 506 ± 49; 17: 1.0 ± 0.07



Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 0.23 ± 0.044 nmol/mL

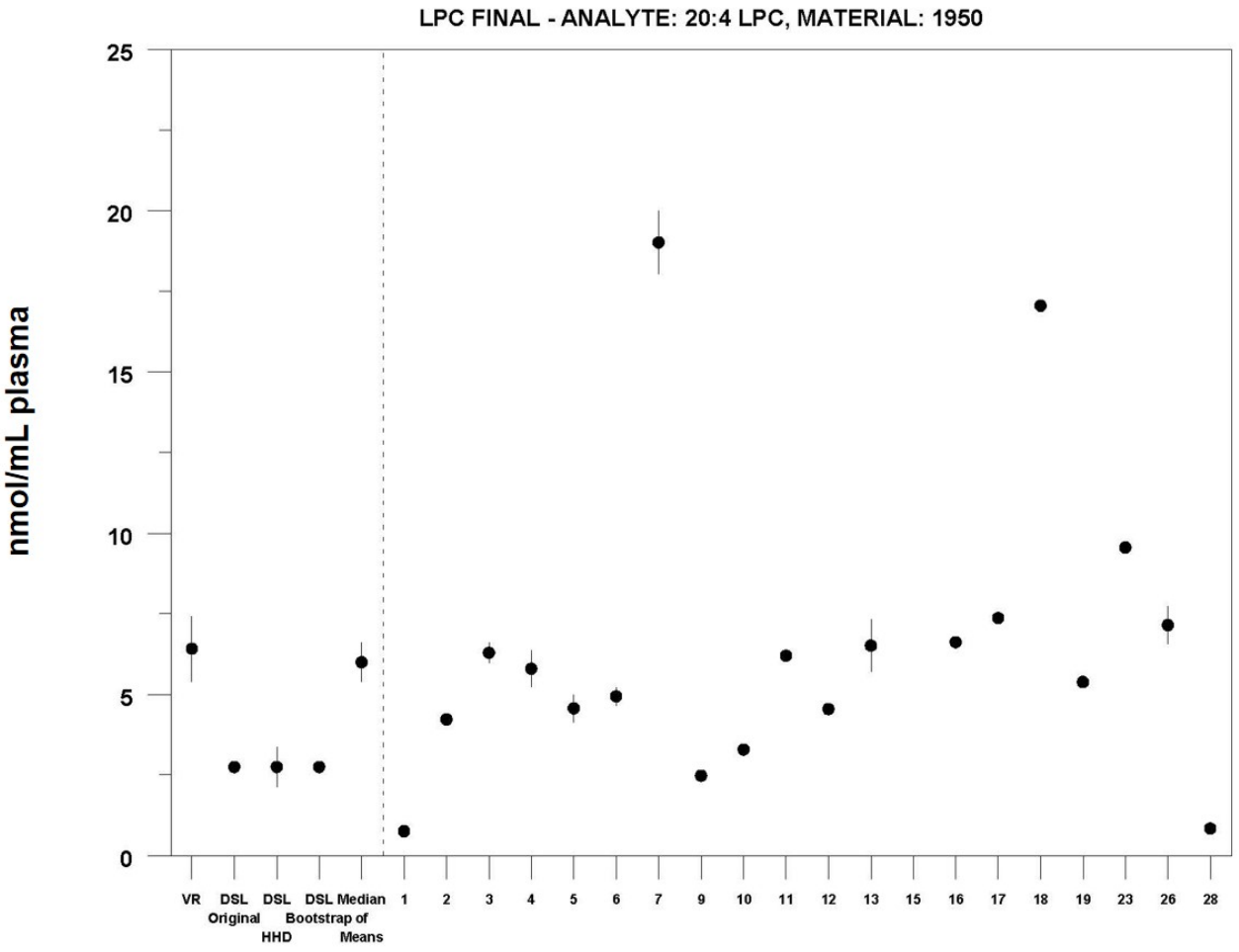
15: 1472 ± 233



Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 1.8 ± 0.26 nmol/mL

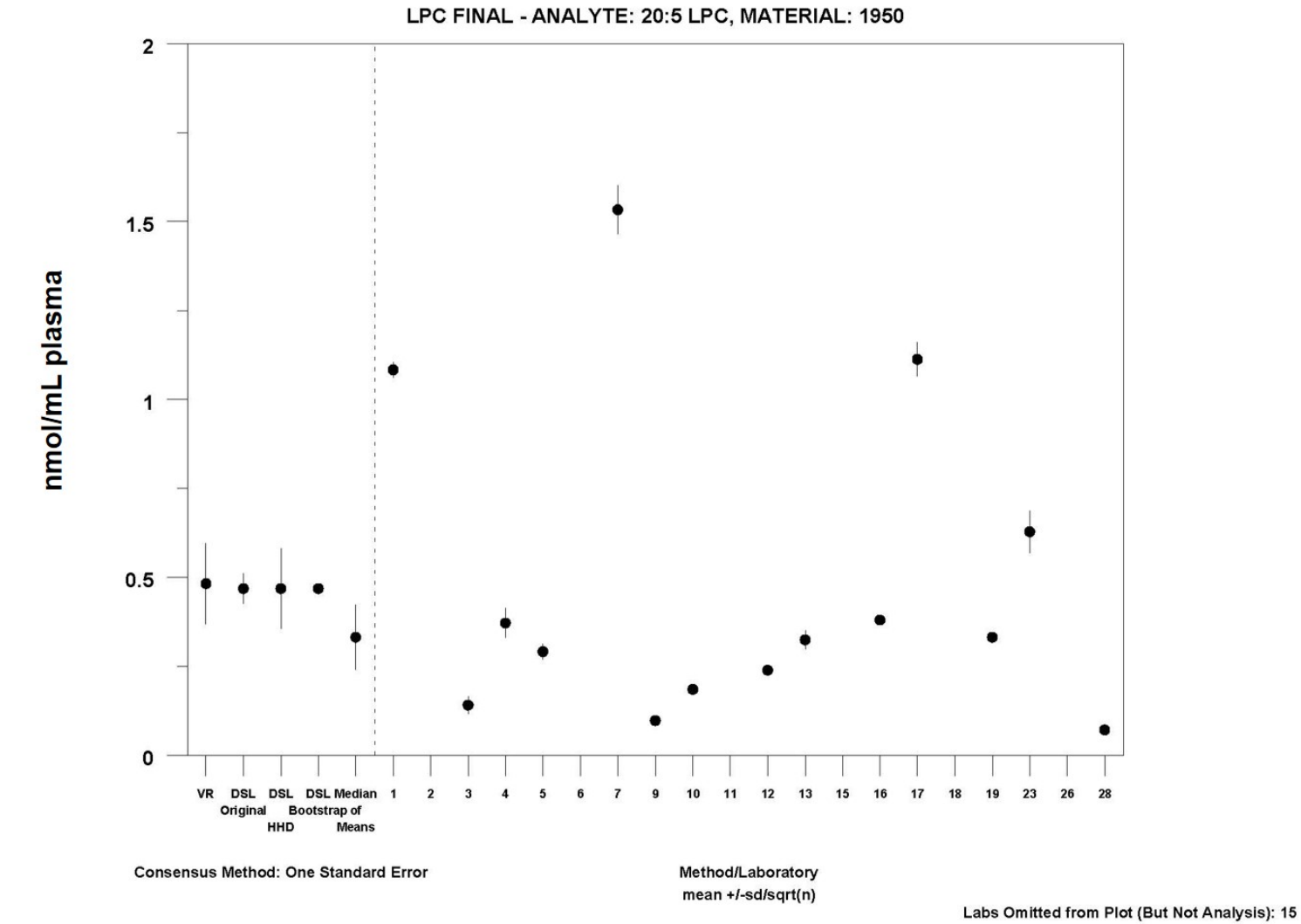
15: 7218 ± 1758

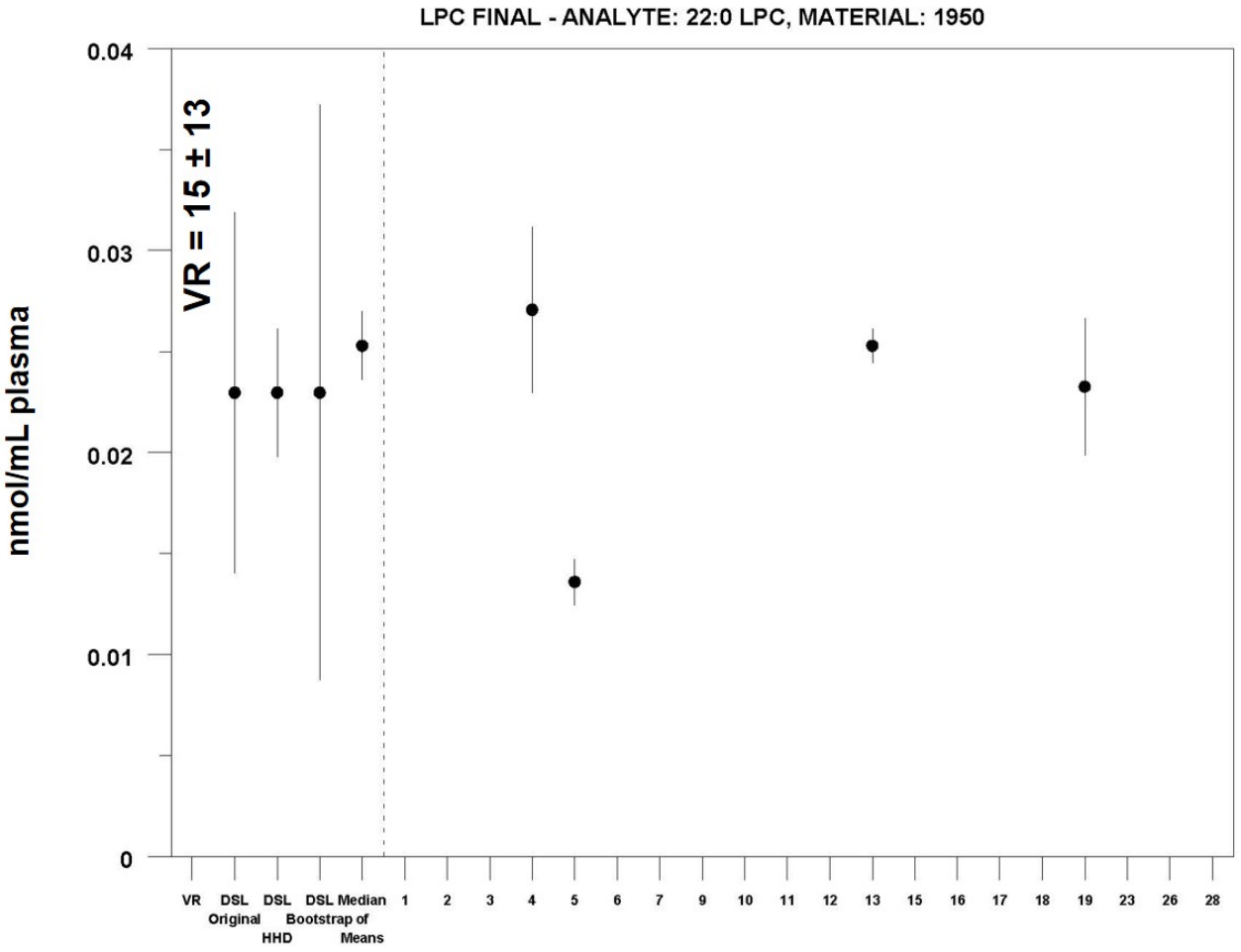


Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 6.0 ± 0.60 nmol/mL

15: 24064 ± 4872

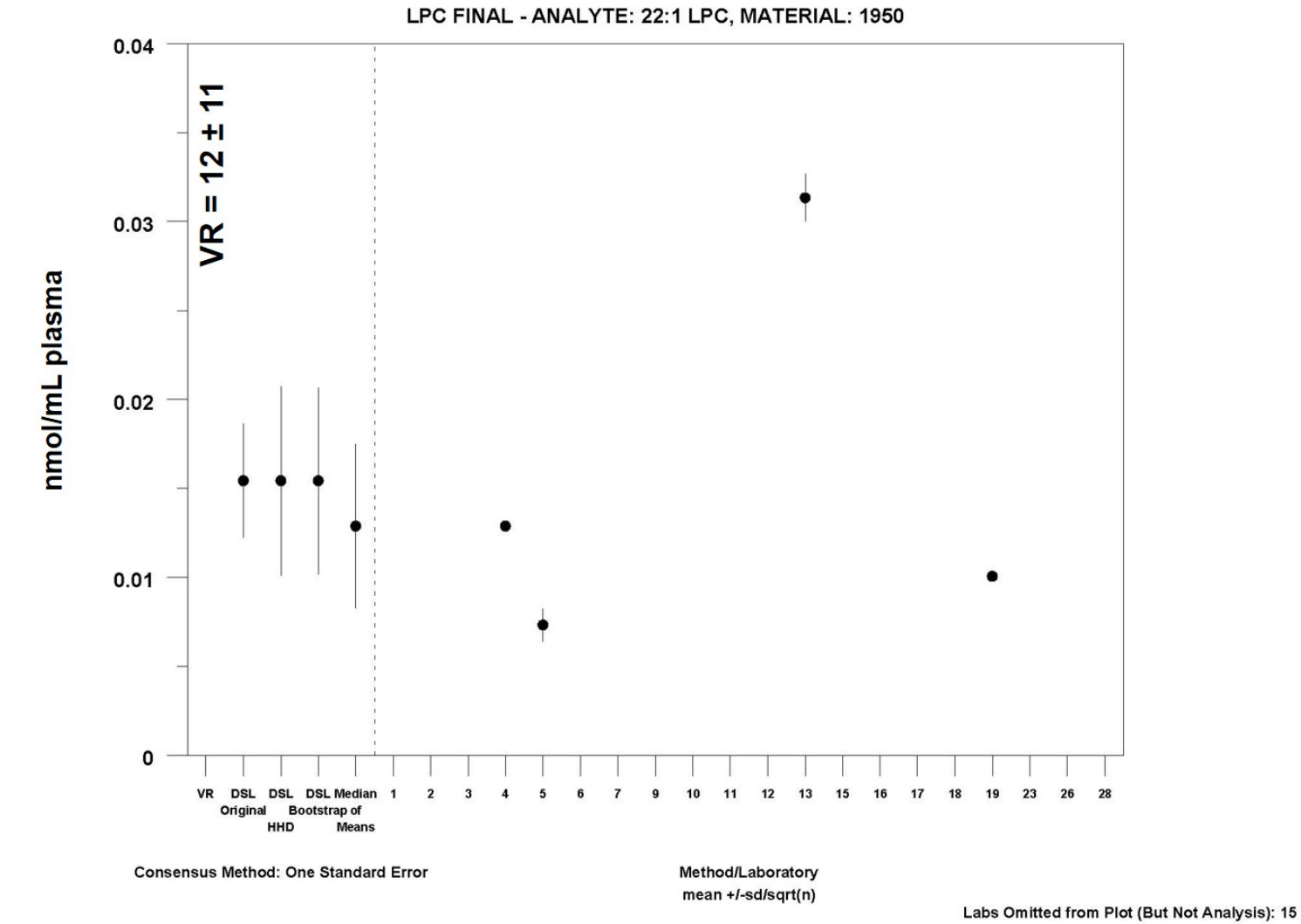


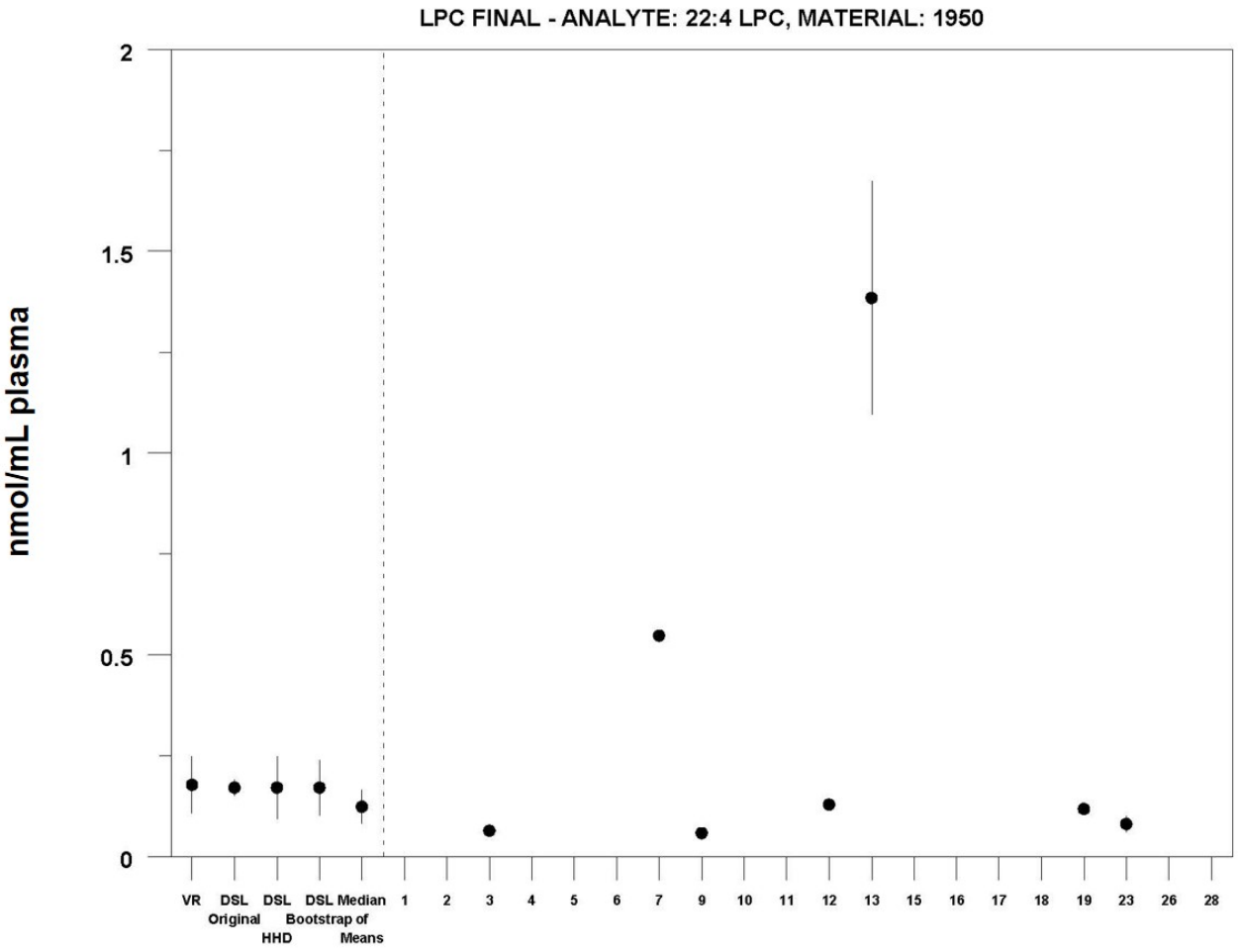


Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 0.025 ± 0.0017 nmol/mL

15: 73 ± 5

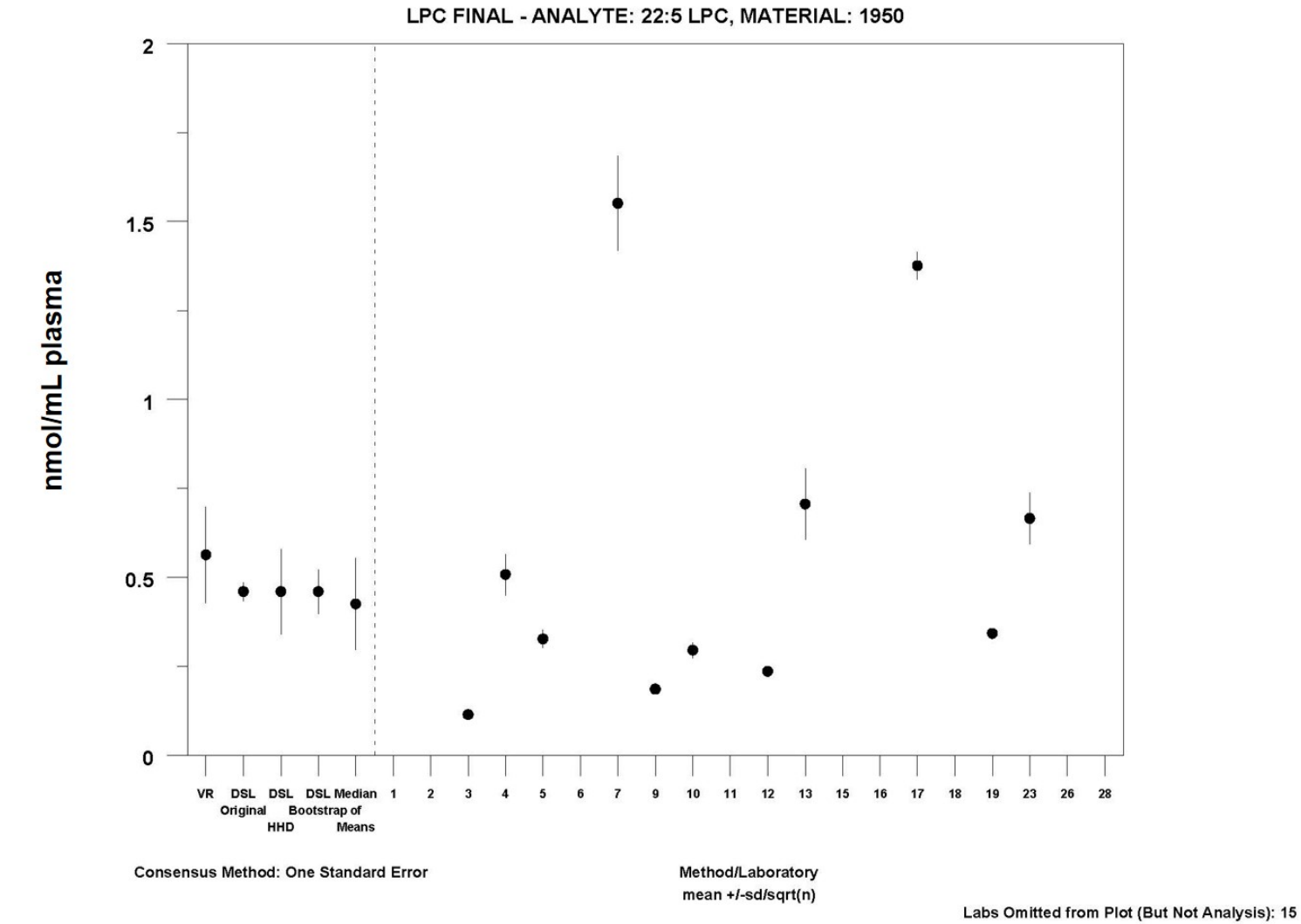


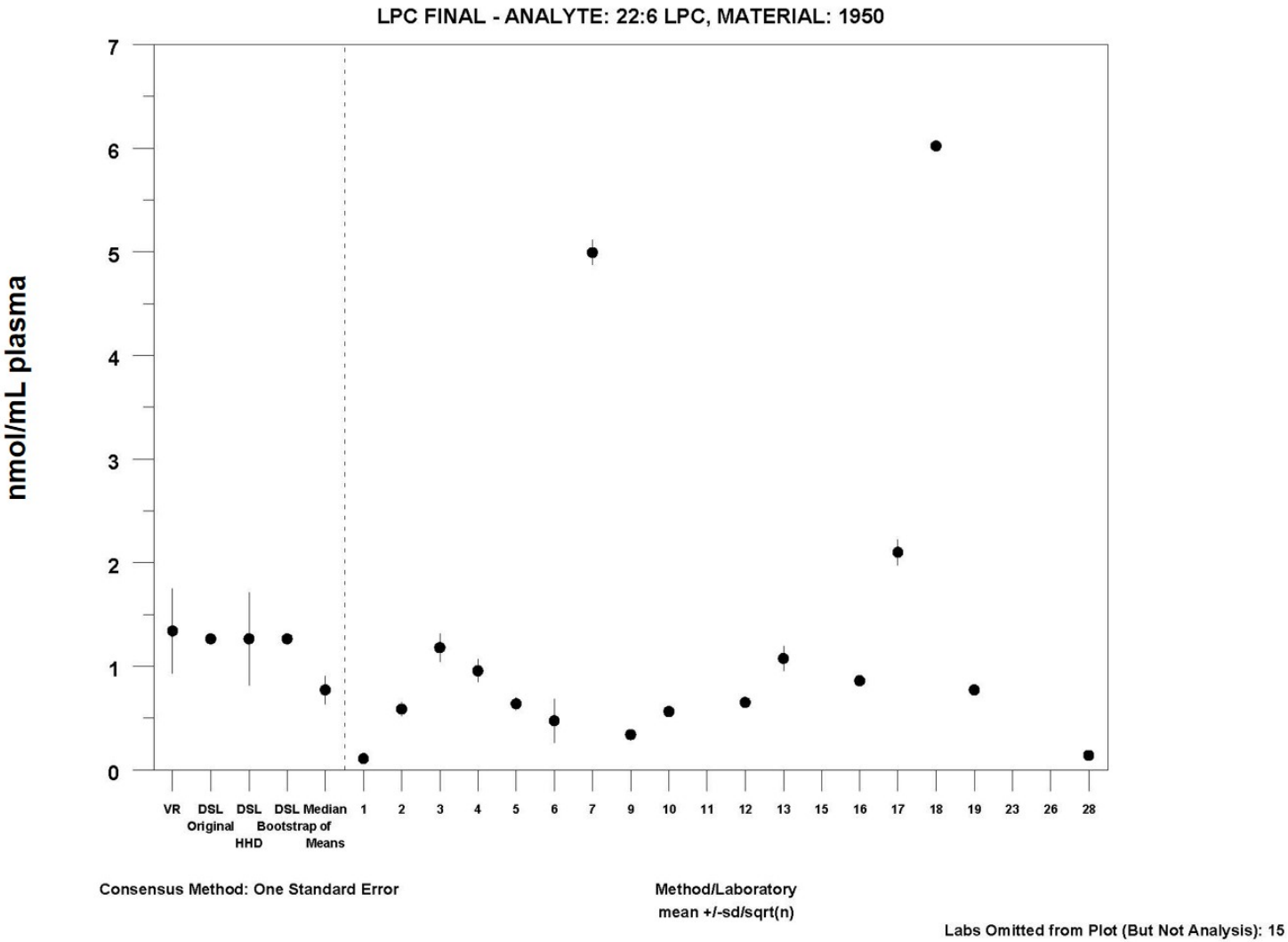


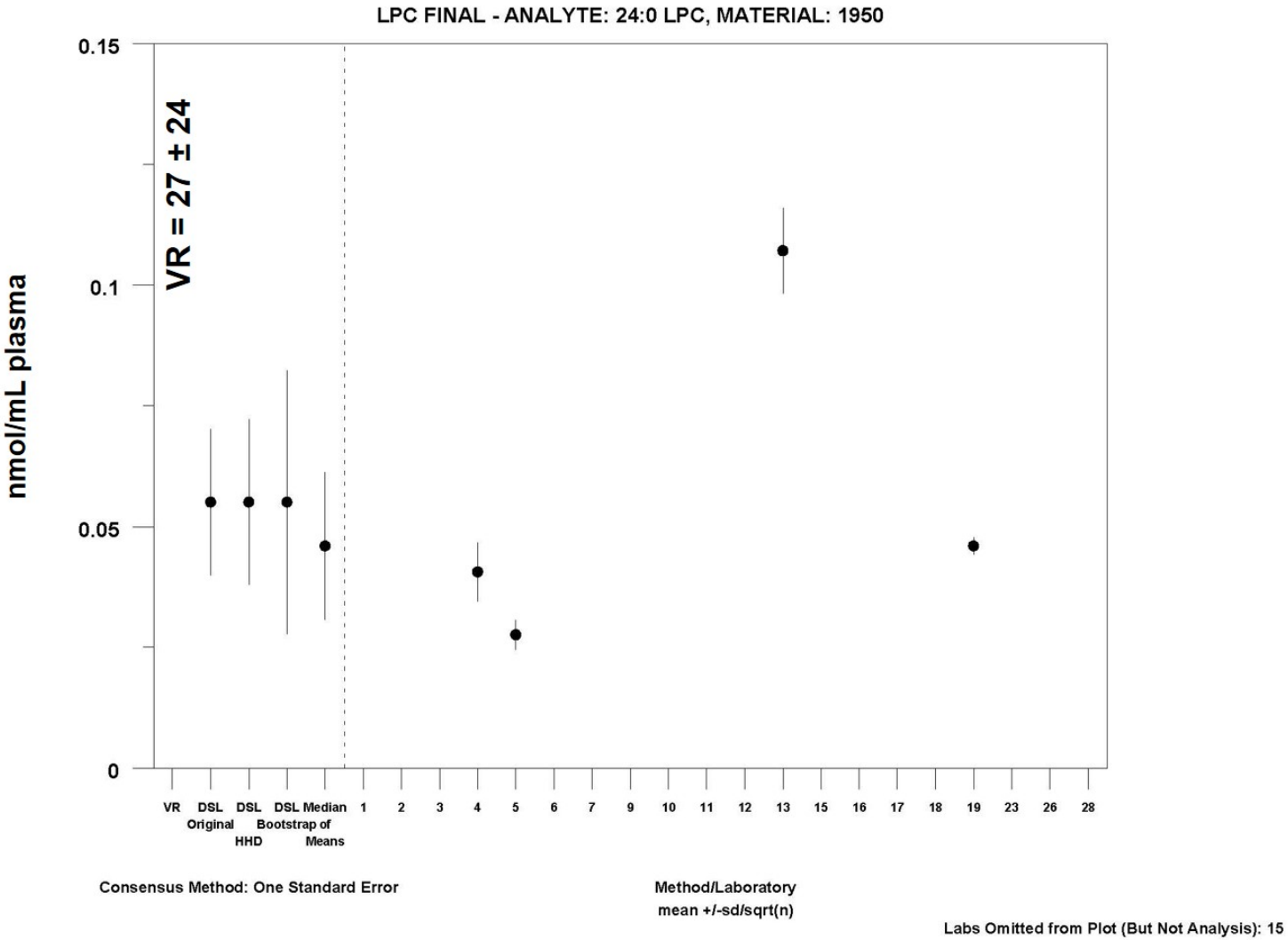
Labs Omitted from Plot (But Not Analysis): 15

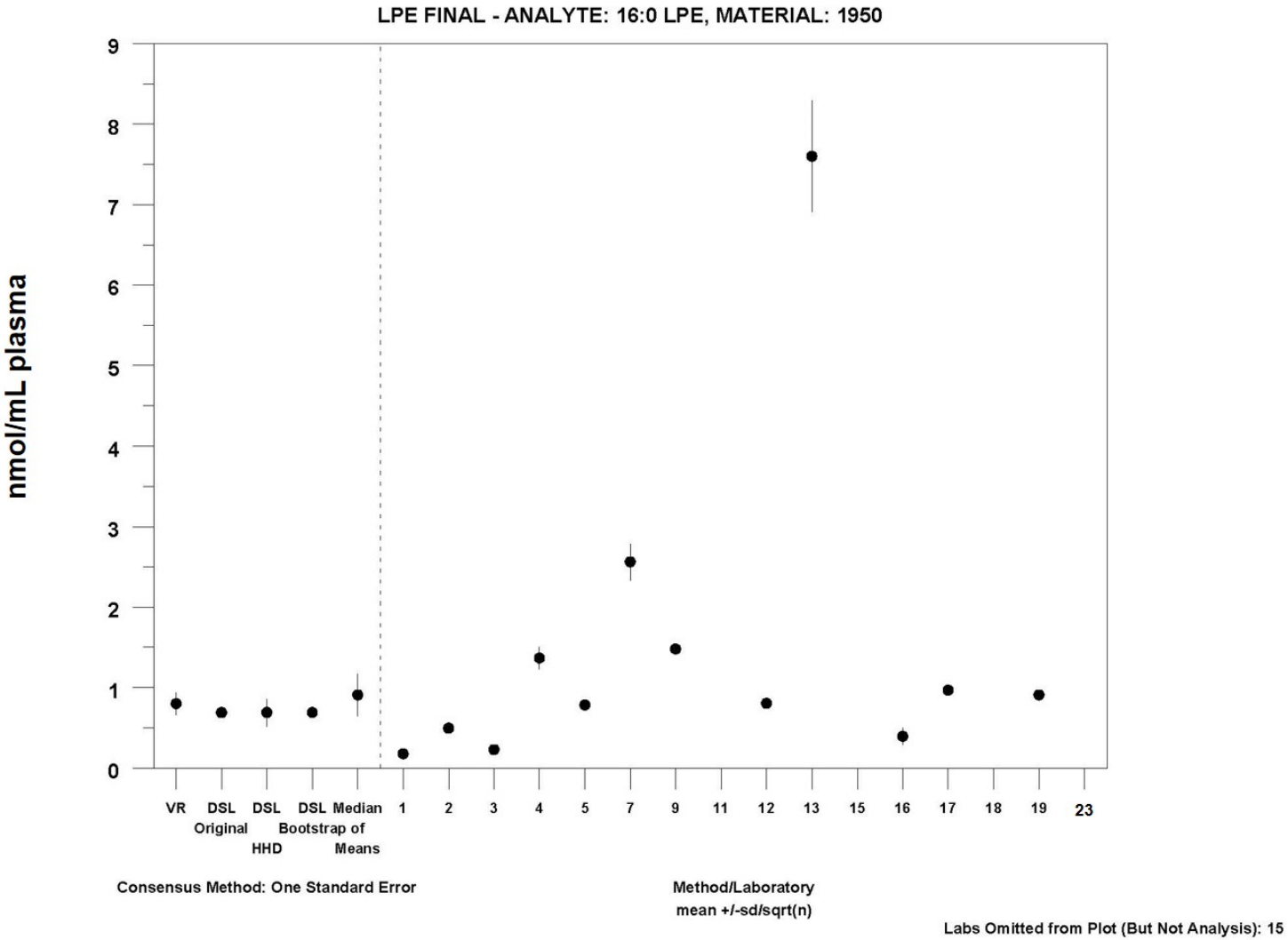
MEDM Location: 0.12 ± 0.041 nmol/mL

15: 444 ± 298





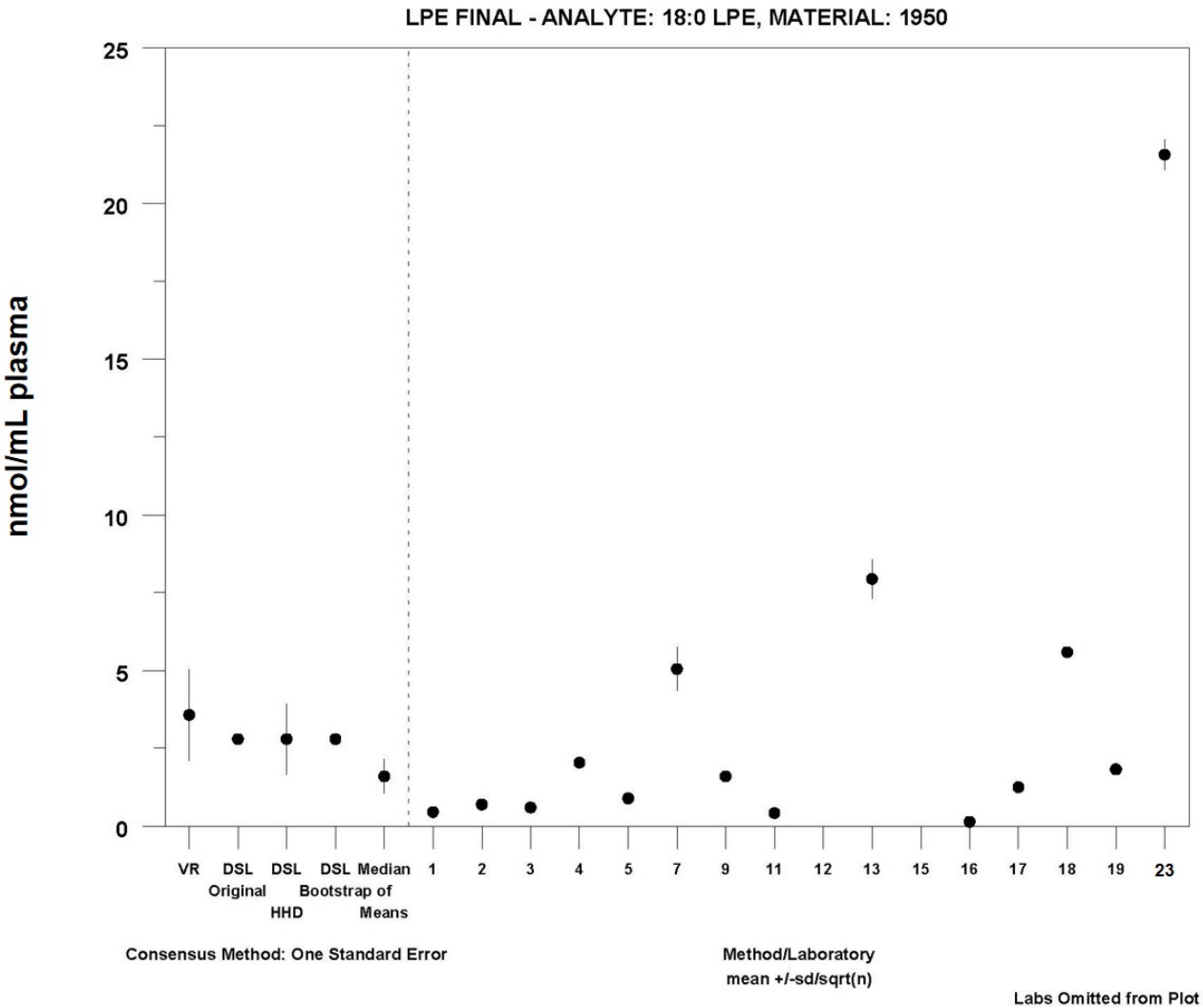




Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 0.91 ± 0.27 nmol/mL

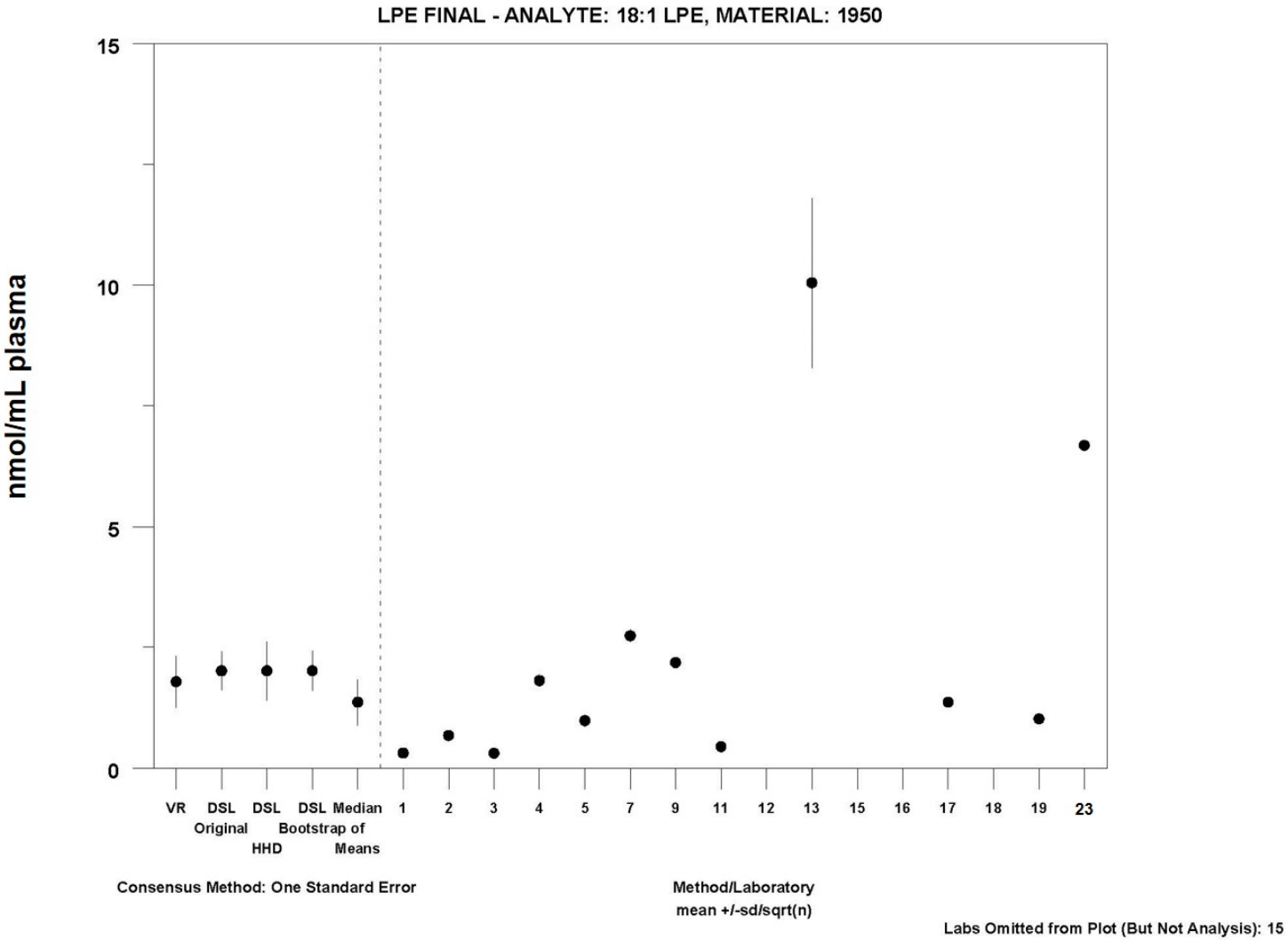
15: 179 ± 22

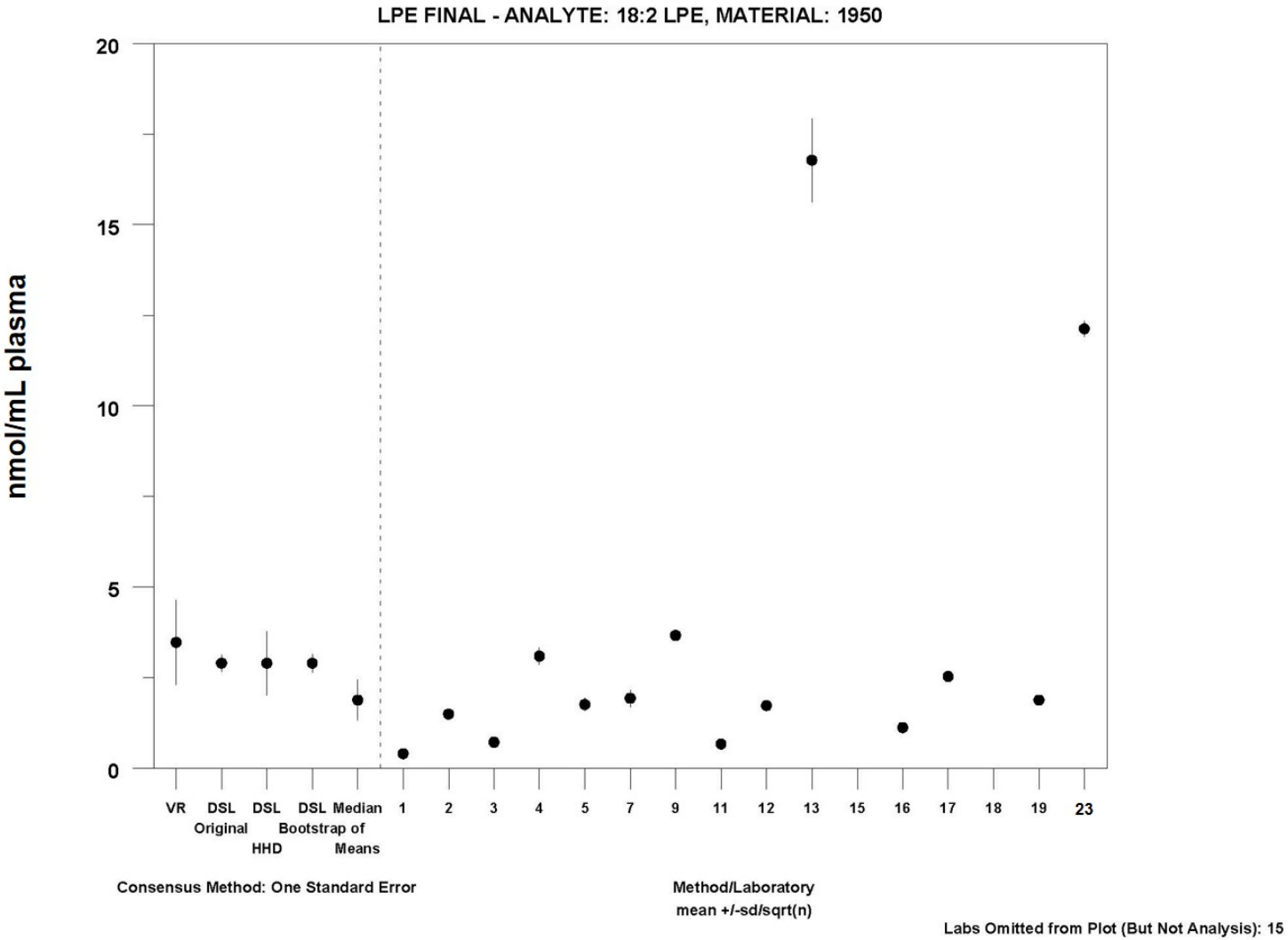


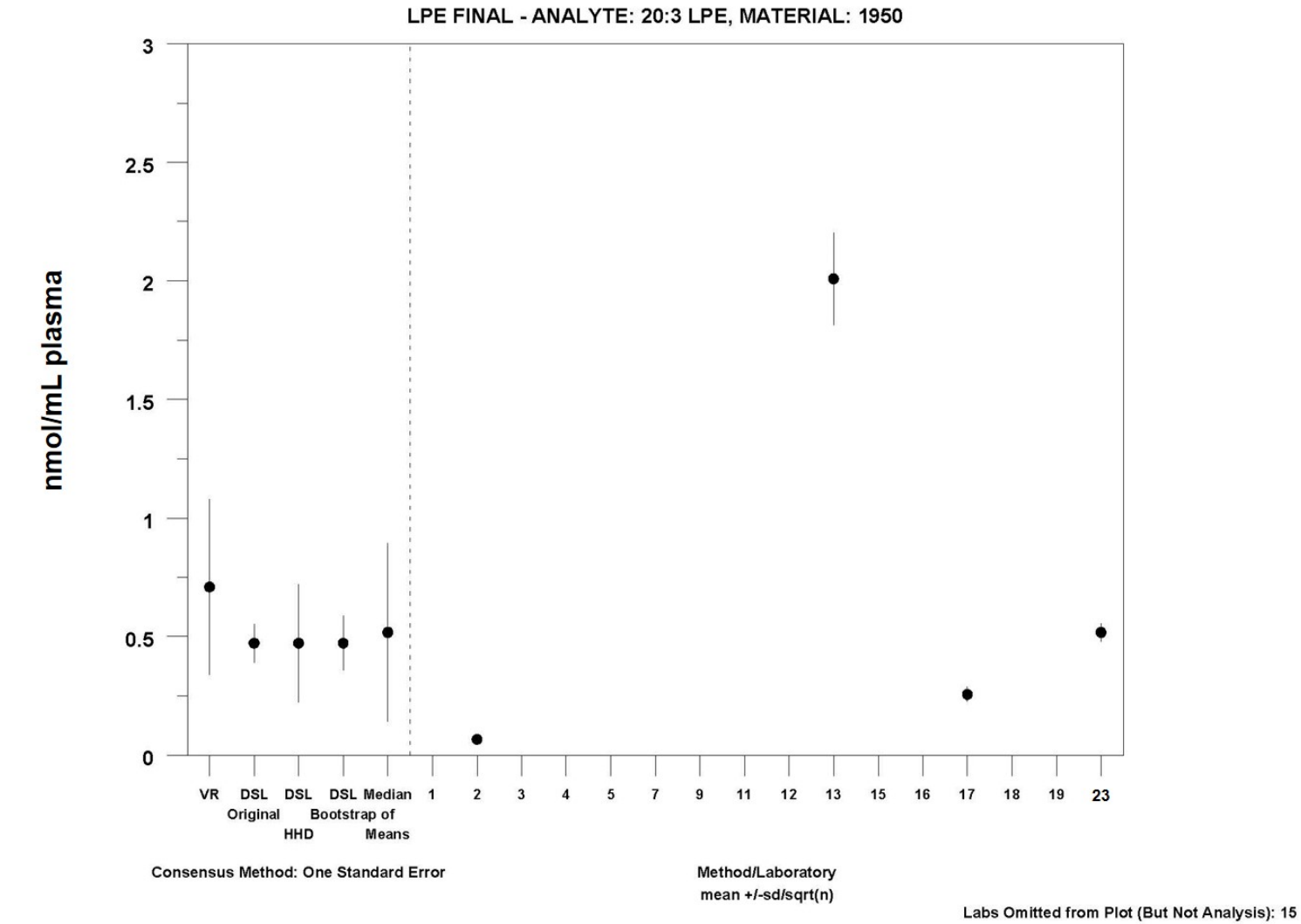
Labs Omitted from Plot (But Not Analysis): 15

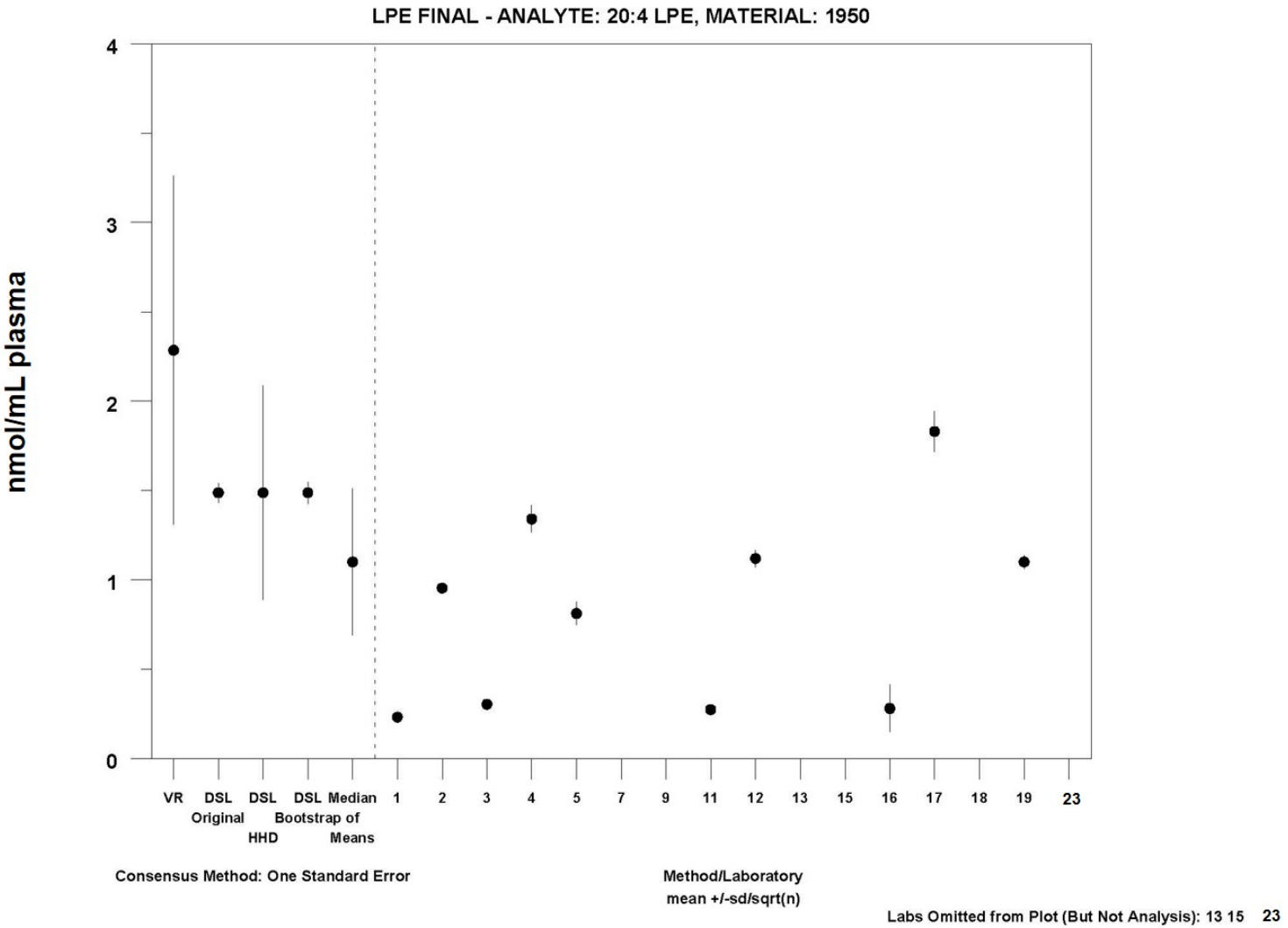
MEDM Location: 1.6 ± 0.55 nmol/mL

15: 449 ± 70





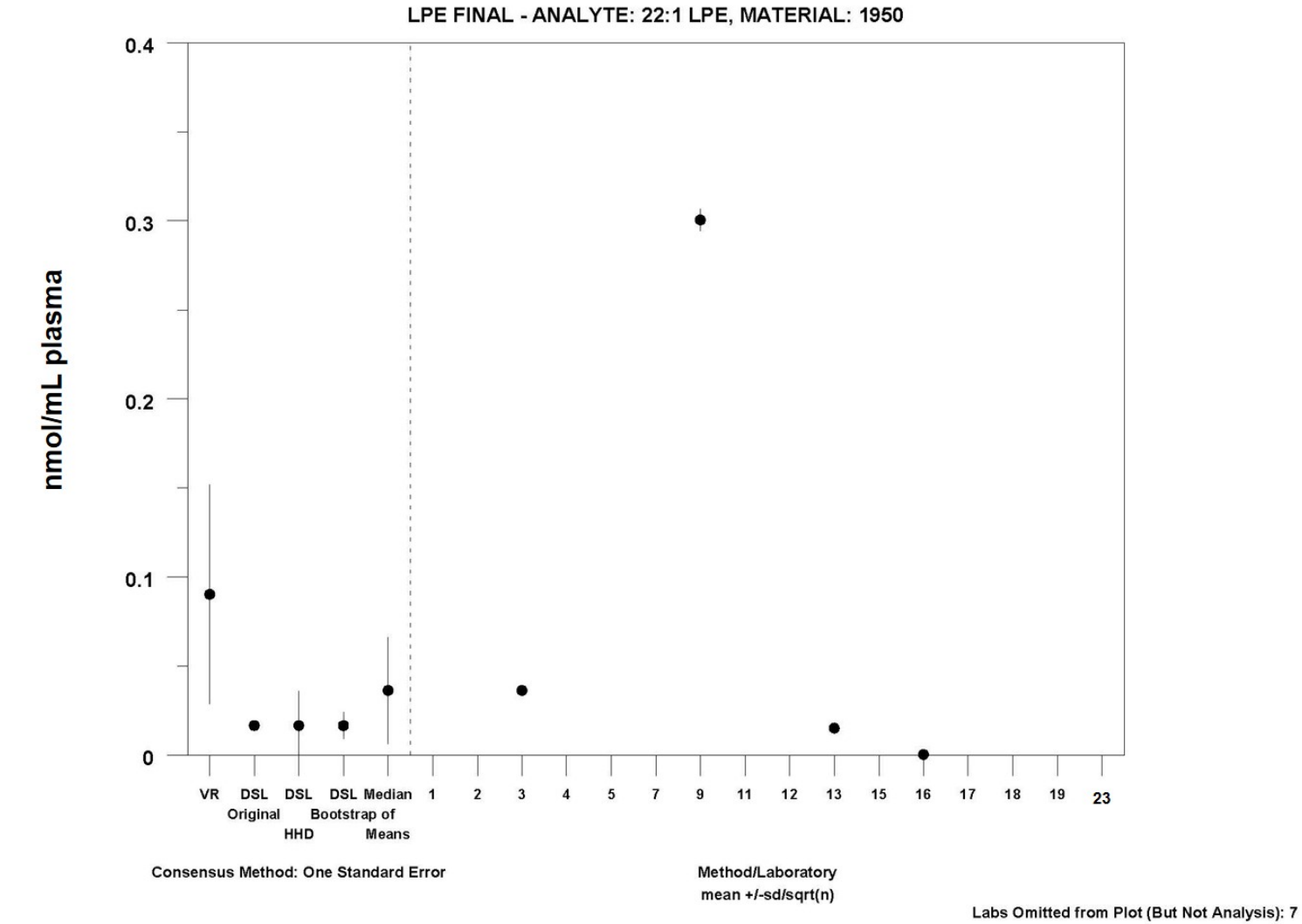


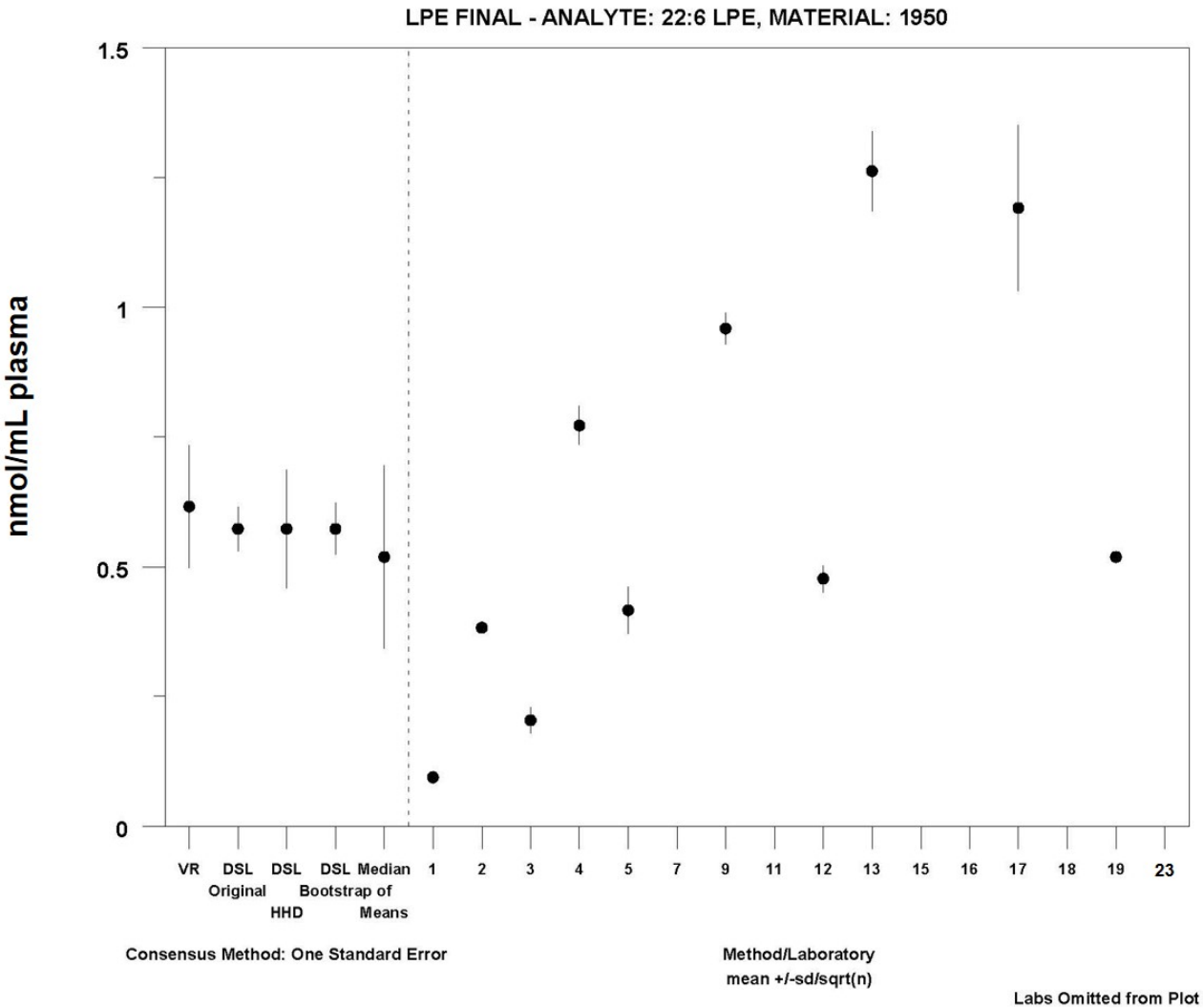


MEDM Location: 1.1 ± 0.41 nmol/mL

Labs Omitted from Plot (But Not Analysis): 13 15 23

13: 11.8 ± 0.8; 15: 196 ± 29, 23: 7.4 ± 0.1

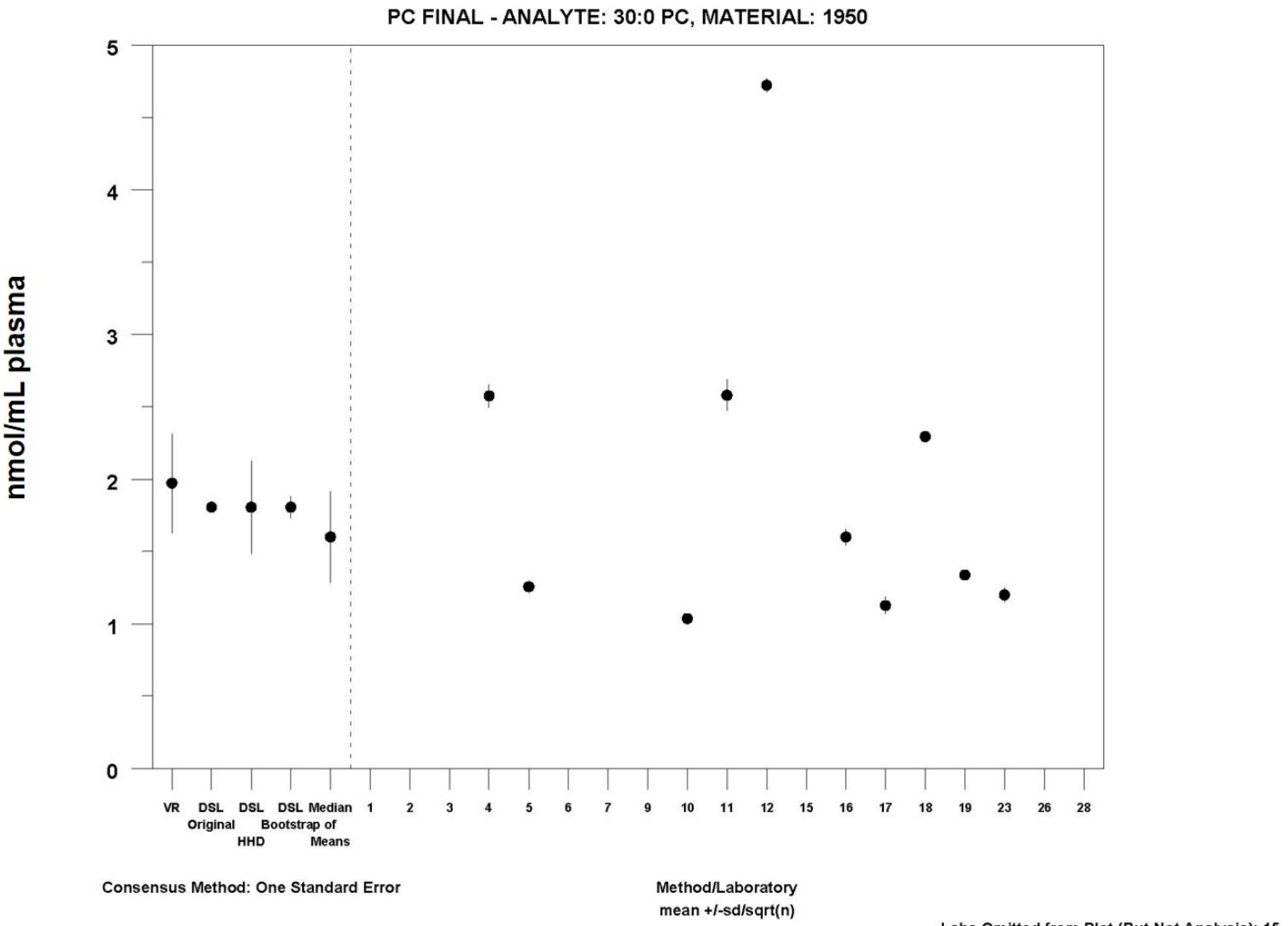


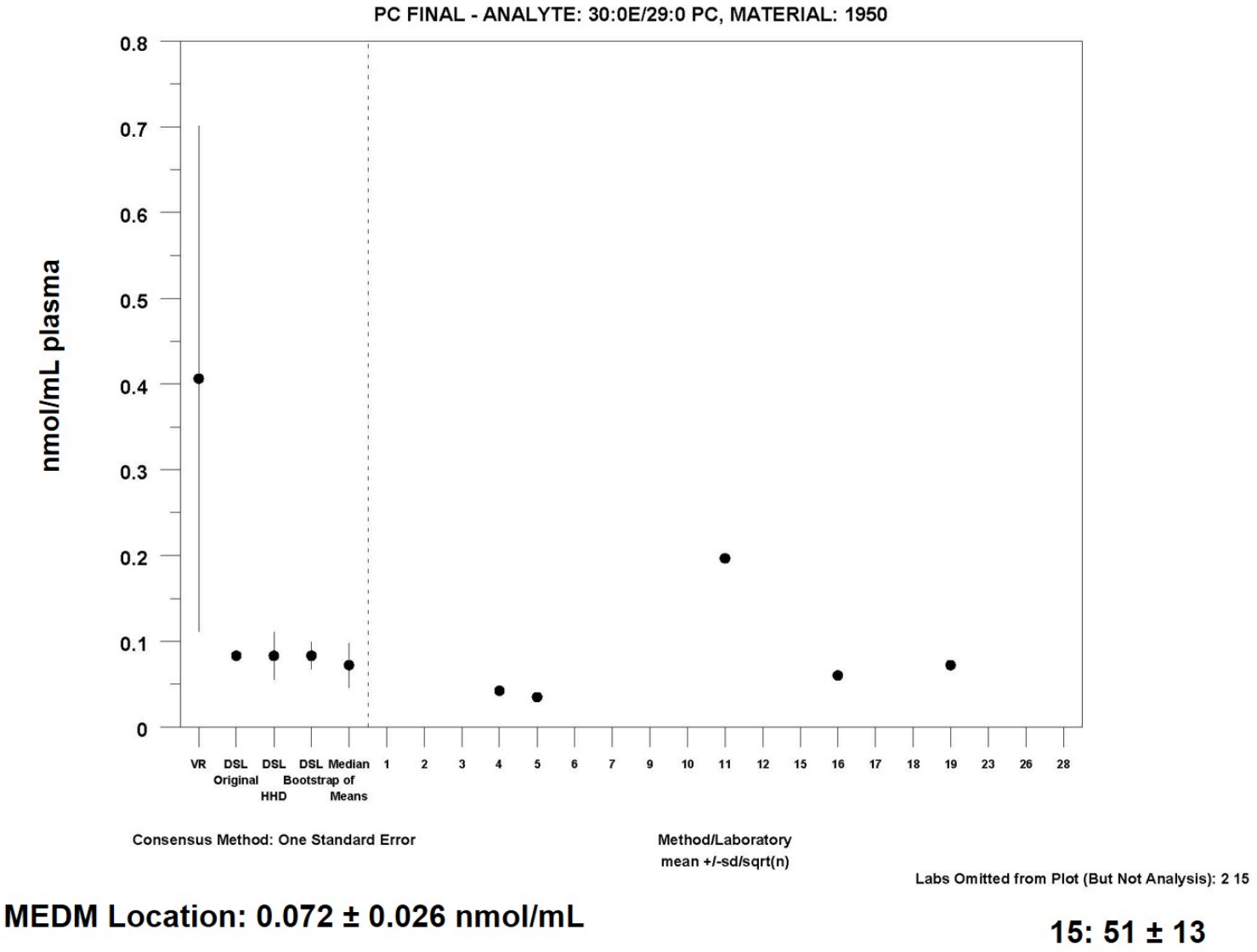


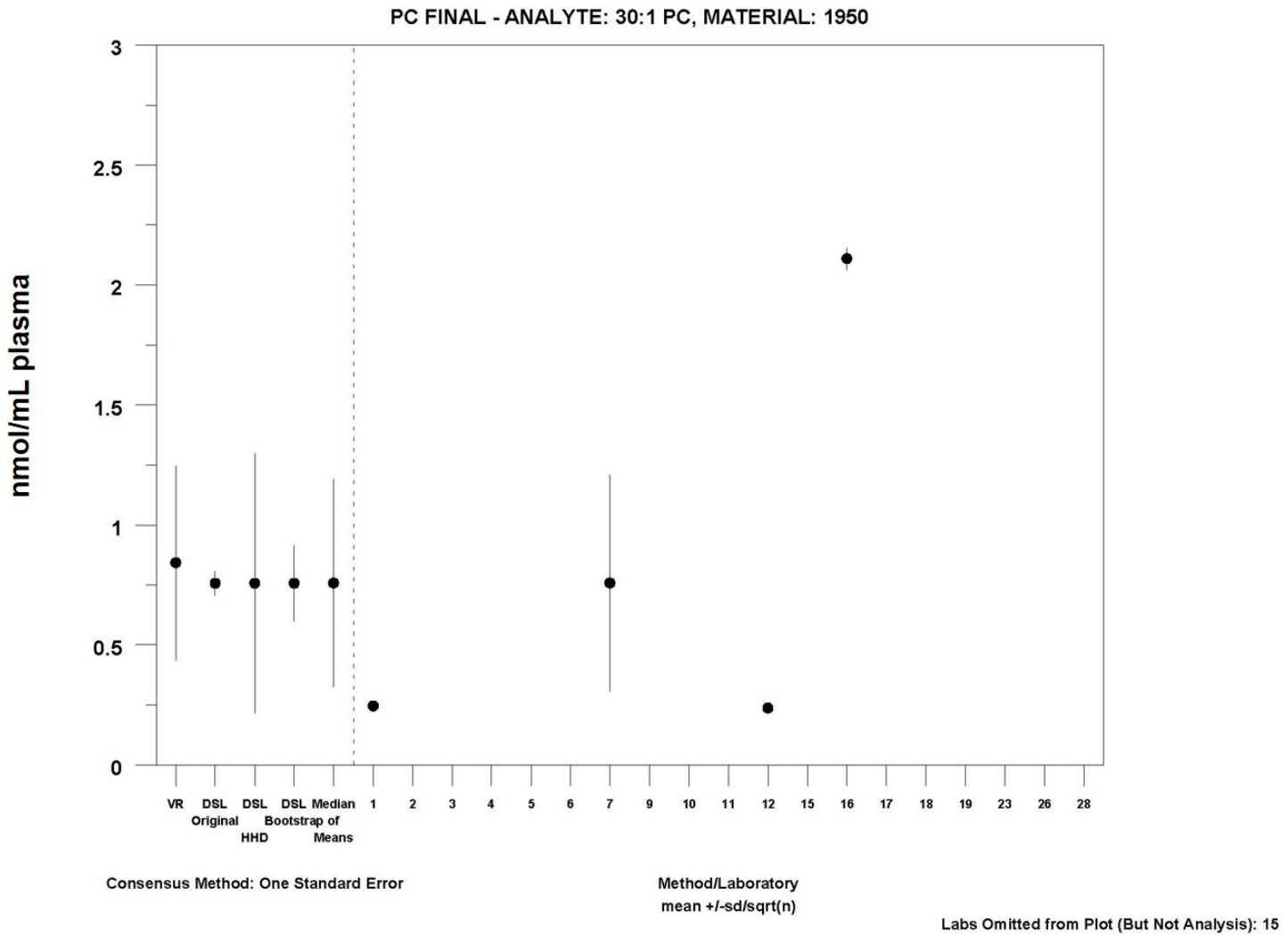
Labs Omitted from Plot (But Not Analysis): 15

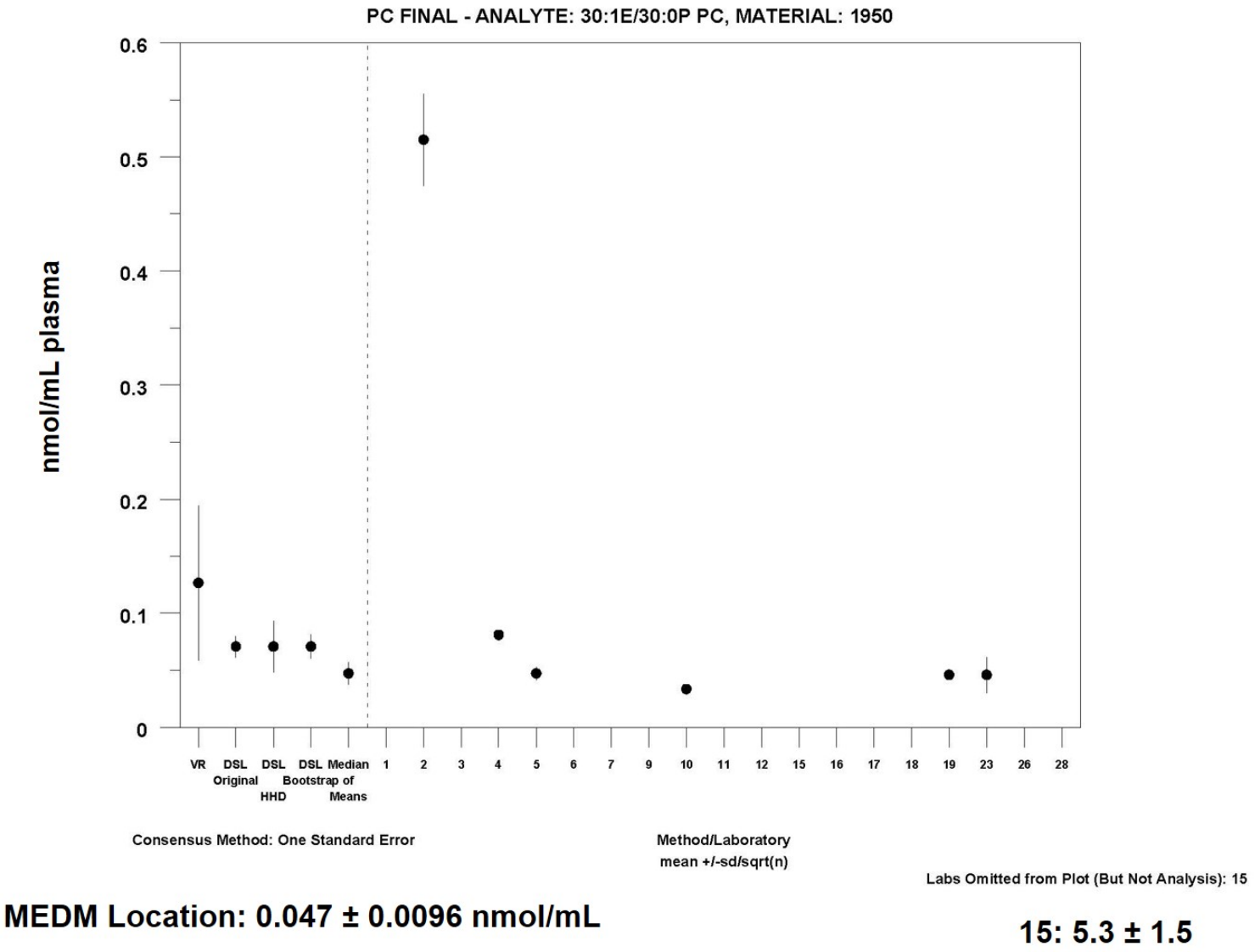
MEDM Location: 0.52 ± 0.18 nmol/mL

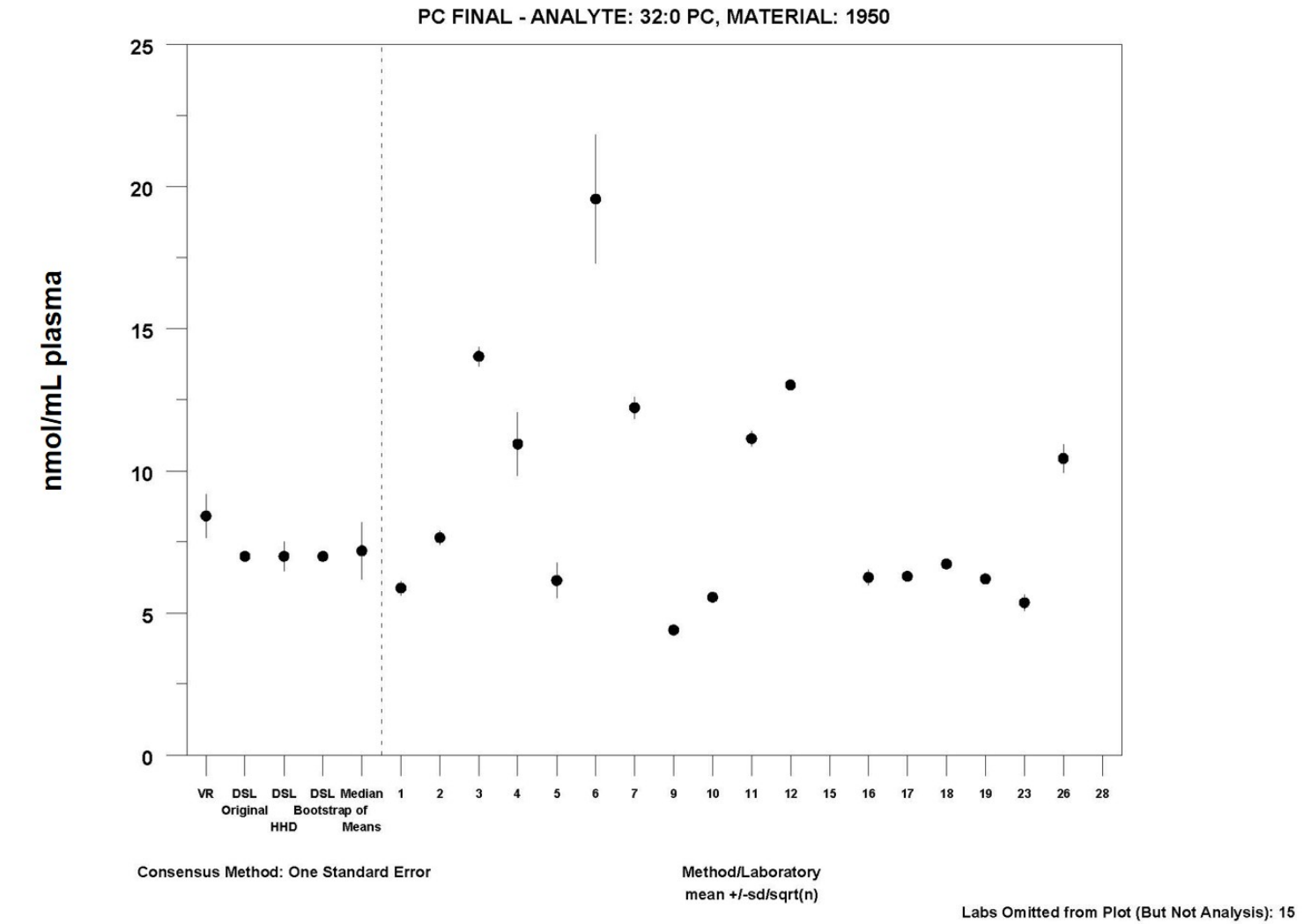
15: 64 ± 17

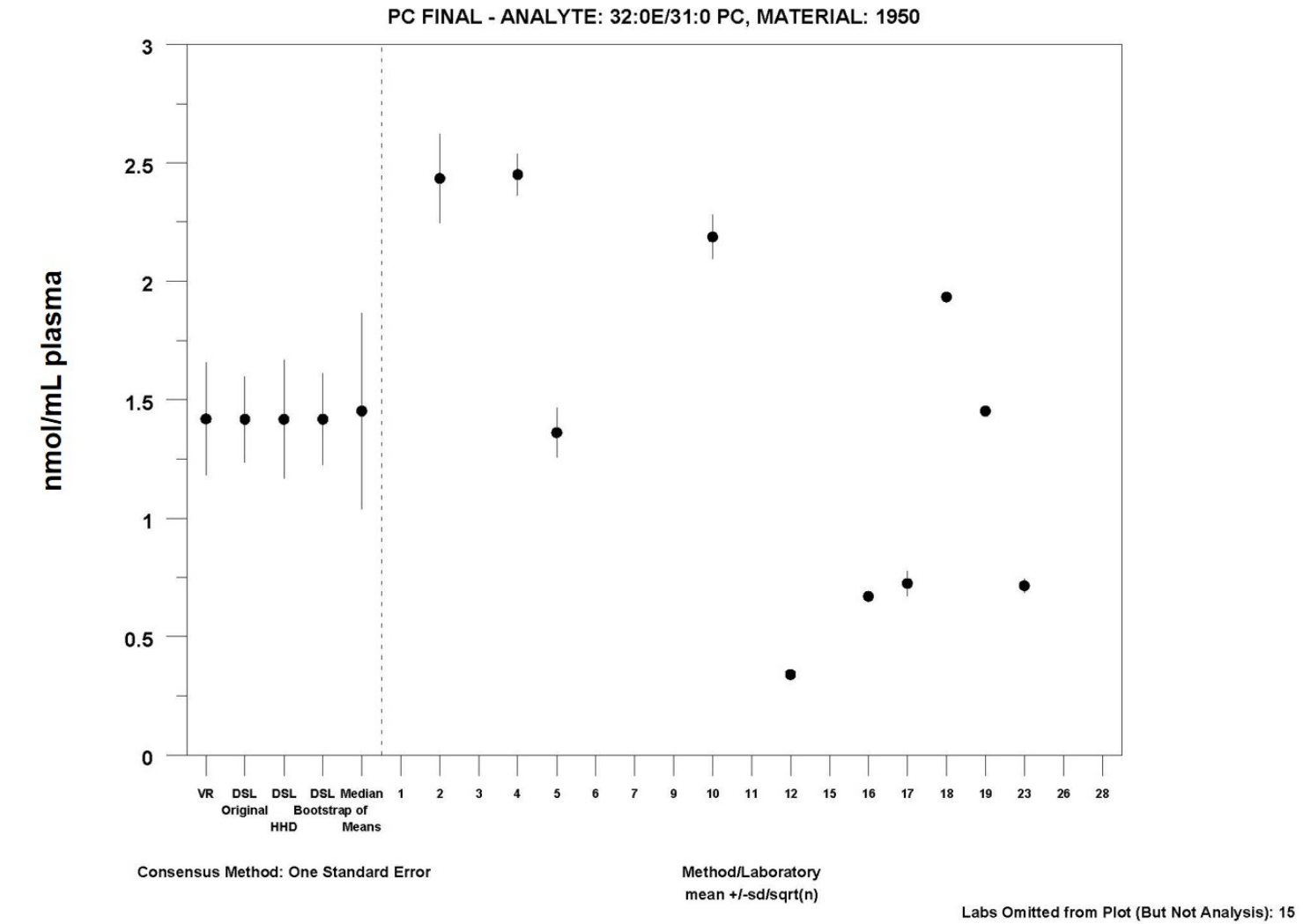


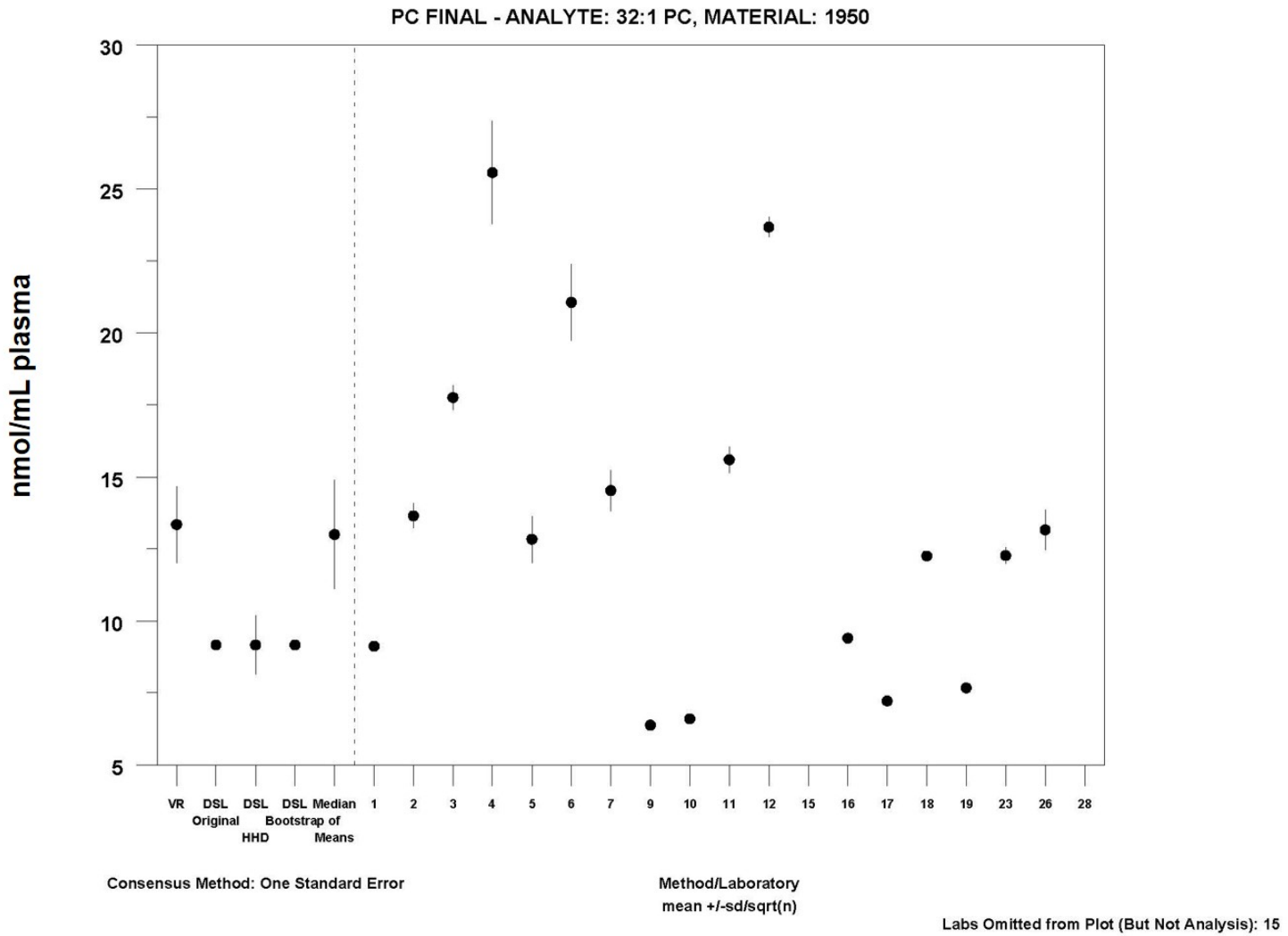


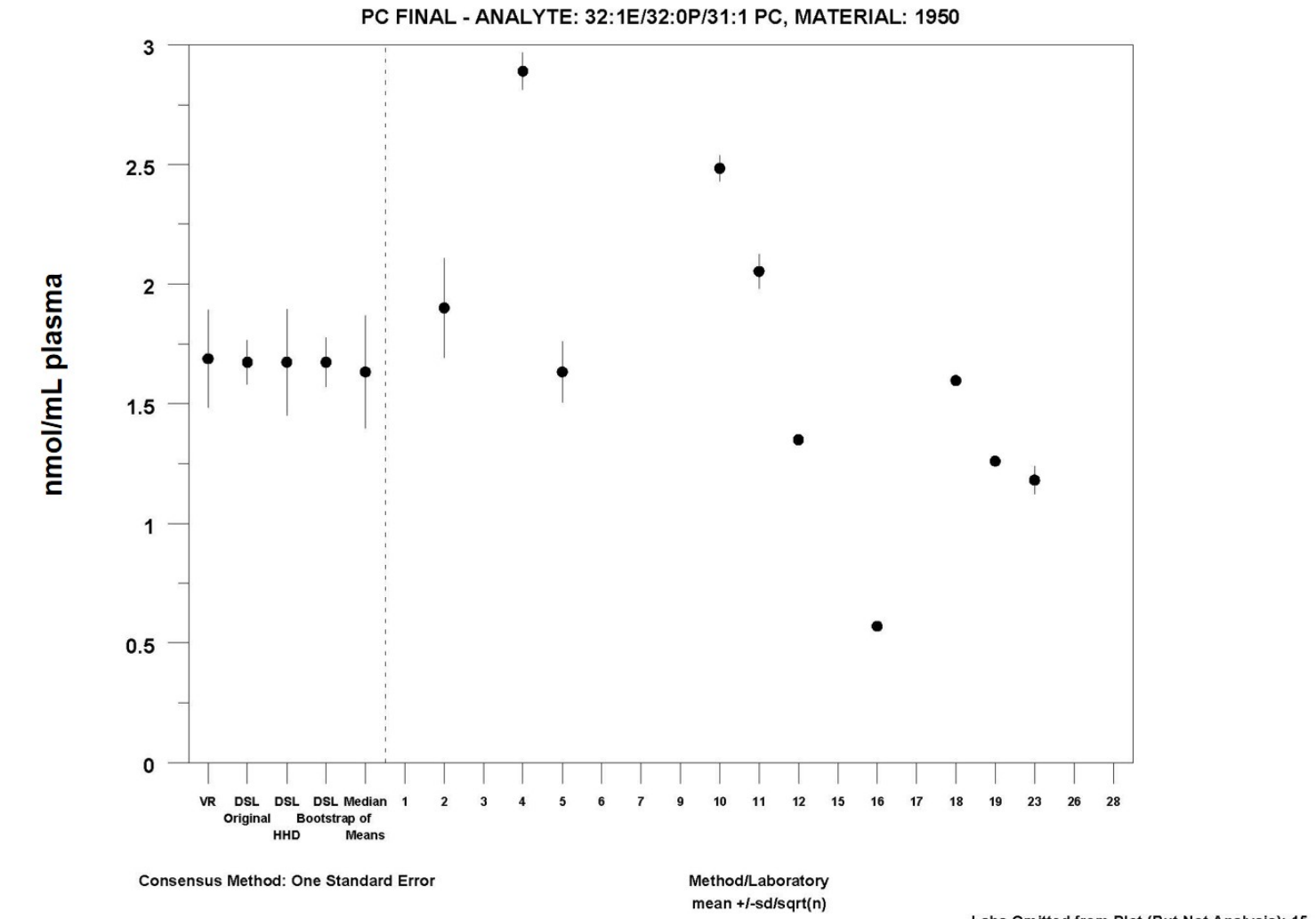


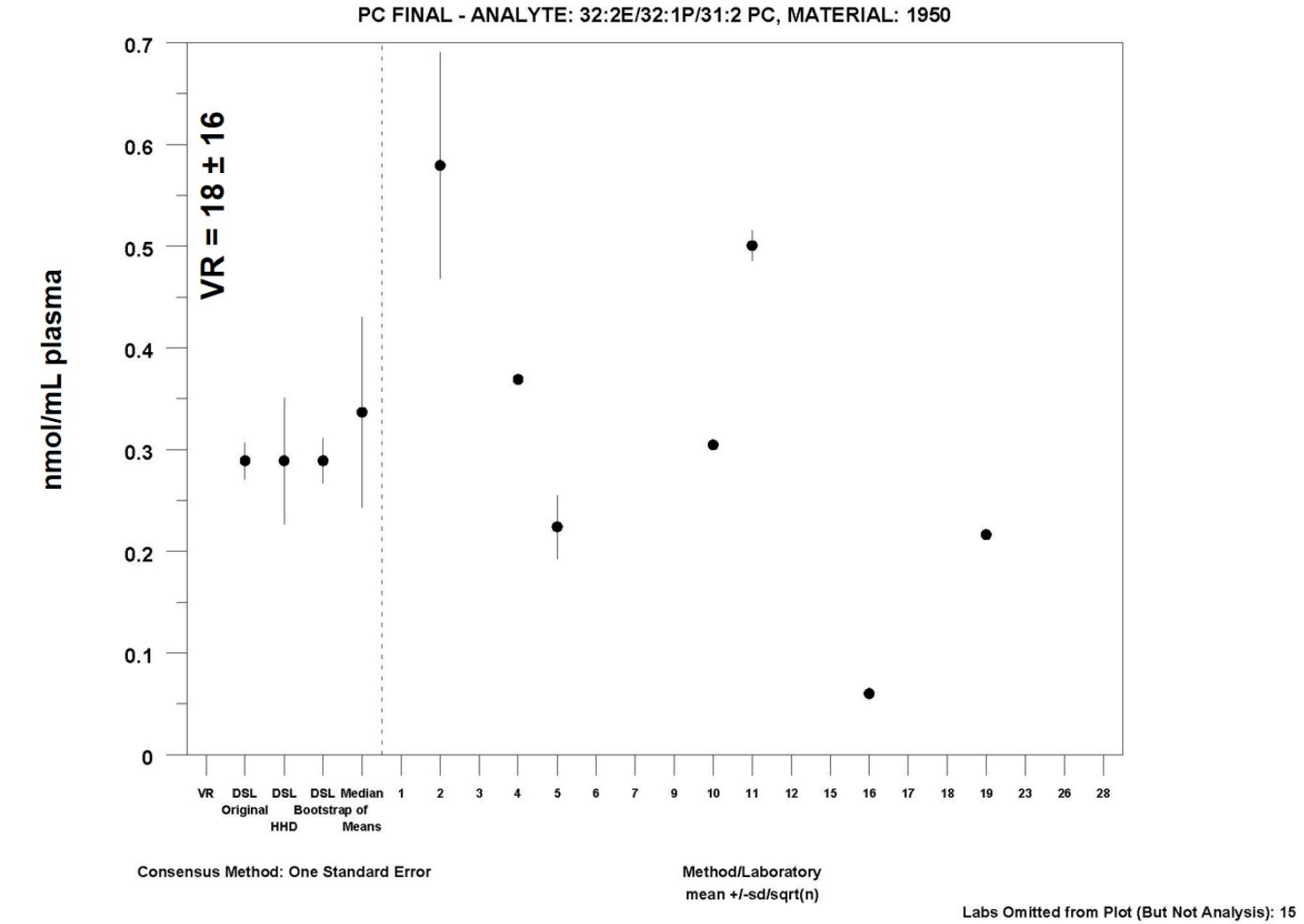


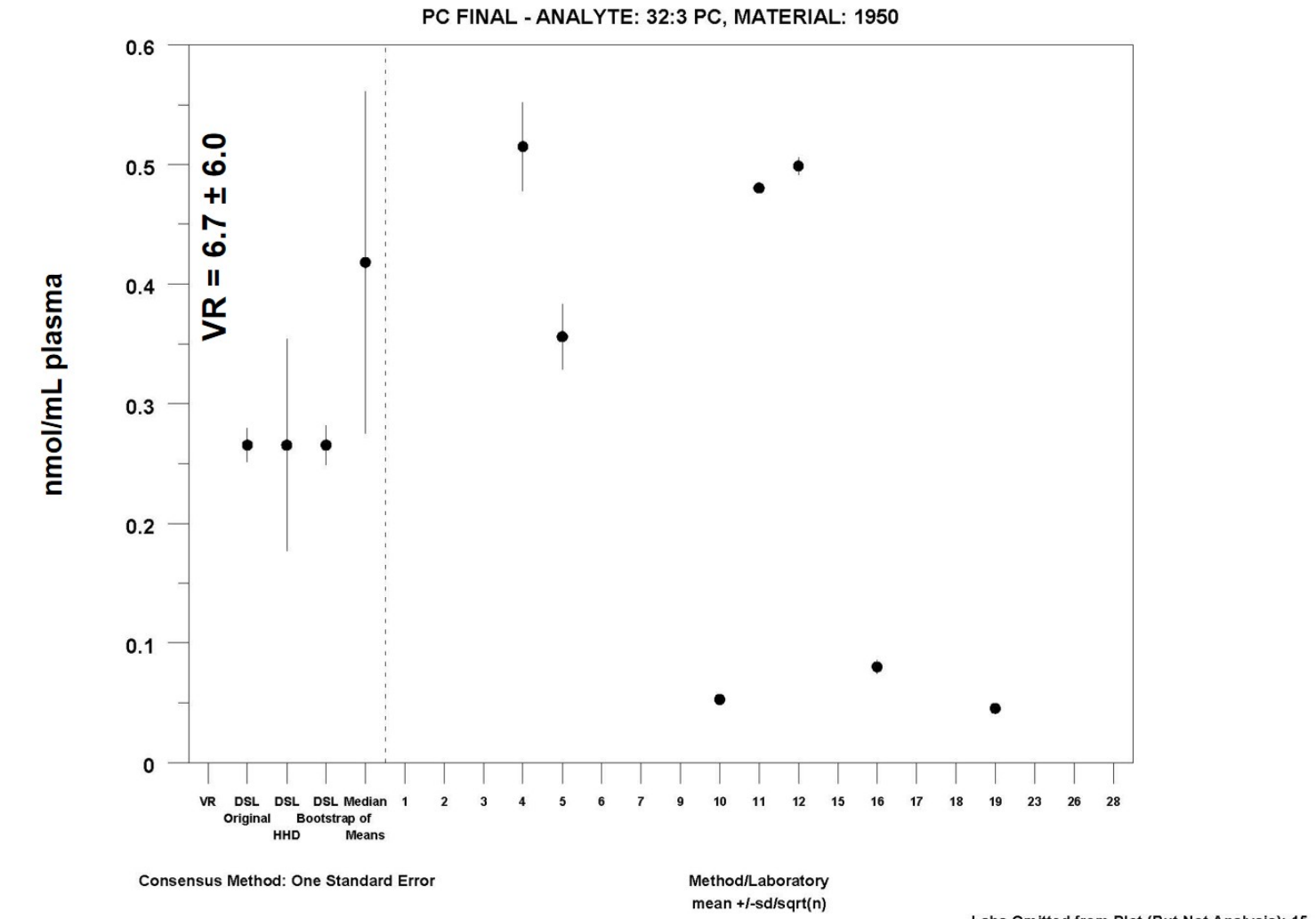


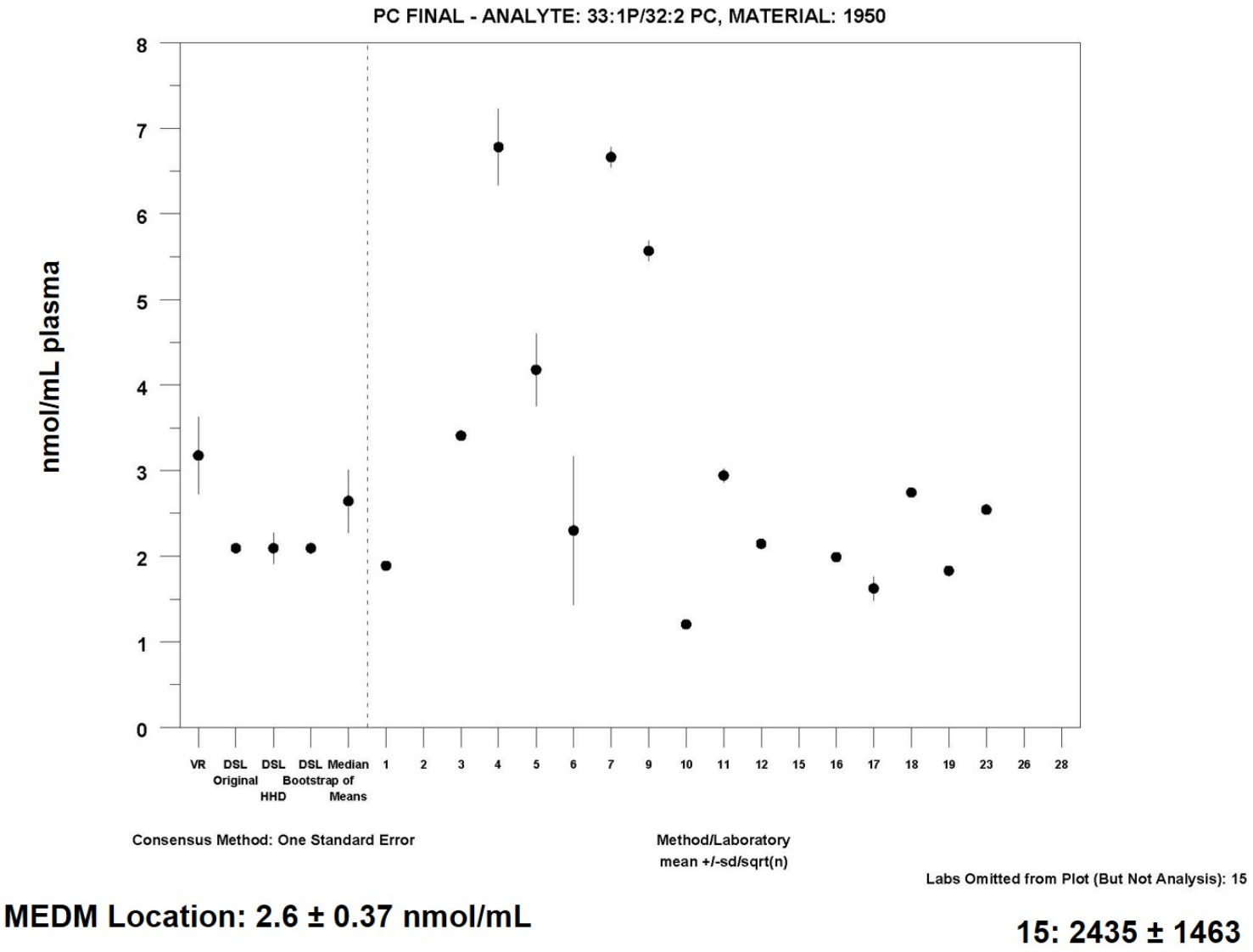


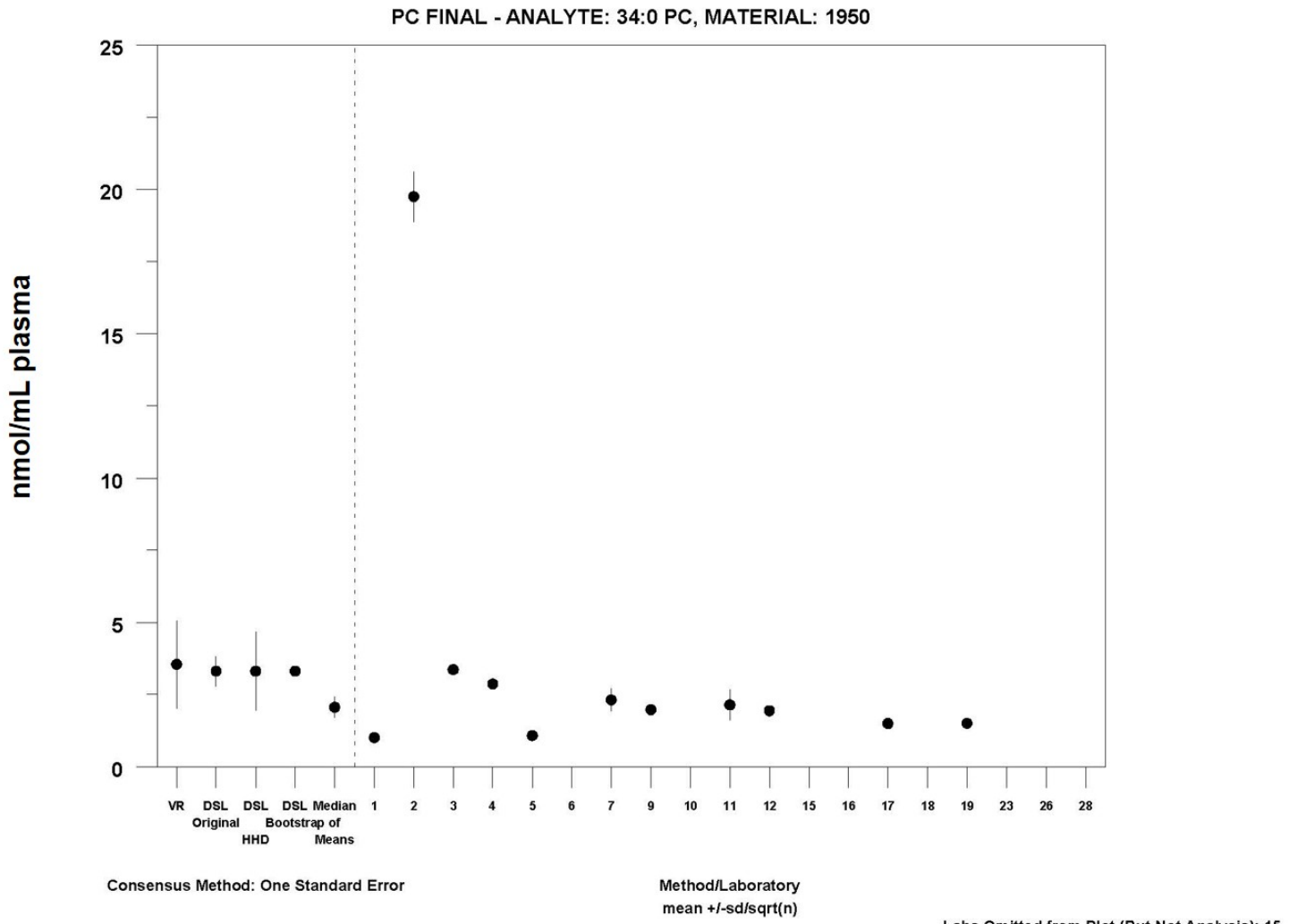


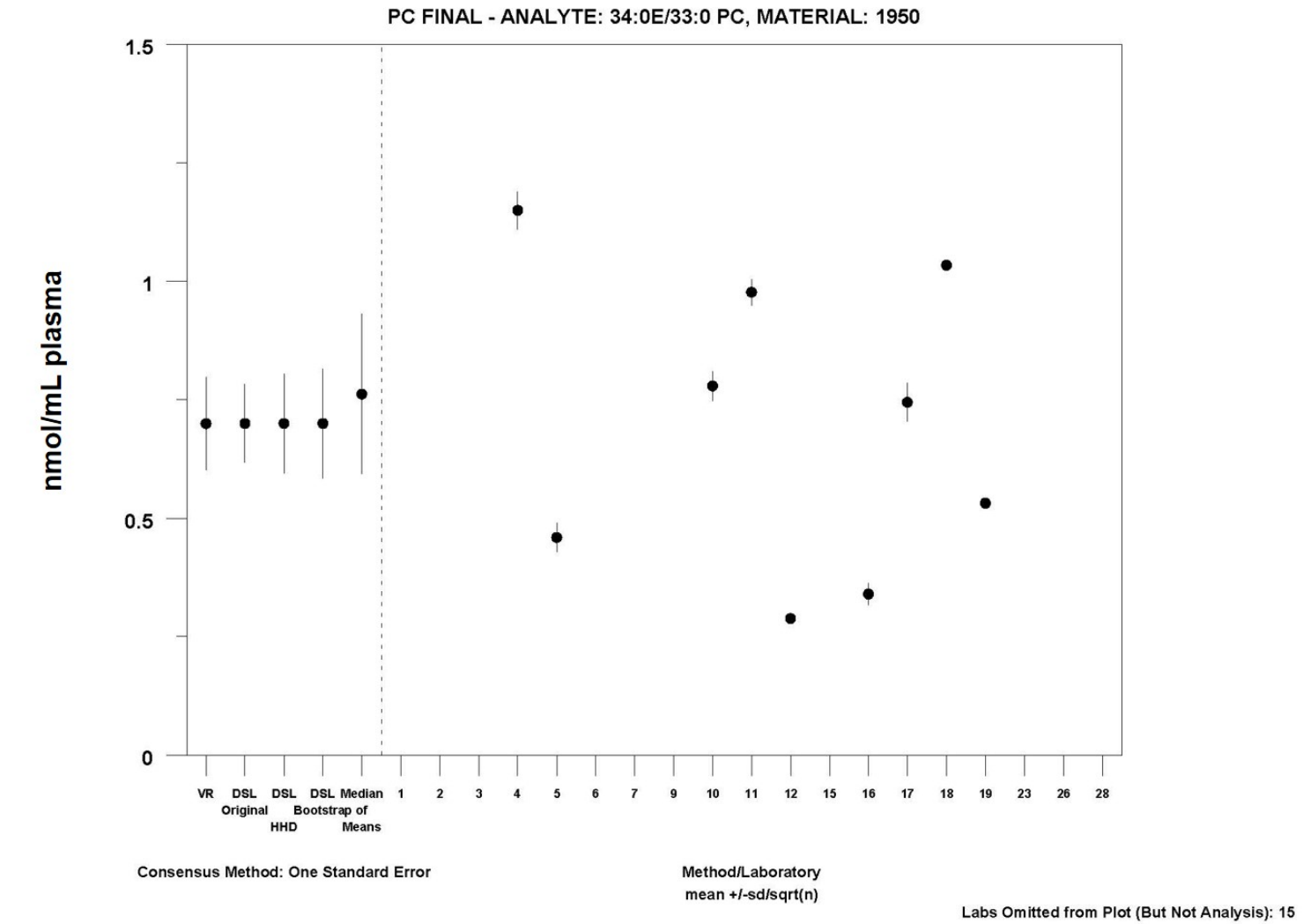


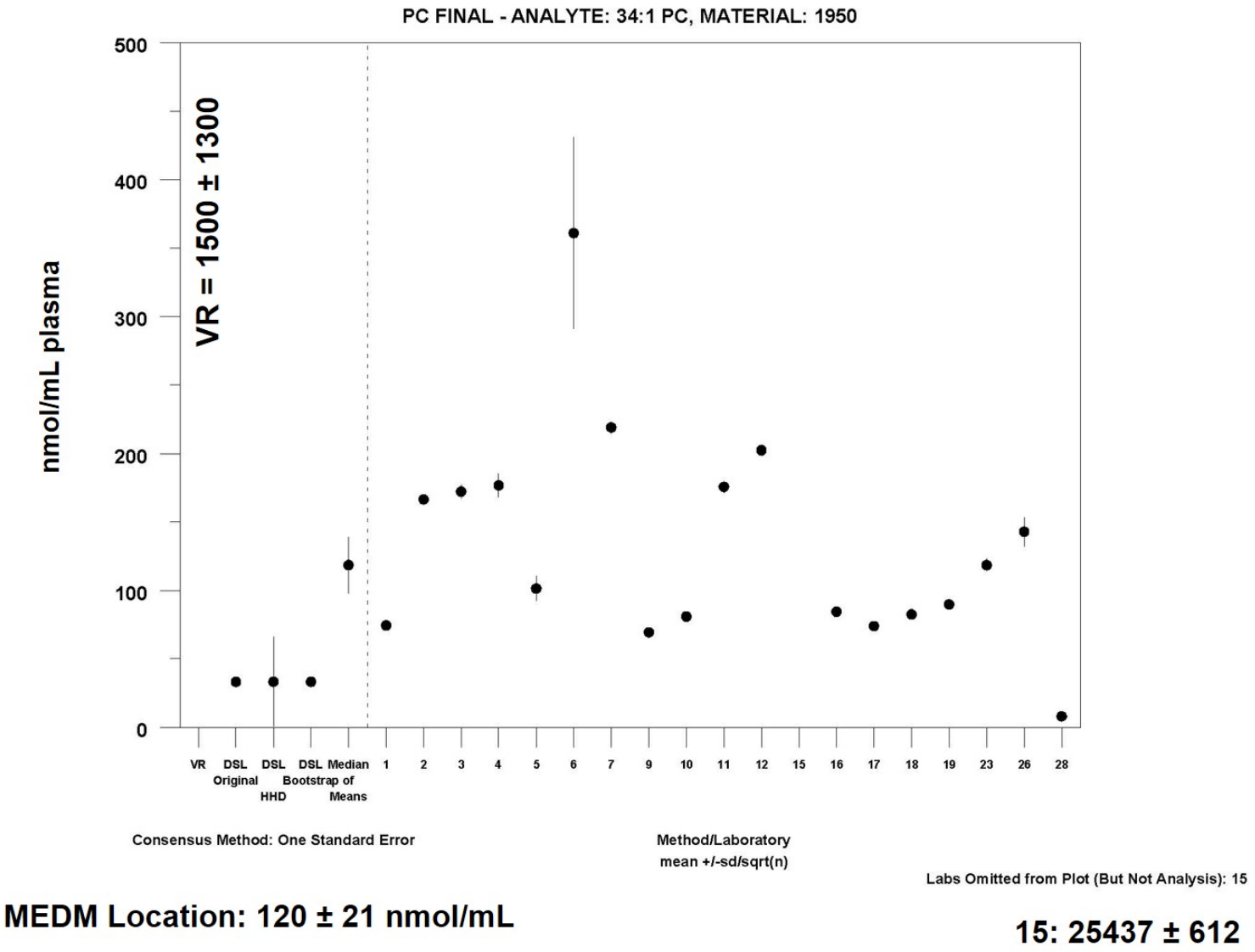


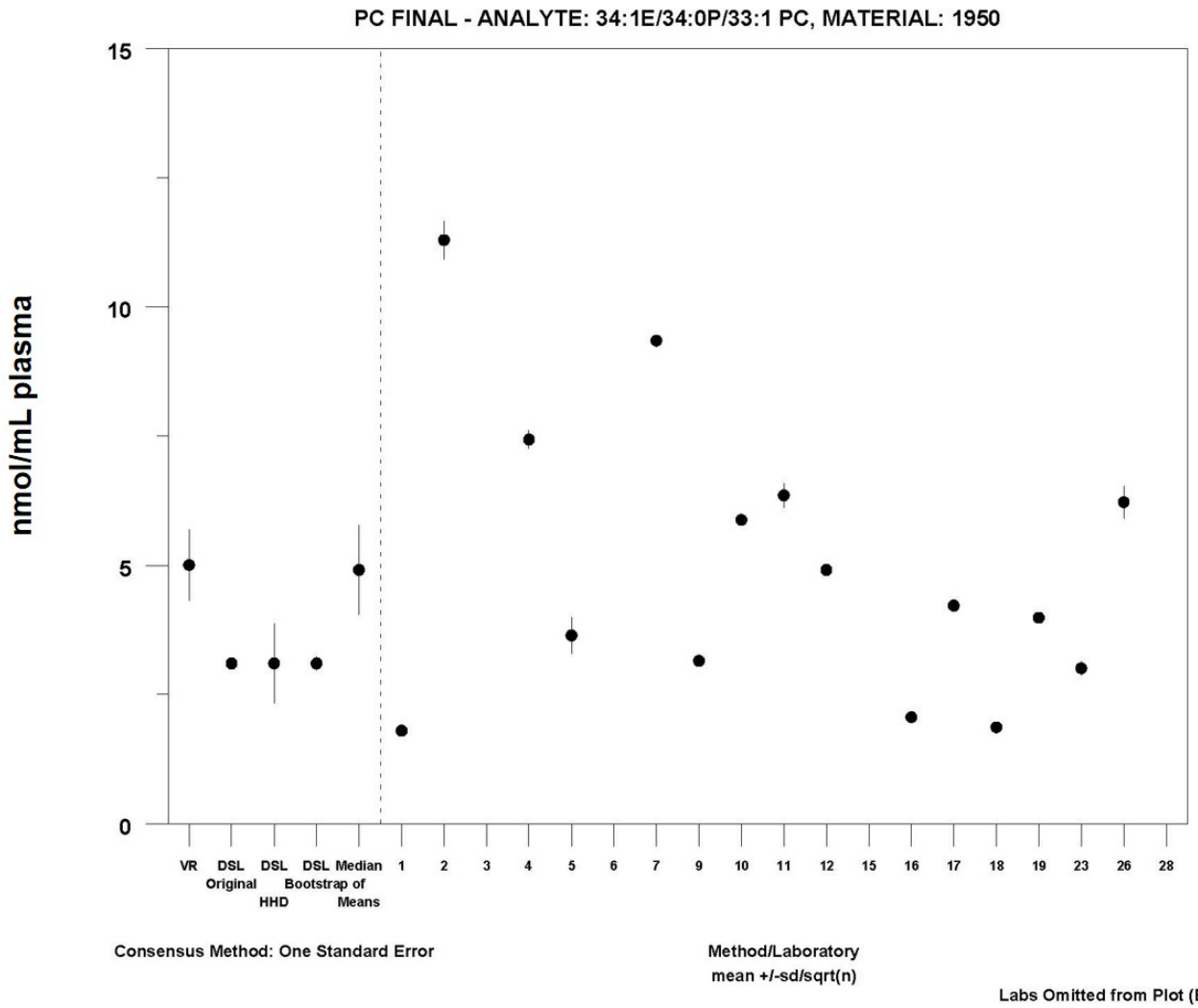






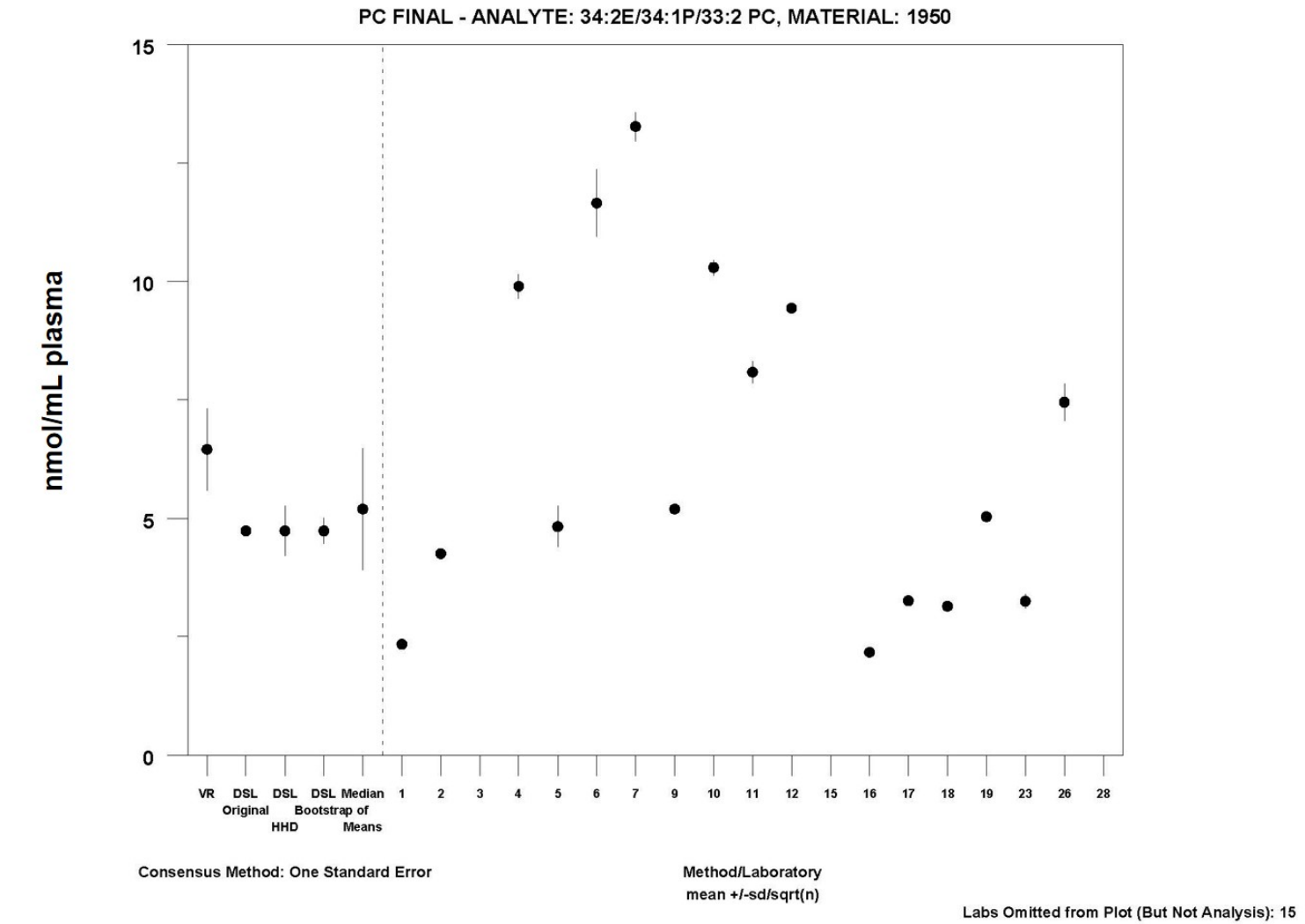


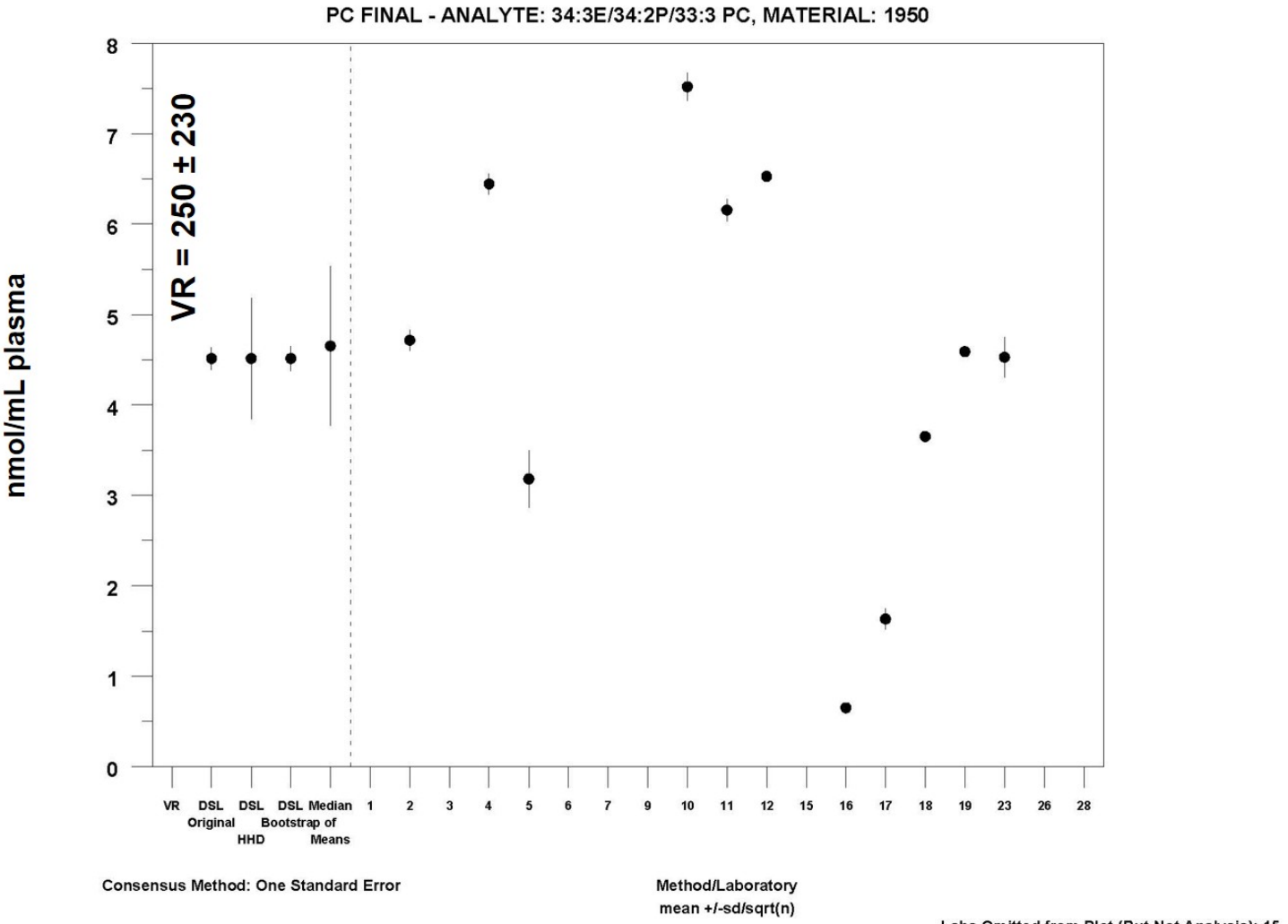


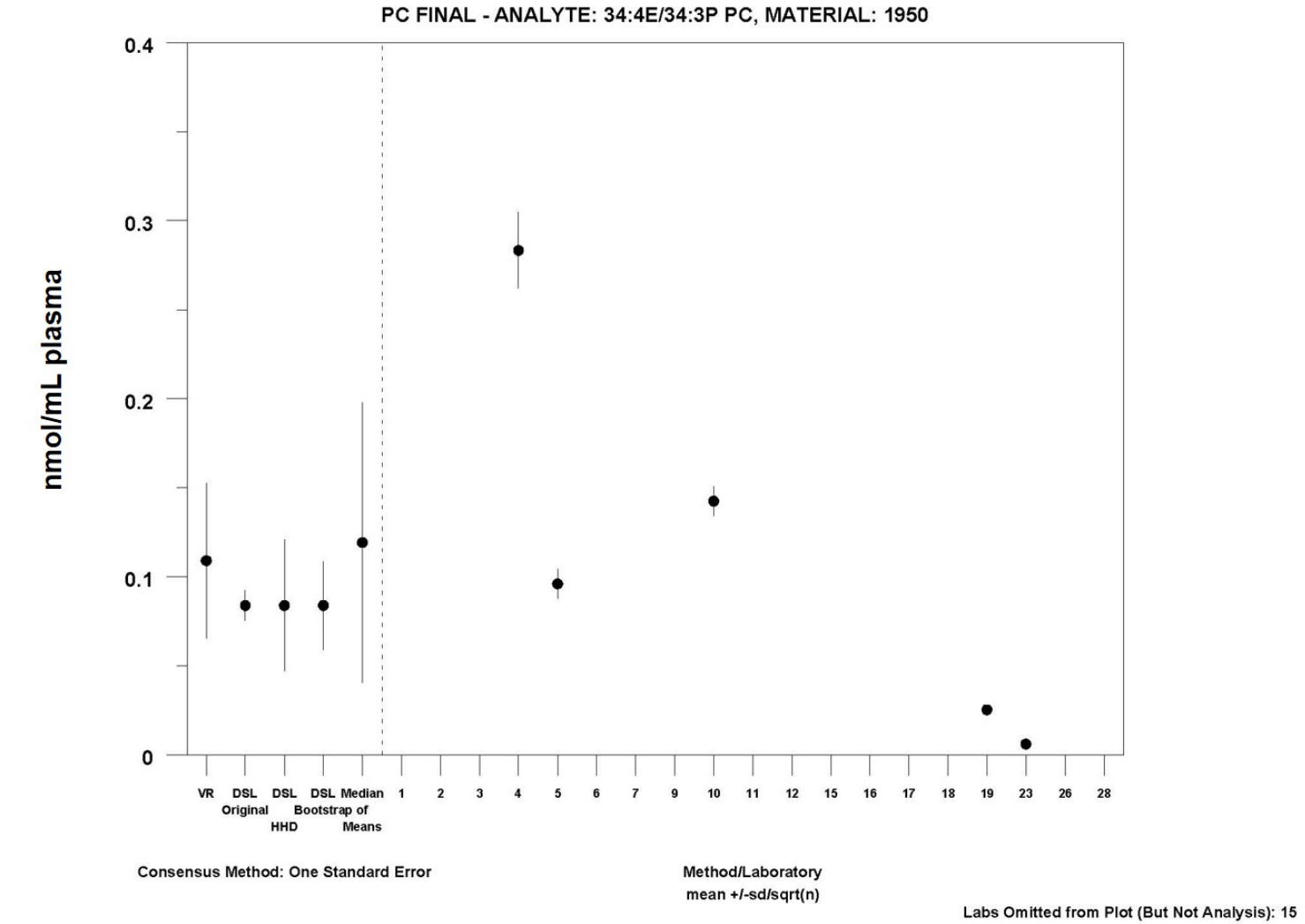


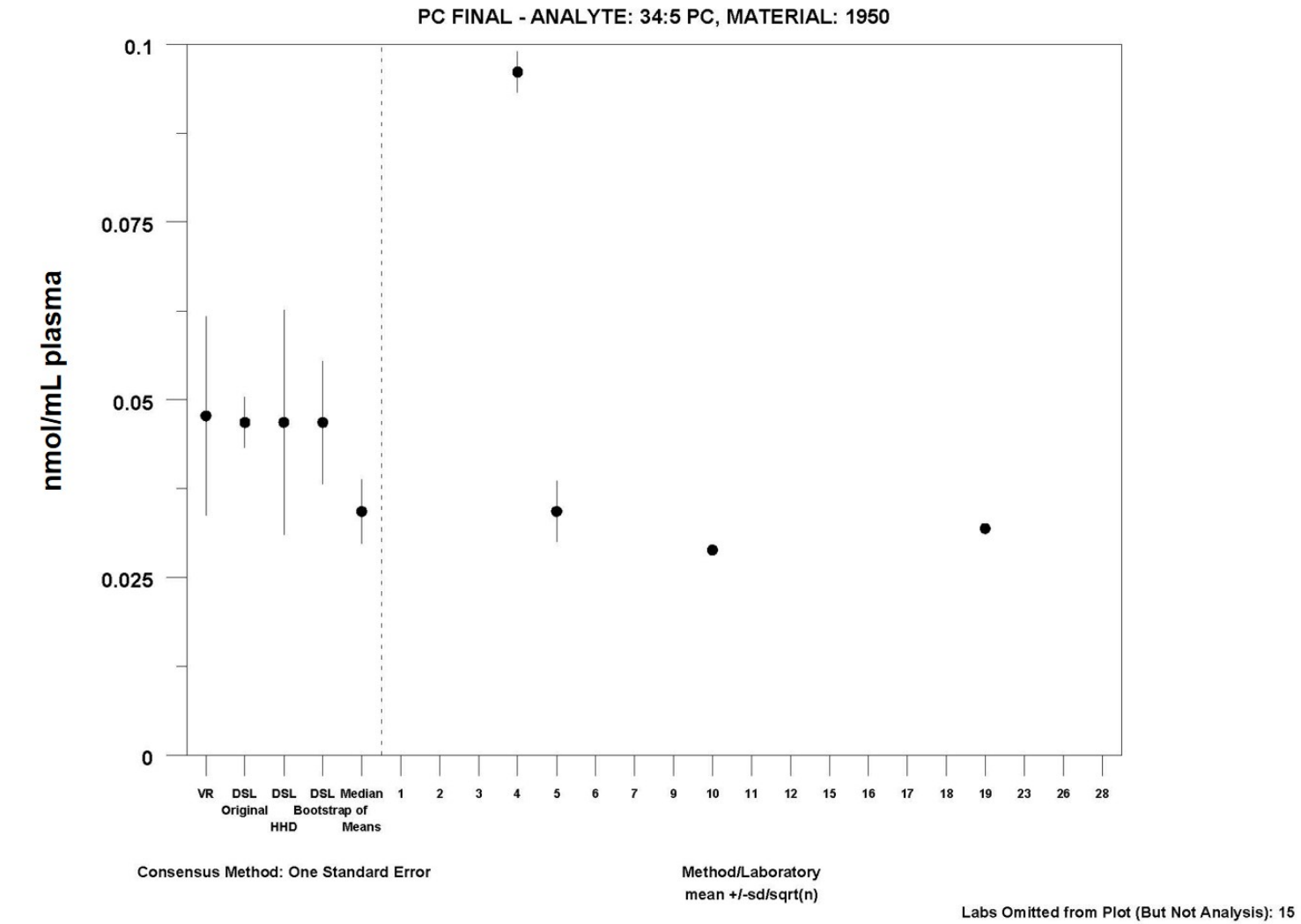
MEDM Location: 4.9 ± 0.86 nmol/mL

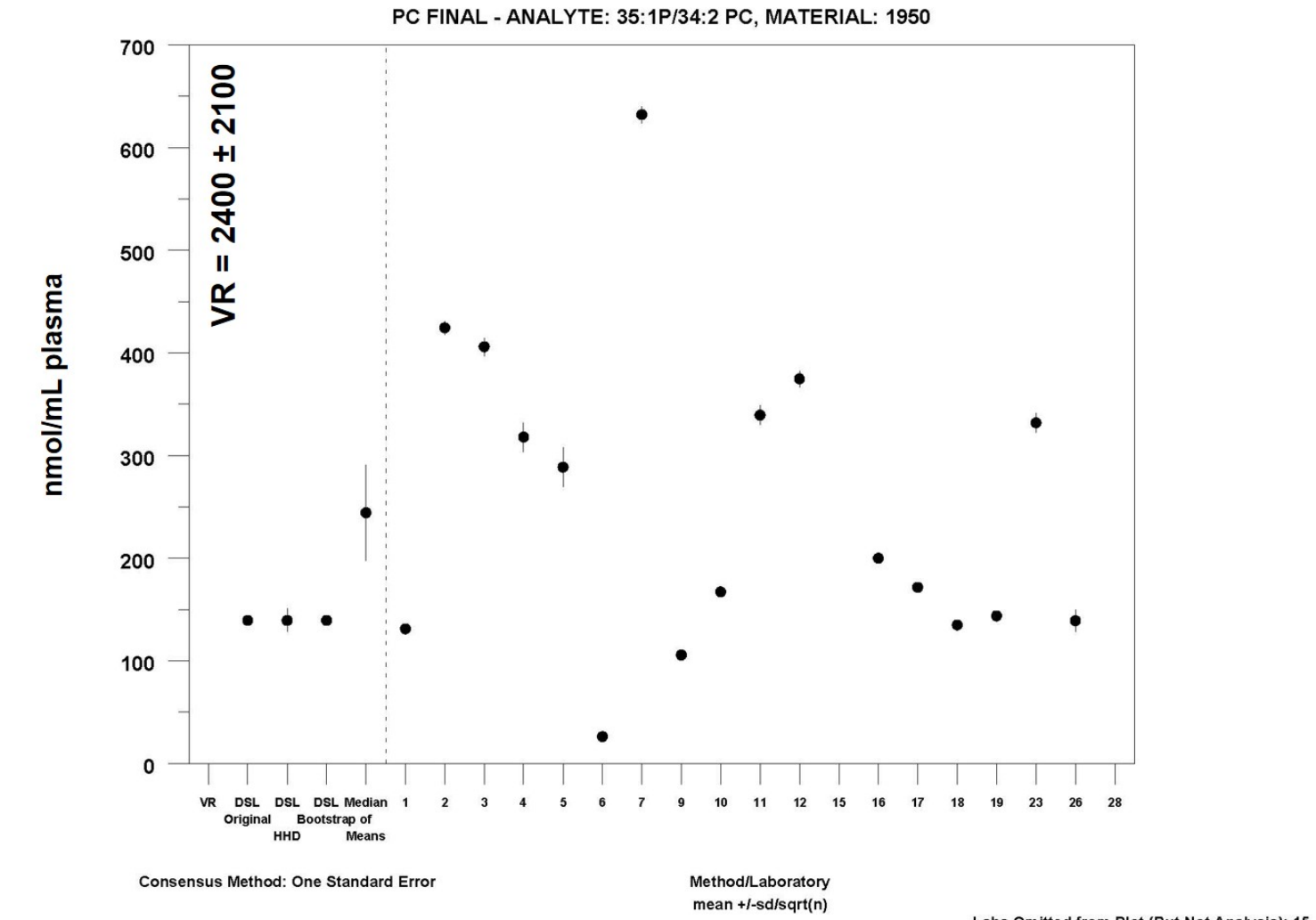
6: 662 ± 67; 15: 3144 ± 540

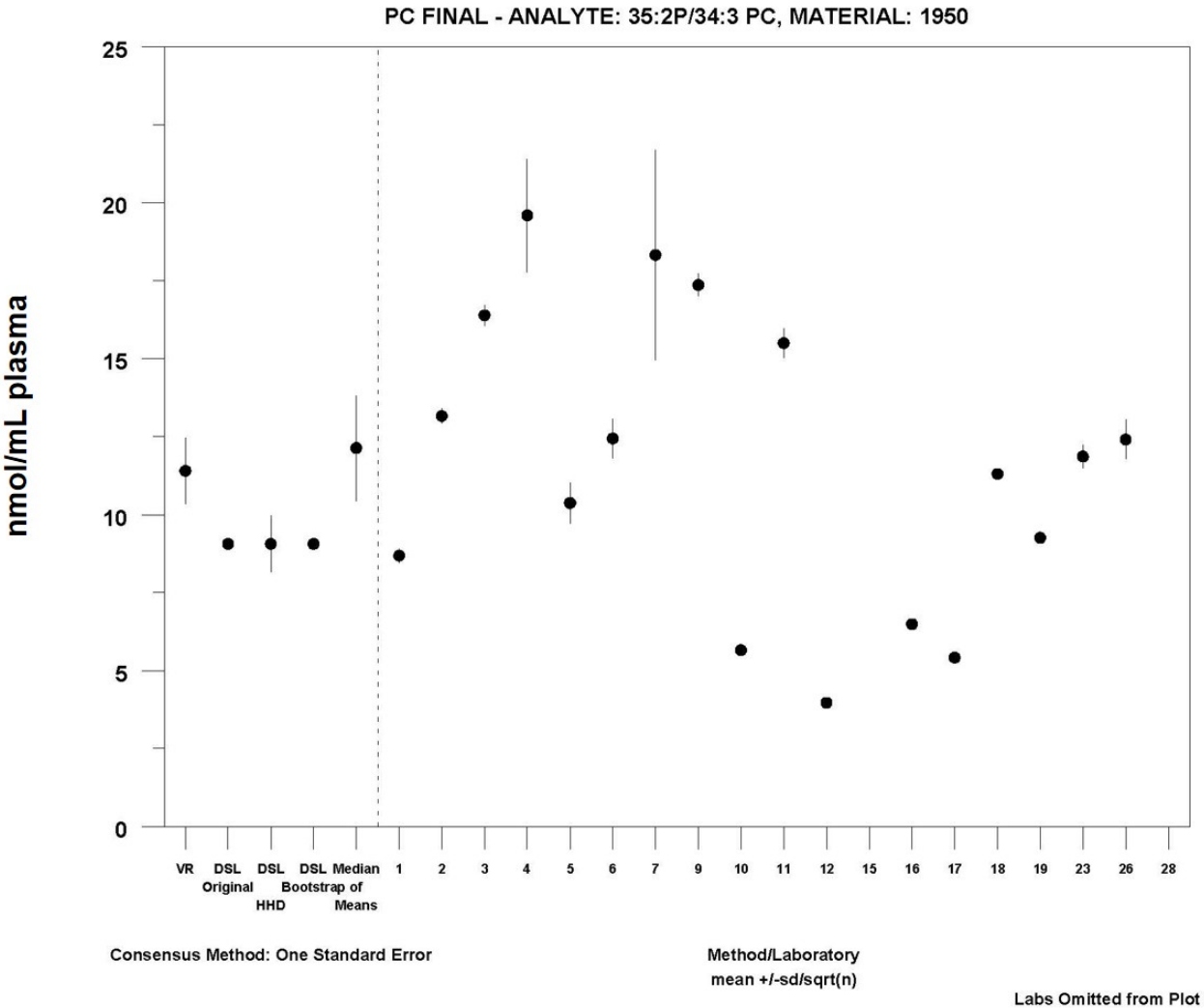


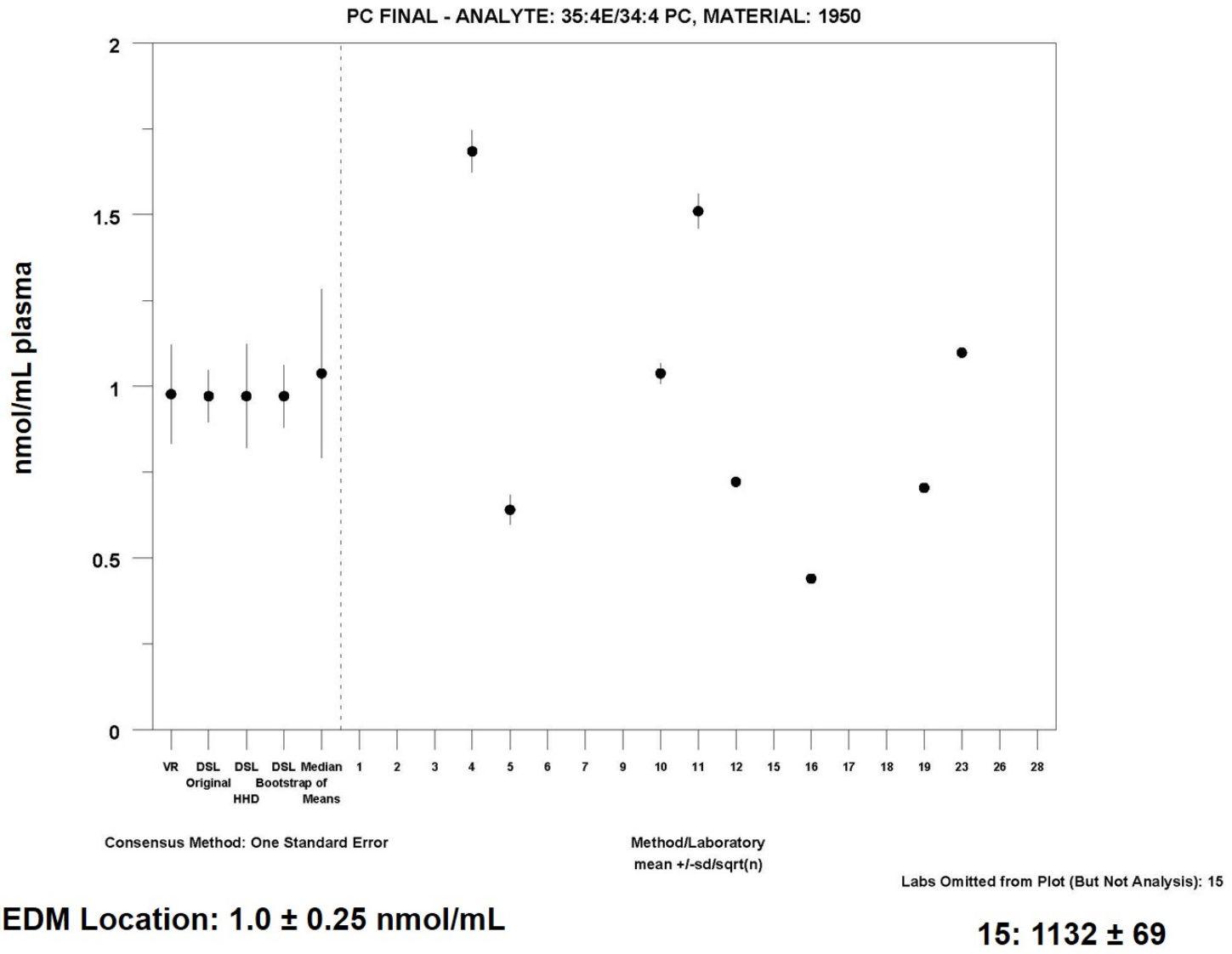


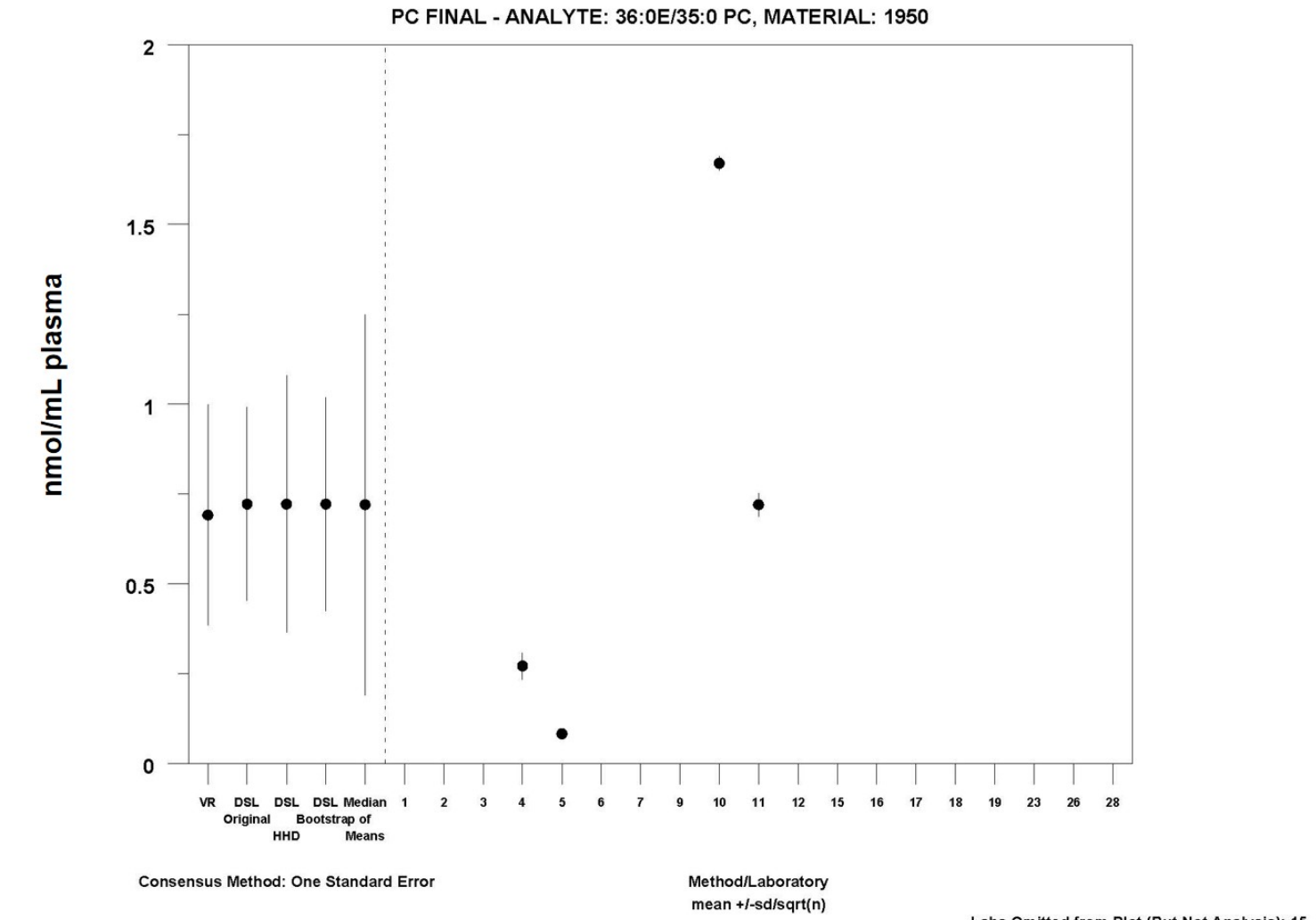


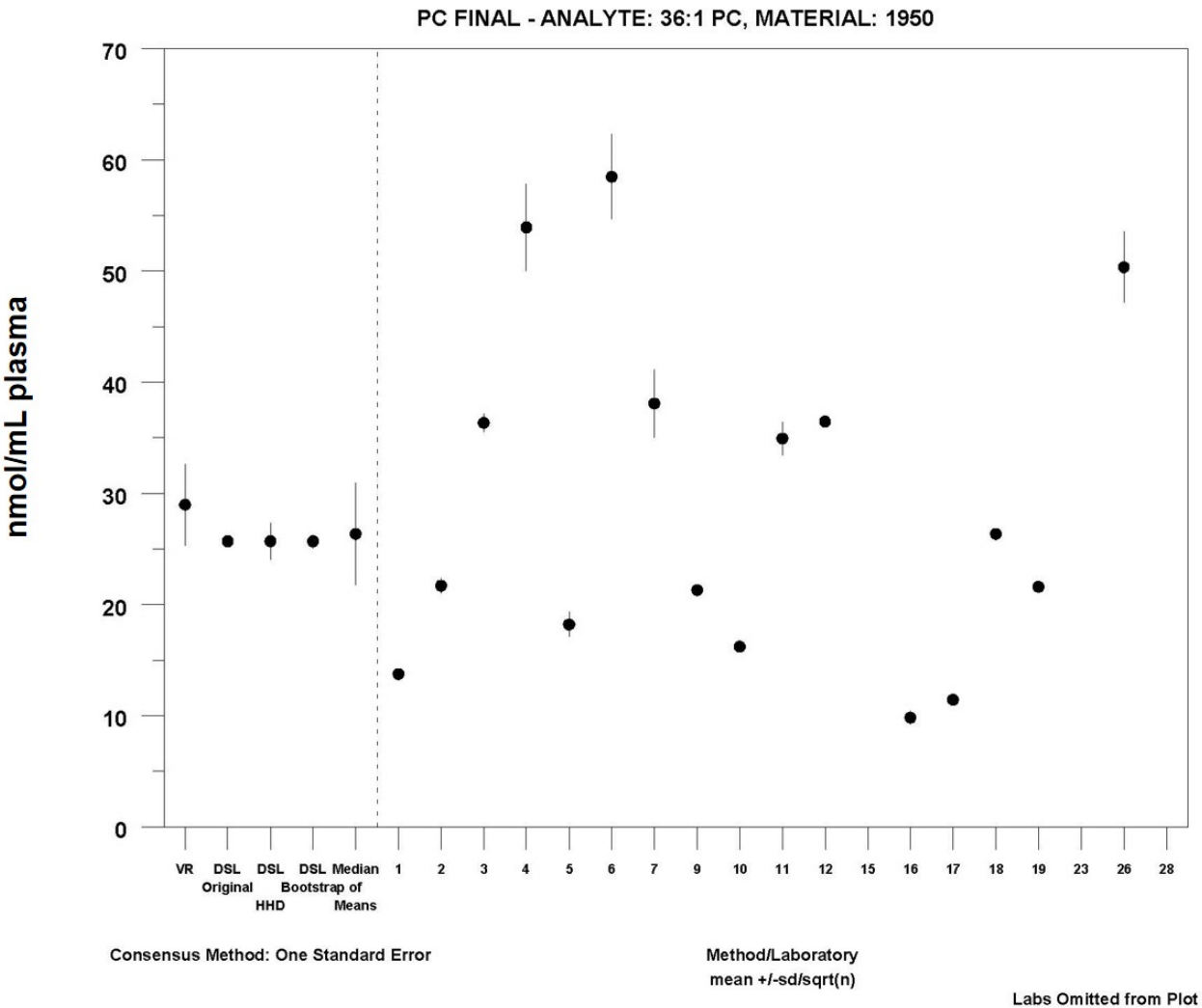


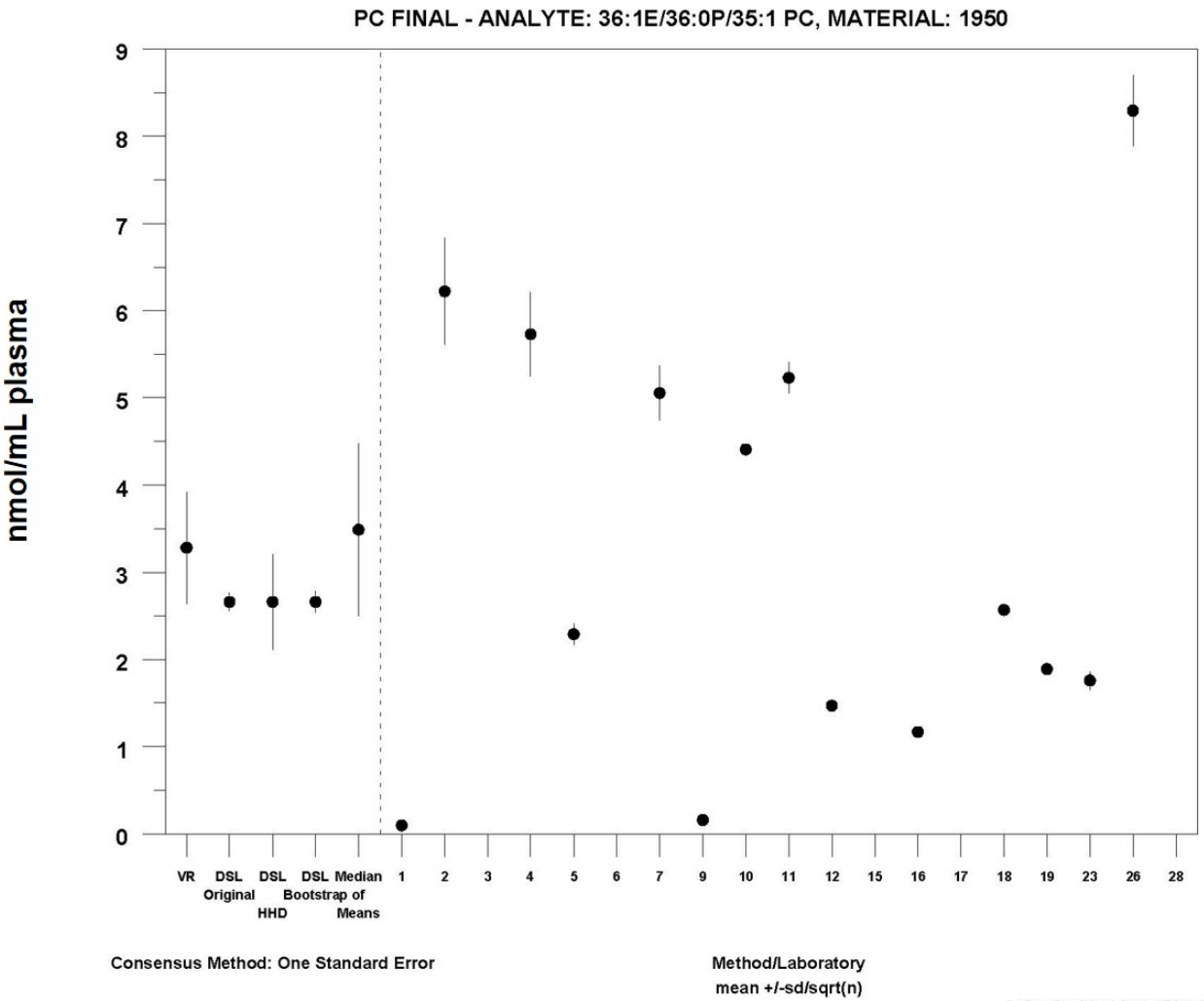








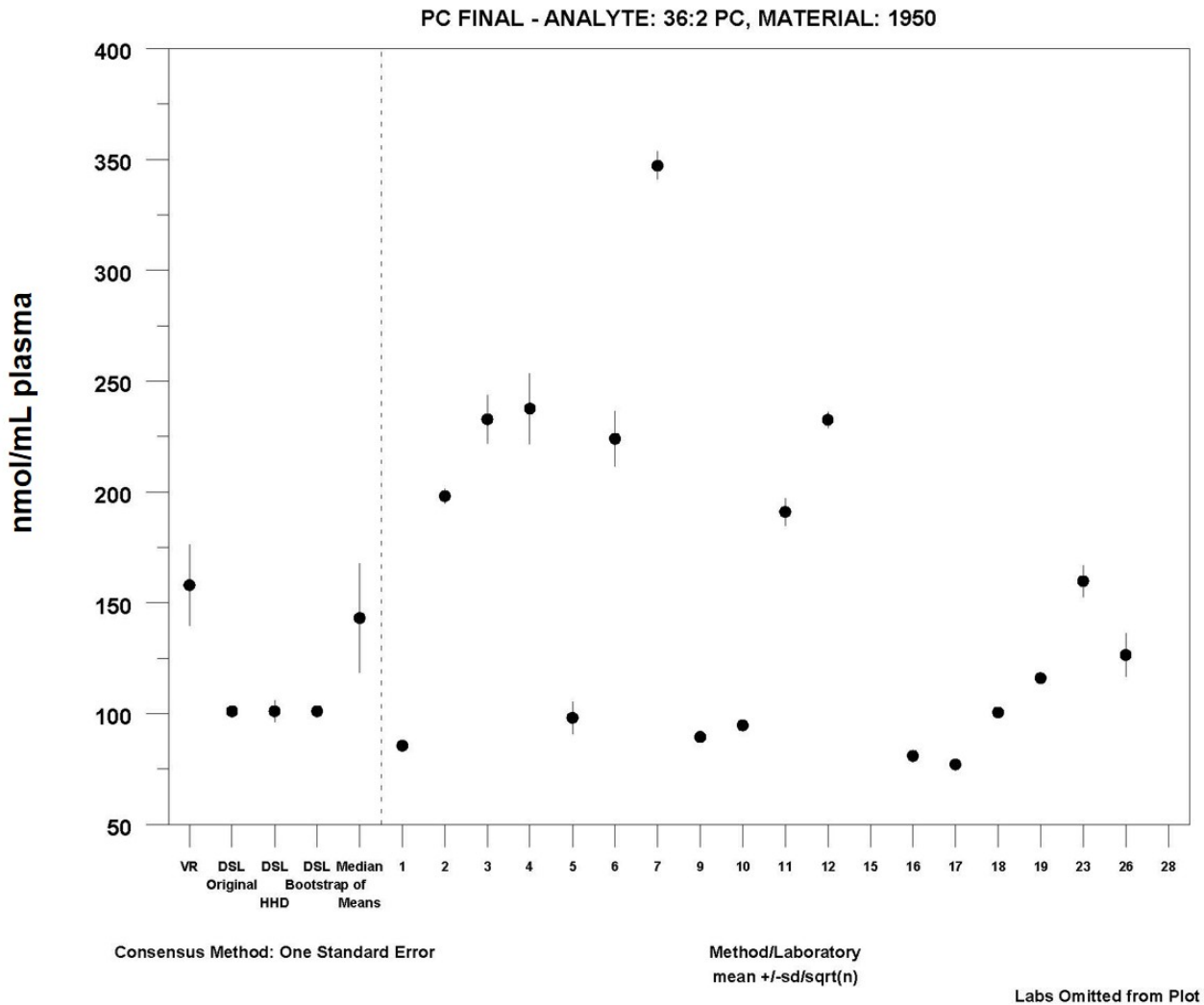


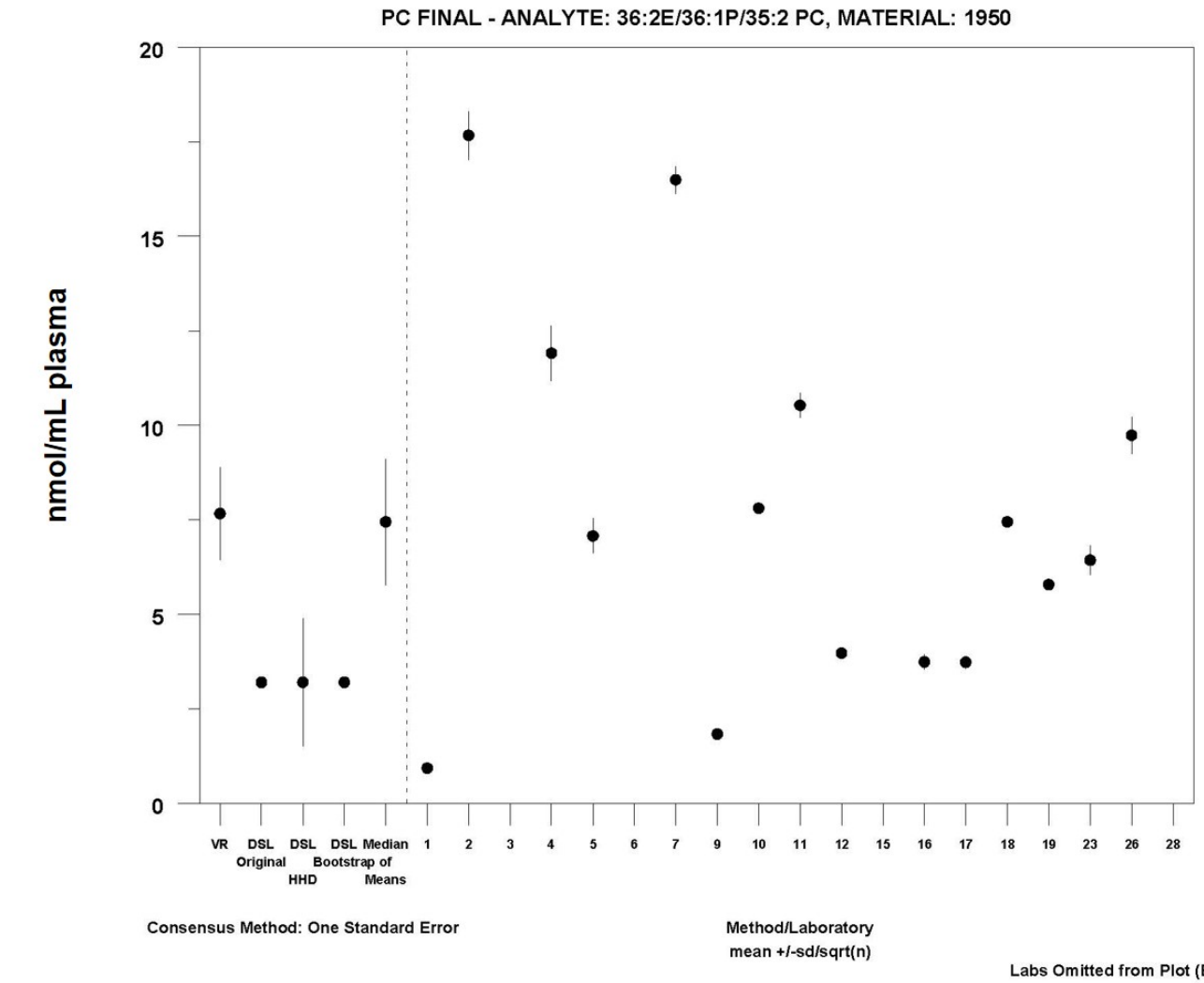


Labs Omitted from Plot (But Not Analysis): 6 15

MEDM Location: 3.5 ± 0.99 nmol/mL

6: 406 ± 32; 15: 928 ± 337

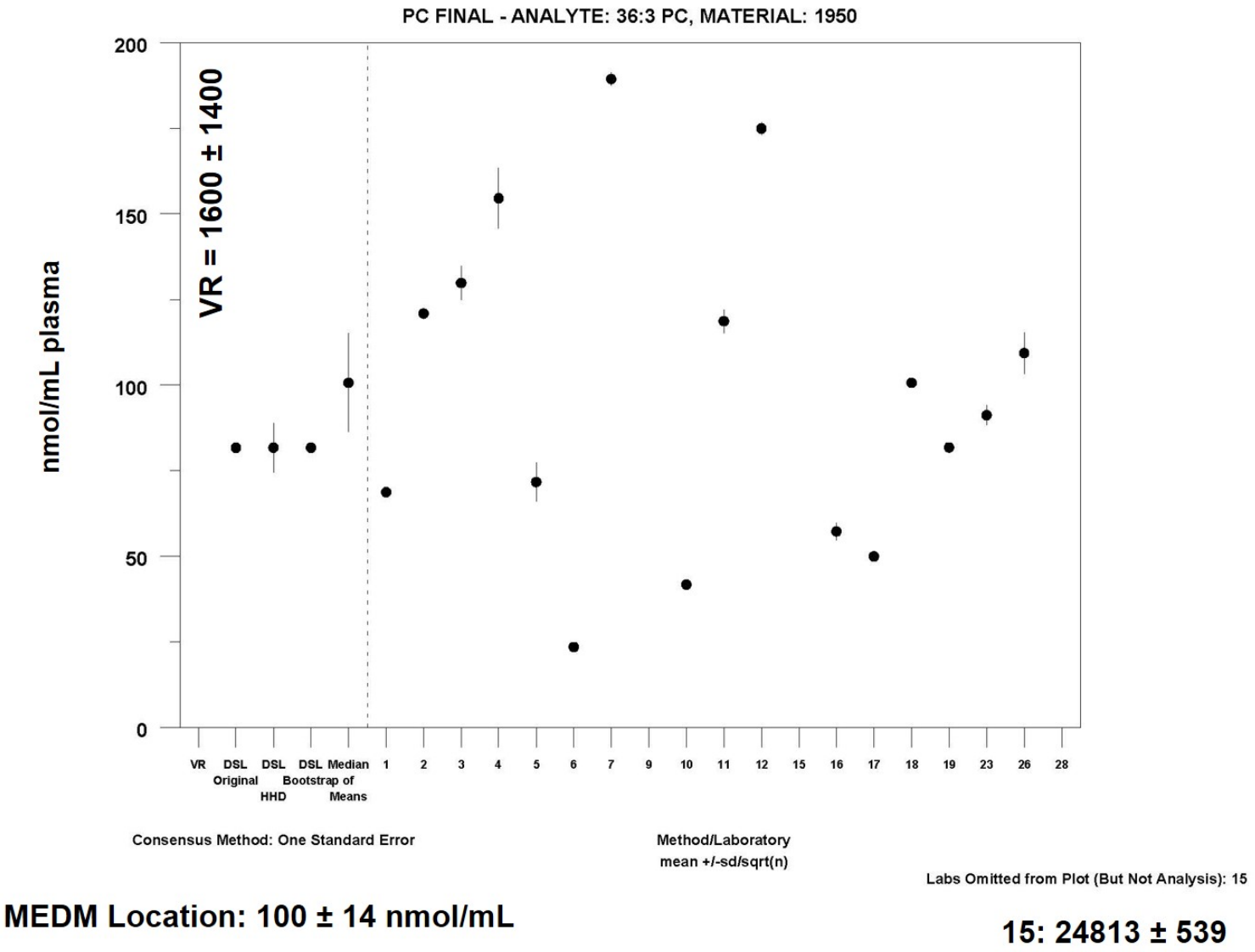


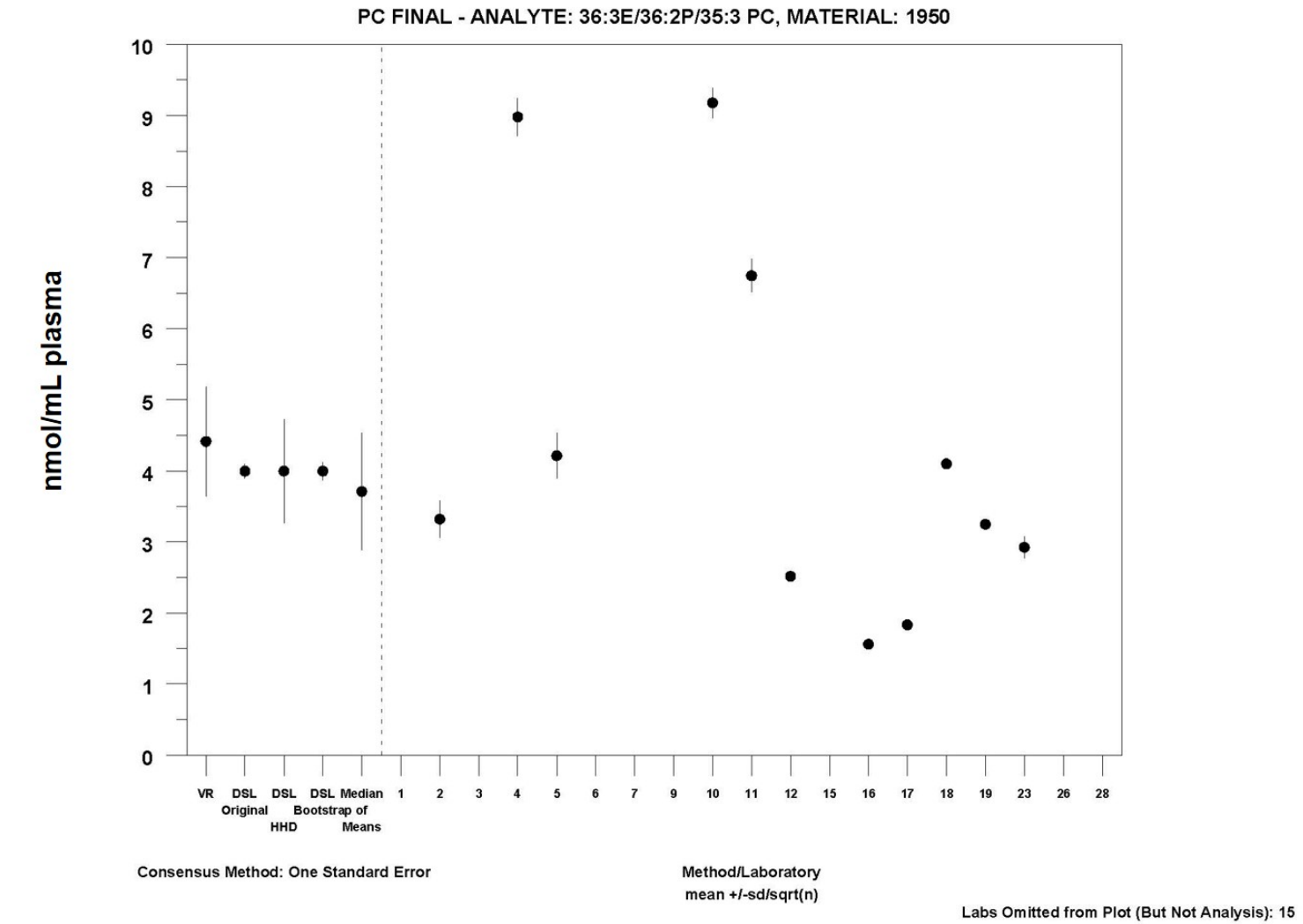


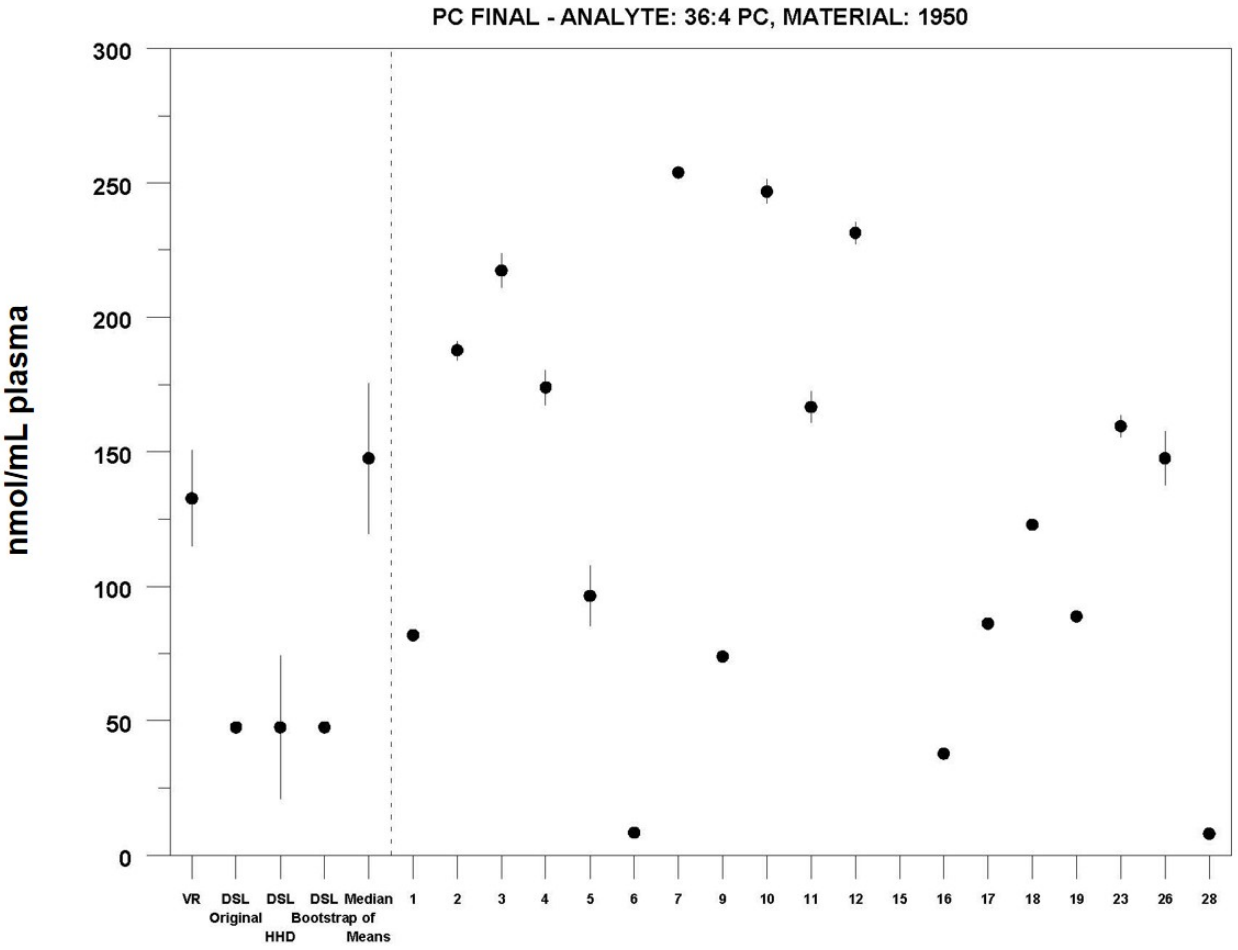
Labs Omitted from Plot (But Not Analysis): 6 15

MEDM Location: 7.4 ± 1.7 nmol/mL

6: 305 ± 27; 15: 4496 ± 448



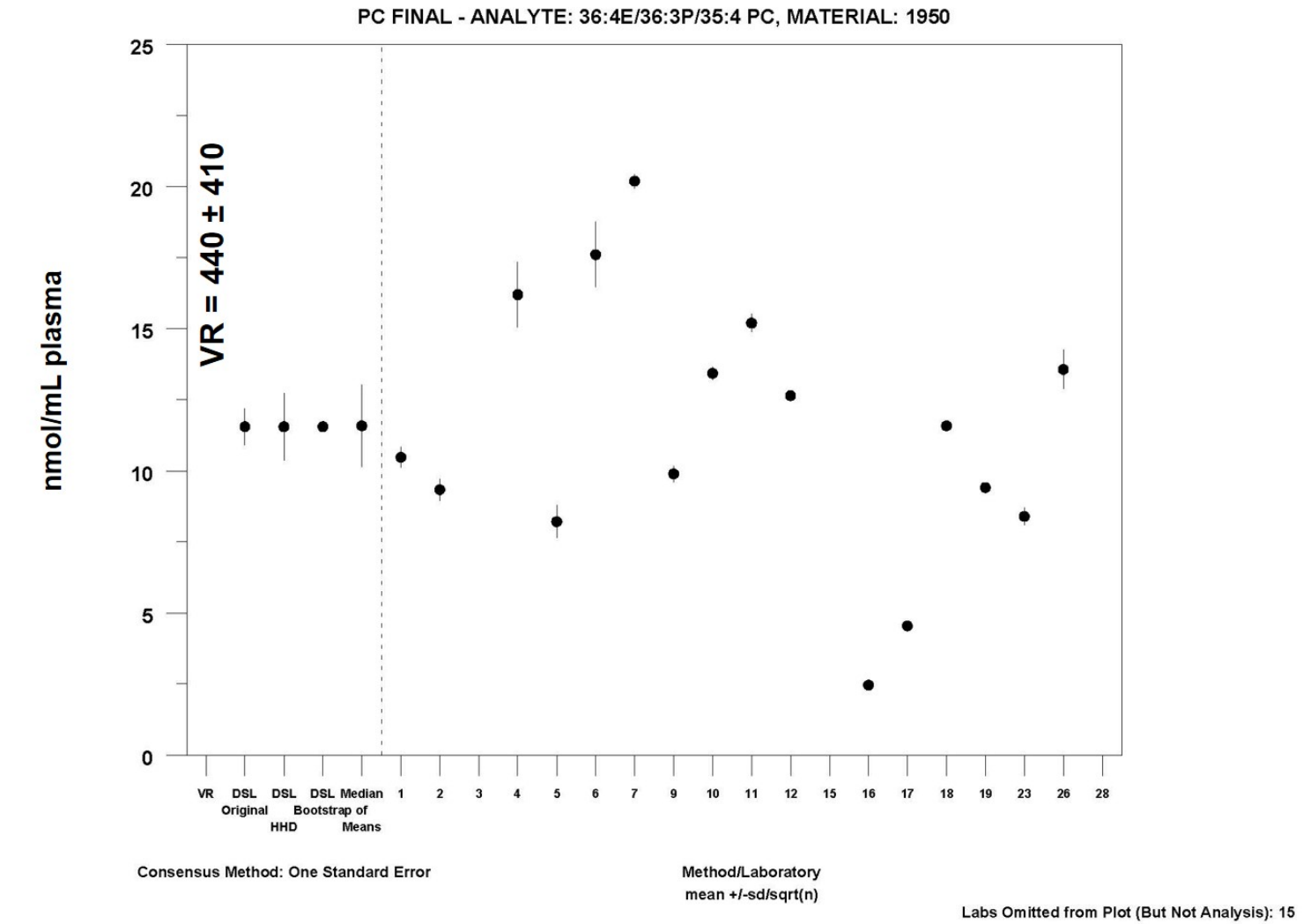


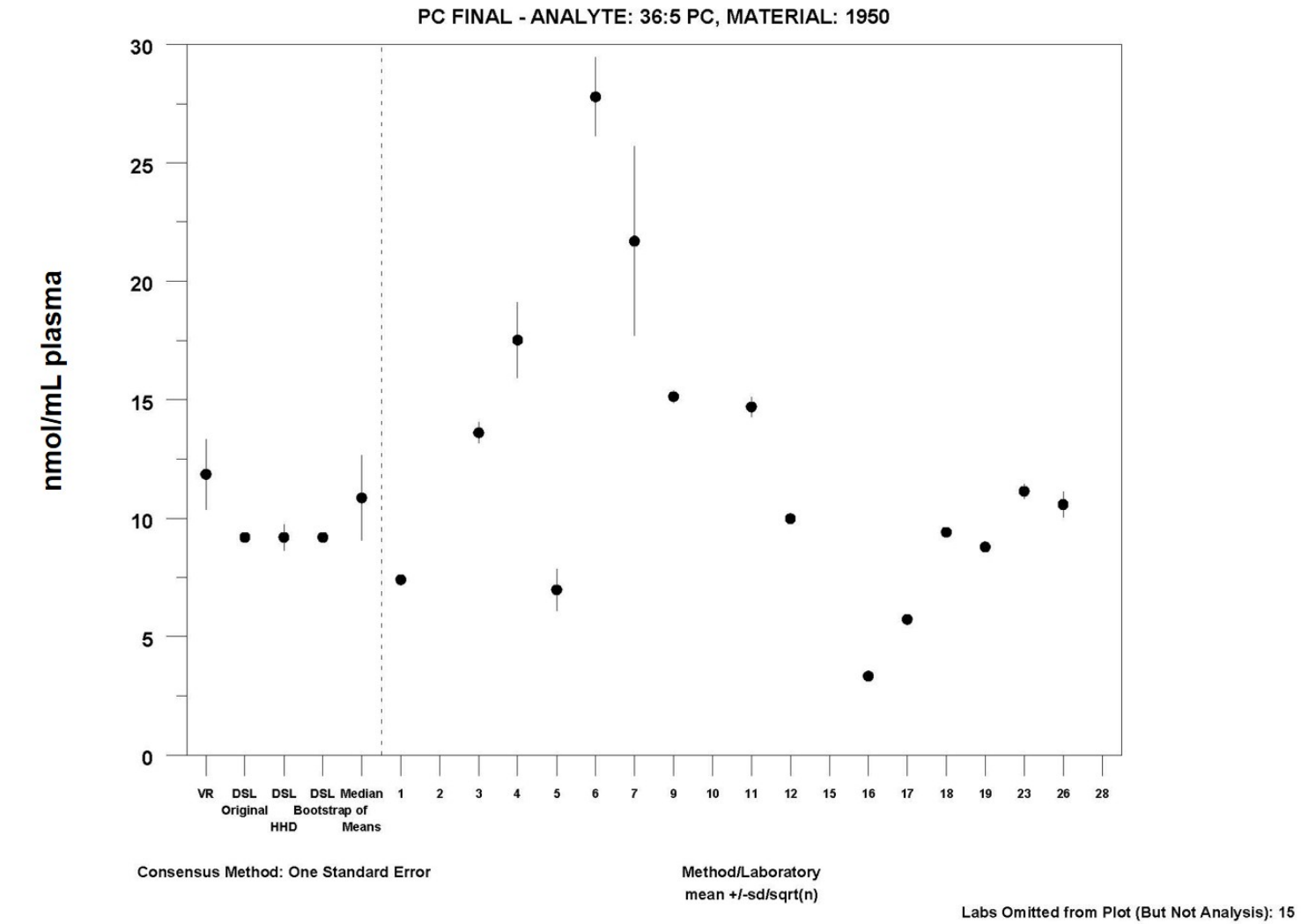


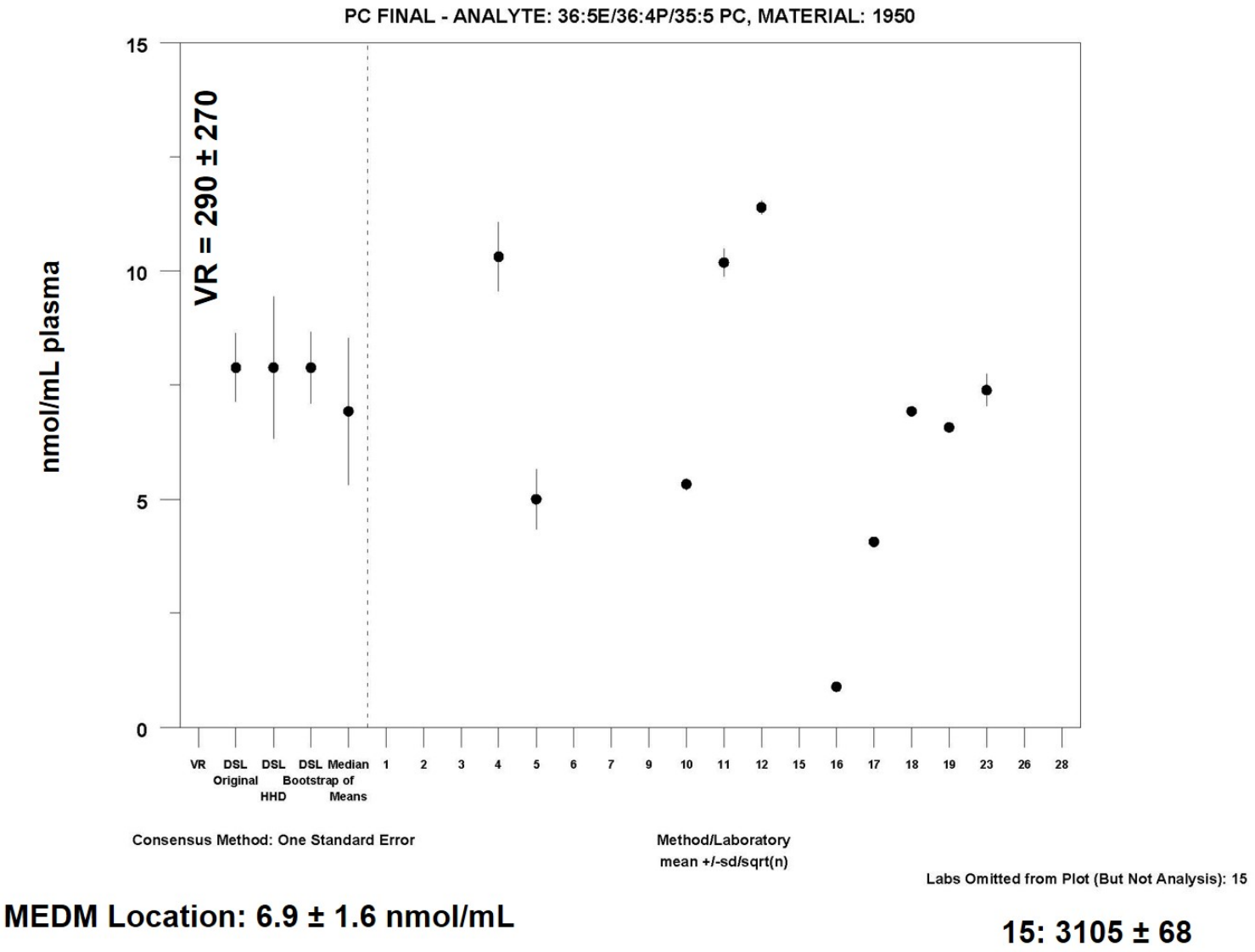
Labs Omitted from Plot (But Not Analysis): 15

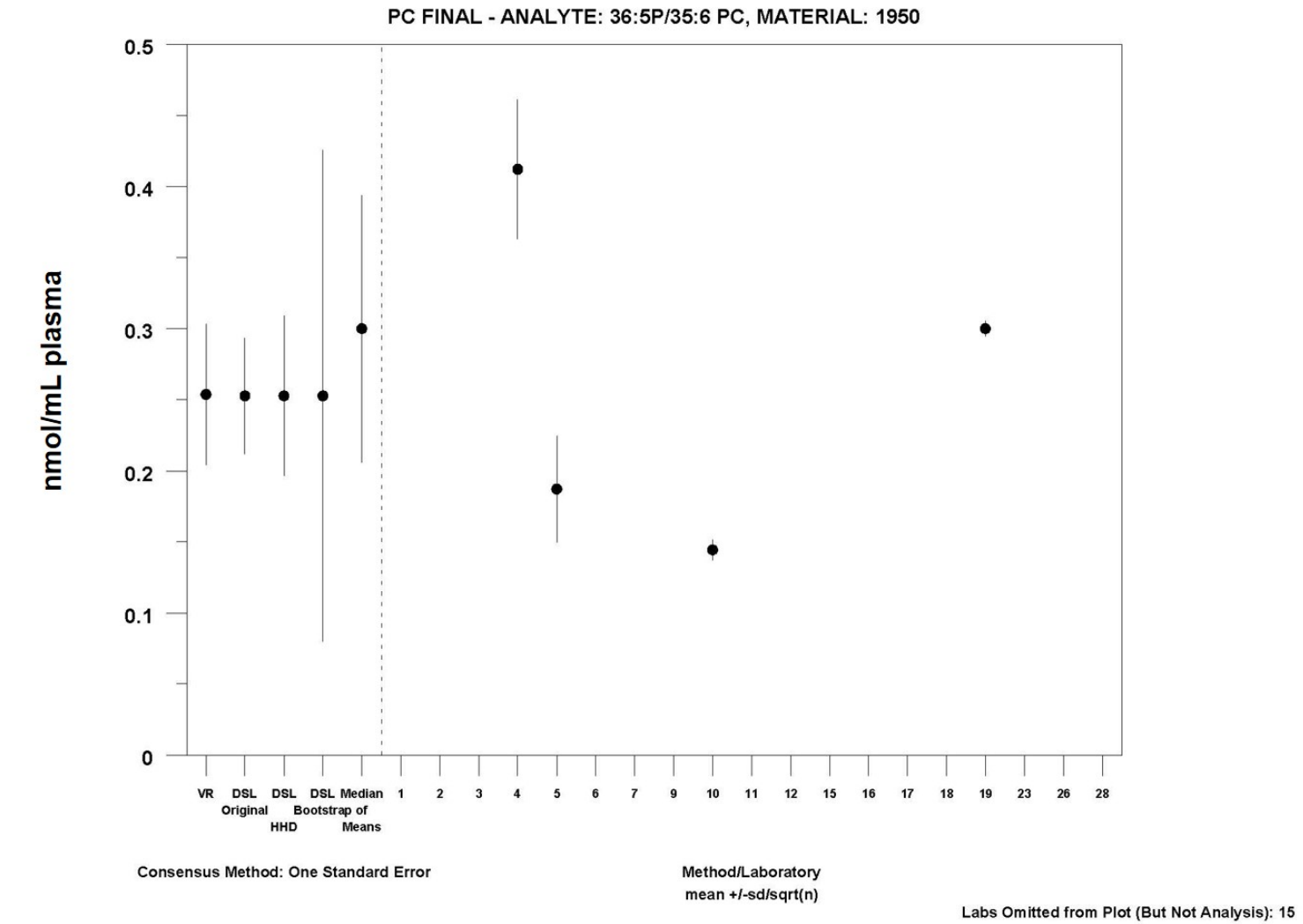
MEDM Location: 150 ± 28 nmol/mL

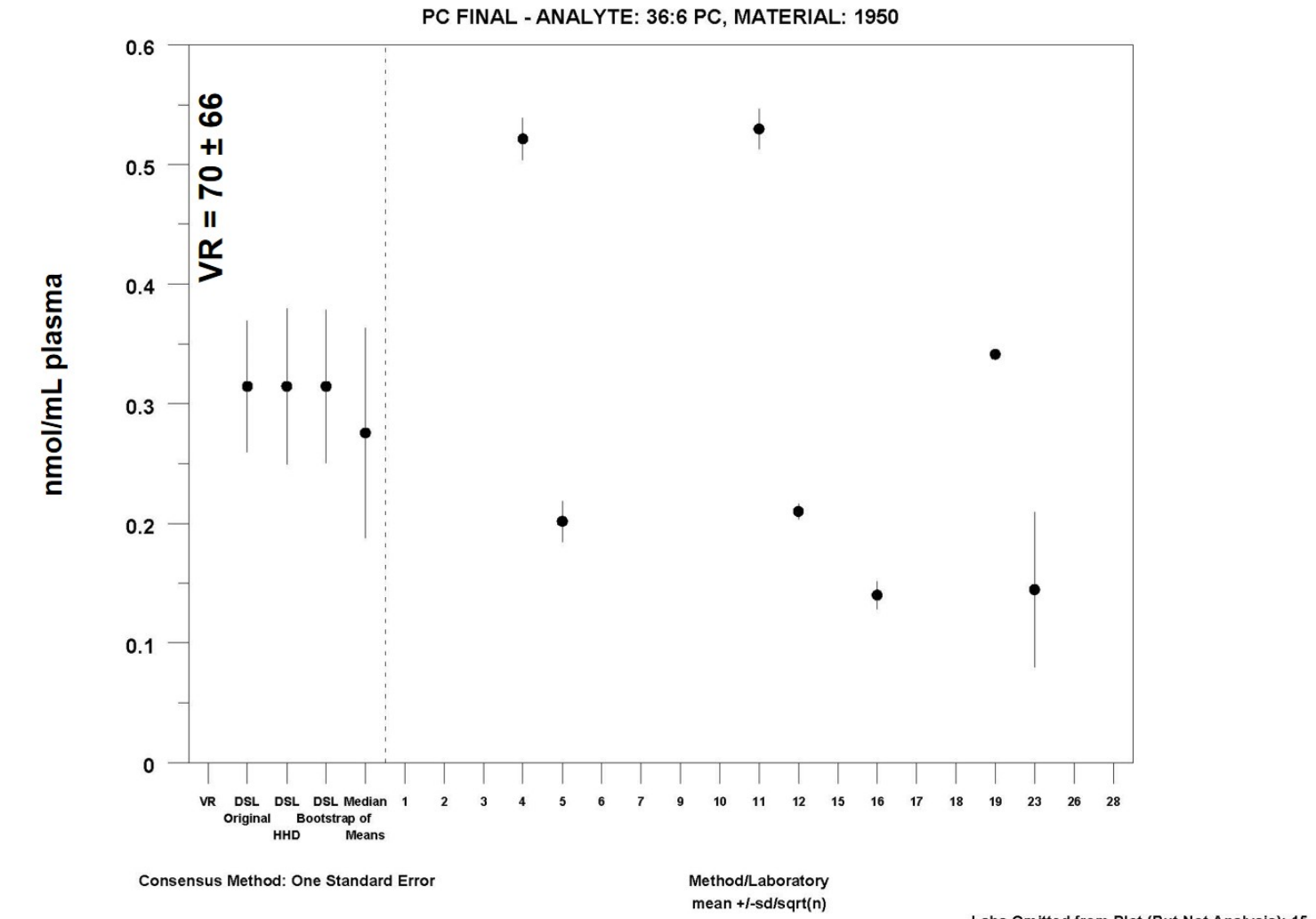
15: 33029 ± 3652

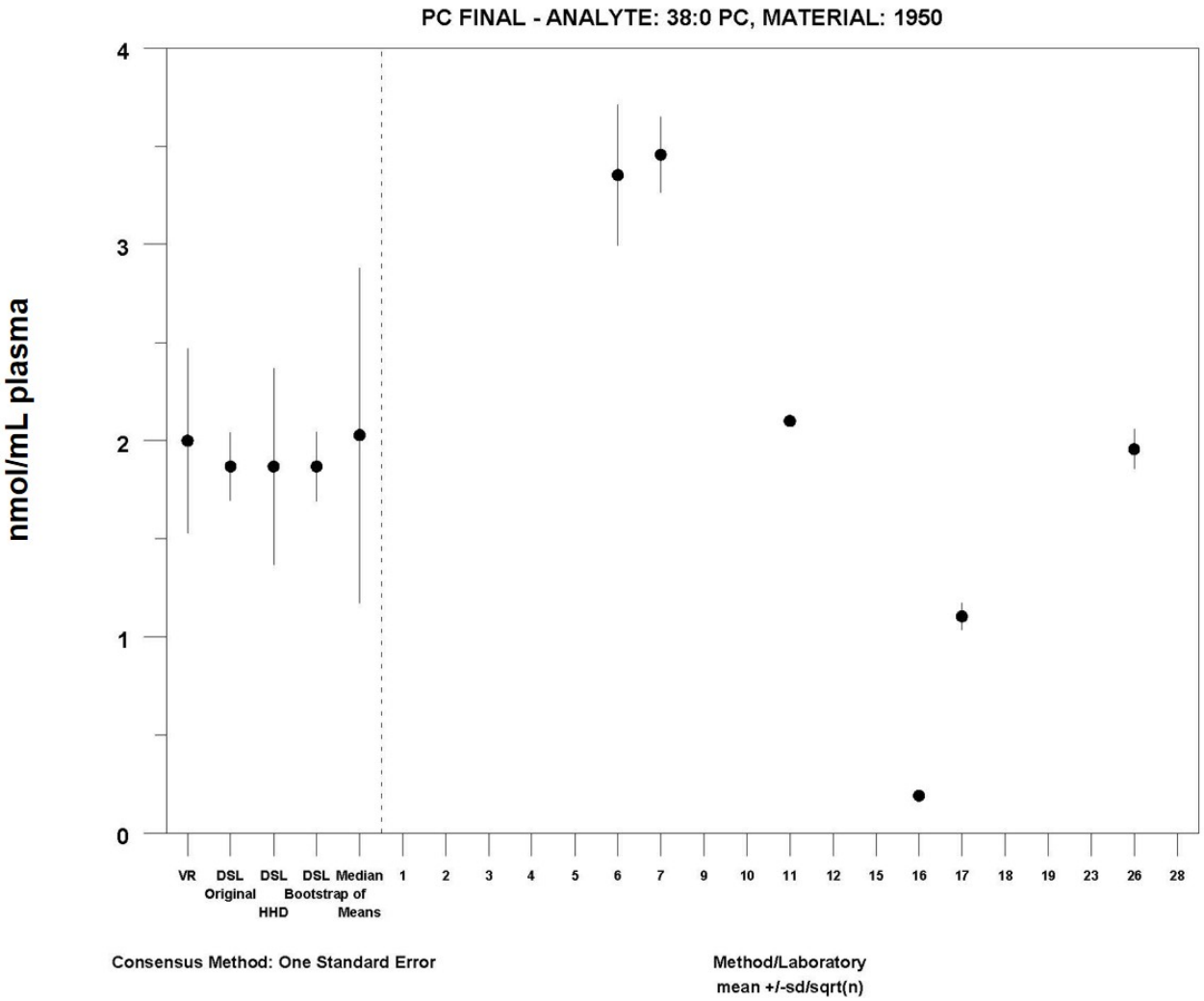




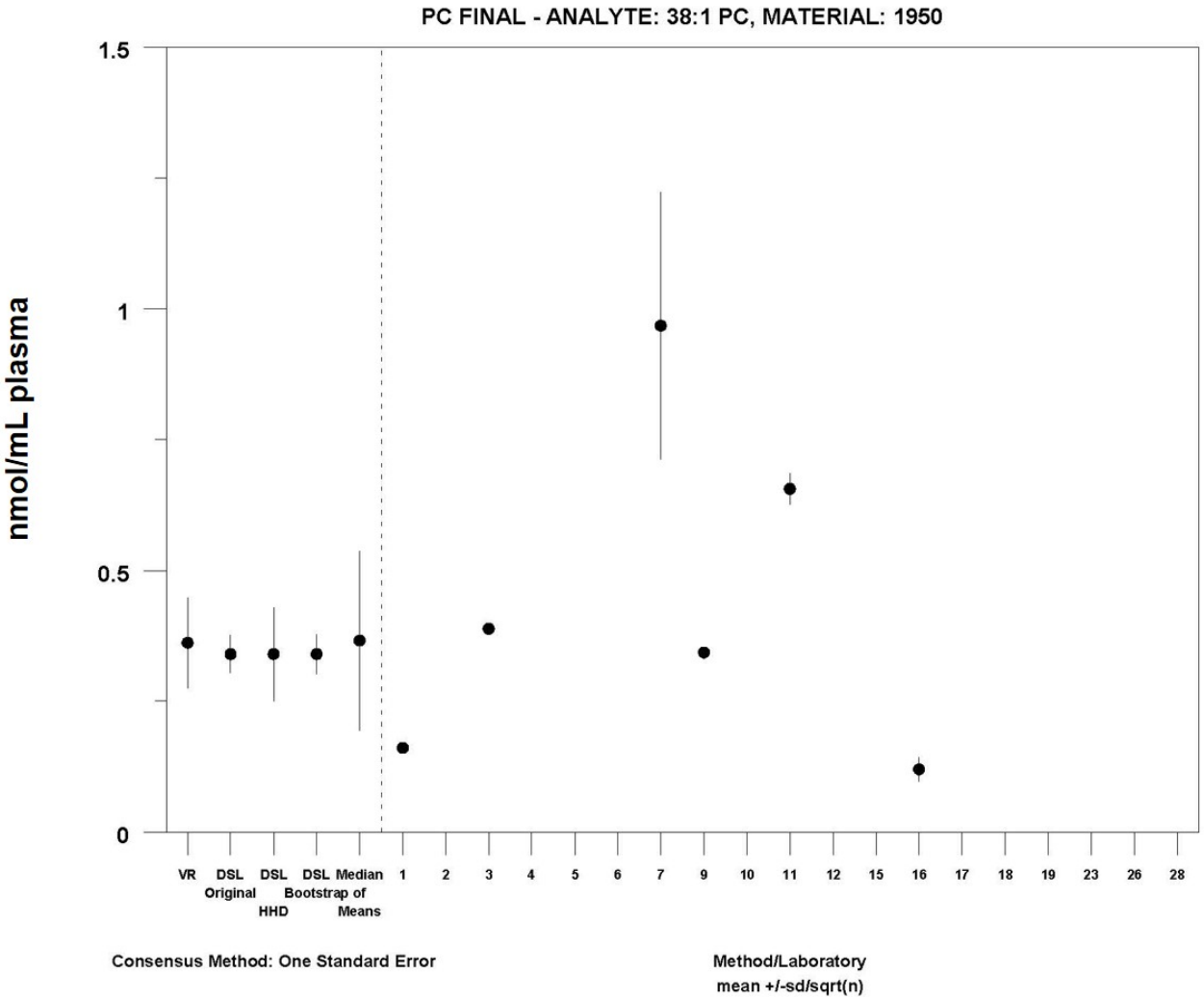




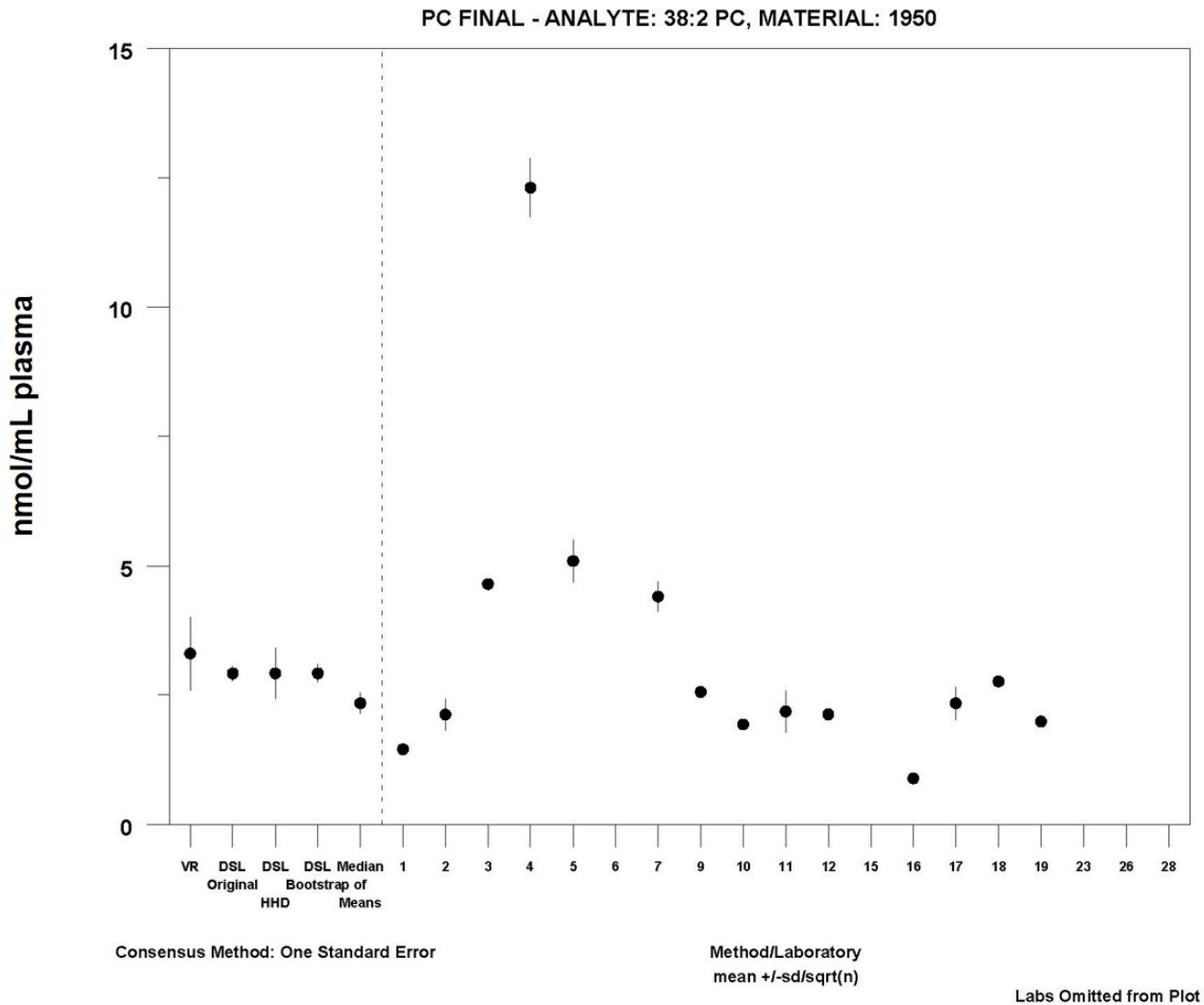


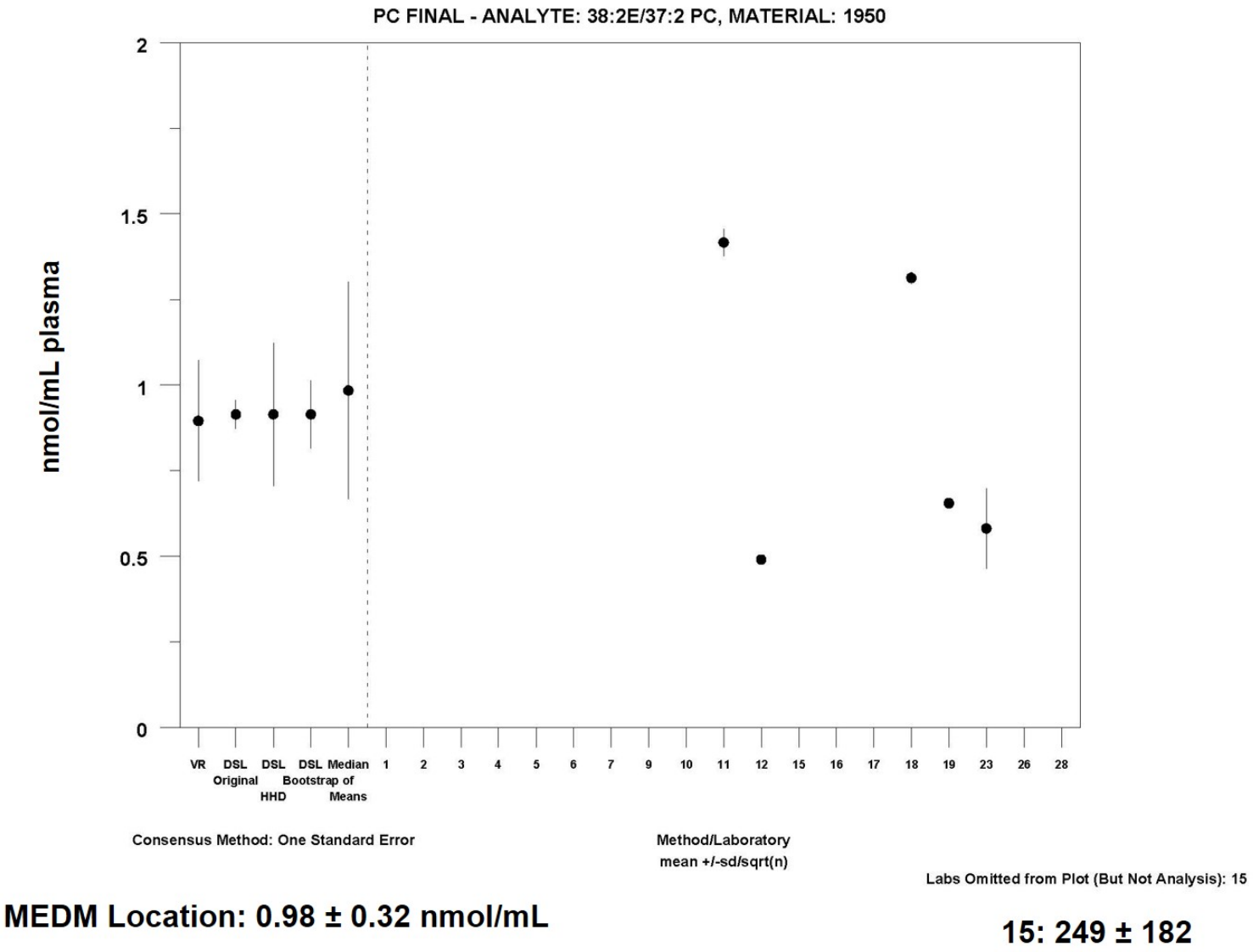


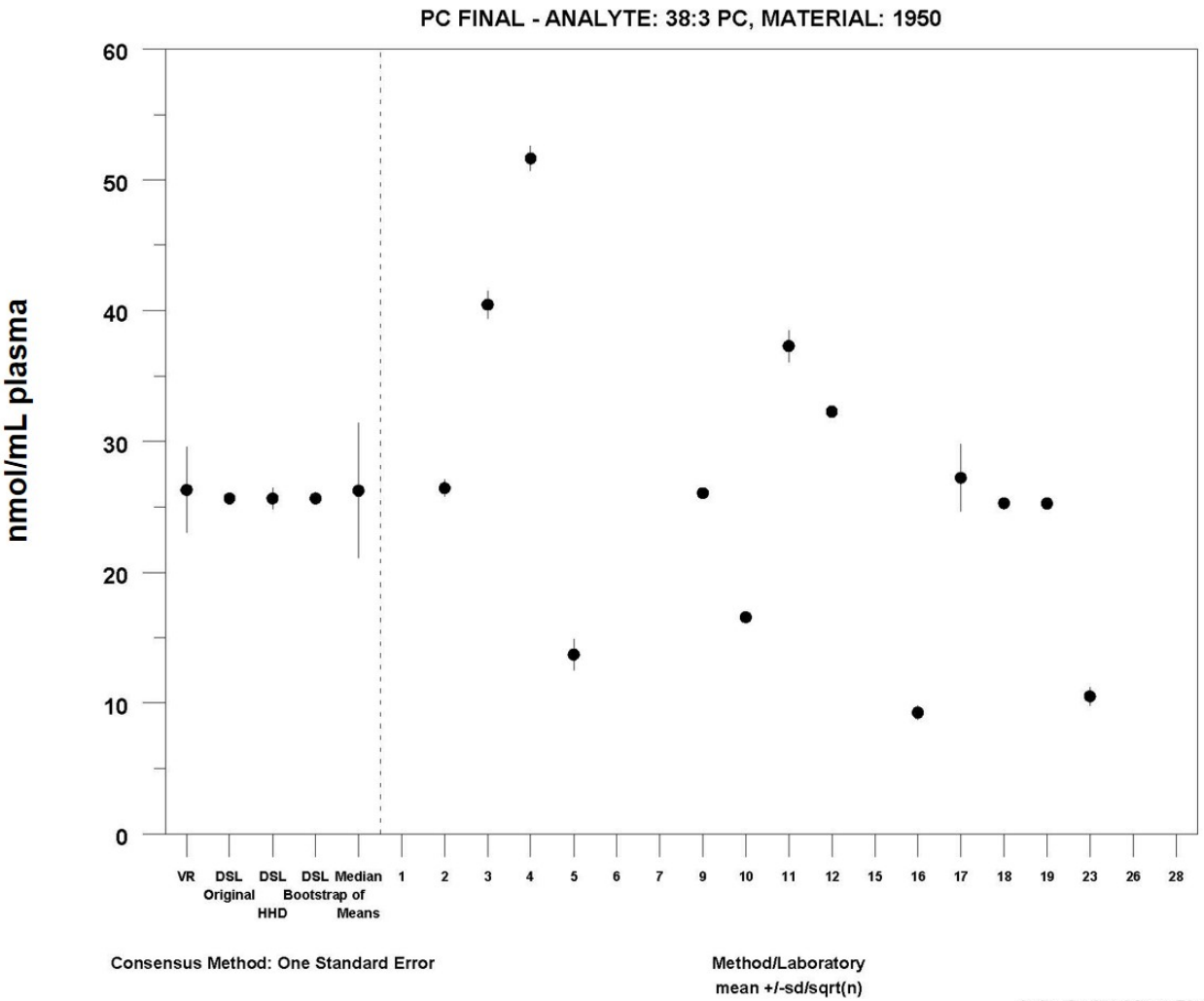
MEDM Location: 2.0 ± 0.85 nmol/mL

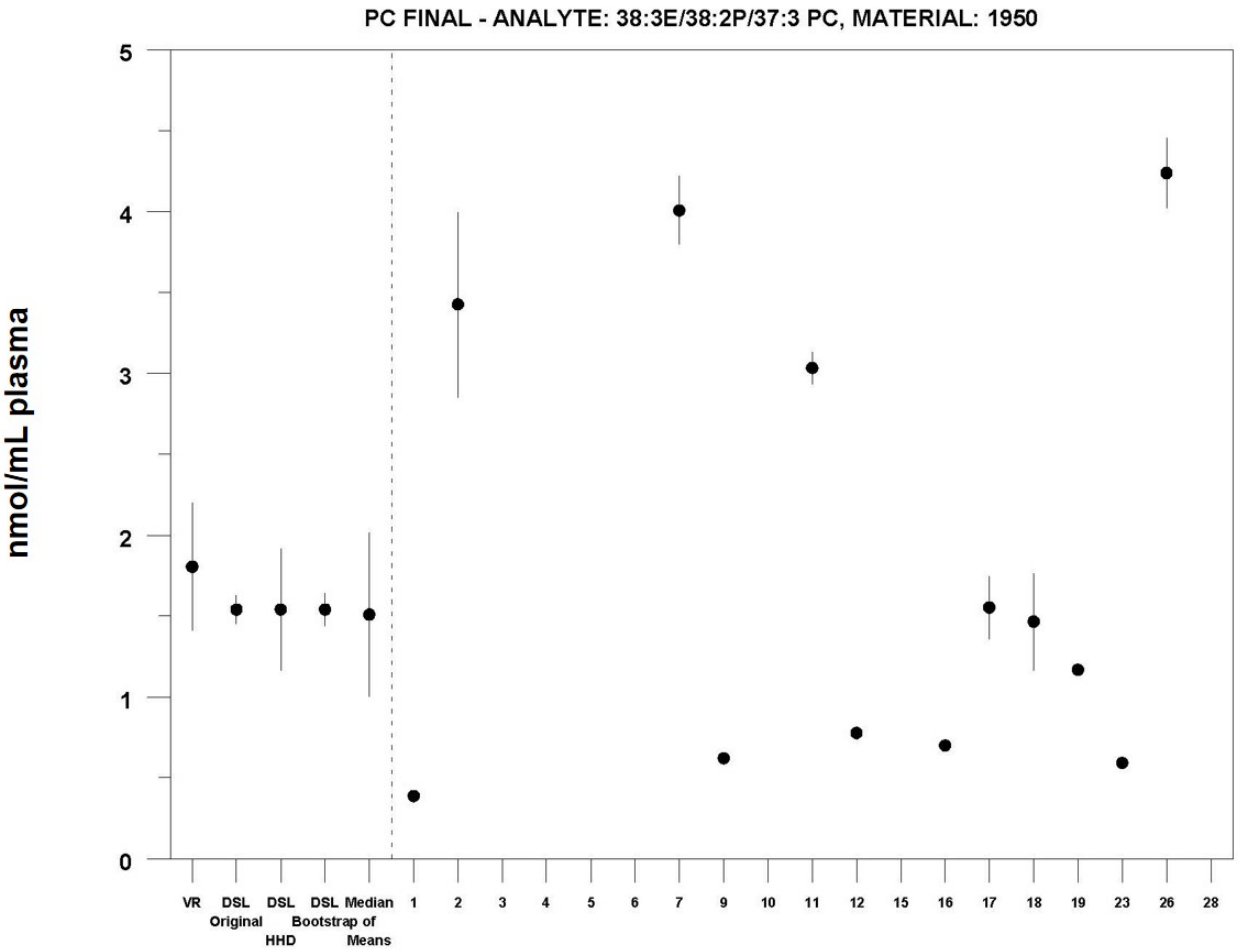


MEDM Location: 0.37 ± 0.17 nmol/mL





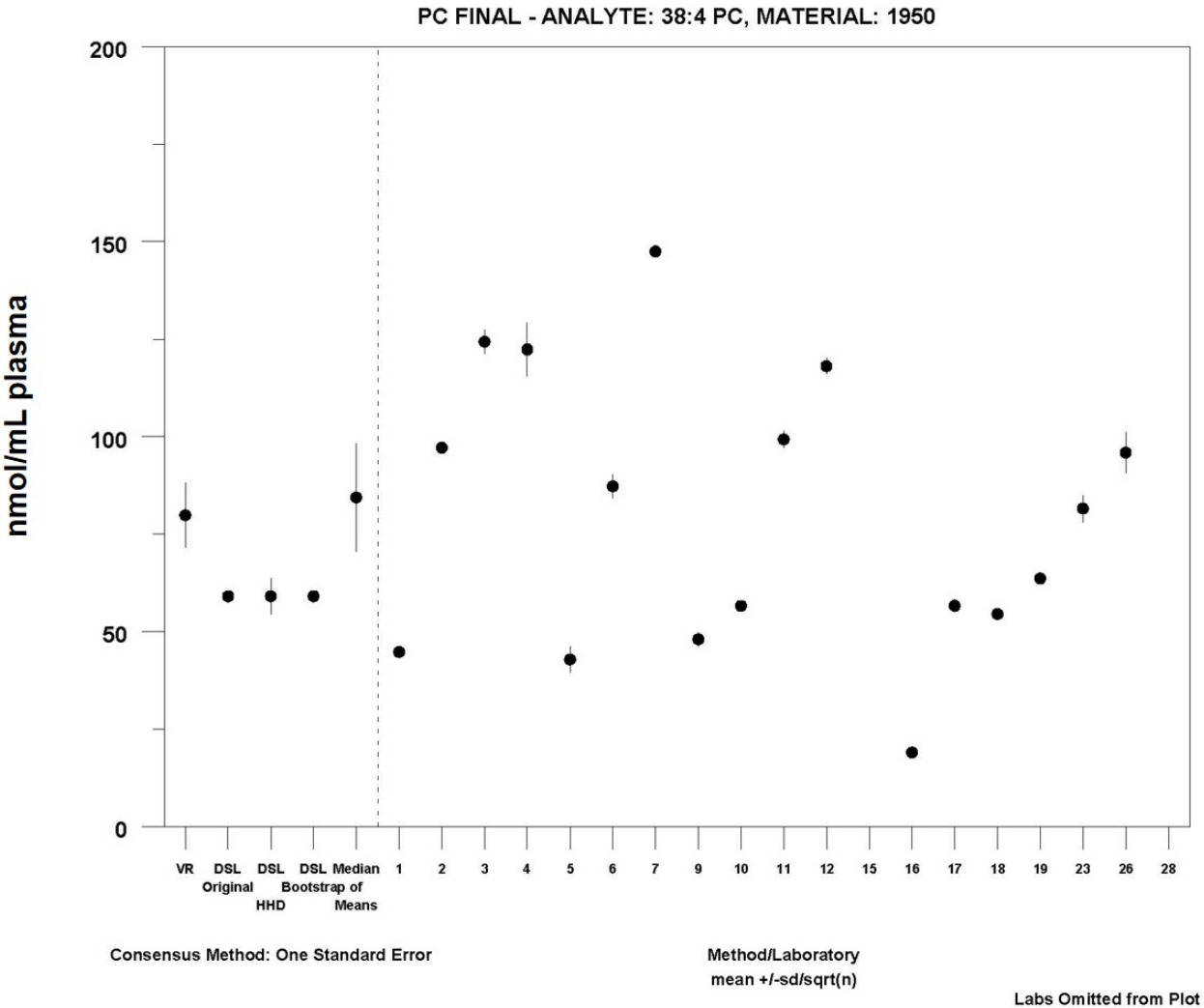


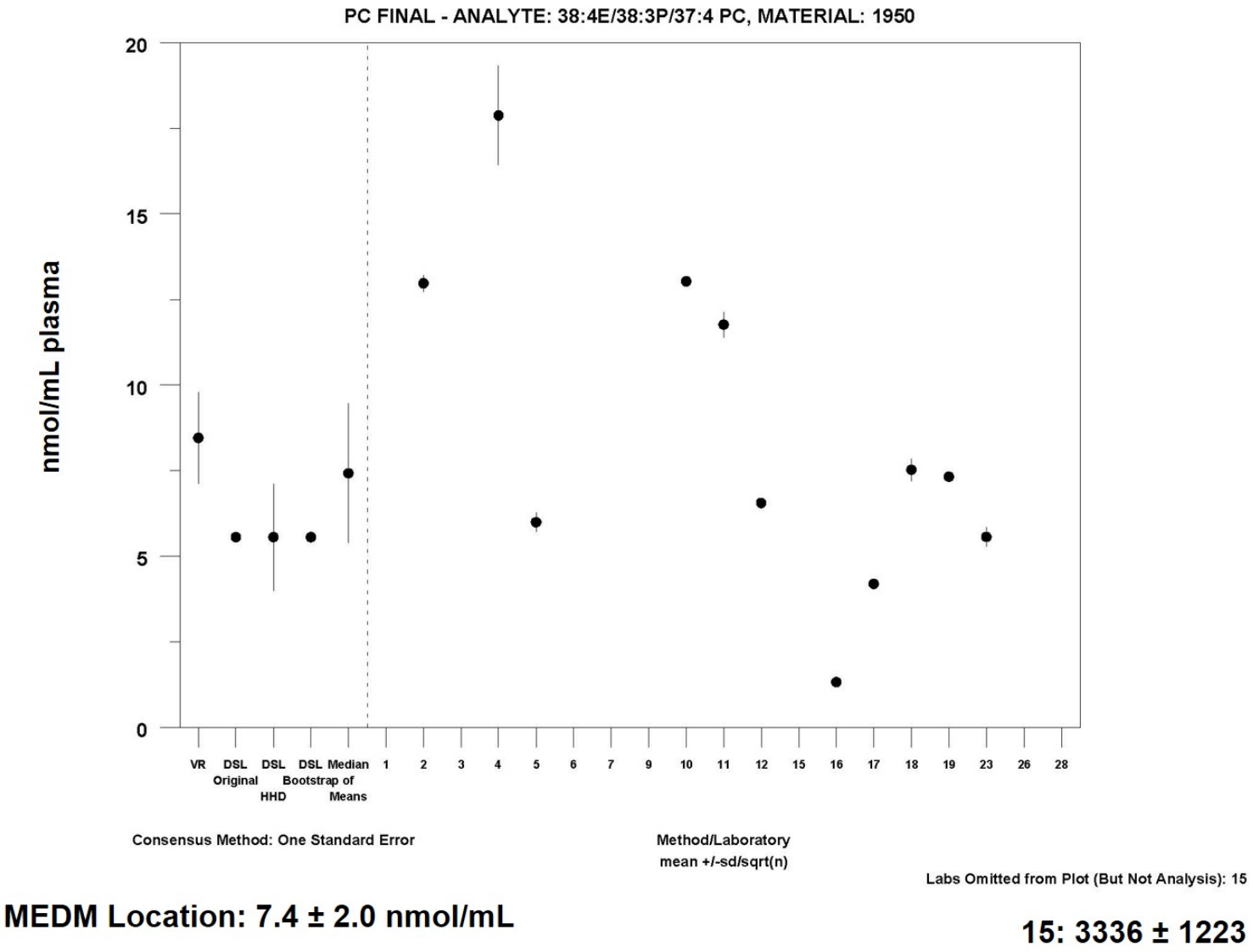


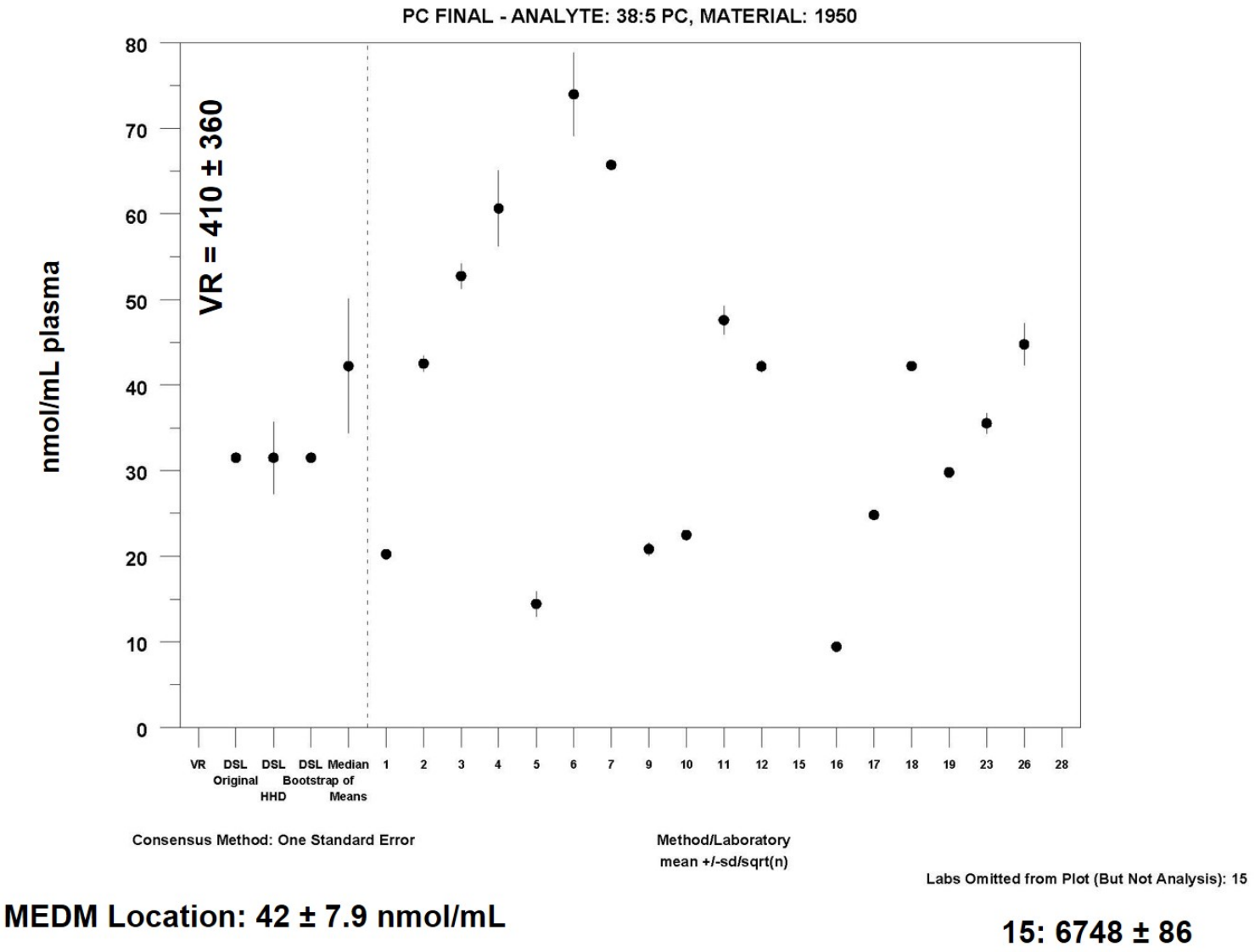
Labs Omitted from Plot (But Not Analysis): 6 15

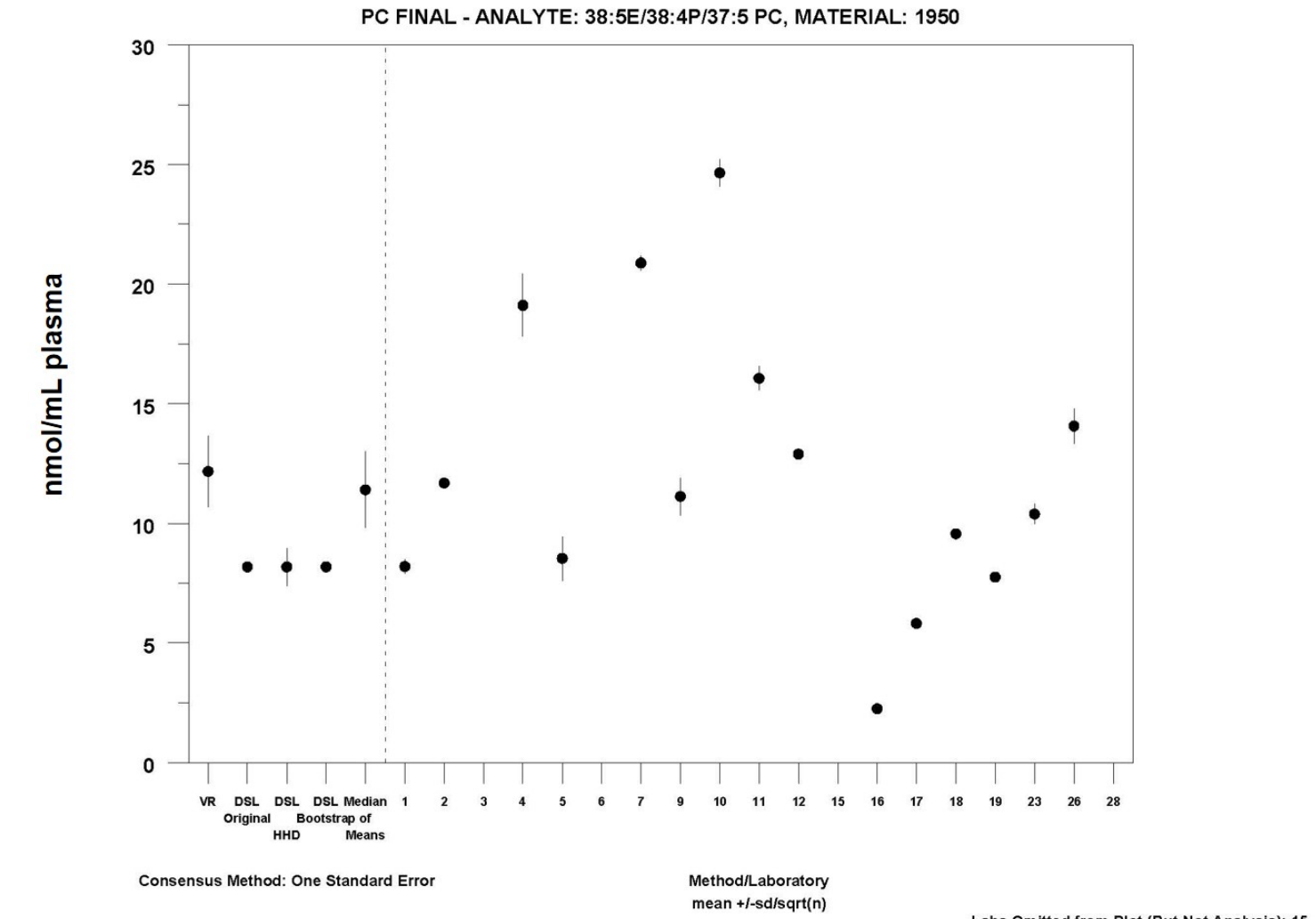
MEDM Location: 1.5 ± 0.51 nmol/mL

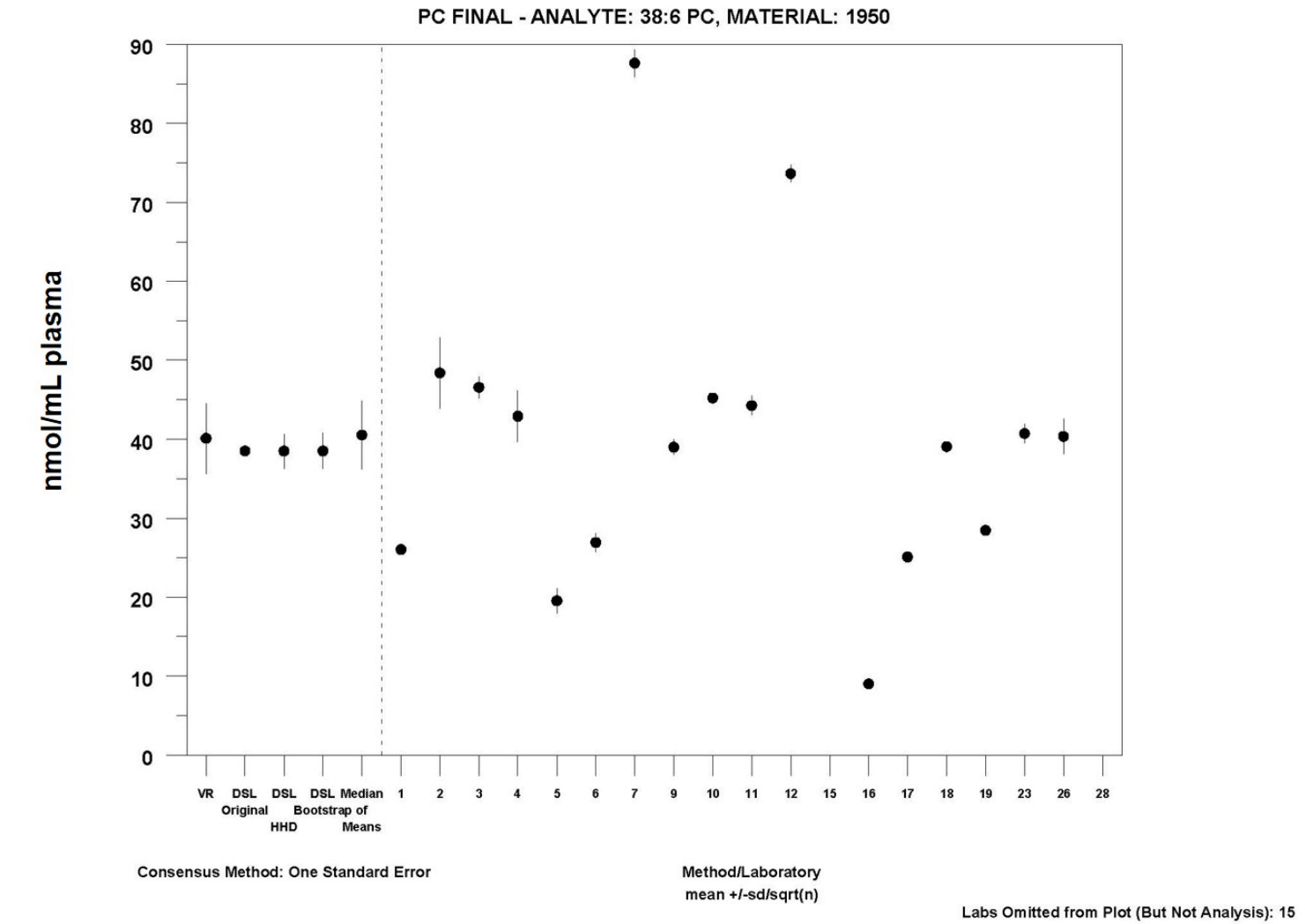
6: 194 ± 21; 15: 585 ± 67

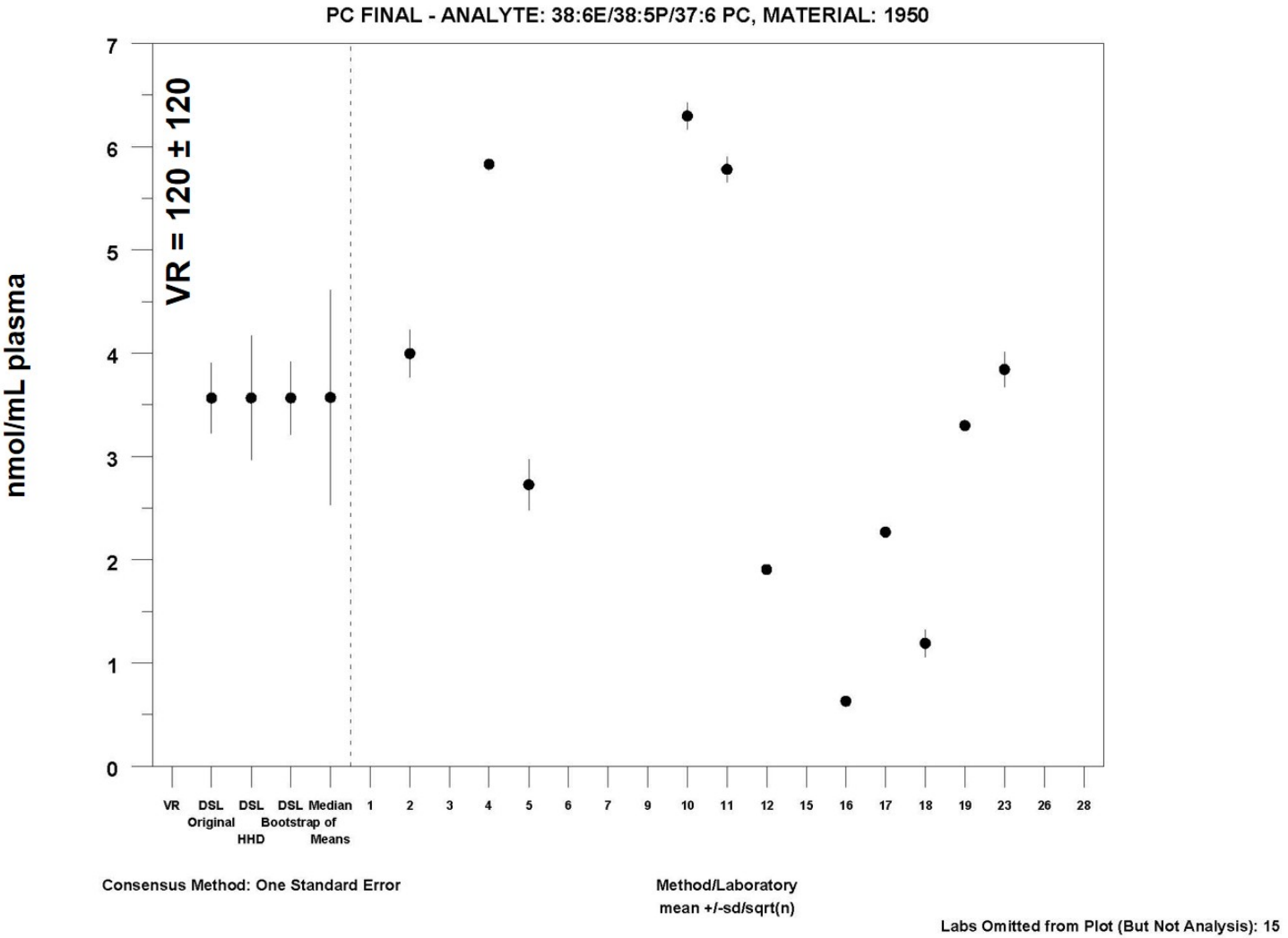


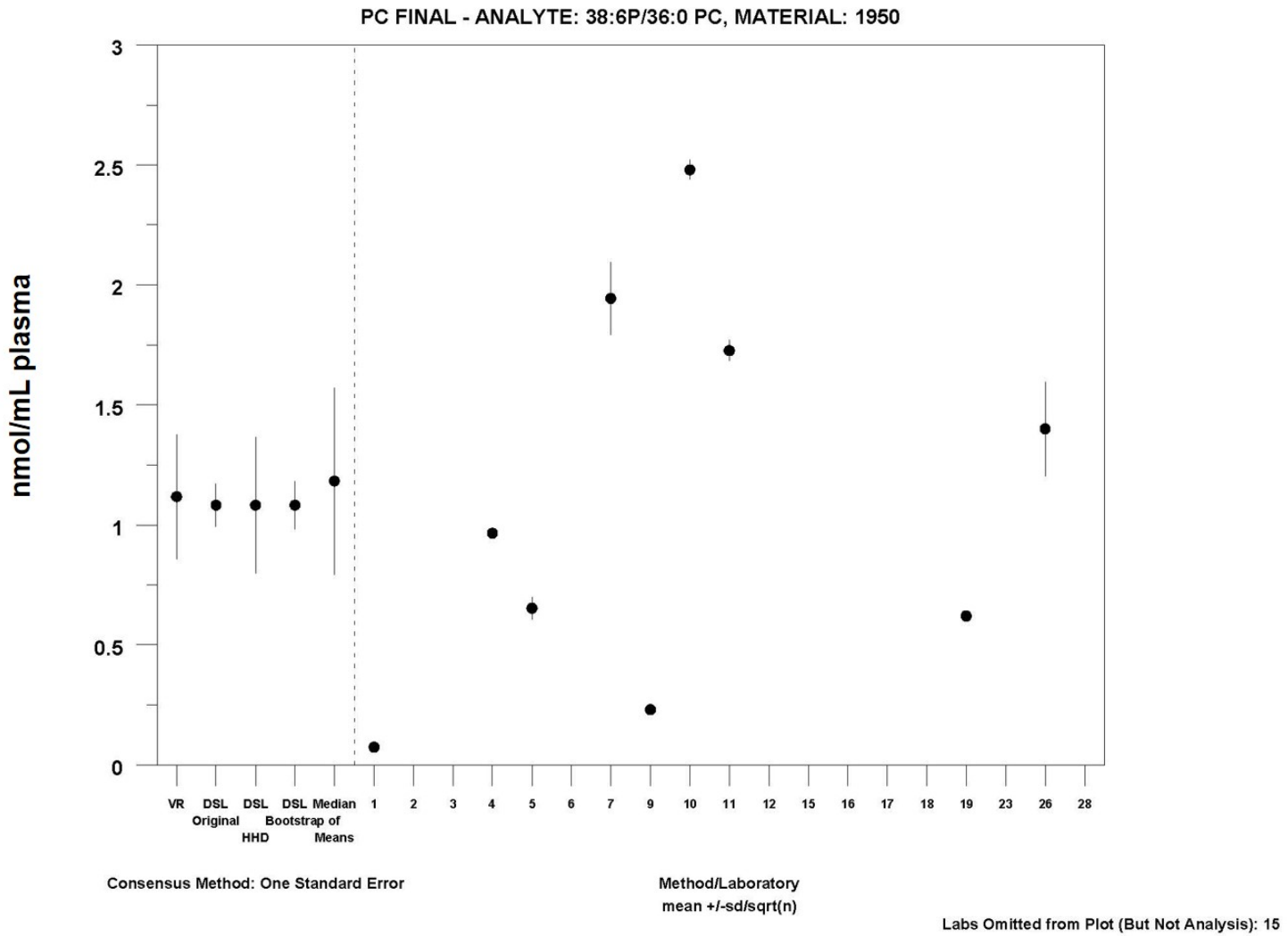


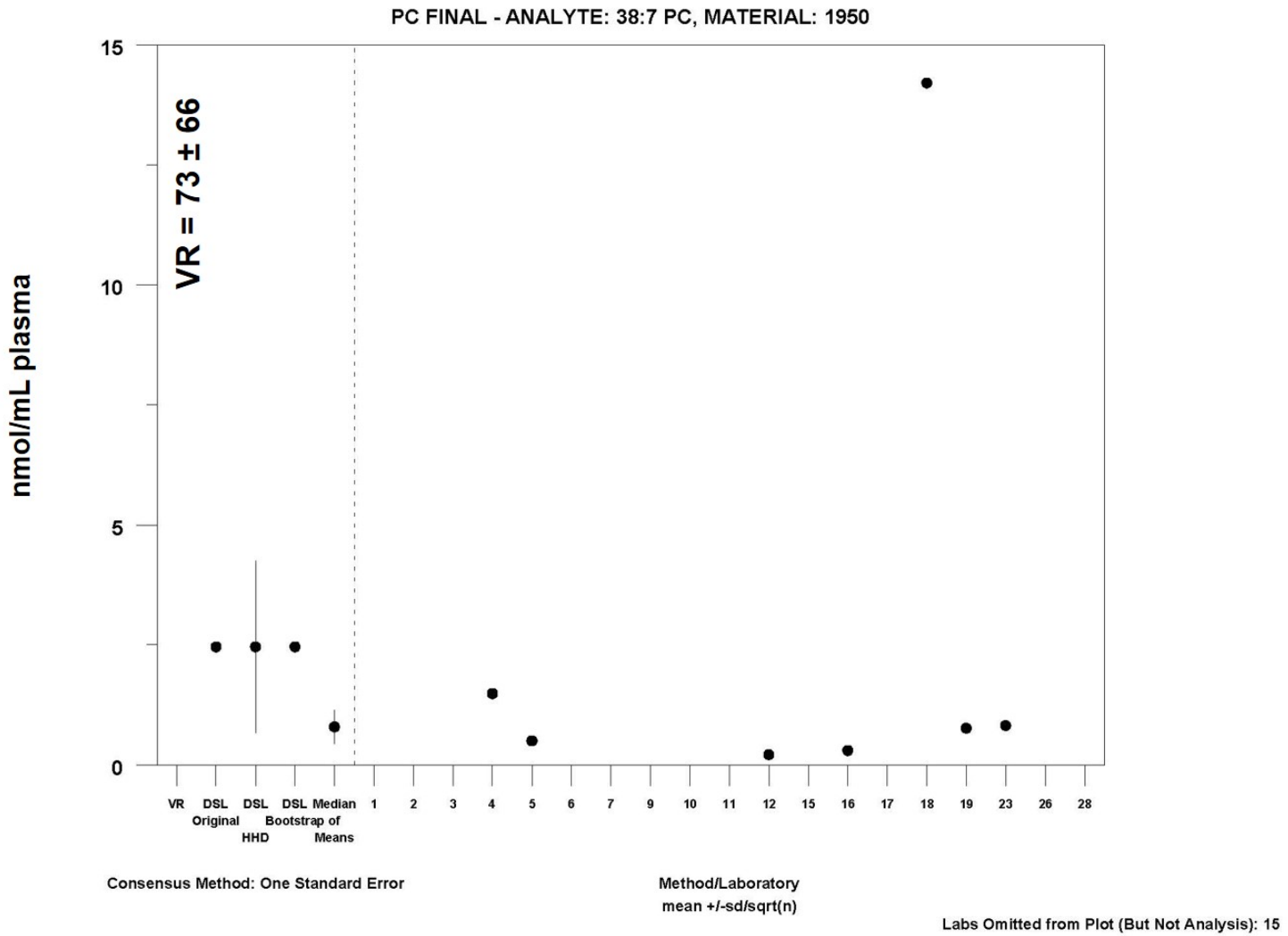


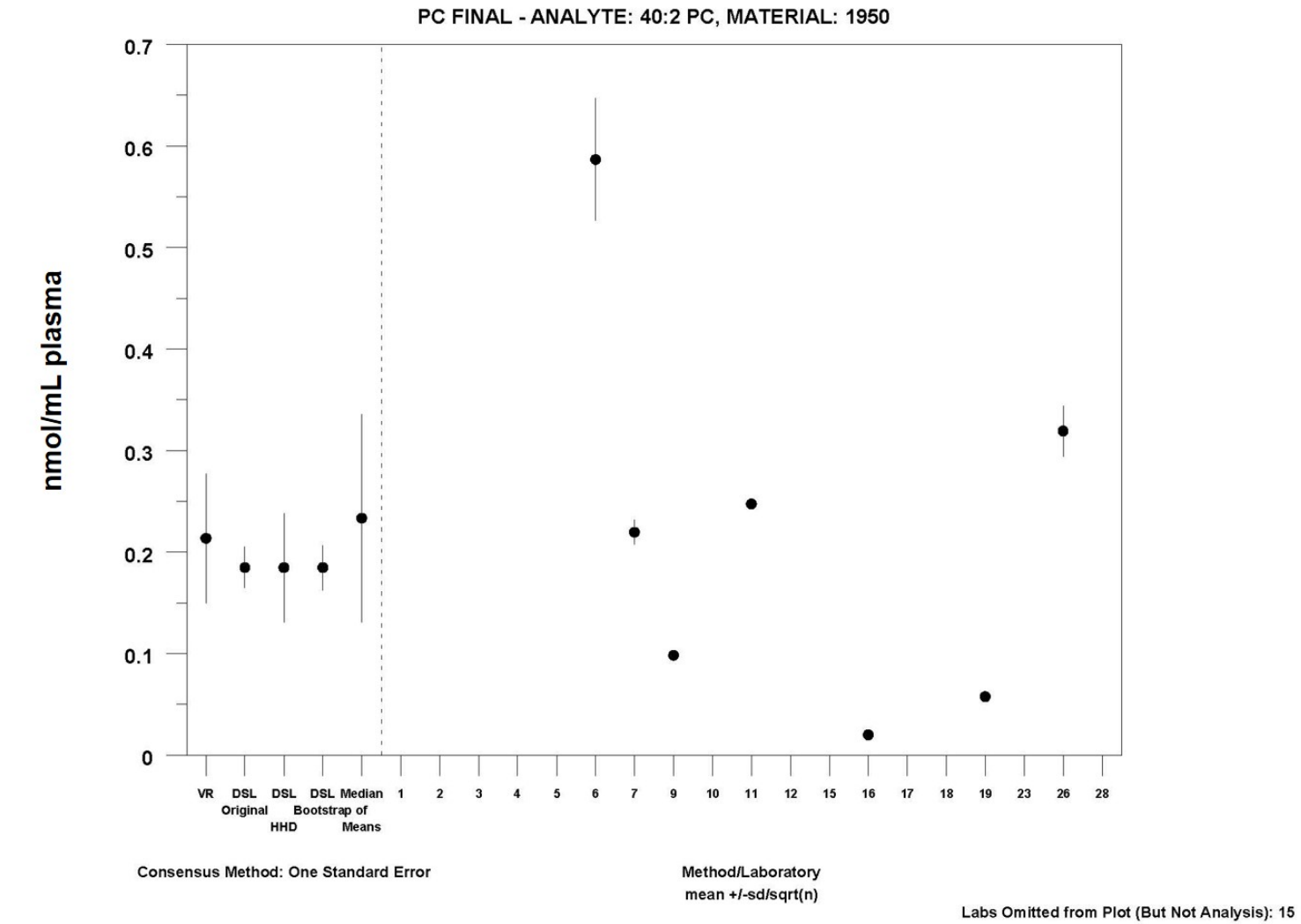






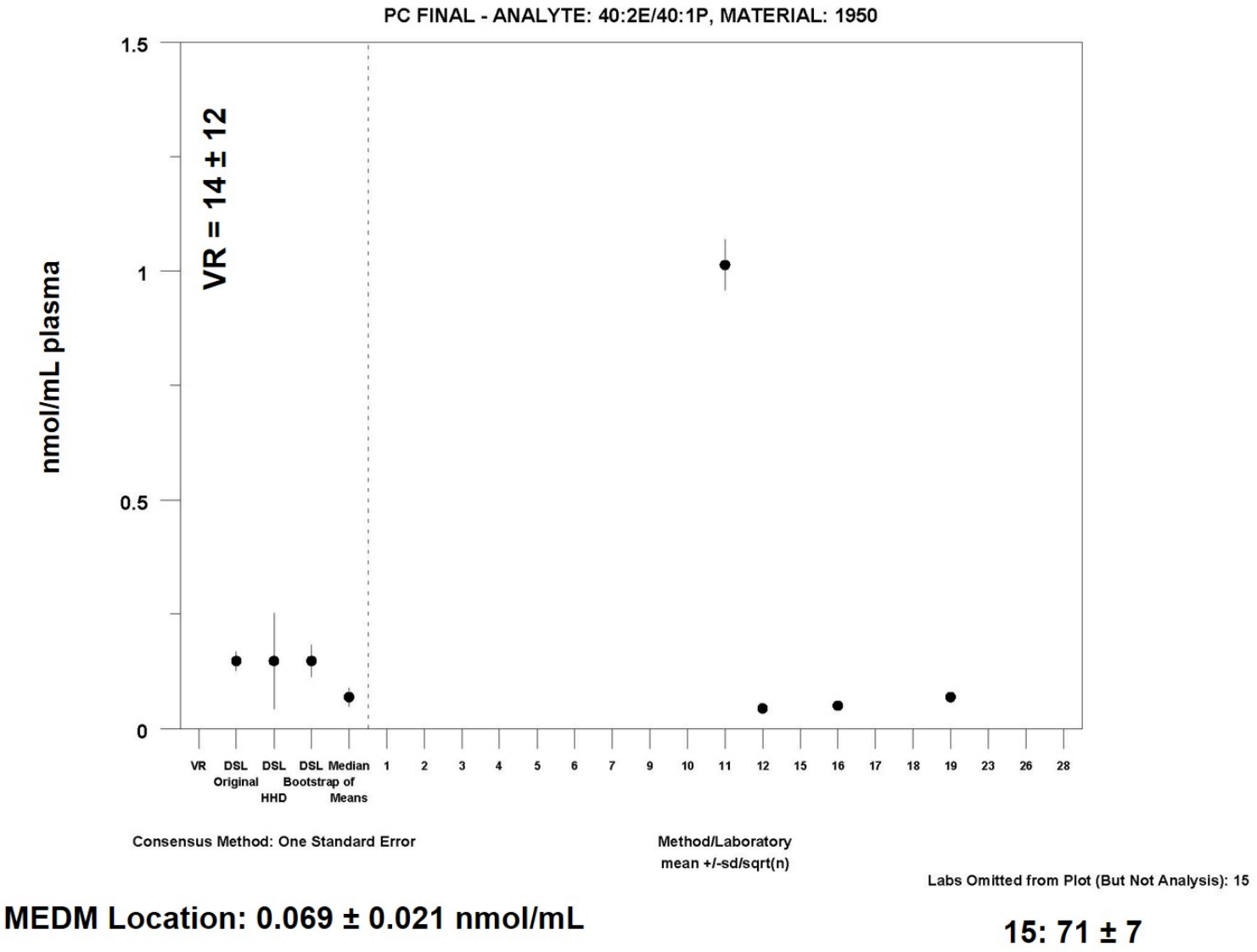


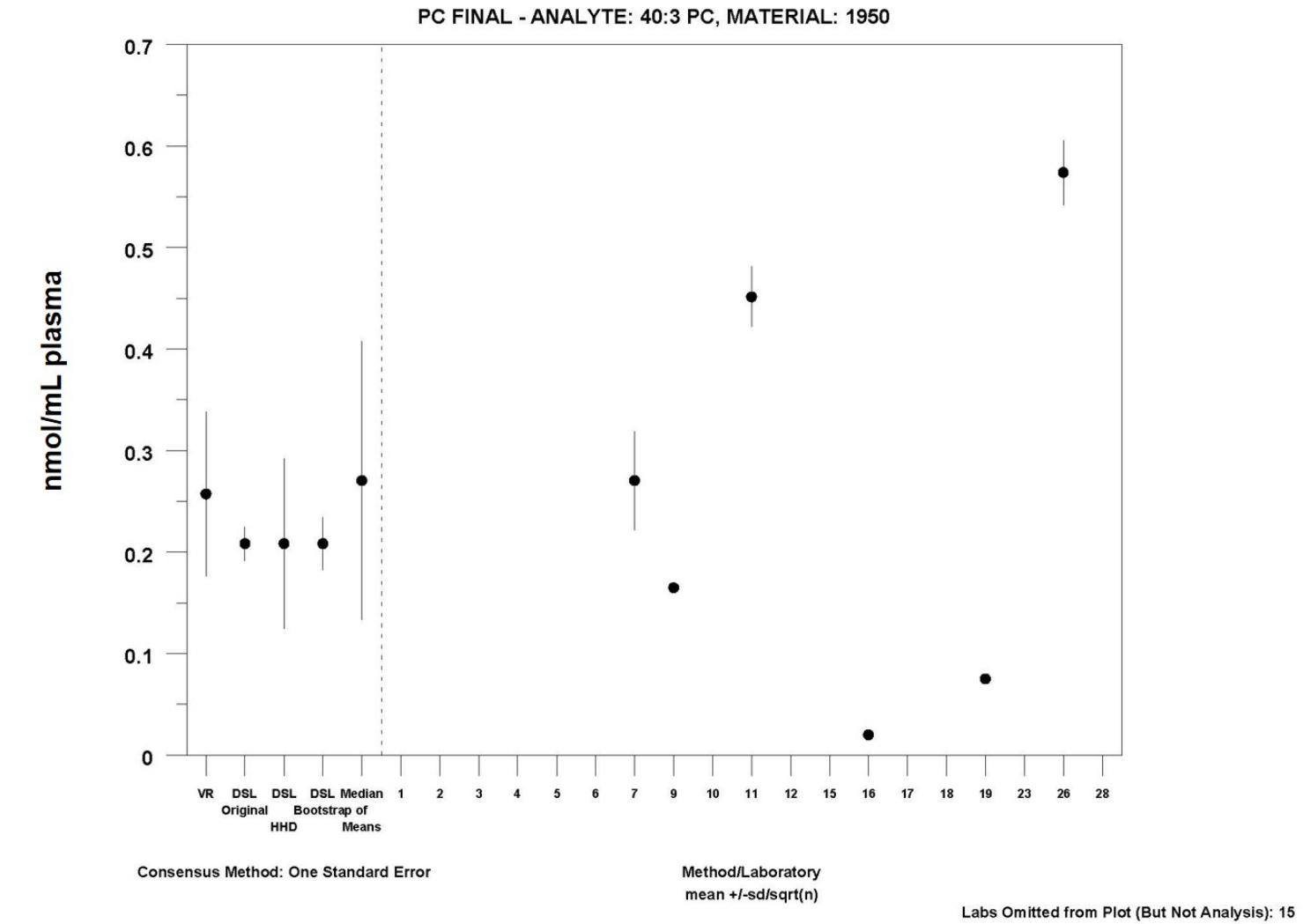


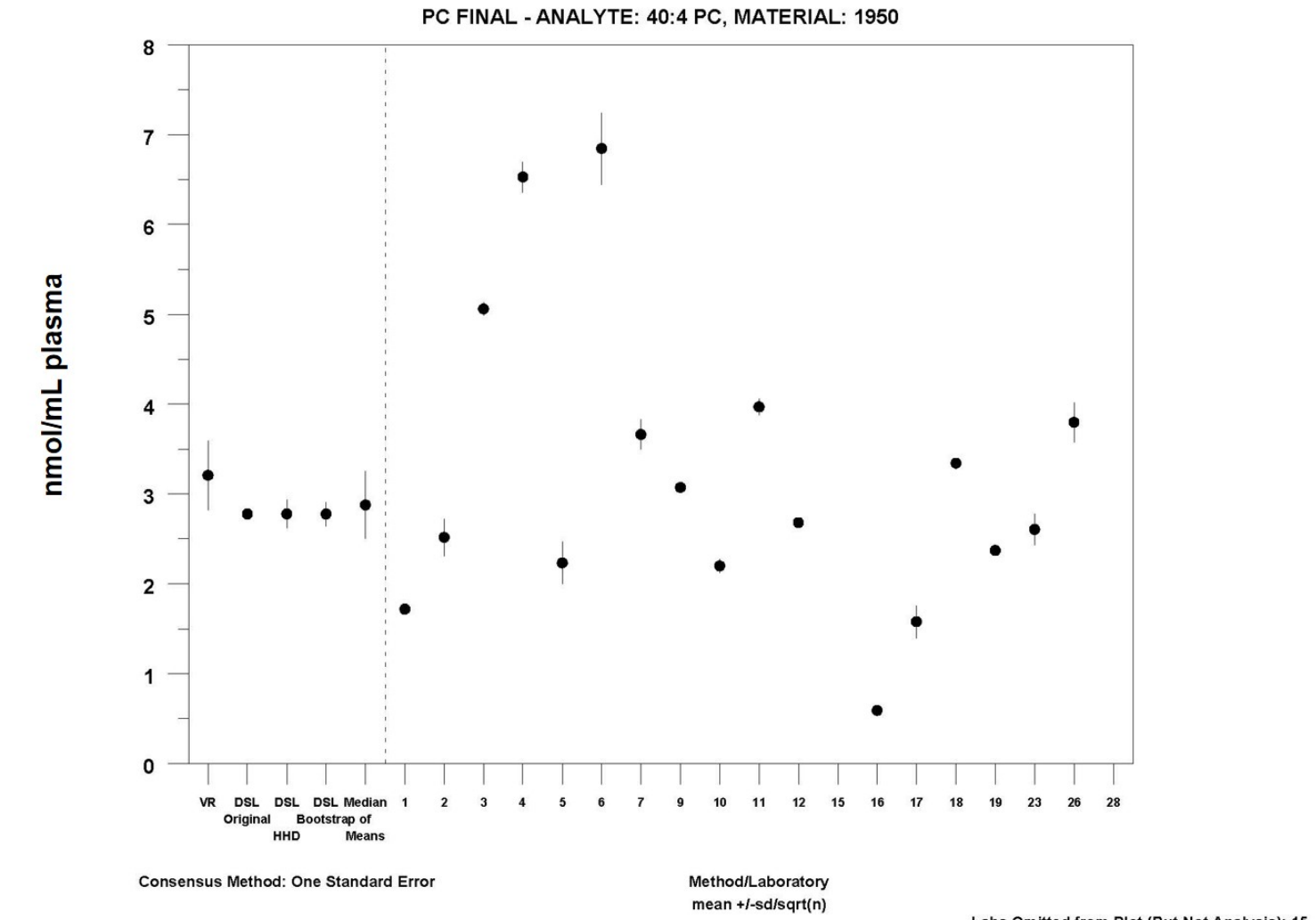


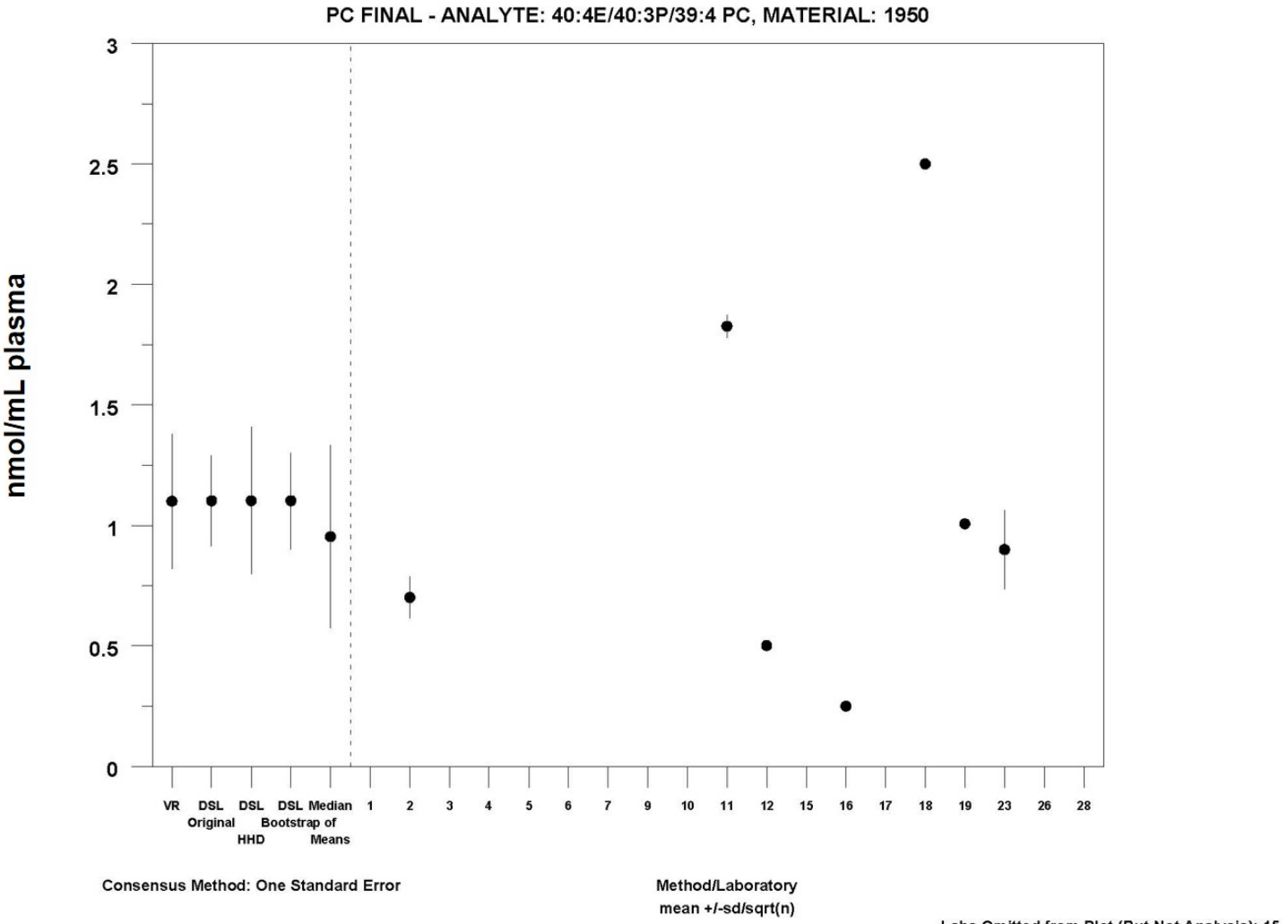
MEDM Location: 0.23 ± 0.10 nmol/mL

15: 20 ± 4



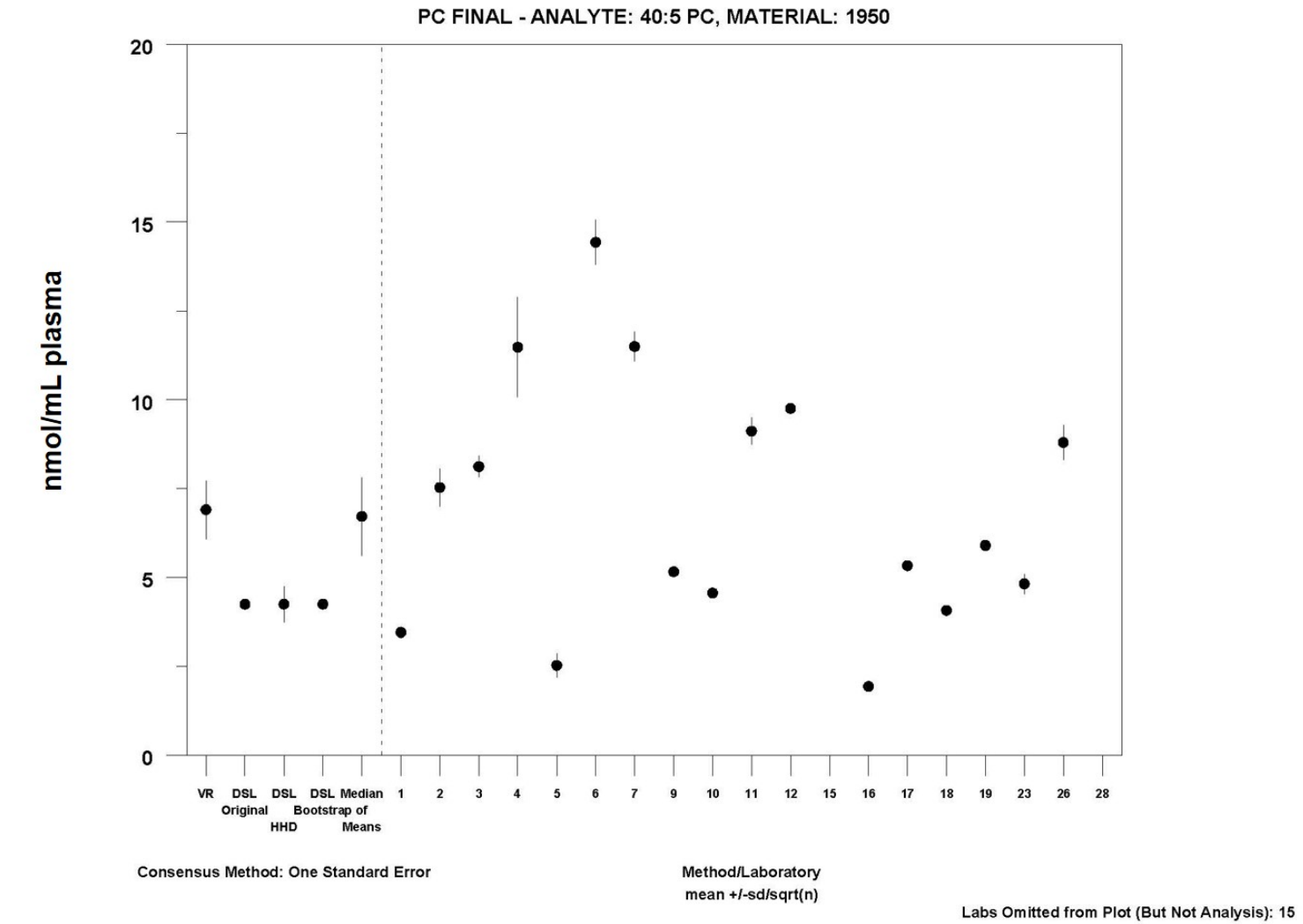


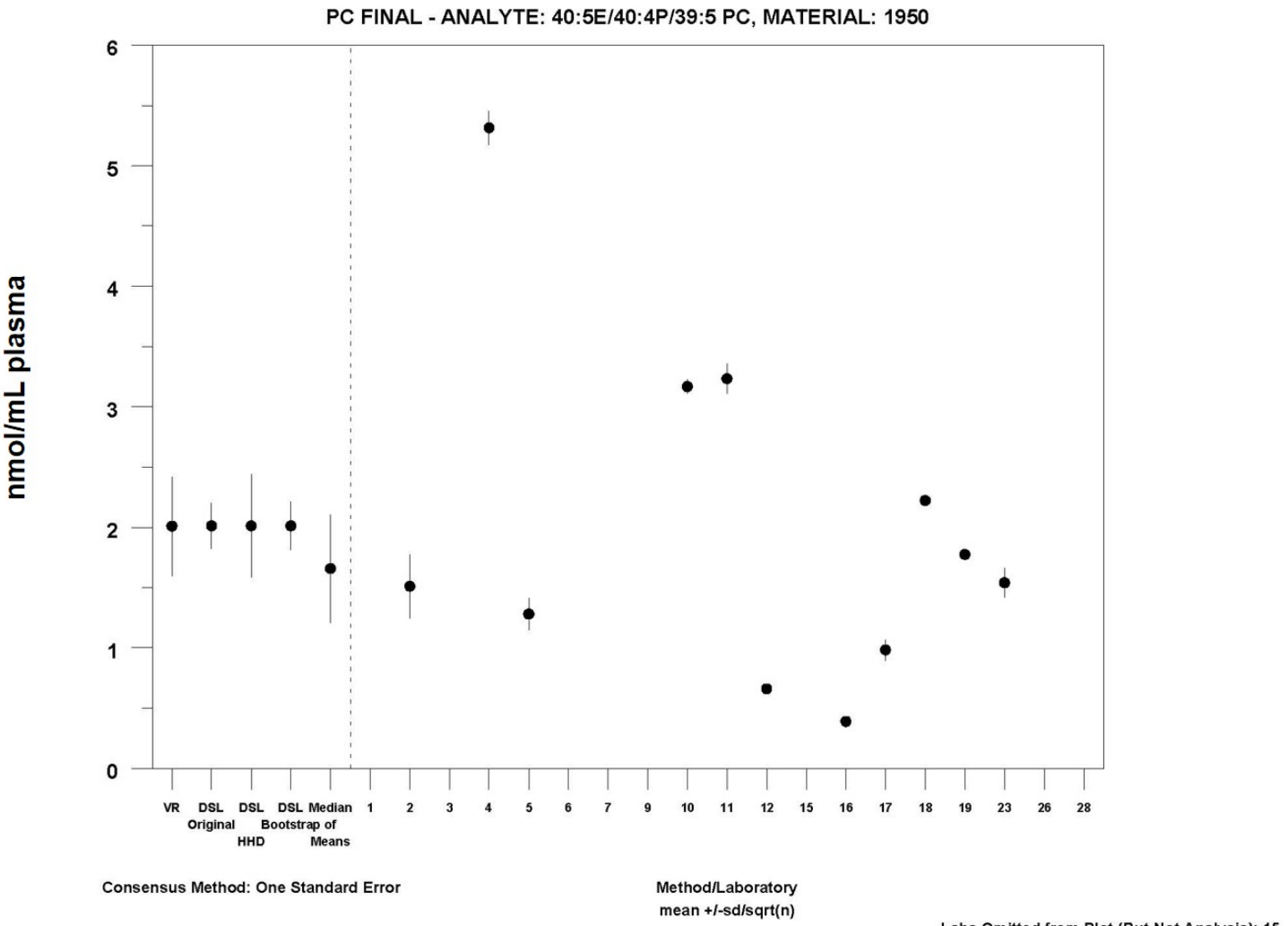


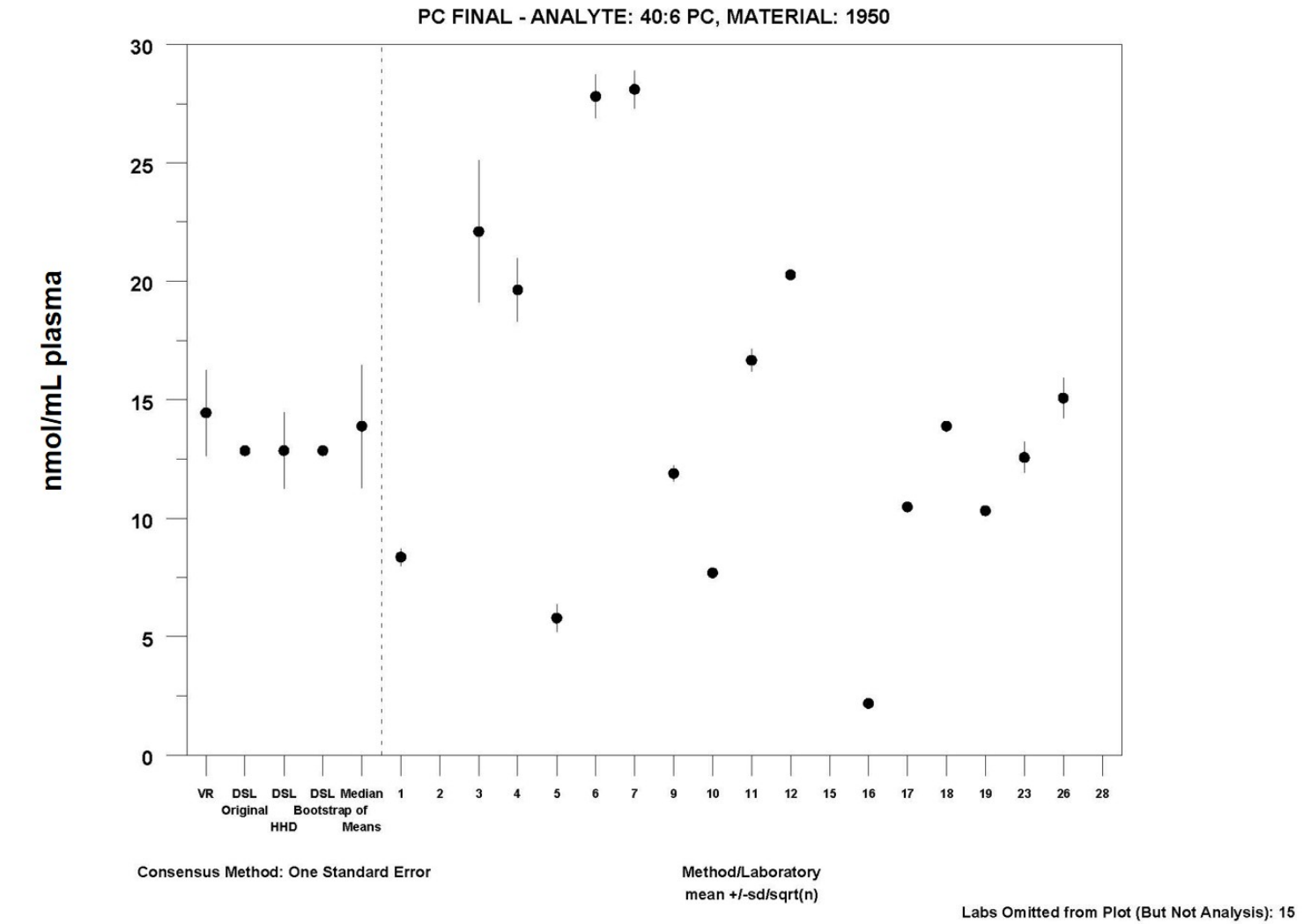


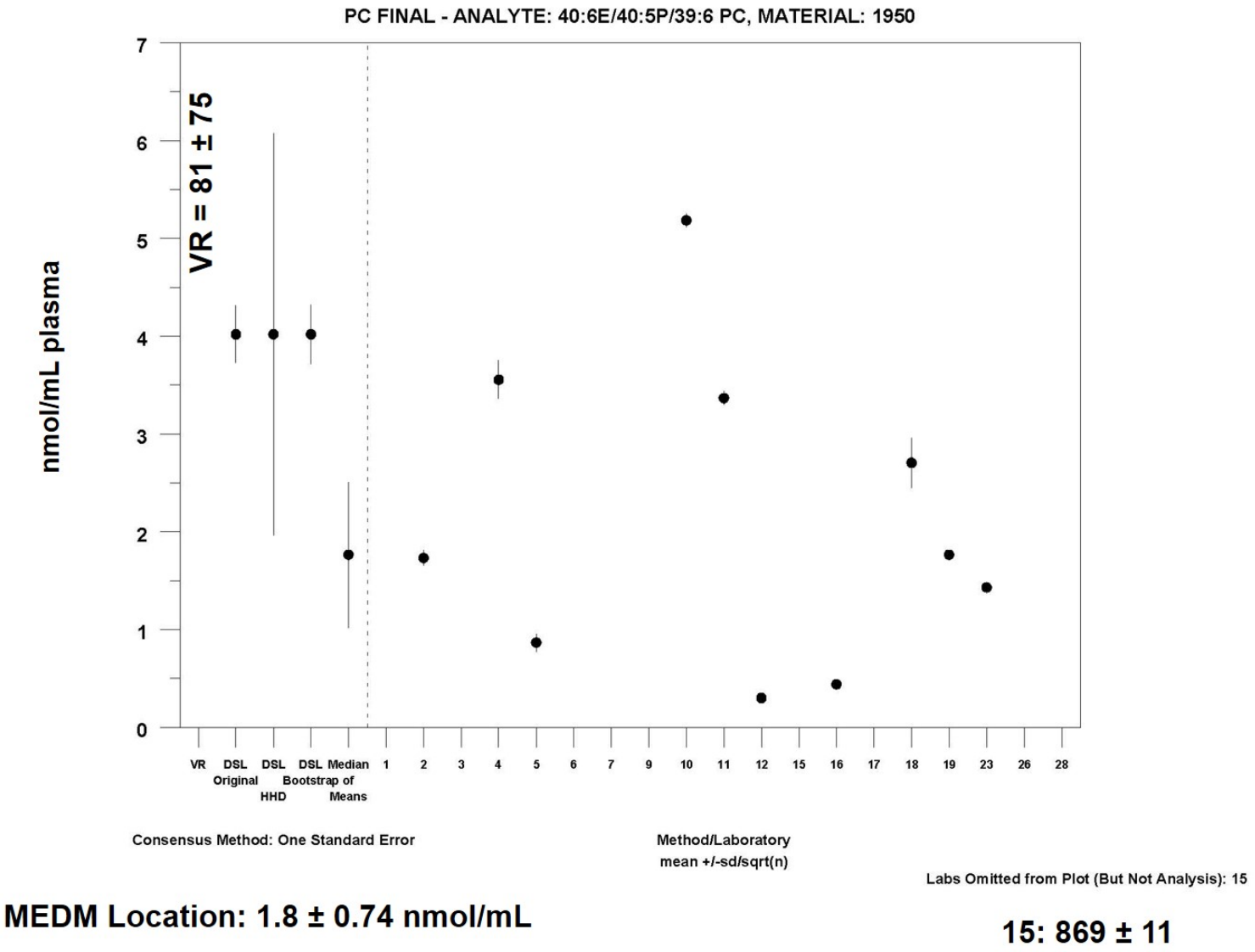
MEDM Location: 0.95 ± 0.38 nmol/mL

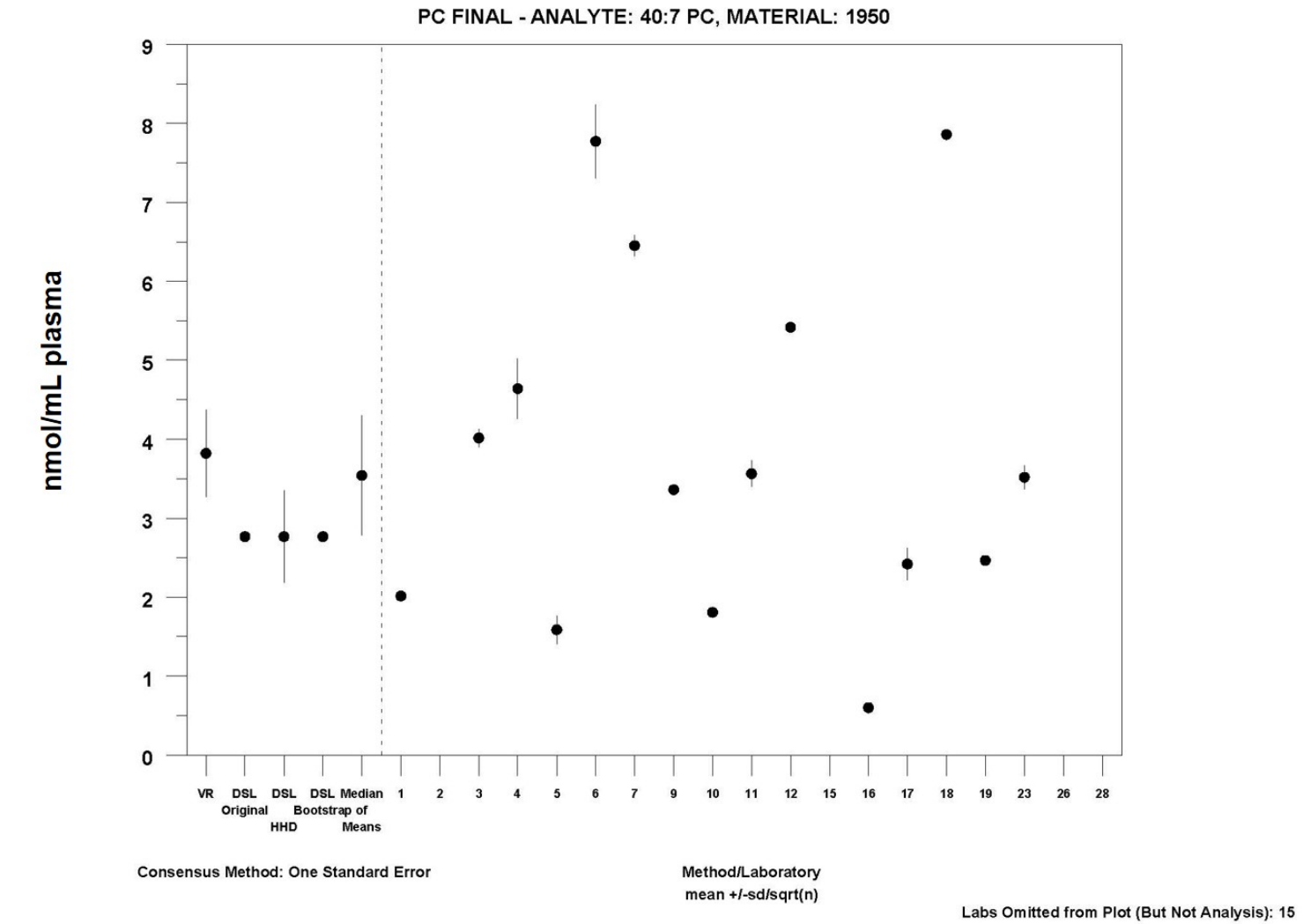
15: 491 ± 273

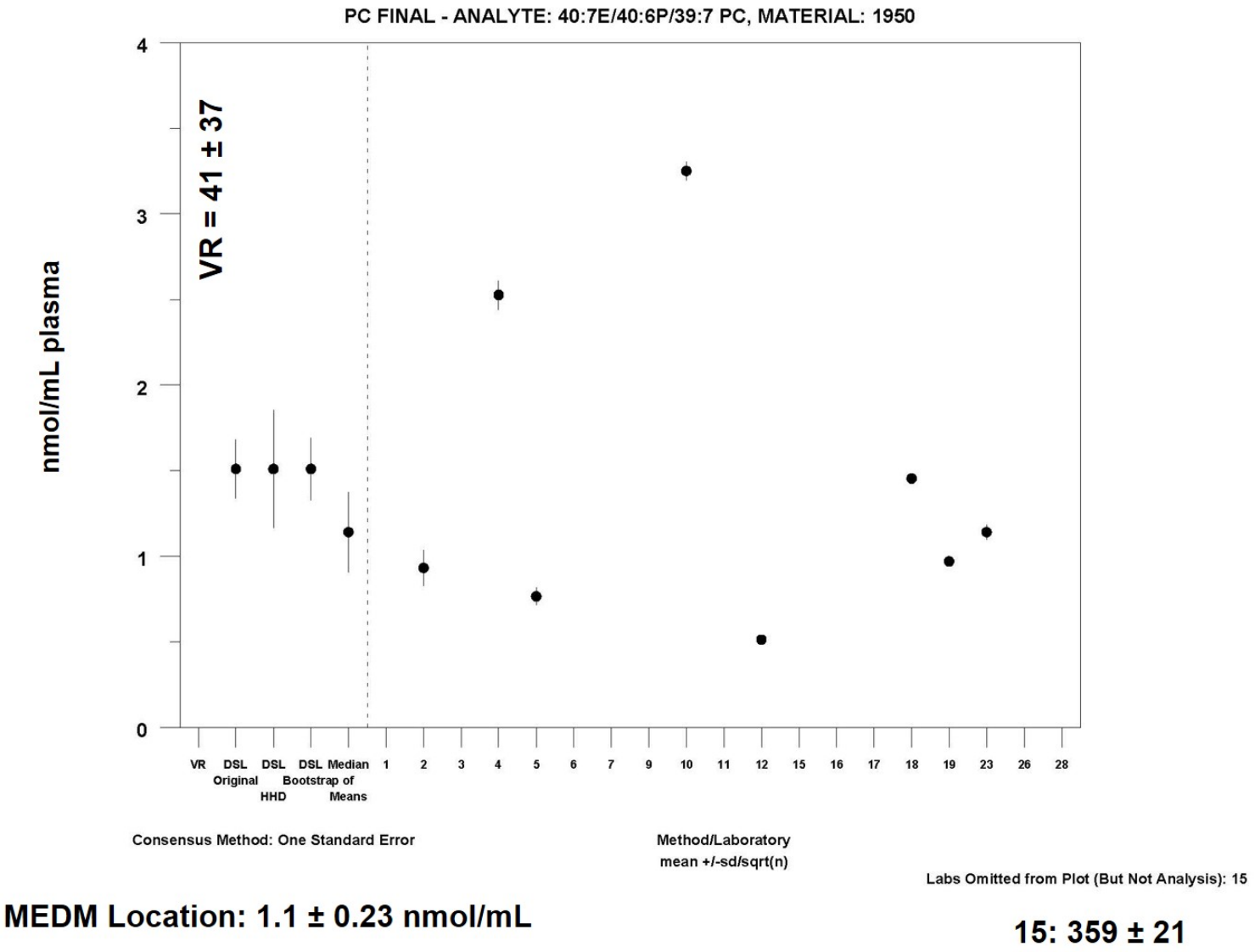


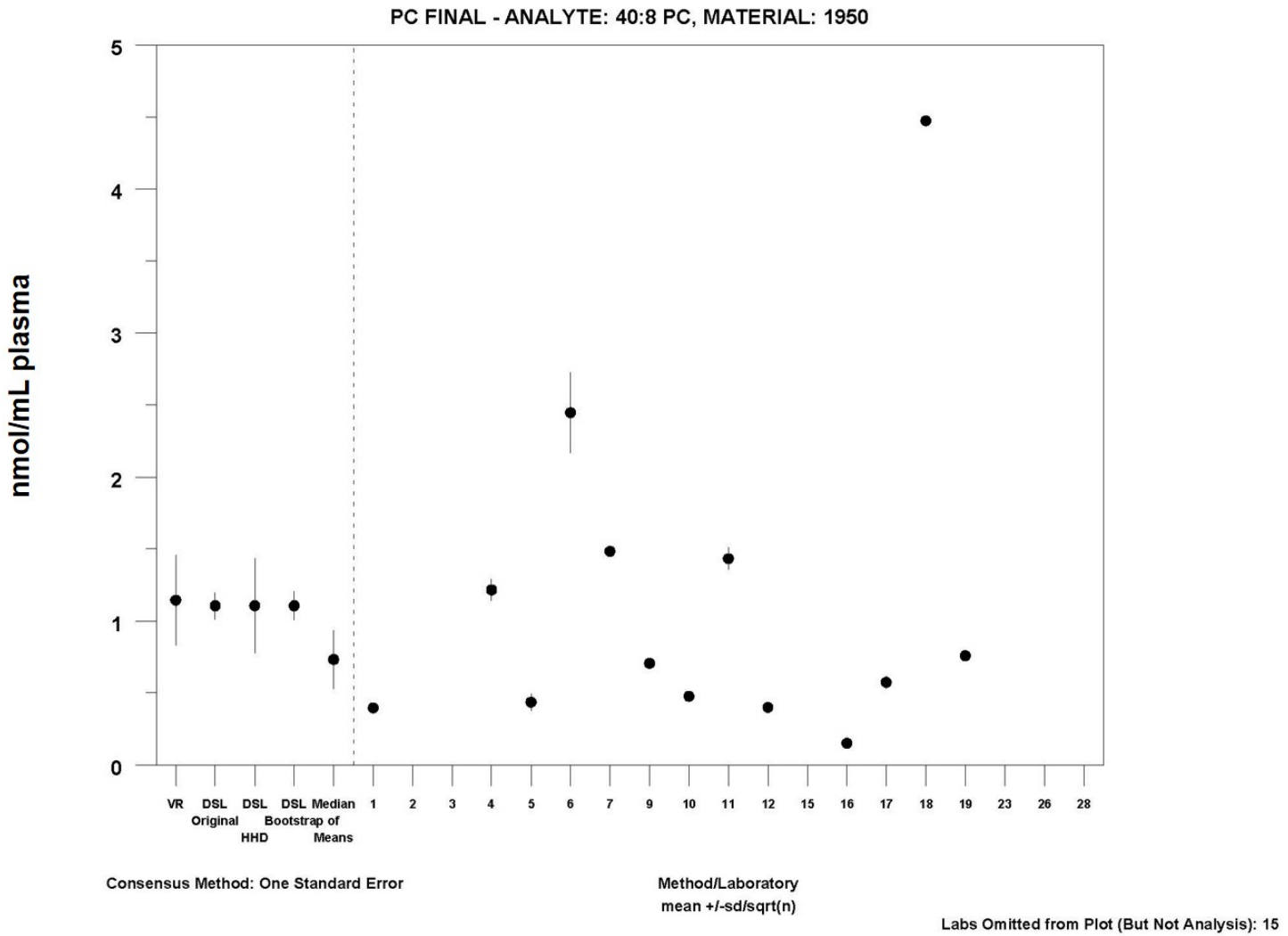


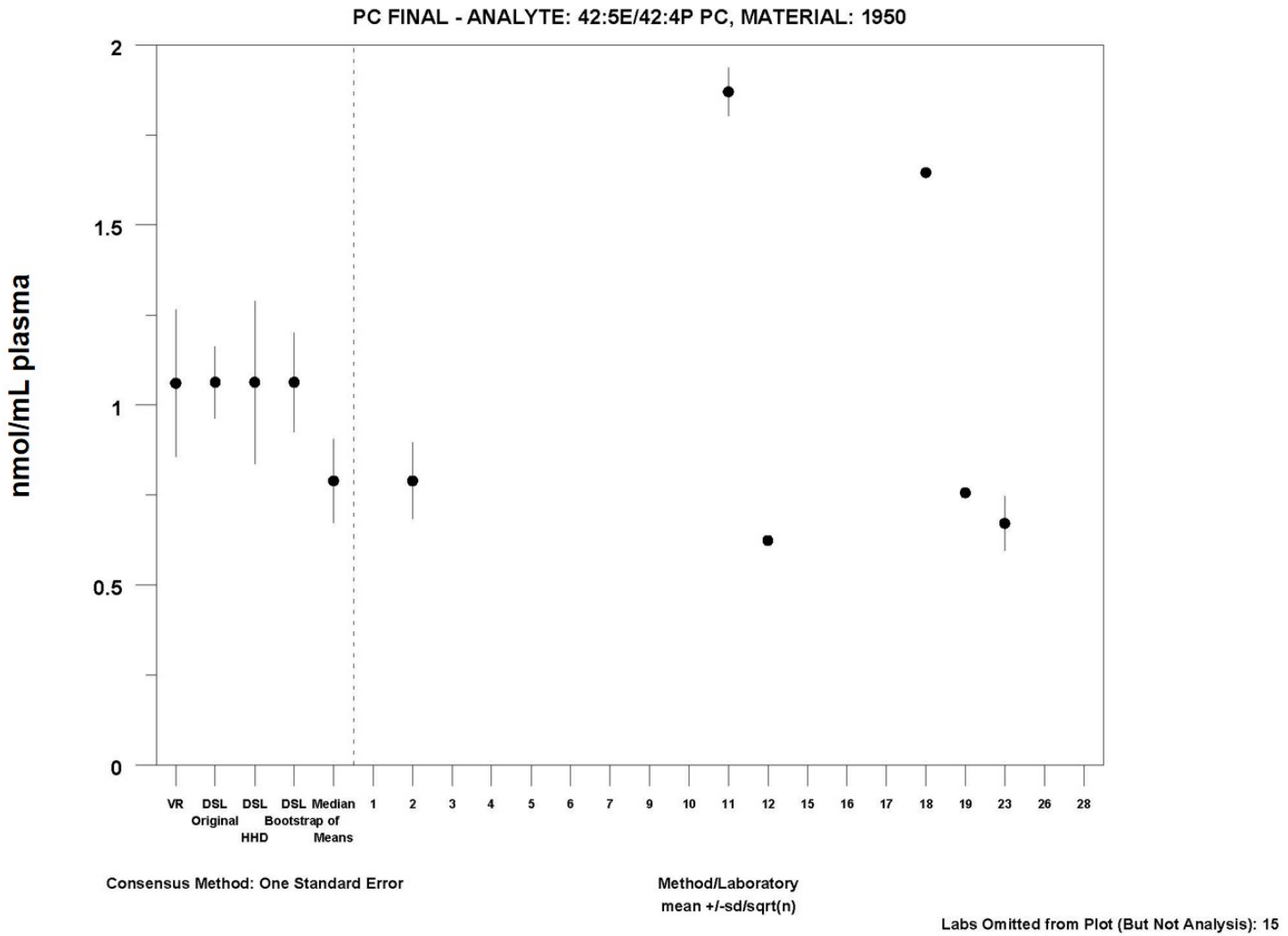


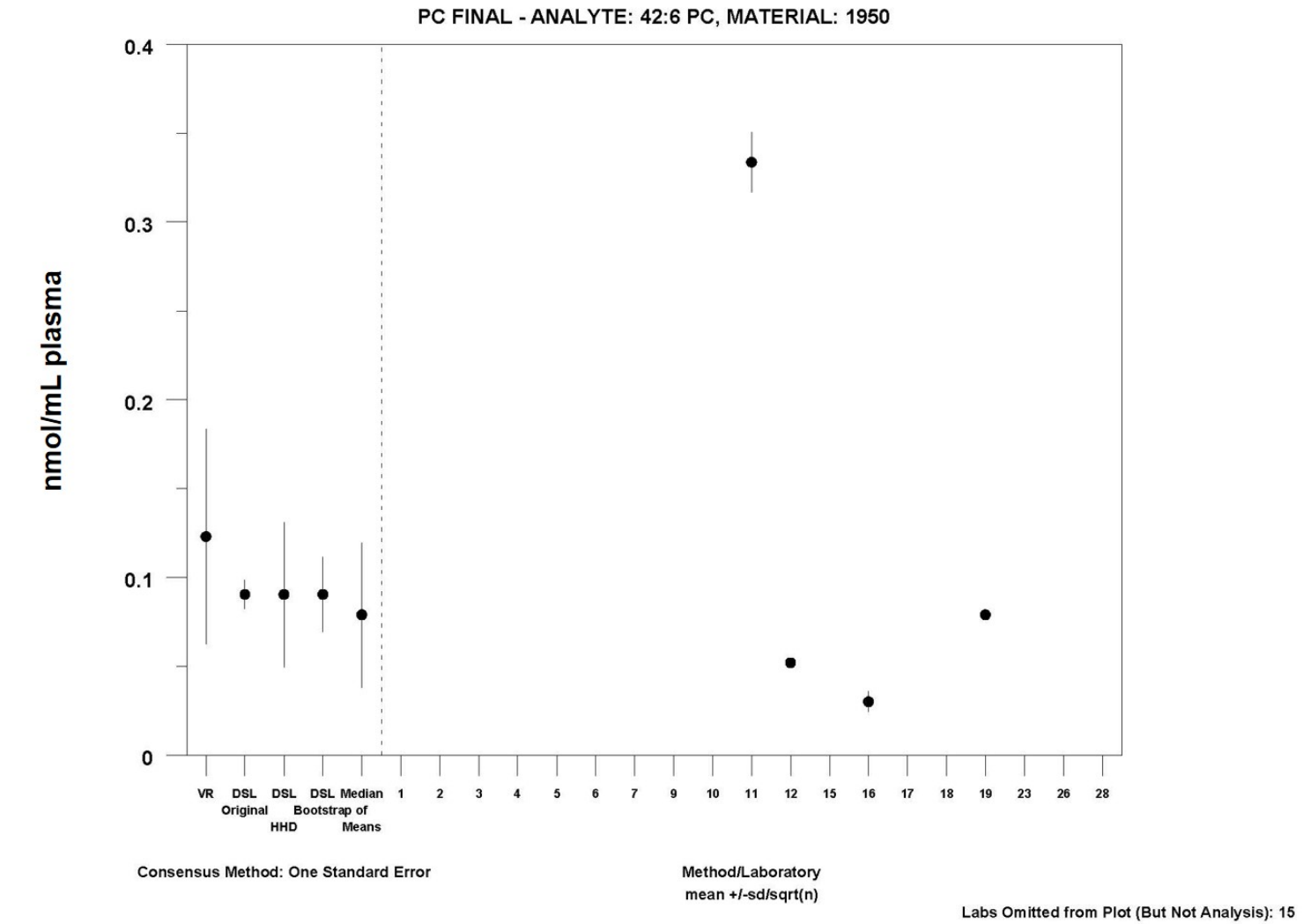


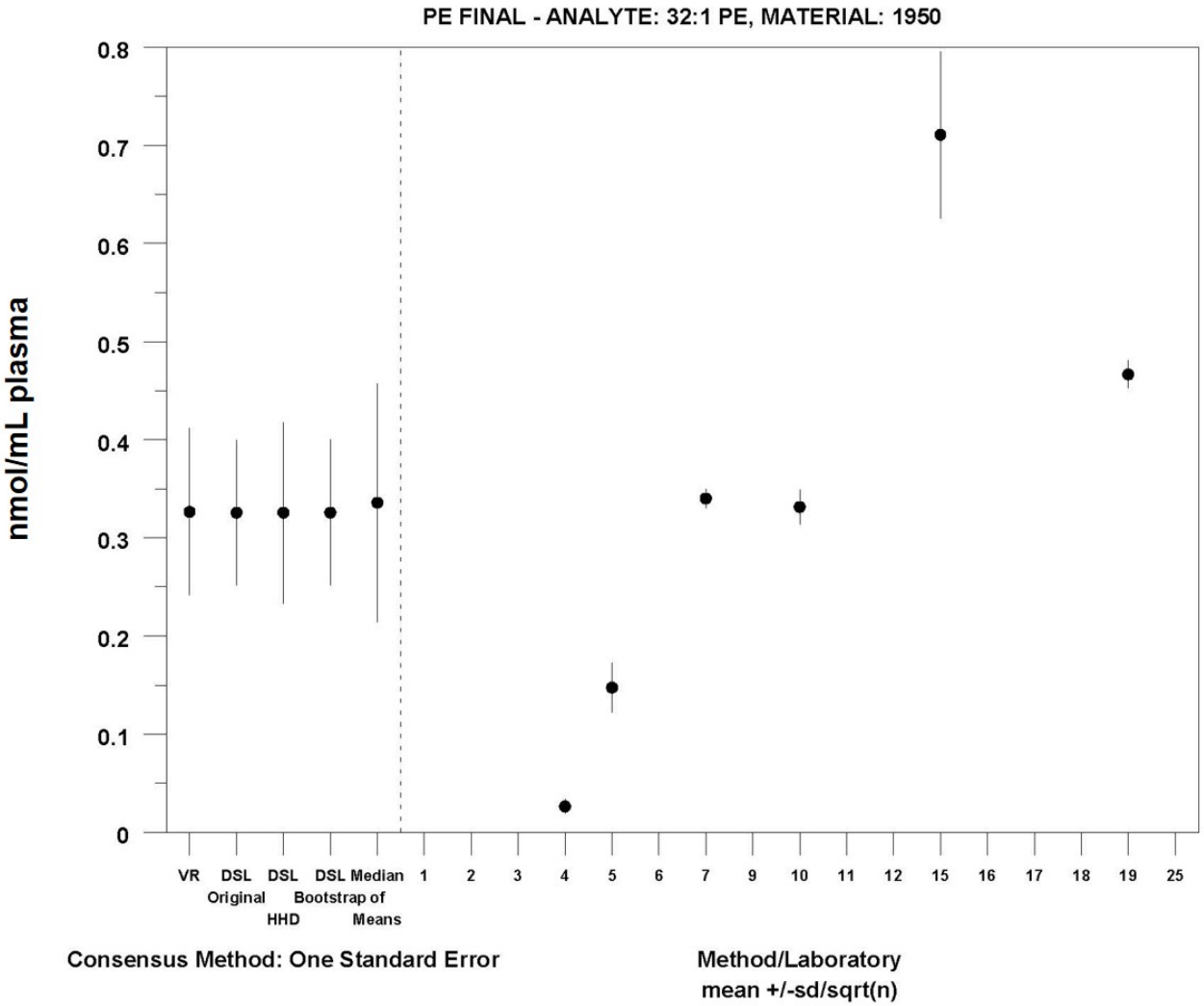




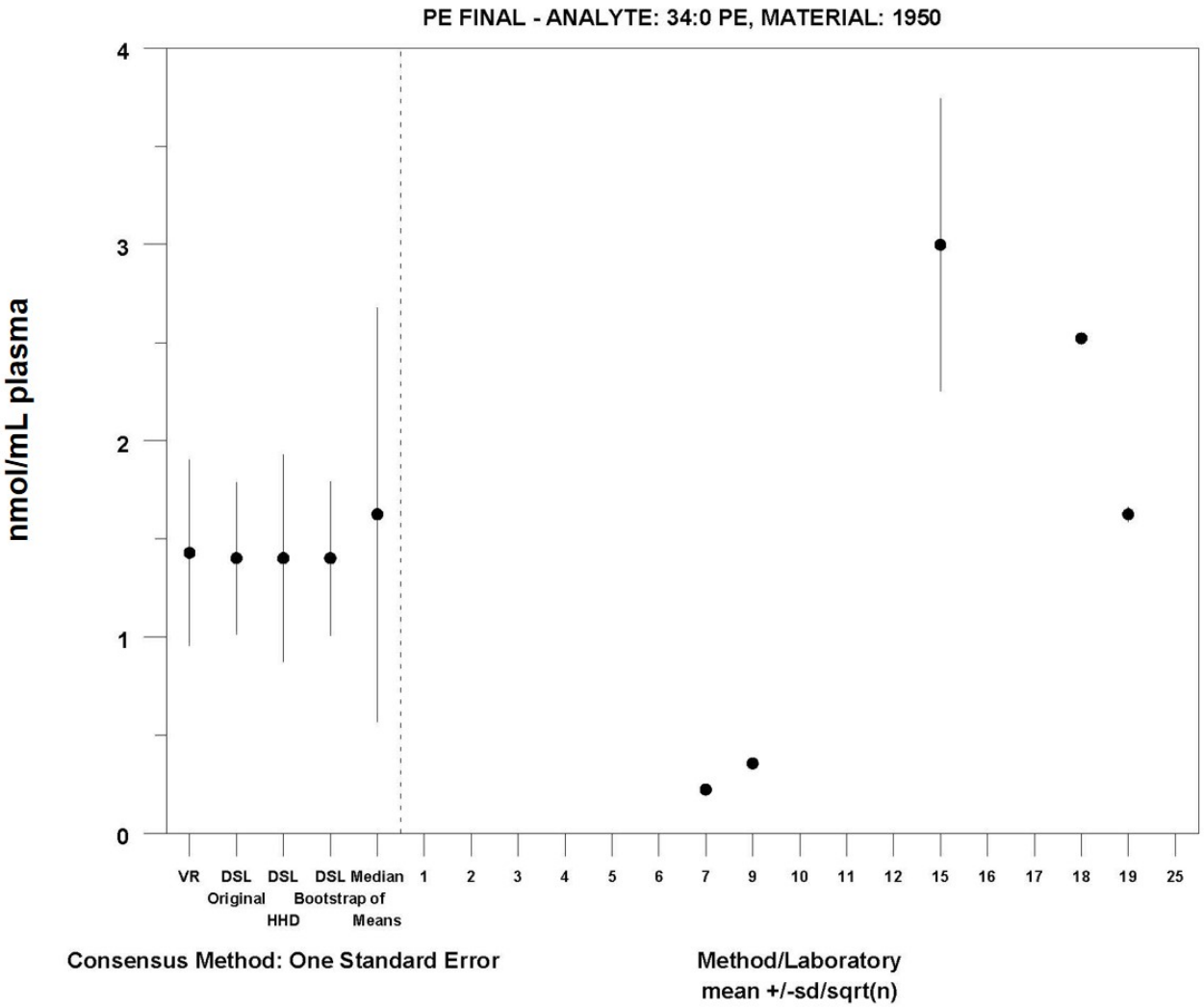




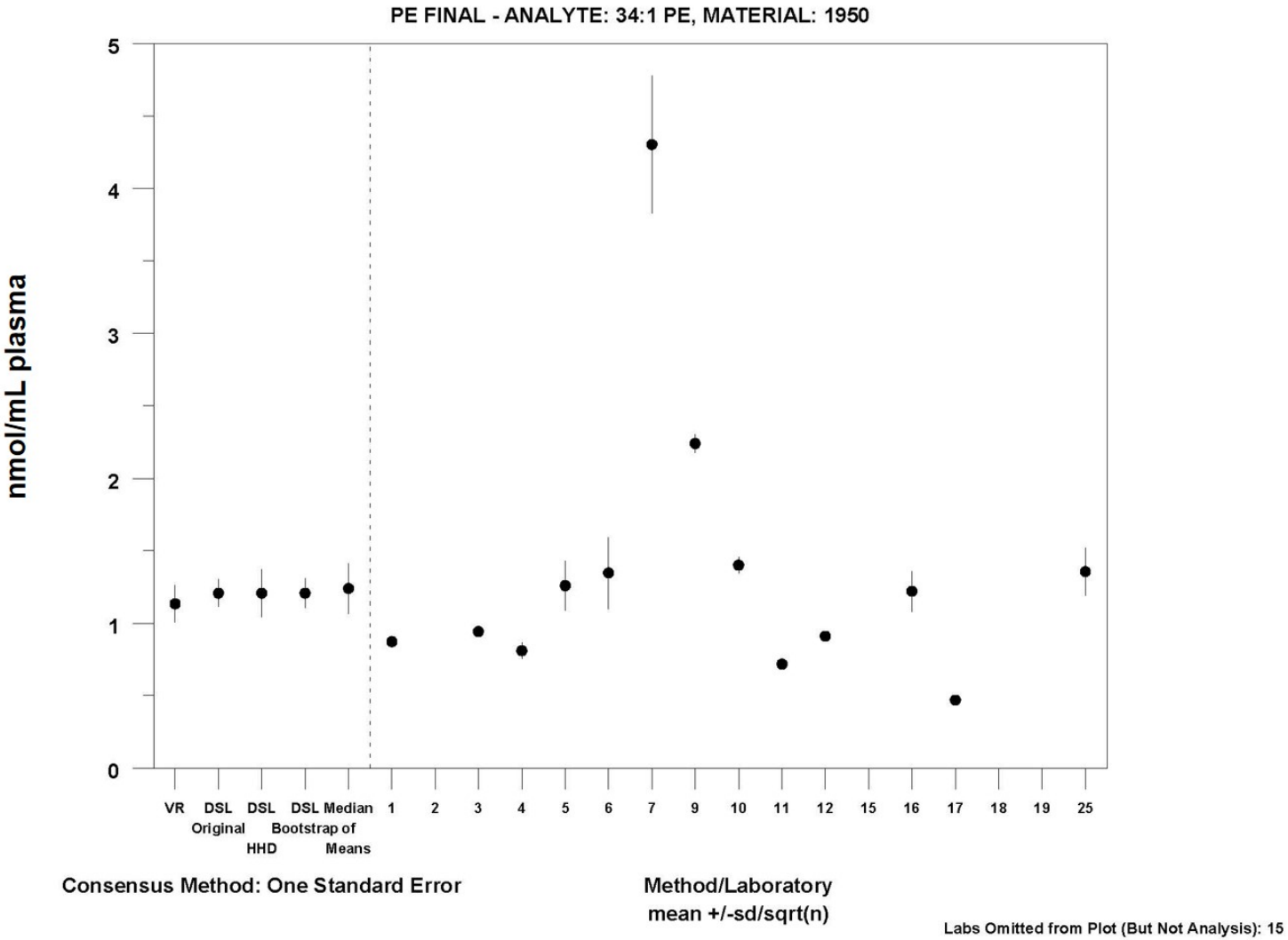


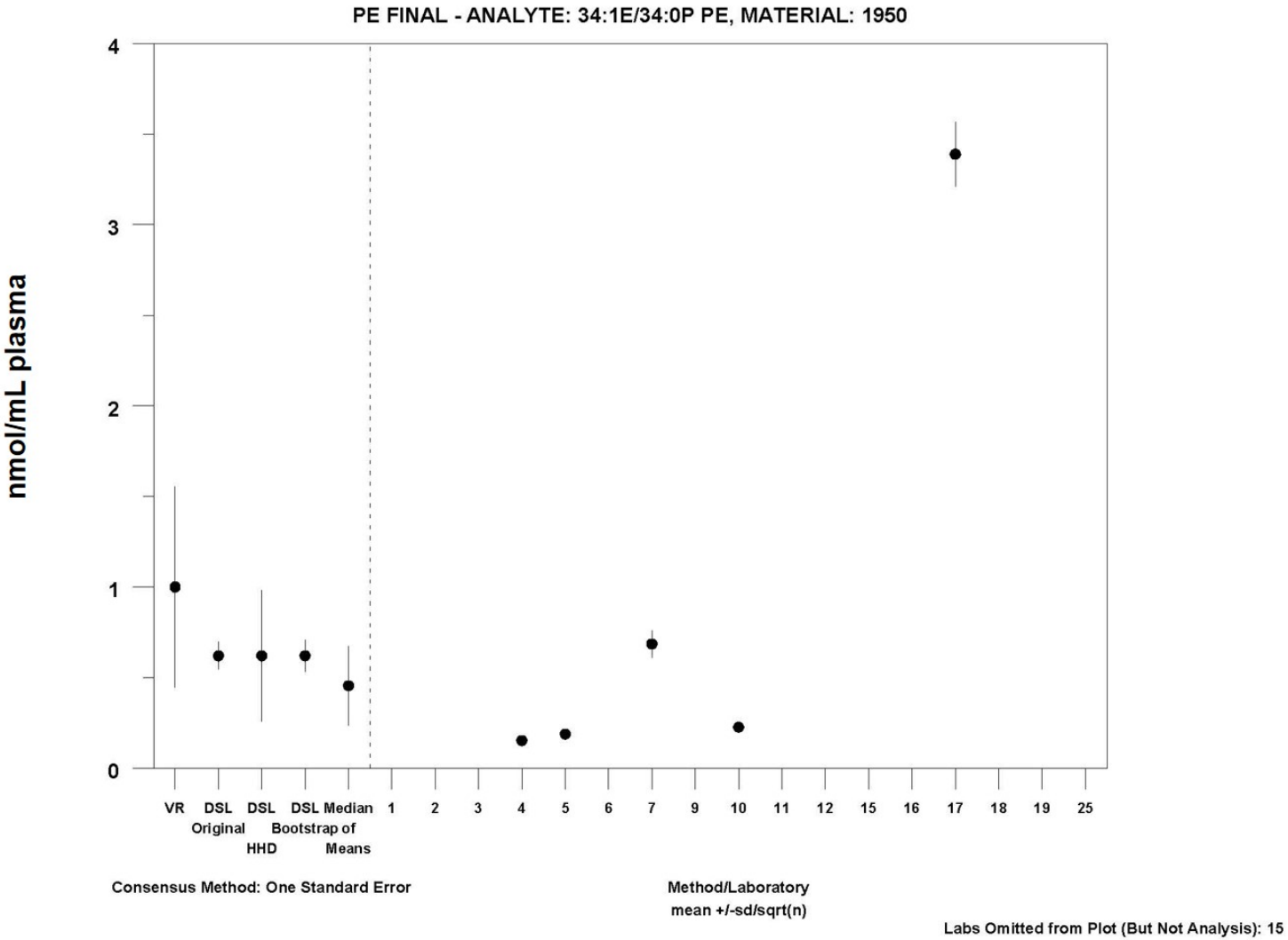


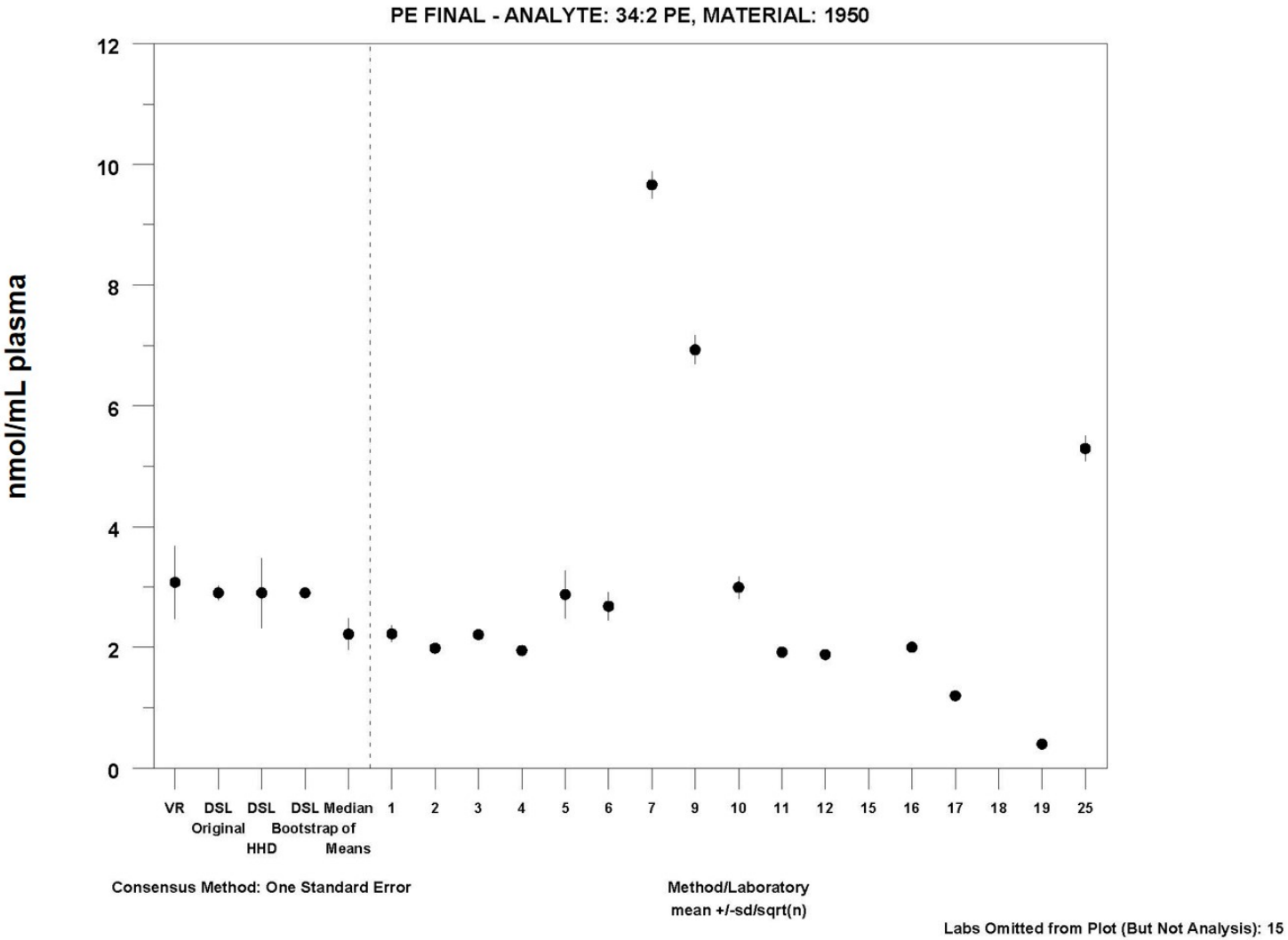
MEDM Location: 0.34 ± 0.12 nmol/mL

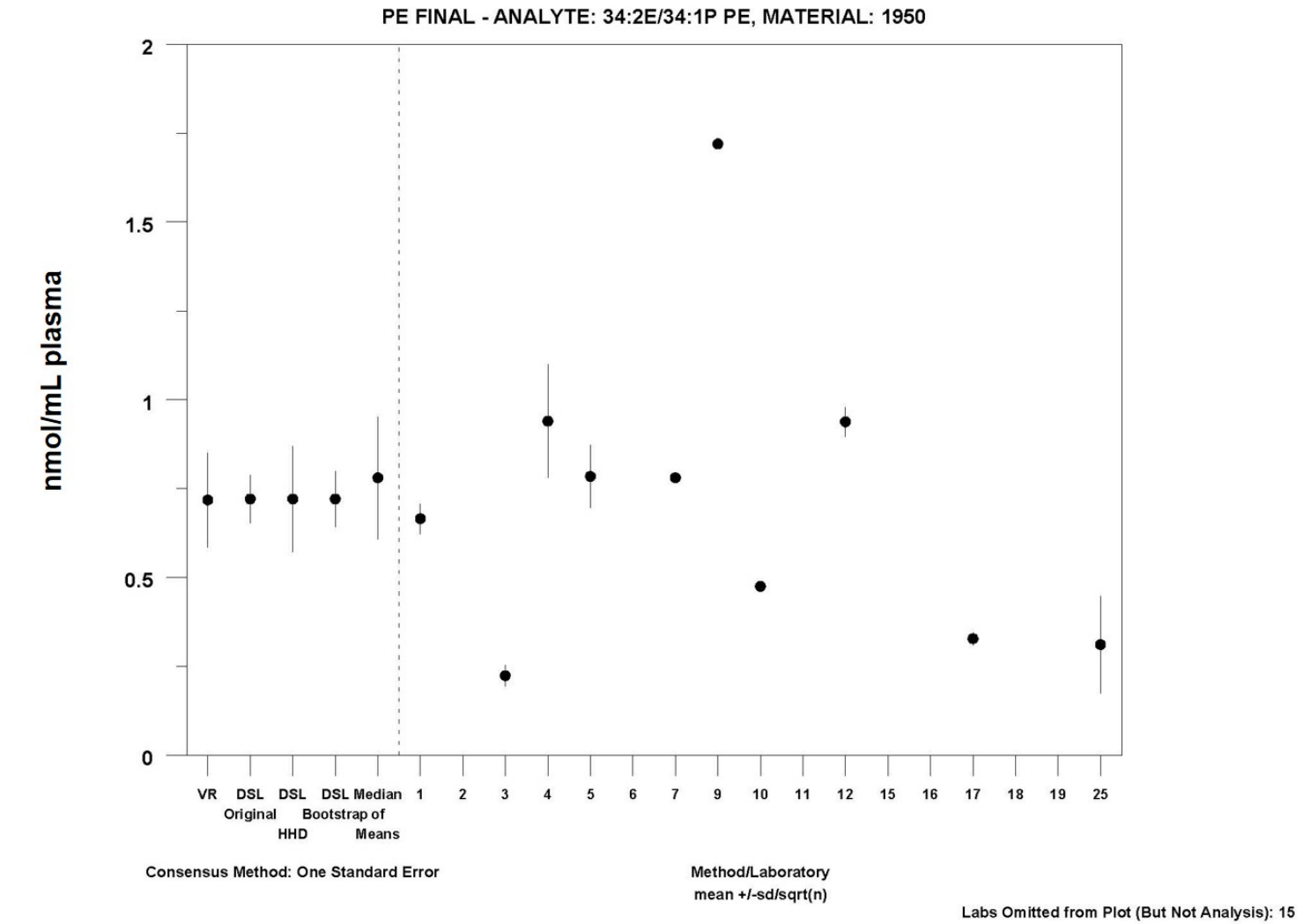


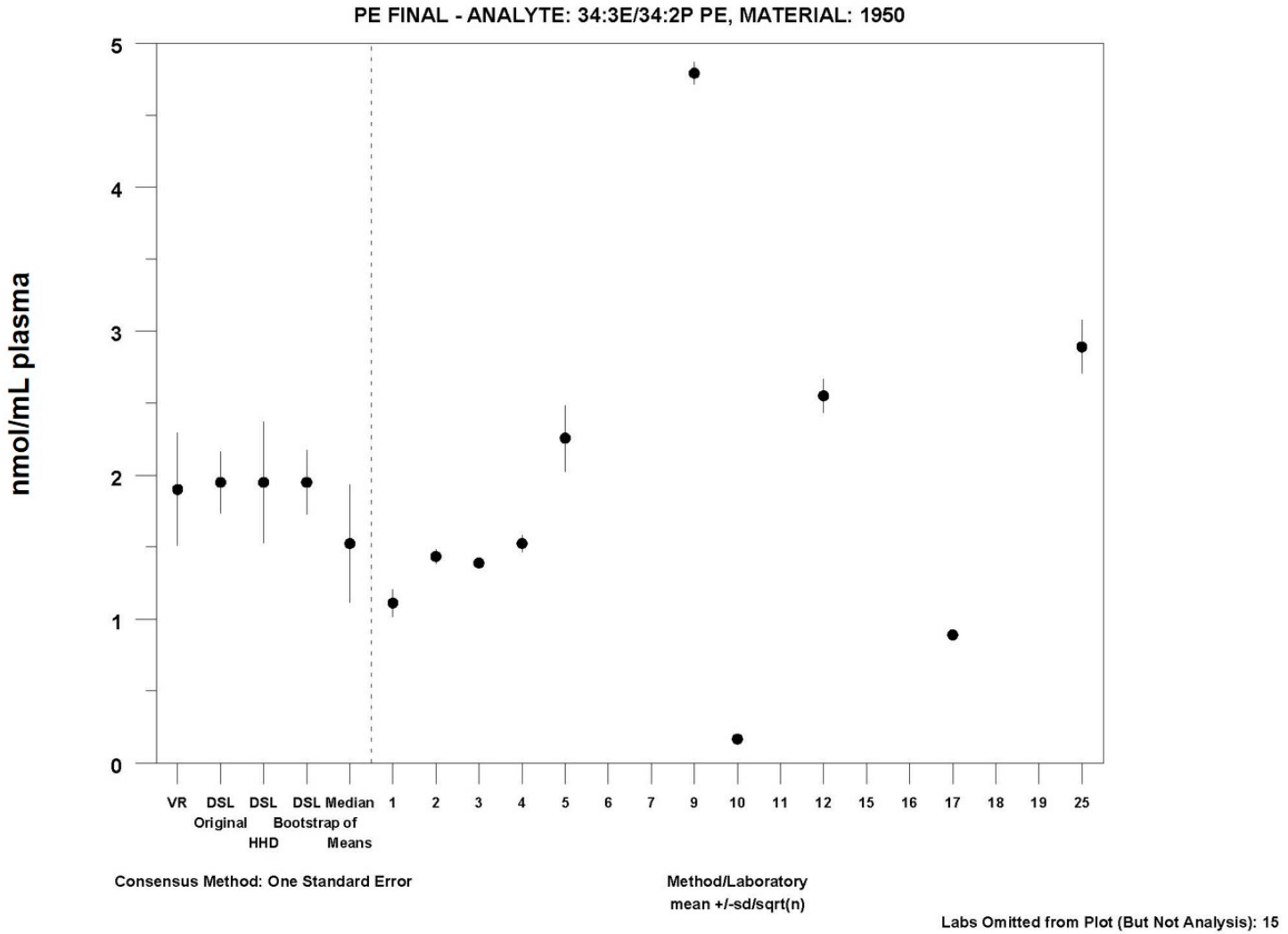
MEDM Location: 1.6 ± 1.1 nmol/mL

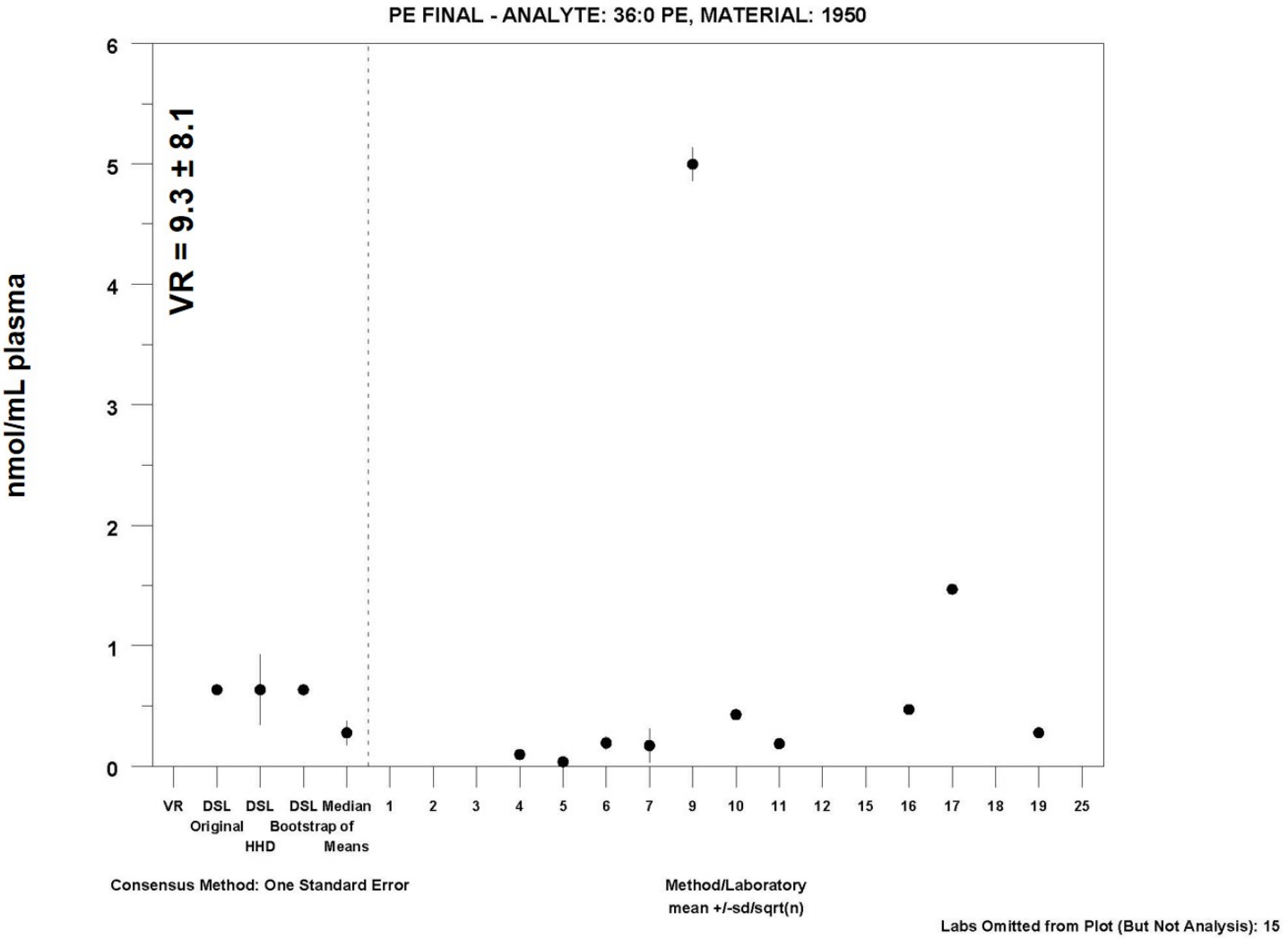


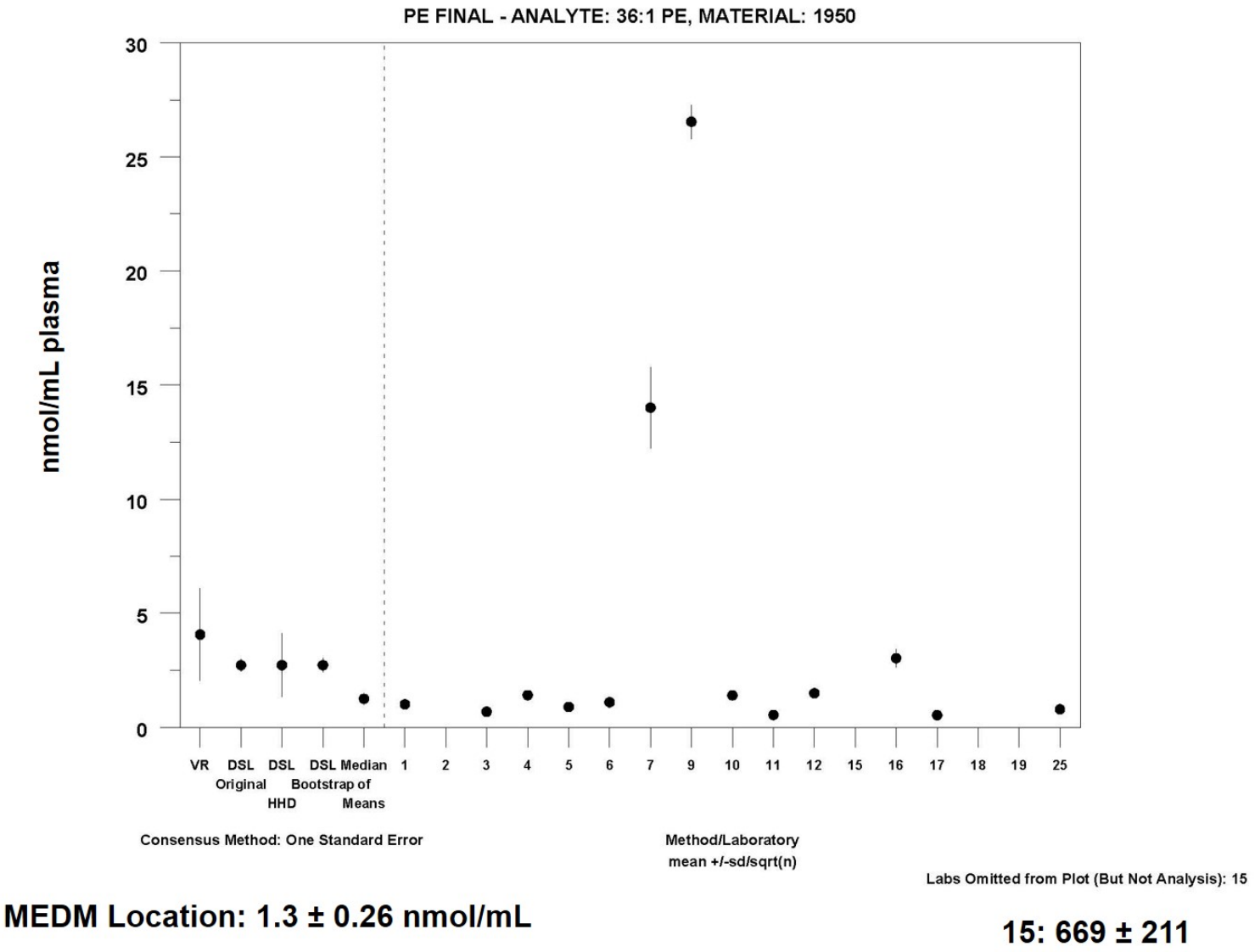


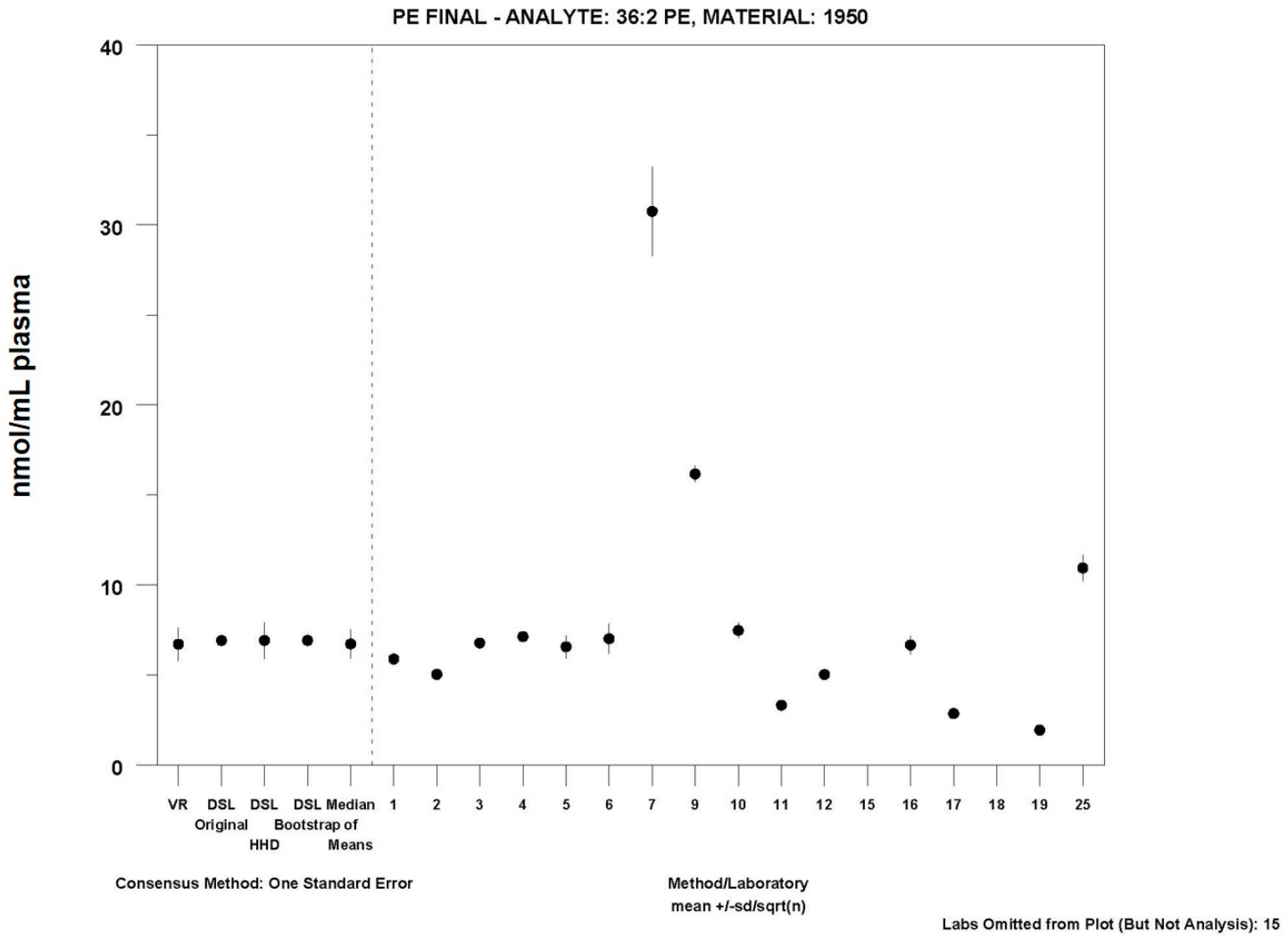


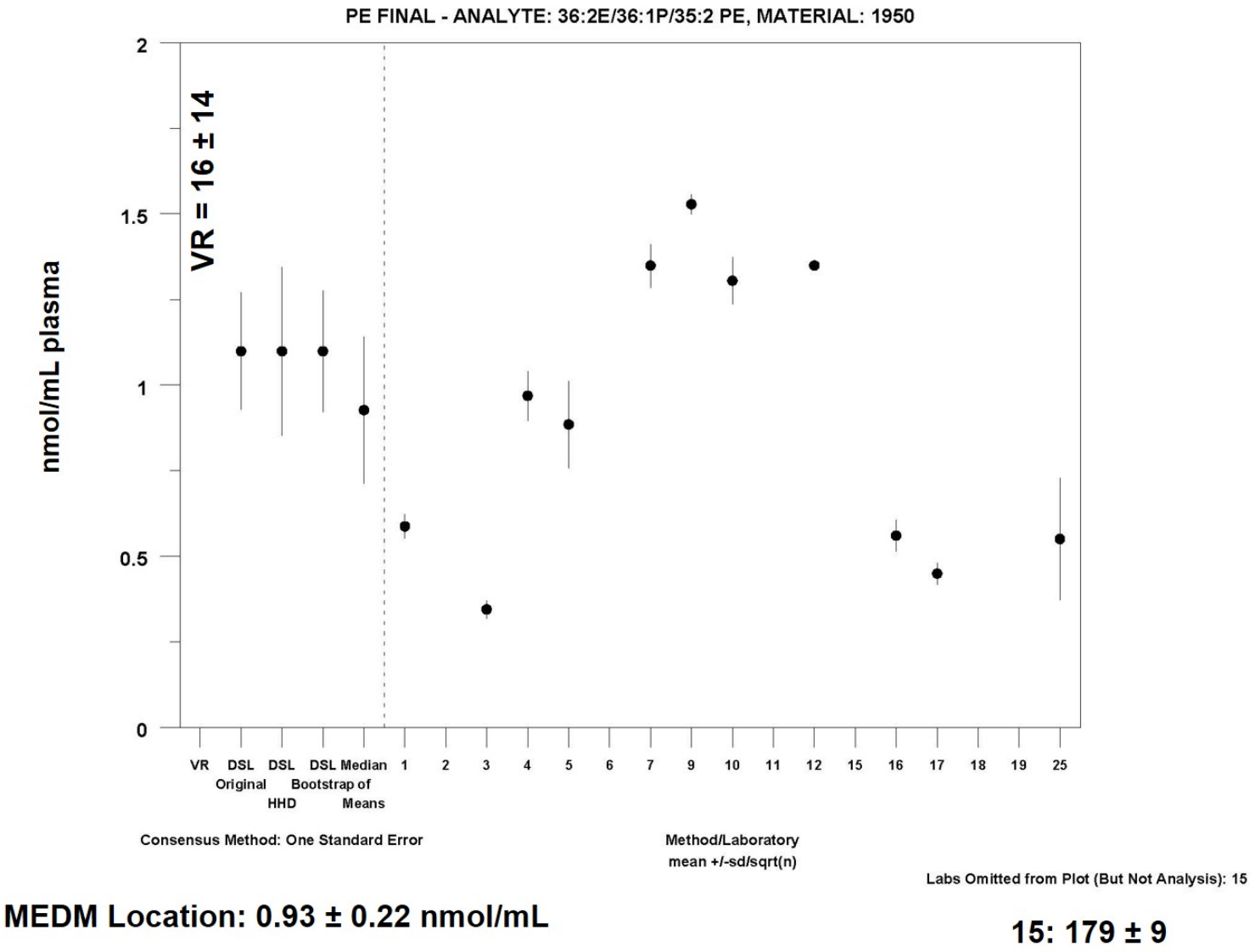


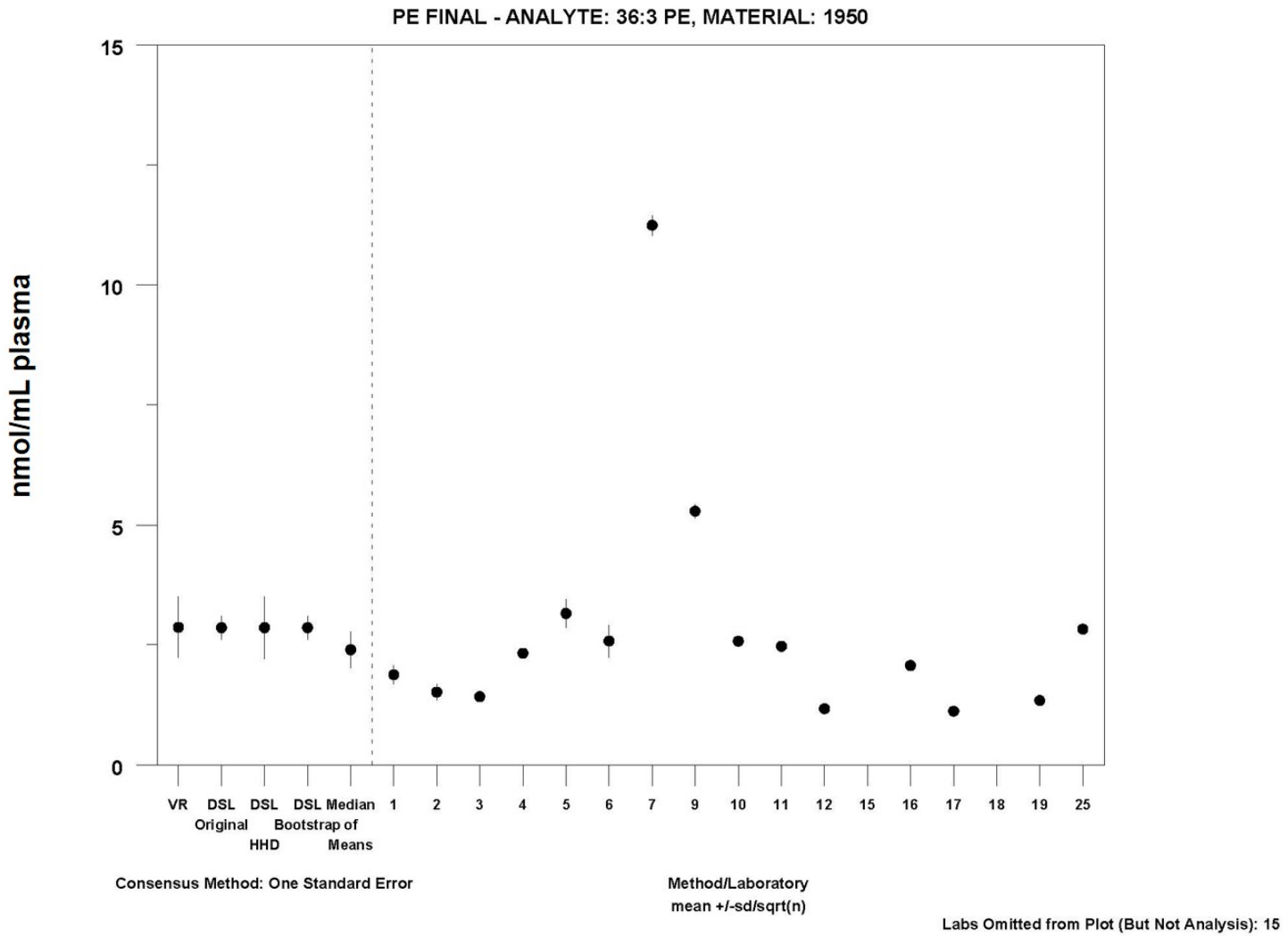


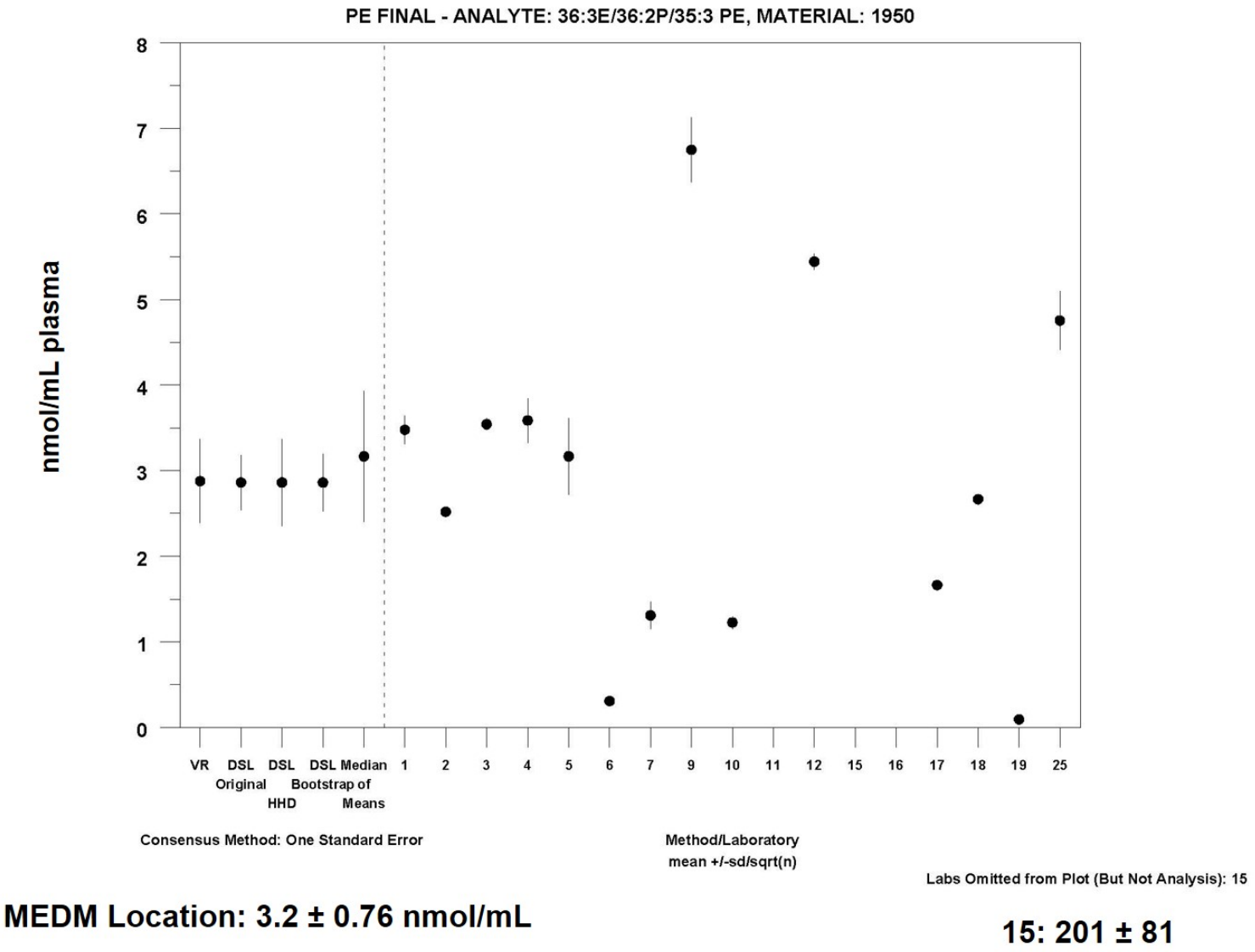


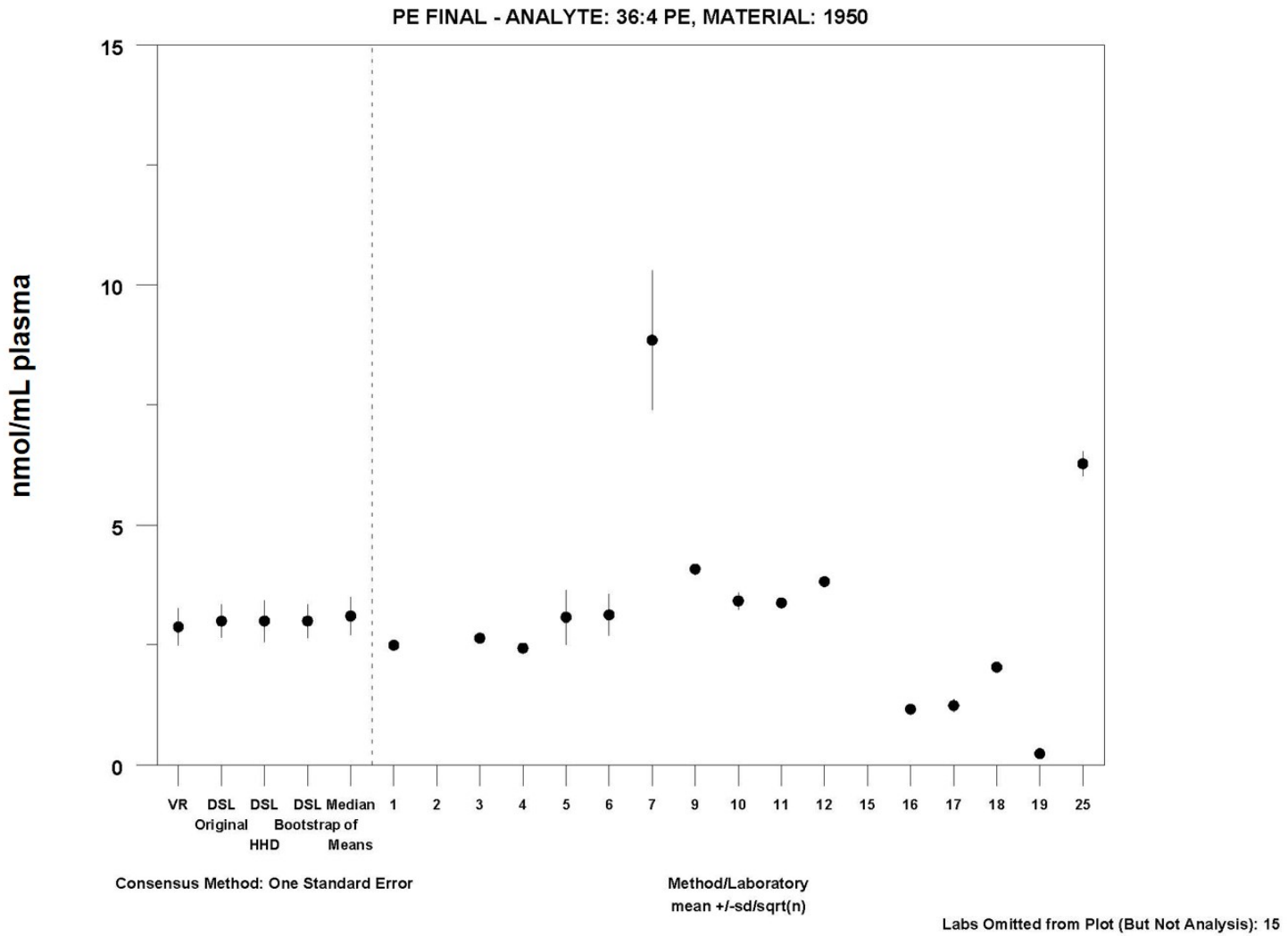


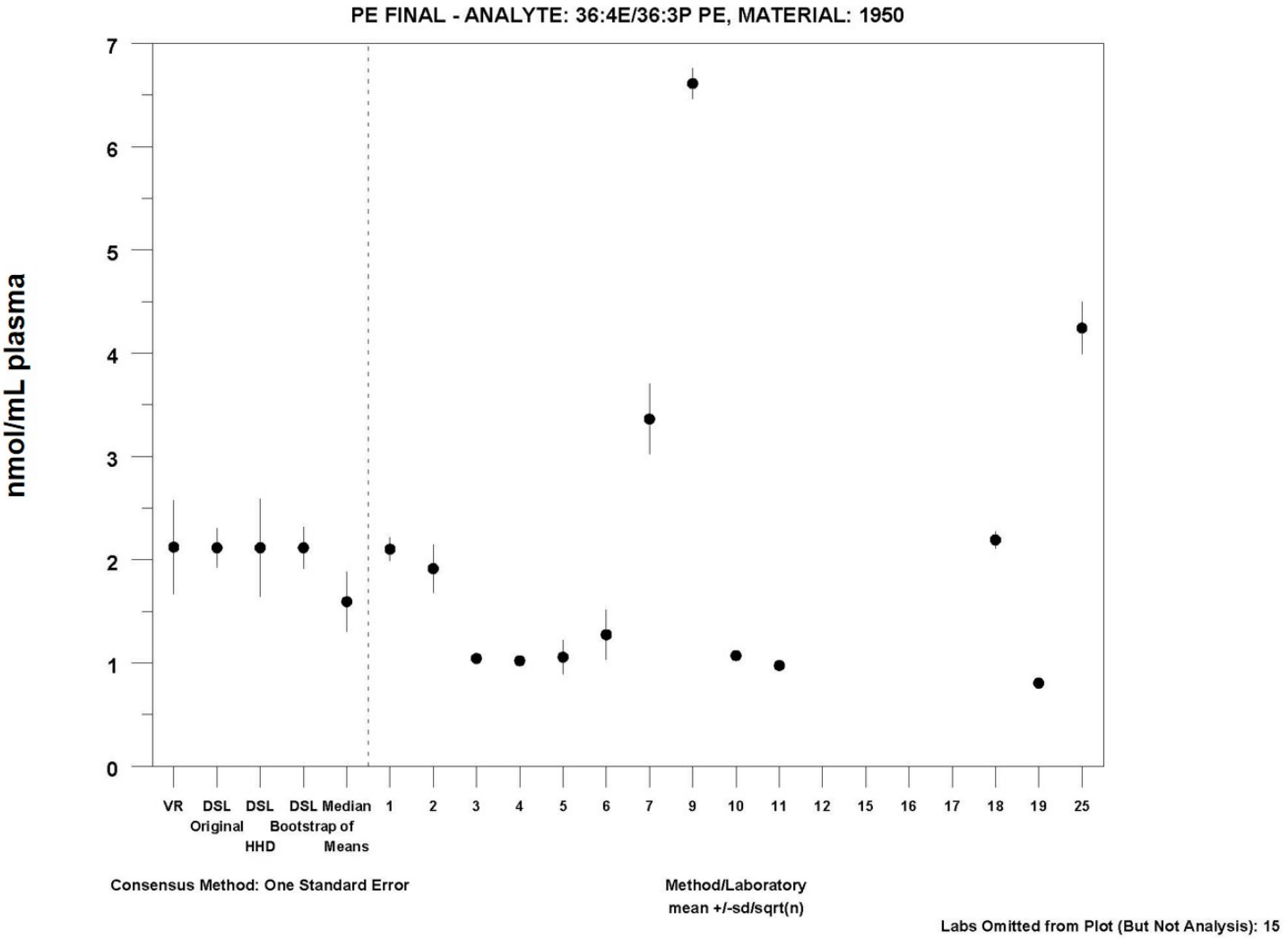


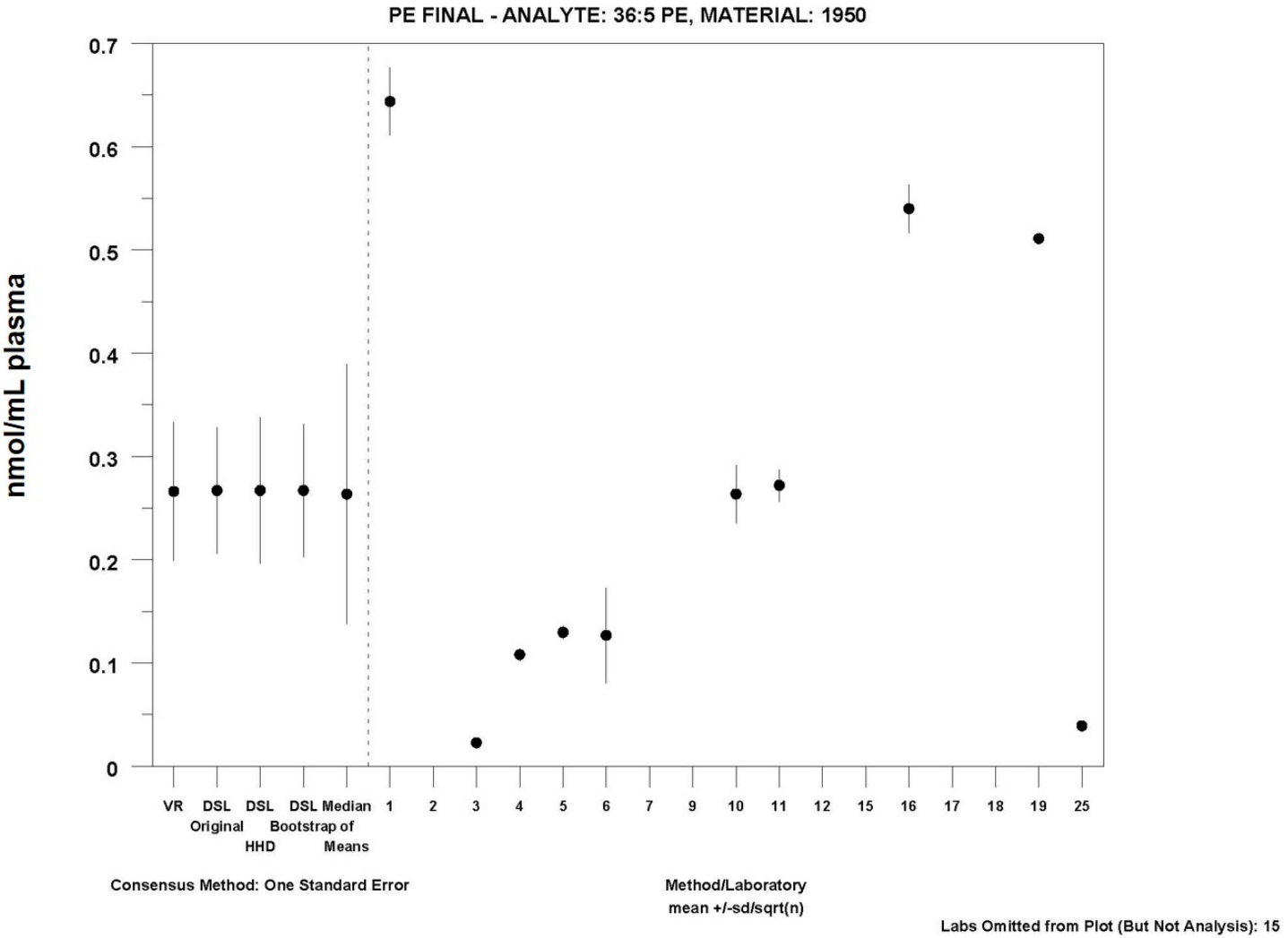


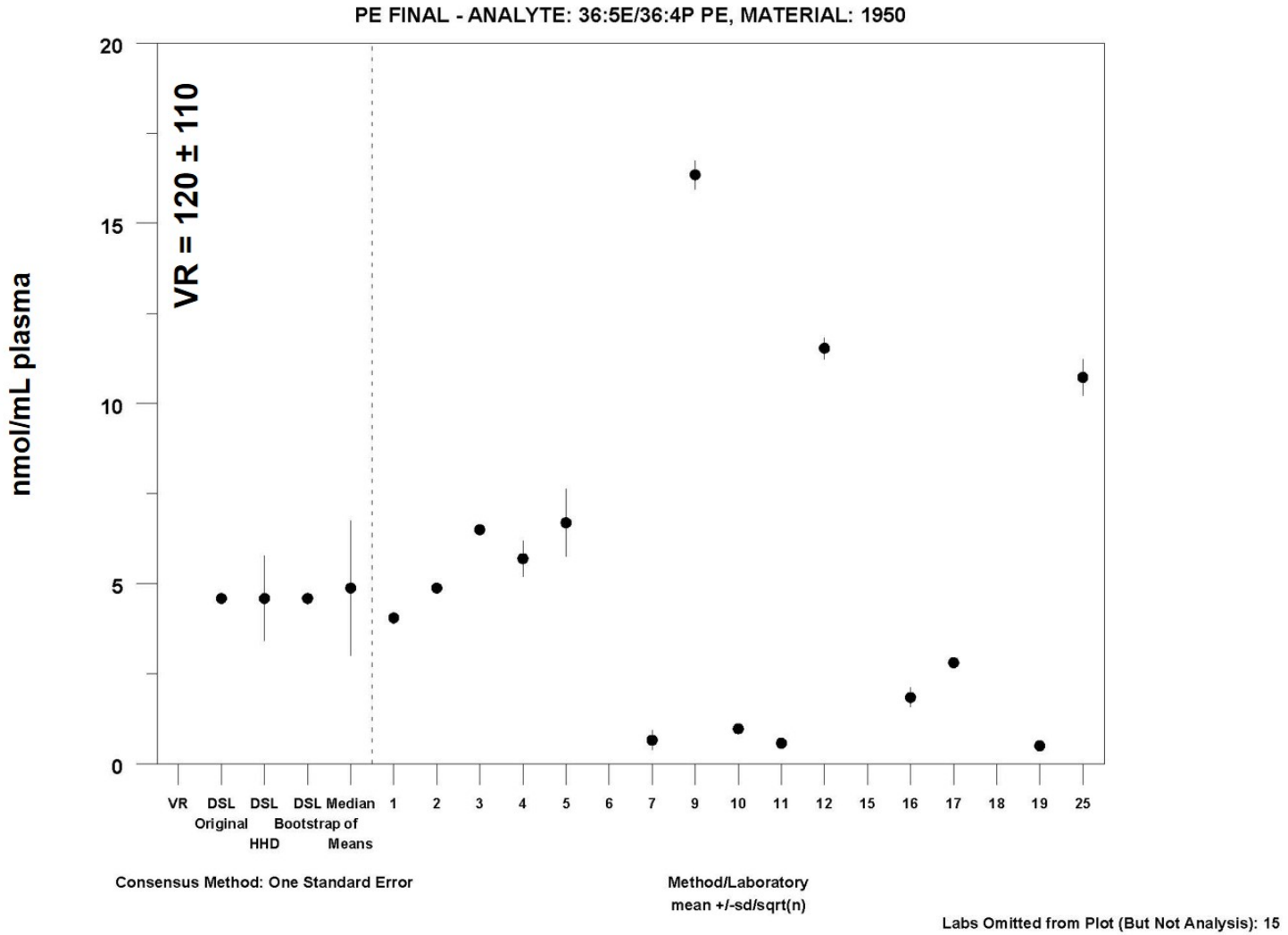


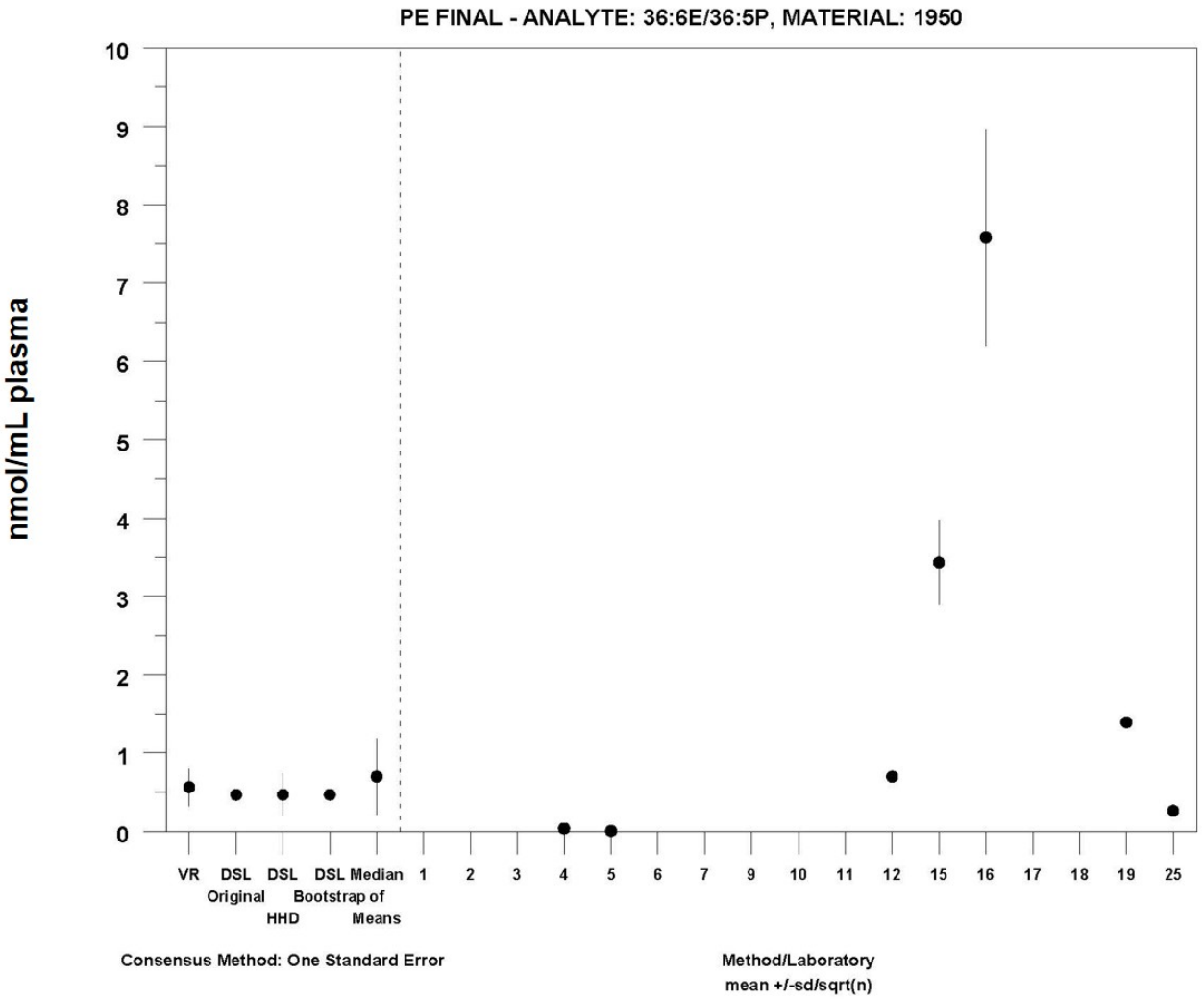




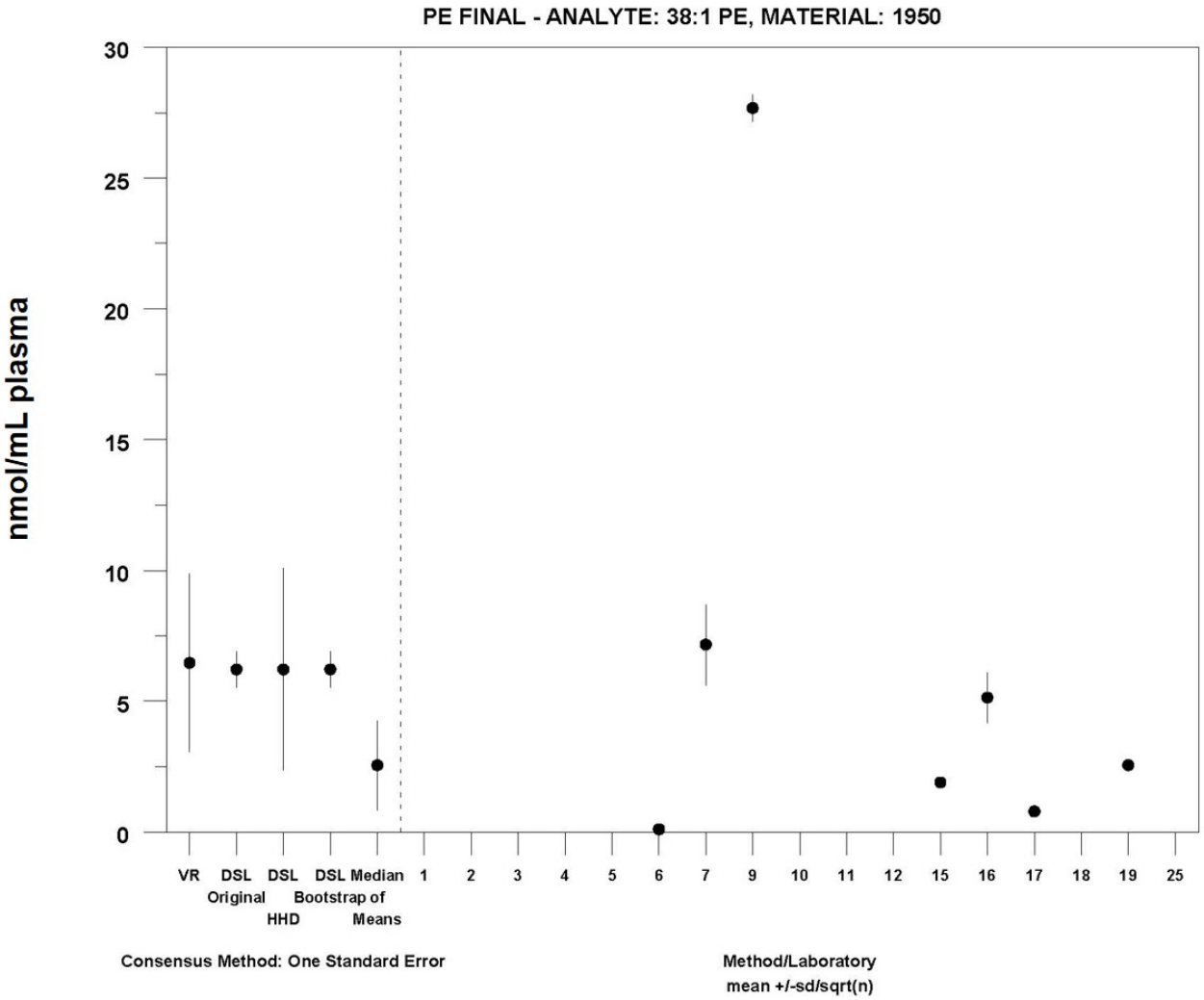




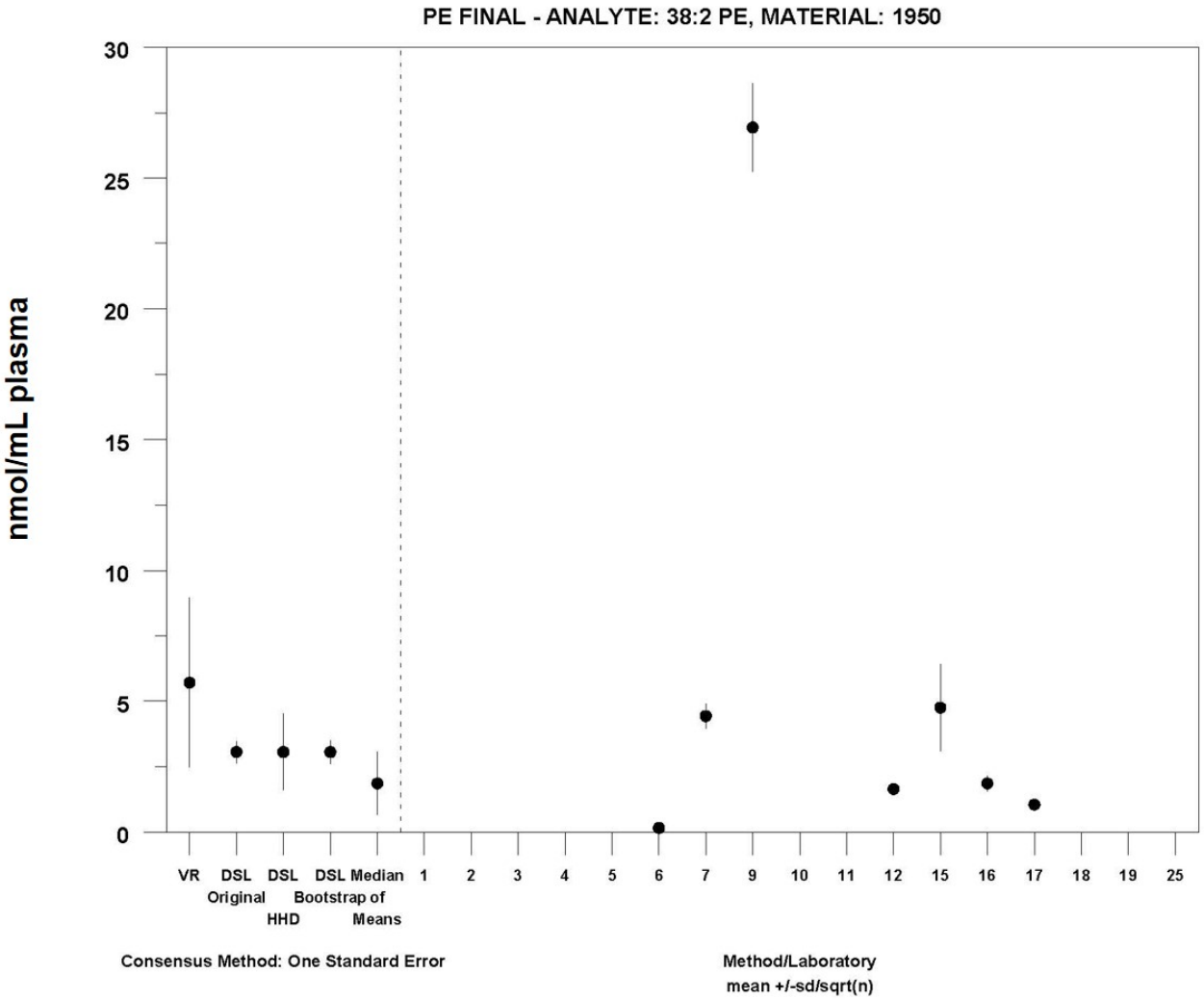




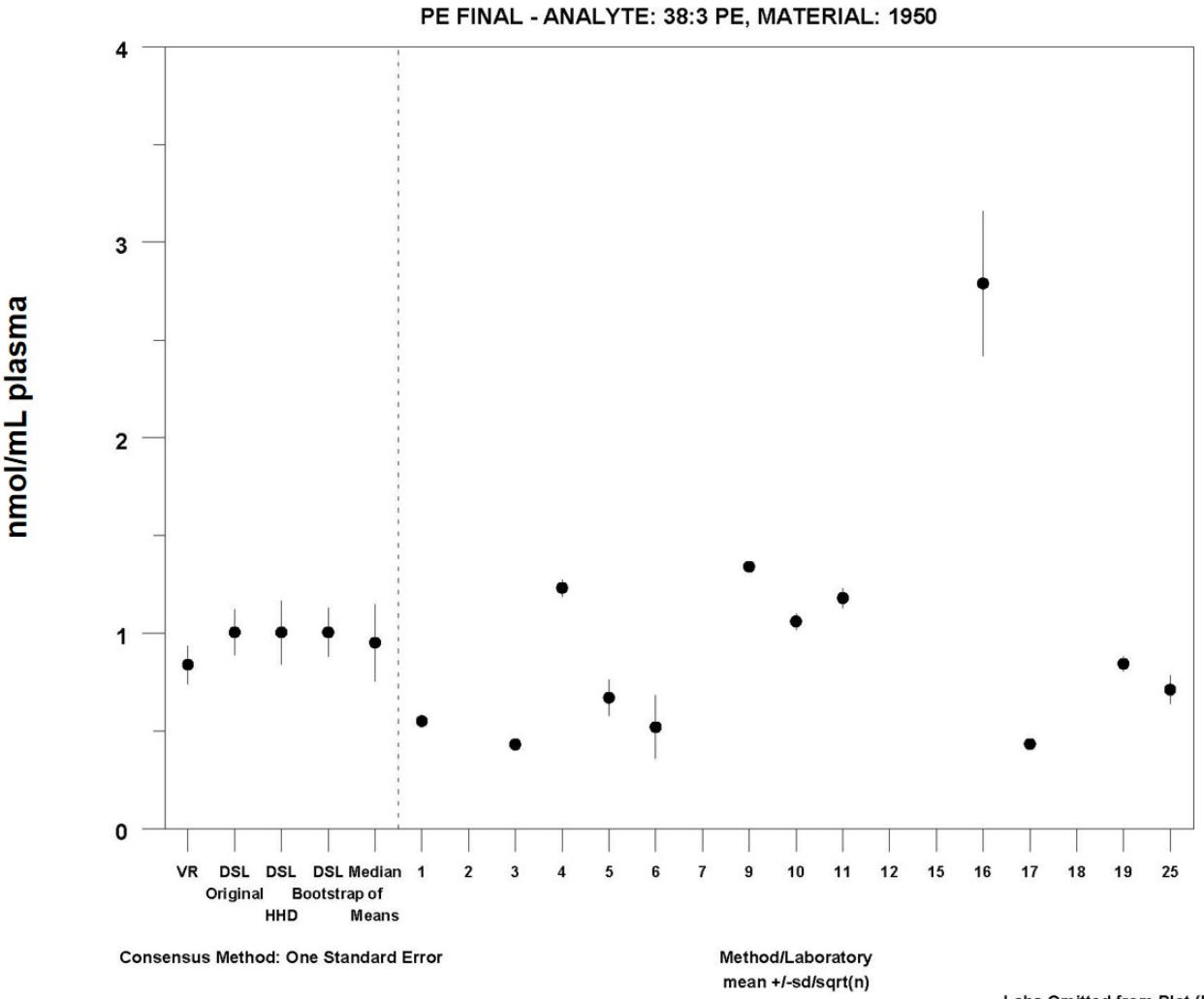
MEDM Location: 0.70 ± 0.49 nmol/mL



MEDM Location: 2.6 ± 1.7 nmol/mL



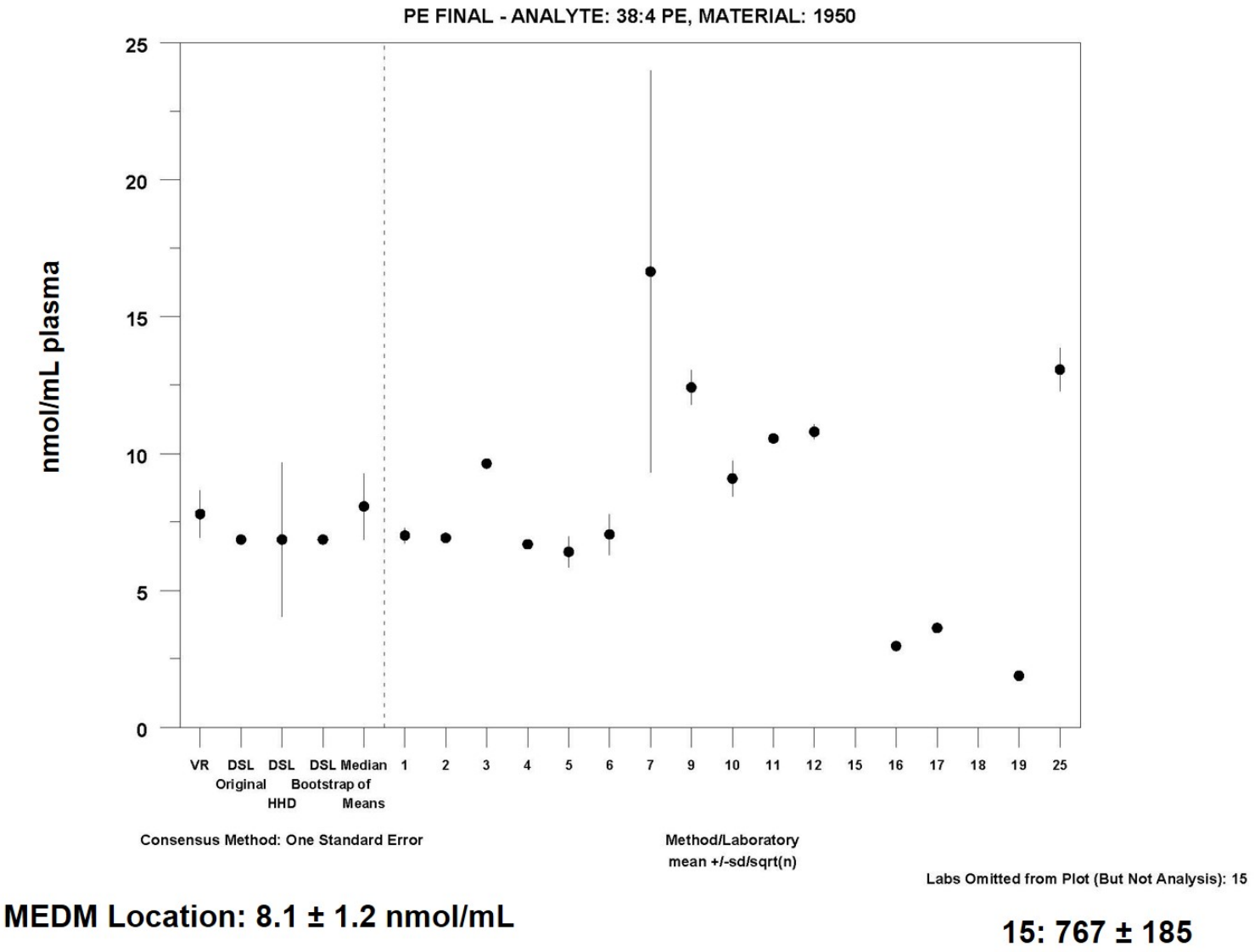
MEDM Location: 1.9 ± 1.2 nmol/mL

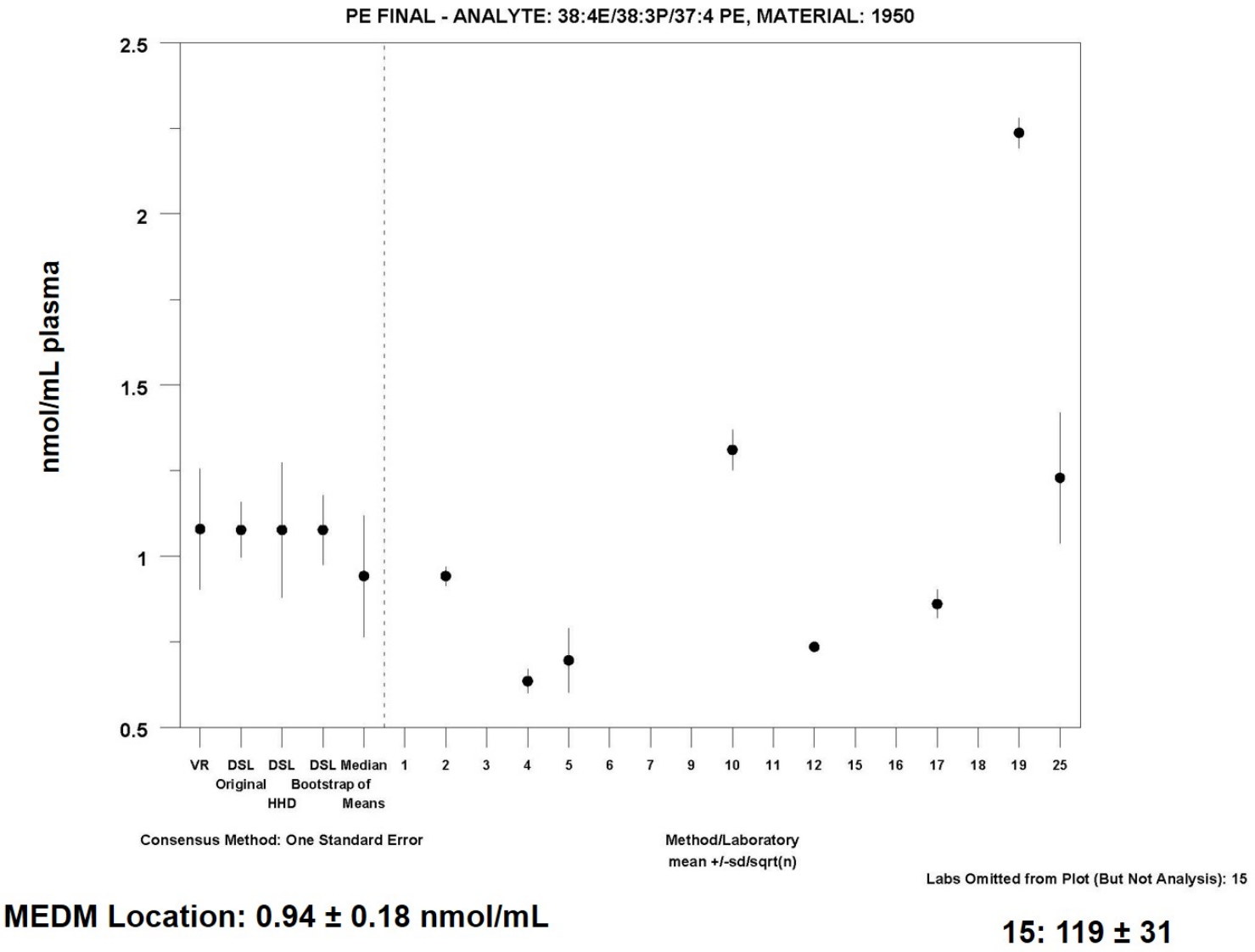


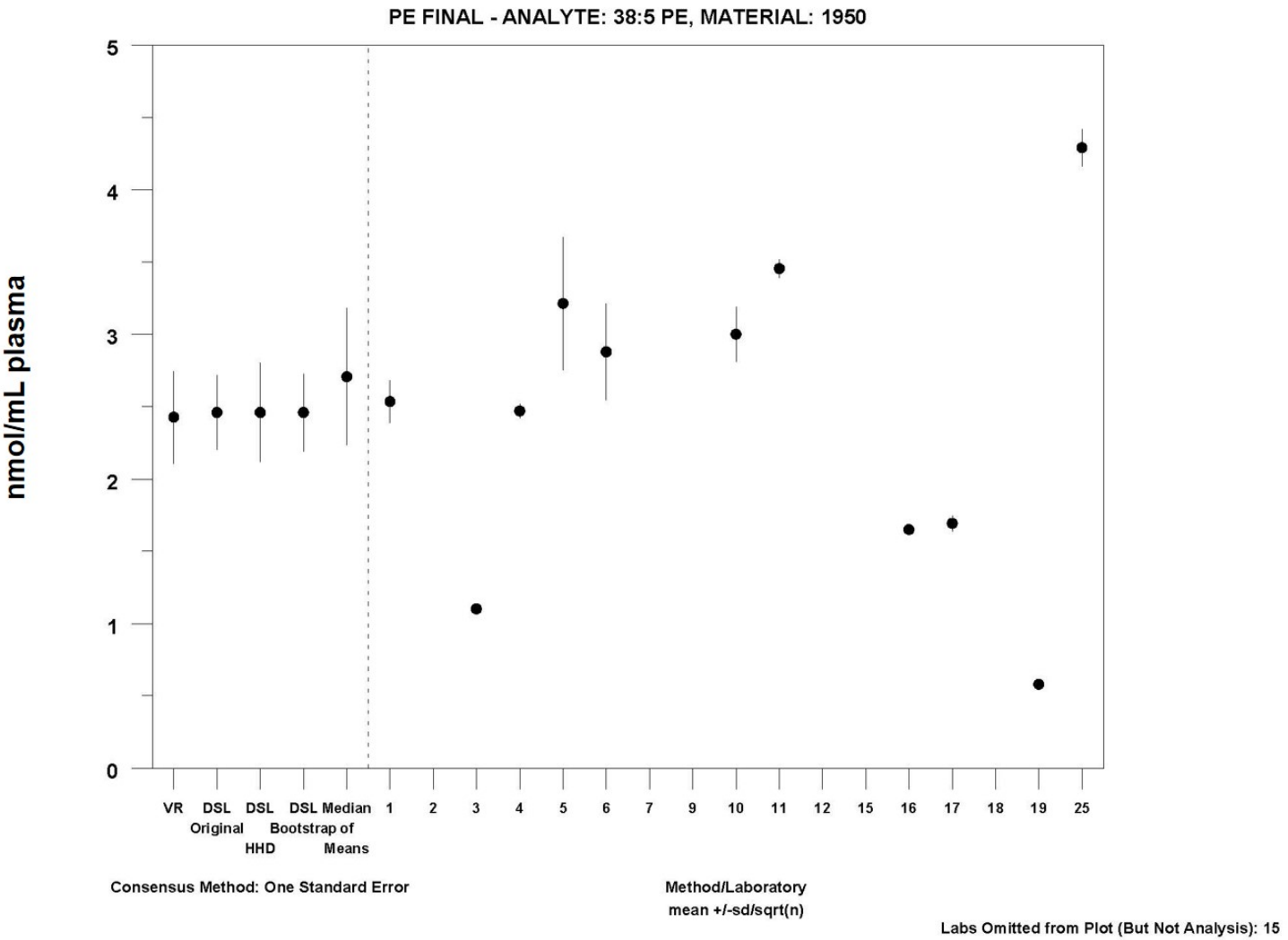
Labs Omitted from Plot (But Not Analysis): 7 15

MEDM Location: 0.95 ± 0.20 nmol/mL

7: 9.5 ± 2; 15: 121 ± 25

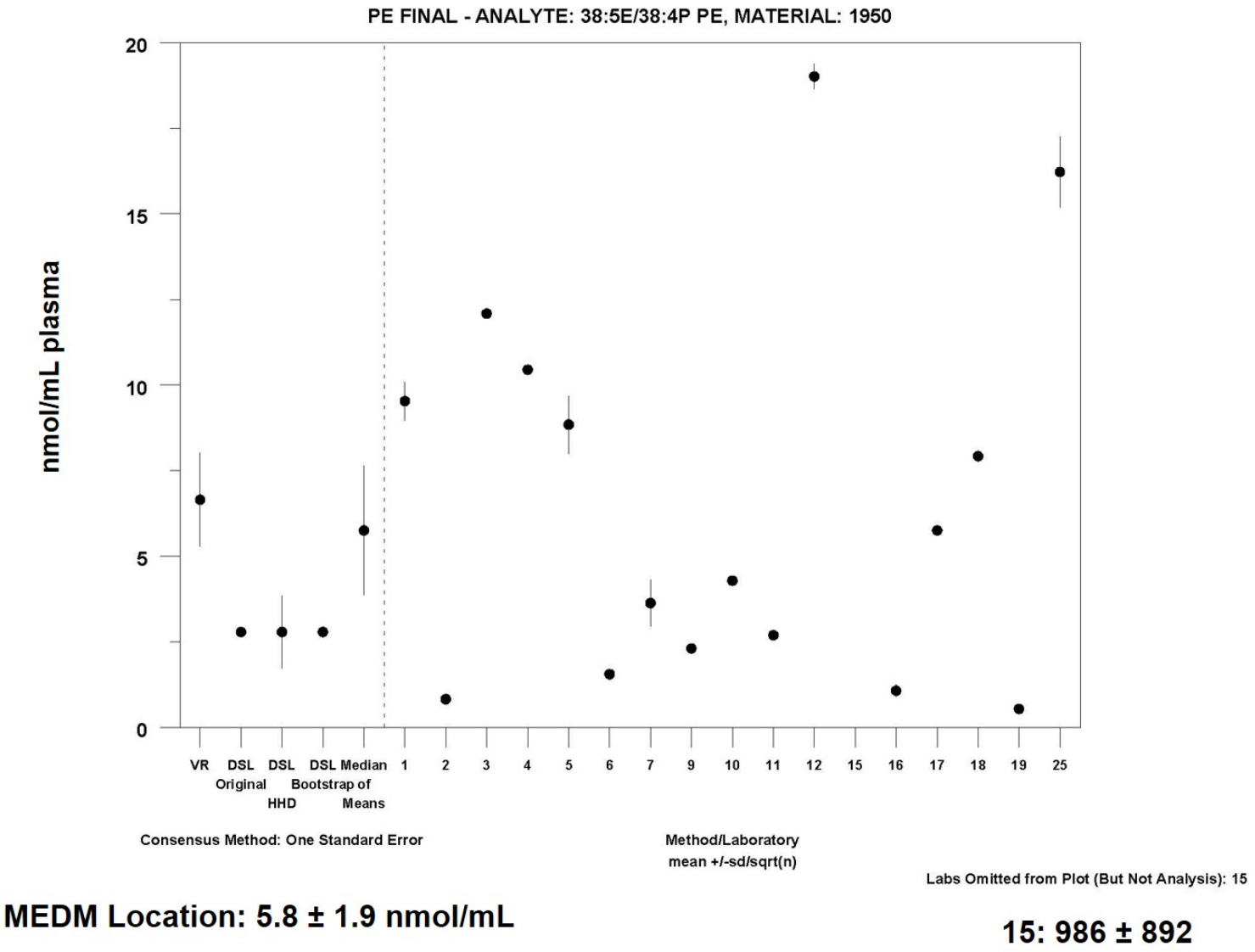


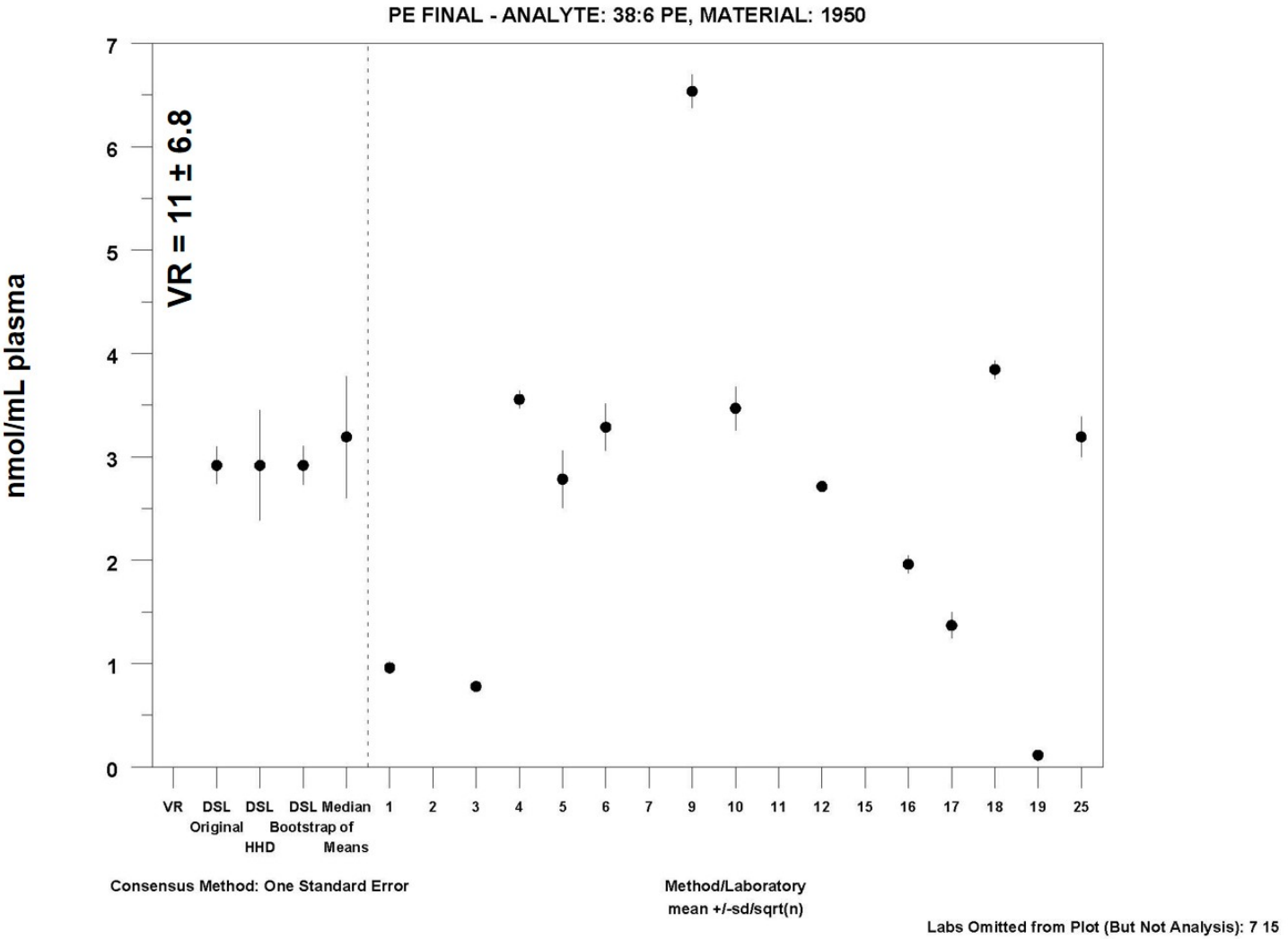


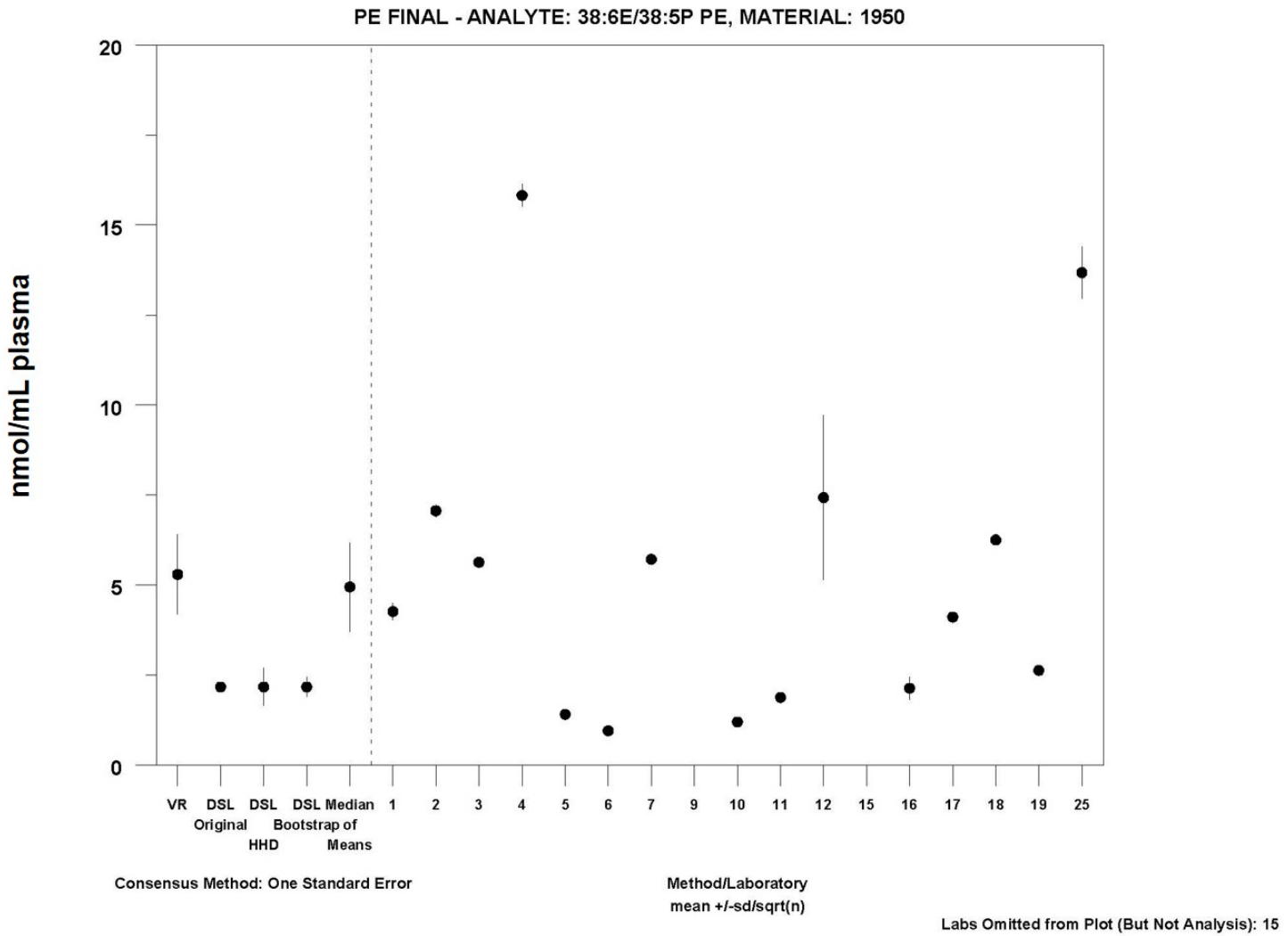


MEDM Location: 2.7 ± 0.47 nmol/mL

15: 74 ± 18

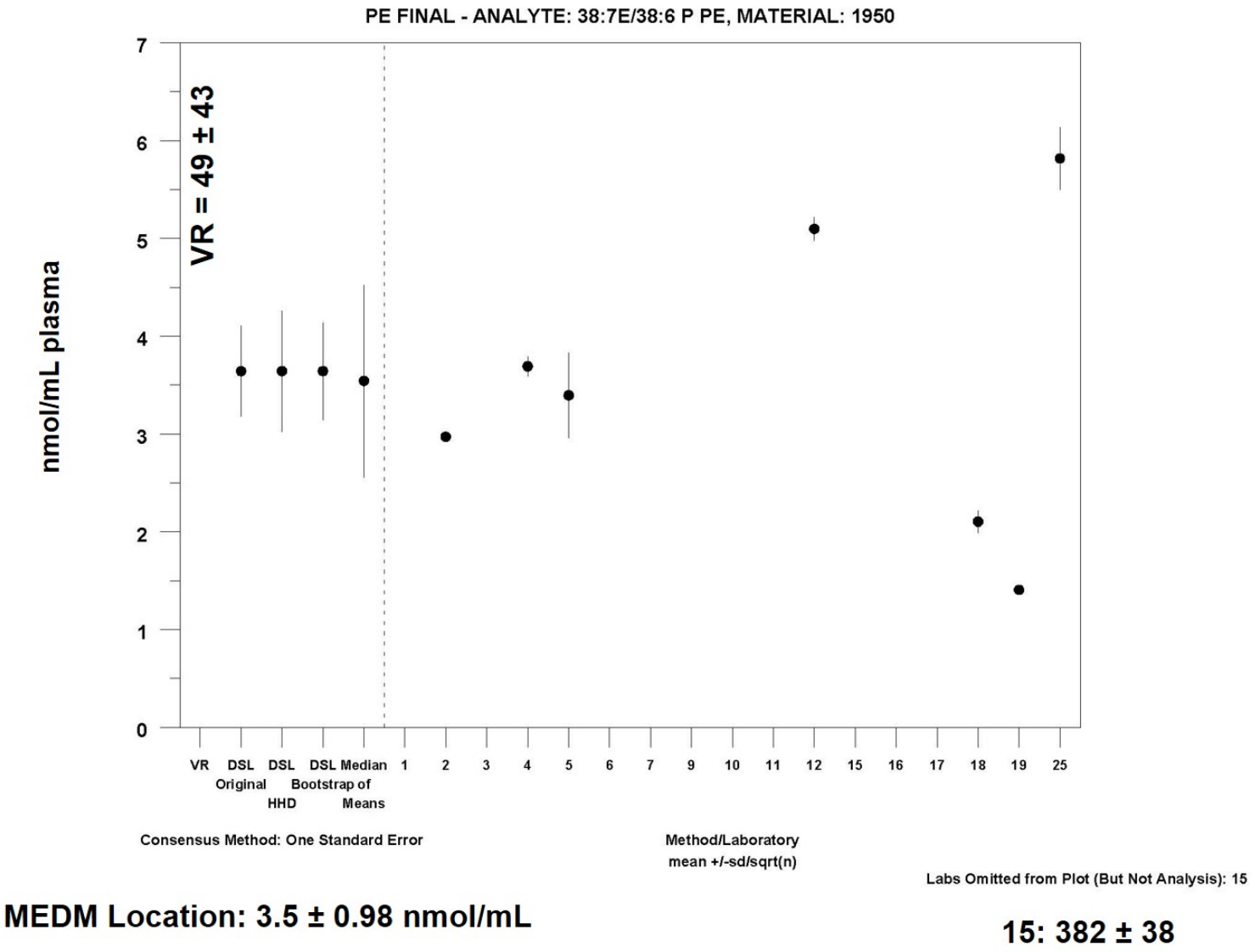


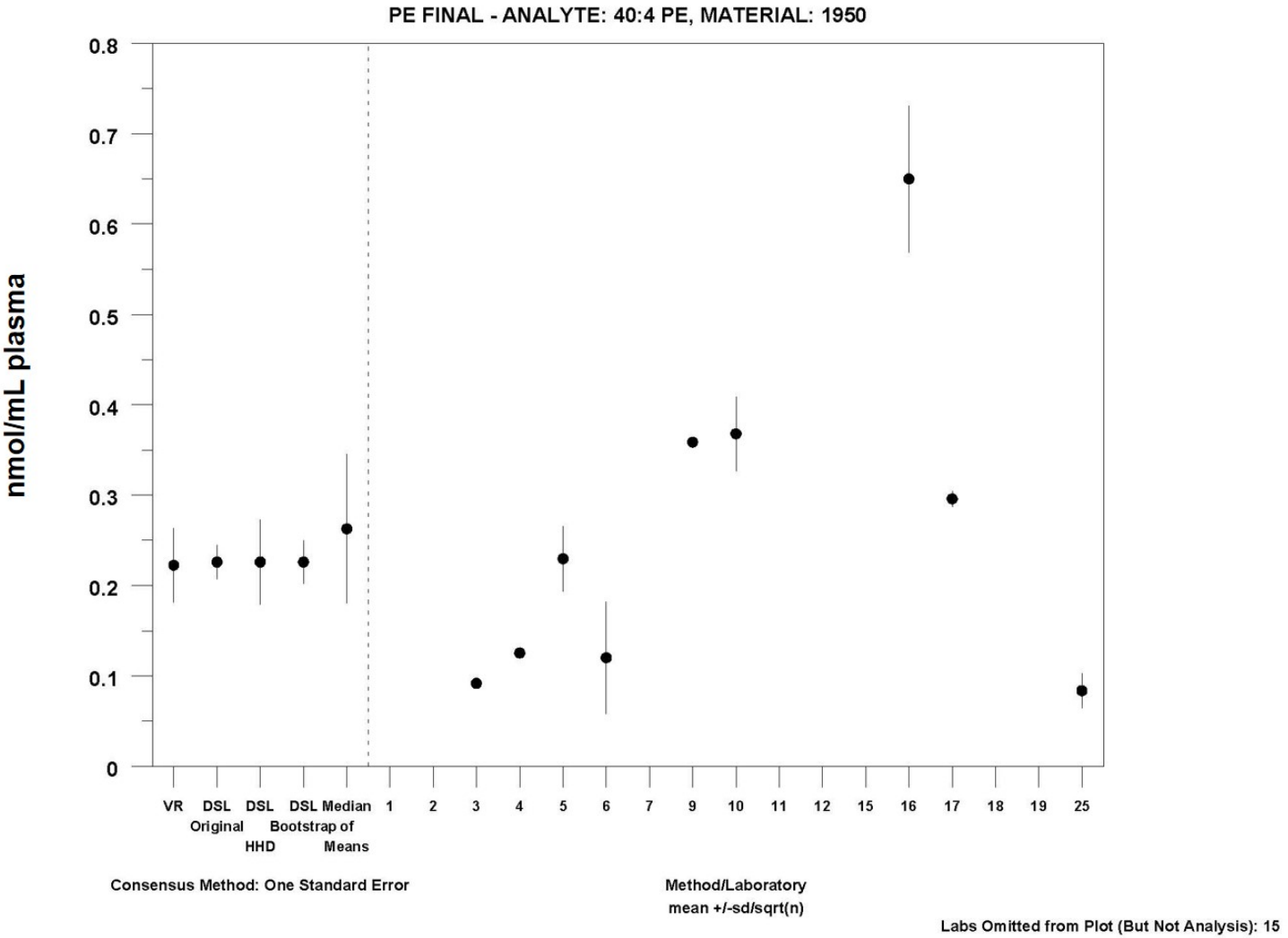


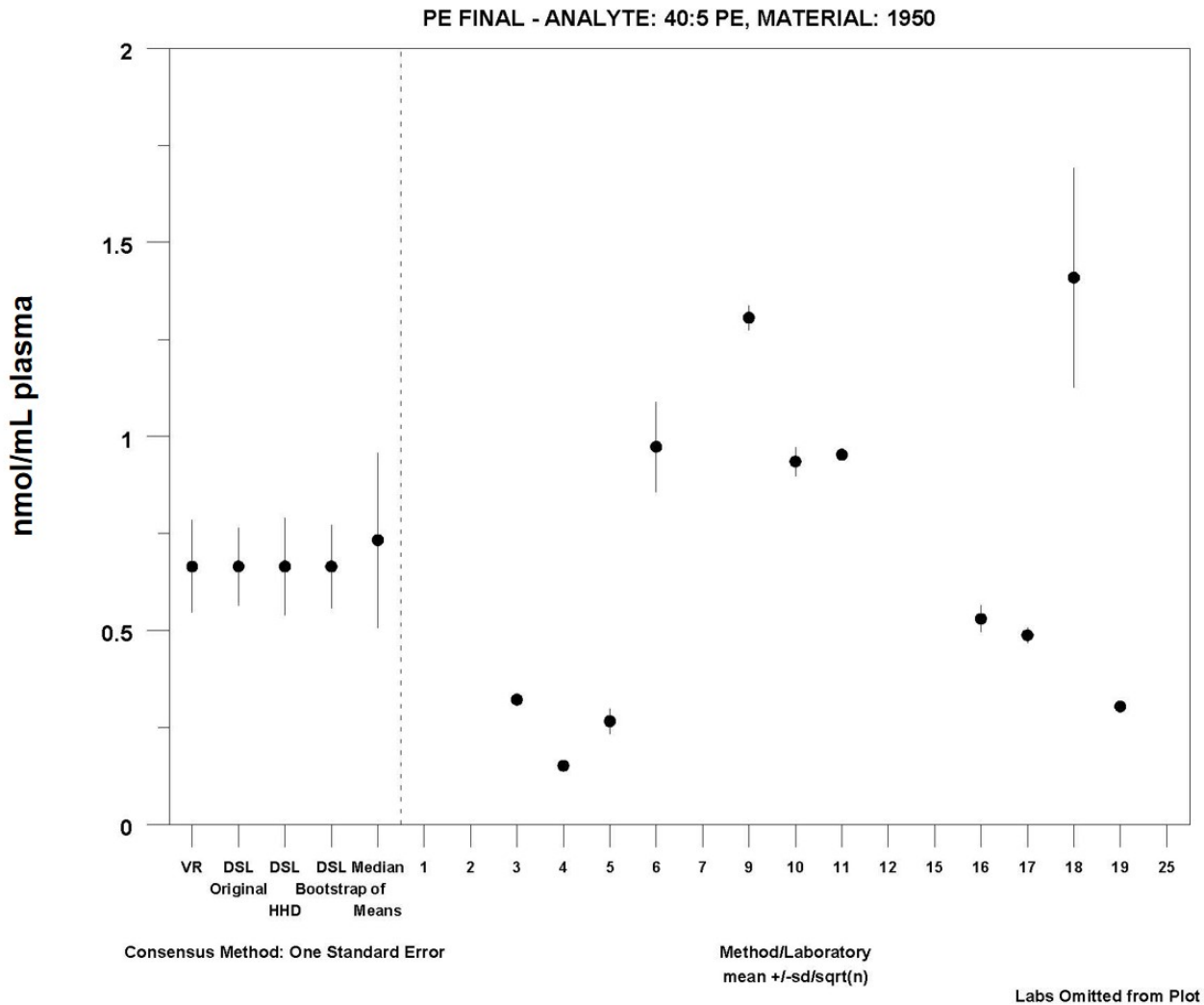


MEDM Location: 4.9 ± 1.2 nmol/mL

15: 2693 ± 651



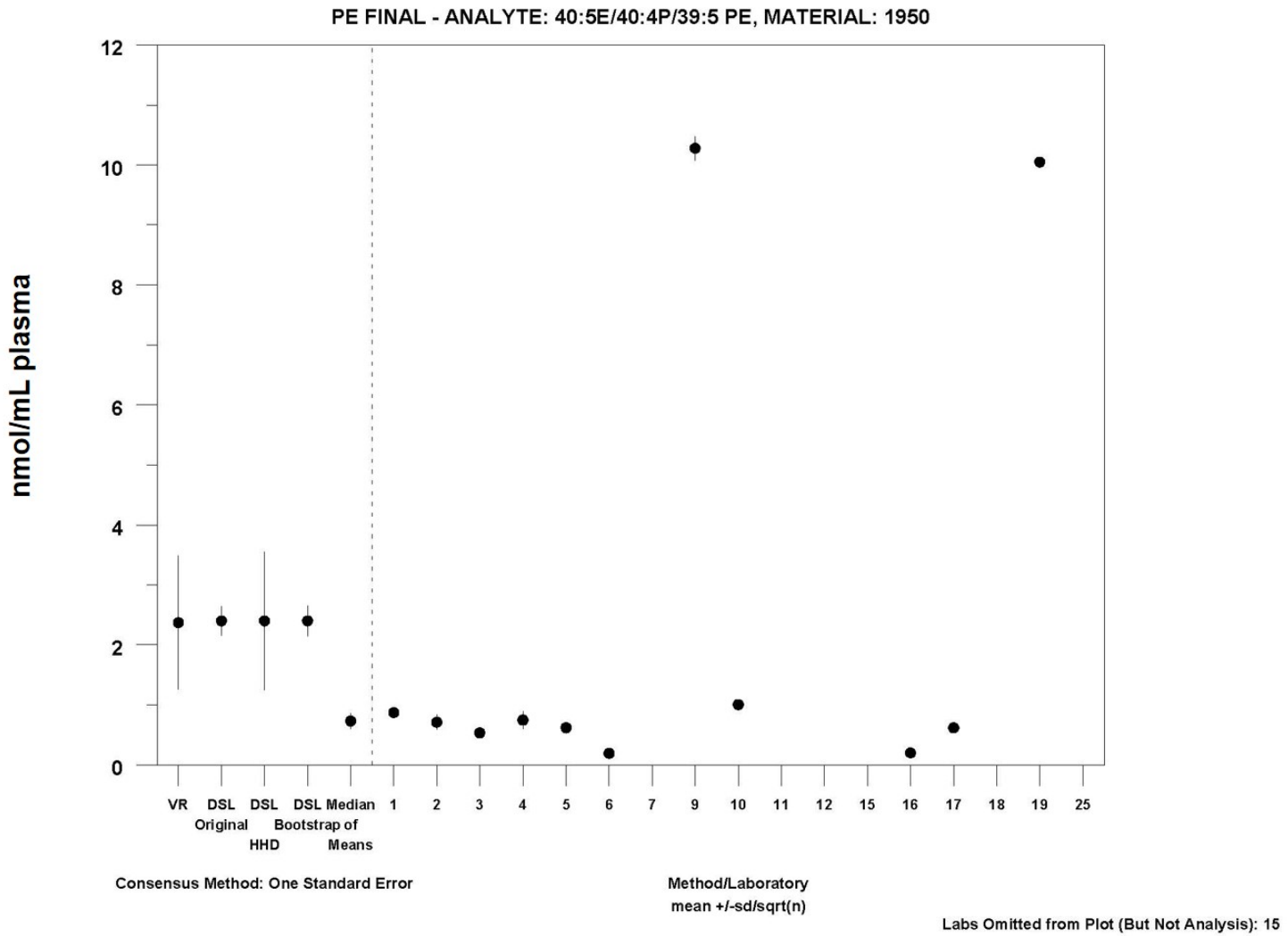


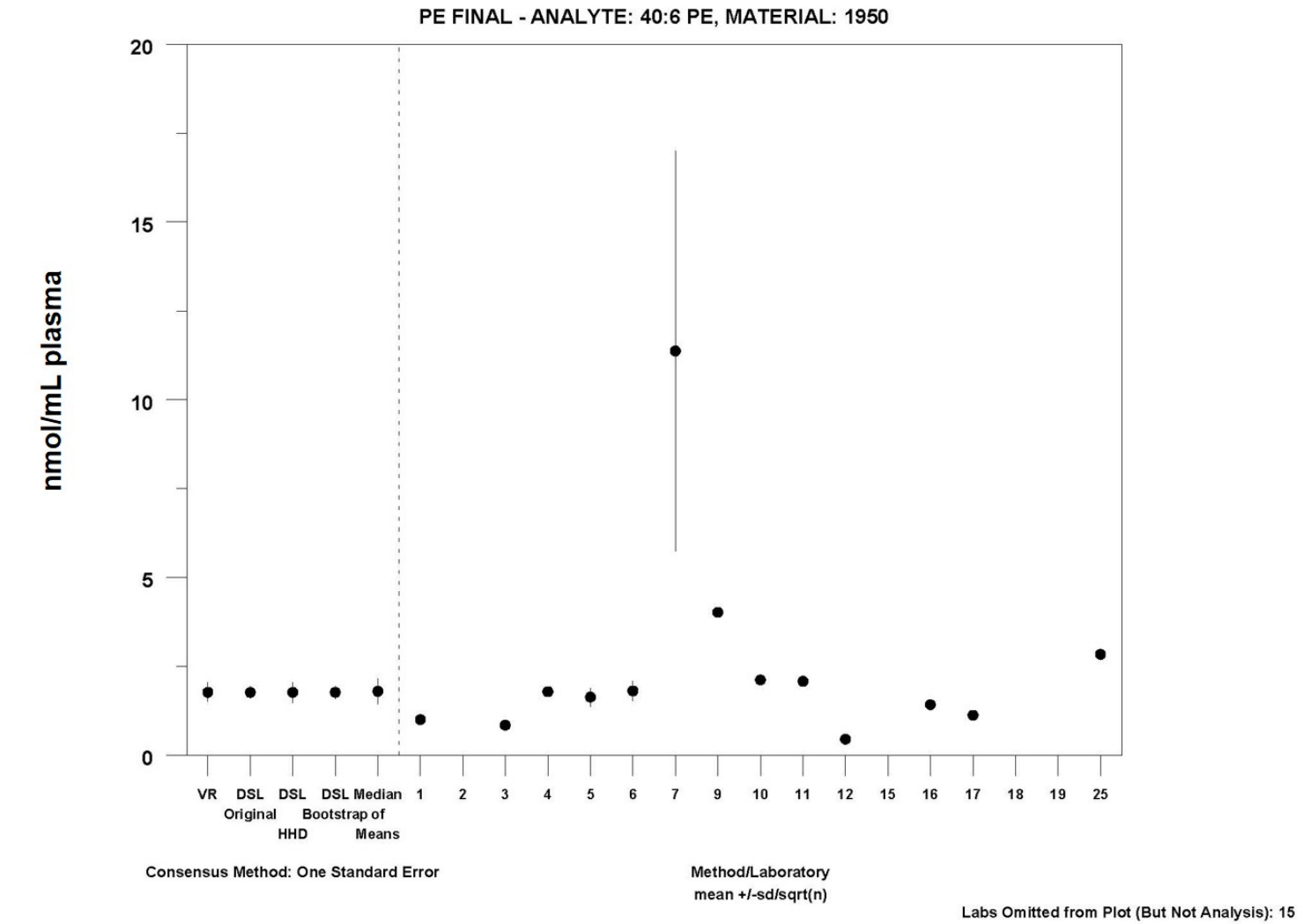


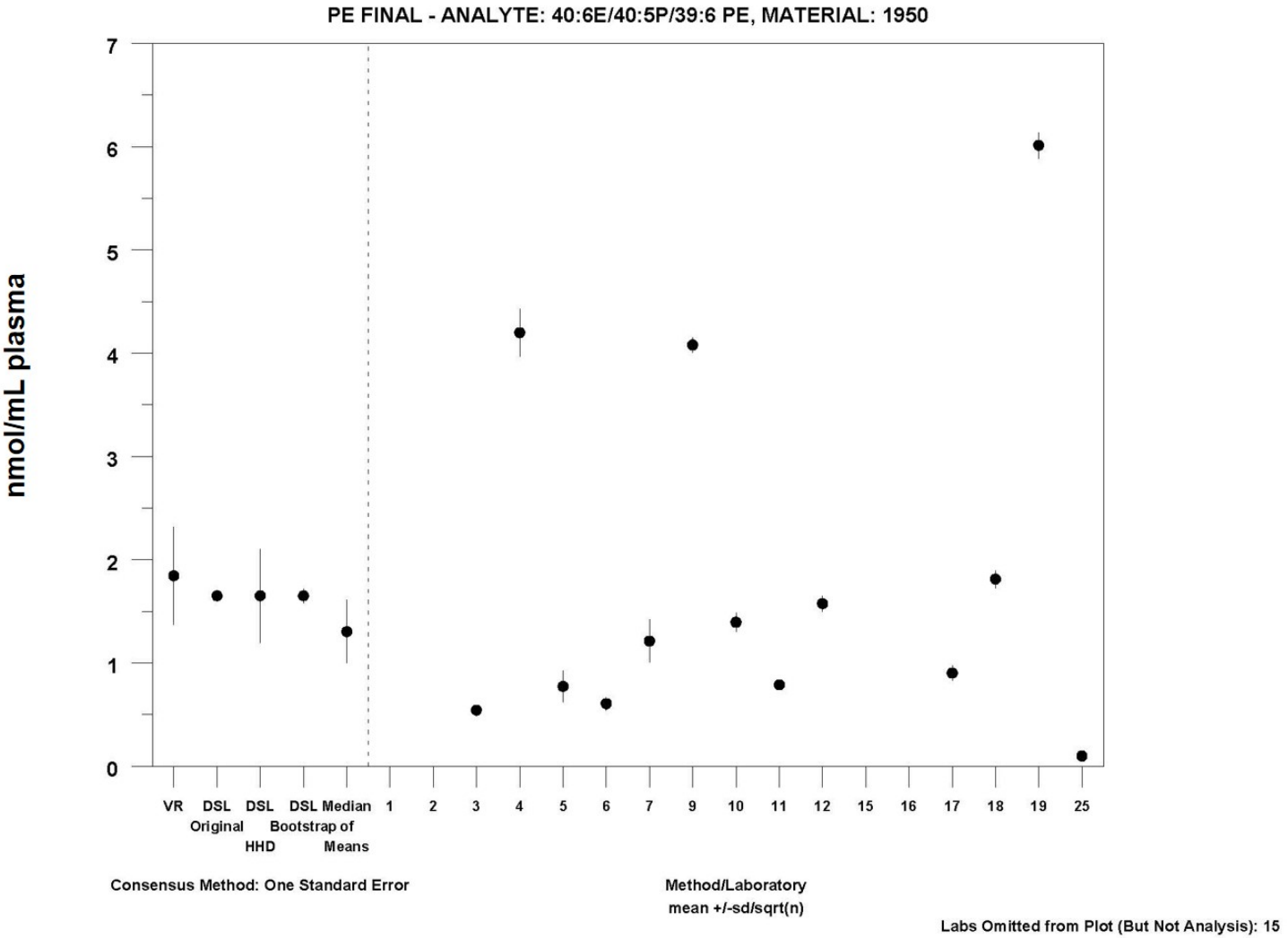
Labs Omitted from Plot (But Not Analysis): 15

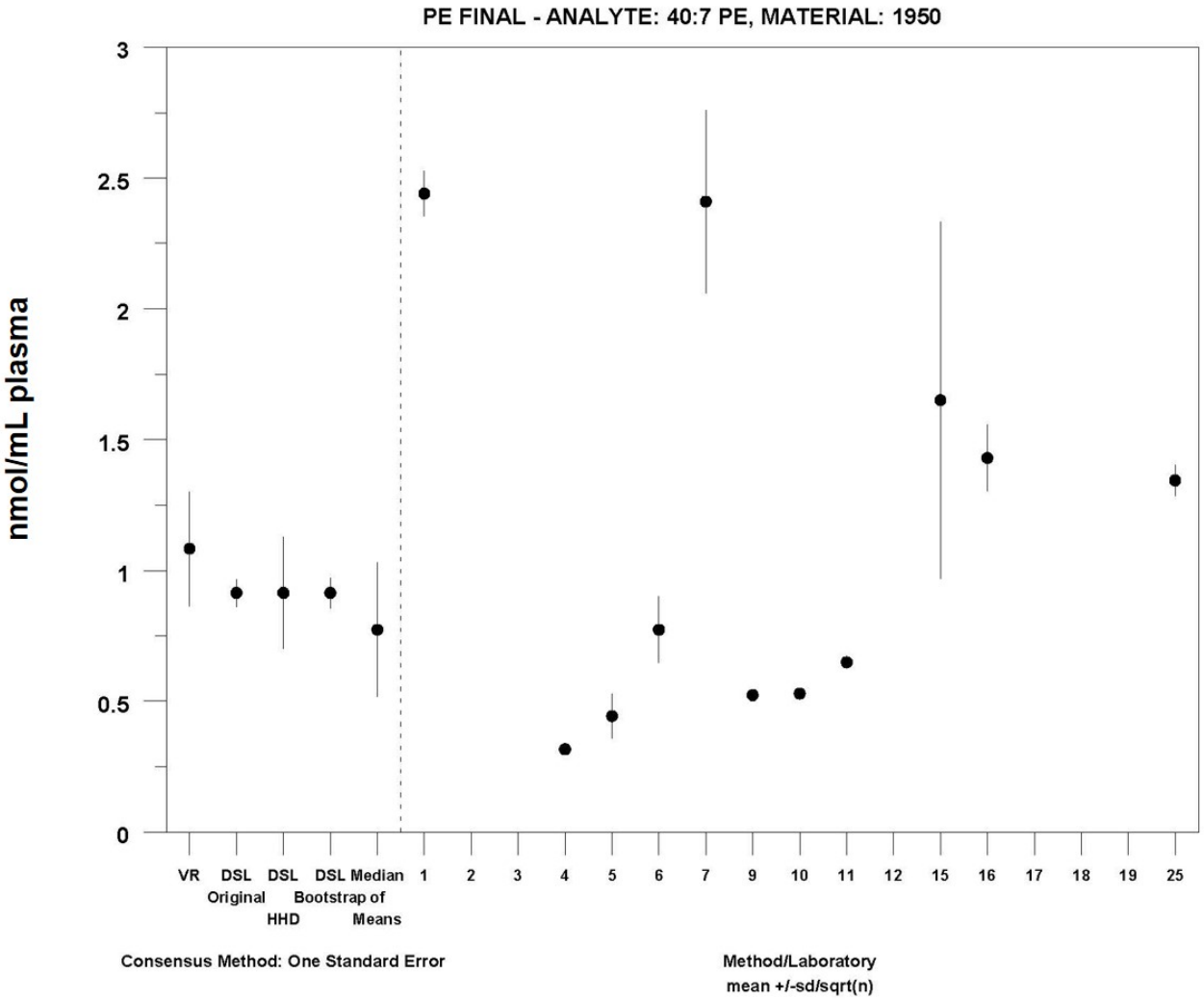
MEDM Location: 0.73 ± 0.23 nmol/mL

15: 35 ± 17

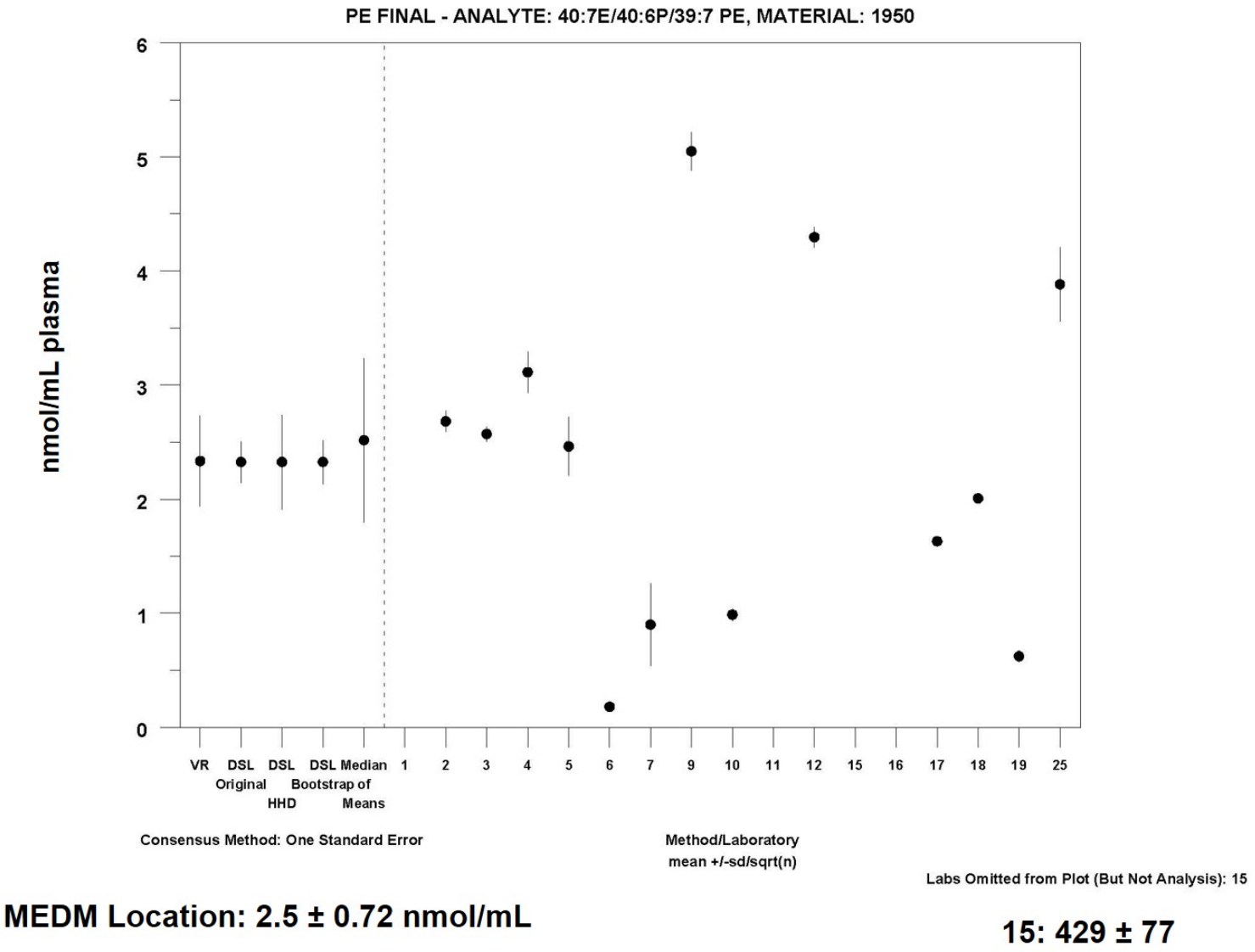


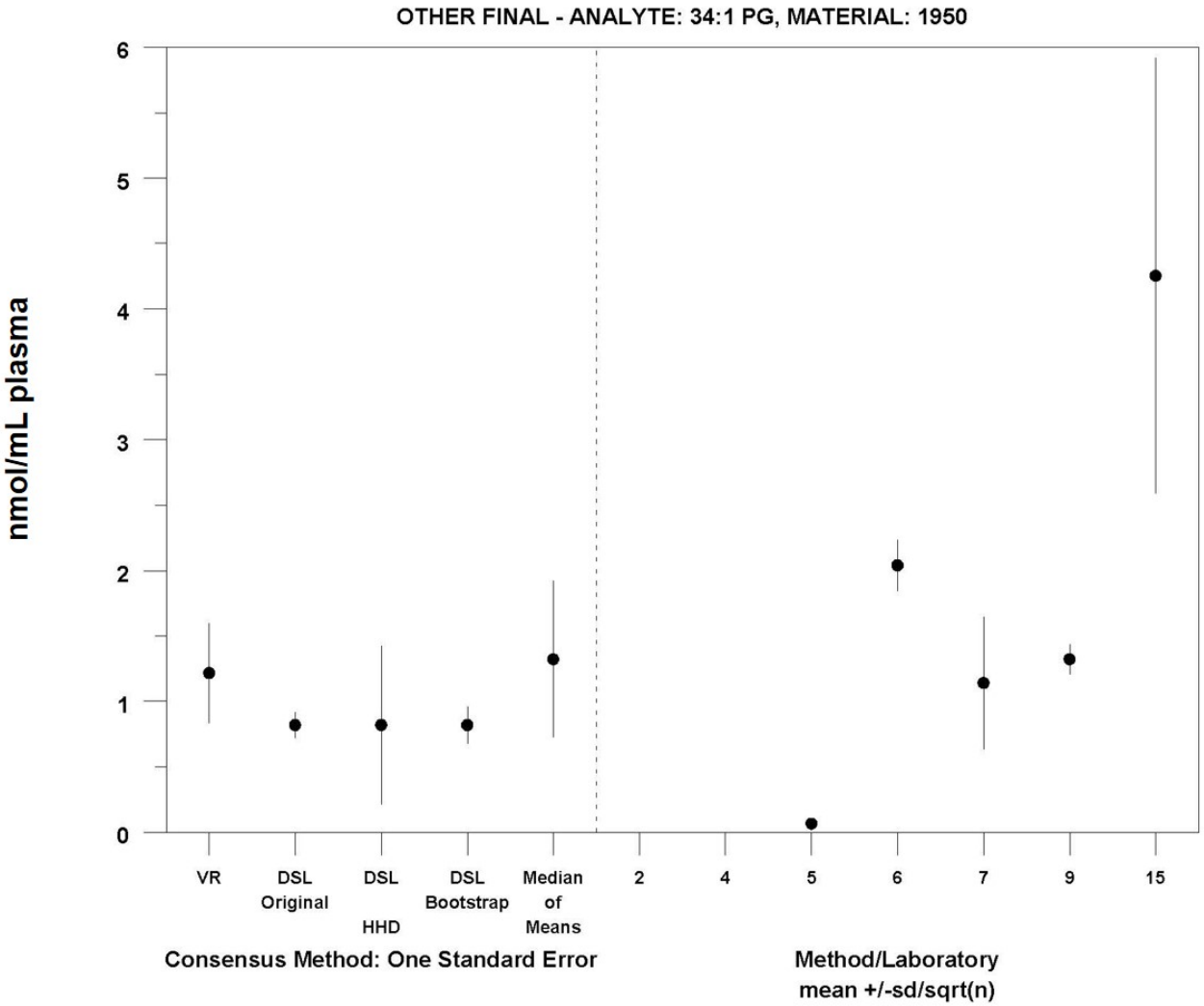




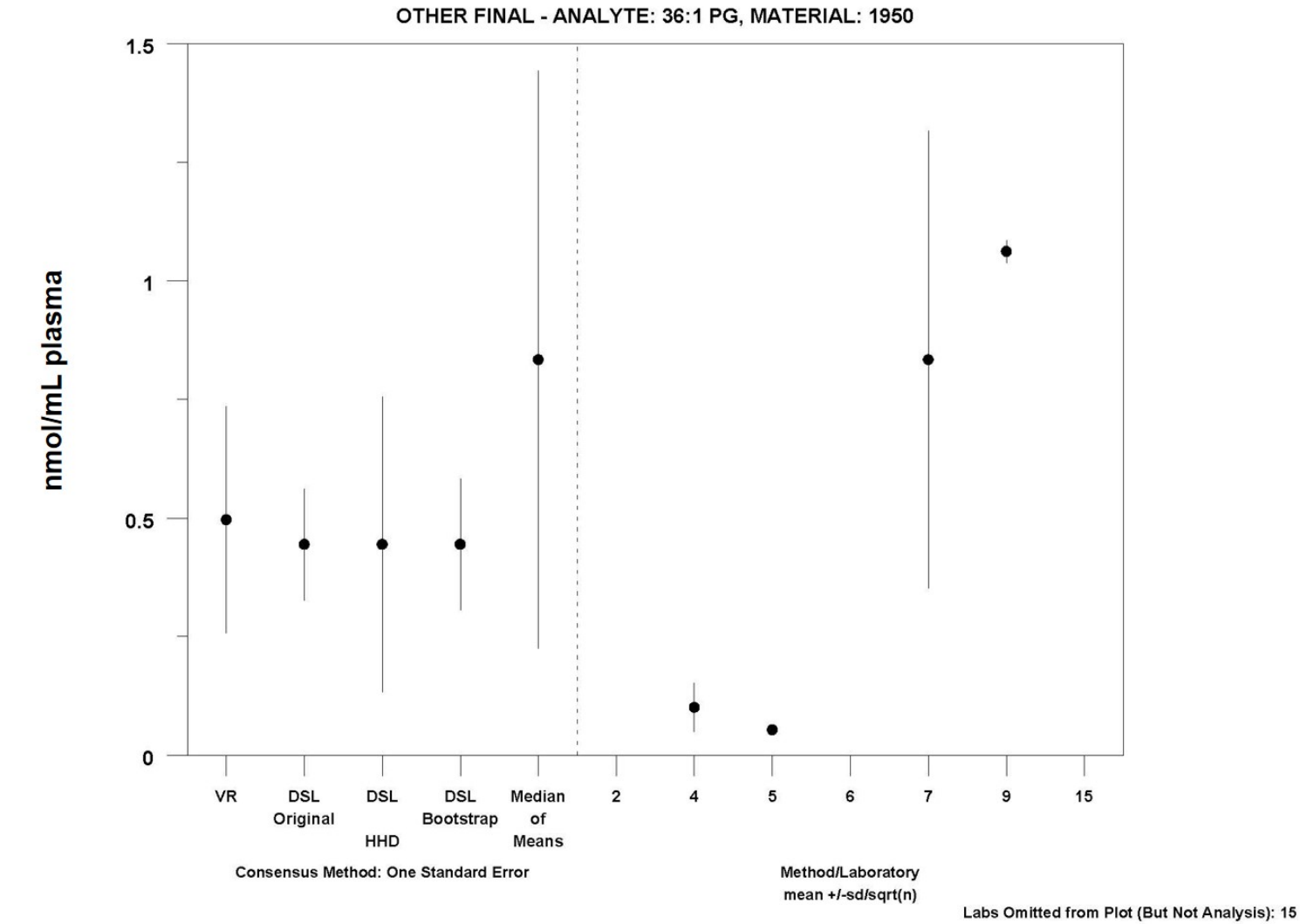


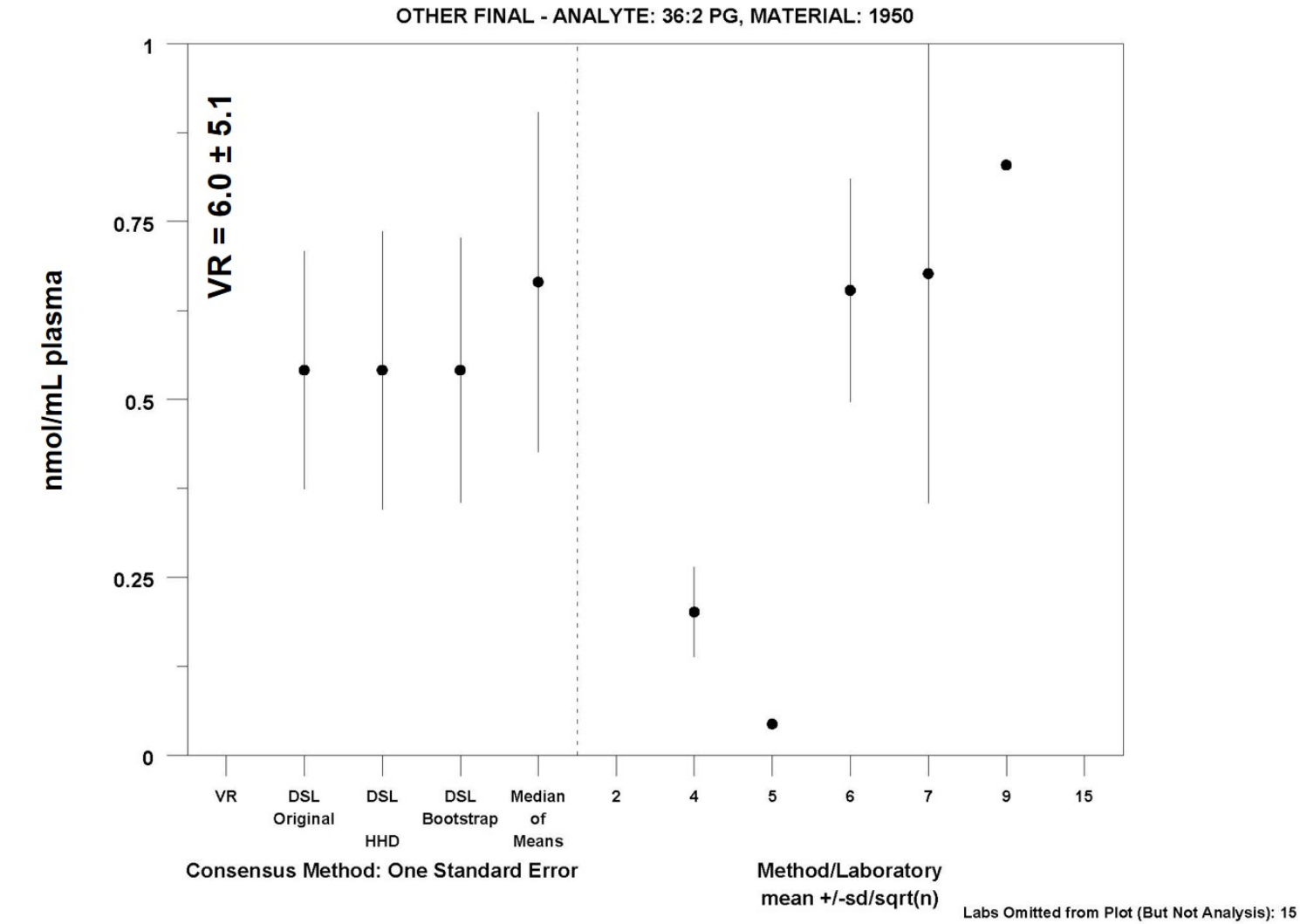
MEDM Location: 0.77 ± 0.26 nmol/mL

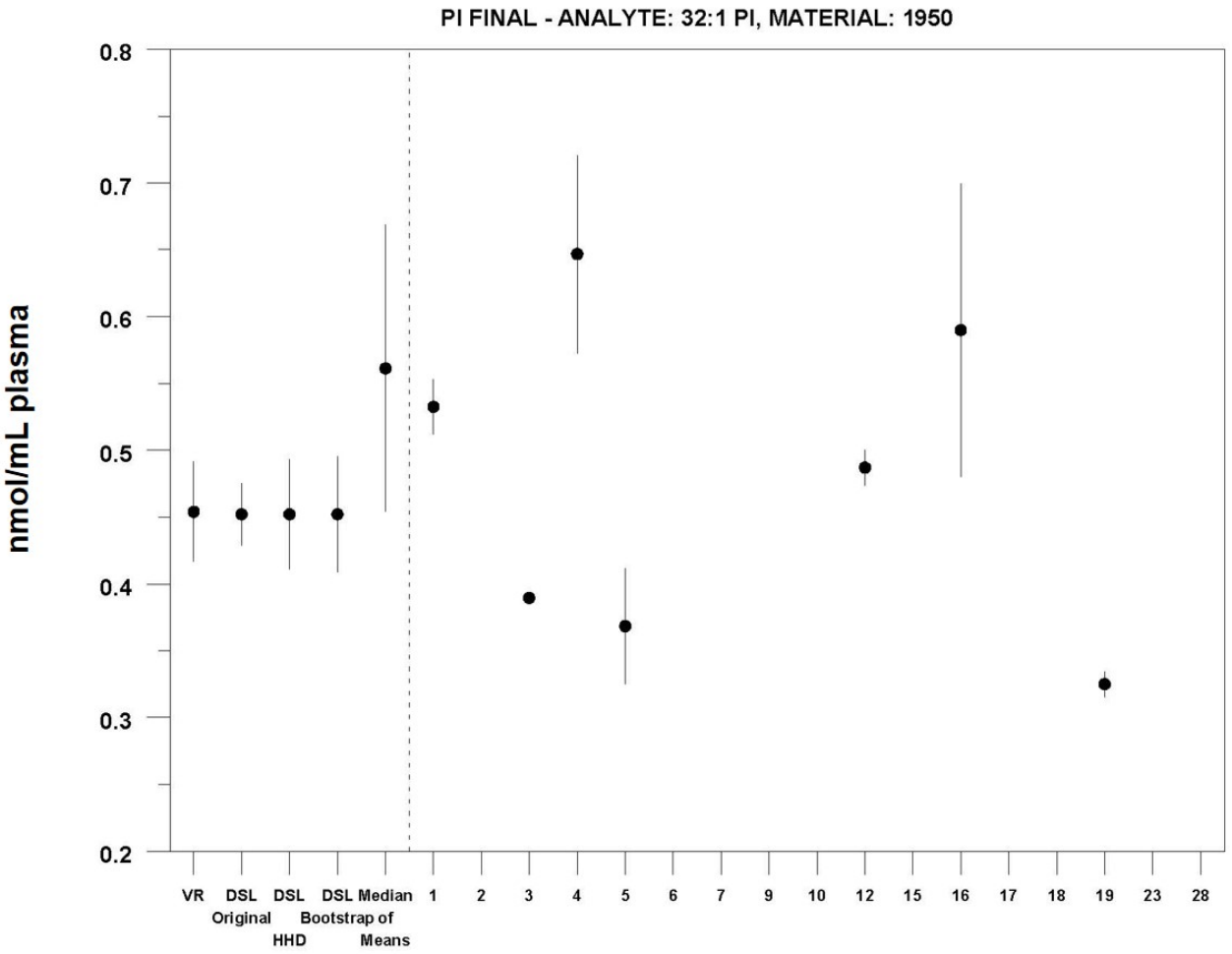




MEDM Location: 1.3 ± 0.60 nmol/mL



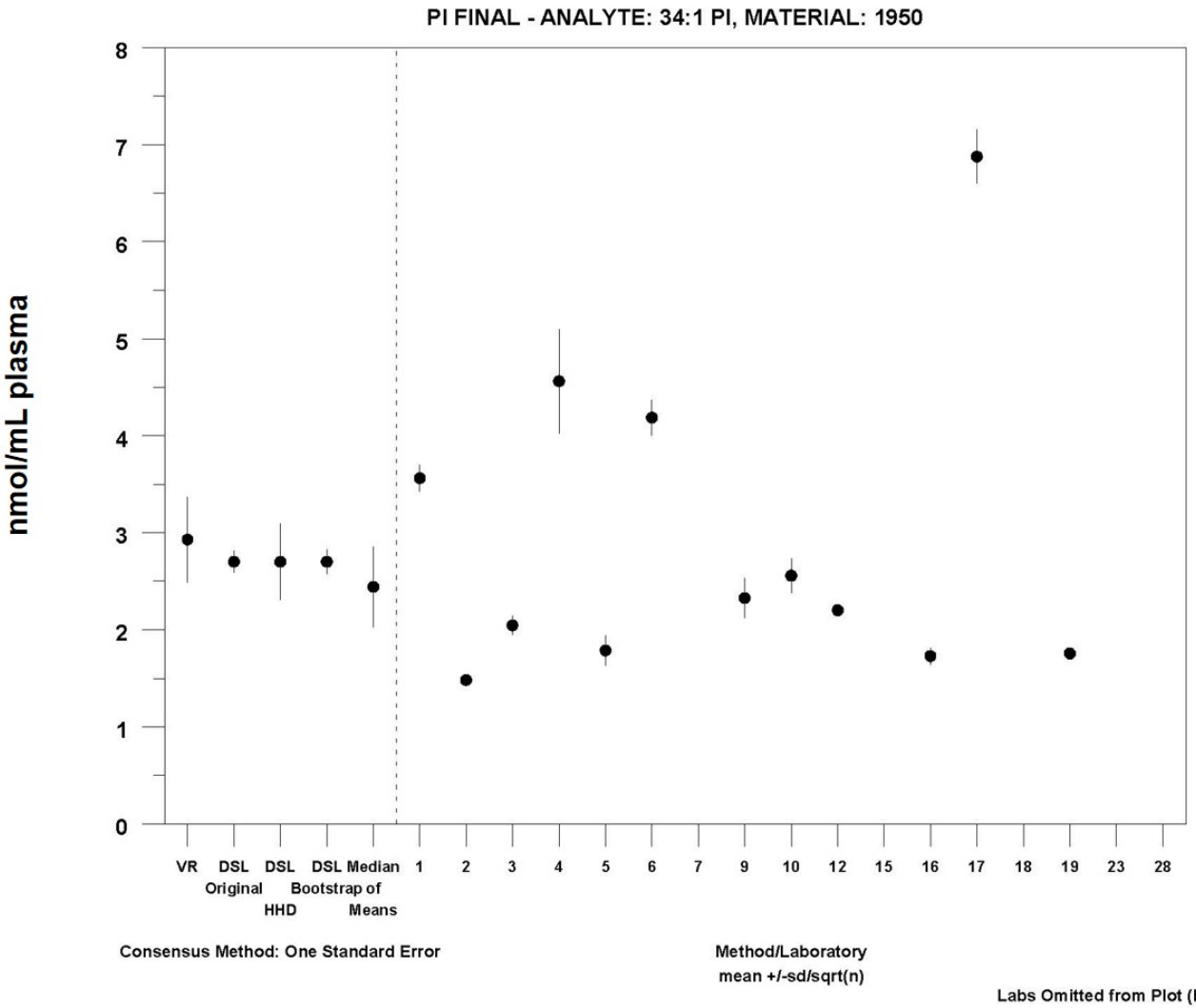




MEDM Location: 0.56 ± 0.11 nmol/mL

Labs Omitted from Plot (But Not Analysis): 7 9 15

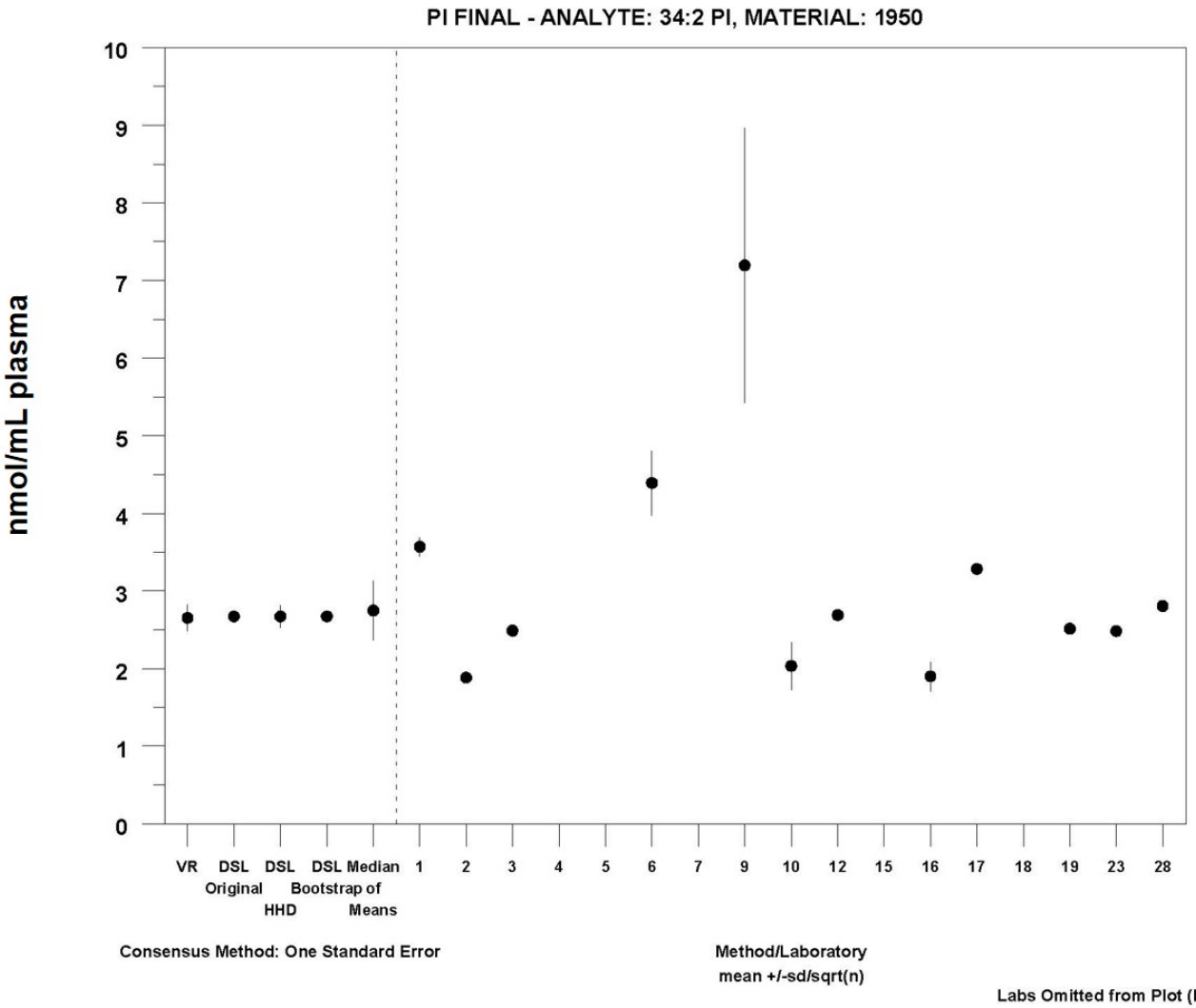
7: 5.1 ± 1.7; 9: 9.3 ± 1.5; 15: 29 ± 16



Labs Omitted from Plot (But Not Analysis): 7 15

MEDM Location: 2.4 ± 0.42 nmol/mL

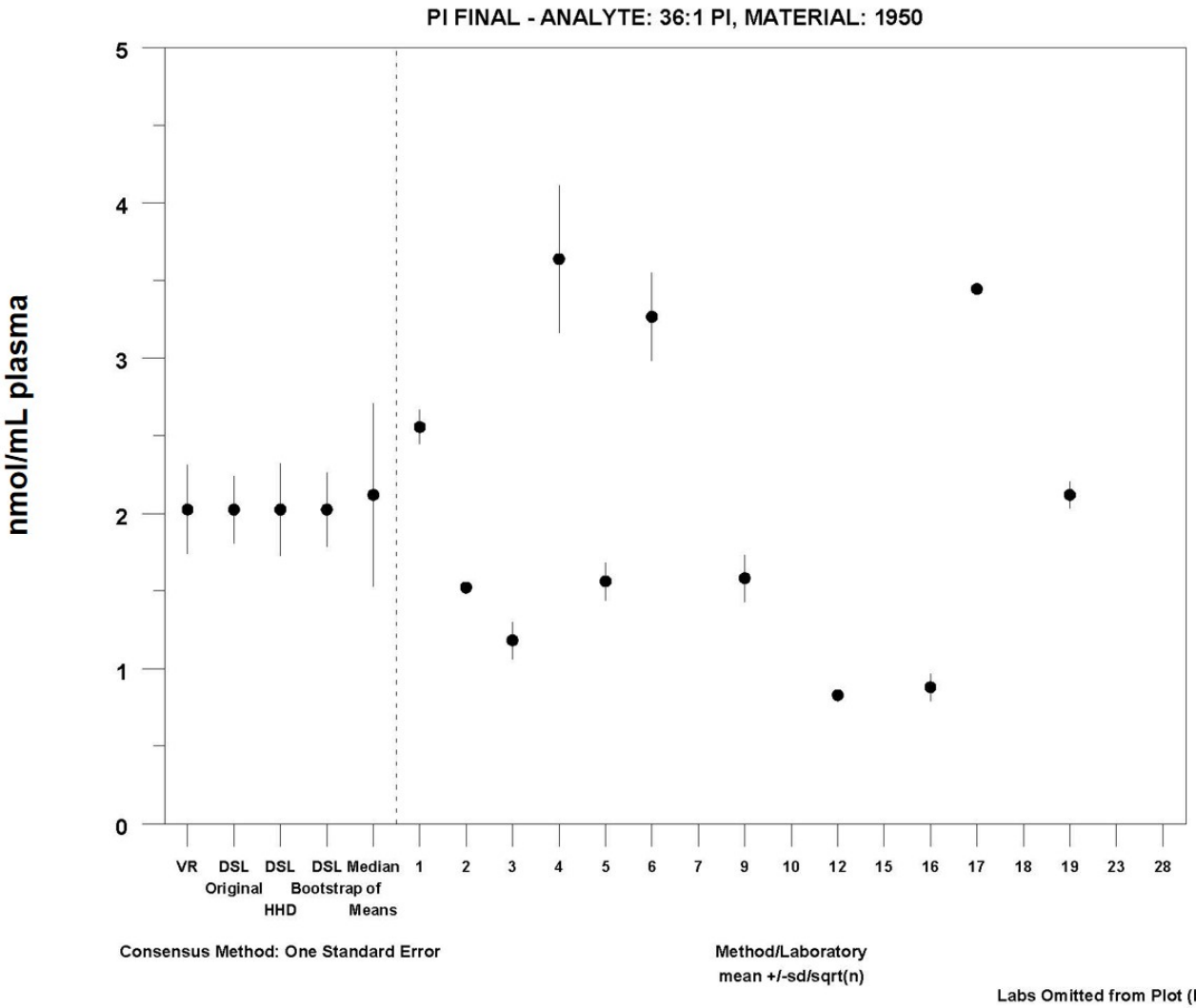
7: 23 ± 9; 15: 63 ± 14



Labs Omitted from Plot (But Not Analysis): 7 15

MEDM Location: 2.8 ± 0.38 nmol/mL

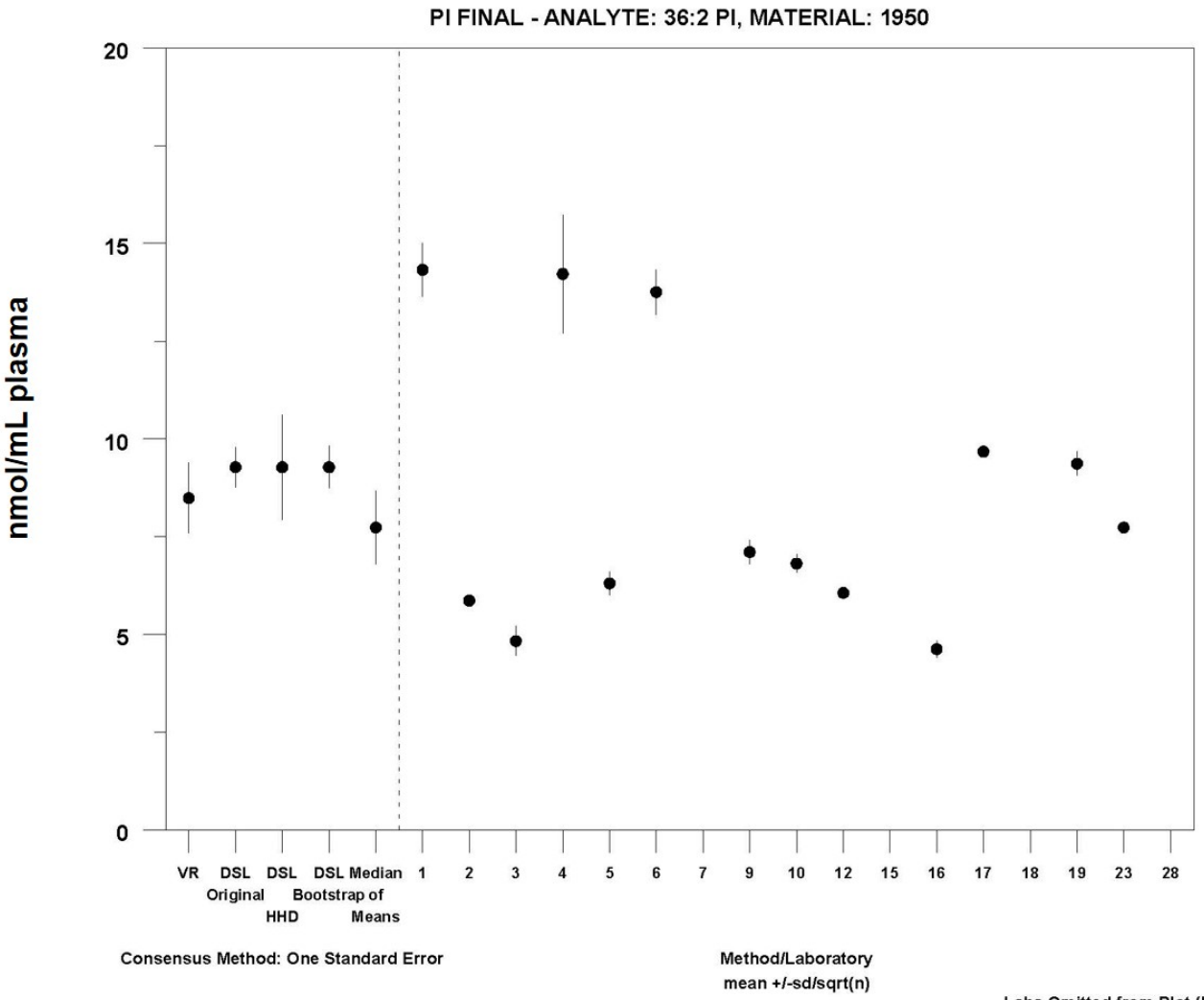
7: 30 ± 13; 15: 144 ± 87



MEDM Location: 2.1 ± 0.59 nmol/mL

Labs Omitted from Plot (But Not Analysis): 7 15

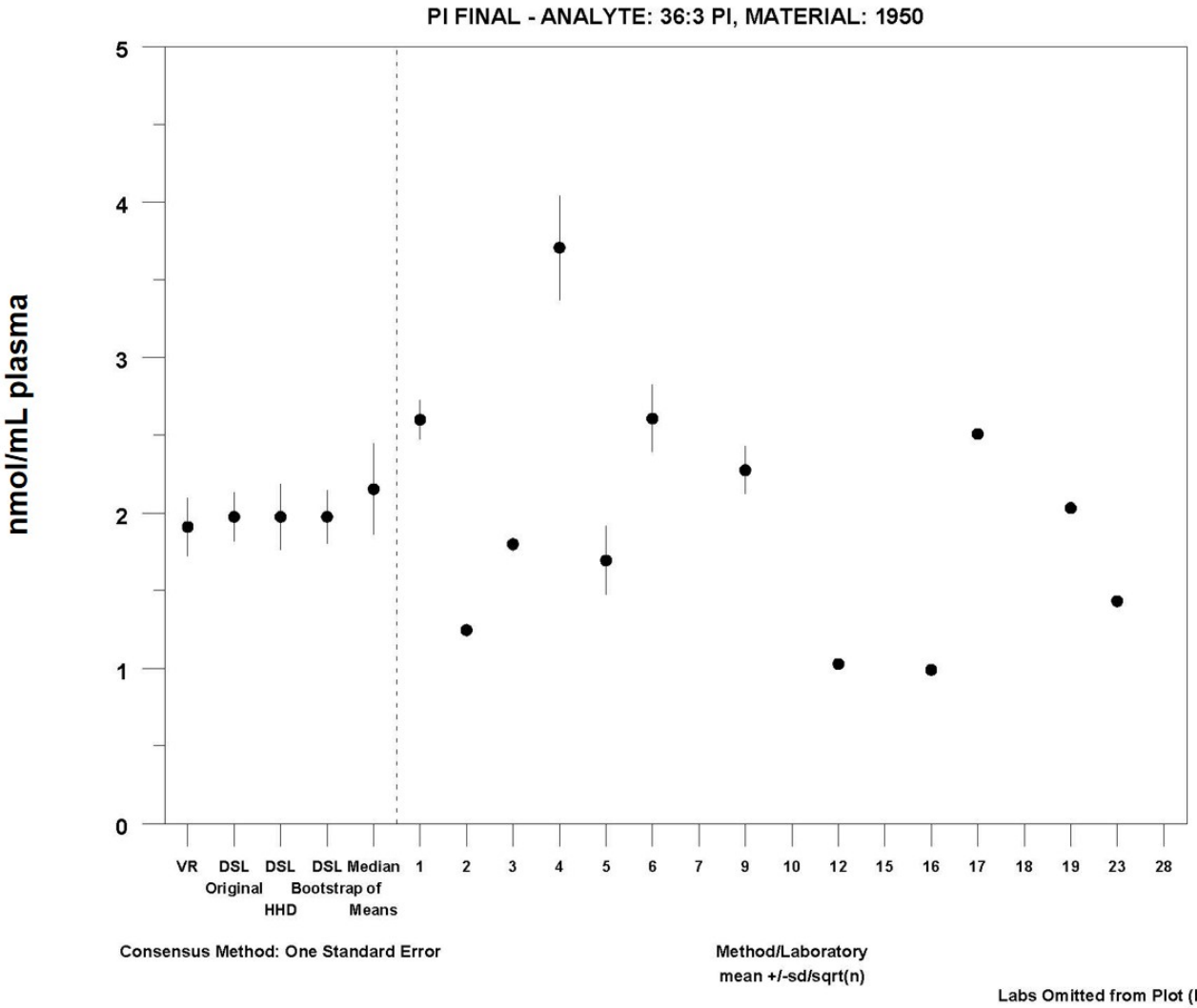
7: 15 ± 11; 15: 172 ± 15



Labs Omitted from Plot (But Not Analysis): 7 15

MEDM Location: 7.7 ± 0.93 nmol/mL

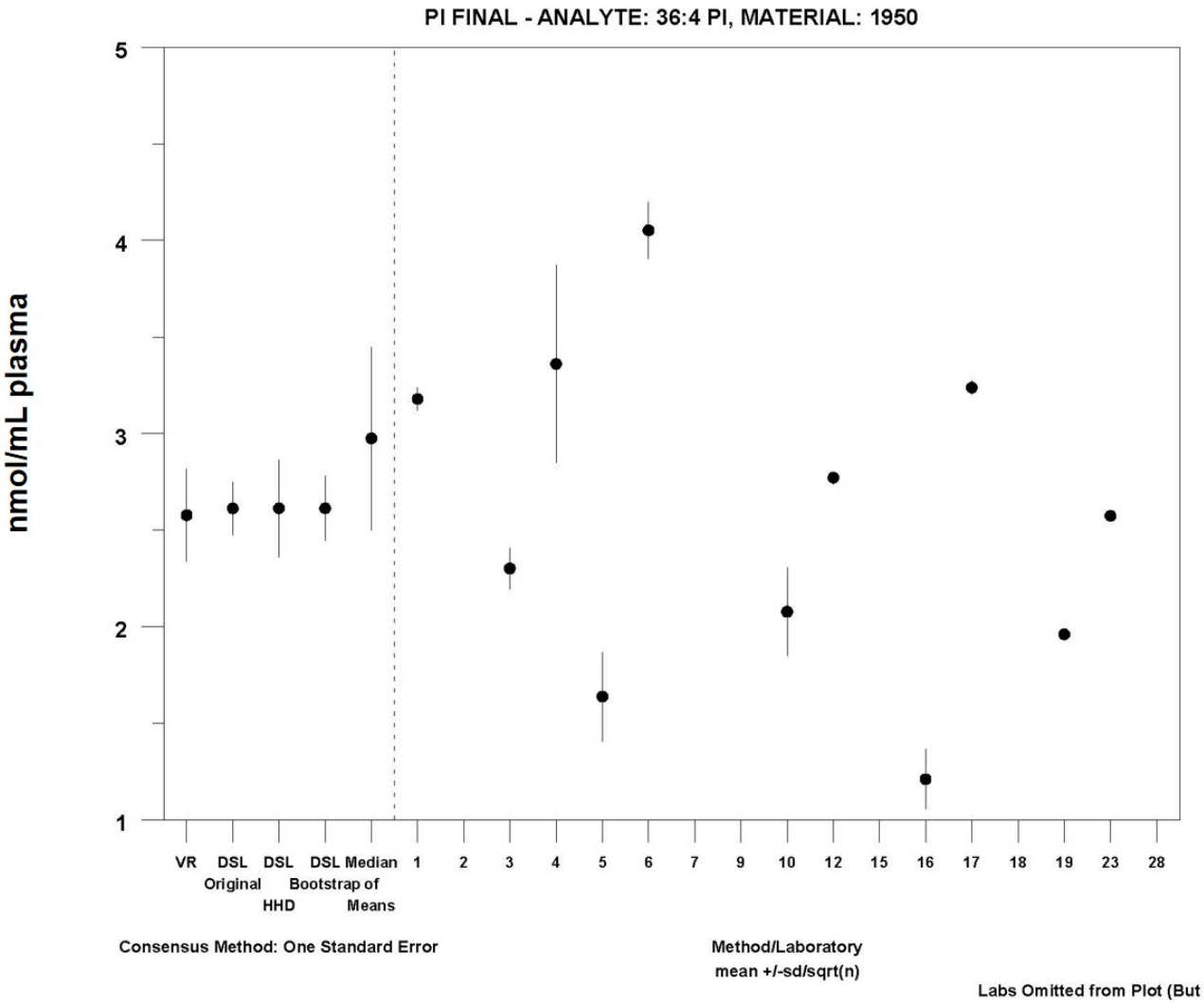
7: 70 ± 27; 15: 54 ± 5



Labs Omitted from Plot (But Not Analysis): 7 15

MEDM Location: 2.2 ± 0.29 nmol/mL

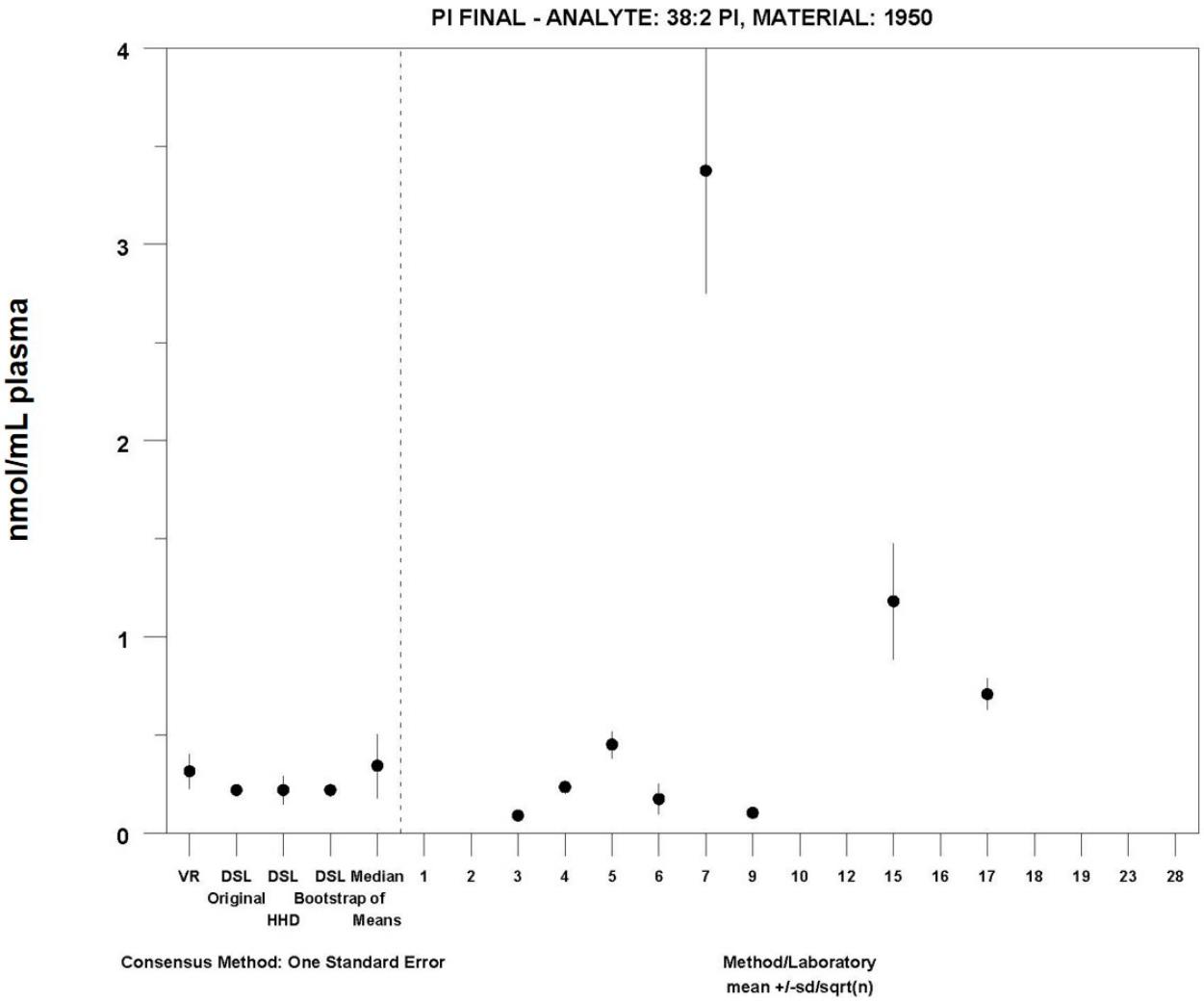
7: 14 ± 7; 15: 136 ± 27



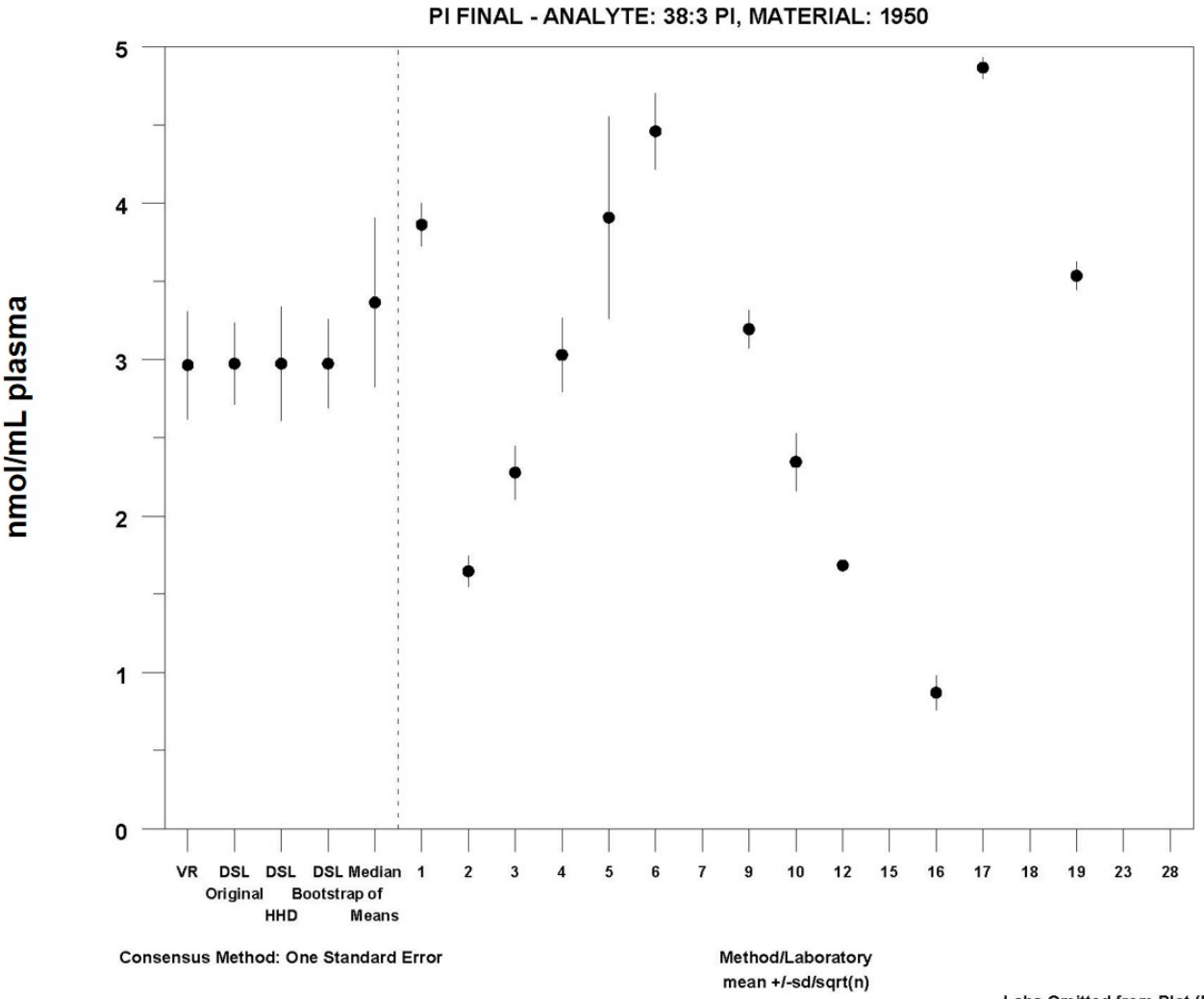
Labs Omitted from Plot (But Not Analysis): 7 9 15

7: 29 ± 13; 9: 51 ± 8; 15: 207 ± 102

MEDM Location: 3.0 ± 0.48 nmol/mL



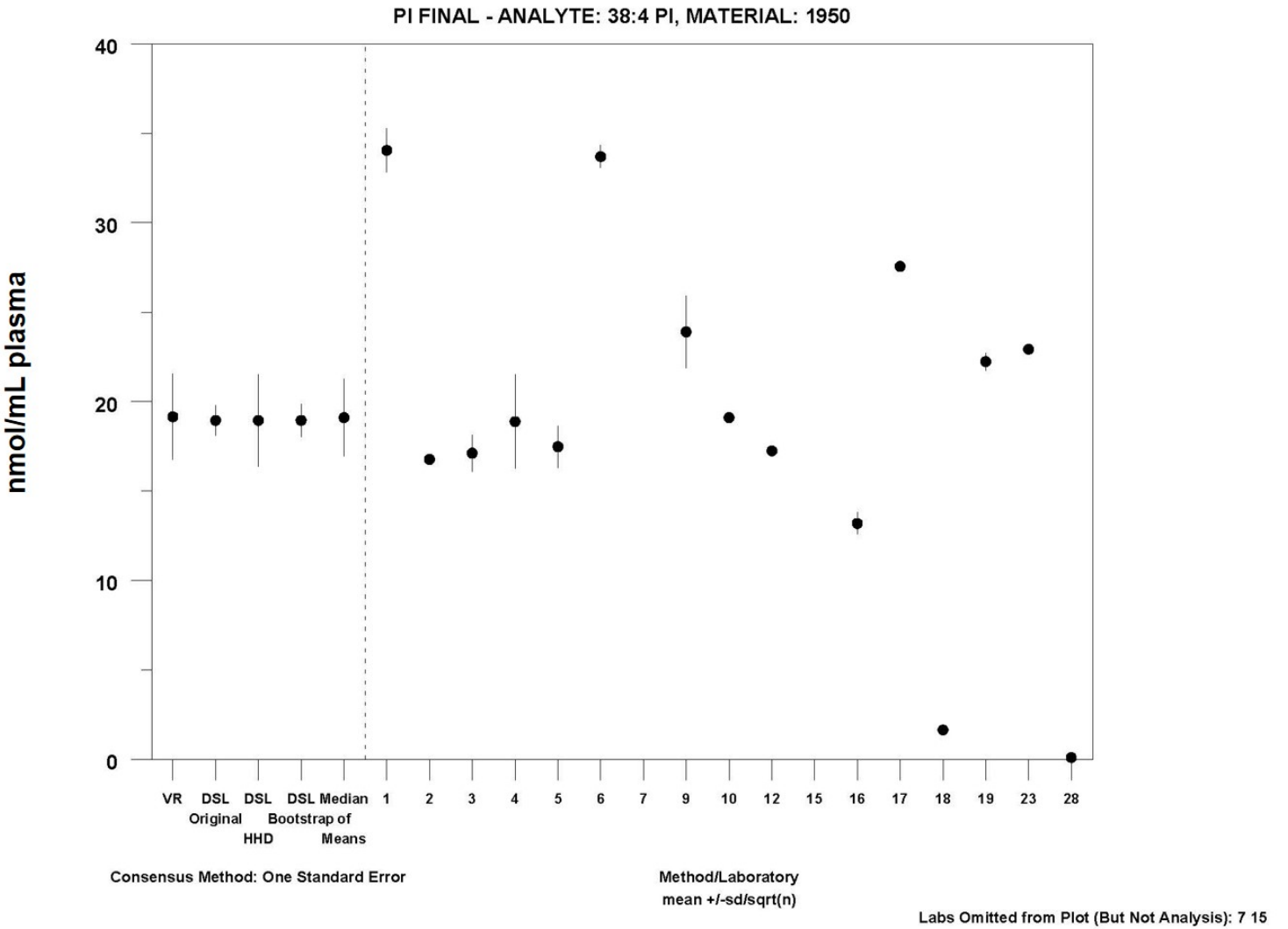
MEDM Location: 0.34 ± 0.16 nmol/mL



Labs Omitted from Plot (But Not Analysis): 7 15

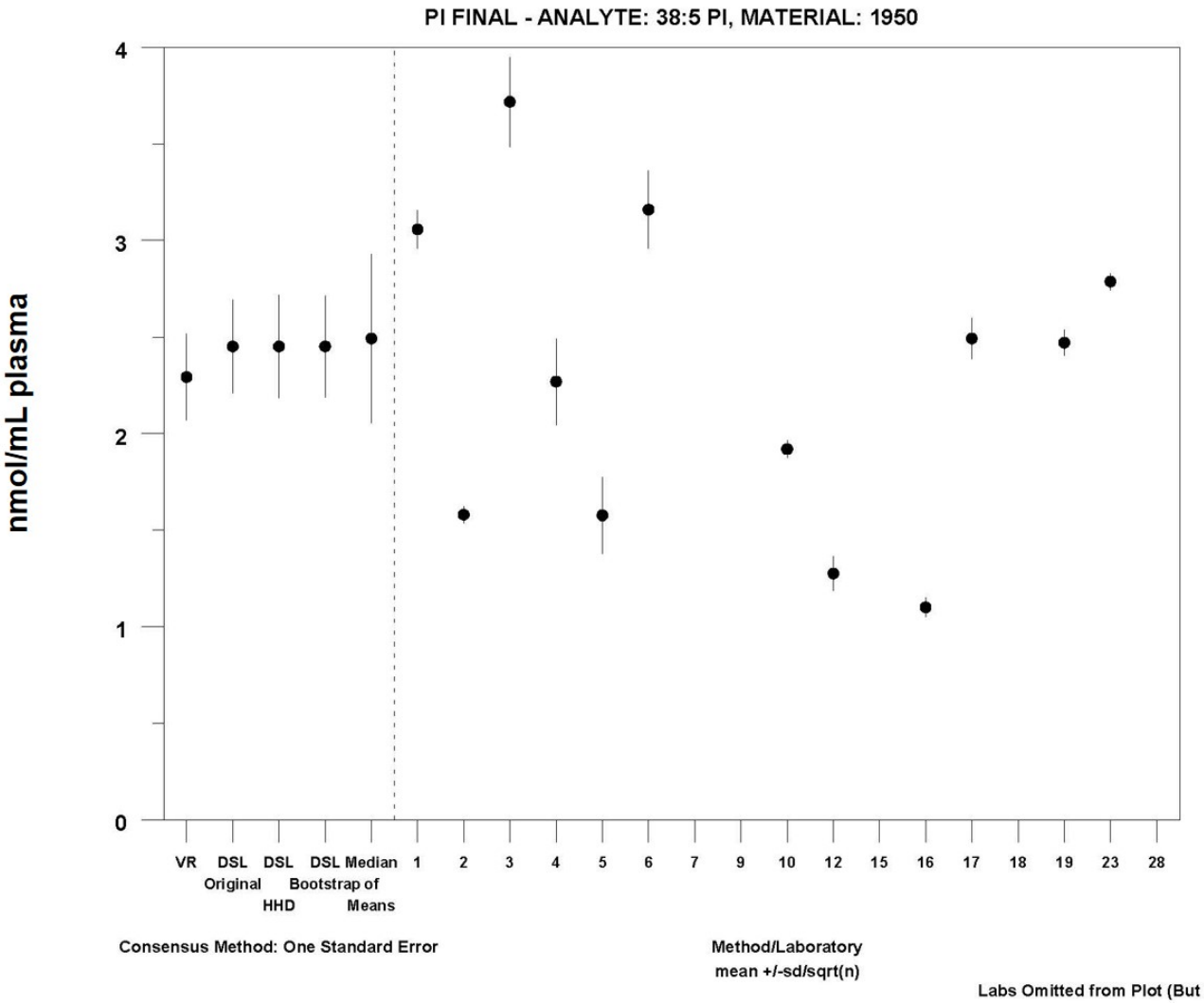
MEDM Location: 3.4 ± 0.54 nmol/mL

7: 32 ± 19; 15: 180 ± 46



MEDM Location: 19 ± 2.2 nmol/mL

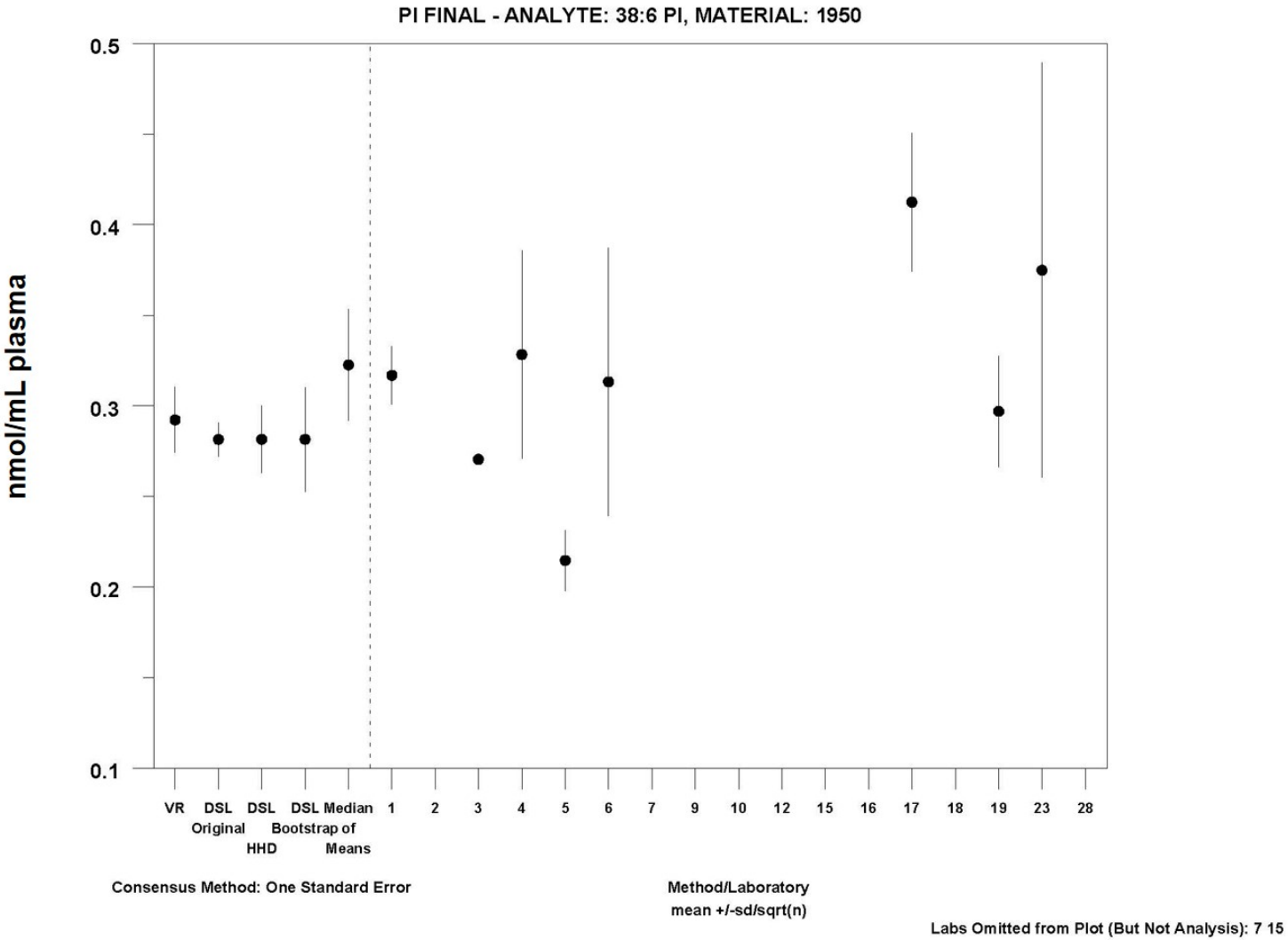
7: 208 ± 83; 15: 353 ± 101



Labs Omitted from Plot (But Not Analysis): 7 9 15

7: 15 ± 5; 9: 16 ± 5; 15: 141 ± 70

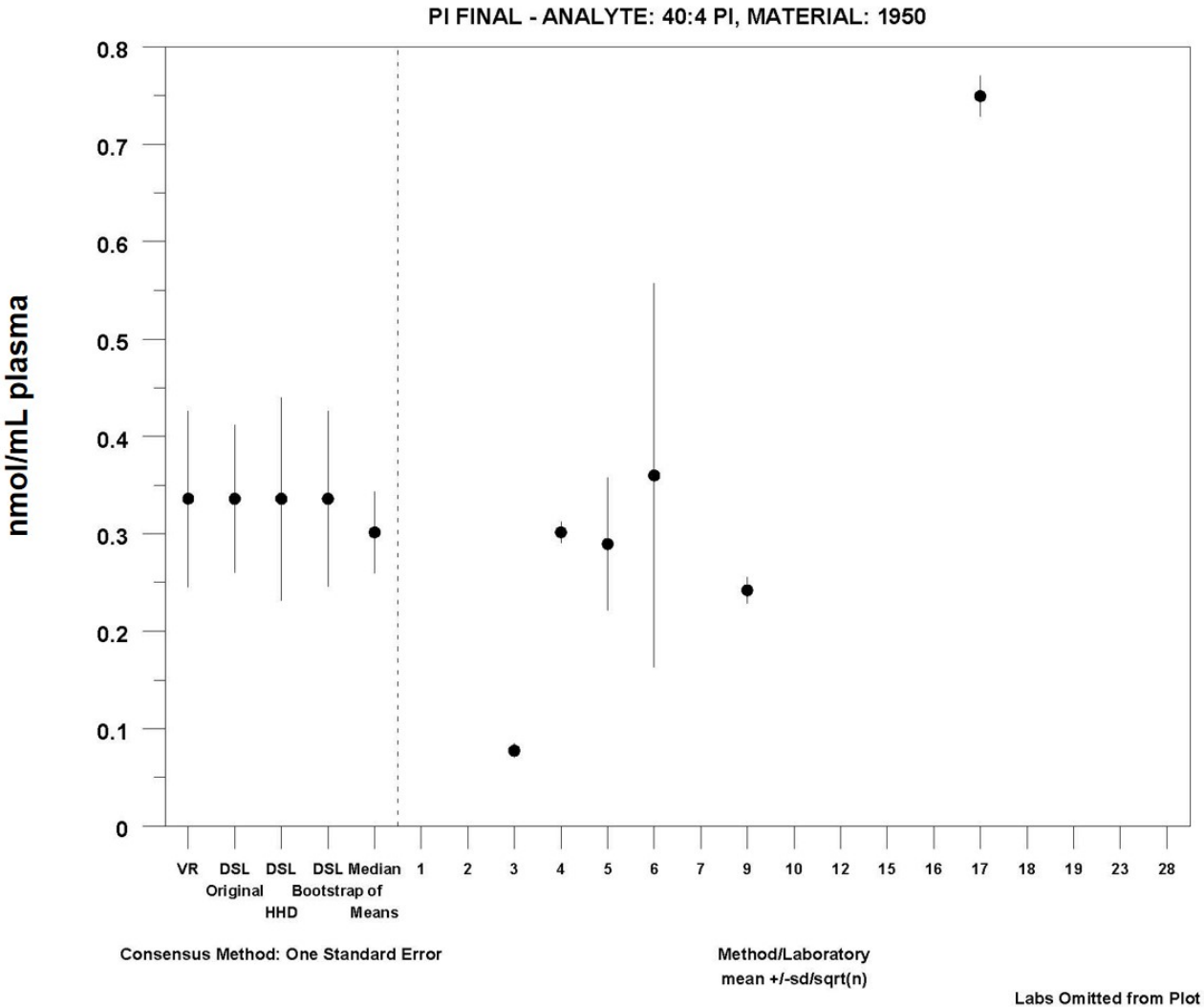
MEDM Location: 2.5 ± 0.44 nmol/mL



Labs Omitted from Plot (But Not Analysis): 7 15

MEDM Location: 0.32 ± 0.031 nmol/mL

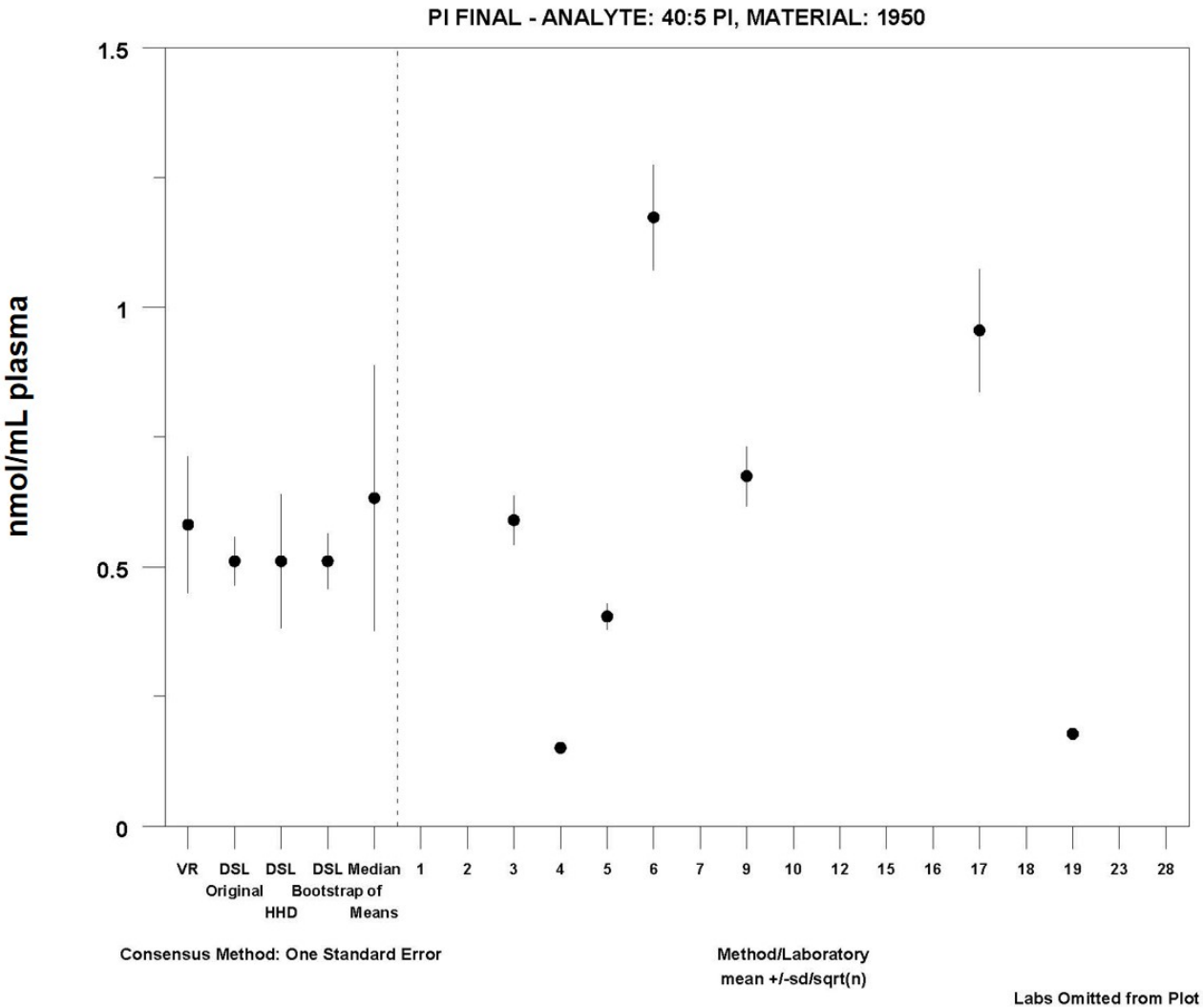
7: 7 ± 3; 15: 32 ± 11



Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 0.30 ± 0.042 nmol/mL

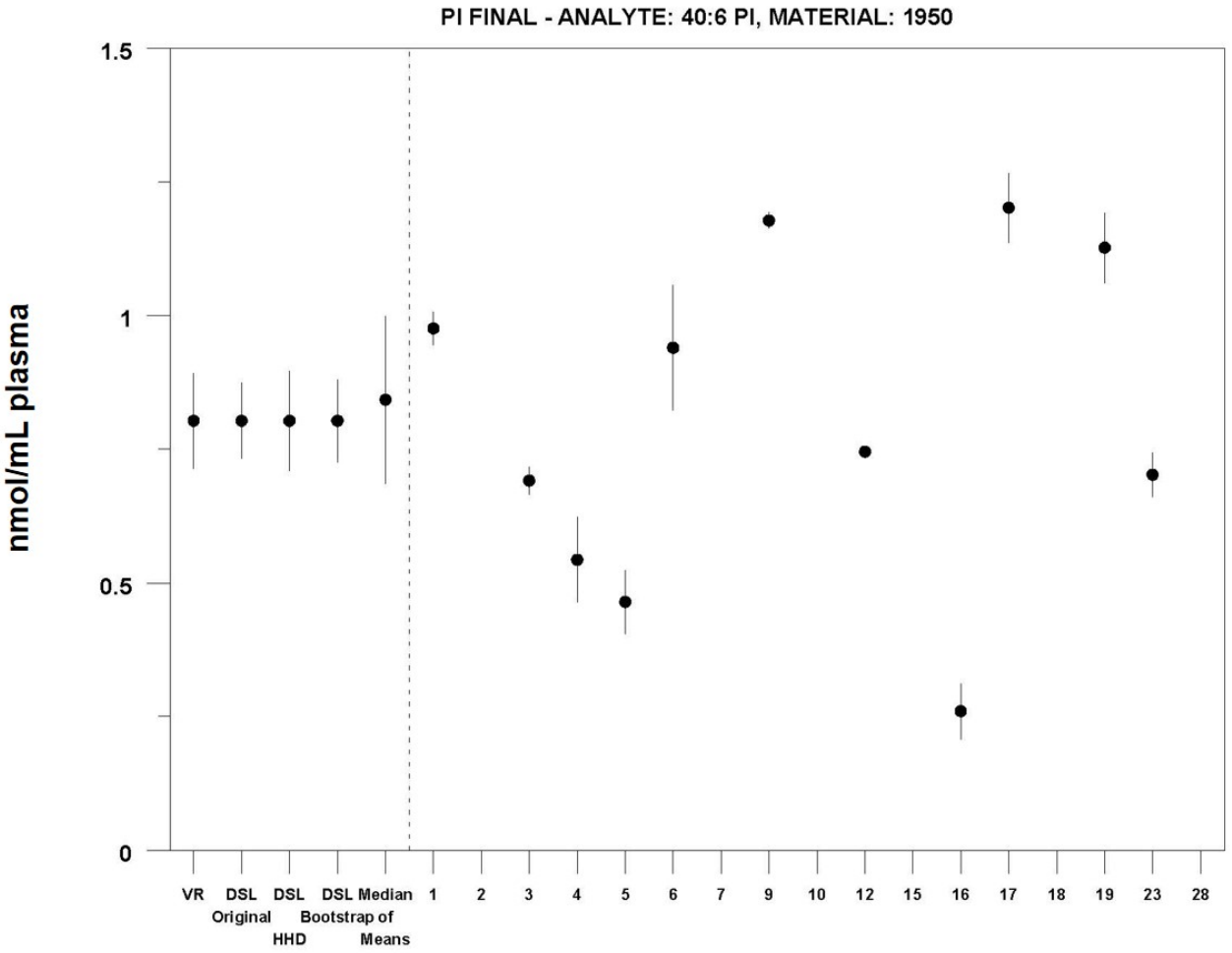
15: 19 ± 14



Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 0.63 ± 0.26 nmol/mL

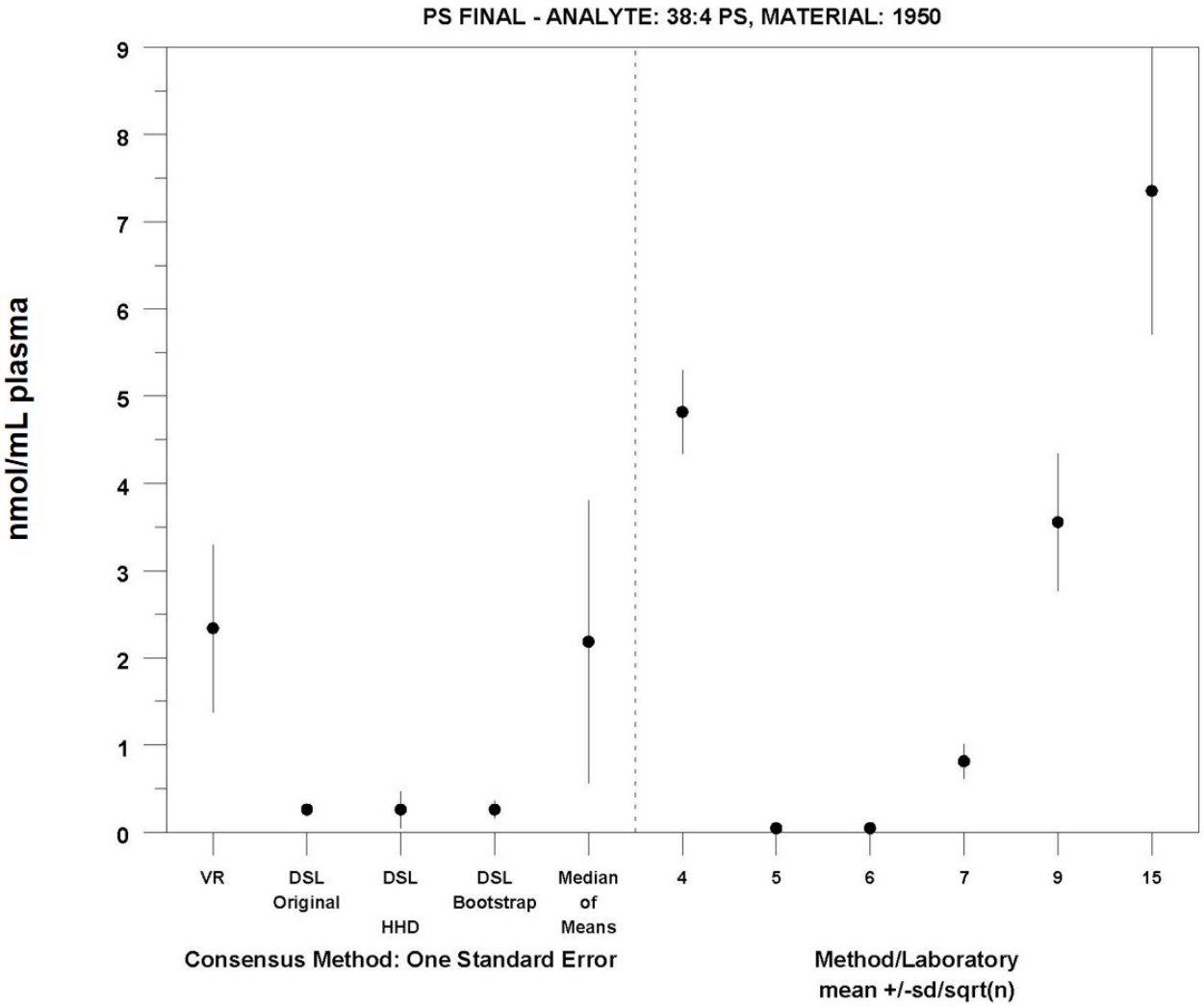
15: 10 ± 4



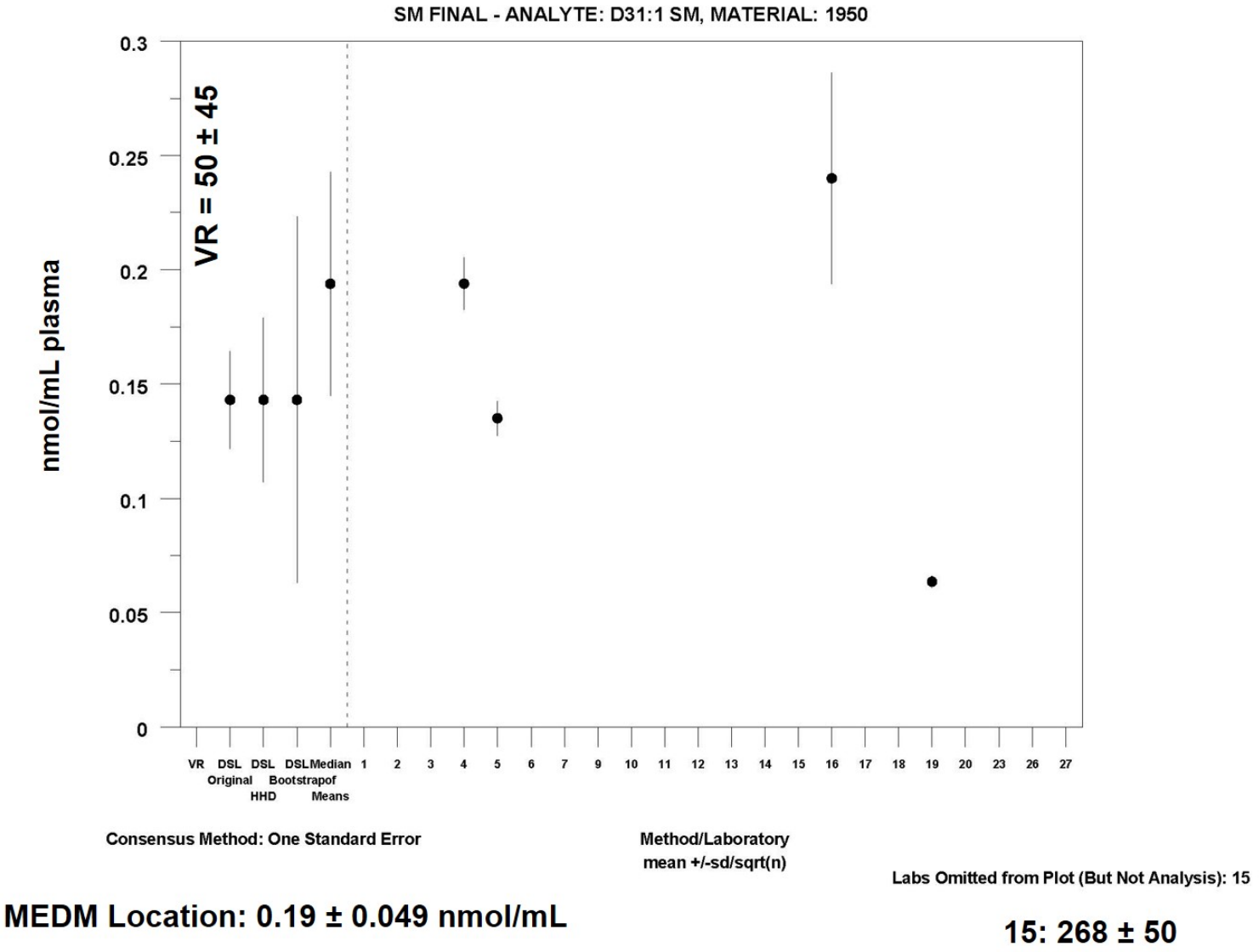
Labs Omitted from Plot (But Not Analysis): 15

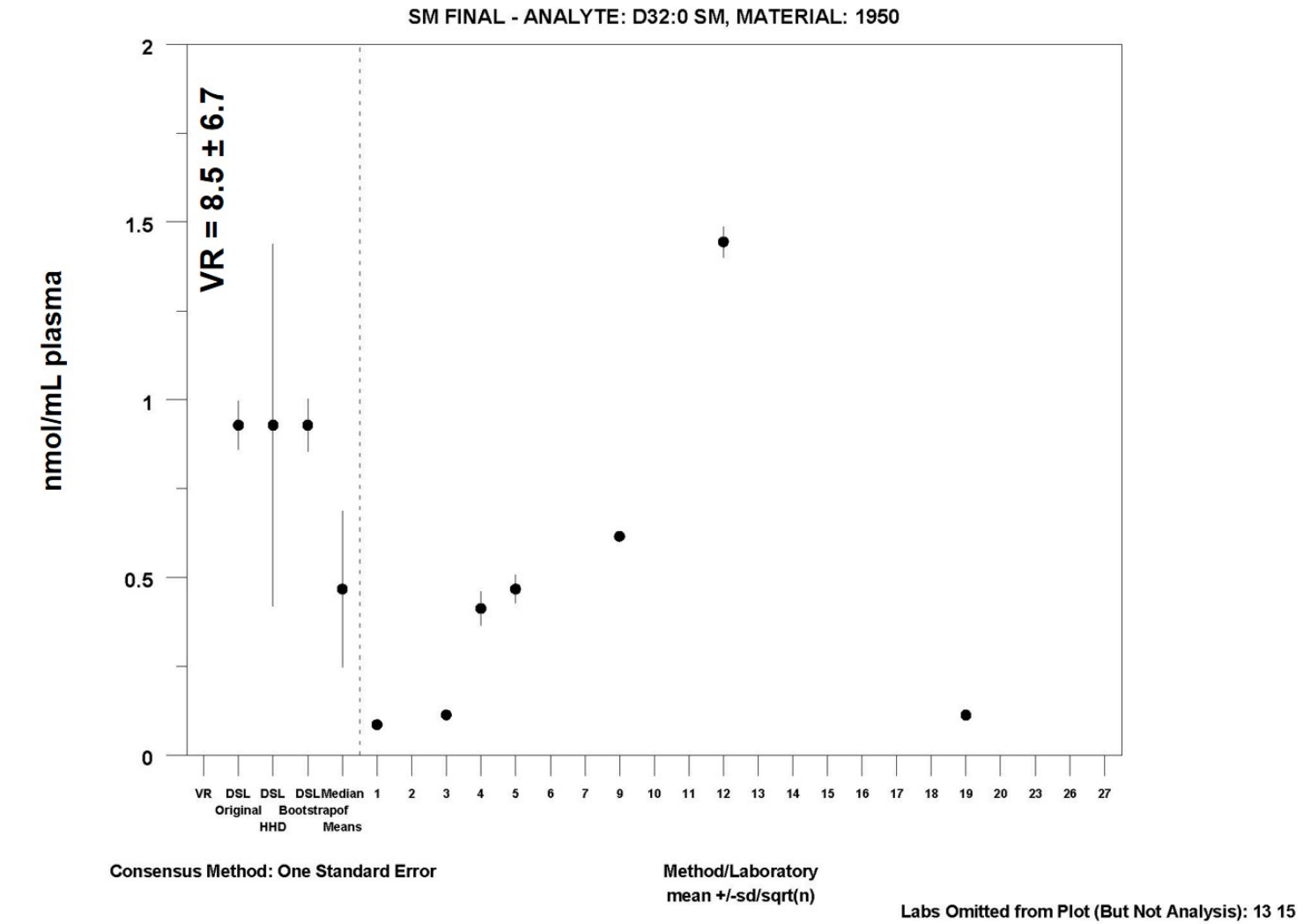
MEDM Location: 0.84 ± 0.16 nmol/mL

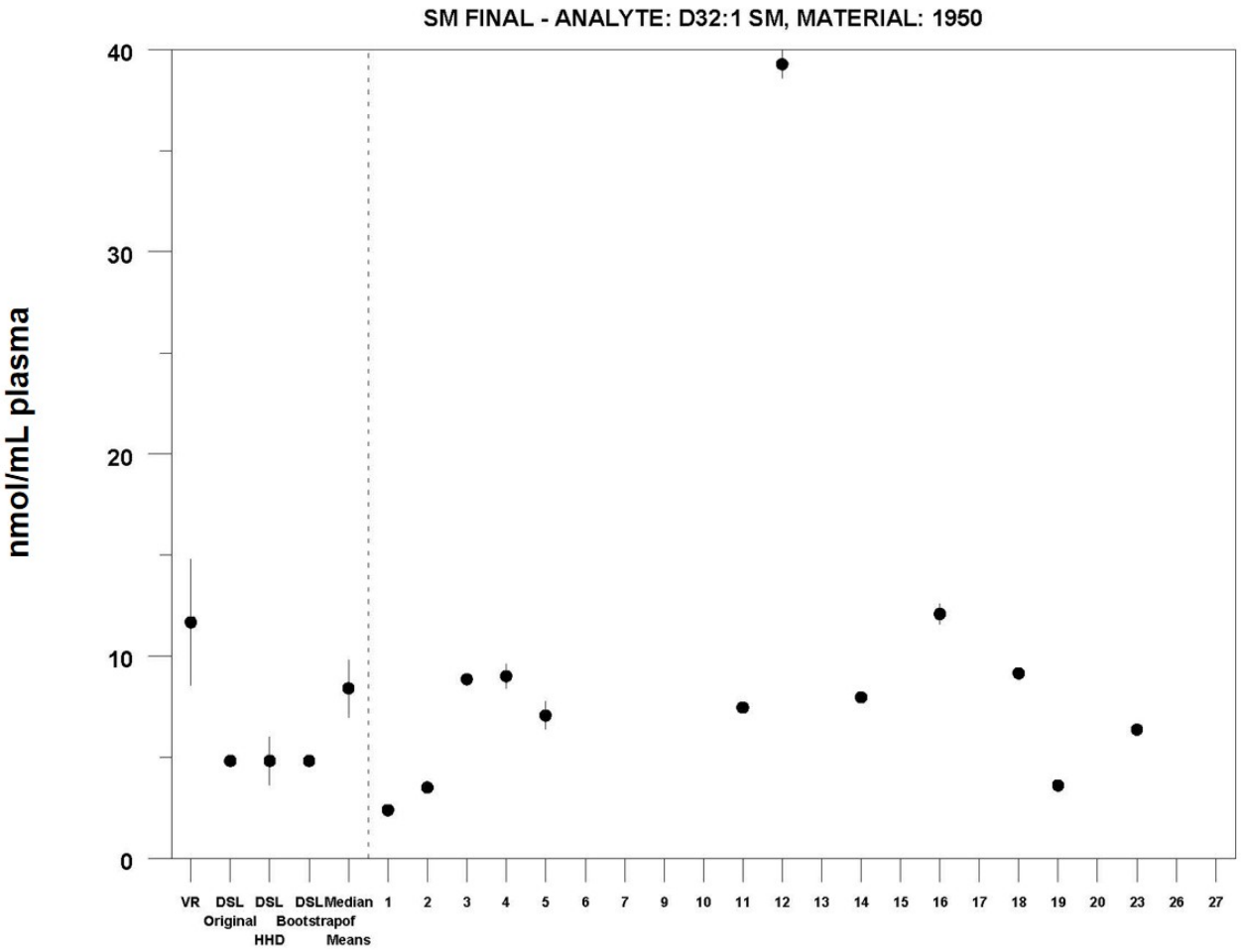
15: 16 ± 14



MEDM Location: 2.2 ± 1.6 nmol/mL



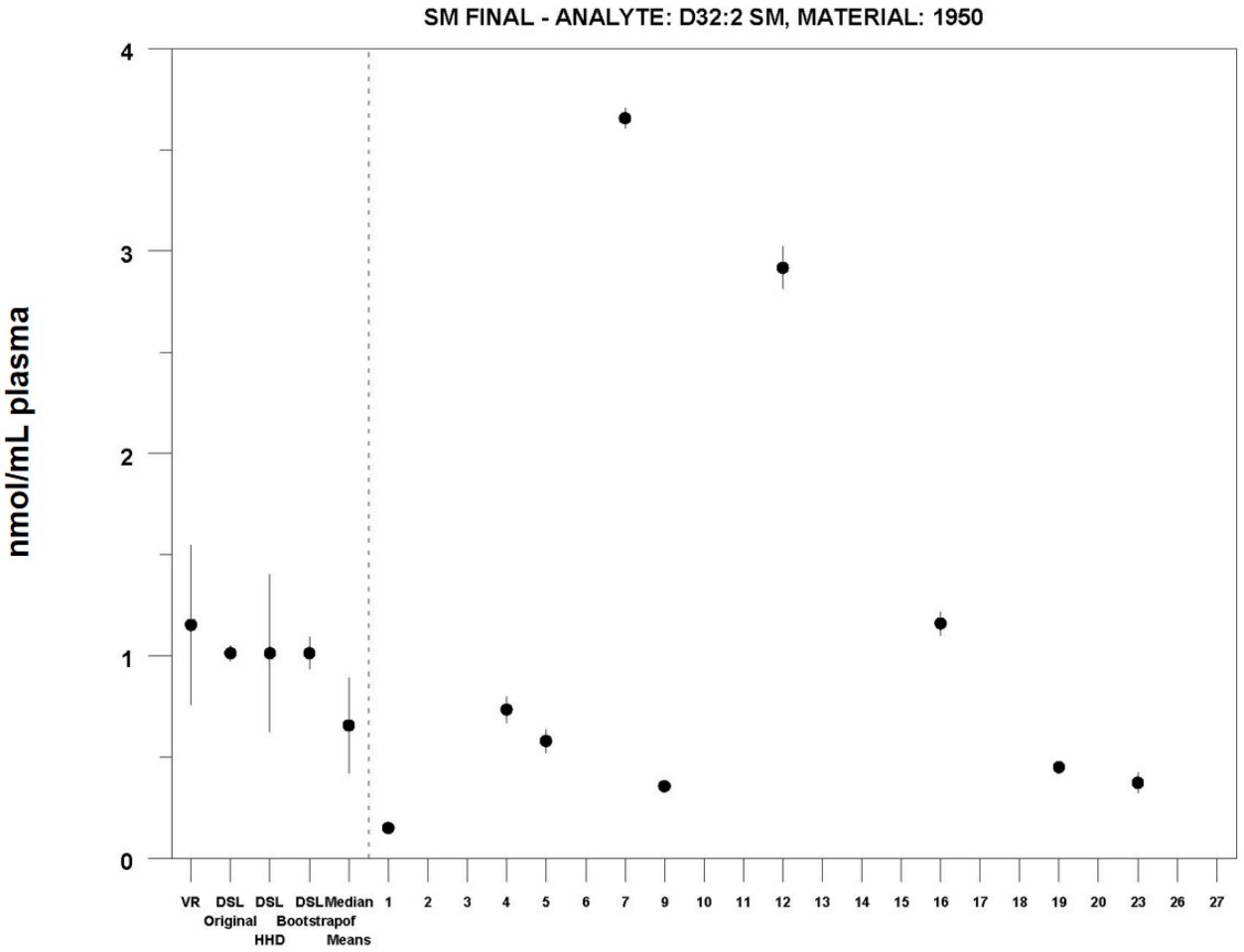


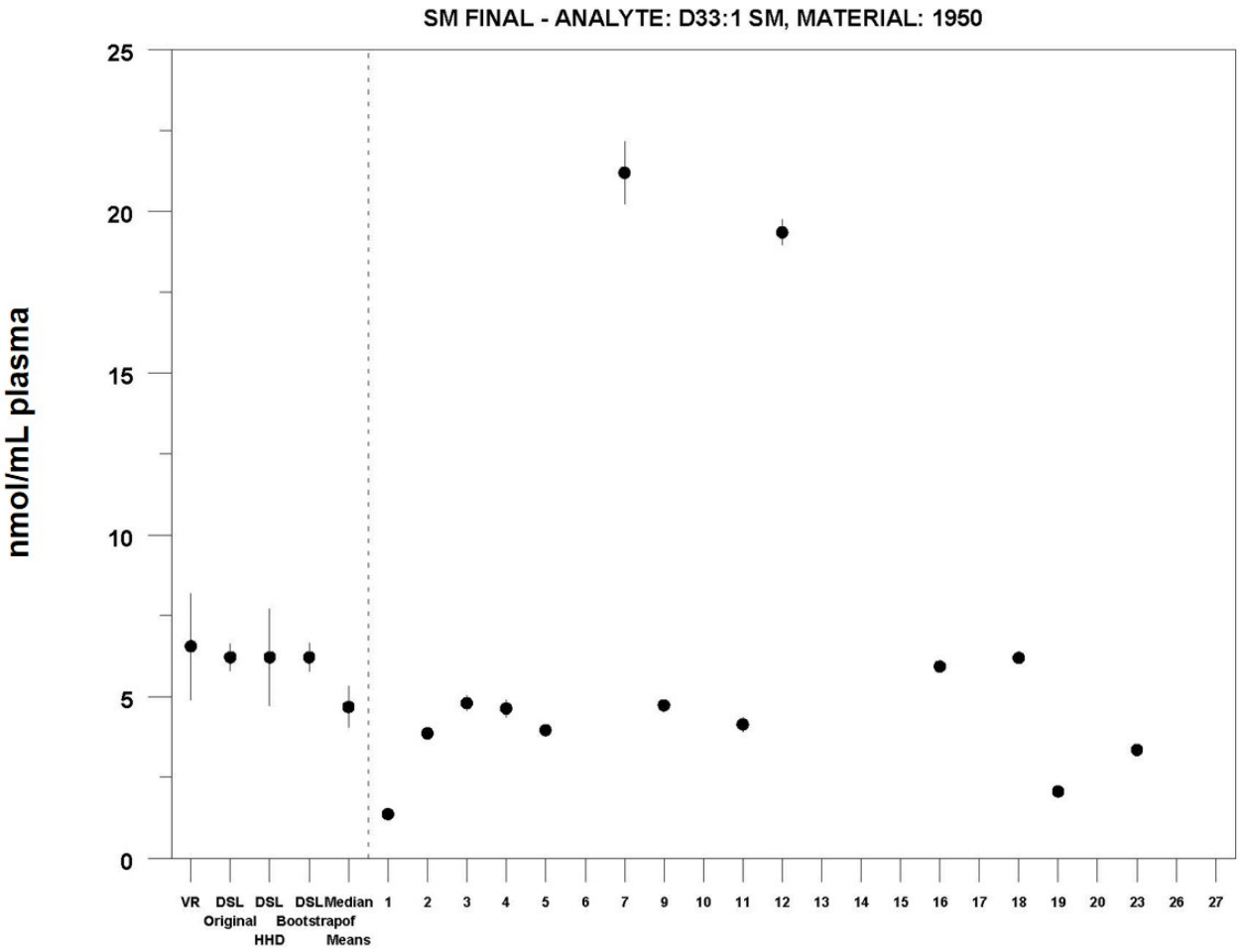


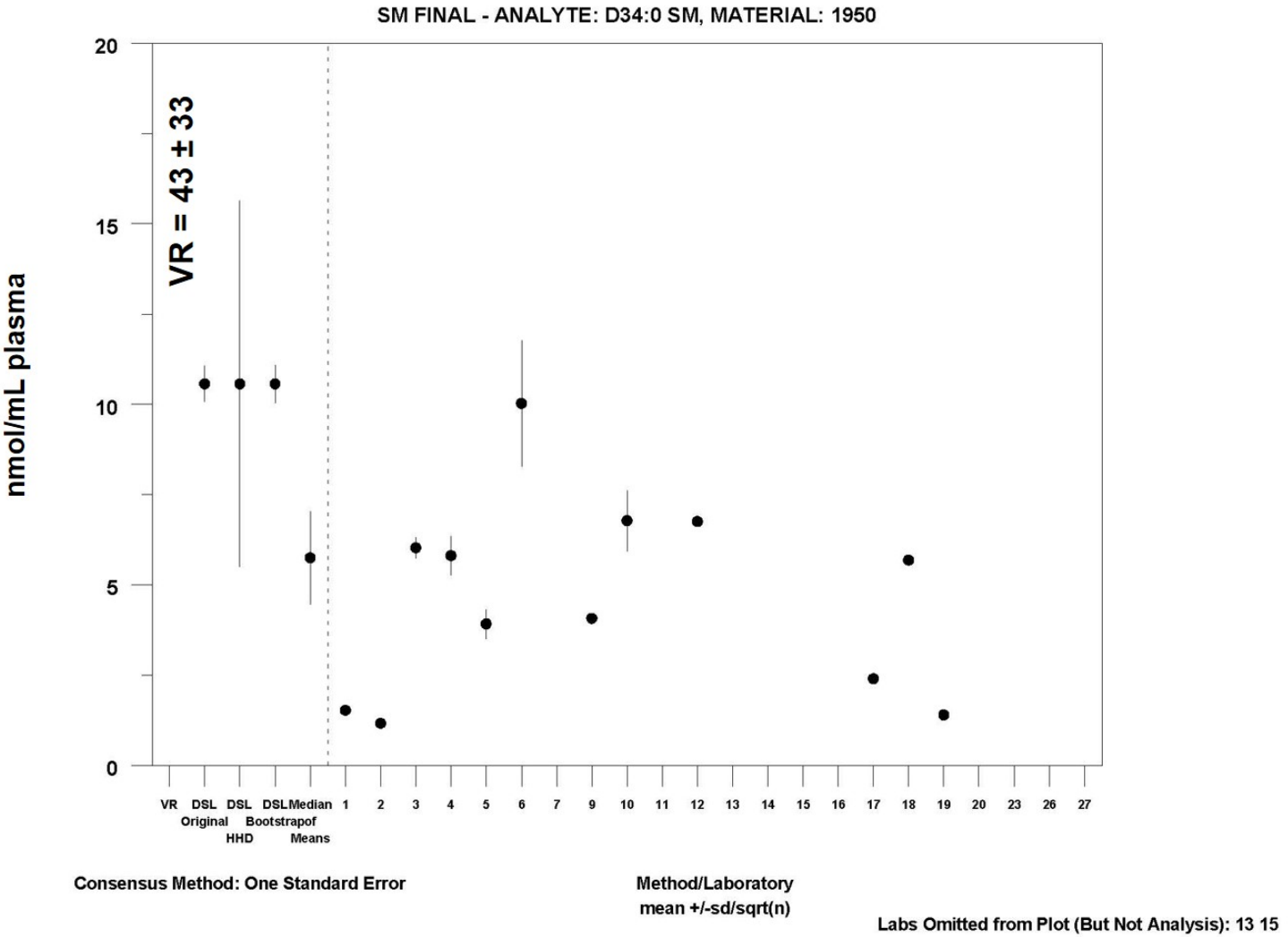
MEDM Location: 8.4 ± 1.4 nmol/mL

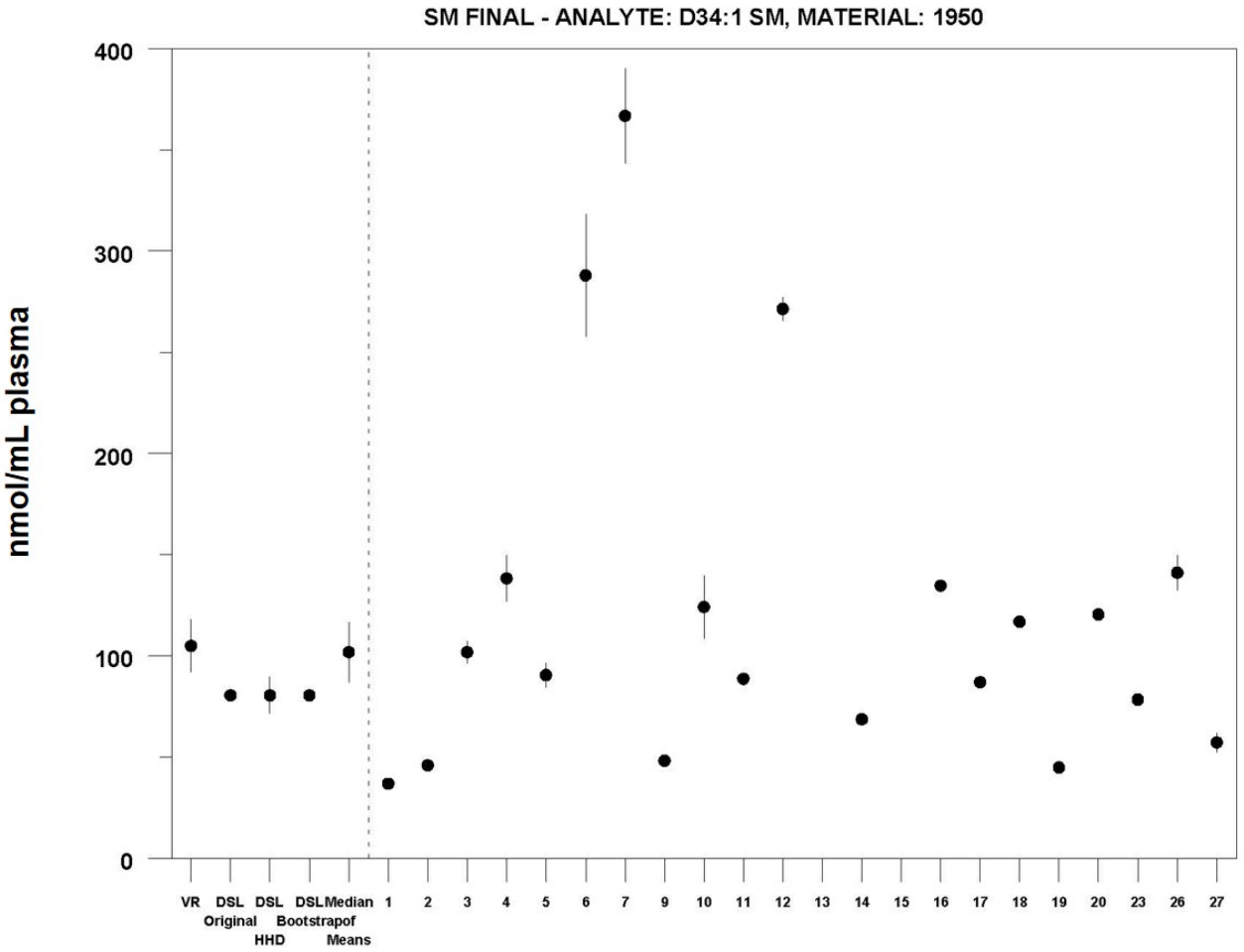
Labs Omitted from Plot (But Not Analysis): 7 15

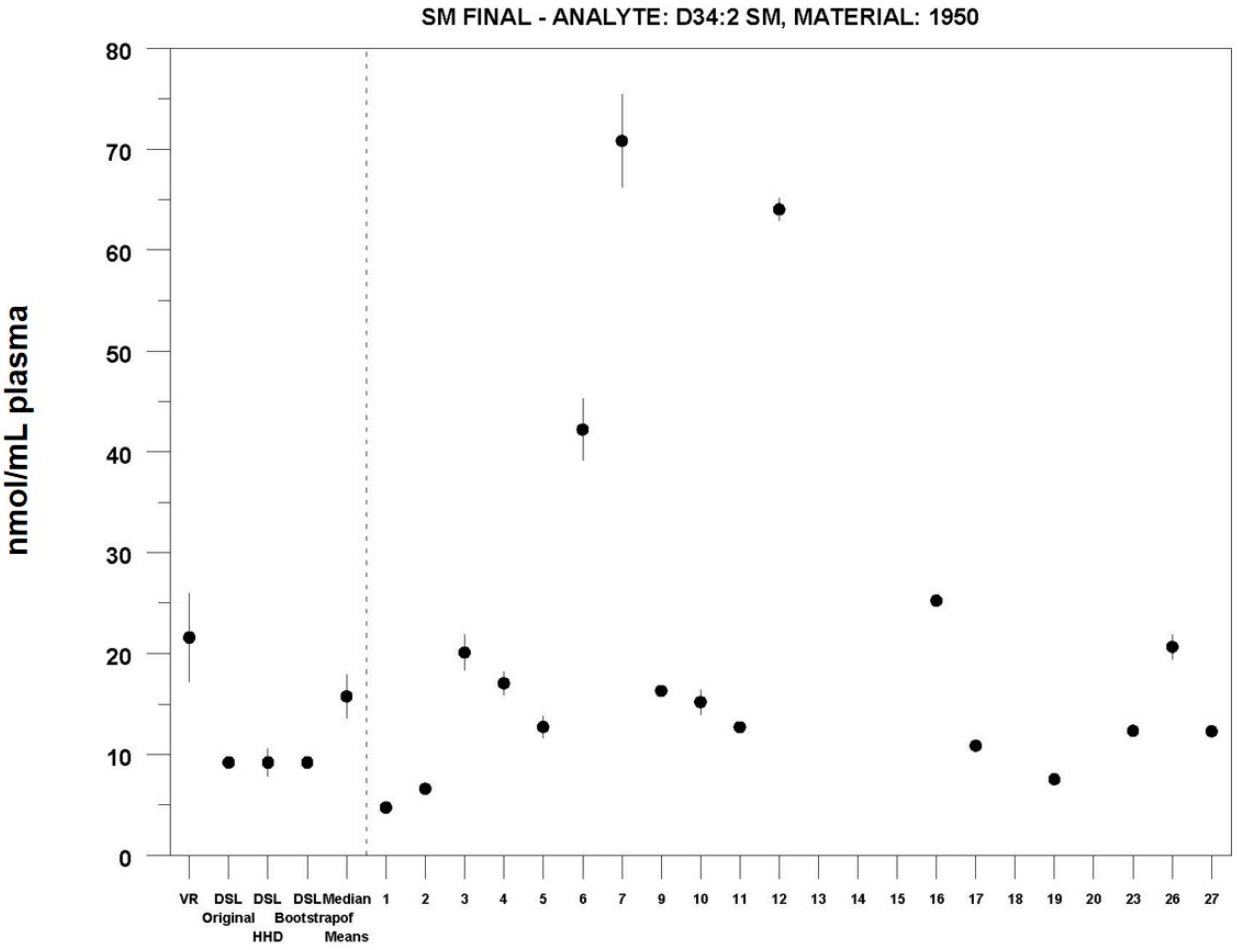
7: 37 ± 6; 15: 3719 ± 1464







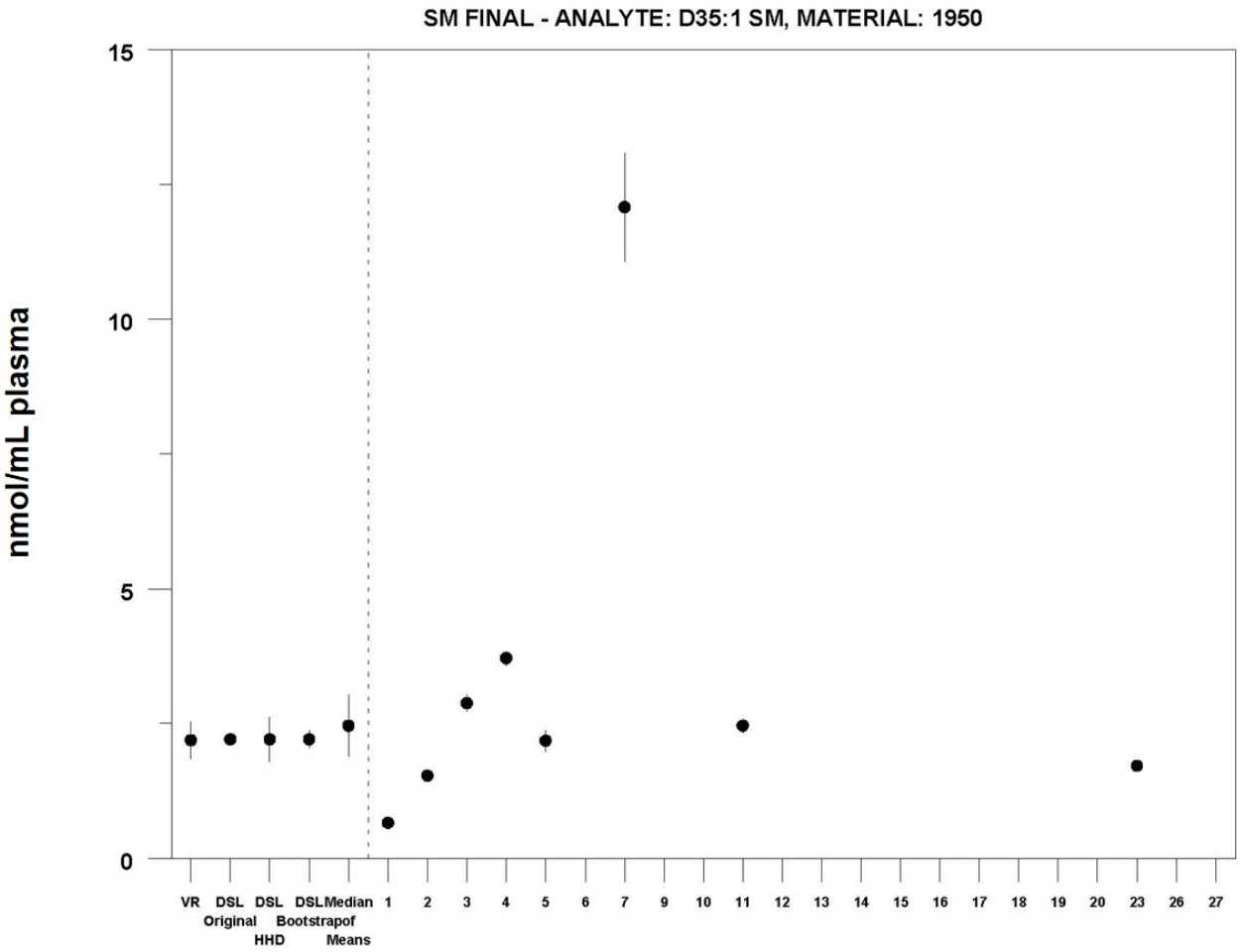




MEDM Location: 16 ± 2.2 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

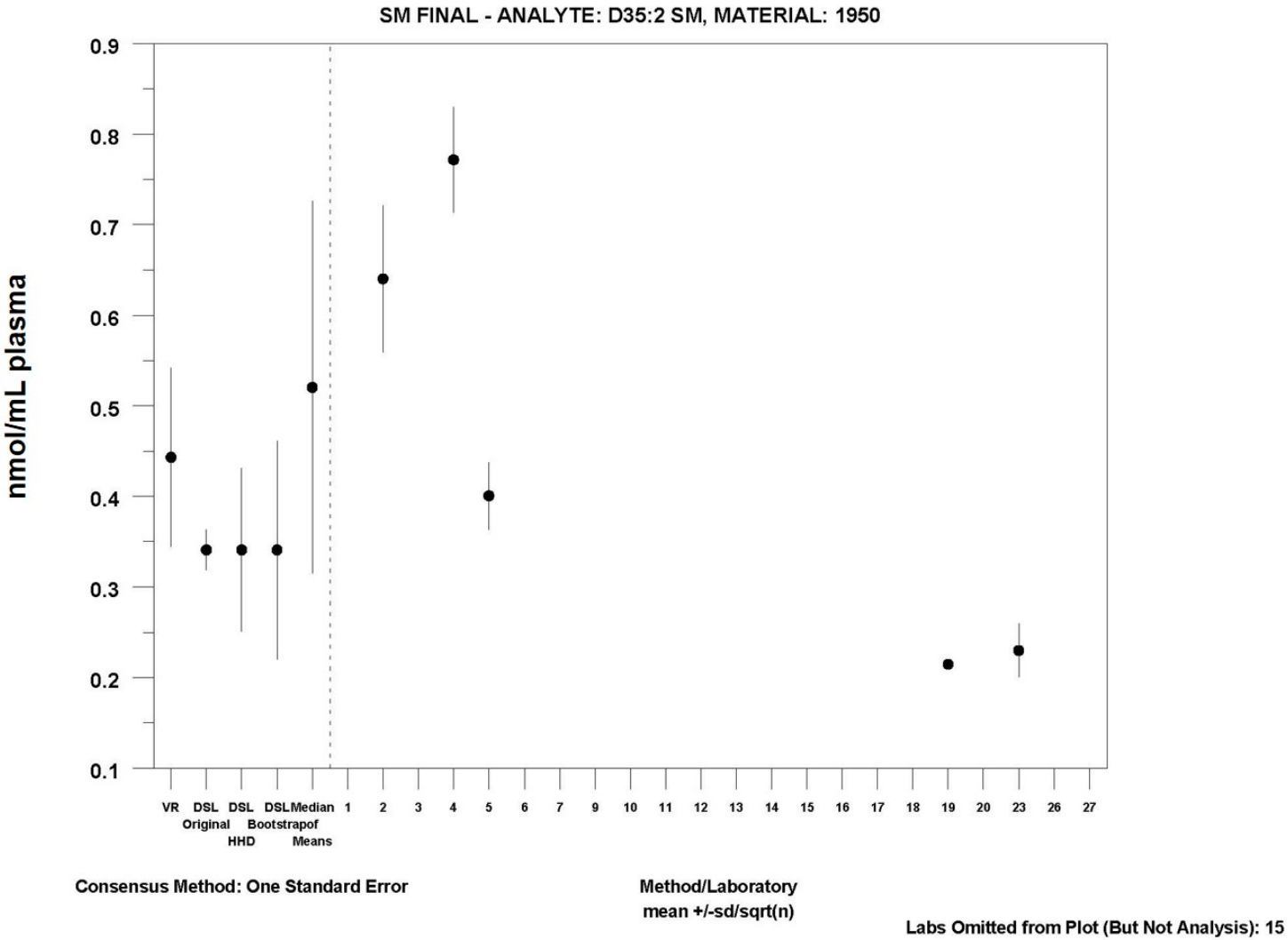
15: 3215 ± 2116

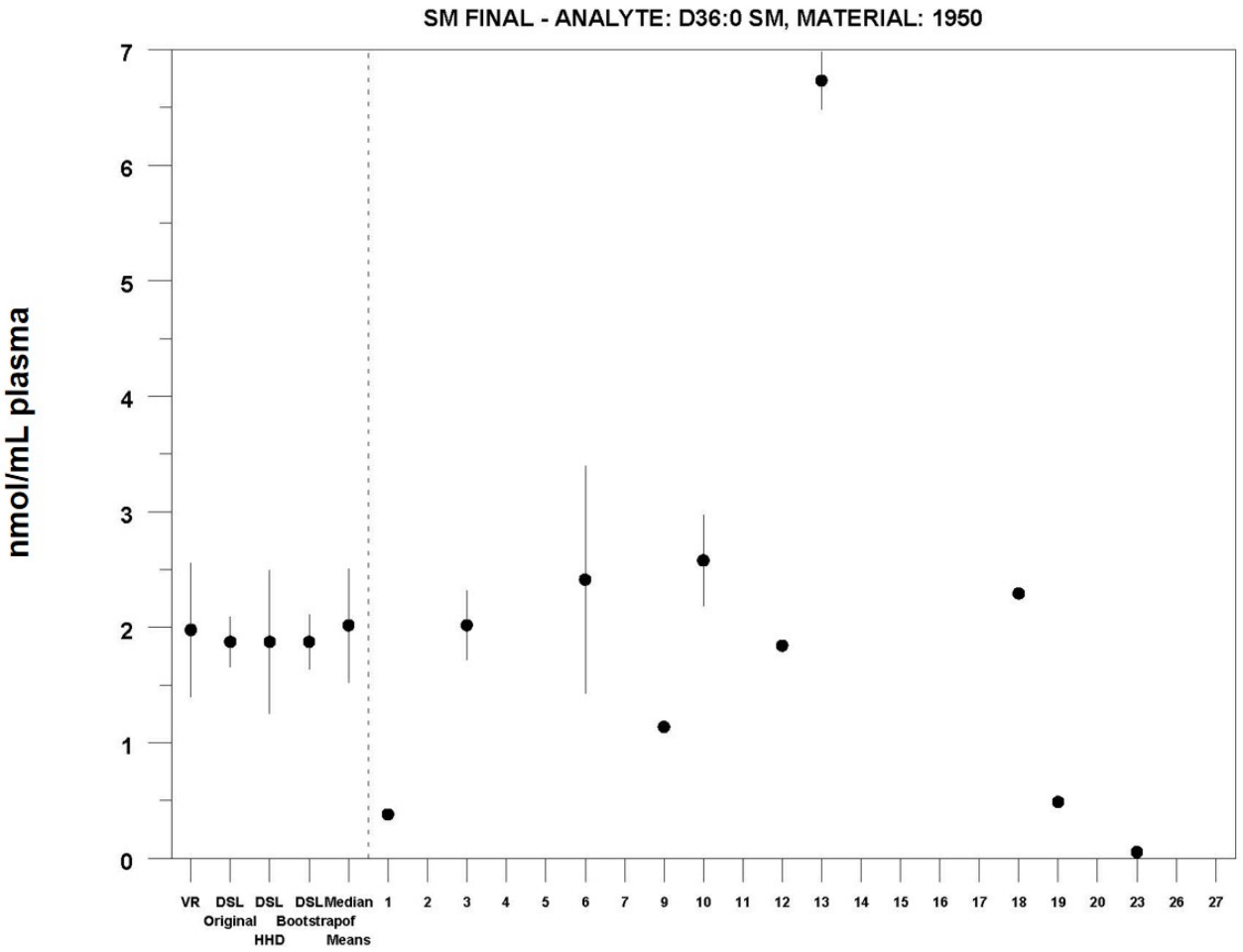


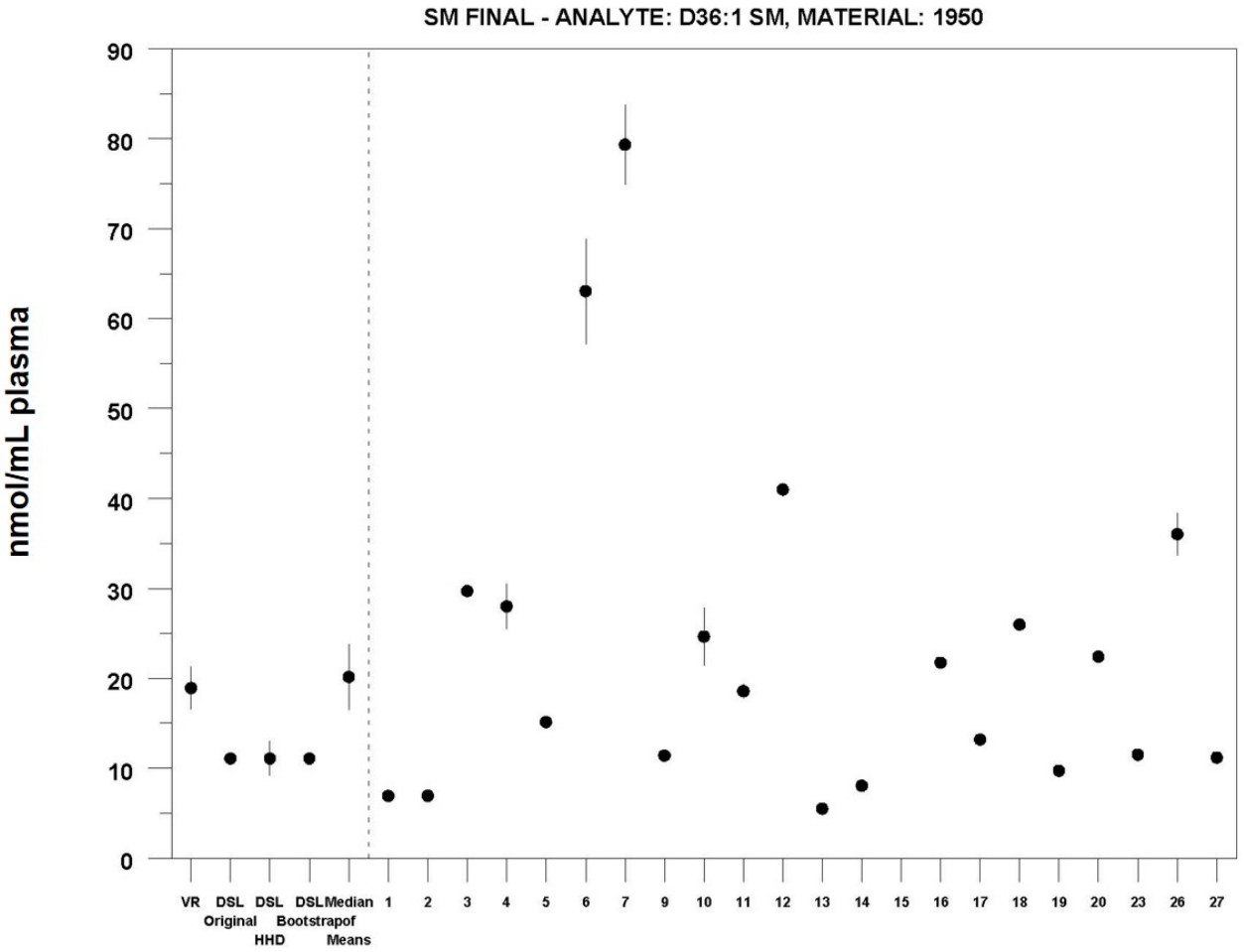
Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 2.5 ± 0.58 nmol/mL

15: 421 ± 59



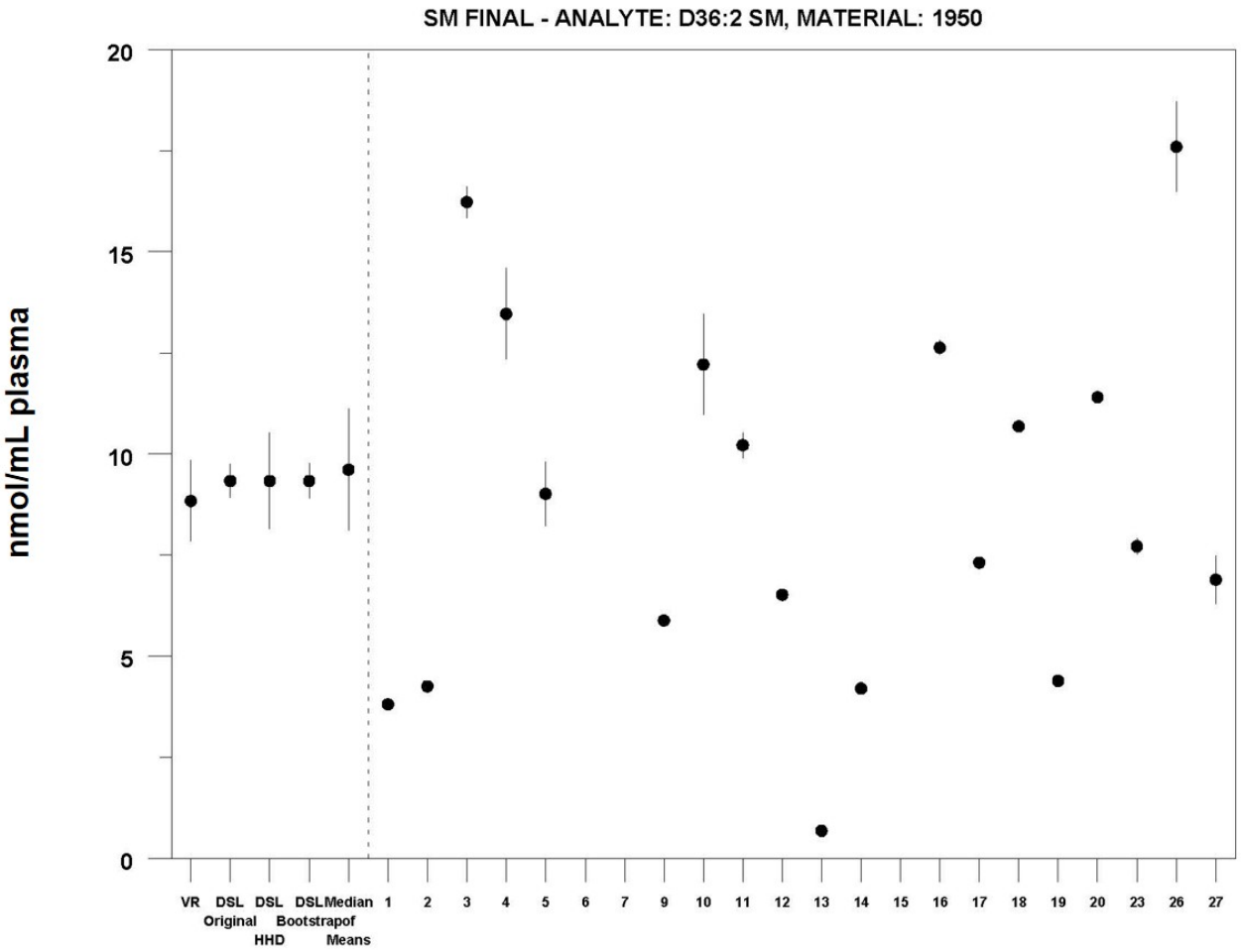




MEDM Location: 20 ± 3.7 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

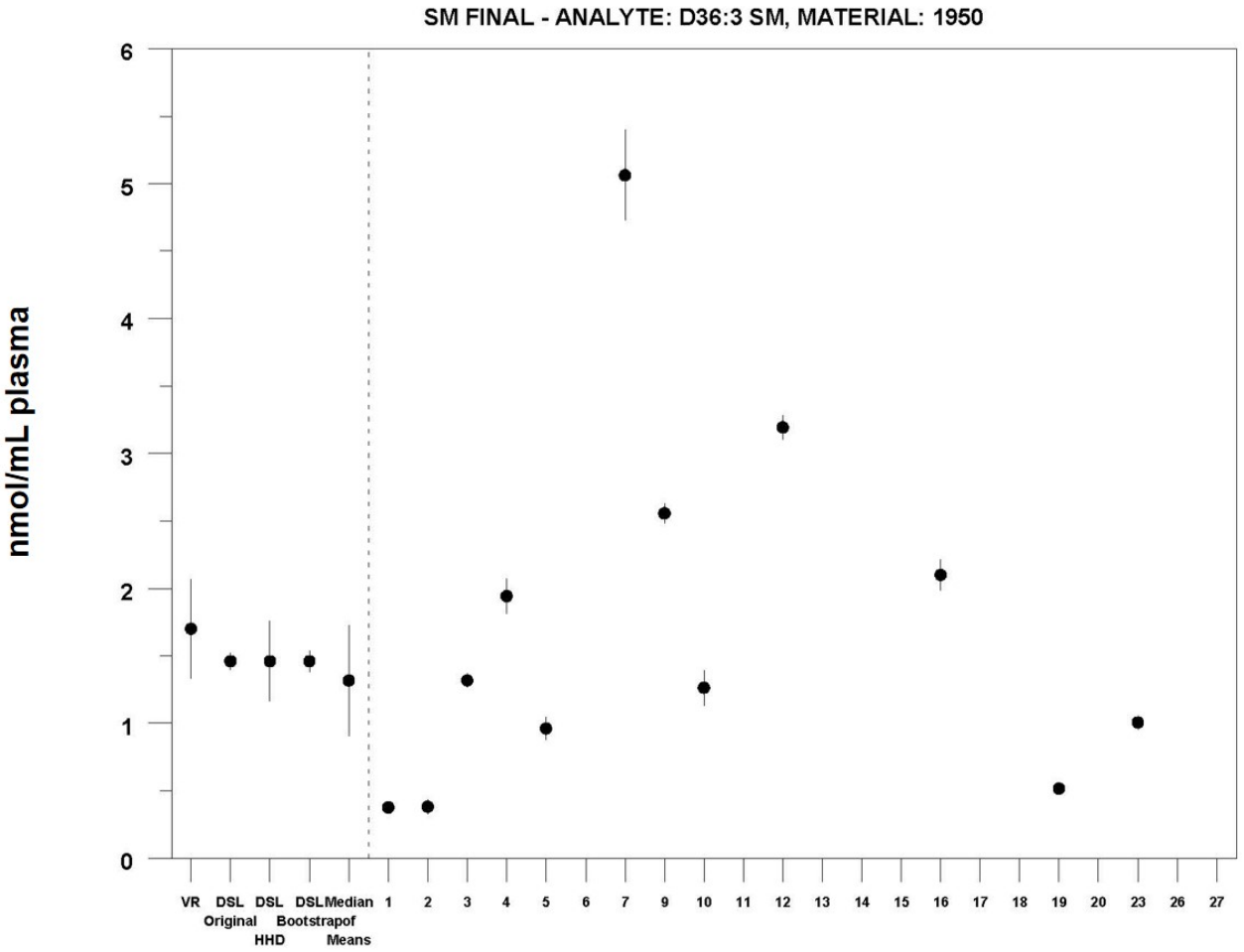
15: 1044 ± 59

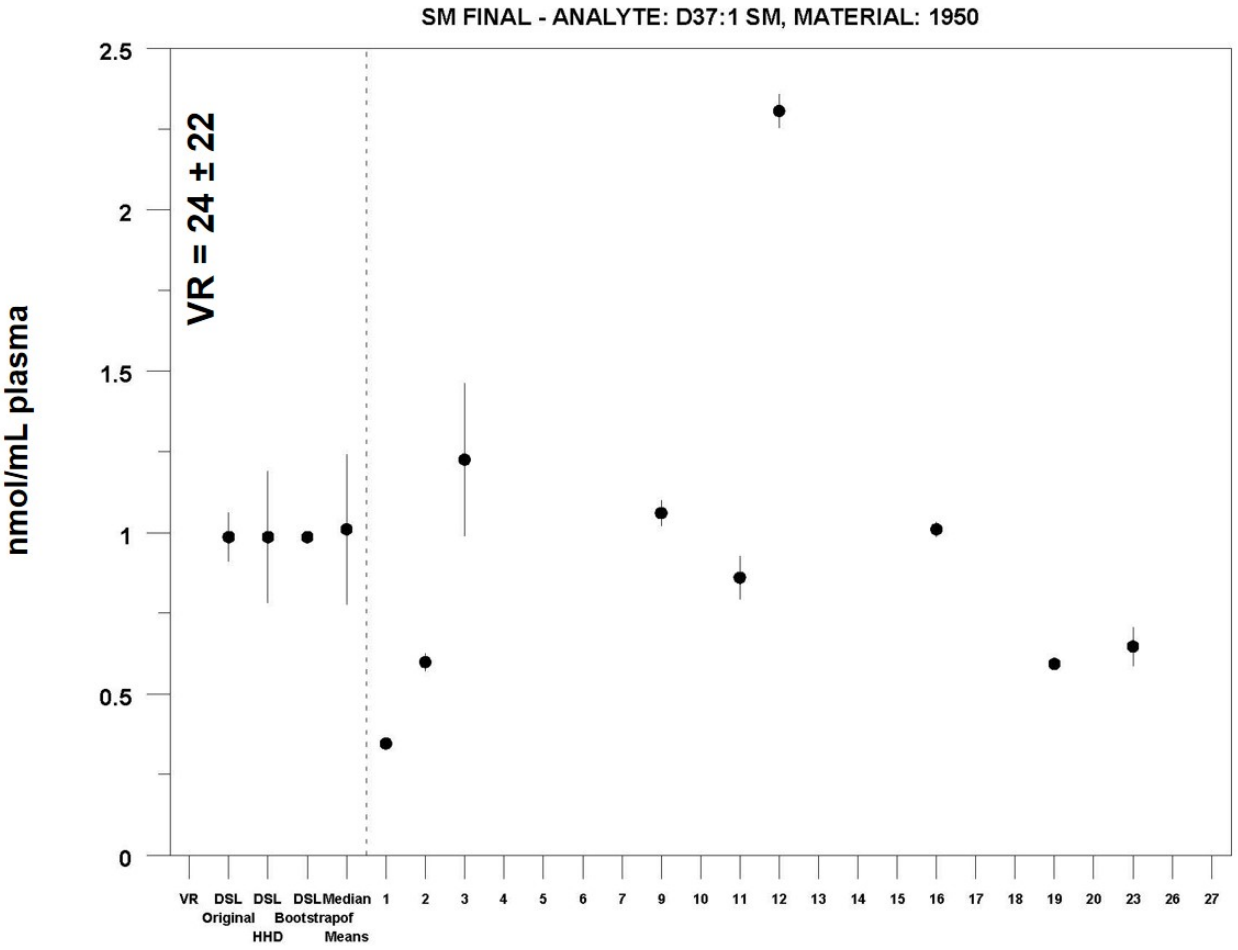


MEDM Location: 9.6 ± 1.5 nmol/mL

Labs Omitted from Plot (But Not Analysis): 6 7 15

6: 33 ± 4; 7: 48 ± 7; 15: 705 ± 88





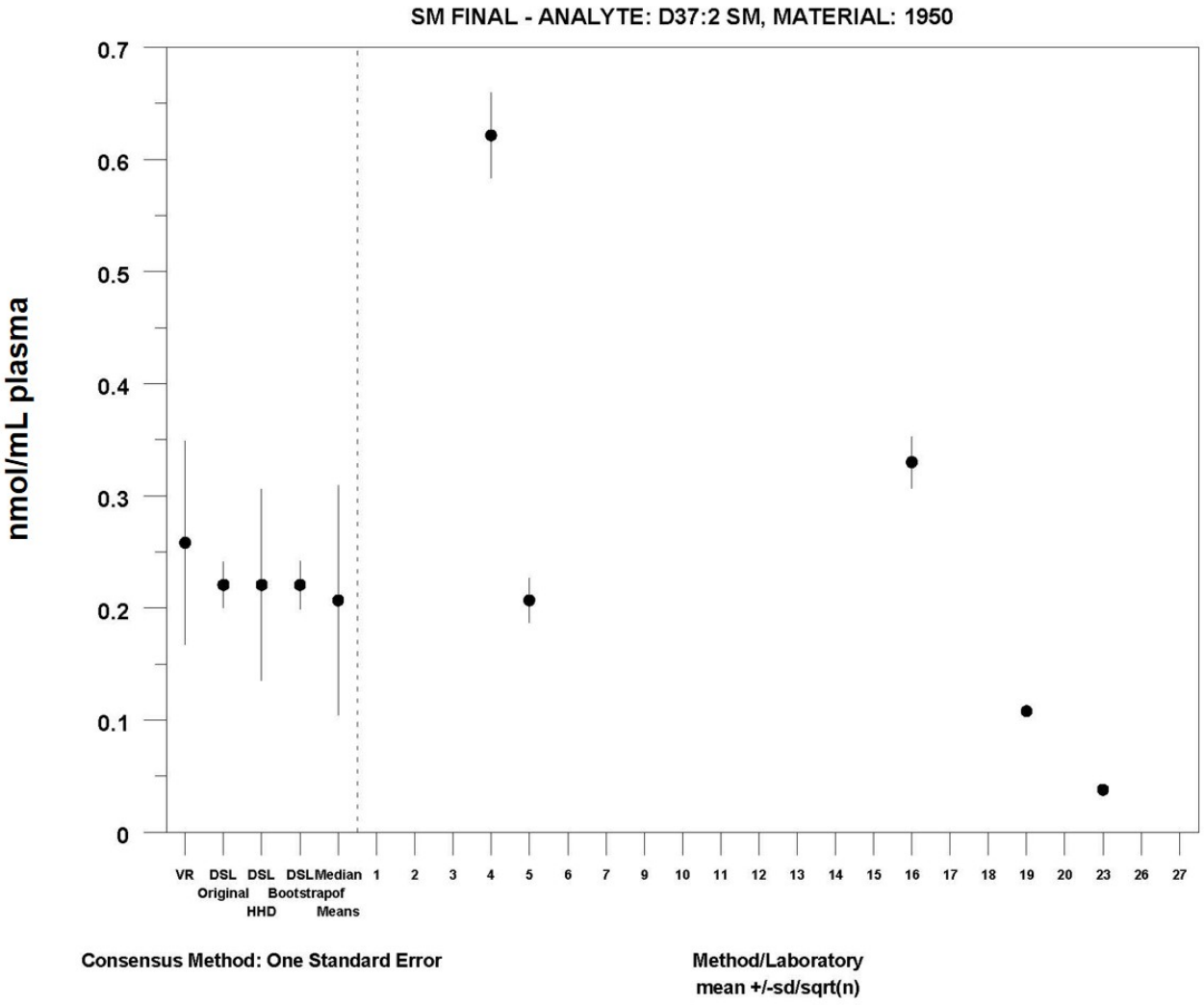
Consensus Method: One Standard Error

Method/Laboratory mean +/-sd/sqrt(n)

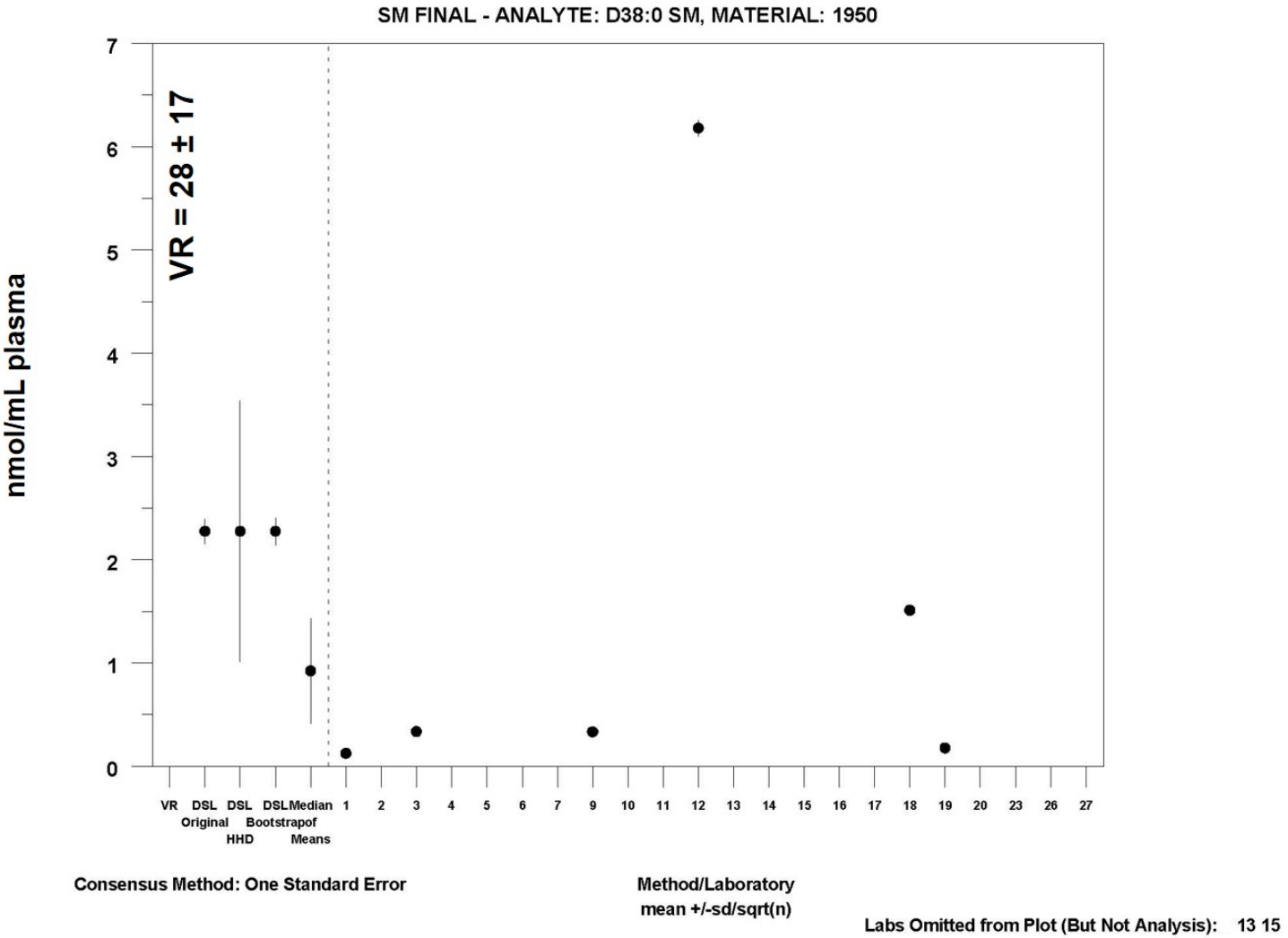
Labs Omitted from Plot (But Not Analysis): 7 15

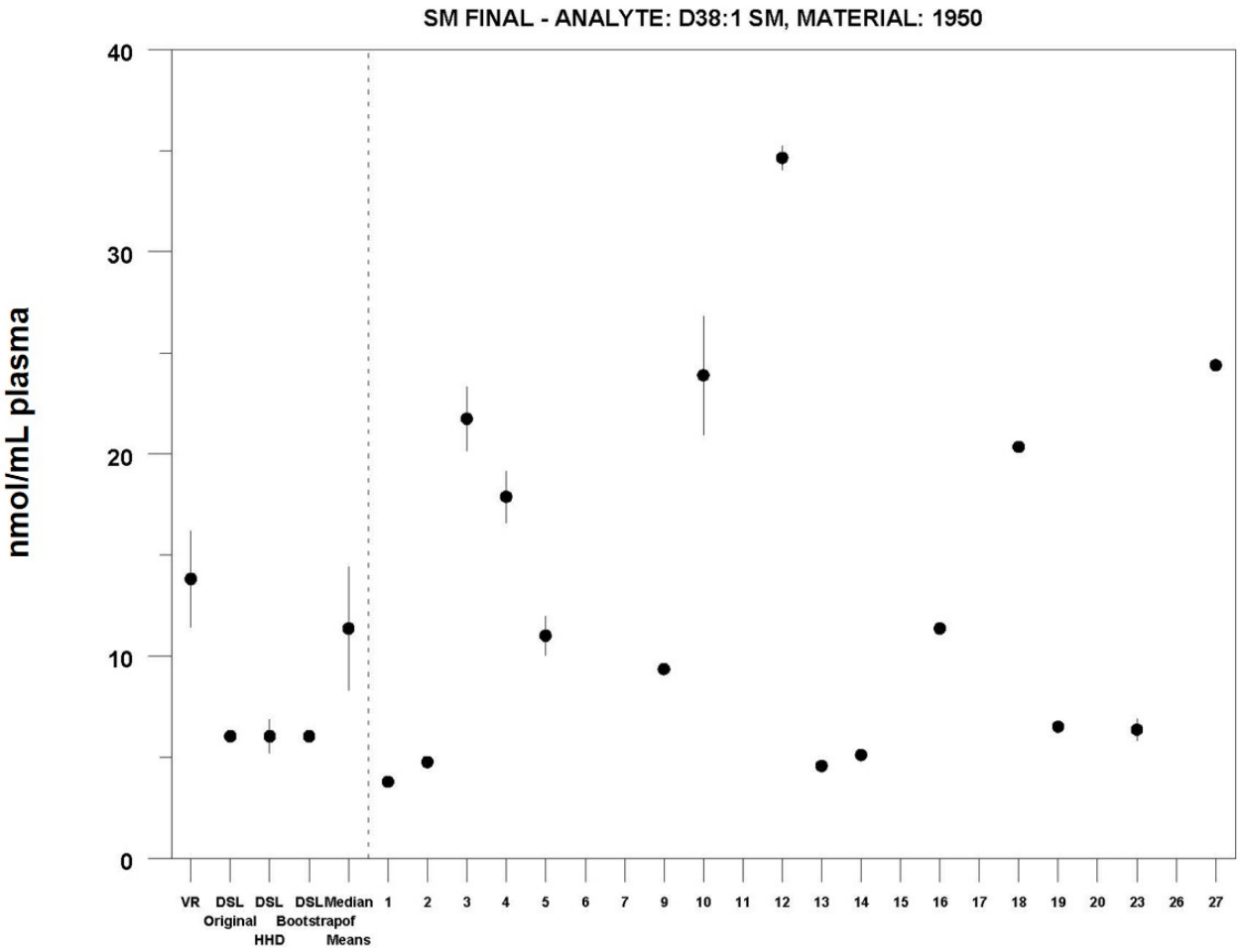
MEDM Location: 1.0 ± 0.23 nmol/mL

7: 9 ± 2; 15: 258 ± 21



MEDM Location: 0.21 ± 0.10 nmol/mL

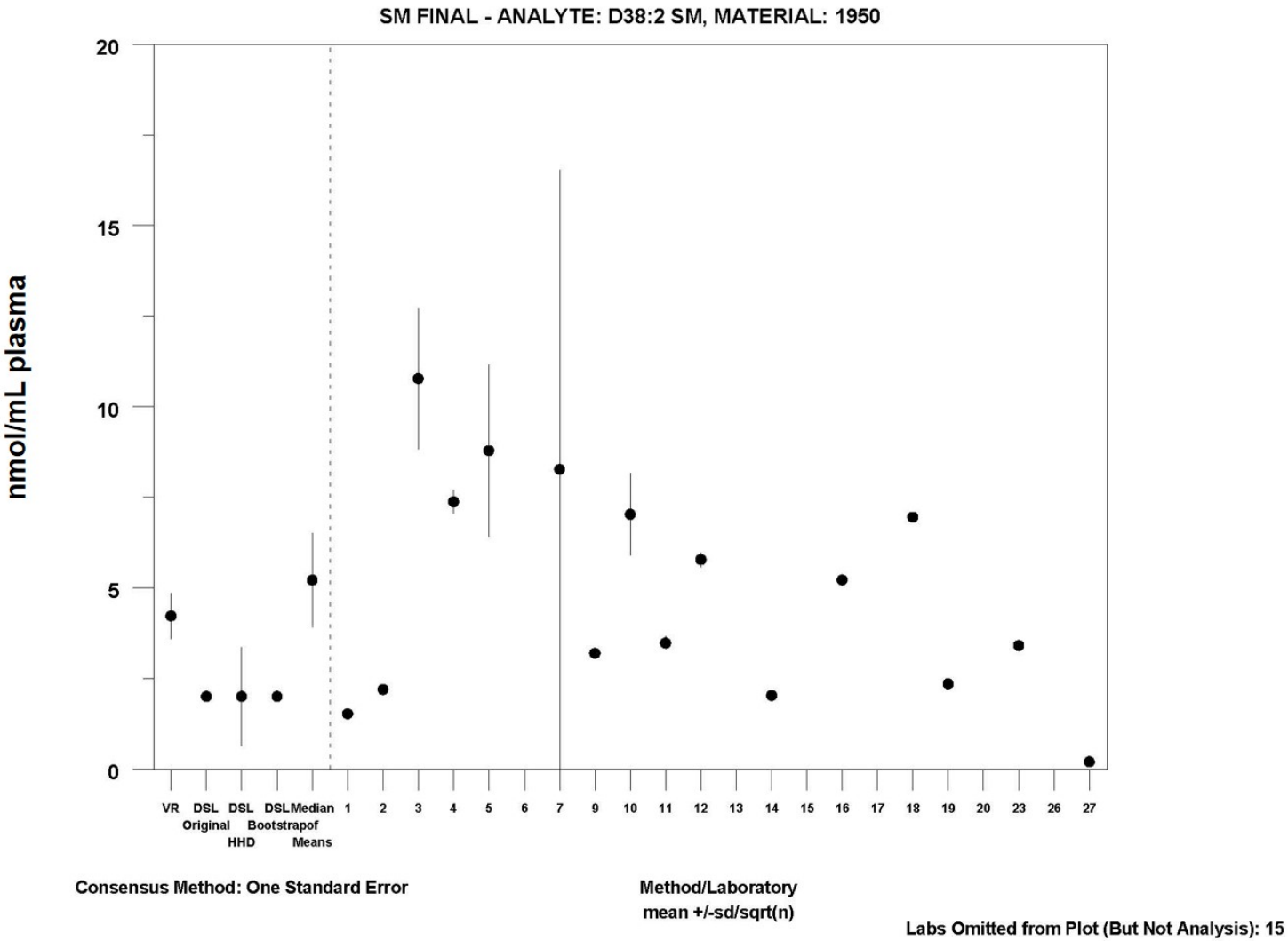


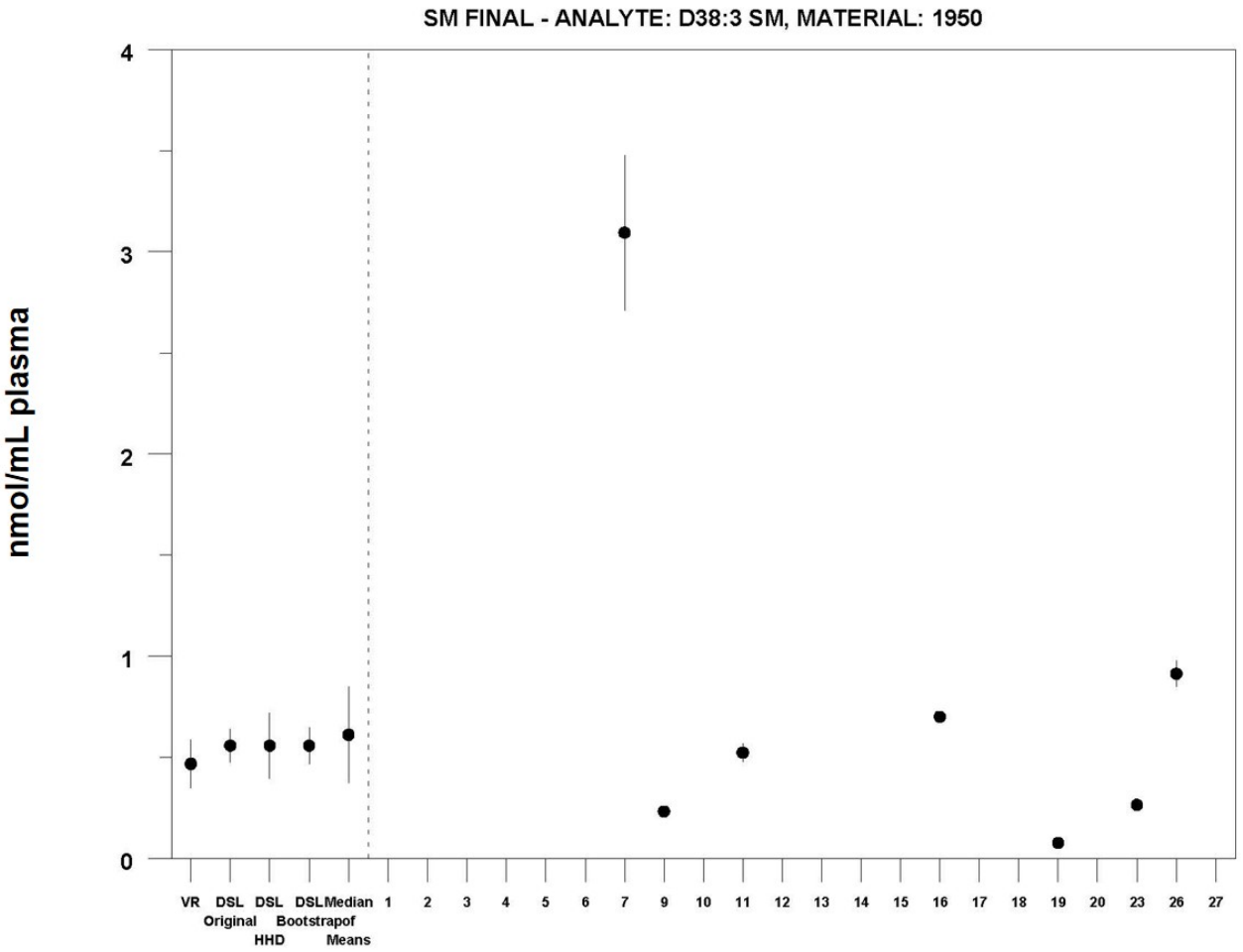


MEDM Location: 11 ± 3.1 nmol/mL

Labs Omitted from Plot (But Not Analysis): 7 15

7: 105 ± 20; 15: 1314 ± 685

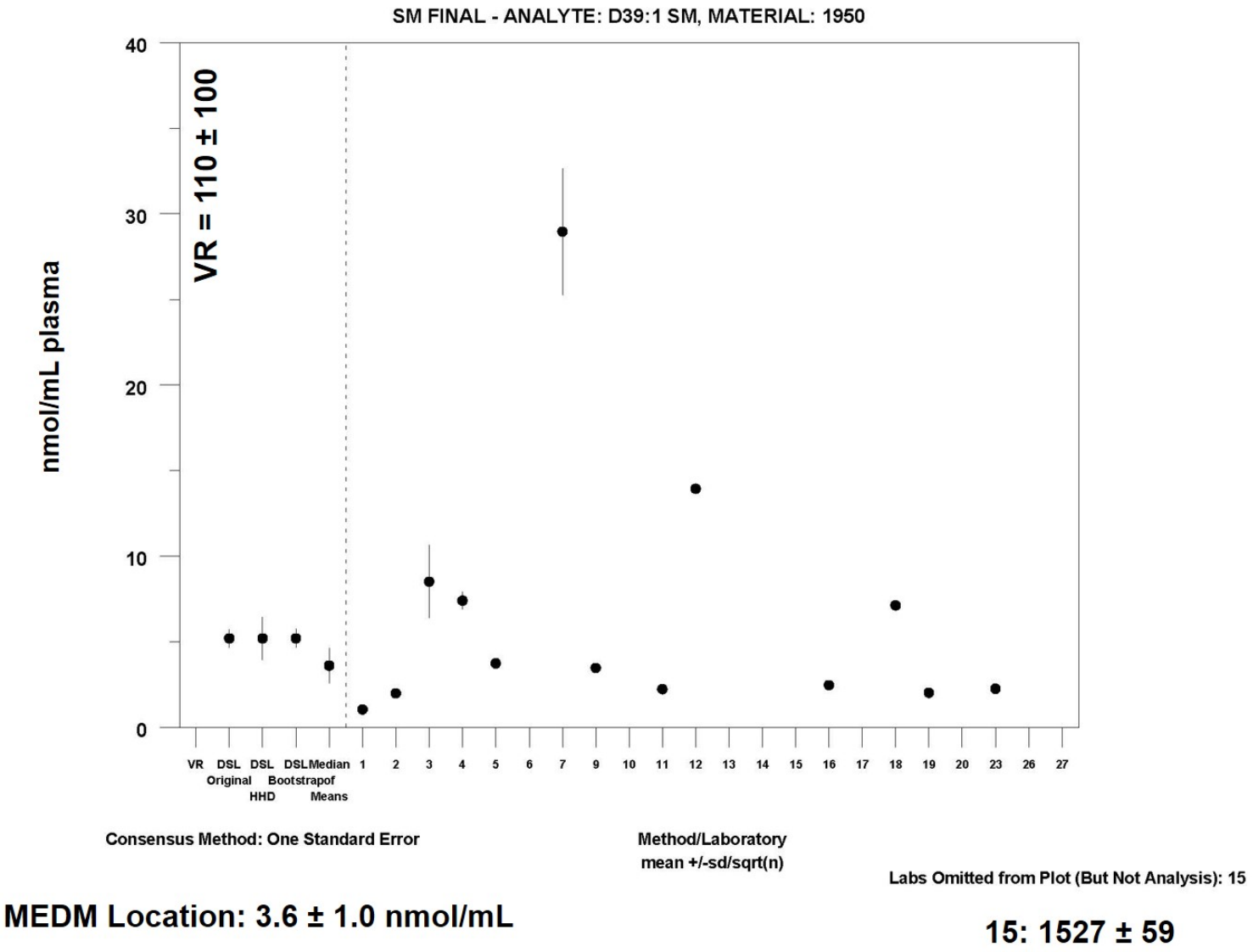


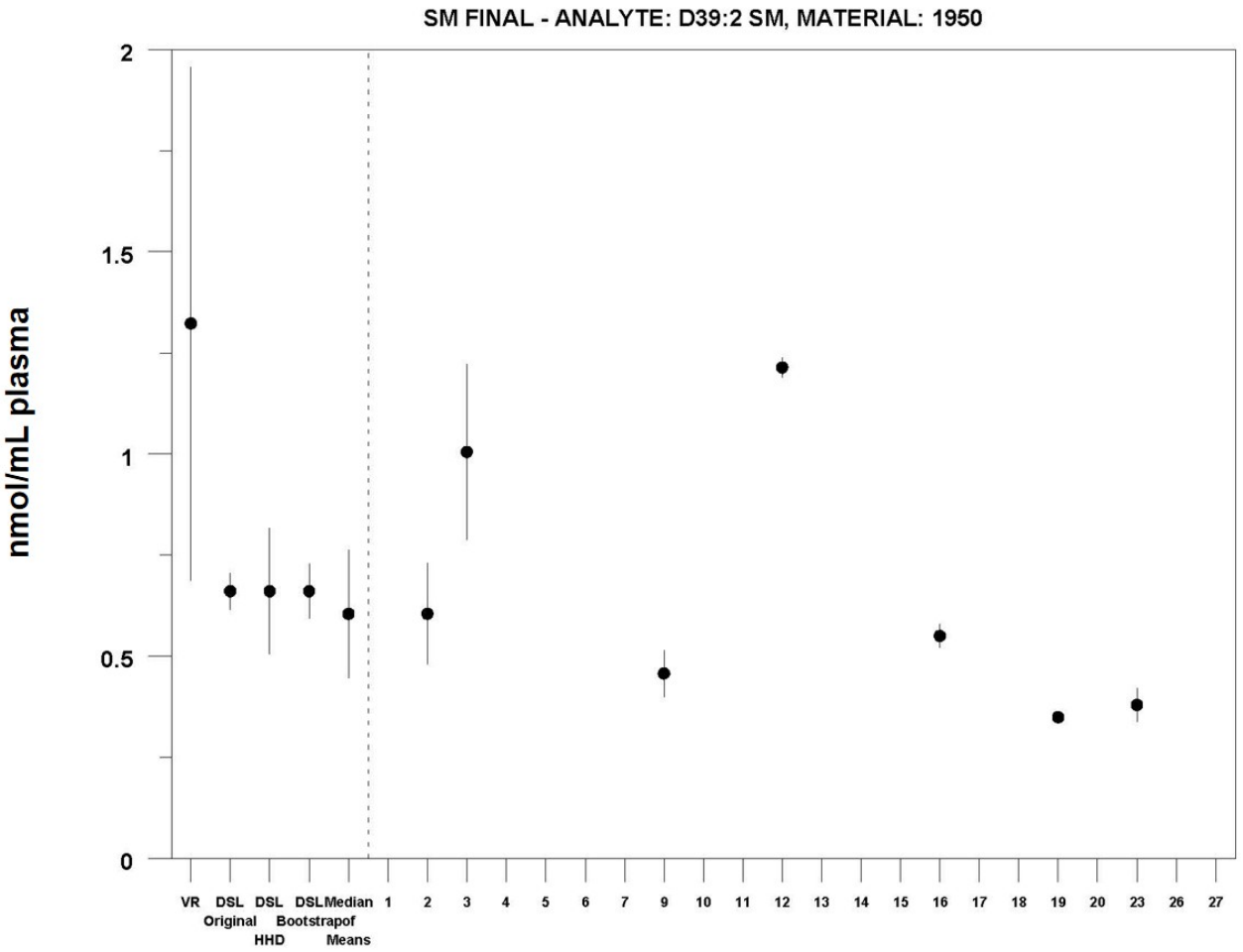


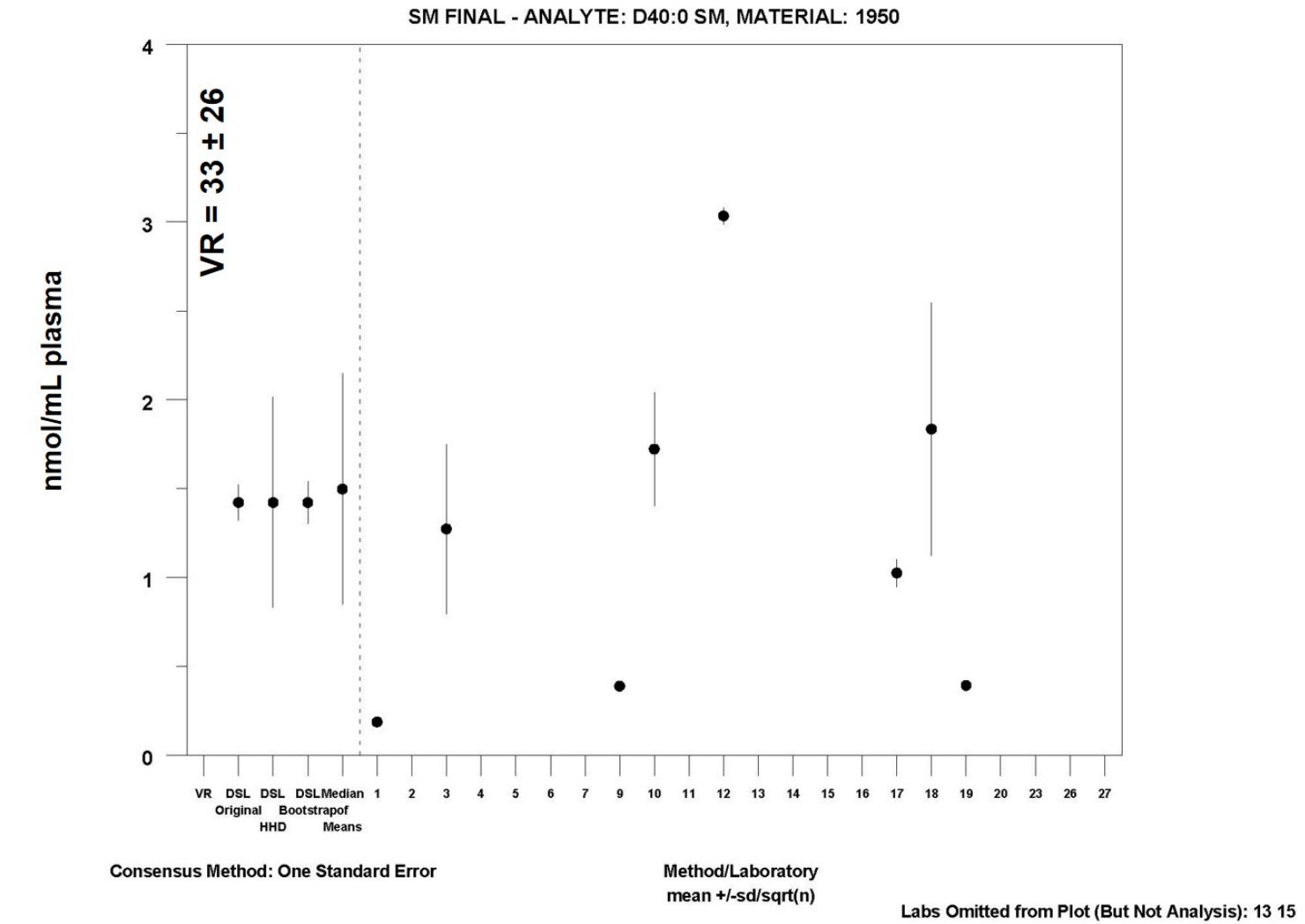
Labs Omitted from Plot (But Not Analysis): 15

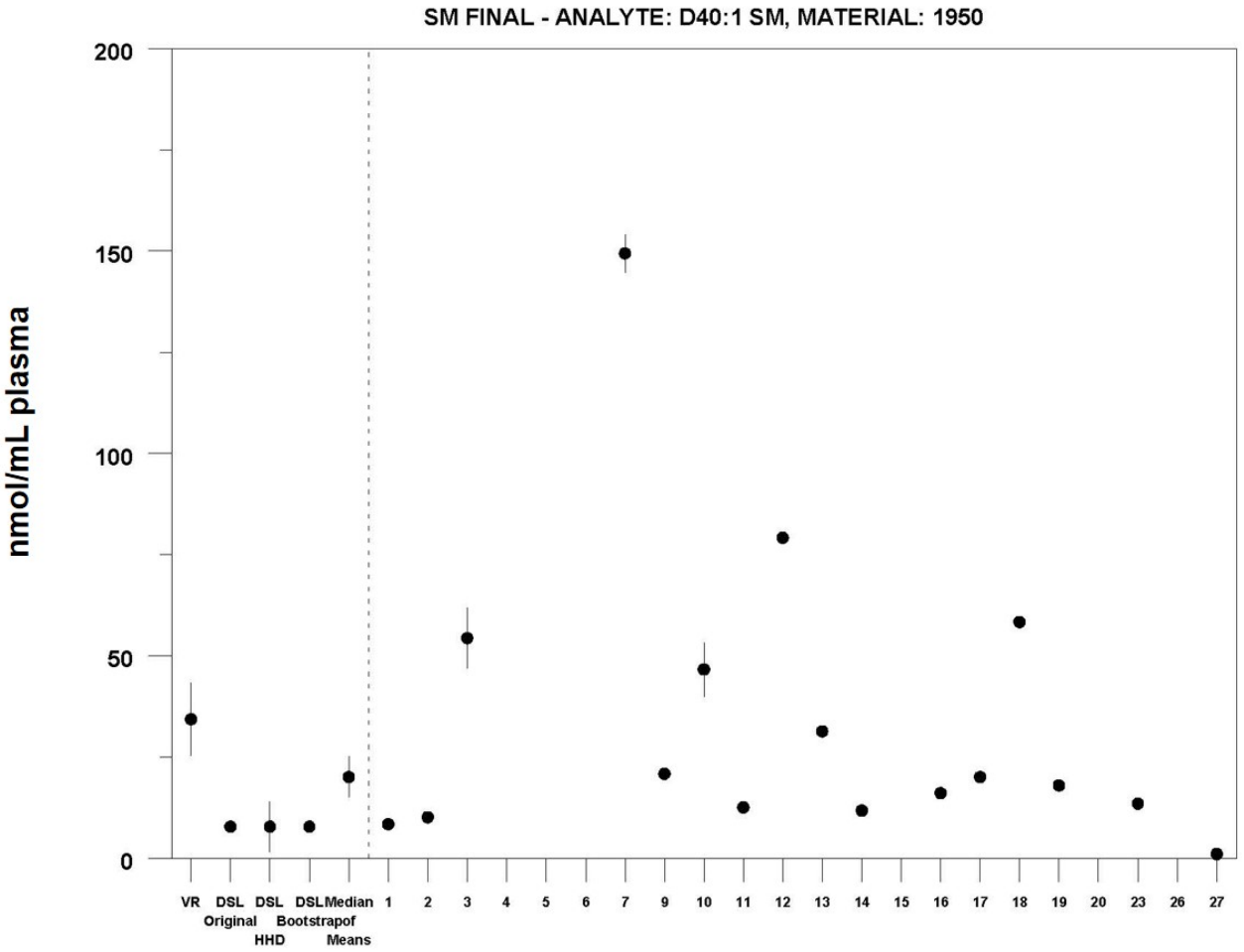
MEDM Location: 0.61 ± 0.24 nmol/mL

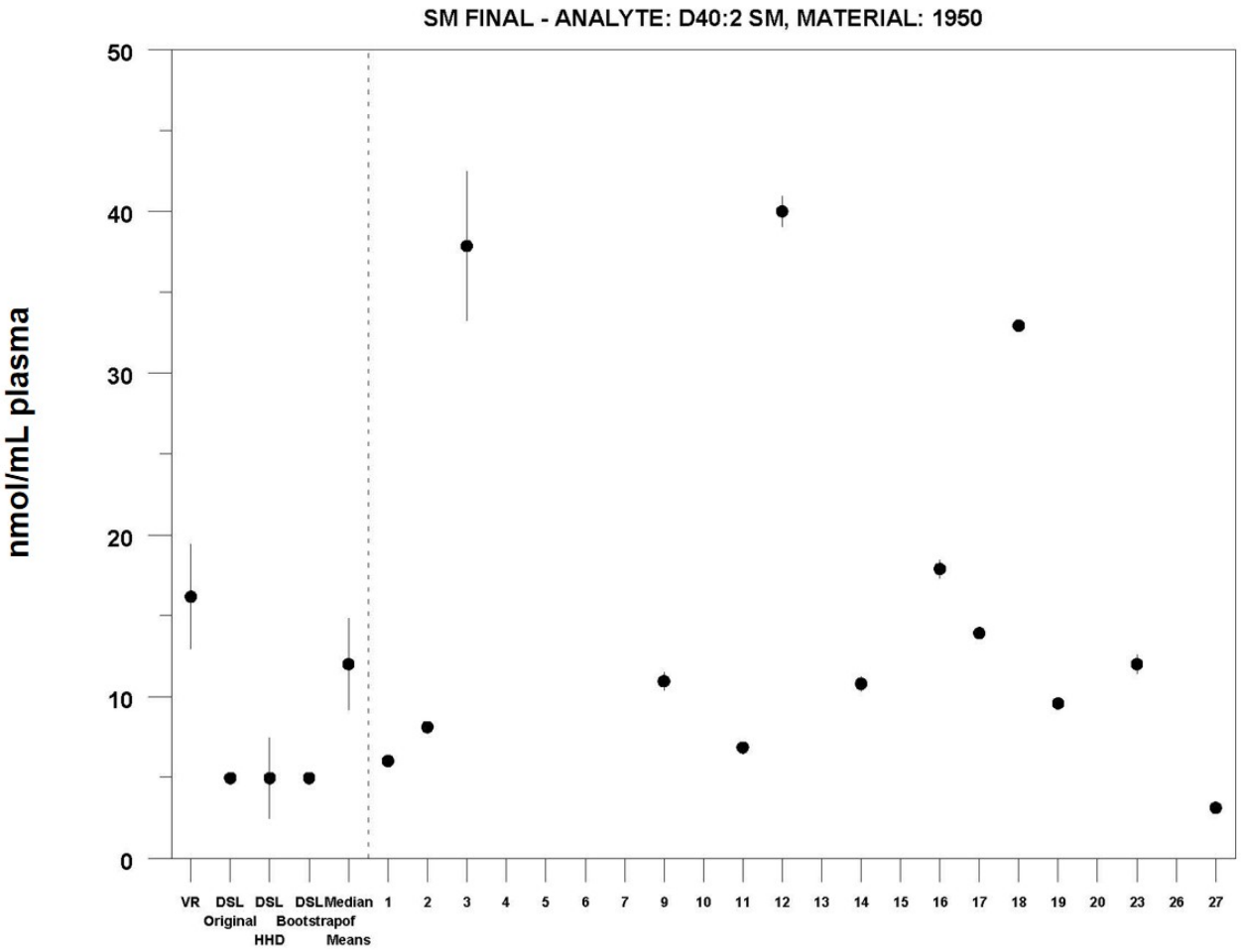
15: 10 ± 3







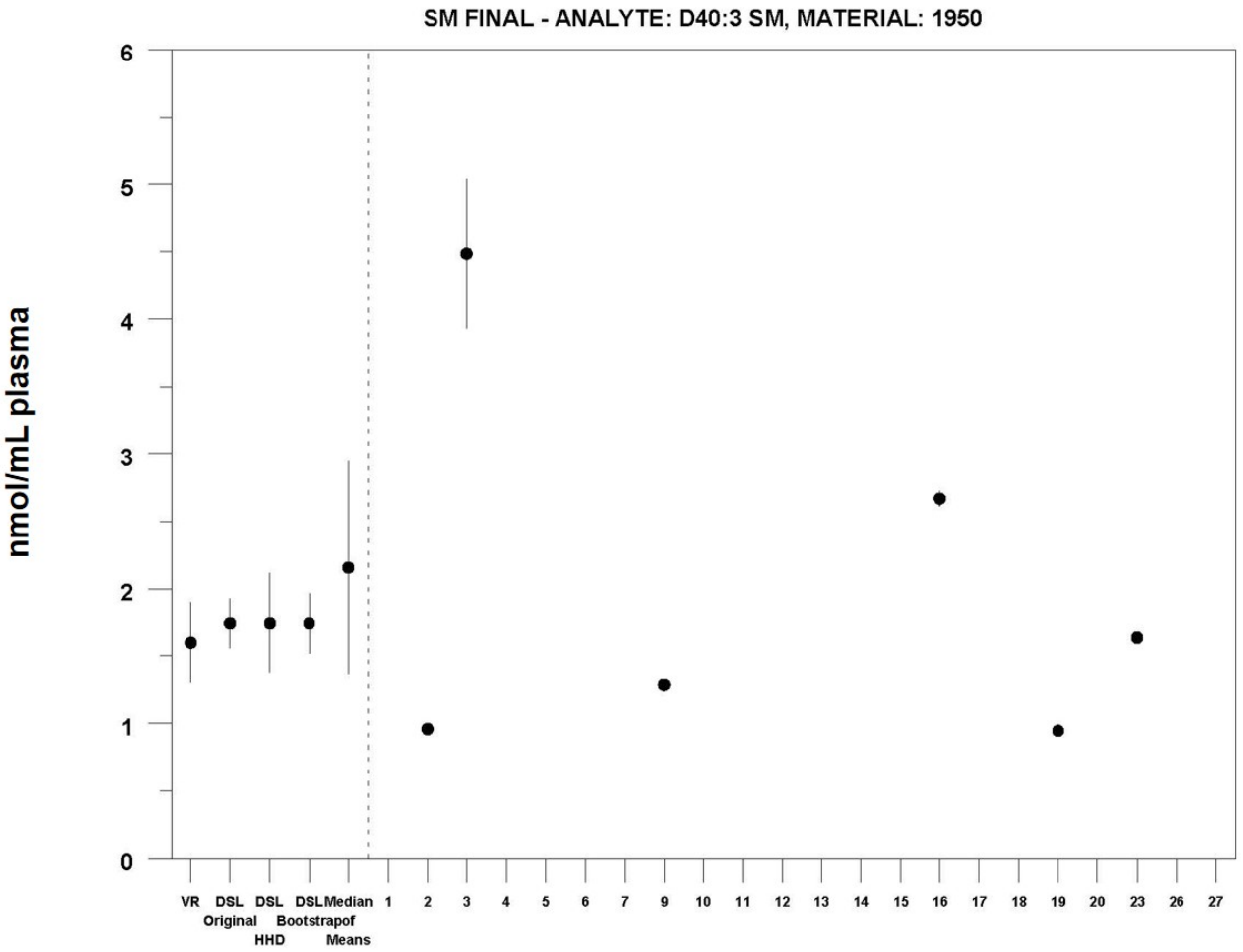




Labs Omitted from Plot (But Not Analysis): 7 15

MEDM Location: 12 ± 2.8 nmol/mL

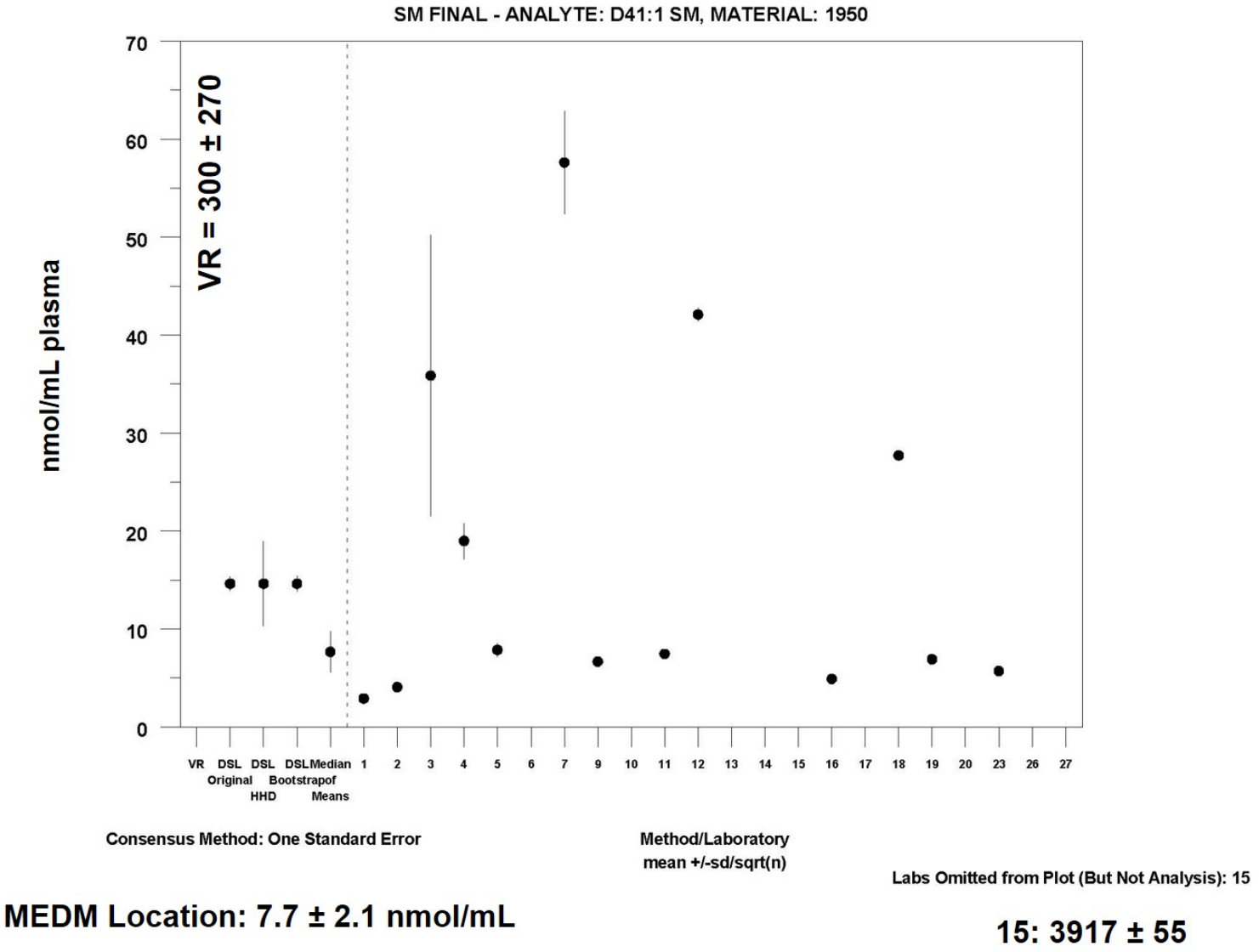
7: 130 ± 23; 15: 2142 ± 551

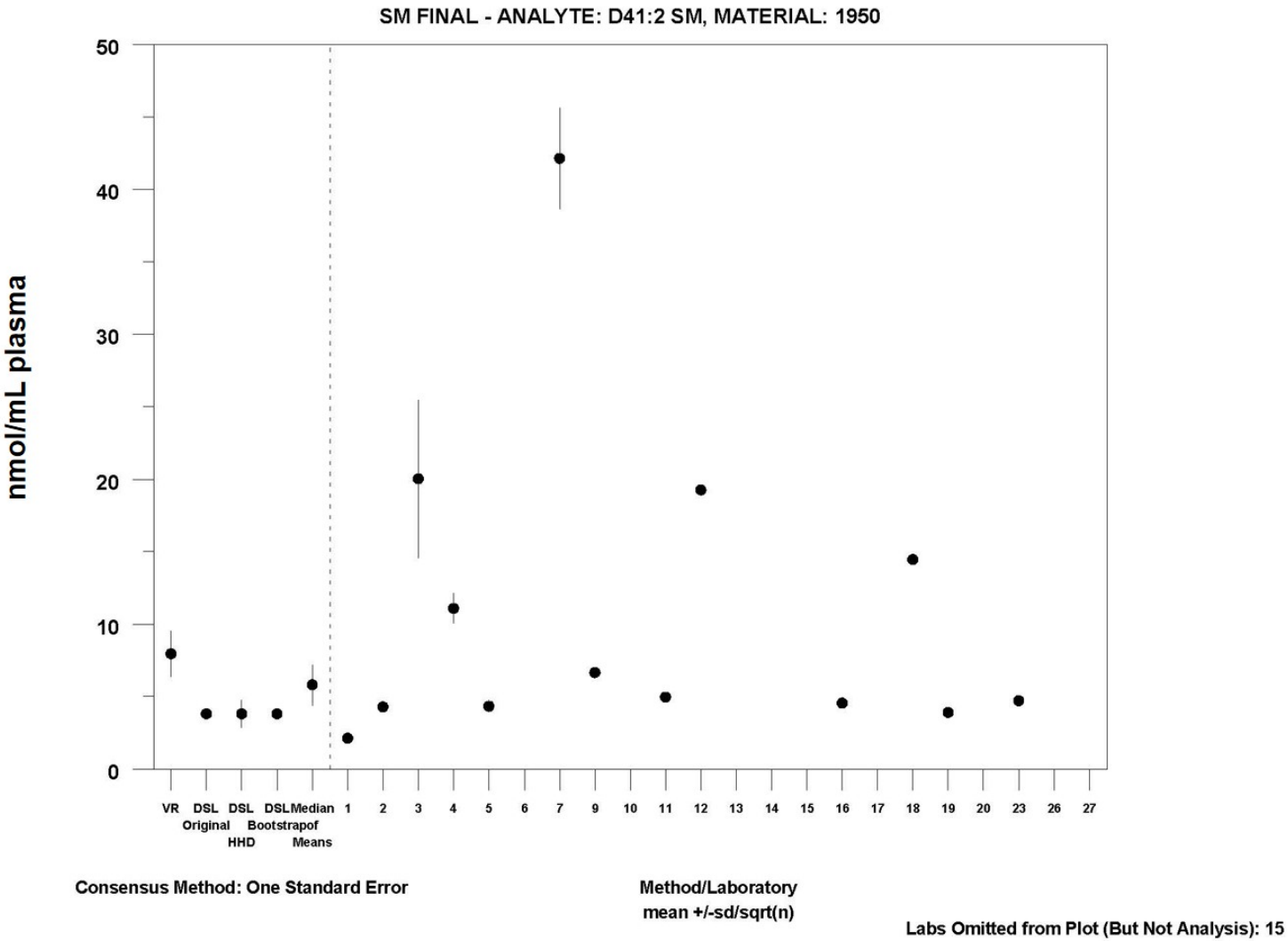


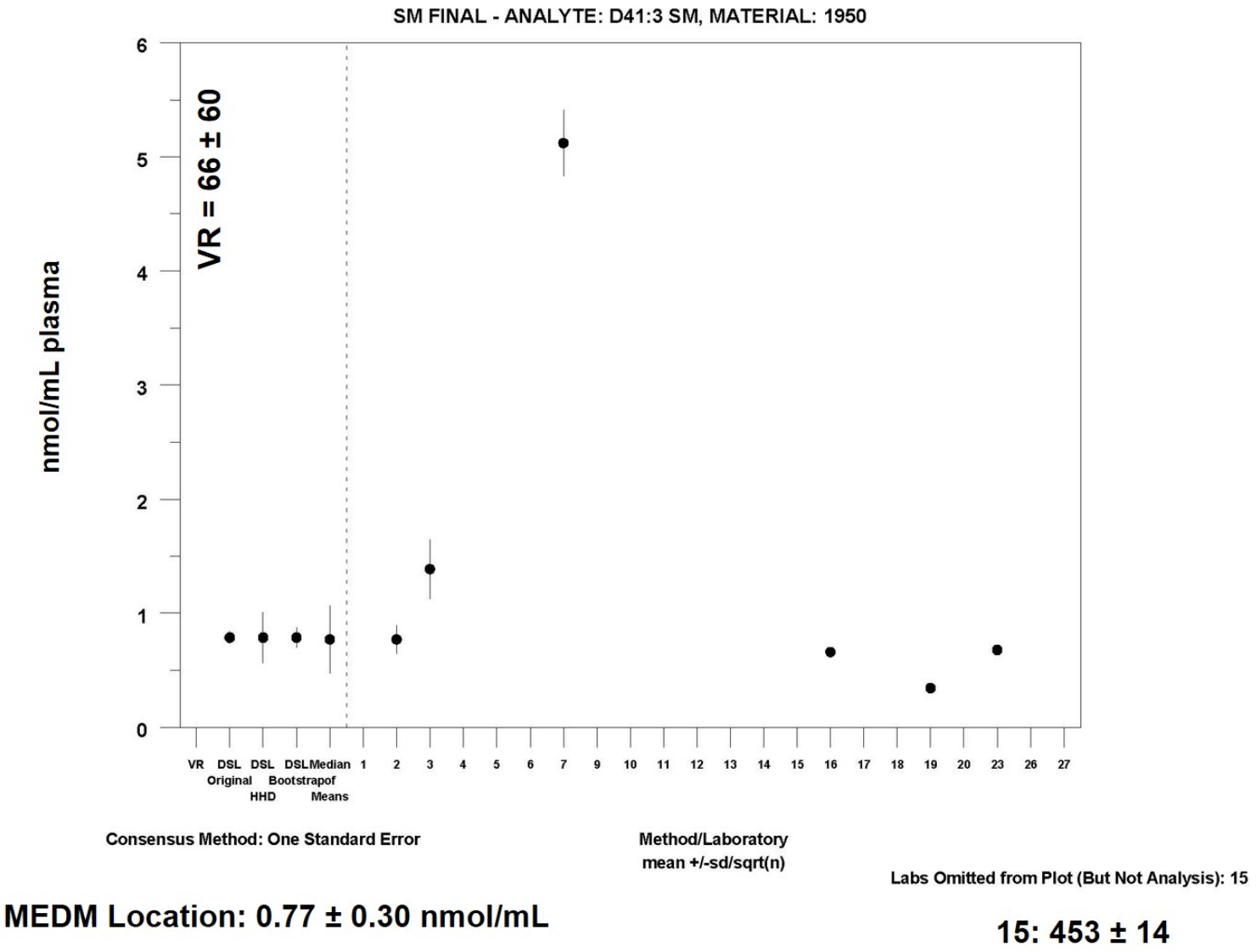
MEDM Location: 2.2 ± 0.79 nmol/mL

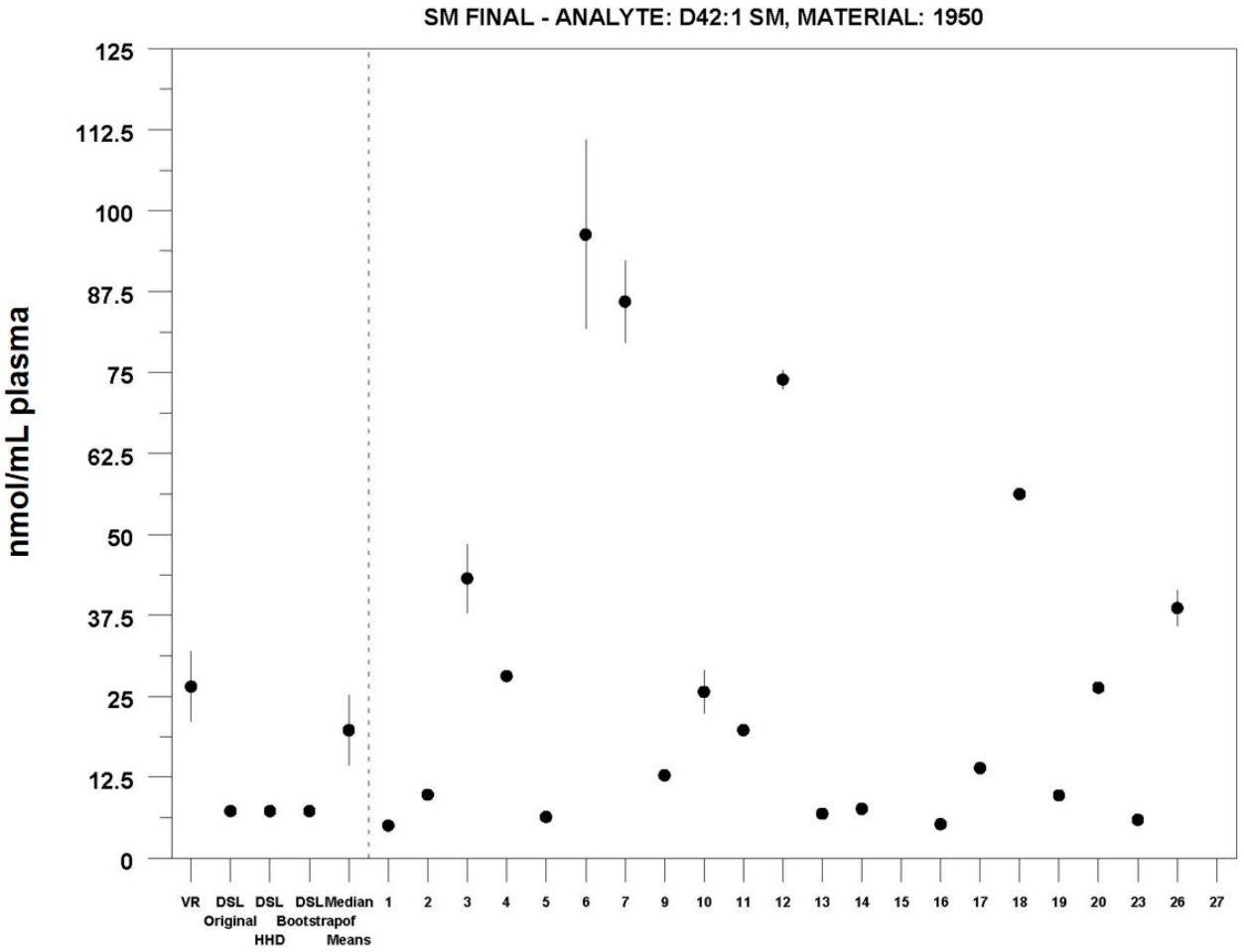
Labs Omitted from Plot (But Not Analysis): 7 15

7: 39 ± 11; 15: 164 ± 31





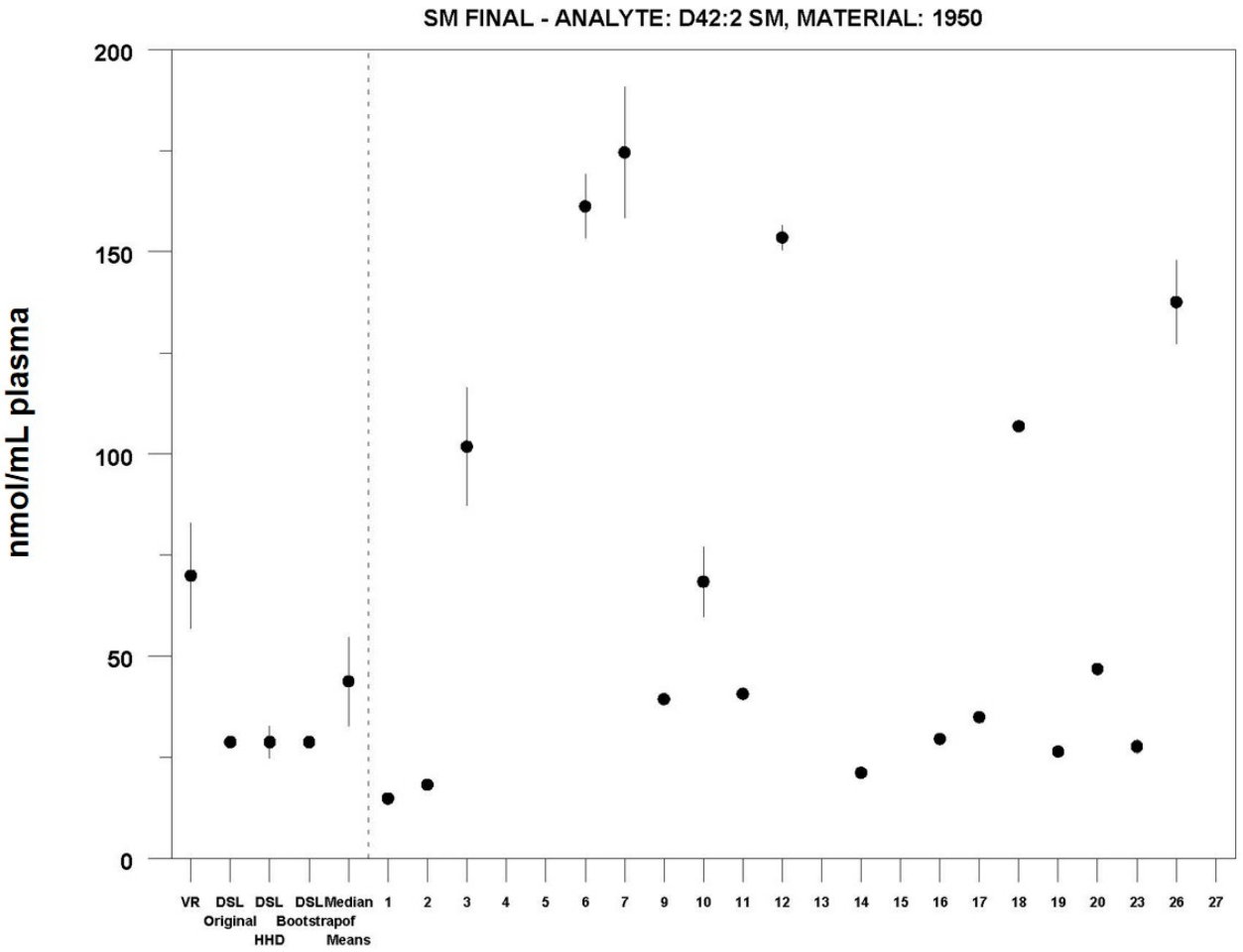


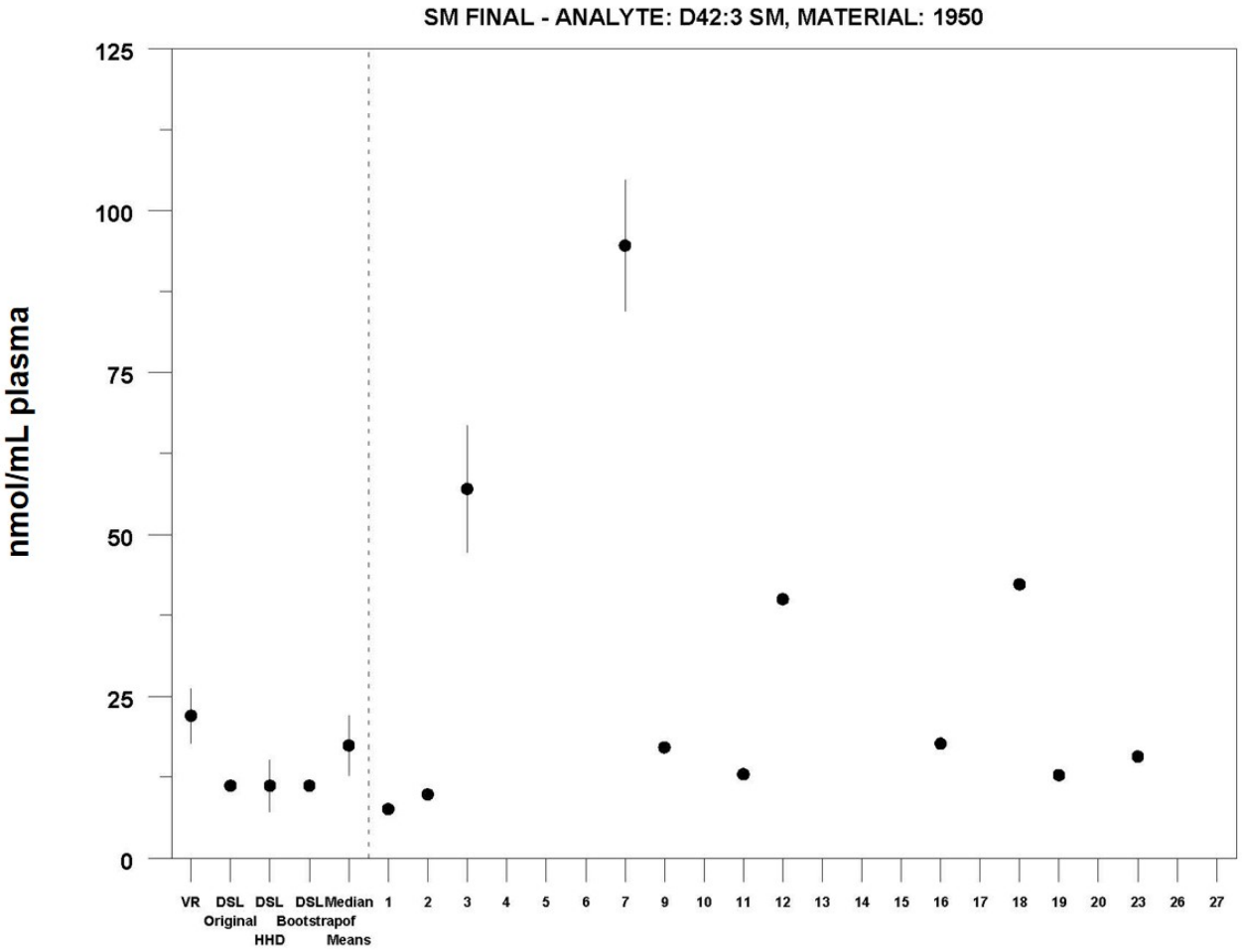


MEDM Location: 20 ± 5.4 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 5189 ± 362

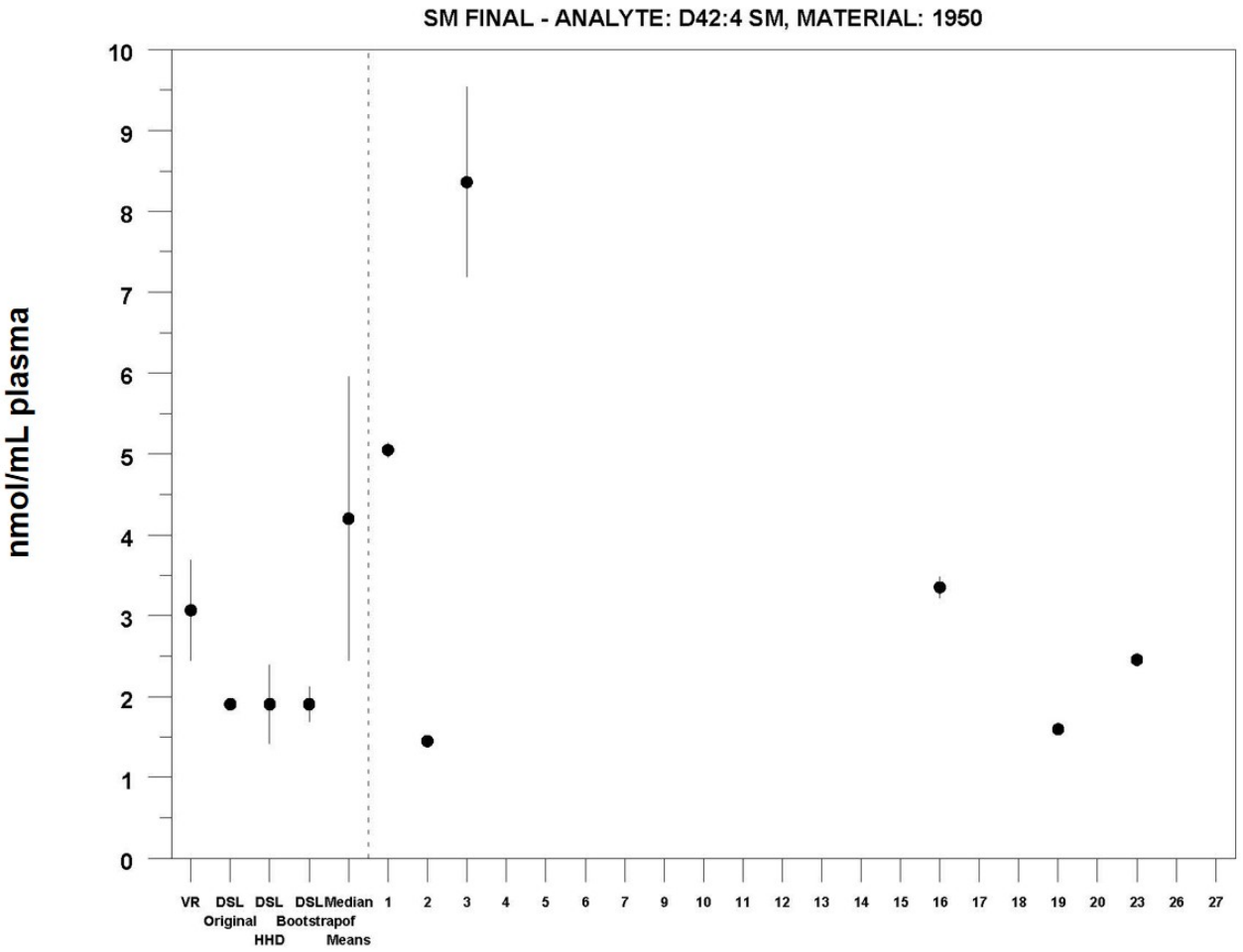




Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 17 ± 4.7 nmol/mL

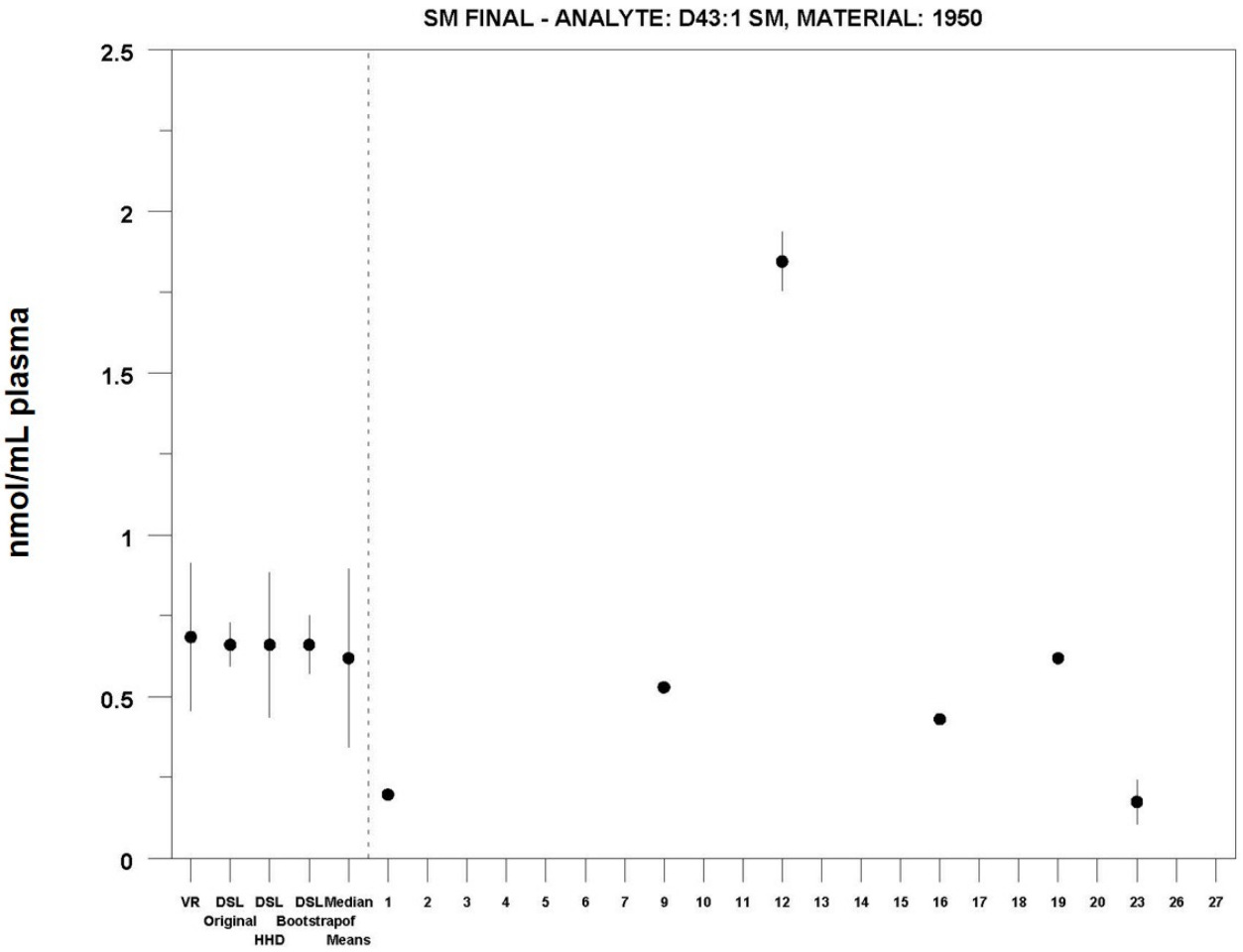
15: 2161 ± 1016



Labs Omitted from Plot (But Not Analysis): 7 15

MEDM Location: 4.2 ± 1.8 nmol/mL

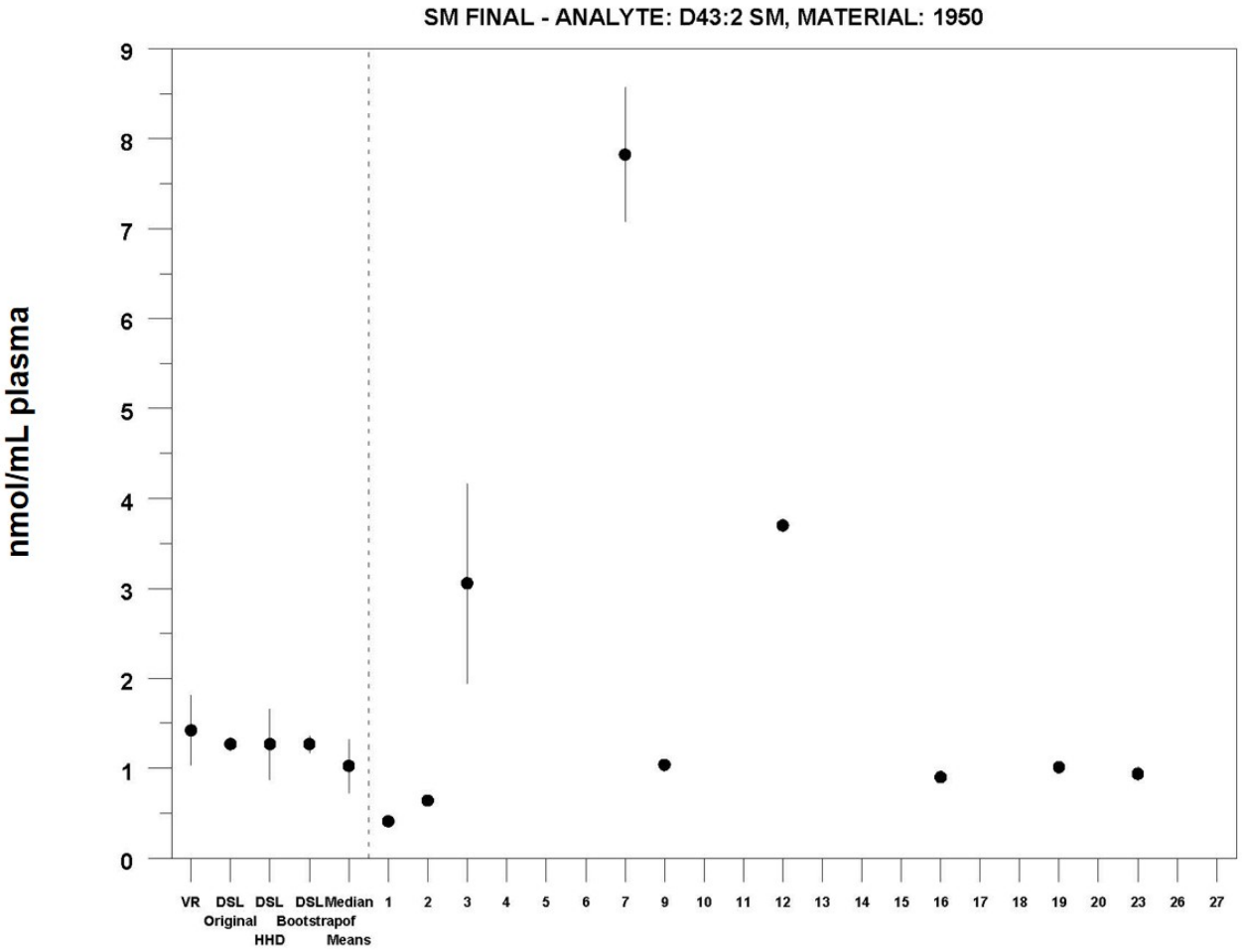
7: 27 ± 8; 15: 235 ± 97



MEDM Location: 0.62 ± 0.28 nmol/mL

Labs Omitted from Plot (But Not Analysis): 3 7 15

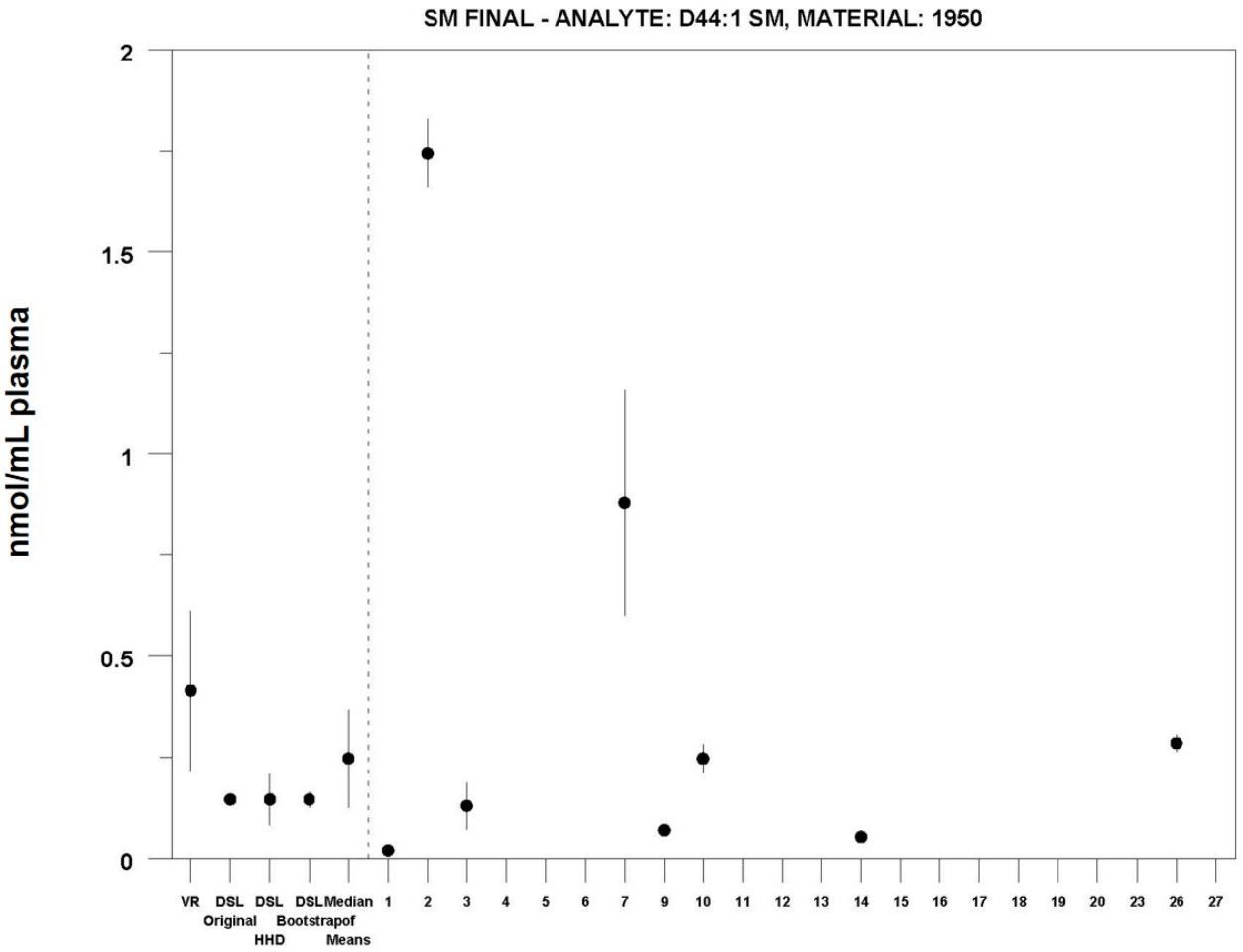
3: 3.0 ± 3.1; 7: 6.8 ± 1.1; 15: 405 ± 67



Labs Omitted from Plot (But Not Analysis): 15

MEDM Location: 1.03 ± 0.588 nmol/mL

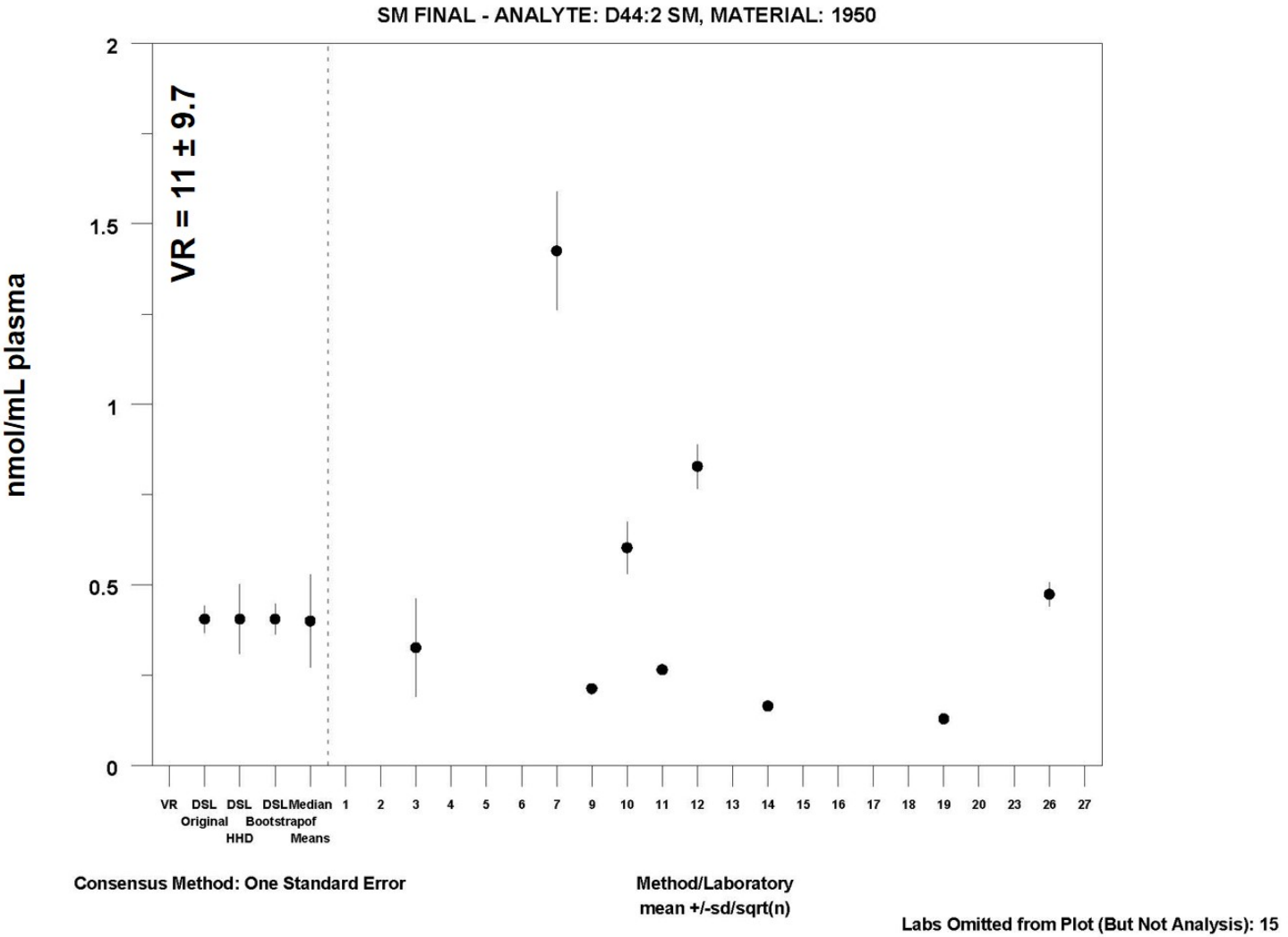
15: 257 ± 218

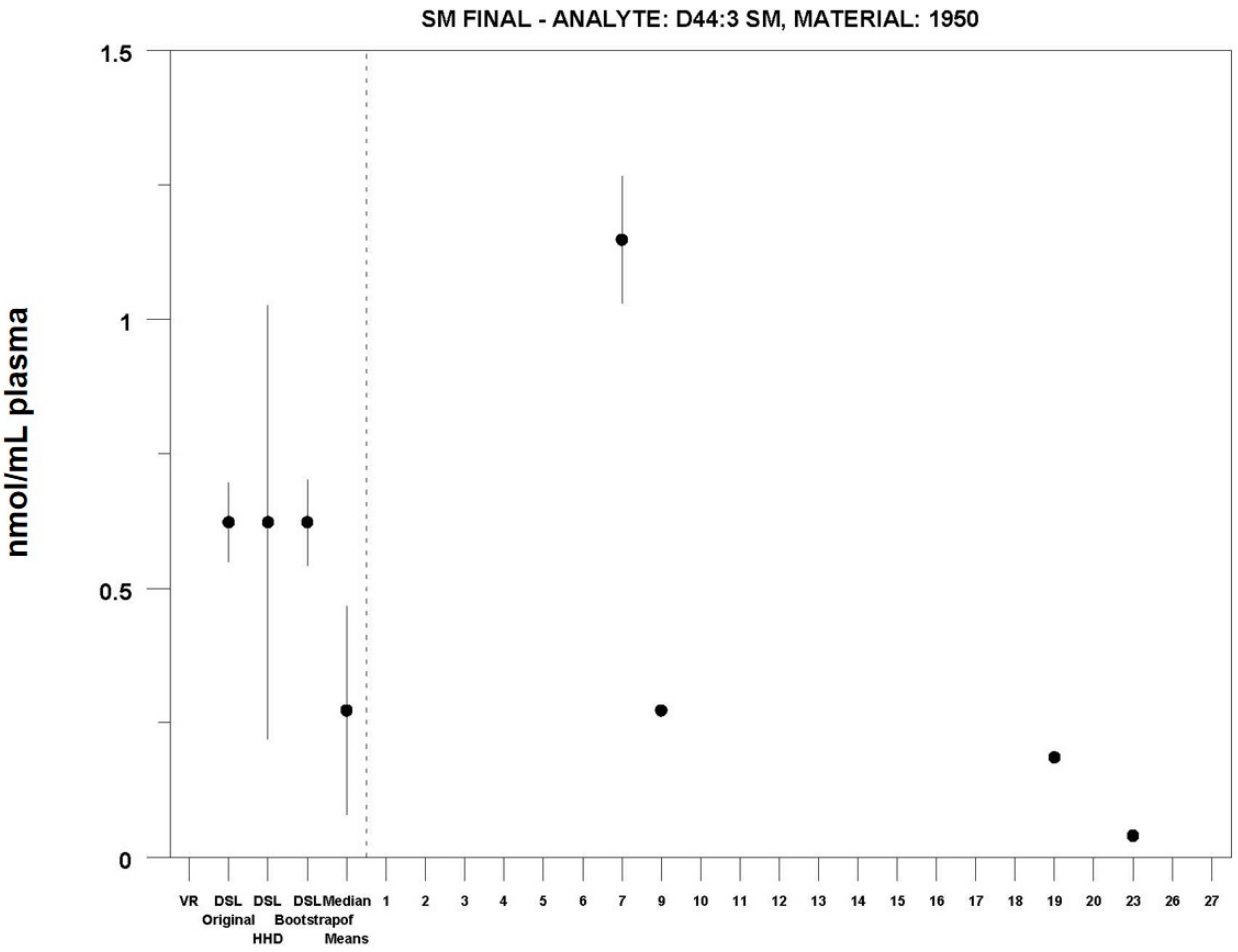


MEDM Location: 0.25 ± 0.12 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 86 ± 31

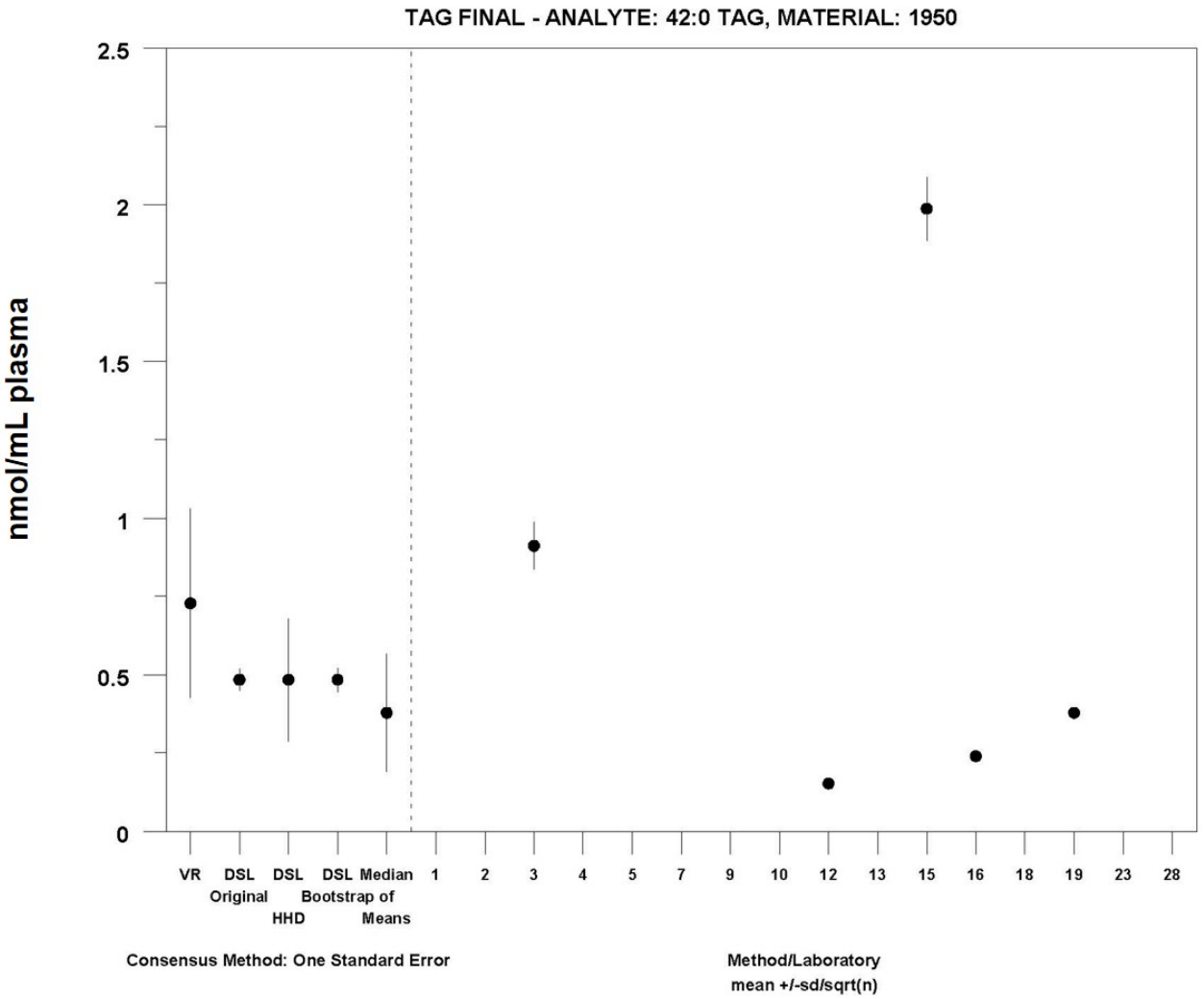




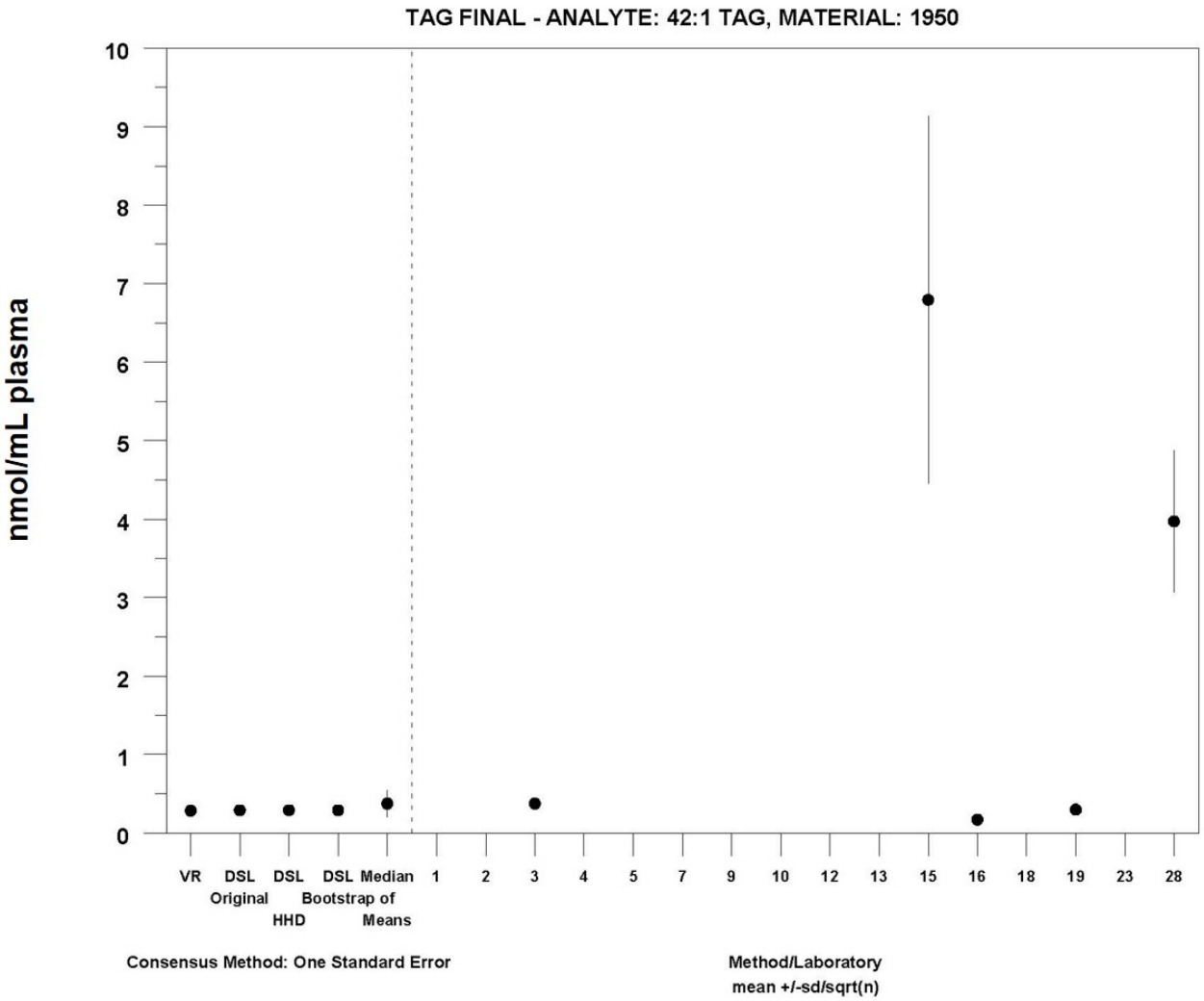
MEDM Location: 0.27 ± 0.19 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

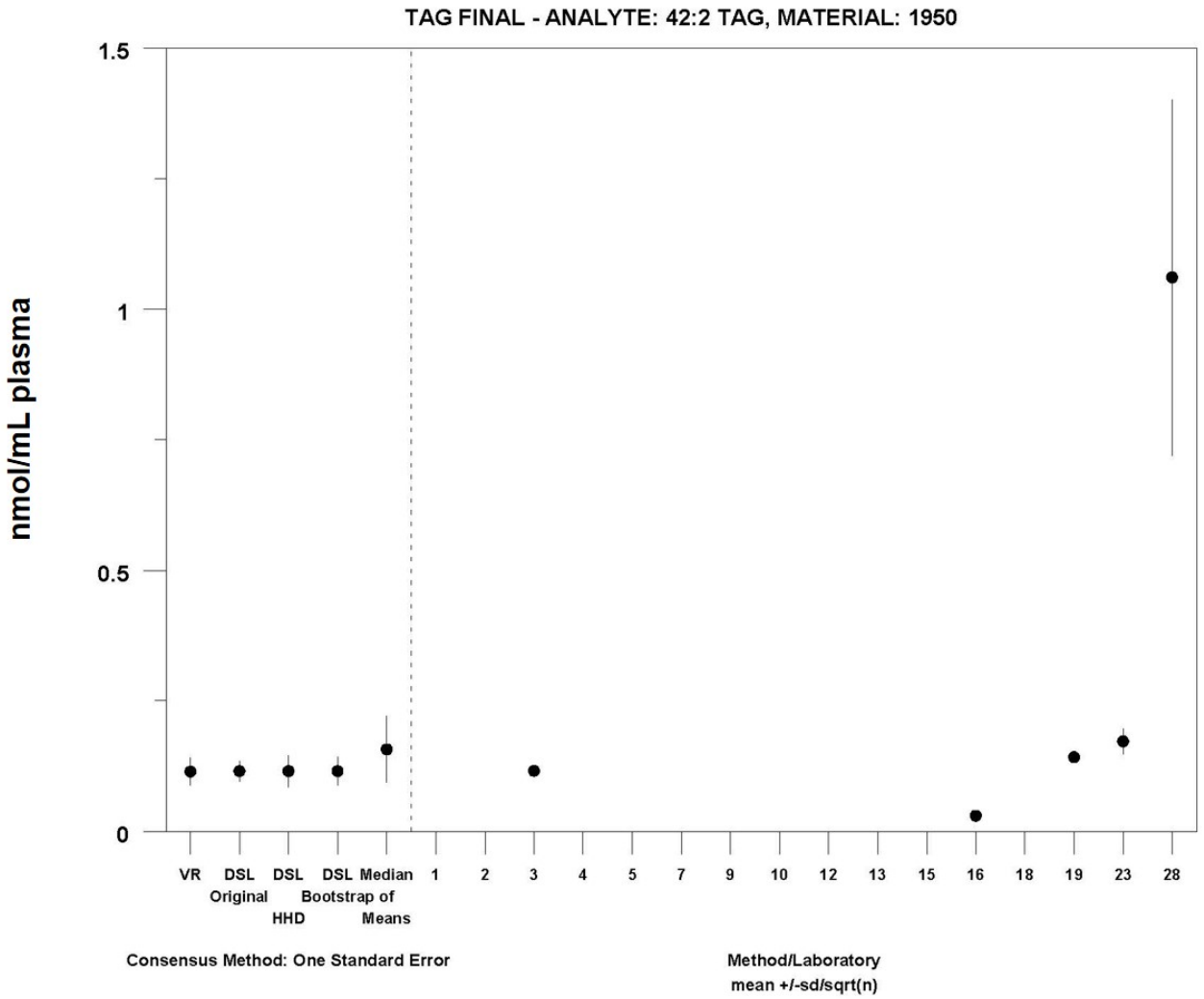
15: 20 ± 1



MEDM Location: 0.38 ± 0.19 nmol/mL



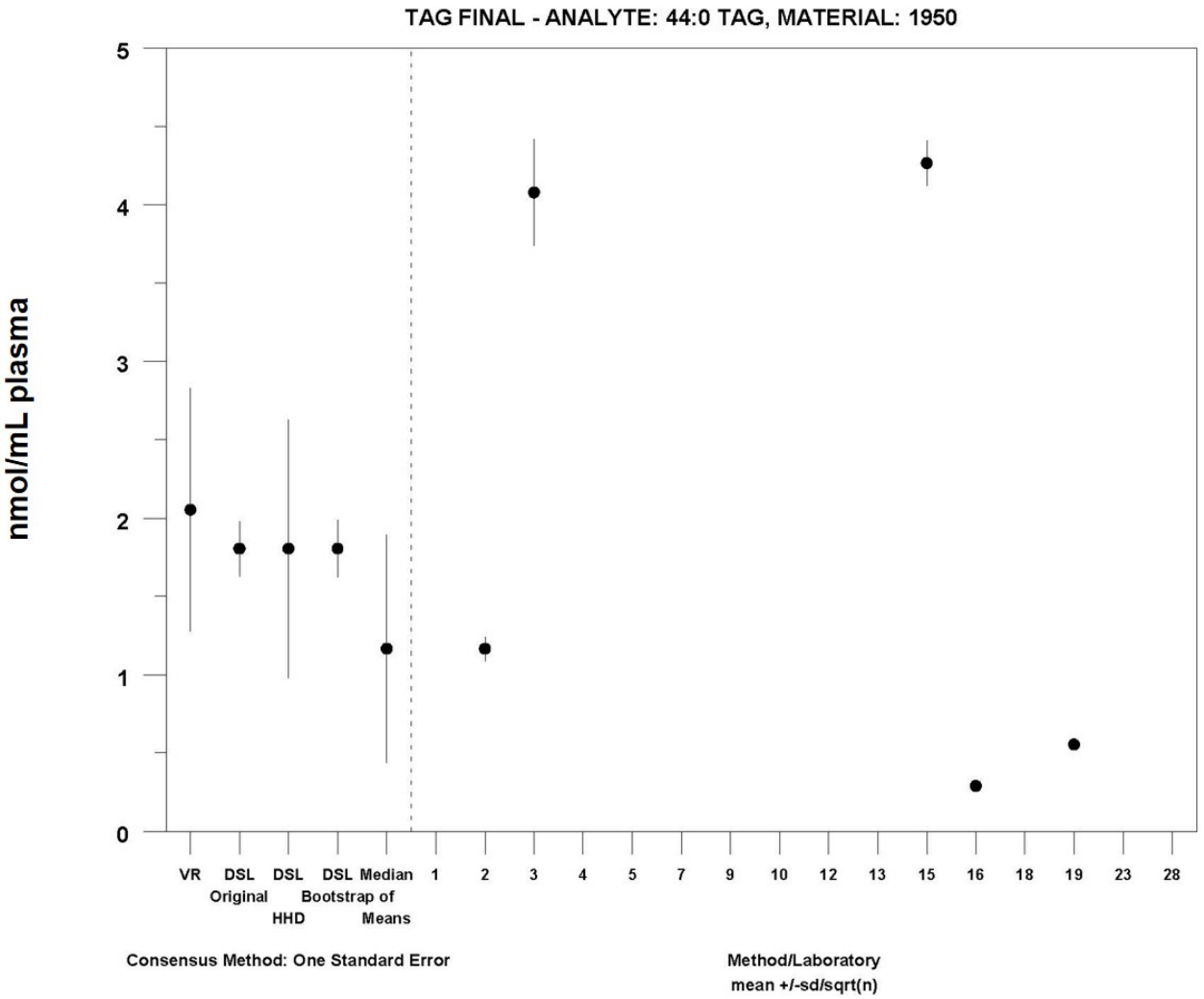
MEDM Location: 0.37 ± 0.17 nmol/mL



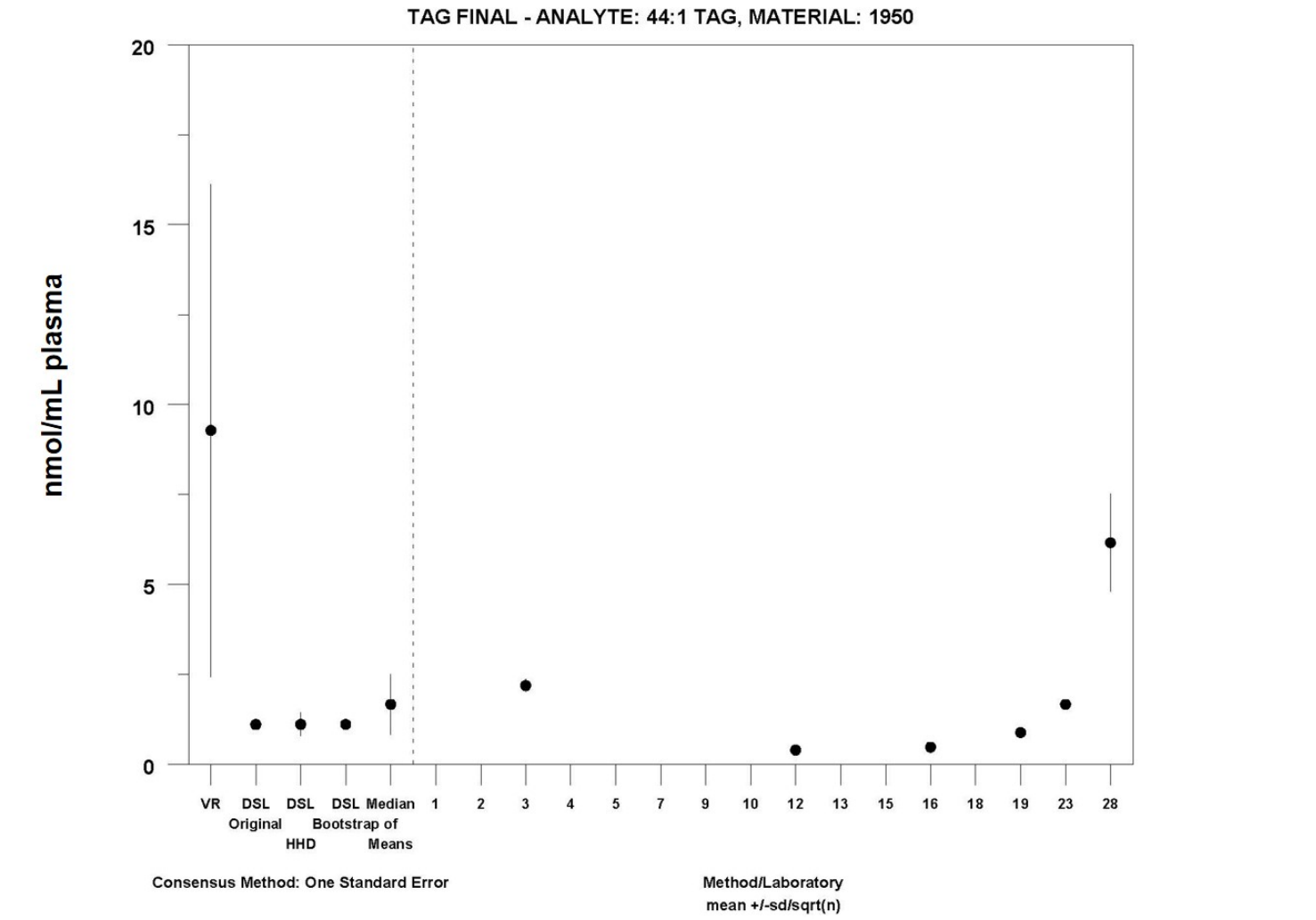
MEDM Location: 0.16 ± 0.064 nmol/mL

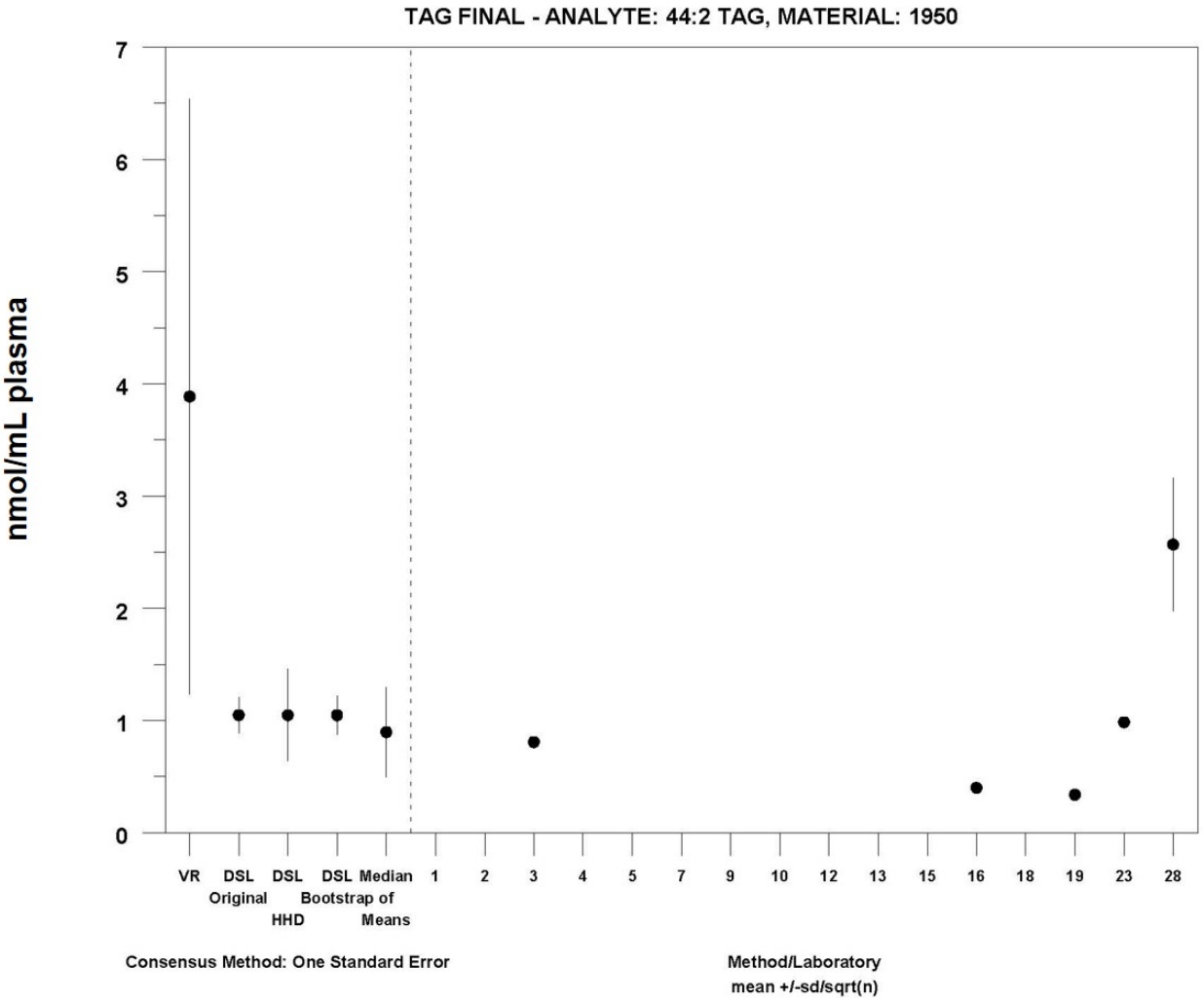
Labs Omitted from Plot (But Not Analysis): 15

15: 4.4 ± 1.9



MEDM Location: 1.2 ± 0.73 nmol/mL

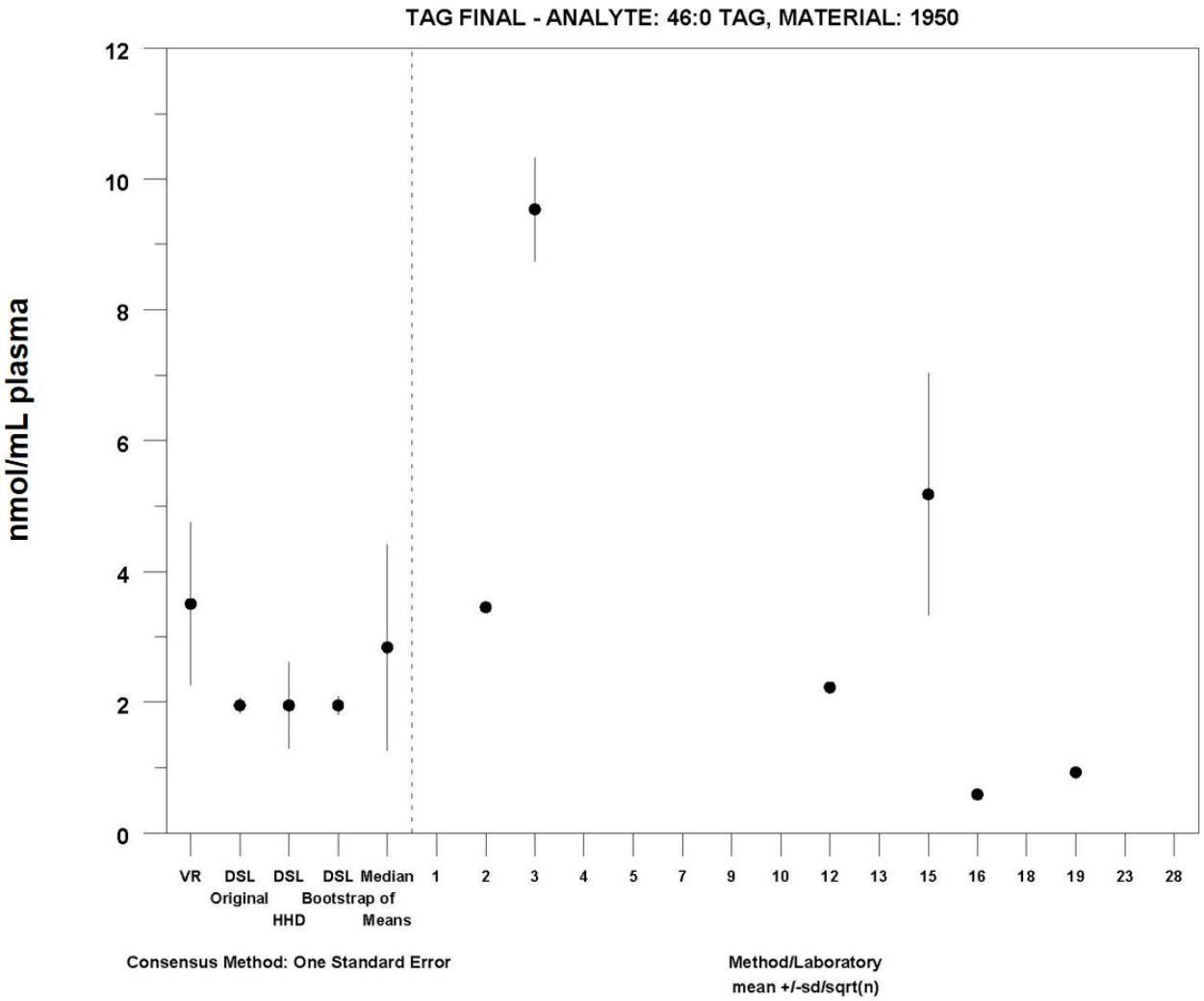




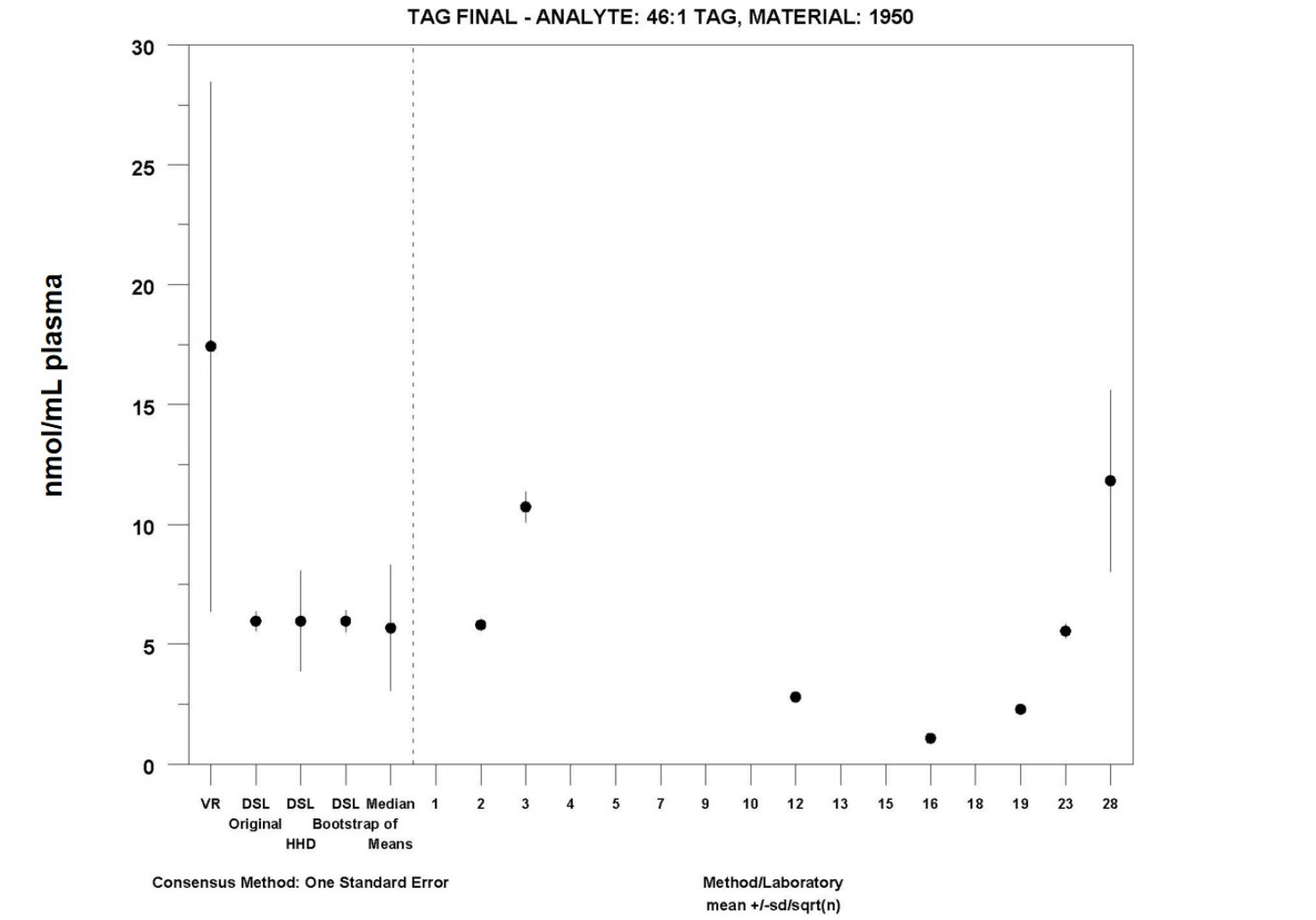
MEDM Location: 0.90 ± 0.40 nmol/mL

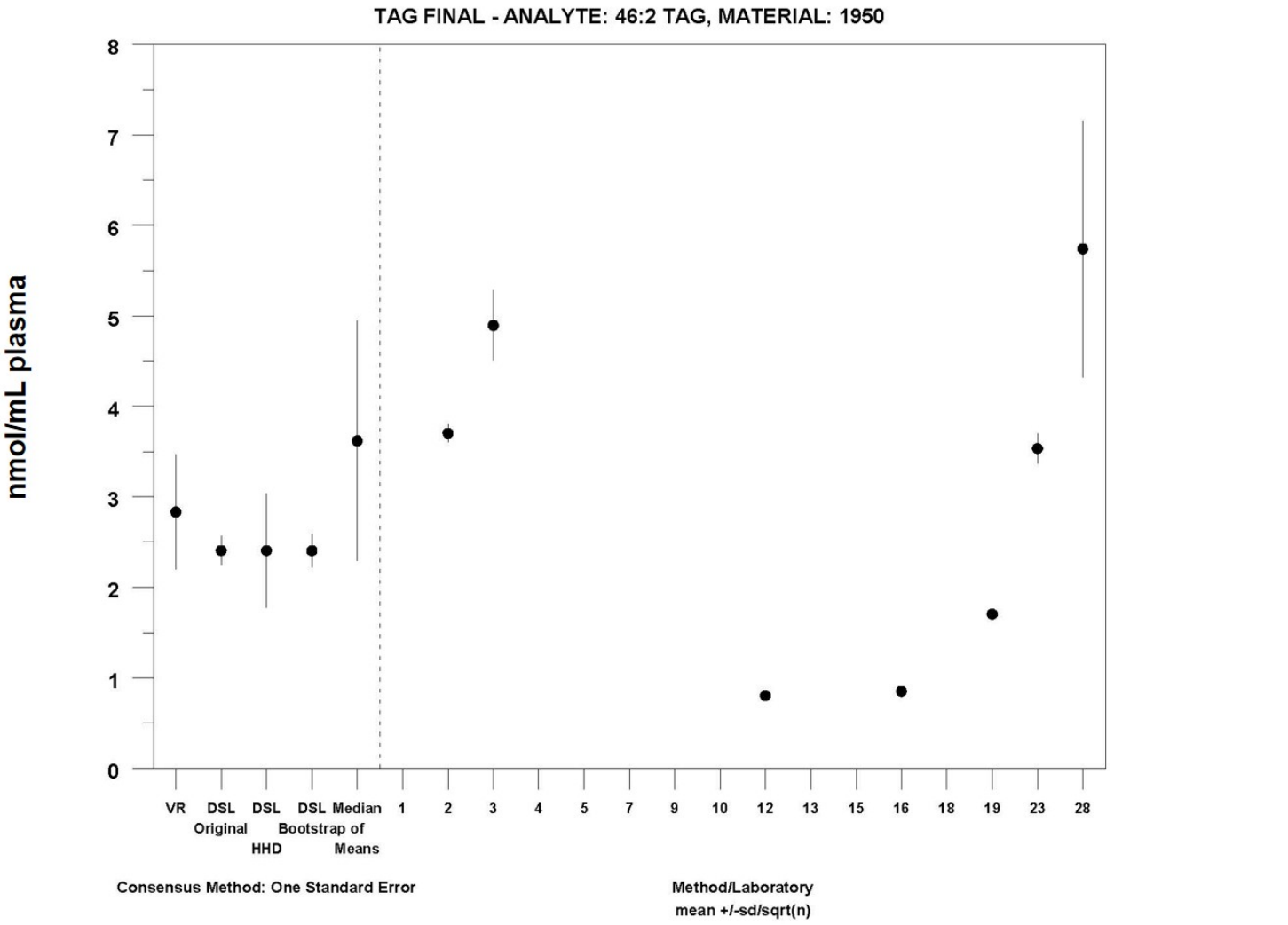
Labs Omitted from Plot (But Not Analysis): 15

15: 19 ± 2



MEDM Location: 2.8 ± 1.6 nmol/mL

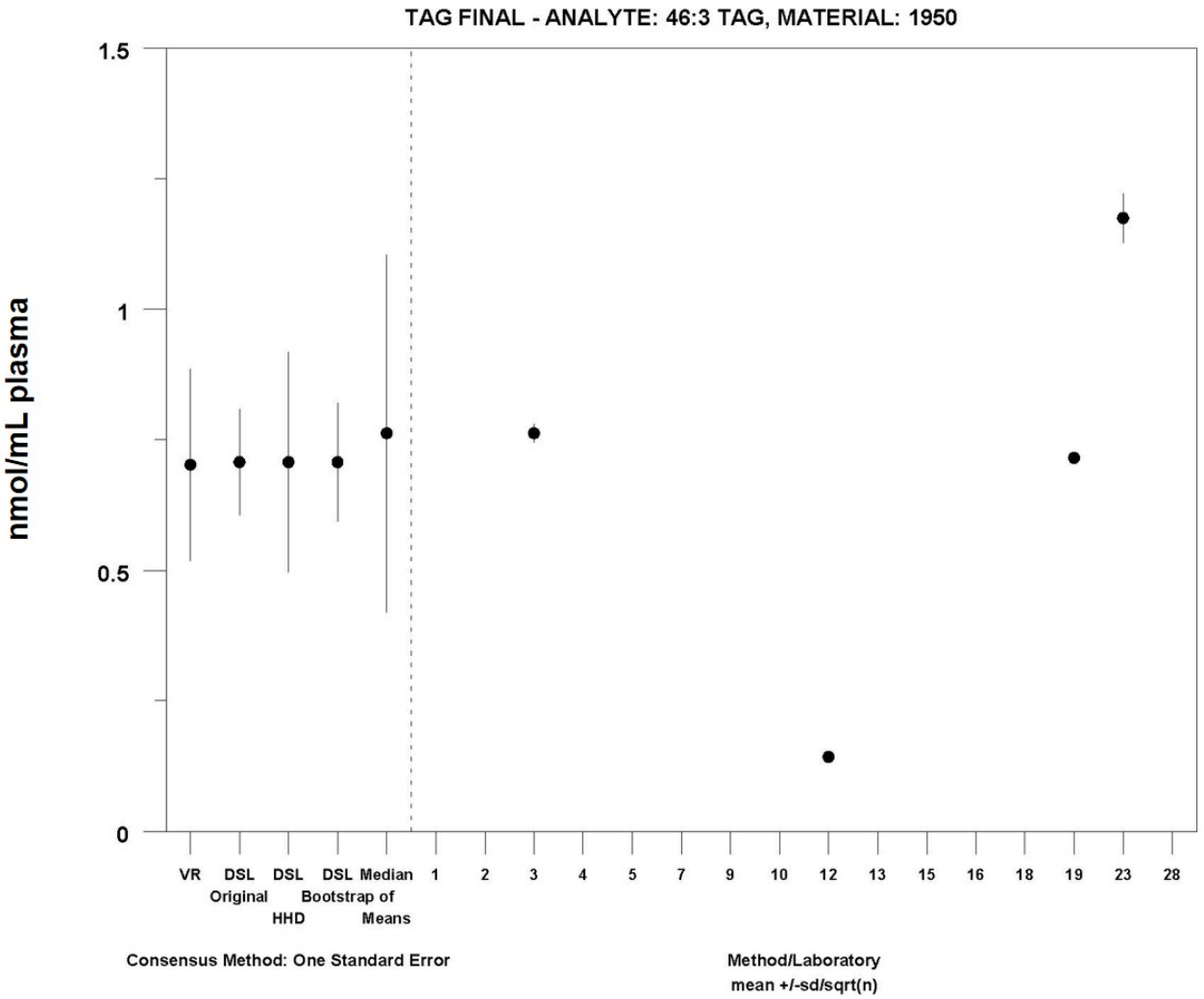




MEDM Location: 3.6 ± 1.3 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

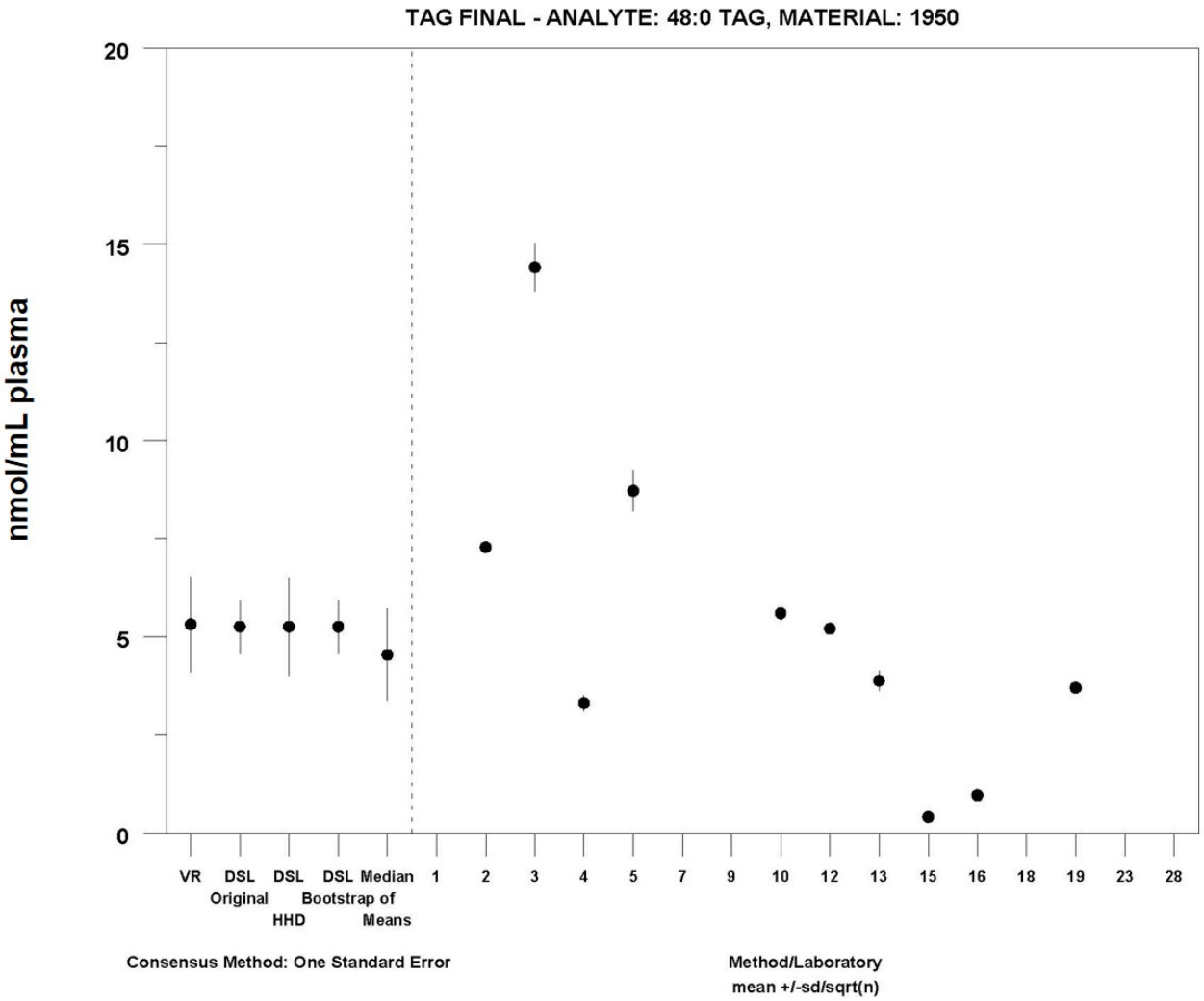
15: 60 ± 9



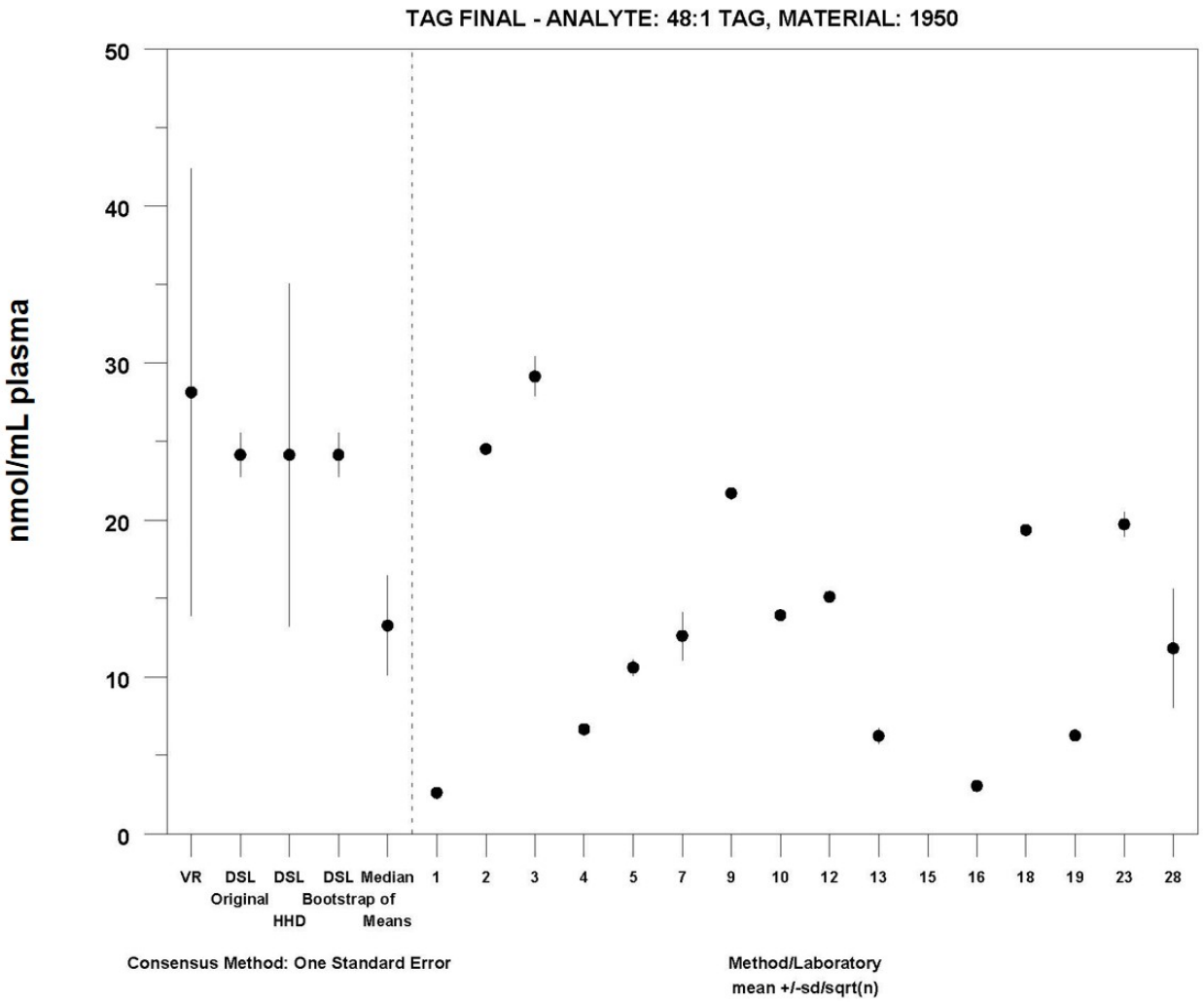
MEDM Location: 0.76 ± 0.34 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 18 ± 6



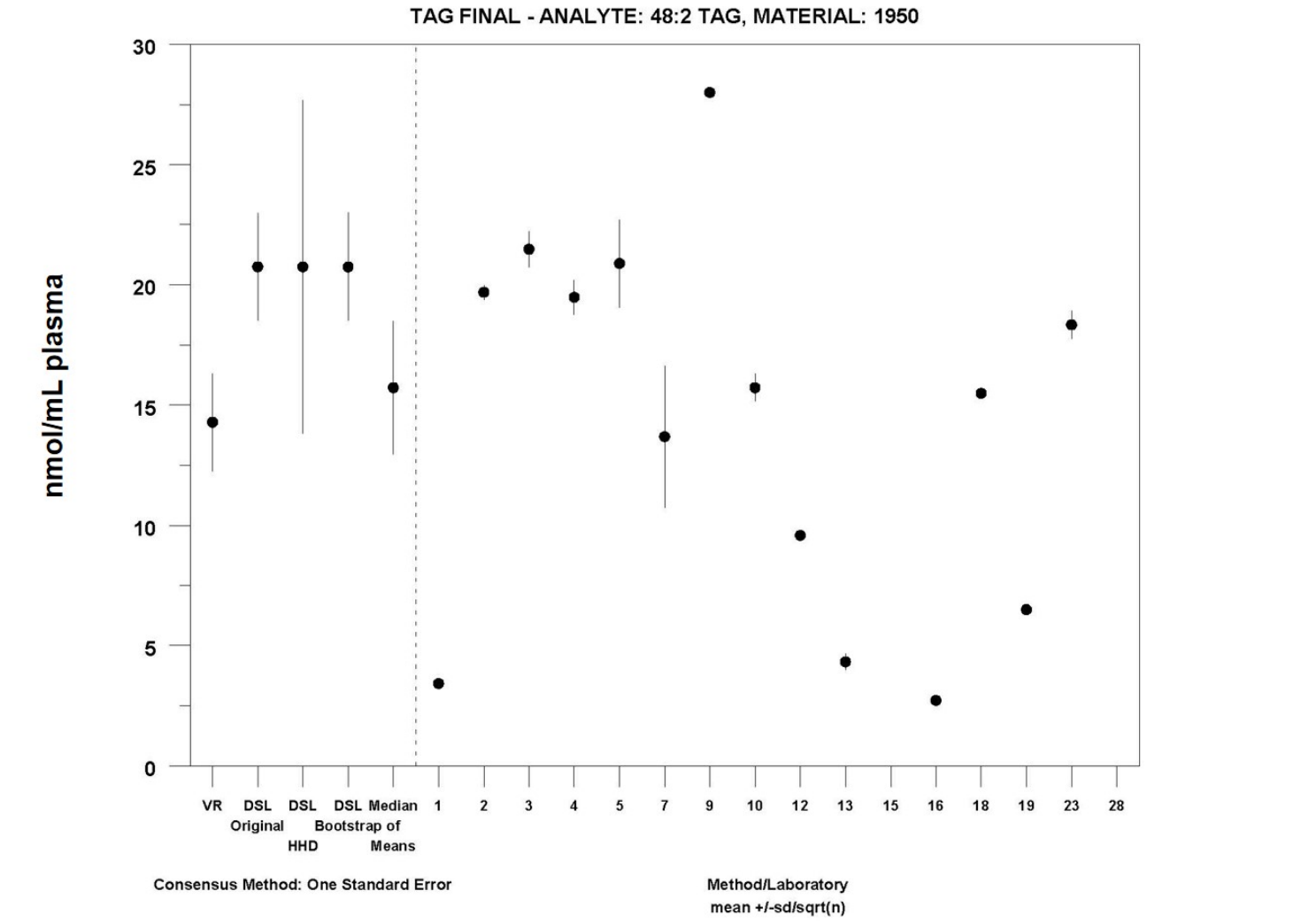
MEDM Location: 4.5 ± 1.2 nmol/mL



MEDM Location: 13 ± 3.2 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

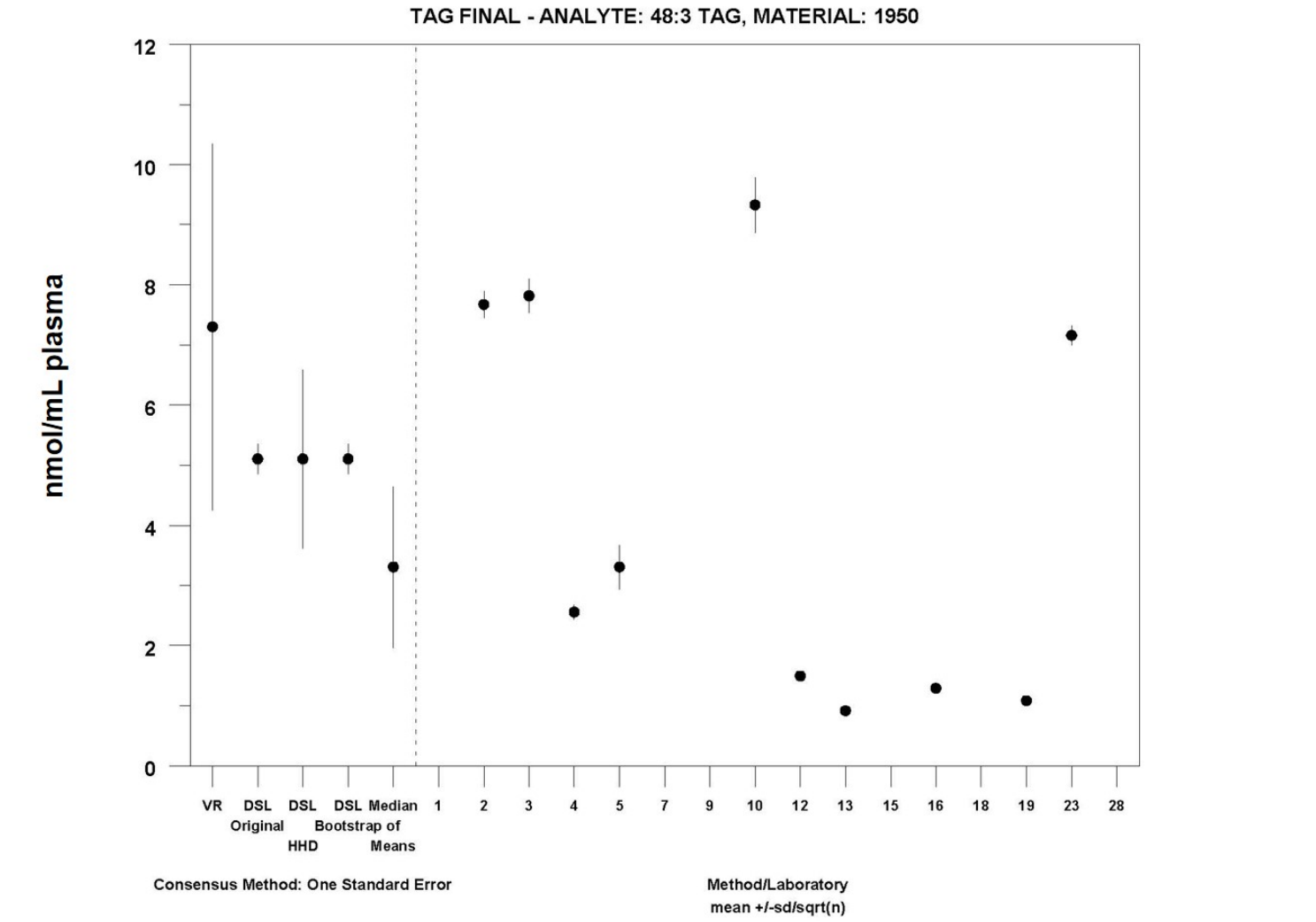
15: 248 ± 6



MEDM Location: 16 ± 2.8 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

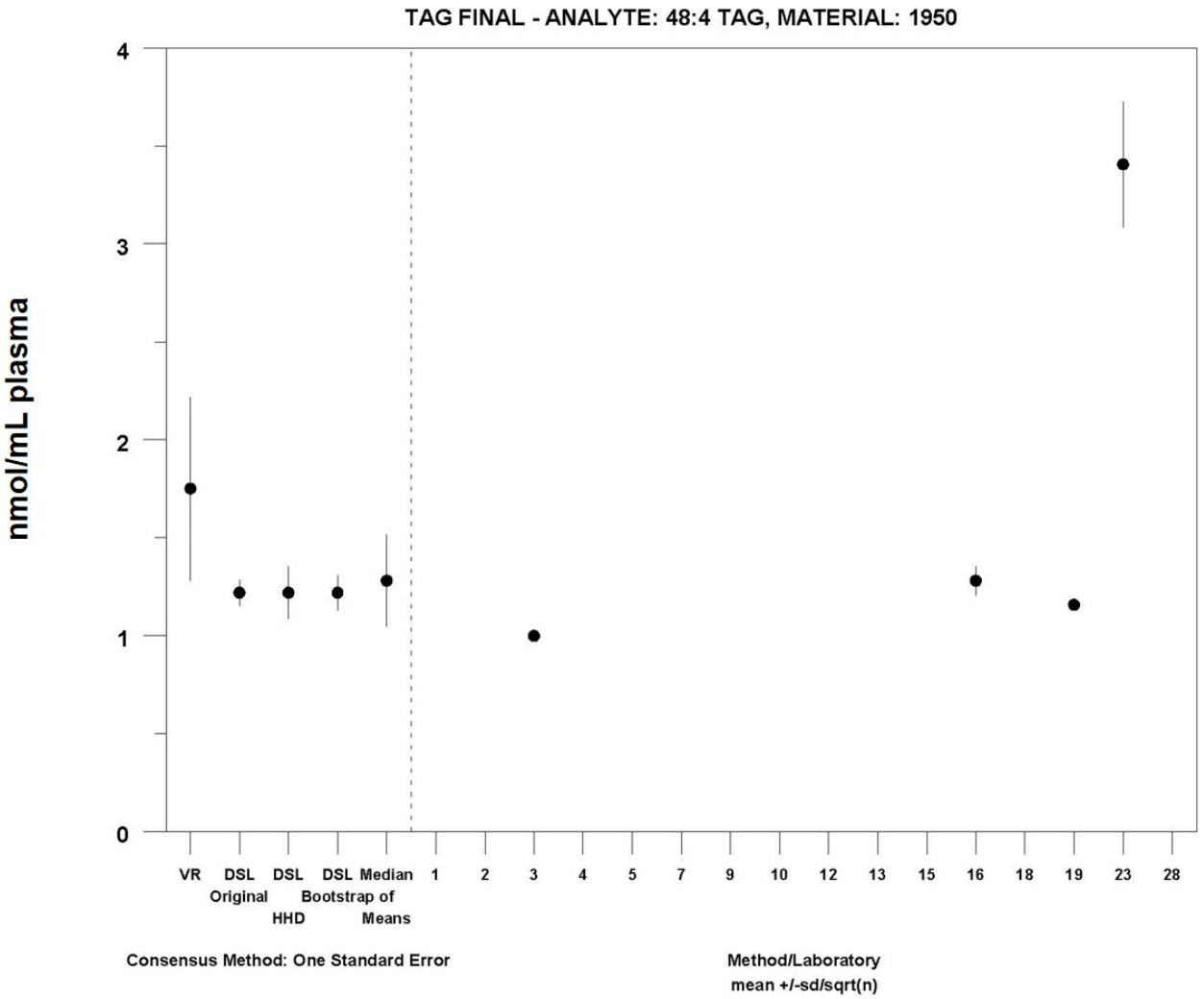
15: 170 ± 12



MEDM Location: 3.3 ± 1.3 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

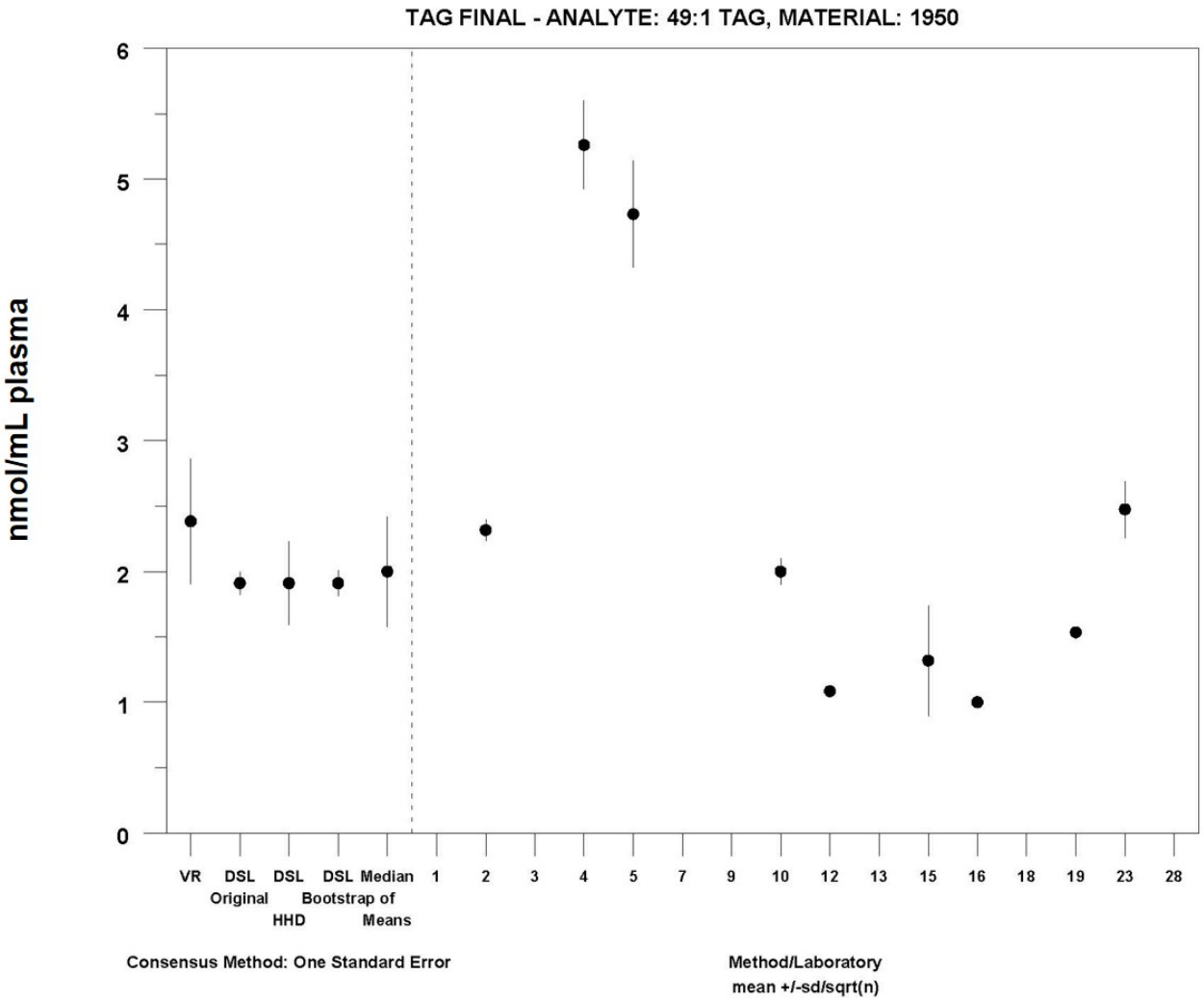
15: 38 ± 2



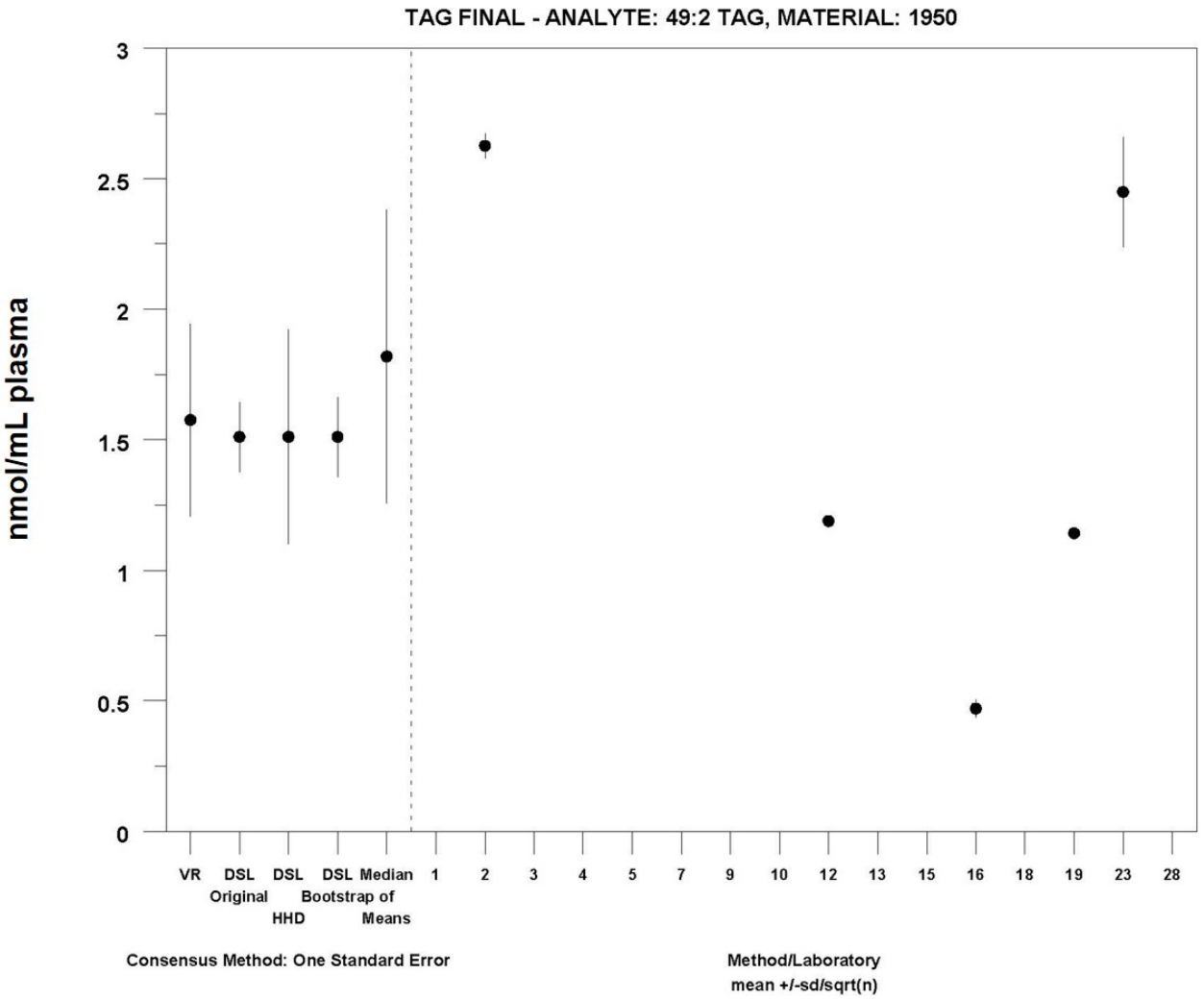
MEDM Location: 1.3 ± 0.23 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 7.5 ± 3.8



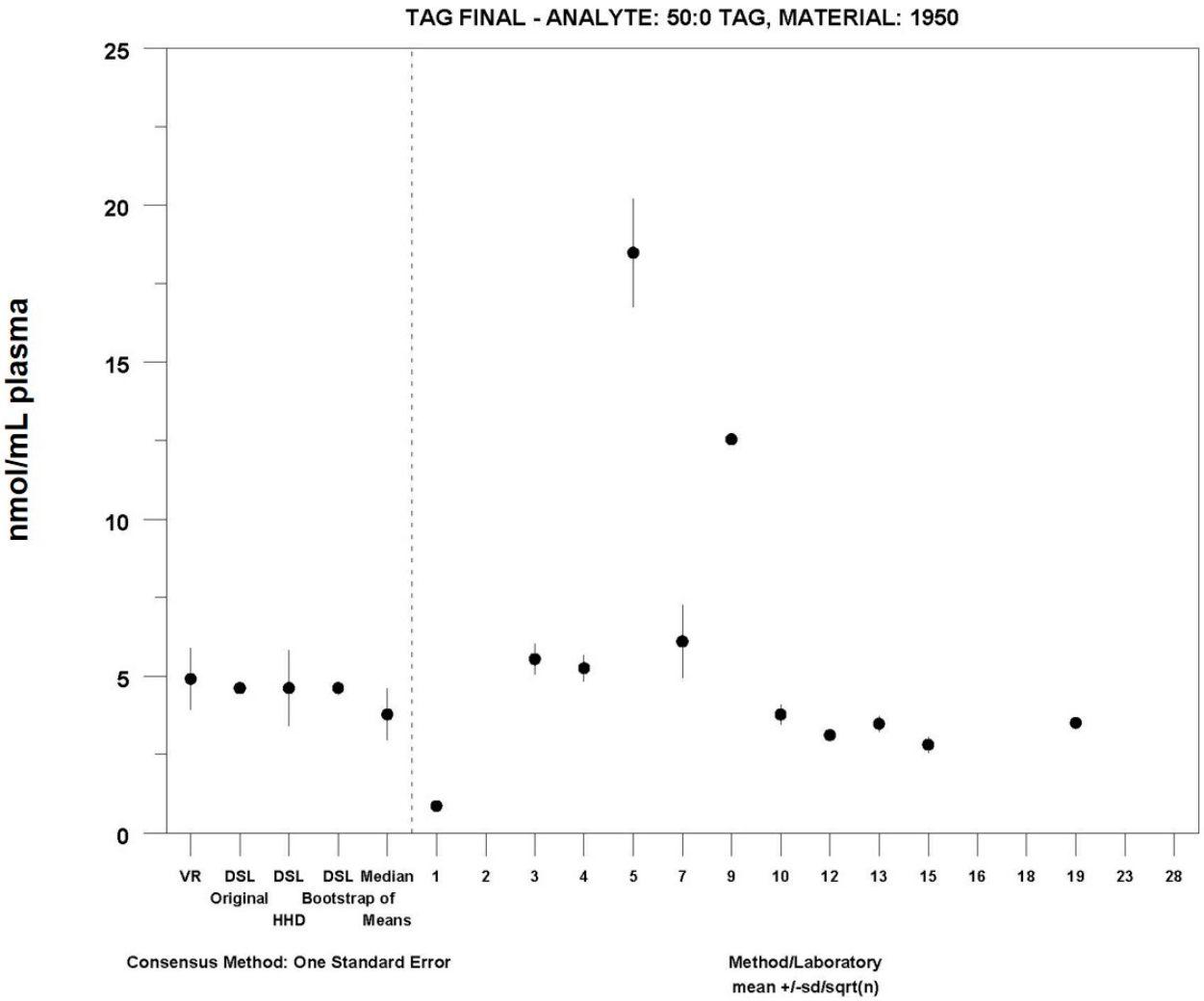
MEDM Location: 2.0 ± 0.42 nmol/mL



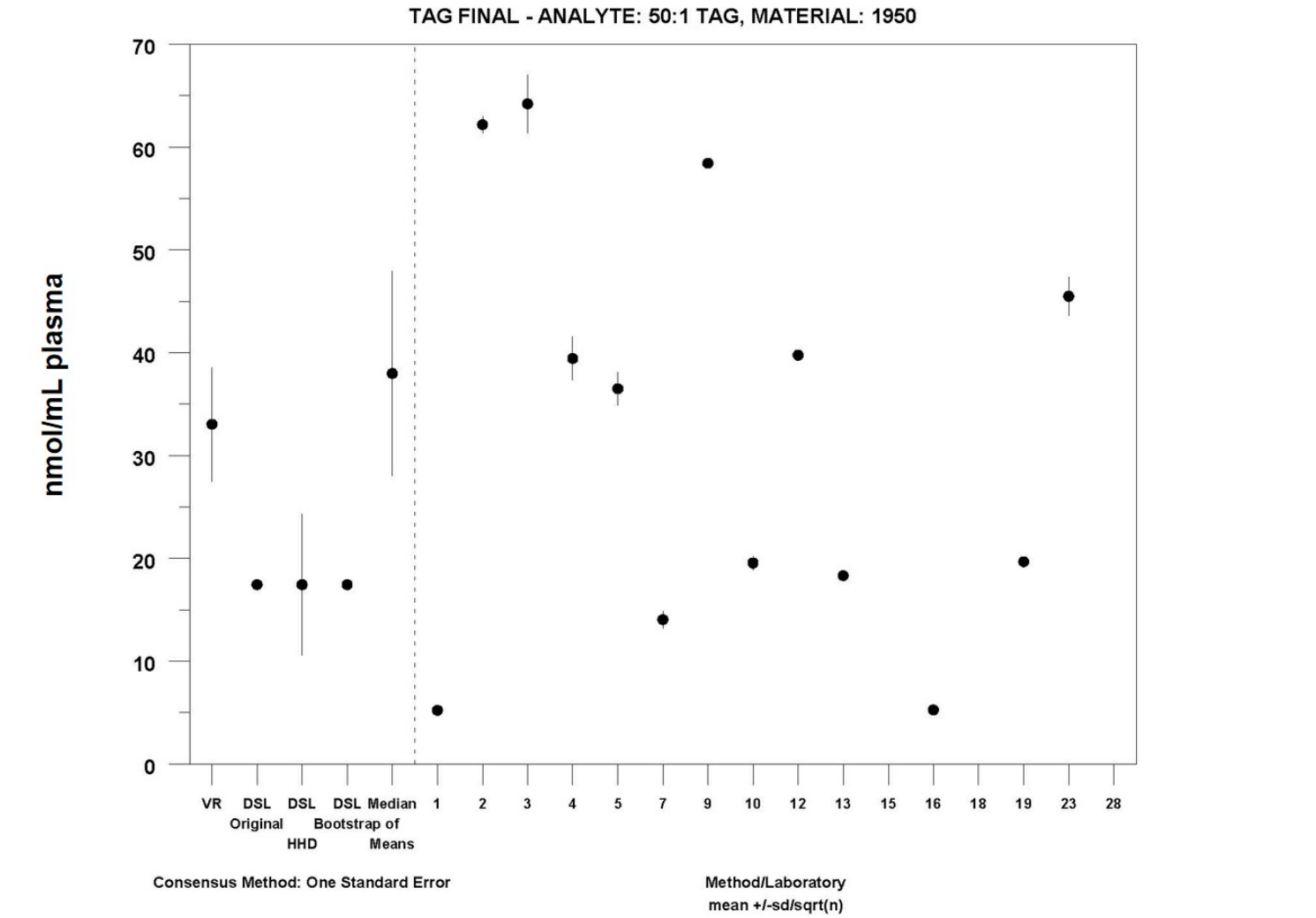
MEDM Location: 1.8 ± 0.56 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 30 ± 17



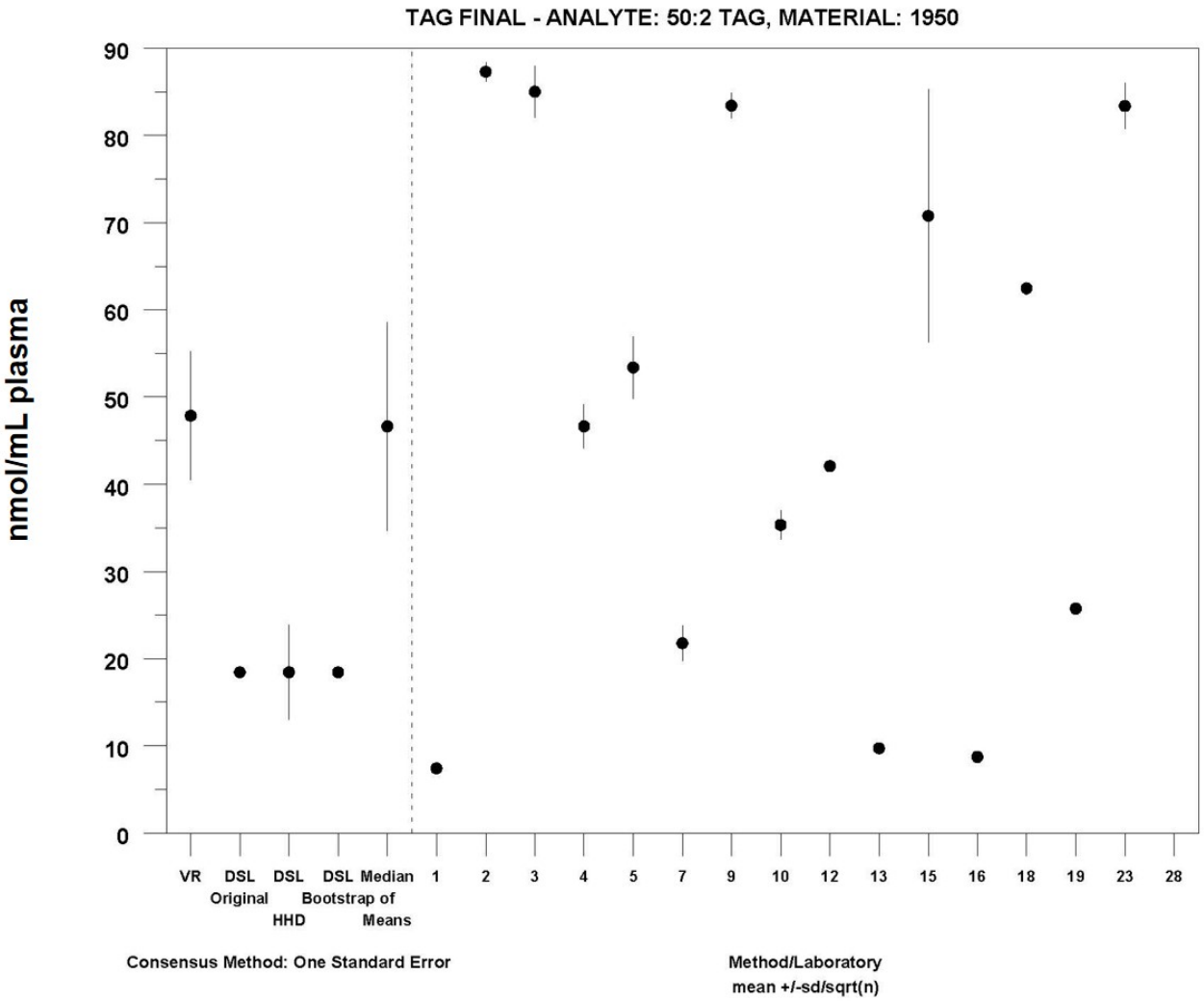
MEDM Location: 3.8 ± 0.83 nmol/mL



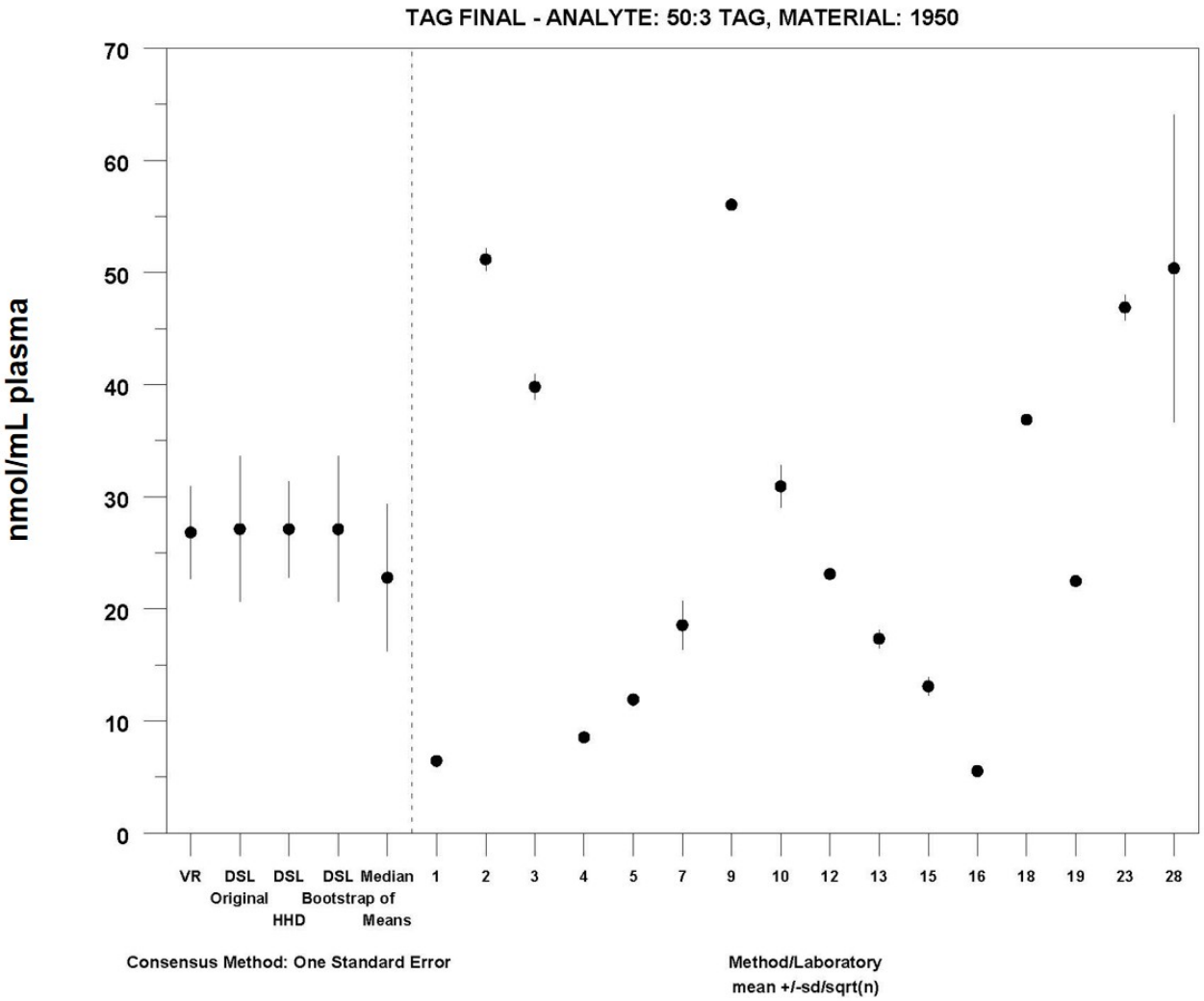
MEDM Location: 38 ± 10.0 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

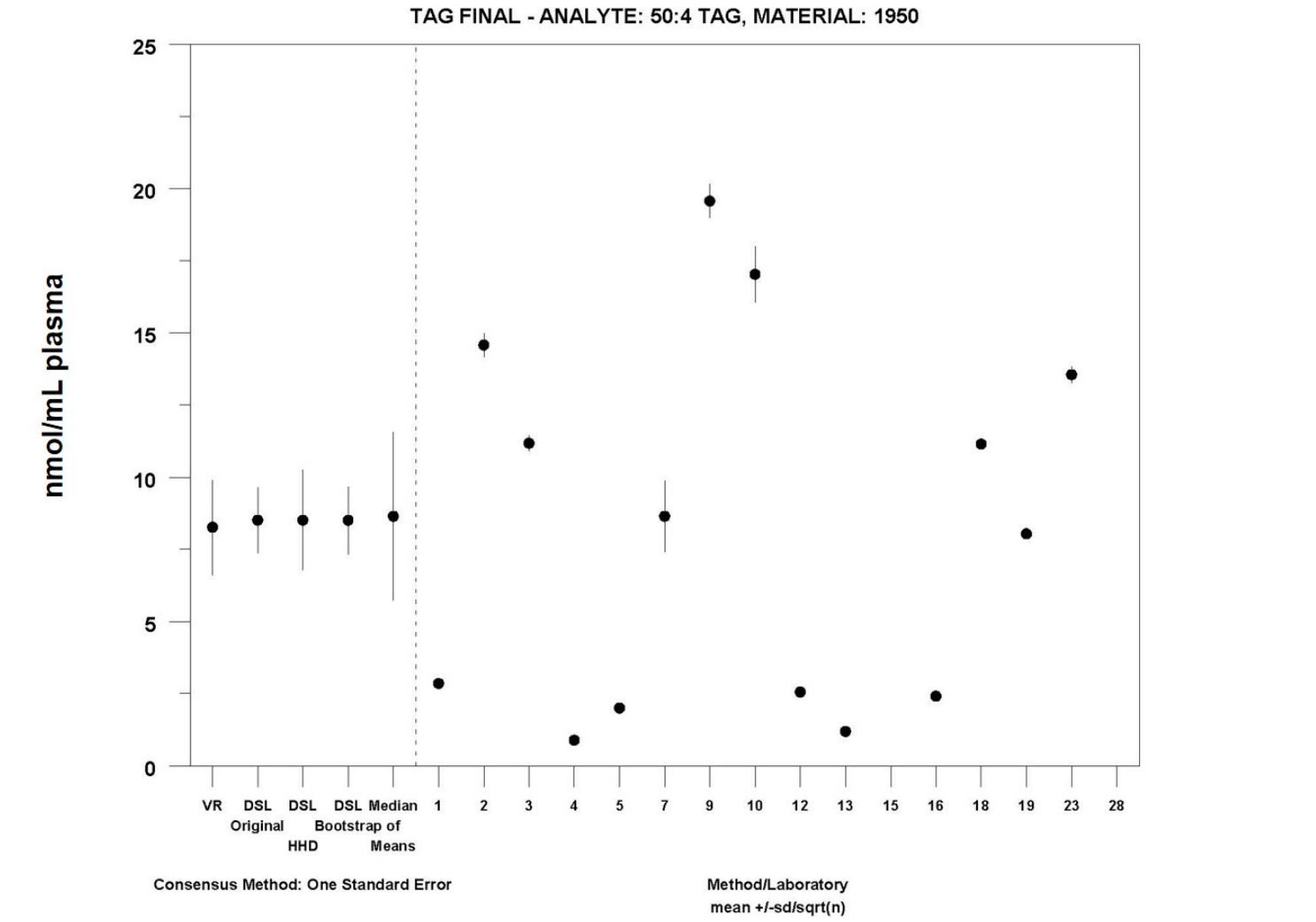
15: 506 ± 156



MEDM Location: 47 ± 12 nmol/mL



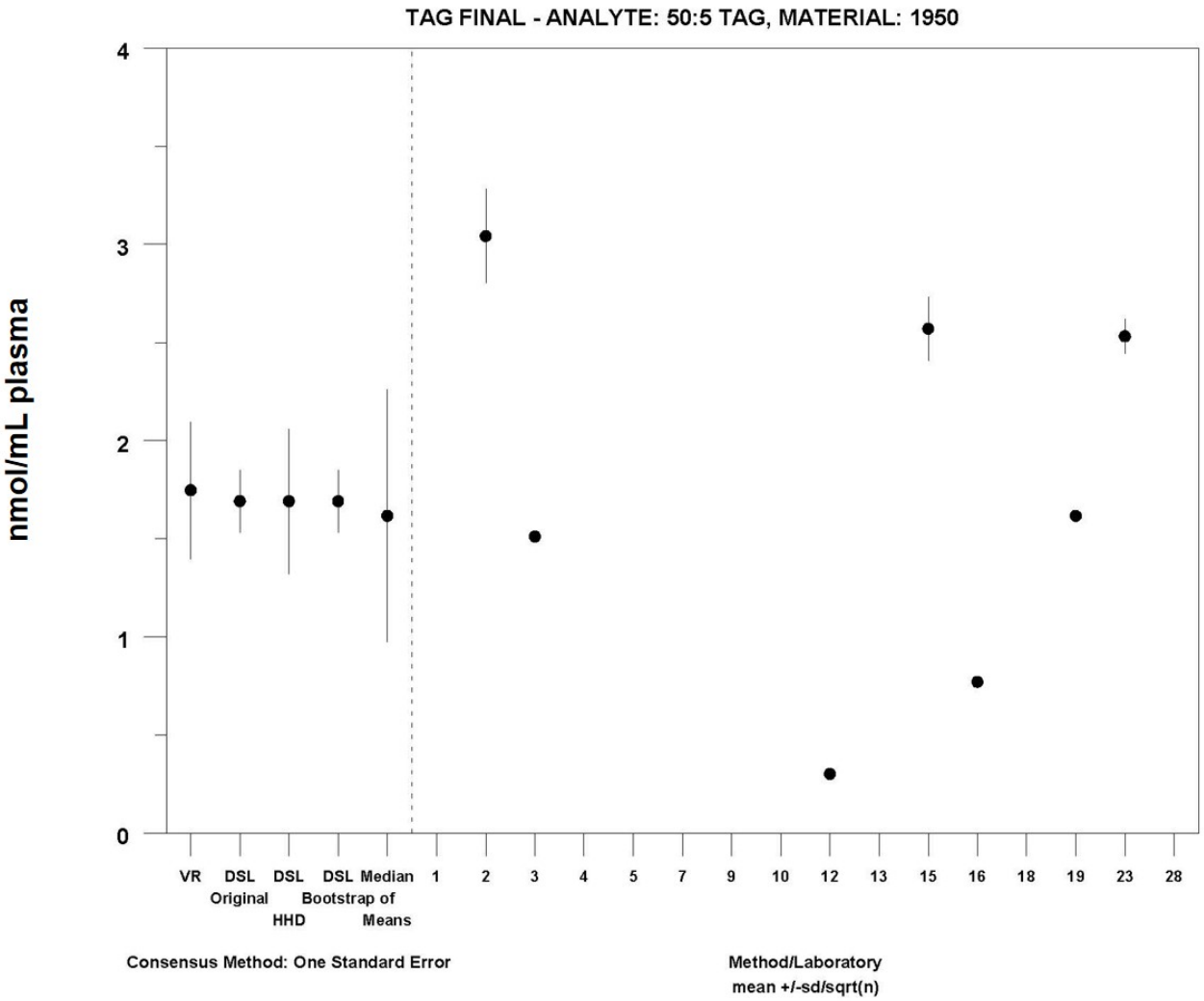
MEDM Location: 23 ± 6.6 nmol/mL



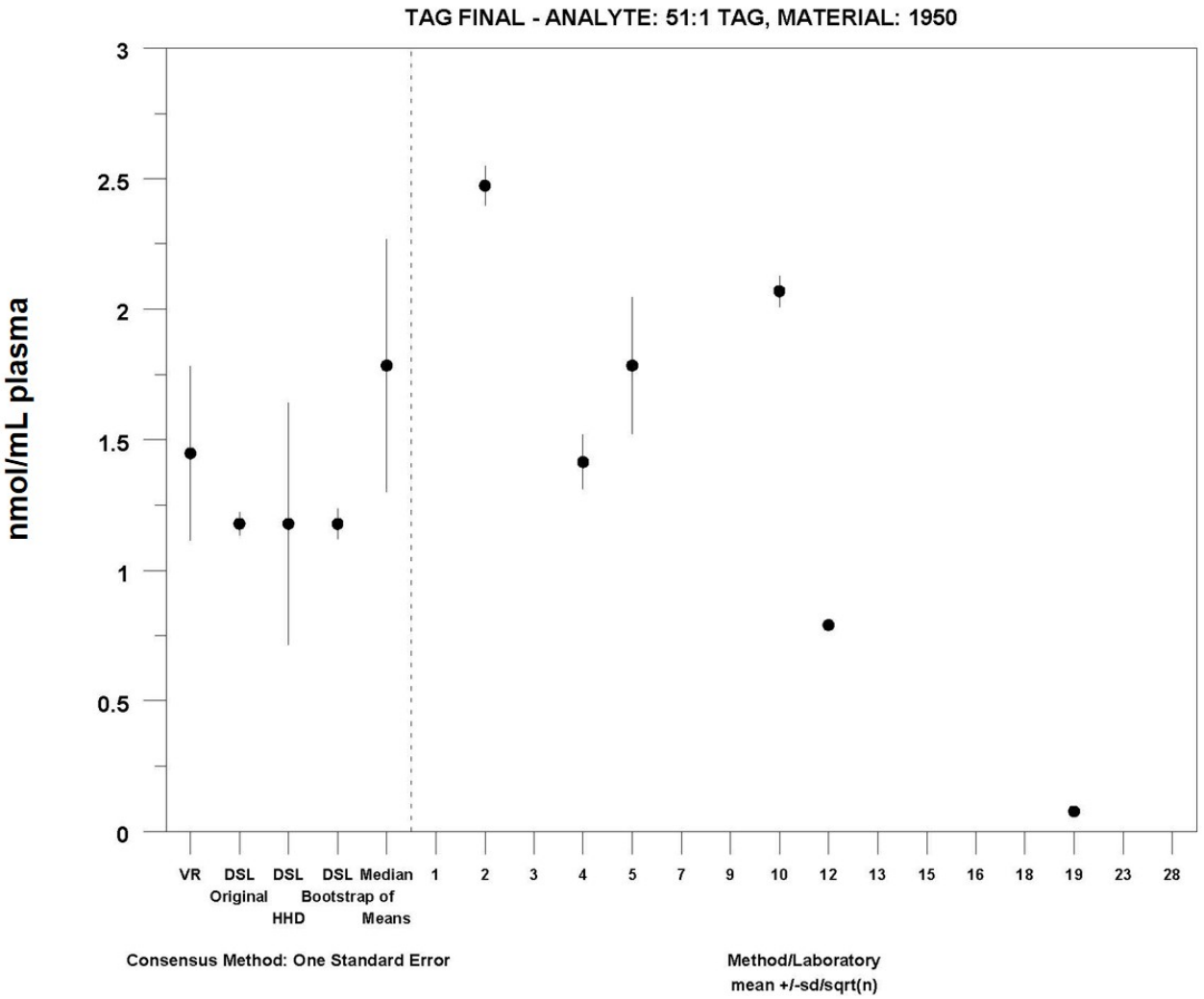
MEDM Location: 8.7 ± 2.9 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 250 ± 55



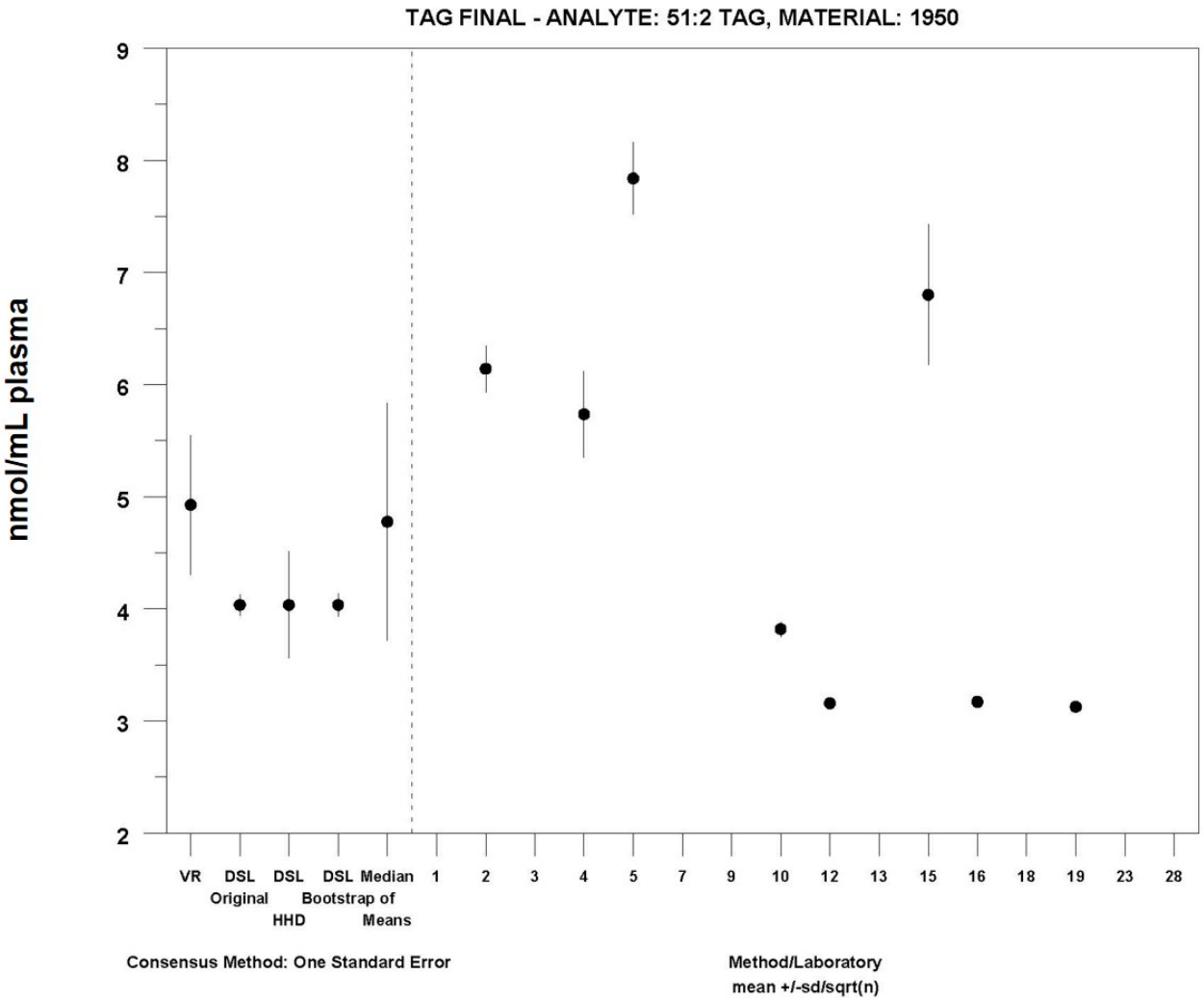
MEDM Location: 1.6 ± 0.64 nmol/mL



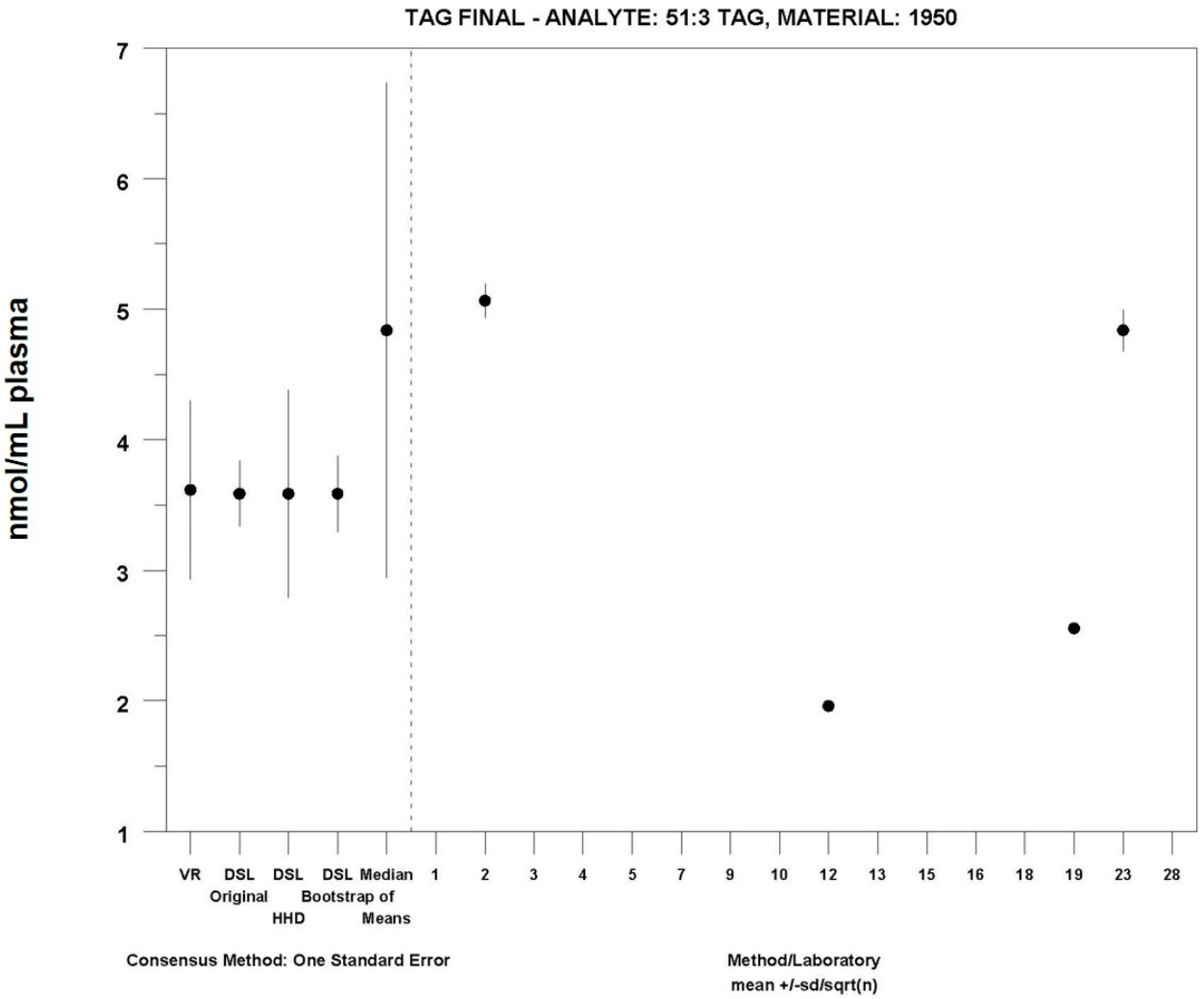
MEDM Location: 1.8 ± 0.48 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 15 ± 7



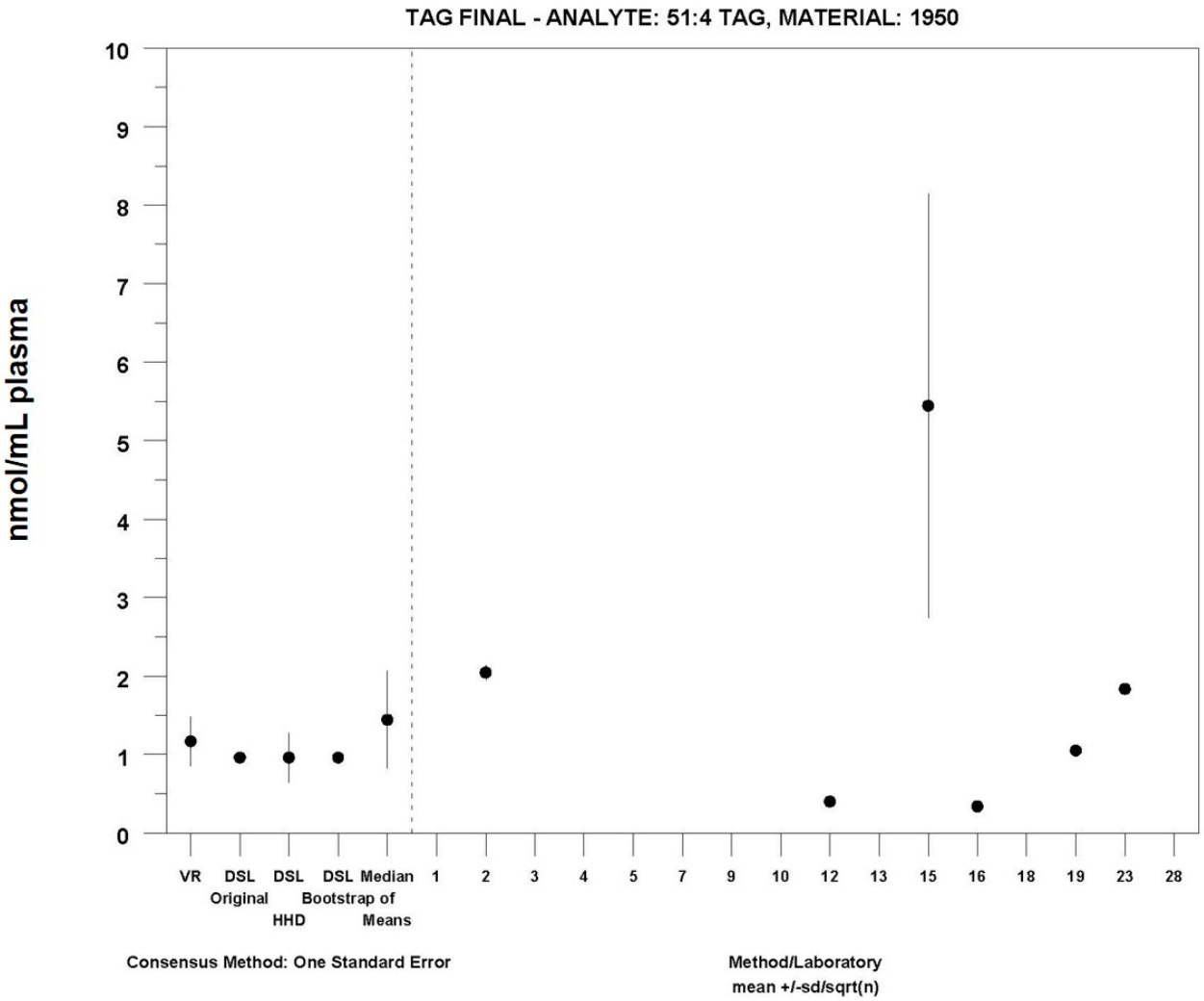
MEDM Location: 4.8 ± 1.1 nmol/mL



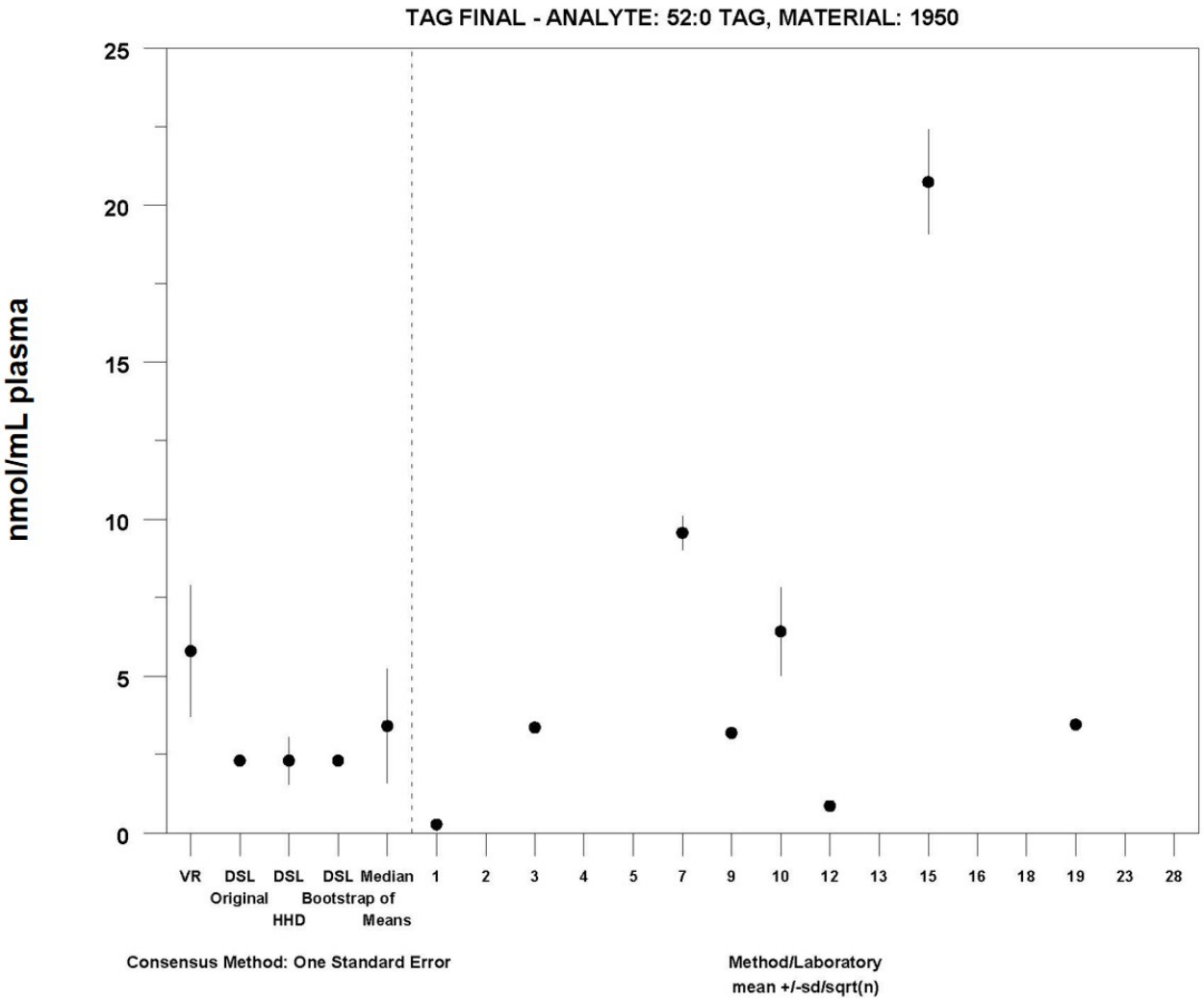
MEDM Location: 4.8 ± 1.9 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

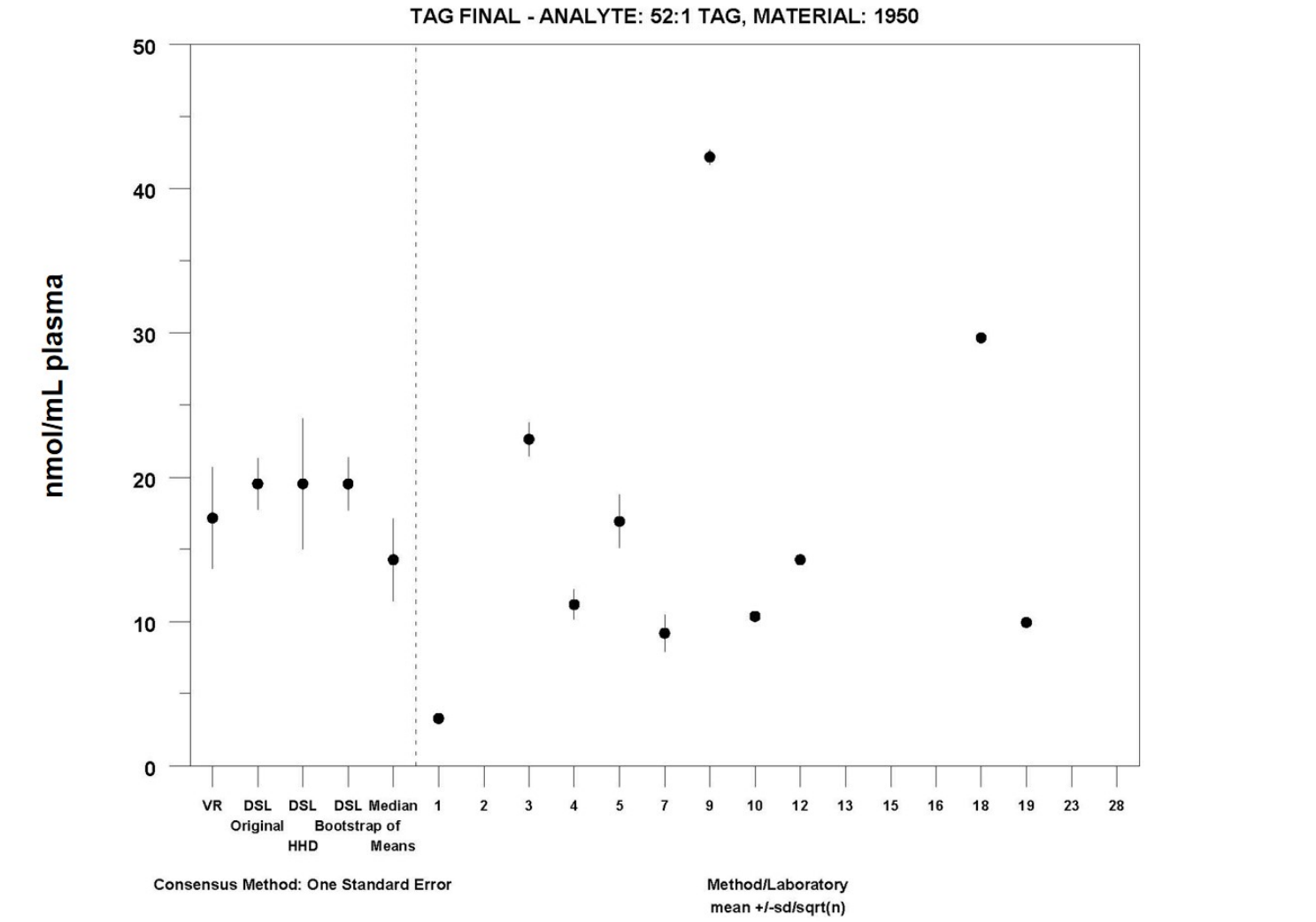
15: 74 ± 19



MEDM Location: 1.4 ± 0.62 nmol/mL



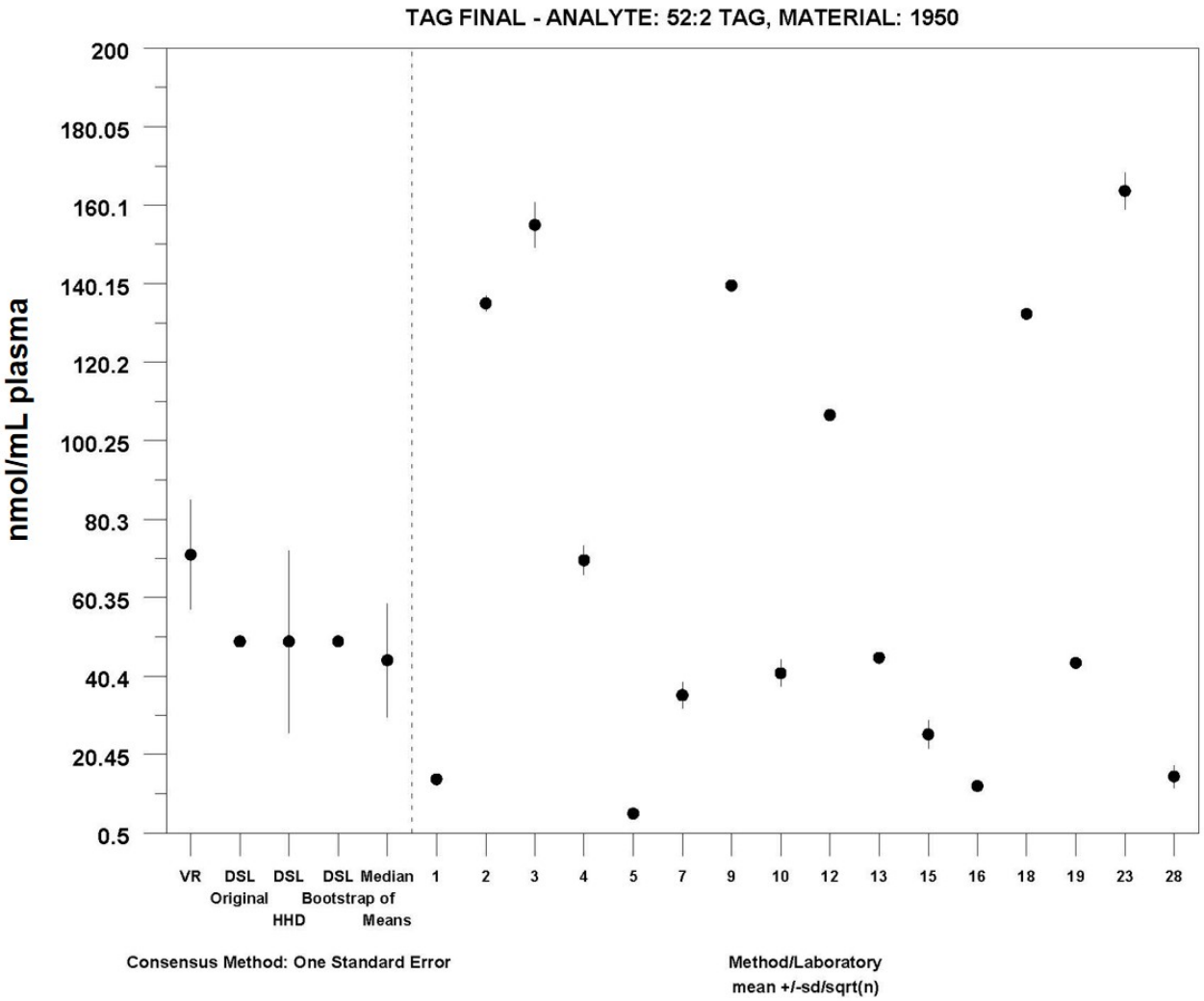
MEDM Location: 3.4 ± 1.8 nmol/mL



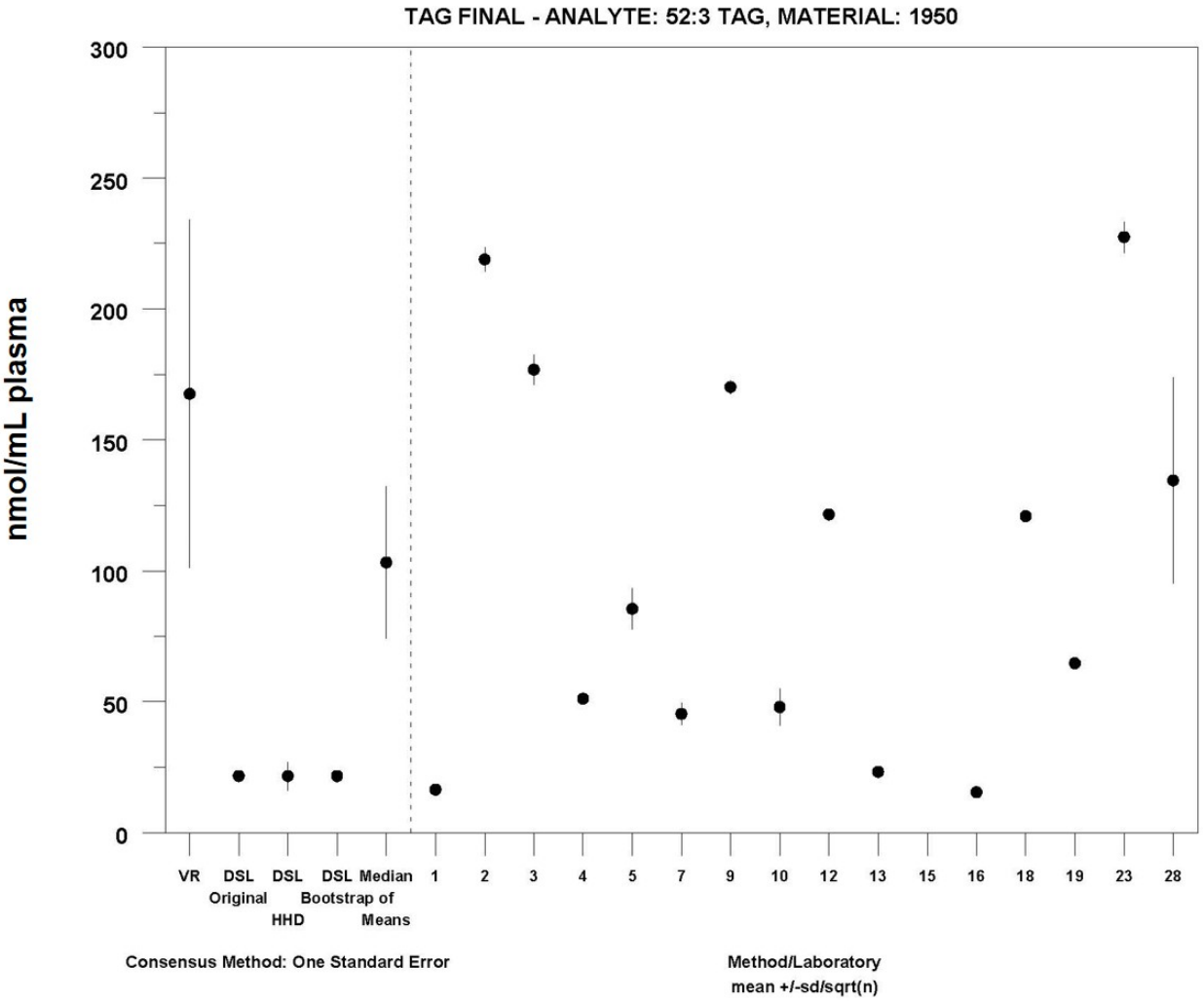
MEDM Location: 14 ± 2.9 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 200 ± 24



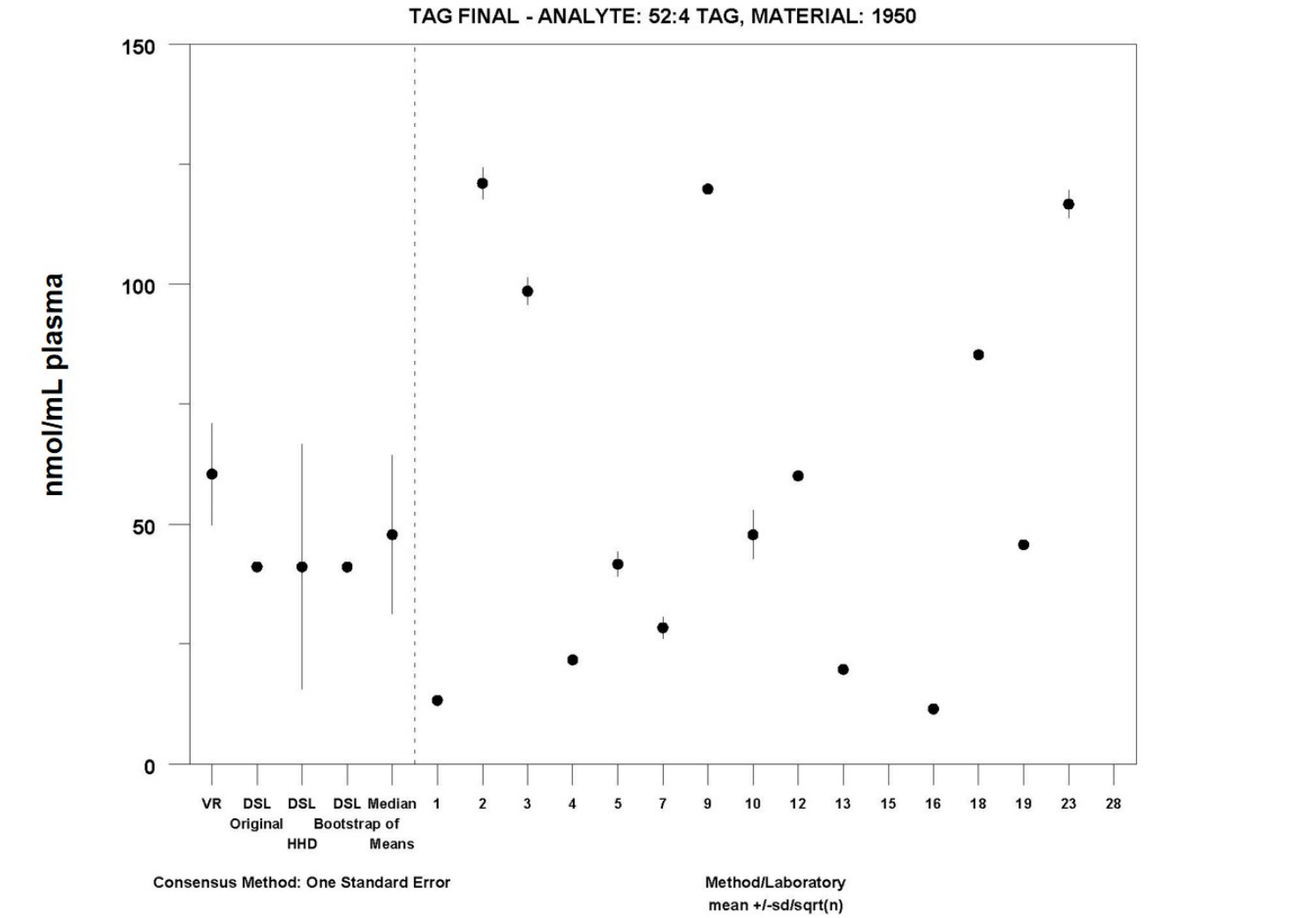
MEDM Location: 44 ± 14 nmol/mL



MEDM Location: 100 ± 29 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

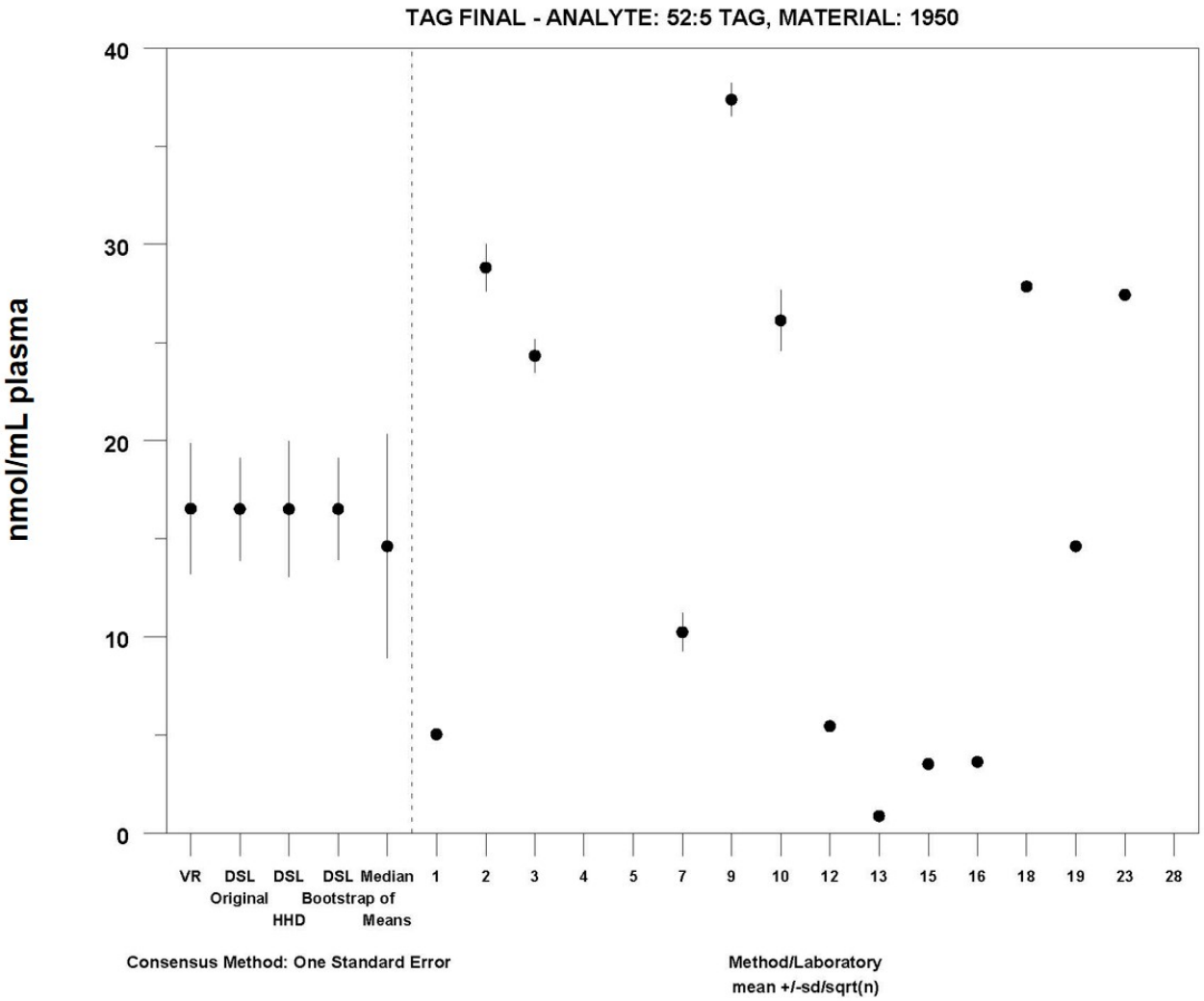
15: 1166 ± 35



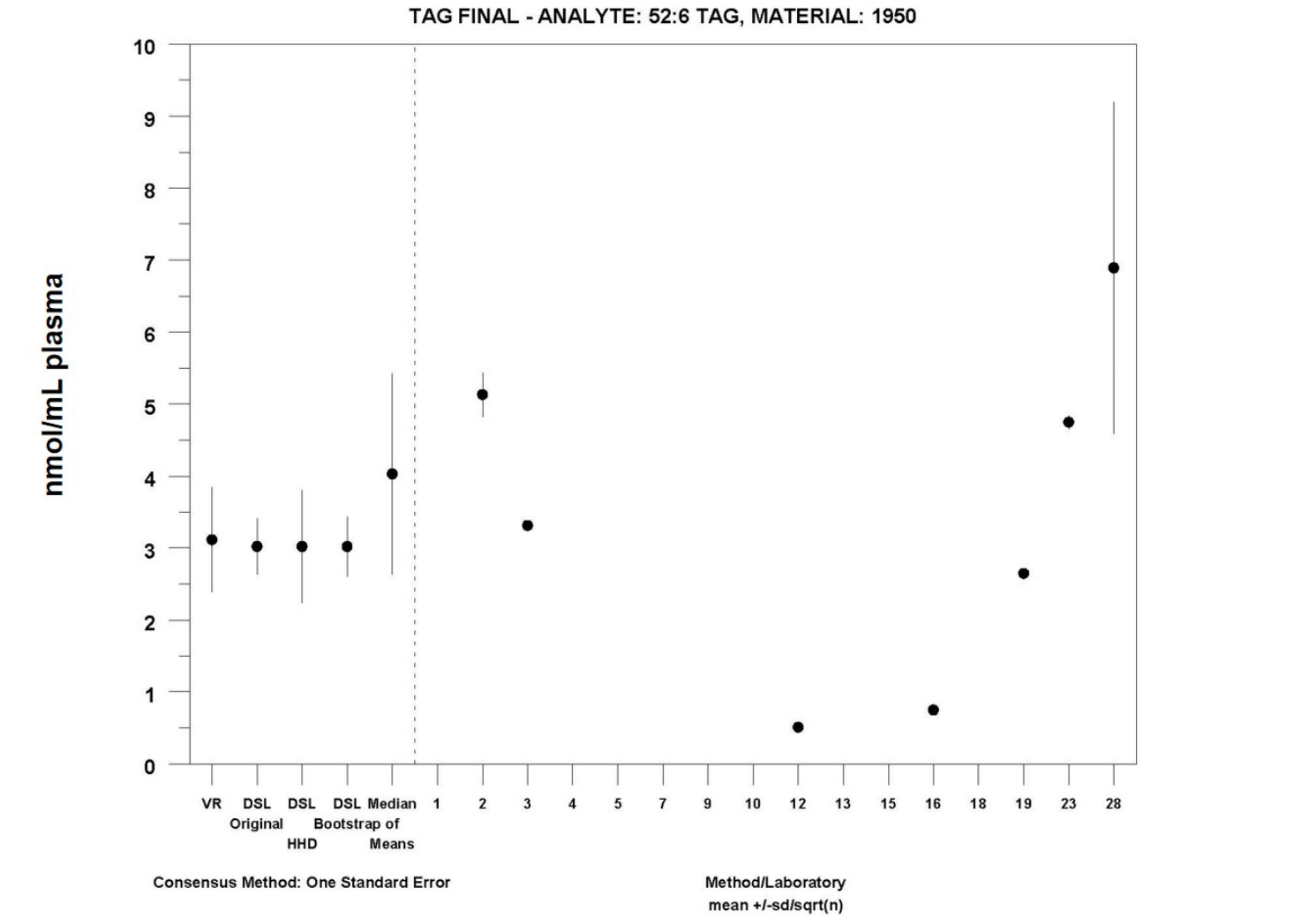
MEDM Location: 48 ± 17 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 350 ± 105



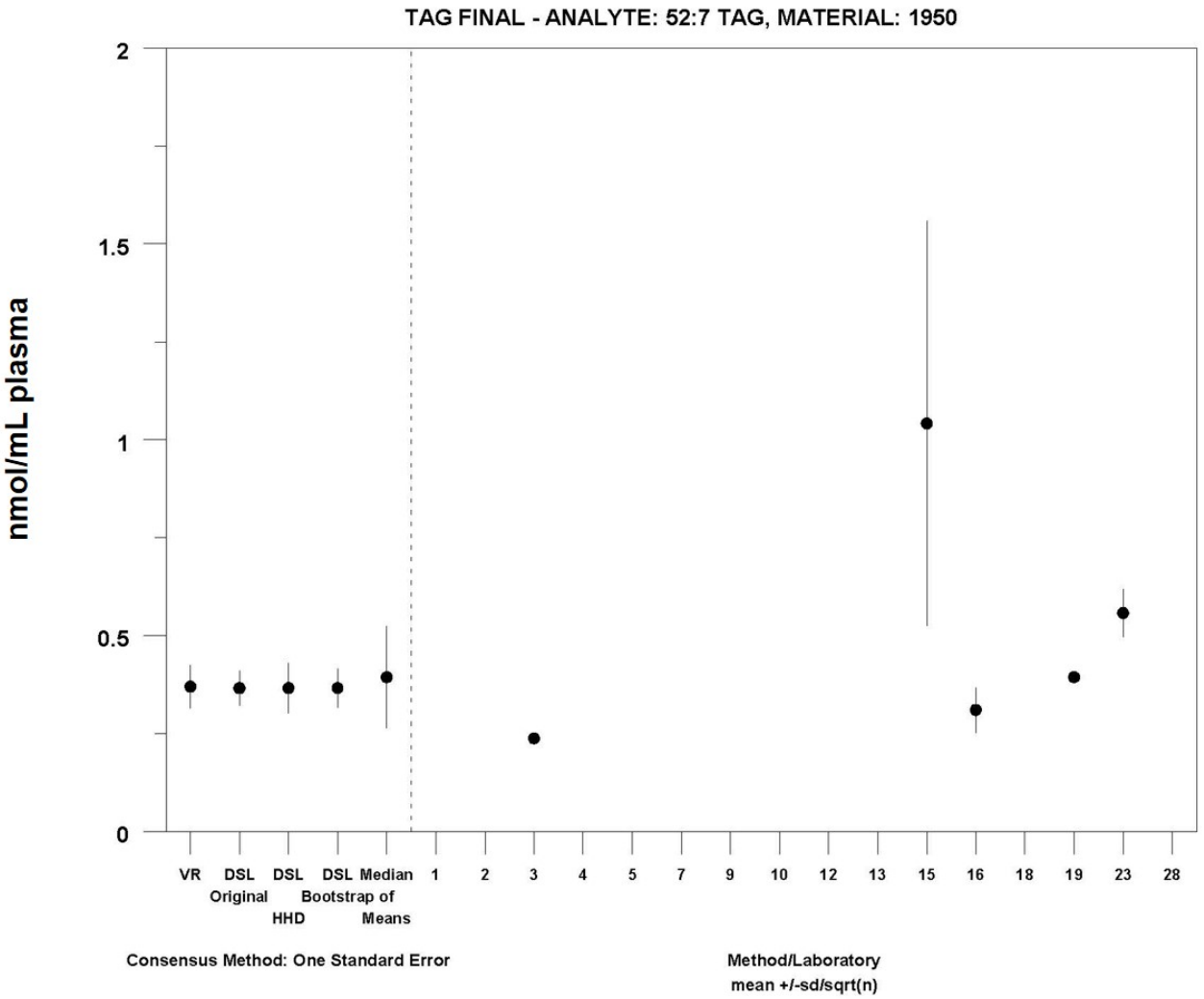
MEDM Location: 15 ± 5.7 nmol/mL



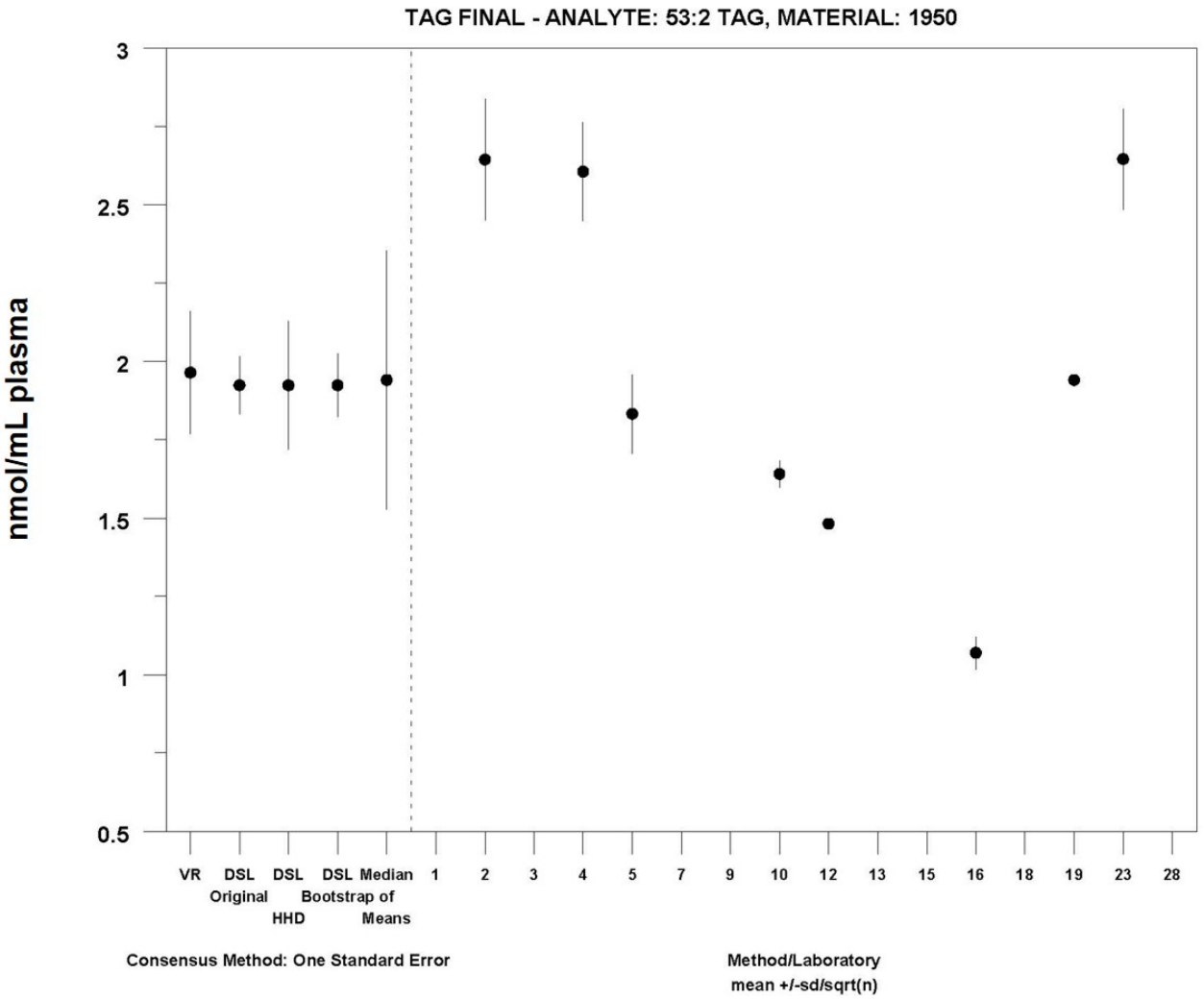
MEDM Location: 4.0 ± 1.4 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 29 ± 10



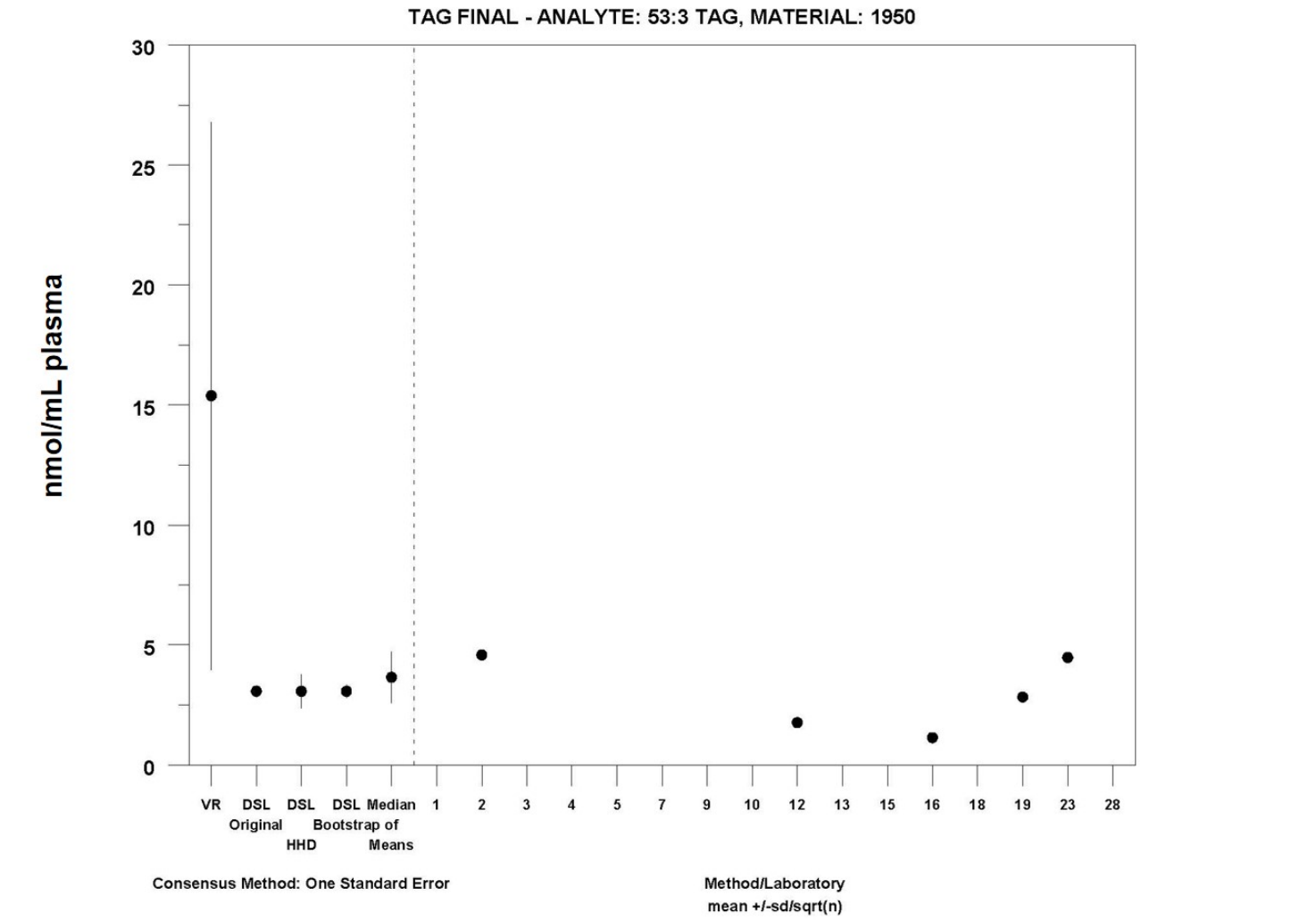
MEDM Location: 0.39 ± 0.13 nmol/mL

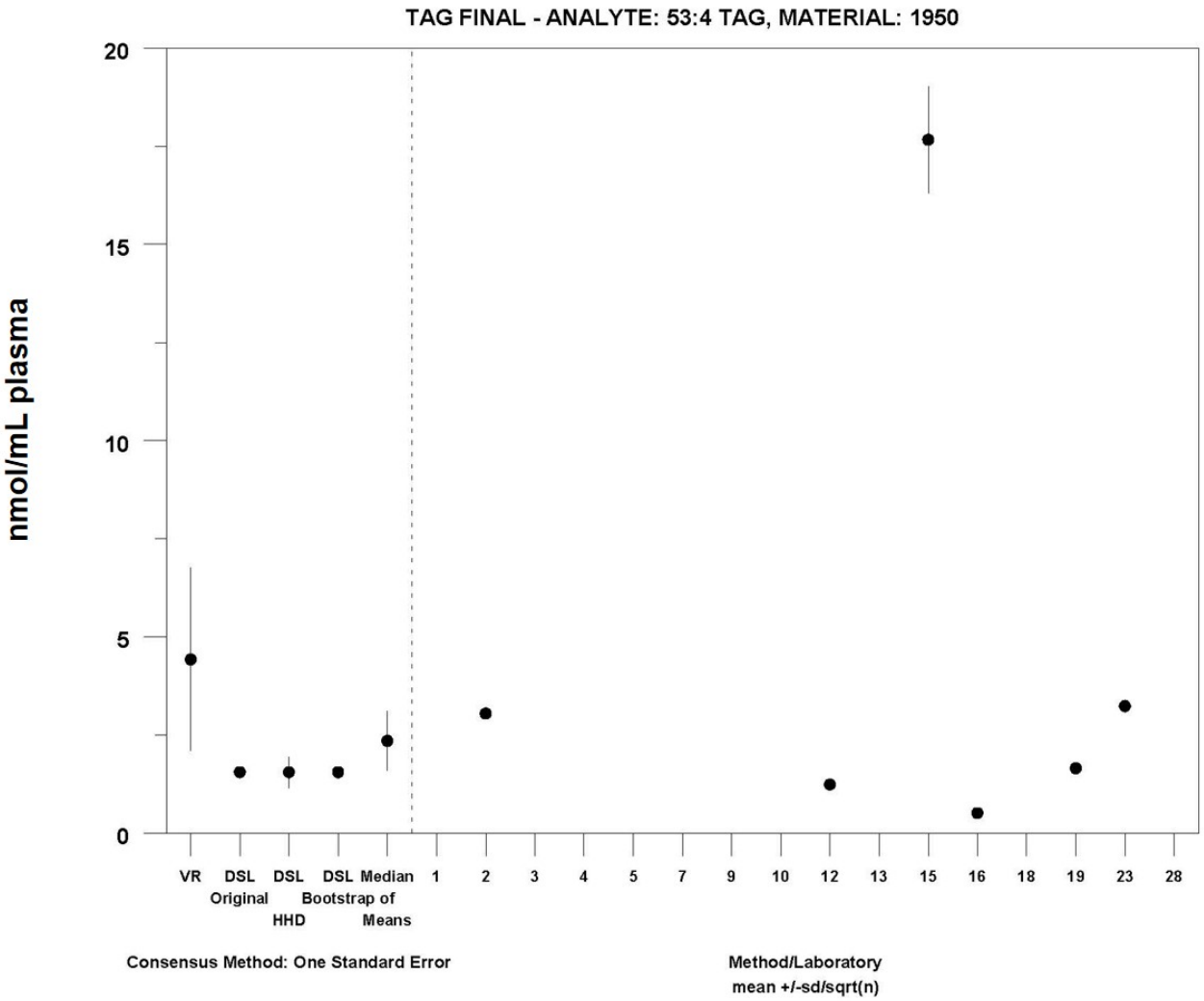


MEDM Location: 1.9 ± 0.41 nmol/mL

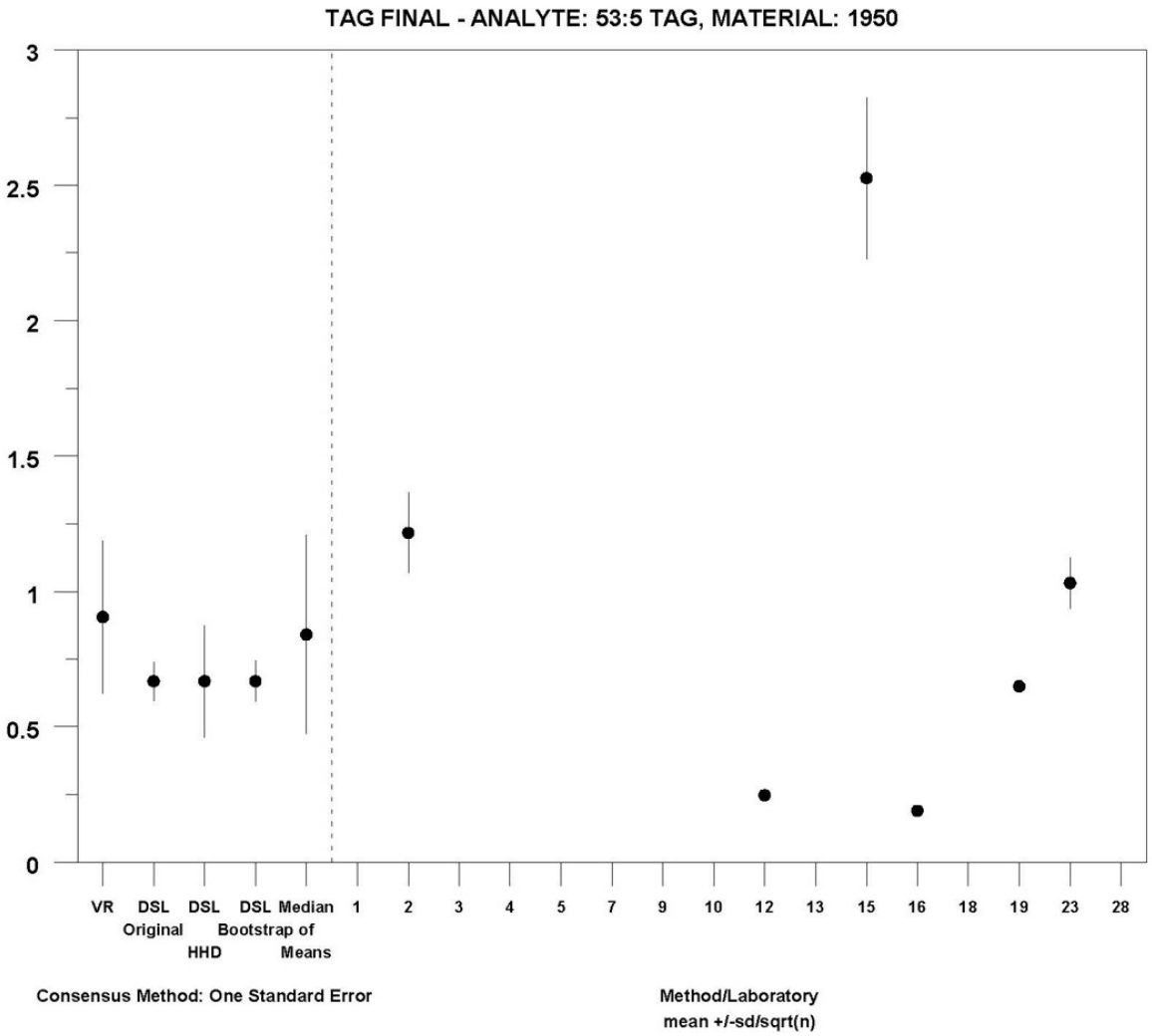
Labs Omitted from Plot (But Not Analysis): 15

15: 40 ± 6

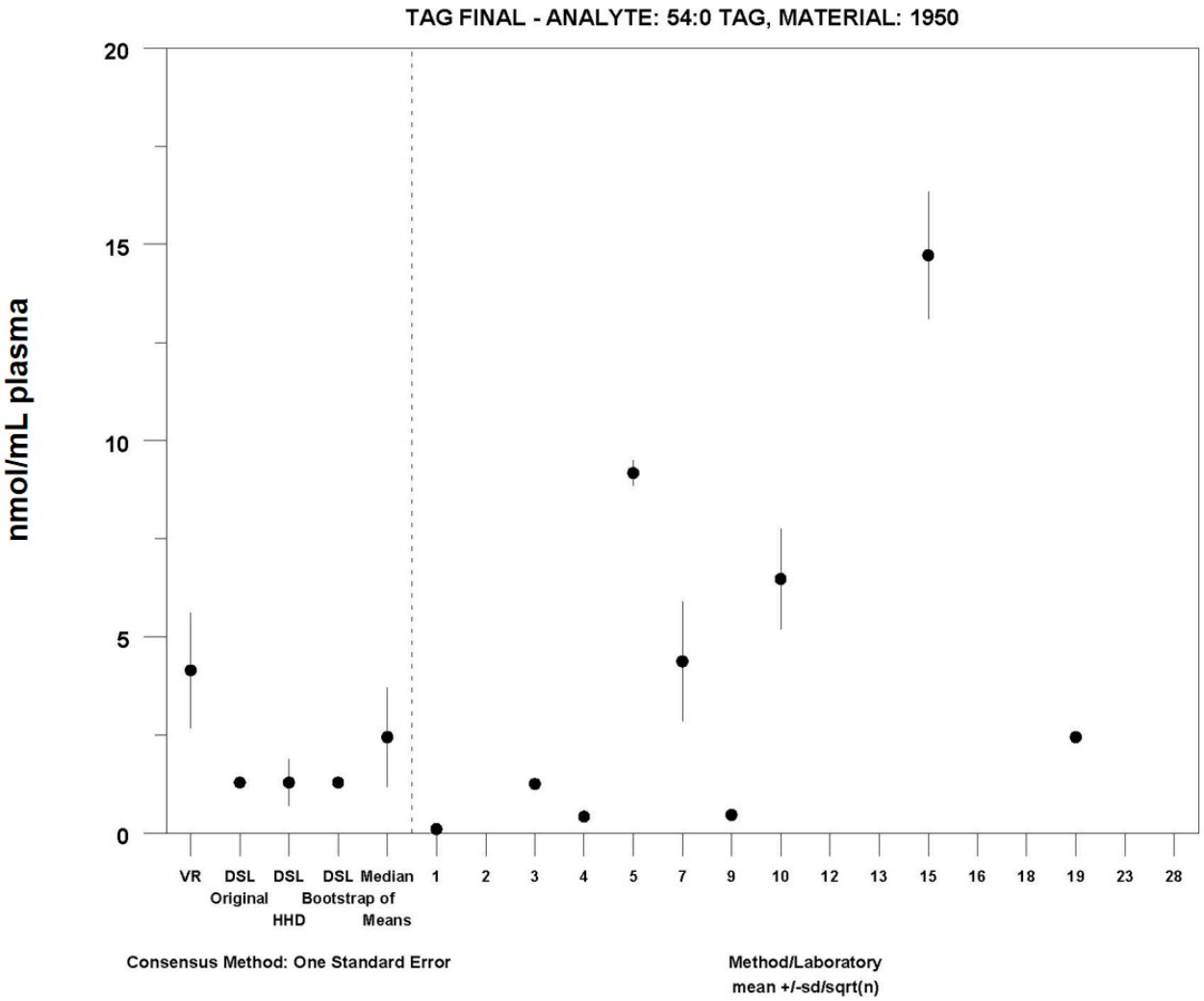




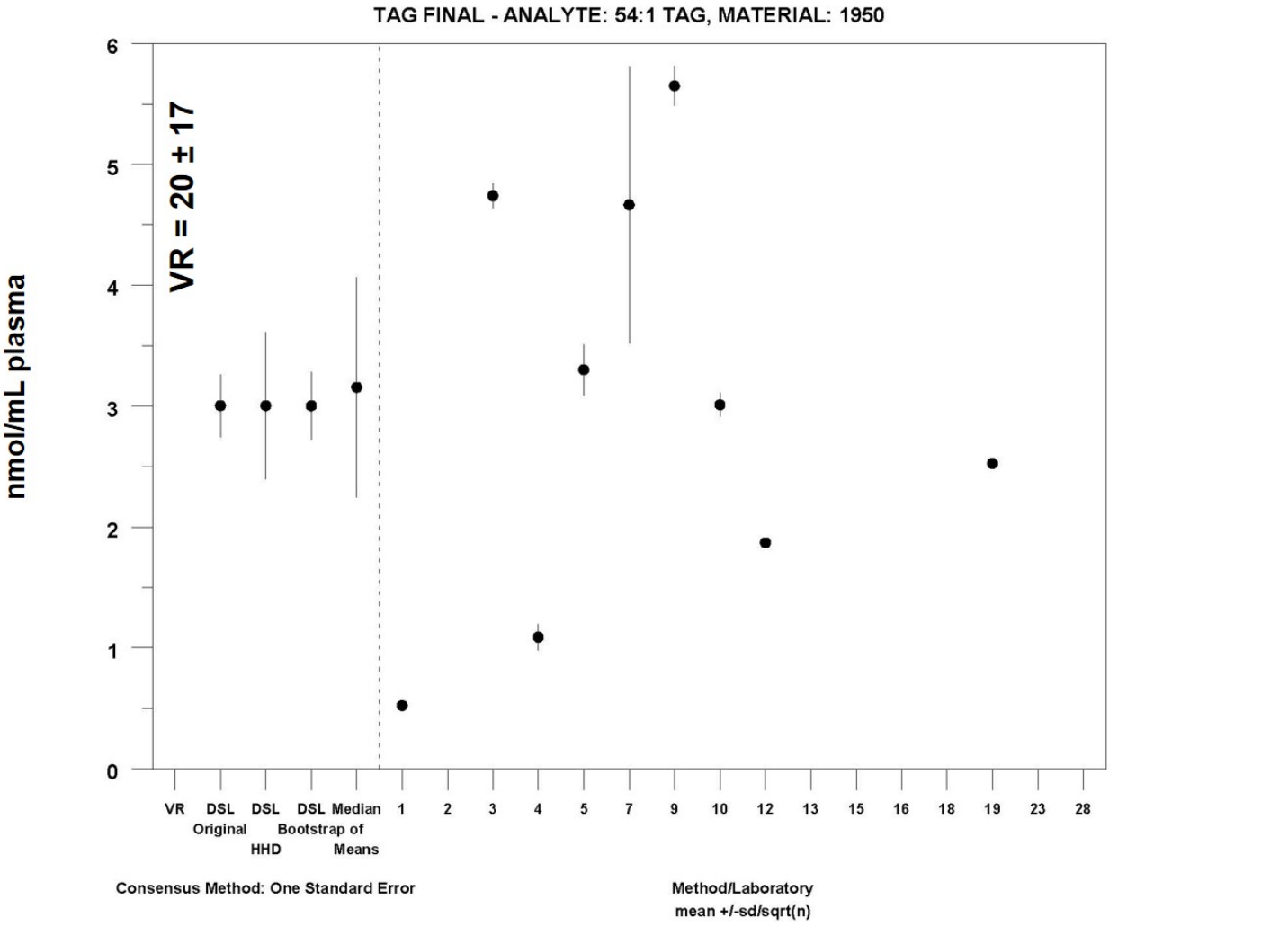
MEDM Location: 2.4 ± 0.76 nmol/mL



MEDM Location: 0.84 ± 0.37 nmol/mL



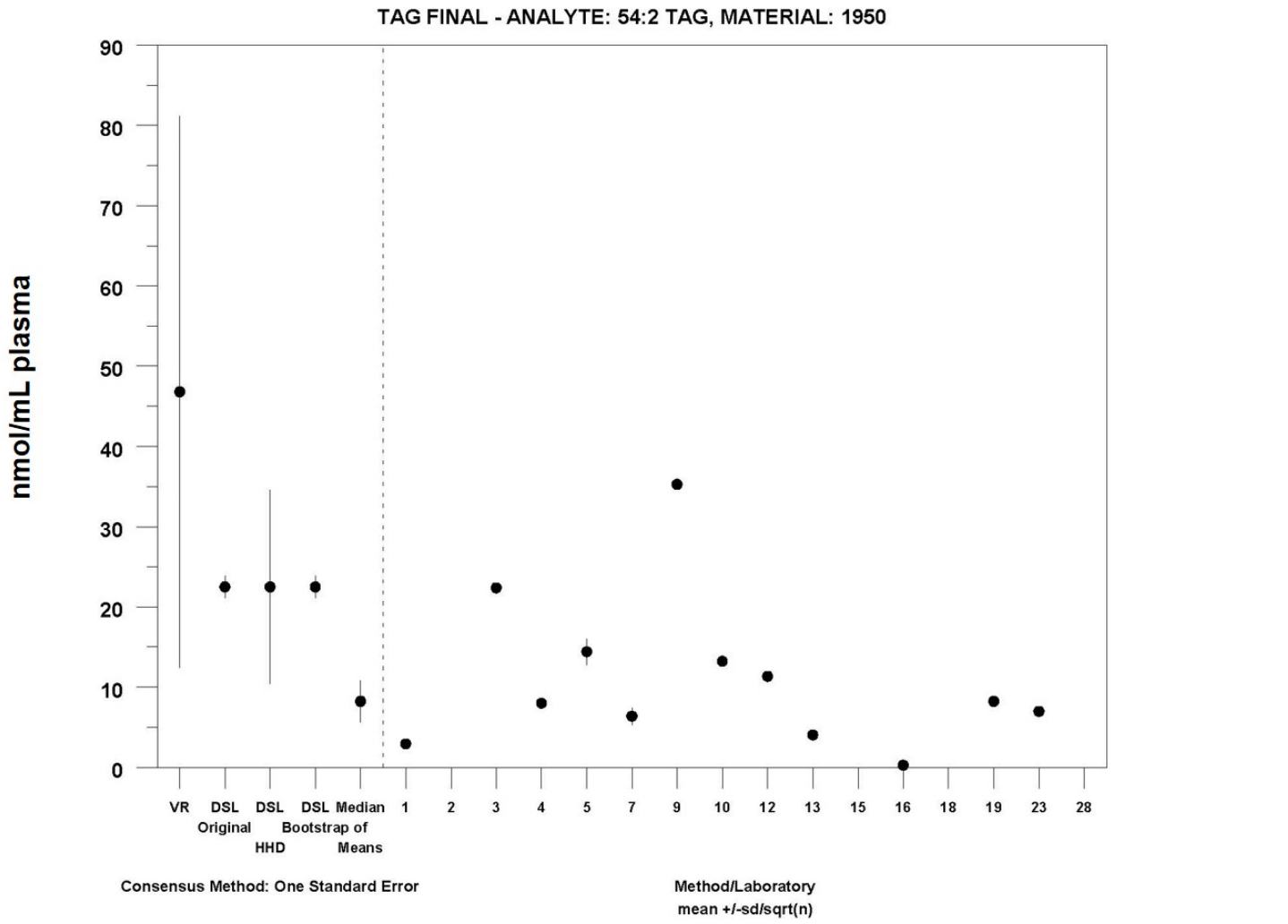
MEDM Location: 2.4 ± 1.3 nmol/mL



MEDM Location: 3.2 ± 0.91 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

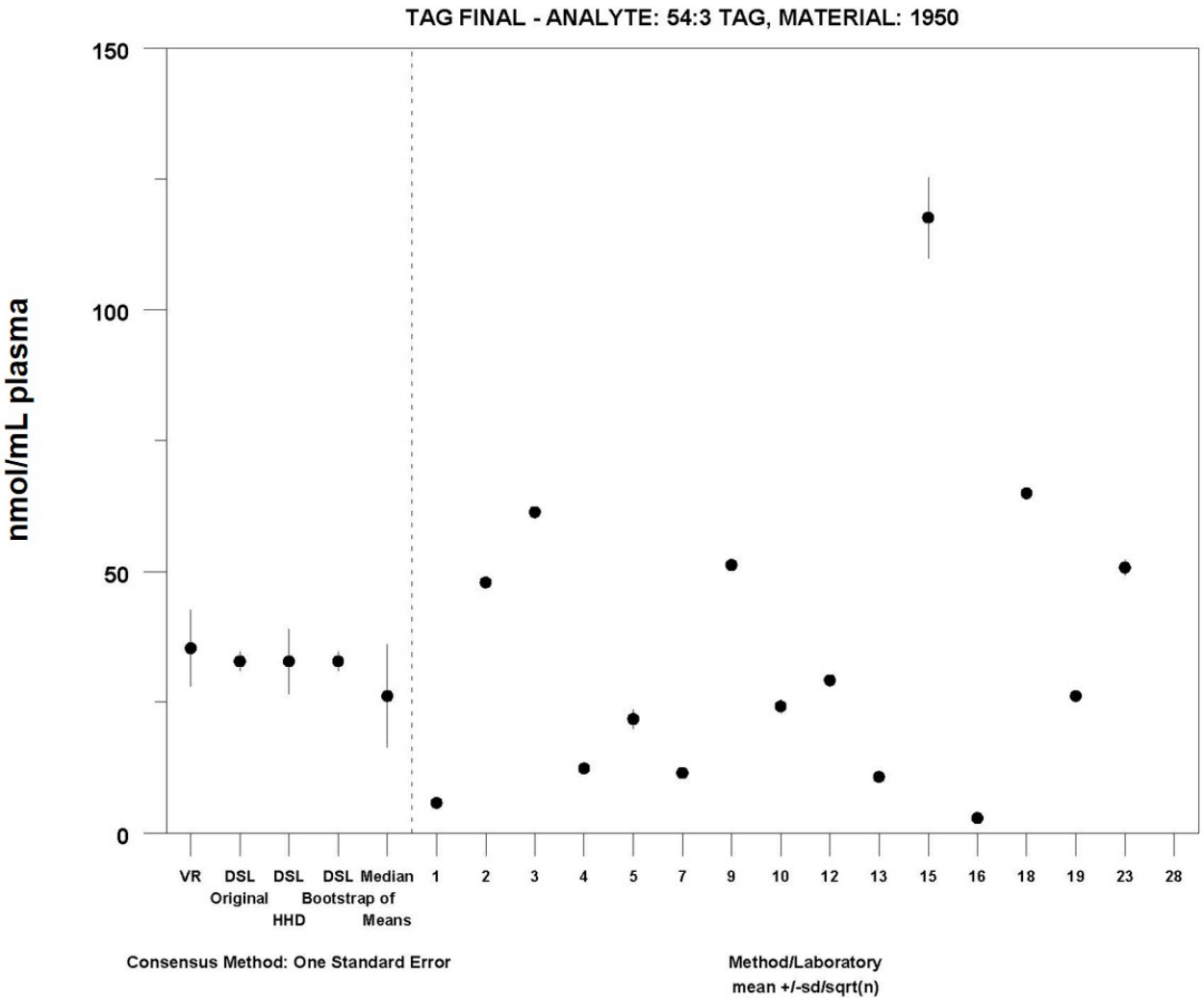
15: 184 ± 18



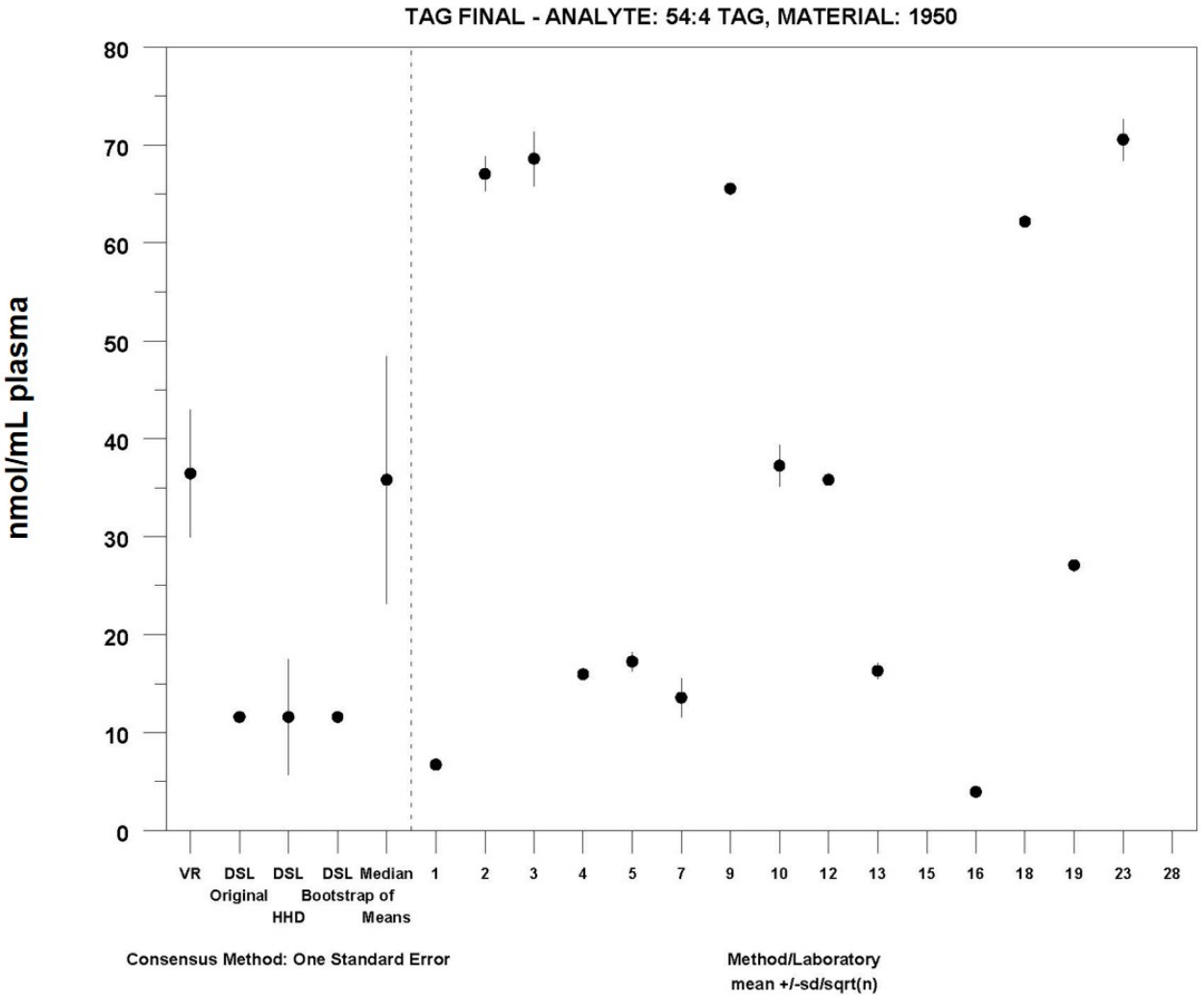
MEDM Location: 8.2 ± 2.6 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 477 ± 13



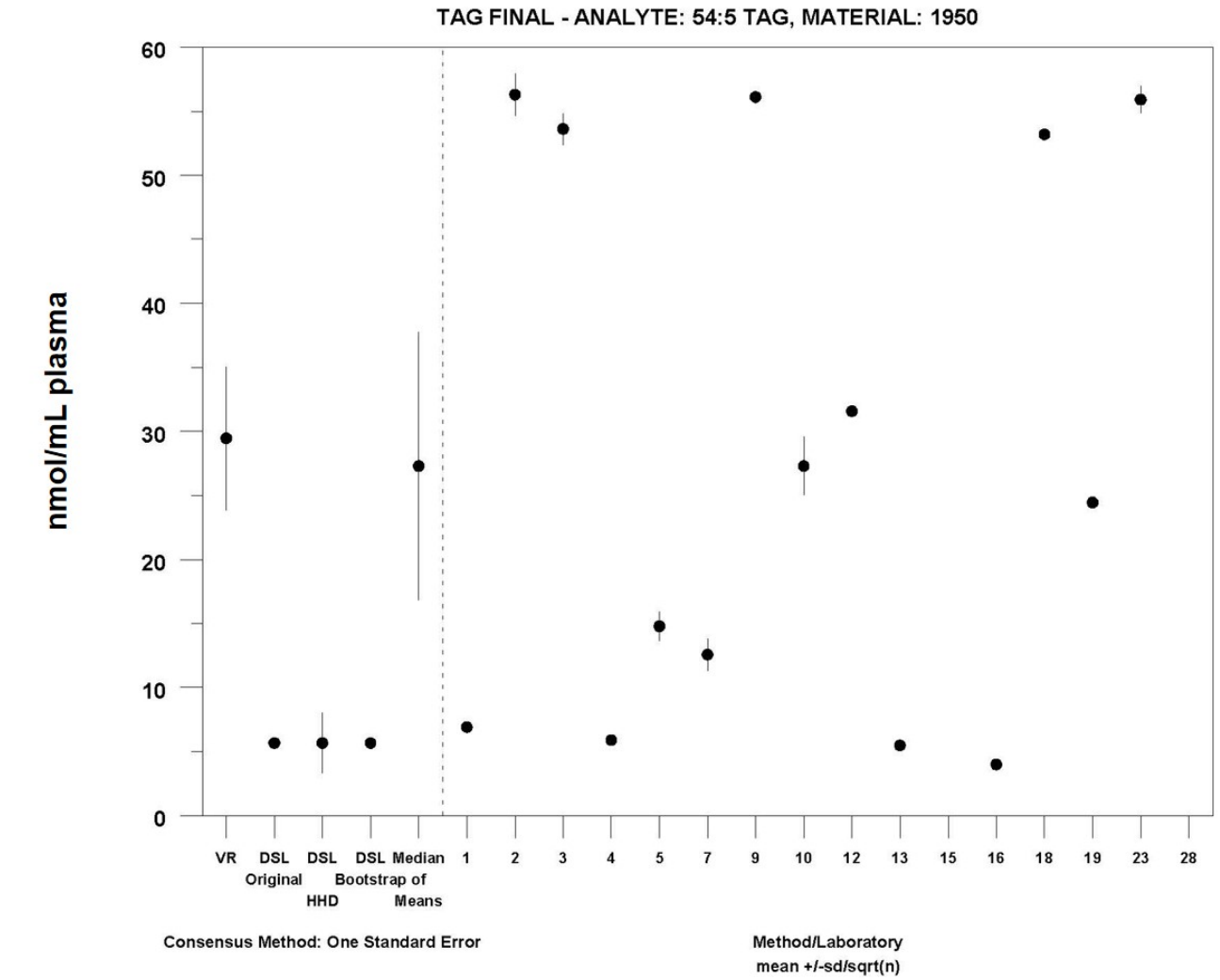
MEDM Location: 26 ± 9.8 nmol/mL



MEDM Location: 36 ± 13 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

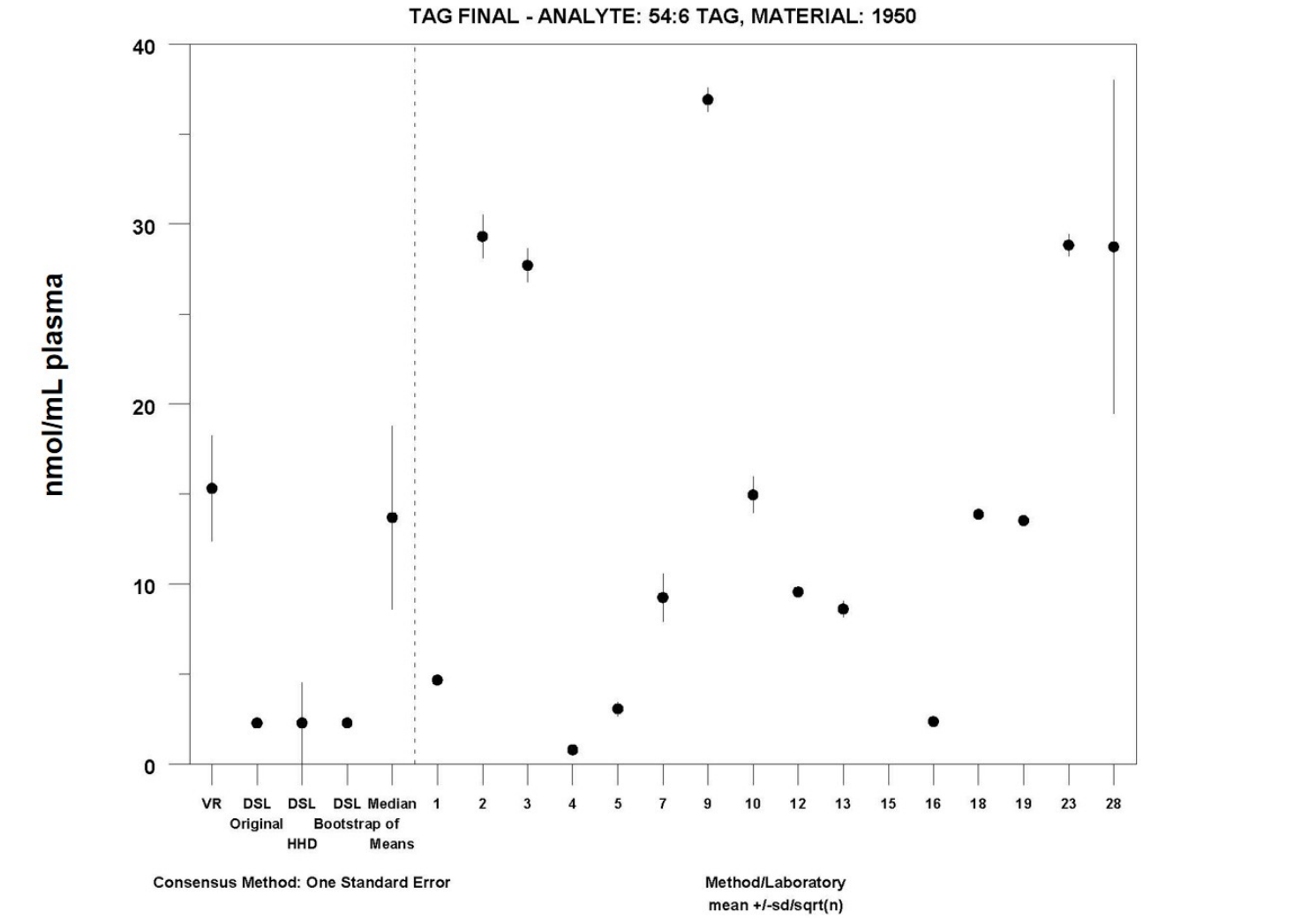
15: 399 ± 318



MEDM Location: 27 ± 11 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

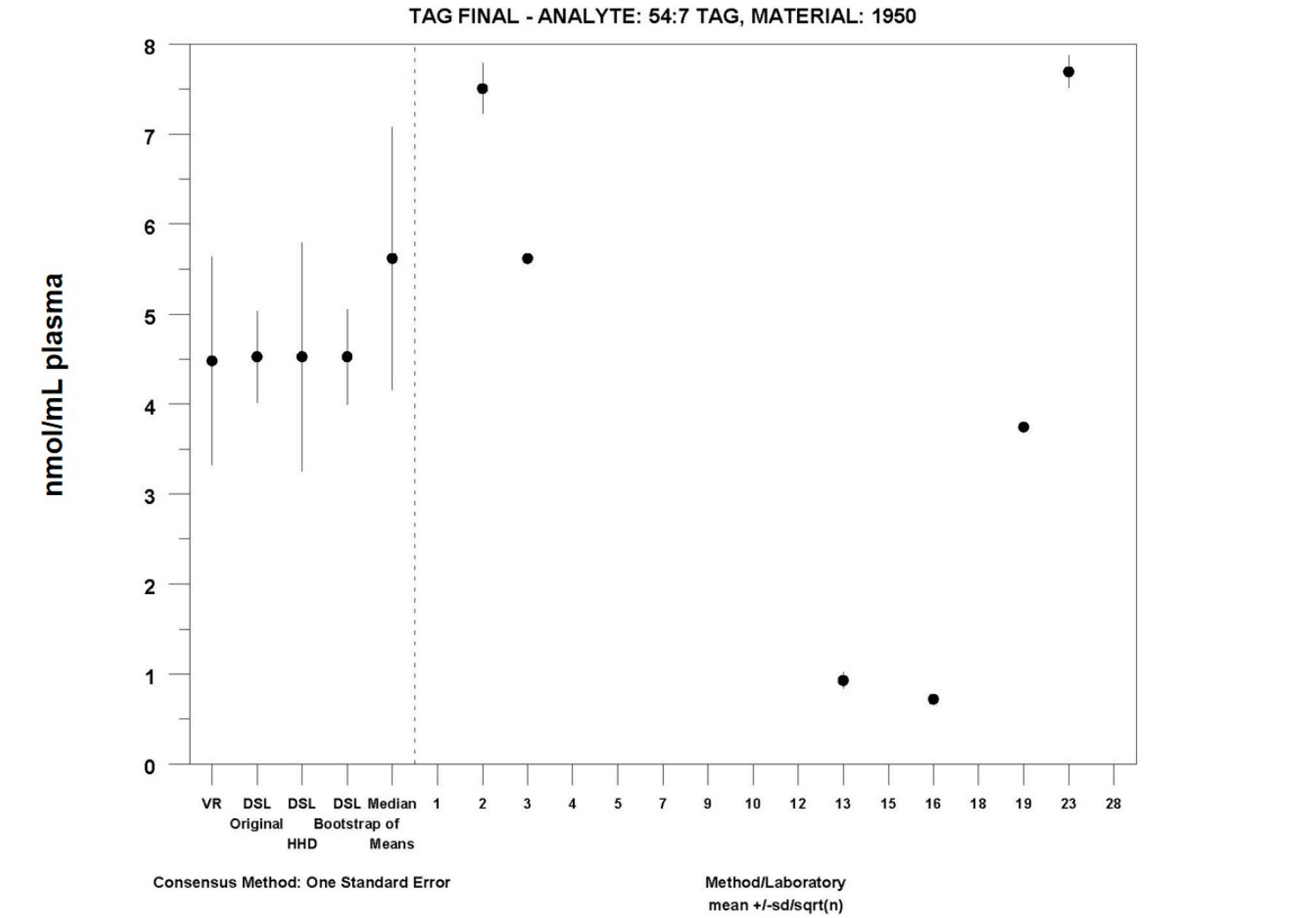
15: 270 ± 126



MEDM Location: 14 ± 5.1 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

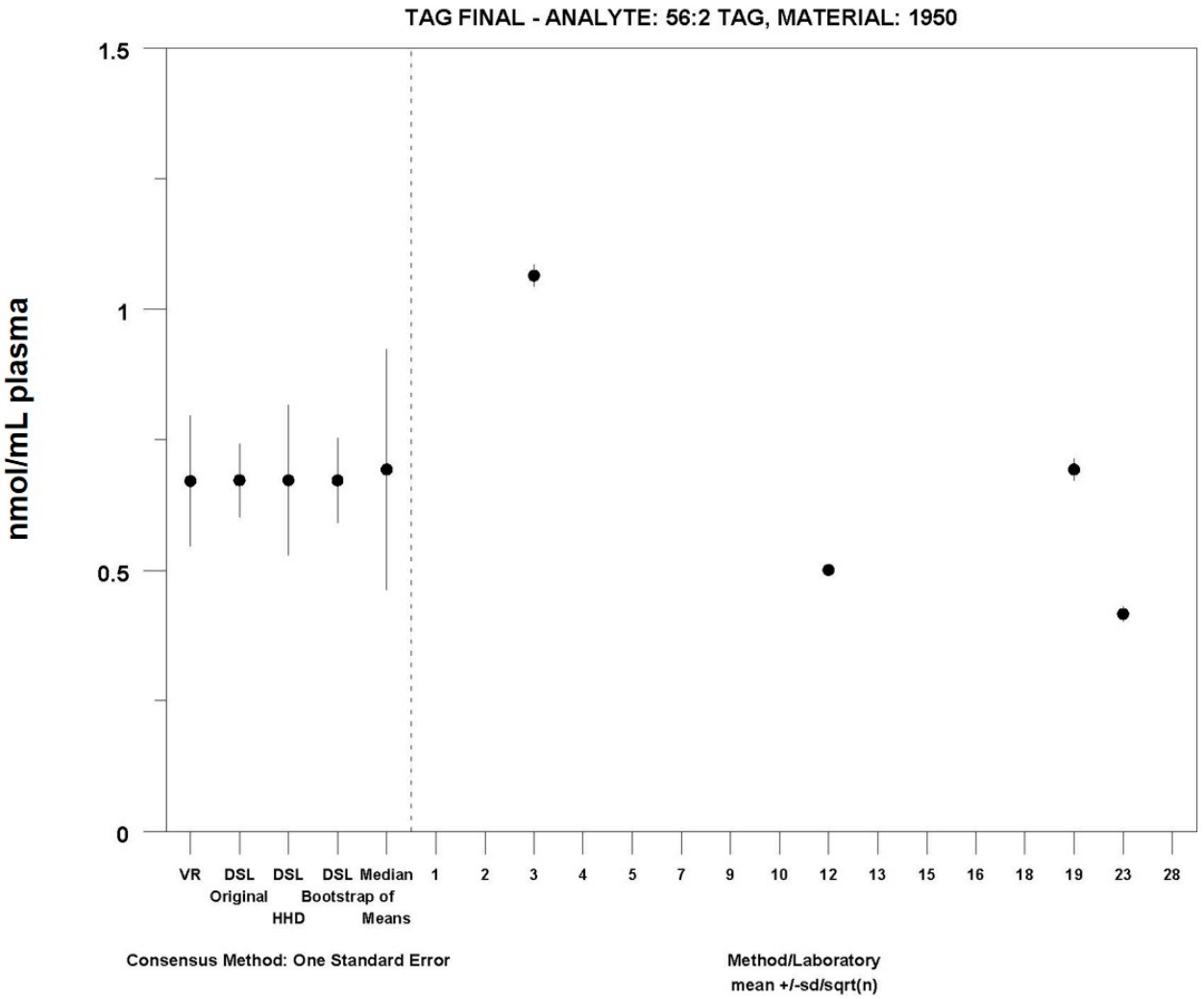
15: 93 ± 69



MEDM Location: 5.6 ± 1.5 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

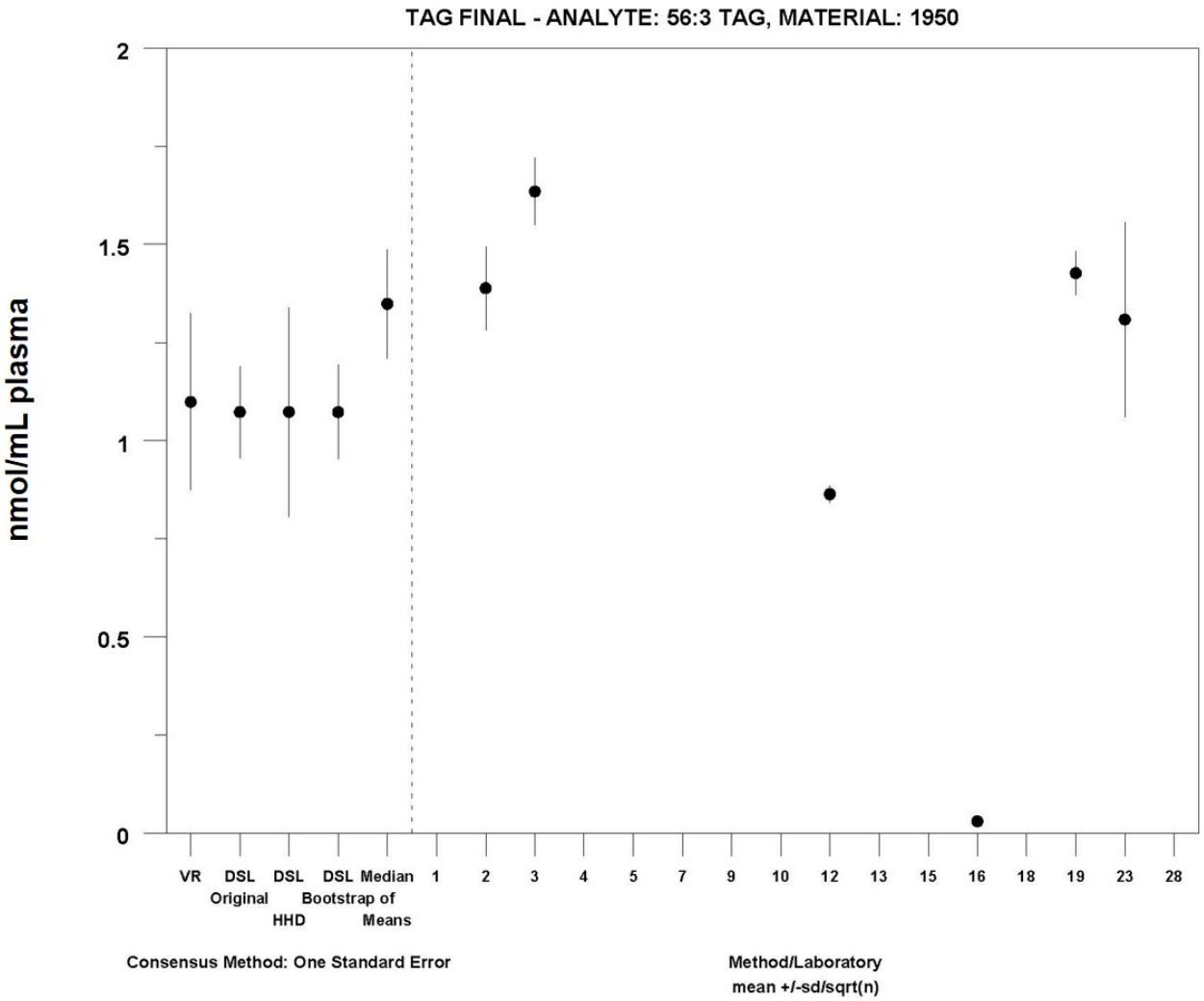
15: 36 ± 11



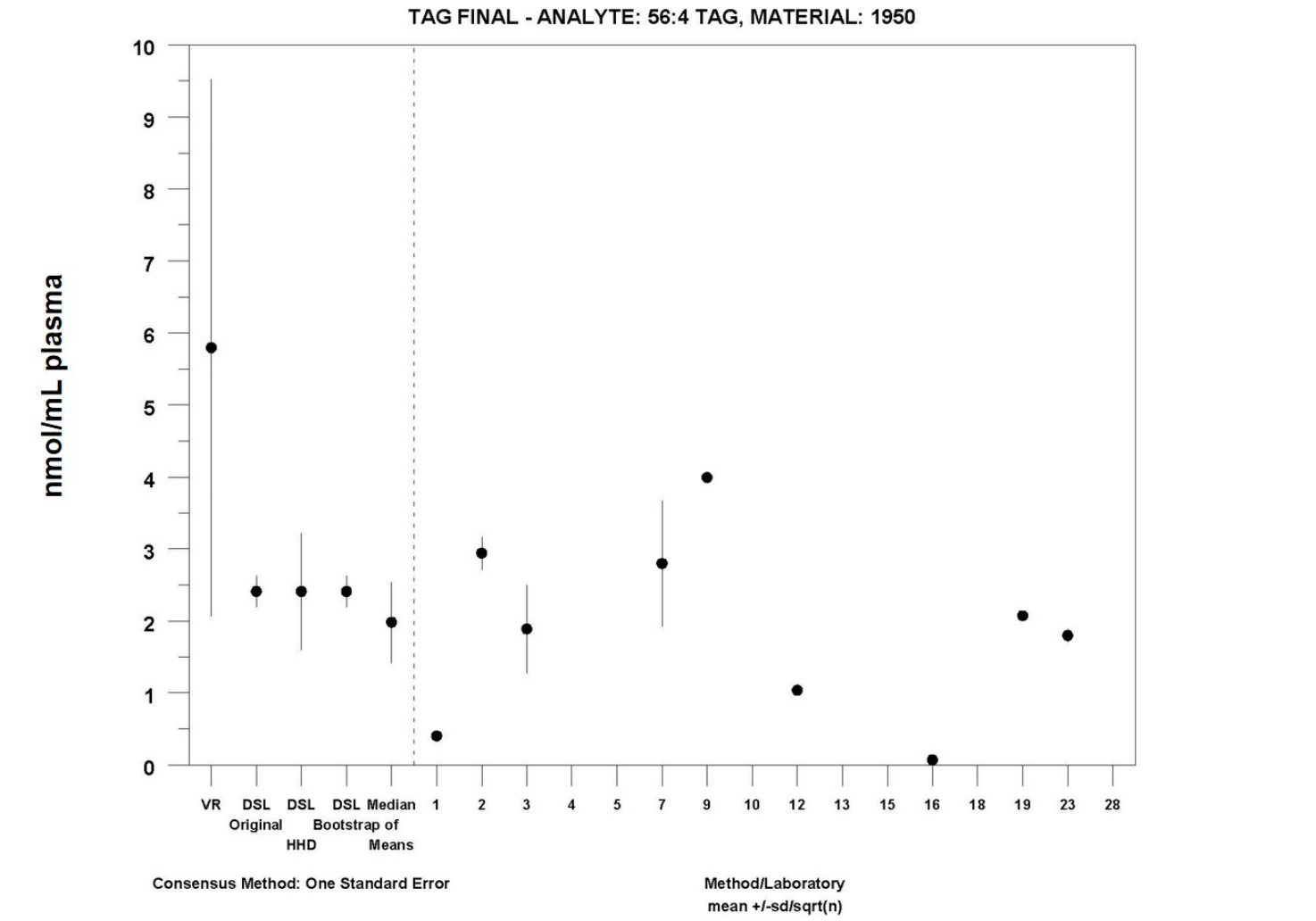
MEDM Location: 0.69 ± 0.23 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 15 ± 6



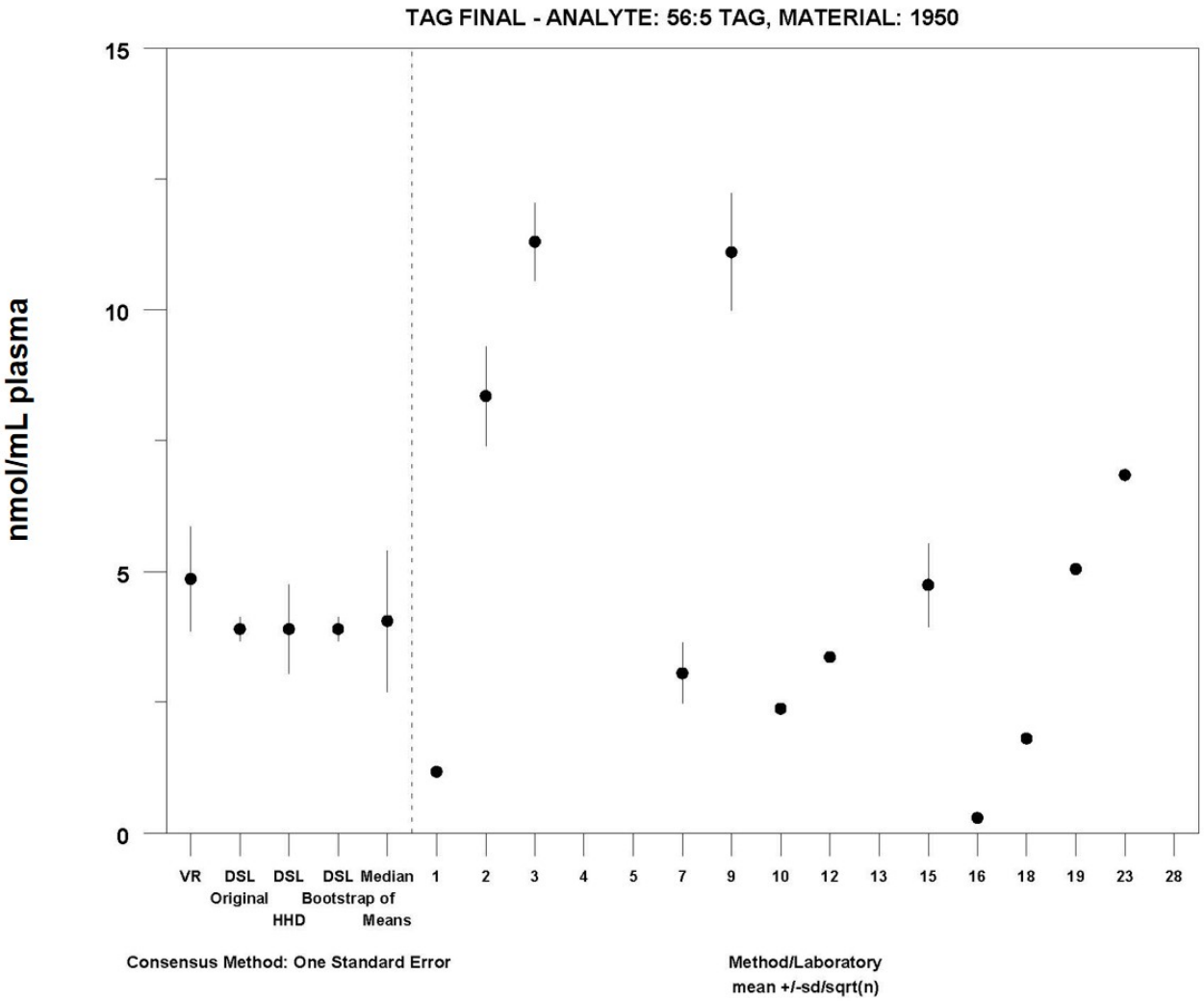
MEDM Location: 1.4 ± 0.14 nmol/mL



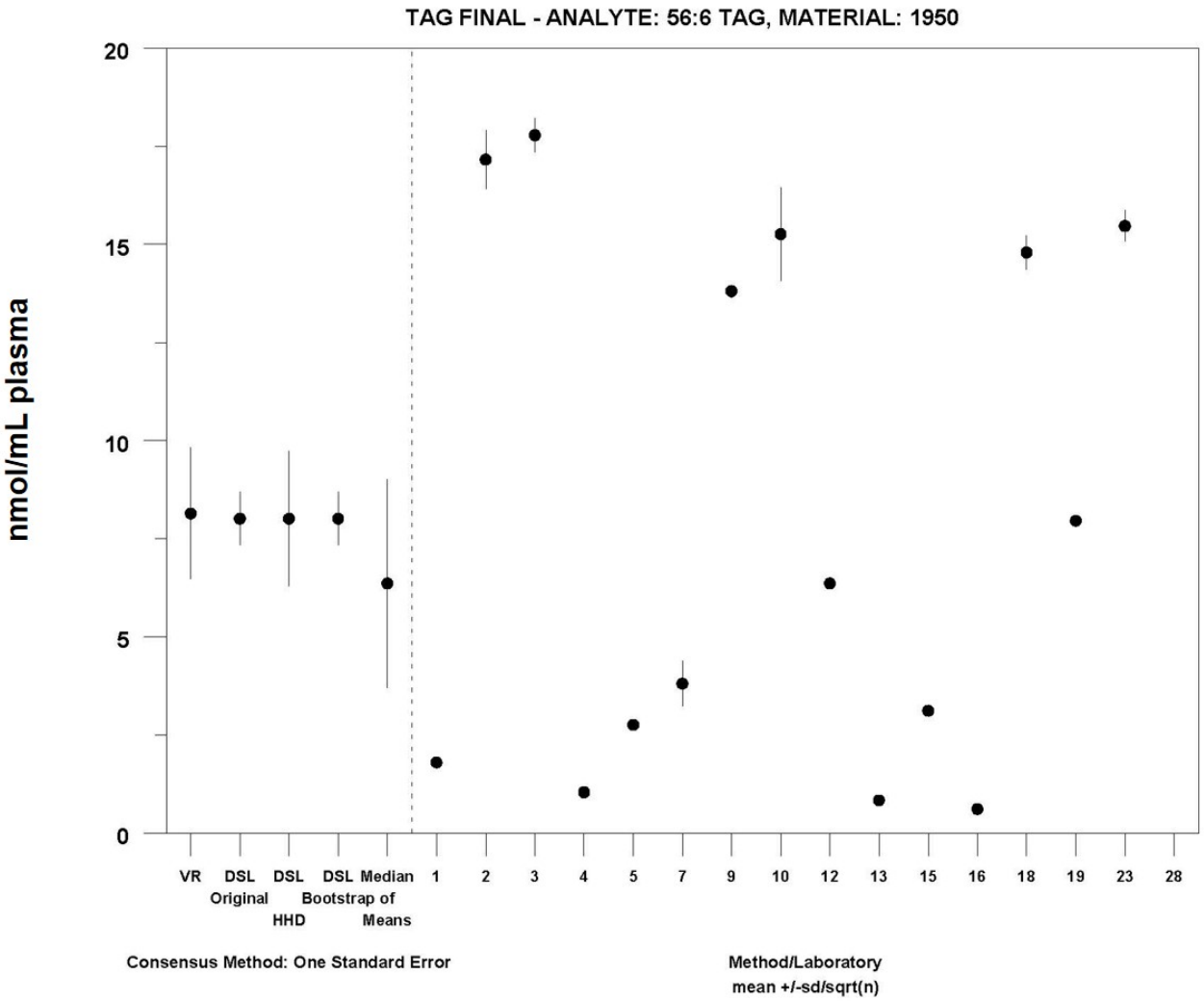
MEDM Location: 2.0 ± 0.56 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

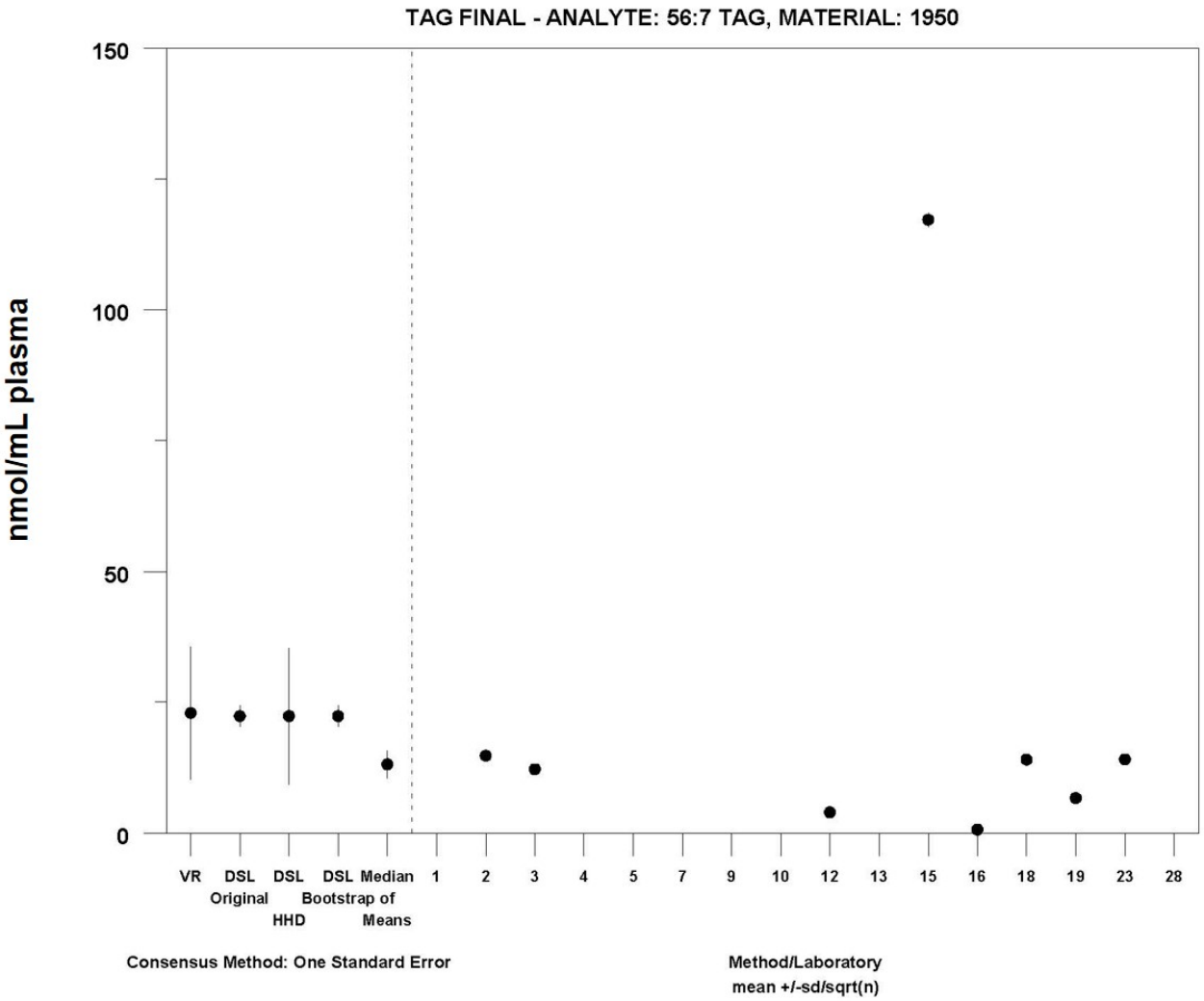
15: 42 ± 3



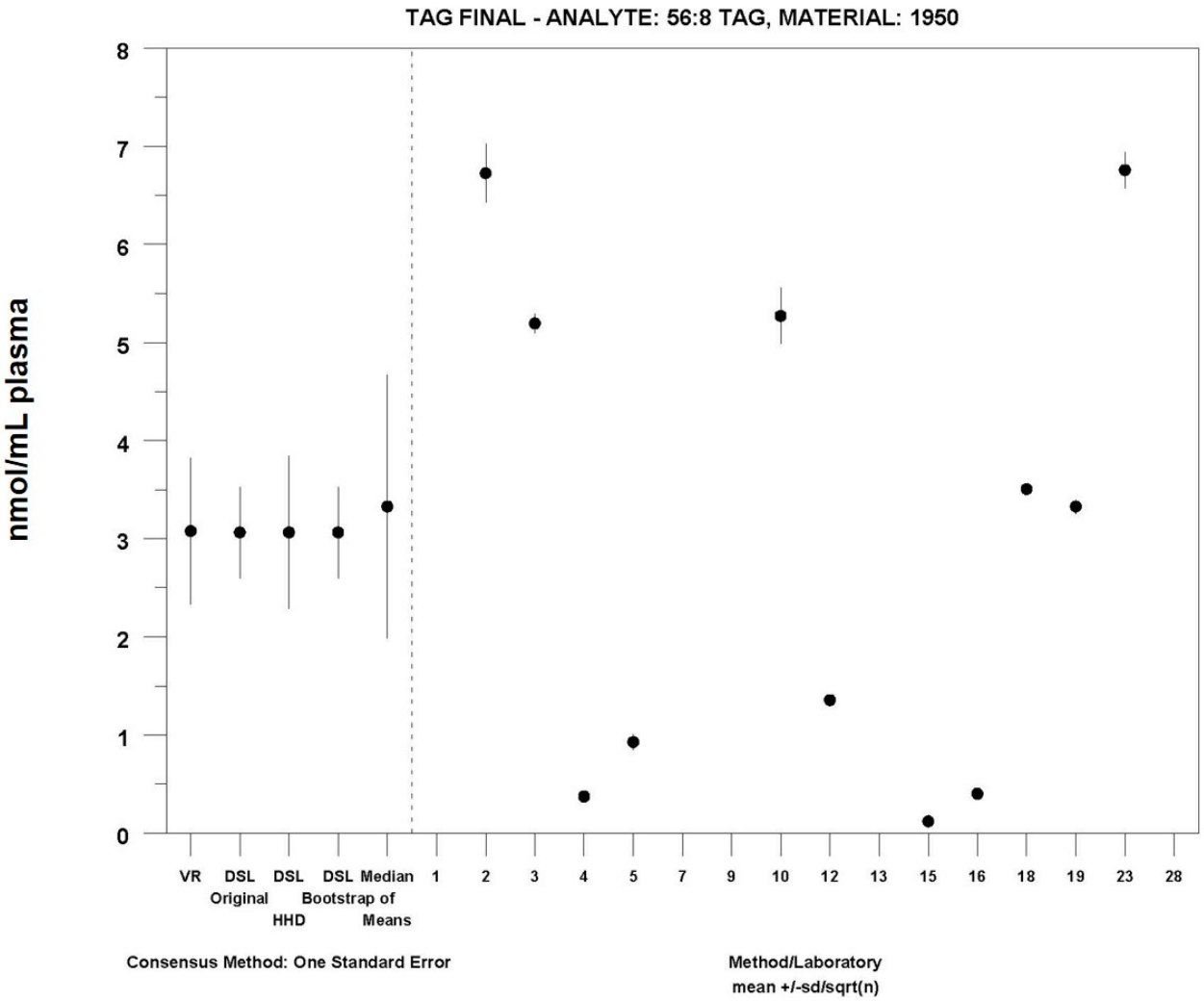
MEDM Location: 4.1 ± 1.4 nmol/mL



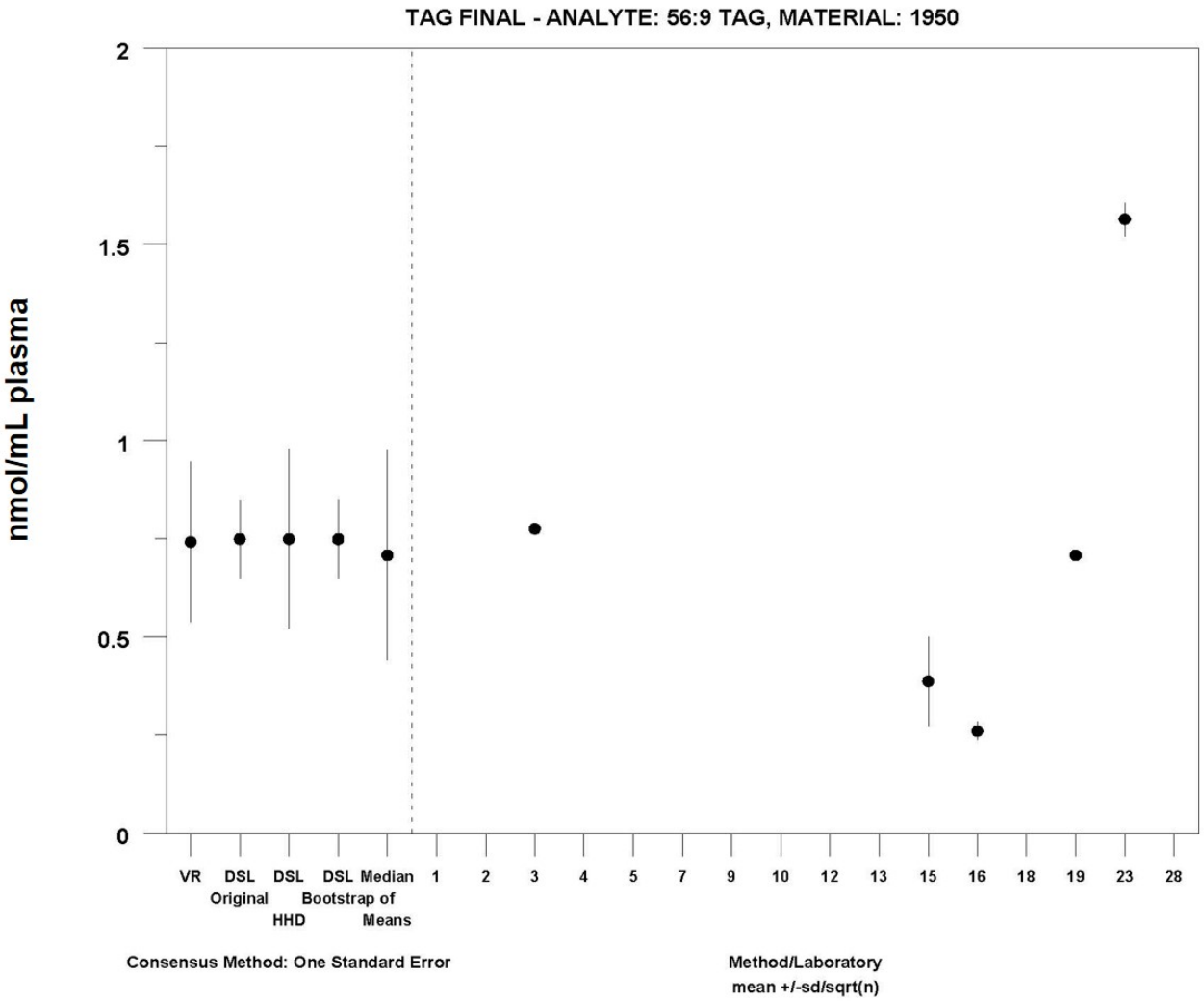
MEDM Location: 6.4 ± 2.7 nmol/mL



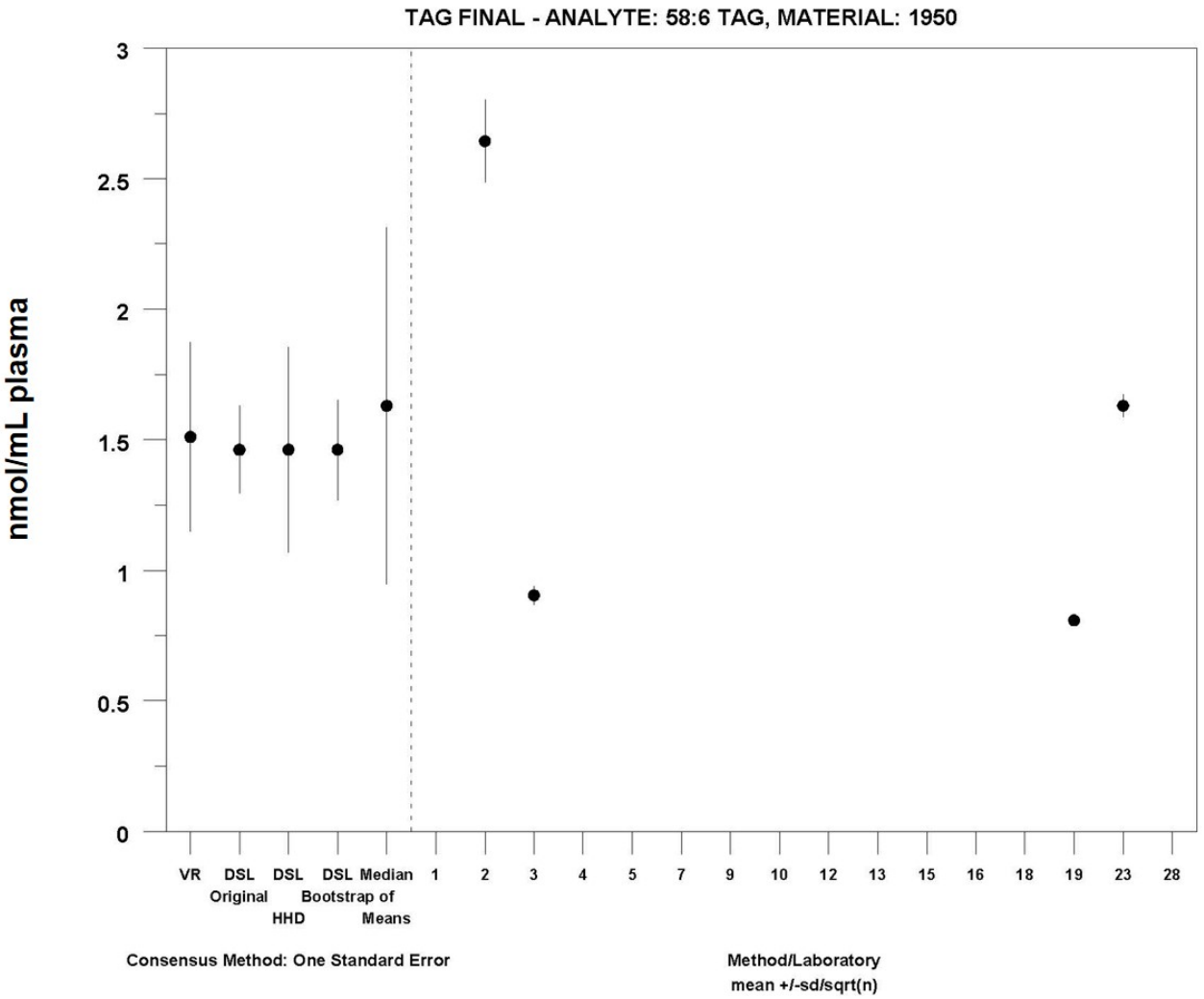
MEDM Location: 13 ± 2.7 nmol/mL



MEDM Location: 3.3 ± 1.3 nmol/mL



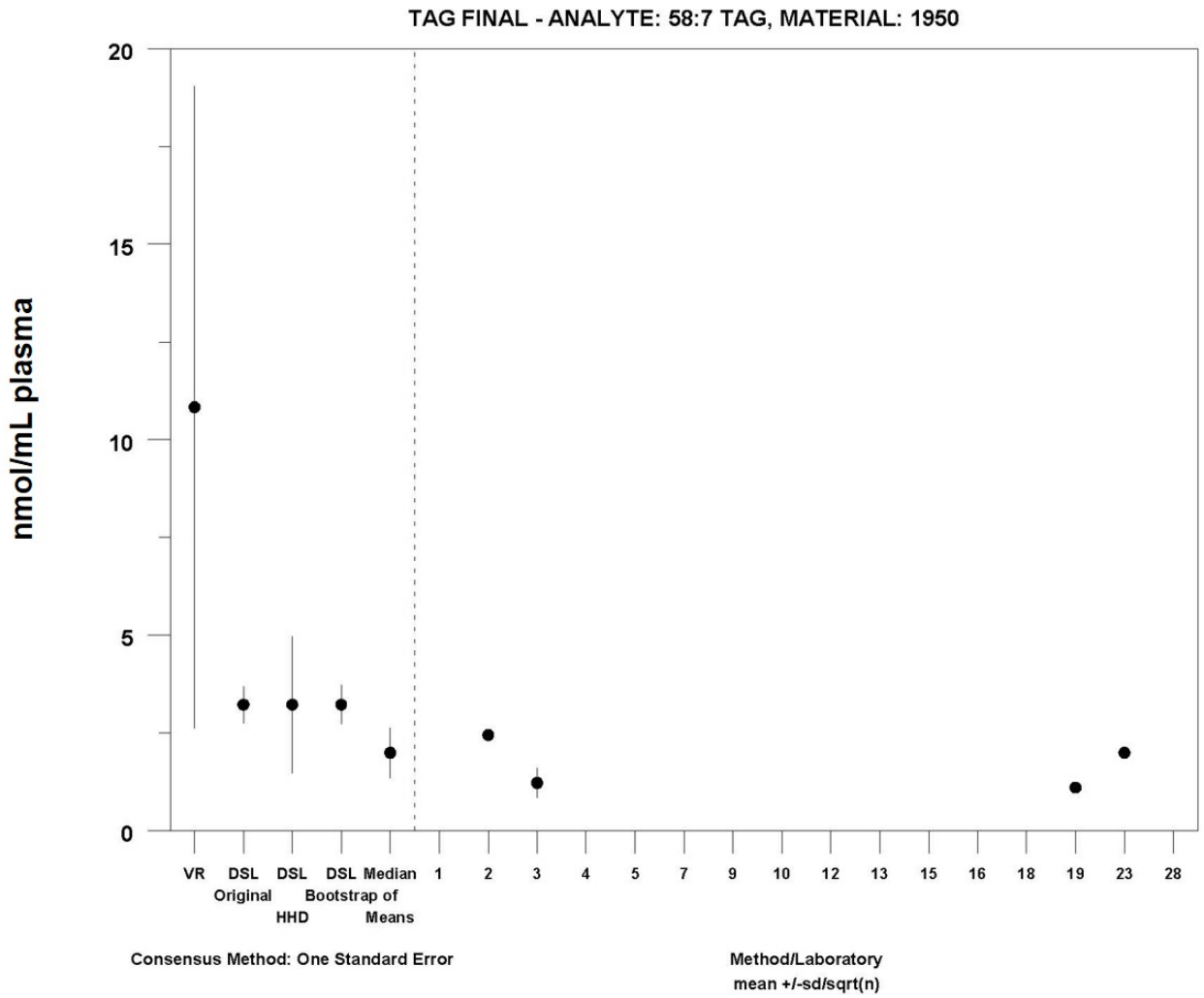
MEDM Location: 0.71 ± 0.27 nmol/mL



MEDM Location: 1.6 ± 0.68 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

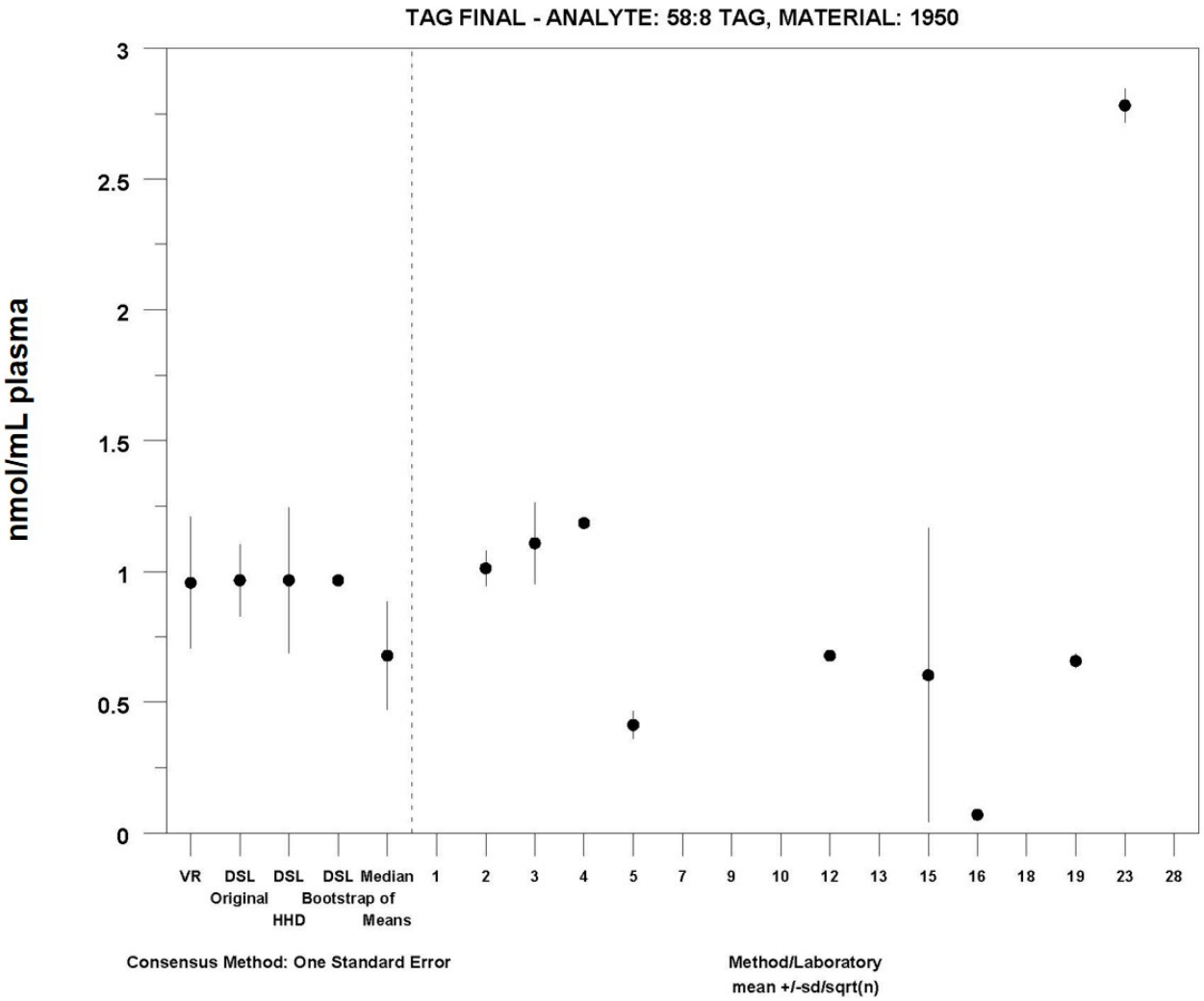
15: 13 ± 7



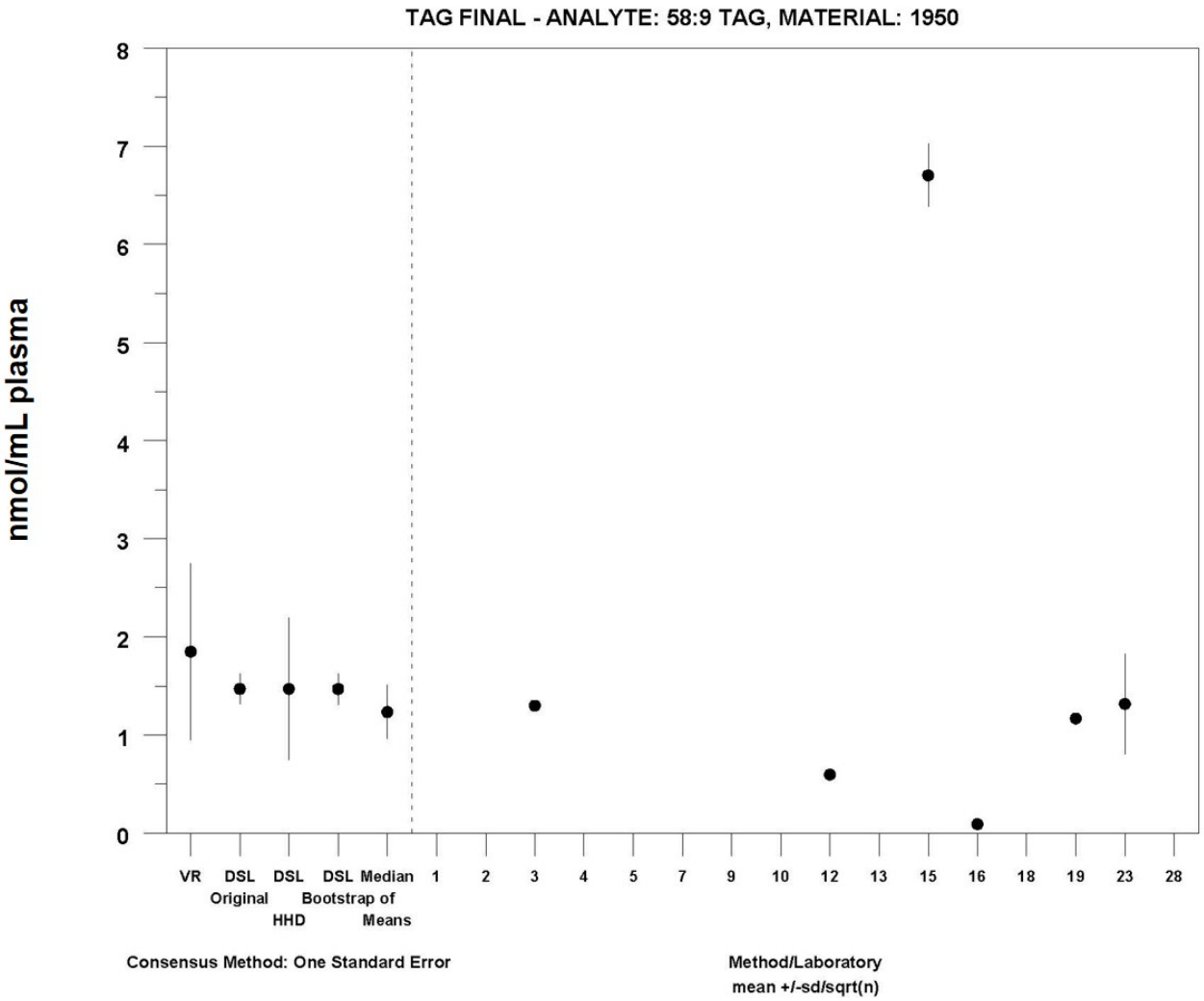
MEDM Location: 2.0 ± 0.64 nmol/mL

Labs Omitted from Plot (But Not Analysis): 15

15: 48 ± 4



MEDM Location: 0.68 ± 0.21 nmol/mL



MEDM Location: 1.2 ± 0.27 nmol/mL

Table S14. Top-50 ranked MEDM locations by concentration (nmol/mL) in SRM 1950

Lipid	# of Labs	MEDM Location (nmol/mL)	COD (%)
TAG 54:6	16	13.7	37
PC 40:6	17	13.9	19
TAG 52:1	11	14.3	20
FFA 18:0	5	14.5	62
TAG 52:5	13	14.6	39
CE 18:0	7	15.2	25
SM d34:2	17	15.7	14
TAG 48:2	15	15.7	18
CE 14:0	7	16.0	37
SM d42:3	12	17.4	27
LPC 18:1	19	18.4	13
SM d42:1	21	19.8	28
SM d40:1	17	20.0	25
SM d36:1	22	20.2	18
LPC 18:2	19	22.1	13
TAG 50:3	16	22.8	29
TAG 54:3	15	26.2	37
PC 38:3	14	26.2	20
PC 36:1	17	26.3	17
LPC 18:0	20	26.9	12
TAG 54:5	15	27.3	38
CE 20:3	13	35.0	35
TAG 54:4	15	35.8	35
CE 22:6	11	37.0	26
CE 20:5	12	37.6	23
TAG 50:1	14	38.0	26
PC 38:6	18	40.5	11
PC 38:5	18	42.2	19
FFA 16:0	5	42.5	31
SM d42:2	18	43.8	25
FFA 18:2	6	44.3	49
TAG 52:2	16	44.4	33
TAG 50:2	15	46.6	26
TAG 52:4	15	47.8	35
LPC 16:0	20	72.9	15
CE 18:3	13	84.1	28

PC 38:4	18	84.4	17
PC 36:3	17	101	14
CE 16:1	11	102	27
SM d34:1	21	102	15
TAG 52:3	16	103	28
FFA 18:1	6	110	48
PC 34:1	19	119	17
PC 36:2	18	143	17
PC 36:4	19	148	19
CE 16:0	13	205	28
PC P-35:1/34:2	18	244	19
CE 20:4	14	345	17
CE 18:1	14	453	25
CE 18:2	14	1,660	26
Mean	15		26
Standard Dev.	4		11

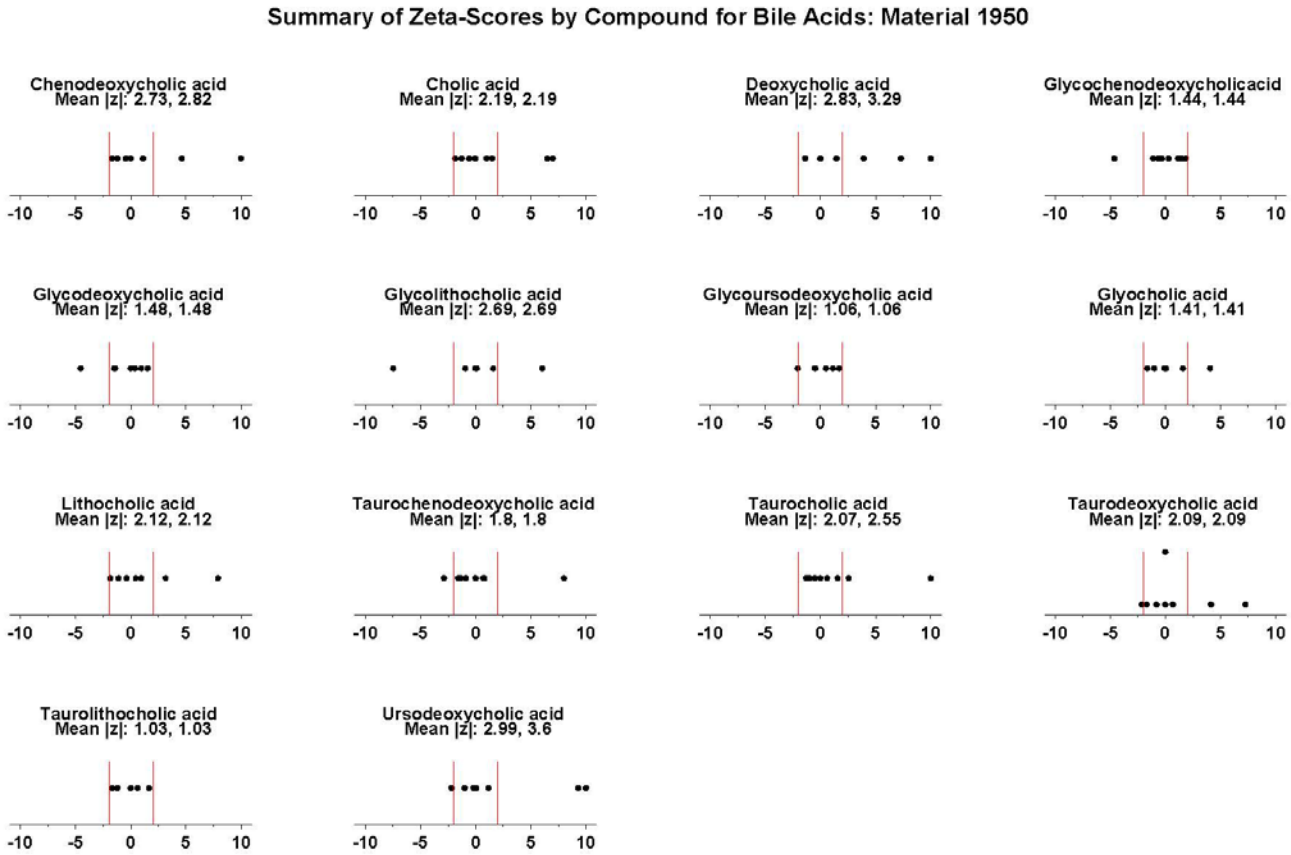
Table S15. Bottom-50 ranked MEDM locations by concentration (nmol/mL) in SRM 1950

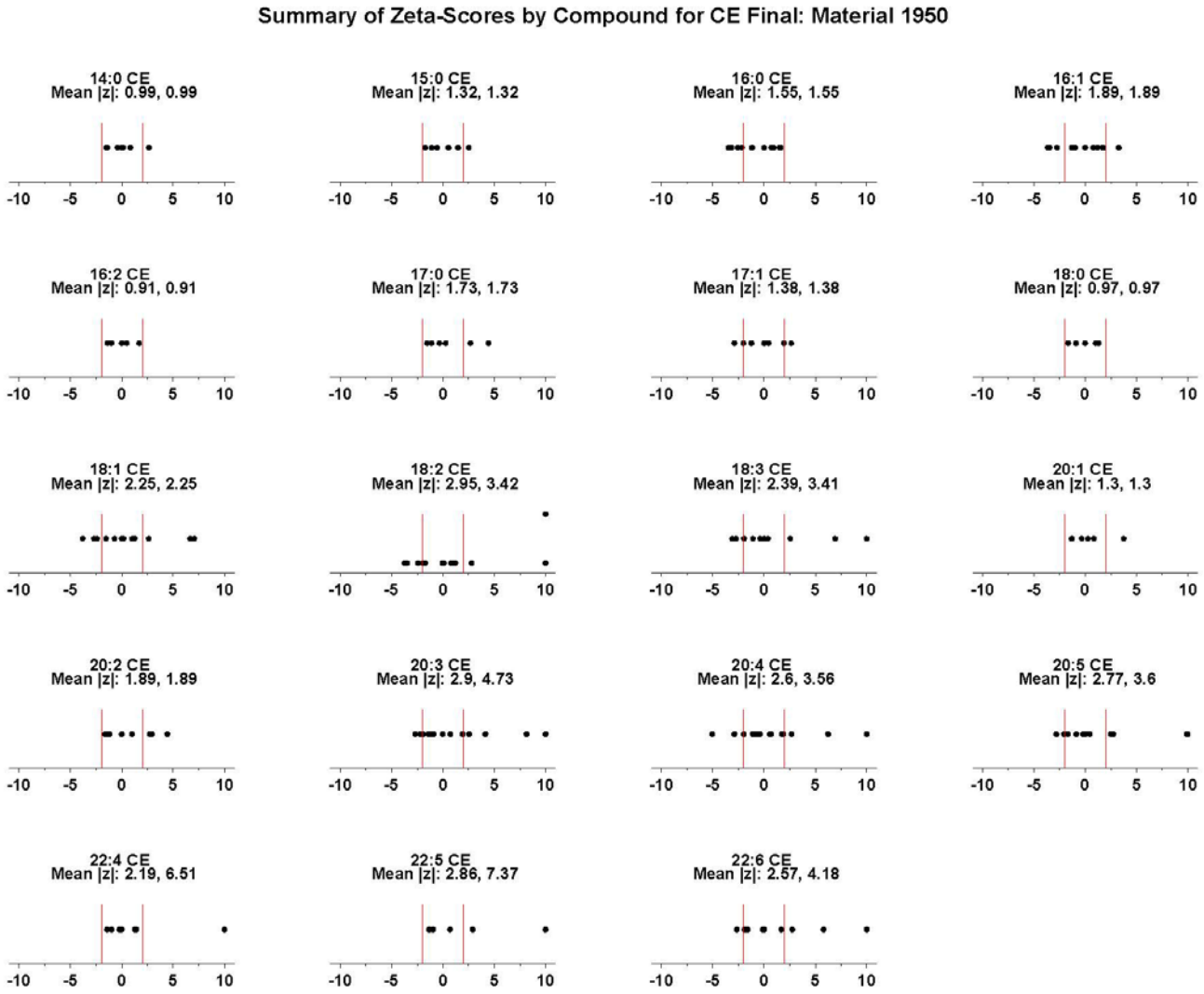
Lipid	# of Labs	MEDM Location (nmol/mL)	COD (%)
15-HETE	5	0.00239	27
TLCA	5	0.00269	26
12-HETE	5	0.00680	23
5-HETE	5	0.0102	13
LPC 22:1	5	0.0129	36
LCA	8	0.0141	26
TAG 42:2	6	0.157	41
GLCA	6	0.0245	7
LPC 22:0	5	0.0253	7
CER d36:2	7	0.0256	56
TCA	9	0.0260	22
PC 34:5	5	0.0343	13
LPE 22:1	5	0.0363	82
TDCA	8	0.0402	16
CER d44:2	7	0.0442	49
CER d34:0	5	0.0450	70
LPC 24:0	5	0.0460	33
PC O-30:1/P-30:0	7	0.0473	20
CER d32:1	8	0.0513	42
CER d44:1	7	0.0631	49
PC O-40:2/P-40:1	5	0.0688	30
PC O-30:0/29:0	7	0.0720	36
PC 42:6	5	0.0790	52
DAG 40:5	5	0.0838	63
TCDCA	9	0.0839	6
LPC 20:0	7	0.100	34
UDCA	8	0.106	22
CER d38:1	16	0.109	20
PC O-34:4/P-34:3	6	0.119	66
CER d36:1	14	0.122	17
CA	9	0.122	28
LPC 22:4	8	0.123	33
HexCer d36:1	5	0.127	34
CER d40:2	6	0.145	14
GUDCA	6	0.146	16
LPC O-18:0	6	0.158	36
LPC 20:1	13	0.194	12
SM d31:1	5	0.194	25
SM d37:2	5	0.207	50
CER d42:3	5	0.228	62

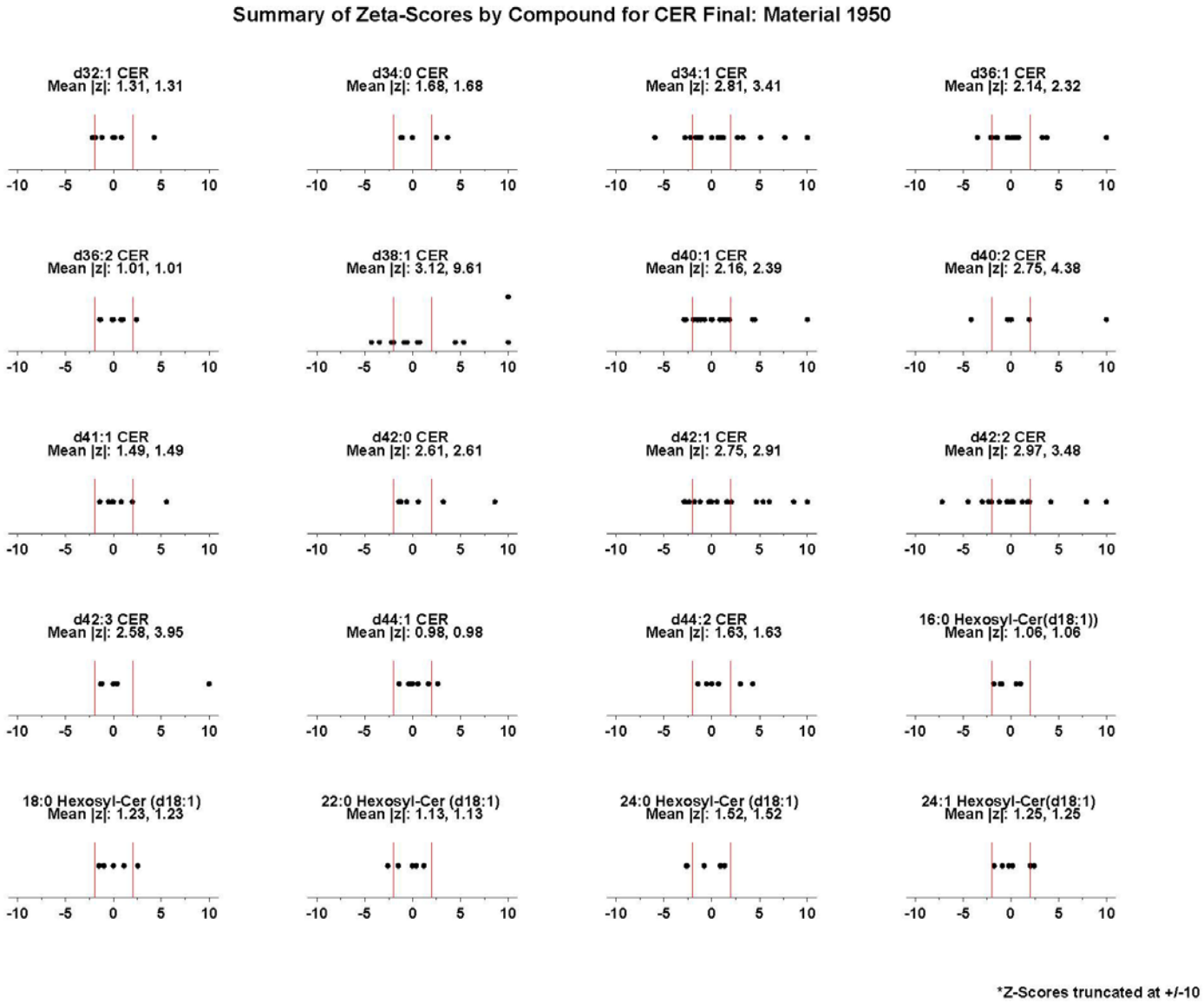
LPC 20:2	9	0.231	19
PC 40:2	8	0.233	44
DAG 38:0	7	0.240	55
GCA	6	0.242	29
SM d44:1	9	0.247	49
LPC 17:1	6	0.249	29
PE 40:4	10	0.263	31
PE 36:5	11	0.264	48
PC 40:3	7	0.270	51
SM d44:3	5	0.273	71
Mean	7		35
Standard Dev.	2		19

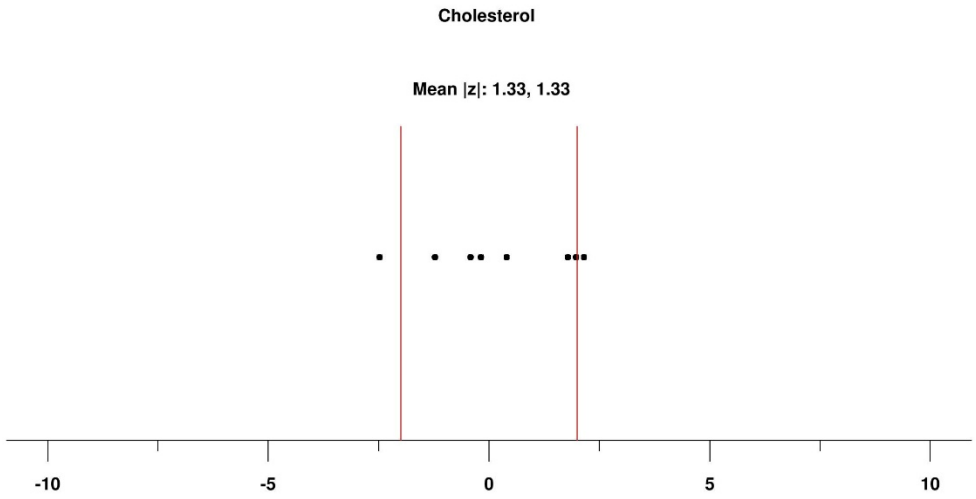
Appendix E: Zeta-Score Organized by Lipid Species

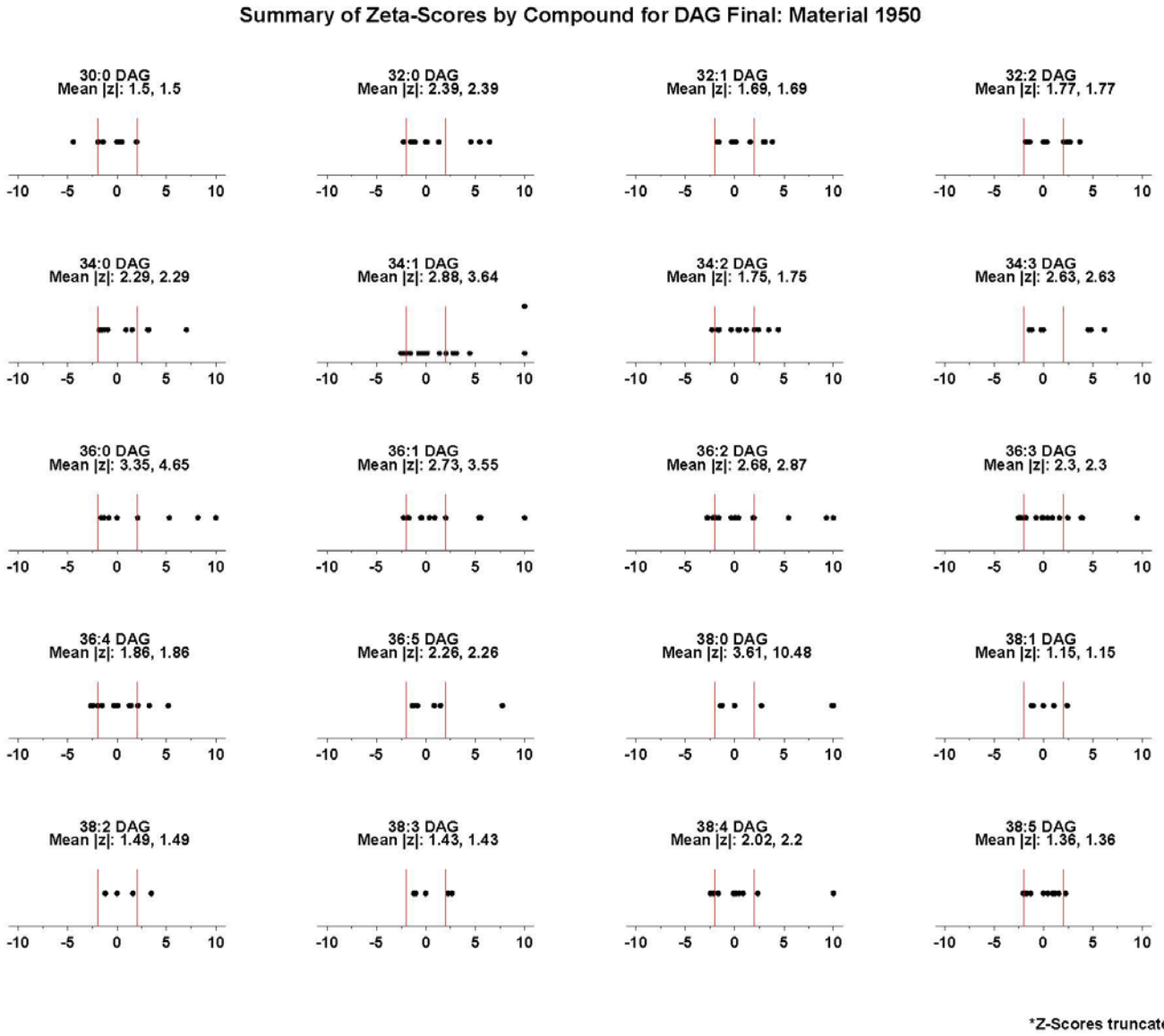
Zeta-score plots are provided for lipids organized by lipid (measured by at least five participating laboratories). Each dot represents a single laboratory measurement for that lipid. The ζ-scores were calculated using the MEDM location as the target. The distance for each point from the mean indicates how many *x times the number of combined standard uncertainties* the submitted value is above or below the MEDM location. The plots were truncated at ± 10 to maintain visual resolution. Absolute value mean ζ-scores were calculated two ways: (1) setting truncated values to 10 (first ζ-score average listed) and (2) using the original outlier ζ-score in the calculation.

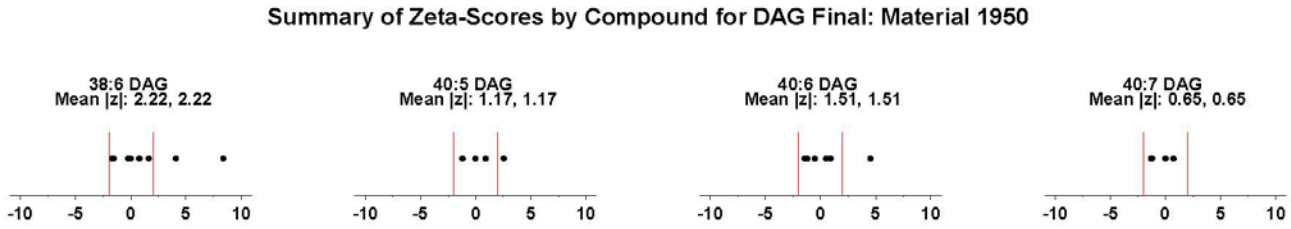


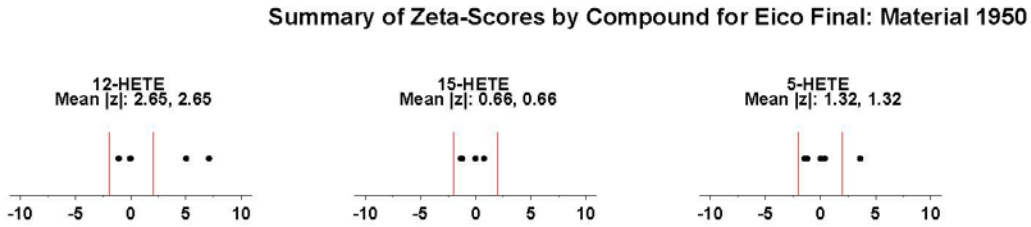


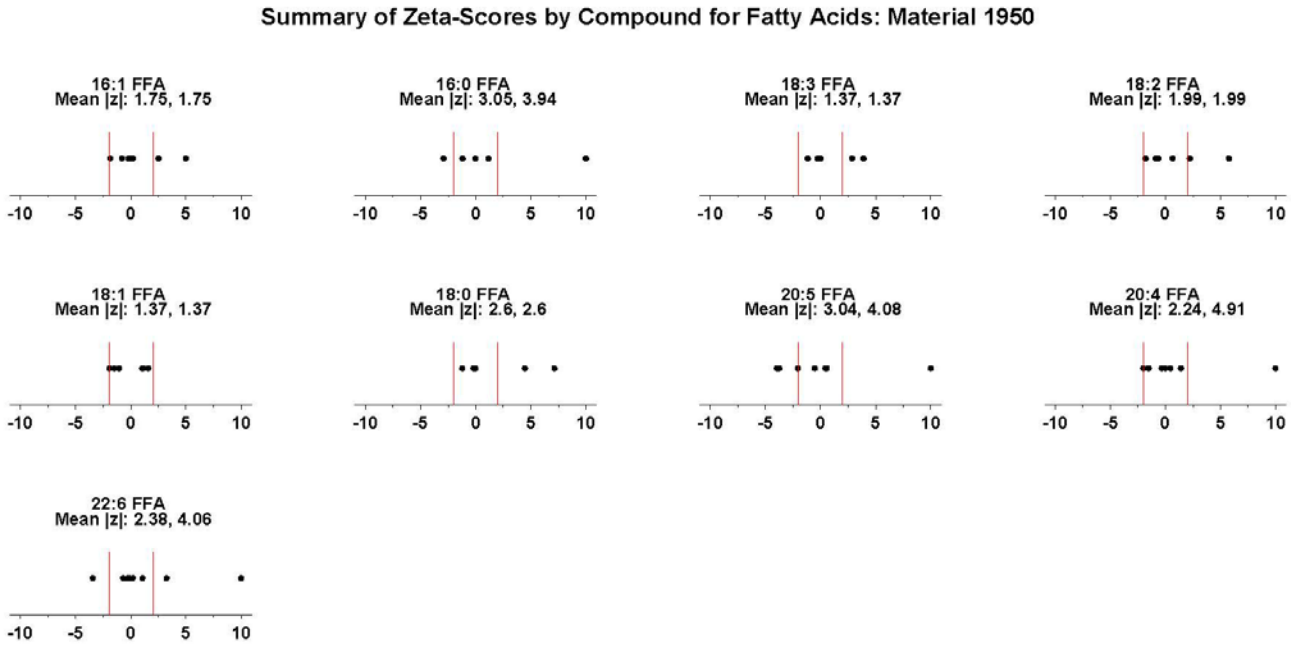


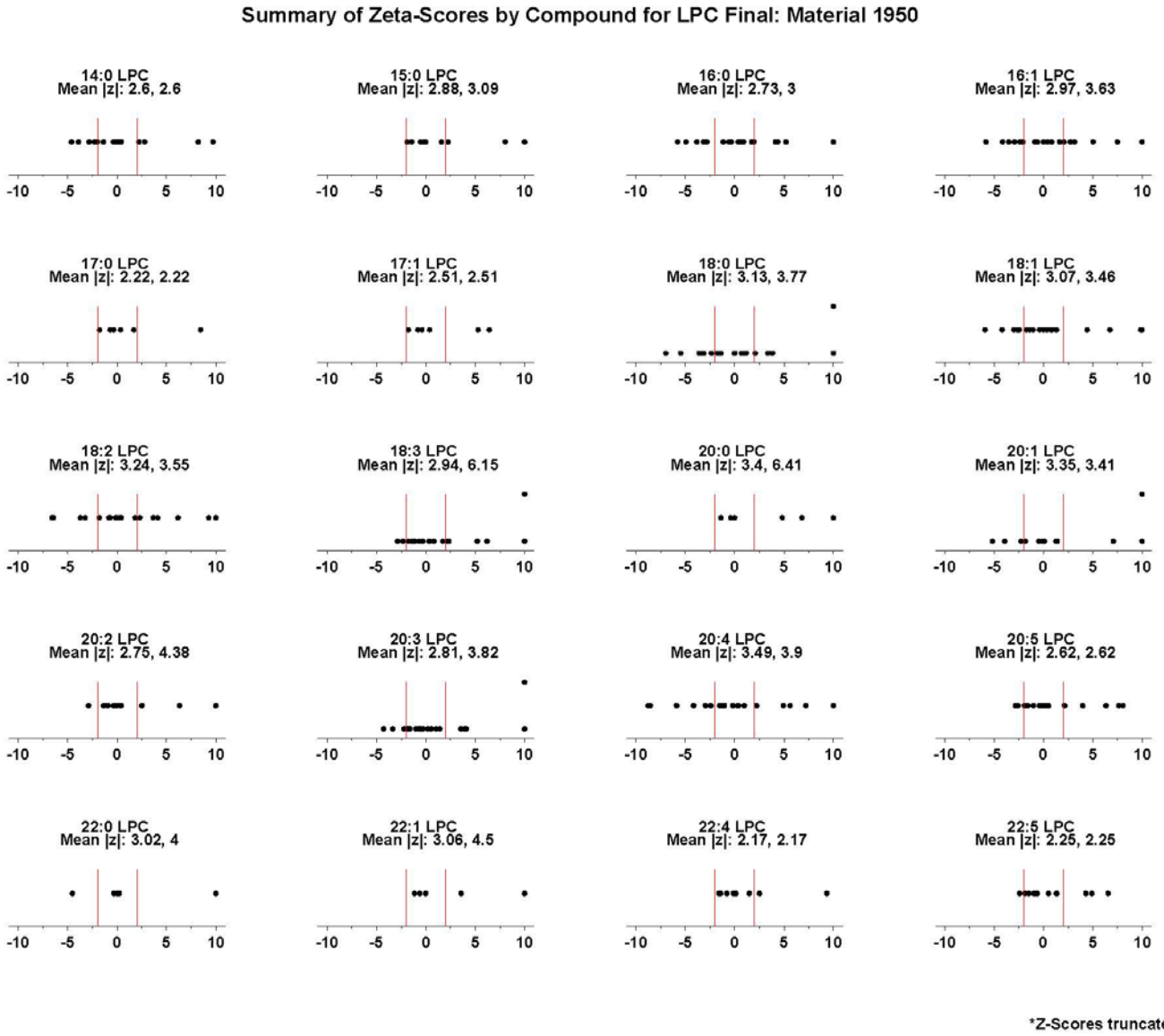


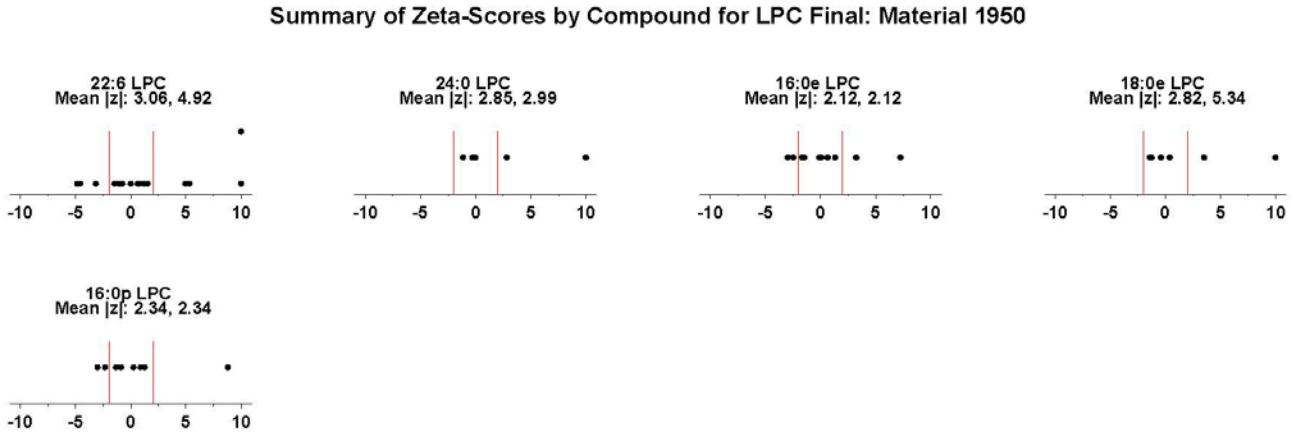


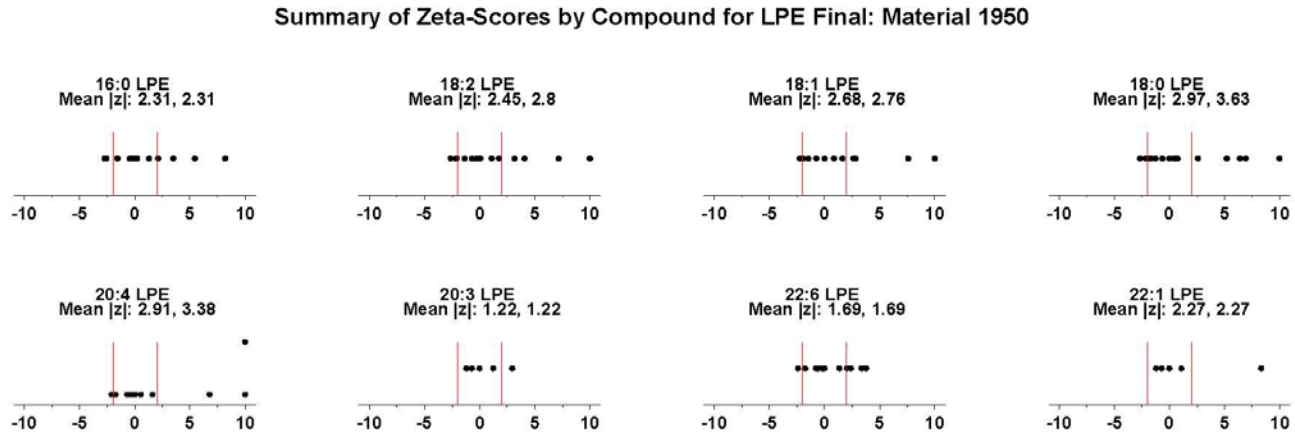


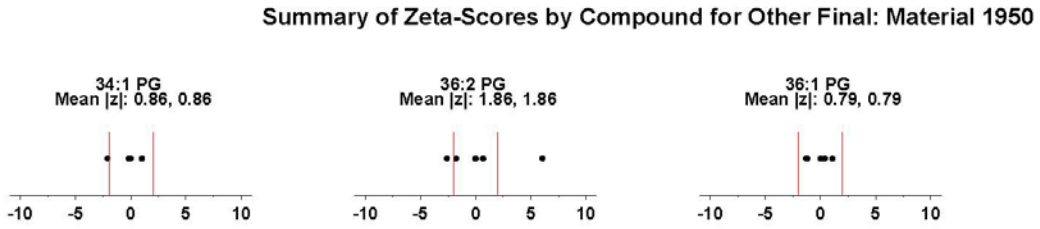


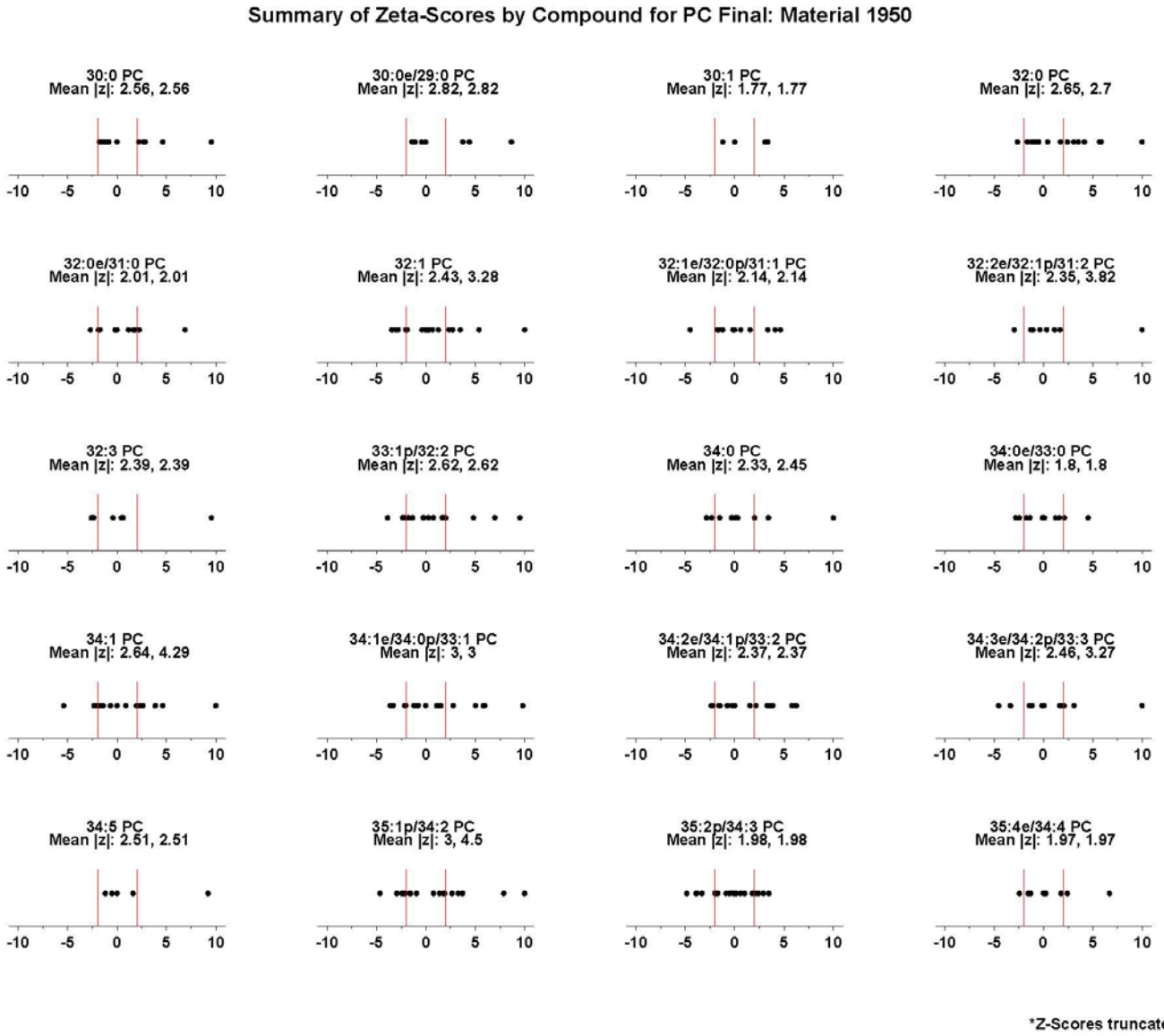


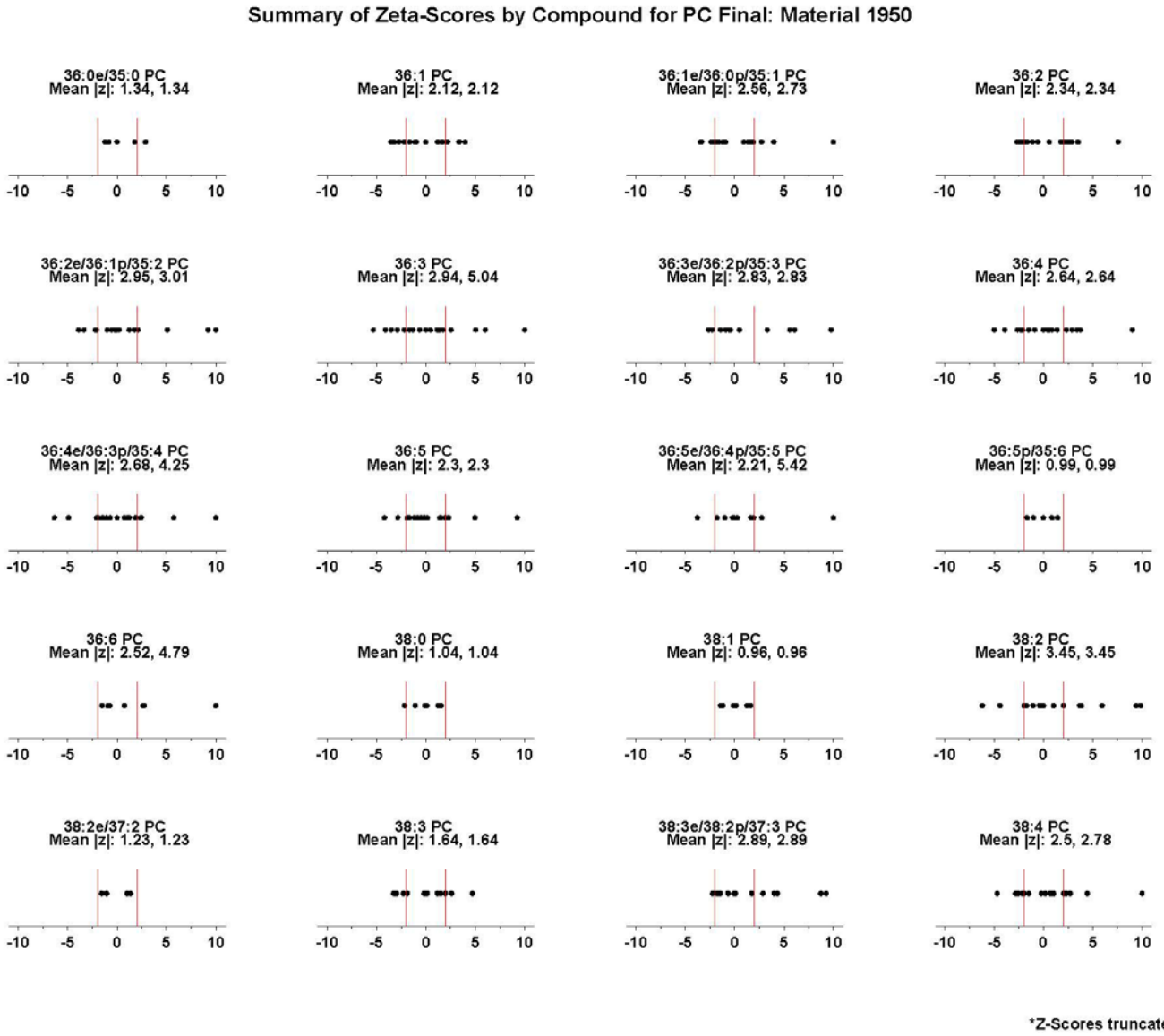


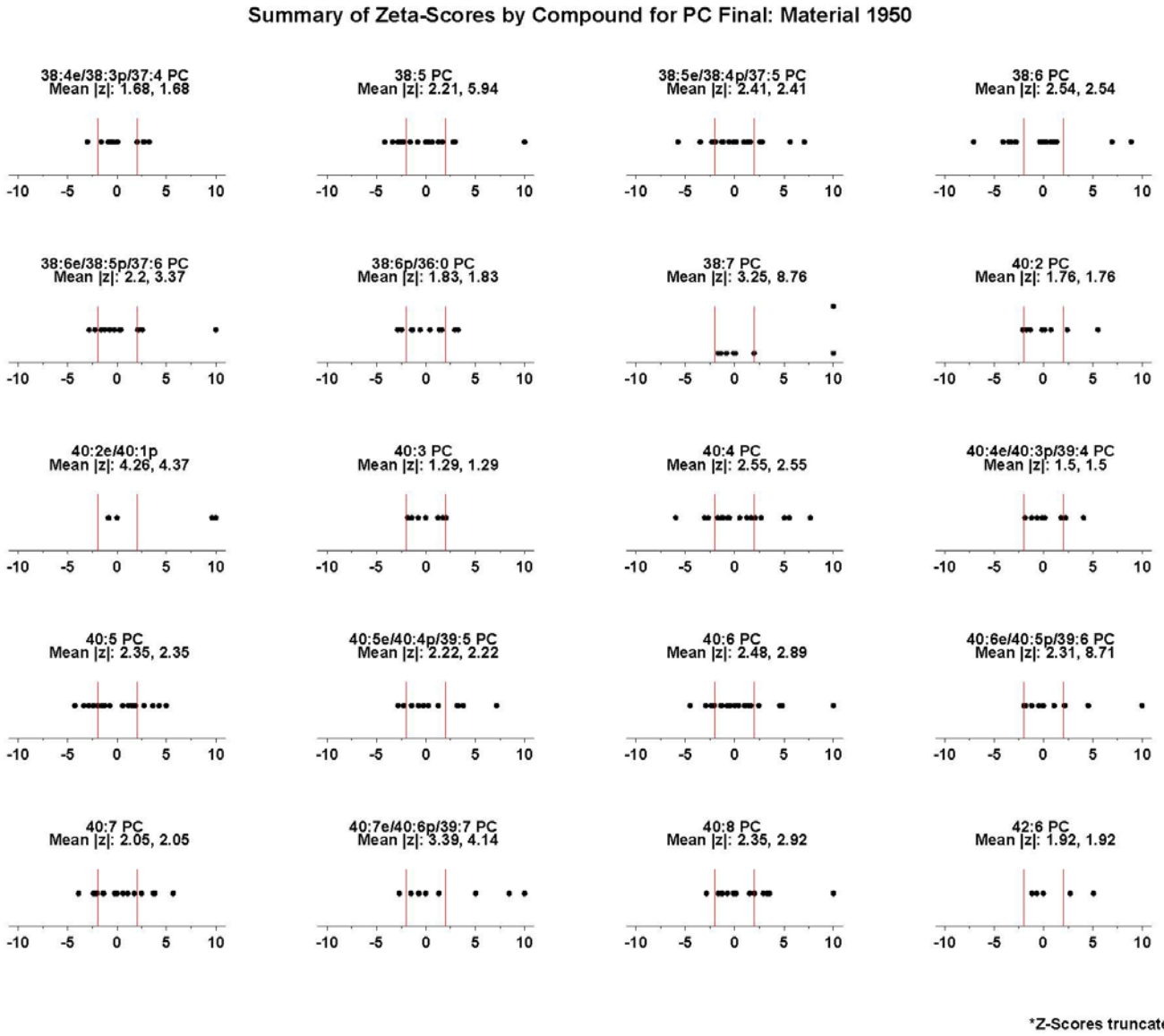


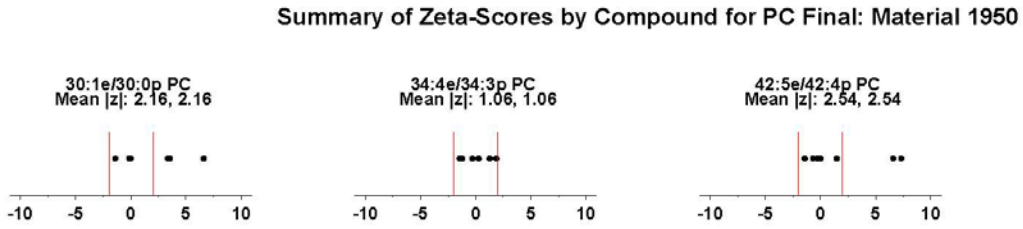


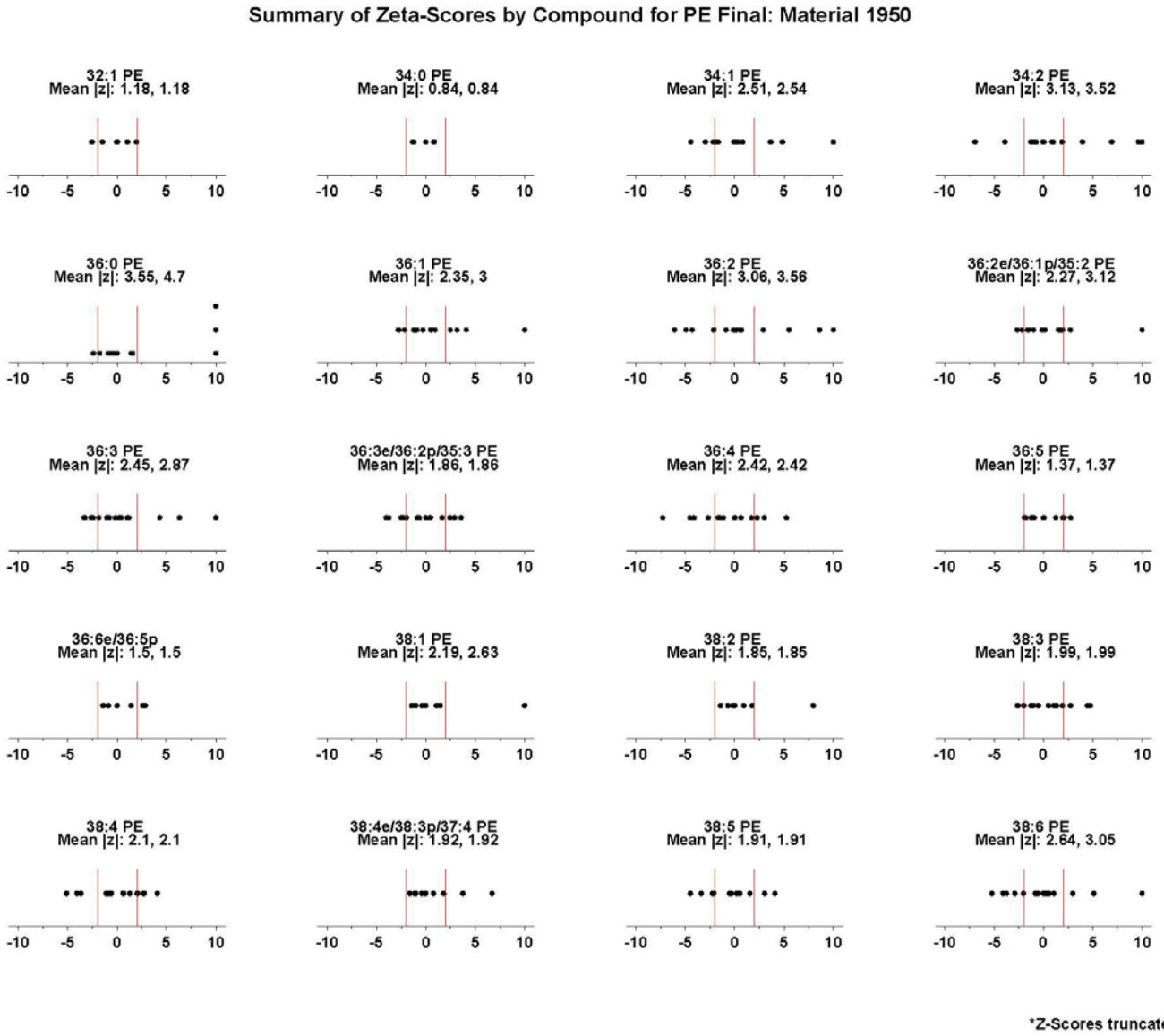


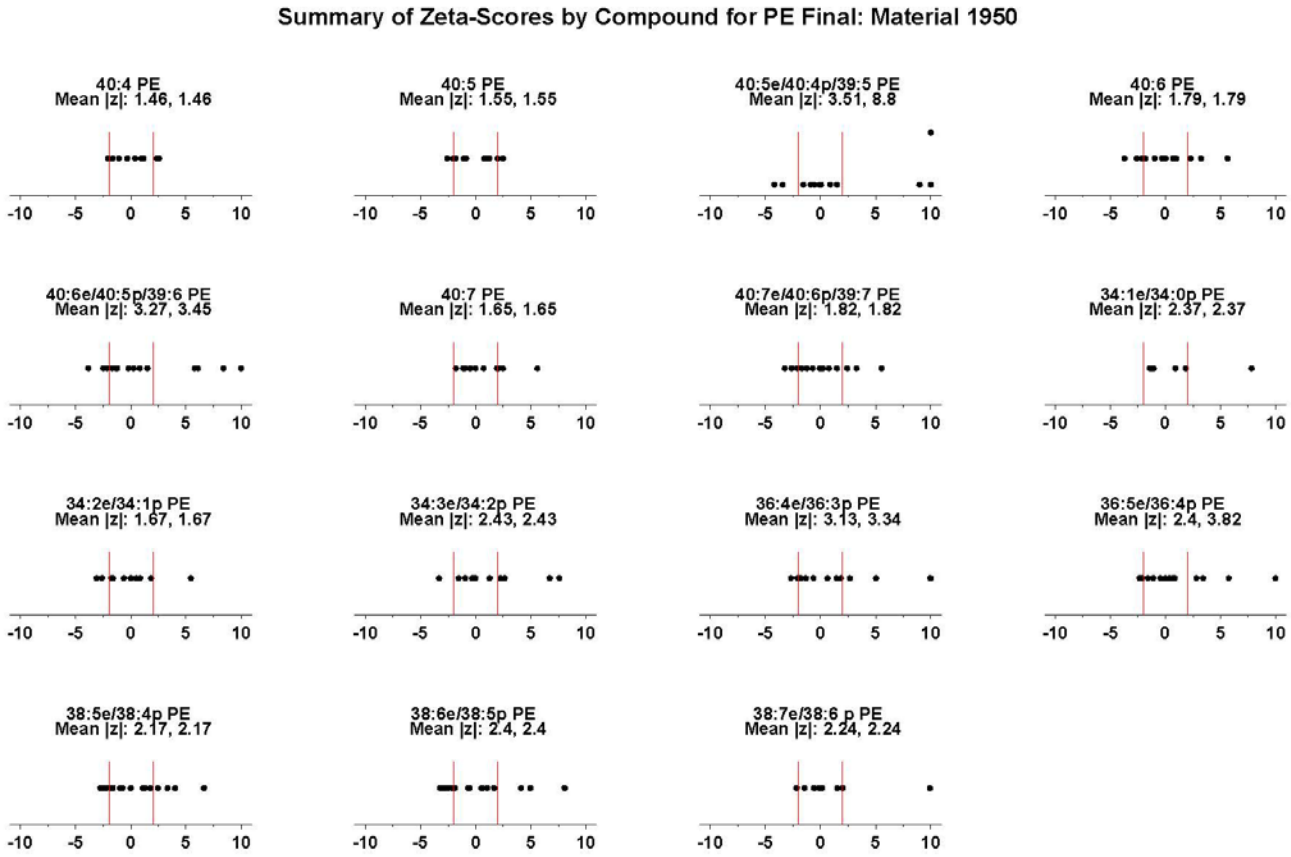


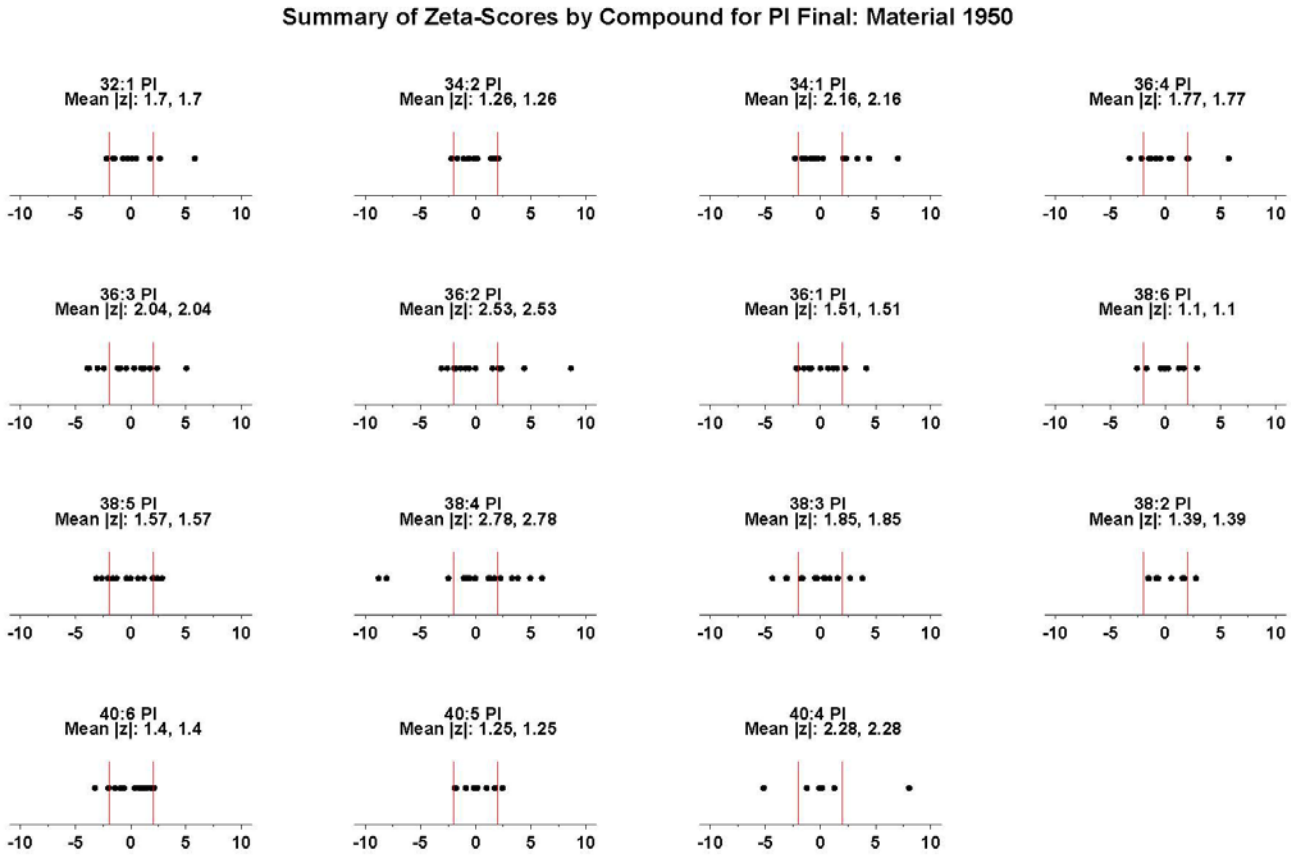


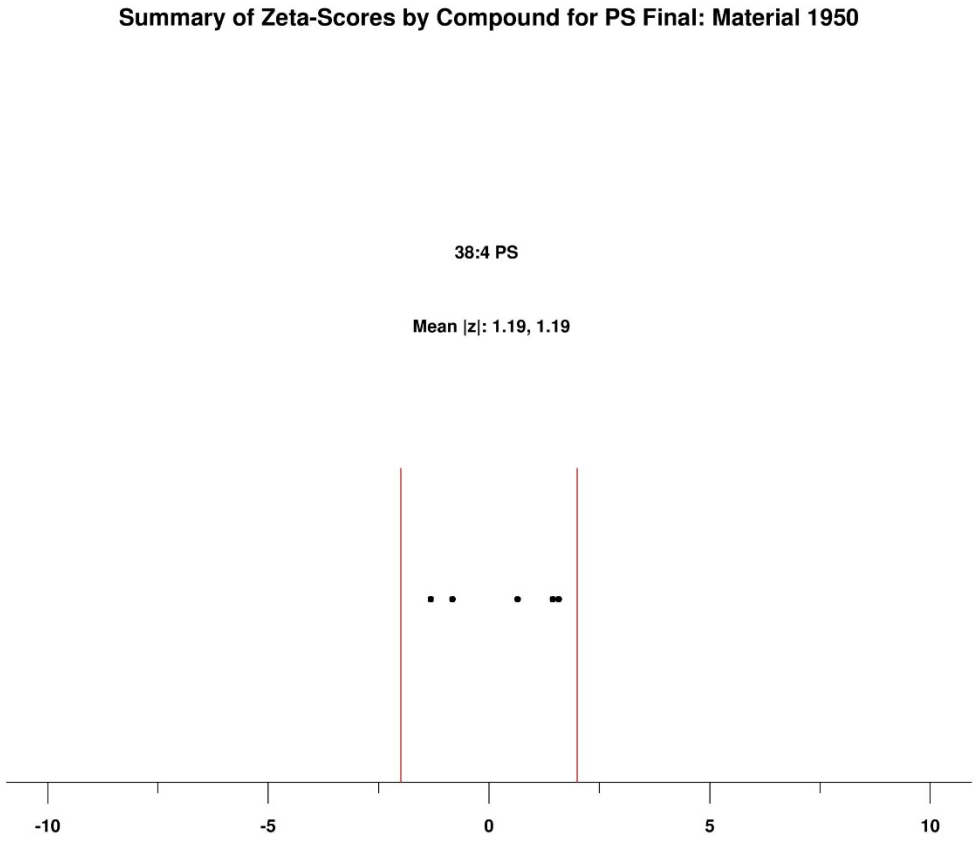


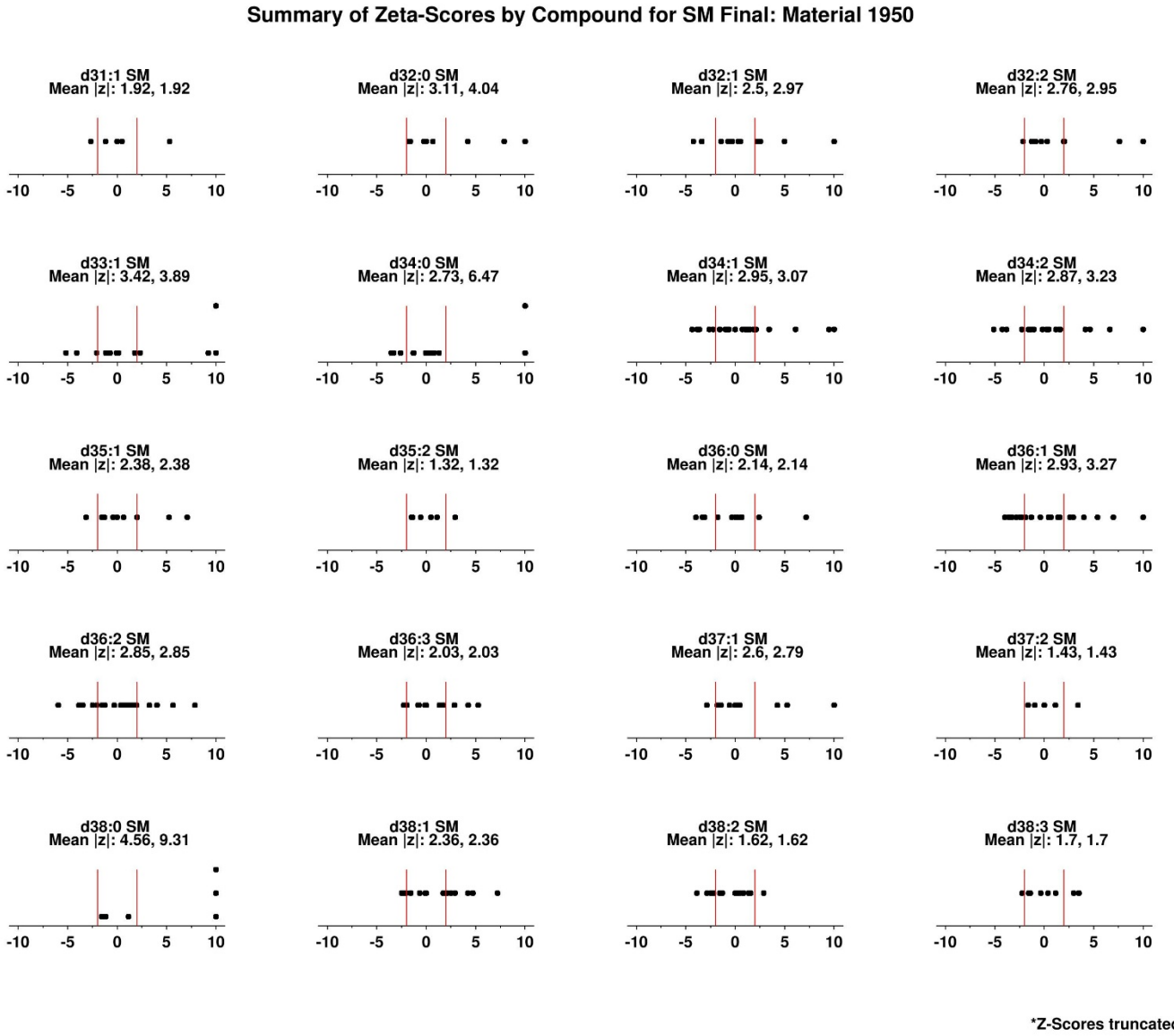


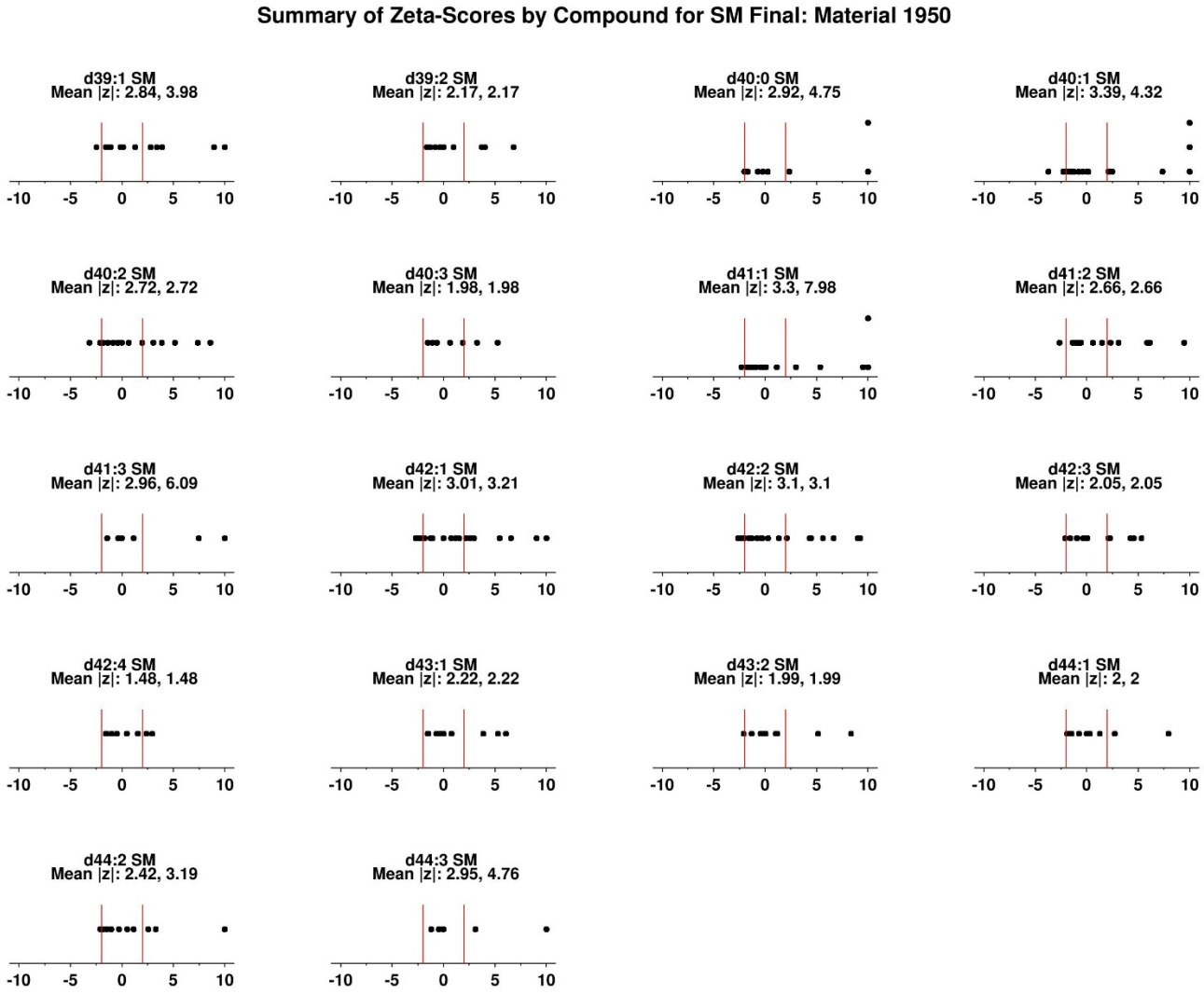


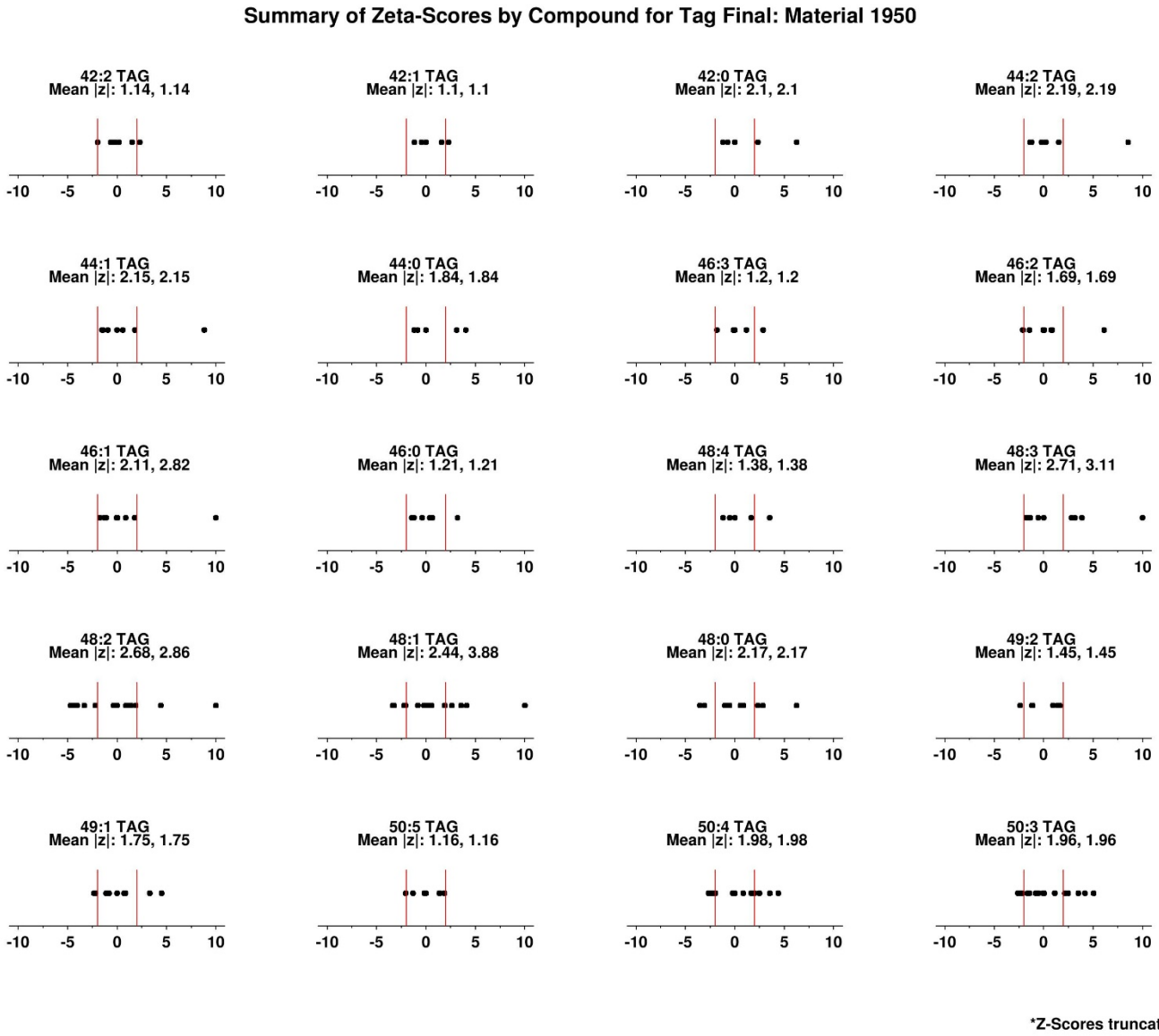


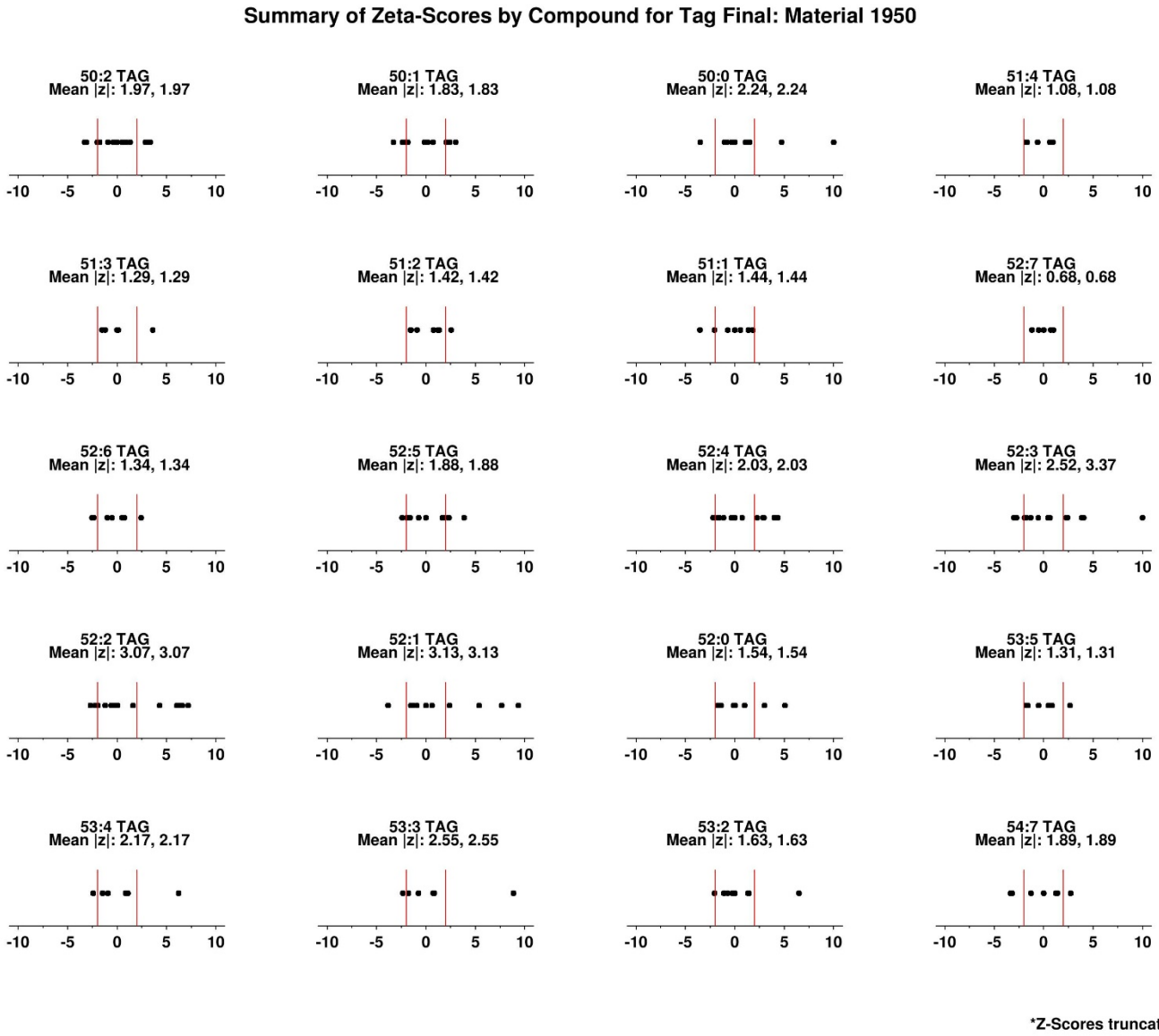


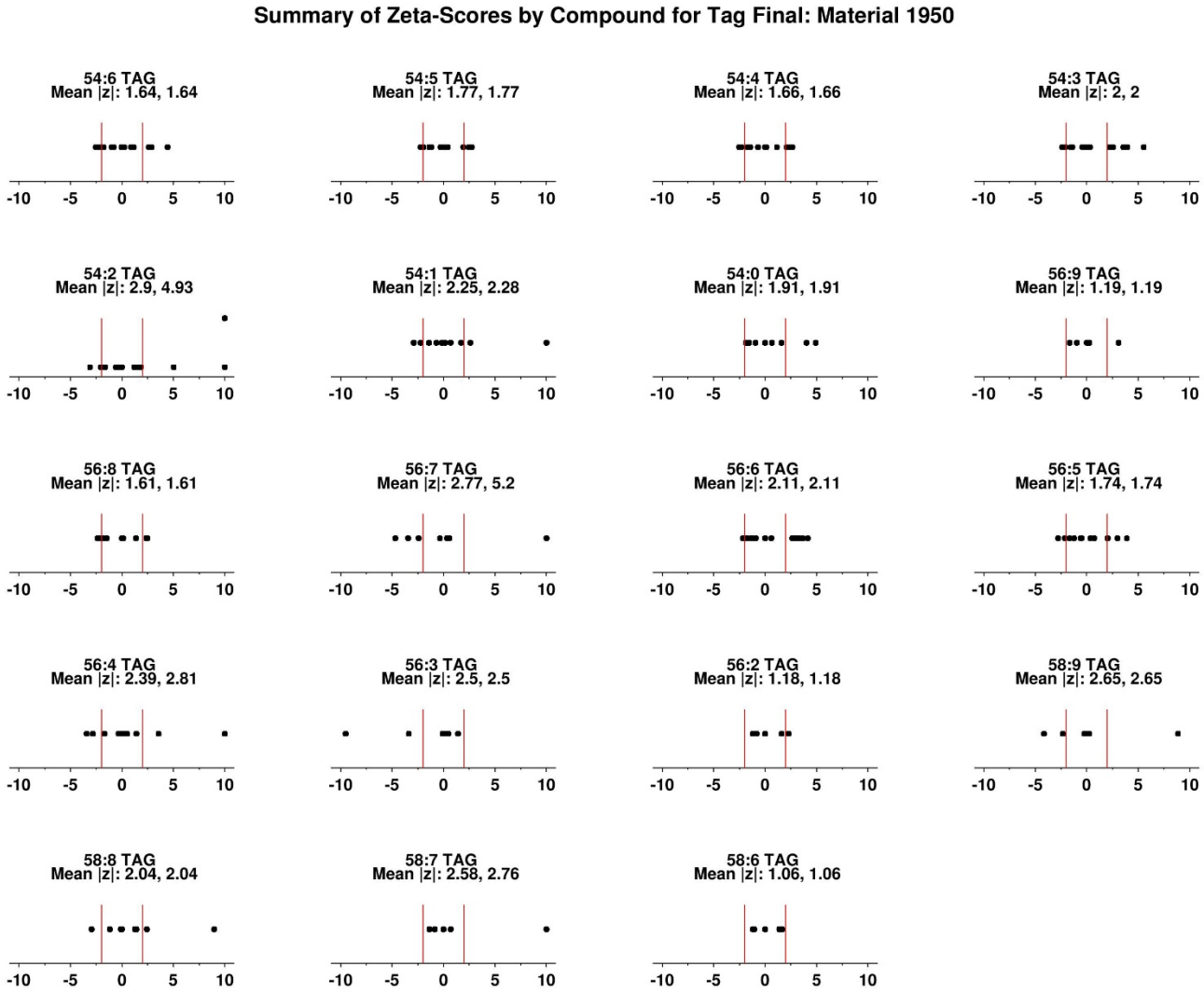








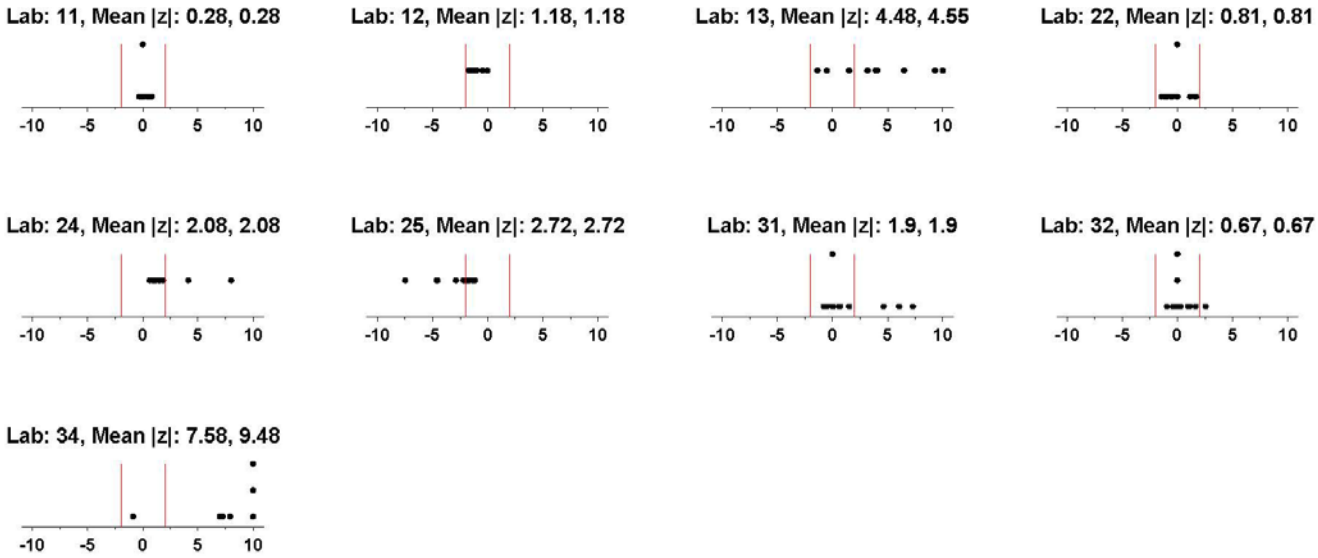




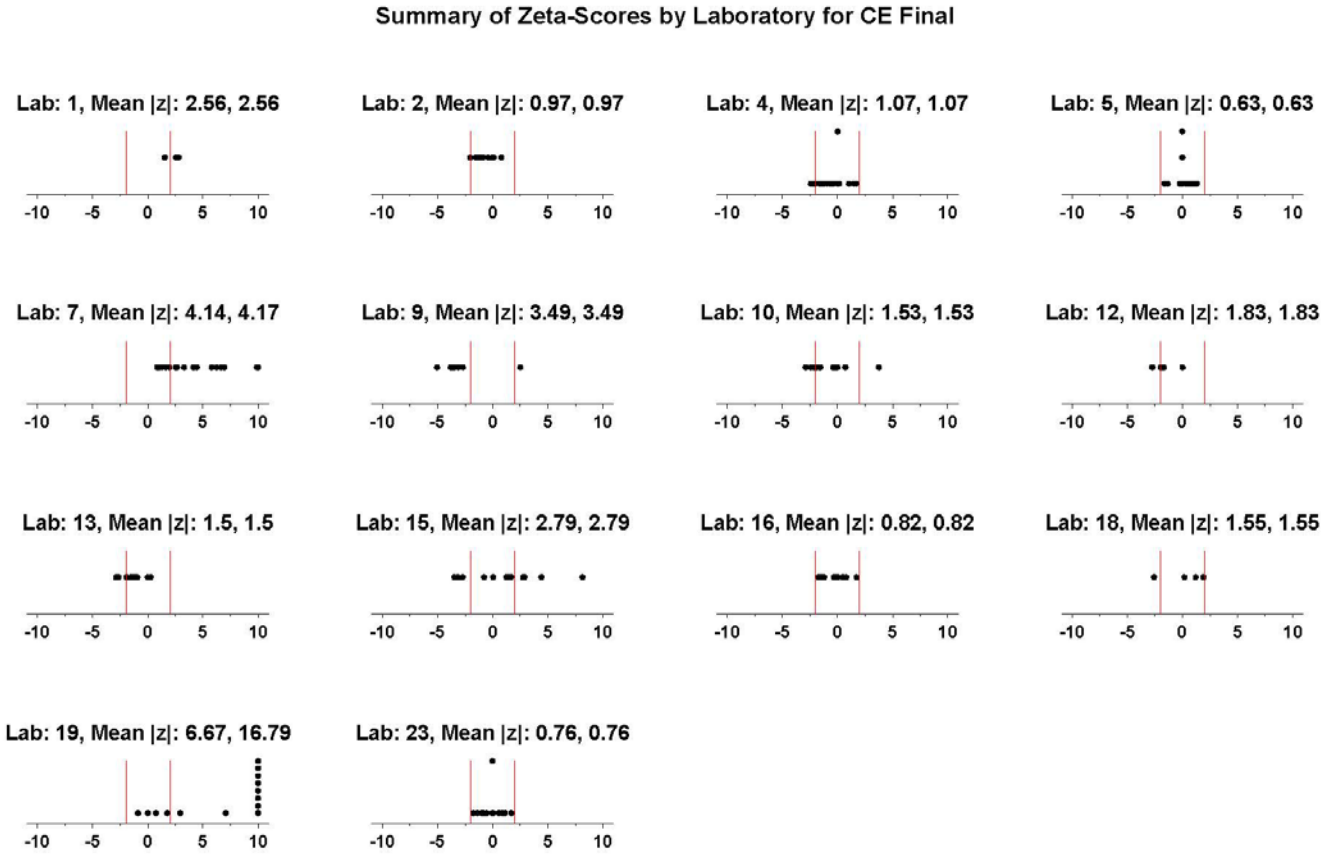
Appendix F: Zeta-Scores Organized by Laboratory

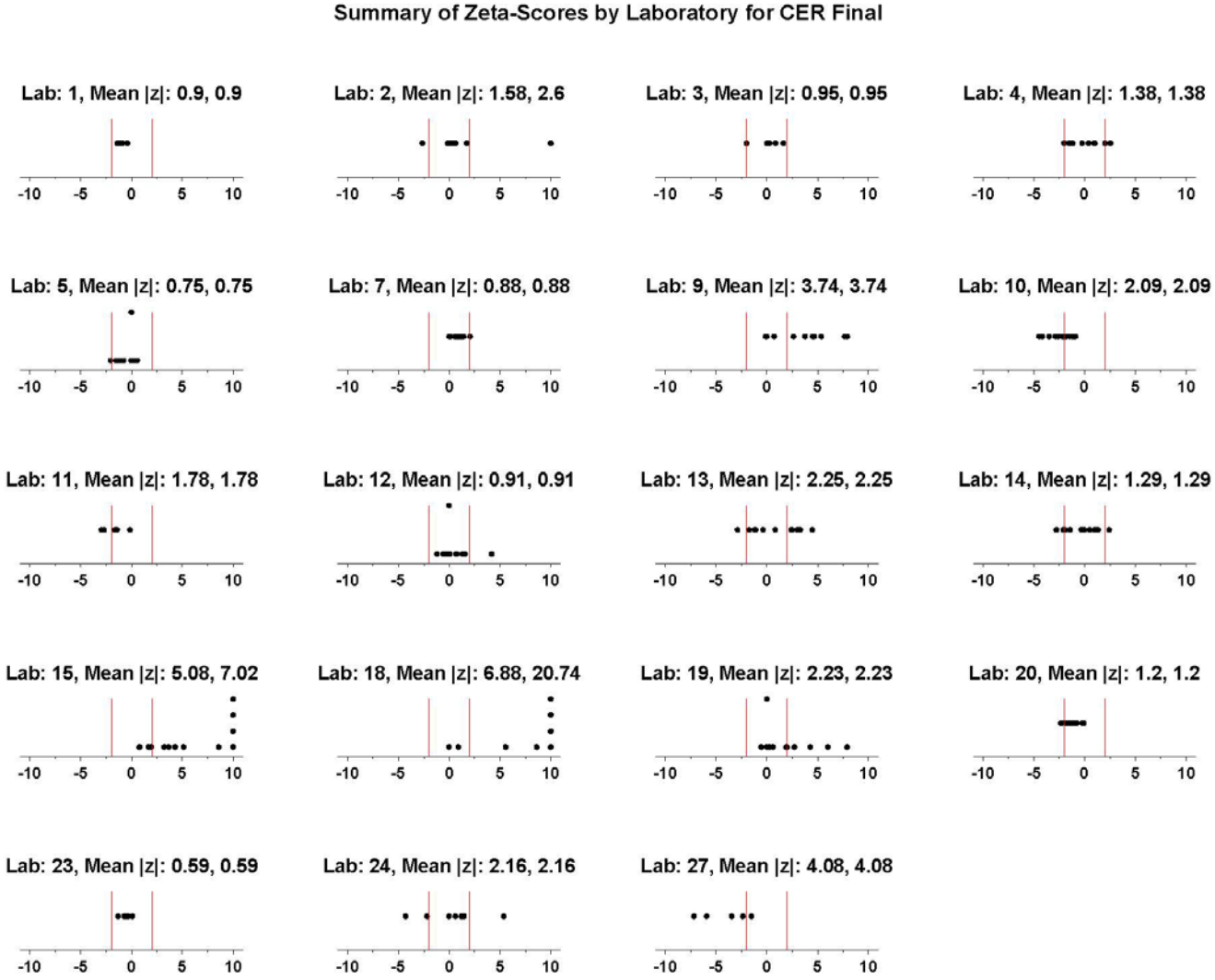
Zeta-score plots provided for all consensus lipids (n ≥ 5 participating laboratories reporting), organized by participating laboratory and presented on a lipid class basis. Each dot represents a single laboratory measurement for a reported lipid using the MEDM location as the target. The distance for each point from the mean indicates that the measurement is *x times the number of combined standard uncertainties* the submitted values is above or below the MEDM location. The plots were truncated at ± 10 to maintain visual resolution. Absolute value mean ζ-scores were calculated two ways: (1) setting truncated values to 10 (first ζ-score average listed) and (2) using the original outlier ζ-score in the calculation. The purpose of this organization was to identify the laboratories that consistently measured outside the consensus location with high frequency and magnitude.

Summary of Zeta-Scores by Laboratory for Bile Acids

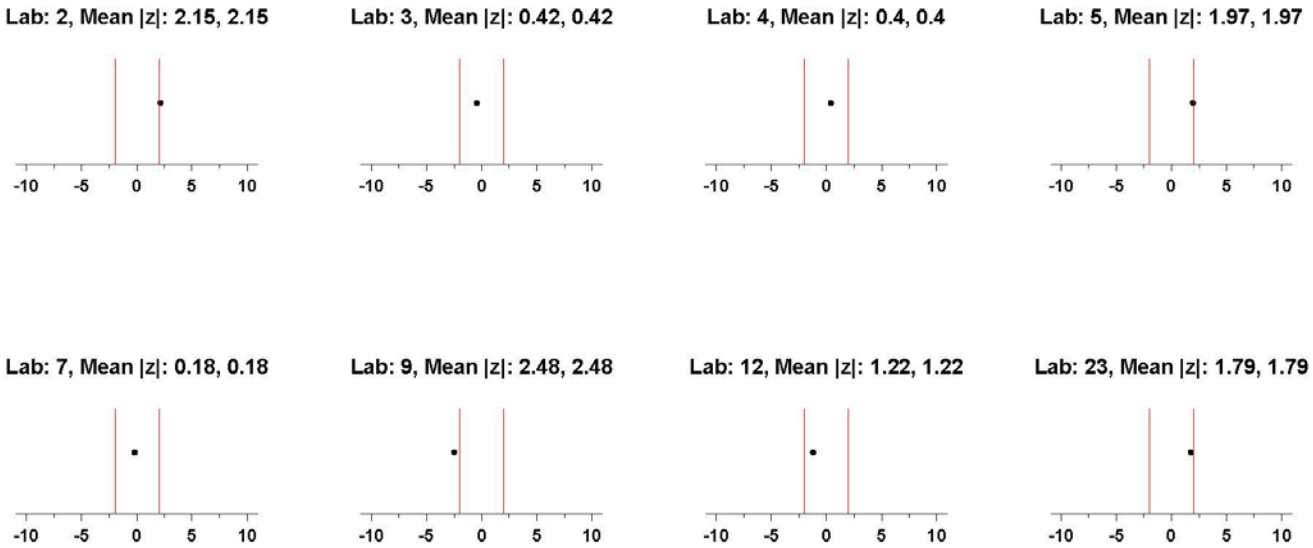


*Z-Scores truncated at +/-10

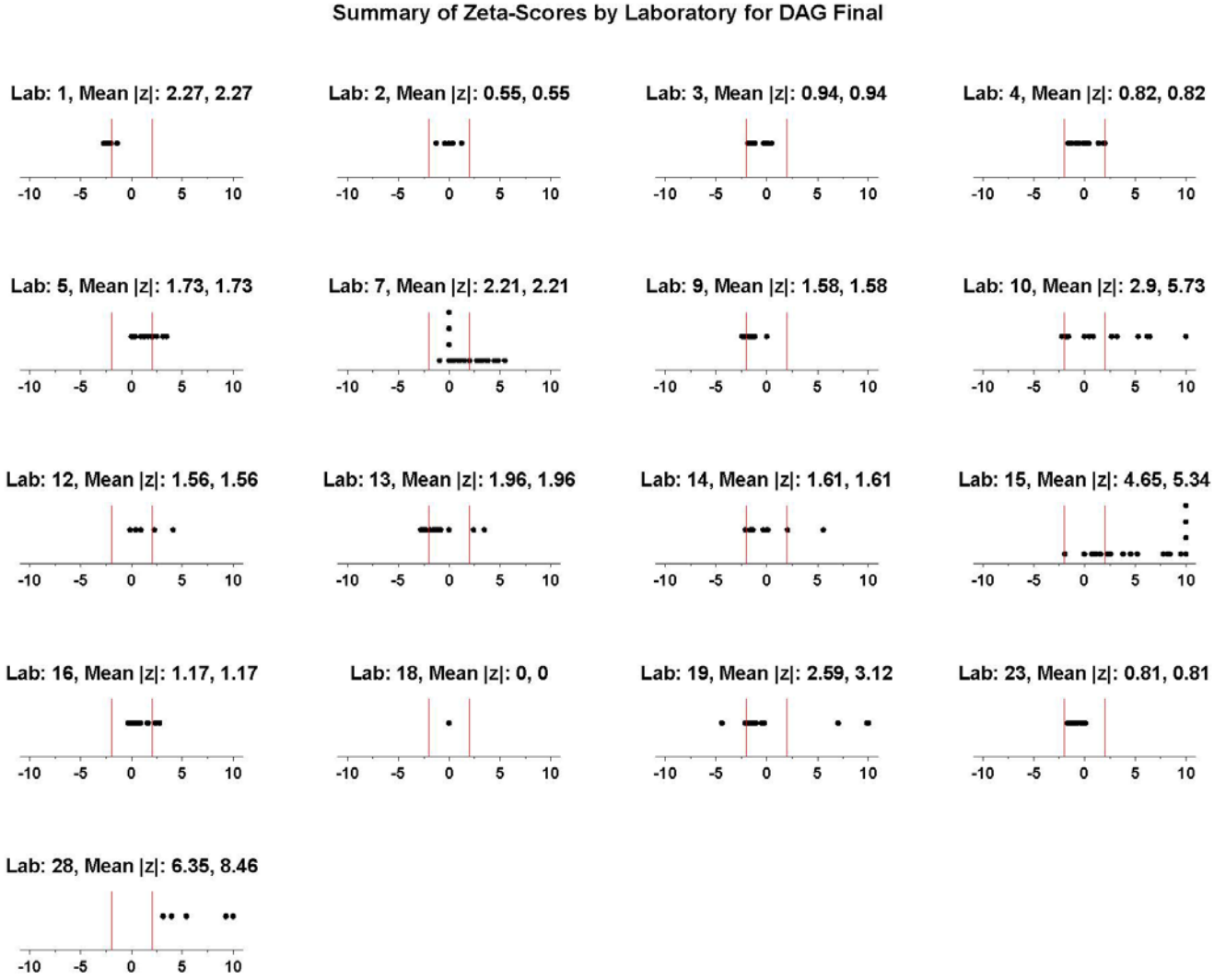




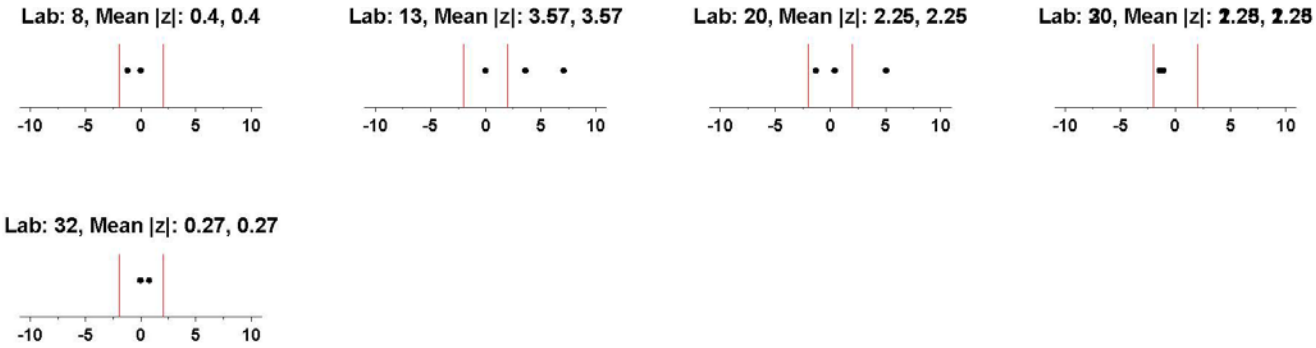
Summary of Zeta-Scores by Laboratory for Cholesterol Final



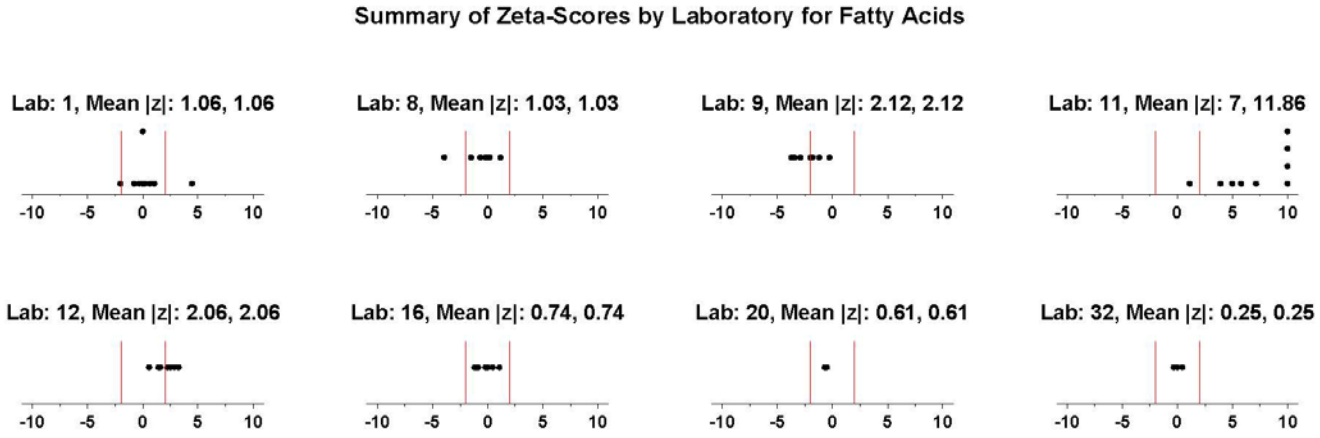
*Zeta-Scores truncated at +/-10

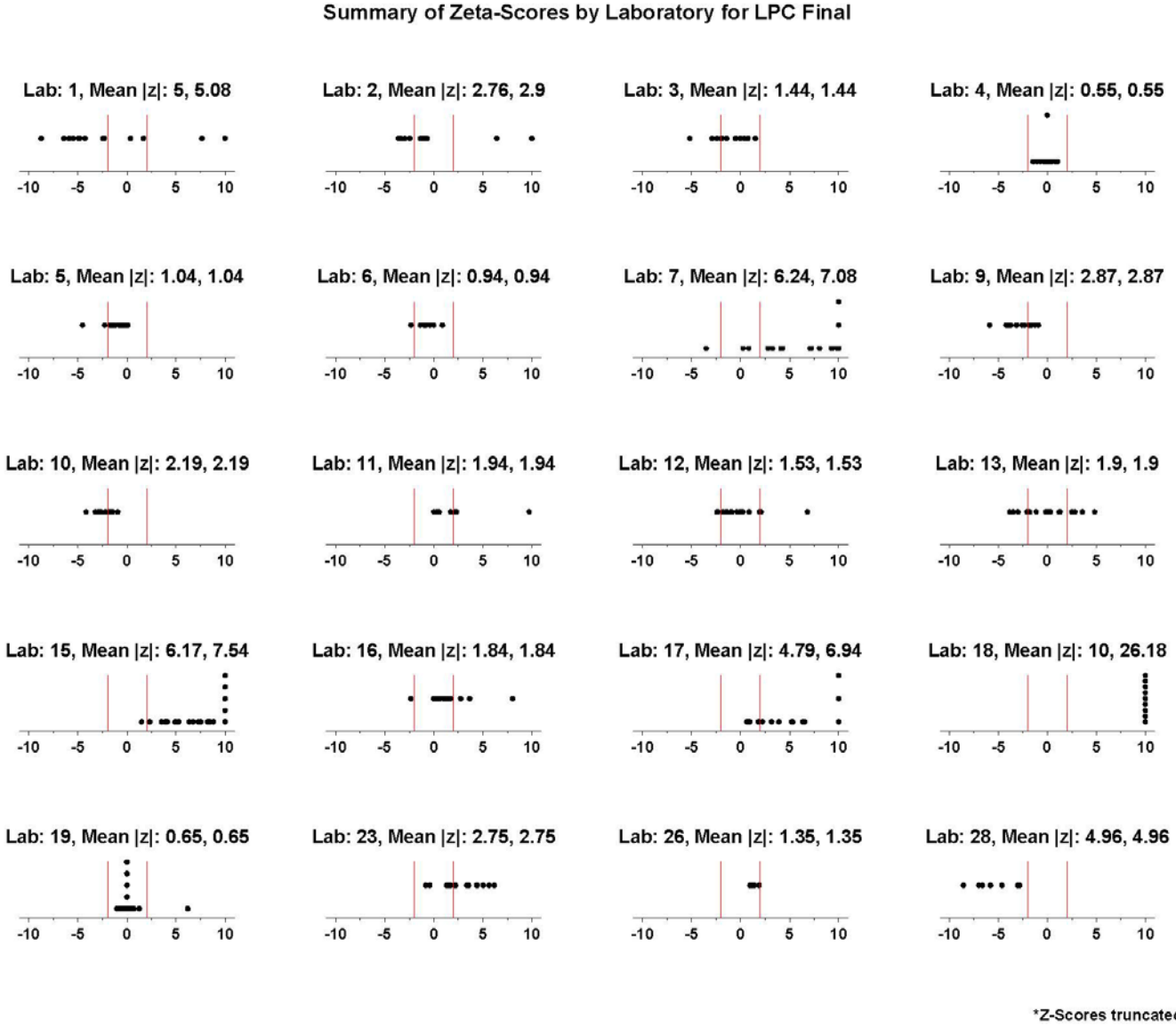


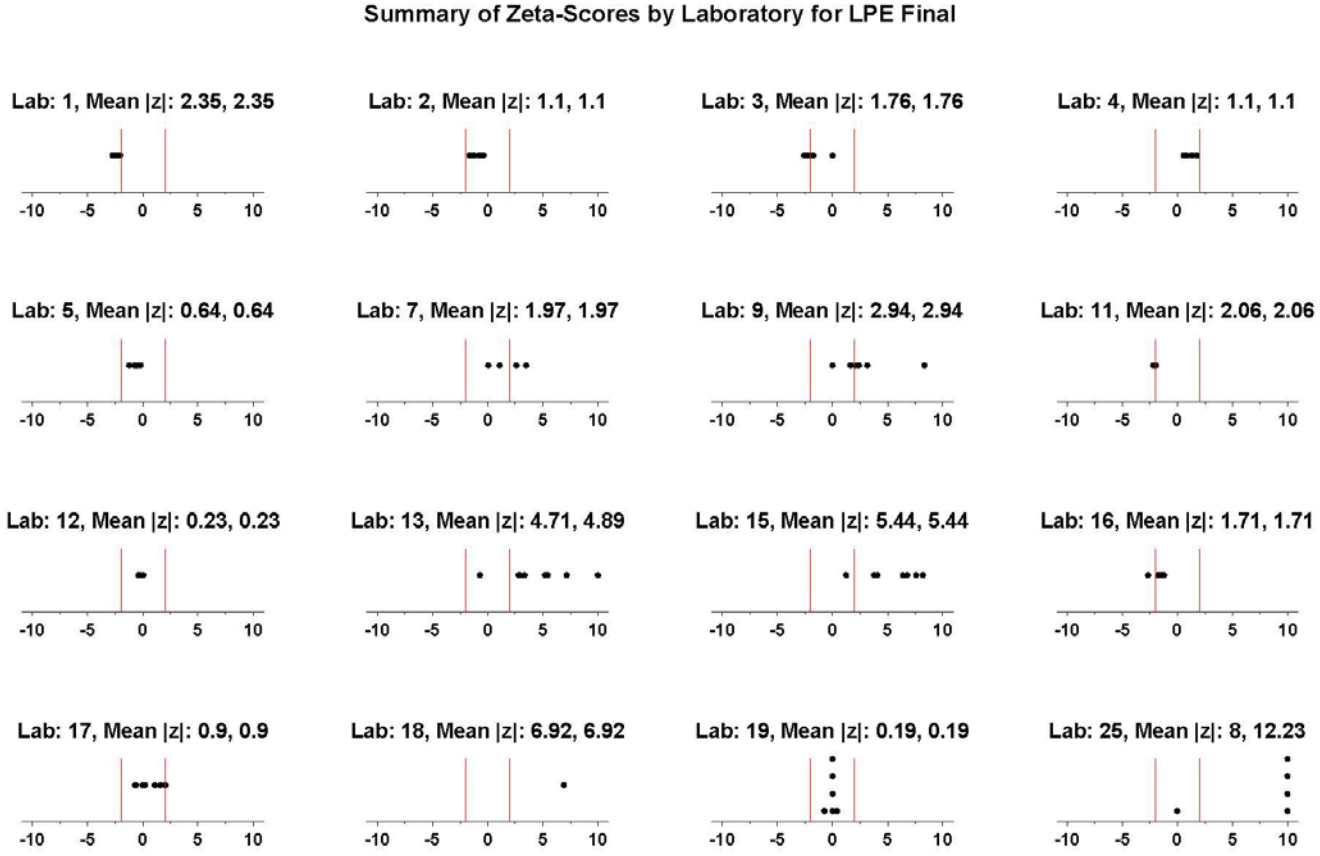
Summary of Zeta-Scores by Laboratory for Eico Final



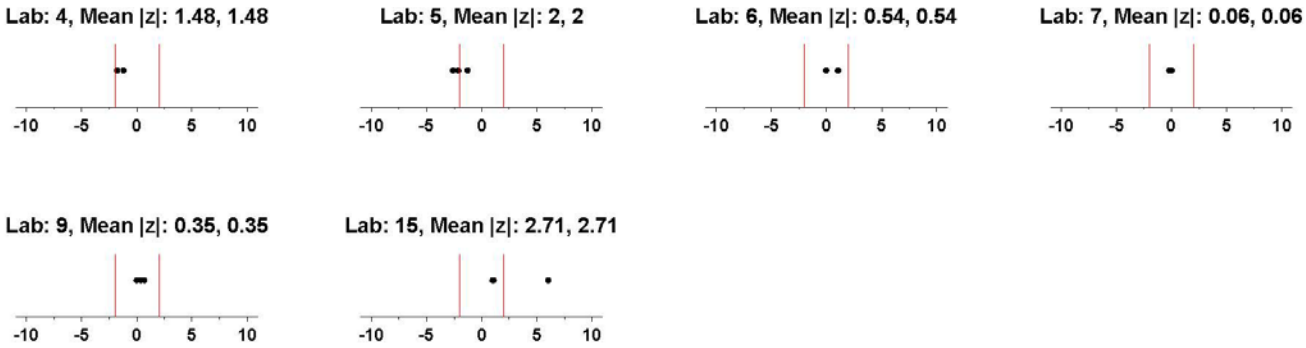
*Z-Scores truncated at +/-10



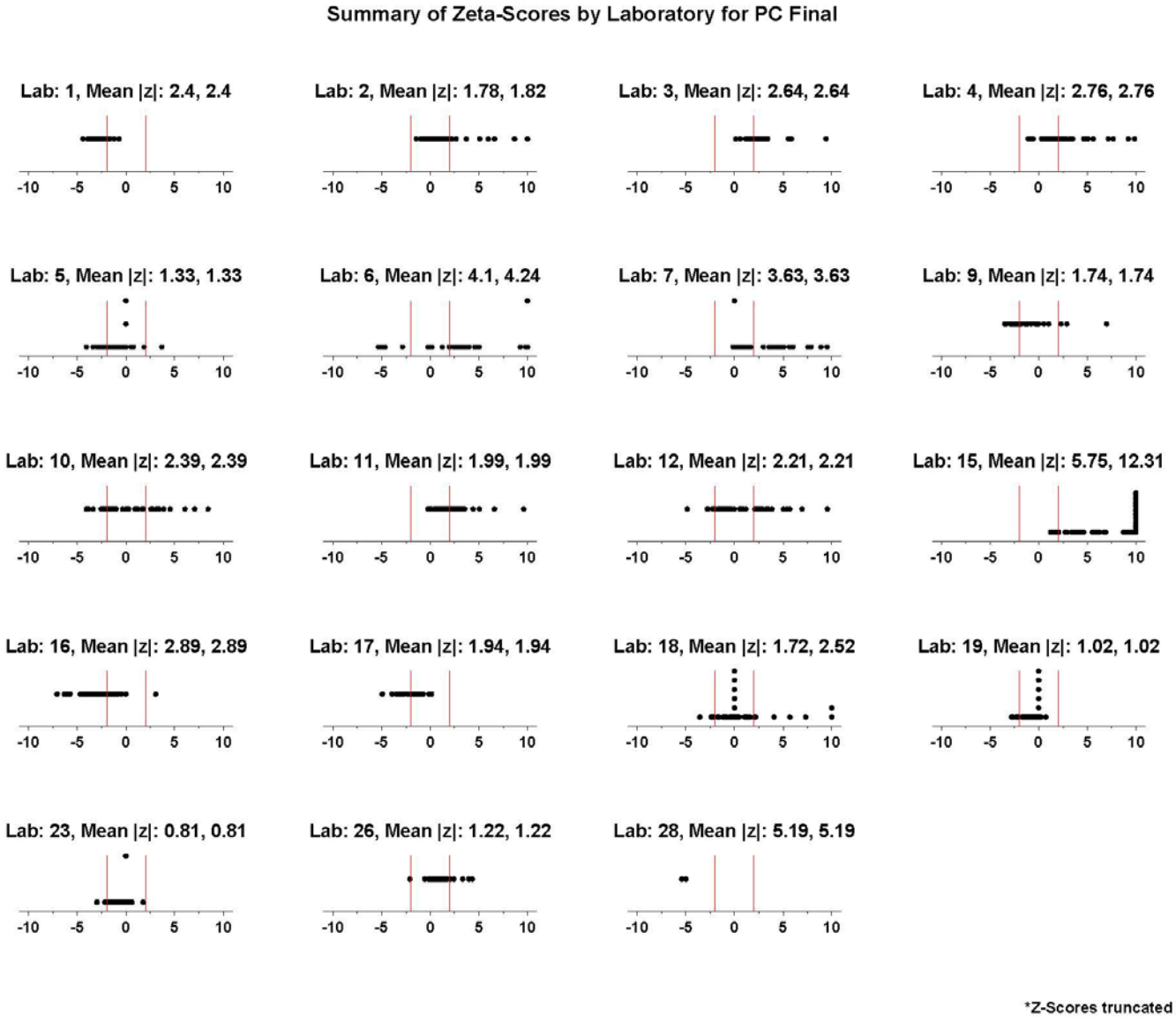


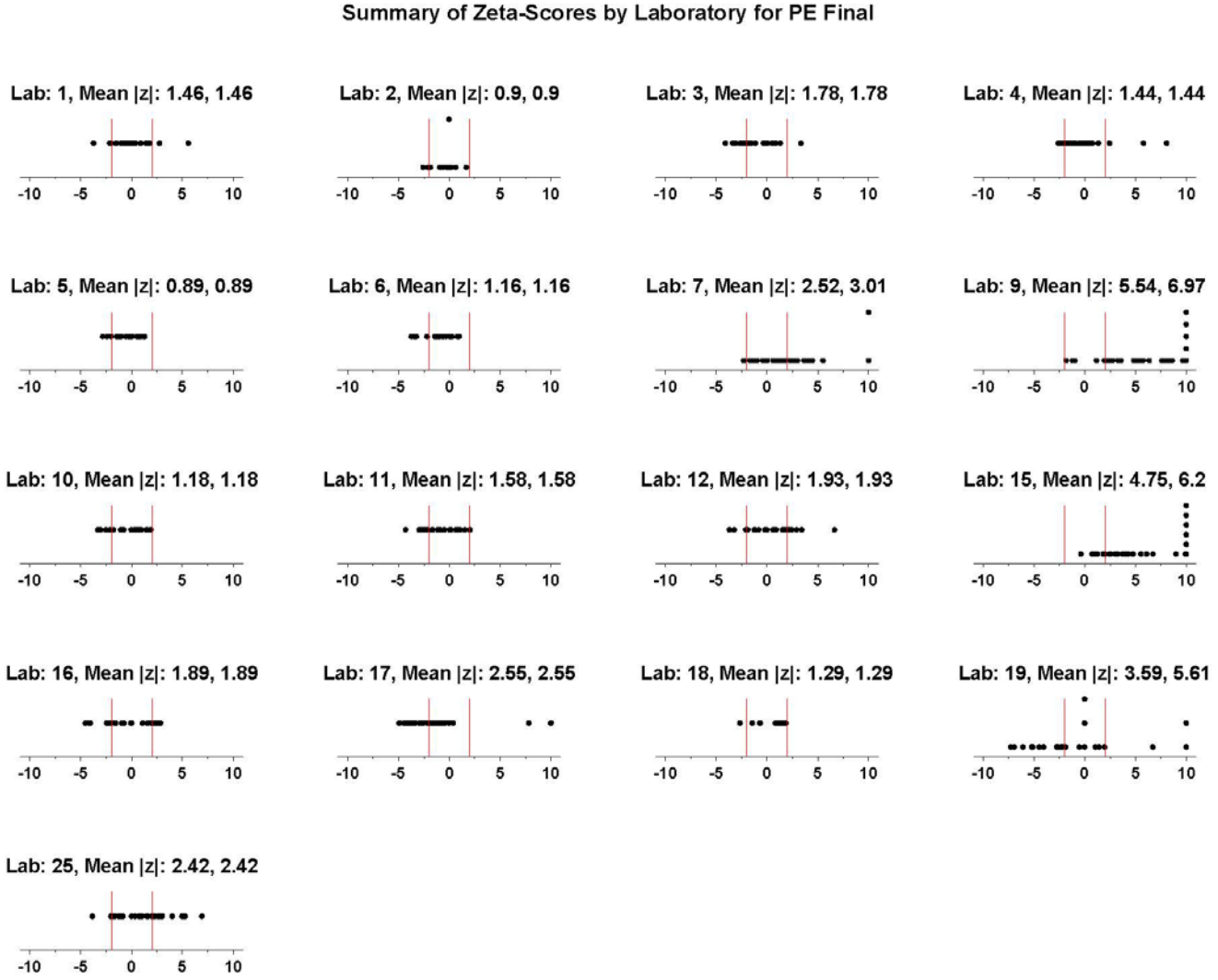


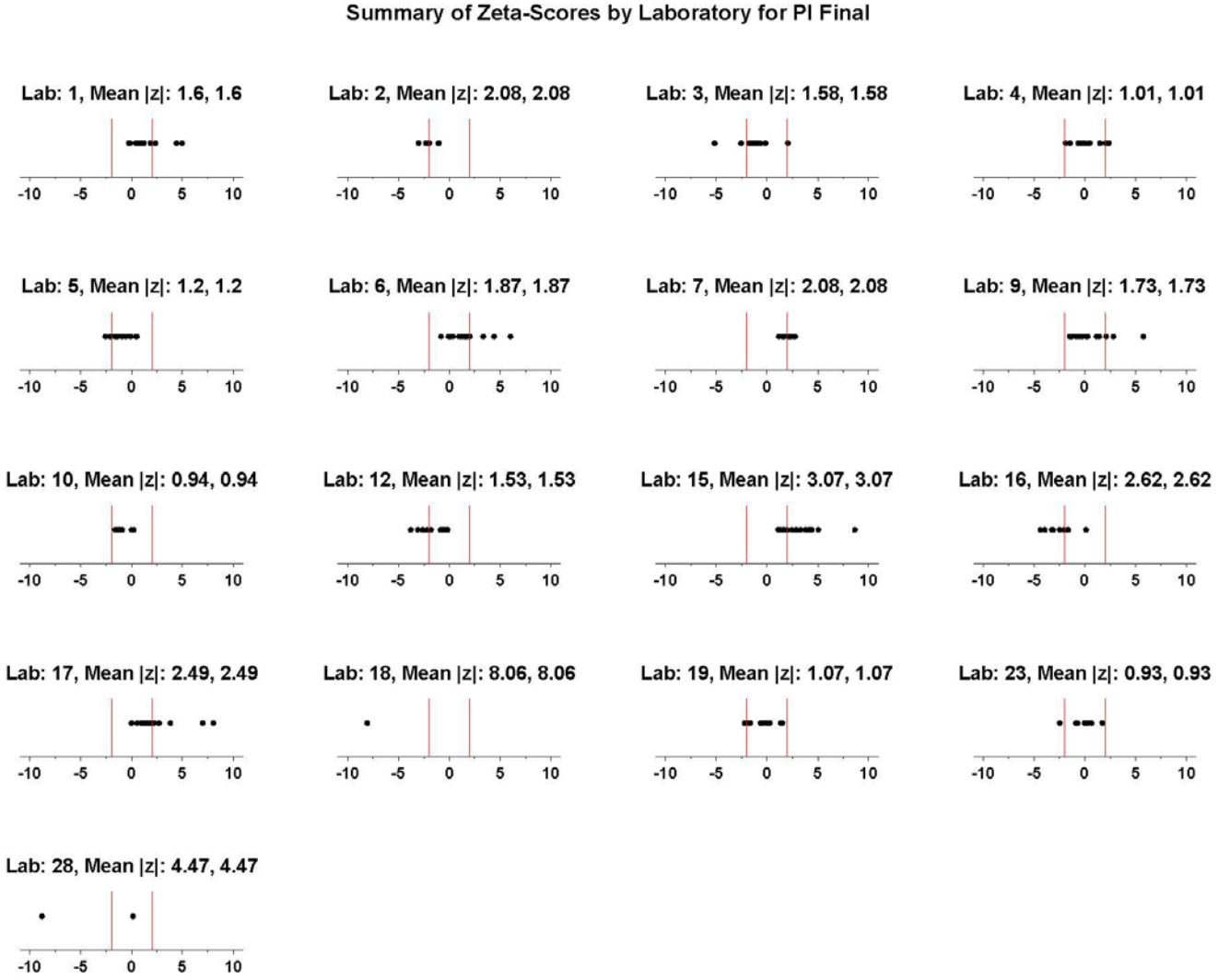
Summary of Zeta-Scores by Laboratory for Other Final



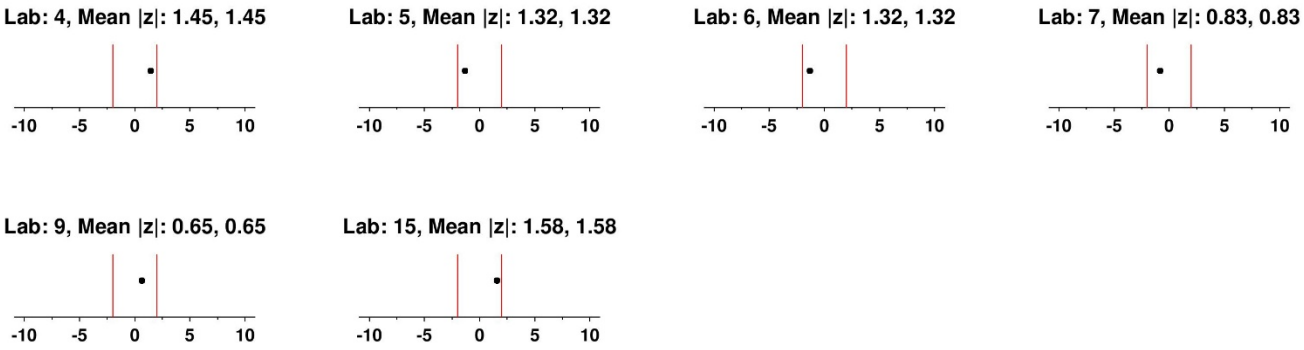
*Z-Scores truncated at +/-10



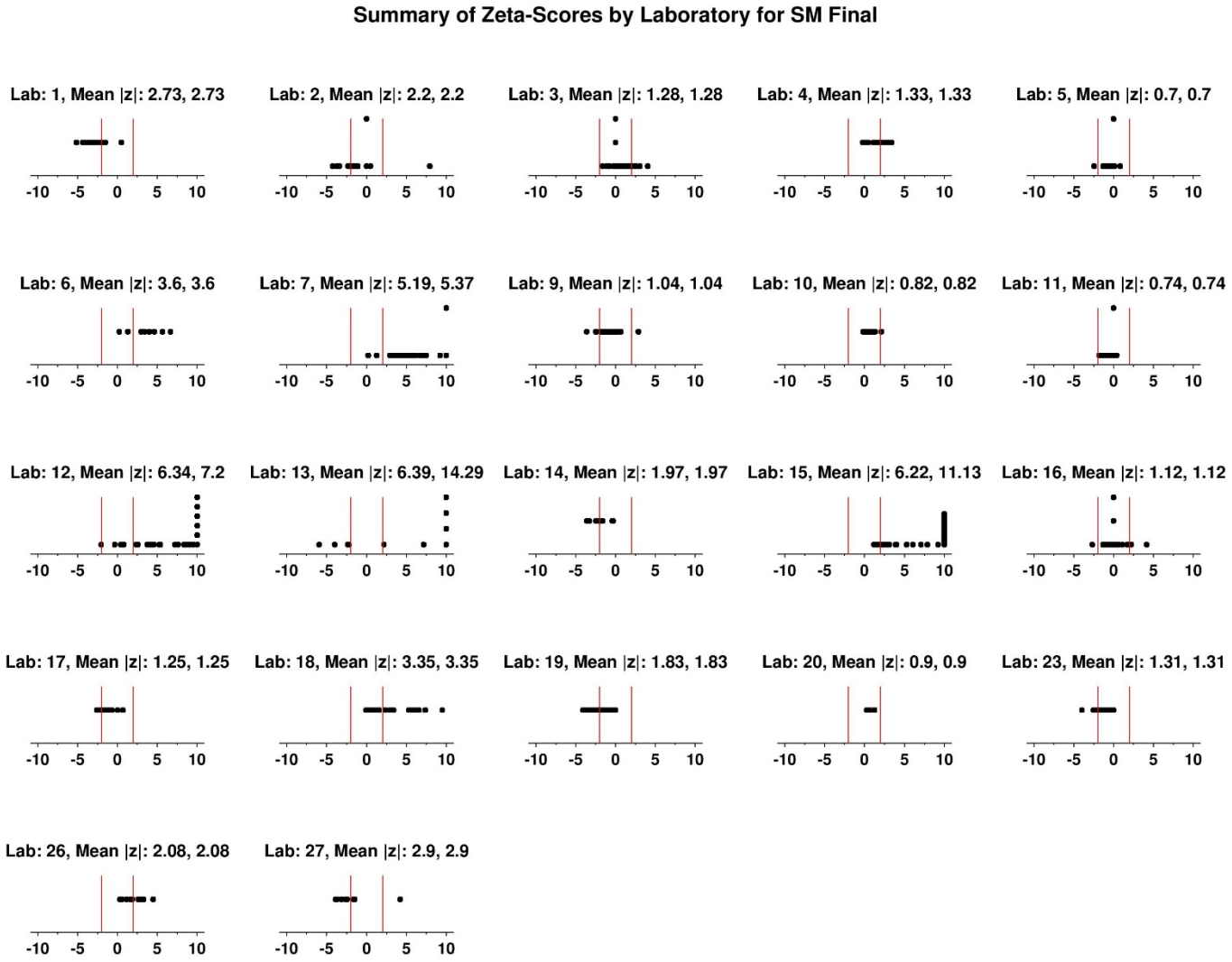


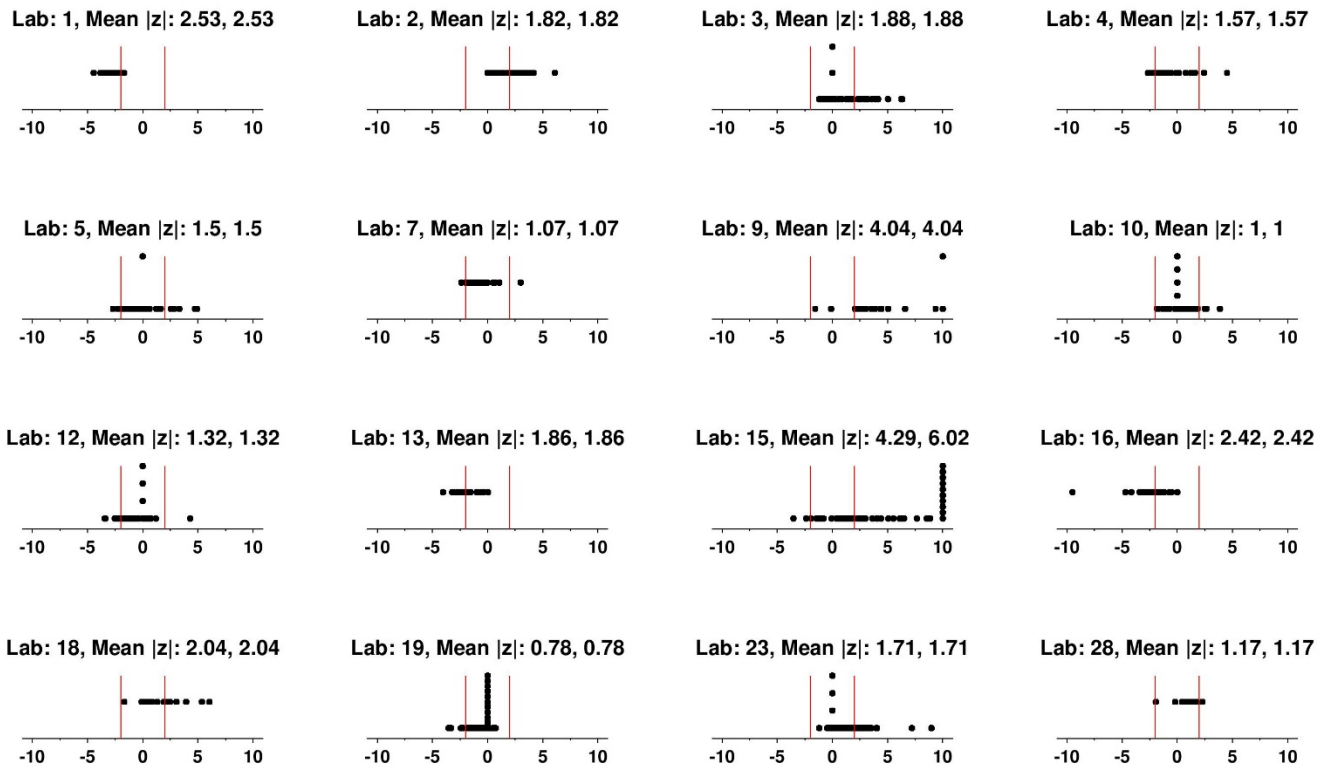


Summary of Zeta-Scores by Laboratory for PS Final



*Z-Scores truncated at +/-10





Appendix G: Interlaboratory Exercise Participants

For this exercise, lipid data was submitted from the following laboratories with contributing investigators listed (see below). The order of the listing does **NOT** correspond to the laboratory number identification codes used in this report, which were randomly assigned upon receipt of data.

The Roskamp Institute
2040 Whitfield Avenue
Sarasota, FL, 34243 USA
Laila Abdullah

Steno Diabetes Center
Copenhagen
DK-2820 Gentofte, Denmark
Linda Ahonen

Department of Pharmaceutical Sciences
986025 Nebraska Medical Center
Omaha, NE 68198-6025 USA
Yazen Alnouti, Rhishikesh Thakare

Department of Chemistry and Biochemistry and Department of Pharmacology
School of Medicine
University of California, San Diego
9500 Gilman Drive
La Jolla, CA 92093-0601 USA
Aaron Armando, Edward A. Dennis, Jiang Jiang

Department of Medicine and Department of Pharmacology
School of Medicine, University of California, San Diego
9500 Gilman Drive, La Jolla, CA 92093-0601 USA
Oswald Quehenberger

Division of Signal Transduction
Beth Israel Deaconess Medical Center
Boston, MA USA
John M. Asara, Min Yuan, Susanne B. Breitkopf

Division of Metabolomics
Research Center for Transomics Medicine

Medical Institute of Bioregulation
Kyushu University
3-1-1 Maidashi, Higashi-ku
Fukuoka, Fukuoka 812-8582 Japan
Takeshi Bamba, Yoshihiro Izumi, Hiroaki Takeda

Division of Laboratory Sciences
National Center for Environmental Health
Centers for Disease Control and Prevention
4770 Buford Hwy MS-F50
Atlanta, GA 30341 USA
John R. Barr, Zsuzsanna Kuklenyik, Jon Rees, Michael S. Gardner, Kayla Carter

Department of Chemistry-BMC
Analytical Chemistry
Uppsala University, Sweden
Kumari Ubhayasekera, Jonas Bergquist

Department of Biochemistry and Molecular Biology
Medical University South Carolina
173 Ashley Ave. Charleston, SC 29425 USA
Jason S. Pierce, Barbara Rembiesa

University of Victoria-Genome British Columbia Proteomics Centre
University of Victoria
3101-4464 Markham Street, Victoria, BC V8Z 7X8 Canada
Christoph H. Borchers, Karen Lin, Jun Han

University of Southampton, Faculty of Medicine
Academic Unit of Clinical & Experimental Sciences
Southampton General Hospital, Tremona Road
Southampton, SO16 6YD, UK
Anthony D. Postle, Joost Brandsma, Grielof Koster

NIH West Coast Metabolomics Center
UC Davis Genome Center
451 Health Sci Drive
Davis, CA 95616 USA
Oliver Fiehn, Tomas Cajka

National University of Singapore
Yong Loo Lin School of Medicine
Department of Biochemistry
SLING, 28 Medical Drive 03-03, 117456 Singapore
Markus R Wenk, Amaury Cazenave-Gassiot, Federico Torta, Aveline Huipeng Neo
Division of Physiological Chemistry 2

Department of Medical Biochemistry and Biophysics
Karolinska Institutet
Stockholm, 171 77, Sweden
Craig E. Wheelock, Antonio Checa, Johan Kolmert, Alexander Fauland

Baker Heart and Diabetes Institute
75 Commercial Road
Melbourne VIC 3004, Australia
Peter J. Meikle, Michelle A Cinel, Natalie A. Mellett, Jacquelyn M. Weir

Center for Experimental Therapeutics and Reperfusion Injury
Department of Anesthesiology
Perioperative and Pain Medicine
Blg for Transformative Medicine
Brigham and Women's Hospital and Harvard Medical School
Boston, Massachusetts 02115, USA
Charles N. Serhan, Romain A. Colas

Biomarker Core Laboratory
Irving Institute for Clinical and Translational Research
Columbia University Medical Center, 630 West 168th Street
New York, NY 10032, USA
Serge Cremers, Renu Nandakumar, Hongfeng Jiang, William Blaner

University of Florida
Department of Pathology
Immunology and Laboratory Medicine
Gainesville, FL 32610 USA
Tim Garrett, Jeremy Koelmel, Danielle McDougall, Rainey Patterson

Department of Pharmacology
New York Medical College School of Medicine
15 Dana Road, Valhalla, NY 10595 USA
Houli Jiang, Katherine H. Gotlinger, Michal Laniado Schwartzman

Thermo Fisher Scientific
355 River Oaks Parkway
San Jose, CA 95134 USA
David Peake, Yingying Huang, Reiko Kiyonami

Department of Chemistry
Örebro University
702 81 Örebro, Sweden
Tuulia Hyötyläinen

Metabolomics Core, BRCF
University of Michigan
1000 Wall St
Ann Arbor, MI 48105-5714 USA
Maureen Kachman

Biocrates Life Sciences AG
Eduard-Bodem-Gasse 8
6020 Innsbruck, Austria
Kristaps Klavins, Therese Koal

Lipotype GmbH
Tatzberg 47
01307 Dresden, Germany
Christian Klose, Michal A. Surma

Core Facility for Mass Spectrometry
Medical University of Graz, ZMF
Stiftingtalstrasse 24, 8010 Graz, Austria
Harald C. Köfeler, Alexander Triebl, Martin Trötzmüller

Stable Isotope and Metabolomics Core Facility
Diabetes Research Center
Albert Einstein College of Medicine
1301 Morris Park Ave
Bronx, NY 10461 USA
Irwin J. Kurland, Yunping Qiu, Xueqing Heather Zhao

Analytical Facility of Bioactive Molecules
The Hospital for Sick Children Research Institute
686 Bay Street, Toronto, ON, M5G 0A4, Canada
Michael Leadley, Martin Post, Denis Reynaud

Lipidomics Core Facility and Department of Pathology
Wayne State University
5101 Cass Avenue
Detroit, MI 48202 USA
Krishna Rao Maddipati, Senlin Zhou

Department of Chemistry and Biochemistry
Concordia University
7141 Sherbrooke Street West
Montréal, QC, H4B 1R6, Canada
Dajana Vuckovic, Cian Monnin, Parsram Ramrup

Proteomics and Metabolomics Shared Resource
Duke University School of Medicine, B02 Levine Science Research Center
450 Research Drive
Durham, NC 27710 USA
M. Arthur Moseley, Lisa St. John-Williams, J. Will Thompson

Turku Centre for Biotechnology
University of Turku and Åbo Akademi University
FI-20520 Turku, Finland
Matej Oresic

Max Planck Institute of Molecular Cell Biology and Genetics
Pfotenhauerstr. 108
01307 Dresden, Germany
Andrej Shevchenko, Susanne Sales, Kai Schuhmann

Medical University of South Carolina
Hollings Marine Laboratory
311 Fort Johnson Road
Charleston, SC 29412 USA
Stephen E. Somerville

Kansas Lipidomics Research Center
Division of Biology
Kansas State University
Ackert Hall, 1717 Claflin Rd.
Manhattan, KS 66506 USA
Ruth Welti, Mary R. Roth, Libin Yao