

California Environmental Protection Agency



**PARALLEL STUDY OF DATA FROM AMBIENT AIR
SAMPLES ANALYZED BY METHODS MLD052
MLD057, AND MLD058 FOR 1,3-BUTADIENE,
AROMATIC, AND HALOGENATED COMPOUNDS**

Northern Laboratory Branch
Monitoring and Laboratory Division

Initial Revision Date: August 31, 2000
Initial Revision Number: 1.00 [**DRAFT**]
Revision Date: June 25, 2002
Revision Number: 2.00

DISCLAIMER: Mention of any trade name or commercial product in this Standard Operating Procedure does not constitute endorsement or recommendation of this product by the Air Resources Board. Specific brand names and instrument descriptions listed in the Standard Operating Procedure are for equipment used by the ARB laboratory.

This Page Left Intentionally Blank

Prepared by:

Steven C. Madden, Spectroscopist

Nati Lapurga, Public Health Chemist
Pamela Gupta, Air Pollution Specialist
Lynn Yeung, Air Pollution Specialist

Organic Laboratory Section
Northern Laboratory Branch
Monitoring and Laboratory Division
California Air resources Board

Reviewed and Approved by:

William V. Loscutoff, Chief, Monitoring and Laboratory Division

Michael Poore, Chief, Northern Laboratory Branch

Hieu M. Le, Manager, Organic Laboratory Section

This Page Left Intentionally Blank

Table of Contents

1. PURPOSE.....	1
2. BACKGROUND.....	1
3. METHOD MLD058.....	2
4. DATA.....	3
5. DATA ANALYSIS.....	4
Less than Published LOD Points.....	4
Rejected Points.....	4
6. DATA TREATMENT.....	6
7. OBSERVATIONS.....	6
Benzene.....	6
1,3-Butadiene.....	6
Carbon tetrachloride.....	6
<i>p</i> -Dichlorobenzene.....	7
Perchloroethylene.....	7
Dichloromethane.....	7
Chloroform.....	7
Trichloroethylene.....	7
1,1,1-Trichloroethane.....	8
Toluene.....	8

Table of Contents

Ethylbenzene	8
<i>m/p</i> -Xylene	8
<i>o</i> -Xylene	9
Styrene	9
<i>o</i> -Dichlorobenzene	9
8. CONCLUSIONS.....	10
No Conclusion Available	10
Ethylbenzene	10
<i>o</i> -Dichlorobenzene.....	10
Dichloromethane.....	10
<i>p</i> -Dichlorobenzene.....	10
No Data Correction	10
Carbon Tetrachloride.....	10
Benzene	11
Perchloroethylene.....	11
<i>o</i> -Xylene	12
1,1,1-Trichloroethane.....	13
Trichloroethylene.....	14
Possible Data Correction.....	14
<i>m/p</i> -Xylene	14

Table of Contents

Toluene	15
Chloroform	16
1,3-Butadiene.....	17
Styrene	18
9. COMMENTS	19

This Page Left Intentionally Blank

List of Tables

Table 1: SOPs for the Analysis of 1,3-Butadiene	21
Table 2: SOPs for the Analysis of Benzene.....	22
Table 3: SOPs for the Analysis of Volatile Halogenated and/or Aromatic Hydrocarbons .	23
Table 4: NIST ALM046027 Compound Concentrations	25
Table 5: Published Limit of Detection (LOD).....	26
Table 6: Rejected Points	27
Table 7: Corrected GC/MS Concentrations (Part 1).....	29
Table 8: Corrected GC/MS Concentrations (Part 2).....	31
Table 9: Corrected GC/MS Concentrations (Part 3).....	33

List of Figures

Figure 1: NIST Standard ALM046027	35
Figure 2: Mass Spectrum of Benzene from ALM046027 at 18.661 Minutes.....	36
Figure 3: Benzene - GC (PID) vs. Full Scan GC/MS	37
Figure 4: 1,3-Butadiene - GC (PID) vs. Full Scan GC/MS.....	38
Figure 5: Carbon Tetrachloride - GC (PID) vs. Full Scan GC/MS.....	39
Figure 6: <i>p</i> -Dichlorobenzene - GC (ECD) vs. Full Scan GC/MS	40
Figure 7: Perchloroethylene - GC (ECD) vs. Full Scan GC/MS	41
Figure 8: Dichloromethane - GC (ECD) vs. Full Scan GC/MS	42
Figure 9: Chloroform - GC (ECD) vs. Full Scan GC/MS	43
Figure 10: Chloroform with 2 nd Distribution - GC (ECD) vs. Full Scan GC/MS.....	44
Figure 11: Trichloroethylene - GC (PID) vs. Full Scan GC/MS	45
Figure 12: Trichloroethylene - LOW RANGE - GC (PID) vs. Full Scan GC/MS	46
Figure 13: 1,1,1-Trichloroethane - GC (ECD) vs. Full Scan GC/MS	47
Figure 14: 1,1,1-Trichloroethane - LOW RANGE - GC (ECD) vs. Full Scan GC/MS.....	48
Figure 15: Toluene - GC (PID) vs. Full Scan GC/MS	49
Figure 16: <i>m/p</i> -Xylene - GC (PID) vs. Full Scan GC/MS.....	50
Figure 17: <i>o</i> -Xylene - GC (PID) vs. Full Scan GC/MS	51
Figure 18: Styrene - GC (PID) vs. Full Scan GC/MS.....	52
Figure 19: Styrene - LOW RANGE - GC (PID) vs. Full Scan GC/MS	53
Figure 20: Benzene - RPD - GC (PID) vs. Full Scan GC/MS.....	54
Figure 21: 1,3-Butadiene - RPD - GC (PID) vs. Full Scan GC/MS.....	55
Figure 22: Carbon Tetrachloride - RPD - GC (ECD) vs. Full Scan GC/MS	56
Figure 23: Perchloroethylene - RPD - GC (ECD) vs. Full Scan GC/MS	57
Figure 24: Chloroform - RPD - GC (ECD) vs. Full Scan GC/MS	58

List of Figures

Figure 25: Trichloroethylene - RPD - GC (ECD) vs. Full Scan GC/MS.....	59
Figure 26: Trichloroethane - RPD - GC (ECD) vs. Full Scan GC/MS.....	60
Figure 27: Toluene - RPD - GC (PID) vs. Full Scan GC/MS.....	61
Figure 28: <i>m/p</i> -Xylene - RPD - GC (PID) vs. Full Scan GC/MS	62
Figure 29: <i>o</i> -Xylene - RPD - GC (PID) vs. Full Scan GC/MS	63
Figure 30: Styrene - RPD - GC (PID) vs. Full Scan GC/MS	64

This Page Left Intentionally Blank

1. PURPOSE

The Organic Laboratory Section has implemented a change in the procedure used for the analysis of aromatic and halogenated Toxic Air Contaminants (TACs) in ambient air. The new procedure, MLD058, titled "Standard Operating Procedure for the Analysis of Aromatic and Halogenated Hydrocarbons in Ambient Air Using Summa Canister Sampling and Gas Chromatographic/Mass Spectrometric Analysis", was implemented for Southern TAC monitoring sites on February 1, 2001, and for all TAC monitoring sites on May 1, 2001.

The previous procedures were:

MLD057 - "Standard Operating Procedure for the Determination of 1,3-Butadiene and Benzene in Ambient Air by Capillary Column Gas Chromatography with Photoionization Detector", and;

MLD052 - "Standard Operating Procedure for the Determination of Volatile Aromatic and Halogenated Compounds in Ambient Air by Gas Chromatography Using Capillary Column with Photoionization and Electron Capture Detectors."

The purpose of this parallel study is to compare results obtained from the analysis of ambient air samples by the two gas chromatography detector oriented methods, MLD057 and MLD052, and the new GC Mass Spectral Detector oriented method, MLD058. If warranted, procedures for temporarily offsetting any discontinuity in the historical data set caused by changing analytical Methods will be discussed.

2. BACKGROUND

Lists of the various SOPs used since 1985 for the analysis of 1,3-butadiene, benzene, and other halogenated and aromatic hydrocarbons are given in Tables [Table 1](#), [Table 2](#), and [Table 3](#). Although many methods have been developed, the procedures for these compounds have remained relatively constant since 1994. Method MLD051, for the analysis of 1,3-butadiene, and Method MLD052, for the analysis of volatile halogenated and aromatic compounds, were both implemented on March 1, 1994. Method MLD051 was amended to include benzene as a target analyte on January 1, 1997. Method MLD057 replaced MLD051 on January 1, 1999, where single-point calibration was replaced by a multipoint, non-linear calibration curve.

All three methods utilize an automated sampling system, including a single stage cryogenic concentrator, for transferring samples to the gas chromatograph (GC). The analytical column is a 75-meter by 0.44-mm internal diameter (i.d.) DB-VRX fused silica capillary, with a 2.55 μm film thickness. A Photoionization Detector (PID) is used for detection and quantitation of aromatic compounds, and an Electron Capture Detector (ECD) is used for halogenated compounds.

The major physical difference between the methods is the volume of sample concentrated. A sample volume of 400 cm³ is used in MLD051, compared to 150 cm³ in MLD052. The larger volume is required for the analysis of 1,3-butadiene, because the PID is less sensitive to it than to aromatic compounds. Benzene was added to the MLD051 to achieve a lower detection limit, because the larger sample volume was not feasible for MLD052. While the PID has a relatively long calibration range, the ECD is an extremely sensitive detector with a short calibration range.

MLD057 utilizes the same physical settings as MLD051, but differs in the calibration method. A multipoint, non-linear calibration is used in place of a single-point response factor.

3. METHOD MLD058

The new method also uses an automated sampling system similar to the previous methods. A two stage, rather than single stage, cryogenic concentration is performed. A 150 ml aliquot of the sample is first cryogenically trapped on an 1/8 inch packed cryotrap, followed by a second trap cycle onto a smaller, 1/16 inch cryofocuser. The concentrated sample is injected onto the GC column from the cryofocuser. This two-stage system is necessary because the GC column is a 60-meter by 0.25-mm id DB-VRX fused silica capillary, with a 1.40 µm film thickness. Although the separatory phase is the same, the smaller column i.d. uses lower flow rate and yields narrower chromatographic peaks. Both of these conditions are better suited for the GC/MS System.

The biggest difference is the change in detectors. Previous methods used GC detectors that exhibit either specificity/selectivity or higher proportional response to certain compound classes. The PID shows specificity/selectivity to species having ionization potentials at or below 10.2 eV. Aromatics, such as benzene and toluene, have much higher proportional responses to the PID. Compounds with double bonds, like 1,3-butadiene, have less response than aromatics, but the response is clearly more specific/selective than it is for butane or trichloroethane. The ECD is extremely sensitive and selective to electron capturing compounds, such as carbon tetrachloride and trichloroethane. Both detectors respond to compounds like trichloroethylene and perchloroethylene, but the ECD shows a much greater proportional response.

With these detectors, the combination of the specific/selective response and the chromatographic retention time is used to qualitatively identify the compound. The magnitude of the response is used for quantitation.

The Mass Spectral, or Mass Selective, Detector (MSD) used in method MLD058 is a more universal detector. After eluting from the GC column, molecules entering the detector are bombarded by a stream of 70 eV electrons. The resulting collisions ionize and fragment the parent molecules, which are filtered/sorted by mass to

charge ration (mz) to produce a response. Any compound that passes from the GC column into the MSD and can be ionized and fragmented by the electron beam is detected.

As an illustration of the chromatography and the specificity/selectivity and proportional response of the various detectors, [Figure 1](#) shows chromatograms from the ECD, PID, and a Total Ion Chromatogram (TIC) from the analysis of NIST Standard ALM046027. The response scales for all plots are normalized to the highest peak in each chromatogram/TIC. The time axis for the GC runs cover approximately 30 minutes, while the TIC covers only 22 minutes. The concentrations of compounds in ALM046027 are given in [Table 4](#).

The elution order, which is primarily a property of the chromatographic phase, is the same, since the phase is the same, for all plots. The total time to elute all compounds of interest is shorter for the GC/MS. This is consistent with the smaller internal diameter column used the GC/MS. The added benefit is sharper, narrower peaks with correspondingly larger peak heights.

The higher proportional response of the ECD to halogenated compounds is shown by the higher peaks for trichloroethane, carbon tetrachloride, and perchloroethylene when compared to the PID and MSD. Their concentrations are 0.91, 0.08, and 0.34 ppbv (**parts per billion by volume**) respectively. The specificity/selectivity of the detectors is shown by variable response to carbon tetrachloride. It has a very high response the ECD, none to the PID, and a smaller response to the MSD. For m/p-xylene, the ECD does not respond, while both the PID and MSD respond well.

In addition to producing a total response at a particular chromatographic retention time, the detector also produces a mass spectrum at fixed intervals during the run. The spectrum represents the relative response of each fragment ion produced by the detector to it's mass, and is compared to the total response. This mass "fingerprint" is specific by compound, and is used, with the chromatographic retention time, to qualitatively identify the compound. The response of one mass fragment, chosen to be as specific to the parent compound as possible, is used for quantitation. [Figure 2](#) shows both a typical mass spectrum and an Extracted Ion Chromatogram (EIC) for benzene. The mass 78 ion is the primary quantitation ion for benzene.

4. DATA

The results of analysis performed on 56 ambient air samples, which were sampled at Toxic Air Contaminant monitoring sites between July 23, 2000 and October 15, 2000, were used in this study. The samples were analyzed by methods MLD052, MLD057, and MLD058 for the 15 compounds shown in [Table 4](#). Each method was performed as dictated by its corresponding SOP. All applicable QC procedures were followed.

The results for the GC procedures were obtained from the Laboratory Information Management System (LIMS), since this was the data for record for these samples. The GC/MS data was obtained directly from the GC/MS reports.

5. DATA ANALYSIS

After it was compiled, the data was checked for completeness. The maximum number of data pairs available from the analysis of 56 ambient air samples for 15 compounds by both GC and GC/MS was 840. This represents a maximum of 1680 individual data points.

Less than Published LOD Points

No data points where one or both of the GC or GC/MS results were less than the Published Limit of Detection (LOD) were used in this study. The Published LODs are shown in [Table 5](#).

There were 306 data pairs, or 612 data points, where both the GC and GC/MS values were less than the Published LOD. There were 42 data pairs, or 86 data points, where one of the values was less than the Published LOD. Of these 42 data pairs, there were four (4) data pairs, or eight (8) data points, where the GC value was greater than the Published LOD but the GC/MS value was not. All four of these points were results from o-dichlorobenzene analyses.

There were 38 data pairs, or 76 data points, where the GC/MS value was greater than the Published LOD but the GC value was not. For five (5) of these data pairs, or 10 data points, the GC value for styrene was Not Available (NA), although the GC/MS value exceeded the Published LOD.

A total of 348 data pairs, or 696 data points, were found to have values less than the Published LOD. Since the Published LOD is the lower limit for all reported data, none of these data pairs/data points was used in this study. After this evaluation, 41.4% of the potentially available data was removed. The remaining 492 data pairs, or 58.6%, passed into the next stage of evaluation. A list of these data points is not included.

Rejected Points

After removing the data points described in [Less than Published LOD Points](#) above, the Percent Difference and the Relative Percent Difference was calculated for each remaining data pair, by compound. For this study, Percent Difference, or PD, is defined as:

$$PD = \frac{(GC/MS \text{ Concentration} - GC \text{ Concentration})}{GC/MS \text{ Concentration}} \times 100 \quad (1)$$

The Relative Percent Difference, or RPD, is defined as:

$$\text{RPD} = \frac{(\text{GC / MS Concentration} - \text{GC Concentration})}{\frac{(\text{GC / MS Concentration} + \text{GC Concentration})}{2}} \times 100 \quad (2)$$

The Mean and Standard Deviation of both the PD and RPD results were calculated for each compound data set. Data pairs with either a PD or a RPD Z-Score greater than 4.0 were eliminated, and the Mean and Standard Deviation recalculated. For this study, the Z-Score, is defined as:

$$\text{Z - score} = \frac{|(X_{\text{PD}} - \text{Mean}_{\text{PD}})|}{\text{SD}_{\text{PD}}} \quad \text{or} \quad \frac{|(X_{\text{RPD}} - \text{Mean}_{\text{RPD}})|}{\text{SD}_{\text{RPD}}} \quad (3)$$

where

SD = Standard Deviation

The Z-score is essentially the number of Standard Deviation units a value lies from the Mean. This process was repeated until there were no remaining data pairs with a PD or RPD Z-score greater than 4.0. Seven (7) data pairs were rejected and then eliminated by this procedure.

Two styrene data pairs were rejected and eliminated with Z-scores between 2.2 and 3.1. This case is discussed further in [Styrene](#), on page 9, below.

The chloroform data presented an unusual situation. Initially, only two data pairs had PD or RPD Z-scores greater than two. Using the iterative process, 12 additional data pairs were tested for removal. Their Z-scores also hovered around two. Removing these data pairs significantly helped the distribution of the remaining data pairs. These 14 data pairs were eliminated from the primary chloroform distribution, but were appeared to be part of a second distribution. This is discussed further in [Chloroform](#), on page 7, below.

This portion of the evaluation resulted in an additional 23 data pairs, or 46 data points, being rejected for specific reasons. Fourteen data pairs, or 28 data points, from chloroform were rejected from the primary distribution but were held and evaluated as a possible second chloroform distribution. The points rejected, and the reason for their rejection, are given in [Table 6](#).

6. DATA TREATMENT

A total of 371 data pairs, or 742 data points, were removed from the data set following Data Analysis. This left 469 data pairs, or 938 data points, for evaluation. This represents 55.8% of the original data.

The data obtained from the GC analyses were plotted against the data obtained from the GC/MS analyses for each of the 15 compounds. These plots are shown in [Figure 3](#) through [Figure 19](#). Each plot shows the 1st Order Regression line, its associated equation, and coefficient of determination (R^2), and the Published LOD for the compound. In addition, a straight line between the origin and the intersection of the highest concentration values is provided to illustrate a 1:1 relationship.

The Percent Difference (PD) between the GC/MS results and the GC results with respect to the GC/MS results was plotted against the GC/MS results for each of the 15 compounds. These plots are shown in through [Figure 30](#). Each plot shows the zero percentage line, the $\pm 15\%$ from zero lines, and the mean PD.

7. OBSERVATIONS

Benzene

The benzene data exhibits excellent correlation between the GC and GC/MS results, as shown in [Figure 3](#). The intercept is near zero, the slope close to one and the 1st Order Regression line is very close to the ideal 1:1 line. As shown in [Figure 20](#), the mean RPD is -2.1%, with 87.2% of the values within $\pm 15\%$ of the mean. The only points outside that range had values less than five (5) times the Published LOD. The cluster of benzene values around 0.03 to 0.40 ppb, plus the negative mean RPD show a slight bias to lower values for benzene by GC/MS.

1,3-Butadiene

The butadiene data shows good correlation between the GC and GC/MS results, as shown in [Figure 4](#). The 1st Order Regression line does not follow the ideal 1:1 line well. The mean RPD, shown in [Figure 21](#), is 20.4% with 61.7% of the values within $\pm 15\%$ of the mean. The wider distribution of points near the LOD, between 0.04 and 0.01 ppb (approximately 2,5 times the LOD) is reasonable, but the trend throughout the concentration range shows a bias towards higher values by GC/MS.

Carbon tetrachloride

As shown in [Figure 5](#), a correlation plot is not applicable to the carbon tetrachloride data. Since the ambient values are so tightly clustered, the RPD plot, [Figure 22](#), is much more informative. For carbon tetrachloride, 94.6% of the RPD values are within $\pm 15\%$ of the mean. The cluster of values between 0.90 and 1.0 ppb and the

positive mean RPD of 1.3% show an almost negligible bias towards higher GC/MS values.

p-Dichlorobenzene

As seen in [Figure 6](#), there are only four results available for p-dichlorobenzene.

Perchloroethylene

The perchloroethylene data exhibits excellent correlation between the GC and GC/MS results, as shown in [Figure 7](#). The intercept is near zero, the slope close to one and the 1st Order Regression line is very close to the ideal 1:1 line. As shown in [Figure 23](#), the mean RPD is 2.6%, with 98.0% of the values within $\pm 15\%$ of the mean. The positive mean RPD shows a slight bias towards higher GC/MS values.

Dichloromethane

[Figure 8](#) shows there are only five results for dichloromethane greater than the Published LOD.

Chloroform

The initial correlation plot for chloroform, shown in [Figure 9](#), demonstrates very poor correlation between the GC and GC/MS results. The outlier points on the plot could not be eliminated using the iterative procedure described in [Rejected Points](#). After further inspection, the outlier points were reevaluated as a second distribution. The plot of both distributions is shown in [Figure 10](#). Creating the second distribution improved the correlation among the remaining data, but there is NO determinate reason for the occurrence of the second distribution.

The primary distribution does show correlation between the GC and GC/MS results. The 1st Order Regression line does not follow the ideal 1:1 line well, and crosses it at 0.04 ppb. The mean RPD, shown in [Figure 24](#), is -0.6%, with 66.7% of the values within $\pm 15\%$ of the mean. The slightly negative mean RPD shows that the points are well distributed around the mean, with essentially no bias towards GC or GC/MS values. Values between the Published LOD and 0.04 ppb, two times the LOD, tend towards higher GC concentrations. Values from 0.04 ppb to 0.12 ppb, the highest value at six times the LOD, tend towards higher GC/MS concentrations.

Trichloroethylene

The trichloroethylene data shows excellent correlation between the GC and GC/MS results, as shown in [Figure 11](#) and [Figure 12](#). The intercept is near zero, the slope close to one and the 1st Order Regression line is very close to the ideal 1:1 line. [Figure 25](#) shows that the ambient values for trichloroethylene are clustered over a

narrow concentration range around the Published LOD. This is similar to the carbon tetrachloride distribution, with eight higher range points for consideration. The mean RPD is 5.1%, with 61.8% of the values less than $\pm 15\%$. Using a wider range of $\pm 25\%$, 88.2% of the values are less than $\pm 25\%$. With so many values near the Published LOD, the 1st Order Regression line moves towards higher GC/MS values at higher concentrations. The mean RPD also shows a slight bias towards higher GC/MS concentrations.

1,1,1-Trichloroethane

The 1,1,1-trichloroethane data shows excellent correlation between the GC and GC/MS results, as shown in [Figure 13](#) and [Figure 14](#). The intercept is near zero, the slope close to one and the 1st Order Regression line is very close to the ideal 1:1 line. [Figure 26](#) shows that the ambient values for 1,1,1-trichloroethane are clustered in the range between 0.045 and 0.08 ppb with one high value. This is similar to the trichloroethylene distribution with fewer higher values. Unlike the latter, the 1st Order Regression line lies closer to the ideal line at the high end. The mean RPD is 9.8%, with 100.0% of the values less than $\pm 15\%$. The mean RPD also shows a slight bias towards higher GC/MS concentrations

Toluene

Like benzene, the toluene data exhibits excellent correlation between the GC and GC/MS results, as shown in [Figure 15](#). The slope is close to one, but the intercept is further from zero. The 1st Order Regression line is parallel to the ideal 1:1 line, but is biased towards higher GC/MS concentrations throughout the range. As shown in [Figure 27](#), the mean RPD is 14.9%, with 96.3% of the values within $\pm 15\%$ of the mean. This shows a bias towards higher values for toluene by GC/MS. The bias is not distributed evenly across the concentration range. At lower concentrations, between 0.2 ppb, the Published LOD, and 1.0, five times the Published LOD, the mean bias appears higher than the overall mean bias. At higher concentrations, the mean bias appears less than the overall mean bias. Overall, the results for toluene show a bias towards higher GC/MS values.

Ethylbenzene

No ethylbenzene results exceeded the Published LOD.

m/p-Xylene

The data for *m/p*-xylene shows good correlation between the GC and GC/MS results, as shown in [Figure 16](#). The intercept is almost zero. The 1st Order Regression line increasingly diverges from the ideal 1:1 line as the concentration increases. [Figure 28](#) shows that the mean RPD is 8.7%, with 89.7% of the values within $\pm 15\%$ of the mean. This shows some bias towards higher GC/MS values.

o-Xylene

Like toluene, the *o*-xylene data exhibits excellent correlation between the GC and GC/MS results, as shown in [Figure 17](#). The slope is close to one and the intercept is closer from zero. The 1st Order Regression line is parallel to the ideal 1:1 line and is biased towards higher GC/MS concentrations throughout the range. As shown in [Figure 29](#), the mean RPD is 11.5%, with 52.5% of the values within $\pm 15\%$ of the mean. The scatter of the data is greater than for toluene, so the bias towards higher values is not as great as for toluene. As with toluene, although not a pronounced, the mean bias appears less than the overall mean bias at higher concentrations.

It should be noted, as discussed under styrene, below, that the GC method may have slightly overestimated the *o*-xylene concentration. The *o*-xylene bias may be reduced slightly because of this tendency. Overall, the results for *o*-xylene show a bias towards higher GC/MS values.

Styrene

The styrene data set has only 15 points above the Published LOD. Most of these values are in the range from 0.1 to 0.6 ppb. There is one point at a significantly higher concentration. The data shows good correlation between the GC and GC/MS results, as shown in [Figure 18](#) and [Figure 19](#). The 1st Order Regression line does not follow the ideal 1:1 line well, and crosses it at 0.23 ppb. This is very similar to the primary chloroform distribution discussed on page [7](#). The mean RPD, shown in [Figure 30](#), is 4.8%, with only 33.3% of the values within $\pm 15\%$ of the mean. The available data is actually scattered quite uniformly around 0% RPD.

It should be noted that the separation between styrene, which elutes first, and *o*-xylene has been difficult by GC method MLD052. With the ambient concentration of *o*-xylene predominantly greater than the styrene concentration, it is entirely possible that the GC method has tended to underestimate the styrene concentration and slightly overestimate the *o*-xylene concentration. The better chromatographic separation of the GC/MS system and the ability of the MS to better isolate the styrene/*o*-xylene response will probably yield higher styrene results.

Although the mean RPD shows a bias towards higher concentrations by GC/MS, this tendency may be overestimated because so few data points are available. In addition, this bias may effectively be less due to the GC methods difficulty with the styrene/*o*-xylene separation.

o-Dichlorobenzene

Only one *o*-dichlorobenzene result exceeded the Published LOD.

8. CONCLUSIONS

No Conclusion Available

Ethylbenzene
o-Dichlorobenzene
Dichloromethane
p-Dichlorobenzene

Of the 15 compounds evaluated in this comparison, ethylbenzene and o-dichlorobenzene had zero and one point respectively, and dichloromethane and p-dichlorobenzene had four and five points respectively. Two of the p-dichlorobenzene points lie between the old Published LOD of 0.2 ppb and the new Published LOD of 0.3 ppb. With so little available data, it is not possible to make any comparison between the GC and GC/MS methods for these compounds.

To acquire enough useable points for these compounds, the study period would have needed to be lengthened by approximately 9 months. Unfortunately, the Gas Chromatographic Systems used in Methods MLD052 and MLD057 were reaching the end of their useful life. They were experiencing increasingly frequent and more serious problems.

Also, between January 4, 1997 and April 19, 2001, an average of 13.5% of the ambient results for these four compounds exceeded the Published LOD. This is in contrast to the remaining 11 compounds, that had an average of 75.7% of the results exceeding the Published LOD for the same period.

The prospect of complete failure of the analytical equipment, plus the long lead time in acquiring and setting up the new GC/MS based equipment, coupled with the low incidence of greater than Published LOD values for these compounds, made the acquisition of additional data impossible.

No Data Correction

Carbon Tetrachloride

The GC and GC/MS carbon tetrachloride results compare extremely well. Although all data points are less than five (5) times the Published LOD, 94.6% of all data pairs lie within $\pm 15\%$ of the mean RPD. This actually exceeds the ambient duplicate analysis RPD criteria.

There should be no discontinuity in the historical data, so no data correction procedure is recommended.

Benzene

With the mean RPD for benzene showing a slight bias towards lower GC/MS than GC results, the linear correlation equation, as given on [Figure 3](#), was evaluated for use in data "correction". The ambient benzene values between January 4, 1997 and April 19, 2001 had a peak value of approximately 16 ppb, with 98% of the detected values ranging from the Published LOD of 0.2 ppb to 4.0 ppb. Applying the linear regression equation to potential GC/MS values ranging from the LOD to 16 ppb, yielded the "corrected" values shown in [Table 7](#).

The RPD between "corrected" and raw values ranges from +4.85% down to +0.74% for concentrations from the Published LOD to five (5) times the Published LOD, and less than $\pm 0.64\%$ at higher concentrations. This is well within the allowable $\pm 15\%$ RPD between ambient duplicate sample analyses.

There should be no discontinuity in the historical data, so no data correction procedure is recommended.

If a data user, however, feels that data correction should be applied, either of the following 1st Order Regression equations could be used to correct the concentration data. Equation (4) corrects observed GC/MS results to the lower GC results, and equation (5) corrects GC results to the higher GC/MS results.

$$\text{CONC}_{(\text{Corrected}=\text{GC})} = 0.996853 * \text{CONC}_{\text{GC/MS}} + 0.0105668 \quad (4)$$

Or

$$\text{CONC}_{(\text{Corrected}=\text{GC/MS})} = 0.982963 * \text{CONC}_{\text{GC}} + 0.0007253 \quad (5)$$

Perchloroethylene

The positive mean RPD for perchloroethylene shows a slight bias towards higher GC/MS than GC values. The linear correlation equation, as given on [Figure 7](#), was evaluated for use in data "correction". Ambient perchloroethylene values, between January 4, 1997 and April 19, 2001, had a peak value of approximately 2.2 ppb, with 98% of the detected values ranging from the Published LOD of 0.01 ppb to 0.6 ppb. Applying the linear regression equation to potential GC/MS values ranging from the LOD to 3.0 ppb, yields the "corrected" values shown in [Table 7](#).

The RPD between "corrected" and raw values ranges from -10.6% up to -2.3% for concentrations from the Published LOD to five (5) times the Published LOD, from -2.3% up to -1.0% for concentrations up to 1.4 ppb, and less than -1.0% at higher concentrations. This is well within the allowable $\pm 15\%$ RPD between ambient duplicate sample analyses.

There should be no discontinuity in the historical data, so no data correction procedure is recommended.

If a data user, however, feels that data correction should be applied, either of the following 1st Order Regression equations could be used to correct the concentration data. Equation (14) corrects observed GC/MS results to the lower GC results, and equation (15) corrects GC results to the higher GC/MS results.

$$\text{Or } \text{CONC}_{(\text{Corrected}=\text{GC})} = 0.996853 * \text{CONC}_{\text{GC/MS}} + 0.0105668 \quad (6)$$

$$\text{CONC}_{(\text{Corrected}=\text{GC/MS})} = 0.992623 * \text{CONC}_{\text{GC}} + 0.00170756 \quad (7)$$

o-Xylene

With the mean RPD for o-xylene showing a bias towards higher GC/MS than GC results, the linear correlation equation, as given on [Figure 17](#), was evaluated for use in data "correction". Ambient o-xylene values, between January 4, 1997 and April 19, 2001, had a peak value of approximately 13 ppb with 98% of the detected values ranged from the Published LOD of 0.1 ppb to 2.0 ppb. Applying the linear regression formula as given on , to potential GC/MS values ranging from the LOD to 3.0 ppb, yields the "corrected" values shown in [Table 7](#).

The RPD between "corrected" and raw values ranges from -24.9% up to -5.0% for concentrations from the Published LOD to five (5) times the Published LOD, from -4.2% up to -2.1% for concentrations up to 1.4 ppb, and less than -2.0% at higher concentrations. Aside from the value at the LOD, these percentages are well within the allowable ±15% RPD between ambient duplicate sample analyses. At values below five (5) times the Published LOD, the RPD is known to exceed the ±15% criteria.

There should be no discontinuity in the historical data, so no data correction procedure is recommended.

If a data user, however, feels that data correction should be applied, either of the following 1st Order Regression equations could be used to correct the concentration data. Equation 0 corrects observed GC/MS results to the lower GC results, and equation (9) corrects GC results to the higher GC/MS results.

$$\text{Or } \text{CONC}_{(\text{Corrected}=\text{GC})} = 0.994691 * \text{CONC}_{\text{GC/MS}} + (-0.0216193) \quad (8)$$

$$\text{CONC}_{(\text{Corrected}=\text{GC/MS})} = 0.958415 * \text{CONC}_{\text{GC}} + 0.0348355 \quad (9)$$

1,1,1-Trichloroethane

The positive mean RPD for 1,1,1-trichloroethane shows a bias towards higher GC/MS than GC values. The linear correlation equation, as given on [Figure 11](#), was evaluated for use in data "correction". Ambient 1,1,1-trichloroethane values, between January 4, 1997 and April 19, 2001, had a peak value of approximately 15 ppb with 96% of the detected values ranged from the Published LOD of 0.01 ppb to 1.0 ppb. Applying the linear regression formula as given on [Figure 13](#), to potential GC/MS values ranging from the LOD to 16 ppb, yields the "corrected" values shown in [Table 7](#).

The RPD between "corrected" and raw values ranges from -100% up to -13.5% for concentrations from the Published LOD to five (5) times the Published LOD, from -11.0% up to -1.4% for concentrations up to 0.3 ppb, and less than $\pm 1.0\%$ at higher concentrations. At concentrations greater than five (5) times the Published LOD, these percentages are well within the allowable $\pm 15\%$ RPD between ambient duplicate sample analyses. At values below five (5) times the Published LOD, the RPD is known to exceed the $\pm 15\%$ criteria. Even so, GC/MS values at 0.01 and 0.02 ppb seem much higher than expected.

Since there are no 1,1,1-trichloroethane values in the data set below 0.04 ppb, there is a high probability that the calculated linear correlation equation loses validity below 0.04 ppb. A check of reported values between January 4, 1997 and April 19, 2001 show only one sample with a concentration between the Published LOD and 0.02 ppb. There were five samples with concentrations between 0.02 and 0.03 ppb.

With so little existing data historical data, at least in the last $4\frac{1}{3}$ years, and the possibility that the potential correction equation loses validity below 0.04 ppb, it is recommended that no data correction procedure be performed.

If a data user, however, feels that data correction should be applied, either of the following 1st Order Regression equations could be used to correct the concentration data. Equation (10) corrects observed GC/MS results to the lower GC results, and equation (11) corrects GC results to the higher GC/MS results.

Or

$$\text{CONC}_{(\text{Corrected}=\text{GC})} = 1.008773 * \text{CONC}_{\text{GC/MS}} + (1.008773) \quad (10)$$

$$\text{CONC}_{(\text{Corrected}=\text{GC/MS})} = 0.990295 * \text{CONC}_{\text{GC}} + 0.00677546 \quad (11)$$

Trichloroethylene

With the mean RPD for trichloroethylene showing a slight bias towards higher GC/MS than GC results, the linear correlation equation, as given on [Figure 11](#), was evaluated for use in data "correction". The ambient trichloroethylene values between January 4, 1997 and April 19, 2001 had a peak value of approximately 8.6 ppb, with 98% of the detected values ranged from the Published LOD of 0.02 ppb to 0.9 ppb. Applying the linear regression equation to potential GC/MS values ranging from the LOD to 9 ppb, yielded the "corrected" values shown in [Table 8](#).

The RPD between "corrected" and raw values ranges from -17.7% up to -5.6% for concentrations from the Published LOD to five (5) times the Published LOD, and up to -2.8% at higher concentrations. Aside from the value at the LOD, these percentages are well within the allowable $\pm 15\%$ RPD between ambient duplicate sample analyses. At values below five (5) times the Published LOD, and especially at the LOD value, the RPD is known to exceed the $\pm 15\%$ criteria.

Examination of the trichloroethylene "Change ppb" column (Δ ppb) in [Table 8](#) shows that the actual ppb change between 0.10 and 0.40 ppb is approximately -0.01 ppb. From 0.5 to 0.9 ppb, it is approximately -0.03 ppb, from 1.0 to 5.0 ppb it is approximately -0.1 ppb, and from 6.0 to 9.0 ppb it is approximately -0.2 ppb. Twenty-one percent of the detected values lie within this range. For concentration values from the Published LOD of 0.020 ppb to just under five (5) times the LOD, at 0.095 ppb, the Δ ppb ranges from -0.003 to -0.005 ppb.

Changes this small should not cause a discontinuity in the historical data, so no data correction procedure is recommended.

If a data user, however, feels that data correction should be applied, either of the following 1st Order Regression equations could be used to correct the concentration data. Equation (12) corrects observed GC/MS results to the lower GC results, and equation (13) corrects GC results to the higher GC/MS results.

$$\text{Or } \text{CONC}_{(\text{Corrected}=\text{GC})} = 0.972375 * \text{CONC}_{\text{GC/MS}} + (-0.00269440) \quad (12)$$

$$\text{CONC}_{(\text{Corrected}=\text{GC/MS})} = 1.021626 * \text{CONC}_{\text{GC}} + 0.00338751 \quad (13)$$

Possible Data Correction

m/p-Xylene

Since m- and p-xylene cannot be separated by either Method 52 or Method 58, and the Mass Spectrums of the two compounds are nearly indistinguishable, the

two independent compounds are measured as one. The mean RPD for the *m/p*-xylene pair shows some bias towards higher GC/MS than GC results. The linear correlation equation given on [Figure 16](#) was evaluated for use in data "correction". The ambient values between January 4, 1997 and April 19, 2001 had a peak value of approximately 53 ppb. The next lowest value was 26 ppb. Of all detected points, 98% of the values ranged from the Published LOD of 0.6 ppb to 9.0 ppb. Applying the linear regression equation to potential GC/MS values ranging from the LOD to 60 ppb, yielded the "corrected" values shown in [Table 8](#).

The RPD between the "corrected" and raw values is a constant -8.9%. The cause can be seen on [Figure 16](#) where the linear correlation line diverges from the ideal 1:1 line in a constant manner towards higher GC/MS results. This yields a constant percentage instead of the more common constant, or nearly constant, amount. The constant percentage change yields concentrations that are still within the allowable $\pm 15\%$ RPD between ambient duplicate sample analyses. At values below five (5) times the Published LOD, and especially at the LOD value, the RPD is known to exceed the $\pm 15\%$ criteria.

Only 52% of the ambient samples analyzed in this study had useable *m/p*-xylene values for this evaluation. Since the observed bias is within the allowable duplicate analytical range, no data correction is recommended. However, if a data user feels the differences are consistent enough and show a large enough discontinuity in the historical data to justify correction, either of the following 1st Order Regression equations could be used to correct the concentration data. Equation (14) corrects observed GC/MS results to the lower GC results, and equation (15) corrects GC results to the higher GC/MS results.

$$\text{CONC}_{(\text{Corrected}=\text{GC})} = 0.915157 * \text{CONC}_{\text{GC/MS}} + (-0.000328637) \quad (14)$$

Or

$$\text{CONC}_{(\text{Corrected}=\text{GC/MS})} = 1.072825 * \text{CONC}_{\text{GC}} + 0.0257000 \quad (15)$$

Toluene

The mean RPD for toluene shows a bias towards higher GC/MS than GC results, especially at lower concentrations. The linear correlation equation given on [Figure 15](#) was evaluated for use in data "correction". The ambient values between January 4, 1997 and April 19, 2001 had a peak value of approximately 39 ppb with 98% of the detected values ranging from the Published LOD of 0.2 ppb to 9.0 ppb. Applying the linear regression equation to potential GC/MS values ranging from the LOD to 40 ppb, yielded the "corrected" values shown in [Table 8](#).

The RPD between "corrected" and raw values ranges is similar to trichloroethylene, although of a larger magnitude. It ranges from -96.8% up to -16.1% for con-

concentrations from the Published LOD to five (5) times the Published LOD, -9.0% up to -5.0% from 2.0 to 5.0 ppb, and -5.0% up to -2.7 % from 5.0 to 40 ppb. At concentrations above five (5) times the LOD, the percentages are within the allowable $\pm 15\%$ RPD between ambient duplicate sample analyses. Although the RPD is known to exceed the $\pm 15\%$ criteria at values below five (5) times the Published LOD, toluene values exceed the criteria by 1.5 to 6.4 times from .70 ppb down to 0.2 ppb.

Ninety-six point four percent (96.4%) of the ambient samples analyzed in this study had useable toluene values for evaluation. Since the observed bias is within the allowable duplicate analytical range above five (5) times the Published LOD, no data correction is recommended in this range. The data does show bias at concentrations below the five (5) times the Published LOD. However, if a data user feels the differences are consistent enough and show a large enough discontinuity in the historical data to justify correction, either of the following 1st Order Regression equations could be used to correct the concentration data. Equation (16) corrects observed GC/MS results to the lower GC results, and equation (17) corrects GC results to the higher GC/MS results.

$$\text{CONC}_{(\text{Corrected}=\text{GC})} = 0.976670 * \text{CONC}_{\text{GC/MS}} + (-0.125762) \quad (16)$$

Or

$$\text{CONC}_{(\text{Corrected}=\text{GC/MS})} = 1.020497 * \text{CONC}_{\text{GC}} + 0.133819 \quad (17)$$

Chloroform

The chloroform data is unusual, since two distributions were found (See [Chloroform](#), on page 7). The RPD showed negligible bias towards either GC or GC/MS values. The data has a high degree of scatter and a relatively poor coefficient of determination (R^2). Although the fit is not good, the linear correlation equation, for the primary distribution, as given on [Figure 9](#), was evaluated for use in data "correction". Ambient chloroform values, between January 4, 1997 and April 19, 2001, had a peak value of approximately 0.44 ppb, with 98% of the detected values ranged from the Published LOD of 0.02 ppb to 0.19 ppb. Applying the linear regression equation to potential GC/MS values ranging from the LOD to 0.44 ppb, yields the "corrected" values shown in [Table 8](#).

The linear correlation line crosses the ideal 1:1 line at 0.039 ppb and diverges towards higher GC/MS results. Between the Published LOD and five (5) times the Published LOD, the RPD ranges from +15.9% down to 0.0%, and then down to -12.1%. These percentages are within the allowable $\pm 15\%$ RPD between ambient duplicate sample analyses. The corresponding Δ ppb values are 0.003 ppb, 0 ppb, and -0.01 ppb. Ninety-four percent (94%) of the ambient chloroform val-

ues lie in this region. Since the observed bias is within the allowable duplicate analytical range in this region, no data correction is recommended in this range.

At concentrations exceeding 0.12 ppb, the RPD ranges from -13.5% down to -18.4%. Approximately 6% of ambient chloroform values lie above 0.10 ppb. The data does show bias towards higher GC/MS at concentrations above 0.12 ppb.

The linear correlation equation does not demonstrate a good fit to the data. Because of this, it is recommended that no data correction procedure be performed. If, however, a data user feels the differences are consistent enough and show a large enough discontinuity in the historical data to justify correction, either of the following 1st Order Regression equations could be used to correct the concentration data. Equation (18) corrects observed GC/MS results to the higher or lower GC results, and equation (19) corrects GC results to the lower or higher GC/MS results.

$$\text{CONC}_{(\text{Corrected}=\text{GC})} = 0.814279 * \text{CONC}_{\text{GC/MS}} + 0.00716047 \quad (18)$$

Or

$$\text{CONC}_{(\text{Corrected}=\text{GC/MS})} = 1.103212 * \text{CONC}_{\text{GC}} + (-0.0036475) \quad (19)$$

1,3-Butadiene

The positive mean RPD for 1,3-butadiene shows a bias towards higher GC/MS than GC values. The linear correlation equation, as given on [Figure 4](#), was evaluated for use in data "correction". Ambient values, between January 4, 1997 and April 19, 2001, had a peak value of approximately 6.0 ppb, with 98% of the detected values ranged from the Published LOD of 0.04 ppb to 1.0 ppb. Applying the linear regression equation to potential GC/MS values ranging from the LOD to 6.0 ppb, yields the "corrected" values shown in [Table 9](#).

The RPD between "corrected" and raw values ranges is similar in some respects to *m/p*-xylene, although the RPD is not as constant. The linear correlation line diverges from the ideal 1:1 line towards higher GC/MS results. It ranges from -26.8% up to -17.6% for concentrations from the Published LOD to five (5) times the Published LOD and -17.5% up to -15.5 % from 0.2 to 6 ppb. The RPD exceeds the allowable $\pm 15\%$ RPD between ambient duplicate sample analyses throughout the range of concentrations.

Eighty-nine point three percent (89.3%) of the ambient samples analyzed in this study had useable 1,3-butadiene values for evaluation. Since the data does show a bias towards higher GC/MS than GC values throughout the entire concentration range, a large enough discontinuity in the historical data set may result which could justify data correction. If a data user feels data correction is justified, either

of the following 1st Order Regression equations could be used to correct the concentration data. Equation (20) corrects observed GC/MS results to the lower GC results, and equation (21) corrects GC results to the higher GC/MS results.

$$\text{CONC}_{(\text{Corrected}=\text{GC})} = 0.856982 * \text{CONC}_{\text{GC/MS}} + (-0.00374499) \quad (20)$$

Or

$$\text{CONC}_{(\text{Corrected}=\text{GC/MS})} = 1.106391 * \text{CONC}_{\text{GC}} + 0.0118791 \quad (21)$$

Styrene

The mean RPD for styrene shows a small bias towards higher GC/MS than GC values. The linear correlation equation, as given on [Figure 18](#), was evaluated for use in data "correction". Ambient styrene values, between January 4, 1997 and April 19, 2001, had a peak value of approximately 2.7 ppb, with 98% of the detected values ranged from the Published LOD of 0.10 ppb to 1.6 ppb. Applying the linear regression equation to potential GC/MS values ranging from the LOD to 2.6 ppb, yields the "corrected" values shown in [Table 9](#).

The RPD between "corrected" and raw values ranges is similar in some respects to 1,3-butadiene, although of a larger magnitude. Because the linear correlation line crosses the ideal 1:1 line at 0.23 ppb and diverges towards higher GC/MS results, the RPD goes from 27.9% down to 0% between the Published LOD and 0.23 ppb. It then goes down to -14.1% at 0.5 ppb, five (5) times the Published LOD, and continues down to -25.1% at 2.6 ppb. Aside from the value at the LOD, the RPD for concentrations below five (5) times the Published LOD are within the allowable $\pm 15\%$ RPD between ambient duplicate sample analyses. For results at higher concentrations, the data does show bias towards higher GC/MS concentrations.

Only 26.8% of the ambient samples analyzed in this study had useable styrene values for evaluation. With so little data, there is a reasonable probability that the calculated linear correlation equation loses validity, especially at higher concentrations. Since the data does show, however, a bias towards higher GC/MS than GC values throughout the entire concentration range, a large enough discontinuity in the historical data set may result which could justify data correction. If a data user feels data correction is justified, either of the following 1st Order Regression equations could be used to correct the concentration data. Equation (22) corrects observed GC/MS results to the higher or lower GC results, and equation (23) corrects GC results to the lower or higher GC/MS results.

$$\text{CONC}_{(\text{Corrected}=\text{GC})} = 0.754806 * \text{CONC}_{\text{GC/MS}} + 0.0568869 \quad (22)$$

Or

$$\text{CONC}_{(\text{Corrected}=\text{GC/MS})} = 1.303298 * \text{CONC}_{\text{GC}} + (-0.0670467) \quad (23)$$

9. COMMENTS

Only one of the 15 compounds in this study is a candidate for possible data correction because of potential discontinuities in the historical database. If data correction is performed, the following caveats should be noted.

- The linear equations provided for possible data correction truly apply only to the data actually included in the study.
- The application of data correction is a **short term** procedure for comparing historical data compiled from methods MLD052 and MLD057 with new data derived from method MLD058.
- In the long term, the data should be flagged when methodology is changed and evaluated **without correction**.

This Page Left Intentionally Blank

Table 1: SOPs for the Analysis of 1,3-Butadiene

SOP #	Name	Effective Date	Basic Description
MLD013	Standard Operating Procedure for the Determination of 1,3-Butadiene in Ambient Air," Revision 3.0	1/1/1990	- Carbopack C trapping - thermal desorption - packed GC column - PID/FID
MLD042	Standard Operating Procedure for the Determination of Volatile Organic Compounds in Ambient Air Using Cryogenic Preconcentration Techniques and Gas Chromatography with Photoionization and Electron Capture Detectors, Revision 1.0	1/1/1993	- cryogenic trapping/concentration - thermal desorption - large bore capillary GC column - PID/ECD
MLD051	Standard Operating Procedure for the Determination of 1,3-Butadiene and Benzene in Ambient Air by Capillary Column Gas Chromatography with Photoionization Detector", Revision 1.0	3/1/1994	- Cryogenic trapping/concentration - thermal desorption - large bore capillary GC column - PID
MLD057	Standard Operating Procedure for the Determination of 1,3-Butadiene and Benzene in Ambient Air by Capillary Column Gas Chromatography with Photoionization Detector", Revision 1.0	1/1/1999	- cryogenic trapping/concentration - thermal desorption - large bore capillary GC column - PID

Table 2: SOPs for the Analysis of Benzene

SOP #	Name	Effective Date	Basic Description
ADDL001	Standard Operating Procedure for the Determination of Volatile Organics in Ambient Air Using Tenax Trap Preconcentration Gas Chromatography with Mass Spectrometer Detector, Preliminary Draft 3	8/11/1986	- Tenax trapping - thermal desorption - capillary GC column - MSD
ADDL004	Method for Determination of Benzene, Xylenes, Toluene and Ethyl Benzene in Ambient Air Using Tenax Preconcentration and Gas Chromatography/Photoionization Detection, Preliminary Draft 4	8/27/1985	- Tenax trapping - thermal desorption - packed GC column - PID
ADDL008	Determination of Aromatic Hydrocarbons Using Charcoal Adsorbent and Capillary Gas Chromatography, Preliminary Draft 1	10/12/1985	- charcoal adsorbent tube - carbon disulfide extraction - capillary GC column - FID
MLD002	Standard Operating Procedure for the Determination of Volatile Organic Compounds in Ambient Air Using Tenax Trap Preconcentration Gas Chromatography and Tandem Photoionization/Electron Capture Detectors, Revision 4.0	3/1/1990	- Tenax trapping - thermal desorption - packed GC column - PID/ECD
MLD012	Standard Operating Procedure for the Determination of Volatile Organic Compounds in Ambient Air Using Tenax Preconcentration Capillary Gas Chromatography with Photoionization Detector, Revision 2.0	7/1/1991	- Tenax trapping - thermal desorption - capillary GC column - PID
MLD042	Standard Operating Procedure for the Determination of Volatile Organic Compounds in Ambient Air Using Cryogenic Preconcentration Techniques and Gas Chromatography with Photoionization and Electron Capture Detectors, Revision 1.0	1/1/1993	- cryogenic trapping/concentration - thermal desorption - large bore capillary GC column - PID/ECD
MLD051	Standard Operating Procedure for the Determination of 1,3-Butadiene and Benzene in Ambient Air by Capillary Column Gas Chromatography with Photoionization Detector", Revision 1.0	3/1/1994	- Cryogenic trapping/concentration - thermal desorption - large bore capillary GC column - PID
MLD057	Standard Operating Procedure for the Determination of 1,3-Butadiene and Benzene in Ambient Air by Capillary Column Gas Chromatography with Photoionization Detector", Revision 1.0	1/1/1999	- cryogenic trapping/-concentration - thermal desorption - large bore capillary GC column - PID

Table 3: SOPs for the Analysis of Volatile Halogenated and/or Aromatic Hydrocarbons

SOP #	Name	Effective Date	Basic Description
ADDL001	Standard Operating Procedure for the Determination of Volatile Organics in Ambient Air Using Tenax Trap Preconcentration Gas Chromatography with Mass Spectrometer Detector, Preliminary Draft 3	8/11/1986	- Tenax trapping - thermal desorption - capillary GC column - MSD
ADDL004	Method for Determination of Benzene, Xylenes, Toluene and Ethyl Benzene in Ambient Air Using Tenax Preconcentration and Gas Chromatography/Photoionization Detection, Preliminary Draft 4	8/27/1985	- Tenax trapping - thermal desorption - packed GC column - PID
ADDL008	Determination of Aromatic Hydrocarbons Using Charcoal Adsorbent and Capillary Gas Chromatography, Preliminary Draft 1	10/12/1985	- charcoal adsorbent tube - carbon disulfide extraction - capillary GC column - FID
MLD002	Standard Operating Procedure for the Determination of Volatile Organic Compounds in Ambient Air Using Tenax Trap Preconcentration Gas Chromatography and Tandem Photoionization/Electron Capture Detectors, Revision 4.0	3/1/1990	- Tenax trapping - thermal desorption - packed GC column - PID/ECD
MLD012	Standard Operating Procedure for the Determination of Volatile Organic Compounds in Ambient Air Using Tenax Preconcentration Capillary Gas Chromatography with Photoionization Detector, Revision 2.0	7/1/1991	- Tenax trapping - thermal desorption - capillary GC column - PID
MLD042	Standard Operating Procedure for the Determination of Volatile Organic Compounds in Ambient Air Using Cryogenic Preconcentration Techniques and Gas Chromatography with Photoionization and Electron Capture Detectors, Revision 1.0	1/1/1993	- cryogenic trapping/concentration - thermal desorption - large bore capillary GC column - PID/ECD
MLD052	Standard Operating Procedure for the Determination of Volatile Aromatic and Halogenated Compounds Ambient Air by Capillary Column Gas Chromatography with Photoionization and Electron Capture Detectors", Revision 1.0	10/1/1994	- Cryogenic trapping/-concentration - thermal desorption - large bore capillary GC column - PID

This Page Left Intentionally Blank

Table 4: NIST ALM046027 Compound Concentrations

Compound Name	Abbreviation	ALM046027 ppbv
Method MLD057-PID and Method MLD058		
1,3-Butadiene	Buta	0.84
Benzene	Benz	2.02
Method MLD052-ECD and Method MLD058		
Dichloromethane	DCM	2.80
Chloroform	CHCl ₃	0.24
1,1,1-Trichloroethane	TCEA	0.91
Carbon tetrachloride	CCl ₄	0.08
Trichloroethylene	TCE	0.56
Perchloroethylene	PERC	0.34
Method MLD052-PID and Method MLD058		
Toluene	Tol	4.82
Ethylbenzene	EtBenz	4.72
m/p-Xylene	m/p-Xyl	5.58
Styrene	Styr	4.10
o-Xylene	o-Xyl	2.81
p-Dichlorobenzene	p-DCB	5.16
o-Dichlorobenzene	o-DCB	4.41

Table 5: Published Limit of Detection (LOD)

Compound Name	Abbreviation	Published LOD (ppbv)
1,3-Butadiene	Buta	0.04
Benzene	Benz	0.2
Dichloromethane	DCM	1.0
Chloroform	CHCl ₃	0.02
1,1,1-Trichloroethane	TCEA	0.01
Carbon tetrachloride	CCl ₄	0.02
Trichloroethylene	TCE	0.02
Perchloroethylene	PERC	0.01
Toluene	Tol	0.2
Ethylbenzene	EtBenz	0.6
m/p-Xylene	m/p-Xyl	0.6
Styrene	Styr	0.1
o-Xylene	o-Xyl	0.1
p-Dichlorobenzene	p-DCB	0.2
o-Dichlorobenzene	o-DCB	0.1

Table 6: Rejected Points

Component	Points Rejected	Sample ID	GC Conc. (ppb)	GC/MS Conc. (ppb)	PD ⁽¹⁾	RPD ⁽²⁾	Reason
1,1,1-Trichloroethane	8	TX003092	0.092	0.043	-114.0%	-72.6%	PD Z-S = 5.9; RPD Z-S = 5.2 ⁽³⁾
		TX003117	0.079	0.052	-51.9%	-41.2%	PD Z-S = 4.8; RPD Z-S = 4.5 ⁽³⁾
		TX003089	0.067	0.050	-34.0%	-29.6%	PD Z-S = 4.5; RPD Z-S = 4.3 ⁽³⁾
		TX003084	0.071	0.052	-36.5%	-30.9%	PD Z-S = 6.1; RPD Z-S = 5.7 ⁽³⁾
Benzene	2	TX003085	0.93	1.50	37.8%	46.6%	PD Z-S = 3.7; RPD Z-S = 4.2 ⁽³⁾
Perchloroethylene	4	TX003110	0.021	0.011	-46.2%	-62.5%	PD Z-S = 5.6; RPD Z-S = 4.9 ⁽³⁾
		TX003105	0.019	0.013	-90.9%	-37.5%	PD Z-S = 4.7; RPD Z-S = 4.2 ⁽³⁾
Styrene	4	TX003195	0.69	0.29	-135.5%	-80.8%	PD Z-S = 3.1; RPD Z-S = 2.5 ⁽³⁾
		TX003207	0.59	0.35	-68.6%	-51.1%	PD Z-S = 2.6; RPD Z-S = 2.2 ⁽³⁾
Chloroform	28	TX003028	0.089	0.055	-61.8%	-47.2%	These points were rejected from the primary distribution because they appeared to be part of a second distribution.
		TX003080	0.035	0.019	-84.2%	-59.3%	
		TX003094	0.040	0.019	-110.5%	-71.2%	
		TX003106	0.060	0.028	-114.3%	-72.7%	
		TX003099	0.061	0.027	-125.9%	-77.3%	
		TX003111	0.061	0.036	-69.4%	-51.6%	
		TX003120	0.095	0.036	-163.9%	-90.1%	
		TX003105	0.044	0.021	-109.5%	-70.8%	
		TX003110	0.083	0.035	-137.1%	-81.4%	
		TX003176	0.049	0.017	-188.2%	-97.0%	
		TX003178	0.035	0.022	-59.1%	-45.6%	

Table 6: Rejected Points

Component	Points Rejected	Sample ID	GC Conc. (ppb)	GC/MS Conc. (ppb)	PD ⁽¹⁾	RPD ⁽²⁾	Reason
		TX003190	0.039	0.025	-56.0%	-43.8%	
		TX003193	0.076	0.039	-94.9%	-64.4%	
		TX003197	0.090	0.043	-109.3%	-70.7%	
Total Rejected:	46						

⁽¹⁾ Percent Difference

⁽²⁾ Relative Percent Difference

⁽³⁾ See page 5 for a definition of Z-S = Z-Score

Table 7: Corrected GC/MS Concentrations (Part 1)

BENZENE				PERCHLOROETHYLENE				o-XYLENE				1,1,1-TRICHLOROETHANE			
GC/MS				GC/MS				GC/MS				GC/MS			
Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD
ppb	ppb	ppb	%	ppb	ppb	ppb	%	ppb	ppb	ppb	%	ppb	ppb	ppb	%
0.20	0.21	0.01	4.8%	0.010	0.009	-0.001	-10.6%	0.10	0.08	-0.02	-24.9%	0.010	0.003	-0.007	-100.2%
0.30	0.31	0.01	3.2%	0.020	0.019	-0.001	-5.3%	0.20	0.18	-0.02	-12.0%	0.020	0.013	-0.007	-39.4%
0.40	0.41	0.01	2.3%	0.030	0.029	-0.001	-3.6%	0.30	0.28	-0.02	-8.0%	0.030	0.024	-0.006	-24.3%
0.50	0.51	0.01	1.8%	0.040	0.039	-0.001	-2.8%	0.40	0.38	-0.02	-6.1%	0.040	0.034	-0.006	-17.4%
0.60	0.61	0.01	1.4%	0.050	0.049	-0.001	-2.3%	0.50	0.48	-0.02	-5.0%	0.050	0.044	-0.006	-13.5%
0.70	0.71	0.01	1.2%	0.060	0.059	-0.001	-2.0%	0.60	0.58	-0.02	-4.2%	0.060	0.054	-0.006	-11.0%
0.80	0.81	0.01	1.0%	0.070	0.069	-0.001	-1.7%	0.70	0.67	-0.03	-3.7%	0.070	0.064	-0.006	-9.2%
0.90	0.91	0.01	0.9%	0.080	0.079	-0.001	-1.5%	0.80	0.77	-0.03	-3.3%	0.080	0.074	-0.006	-7.9%
1.0	1.0	0.0	0.7%	0.090	0.089	-0.001	-1.4%	0.90	0.87	-0.03	-3.0%	0.090	0.084	-0.006	-6.9%
1.1	1.1	0.0	0.6%	0.100	0.099	-0.001	-1.3%	1.00	0.97	-0.03	-2.7%	0.100	0.094	-0.006	-6.1%
1.2	1.2	0.0	0.6%	0.11	0.11	0.00	-1.2%	1.1	1.1	0.0	-2.5%	0.11	0.10	-0.01	-5.4%
1.3	1.3	0.0	0.5%	0.12	0.12	0.00	-1.1%	1.2	1.2	0.0	-2.4%	0.20	0.19	-0.01	-2.5%
1.4	1.4	0.0	0.4%	0.13	0.13	0.00	-1.1%	1.3	1.3	0.0	-2.2%	0.30	0.30	0.00	-1.4%
1.5	1.5	0.0	0.4%	0.14	0.14	0.00	-1.0%	1.4	1.4	0.0	-2.1%	0.40	0.40	0.00	-0.8%
1.6	1.6	0.0	0.3%	0.15	0.15	0.00	-1.0%	1.5	1.5	0.0	-2.0%	0.50	0.50	0.00	-0.5%
1.7	1.7	0.0	0.3%	0.16	0.16	0.00	-0.9%	1.6	1.6	0.0	-1.9%	0.60	0.60	0.00	-0.2%
1.8	1.8	0.0	0.3%	0.17	0.17	0.00	-0.9%	1.7	1.7	0.0	-1.8%	0.70	0.70	0.00	-0.1%
1.9	1.9	0.0	0.2%	0.18	0.18	0.00	-0.9%	1.8	1.8	0.0	-1.7%	0.80	0.80	0.00	0.0%
2.0	2.0	0.0	0.2%	0.19	0.19	0.00	-0.8%	1.9	1.9	0.0	-1.7%	0.90	0.90	0.00	0.1%
2.5	2.5	0.0	0.1%	0.20	0.20	0.00	-0.8%	2.0	2.0	0.0	-1.6%	1.0	1.0	0.0	0.2%
3.0	3.0	0.0	0.0%	0.21	0.21	0.00	-0.8%	2.2	2.2	0.0	-1.5%	2.0	2.0	0.0	0.5%
3.5	3.5	0.0	0.0%	0.22	0.22	0.00	-0.8%	2.4	2.4	0.0	-1.4%	3.0	3.0	0.0	0.6%
4.0	4.0	0.0	-0.1%	0.23	0.23	0.00	-0.7%	2.6	2.6	0.0	-1.4%	4.0	4.0	0.0	0.7%
5.0	5.0	0.0	-0.1%	0.24	0.24	0.00	-0.7%	2.8	2.8	0.0	-1.3%	5.0	5.0	0.0	0.7%

Table 7: Corrected GC/MS Concentrations (Part 1)

BENZENE				PERCHLOROETHYLENE				o-XYLENE				1,1,1-TRICHLOROETHANE			
GC/MS				GC/MS				GC/MS				GC/MS			
Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD
ppb	ppb	ppb	%	ppb	ppb	ppb	%	ppb	ppb	ppb	%	ppb	ppb	ppb	%
6.0	6.0	0.0	-0.1%	0.25	0.25	0.00	-0.7%	3.0	3.0	0.0	-1.3%	6.0	6.0	0.0	0.8%
7.0	7.0	0.0	-0.2%	0.26	0.26	0.00	-0.7%	4.0	4.0	0.0	-1.1%	7.0	7.1	0.1	0.8%
8.0	8.0	0.0	-0.2%	0.27	0.27	0.00	-0.7%	5.0	5.0	0.0	-1.0%	8.0	8.1	0.1	0.8%
9.0	9.0	0.0	-0.2%	0.28	0.28	0.00	-0.7%	6.0	5.9	-0.1	-0.9%	9.0	9.1	0.1	0.8%
10.0	10.0	0.0	-0.2%	0.29	0.29	0.00	-0.6%	7.0	6.9	-0.1	-0.8%	10.0	10.1	0.1	0.8%
11.0	11.0	0.0	-0.2%	0.30	0.30	0.00	-0.6%	8.0	7.9	-0.1	-0.8%	11.0	11.1	0.1	0.8%
12.0	12.0	0.0	-0.2%	0.40	0.40	0.00	-0.6%	9.0	8.9	-0.1	-0.8%	12.0	12.1	0.1	0.8%
13.0	13.0	0.0	-0.2%	0.50	0.50	0.00	-0.5%	10.0	9.9	-0.1	-0.7%	13.0	13.1	0.1	0.8%
14.0	14.0	0.0	-0.2%	1.0	1.0	0.0	-0.4%	11.0	10.9	-0.1	-0.7%	14.0	14.1	0.1	0.8%
15.0	15.0	0.0	-0.2%	2.0	2.0	0.0	-0.4%	12.0	11.9	-0.1	-0.7%	15.0	15.1	0.1	0.8%
16.0	16.0	0.0	-0.2%	3.0	3.0	0.0	-0.3%	13.0	12.9	-0.1	-0.7%	16.0	16.1	0.1	0.8%

Corr.: Corrected Value

Δ: Change

Table 8: Corrected GC/MS Concentrations (Part 2)

TRICHLOROETHYLENE				<i>m/p</i> -XYLENE				TOLUENE				CHLOROFORM			
GC/MS				GC/MS				GC/MS				GC/MS			
Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD
ppb	ppb	ppb	%	ppb	ppb	ppb	%	ppb	ppb	ppb	%	ppb	ppb	ppb	%
0.020	0.017	-0.003	-17.7%	0.60	0.55	-0.05	-8.92%	0.20	0.07	-0.13	-96.8%	0.020	0.023	0.003	15.9%
0.030	0.026	-0.004	-12.5%	0.70	0.64	-0.06	-8.91%	0.25	0.12	-0.13	-71.4%	0.030	0.032	0.002	5.2%
0.040	0.036	-0.004	-10.0%	0.80	0.73	-0.07	-8.90%	0.30	0.17	-0.13	-56.8%	0.040	0.040	0.000	-0.7%
0.050	0.046	-0.004	-8.5%	0.90	0.82	-0.08	-8.90%	0.40	0.26	-0.14	-40.6%	0.050	0.048	-0.002	-4.3%
0.060	0.056	-0.004	-7.5%	1.00	0.91	-0.09	-8.90%	0.50	0.36	-0.14	-31.9%	0.060	0.056	-0.004	-6.9%
0.070	0.065	-0.005	-6.8%	1.1	1.0	-0.1	-8.89%	0.60	0.46	-0.14	-26.4%	0.070	0.064	-0.006	-8.7%
0.080	0.075	-0.005	-6.3%	1.2	1.1	-0.1	-8.89%	0.70	0.56	-0.14	-22.6%	0.080	0.072	-0.008	-10.1%
0.090	0.085	-0.005	-5.9%	1.3	1.2	-0.1	-8.89%	0.80	0.66	-0.14	-19.8%	0.090	0.080	-0.010	-11.2%
0.100	0.095	-0.005	-5.6%	1.4	1.3	-0.1	-8.89%	0.90	0.75	-0.15	-17.8%	0.10	0.09	-0.01	-12.1%
0.11	0.10	-0.01	-5.4%	1.5	1.4	-0.1	-8.88%	1.0	0.9	-0.1	-16.1%	0.11	0.10	-0.01	-12.8%
0.12	0.11	-0.01	-5.1%	1.6	1.5	-0.1	-8.88%	2.0	1.8	-0.2	-9.0%	0.12	0.10	-0.02	-13.5%
0.13	0.12	-0.01	-5.0%	1.7	1.6	-0.1	-8.88%	2.2	2.0	-0.2	-8.4%	0.13	0.11	-0.02	-14.0%
0.14	0.13	-0.01	-4.8%	1.8	1.6	-0.2	-8.88%	2.4	2.2	-0.2	-7.9%	0.14	0.12	-0.02	-14.4%
0.15	0.14	-0.01	-4.7%	1.9	1.7	-0.2	-8.88%	2.6	2.4	-0.2	-7.4%	0.15	0.13	-0.02	-14.8%
0.16	0.15	-0.01	-4.5%	2.0	1.8	-0.2	-8.88%	2.8	2.6	-0.2	-7.1%	0.16	0.14	-0.02	-15.2%
0.17	0.16	-0.01	-4.4%	2.1	1.9	-0.2	-8.88%	3.0	2.8	-0.2	-6.7%	0.17	0.15	-0.02	-15.5%
0.18	0.17	-0.01	-4.4%	2.2	2.0	-0.2	-8.88%	3.1	2.9	-0.2	-6.6%	0.18	0.15	-0.03	-15.7%
0.19	0.18	-0.01	-4.3%	2.3	2.1	-0.2	-8.88%	3.2	3.0	-0.2	-6.5%	0.19	0.16	-0.03	-16.0%
0.20	0.19	-0.01	-4.2%	2.4	2.2	-0.2	-8.88%	3.3	3.1	-0.2	-6.3%	0.20	0.17	-0.03	-16.2%
0.30	0.29	-0.01	-3.7%	2.5	2.3	-0.2	-8.87%	3.4	3.2	-0.2	-6.2%	0.21	0.18	-0.03	-16.4%
0.40	0.39	-0.01	-3.5%	2.6	2.4	-0.2	-8.87%	3.5	3.3	-0.2	-6.1%	0.22	0.19	-0.03	-16.6%
0.50	0.48	-0.02	-3.4%	2.8	2.6	-0.2	-8.87%	3.6	3.4	-0.2	-6.0%	0.23	0.19	-0.04	-16.8%
0.60	0.58	-0.02	-3.3%	3.0	2.7	-0.3	-8.87%	3.7	3.5	-0.2	-5.9%	0.24	0.20	-0.04	-16.9%
0.70	0.68	-0.02	-3.2%	4.0	3.7	-0.3	-8.87%	3.8	3.6	-0.2	-5.8%	0.25	0.21	-0.04	-17.0%

Table 8: Corrected GC/MS Concentrations (Part 2)

TRICHLOROETHYLENE				<i>m/p</i> -XYLENE				TOLUENE				CHLOROFORM			
GC/MS				GC/MS				GC/MS				GC/MS			
Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD
ppb	ppb	ppb	%	ppb	ppb	ppb	%	ppb	ppb	ppb	%	ppb	ppb	ppb	%
0.80	0.78	-0.02	-3.1%	5.0	4.6	-0.4	-8.87%	3.9	3.7	-0.2	-5.7%	0.26	0.22	-0.04	-17.2%
0.90	0.87	-0.03	-3.1%	6.0	5.5	-0.5	-8.87%	4.0	3.8	-0.2	-5.6%	0.27	0.23	-0.04	-17.3%
1.00	0.97	-0.03	-3.1%	7.0	6.4	-0.6	-8.87%	5.0	4.8	-0.2	-5.0%	0.28	0.24	-0.04	-17.4%
2.0	1.9	-0.1	-2.9%	8.0	7.3	-0.7	-8.86%	6.0	5.7	-0.3	-4.5%	0.30	0.25	-0.05	-17.6%
3.0	2.9	-0.1	-2.9%	9.0	8.2	-0.8	-8.86%	7.0	6.7	-0.3	-4.2%	0.32	0.27	-0.05	-17.8%
4.0	3.9	-0.1	-2.9%	10.0	9.2	-0.8	-8.86%	8.0	7.7	-0.3	-4.0%	0.34	0.28	-0.06	-17.9%
5.0	4.9	-0.1	-2.9%	20.0	18.3	-1.7	-8.86%	9.0	8.7	-0.3	-3.8%	0.36	0.30	-0.06	-18.1%
6.0	5.8	-0.2	-2.8%	30.0	27.5	-2.5	-8.86%	10.0	9.6	-0.4	-3.7%	0.38	0.32	-0.06	-18.2%
7.0	6.8	-0.2	-2.8%	40.0	36.6	-3.4	-8.86%	20.0	19.4	-0.6	-3.0%	0.40	0.33	-0.07	-18.3%
8.0	7.8	-0.2	-2.8%	50.0	45.8	-4.2	-8.86%	30.0	29.2	-0.8	-2.8%	0.42	0.35	-0.07	-18.4%
9.0	8.7	-0.3	-2.8%	60.0	54.9	-5.1	-8.86%	40.0	38.9	-1.1	-2.7%	0.44	0.37	-0.07	-18.5%

Corr.: Corrected Value

Δ: Change

Table 9: Corrected GC/MS Concentrations (Part 3)

1,3-BUTADIENE				STYRENE			
GC/MS				GC/MS			
Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD
ppb	ppb	ppb	%	ppb	ppb	ppb	%
0.040	0.031	-0.009	-26.8%	0.10	0.13	0.03	27.9%
0.050	0.039	-0.011	-24.5%	0.15	0.17	0.02	12.6%
0.060	0.048	-0.012	-22.9%	0.20	0.21	0.01	3.8%
0.070	0.056	-0.014	-21.8%	0.25	0.25	0.00	-1.8%
0.080	0.065	-0.015	-21.0%	0.30	0.28	-0.02	-5.7%
0.090	0.073	-0.017	-20.3%	0.35	0.32	-0.03	-8.6%
0.10	0.08	-0.02	-19.8%	0.40	0.36	-0.04	-10.9%
0.11	0.09	-0.02	-19.4%	0.45	0.40	-0.05	-12.6%
0.12	0.10	-0.02	-19.1%	0.50	0.43	-0.07	-14.1%
0.13	0.11	-0.02	-18.8%	0.55	0.47	-0.08	-15.3%
0.14	0.12	-0.02	-18.6%	0.60	0.51	-0.09	-16.3%
0.15	0.12	-0.03	-18.3%	0.65	0.55	-0.10	-17.1%
0.16	0.13	-0.03	-18.2%	0.70	0.59	-0.11	-17.9%
0.17	0.14	-0.03	-18.0%	0.75	0.62	-0.13	-18.5%
0.18	0.15	-0.03	-17.8%	0.80	0.66	-0.14	-19.1%
0.19	0.16	-0.03	-17.7%	0.85	0.70	-0.15	-19.6%
0.20	0.17	-0.03	-17.6%	0.90	0.74	-0.16	-20.0%
0.21	0.18	-0.03	-17.5%	0.95	0.77	-0.18	-20.4%
0.22	0.18	-0.04	-17.4%	1.0	0.8	-0.2	-20.8%
0.23	0.19	-0.04	-17.3%	1.1	0.9	-0.2	-21.4%
0.24	0.20	-0.04	-17.2%	1.2	1.0	-0.2	-21.9%
0.25	0.21	-0.04	-17.2%	1.3	1.0	-0.3	-22.4%
0.26	0.22	-0.04	-17.1%	1.4	1.1	-0.3	-22.8%
0.27	0.23	-0.04	-17.0%	1.5	1.2	-0.3	-23.1%

Table 9: Corrected GC/MS Concentrations (Part 3)

1,3-BUTADIENE				STYRENE			
GC/MS				GC/MS			
Raw	Corr.	Δ	RPD	Raw	Corr.	Δ	RPD
ppb	ppb	ppb	%	ppb	ppb	ppb	%
0.28	0.24	-0.04	-17.0%	1.6	1.3	-0.3	-23.4%
0.29	0.24	-0.05	-16.9%	1.7	1.3	-0.4	-23.7%
0.30	0.25	-0.05	-16.9%	1.8	1.4	-0.4	-23.9%
0.40	0.34	-0.06	-16.5%	1.9	1.5	-0.4	-24.1%
0.50	0.42	-0.08	-16.3%	2.0	1.6	-0.4	-24.3%
0.60	0.51	-0.09	-16.1%	2.1	1.6	-0.5	-24.5%
0.80	0.68	-0.12	-15.9%	2.2	1.7	-0.5	-24.6%
1.0	0.9	-0.1	-15.8%	2.3	1.8	-0.5	-24.8%
2.0	1.7	-0.3	-15.6%	2.4	1.9	-0.5	-24.9%
4.0	3.4	-0.6	-15.5%	2.5	1.9	-0.6	-25.0%
6.0	5.1	-0.9	-15.5%	2.6	2.0	-0.6	-25.1%

Corr.: Corrected Value

Δ : Change

Figure 1: NIST Standard ALM046027

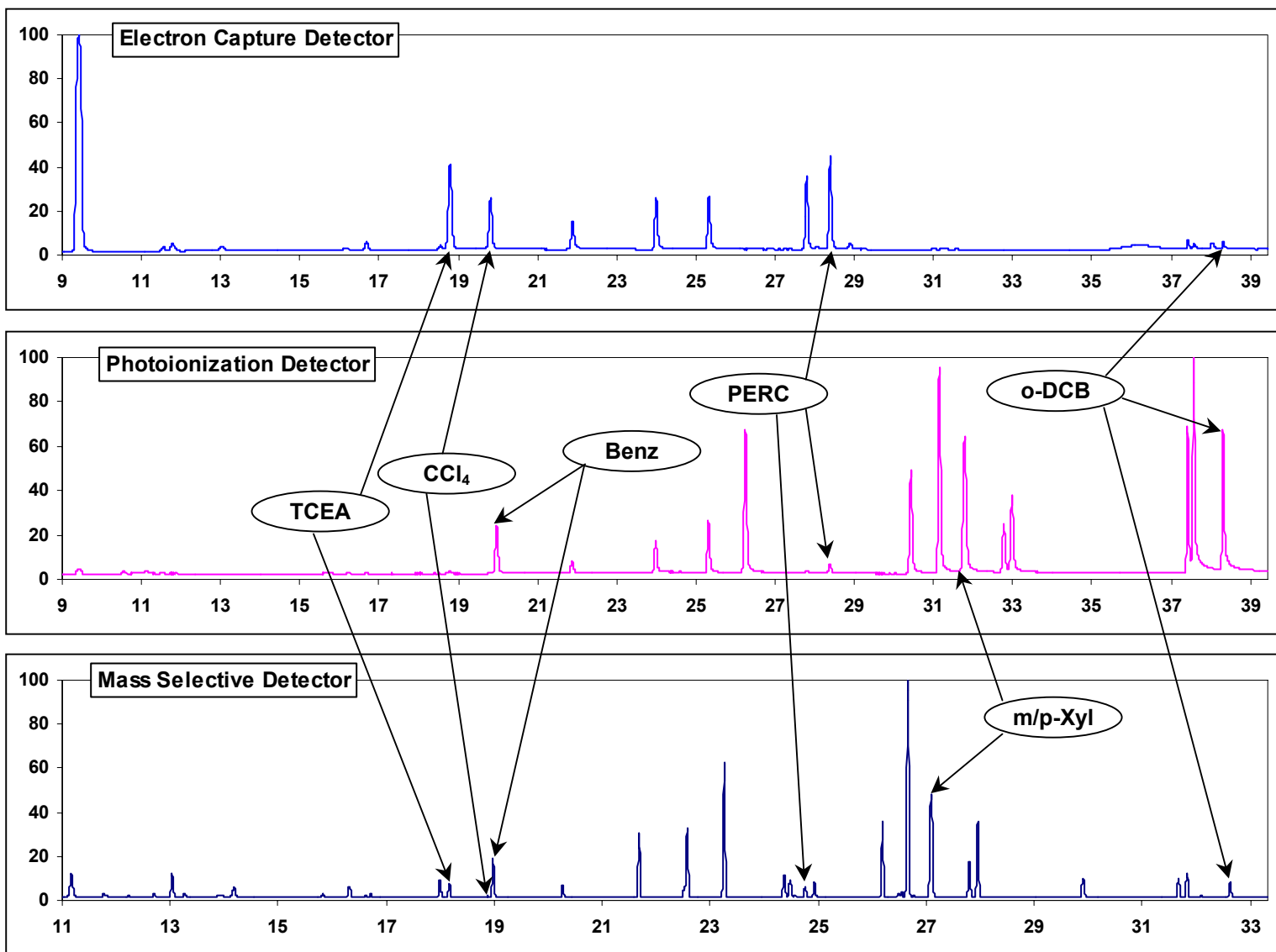


Figure 2: Mass Spectrum of Benzene from ALM046027 at 18.661 Minutes

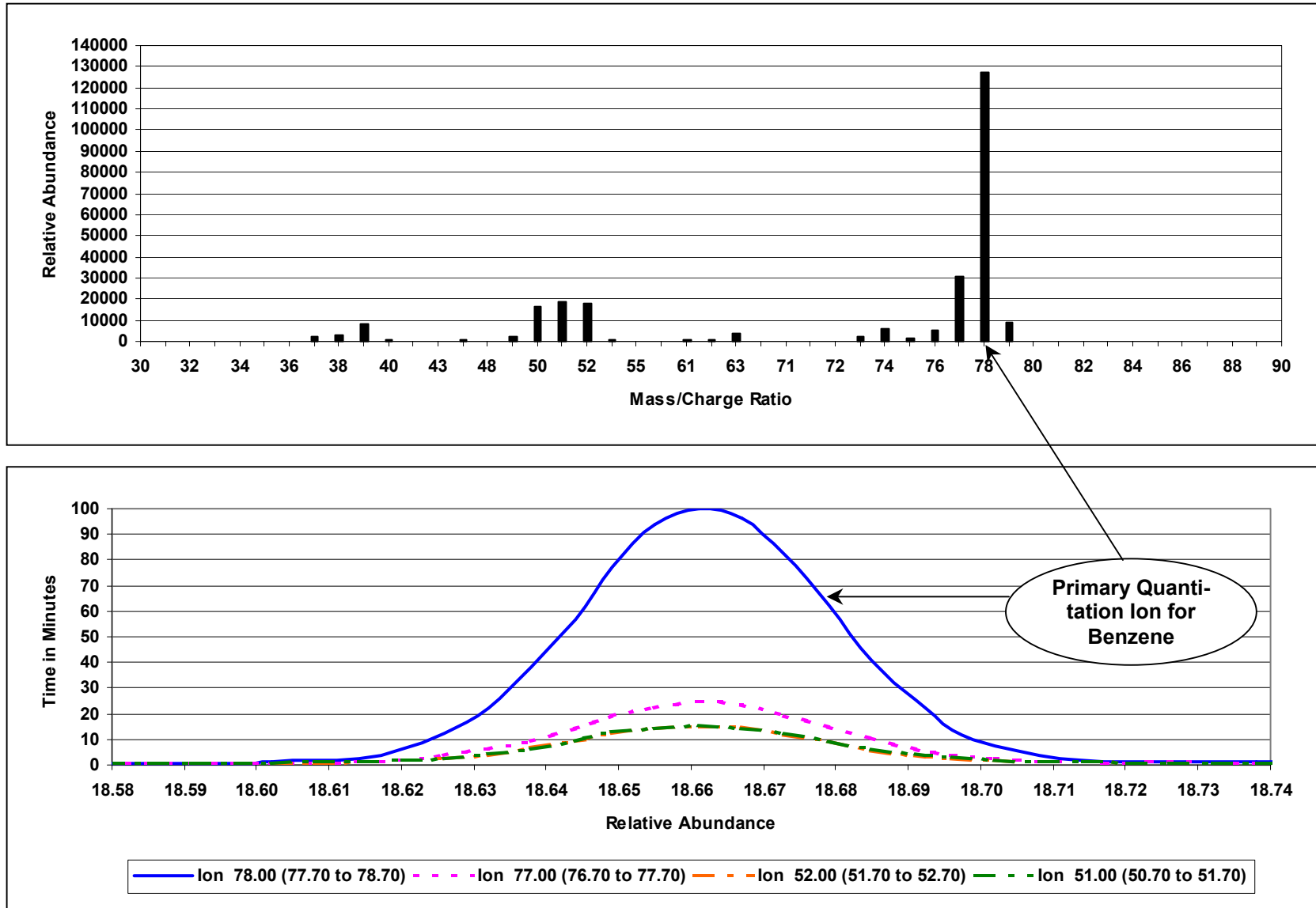


Figure 3: Benzene - GC (PID) vs. Full Scan GC/MS

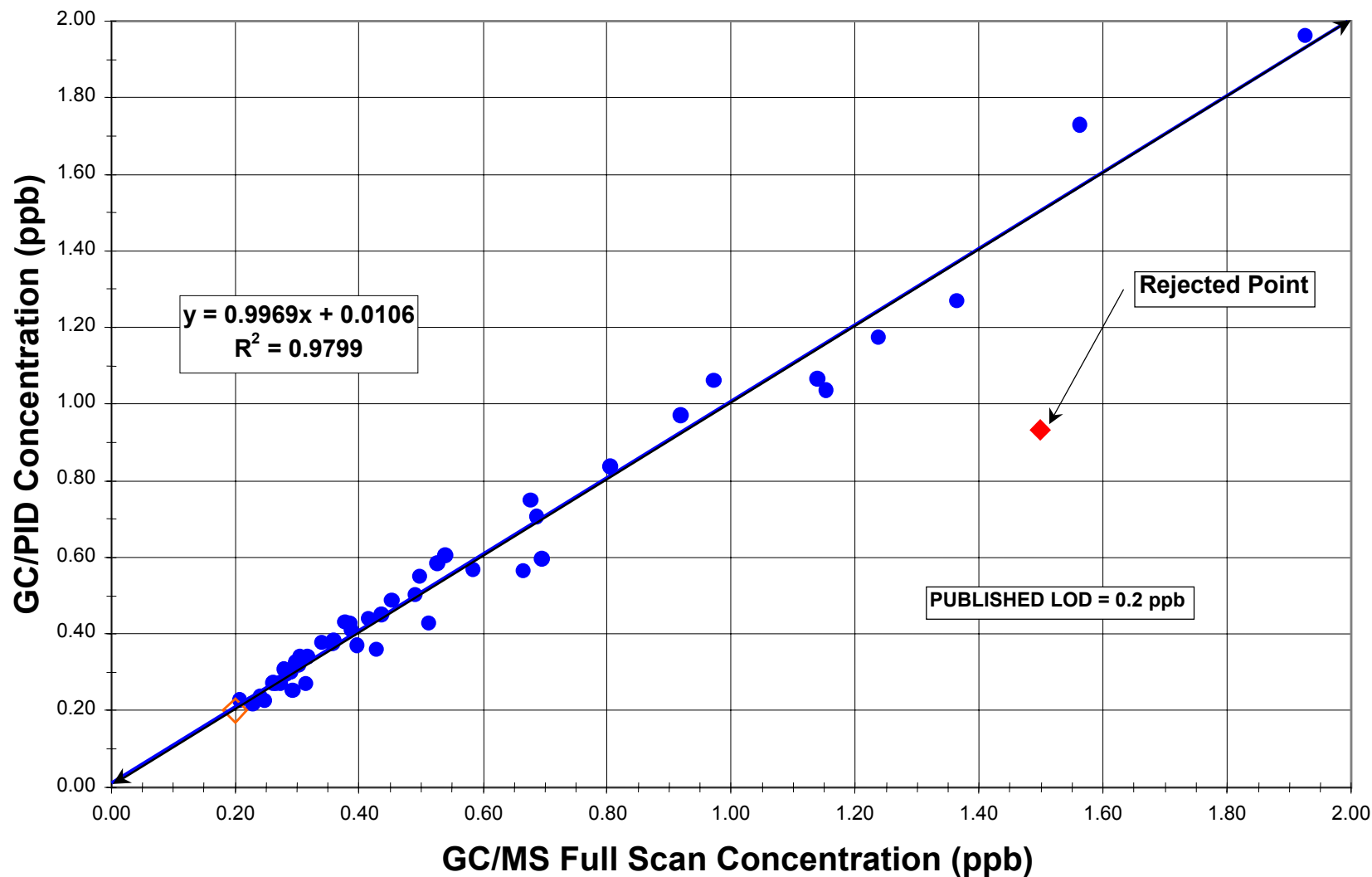


Figure 4: 1,3-Butadiene - GC (PID) vs. Full Scan GC/MS

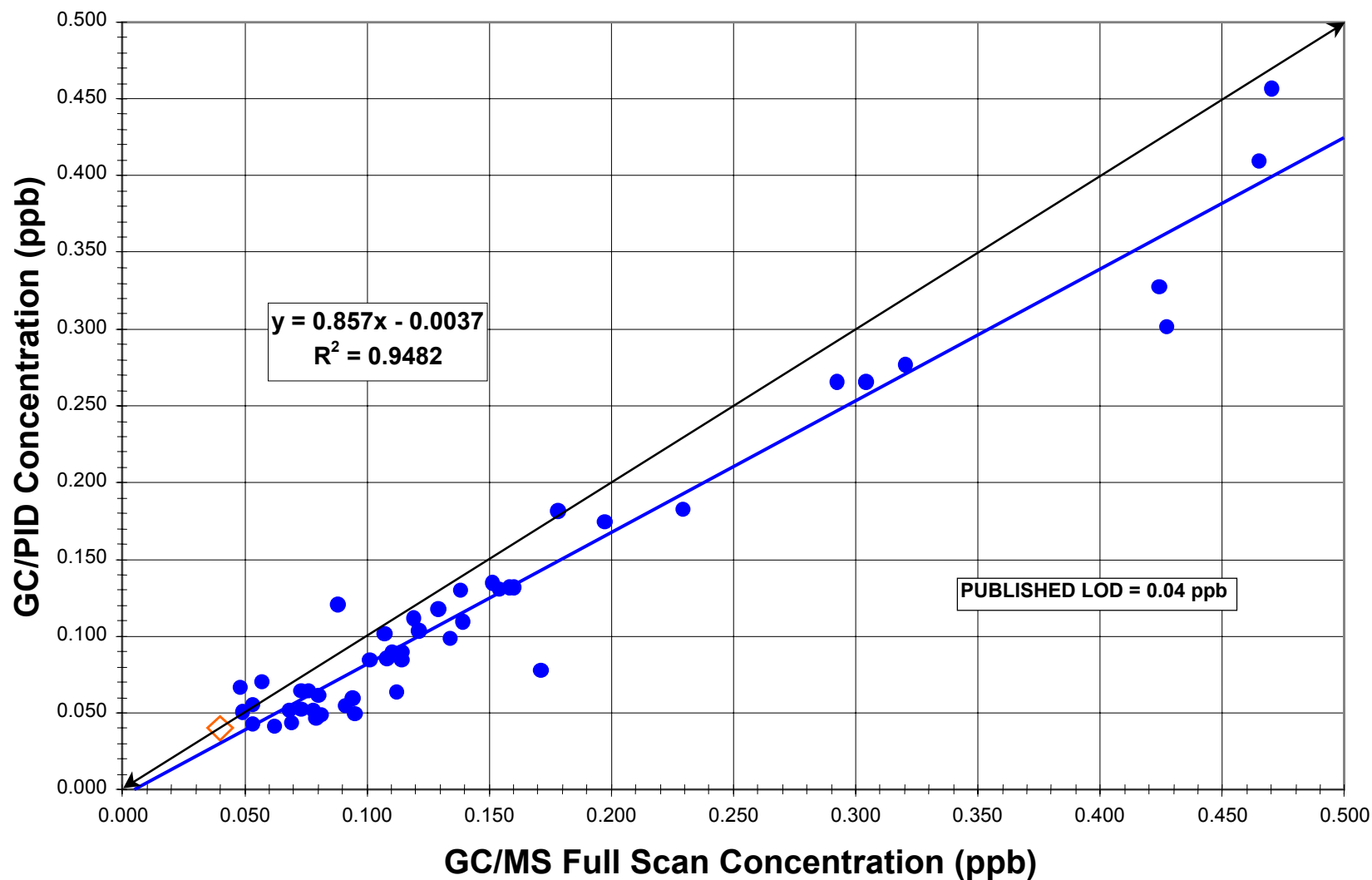


Figure 5: Carbon Tetrachloride - GC (PID) vs. Full Scan GC/MS

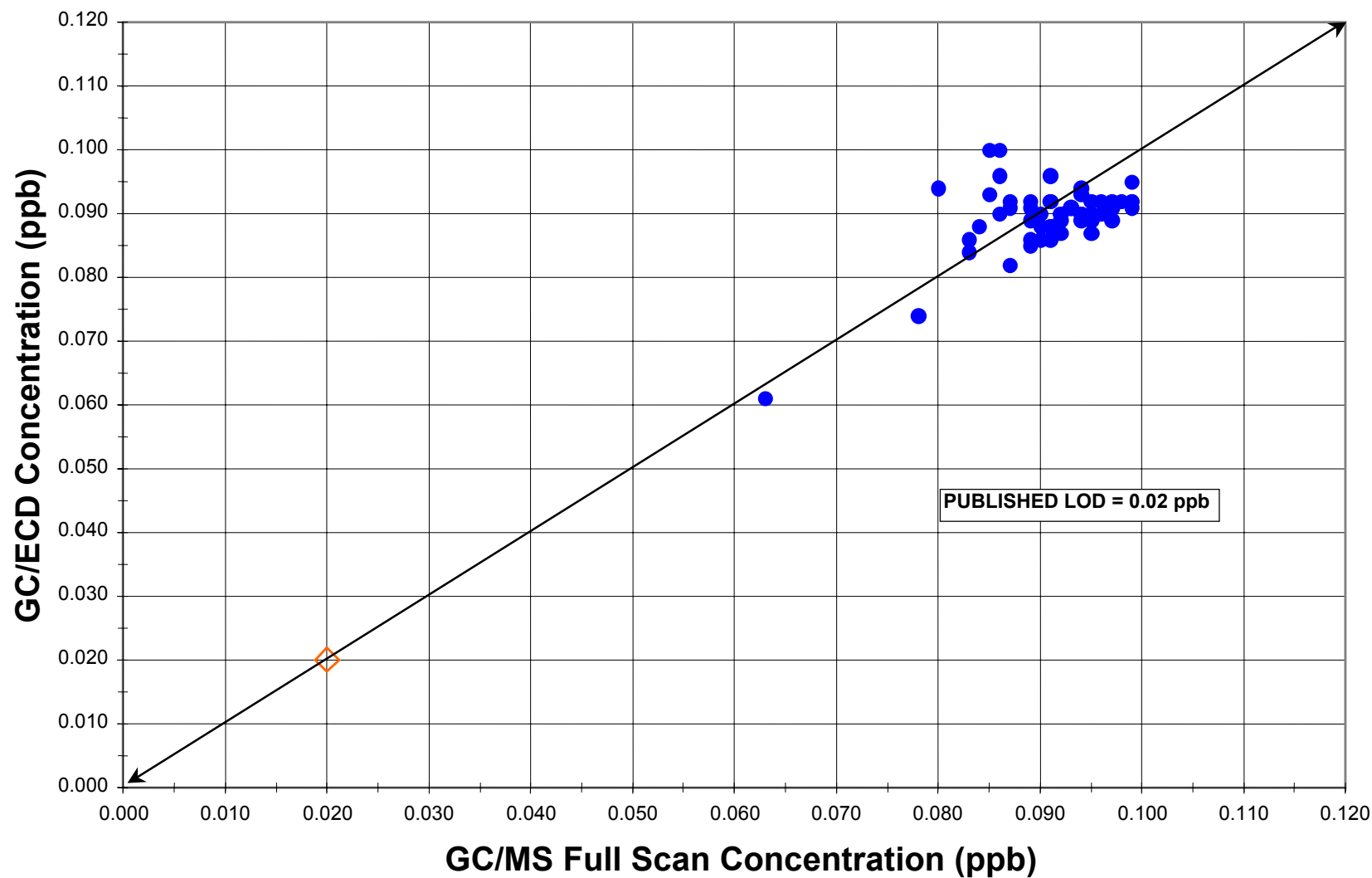


Figure 6: *p*-Dichlorobenzene - GC (ECD) vs. Full Scan GC/MS

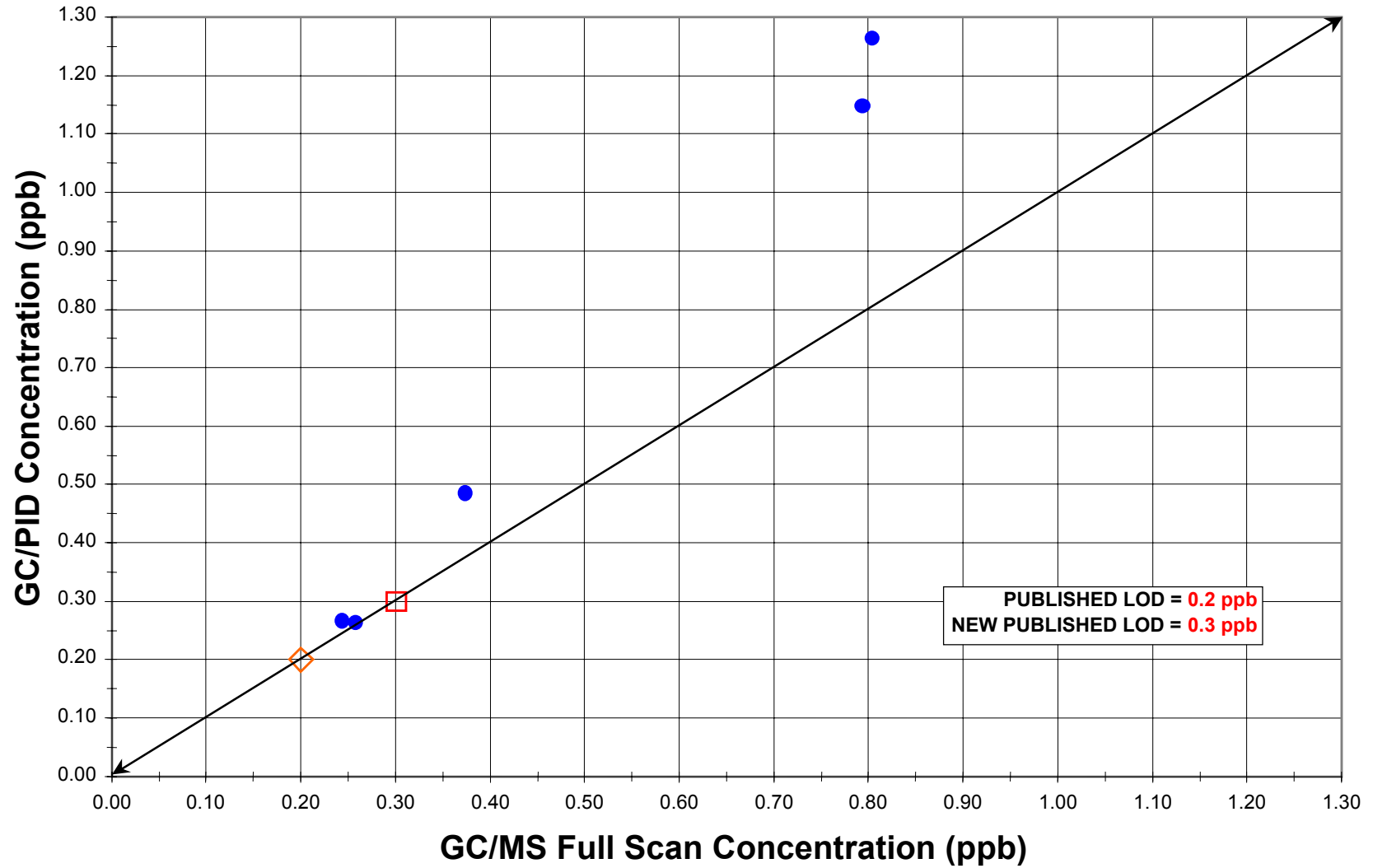


Figure 7: Perchloroethylene - GC (ECD) vs. Full Scan GC/MS

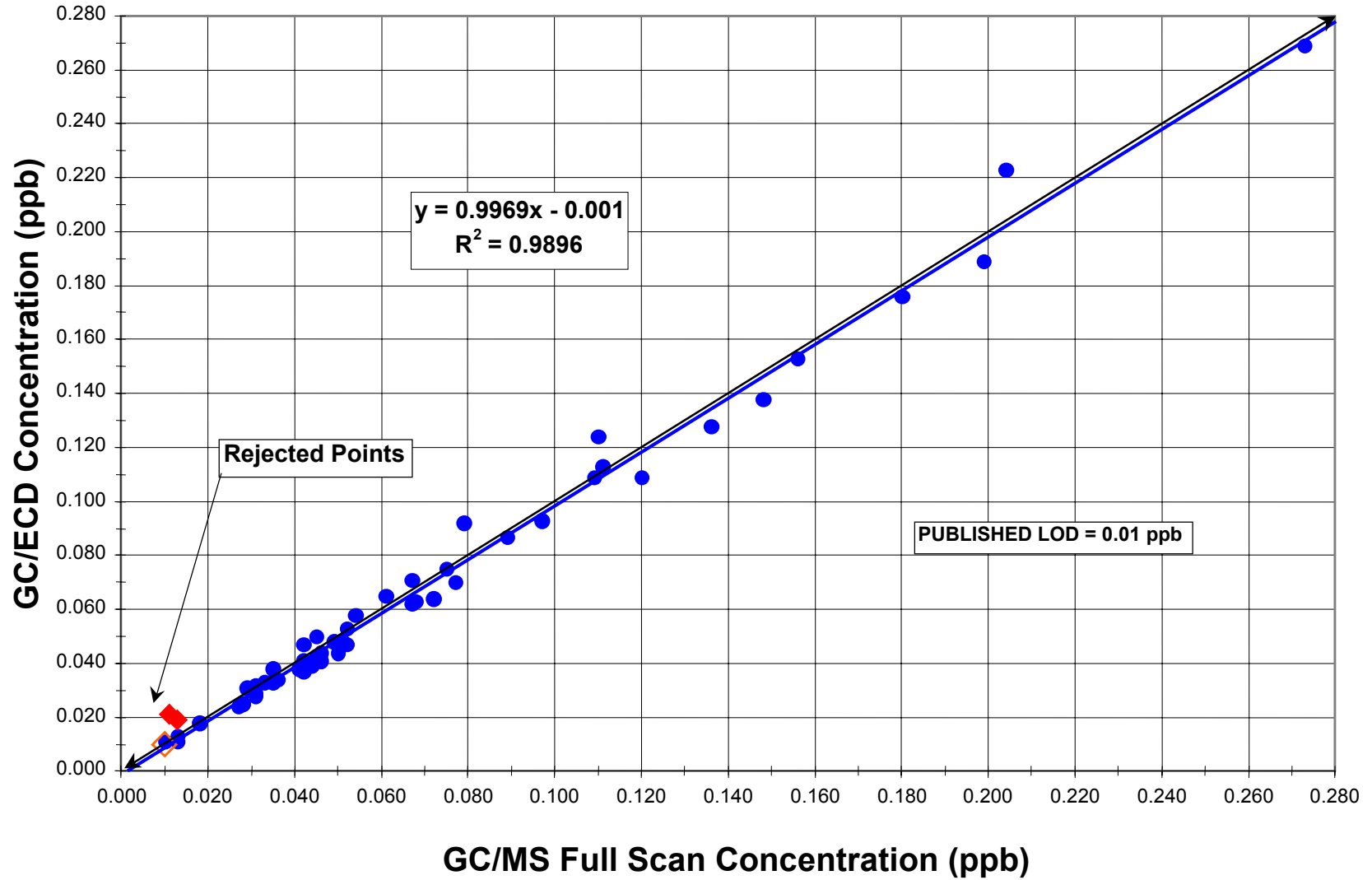


Figure 8: Dichloromethane - GC (ECD) vs. Full Scan GC/MS

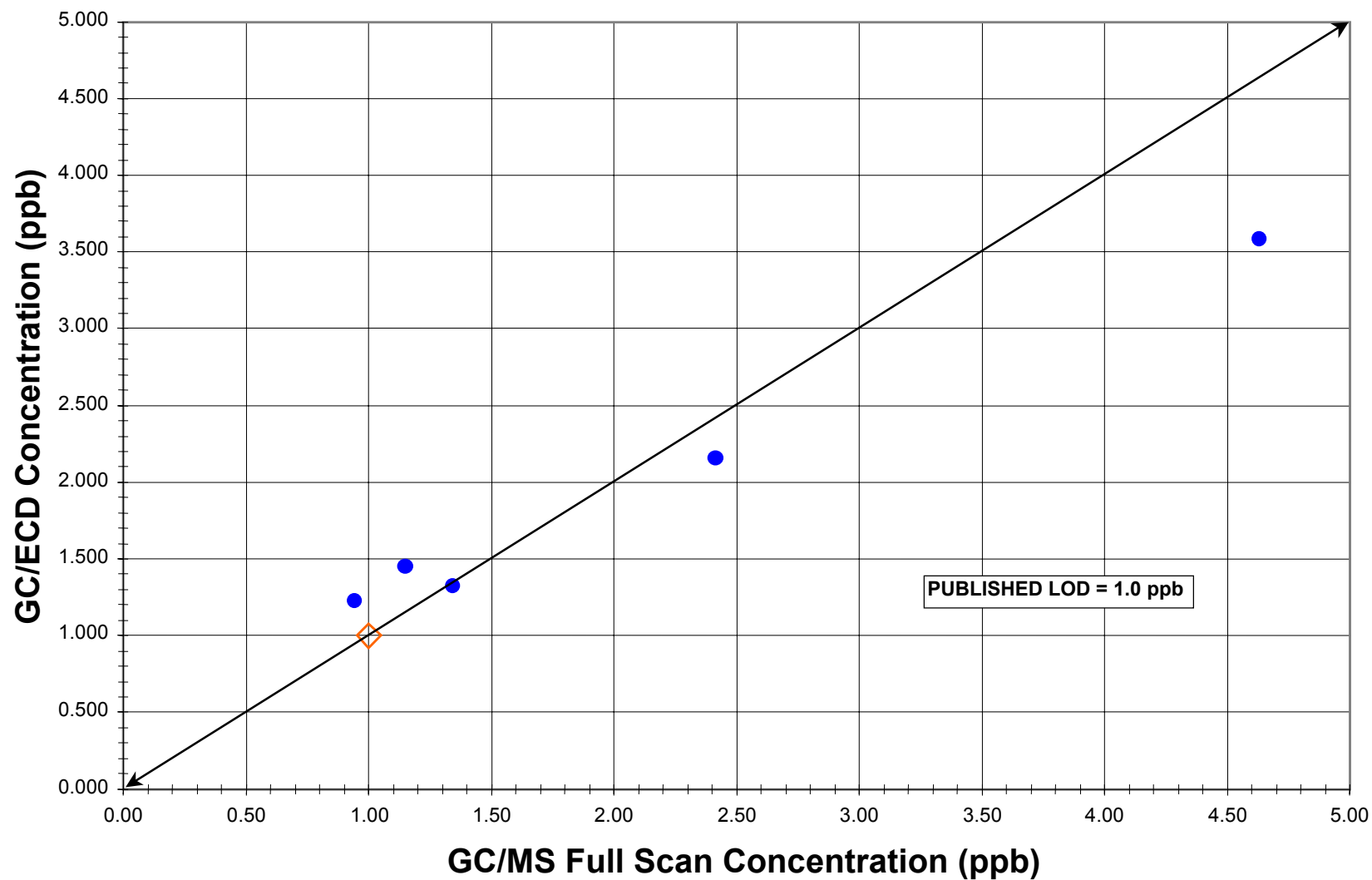


Figure 9: Chloroform - GC (ECD) vs. Full Scan GC/MS

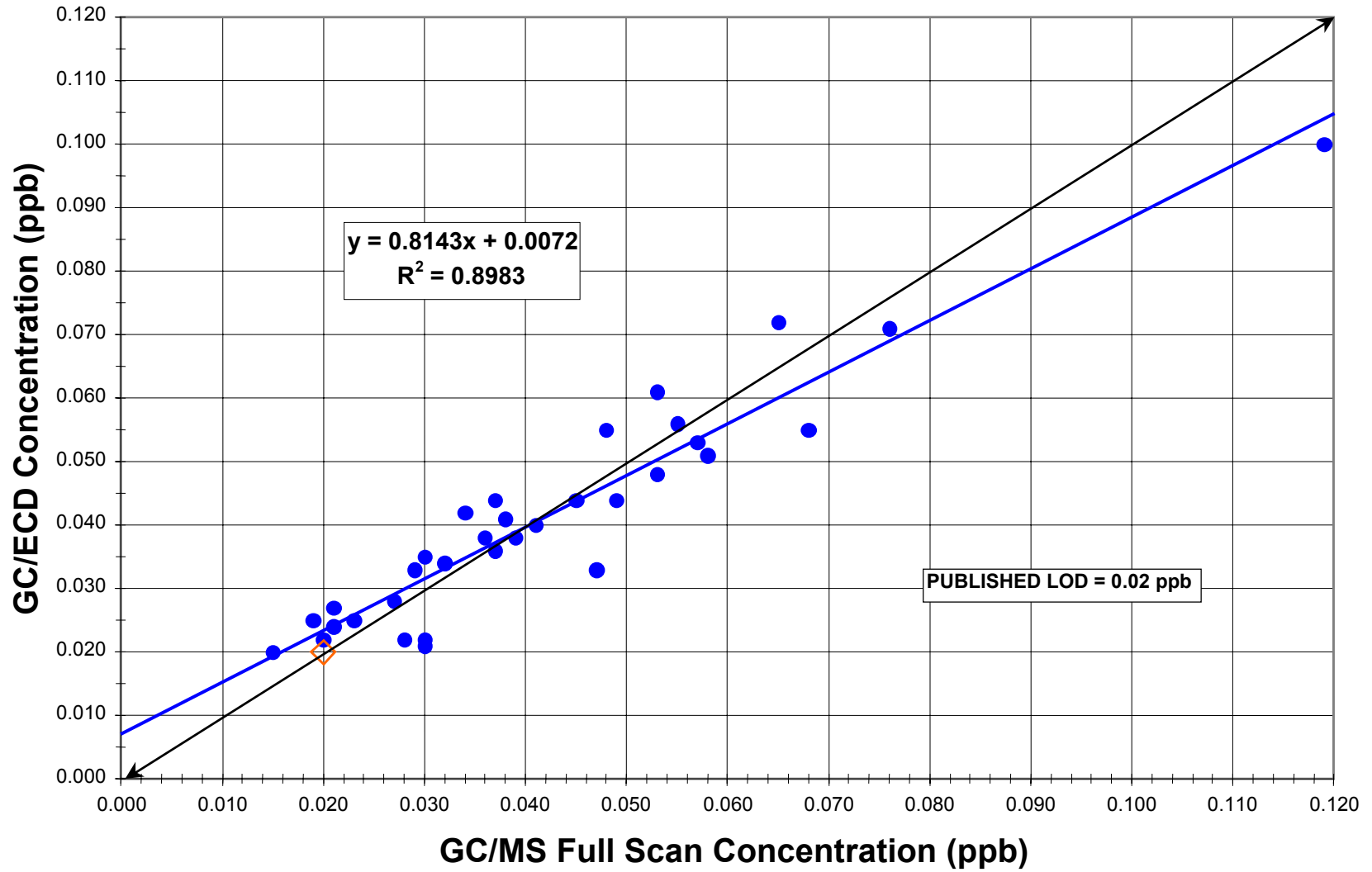


Figure 10: Chloroform with 2nd Distribution - GC (ECD) vs. Full Scan GC/MS

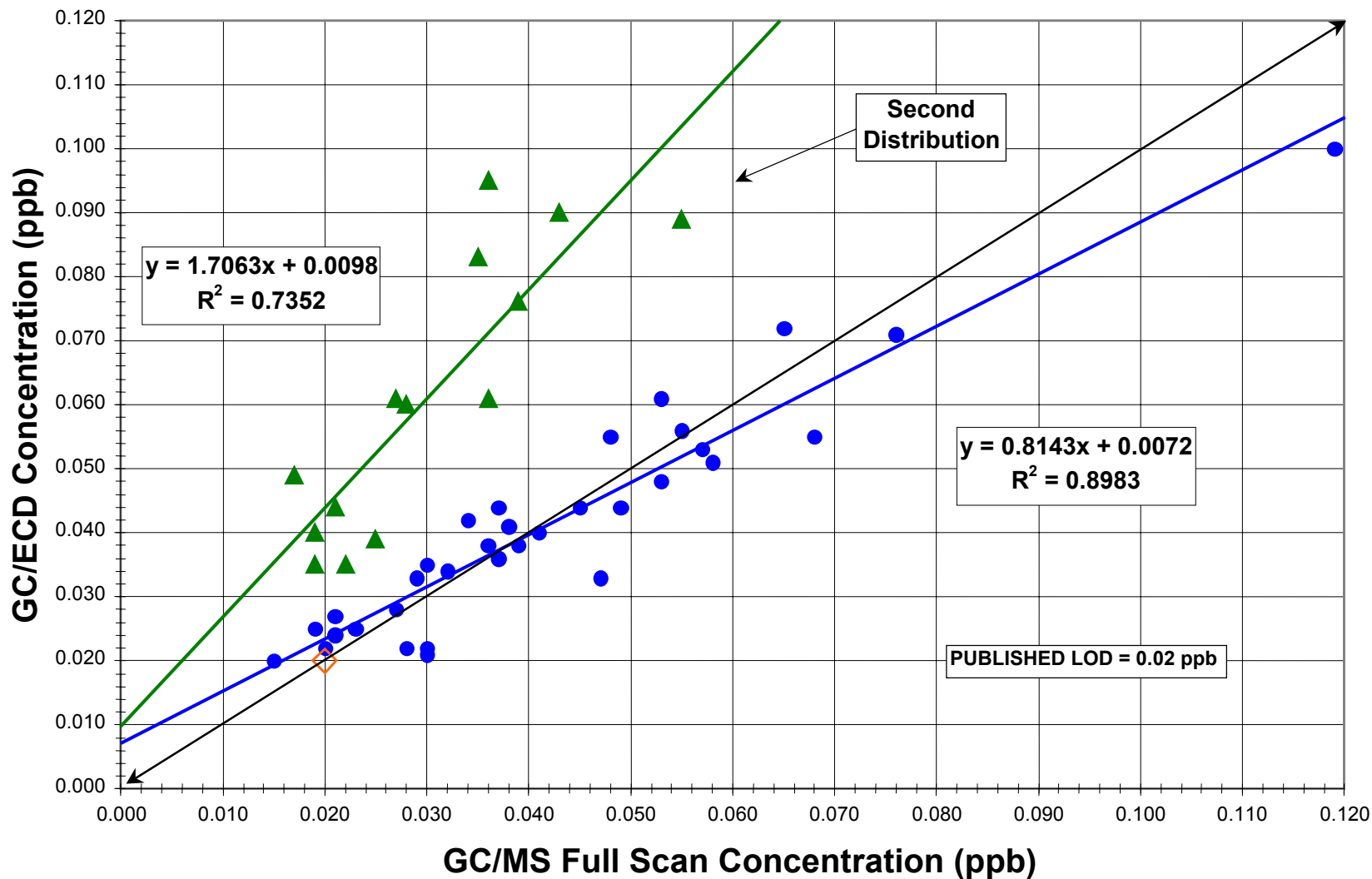


Figure 11: Trichloroethylene - GC (PID) vs. Full Scan GC/MS

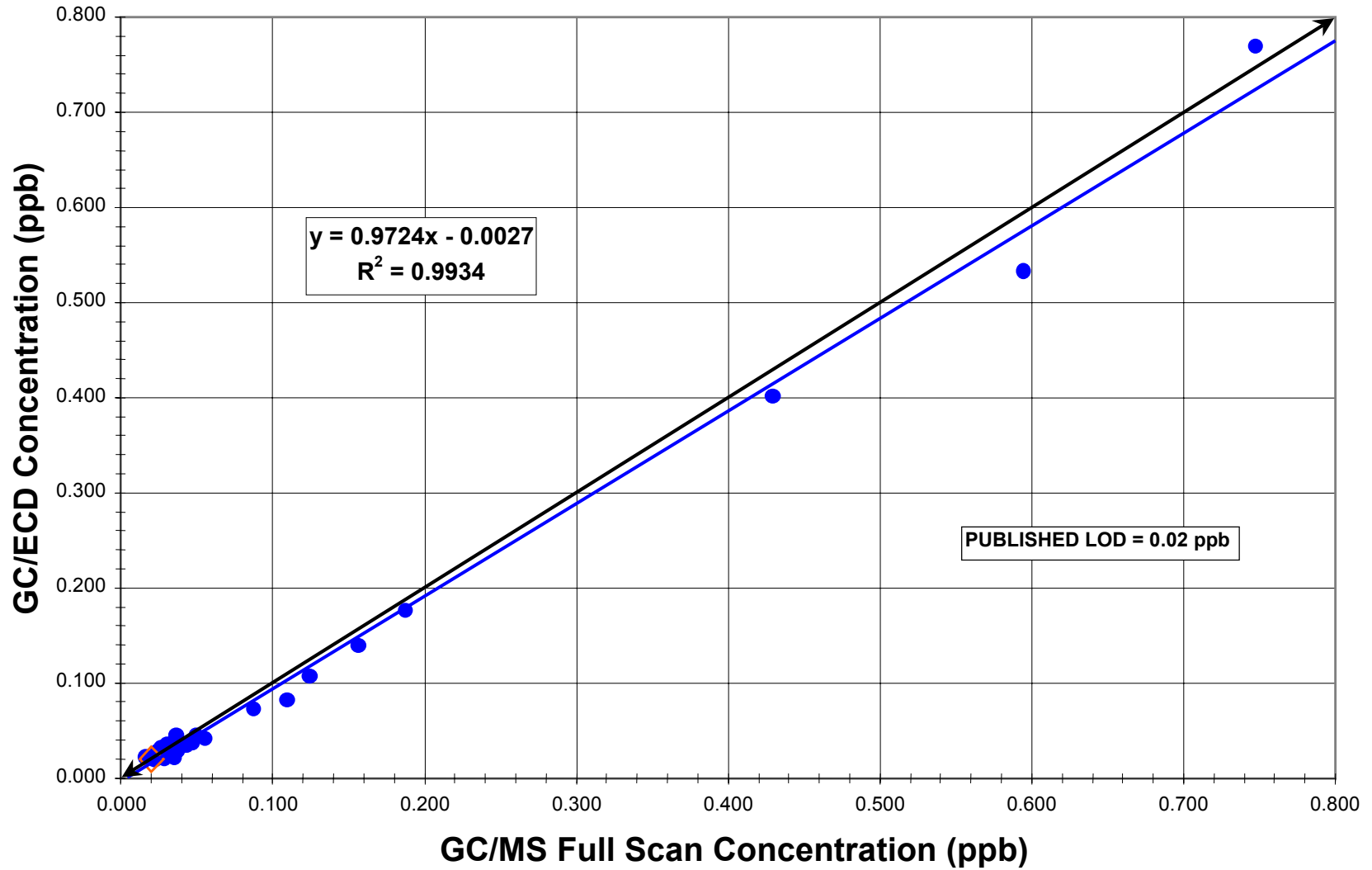


Figure 12: Trichloroethylene - LOW RANGE - GC (PID) vs. Full Scan GC/MS

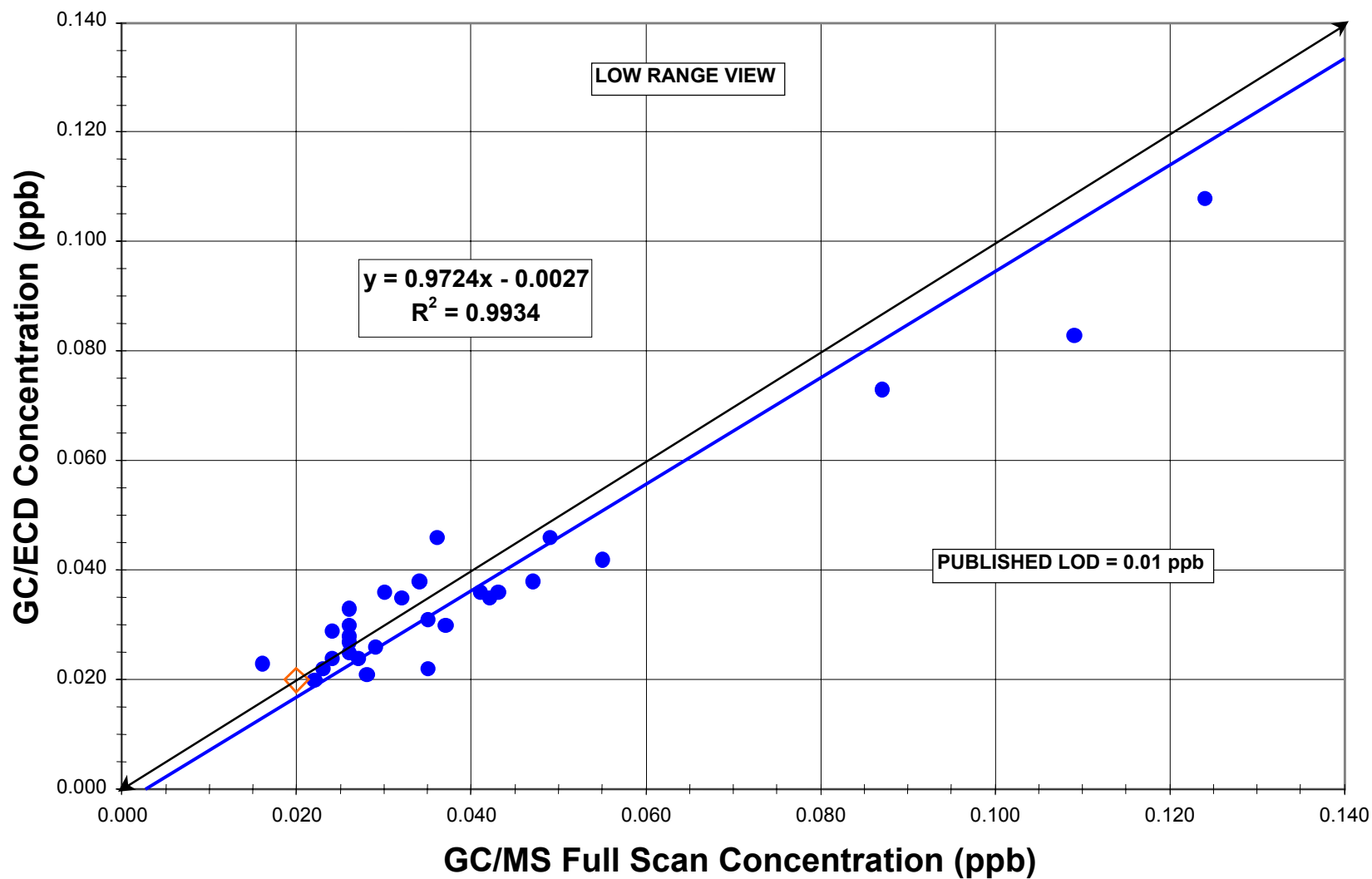


Figure 13: 1,1,1-Trichloroethane - GC (ECD) vs. Full Scan GC/MS

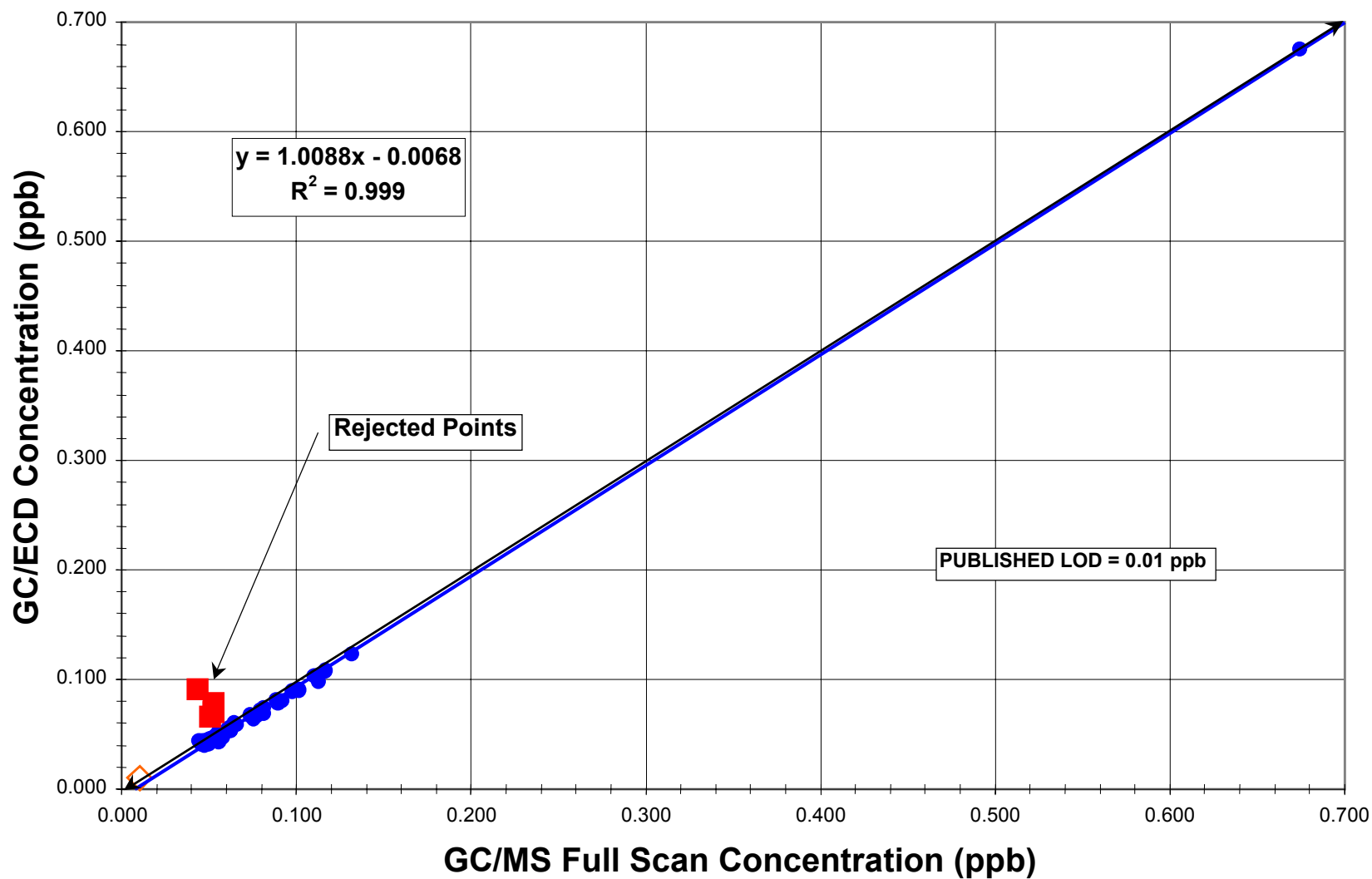


Figure 14: 1,1,1-Trichloroethane - LOW RANGE - GC (ECD) vs. Full Scan GC/MS

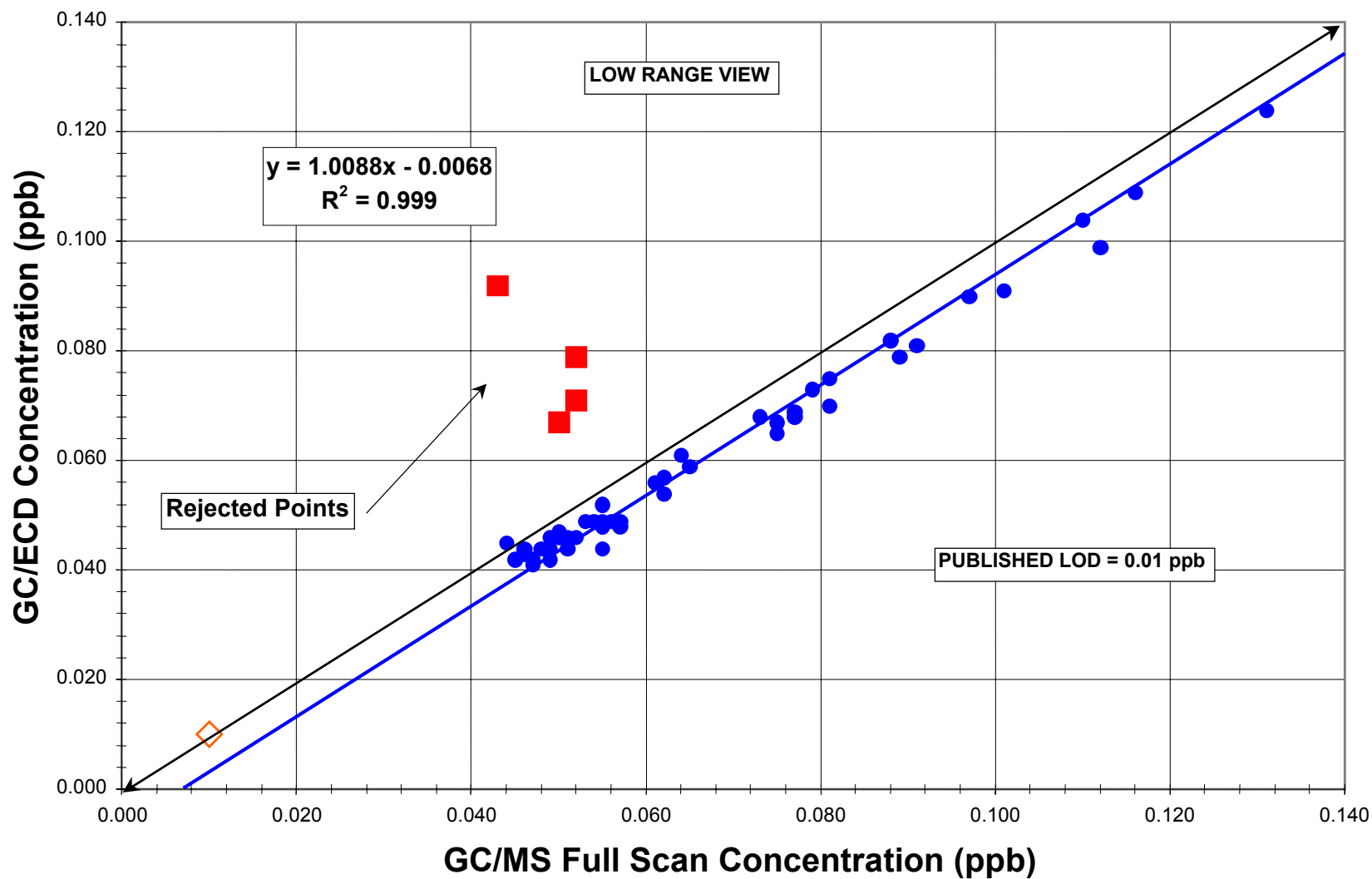


Figure 15: Toluene - GC (PID) vs. Full Scan GC/MS

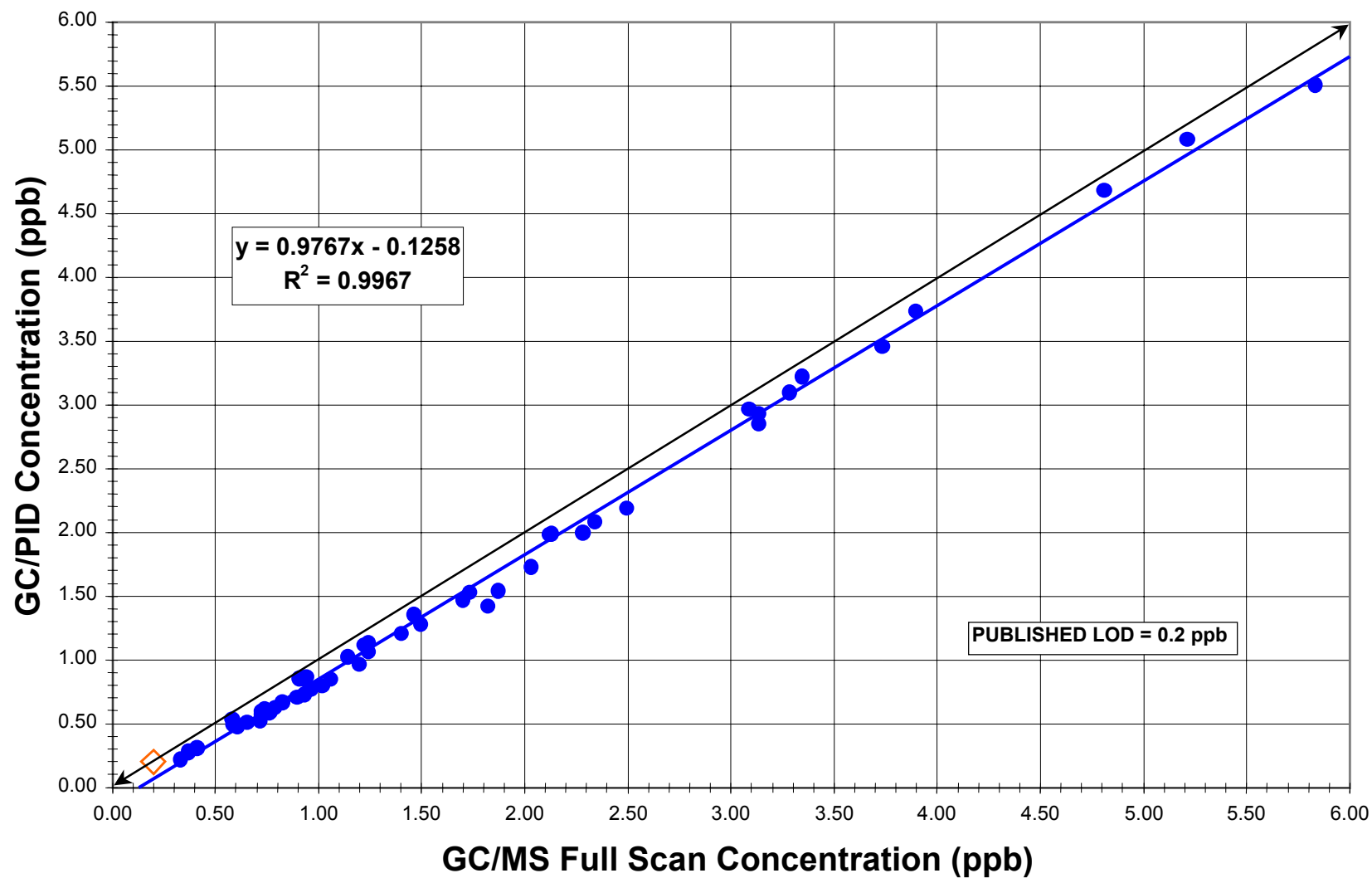


Figure 16: *m/p*-Xylene - GC (PID) vs. Full Scan GC/MS

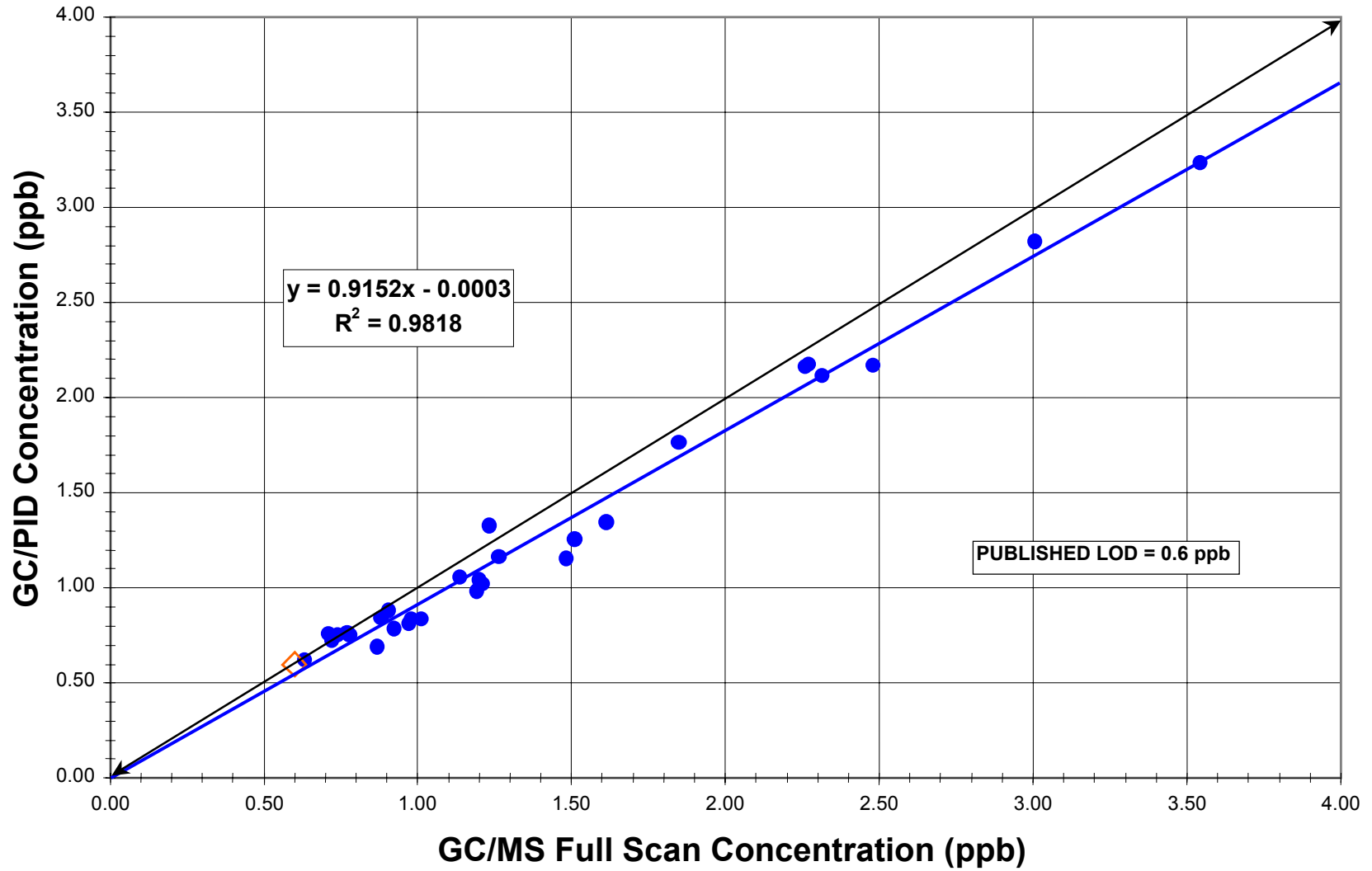


Figure 17: o-Xylene - GC (PID) vs. Full Scan GC/MS

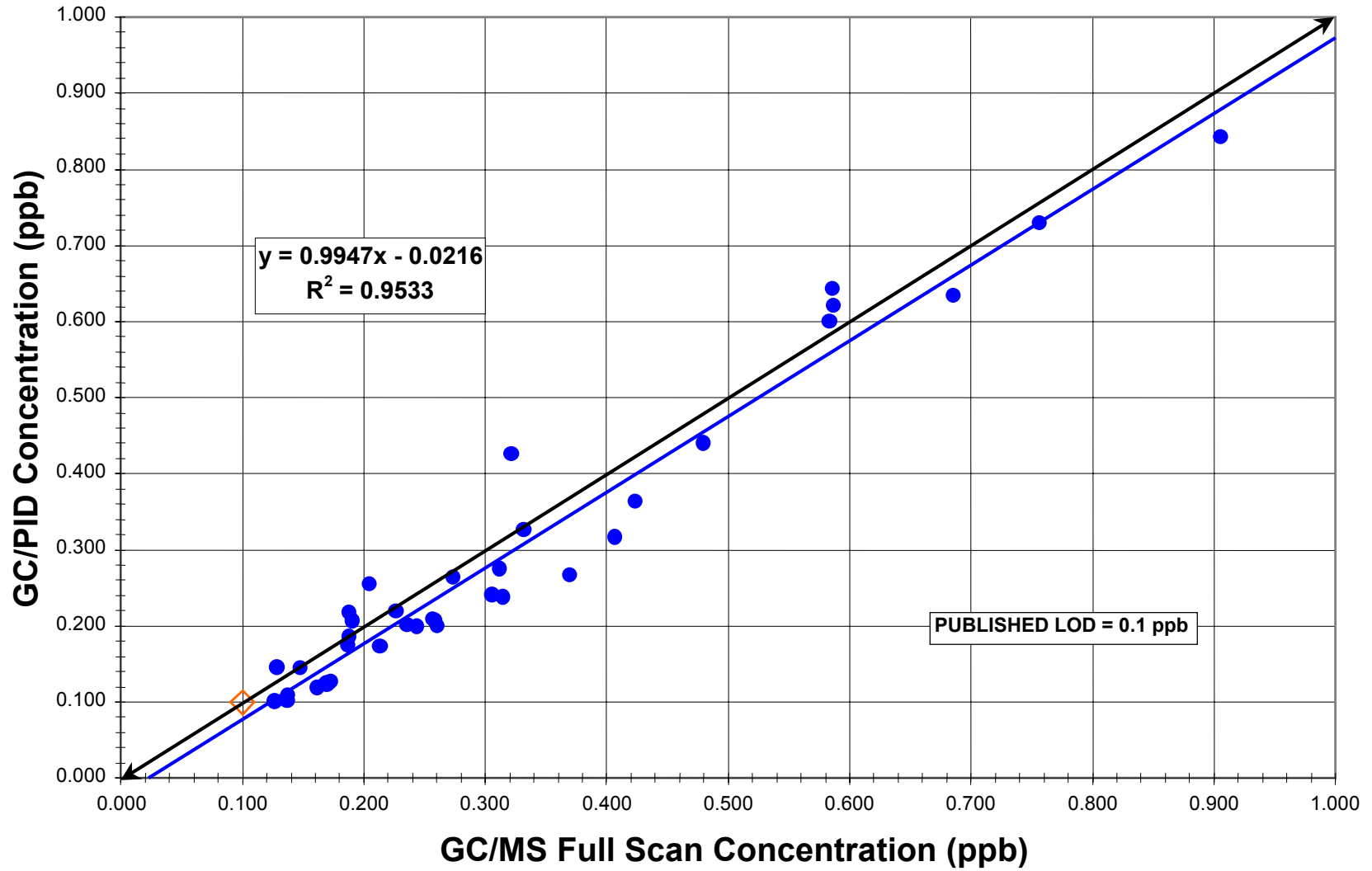


Figure 18: Styrene - GC (PID) vs. Full Scan GC/MS

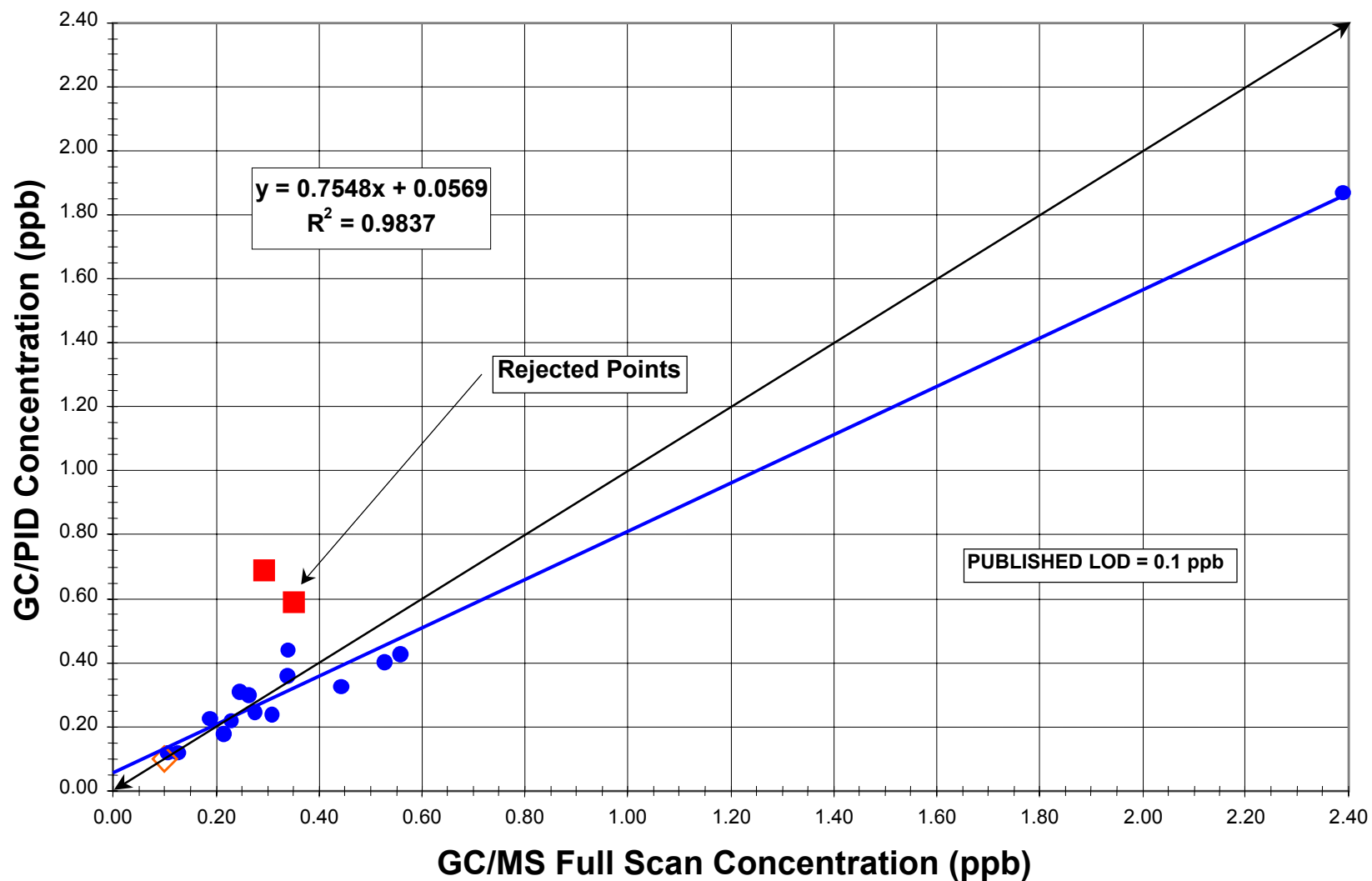


Figure 19: Styrene - LOW RANGE - GC (PID) vs. Full Scan GC/MS

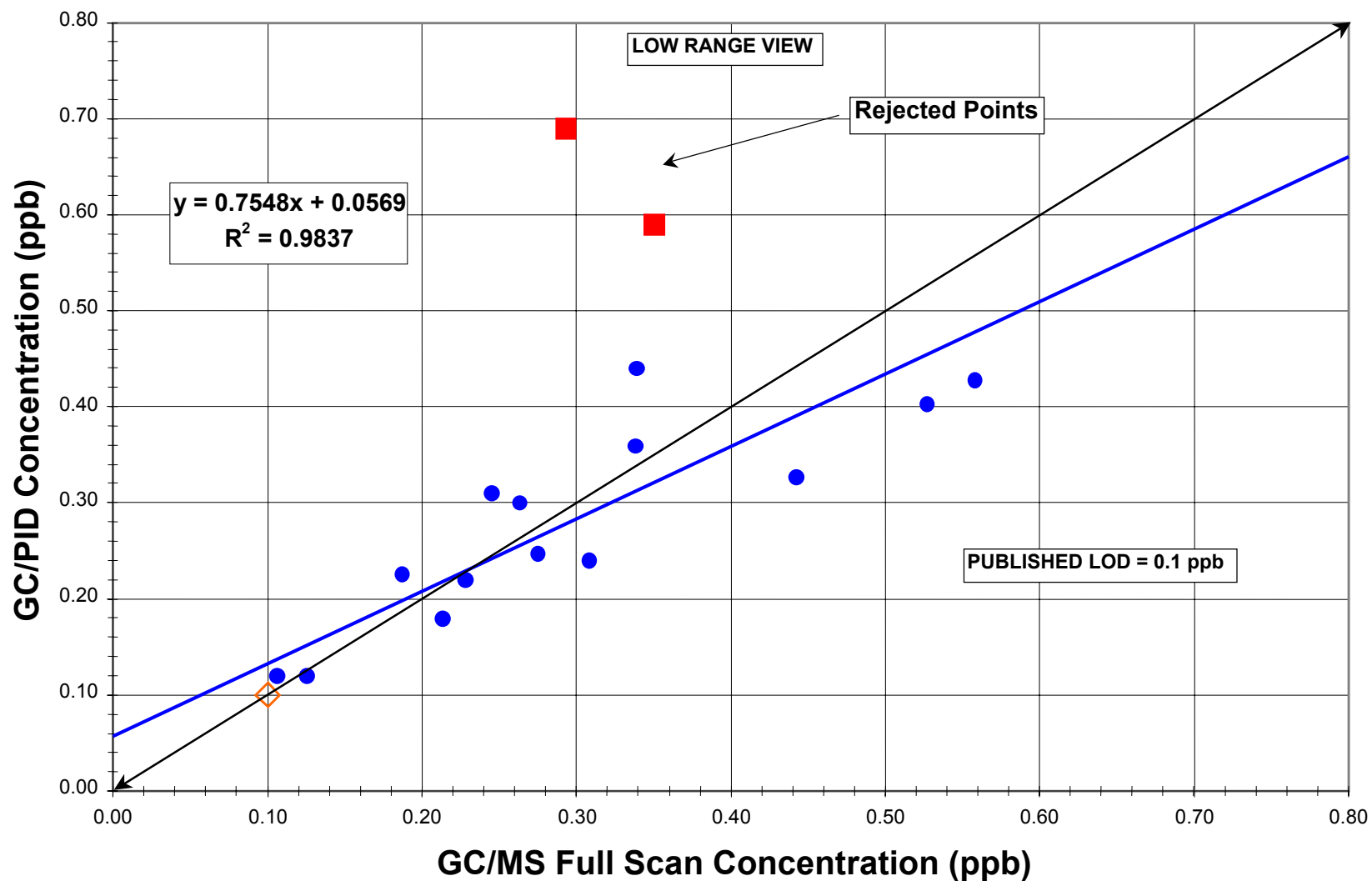


Figure 20: Benzene - RPD - GC (PID) vs. Full Scan GC/MS

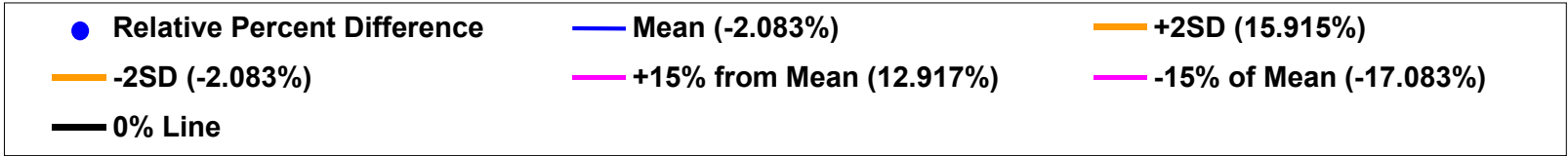
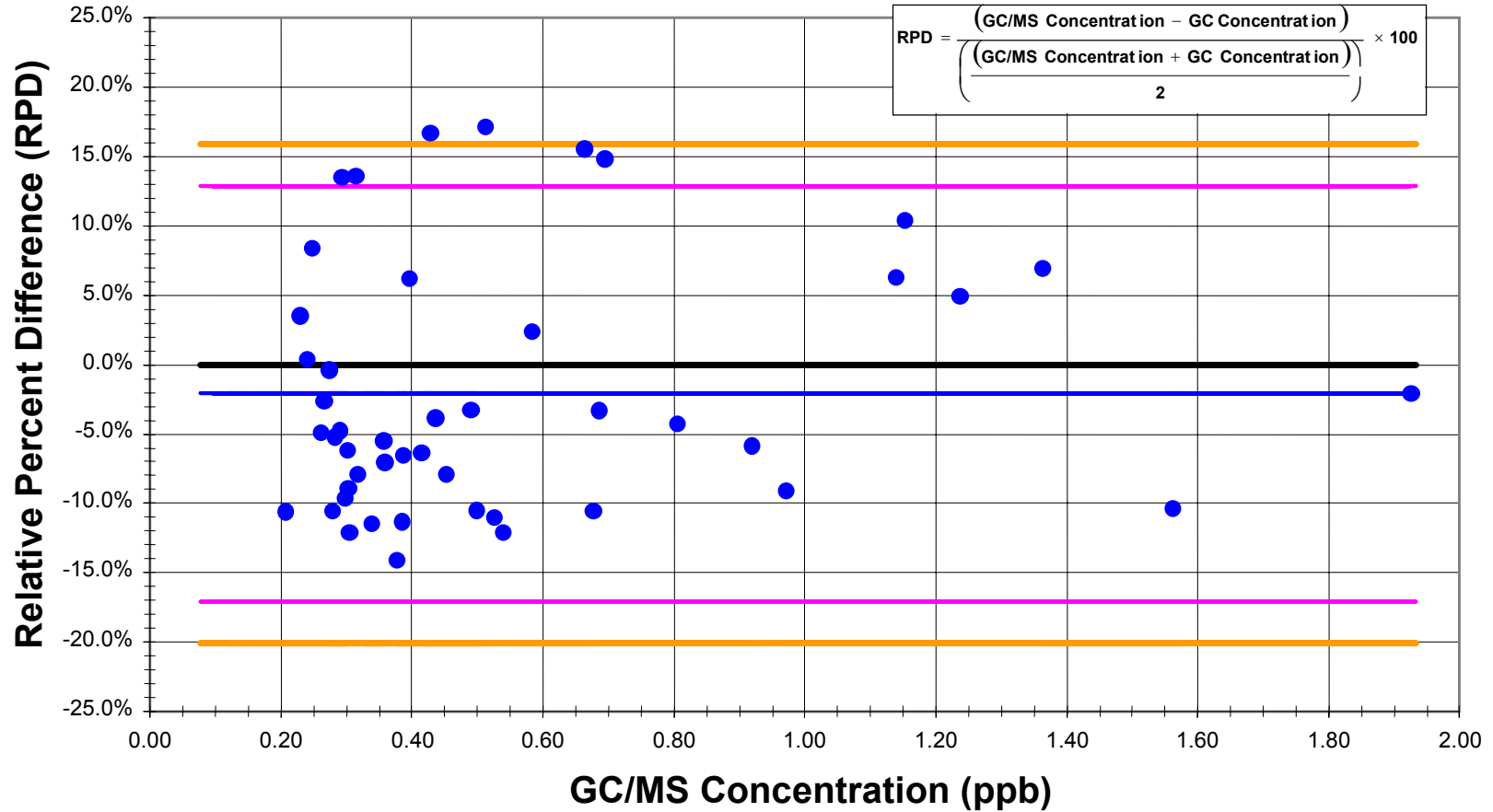


Figure 21: 1,3-Butadiene - RPD - GC (PID) vs. Full Scan GC/MS

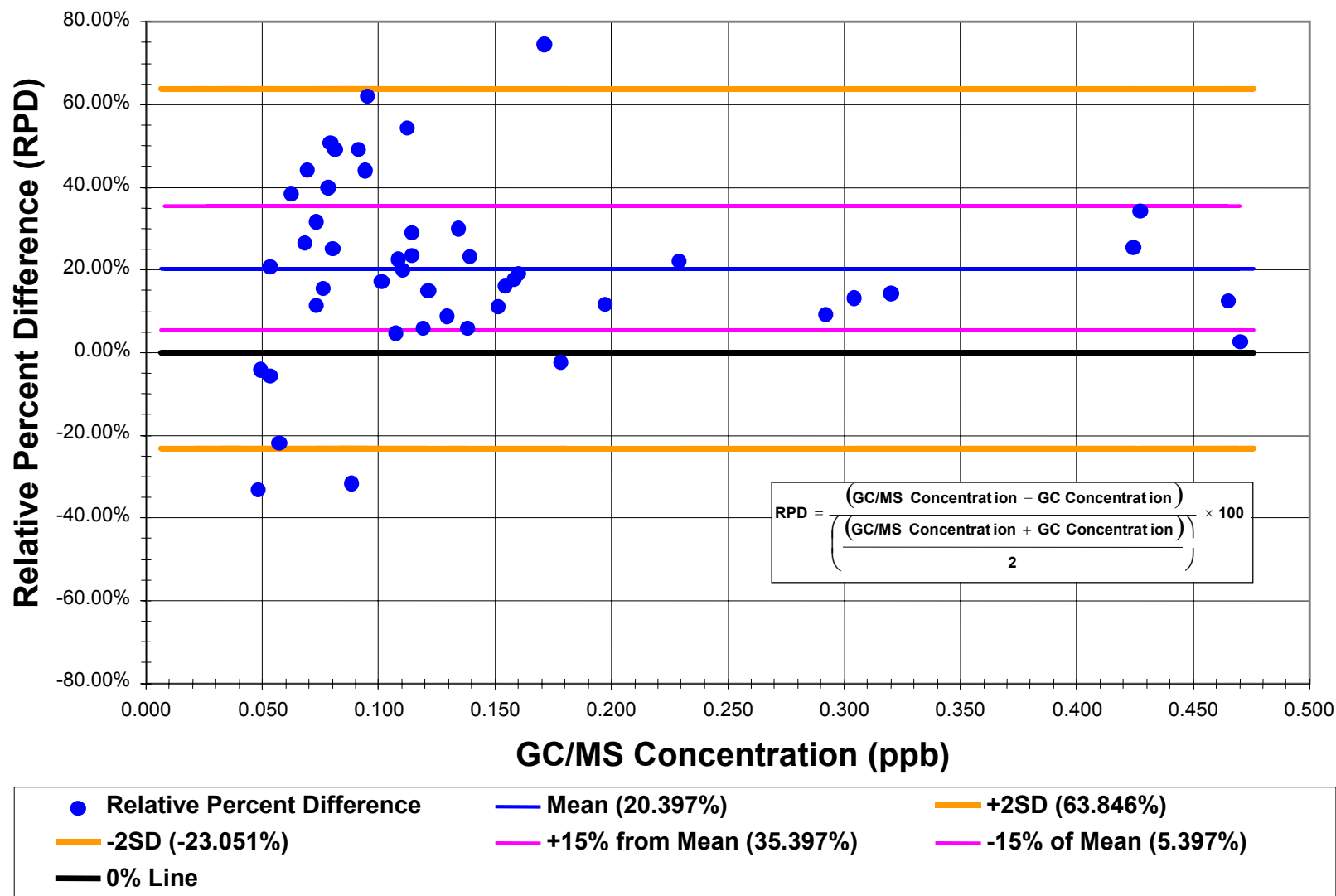


Figure 22: Carbon Tetrachloride - RPD - GC (ECD) vs. Full Scan GC/MS

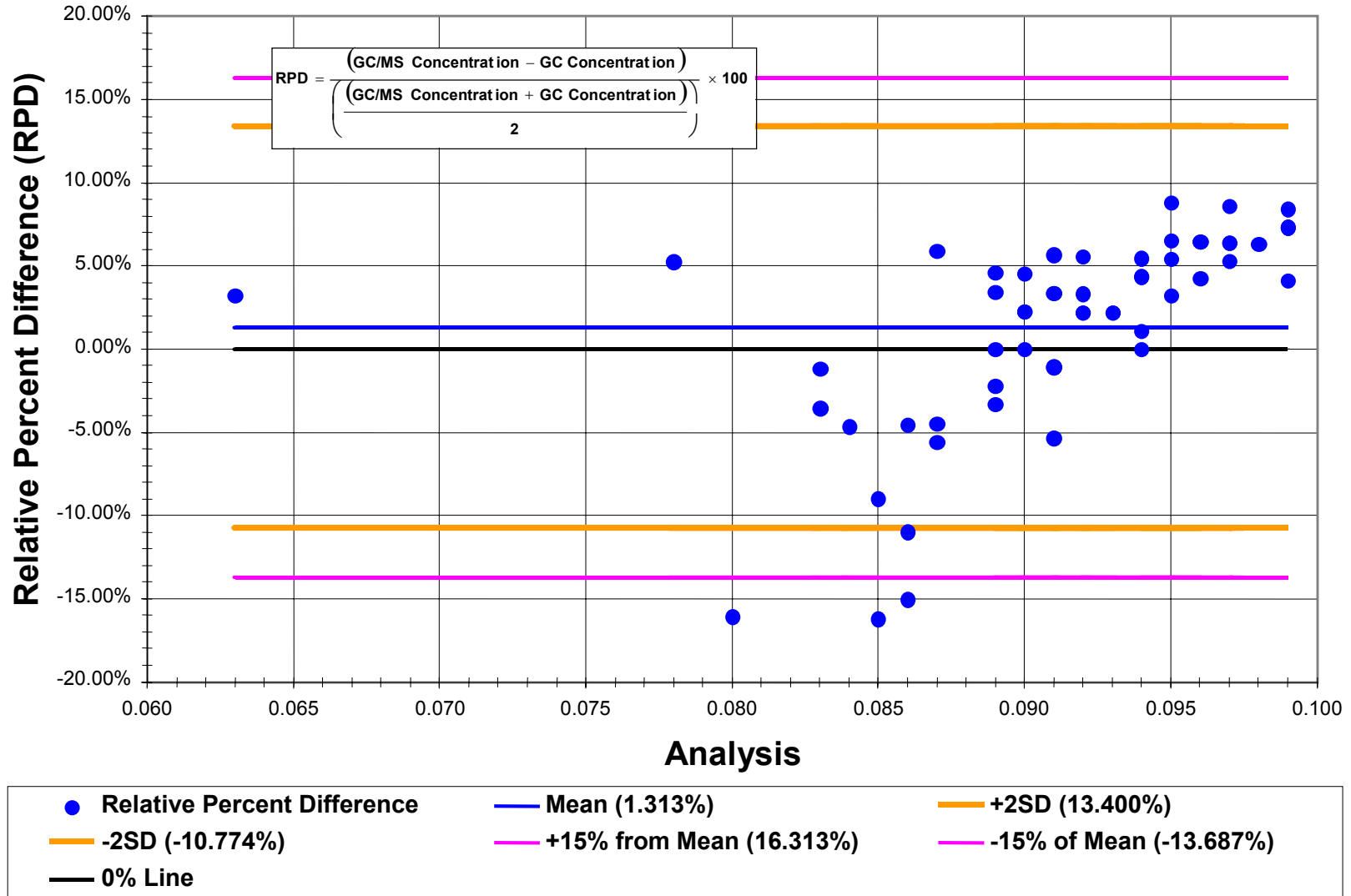


Figure 23: Perchloroethylene - RPD - GC (ECD) vs. Full Scan GC/MS

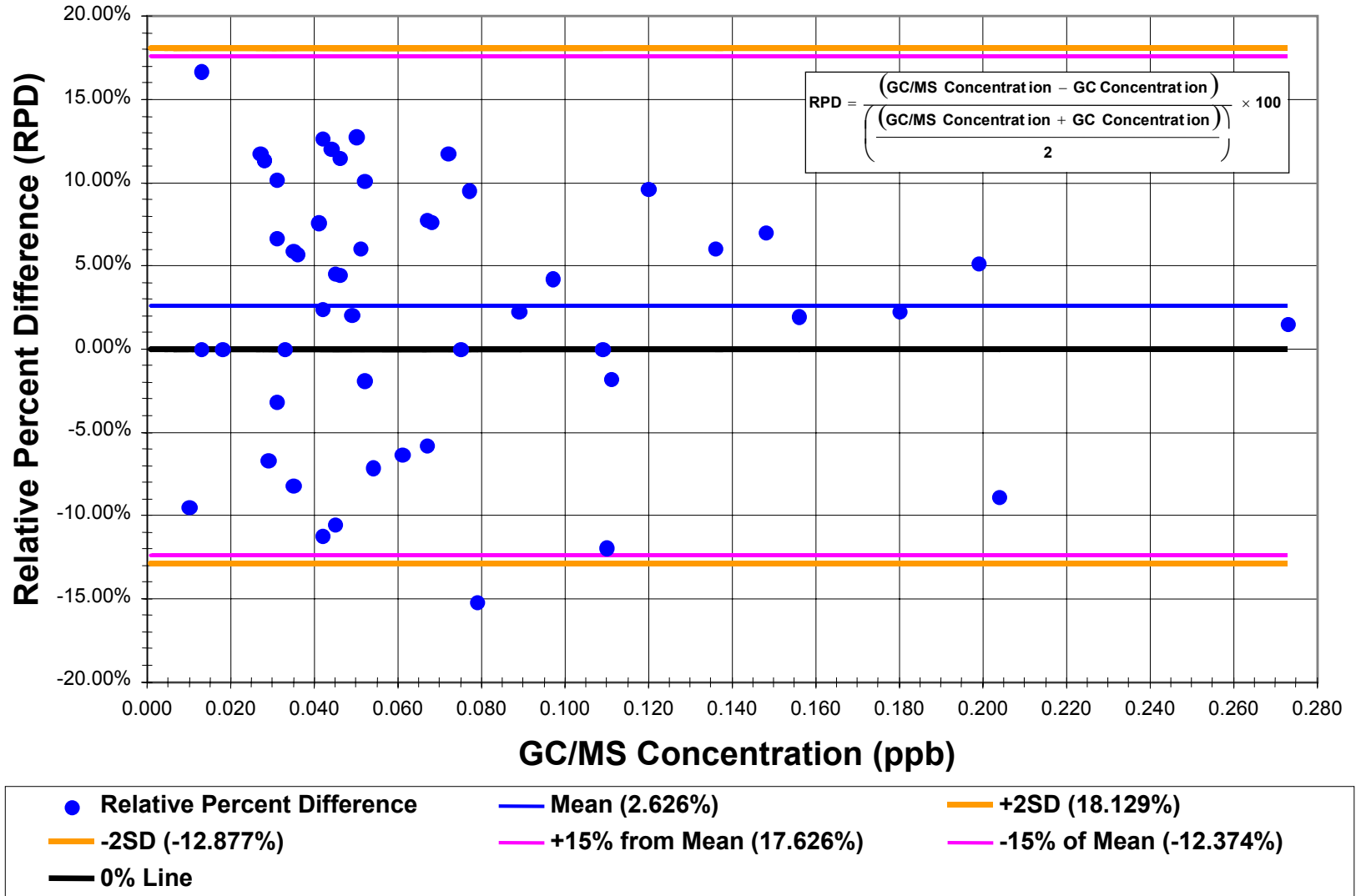


Figure 24: Chloroform - RPD - GC (ECD) vs. Full Scan GC/MS

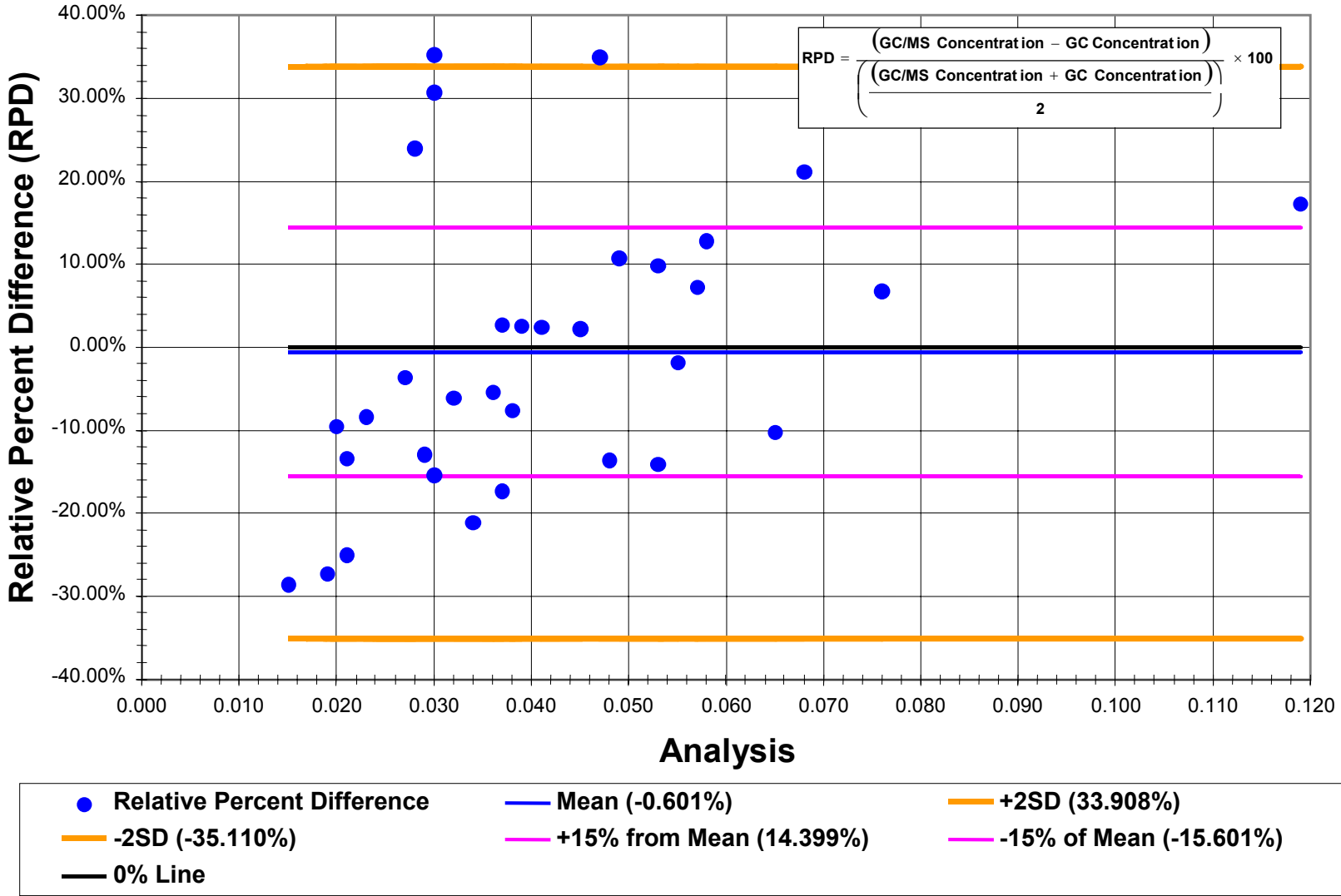


Figure 25: Trichloroethylene - RPD - GC (ECD) vs. Full Scan GC/MS

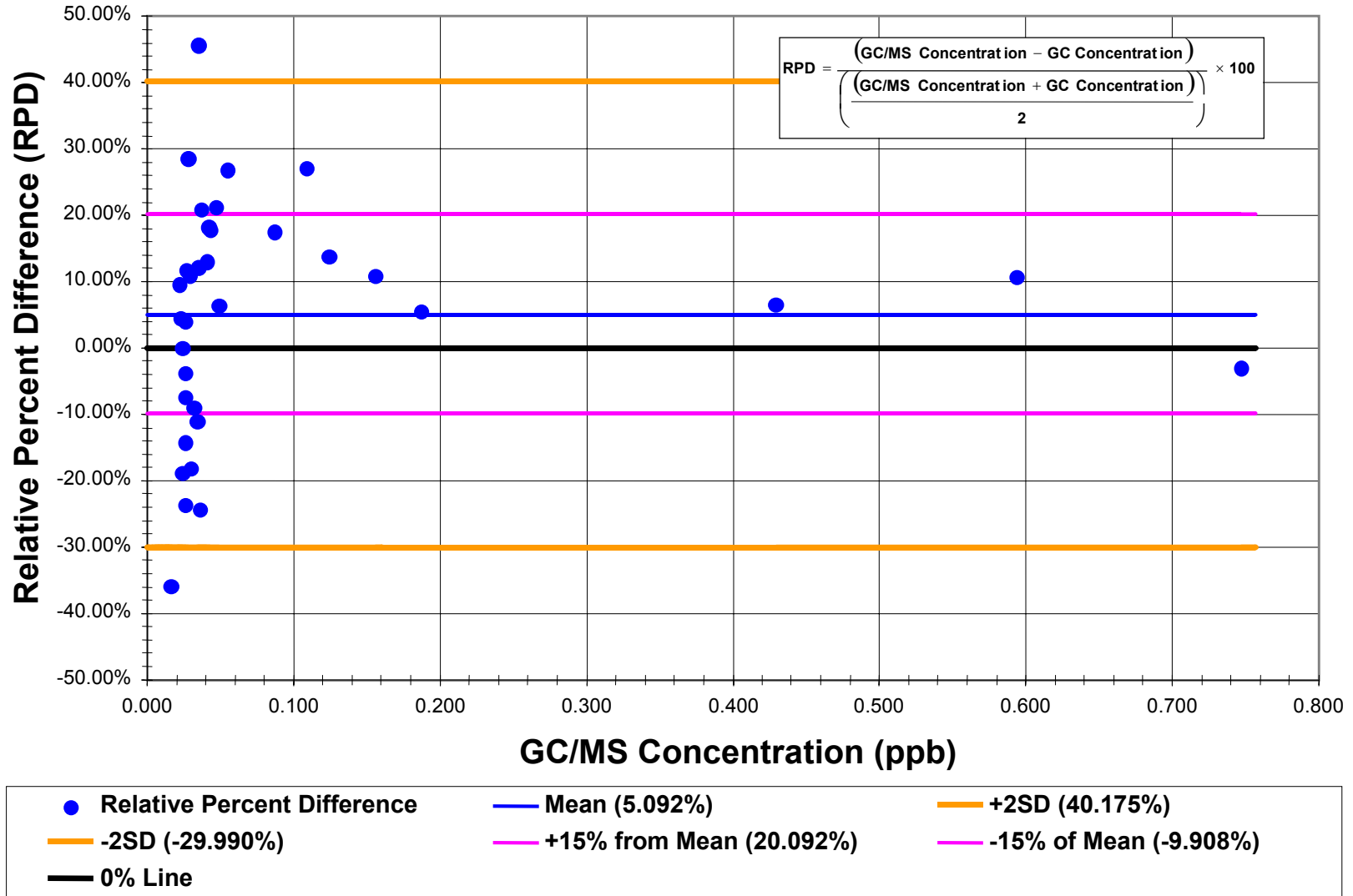


Figure 26: Trichloroethane - RPD - GC (ECD) vs. Full Scan GC/MS

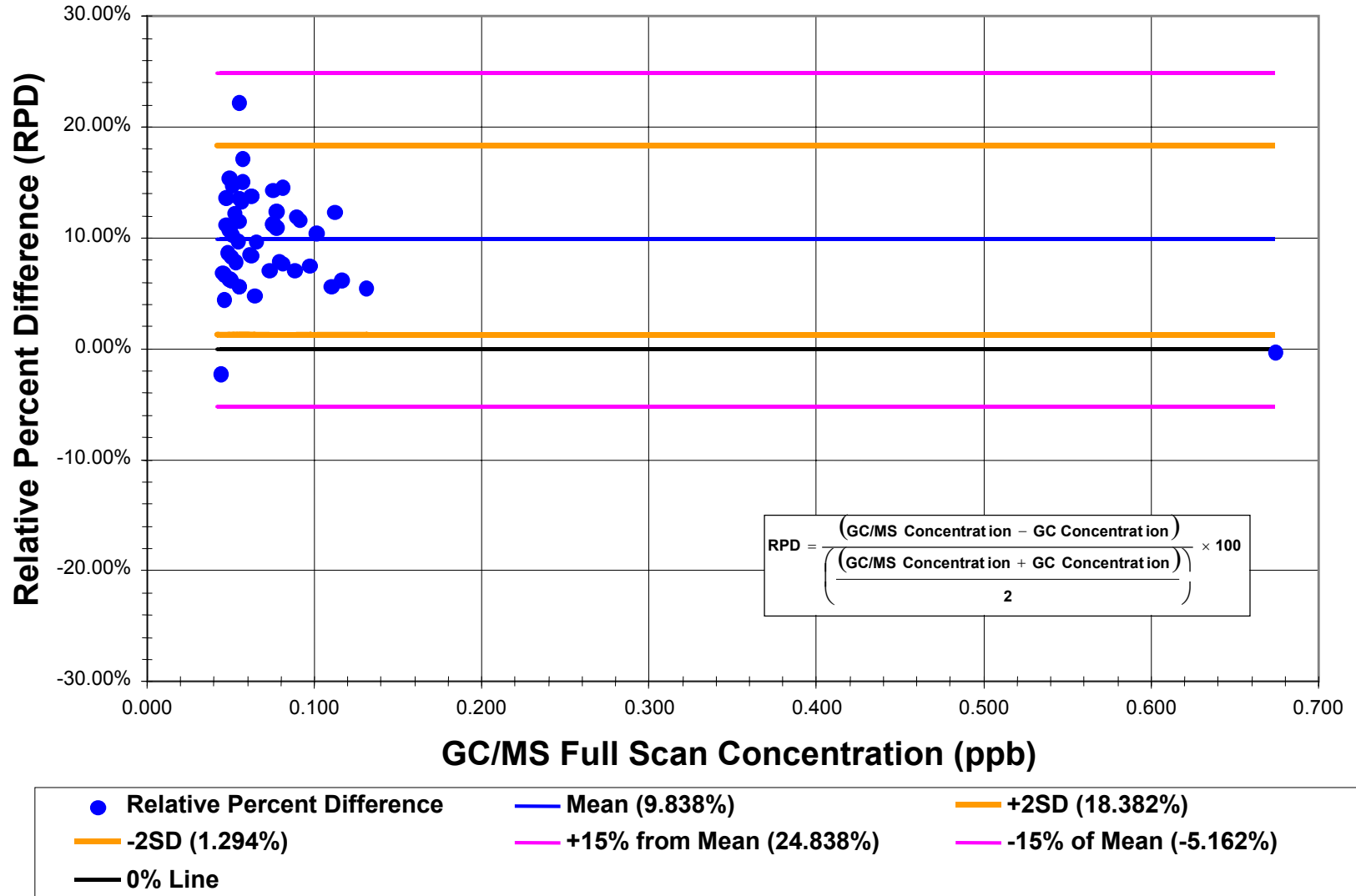


Figure 27: Toluene - RPD - GC (PID) vs. Full Scan GC/MS

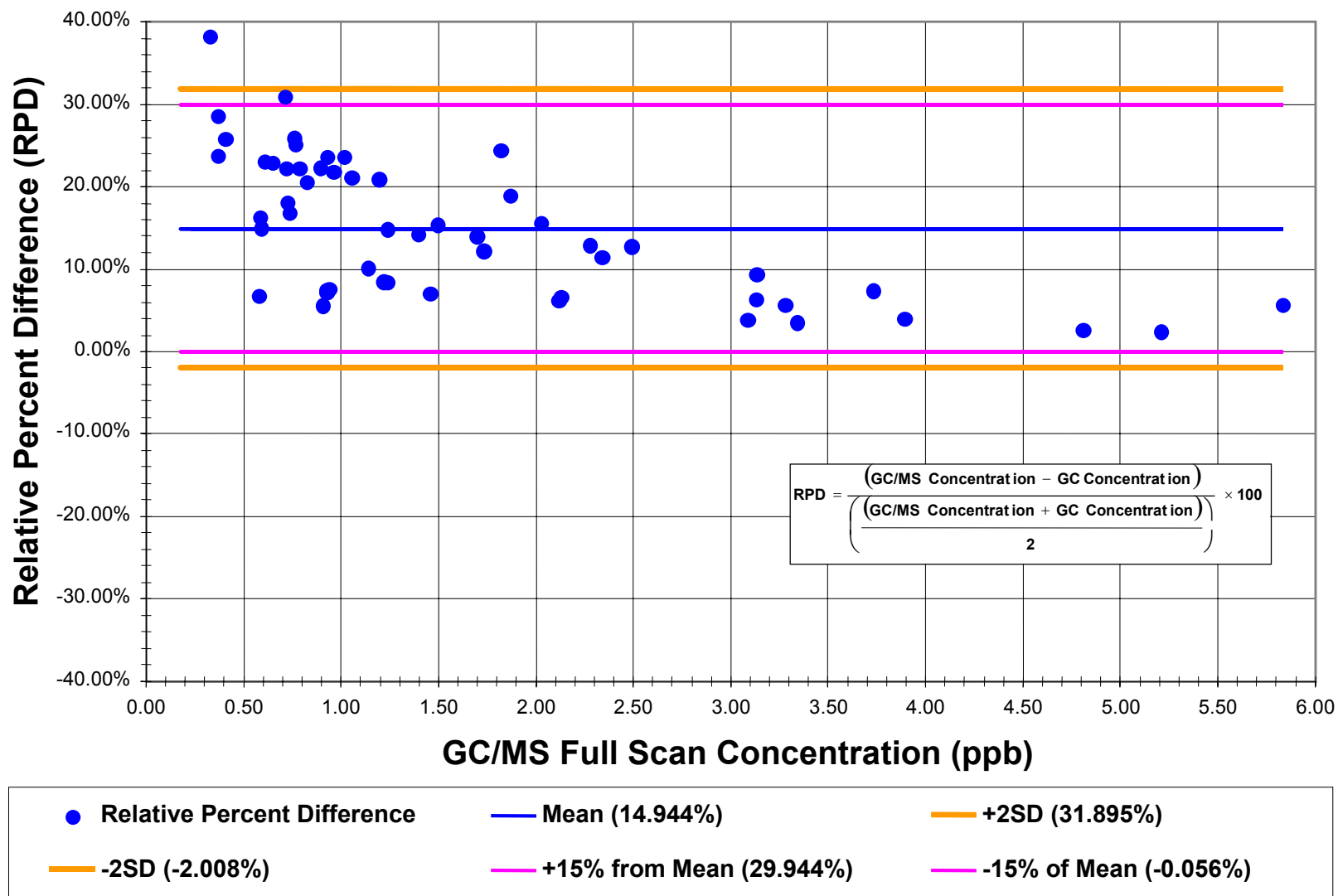


Figure 28: *m/p*-Xylene - RPD - GC (PID) vs. Full Scan GC/MS

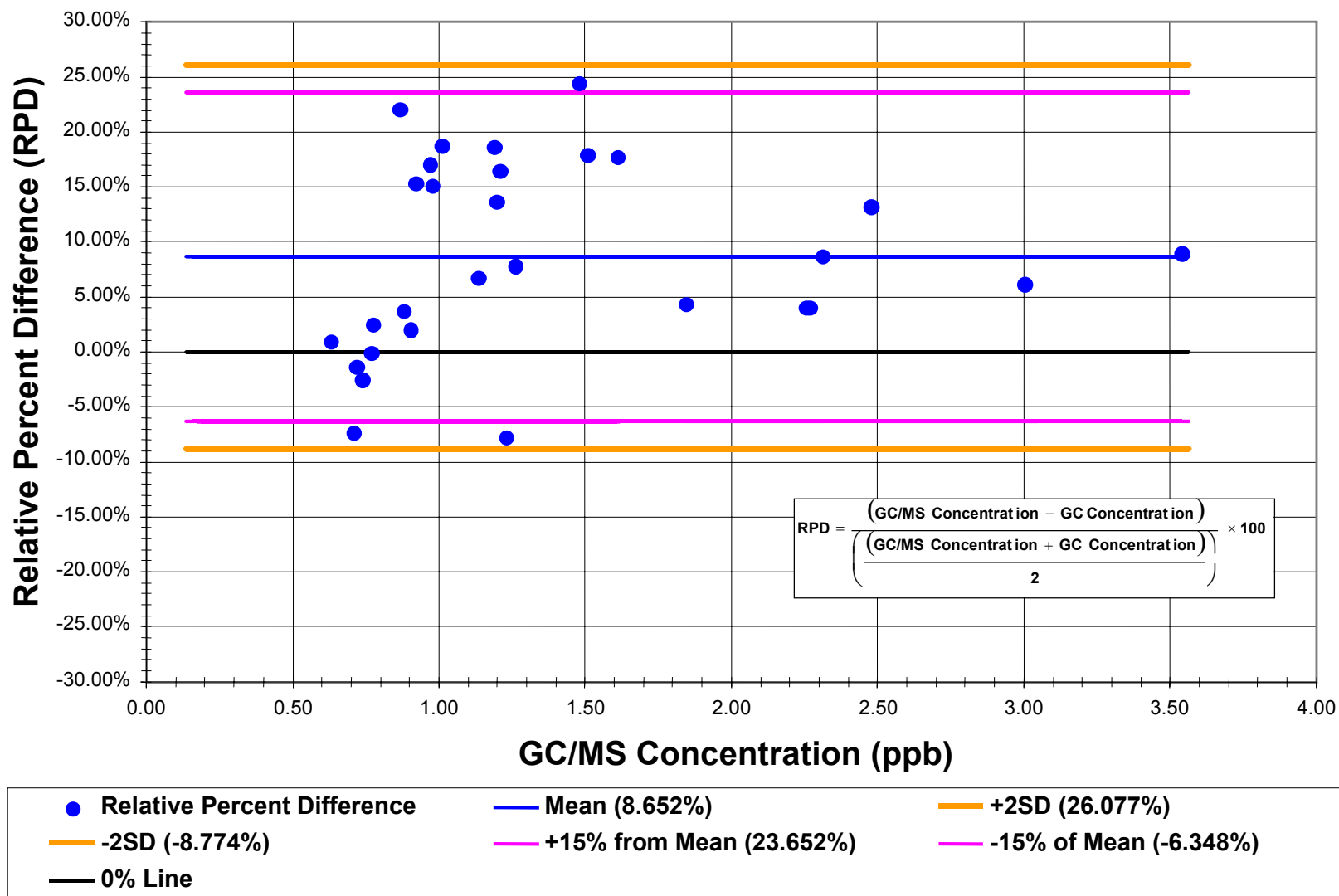


Figure 29: o-Xylene - RPD - GC (PID) vs. Full Scan GC/MS

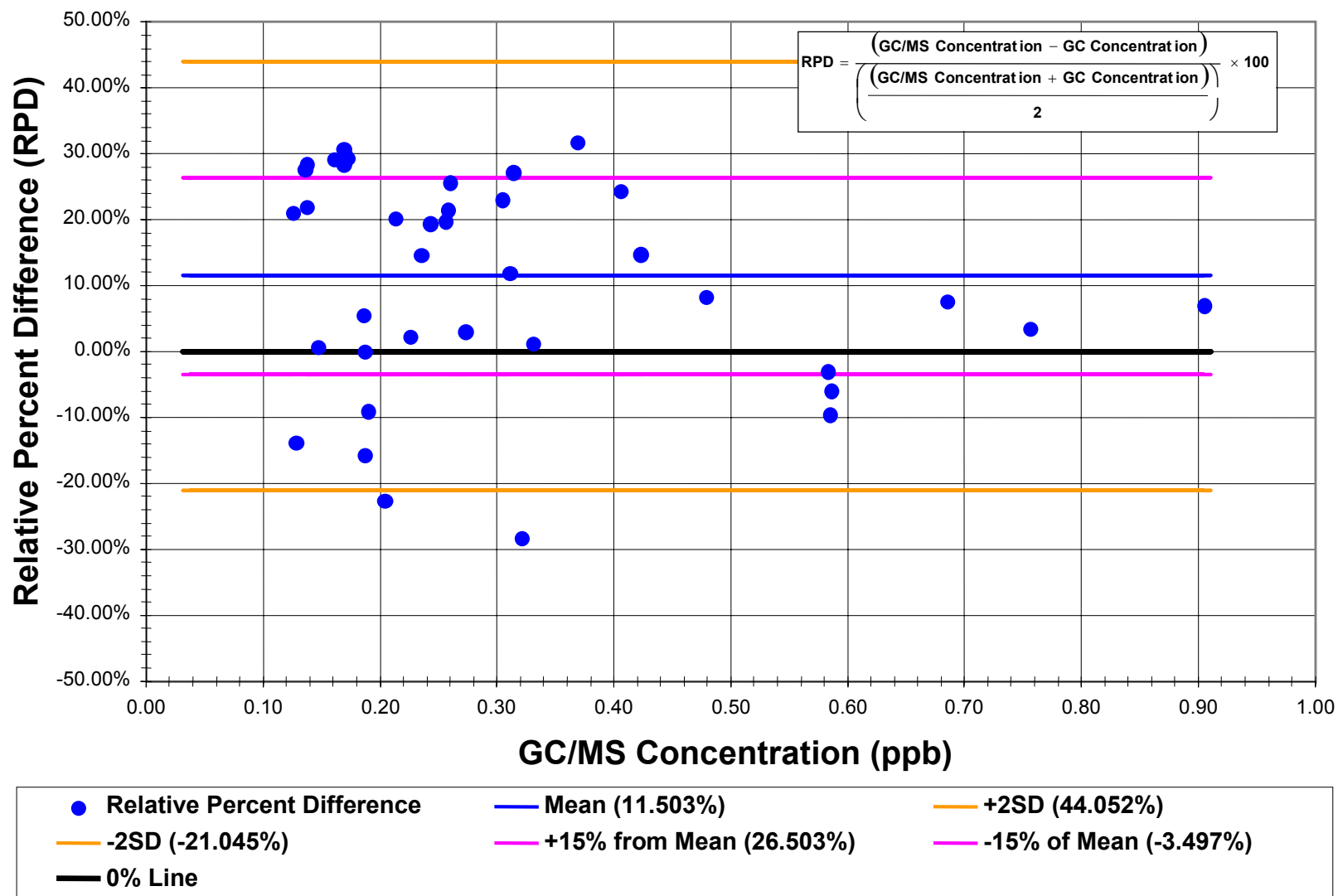
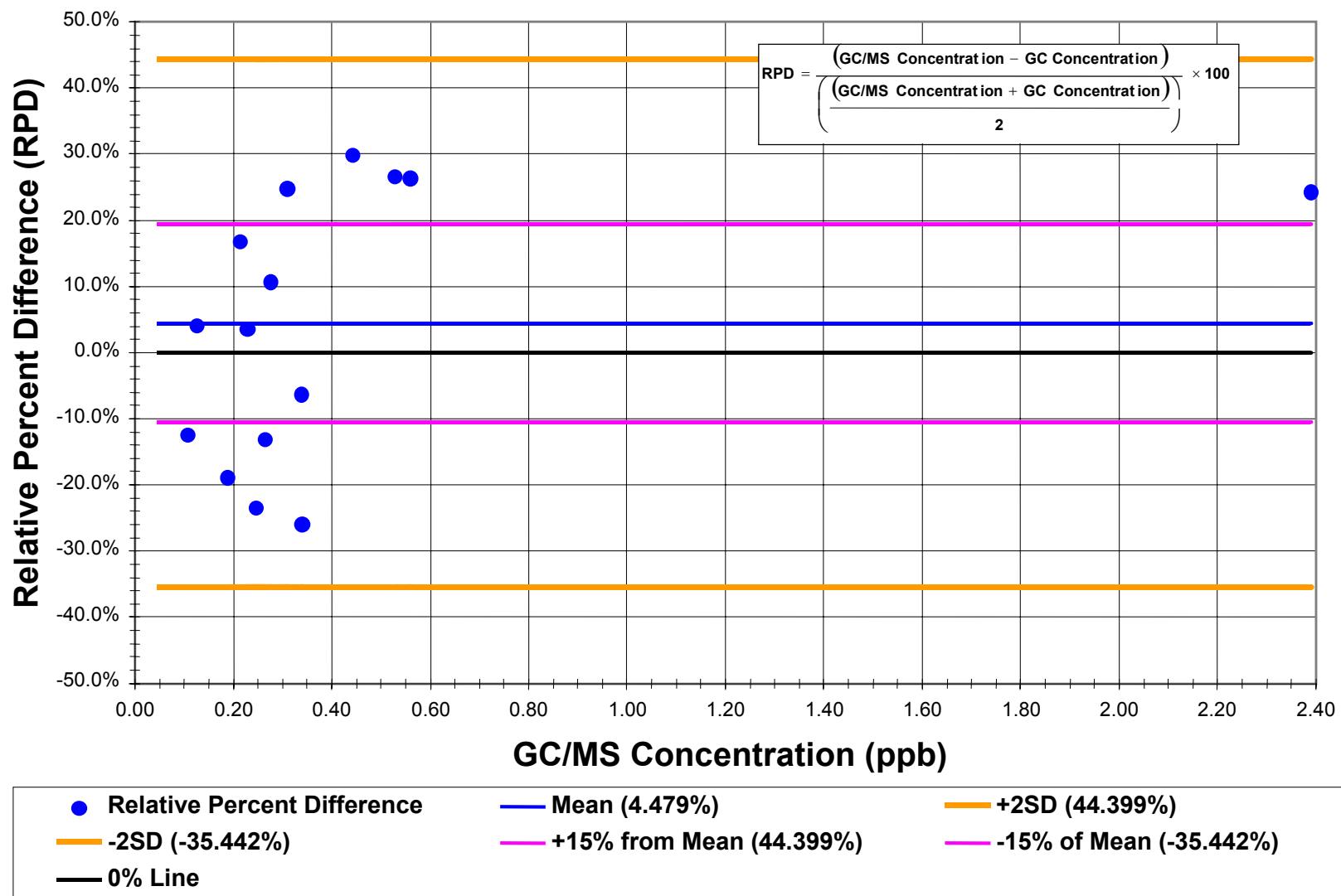


Figure 30: Styrene - RPD - GC (PID) vs. Full Scan GC/MS



This Page Left Intentionally Blank

